Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 04:18 AM EDT

PDB ID	:	8FC2 / pdb_00008fc2
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and azithromycin at 2.50A resolution
Authors	:	Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on	:	2022-12-01
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

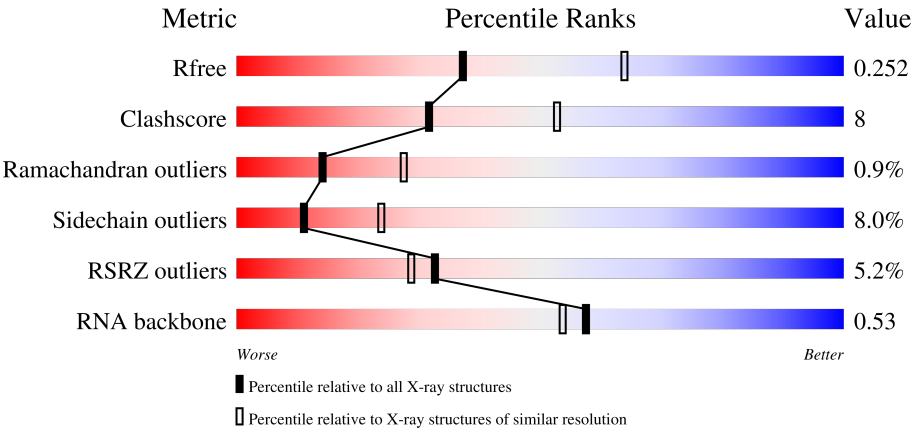
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 68% 25% 6%
1	2A	2915	4% 62% 29% 7%
2	1B	121	% 71% 23% 5%
2	2B	121	2% 59% 35% 6%

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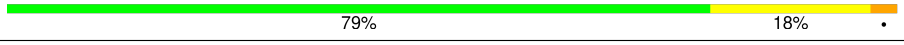
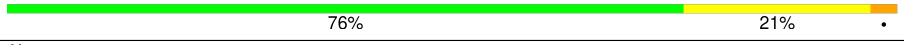
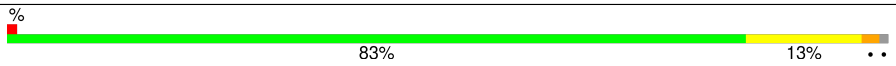
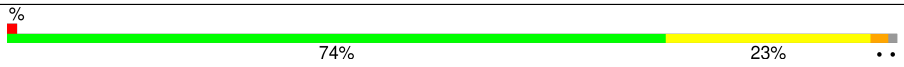
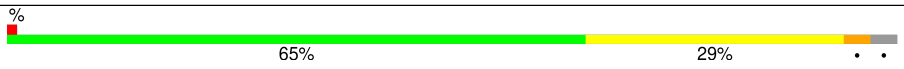
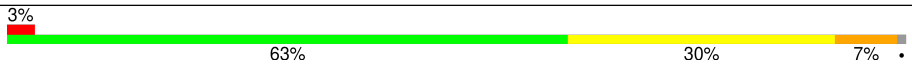
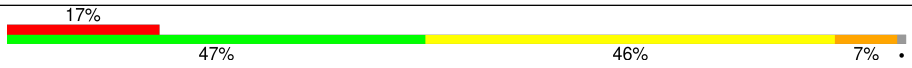
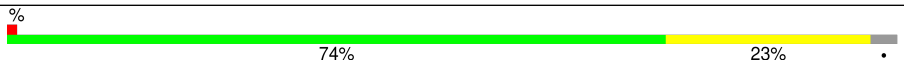
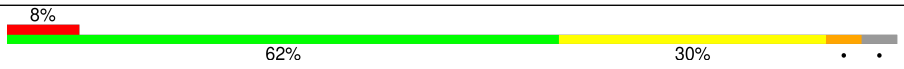
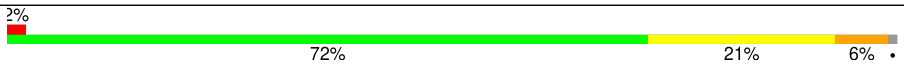
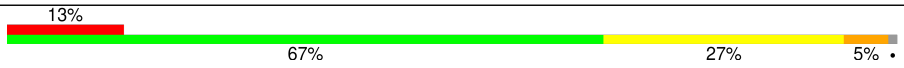
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
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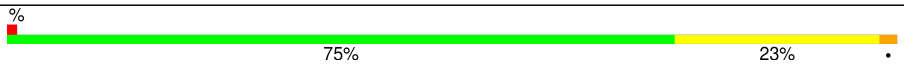
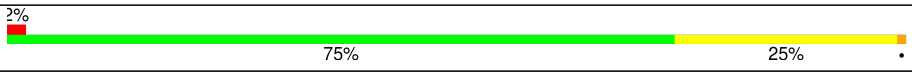
9	2N	140	
10	1O	122	
10	2O	122	
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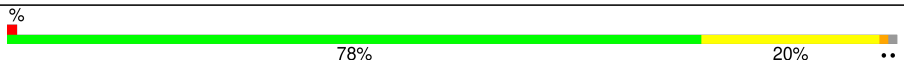
11	2P	150	
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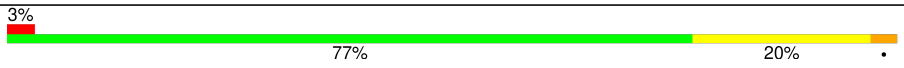
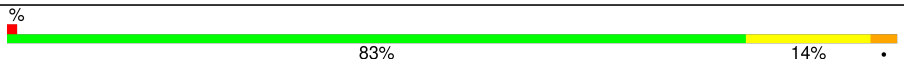
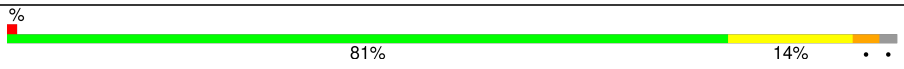
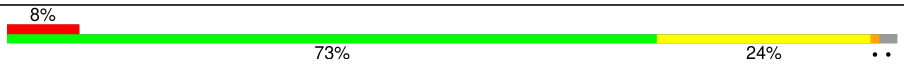
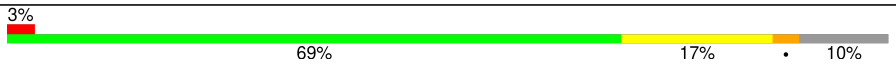
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
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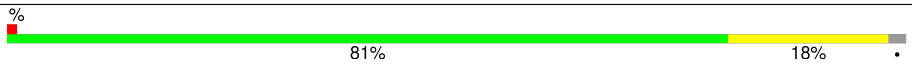
16	2U	118	
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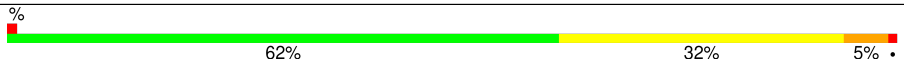
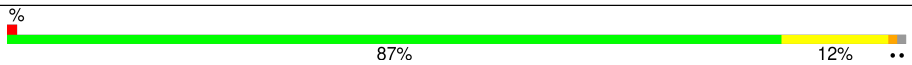
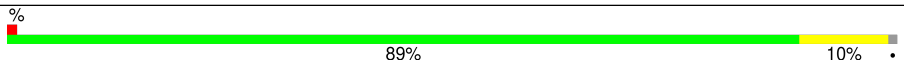
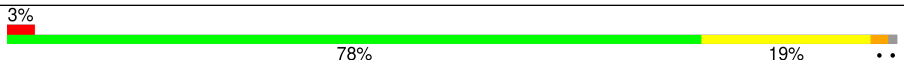
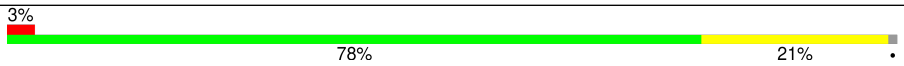
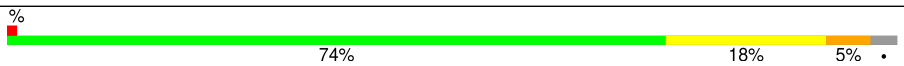
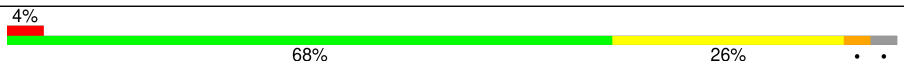
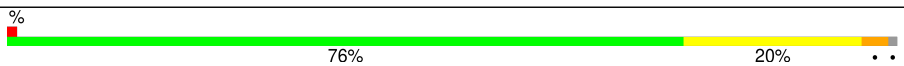
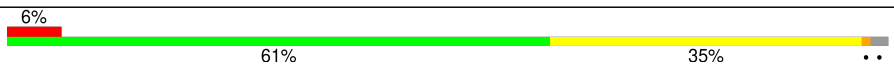
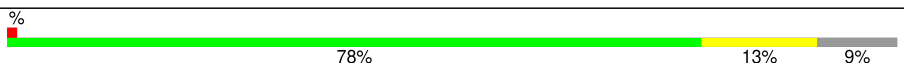
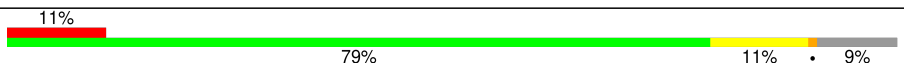
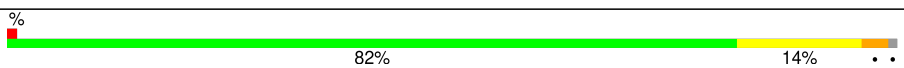
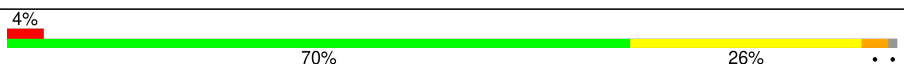
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
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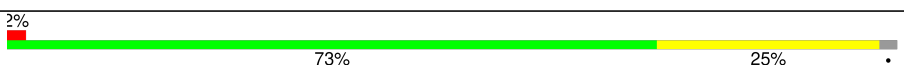
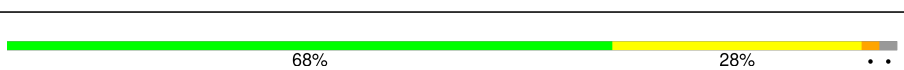
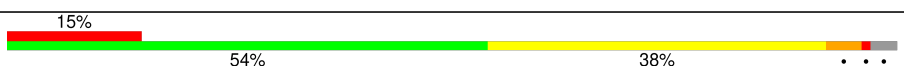
24	22	72	
25	13	60	
25	23	60	
26	14	71	
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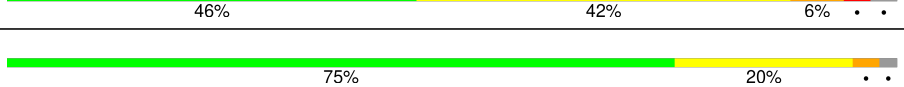
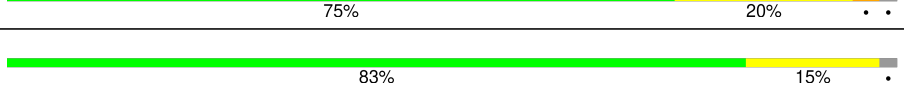
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
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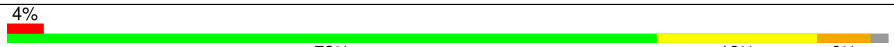
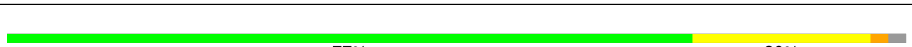
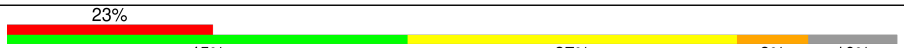
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
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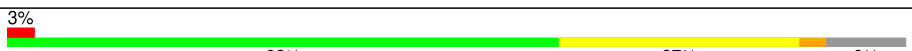
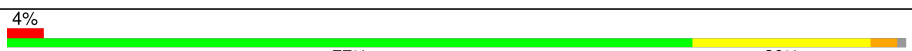
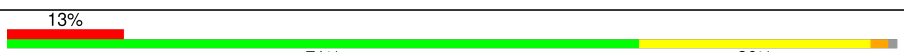
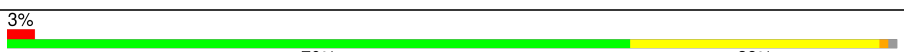
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	45% 47% 45% 6%
41	1j	105	28% 64% 26% 8%
41	2j	105	33% 53% 34% 9%
42	1k	129	2% 66% 22% 12%
42	2k	129	4% 69% 15% 5% 12%
43	1l	132	3% 65% 27% 8%
43	2l	132	3% 76% 17% 8%
44	1m	126	6% 54% 37% 8%
44	2m	126	32% 51% 37% 10%
45	1n	61	3% 62% 34%
45	2n	61	36% 52% 43%
46	1o	89	2% 71% 22% 6%
46	2o	89	3% 72% 25%
47	1p	88	10% 64% 28% 7%
47	2p	88	7% 60% 28% 5% 7%
48	1q	105	3% 70% 25% 6%
48	2q	105	3% 70% 24% 6%
49	1r	88	3% 61% 16% 23%
49	2r	88	% 60% 17% 23%
50	1s	93	8% 57% 31% 11%
50	2s	93	31% 48% 37% 11%
51	1t	106	8% 61% 27% 9%
51	2t	106	9% 70% 22% 8%
52	1u	27	22% 74% 11% 15%
52	2u	27	37% 63% 22% 15%

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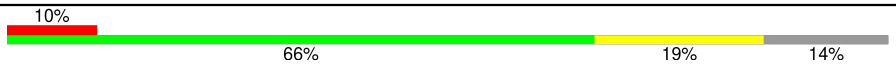
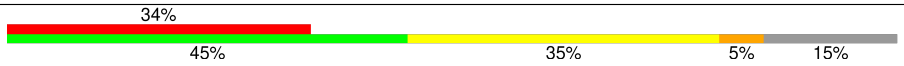
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	SF4	1d	305	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 296715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total 1135	C 706	N 230	O 196	S 3	0	0	0
11	2P	149	Total 1135	C 706	N 230	O 196	S 3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0
12	2Q	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total 968	C 604	N 203	O 160	S 1	0	0	0
13	2R	118	Total 968	C 604	N 203	O 160	S 1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total 877	C 553	N 175	O 149	0	0	0
14	2S	110	Total 870	C 549	N 173	O 148	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total 1091	C 680	N 225	O 185	S 1	0	0	0
15	2T	131	Total 1083	C 675	N 224	O 183	S 1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total 764	C 478	N 144	O 139	S 3	0	0	0
53	2y	96	Total 749	C 468	N 141	O 137	S 3	0	0	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1021	Total 1021	Mg 1021	0	0
54	1B	29	Total 29	Mg 29	0	0
54	1D	20	Total 20	Mg 20	0	0
54	1E	10	Total 10	Mg 10	0	0
54	1F	17	Total 17	Mg 17	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	4	Total 4	Mg 4	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	5	Total 5	Mg 5	0	0
54	1Q	5	Total 5	Mg 5	0	0
54	1R	8	Total 8	Mg 8	0	0
54	1T	3	Total 3	Mg 3	0	0
54	1U	6	Total 6	Mg 6	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	4	Total 4	Mg 4	0	0
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	10	8	Total Mg 8 8	0	0
54	11	5	Total Mg 5 5	0	0
54	13	3	Total Mg 3 3	0	0
54	14	1	Total Mg 1 1	0	0
54	15	8	Total Mg 8 8	0	0
54	17	6	Total Mg 6 6	0	0
54	18	2	Total Mg 2 2	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	281	Total Mg 281 281	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	4	Total Mg 4 4	0	0
54	1e	4	Total Mg 4 4	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	2	Total Mg 2 2	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1k	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1m	1	Total Mg 1 1	0	0
54	1n	2	Total Mg 2 2	0	0
54	1o	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	1	Total Mg 1 1	0	0
54	1y	3	Total Mg 3 3	0	0
54	2A	729	Total Mg 729 729	0	0
54	2B	16	Total Mg 16 16	0	0
54	2D	12	Total Mg 12 12	0	0
54	2E	7	Total Mg 7 7	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	2	Total Mg 2 2	0	0
54	2I	2	Total Mg 2 2	0	0
54	2O	2	Total Mg 2 2	0	0
54	2P	2	Total Mg 2 2	0	0
54	2Q	3	Total Mg 3 3	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	4	Total Mg 4 4	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	3	Total Mg 3 3	0	0
54	2W	3	Total Mg 3 3	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	3	Total Mg 3 3	0	0
54	21	1	Total Mg 1 1	0	0

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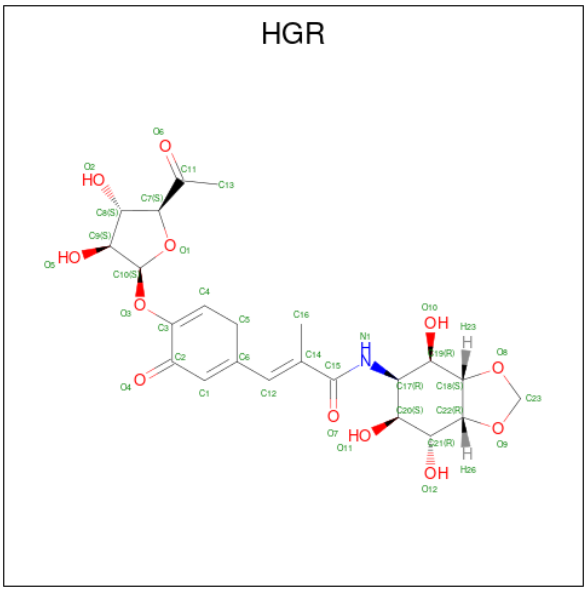
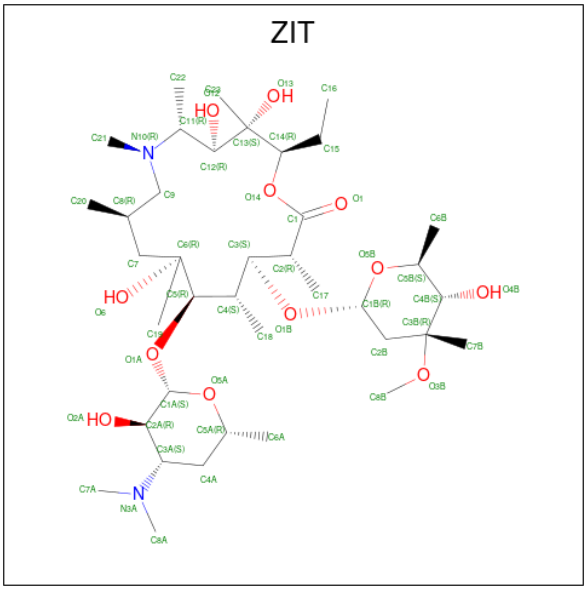
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	23	1	Total Mg 1 1	0	0
54	25	3	Total Mg 3 3	0	0
54	27	3	Total Mg 3 3	0	0
54	28	3	Total Mg 3 3	0	0
54	2a	193	Total Mg 193 193	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2o	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



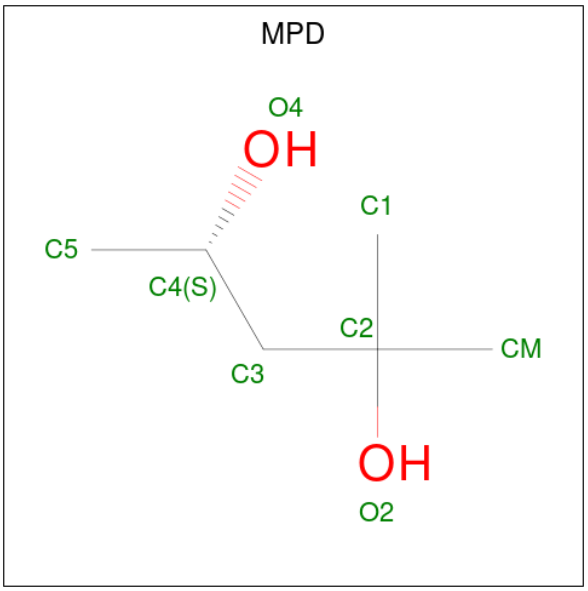
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 36 23 1 12	0	0
55	2A	1	Total C N O 36 23 1 12	0	0

- Molecule 56 is AZITHROMYCIN (CCD ID: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$) (labeled as "Ligand of Interest" by depositor).



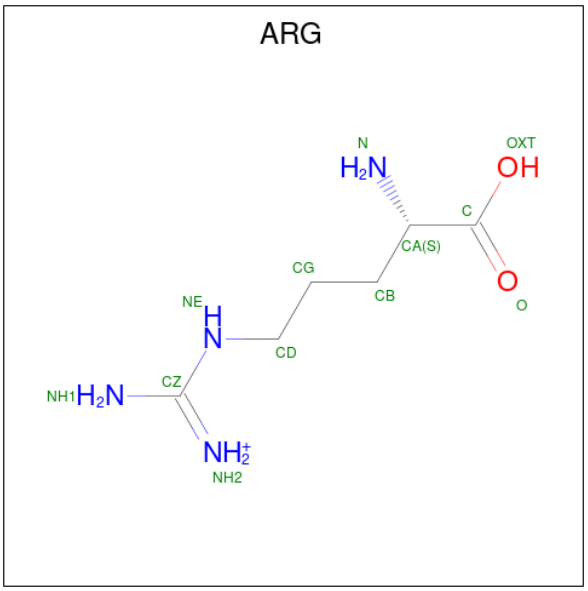
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total C N O 52 38 2 12	0	0
56	2A	1	Total C N O 52 38 2 12	0	0

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	1	Total C N O 12 6 4 2	0	0
58	1F	1	Total C N O 12 6 4 2	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0

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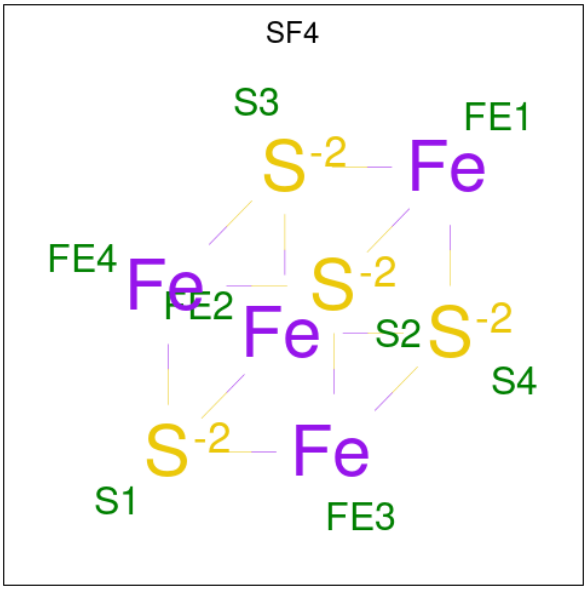
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3943	Total O 3943 3943	0	0
61	1B	106	Total O 106 106	0	0
61	1D	106	Total O 106 106	0	0
61	1E	75	Total O 75 75	0	0
61	1F	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	15	Total O 15 15	0	0
61	1H	13	Total O 13 13	0	0
61	1I	6	Total O 6 6	0	0
61	1N	50	Total O 50 50	0	0
61	1O	23	Total O 23 23	0	0
61	1P	56	Total O 56 56	0	0
61	1Q	38	Total O 38 38	0	0
61	1R	37	Total O 37 37	0	0
61	1S	11	Total O 11 11	0	0
61	1T	39	Total O 39 39	0	0
61	1U	43	Total O 43 43	0	0
61	1V	36	Total O 36 36	0	0
61	1W	29	Total O 29 29	0	0
61	1X	26	Total O 26 26	0	0
61	1Y	16	Total O 16 16	0	0
61	1Z	12	Total O 12 12	0	0
61	10	21	Total O 21 21	0	0
61	11	24	Total O 24 24	0	0
61	12	12	Total O 12 12	0	0
61	13	19	Total O 19 19	0	0
61	14	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	24	Total O 24 24	0	0
61	16	19	Total O 19 19	0	0
61	17	14	Total O 14 14	0	0
61	18	25	Total O 25 25	0	0
61	19	2	Total O 2 2	0	0
61	1a	465	Total O 465 465	0	0
61	1b	1	Total O 1 1	0	0
61	1d	8	Total O 8 8	0	0
61	1e	4	Total O 4 4	0	0
61	1f	1	Total O 1 1	0	0
61	1h	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	4	Total O 4 4	0	0
61	1o	4	Total O 4 4	0	0
61	1t	1	Total O 1 1	0	0
61	1u	1	Total O 1 1	0	0
61	1y	3	Total O 3 3	0	0
61	2A	1664	Total O 1664 1664	0	0
61	2B	25	Total O 25 25	0	0
61	2D	38	Total O 38 38	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2E	18	Total O 18 18	0	0
61	2F	18	Total O 18 18	0	0
61	2G	4	Total O 4 4	0	0
61	2H	1	Total O 1 1	0	0
61	2I	1	Total O 1 1	0	0
61	2N	2	Total O 2 2	0	0
61	2O	11	Total O 11 11	0	0
61	2P	11	Total O 11 11	0	0
61	2Q	10	Total O 10 10	0	0
61	2R	16	Total O 16 16	0	0
61	2T	7	Total O 7 7	0	0
61	2U	8	Total O 8 8	0	0
61	2V	5	Total O 5 5	0	0
61	2W	17	Total O 17 17	0	0
61	2X	3	Total O 3 3	0	0
61	2Y	3	Total O 3 3	0	0
61	2Z	3	Total O 3 3	0	0
61	20	6	Total O 6 6	0	0
61	21	12	Total O 12 12	0	0
61	23	1	Total O 1 1	0	0
61	25	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	26	5	Total O 5 5	0	0
61	27	5	Total O 5 5	0	0
61	28	8	Total O 8 8	0	0
61	2a	245	Total O 245 245	0	0
61	2d	2	Total O 2 2	0	0
61	2e	1	Total O 1 1	0	0
61	2f	3	Total O 3 3	0	0
61	2l	3	Total O 3 3	0	0
61	2m	1	Total O 1 1	0	0
61	2o	2	Total O 2 2	0	0
61	2q	2	Total O 2 2	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2y	2	Total O 2 2	0	0

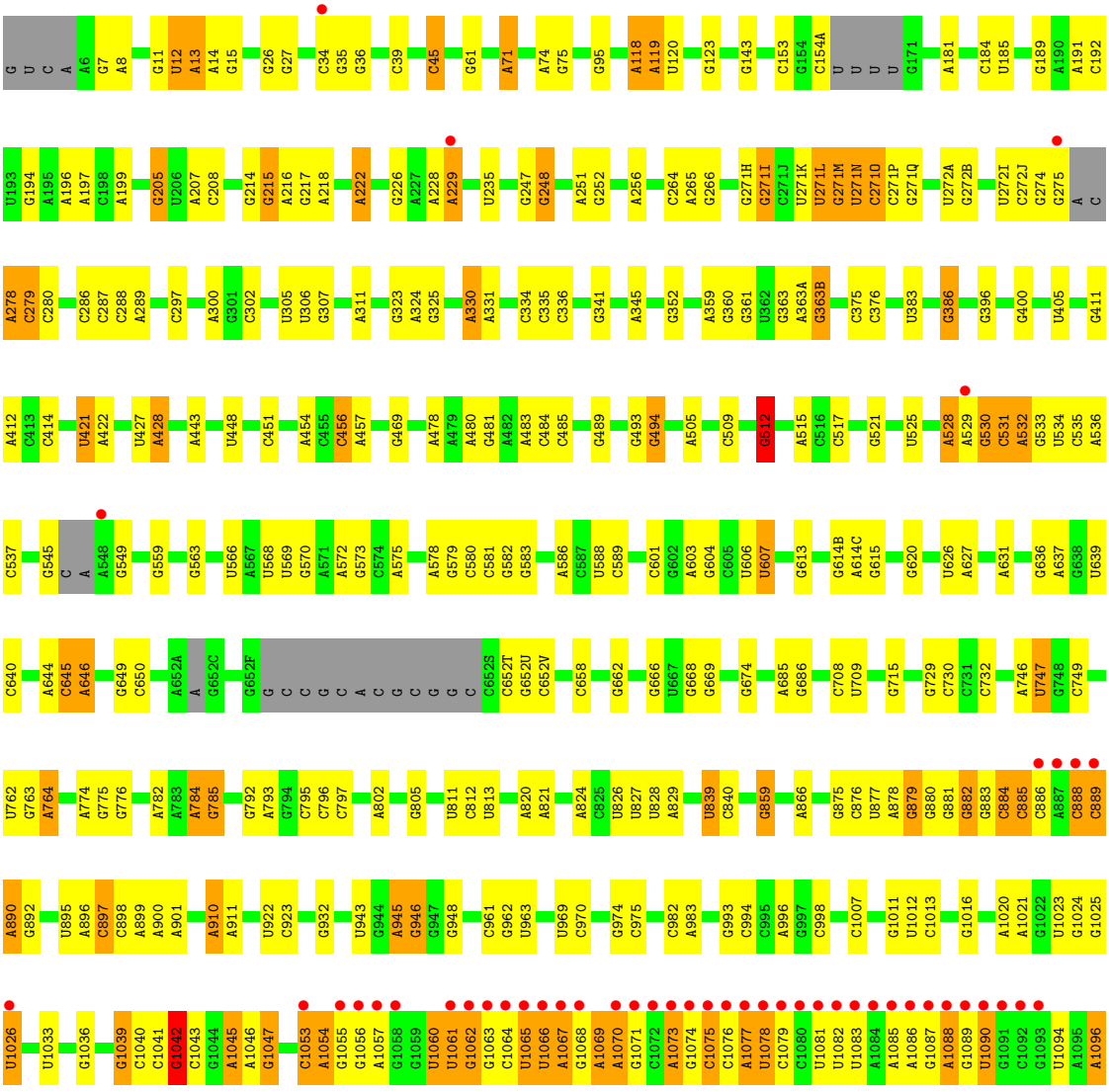
3 Residue-property plots (i)

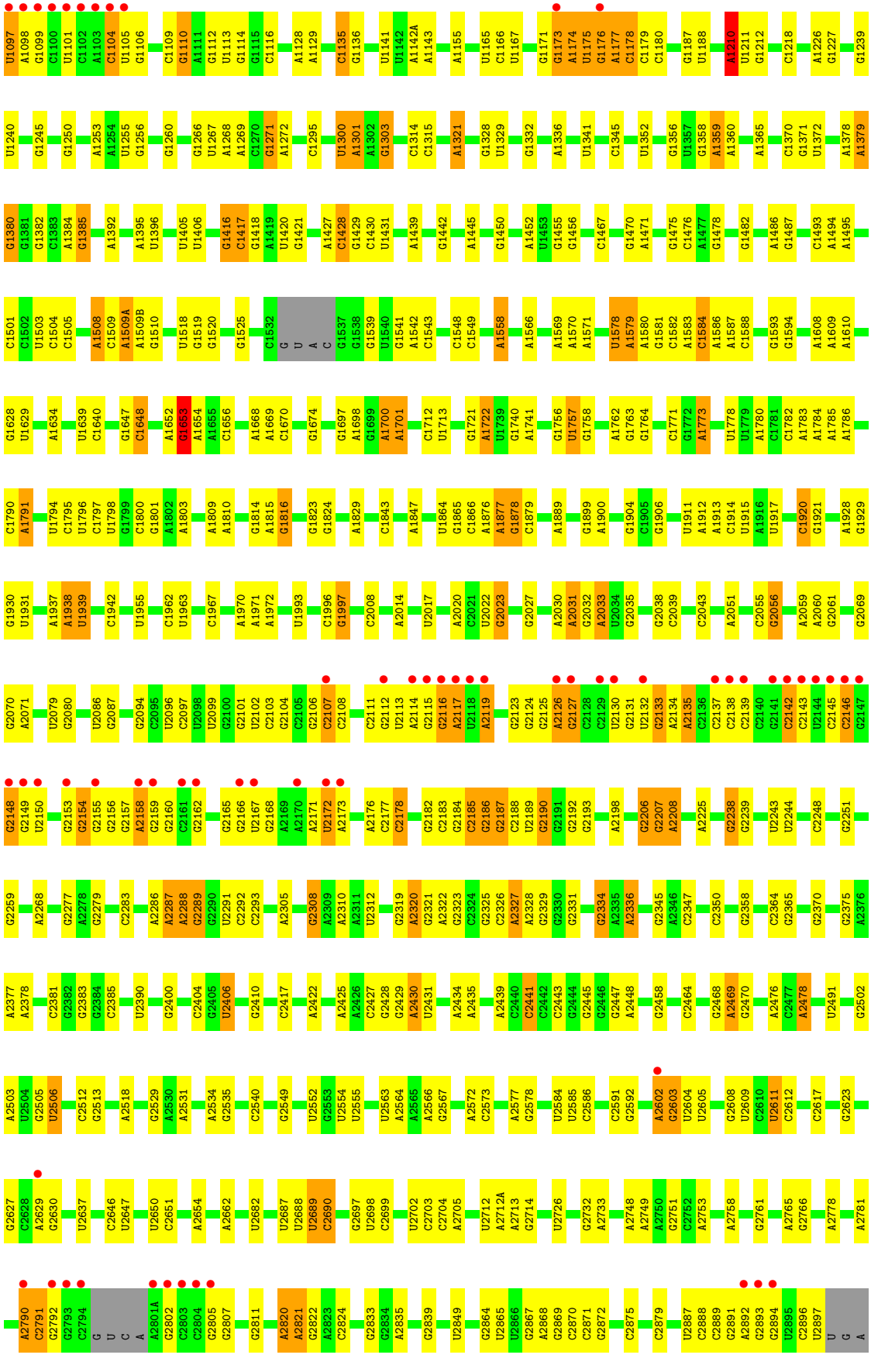
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S Ribosomal RNA

Chain 1A:





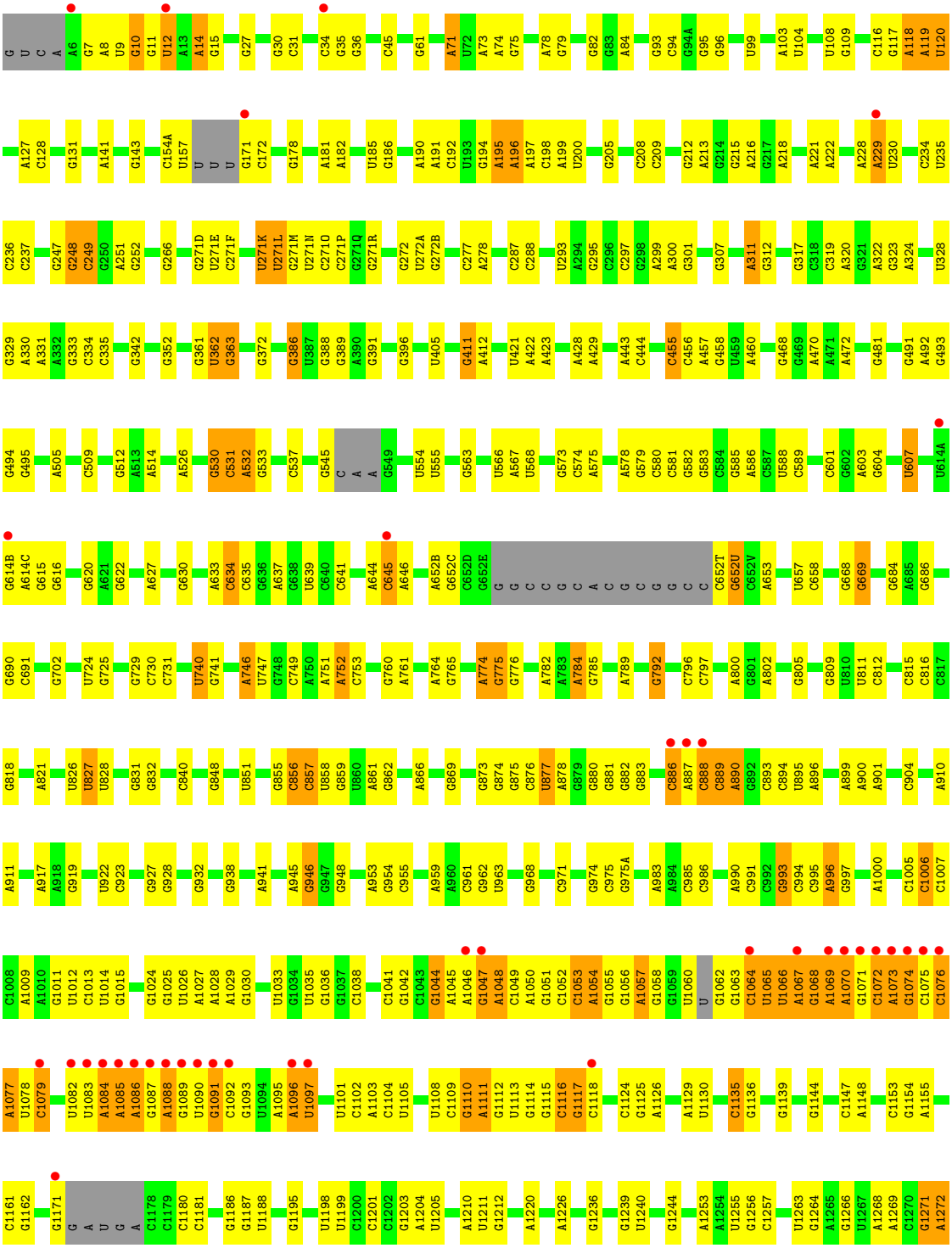


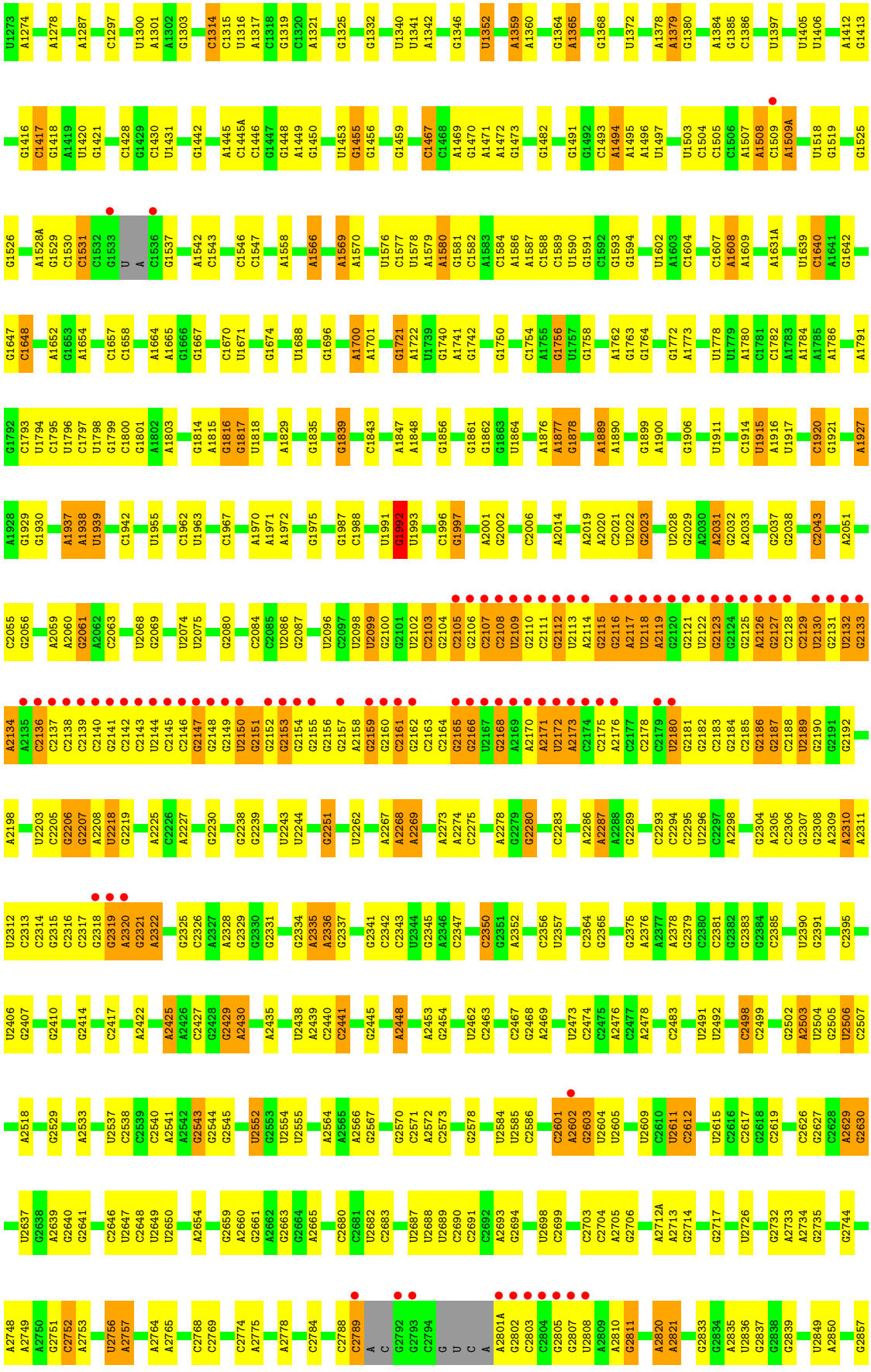


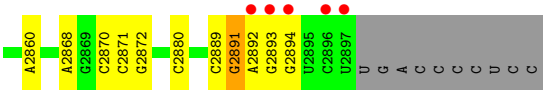
• Molecule 1: 23S Ribosomal RNA

Chain 2A:





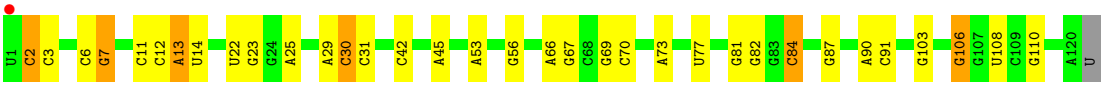

U1273 A1274 A1278 A1287 C1297 U1300 A1301 A1302 G1303 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 G1325 G1332 U1340 U1341 A1342 G1346 U1362 A1359 A1360 G1364 A1365 G1368 U1372 A1378 A1379 G1380 A1384 G1385 C1386 U1397 U1405 U1406 A1412 G1413
G1416 C1417 G1418 A1419 U1420 G1421 C1428 G1429 C1430 U1431 G1442 A1445 C1445A C1446 G1447 G1448 A1449 G1450 U1453 G1455 G1456 G1459 C1467 C1468 A1469 G1470 A1471 A1472 G1473 G1482 G1491 G1492 C1493 A1494 A1495 A1496 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A U1518 G1519 G1525
G1526 A1528A G1529 C1530 C1531 C1532 G1533 U A C1536 G1537 A1542 C1543 C1546 C1547 A1558 A1566 A1569 A1570 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 U1602 A1603 C1604 C1607 A1608 A1609 A1631A U1639 C1640 A1641 G1642
G1647 C1648 A1652 G1653 A1654 C1657 C1658 A1664 A1665 G1666 G1667 C1670 U1671 G1674 U1688 G1696 A1700 A1701 G1721 A1722 U1739 G1740 A1741 G1742 G1750 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1791
G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 G1814 A1815 G1816 G1817 U1818 A1829 G1835 G1839 C1843 A1847 A1848 G1856 G1861 G1862 G1863 U1864 A1876 A1877 G1878 A1889 A1890 G1899 A1900 G1906 U1911 C1914 U1915 A1916 U1917 C1920 G1921 A1927
A1928 G1929 C1930 A1937 A1938 U1939 C1942 U1955 C1962 U1963 C1967 A1970 A1971 A1972 G1975 G1987 C1988 U1991 G1992 U1993 C1996 G1997 A2001 G2002 C2006 A2014 A2019 A2020 C2021 U2022 G2023 U2028 G2029 A2030 A2031 G2032 A2033 G2037 G2038 C2043 A2051
C2055 G2056 A2059 A2060 G2061 A2062 C2063 U2068 G2069 U2074 U2075 G2080 C2084 C2085 U2086 G2087 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133
A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 C2156 G2157 A2158 G2159 G2160 C2161 C2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 C2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192
A2198 U2203 C2205 G2206 G2207 A2208 U2218 G2219 A2225 C2226 A2227 G2230 G2238 G2239 U2243 U2244 G2251 U2262 A2267 A2268 A2269 A2273 A2274 C2275 A2278 G2279 G2280 C2283 A2286 A2287 A2288 G2289 C2293 C2294 C2295 U2296 C2297 A2298 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311
U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 A2322 G2325 C2326 A2327 A2328 G2329 G2330 G2331 C2334 A2335 A2336 G2337 G2341 C2342 C2343 U2344 C2345 A2346 C2347 C2350 G2351 A2352 C2356 U2357 C2364 G2365 G2375 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 U2390 G2391 C2396
U2406 G2407 G2410 G2414 C2417 A2422 A2425 A2426 C2427 G2428 G2429 A2430 A2435 U2438 A2439 C2440 C2441 G2445 A2448 A2453 G2454 U2462 C2463 C2467 G2468 A2469 U2473 C2474 C2475 A2476 C2477 A2478 C2483 U2491 U2492 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507
A2518 G2529 A2533 U2537 C2538 C2539 C2540 A2541 A2542 G2543 G2544 G2545 U2552 G2553 U2554 U2555 A2564 A2565 A2566 G2567 G2570 C2571 A2572 C2573 G2578 U2584 U2585 C2586 C2601 A2602 G2603 U2604 U2605 U2609 C2610 U2611 C2612 U2615 C2616 C2617 G2618 C2619 C2626 G2627 C2628 A2629 G2630
U2637 G2638 A2639 G2640 C2641 C2646 U2647 C2648 U2649 U2650 A2654 G2659 A2660 C2661 A2662 G2663 G2664 A2665 C2680 C2681 U2682 C2683 U2687 U2688 U2689 C2690 C2691 C2692 A2693 G2694 U2698 C2699 C2703 C2704 A2705 G2706 A2712A A2713 G2714 G2717 U2726 G2732 A2733 A2734 G2735 G2744
A2748 A2749 A2750 G2751 C2752 A2753 U2756 A2757 A2764 A2765 C2768 C2769 C2774 A2775 A2778 C2784 C2788 C2789 A C G2792 G2793 C2794 G U C A A2801A G2802 C2803 C2804 G2805 G2807 U2808 A2809 A2810 G2811 A2820 A2821 G2833 G2834 A2835 U2836 G2837 G2838 G2839 U2849 A2850 G2857



• Molecule 2: 5S Ribosomal RNA

Chain 1B:

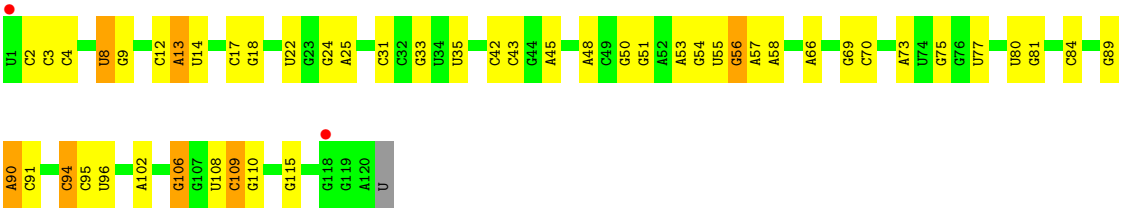




• Molecule 2: 5S Ribosomal RNA

Chain 2B:

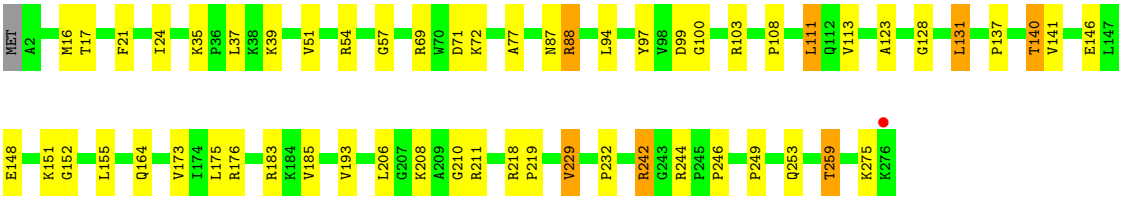




• Molecule 3: 50S ribosomal protein L2

Chain 1D:

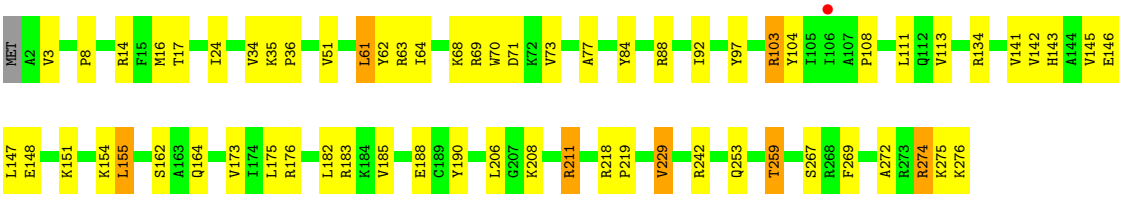




• Molecule 3: 50S ribosomal protein L2

Chain 2D:

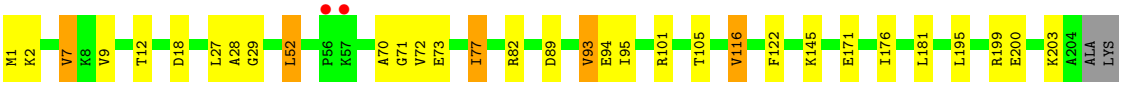




• Molecule 4: 50S ribosomal protein L3

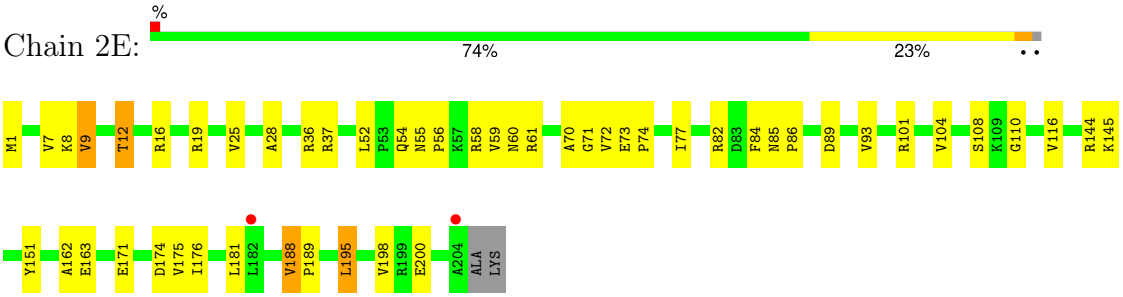
Chain 1E:





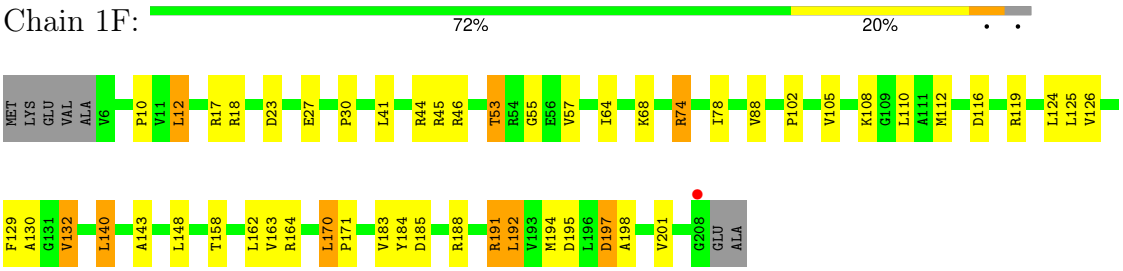
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



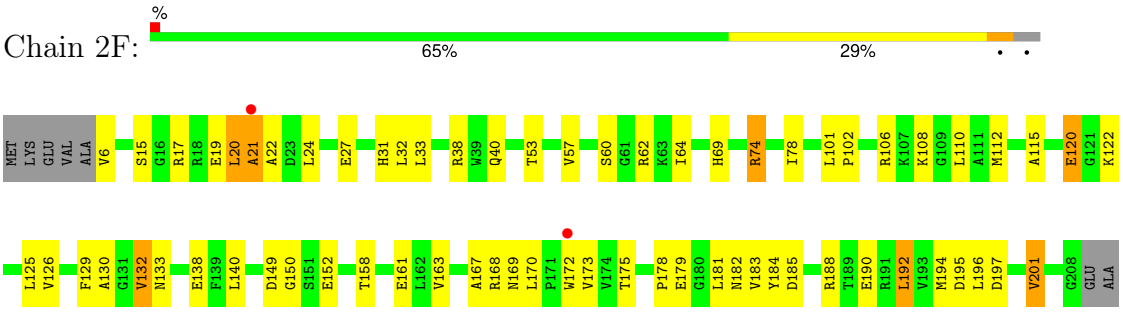
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



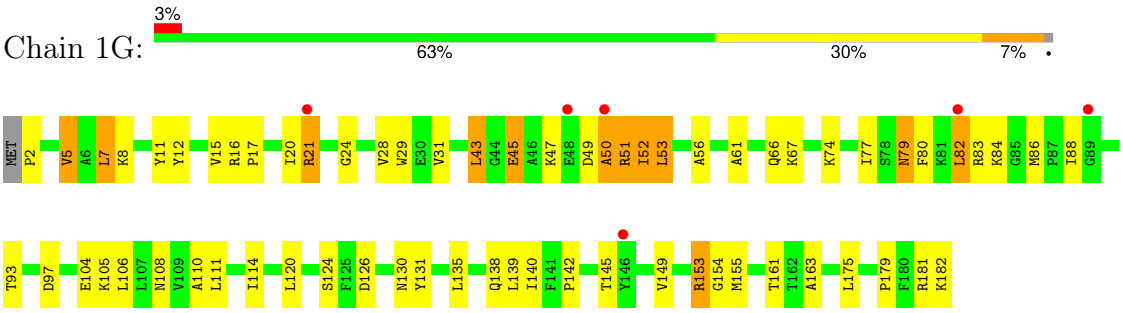
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



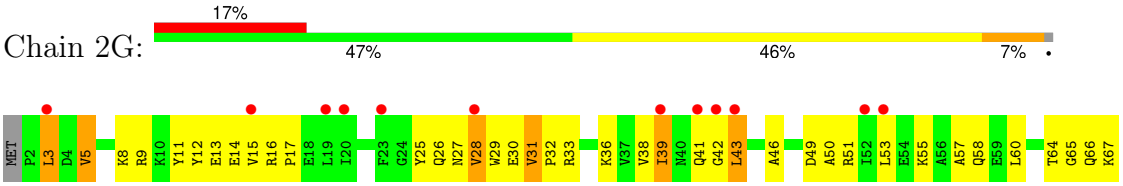
• Molecule 6: 50S ribosomal protein L5

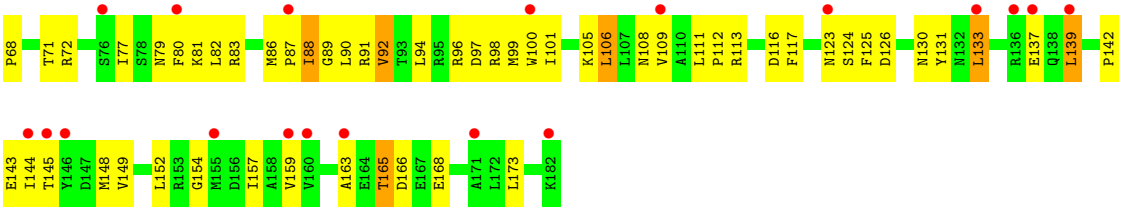
Chain 1G:



• Molecule 6: 50S ribosomal protein L5

Chain 2G:





• Molecule 7: 50S ribosomal protein L6

Chain 1H:

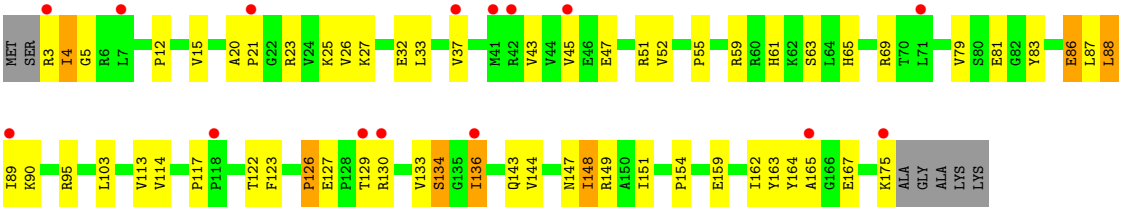




• Molecule 7: 50S ribosomal protein L6

Chain 2H:

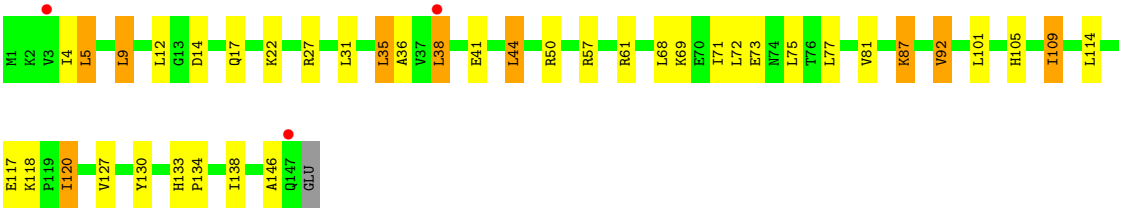




• Molecule 8: 50S ribosomal protein L9

Chain 1I:

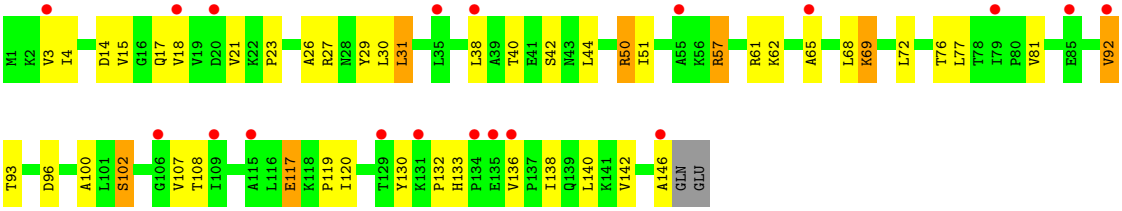




• Molecule 8: 50S ribosomal protein L9

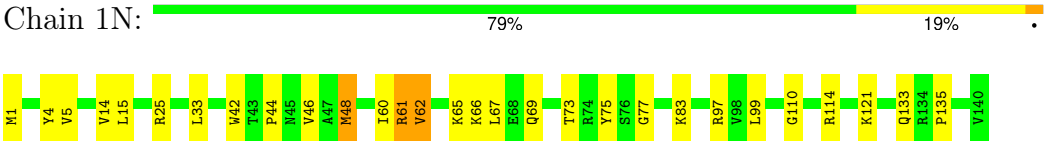
Chain 2I:





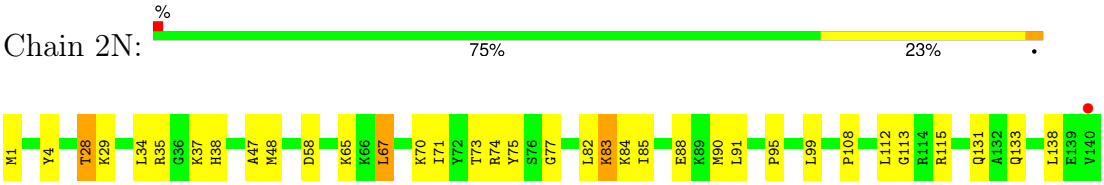
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



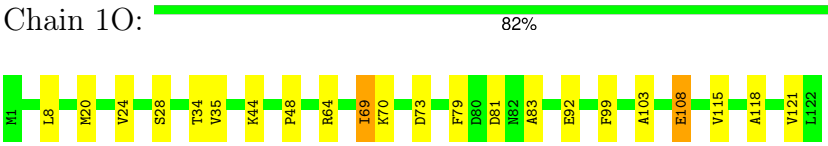
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



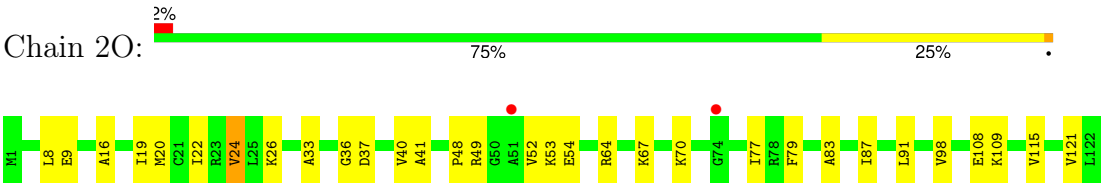
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



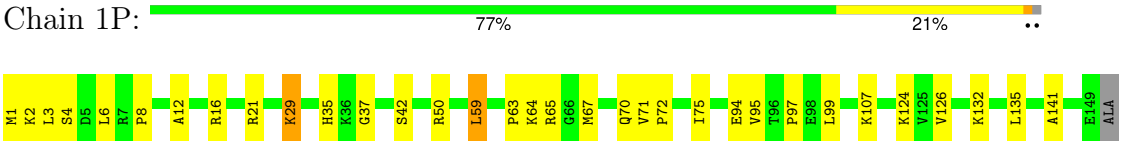
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



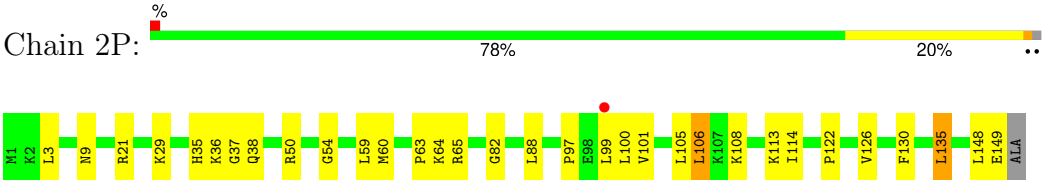
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



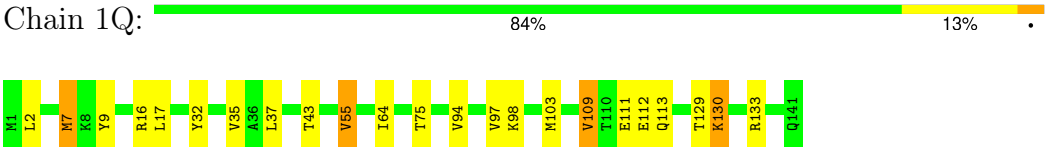
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



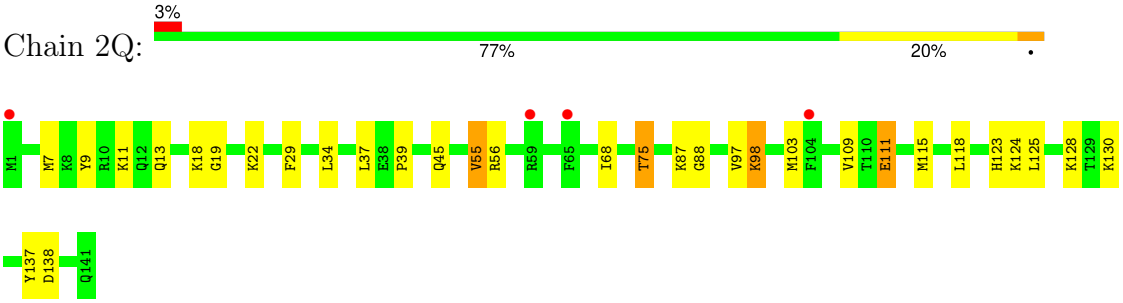
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



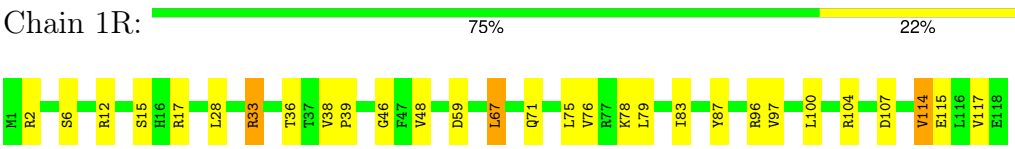
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



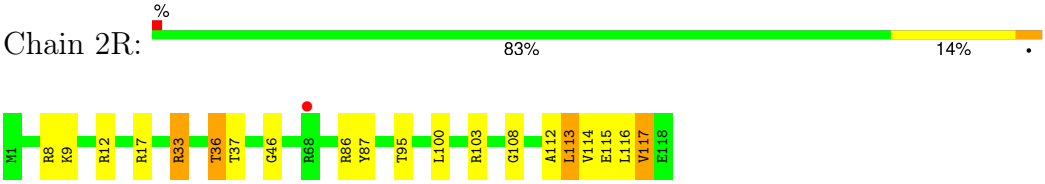
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



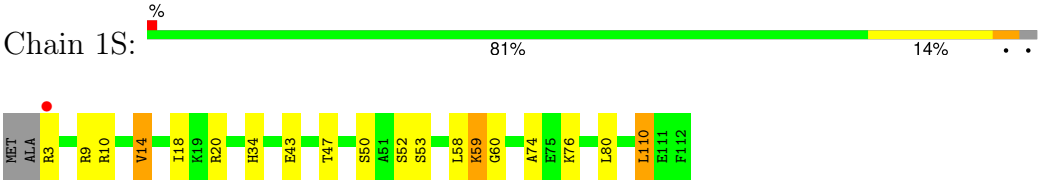
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



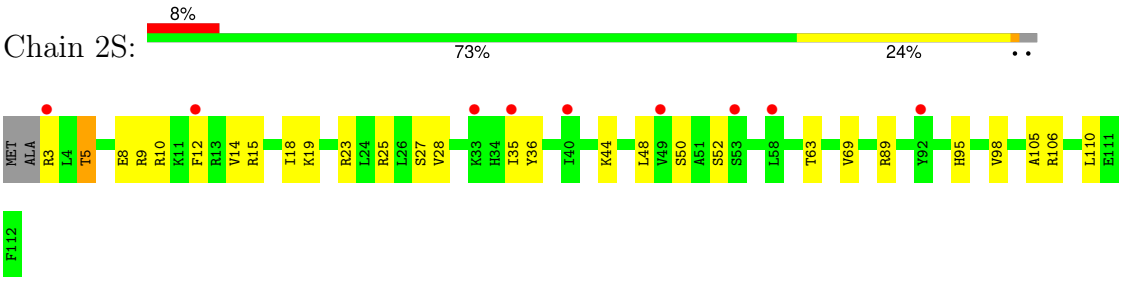
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



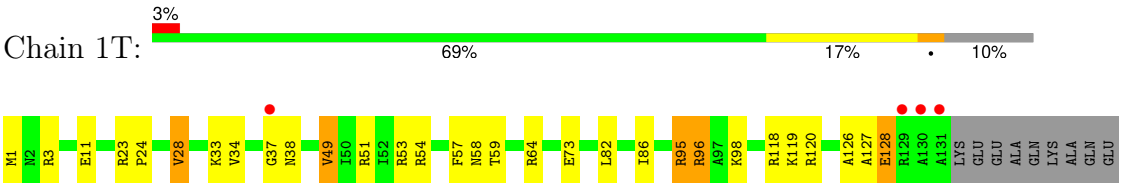
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



• Molecule 15: 50S ribosomal protein L19

Chain 1T:





• Molecule 15: 50S ribosomal protein L19

Chain 2T:



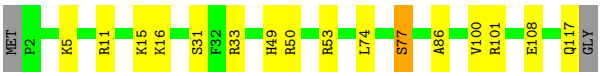




• Molecule 16: 50S ribosomal protein L20

Chain 1U:

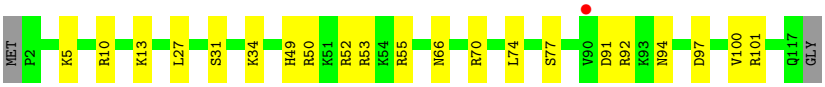




• Molecule 16: 50S ribosomal protein L20

Chain 2U:





• Molecule 17: 50S ribosomal protein L21

Chain 1V:

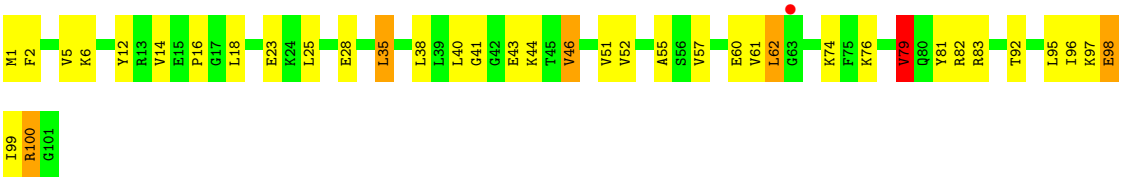




• Molecule 17: 50S ribosomal protein L21

Chain 2V:





• Molecule 18: 50S ribosomal protein L22

Chain 1W:

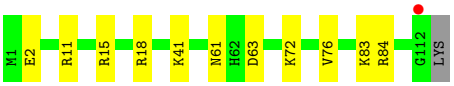




• Molecule 18: 50S ribosomal protein L22

Chain 2W:

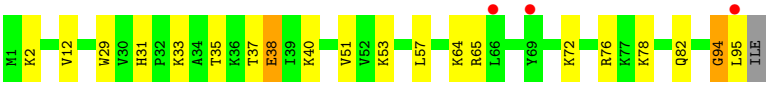




• Molecule 19: 50S ribosomal protein L23

Chain 1X:

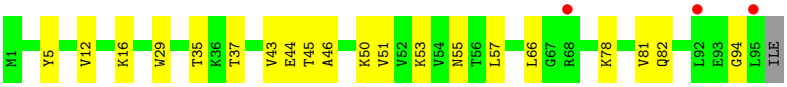




• Molecule 19: 50S ribosomal protein L23

Chain 2X:

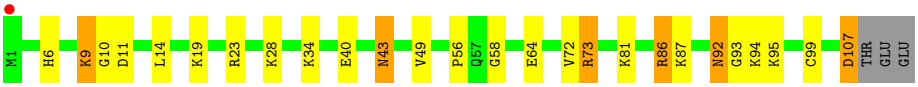




• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

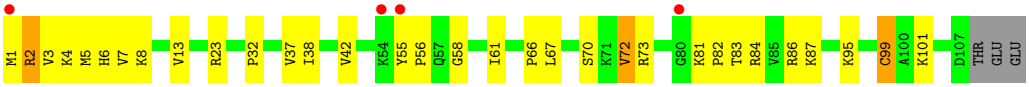




• Molecule 20: 50S ribosomal protein L24

Chain 2Y:

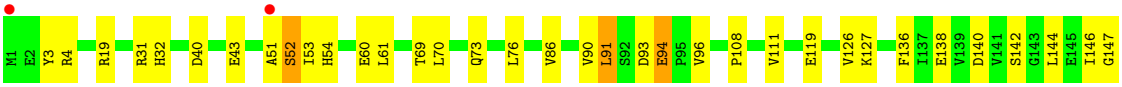


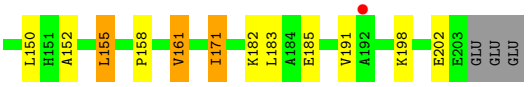


• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



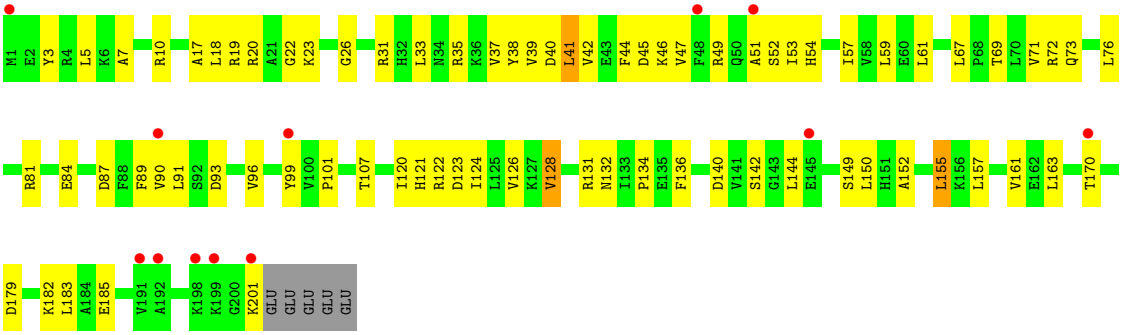




• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

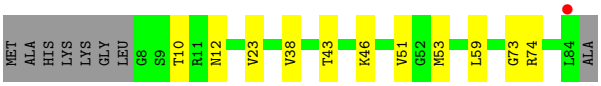




• Molecule 22: 50S ribosomal protein L27

Chain 10:

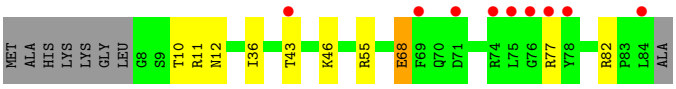




• Molecule 22: 50S ribosomal protein L27

Chain 20:

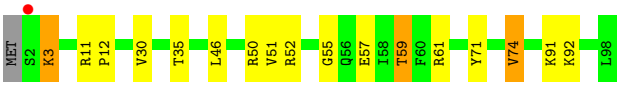




• Molecule 23: 50S ribosomal protein L28

Chain 11:

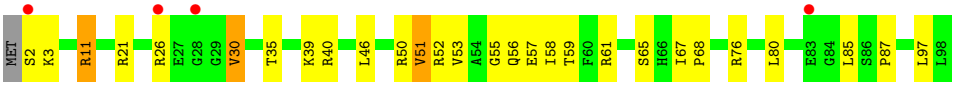




• Molecule 23: 50S ribosomal protein L28

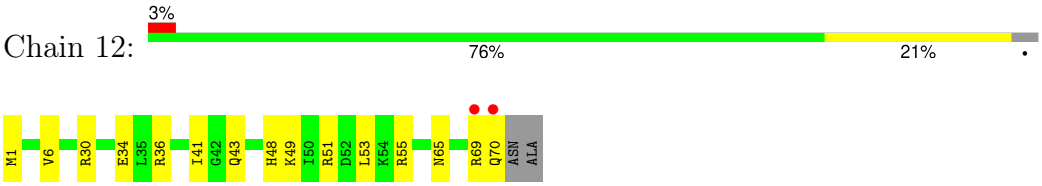
Chain 21:





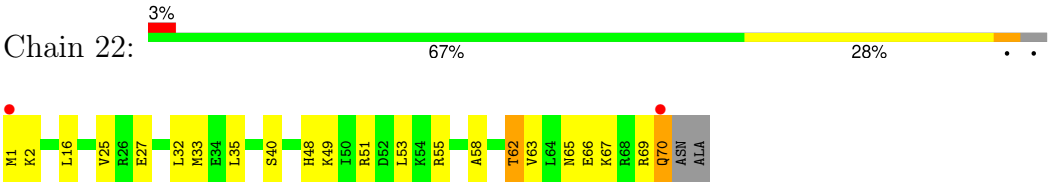
• Molecule 24: 50S ribosomal protein L29

Chain 12:



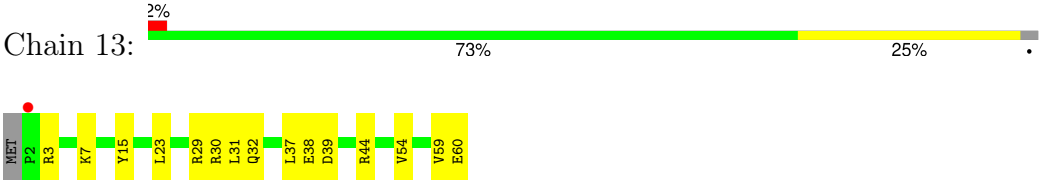
• Molecule 24: 50S ribosomal protein L29

Chain 22:



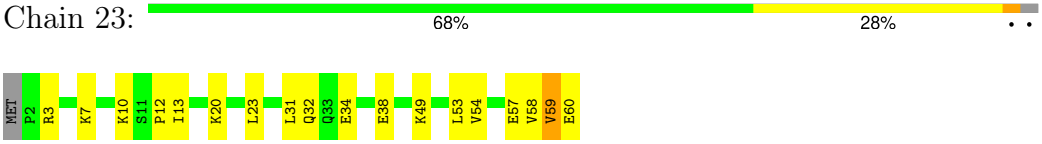
• Molecule 25: 50S ribosomal protein L30

Chain 13:



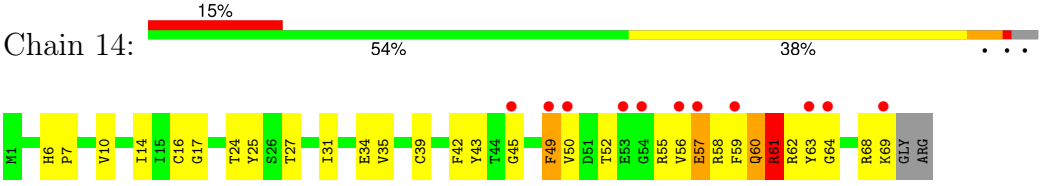
• Molecule 25: 50S ribosomal protein L30

Chain 23:



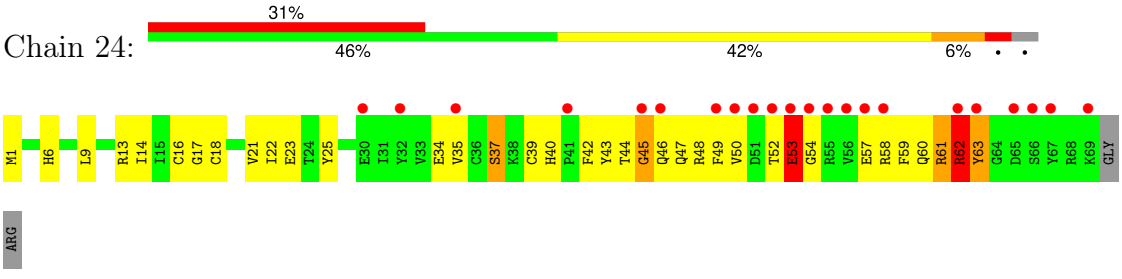
• Molecule 26: 50S ribosomal protein L31

Chain 14:



• Molecule 26: 50S ribosomal protein L31

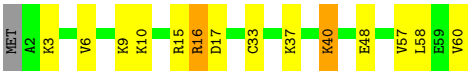
Chain 24:



• Molecule 27: 50S ribosomal protein L32

Chain 15:

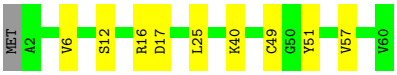




• Molecule 27: 50S ribosomal protein L32

Chain 25:





• Molecule 28: 50S ribosomal protein L33

Chain 16:

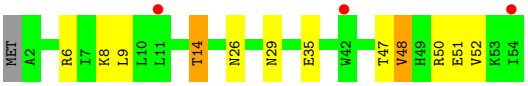




• Molecule 28: 50S ribosomal protein L33

Chain 26:

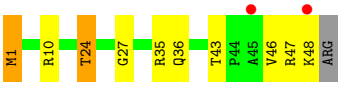




• Molecule 29: 50S ribosomal protein L34

Chain 17:

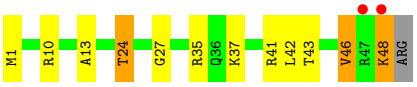




• Molecule 29: 50S ribosomal protein L34

Chain 27:

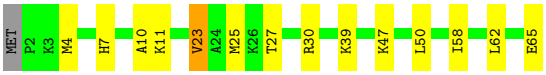




• Molecule 30: 50S ribosomal protein L35

Chain 18:





• Molecule 30: 50S ribosomal protein L35

Chain 28:

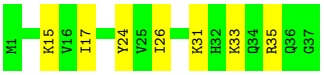




• Molecule 31: 50S ribosomal protein L36

Chain 19:

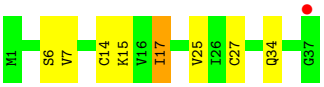




• Molecule 31: 50S ribosomal protein L36

Chain 29:

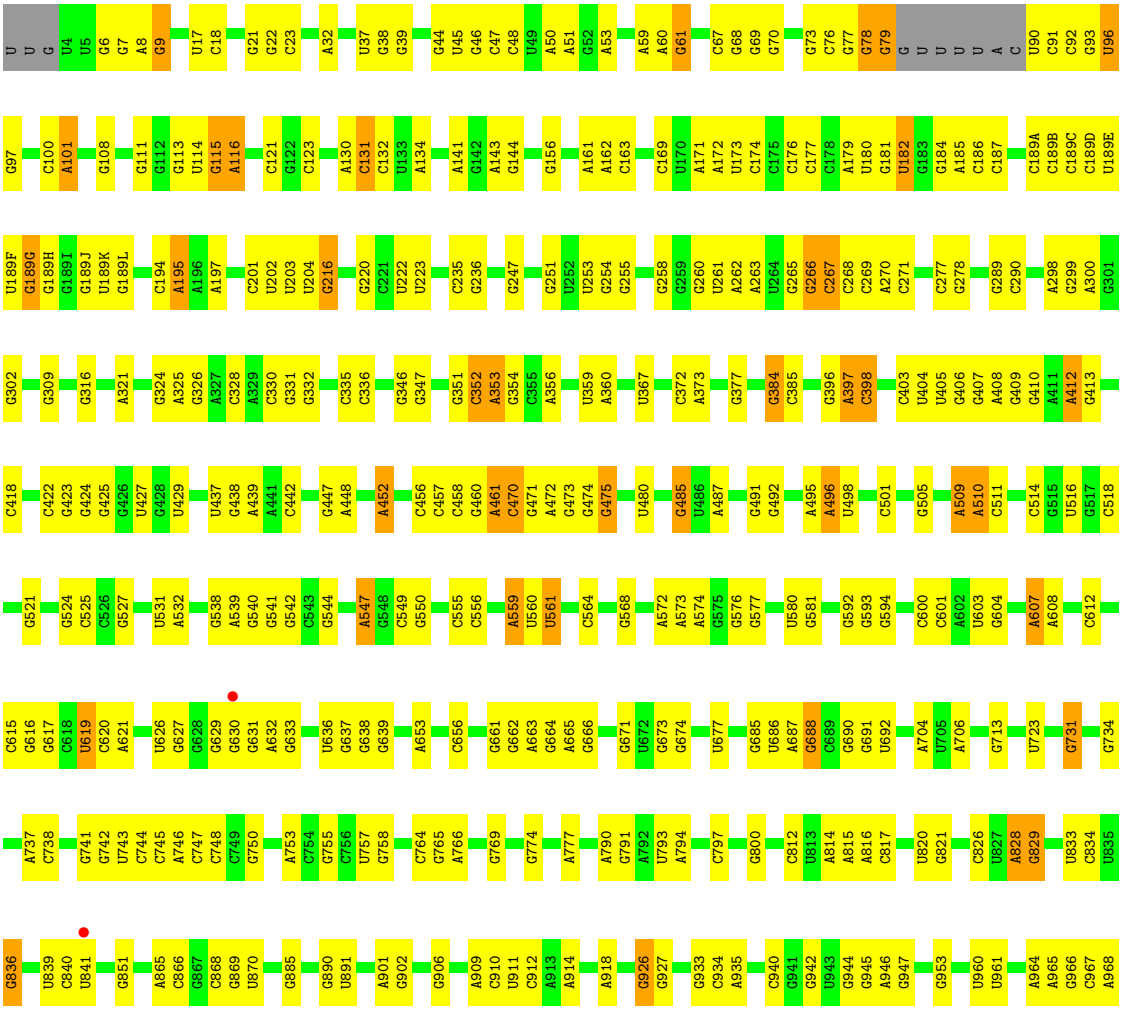


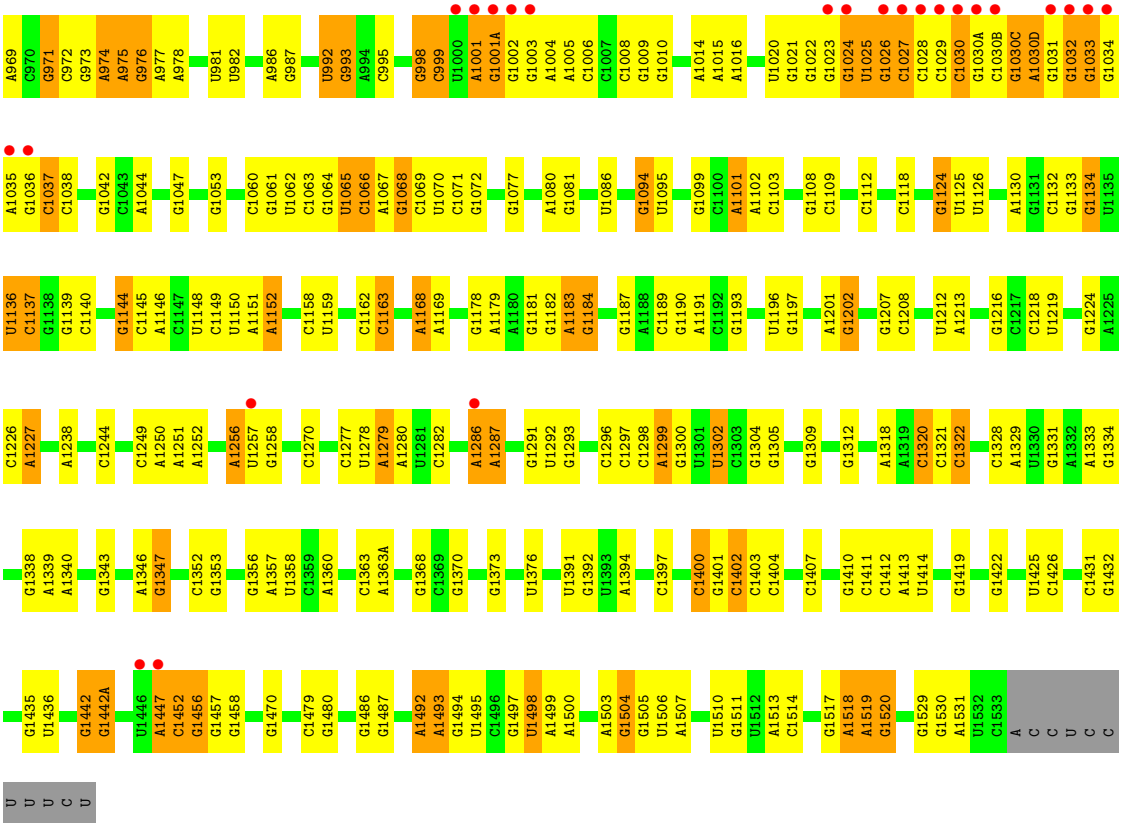


• Molecule 32: 16S Ribosomal RNA

Chain 1a:



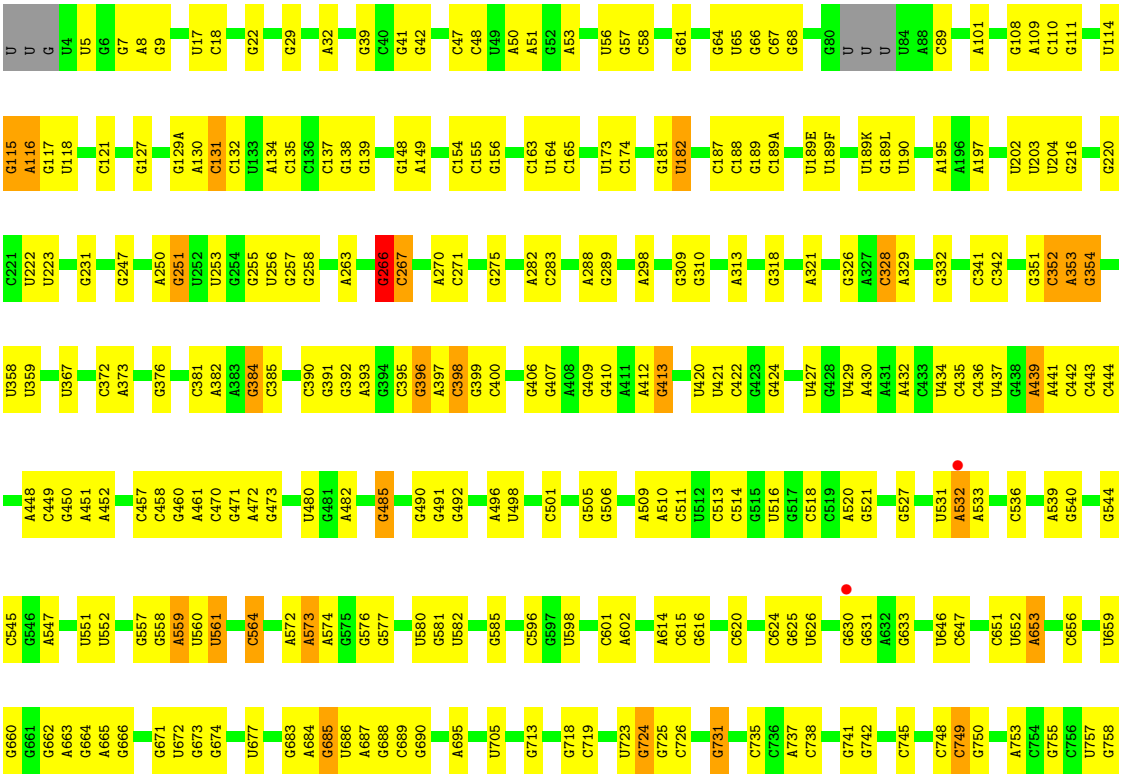


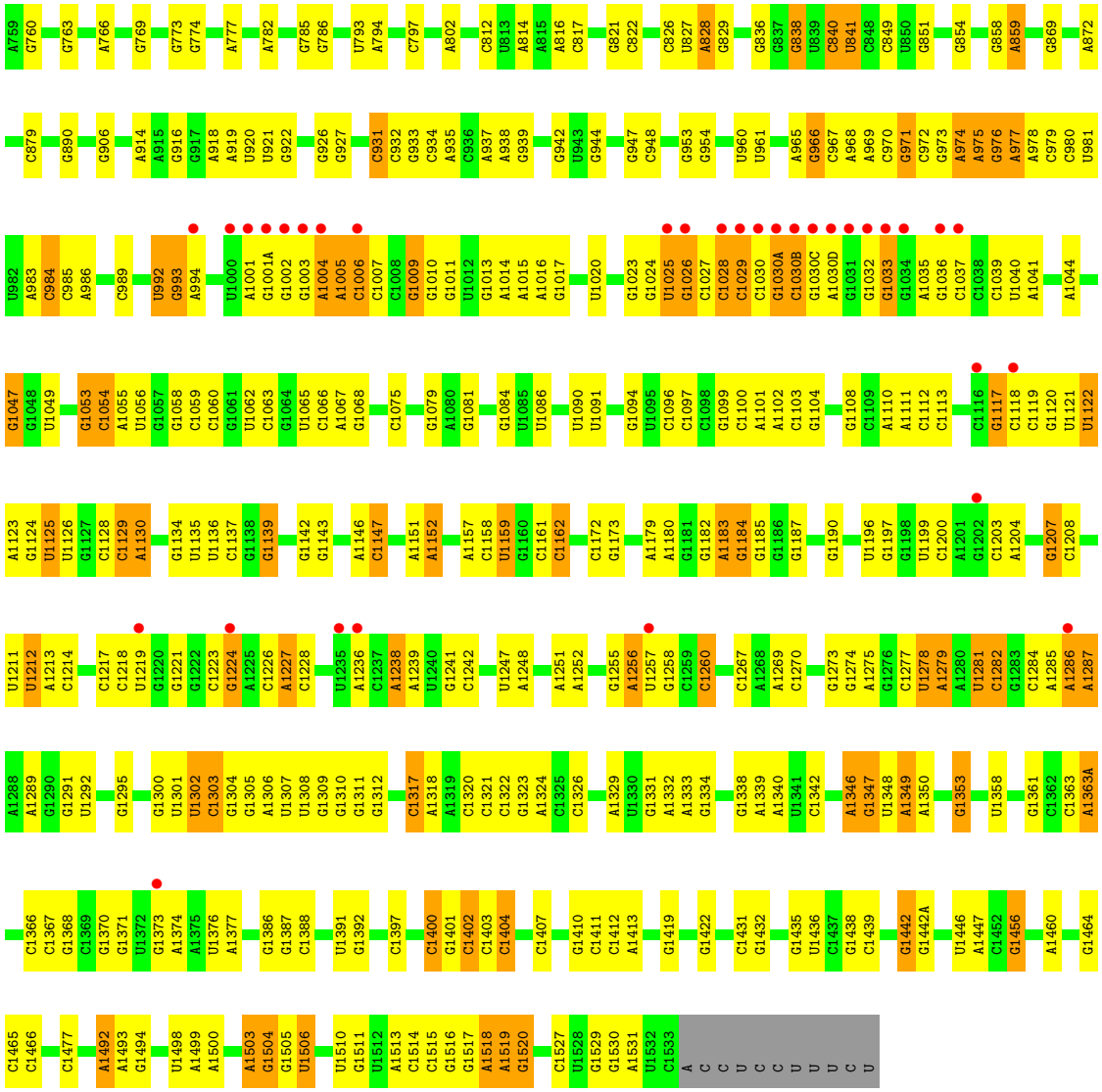


• Molecule 32: 16S Ribosomal RNA

Chain 2a:



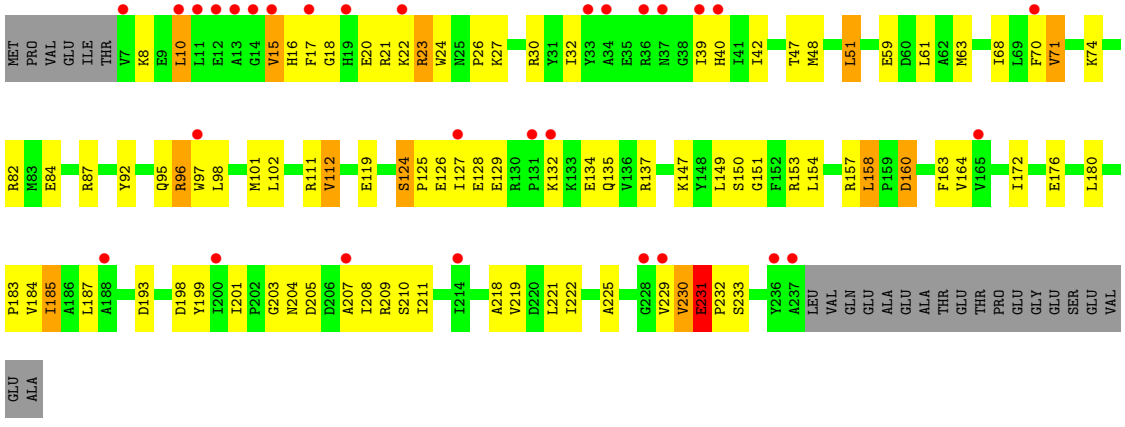




• Molecule 33: 30S ribosomal protein S2

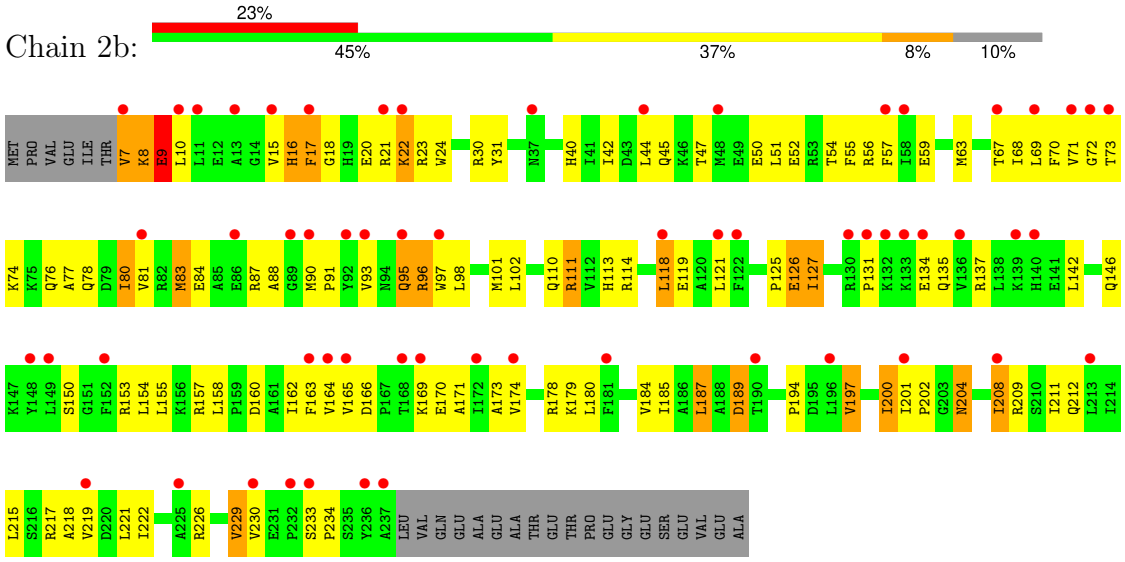
Chain 1b:





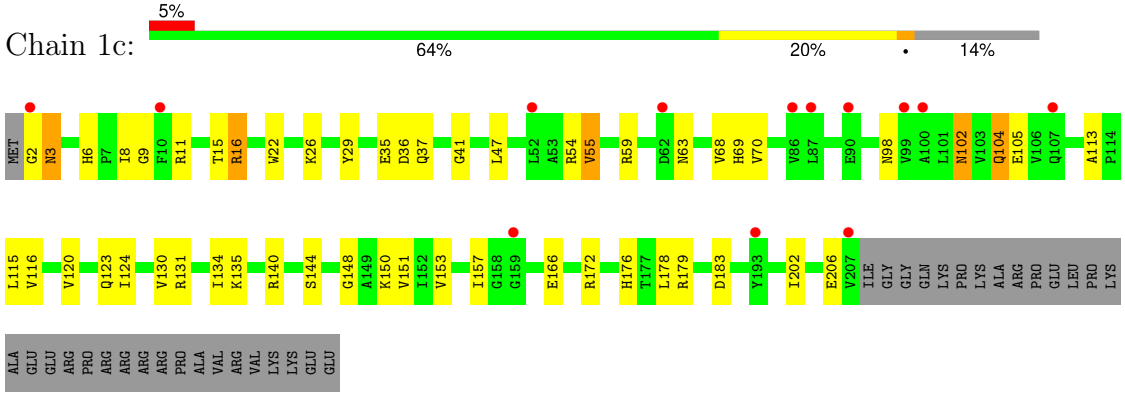
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



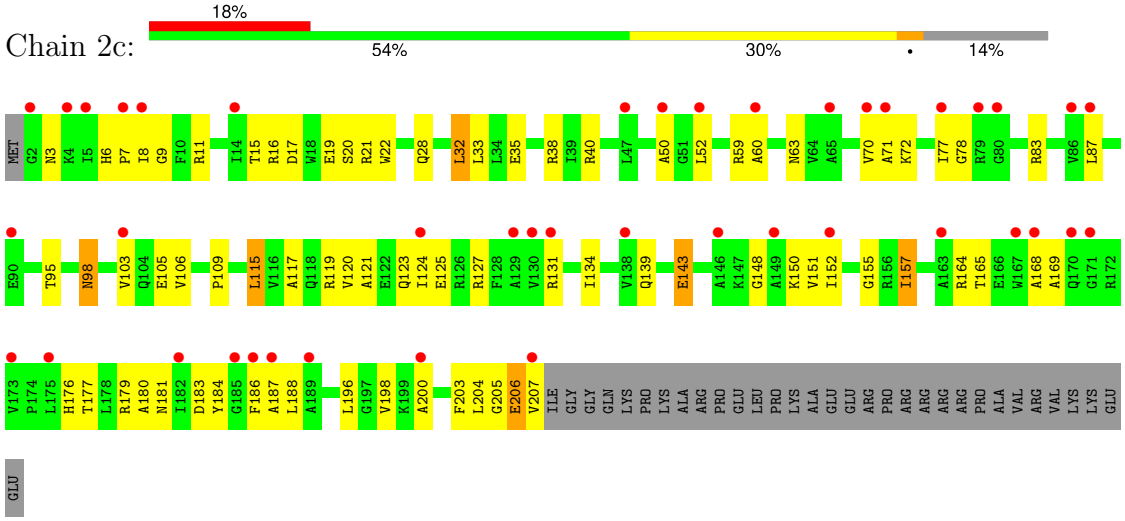
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



• Molecule 34: 30S ribosomal protein S3

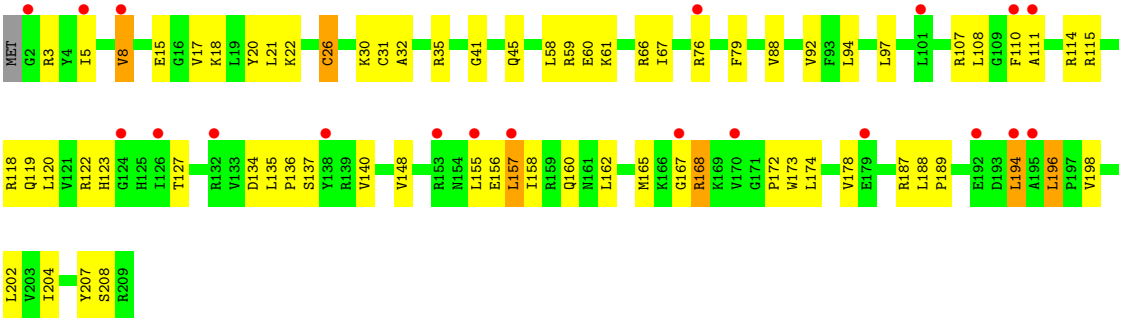
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

Chain 1d:

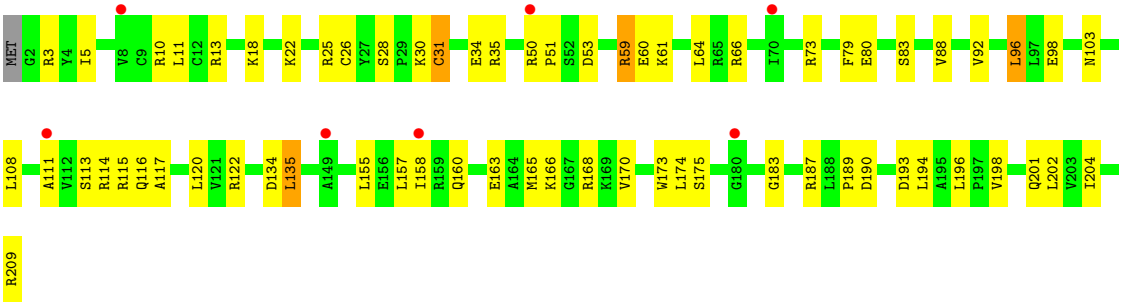




• Molecule 35: 30S ribosomal protein S4

Chain 2d:

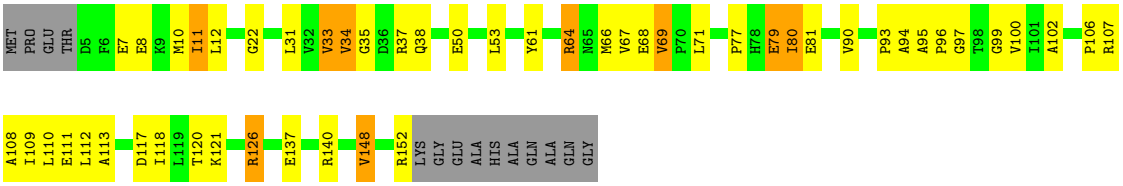




• Molecule 36: 30S ribosomal protein S5

Chain 1e:

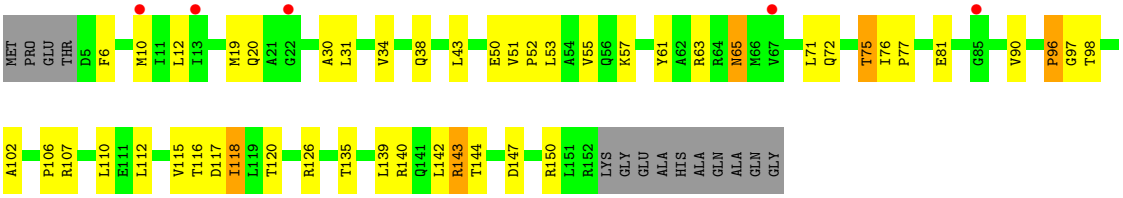




• Molecule 36: 30S ribosomal protein S5

Chain 2e:

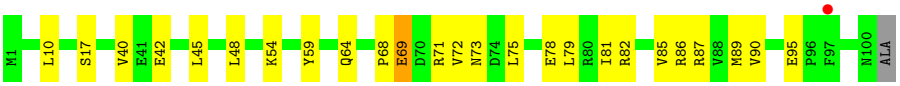




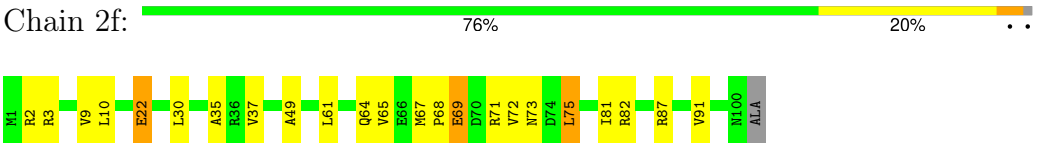
• Molecule 37: 30S ribosomal protein S6

Chain 1f:

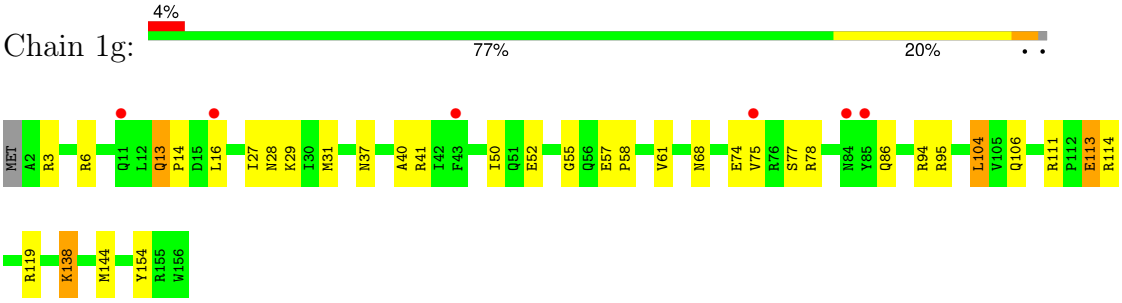




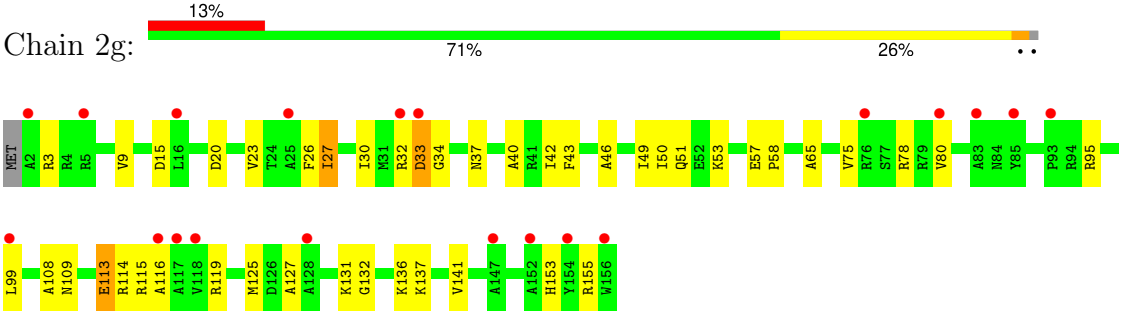
• Molecule 37: 30S ribosomal protein S6



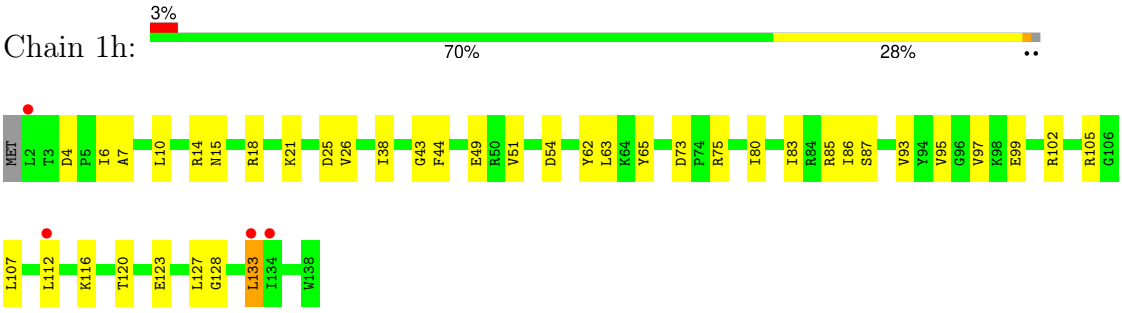
• Molecule 38: 30S ribosomal protein S7



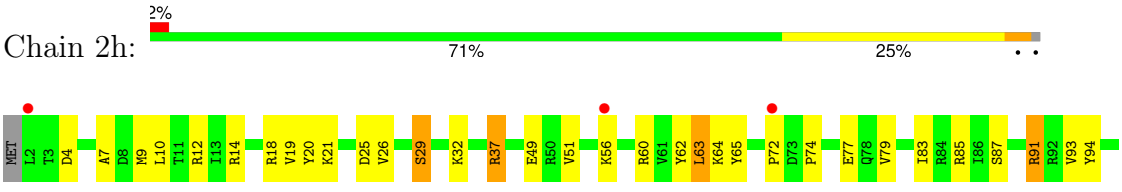
• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8



• Molecule 39: 30S ribosomal protein S8

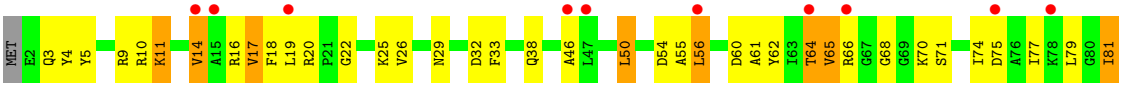


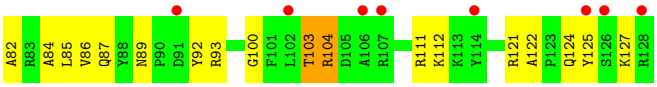


• Molecule 40: 30S ribosomal protein S9

Chain 1i:



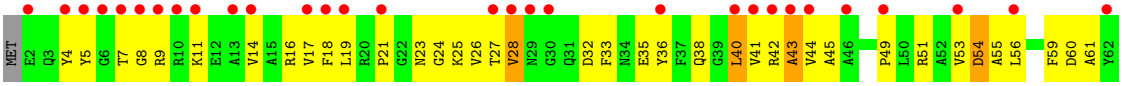


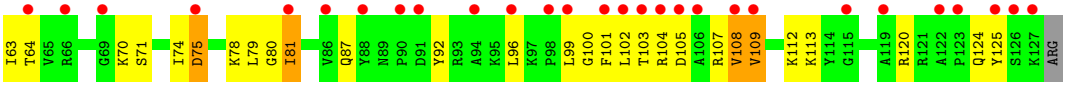


• Molecule 40: 30S ribosomal protein S9

Chain 2i:



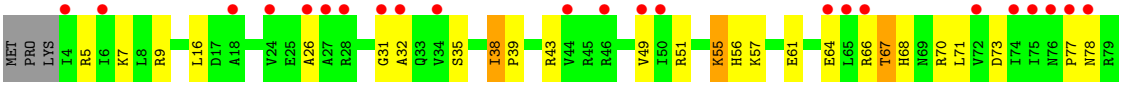


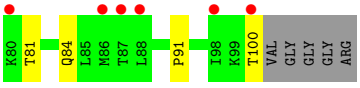


• Molecule 41: 30S ribosomal protein S10

Chain 1j:



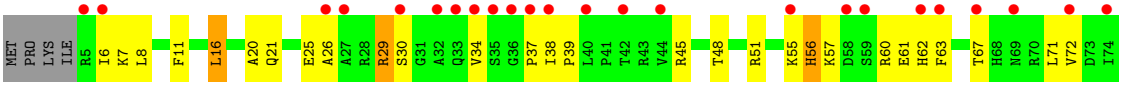


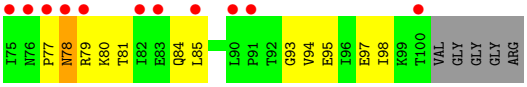


• Molecule 41: 30S ribosomal protein S10

Chain 2j:



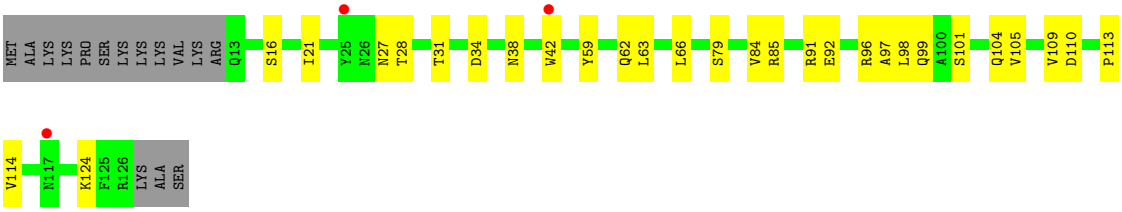




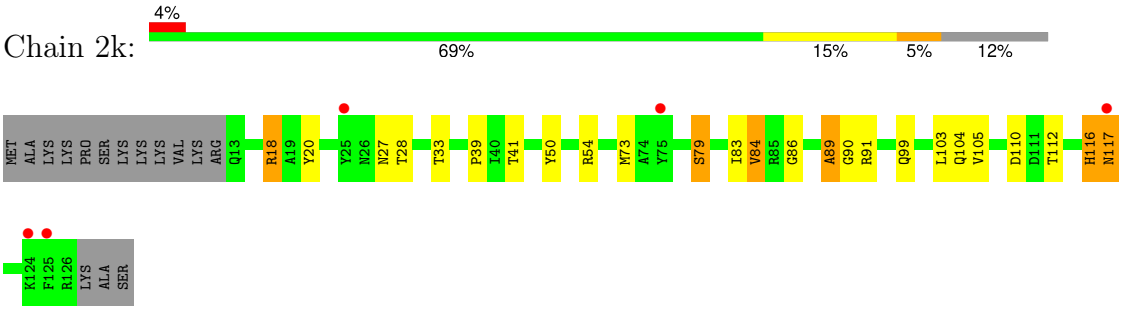
• Molecule 42: 30S ribosomal protein S11

Chain 1k:

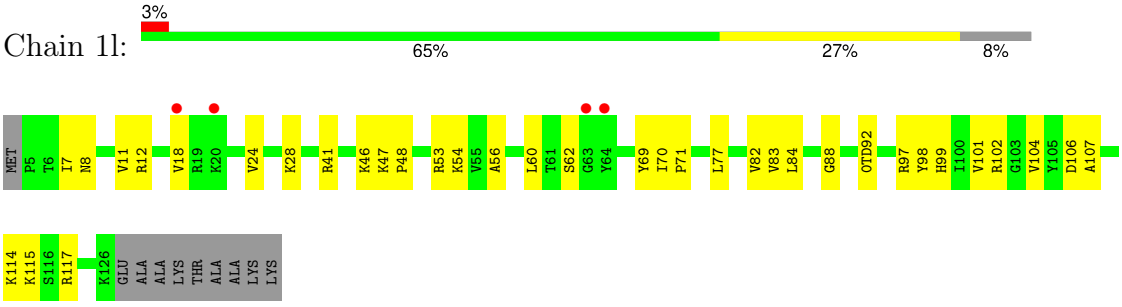




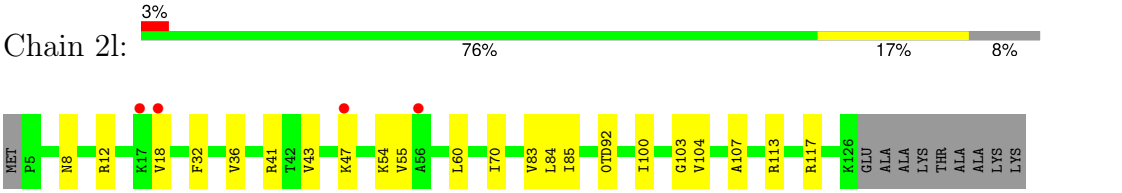
• Molecule 42: 30S ribosomal protein S11



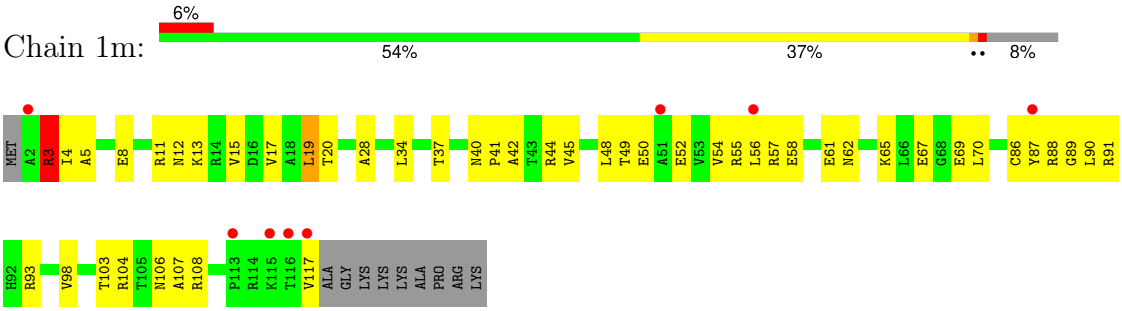
• Molecule 43: 30S ribosomal protein S12



• Molecule 43: 30S ribosomal protein S12

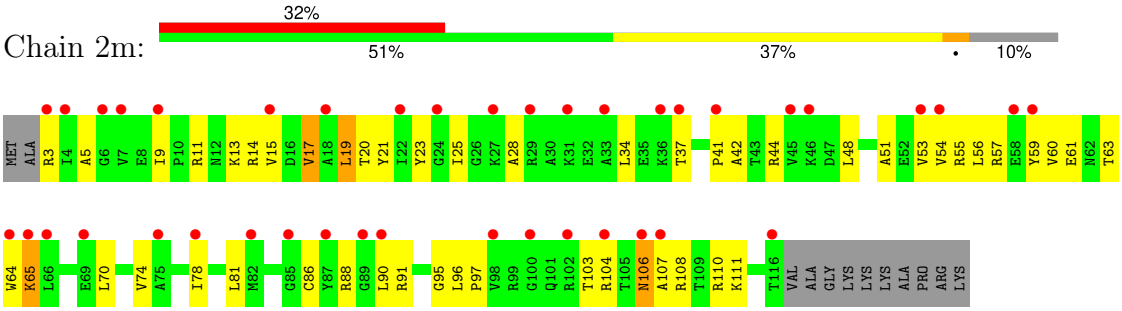


• Molecule 44: 30S ribosomal protein S13



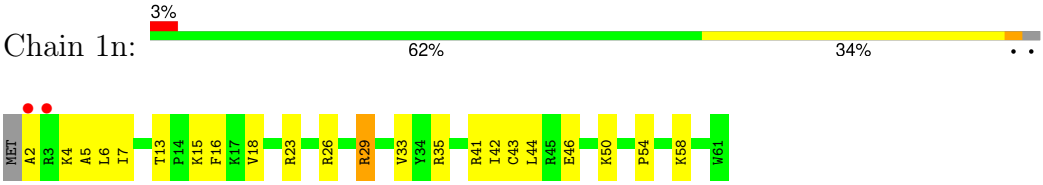
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



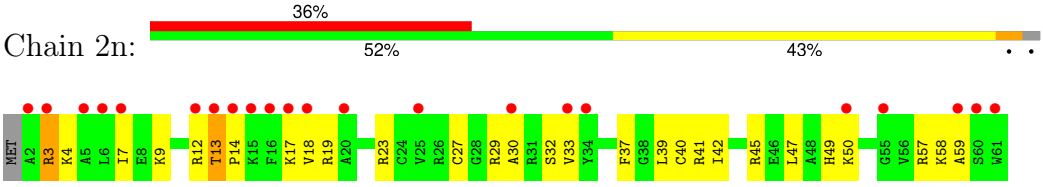
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



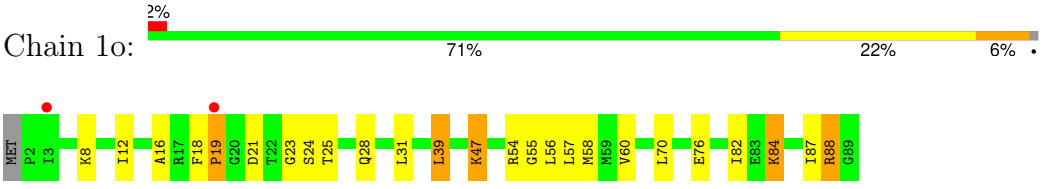
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



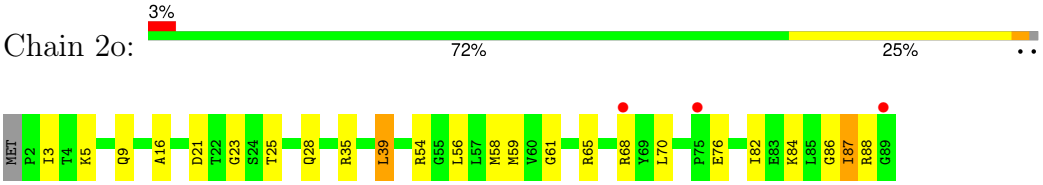
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



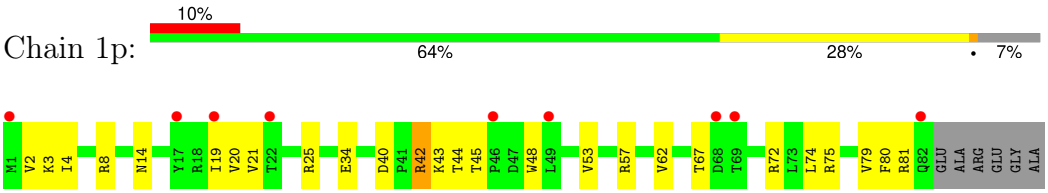
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



• Molecule 47: 30S ribosomal protein S16

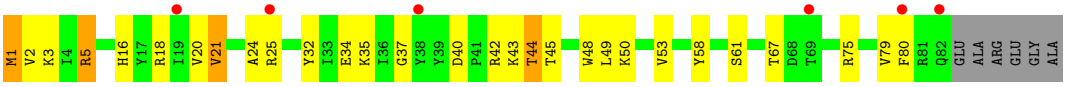
Chain 1p:



• Molecule 47: 30S ribosomal protein S16

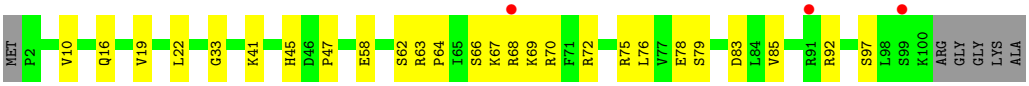
Chain 2p:





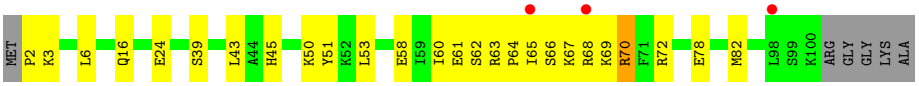
• Molecule 48: 30S ribosomal protein S17





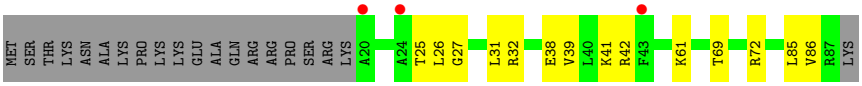
• Molecule 48: 30S ribosomal protein S17





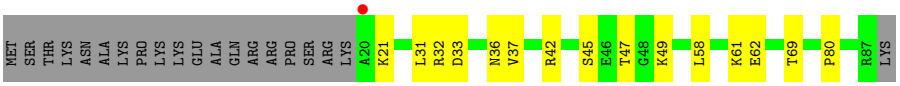
• Molecule 49: 30S ribosomal protein S18





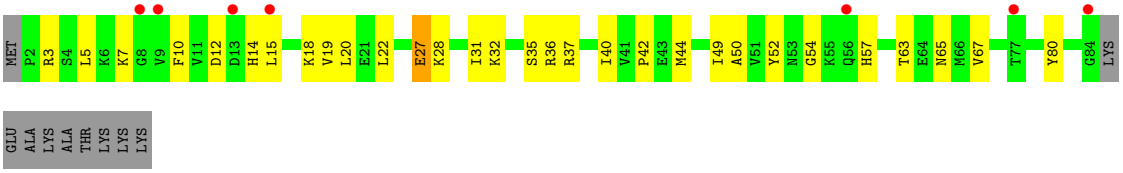
• Molecule 49: 30S ribosomal protein S18





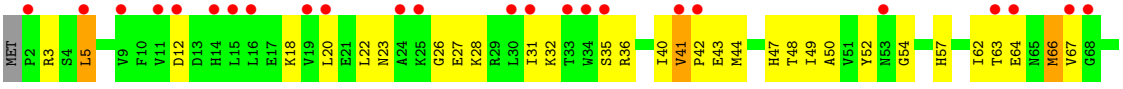
• Molecule 50: 30S ribosomal protein S19

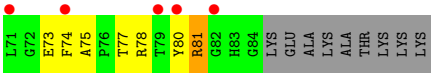




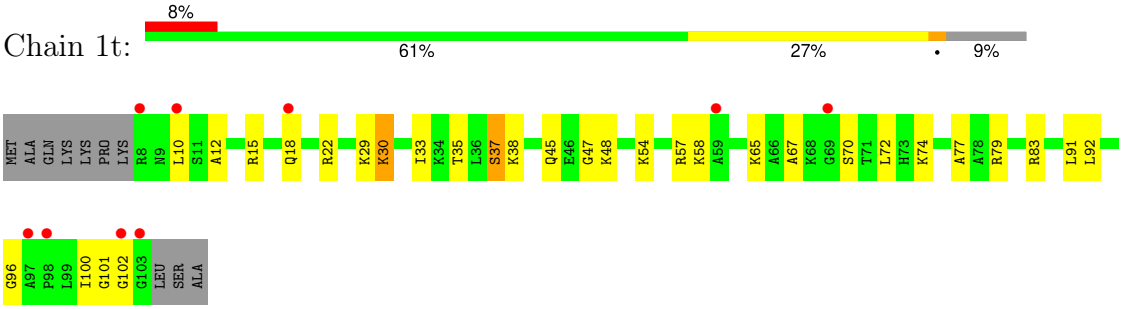
• Molecule 50: 30S ribosomal protein S19



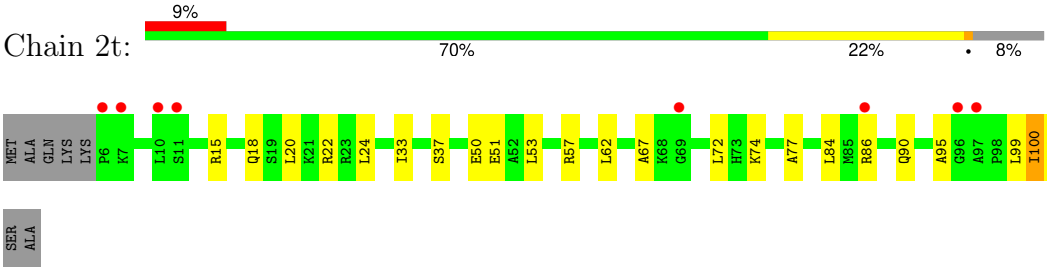




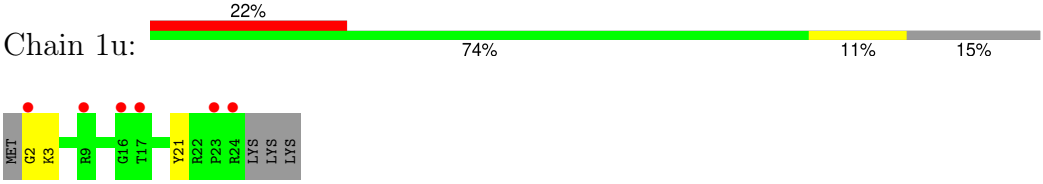
• Molecule 51: 30S ribosomal protein S20



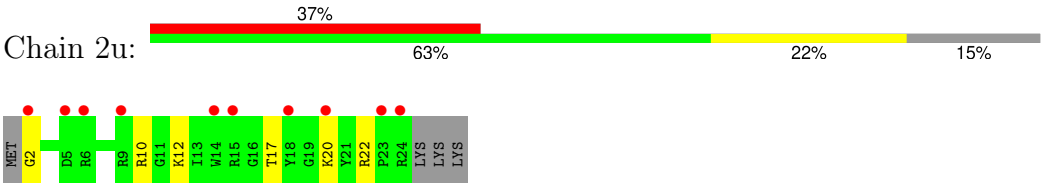
• Molecule 51: 30S ribosomal protein S20



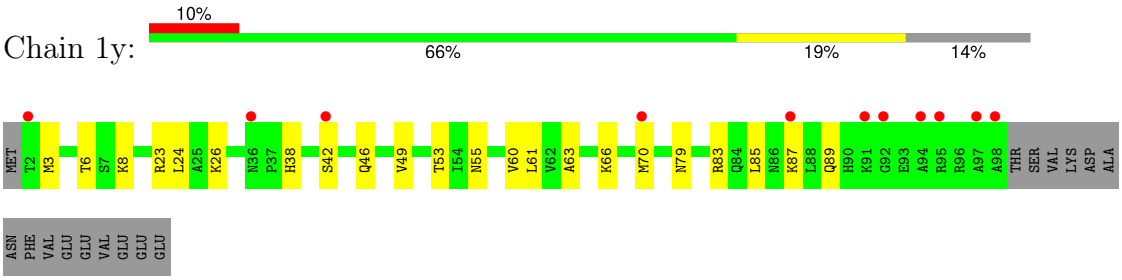
• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx

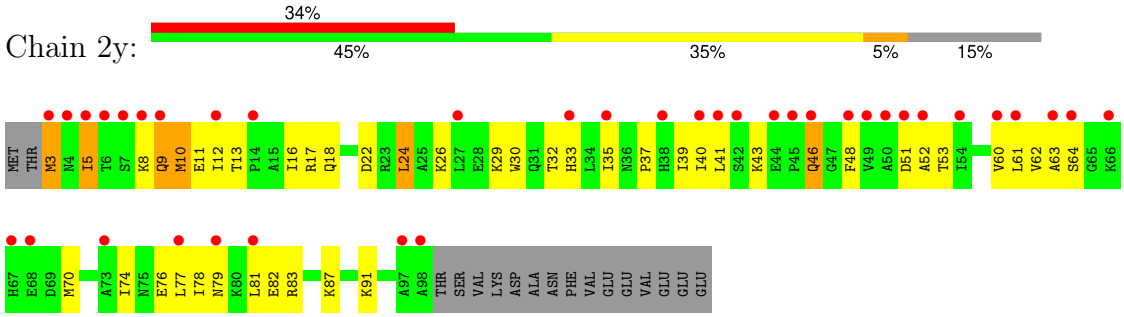


• Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:


34%
45%
35%
5%
15%
MET THR M3 N4 I5 T6 S7 K8 Q9 M10 E11 I12 T13 P14 A15 I16 R17 Q18 D22 R23 L24 A25 K26 L27 E28 K29 W30 Q31 T32 H33 L34 I35 N36 P37 H38 I39 I40 L41 S42 K43 E44 P45 Q46 G47 F48 V49 A50 D51 A52 T53 I54 V60 L61 V62 A63 S64 G65 K66
H67 E68 D69 M70 A73 I74 N75 E76 L77 I78 N79 K80 L81 E82 R83 K87 K91 A97 A98 THR SER VAL LYS ASP ALA ASN PHE VAL GLU GLU VAL GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.90Å 450.73Å 622.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.04 – 2.50 174.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (174.04-2.50) 99.8 (174.04-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.250 0.209 , 0.252	Depositor DCC
R_{free} test set	100475 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	296715	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, UR3, MA6, 2MU, 2MA, MPD, MG, ZN, M2G, ZIT, HGR, 2MG, G7M, SF4, OMC, 4OC, PSU, 5MC, 5MU, 0TD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1A	0.29	0/69030	0.49	5/107750 (0.0%)
1	2A	0.23	0/68902	0.43	2/107548 (0.0%)
2	1B	0.24	0/2876	0.44	0/4486
2	2B	0.20	0/2878	0.39	0/4490
3	1D	0.28	0/2181	0.53	0/2940
3	2D	0.24	0/2186	0.50	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.22	0/1451	0.43	0/1961
6	2G	0.21	0/1449	0.41	0/1957
7	1H	0.22	0/1356	0.44	0/1834
7	2H	0.19	0/1350	0.42	0/1826
8	1I	0.20	0/1109	0.43	0/1512
8	2I	0.18	0/1091	0.38	0/1490
9	1N	0.25	0/1148	0.46	0/1547
9	2N	0.21	0/1144	0.39	0/1543
10	1O	0.27	0/943	0.51	0/1269
10	2O	0.22	0/943	0.43	0/1269
11	1P	0.27	0/1152	0.51	0/1533
11	2P	0.24	0/1152	0.51	2/1533 (0.1%)
12	1Q	0.27	0/1143	0.50	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.30	0/982	0.53	0/1312
13	2R	0.23	0/982	0.47	0/1312
14	1S	0.23	0/887	0.47	0/1180
14	2S	0.21	0/880	0.42	0/1172
15	1T	0.27	0/1105	0.52	0/1477
15	2T	0.22	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.27	0/786	0.48	0/1053
17	2V	0.20	0/782	0.42	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.22	0/897	0.43	0/1205
19	1X	0.27	0/764	0.52	0/1025
19	2X	0.22	0/764	0.43	0/1025
20	1Y	0.26	0/823	0.55	0/1099
20	2Y	0.20	0/823	0.48	0/1100
21	1Z	0.23	0/1620	0.45	0/2200
21	2Z	0.19	0/1590	0.41	0/2162
22	10	0.27	0/616	0.48	0/821
22	20	0.21	0/616	0.46	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.25	0/766	0.43	0/1018
24	12	0.25	0/590	0.43	0/781
24	22	0.20	0/594	0.38	0/785
25	13	0.29	0/474	0.51	0/635
25	23	0.21	0/469	0.46	0/630
26	14	0.26	0/559	0.66	0/754
26	24	0.29	0/549	0.63	0/741
27	15	0.31	0/473	0.55	0/639
27	25	0.22	0/469	0.46	0/635
28	16	0.26	0/460	0.50	0/613
28	26	0.22	0/456	0.40	0/608
29	17	0.31	0/426	0.55	0/561
29	27	0.27	0/426	0.48	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.28	0/310	0.51	0/407
31	29	0.22	0/310	0.45	0/407
32	1a	0.21	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	0/35890	0.38	2/56012 (0.0%)
33	1b	0.22	0/1876	0.48	0/2533
33	2b	0.23	0/1860	0.47	0/2518
34	1c	0.20	0/1582	0.41	0/2137
34	2c	0.21	0/1566	0.41	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.19	0/1698	0.41	0/2277
36	1e	0.22	0/1149	0.45	0/1548
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/827	0.39	0/1120
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1254	0.38	0/1683
38	2g	0.20	0/1248	0.39	0/1676
39	1h	0.20	0/1118	0.43	0/1506
39	2h	0.18	0/1108	0.45	0/1494
40	1i	0.21	0/1005	0.47	0/1351
40	2i	0.22	0/985	0.50	0/1329
41	1j	0.29	0/732	0.44	0/993
41	2j	0.21	0/723	0.47	0/984
42	1k	0.18	0/849	0.39	0/1150
42	2k	0.19	0/848	0.45	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.20	0/924	0.50	0/1242
44	2m	0.21	0/905	0.48	0/1217
45	1n	0.21	0/501	0.46	0/664
45	2n	0.20	0/501	0.44	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.20	0/739	0.38	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.21	0/693	0.45	0/935
48	1q	0.21	0/836	0.42	0/1117
48	2q	0.21	0/836	0.43	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.20	0/560	0.39	0/746
50	1s	0.21	0/663	0.44	0/895
50	2s	0.20	0/660	0.42	0/893
51	1t	0.20	0/734	0.45	0/969
51	2t	0.20	0/736	0.43	0/976
52	1u	0.19	0/203	0.41	0/266
52	2u	0.21	0/203	0.49	0/266
53	1y	0.19	0/776	0.38	0/1048
53	2y	0.19	0/761	0.36	0/1030
All	All	0.24	0/309939	0.44	14/463231 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	1T	0	1
21	2Z	0	1
26	14	0	1
33	1b	0	1
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1042	G	OP1-P-O3'	-9.62	79.13	108.00
1	2A	1992	G	C2'-C3'-O3'	6.32	118.99	109.50
1	1A	1042	G	OP2-P-O3'	-6.13	89.60	108.00
1	1A	1653	G	C2'-C3'-O3'	5.56	117.84	109.50
11	2P	36	LYS	CA-C-N	-5.54	116.60	122.30
11	2P	36	LYS	C-N-CA	-5.54	116.60	122.30
32	2a	266	G	C2'-C3'-O3'	5.49	117.73	109.50
1	1A	1210	A	C4'-C3'-O3'	5.35	117.43	109.40
1	1A	512	G	O4'-C1'-N9	5.24	116.06	108.20
5	2F	21	ALA	CA-C-N	5.21	131.07	121.70
5	2F	21	ALA	C-N-CA	5.21	131.07	121.70
32	2a	266	G	P-O3'-C3'	5.19	127.98	120.20
1	2A	752	A	C2'-C3'-O3'	5.18	117.26	109.50
32	1a	1067	A	P-O3'-C3'	5.12	127.87	120.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
11	1P	35	HIS	Peptide
15	1T	95	ARG	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	Peptide
21	2Z	136	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31206	540	0
1	2A	61758	0	31152	675	0
2	1B	2572	0	1305	26	0
2	2B	2573	0	1306	33	0
3	1D	2131	0	2207	38	0
3	2D	2136	0	2218	44	0
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	31	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	42	0
6	1G	1426	0	1445	51	0
6	2G	1424	0	1441	71	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	34	0
8	1I	1094	0	1127	32	0
8	2I	1076	0	1094	27	0
9	1N	1121	0	1195	15	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	15	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	26	0
11	2P	1135	0	1212	19	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	14	0
14	1S	877	0	938	13	0
14	2S	870	0	923	17	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	16	0
17	1V	775	0	841	16	0
17	2V	771	0	830	23	0
18	1W	886	0	940	8	0
18	2W	886	0	940	7	0
19	1X	750	0	814	15	0
19	2X	750	0	814	12	0
20	1Y	810	0	892	20	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	28	0
21	2Z	1557	0	1564	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	608	0	622	9	0
22	20	608	0	622	5	0
23	11	754	0	823	12	0
23	21	759	0	837	19	0
24	12	588	0	643	8	0
24	22	592	0	654	11	0
25	13	469	0	518	7	0
25	23	464	0	514	11	0
26	14	546	0	522	19	0
26	24	536	0	514	39	0
27	15	459	0	476	10	0
27	25	455	0	465	6	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	6	0
29	27	418	0	467	9	0
30	18	517	0	582	14	0
30	28	517	0	582	12	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	401	0
32	2a	32331	0	16338	414	0
33	1b	1842	0	1862	58	0
33	2b	1825	0	1828	80	0
34	1c	1558	0	1557	32	0
34	2c	1542	0	1517	62	0
35	1d	1665	0	1687	52	0
35	2d	1668	0	1703	38	0
36	1e	1133	0	1191	35	0
36	2e	1133	0	1191	31	0
37	1f	814	0	808	11	0
37	2f	816	0	808	11	0
38	1g	1235	0	1249	20	0
38	2g	1229	0	1238	25	0
39	1h	1098	0	1143	22	0
39	2h	1088	0	1126	24	0
40	1i	986	0	990	52	0
40	2i	966	0	953	51	0
41	1j	719	0	672	18	0
41	2j	710	0	661	26	0
42	1k	834	0	838	16	0
42	2k	833	0	836	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	18	0
43	2l	932	0	981	11	0
44	1m	914	0	954	30	0
44	2m	895	0	920	38	0
45	1n	492	0	529	18	0
45	2n	492	0	529	20	0
46	1o	728	0	760	16	0
46	2o	728	0	760	15	0
47	1p	681	0	697	13	0
47	2p	677	0	686	20	0
48	1q	823	0	891	16	0
48	2q	823	0	891	15	0
49	1r	555	0	618	8	0
49	2r	555	0	618	9	0
50	1s	648	0	658	26	0
50	2s	645	0	635	33	0
51	1t	732	0	809	22	0
51	2t	733	0	795	14	0
52	1u	199	0	208	3	0
52	2u	199	0	208	5	0
53	1y	764	0	786	16	0
53	2y	749	0	757	34	0
54	10	8	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	6	0	0	0	0
54	18	2	0	0	0	0
54	19	2	0	0	0	0
54	1A	1021	0	0	0	0
54	1B	29	0	0	0	0
54	1D	20	0	0	0	0
54	1E	10	0	0	0	0
54	1F	17	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1T	3	0	0	0	0
54	1U	6	0	0	0	0
54	1V	6	0	0	0	0
54	1W	4	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	281	0	0	0	0
54	1b	1	0	0	0	0
54	1d	4	0	0	0	0
54	1e	4	0	0	0	0
54	1f	2	0	0	0	0
54	1g	2	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	2	0	0	0	0
54	1t	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	3	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	3	0	0	0	0
54	28	3	0	0	0	0
54	2A	729	0	0	0	0
54	2B	16	0	0	0	0
54	2D	12	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	2	0	0	0	0
54	2O	2	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	2	0	0	0	0
54	2T	4	0	0	0	0
54	2U	1	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	193	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2o	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	36	0	29	1	0
55	2A	36	0	29	2	0
56	1A	52	0	72	0	0
56	2A	52	0	72	2	0
57	18	8	0	14	1	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	12	5	0
57	2A	16	0	28	1	0
57	2B	8	0	14	0	0
58	1B	12	0	12	2	0
58	1F	12	0	12	2	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	10	21	0	0	0	0
61	11	24	0	0	0	0
61	12	12	0	0	1	0
61	13	19	0	0	0	0
61	14	3	0	0	0	0
61	15	24	0	0	2	0
61	16	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	17	14	0	0	1	0
61	18	25	0	0	2	0
61	19	2	0	0	0	0
61	1A	3943	0	0	95	0
61	1B	106	0	0	6	0
61	1D	106	0	0	1	0
61	1E	75	0	0	1	0
61	1F	62	0	0	1	0
61	1G	15	0	0	0	0
61	1H	13	0	0	0	0
61	1I	6	0	0	0	0
61	1N	50	0	0	0	0
61	1O	23	0	0	0	0
61	1P	56	0	0	3	0
61	1Q	38	0	0	1	0
61	1R	37	0	0	1	0
61	1S	11	0	0	1	0
61	1T	39	0	0	3	0
61	1U	43	0	0	4	0
61	1V	36	0	0	3	0
61	1W	29	0	0	0	0
61	1X	26	0	0	1	0
61	1Y	16	0	0	2	0
61	1Z	12	0	0	0	0
61	1a	465	0	0	16	0
61	1b	1	0	0	0	0
61	1d	8	0	0	0	0
61	1e	4	0	0	1	0
61	1f	1	0	0	0	0
61	1h	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	4	0	0	0	0
61	1o	4	0	0	0	0
61	1t	1	0	0	0	0
61	1u	1	0	0	0	0
61	1y	3	0	0	1	0
61	20	6	0	0	0	0
61	21	12	0	0	1	0
61	23	1	0	0	1	0
61	25	6	0	0	0	0
61	26	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	27	5	0	0	0	0
61	28	8	0	0	0	0
61	2A	1664	0	0	82	0
61	2B	25	0	0	4	0
61	2D	38	0	0	0	0
61	2E	18	0	0	0	0
61	2F	18	0	0	1	0
61	2G	4	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	2	0	0	0	0
61	2O	11	0	0	1	0
61	2P	11	0	0	1	0
61	2Q	10	0	0	0	0
61	2R	16	0	0	2	0
61	2T	7	0	0	0	0
61	2U	8	0	0	1	0
61	2V	5	0	0	0	0
61	2W	17	0	0	0	0
61	2X	3	0	0	0	0
61	2Y	3	0	0	0	0
61	2Z	3	0	0	0	0
61	2a	245	0	0	20	0
61	2d	2	0	0	0	0
61	2e	1	0	0	0	0
61	2f	3	0	0	0	0
61	2l	3	0	0	0	0
61	2m	1	0	0	0	0
61	2o	2	0	0	0	0
61	2q	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2y	2	0	0	0	0
All	All	296715	0	194718	3790	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3790) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2139:C:N4	1:2A:2152:G:H1	1.50	1.07
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.20	1.06
1:1A:2137:C:N4	1:1A:2154:G:H1	1.55	1.03
1:1A:1054:A:H61	1:1A:1105:U:H3	1.07	0.99
1:1A:1082:U:H3	1:1A:1086:A:H61	1.04	0.99
1:1A:2137:C:H42	1:1A:2154:G:H1	1.08	0.97
1:2A:2131:G:H5"	1:2A:2132:U:H5'	1.48	0.96
1:2A:962:G:OP1	61:2A:3803:HOH:O	1.83	0.95
1:2A:2499:C:OP1	61:2A:3804:HOH:O	1.84	0.94
1:1A:1082:U:O4	1:1A:1086:A:N1	2.00	0.93
1:2A:2122:U:H3	1:2A:2176:A:H61	1.17	0.93
1:1A:1082:U:H3	1:1A:1086:A:N6	1.65	0.93
1:1A:962:G:OP1	61:1A:4103:HOH:O	1.88	0.92
1:2A:2104:G:N7	1:2A:2186:G:N2	2.18	0.91
22:10:10:THR:HG22	22:10:12:ASN:H	1.36	0.91
1:1A:2137:C:N3	1:1A:2154:G:N2	2.19	0.91
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.49	0.91
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.53	0.90
29:27:24:THR:HG22	29:27:27:GLY:H	1.35	0.90
32:2a:1318:A:H5"	50:2s:3:ARG:HH22	1.36	0.90
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.52	0.90
1:2A:2100:G:H1	1:2A:2189:U:H3	1.15	0.90
1:1A:1670:C:OP2	61:1A:4104:HOH:O	1.90	0.89
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.35	0.89
1:2A:194:G:OP2	61:2A:3805:HOH:O	1.91	0.89
16:1U:33:ARG:NH1	61:1U:301:HOH:O	2.04	0.89
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.06	0.89
39:2h:51:VAL:HG11	39:2h:60:ARG:HD2	1.56	0.88
1:2A:2602:A:H1'	1:2A:2603:G:H5"	1.56	0.87
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.57	0.87
32:1a:1086:U:H3	32:1a:1099:G:H22	1.21	0.87
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.40	0.86
1:2A:1602:U:O4	61:2A:3806:HOH:O	1.92	0.86
32:2a:977:A:N6	32:2a:1224:G:OP1	2.08	0.85
1:2A:2427:C:OP1	61:2A:3807:HOH:O	1.92	0.85
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.10	0.85
1:2A:2139:C:N3	1:2A:2152:G:N2	2.23	0.85
32:2a:758:G:N7	61:2a:3203:HOH:O	2.08	0.85
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.42	0.84
1:1A:2822:G:OP2	61:1A:4105:HOH:O	1.96	0.83
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.60	0.83
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.62	0.82
32:1a:201:C:H42	32:1a:216:G:H1	1.27	0.82
32:1a:664:G:H22	32:1a:741:G:H1	1.27	0.82
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.61	0.82
4:2E:110:GLY:O	61:2R:301:HOH:O	1.97	0.82
33:2b:178:ARG:HB3	39:2h:72:PRO:HA	1.61	0.81
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.13	0.81
33:1b:21:ARG:O	33:1b:23:ARG:N	2.13	0.81
1:2A:1342:A:OP2	61:2A:3806:HOH:O	1.98	0.81
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.63	0.81
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.53	0.81
32:2a:975:A:H4'	32:2a:976:G:H5"	1.63	0.81
32:1a:975:A:H4'	32:1a:976:G:H5"	1.61	0.80
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.63	0.80
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.62	0.80
1:2A:2156:G:N7	1:2A:2157:G:N2	2.30	0.80
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.14	0.79
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.63	0.79
1:1A:2821:A:OP2	61:1A:4105:HOH:O	2.00	0.79
1:2A:993:G:N2	17:2V:23:GLU:OE2	2.15	0.79
1:1A:1054:A:N6	1:1A:1105:U:H3	1.79	0.79
1:2A:826:U:OP1	61:2A:3807:HOH:O	1.99	0.79
1:2A:2807:G:N2	1:2A:2893:G:O6	2.14	0.79
1:2A:1647:G:OP1	61:2A:3809:HOH:O	1.99	0.79
1:2A:2141:G:O6	1:2A:2150:U:O2	2.01	0.79
1:2A:2448:A:OP1	61:2A:3804:HOH:O	1.98	0.78
5:1F:197:ASP:N	5:1F:197:ASP:OD1	2.16	0.78
1:2A:991:C:OP2	61:2A:3810:HOH:O	2.00	0.78
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.16	0.78
34:2c:35:GLU:HA	34:2c:38:ARG:HD2	1.66	0.78
1:1A:2464:C:O2'	61:1A:4106:HOH:O	2.02	0.78
22:20:10:THR:HG22	22:20:12:ASN:H	1.47	0.78
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.66	0.78
34:1c:179:ARG:NH1	34:1c:206:GLU:OE1	2.18	0.77
3:2D:134:ARG:NH1	3:2D:188:GLU:OE2	2.16	0.77
32:1a:73:G:H1	32:1a:96:U:H3	1.32	0.77
1:1A:1039:G:O6	1:1A:1116:C:N4	2.16	0.77
1:1A:1647:G:OP1	61:1A:4107:HOH:O	2.03	0.76
1:1A:2116:G:OP2	1:1A:2166:G:N2	2.17	0.76
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.18	0.76
53:1y:3:MET:HE3	53:1y:24:LEU:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1006:C:OP2	61:2A:3811:HOH:O	2.03	0.76
32:1a:612:C:O2	32:1a:629:G:N2	2.19	0.76
26:24:48:ARG:HB3	26:24:52:THR:HA	1.66	0.76
32:2a:559:A:H4'	32:2a:560:U:H3'	1.66	0.76
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.17	0.76
32:2a:954:G:H21	32:2a:1227:A:H62	1.34	0.76
36:2e:50:GLU:HB2	36:2e:53:LEU:HD13	1.67	0.76
20:2Y:81:LYS:HD3	20:2Y:82:PRO:HD2	1.67	0.76
40:2i:9:ARG:HB2	40:2i:104:ARG:HE	1.49	0.76
1:2A:1057:A:N6	1:2A:1087:G:OP1	2.19	0.76
1:2A:2122:U:H3	1:2A:2176:A:N6	1.83	0.76
1:1A:1701:A:OP2	61:1A:4108:HOH:O	2.04	0.76
32:2a:1500:A:OP2	61:2a:3201:HOH:O	2.04	0.75
1:1A:2447:G:OP2	61:1A:4109:HOH:O	2.05	0.75
19:1X:76:ARG:NH1	61:1X:101:HOH:O	2.18	0.75
1:2A:2429:G:OP1	61:2A:3807:HOH:O	2.04	0.75
36:2e:140:ARG:O	36:2e:143:ARG:NH2	2.19	0.75
32:1a:1025:U:C2	32:1a:1036:G:O6	2.39	0.75
32:1a:1026:G:H5'	32:1a:1027:C:H5	1.51	0.75
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.68	0.75
32:1a:330:C:OP2	61:1a:1902:HOH:O	2.03	0.75
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.20	0.75
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.69	0.75
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.51	0.75
6:2G:65:GLY:HA3	26:24:9:LEU:HD11	1.67	0.75
40:2i:53:VAL:O	40:2i:55:ALA:N	2.19	0.75
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.20	0.74
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.23	0.74
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.20	0.74
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.20	0.74
1:2A:1009:A:OP2	61:2A:3812:HOH:O	2.04	0.74
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.70	0.74
1:1A:1315:C:OP2	61:1A:4111:HOH:O	2.05	0.74
32:1a:814:A:OP2	61:1a:1903:HOH:O	2.05	0.74
1:2A:881:G:H1	1:2A:895:U:H3	1.35	0.74
1:2A:2102:U:O2	1:2A:2187:G:O6	2.05	0.74
1:1A:1669:A:OP2	61:1A:4104:HOH:O	2.05	0.74
32:2a:427:U:OP1	35:2d:13:ARG:NH2	2.21	0.74
32:1a:1495:U:OP1	53:1y:23:ARG:NH2	2.18	0.74
51:1t:33:ILE:O	51:1t:37:SER:OG	2.04	0.74
32:1a:800:G:N7	61:1a:1915:HOH:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:18:LYS:NZ	35:1d:31:CYS:SG	2.58	0.74
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.70	0.74
1:2A:1057:A:H62	1:2A:1086:A:H3'	1.54	0.73
1:1A:1634:A:OP2	61:1A:4112:HOH:O	2.05	0.73
1:1A:998:C:OP1	61:1A:4110:HOH:O	2.05	0.73
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.71	0.73
32:1a:1069:C:OP2	61:1a:1904:HOH:O	2.05	0.73
32:2a:1492:A:H5"	43:2l:47:LYS:HD3	1.70	0.73
1:2A:14:A:OP2	61:2A:3814:HOH:O	2.06	0.73
1:2A:2123:G:O6	1:2A:2175:C:N3	2.22	0.73
2:1B:82:G:N3	61:1B:304:HOH:O	2.21	0.73
32:2a:580:U:OP2	61:2a:3202:HOH:O	2.06	0.73
33:2b:74:LYS:O	33:2b:78:GLN:N	2.22	0.73
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.71	0.73
1:2A:1063:G:H2'	1:2A:1065:U:H6	1.51	0.73
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.54	0.73
32:1a:352:C:OP2	61:1a:1905:HOH:O	2.05	0.73
1:2A:1024:G:OP2	61:2A:3813:HOH:O	2.06	0.73
1:2A:2125:G:H22	1:2A:2172:U:H3'	1.54	0.73
21:2Z:72:ARG:HG2	21:2Z:89:PHE:HB2	1.70	0.72
1:1A:11:G:H2'	1:1A:12:U:H5"	1.68	0.72
1:1A:1143:A:OP1	9:1N:25:ARG:NH2	2.22	0.72
40:1i:16:ARG:H	40:1i:64:THR:HG22	1.52	0.72
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.72	0.72
1:2A:331:A:N1	61:2A:3858:HOH:O	2.22	0.72
1:1A:1026:U:OP1	61:1A:4113:HOH:O	2.07	0.72
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.22	0.72
26:24:59:PHE:HA	26:24:61:ARG:N	2.04	0.72
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.36	0.72
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.23	0.72
1:2A:1314:C:OP1	61:2A:3815:HOH:O	2.08	0.72
1:1A:1771:C:OP1	61:1A:4116:HOH:O	2.08	0.72
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.55	0.72
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.54	0.71
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.72	0.71
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.72	0.71
1:1A:1024:G:OP2	61:1A:4113:HOH:O	2.07	0.71
6:1G:83:ARG:H	6:1G:86:MET:HE3	1.56	0.71
1:2A:1041:C:H42	1:2A:1114:G:H1	1.38	0.71
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.23	0.71
1:1A:749:C:OP2	61:1A:4115:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2427:C:OP1	61:1A:4114:HOH:O	2.07	0.71
1:2A:2706:G:N7	61:2A:3865:HOH:O	2.23	0.71
32:2a:17:U:H2'	32:2a:18:C:C6	2.26	0.71
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.55	0.71
1:1A:297:C:N4	61:1A:4124:HOH:O	2.22	0.71
1:1A:2116:G:H1	1:1A:2165:G:H22	1.36	0.71
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.71	0.71
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.24	0.71
32:1a:964:A:OP1	61:1a:1906:HOH:O	2.09	0.71
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.71
32:2a:1505:G:OP1	61:2a:3204:HOH:O	2.08	0.71
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	1.72	0.71
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.55	0.71
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.24	0.71
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.73	0.71
1:1A:1321:A:N1	61:1A:4172:HOH:O	2.22	0.71
1:2A:2107:C:H42	1:2A:2182:G:H1	1.38	0.71
33:2b:118:LEU:HD22	33:2b:142:LEU:HB2	1.72	0.71
1:1A:2602:A:N7	61:1A:4181:HOH:O	2.24	0.70
1:1A:2879:C:OP2	61:1A:4117:HOH:O	2.09	0.70
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.23	0.70
1:2A:568:U:O4	61:2A:3816:HOH:O	2.09	0.70
32:1a:1025:U:O2	32:1a:1036:G:O6	2.08	0.70
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.24	0.70
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.22	0.70
38:2g:95:ARG:HE	38:2g:99:LEU:HD11	1.56	0.70
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.72	0.70
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.24	0.70
32:1a:656:C:O2'	46:1o:28:GLN:NE2	2.22	0.70
1:2A:601:C:OP1	5:2F:108:LYS:NZ	2.24	0.70
50:2s:20:LEU:HA	50:2s:23:ASN:HD22	1.54	0.70
1:1A:859:G:O6	61:1A:4123:HOH:O	2.09	0.70
1:1A:271(M):G:H21	8:1I:50:ARG:HD3	1.56	0.70
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.08	0.70
1:2A:2139:C:H42	1:2A:2152:G:H1	0.77	0.70
32:2a:937:A:OP2	61:2a:3205:HOH:O	2.09	0.70
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.74	0.70
1:1A:2623:G:OP1	61:1A:4119:HOH:O	2.09	0.70
1:2A:2104:G:N2	1:2A:2105:C:N3	2.39	0.70
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.57	0.70
32:2a:673:G:H2'	32:2a:674:G:C8	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1401:G:N7	53:2y:83:ARG:NH1	2.36	0.70
33:2b:15:VAL:O	33:2b:17:PHE:N	2.24	0.70
1:1A:1175:U:OP1	1:1A:1177:A:N6	2.25	0.69
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.25	0.69
1:2A:1056:G:H5"	1:2A:1057:A:H5'	1.74	0.69
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.73	0.69
46:1o:82:ILE:HD12	46:1o:88:ARG:HB2	1.74	0.69
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.39	0.69
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.73	0.69
53:1y:79:ASN:OD1	61:1y:301:HOH:O	2.10	0.69
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.75	0.69
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.75	0.69
1:1A:2534:A:N7	61:1A:4188:HOH:O	2.25	0.69
1:2A:1346:G:OP2	61:2A:3818:HOH:O	2.11	0.69
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.08	0.69
1:1A:1271:G:OP2	61:1A:4107:HOH:O	2.10	0.69
1:1A:1382:G:N7	61:1A:4186:HOH:O	2.25	0.69
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.74	0.69
1:2A:1648:C:OP1	61:2A:3809:HOH:O	2.09	0.69
1:2A:2111:C:H42	1:2A:2147:G:H22	1.40	0.69
28:16:13:CYS:SG	28:16:47:THR:HG21	2.33	0.69
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.26	0.69
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.74	0.69
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.75	0.69
1:2A:2837:G:N7	61:2A:3886:HOH:O	2.26	0.69
4:2E:77:ILE:HG21	4:2E:195:LEU:HD21	1.74	0.69
33:2b:18:GLY:HA2	33:2b:42:ILE:HD12	1.74	0.69
42:2k:79:SER:HB2	42:2k:104:GLN:HB3	1.74	0.69
1:1A:1023:U:OP2	61:1A:4113:HOH:O	2.10	0.69
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.10	0.69
37:1f:95:GLU:O	49:1r:32:ARG:NH1	2.25	0.69
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.25	0.69
17:1V:1:MET:HE1	17:1V:43:GLU:HB2	1.75	0.69
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.25	0.69
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.75	0.69
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.27	0.68
1:2A:1938:A:OP2	61:2A:3819:HOH:O	2.11	0.68
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.73	0.68
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.23	0.68
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.27	0.68
32:1a:1292:U:OP2	38:1g:41:ARG:NH2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1271:G:OP2	61:2A:3809:HOH:O	2.10	0.68
34:2c:6:HIS:CD2	45:2n:49:HIS:HB3	2.28	0.68
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.75	0.68
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.26	0.68
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.75	0.68
1:2A:775:G:O3'	61:2A:3820:HOH:O	2.11	0.68
1:2A:1642:G:N7	61:2A:3885:HOH:O	2.26	0.68
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.74	0.68
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.75	0.68
32:1a:60:A:H4'	32:1a:61:G:H5'	1.76	0.68
1:2A:1153:C:OP2	61:2A:3817:HOH:O	2.10	0.68
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.27	0.68
1:1A:601:C:OP2	61:1A:4122:HOH:O	2.09	0.68
1:1A:2114:A:H3'	1:1A:2115:G:H8	1.58	0.68
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.58	0.68
25:23:13:ILE:O	61:23:201:HOH:O	2.11	0.68
32:1a:1414:U:H3	32:1a:1486:G:H1	1.41	0.68
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.74	0.68
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.40	0.68
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.59	0.68
7:2H:52:VAL:HG21	7:2H:69:ARG:HB2	1.76	0.68
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.74	0.68
1:2A:948:G:OP1	61:2A:3803:HOH:O	2.12	0.67
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.76	0.67
44:2m:81:LEU:HD13	44:2m:88:ARG:HD2	1.76	0.67
1:2A:1670:C:OP1	61:2A:3821:HOH:O	2.11	0.67
32:2a:660:G:H1	32:2a:745:C:H42	1.41	0.67
32:2a:1005:A:OP2	32:2a:1024:G:N2	2.27	0.67
37:2f:35:ALA:HB2	37:2f:67:MET:HE2	1.74	0.67
35:1d:172:PRO:HB2	35:1d:187:ARG:HH21	1.59	0.67
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.13	0.67
1:2A:585:G:OP2	61:2A:3823:HOH:O	2.12	0.67
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.76	0.67
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.22	0.67
1:1A:1648:C:OP1	61:1A:4107:HOH:O	2.13	0.67
1:1A:2400:G:O6	61:1A:4118:HOH:O	2.09	0.67
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.10	0.67
1:1A:1295:C:OP2	61:1A:4125:HOH:O	2.12	0.67
1:1A:2133:G:H3'	1:1A:2157:G:H21	1.59	0.67
32:2a:656:C:O2'	46:2o:28:GLN:NE2	2.28	0.67
1:1A:826:U:O4	61:1A:4121:HOH:O	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.27	0.67
32:1a:194:C:H2'	32:1a:195:A:H5"	1.76	0.67
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.60	0.67
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.28	0.67
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.27	0.67
9:2N:85:ILE:HG21	9:2N:90:MET:HE2	1.77	0.67
40:1i:18:PHE:HB2	40:1i:62:TYR:HB3	1.77	0.67
1:1A:580:C:OP1	61:1A:4127:HOH:O	2.12	0.66
1:2A:1647:G:OP2	61:2A:3826:HOH:O	2.13	0.66
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.95	0.66
2:2B:66:A:H61	2:2B:109:C:H5'	1.60	0.66
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.28	0.66
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.28	0.66
1:1A:963:U:OP2	61:1A:4103:HOH:O	2.11	0.66
1:1A:2404:C:OP2	61:1A:4128:HOH:O	2.13	0.66
32:2a:812:C:N3	61:2a:3223:HOH:O	2.28	0.66
32:2a:1401:G:O6	53:2y:83:ARG:NH2	2.29	0.66
1:1A:1016:G:N7	61:1A:4218:HOH:O	2.29	0.66
32:1a:1178:G:OP2	40:1i:93:ARG:NH2	2.29	0.66
1:2A:2115:G:H21	1:2A:2171:A:H61	1.41	0.66
11:2P:54:GLY:O	61:2P:301:HOH:O	2.12	0.66
34:2c:6:HIS:HD2	45:2n:49:HIS:HB3	1.59	0.66
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.76	0.66
41:1j:16:LEU:HD22	41:1j:68:HIS:HB2	1.75	0.66
1:1A:826:U:OP1	61:1A:4114:HOH:O	2.13	0.66
1:1A:1757:U:OP1	61:1A:4129:HOH:O	2.13	0.66
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.77	0.66
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.77	0.66
32:1a:324:G:N7	61:1a:1924:HOH:O	2.28	0.66
1:1A:1865:G:OP1	61:1A:4126:HOH:O	2.12	0.66
15:1T:1:MET:HE2	15:1T:3:ARG:HG2	1.78	0.66
44:1m:65:LYS:HE2	44:1m:69:GLU:HG2	1.78	0.66
1:1A:2319:G:N2	14:1S:3:ARG:HD3	2.04	0.66
1:2A:1470:G:N7	61:2A:3900:HOH:O	2.29	0.66
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.28	0.66
3:1D:39:LYS:NZ	3:1D:57:GLY:O	2.28	0.66
35:2d:189:PRO:HB2	35:2d:194:LEU:HD11	1.78	0.66
38:2g:113:GLU:HG3	38:2g:119:ARG:HG2	1.78	0.66
33:1b:63:MET:HG3	33:1b:225:ALA:HB1	1.76	0.66
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.31	0.66
32:2a:986:A:N3	50:2s:52:TYR:OH	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1054:C:H41	53:2y:46:GLN:HG3	1.61	0.66
32:1a:1373:G:N7	40:1i:11:LYS:NZ	2.42	0.65
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.78	0.65
1:2A:607:U:OP1	5:2F:102:PRO:HA	1.96	0.65
21:2Z:126:VAL:HG11	21:2Z:161:VAL:HG13	1.78	0.65
32:2a:1388:C:O2'	61:2a:3208:HOH:O	2.14	0.65
1:1A:1456:G:OP2	61:1A:4132:HOH:O	2.14	0.65
32:2a:1500:A:OP1	61:2a:3204:HOH:O	2.14	0.65
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.62	0.65
1:1A:763:G:OP1	61:1A:4131:HOH:O	2.14	0.65
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.13	0.65
1:2A:1063:G:H1	1:2A:1075:C:N4	1.94	0.65
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.78	0.65
32:2a:1527:C:OP1	61:2a:3206:HOH:O	2.14	0.65
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.79	0.65
23:11:52:ARG:NH2	23:11:55:GLY:O	2.29	0.65
1:2A:1186:G:OP2	61:2A:3810:HOH:O	2.14	0.65
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.78	0.65
41:2j:55:LYS:O	41:2j:57:LYS:N	2.29	0.65
1:1A:2008:C:OP2	61:1A:4134:HOH:O	2.15	0.65
40:1i:10:ARG:HG3	40:1i:11:LYS:H	1.62	0.65
1:2A:1937:A:O2'	61:2A:3825:HOH:O	2.13	0.65
20:1Y:28:LYS:HG3	20:1Y:40:GLU:HG2	1.78	0.65
32:1a:396:G:O2'	32:1a:398:C:OP1	2.13	0.65
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.29	0.65
1:2A:684:G:O3'	61:2A:3808:HOH:O	2.14	0.65
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.61	0.65
53:2y:5:ILE:HG23	53:2y:39:ILE:HB	1.79	0.65
1:1A:2102:U:O2	1:1A:2187:G:O6	2.14	0.65
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.29	0.65
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.28	0.65
35:2d:187:ARG:NH2	35:2d:193:ASP:OD2	2.30	0.65
35:1d:18:LYS:NZ	60:1d:305:SF4:S1	2.69	0.65
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.79	0.65
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.62	0.64
32:1a:945:G:OP1	61:1a:1908:HOH:O	2.15	0.64
33:1b:15:VAL:HG22	33:1b:209:ARG:HB3	1.79	0.64
32:2a:492:G:OP2	61:2a:3211:HOH:O	2.15	0.64
32:2a:574:A:OP2	61:2a:3207:HOH:O	2.14	0.64
32:2a:1030(A):G:H21	32:2a:1030(C):G:H3'	1.61	0.64
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.29	0.64
53:2y:53:THR:HG22	53:2y:62:VAL:HG22	1.80	0.64
1:1A:2070:G:OP2	61:1A:4133:HOH:O	2.15	0.64
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.31	0.64
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.63	0.64
2:2B:58:A:OP2	61:2B:301:HOH:O	2.15	0.64
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.78	0.64
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.28	0.64
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.79	0.64
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.80	0.64
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.30	0.64
28:26:8:LYS:NZ	61:26:601:HOH:O	2.25	0.64
2:1B:22:U:O4	61:1B:301:HOH:O	2.10	0.64
28:16:2:ALA:N	61:16:601:HOH:O	2.31	0.64
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.33	0.64
43:2l:103:GLY:N	43:2l:107:ALA:O	2.26	0.64
1:1A:248:G:OP1	61:1A:4135:HOH:O	2.15	0.64
32:2a:1504:G:OP1	61:2a:3209:HOH:O	2.15	0.64
1:1A:1069:A:H4'	1:1A:1070:A:H5"	1.80	0.64
26:24:13:ARG:HH12	26:24:23:GLU:HG2	1.61	0.64
25:13:59:VAL:HG23	25:13:60:GLU:HG2	1.79	0.64
12:2Q:29:PHE:O	21:2Z:122:ARG:NH2	2.30	0.64
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.45	0.64
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.80	0.64
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.80	0.63
1:2A:1803:A:O2'	3:2D:259:THR:HG21	1.98	0.63
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.28	0.63
61:1A:4197:HOH:O	18:1W:83:LYS:NZ	2.30	0.63
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.46	0.63
37:1f:69:GLU:OE1	37:1f:69:GLU:N	2.32	0.63
1:2A:1315:C:OP2	61:2A:3815:HOH:O	2.15	0.63
1:1A:286:C:H2'	1:1A:287:C:H6	1.64	0.63
1:1A:878:A:H2'	1:1A:879:G:H5'	1.80	0.63
11:1P:42:SER:O	61:1P:301:HOH:O	2.16	0.63
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.31	0.63
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.61	0.63
1:2A:2453:A:OP1	61:2A:3828:HOH:O	2.15	0.63
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.78	0.63
1:1A:2115:G:H2'	1:1A:2117:A:N6	2.14	0.63
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.33	0.63
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2135:A:H62	1:1A:2156:G:H21	1.45	0.63
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.34	0.63
32:2a:1004:A:H5"	32:2a:1025:U:C5	2.33	0.63
32:2a:1291:G:OP1	38:2g:37:ASN:ND2	2.31	0.63
34:2c:8:ILE:HD12	34:2c:16:ARG:HD2	1.81	0.63
39:2h:14:ARG:NH1	39:2h:83:ILE:O	2.31	0.63
1:1A:578:A:H3'	61:1A:4594:HOH:O	1.98	0.63
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.33	0.63
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	1.81	0.63
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	1.81	0.63
33:2b:91:PRO:HG3	33:2b:155:LEU:HD13	1.79	0.63
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.79	0.63
1:1A:2133:G:C2	1:1A:2157:G:H2'	2.34	0.63
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.79	0.63
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.81	0.63
61:2A:3850:HOH:O	11:2P:37:GLY:HA3	1.99	0.62
32:2a:222:U:H2'	32:2a:223:U:C6	2.34	0.62
32:1a:992:U:H4'	32:1a:993:G:H5'	1.81	0.62
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.34	0.62
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.47	0.62
21:2Z:5:LEU:HD11	21:2Z:39:VAL:HB	1.79	0.62
32:2a:1291:G:O2'	40:2i:38:GLN:OE1	2.17	0.62
9:1N:65:LYS:HE2	9:1N:69:GLN:HE22	1.63	0.62
2:2B:106:G:OP1	21:2Z:31:ARG:NH1	2.32	0.62
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.82	0.62
21:2Z:152:ALA:HA	21:2Z:155:LEU:HD13	1.80	0.62
34:2c:28:GLN:HG2	34:2c:32:LEU:HD13	1.81	0.62
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.35	0.62
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.80	0.62
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.14	0.62
1:2A:848:G:OP1	61:2A:3829:HOH:O	2.16	0.62
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.00	0.62
32:1a:78:G:H1	32:1a:91:C:H42	1.45	0.62
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.65	0.62
1:2A:2230:G:N7	61:2A:3910:HOH:O	2.31	0.62
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.80	0.62
32:2a:1075:C:H5"	33:2b:179:LYS:HE2	1.81	0.62
5:1F:164:ARG:HD2	58:1F:318:ARG:HH12	1.64	0.62
21:1Z:152:ALA:HA	21:1Z:155:LEU:HD22	1.82	0.62
32:1a:222:U:H2'	32:1a:223:U:C6	2.35	0.62
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.33	0.62
21:2Z:179:ASP:O	21:2Z:182:LYS:HG2	2.00	0.62
32:2a:651:C:N4	32:2a:753:A:OP2	2.32	0.62
32:2a:1129:C:N4	32:2a:1143:G:H1	1.98	0.62
50:2s:31:ILE:HB	50:2s:49:ILE:HG22	1.80	0.62
1:1A:572:A:OP2	17:1V:78:LYS:NZ	2.32	0.62
1:1A:1073:A:H2	1:1A:1074:G:C8	2.18	0.62
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.35	0.62
10:1O:20:MET:HE3	10:1O:44:LYS:HE3	1.82	0.62
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.30	0.62
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.82	0.62
20:2Y:82:PRO:O	20:2Y:101:LYS:NZ	2.31	0.62
26:14:16:CYS:SG	26:14:17:GLY:N	2.73	0.62
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.80	0.62
1:2A:1352:U:OP2	61:2A:3830:HOH:O	2.16	0.62
1:2A:2099:U:H3	1:2A:2190:G:H1	1.48	0.62
26:24:34:GLU:HG2	26:24:35:VAL:HG12	1.81	0.62
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.34	0.61
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.14	0.61
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.17	0.61
32:1a:1183:A:H3'	32:1a:1184:G:H5"	1.82	0.61
6:1G:181:ARG:HG3	6:1G:182:LYS:H	1.65	0.61
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.33	0.61
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.82	0.61
1:2A:1075:C:H2'	1:2A:1076:C:H5'	1.81	0.61
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.34	0.61
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.65	0.61
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.33	0.61
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.00	0.61
1:1A:2142:C:C2	1:1A:2149:G:N1	2.69	0.61
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.35	0.61
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.15	0.61
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.34	0.61
1:2A:2103:C:N4	1:2A:2185:C:H42	1.98	0.61
1:2A:2137:C:O2	1:2A:2154:G:N1	2.33	0.61
2:2B:56:G:O2'	61:2B:302:HOH:O	2.16	0.61
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.82	0.61
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.30	0.61
32:1a:1124:G:N2	32:1a:1125:U:O4	2.33	0.61
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.83	0.61
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.32	0.61
42:1k:31:THR:HG22	42:1k:42:TRP:HB2	1.83	0.61
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.36	0.61
32:2a:920:U:H2'	32:2a:921:U:C6	2.36	0.61
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.83	0.61
1:1A:889:C:O2'	1:1A:890:A:O5'	2.17	0.61
1:1A:2577:A:H5'	27:15:3:LYS:HE3	1.82	0.61
6:1G:12:TYR:HA	6:1G:16:ARG:HG3	1.81	0.61
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.83	0.61
32:1a:460:G:N2	32:1a:471:G:N7	2.49	0.61
7:2H:5:GLY:HA3	7:2H:65:HIS:HD2	1.65	0.61
32:2a:115:G:OP1	61:2a:3212:HOH:O	2.16	0.61
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.33	0.61
32:1a:1027:C:N3	32:1a:1034:G:O6	2.33	0.61
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.82	0.61
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.34	0.61
6:1G:77:ILE:HB	6:1G:82:LEU:HB2	1.83	0.61
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.09	0.61
1:2A:855:G:O6	61:2A:3827:HOH:O	2.14	0.61
32:2a:1005:A:OP1	32:2a:1006:C:N4	2.33	0.61
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.35	0.60
32:1a:1108:G:O6	61:1a:1907:HOH:O	2.12	0.60
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.66	0.60
1:1A:2126:A:H4'	1:1A:2127:G:O5'	2.00	0.60
32:1a:1030:C:N4	32:1a:1032:G:O6	2.33	0.60
1:2A:1062:G:C5	1:2A:1070:A:H1'	2.36	0.60
1:2A:2504:U:OP2	61:2A:3832:HOH:O	2.17	0.60
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.33	0.60
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.82	0.60
39:2h:37:ARG:NH2	39:2h:118:VAL:O	2.34	0.60
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.82	0.60
53:2y:18:GLN:NE2	53:2y:22:ASP:OD1	2.35	0.60
1:1A:2712:U:H2'	1:1A:2714:G:H5"	1.82	0.60
29:17:24:THR:HG22	29:17:27:GLY:H	1.66	0.60
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.36	0.60
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.32	0.60
32:2a:662:G:H2'	32:2a:663:A:C8	2.35	0.60
33:1b:157:ARG:HG2	33:1b:158:LEU:H	1.66	0.60
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.37	0.60
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.36	0.60
32:2a:164:U:H2'	32:2a:165:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:171:ALA:HA	33:2b:174:VAL:HG12	1.83	0.60
1:1A:2114:A:H3'	1:1A:2115:G:C8	2.36	0.60
1:1A:2143:C:N3	1:1A:2148:G:O6	2.34	0.60
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.34	0.60
32:2a:117:G:OP2	61:2a:3213:HOH:O	2.16	0.60
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.37	0.60
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.48	0.60
1:1A:1078:U:C5	1:1A:1088:A:H5"	2.36	0.60
1:1A:2390:U:OP2	61:1A:4136:HOH:O	2.16	0.60
35:1d:165:MET:HA	35:1d:168:ARG:HB2	1.83	0.60
1:2A:1063:G:H2'	1:2A:1065:U:C6	2.35	0.60
26:24:59:PHE:CE2	50:2s:64:GLU:HB2	2.36	0.60
32:2a:1146:A:H3'	32:2a:1147:C:H5"	1.83	0.60
39:2h:29:SER:HB3	39:2h:32:LYS:HD2	1.84	0.60
6:1G:49:ASP:O	6:1G:51:ARG:N	2.35	0.60
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.83	0.60
1:2A:2161:C:O2'	1:2A:2173:A:O2'	2.19	0.60
5:2F:74:ARG:HD2	61:2F:415:HOH:O	2.01	0.60
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.37	0.60
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.37	0.60
5:2F:122:LYS:NZ	5:2F:152:GLU:OE2	2.31	0.60
31:29:15:LYS:HE2	31:29:17:ILE:HD11	1.84	0.60
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.50	0.60
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.34	0.60
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.36	0.60
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.67	0.60
32:2a:1129:C:H42	32:2a:1143:G:H1	1.50	0.60
40:2i:42:ARG:NH1	40:2i:71:SER:O	2.35	0.60
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.34	0.59
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.37	0.59
50:1s:18:LYS:HD3	50:1s:31:ILE:HD12	1.83	0.59
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.67	0.59
1:2A:668:G:H5'	1:2A:669:G:OP2	2.02	0.59
1:2A:2134:A:H8	1:2A:2156:G:H21	1.48	0.59
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.36	0.59
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.67	0.59
32:2a:1278:U:H5"	32:2a:1279:A:H5'	1.83	0.59
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.35	0.59
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.35	0.59
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.84	0.59
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.36	0.59
1:2A:1754:C:P	15:2T:96:ARG:HH12	2.25	0.59
35:2d:111:ALA:HB2	35:2d:120:LEU:HD22	1.84	0.59
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.84	0.59
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.34	0.59
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.32	0.59
32:1a:1401:G:N7	53:1y:83:ARG:NH1	2.49	0.59
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.35	0.59
26:24:59:PHE:HA	26:24:60:GLN:C	2.28	0.59
32:1a:7:G:H5'	32:1a:298:A:O4'	2.01	0.59
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.35	0.59
15:2T:1:MET:HE2	15:2T:3:ARG:HG2	1.83	0.59
53:2y:61:LEU:HB3	53:2y:81:LEU:HD22	1.84	0.59
1:1A:1300:U:H4'	1:1A:1301:A:H5'	1.84	0.59
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	2.02	0.59
1:1A:1541:G:O6	61:1A:4130:HOH:O	2.13	0.59
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.84	0.59
32:2a:1182:G:H4'	32:2a:1183:A:H3'	1.82	0.59
1:1A:762:U:OP1	61:1A:4137:HOH:O	2.16	0.59
1:1A:1332:G:OP1	61:1A:4111:HOH:O	2.16	0.59
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.01	0.59
32:1a:1047:G:H5"	45:1n:4:LYS:HE3	1.85	0.59
33:1b:42:ILE:HD12	33:1b:203:GLY:HA2	1.85	0.59
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.67	0.59
21:2Z:157:LEU:HD23	21:2Z:161:VAL:HG12	1.84	0.59
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.18	0.59
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.66	0.59
51:2t:50:GLU:HG3	51:2t:100:ILE:HD11	1.84	0.59
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.68	0.59
39:1h:86:ILE:HG21	39:1h:133:LEU:HD13	1.85	0.59
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.84	0.59
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	1.83	0.59
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.83	0.59
32:2a:64:G:H4'	32:2a:65:U:H3'	1.84	0.59
32:2a:1503:A:H5'	32:2a:1531:A:H1'	1.83	0.59
1:1A:1007:C:OP2	61:1A:4138:HOH:O	2.17	0.59
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.38	0.59
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.36	0.59
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.85	0.59
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.85	0.59
39:1h:97:VAL:HG21	39:1h:128:GLY:HA2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.35	0.59
21:2Z:17:ALA:HA	21:2Z:20:ARG:HE	1.66	0.59
50:2s:27:GLU:OE1	50:2s:47:HIS:NE2	2.36	0.59
1:1A:61:G:OP1	24:12:51:ARG:NH2	2.36	0.59
1:2A:1793:C:OP1	61:2A:3833:HOH:O	2.17	0.59
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.36	0.59
32:2a:664:G:H22	32:2a:741:G:H1	1.51	0.59
42:2k:84:VAL:HG12	42:2k:110:ASP:HA	1.85	0.59
1:1A:948:G:OP1	61:1A:4103:HOH:O	2.17	0.58
6:1G:16:ARG:CZ	6:1G:31:VAL:HG21	2.34	0.58
32:1a:501:C:H1'	32:1a:549:C:H1'	1.84	0.58
1:2A:2306:C:N4	6:2G:42:GLY:O	2.36	0.58
21:2Z:91:LEU:HD11	21:2Z:96:VAL:HG11	1.84	0.58
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.68	0.58
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.85	0.58
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.36	0.58
33:2b:51:LEU:HD21	33:2b:201:ILE:HG23	1.85	0.58
1:1A:286:C:H2'	1:1A:287:C:C6	2.38	0.58
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.36	0.58
50:2s:41:VAL:HG12	50:2s:44:MET:HG3	1.85	0.58
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.20	0.58
49:1r:38:GLU:HA	49:1r:41:LYS:HD2	1.85	0.58
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.36	0.58
42:2k:86:GLY:N	42:2k:112:THR:OG1	2.25	0.58
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.18	0.58
32:1a:269:C:H2'	32:1a:270:A:C8	2.38	0.58
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.27	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.68	0.58
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.21	0.58
43:1l:84:LEU:HB3	43:1l:104:VAL:HG21	1.85	0.58
1:2A:2109:U:H2'	1:2A:2110:G:C8	2.38	0.58
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.84	0.58
48:2q:67:LYS:O	48:2q:69:LYS:N	2.36	0.58
1:1A:1175:U:O2'	1:1A:1176:G:O5'	2.21	0.58
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.30	0.58
28:16:15:GLU:OE1	28:16:45:LYS:NZ	2.36	0.58
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.38	0.58
1:2A:634:C:H2'	1:2A:635:C:C6	2.38	0.58
1:2A:1671:U:OP2	61:2A:3821:HOH:O	2.16	0.58
1:2A:2304:G:H22	1:2A:2312:U:H3	1.52	0.58
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.36	0.58
32:2a:135:C:O2	47:2p:1:MET:N	2.36	0.58
51:1t:47:GLY:HA2	51:1t:48:LYS:HB2	1.86	0.58
1:2A:873:G:H1	1:2A:904:C:H42	1.52	0.58
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.68	0.58
5:1F:12:LEU:HD22	5:1F:124:LEU:HD21	1.86	0.58
32:1a:77:G:H2'	32:1a:78:G:H5'	1.85	0.58
32:1a:973:G:H3'	32:1a:974:A:H5"	1.86	0.58
1:2A:495:G:OP2	61:2A:3834:HOH:O	2.17	0.58
1:2A:2717:G:N7	61:2A:3918:HOH:O	2.32	0.58
53:2y:3:MET:HB2	53:2y:37:PRO:HG2	1.84	0.58
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.85	0.58
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.68	0.58
1:2A:963:U:OP2	61:2A:3803:HOH:O	2.16	0.58
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.84	0.58
32:2a:677:U:H3	32:2a:713:G:H22	1.50	0.58
1:1A:614(C):A:OP2	61:1A:4139:HOH:O	2.17	0.58
2:1B:25:A:OP2	61:1B:302:HOH:O	2.17	0.58
35:1d:148:VAL:HG11	35:1d:158:ILE:HD12	1.86	0.58
40:1i:16:ARG:O	40:1i:64:THR:N	2.33	0.58
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.86	0.58
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.39	0.58
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.20	0.58
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.36	0.58
3:1D:137:PRO:O	3:1D:140:THR:HG23	2.04	0.58
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.36	0.58
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	1.85	0.58
32:2a:992:U:H4'	32:2a:993:G:O5'	2.04	0.58
35:2d:165:MET:SD	35:2d:168:ARG:NH1	2.77	0.58
1:1A:1064:C:H3'	1:1A:1065:U:H5"	1.86	0.57
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.86	0.57
32:1a:1158:C:H5	32:1a:1181:G:H1	1.52	0.57
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.68	0.57
2:2B:102:A:OP2	61:2B:303:HOH:O	2.17	0.57
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.37	0.57
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.39	0.57
8:1I:4:ILE:HD11	8:1I:44:LEU:HD13	1.86	0.57
1:2A:249:C:O2'	11:2P:64:LYS:NZ	2.34	0.57
1:2A:2137:C:N3	1:2A:2154:G:O6	2.37	0.57
32:2a:1256:A:H61	32:2a:1278:U:C1'	2.16	0.57
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:346:G:H5”	57:1a:1882:MPD:H4	1.85	0.57
32:1a:1304:G:OP2	61:1a:1909:HOH:O	2.17	0.57
33:1b:27:LYS:O	33:1b:30:ARG:NH1	2.37	0.57
34:1c:35:GLU:OE2	34:1c:59:ARG:NH2	2.37	0.57
6:2G:123:ASN:O	6:2G:125:PHE:N	2.33	0.57
50:2s:22:LEU:HD13	50:2s:28:LYS:H	1.67	0.57
1:1A:2096:U:H2’	1:1A:2097:C:C6	2.40	0.57
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.37	0.57
35:1d:59:ARG:HH12	35:1d:66:ARG:HH12	1.52	0.57
1:2A:1503:U:H2’	1:2A:1504:C:C6	2.39	0.57
44:2m:51:ALA:O	44:2m:55:ARG:HB2	2.04	0.57
1:1A:1721:G:H8	1:1A:1741:A:H62	1.50	0.57
1:1A:2079:U:O3’	23:11:35:THR:OG1	2.22	0.57
14:1S:59:LYS:HE2	14:1S:60:GLY:H	1.69	0.57
32:1a:96:U:H2’	32:1a:97:G:C8	2.39	0.57
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.28	0.57
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.38	0.57
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.85	0.57
42:2k:86:GLY:H	42:2k:112:THR:HG1	1.51	0.57
53:2y:3:MET:HE3	53:2y:5:ILE:HG12	1.86	0.57
1:1A:2243:U:H2’	1:1A:2244:U:C6	2.39	0.57
1:2A:2084:C:O2	61:2A:3822:HOH:O	2.11	0.57
21:2Z:18:LEU:HG	21:2Z:23:LYS:HB2	1.86	0.57
26:24:62:ARG:H	26:24:62:ARG:HD2	1.69	0.57
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.87	0.57
1:1A:2563:U:H4’	10:1O:28:SER:HA	1.86	0.57
4:1E:29:GLY:HA3	61:1E:416:HOH:O	2.03	0.57
44:1m:11:ARG:O	44:1m:13:LYS:N	2.36	0.57
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE3	1.87	0.57
32:2a:256:U:H2’	32:2a:257:G:C8	2.40	0.57
32:2a:1269:A:N1	32:2a:1312:G:O2’	2.32	0.57
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.04	0.57
32:1a:79:G:N1	32:1a:90:U:N3	2.53	0.57
1:2A:1359:A:N3	1:2A:1359:A:H5’	2.20	0.57
1:2A:2206:G:H5”	1:2A:2207:G:N7	2.20	0.57
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.87	0.57
32:2a:890:G:O2’	32:2a:906:G:O6	2.20	0.57
7:1H:86:GLU:OE1	7:1H:130:ARG:HD2	2.05	0.57
32:1a:78:G:H1	32:1a:91:C:N4	2.02	0.57
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.37	0.57
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.40	0.57
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.38	0.57
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.37	0.57
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.28	0.57
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.87	0.57
11:1P:70:GLN:NE2	61:1P:303:HOH:O	2.37	0.57
39:1h:44:PHE:HB3	39:1h:80:ILE:HD11	1.87	0.57
51:1t:79:ARG:HD2	51:1t:83:ARG:HH21	1.68	0.57
1:2A:1332:G:OP1	61:2A:3815:HOH:O	2.18	0.57
1:1A:2145:C:H5"	1:1A:2146:C:C5	2.39	0.56
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.86	0.56
20:1Y:23:ARG:HD3	61:1Y:301:HOH:O	2.05	0.56
32:1a:377:G:OP1	47:1p:3:LYS:NZ	2.32	0.56
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.05	0.56
1:1A:1356:G:N3	61:1A:4253:HOH:O	2.32	0.56
32:1a:67:C:H2'	32:1a:68:G:C8	2.40	0.56
33:1b:74:LYS:NZ	33:1b:205:ASP:O	2.37	0.56
36:1e:110:LEU:HD13	36:1e:118:ILE:HD13	1.87	0.56
1:2A:295:G:H4'	20:2Y:1:MET:HE2	1.86	0.56
1:2A:1053:C:H2'	1:2A:1054:A:C8	2.40	0.56
32:2a:134:A:N6	47:2p:25:ARG:HH22	2.04	0.56
1:1A:428:A:OP1	61:1A:4142:HOH:O	2.18	0.56
1:1A:2059:A:OP2	61:1A:4140:HOH:O	2.17	0.56
3:1D:164:GLN:OE1	3:1D:176:ARG:NH2	2.38	0.56
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.21	0.56
32:1a:38:G:H22	32:1a:397:A:H5'	1.70	0.56
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.32	0.56
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.43	0.56
1:2A:971:C:OP2	61:2A:3838:HOH:O	2.18	0.56
2:2B:14:U:OP2	2:2B:70:C:O2'	2.22	0.56
13:2R:33:ARG:HD2	13:2R:113:LEU:HD13	1.86	0.56
15:2T:108:ARG:NH1	32:2a:1464:G:OP1	2.38	0.56
40:2i:42:ARG:NH1	40:2i:75:ASP:OD1	2.38	0.56
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.70	0.56
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.41	0.56
32:1a:1027:C:N3	32:1a:1034:G:C6	2.74	0.56
40:1i:5:TYR:H	40:1i:87:GLN:NE2	2.03	0.56
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.38	0.56
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.87	0.56
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.36	0.56
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.31	0.56
34:2c:180:ALA:HA	34:2c:206:GLU:HA	1.86	0.56
38:2g:46:ALA:HA	38:2g:49:ILE:HD12	1.87	0.56
1:1A:529:A:OP2	9:1N:114:ARG:NH2	2.39	0.56
9:1N:73:THR:HA	9:1N:83:LYS:O	2.06	0.56
21:1Z:150:LEU:O	21:1Z:171:ILE:HG13	2.05	0.56
32:1a:404:U:H2'	32:1a:405:U:C6	2.41	0.56
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.20	0.56
40:1i:18:PHE:N	40:1i:62:TYR:O	2.31	0.56
1:2A:362:U:O2'	1:2A:363:G:H5'	2.06	0.56
1:2A:2115:G:N2	1:2A:2171:A:H61	2.04	0.56
1:1A:1721:G:H5'	1:1A:1722:A:OP2	2.05	0.56
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.39	0.56
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.88	0.56
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.88	0.56
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.31	0.56
1:2A:1456:G:OP2	61:2A:3836:HOH:O	2.18	0.56
1:2A:2850:A:O2'	61:2A:3837:HOH:O	2.18	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.56
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.40	0.56
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.54	0.56
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.88	0.56
6:1G:5:VAL:HG13	6:1G:8:LYS:HE2	1.88	0.56
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.54	0.56
1:2A:342:G:O6	61:2A:3839:HOH:O	2.18	0.56
1:2A:530:G:O6	61:2A:3831:HOH:O	2.16	0.56
1:2A:586:A:N1	1:2A:809:G:O2'	2.35	0.56
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.88	0.56
32:2a:266:G:O2'	32:2a:267:C:OP2	2.19	0.56
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.87	0.56
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.41	0.56
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.88	0.56
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.37	0.56
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.05	0.56
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.41	0.56
33:1b:95:GLN:HG3	33:1b:147:LYS:O	2.05	0.56
1:2A:2138:C:N3	1:2A:2153:G:O6	2.39	0.56
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.28	0.56
24:22:16:LEU:O	24:22:67:LYS:NZ	2.39	0.56
32:2a:1212:U:H4'	32:2a:1213:A:C8	2.41	0.56
35:2d:114:ARG:HA	35:2d:117:ALA:HB3	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:16:LEU:HD23	41:2j:94:VAL:HG22	1.87	0.56
1:1A:279:C:H42	1:1A:361:G:H1	1.54	0.55
1:1A:469:G:OP1	61:1A:4143:HOH:O	2.18	0.55
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.05	0.55
1:1A:900:A:H2'	1:1A:901:A:H8	1.71	0.55
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.87	0.55
1:1A:2116:G:P	1:1A:2166:G:H21	2.29	0.55
8:1I:87:LYS:H	8:1I:87:LYS:HD2	1.71	0.55
32:1a:673:G:H2'	32:1a:674:G:C8	2.40	0.55
32:1a:1297:C:O2'	38:1g:114:ARG:NH1	2.37	0.55
6:2G:145:THR:HG22	6:2G:148:MET:HG2	1.88	0.55
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.71	0.55
33:2b:119:GLU:OE2	33:2b:153:ARG:NH1	2.39	0.55
42:2k:18:ARG:NH1	42:2k:20:TYR:OH	2.39	0.55
58:1B:230:ARG:N	61:1B:309:HOH:O	2.39	0.55
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.88	0.55
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.07	0.55
36:1e:11:ILE:HD11	36:1e:108:ALA:HB3	1.89	0.55
45:1n:15:LYS:HG2	45:1n:16:PHE:CZ	2.40	0.55
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.21	0.55
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.87	0.55
36:2e:75:THR:OG1	36:2e:117:ASP:O	2.17	0.55
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.06	0.55
32:1a:353:A:H5'	32:1a:353:A:H8	1.71	0.55
35:1d:156:GLU:O	35:1d:160:GLN:HG2	2.06	0.55
42:1k:98:LEU:O	42:1k:101:SER:OG	2.20	0.55
1:2A:154(A):C:H42	1:2A:171:G:H1	1.55	0.55
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.06	0.55
1:2A:922:U:H2'	1:2A:923:C:C6	2.41	0.55
5:2F:24:LEU:HD13	5:2F:115:ALA:HA	1.88	0.55
34:2c:148:GLY:HA3	34:2c:203:PHE:HB3	1.89	0.55
1:1A:588:U:H2'	1:1A:589:C:C6	2.40	0.55
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.06	0.55
1:2A:1920:OMC:HM22	1:2A:1921:G:H5'	1.88	0.55
1:2A:2125:G:O2'	1:2A:2173:A:N6	2.40	0.55
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.42	0.55
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.42	0.55
6:2G:11:TYR:HA	6:2G:15:VAL:HG22	1.88	0.55
32:2a:921:U:O2	36:2e:19:MET:HB2	2.06	0.55
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.41	0.55
33:2b:146:GLN:O	33:2b:150:SER:OG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:747:C:OP2	32:1a:748:C:N4	2.31	0.55
38:1g:13:GLN:HE21	38:1g:14:PRO:HD2	1.70	0.55
1:2A:588:U:H2'	1:2A:589:C:C6	2.42	0.55
6:2G:126:ASP:HB2	6:2G:130:ASN:HB2	1.89	0.55
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.89	0.55
32:2a:1004:A:N7	32:2a:1037:C:H2'	2.21	0.55
1:1A:1075:C:N4	1:1A:1077:A:N1	2.55	0.55
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.89	0.55
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.41	0.55
1:2A:1096:A:C8	1:2A:1097:U:H5	2.24	0.55
32:2a:67:C:H2'	32:2a:68:G:C8	2.41	0.55
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.06	0.55
1:1A:271(L):U:OP1	8:1I:50:ARG:NH2	2.37	0.55
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.55
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.71	0.55
32:1a:270:A:H2'	32:1a:271:C:C6	2.42	0.55
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.21	0.55
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.39	0.55
4:2E:8:LYS:HD2	4:2E:188:VAL:HG12	1.88	0.55
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.72	0.55
1:1A:1300:U:H4'	1:1A:1301:A:C5'	2.36	0.55
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.39	0.55
6:2G:97:ASP:HA	6:2G:100:TRP:CD1	2.41	0.55
32:2a:854:G:O6	61:2a:3210:HOH:O	2.15	0.55
32:2a:1005:A:H1'	32:2a:1025:U:C2	2.42	0.55
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.72	0.55
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.89	0.55
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.40	0.55
53:1y:23:ARG:NH1	53:1y:26:LYS:HD2	2.22	0.55
1:2A:1067:A:H4'	1:2A:1068:G:OP2	2.06	0.55
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.40	0.55
1:1A:265:A:N1	1:1A:427:U:O2'	2.38	0.55
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.43	0.55
32:1a:92:C:H2'	32:1a:93:G:C8	2.42	0.55
32:1a:1010:G:H22	32:1a:1020:U:H1'	1.72	0.55
33:1b:59:GLU:HB3	33:1b:221:LEU:HD21	1.89	0.55
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.41	0.55
6:2G:11:TYR:OH	6:2G:33:ARG:HG2	2.07	0.55
28:26:14:THR:OG1	28:26:48:VAL:O	2.25	0.55
32:2a:490:G:H2'	32:2a:491:G:C8	2.41	0.55
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2y:52:ALA:HB1	53:2y:81:LEU:HD11	1.89	0.55
1:1A:330:A:H2	1:1A:1210:A:O2'	1.90	0.54
61:1A:4498:HOH:O	11:1P:37:GLY:HA3	2.07	0.54
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.88	0.54
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.42	0.54
1:2A:2103:C:H42	1:2A:2185:C:H42	1.53	0.54
32:2a:984:C:H2'	32:2a:985:C:H6	1.72	0.54
1:1A:247:G:H4'	1:1A:386:G:C5	2.42	0.54
1:1A:341:G:O6	61:1A:4124:HOH:O	2.12	0.54
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.72	0.54
32:1a:130:A:C8	48:1q:63:ARG:HG3	2.42	0.54
49:1r:42:ARG:HA	49:1r:42:ARG:HE	1.72	0.54
25:23:3:ARG:HG3	25:23:38:GLU:HA	1.90	0.54
50:2s:22:LEU:O	50:2s:26:GLY:N	2.41	0.54
1:1A:278:A:O2'	1:1A:279:C:OP1	2.21	0.54
1:1A:784:A:H5'	1:1A:785:G:OP1	2.08	0.54
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.40	0.54
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.90	0.54
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.42	0.54
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.06	0.54
1:2A:2166:G:O6	1:2A:2171:A:O2'	2.24	0.54
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.42	0.54
32:2a:1002:G:H2'	32:2a:1003:G:C8	2.42	0.54
32:2a:1305:G:OP1	52:2u:2:GLY:N	2.41	0.54
33:2b:174:VAL:O	33:2b:178:ARG:HG2	2.08	0.54
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.43	0.54
1:1A:2137:C:C2	1:1A:2154:G:N2	2.75	0.54
2:1B:66:A:H61	2:1B:108:U:H2'	1.72	0.54
32:1a:266:G:H5"	32:1a:268:C:H41	1.71	0.54
32:1a:316:G:OP2	32:1a:351:G:O2'	2.25	0.54
32:1a:737:A:H2'	32:1a:738:C:C6	2.42	0.54
33:1b:229:VAL:HG12	33:1b:230:VAL:H	1.72	0.54
36:1e:7:GLU:N	36:1e:35:GLY:O	2.39	0.54
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	1.88	0.54
1:2A:1084:A:N6	1:2A:1086:A:N7	2.54	0.54
32:2a:1002:G:N3	32:2a:1003:G:H8	2.05	0.54
32:2a:1223:C:OP2	50:2s:78:ARG:NH2	2.40	0.54
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.41	0.54
35:2d:201:GLN:NE2	36:2e:116:THR:O	2.36	0.54
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.89	0.54
32:1a:347:G:C8	57:1a:1882:MPD:H53	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.43	0.54
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.21	0.54
6:2G:39:ILE:HG21	6:2G:60:LEU:HD11	1.89	0.54
17:2V:35:LEU:HB2	17:2V:57:VAL:HG23	1.90	0.54
26:24:16:CYS:SG	26:24:17:GLY:N	2.81	0.54
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.88	0.54
1:1A:530:G:N1	1:1A:2023:G:OP1	2.32	0.54
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.43	0.54
2:1B:87:G:N2	2:1B:90:A:OP2	2.32	0.54
32:1a:235:C:H2'	32:1a:236:G:H8	1.73	0.54
32:1a:946:A:H2'	32:1a:947:G:C8	2.43	0.54
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.91	0.54
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.88	0.54
47:1p:44:THR:OG1	47:1p:45:THR:N	2.41	0.54
1:2A:657:U:H2'	1:2A:658:C:C6	2.43	0.54
24:22:58:ALA:O	24:22:62:THR:OG1	2.26	0.54
32:2a:1158:C:O2	32:2a:1158:C:H2'	2.08	0.54
40:2i:51:ARG:HG2	40:2i:56:LEU:HD21	1.90	0.54
41:2j:8:LEU:HD12	41:2j:20:ALA:HB2	1.90	0.54
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.90	0.54
32:1a:255:G:H1'	48:1q:16:GLN:NE2	2.23	0.54
32:1a:1400:5MC:C2	53:1y:63:ALA:HA	2.42	0.54
1:2A:2128:C:H3'	1:2A:2129:C:H5"	1.88	0.54
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.55	0.54
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.41	0.54
44:2m:91:ARG:O	44:2m:96:LEU:N	2.40	0.54
1:1A:1094:U:O2'	1:1A:1096:A:N7	2.29	0.54
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.43	0.54
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	1.88	0.54
25:23:59:VAL:HG12	25:23:60:GLU:H	1.73	0.54
32:2a:1030:C:N4	32:2a:1032:G:O6	2.40	0.54
32:2a:1030(A):G:H2'	32:2a:1030(B):C:H5"	1.89	0.54
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.18	0.54
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.43	0.54
50:2s:36:ARG:HH12	50:2s:75:ALA:HB3	1.73	0.54
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.23	0.54
10:1O:118:ALA:O	57:1a:1882:MPD:H12	2.08	0.54
32:1a:1027:C:O2	32:1a:1034:G:N1	2.41	0.54
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.41	0.54
1:2A:749:C:OP2	61:2A:3835:HOH:O	2.17	0.54
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:128:VAL:HG23	21:2Z:161:VAL:HA	1.89	0.54
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.72	0.54
53:2y:43:LYS:HA	53:2y:48:PHE:HA	1.90	0.54
1:1A:2791:C:H5'	1:1A:2893:G:N2	2.24	0.54
19:1X:35:THR:HG22	19:1X:37:THR:H	1.73	0.54
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.89	0.54
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.89	0.54
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.23	0.54
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.43	0.54
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.17	0.54
1:2A:2821:A:OP2	61:2R:301:HOH:O	2.17	0.54
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.41	0.54
8:2I:62:LYS:HG2	8:2I:133:HIS:NE2	2.21	0.54
32:2a:266:G:N3	32:2a:266:G:H5"	2.23	0.54
40:2i:49:PRO:HG2	40:2i:81:ILE:HG23	1.90	0.54
1:1A:456:C:H4'	61:1A:4797:HOH:O	2.08	0.53
44:1m:13:LYS:HA	44:1m:44:ARG:HH11	1.72	0.53
47:1p:4:ILE:HG22	47:1p:19:ILE:HD11	1.90	0.53
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.41	0.53
1:2A:2105:C:N4	1:2A:2106:G:O6	2.41	0.53
23:21:52:ARG:NH1	23:21:55:GLY:O	2.41	0.53
32:2a:1047:G:H5"	45:2n:4:LYS:HE3	1.91	0.53
1:1A:813:U:OP1	61:1A:4148:HOH:O	2.19	0.53
1:1A:2458:G:OP2	61:1A:4141:HOH:O	2.18	0.53
2:1B:7:G:H5"	2:1B:7:G:H8	1.74	0.53
11:1P:64:LYS:NZ	61:1P:302:HOH:O	2.20	0.53
32:1a:79:G:C6	32:1a:90:U:N3	2.75	0.53
47:1p:14:ASN:OD1	47:1p:42:ARG:NH2	2.42	0.53
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.91	0.53
1:2A:2104:G:N7	1:2A:2186:G:C2	2.76	0.53
32:2a:662:G:H2'	32:2a:663:A:H8	1.73	0.53
32:2a:1039:C:H2'	32:2a:1040:U:O4'	2.08	0.53
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.90	0.53
8:1I:27:ARG:HD2	23:11:71:TYR:CE2	2.44	0.53
12:1Q:109:VAL:HG22	12:1Q:113:GLN:CD	2.33	0.53
35:1d:108:LEU:HD12	35:1d:174:LEU:HD13	1.90	0.53
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.09	0.53
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	1.91	0.53
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.44	0.53
1:1A:2259:G:N3	61:1A:4267:HOH:O	2.33	0.53
1:1A:2602:A:H4'	1:1A:2603:G:OP1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:66:ARG:NH1	61:1V:302:HOH:O	2.30	0.53
32:1a:184:G:H2'	32:1a:185:A:H8	1.74	0.53
32:1a:538:G:H5"	43:1l:114:LYS:HB2	1.89	0.53
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.77	0.53
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.41	0.53
38:2g:42:ILE:HD13	38:2g:116:ALA:HB3	1.90	0.53
44:2m:17:VAL:O	44:2m:20:THR:OG1	2.27	0.53
1:1A:217:G:OP2	61:1A:4147:HOH:O	2.19	0.53
1:1A:1267:U:OP1	61:1A:4146:HOH:O	2.19	0.53
1:1A:1583:A:H5'	1:1A:1584:C:OP1	2.08	0.53
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.91	0.53
6:1G:126:ASP:N	6:1G:130:ASN:O	2.41	0.53
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.74	0.53
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.43	0.53
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.44	0.53
1:2A:2218:U:O4'	23:21:52:ARG:NH2	2.41	0.53
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.91	0.53
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.09	0.53
32:2a:1223:C:P	50:2s:78:ARG:HH21	2.31	0.53
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.24	0.53
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.74	0.53
32:1a:269:C:H2'	32:1a:270:A:H8	1.74	0.53
32:1a:309:G:O2'	32:1a:607:A:N1	2.42	0.53
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.74	0.53
1:2A:954:G:H5"	12:2Q:13:GLN:HB3	1.90	0.53
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.43	0.53
1:2A:2128:C:H42	1:2A:2160:G:H1	1.55	0.53
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.38	0.53
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.09	0.53
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.41	0.53
34:2c:19:GLU:HB3	34:2c:40:ARG:HH12	1.74	0.53
45:2n:47:LEU:HA	45:2n:50:LYS:HB2	1.90	0.53
1:1A:639:U:H2'	1:1A:640:C:C6	2.44	0.53
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.08	0.53
26:14:61:ARG:HG3	26:14:62:ARG:H	1.73	0.53
32:1a:403:C:OP1	35:1d:137:SER:OG	2.22	0.53
35:1d:88:VAL:HG13	36:1e:97:GLY:HA2	1.90	0.53
1:2A:886:C:O2'	1:2A:889:C:N4	2.42	0.53
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.43	0.53
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.09	0.53
1:2A:2310:A:H61	6:2G:79:ASN:HD22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:17:C:H2'	2:2B:18:G:O4'	2.08	0.53
4:2E:12:THR:HG21	15:2T:11:GLU:OE2	2.08	0.53
32:2a:17:U:O2'	32:2a:1079:G:H1'	2.09	0.53
32:2a:1226:C:N4	44:2m:104:ARG:HD2	2.23	0.53
33:2b:222:ILE:O	33:2b:226:ARG:HB2	2.08	0.53
15:1T:54:ARG:HA	15:1T:59:THR:HG23	1.91	0.53
32:1a:384:G:H2'	32:1a:385:C:C6	2.44	0.53
32:1a:978:A:O2'	32:1a:1322:C:N3	2.35	0.53
47:1p:57:ARG:HH21	47:1p:79:VAL:HA	1.73	0.53
1:2A:568:U:OP2	61:2A:3841:HOH:O	2.19	0.53
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.07	0.53
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.90	0.53
6:2G:14:GLU:C	6:2G:17:PRO:HD2	2.34	0.53
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.90	0.53
32:2a:624:C:H2'	32:2a:625:G:H8	1.73	0.53
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.41	0.53
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.17	0.53
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.90	0.53
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.91	0.53
61:1A:5517:HOH:O	9:1N:73:THR:HG21	2.09	0.53
16:1U:33:ARG:NH2	61:1U:306:HOH:O	2.41	0.53
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.91	0.53
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.23	0.53
32:1a:1094:G:OP1	61:1a:1911:HOH:O	2.18	0.53
39:1h:116:LYS:HD3	39:1h:127:LEU:HD23	1.90	0.53
1:2A:731:C:OP1	61:2A:3843:HOH:O	2.19	0.53
1:2A:1799:G:N2	3:2D:155:LEU:HD12	2.24	0.53
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.44	0.53
1:2A:2280:G:H5'	21:2Z:201:LYS:HD2	1.91	0.53
1:2A:2810:A:N6	1:2A:2891:G:O2'	2.42	0.53
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.24	0.53
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.90	0.53
1:1A:123:G:OP2	61:1A:4149:HOH:O	2.19	0.53
1:1A:184:C:H2'	1:1A:185:U:C6	2.44	0.53
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.24	0.53
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.74	0.53
23:11:3:LYS:HB3	23:11:61:ARG:HH22	1.74	0.53
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	1.90	0.53
32:1a:1256:A:OP2	32:1a:1279:A:N6	2.41	0.53
1:2A:108:U:OP1	1:2A:293:U:O2'	2.26	0.53
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.37	0.53
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.40	0.53
35:2d:10:ARG:HG3	35:2d:11:LEU:HD12	1.91	0.53
53:2y:48:PHE:CD2	53:2y:70:MET:HB3	2.44	0.53
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.72	0.52
1:2A:1815:A:OP2	61:2A:3842:HOH:O	2.19	0.52
1:2A:2127:G:O6	1:2A:2161:C:N3	2.42	0.52
1:2A:2152:G:H2'	1:2A:2153:G:H8	1.75	0.52
1:2A:2206:G:H8	1:2A:2207:G:N7	2.06	0.52
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG12	2.09	0.52
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.44	0.52
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.44	0.52
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.25	0.52
33:2b:158:LEU:HD21	33:2b:180:LEU:HD13	1.90	0.52
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.44	0.52
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.39	0.52
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.89	0.52
53:2y:12:ILE:HG22	53:2y:17:ARG:HG3	1.92	0.52
1:1A:1094:U:H2'	1:1A:1096:A:OP2	2.09	0.52
21:1Z:108:PRO:HB2	21:1Z:111:VAL:HG23	1.91	0.52
21:1Z:140:ASP:OD1	21:1Z:142:SER:OG	2.27	0.52
29:17:24:THR:CG2	29:17:27:GLY:H	2.22	0.52
32:1a:22:G:H4'	32:1a:885:G:C8	2.44	0.52
32:1a:100:C:H2'	32:1a:101:A:C8	2.44	0.52
51:1t:45:GLN:HA	51:1t:91:LEU:HD22	1.90	0.52
1:2A:1065:U:H4'	1:2A:1066:U:H5'	1.90	0.52
1:2A:1068:G:H3'	1:2A:1096:A:OP2	2.09	0.52
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.45	0.52
21:2Z:140:ASP:OD1	21:2Z:142:SER:OG	2.26	0.52
32:2a:539:A:H2'	32:2a:540:G:C8	2.44	0.52
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.42	0.52
41:2j:78:ASN:O	41:2j:80:LYS:N	2.43	0.52
1:1A:1245:G:N7	61:1A:4271:HOH:O	2.33	0.52
32:1a:600:C:H2'	32:1a:601:C:H6	1.74	0.52
32:1a:626:U:H2'	32:1a:627:G:C8	2.44	0.52
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.44	0.52
35:1d:94:LEU:HA	35:1d:97:LEU:HD12	1.92	0.52
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.44	0.52
44:2m:54:VAL:HA	44:2m:57:ARG:HB3	1.91	0.52
53:2y:87:LYS:O	53:2y:91:LYS:HB2	2.08	0.52
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:2:LYS:HE2	11:1P:4:SER:H	1.74	0.52
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.91	0.52
32:1a:384:G:H2'	32:1a:385:C:H6	1.75	0.52
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.91	0.52
36:1e:8:GLU:HG3	36:1e:34:VAL:HG23	1.92	0.52
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.25	0.52
41:2j:77:PRO:O	41:2j:81:THR:OG1	2.22	0.52
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.90	0.52
1:1A:2697:G:OP1	61:1A:4144:HOH:O	2.18	0.52
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.24	0.52
32:1a:235:C:H2'	32:1a:236:G:C8	2.45	0.52
32:1a:359:U:H2'	32:1a:360:A:C8	2.45	0.52
32:1a:457:C:H42	32:1a:474:G:H1	1.57	0.52
32:1a:1158:C:H5	32:1a:1181:G:N1	2.08	0.52
35:1d:167:GLY:H	35:1d:168:ARG:NH1	2.08	0.52
1:2A:361:G:O2'	1:2A:362:U:H5'	2.10	0.52
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.92	0.52
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.91	0.52
32:2a:127:G:HO2'	48:2q:2:PRO:N	2.08	0.52
33:2b:229:VAL:HG12	33:2b:230:VAL:H	1.75	0.52
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.92	0.52
32:1a:265:G:H2'	32:1a:267:C:H5	1.74	0.52
32:1a:828:A:H2'	32:1a:829:G:O4'	2.09	0.52
34:1c:102:ASN:HD22	34:1c:102:ASN:N	2.08	0.52
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.45	0.52
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.09	0.52
20:2Y:2:ARG:HE	20:2Y:4:LYS:HD3	1.75	0.52
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.43	0.52
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.10	0.52
39:1h:86:ILE:HG13	39:1h:133:LEU:HD22	1.92	0.52
24:22:67:LYS:HA	24:22:70:GLN:NE2	2.24	0.52
26:24:14:ILE:HB	26:24:22:ILE:HD13	1.92	0.52
32:2a:1005:A:H1'	32:2a:1025:U:O2	2.10	0.52
32:2a:1086:U:H3	32:2a:1099:G:H22	1.58	0.52
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.74	0.52
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.92	0.52
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.40	0.52
32:1a:620:C:H2'	32:1a:621:A:O4'	2.10	0.52
40:1i:16:ARG:HB2	40:1i:64:THR:HB	1.91	0.52
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.25	0.52
6:2G:50:ALA:O	6:2G:53:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.39	0.52
32:2a:918:A:H2'	32:2a:919:A:C8	2.44	0.52
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.91	0.52
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.75	0.52
8:1I:9:LEU:HB3	8:1I:12:LEU:HB3	1.90	0.52
12:1Q:43:THR:HA	12:1Q:94:VAL:HG12	1.92	0.52
44:1m:34:LEU:HD13	44:1m:41:PRO:HB3	1.91	0.52
51:1t:92:LEU:O	51:1t:96:GLY:N	2.40	0.52
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.52
32:2a:737:A:H2'	32:2a:738:C:C6	2.45	0.52
1:1A:1036:G:OP2	7:1H:59:ARG:NH2	2.43	0.52
34:1c:120:VAL:O	34:1c:124:ILE:HG12	2.10	0.52
35:1d:173:TRP:CD1	35:1d:189:PRO:HB3	2.45	0.52
1:2A:82:G:N1	1:2A:103:A:OP2	2.41	0.52
1:2A:2104:G:N2	1:2A:2105:C:C4	2.78	0.52
7:2H:12:PRO:O	7:2H:15:VAL:HG22	2.10	0.52
26:24:59:PHE:HB3	26:24:61:ARG:HB3	1.91	0.52
30:28:39:LYS:O	30:28:43:GLN:HG3	2.09	0.52
32:2a:1024:G:H2'	32:2a:1025:U:H5"	1.92	0.52
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.27	0.52
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.91	0.51
32:1a:130:A:H5'	48:1q:63:ARG:HH21	1.75	0.51
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.43	0.51
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.33	0.51
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.45	0.51
32:1a:524:G:H2'	32:1a:525:C:C6	2.45	0.51
32:1a:1024:G:H21	32:1a:1025:U:H5"	1.75	0.51
2:2B:89:G:OP2	2:2B:89:G:H8	1.93	0.51
8:2I:4:ILE:HD11	8:2I:44:LEU:HD23	1.91	0.51
32:2a:420:U:H2'	32:2a:422:C:C5	2.45	0.51
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.11	0.51
32:2a:1346:A:H5"	40:2i:120:ARG:NH1	2.26	0.51
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.92	0.51
1:1A:1056:G:H5"	1:1A:1057:A:O4'	2.11	0.51
1:2A:1073:A:H2'	1:2A:1074:G:C8	2.45	0.51
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.45	0.51
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.45	0.51
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.45	0.51
33:2b:30:ARG:NH2	33:2b:194:PRO:HB2	2.26	0.51
32:1a:359:U:H2'	32:1a:360:A:H8	1.76	0.51
32:1a:404:U:H2'	32:1a:405:U:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1492:A:H4'	32:1a:1493:A:C2	2.45	0.51
47:1p:75:ARG:HG3	47:1p:80:PHE:HD2	1.75	0.51
5:2F:17:ARG:HH12	5:2F:19:GLU:HG2	1.75	0.51
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.93	0.51
33:2b:8:LYS:HA	33:2b:217:ARG:HH11	1.75	0.51
33:2b:121:LEU:O	33:2b:127:ILE:HG12	2.09	0.51
33:2b:134:GLU:HA	33:2b:137:ARG:NH2	2.26	0.51
6:1G:138:GLN:HE22	6:1G:153:ARG:HH21	1.58	0.51
32:1a:1008:C:H2'	32:1a:1009:G:O4'	2.11	0.51
40:1i:26:VAL:HG11	40:1i:33:PHE:HD1	1.75	0.51
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.25	0.51
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.46	0.51
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.51
11:2P:130:PHE:HB2	11:2P:135:LEU:HD12	1.92	0.51
32:2a:1159:U:O4'	32:2a:1182:G:N2	2.44	0.51
40:2i:26:VAL:HA	40:2i:61:ALA:O	2.11	0.51
1:1A:1250:G:H5"	61:1U:331:HOH:O	2.11	0.51
1:1A:2896:C:H2'	1:1A:2897:U:C6	2.46	0.51
3:1D:88:ARG:NH1	61:1D:407:HOH:O	2.43	0.51
25:13:3:ARG:HG2	25:13:38:GLU:HA	1.92	0.51
32:1a:1149:C:OP2	40:1i:9:ARG:NH2	2.43	0.51
33:1b:20:GLU:HG2	33:1b:23:ARG:HH21	1.76	0.51
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.91	0.51
44:1m:11:ARG:C	44:1m:13:LYS:H	2.17	0.51
1:2A:881:G:H2'	1:2A:882:G:C8	2.45	0.51
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.10	0.51
1:2A:2104:G:N2	1:2A:2105:C:C2	2.71	0.51
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.46	0.51
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.09	0.51
1:1A:271(H):G:O2'	1:1A:271(I):G:OP2	2.25	0.51
1:1A:521:G:O6	61:1A:4145:HOH:O	2.18	0.51
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.26	0.51
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.91	0.51
1:2A:579:G:H2'	1:2A:580:C:C6	2.45	0.51
1:2A:1056:G:H21	1:2A:1103:A:H62	1.58	0.51
1:2A:1062:G:H5'	1:2A:1070:A:H5'	1.92	0.51
1:2A:2756:U:H1'	1:2A:2757:A:H5"	1.92	0.51
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.93	0.51
6:2G:144:ILE:HA	6:2G:148:MET:SD	2.51	0.51
32:2a:1117:G:H4'	40:2i:104:ARG:NH1	2.26	0.51
38:2g:27:ILE:HD12	38:2g:40:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:67:ALA:HB2	51:2t:77:ALA:HB2	1.93	0.51
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.93	0.51
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.92	0.51
16:1U:101:ARG:NH2	61:1U:302:HOH:O	2.24	0.51
36:1e:148:VAL:HG21	39:1h:107:LEU:HB3	1.93	0.51
2:2B:115:G:O2'	14:2S:50:SER:OG	2.29	0.51
8:2I:133:HIS:HD2	8:2I:136:VAL:HG23	1.76	0.51
10:2O:77:ILE:HD12	15:2T:74:ARG:HD3	1.93	0.51
32:2a:434:U:H2'	32:2a:435:C:C6	2.46	0.51
1:1A:1082:U:C4	1:1A:1086:A:N1	2.78	0.51
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.46	0.51
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.51
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.46	0.51
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.10	0.51
1:2A:2788:C:N3	1:2A:2789:C:N4	2.58	0.51
32:2a:750:G:N2	46:2o:23:GLY:O	2.29	0.51
32:2a:1303:C:H2'	32:2a:1304:G:H5'	1.92	0.51
1:1A:335:C:H4'	20:1Y:73:ARG:HD2	1.93	0.51
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.20	0.51
1:2A:1047:G:H21	1:2A:1111:A:H62	1.56	0.51
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.11	0.51
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.46	0.51
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.11	0.51
7:2H:59:ARG:O	7:2H:63:SER:OG	2.22	0.51
32:2a:1001:A:H2'	32:2a:1001(A):G:C8	2.46	0.51
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.76	0.51
1:1A:154(A):C:H3'	61:1A:7832:HOH:O	2.10	0.50
1:1A:1341:U:O4'	19:1X:57:LEU:HD23	2.11	0.50
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.23	0.50
32:1a:1401:G:O6	53:1y:83:ARG:NH2	2.36	0.50
32:1a:1470:G:N7	61:1a:1933:HOH:O	2.34	0.50
35:1d:196:LEU:O	35:1d:198:VAL:N	2.39	0.50
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.26	0.50
1:2A:455:C:N3	1:2A:472:A:H2'	2.27	0.50
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.26	0.50
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.12	0.50
32:2a:490:G:H2'	32:2a:491:G:H8	1.76	0.50
38:2g:115:ARG:HD2	38:2g:115:ARG:N	2.26	0.50
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.11	0.50
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	1.93	0.50
21:1Z:136:PHE:CE1	21:1Z:138:GLU:HG3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:30:ARG:NH1	24:12:34:GLU:OE2	2.44	0.50
28:16:19:ARG:NH1	28:16:52:VAL:HG11	2.27	0.50
1:2A:1939:5MU:O5'	61:2A:3825:HOH:O	2.19	0.50
32:2a:757:U:OP1	32:2a:822:C:O2'	2.29	0.50
32:2a:1035:A:HO2'	32:2a:1036:G:H8	1.59	0.50
36:2e:52:PRO:HG2	36:2e:53:LEU:HD12	1.92	0.50
42:2k:33:THR:HG22	42:2k:39:PRO:HA	1.92	0.50
43:2l:84:LEU:HB3	43:2l:104:VAL:HG21	1.93	0.50
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.93	0.50
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.92	0.50
21:1Z:182:LYS:O	21:1Z:185:GLU:HG2	2.12	0.50
27:15:16:ARG:HG3	27:15:17:ASP:N	2.25	0.50
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.43	0.50
32:1a:1003:G:C2	32:1a:1004:A:H1'	2.46	0.50
32:1a:1305:G:OP1	52:1u:2:GLY:N	2.44	0.50
1:2A:1057:A:N7	1:2A:1086:A:H2'	2.26	0.50
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.44	0.50
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.35	0.50
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.42	0.50
1:2A:2138:C:H2'	1:2A:2139:C:C6	2.47	0.50
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.36	0.50
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.93	0.50
1:1A:1141:U:OP1	9:1N:25:ARG:NH1	2.45	0.50
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.27	0.50
21:1Z:198:LYS:HB3	21:1Z:202:GLU:HB3	1.92	0.50
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.46	0.50
51:1t:67:ALA:HB2	51:1t:77:ALA:HB2	1.94	0.50
1:2A:93:G:H2'	1:2A:94:C:C6	2.47	0.50
1:2A:635:C:O2'	1:2A:639:U:OP1	2.25	0.50
1:2A:1155:A:H5"	16:2U:55:ARG:HD3	1.94	0.50
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.26	0.50
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.93	0.50
10:2O:24:VAL:HB	10:2O:33:ALA:HB2	1.92	0.50
32:2a:933:G:O6	38:2g:3:ARG:NH2	2.41	0.50
34:2c:121:ALA:O	34:2c:125:GLU:HG3	2.12	0.50
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.50
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.27	0.50
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.45	0.50
32:1a:179:A:H2'	32:1a:180:U:H6	1.77	0.50
32:1a:1034:G:H3'	32:1a:1035:A:C8	2.46	0.50
32:1a:1148:U:O2'	40:1i:66:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:62:SER:HB3	48:1q:72:ARG:HH11	1.75	0.50
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.12	0.50
1:2A:1939:5MU:H2'	61:2A:3825:HOH:O	2.11	0.50
1:2A:2111:C:N4	1:2A:2147:G:H22	2.08	0.50
32:2a:130:A:O2'	32:2a:131:C:O5'	2.28	0.50
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.45	0.50
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.46	0.50
33:2b:98:LEU:HB2	33:2b:101:MET:HG3	1.94	0.50
34:2c:6:HIS:CE1	34:2c:8:ILE:HB	2.46	0.50
34:2c:121:ALA:HB2	34:2c:187:ALA:HB1	1.93	0.50
50:2s:49:ILE:HG12	50:2s:62:ILE:HD11	1.93	0.50
1:1A:881:G:H2'	1:1A:882:G:O4'	2.11	0.50
1:1A:1054:A:H5'	1:1A:1055:G:OP2	2.11	0.50
1:1A:1920:OMC:HM22	1:1A:1921:G:H5'	1.94	0.50
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.75	0.50
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.46	0.50
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.39	0.50
1:2A:800:A:H8	1:2A:800:A:OP1	1.95	0.50
1:2A:2659:G:O2'	7:2H:175:LYS:HE2	2.11	0.50
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.47	0.50
7:2H:89:ILE:HB	7:2H:129:THR:HA	1.93	0.50
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.12	0.50
32:2a:328:C:H4'	32:2a:329:A:H5'	1.94	0.50
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.11	0.50
53:2y:10:MET:HE3	53:2y:12:ILE:HD11	1.93	0.50
32:1a:1226:C:N4	44:1m:104:ARG:HD2	2.27	0.50
1:2A:300:A:H1'	1:2A:319:C:H1'	1.93	0.50
1:2A:2051:A:OP2	61:2A:3848:HOH:O	2.19	0.50
9:2N:71:ILE:HG21	9:2N:84:LYS:HD3	1.94	0.50
33:2b:78:GLN:NE2	33:2b:95:GLN:OE1	2.45	0.50
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.11	0.50
1:1A:1054:A:N1	1:1A:1105:U:O2	2.45	0.50
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.94	0.50
8:1I:114:LEU:HD12	8:1I:130:TYR:HA	1.93	0.50
15:1T:51:ARG:NH1	61:1T:302:HOH:O	2.45	0.50
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.94	0.50
49:1r:26:LEU:HD22	49:1r:39:VAL:HG13	1.92	0.50
1:2A:212:G:H2'	1:2A:213:A:O4'	2.11	0.50
1:2A:251:A:C5	1:2A:252:G:H1'	2.46	0.50
1:2A:1124:C:OP1	61:2A:3840:HOH:O	2.18	0.50
1:2A:2107:C:N4	1:2A:2182:G:H1	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2629:A:H1'	1:2A:2630:G:H5"	1.94	0.50
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.12	0.50
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.47	0.50
32:2a:1346:A:H5"	40:2i:120:ARG:HH12	1.76	0.50
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.94	0.50
1:1A:228:A:H8	1:1A:229:A:H5'	1.76	0.50
1:1A:1060:U:H4'	1:1A:1061:U:H5'	1.93	0.50
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.77	0.50
13:1R:71:GLN:NE2	61:1R:303:HOH:O	2.44	0.50
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.44	0.50
34:1c:47:LEU:HD13	34:1c:68:VAL:HG11	1.93	0.50
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	1.94	0.50
1:2A:10:G:H1'	1:2A:2801(A):A:C2	2.46	0.50
1:2A:832:G:OP1	61:2A:3850:HOH:O	2.20	0.50
1:2A:1503:U:H2'	1:2A:1504:C:H6	1.77	0.50
6:2G:28:VAL:O	6:2G:31:VAL:HG13	2.12	0.50
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.93	0.50
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.77	0.50
32:2a:1516:G:H2'	32:2a:1518:MA6:OP2	2.12	0.50
33:2b:57:PHE:HE2	33:2b:185:ILE:HD11	1.77	0.50
1:1A:226:G:H21	1:1A:228:A:H62	1.60	0.49
1:1A:2027:G:OP2	61:1A:4150:HOH:O	2.19	0.49
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.12	0.49
32:1a:45:U:H2'	32:1a:46:G:C8	2.47	0.49
32:1a:995:C:O2	45:1n:4:LYS:NZ	2.44	0.49
32:1a:1216:G:H5"	45:1n:5:ALA:HB2	1.94	0.49
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.46	0.49
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.37	0.49
1:2A:2119:A:H61	1:2A:2168:G:H21	1.58	0.49
1:2A:2134:A:H5"	1:2A:2156:G:H22	1.77	0.49
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.29	0.49
26:24:62:ARG:HD2	26:24:62:ARG:N	2.27	0.49
33:2b:73:THR:HG22	33:2b:95:GLN:O	2.12	0.49
41:2j:7:LYS:HB2	41:2j:97:GLU:HB2	1.94	0.49
44:2m:65:LYS:O	44:2m:70:LEU:HD12	2.11	0.49
1:1A:580:C:H2'	1:1A:581:C:C6	2.46	0.49
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.46	0.49
32:1a:96:U:H2'	32:1a:97:G:H8	1.77	0.49
32:1a:626:U:H2'	32:1a:627:G:H8	1.76	0.49
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.94	0.49
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.47	0.49
1:2A:2507:C:OP1	61:2A:3844:HOH:O	2.19	0.49
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.94	0.49
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.47	0.49
32:2a:1347:G:H5"	40:2i:107:ARG:HB3	1.94	0.49
44:2m:59:TYR:CE1	44:2m:63:THR:HG21	2.47	0.49
50:2s:41:VAL:HG22	50:2s:42:PRO:HD2	1.94	0.49
1:1A:2133:G:H1'	1:1A:2158:A:H2	1.77	0.49
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.78	0.49
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.12	0.49
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.48	0.49
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.46	0.49
1:2A:120:U:OP2	61:2A:3849:HOH:O	2.20	0.49
1:2A:247:G:H4'	1:2A:386:G:C5	2.48	0.49
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.12	0.49
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.48	0.49
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.47	0.49
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.12	0.49
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.94	0.49
10:2O:16:ALA:HB2	10:2O:52:VAL:HG21	1.93	0.49
32:2a:376:G:H5"	47:2p:5:ARG:HD3	1.93	0.49
32:2a:1147:C:O2	40:2i:16:ARG:NH2	2.45	0.49
42:2k:99:GLN:HG2	42:2k:105:VAL:HG11	1.94	0.49
1:1A:2149:G:H2'	1:1A:2150:U:O4'	2.13	0.49
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.28	0.49
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.12	0.49
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.47	0.49
24:12:1:MET:HE3	24:12:6:VAL:HG22	1.94	0.49
1:2A:493:G:H2'	1:2A:494:G:O4'	2.12	0.49
1:2A:644:A:H4'	1:2A:645:C:H5	1.77	0.49
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.94	0.49
32:2a:1238:A:OP2	61:2a:3215:HOH:O	2.20	0.49
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.48	0.49
48:2q:43:LEU:HD12	48:2q:68:ARG:HG2	1.93	0.49
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.10	0.49
1:1A:1700:A:OP2	61:1A:4153:HOH:O	2.20	0.49
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD21	1.95	0.49
33:1b:71:VAL:HB	33:1b:164:VAL:HG22	1.95	0.49
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.12	0.49
38:1g:75:VAL:HG11	38:1g:144:MET:HG3	1.94	0.49
40:1i:3:GLN:NE2	40:1i:20:ARG:HH21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:21:ILE:HD12	42:1k:84:VAL:HG22	1.93	0.49
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.47	0.49
1:2A:2128:C:H1'	1:2A:2173:A:H2	1.78	0.49
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.93	0.49
32:2a:410:G:H21	32:2a:432:A:H62	1.61	0.49
32:2a:443:C:H2'	32:2a:444:C:H6	1.78	0.49
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.46	0.49
32:2a:1403:C:C2	32:2a:1404:5MC:HM52	2.47	0.49
34:2c:6:HIS:CD2	34:2c:9:GLY:H	2.30	0.49
44:2m:14:ARG:NE	44:2m:42:ALA:HA	2.28	0.49
47:2p:20:VAL:HG21	47:2p:32:TYR:CG	2.47	0.49
51:2t:57:ARG:HD3	51:2t:101:GLY:O	2.12	0.49
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.48	0.49
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.12	0.49
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.12	0.49
1:1A:2732:G:OP1	4:1E:203:LYS:NZ	2.38	0.49
15:1T:28:VAL:HG13	15:1T:86:ILE:HG23	1.93	0.49
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.48	0.49
32:1a:593:G:H2'	32:1a:594:G:O4'	2.13	0.49
32:1a:1296:C:OP1	44:1m:44:ARG:NH2	2.46	0.49
33:1b:32:ILE:HD13	33:1b:40:HIS:HB3	1.94	0.49
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.45	0.49
1:2A:1721:G:H8	1:2A:1741:A:H62	1.61	0.49
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.46	0.49
1:2A:2113:U:H2'	1:2A:2114:A:O4'	2.13	0.49
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.77	0.49
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.46	0.49
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.61	0.49
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.95	0.49
6:2G:29:TRP:O	6:2G:33:ARG:NH1	2.46	0.49
6:2G:139:LEU:HA	6:2G:144:ILE:HB	1.95	0.49
32:2a:659:U:H5"	46:2o:9:GLN:HE22	1.76	0.49
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.27	0.49
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.47	0.49
32:2a:1292:U:H5'	40:2i:38:GLN:HE22	1.78	0.49
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.95	0.49
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.94	0.49
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.12	0.49
7:1H:3:ARG:HB3	7:1H:6:ARG:HG2	1.93	0.49
1:2A:8:A:H2'	1:2A:9:U:C6	2.48	0.49
1:2A:818:G:OP2	61:2A:3846:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.28	0.49
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.77	0.49
34:2c:6:HIS:NE2	34:2c:8:ILE:HB	2.27	0.49
40:2i:17:VAL:HG21	40:2i:80:GLY:C	2.37	0.49
43:2l:60:LEU:HD21	43:2l:85:ILE:HD11	1.94	0.49
1:1A:143:G:H4'	19:1X:35:THR:HG21	1.94	0.49
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.25	0.49
6:1G:53:LEU:O	6:1G:56:ALA:N	2.46	0.49
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.31	0.49
20:1Y:92:ASN:N	20:1Y:92:ASN:HD22	2.10	0.49
32:1a:176:C:H2'	32:1a:177:C:H6	1.78	0.49
32:1a:662:G:H2'	32:1a:663:A:C8	2.48	0.49
32:1a:890:G:O2'	32:1a:906:G:O6	2.18	0.49
42:1k:92:GLU:HG3	42:1k:96:ARG:NH1	2.28	0.49
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.78	0.49
1:2A:1508:A:H4'	1:2A:1509(A):A:C6	2.48	0.49
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.12	0.49
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.46	0.49
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.48	0.49
2:2B:42:C:N3	6:2G:91:ARG:NH1	2.57	0.49
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.93	0.49
32:2a:443:C:H2'	32:2a:444:C:C6	2.48	0.49
32:2a:1002:G:N3	32:2a:1003:G:C8	2.81	0.49
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.47	0.49
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.48	0.49
32:1a:17:U:H2'	32:1a:18:C:C6	2.48	0.49
32:1a:437:U:H5'	35:1d:155:LEU:HD21	1.94	0.49
1:2A:236:C:H2'	1:2A:237:C:C6	2.47	0.49
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.59	0.49
1:2A:1494:A:H2'	1:2A:1495:A:C8	2.48	0.49
1:2A:1856:G:N7	61:2A:3936:HOH:O	2.35	0.49
1:2A:2251:OMG:H5'	61:2A:4739:HOH:O	2.13	0.49
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.47	0.49
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.78	0.49
6:2G:60:LEU:HD23	6:2G:68:PRO:HG3	1.95	0.49
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.94	0.49
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.13	0.49
32:2a:653:A:C8	39:2h:56:LYS:HG2	2.48	0.49
32:2a:1256:A:N6	32:2a:1278:U:H1'	2.20	0.49
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.95	0.49
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.48	0.49
1:1A:579:G:H2'	1:1A:580:C:C6	2.48	0.49
1:1A:2650:U:H2'	1:1A:2651:C:C6	2.48	0.49
2:1B:2:C:H2'	2:1B:3:C:C6	2.48	0.49
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.78	0.49
32:1a:67:C:O2'	32:1a:171:A:H1'	2.12	0.49
32:1a:560:U:O2'	32:1a:561:U:OP2	2.29	0.49
32:1a:953:G:N7	44:1m:104:ARG:NH2	2.61	0.49
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.47	0.49
36:1e:81:GLU:HG2	36:1e:90:VAL:HG13	1.95	0.49
1:2A:760:G:H2'	1:2A:761:A:O4'	2.13	0.49
1:2A:2506:U:O2	55:2A:3730:HGR:H23	2.12	0.49
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.48	0.49
32:2a:947:G:H2'	32:2a:948:C:O4'	2.12	0.49
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.48	0.49
1:1A:1053:C:N3	1:1A:1106:G:O6	2.46	0.48
1:1A:1066:U:H2'	1:1A:1067:A:C5	2.48	0.48
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.13	0.48
1:1A:2370:G:OP2	61:1A:4151:HOH:O	2.20	0.48
1:1A:2469:A:H5'	1:1A:2470:G:OP2	2.12	0.48
32:1a:600:C:H2'	32:1a:601:C:C6	2.47	0.48
35:1d:8:VAL:HG12	35:1d:22:LYS:HE2	1.94	0.48
35:1d:118:ARG:HG2	35:1d:136:PRO:HB3	1.95	0.48
36:1e:71:LEU:HD11	36:1e:113:ALA:O	2.13	0.48
39:1h:112:LEU:HD23	39:1h:133:LEU:HA	1.95	0.48
41:1j:81:THR:HA	41:1j:84:GLN:HG2	1.94	0.48
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.48	0.48
1:2A:874:G:O2'	21:2Z:120:ILE:HD11	2.13	0.48
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.12	0.48
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.46	0.48
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.45	0.48
17:2V:28:GLU:O	17:2V:61:VAL:HG21	2.13	0.48
23:21:56:GLN:HE21	23:21:87:PRO:HG3	1.78	0.48
32:2a:944:G:N1	32:2a:1338:G:OP2	2.42	0.48
34:2c:181:ASN:N	34:2c:205:GLY:O	2.31	0.48
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.78	0.48
40:2i:43:ALA:C	40:2i:45:ALA:H	2.21	0.48
48:2q:50:LYS:HD2	48:2q:51:TYR:CZ	2.47	0.48
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.48	0.48
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.61	0.48
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:14:ASP:O	8:1I:17:GLN:HB3	2.13	0.48
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.95	0.48
32:1a:1329:A:P	44:1m:28:ALA:HB3	2.53	0.48
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.95	0.48
1:2A:1069:A:C5	1:2A:1095:A:H4'	2.49	0.48
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.28	0.48
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.13	0.48
33:2b:95:GLN:HG3	33:2b:96:ARG:H	1.77	0.48
43:2l:54:LYS:HB3	43:2l:70:ILE:HD12	1.95	0.48
1:1A:7:G:H2'	1:1A:8:A:O4'	2.12	0.48
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.94	0.48
1:1A:1336:A:OP2	19:1X:64:LYS:NZ	2.45	0.48
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.40	0.48
1:1A:2637:U:OP1	4:1E:82:ARG:NH1	2.46	0.48
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.43	0.48
17:1V:85:LYS:NZ	61:1V:301:HOH:O	2.22	0.48
32:1a:1004:A:O2'	32:1a:1038:C:O2	2.24	0.48
32:1a:1014:A:H4'	50:1s:14:HIS:CE1	2.48	0.48
33:1b:84:GLU:O	33:1b:219:VAL:HG11	2.13	0.48
38:1g:28:ASN:HA	38:1g:31:MET:HE2	1.96	0.48
41:1j:67:THR:O	41:1j:67:THR:OG1	2.25	0.48
48:1q:58:GLU:OE2	48:1q:75:ARG:NH2	2.45	0.48
1:2A:1085:A:H2'	1:2A:1085:A:N3	2.26	0.48
1:2A:2417:C:OP1	11:2P:65:ARG:NH2	2.46	0.48
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.96	0.48
32:2a:111:G:OP2	61:2a:3214:HOH:O	2.20	0.48
32:2a:189(L):G:H2'	32:2a:190:U:C6	2.47	0.48
32:2a:253:U:O2	32:2a:275:G:O2'	2.28	0.48
40:2i:108:VAL:HG12	40:2i:109:VAL:H	1.78	0.48
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.49	0.48
1:1A:2748:A:H5'	7:1H:4:ILE:HD13	1.94	0.48
24:12:65:ASN:O	24:12:69:ARG:HG3	2.12	0.48
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.38	0.48
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.14	0.48
32:1a:1004:A:C5	32:1a:1037:C:C2	3.02	0.48
35:1d:3:ARG:NH1	35:1d:5:ILE:HG22	2.29	0.48
35:1d:20:TYR:HA	35:1d:26:CYS:SG	2.54	0.48
36:1e:61:TYR:HA	36:1e:64:ARG:HB2	1.96	0.48
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.94	0.48
45:1n:4:LYS:O	45:1n:7:ILE:HG13	2.14	0.48
1:2A:1055:G:H2'	1:2A:1056:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.43	0.48
17:2V:5:VAL:HG13	17:2V:35:LEU:HB3	1.93	0.48
20:2Y:5:MET:HE2	20:2Y:32:PRO:HA	1.94	0.48
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HG	1.94	0.48
1:1A:2478:A:H5'	31:19:31:LYS:HE2	1.93	0.48
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.95	0.48
6:1G:21:ARG:HA	6:1G:21:ARG:NE	2.29	0.48
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.48	0.48
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	1.94	0.48
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.28	0.48
32:1a:409:G:H2'	32:1a:410:G:O4'	2.13	0.48
32:1a:574:A:OP2	61:1a:1912:HOH:O	2.20	0.48
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	1.95	0.48
1:2A:821:A:H2'	1:2A:946:G:H5"	1.96	0.48
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.47	0.48
1:2A:2104:G:O6	1:2A:2185:C:N3	2.47	0.48
1:2A:2119:A:H61	1:2A:2168:G:N2	2.11	0.48
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.21	0.48
32:2a:977:A:O3'	32:2a:980:C:N4	2.46	0.48
1:1A:620:G:N3	1:1A:620:G:H5'	2.28	0.48
1:1A:910:A:N1	1:1A:2277:G:H1'	2.28	0.48
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.49	0.48
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.49	0.48
32:1a:8:A:N7	35:1d:208:SER:OG	2.43	0.48
50:1s:10:PHE:HE2	50:1s:37:ARG:HD3	1.79	0.48
1:2A:876:C:H2'	1:2A:877:U:O4'	2.14	0.48
1:2A:1843:C:H5'	3:2D:253:GLN:NE2	2.29	0.48
4:2E:36:ARG:NH1	4:2E:86:PRO:O	2.43	0.48
23:21:30:VAL:HG12	61:21:207:HOH:O	2.14	0.48
32:2a:1402:4OC:HM43	53:2y:83:ARG:CZ	2.44	0.48
35:2d:98:GLU:HG3	35:2d:194:LEU:HD21	1.95	0.48
40:2i:42:ARG:CZ	40:2i:71:SER:HB2	2.43	0.48
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.94	0.48
45:2n:29:ARG:HD3	45:2n:40:CYS:SG	2.54	0.48
53:2y:52:ALA:HB2	53:2y:77:LEU:HD21	1.96	0.48
36:1e:69:VAL:O	36:1e:71:LEU:N	2.46	0.48
38:1g:50:ILE:HD11	38:1g:58:PRO:HA	1.96	0.48
44:1m:5:ALA:HB1	44:1m:61:GLU:HG2	1.95	0.48
1:2A:2134:A:O2'	1:2A:2159:G:N3	2.46	0.48
4:2E:104:VAL:HG13	4:2E:198:VAL:HG22	1.96	0.48
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.48	0.48
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.48	0.48
15:2T:53:ARG:HB3	15:2T:53:ARG:HH11	1.78	0.48
33:2b:80:ILE:HD11	33:2b:212:GLN:HA	1.96	0.48
44:2m:107:ALA:HB3	44:2m:111:LYS:HE3	1.95	0.48
1:1A:272(I):U:H3	1:1A:363(A):A:H61	1.61	0.48
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.26	0.48
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.79	0.48
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.14	0.48
1:2A:889:C:HO2'	1:2A:890:A:H8	1.62	0.48
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.48	0.48
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.95	0.48
29:27:35:ARG:HG3	29:27:42:LEU:HD11	1.96	0.48
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.94	0.48
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.49	0.48
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.48	0.48
1:1A:774:A:N3	1:1A:774:A:H2'	2.29	0.48
1:1A:1210:A:H5"	1:1A:1212:G:O4'	2.14	0.48
1:1A:1378:A:OP1	29:17:10:ARG:NH2	2.47	0.48
1:1A:2206:G:H5"	1:1A:2207:G:C5	2.48	0.48
8:1I:31:LEU:HD21	8:1I:38:LEU:HD13	1.96	0.48
11:1P:59:LEU:HG	30:18:58:ILE:HG12	1.95	0.48
32:1a:491:G:H2'	32:1a:492:G:O4'	2.13	0.48
32:1a:1144:G:O2'	32:1a:1145:C:H5'	2.14	0.48
33:1b:185:ILE:HG22	33:1b:199:TYR:CD2	2.48	0.48
34:1c:6:HIS:CD2	34:1c:9:GLY:H	2.32	0.48
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.94	0.48
6:2G:145:THR:HG22	6:2G:148:MET:HE3	1.95	0.48
10:2O:26:LYS:NZ	10:2O:37:ASP:OD2	2.37	0.48
28:26:26:ASN:HB3	28:26:29:ASN:HB2	1.95	0.48
32:2a:560:U:H4'	32:2a:561:U:O5'	2.13	0.48
32:2a:581:G:OP1	46:2o:61:GLY:HA3	2.14	0.48
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.46	0.48
34:2c:119:ARG:O	34:2c:123:GLN:N	2.39	0.48
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.96	0.48
53:2y:74:ILE:O	53:2y:78:ILE:HG12	2.13	0.48
1:1A:606:U:H4'	1:1A:658:C:H4'	1.96	0.48
1:1A:897:C:H2'	1:1A:898:C:C6	2.49	0.48
1:1A:969:U:H2'	1:1A:970:C:C6	2.49	0.48
1:1A:1040:C:H2'	1:1A:1041:C:O4'	2.13	0.48
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.78	0.48
2:1B:82:G:OP2	61:1B:303:HOH:O	2.20	0.48
5:1F:164:ARG:HD2	58:1F:318:ARG:NH1	2.28	0.48
26:14:58:ARG:HG3	50:1s:67:VAL:HB	1.96	0.48
32:1a:299:G:O5'	32:1a:299:G:H8	1.97	0.48
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	1.94	0.48
1:2A:1110:G:H8	1:2A:1110:G:OP2	1.97	0.48
1:2A:1257:C:OP2	61:2A:3845:HOH:O	2.19	0.48
1:2A:1604:C:OP1	61:2A:3852:HOH:O	2.20	0.48
3:2D:36:PRO:HA	3:2D:61:LEU:HD12	1.95	0.48
7:2H:103:LEU:HB2	7:2H:123:PHE:CD2	2.48	0.48
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.49	0.48
26:24:18:CYS:SG	26:24:39:CYS:HB3	2.54	0.48
32:2a:1128:C:H1'	32:2a:1147:C:N4	2.28	0.48
1:1A:626:U:O4	11:1P:107:LYS:HE2	2.14	0.47
1:1A:662:G:OP1	11:1P:16:ARG:NE	2.46	0.47
1:1A:1439:A:OP1	61:1A:4154:HOH:O	2.20	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.14	0.47
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.14	0.47
2:1B:81:G:N7	58:1B:230:ARG:NH2	2.59	0.47
15:1T:51:ARG:HG3	15:1T:98:LYS:HD2	1.96	0.47
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.44	0.47
36:1e:37:ARG:HH12	36:1e:111:GLU:HG2	1.79	0.47
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.96	0.47
1:2A:78:A:H2'	1:2A:79:G:C8	2.49	0.47
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.79	0.47
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.14	0.47
32:2a:187:C:H2'	32:2a:188:C:H6	1.78	0.47
32:2a:840:C:H4'	32:2a:841:U:OP2	2.10	0.47
33:2b:21:ARG:O	33:2b:23:ARG:N	2.40	0.47
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.29	0.47
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.32	0.47
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.72	0.47
23:11:71:TYR:O	23:11:74:VAL:HG22	2.14	0.47
32:1a:539:A:OP2	43:1l:115:LYS:HE2	2.14	0.47
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.36	0.47
32:1a:1183:A:H3'	32:1a:1184:G:C5'	2.43	0.47
33:1b:134:GLU:HG3	33:1b:137:ARG:NH2	2.29	0.47
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.94	0.47
50:1s:36:ARG:NH1	50:1s:52:TYR:O	2.43	0.47
1:2A:307:G:N7	61:2A:3940:HOH:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.95	0.47
1:2A:1115:G:H2'	1:2A:1116:C:C6	2.49	0.47
1:2A:2317:C:N4	1:2A:2318:G:O6	2.47	0.47
1:2A:2430:A:OP2	61:2A:3854:HOH:O	2.20	0.47
2:2B:66:A:N6	2:2B:109:C:H5'	2.29	0.47
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.11	0.47
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.95	0.47
26:24:50:VAL:HB	44:2m:65:LYS:HG3	1.96	0.47
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.32	0.47
1:1A:1021:A:OP1	61:1A:4152:HOH:O	2.20	0.47
1:1A:1026:U:O2	1:1A:1026:U:H2'	2.15	0.47
1:1A:1578:U:H2'	1:1A:1579:A:H5'	1.96	0.47
1:1A:2142:C:N3	1:1A:2149:G:C6	2.82	0.47
26:14:68:ARG:HD3	26:14:69:LYS:H	1.79	0.47
32:1a:1125:U:H4'	41:1j:5:ARG:HH21	1.79	0.47
32:1a:1187:G:H4'	40:1i:111:ARG:HH11	1.80	0.47
32:1a:1302:U:C5	44:1m:17:VAL:HG11	2.49	0.47
32:1a:1368:G:OP2	40:1i:112:LYS:HG3	2.14	0.47
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.14	0.47
1:2A:300:A:H2'	1:2A:334:C:H1'	1.96	0.47
1:2A:2006:C:OP2	61:2A:3851:HOH:O	2.20	0.47
10:2O:64:ARG:HG2	10:2O:83:ALA:HB3	1.96	0.47
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.19	0.47
15:2T:23:ARG:HD3	15:2T:120:ARG:NH1	2.29	0.47
32:2a:116:A:H61	32:2a:313:A:H1'	1.78	0.47
32:2a:189(L):G:H2'	32:2a:190:U:H6	1.79	0.47
32:2a:614:A:H2'	32:2a:615:C:C6	2.49	0.47
33:2b:73:THR:OG1	33:2b:170:GLU:OE2	2.32	0.47
34:2c:7:PRO:O	34:2c:11:ARG:HD2	2.14	0.47
1:1A:185:U:H4'	1:1A:218:A:H4'	1.96	0.47
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.14	0.47
1:1A:2119:A:H2	1:1A:2171:A:H5'	1.80	0.47
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.14	0.47
5:1F:10:PRO:HB3	5:1F:17:ARG:NH2	2.28	0.47
6:1G:43:LEU:C	6:1G:45:GLU:H	2.23	0.47
19:1X:94:GLY:HA3	19:1X:95:LEU:C	2.40	0.47
32:1a:757:U:H2'	32:1a:758:G:O4'	2.15	0.47
32:1a:1068:G:N2	32:1a:1191:A:N3	2.56	0.47
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.14	0.47
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.28	0.47
36:1e:107:ARG:NH1	61:1e:302:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:78:GLU:O	37:1f:81:ILE:HG22	2.15	0.47
1:2A:796:C:H2'	1:2A:797:C:C6	2.49	0.47
5:2F:20:LEU:HD13	5:2F:125:LEU:HD13	1.97	0.47
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.80	0.47
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.95	0.47
32:2a:392:G:H2'	32:2a:393:A:H8	1.79	0.47
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.14	0.47
33:2b:97:TRP:HZ2	33:2b:102:LEU:HD13	1.79	0.47
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.48	0.47
50:2s:20:LEU:HD23	50:2s:23:ASN:HD22	1.79	0.47
1:1A:1041:C:H5'	1:1A:1042:G:OP2	2.14	0.47
32:1a:1020:U:H2'	32:1a:1021:G:H8	1.78	0.47
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.79	0.47
34:1c:63:ASN:HB3	34:1c:98:ASN:HB2	1.96	0.47
35:1d:30:LYS:HG2	35:1d:35:ARG:HH21	1.79	0.47
46:1o:18:PHE:HB2	46:1o:19:PRO:HD2	1.95	0.47
1:2A:234:C:H2'	1:2A:235:U:H6	1.79	0.47
1:2A:236:C:H2'	1:2A:237:C:H6	1.79	0.47
1:2A:323:G:O2'	1:2A:1205:U:N3	2.37	0.47
1:2A:774:A:H2'	1:2A:774:A:N3	2.29	0.47
1:2A:1104:C:H2'	1:2A:1105:U:H6	1.79	0.47
1:2A:1272:A:OP1	61:2A:3853:HOH:O	2.20	0.47
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.80	0.47
1:2A:2188:C:H2'	1:2A:2189:U:O4'	2.15	0.47
2:2B:13:A:N1	2:2B:69:G:O2'	2.28	0.47
6:2G:25:TYR:OH	6:2G:168:GLU:OE1	2.31	0.47
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.49	0.47
32:2a:724:G:C2	32:2a:725:G:C8	3.02	0.47
32:2a:1400:5MC:N3	53:2y:63:ALA:HA	2.29	0.47
33:2b:16:HIS:O	33:2b:18:GLY:N	2.48	0.47
33:2b:83:MET:SD	33:2b:234:PRO:HB2	2.54	0.47
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.78	0.47
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.49	0.47
1:1A:2867:G:OP2	15:1T:119:LYS:NZ	2.29	0.47
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.14	0.47
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.43	0.47
32:1a:21:G:H2'	32:1a:22:G:C8	2.50	0.47
32:1a:79:G:N2	32:1a:90:U:O2	2.47	0.47
32:1a:131:C:H2'	32:1a:132:C:C6	2.49	0.47
32:1a:1003:G:N2	32:1a:1004:A:H1'	2.30	0.47
34:1c:55:VAL:HG13	34:1c:68:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:35:THR:HA	51:1t:38:LYS:HE2	1.97	0.47
1:2A:299:A:N1	1:2A:322:A:O2'	2.41	0.47
1:2A:1065:U:H4'	1:2A:1066:U:C5'	2.44	0.47
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.50	0.47
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.15	0.47
1:2A:2155:G:C2	1:2A:2156:G:H1'	2.49	0.47
1:2A:2267:A:H5"	1:2A:2268:A:H5'	1.95	0.47
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.15	0.47
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.96	0.47
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.80	0.47
18:2W:83:LYS:O	18:2W:84:ARG:HD3	2.14	0.47
32:2a:718:G:H5'	42:2k:117:ASN:OD1	2.15	0.47
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.97	0.47
40:2i:23:ASN:N	40:2i:23:ASN:OD1	2.47	0.47
1:1A:324:A:H2'	1:1A:325:G:O4'	2.15	0.47
1:1A:400:G:N7	61:1A:4295:HOH:O	2.36	0.47
1:1A:636:G:OP1	11:1P:132:LYS:HE2	2.15	0.47
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.41	0.47
1:1A:1843:C:H5'	3:1D:253:GLN:NE2	2.30	0.47
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.14	0.47
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.49	0.47
1:1A:2165:G:H2'	1:1A:2166:G:H8	1.78	0.47
1:1A:2336:A:H61	22:10:43:THR:CG2	2.28	0.47
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.50	0.47
7:1H:3:ARG:HH22	7:1H:66:GLY:H	1.62	0.47
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.97	0.47
18:1W:68:ARG:NH1	18:1W:111:HIS:HA	2.30	0.47
32:1a:141:A:H1'	32:1a:182:U:O2	2.15	0.47
32:1a:706:A:N3	42:1k:31:THR:HG21	2.30	0.47
32:1a:797:C:OP1	42:1k:124:LYS:HD3	2.15	0.47
32:1a:986:A:H1'	50:1s:54:GLY:O	2.15	0.47
32:1a:998:G:H2'	32:1a:999:C:C6	2.50	0.47
36:1e:152:ARG:HB3	39:1h:43:GLY:HA3	1.97	0.47
40:1i:71:SER:HA	40:1i:74:ILE:HD12	1.96	0.47
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.97	0.47
53:1y:6:THR:OG1	53:1y:38:HIS:HE1	1.97	0.47
1:2A:458:G:C8	29:27:37:LYS:HG2	2.49	0.47
1:2A:526:A:O2'	1:2A:2043:C:O2	2.29	0.47
1:2A:1091:G:H2'	1:2A:1091:G:N3	2.30	0.47
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.31	0.47
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.14	0.47
3:2D:275:LYS:HD3	3:2D:276:LYS:O	2.14	0.47
6:2G:25:TYR:CD1	6:2G:30:GLU:HB3	2.50	0.47
6:2G:106:LEU:O	6:2G:111:LEU:HG	2.15	0.47
6:2G:109:VAL:HG11	6:2G:142:PRO:HB3	1.97	0.47
11:2P:100:LEU:HD22	11:2P:105:LEU:HD12	1.95	0.47
20:2Y:7:VAL:HG11	20:2Y:13:VAL:HG11	1.96	0.47
25:23:57:GLU:HG2	25:23:58:VAL:H	1.80	0.47
26:24:46:GLN:O	26:24:48:ARG:N	2.37	0.47
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.15	0.47
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.49	0.47
32:2a:1126:U:O4'	32:2a:1281:U:H1'	2.14	0.47
32:2a:1277:C:O2'	32:2a:1279:A:C8	2.68	0.47
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.30	0.47
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.80	0.47
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.78	0.47
44:2m:86:CYS:HA	50:2s:73:GLU:O	2.15	0.47
45:2n:32:SER:OG	45:2n:41:ARG:HG2	2.14	0.47
1:1A:1494:A:H2'	1:1A:1495:A:C8	2.50	0.47
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.15	0.47
6:1G:74:LYS:O	6:1G:84:LYS:HG3	2.14	0.47
19:1X:35:THR:HG22	19:1X:37:THR:N	2.30	0.47
32:1a:911:U:H2'	32:1a:912:C:C6	2.50	0.47
32:1a:940:C:OP1	38:1g:29:LYS:NZ	2.47	0.47
32:1a:1034:G:C2	32:1a:1035:A:H1'	2.49	0.47
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.96	0.47
1:2A:9:U:O4	1:2A:2629:A:H2	1.97	0.47
1:2A:228:A:H2'	1:2A:229:A:H5'	1.97	0.47
1:2A:460:A:P	29:27:41:ARG:HH22	2.37	0.47
1:2A:747:U:O2	1:2A:2014:A:H1'	2.14	0.47
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.49	0.47
6:2G:3:LEU:HD11	6:2G:97:ASP:HB3	1.96	0.47
6:2G:109:VAL:HG21	26:24:14:ILE:HG21	1.96	0.47
32:2a:7:G:H5'	32:2a:298:A:O4'	2.15	0.47
32:2a:7:G:O2'	36:2e:120:THR:O	2.32	0.47
32:2a:358:U:H2'	32:2a:359:U:H6	1.80	0.47
34:2c:180:ALA:HB1	34:2c:203:PHE:HE1	1.79	0.47
40:2i:78:LYS:HA	40:2i:81:ILE:HG22	1.97	0.47
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.48	0.47
1:1A:207:A:H2'	1:1A:208:C:O4'	2.14	0.47
1:1A:580:C:H2'	1:1A:581:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.49	0.47
1:1A:2096:U:H3	1:1A:2193:G:H1	1.63	0.47
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.79	0.47
12:1Q:7:MET:HE3	12:1Q:7:MET:HB3	1.73	0.47
15:1T:127:ALA:O	15:1T:128:GLU:HB2	2.15	0.47
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.61	0.47
27:15:15:ARG:NH1	61:15:203:HOH:O	2.35	0.47
32:1a:447:G:O6	32:1a:485:G:O2'	2.31	0.47
32:1a:1004:A:OP1	32:1a:1024:G:N2	2.48	0.47
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.29	0.47
32:1a:1226:C:H2'	44:1m:103:THR:HB	1.97	0.47
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.14	0.47
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.30	0.47
40:1i:50:LEU:HB3	40:1i:85:LEU:HD11	1.97	0.47
40:1i:127:LYS:HE2	40:1i:127:LYS:HB3	1.84	0.47
41:1j:7:LYS:HE3	41:1j:9:ARG:NH1	2.29	0.47
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.47	0.47
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.15	0.47
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.49	0.47
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.95	0.47
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.97	0.47
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.15	0.47
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.50	0.47
32:2a:1005:A:O2'	32:2a:1036:G:N2	2.47	0.47
33:2b:114:ARG:O	33:2b:118:LEU:HB2	2.15	0.47
34:2c:183:ASP:OD1	34:2c:184:TYR:N	2.44	0.47
36:2e:96:PRO:O	36:2e:98:THR:N	2.48	0.47
41:2j:63:PHE:HE1	45:2n:58:LYS:HG2	1.80	0.47
1:1A:493:G:H2'	1:1A:494:G:O4'	2.14	0.47
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.49	0.47
1:1A:2143:C:O2	1:1A:2148:G:N1	2.45	0.47
2:1B:13:A:N1	2:1B:69:G:O2'	2.46	0.47
2:1B:84:C:OP1	25:13:15:TYR:OH	2.28	0.47
6:1G:28:VAL:O	6:1G:31:VAL:HG22	2.15	0.47
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.48	0.47
32:1a:673:G:O3'	37:1f:87:ARG:NH2	2.48	0.47
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.30	0.47
35:1d:168:ARG:N	35:1d:168:ARG:HH11	2.13	0.47
1:2A:514:A:N3	1:2A:581:C:O2'	2.44	0.47
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.30	0.47
6:2G:57:ALA:HB2	6:2G:90:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:80:PHE:O	6:2G:82:LEU:N	2.48	0.47
32:2a:109:A:C6	32:2a:326:G:C6	3.03	0.47
32:2a:384:G:H2'	32:2a:385:C:H6	1.80	0.47
32:2a:458:C:H2'	32:2a:460:G:O4'	2.15	0.47
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.49	0.47
32:2a:1151:A:N3	41:2j:39:PRO:HG3	2.29	0.47
33:2b:50:GLU:O	33:2b:54:THR:N	2.37	0.47
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.15	0.47
35:2d:88:VAL:HG22	36:2e:96:PRO:HB2	1.97	0.47
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.80	0.47
38:2g:113:GLU:CG	38:2g:119:ARG:HG2	2.44	0.47
41:2j:6:ILE:HB	41:2j:72:VAL:HG22	1.96	0.47
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.48	0.47
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.50	0.46
1:1A:1175:U:O3'	1:1A:1176:G:H4'	2.15	0.46
1:1A:2142:C:N3	1:1A:2149:G:O6	2.48	0.46
32:1a:677:U:H3	32:1a:713:G:H22	1.62	0.46
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.15	0.46
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.49	0.46
1:2A:99:U:O4	20:2Y:8:LYS:NZ	2.43	0.46
1:2A:234:C:H2'	1:2A:235:U:C6	2.51	0.46
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.29	0.46
1:2A:2227:A:O2'	61:2A:3855:HOH:O	2.21	0.46
6:2G:125:PHE:CE1	6:2G:131:TYR:HB2	2.50	0.46
7:2H:127:GLU:C	7:2H:129:THR:H	2.23	0.46
26:24:42:PHE:HD2	26:24:43:TYR:CD1	2.32	0.46
32:2a:1368:G:H5"	40:2i:112:LYS:HB3	1.97	0.46
33:2b:197:VAL:HG12	33:2b:200:ILE:HG13	1.96	0.46
34:2c:109:PRO:HB3	34:2c:115:LEU:HD23	1.96	0.46
36:2e:110:LEU:HD21	36:2e:139:LEU:HD21	1.96	0.46
40:2i:70:LYS:O	40:2i:74:ILE:HG13	2.16	0.46
46:2o:82:ILE:O	46:2o:86:GLY:N	2.47	0.46
50:2s:40:ILE:HD11	50:2s:74:PHE:HE2	1.79	0.46
1:1A:302:C:OP2	20:1Y:73:ARG:NH2	2.49	0.46
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.30	0.46
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.97	0.46
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.14	0.46
25:13:29:ARG:HG3	25:13:30:ARG:HG3	1.96	0.46
32:1a:161:A:H2'	32:1a:162:A:C8	2.51	0.46
32:1a:688:G:O2'	32:1a:704:A:N1	2.40	0.46
32:1a:1162:C:C2'	32:1a:1163:C:H5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:70:PHE:O	33:1b:92:TYR:HA	2.15	0.46
34:1c:37:GLN:O	34:1c:41:GLY:N	2.44	0.46
40:1i:79:LEU:HD22	40:1i:104:ARG:HB2	1.97	0.46
41:1j:16:LEU:HD21	41:1j:70:ARG:HG2	1.96	0.46
6:2G:112:PRO:HG3	26:24:43:TYR:CE2	2.49	0.46
21:2Z:132:ASN:O	21:2Z:134:PRO:HD3	2.15	0.46
32:2a:381:C:H2'	32:2a:382:A:O4'	2.15	0.46
32:2a:545:C:OP1	35:2d:61:LYS:NZ	2.48	0.46
32:2a:1274:G:H2'	32:2a:1275:A:H8	1.80	0.46
33:2b:59:GLU:HB2	33:2b:221:LEU:HD21	1.96	0.46
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.97	0.46
47:2p:1:MET:HE3	47:2p:3:LYS:HD2	1.98	0.46
1:1A:528:A:OP2	9:1N:114:ARG:NH1	2.46	0.46
1:1A:2014:A:OP2	61:1A:4157:HOH:O	2.20	0.46
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.16	0.46
2:1B:29:A:H2'	2:1B:30:C:O4'	2.15	0.46
6:1G:181:ARG:HG3	6:1G:182:LYS:N	2.29	0.46
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.81	0.46
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.95	0.46
26:14:61:ARG:HH21	50:1s:42:PRO:CD	2.29	0.46
32:1a:1112:C:C2	34:1c:178:LEU:HB2	2.51	0.46
32:1a:1292:U:H5'	40:1i:38:GLN:OE1	2.15	0.46
33:1b:132:LYS:HA	33:1b:135:GLN:OE1	2.15	0.46
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.97	0.46
1:2A:1087:G:H22	1:2A:1102:C:N4	2.13	0.46
1:2A:2136:C:H2'	1:2A:2137:C:C6	2.50	0.46
1:2A:2892:A:N6	1:2A:2893:G:C6	2.83	0.46
2:2B:90:A:N7	2:2B:91:C:H1'	2.30	0.46
6:2G:137:GLU:HG2	6:2G:152:LEU:HD22	1.98	0.46
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.96	0.46
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.49	0.46
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.48	0.46
21:2Z:10:ARG:HD3	21:2Z:37:VAL:O	2.15	0.46
32:2a:138:G:H2'	32:2a:139:G:H8	1.79	0.46
32:2a:564:C:O2'	39:2h:91:ARG:NH2	2.46	0.46
32:2a:620:C:C2	35:2d:135:LEU:HG	2.51	0.46
32:2a:942:G:C2	32:2a:1342:C:C2	3.03	0.46
32:2a:975:A:H61	41:2j:48:THR:HB	1.81	0.46
34:2c:32:LEU:C	34:2c:59:ARG:HH12	2.23	0.46
44:2m:3:ARG:NH1	44:2m:11:ARG:HE	2.12	0.46
50:2s:22:LEU:HB3	50:2s:27:GLU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2y:64:SER:HA	53:2y:77:LEU:HD13	1.97	0.46
1:1A:300:A:H2'	1:1A:334:C:H1'	1.96	0.46
1:1A:2099:U:H3	1:1A:2190:G:H1	1.62	0.46
1:1A:2171:A:N3	1:1A:2172:U:N3	2.64	0.46
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.98	0.46
13:1R:67:LEU:HG	13:1R:76:VAL:HG21	1.97	0.46
23:11:11:ARG:HG3	23:11:12:PRO:HD2	1.98	0.46
32:1a:474:G:H2'	32:1a:475:G:C8	2.50	0.46
33:1b:87:ARG:HD2	33:1b:233:SER:CB	2.45	0.46
50:1s:12:ASP:C	50:1s:14:HIS:H	2.23	0.46
53:1y:49:VAL:HG22	53:1y:66:LYS:HG2	1.98	0.46
1:2A:191:A:H2'	1:2A:192:C:C6	2.50	0.46
1:2A:460:A:OP1	29:27:41:ARG:NH2	2.49	0.46
1:2A:888:C:H2'	1:2A:889:C:N3	2.30	0.46
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.15	0.46
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.97	0.46
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.98	0.46
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.50	0.46
32:2a:1516:G:N2	32:2a:1519:MA6:OP2	2.48	0.46
33:2b:87:ARG:CZ	33:2b:233:SER:HB3	2.45	0.46
33:2b:119:GLU:HG3	33:2b:153:ARG:HH12	1.79	0.46
35:2d:160:GLN:HA	35:2d:163:GLU:HB2	1.96	0.46
48:2q:24:GLU:HG3	48:2q:39:SER:HB3	1.97	0.46
1:1A:1509(B):A:H2'	1:1A:1510:G:O4'	2.16	0.46
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.38	0.46
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.97	0.46
11:1P:67:MET:HE3	11:1P:67:MET:HB2	1.80	0.46
32:1a:266:G:OP2	32:1a:267:C:N4	2.44	0.46
32:1a:1244:C:H42	32:1a:1293:G:H1	1.64	0.46
40:1i:77:ILE:O	40:1i:81:ILE:HG23	2.15	0.46
44:1m:50:GLU:O	44:1m:54:VAL:HG22	2.15	0.46
44:1m:54:VAL:HA	44:1m:57:ARG:HB3	1.97	0.46
2:2B:50:G:OP1	14:2S:63:THR:N	2.45	0.46
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	1.95	0.46
5:2F:102:PRO:O	5:2F:106:ARG:HG3	2.16	0.46
6:2G:46:ALA:HB1	6:2G:51:ARG:HA	1.97	0.46
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	1.97	0.46
32:2a:435:C:H2'	32:2a:436:C:H6	1.81	0.46
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.98	0.46
39:2h:63:LEU:HD23	39:2h:65:TYR:OH	2.14	0.46
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:42:ARG:HA	49:2r:42:ARG:HE	1.80	0.46
1:1A:484:C:H2'	1:1A:485:C:C6	2.51	0.46
1:1A:732:C:OP1	61:1A:4156:HOH:O	2.20	0.46
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.51	0.46
1:1A:2107:C:N3	1:1A:2182:G:O6	2.48	0.46
1:1A:2142:C:O2	1:1A:2149:G:N1	2.48	0.46
6:1G:7:LEU:HD23	6:1G:7:LEU:HA	1.84	0.46
8:1I:75:LEU:HD13	8:1I:105:HIS:CE1	2.51	0.46
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.97	0.46
23:11:3:LYS:O	23:11:12:PRO:HD3	2.15	0.46
32:1a:9:G:OP2	36:1e:121:LYS:NZ	2.38	0.46
32:1a:685:G:O2'	32:1a:686:U:H5'	2.16	0.46
32:1a:744:C:O2'	32:1a:851:G:N2	2.48	0.46
32:1a:1001:A:H2'	32:1a:1001(A):G:C8	2.51	0.46
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.15	0.46
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.98	0.46
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.98	0.46
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.27	0.46
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.15	0.46
1:2A:815:C:H2'	1:2A:816:C:H6	1.81	0.46
1:2A:2127:G:N1	1:2A:2161:C:O2	2.48	0.46
1:2A:2151:G:H2'	1:2A:2152:G:O4'	2.15	0.46
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.97	0.46
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.31	0.46
1:2A:2808:U:H5"	1:2A:2891:G:O6	2.15	0.46
8:2I:69:LYS:HB2	8:2I:69:LYS:HE3	1.76	0.46
32:2a:1366:C:HO2'	41:2j:60:ARG:HH22	1.57	0.46
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.51	0.46
34:2c:70:VAL:HG12	34:2c:72:LYS:N	2.31	0.46
34:2c:120:VAL:HA	34:2c:123:GLN:HB2	1.98	0.46
35:2d:111:ALA:HB1	35:2d:116:GLN:HE21	1.80	0.46
44:2m:3:ARG:HH11	44:2m:11:ARG:HE	1.62	0.46
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.41	0.46
8:1I:57:ARG:O	8:1I:61:ARG:HG2	2.16	0.46
1:2A:10:G:H1'	1:2A:2801(A):A:N1	2.31	0.46
1:2A:320:A:H4'	1:2A:322:A:N7	2.30	0.46
1:2A:1087:G:H2'	1:2A:1088:A:H5'	1.98	0.46
1:2A:2162:G:H4'	1:2A:2172:U:O2'	2.16	0.46
5:2F:132:VAL:O	5:2F:133:ASN:ND2	2.49	0.46
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.98	0.46
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:148:G:H2'	32:2a:149:A:H8	1.80	0.46
32:2a:601:C:H2'	32:2a:602:A:H8	1.80	0.46
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.50	0.46
40:2i:5:TYR:N	40:2i:87:GLN:OE1	2.45	0.46
48:2q:6:LEU:O	48:2q:58:GLU:HA	2.15	0.46
50:2s:12:ASP:OD2	50:2s:35:SER:HB3	2.16	0.46
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.16	0.46
1:1A:2506:U:O2	55:1A:4022:HGR:H23	2.16	0.46
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.97	0.46
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.50	0.46
32:1a:418:C:H1'	32:1a:540:G:O2'	2.16	0.46
32:1a:865:A:H2	32:1a:918:A:H4'	1.81	0.46
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.49	0.46
32:1a:986:A:H2'	32:1a:987:G:O4'	2.15	0.46
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.50	0.46
43:1l:102:ARG:HA	43:1l:102:ARG:HD2	1.76	0.46
1:2A:1084:A:OP1	1:2A:1085:A:H1'	2.15	0.46
1:2A:1117:G:H2'	1:2A:1118:C:C6	2.51	0.46
1:2A:2306:C:H3'	1:2A:2307:G:H2'	1.97	0.46
32:2a:859:A:H2	39:2h:19:VAL:HG11	1.80	0.46
38:2g:23:VAL:HG13	38:2g:43:PHE:CE2	2.51	0.46
1:1A:271(L):U:H5'	8:1I:50:ARG:HH12	1.81	0.46
1:1A:1177:A:H2'	1:1A:1177:A:N3	2.31	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.63	0.46
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.13	0.46
32:1a:179:A:H2'	32:1a:180:U:C6	2.51	0.46
32:1a:347:G:H8	57:1a:1882:MPD:H53	1.79	0.46
32:1a:540:G:H2'	32:1a:541:G:O4'	2.16	0.46
32:1a:636:U:H2'	32:1a:637:G:H8	1.80	0.46
32:1a:812:C:N3	61:1a:1941:HOH:O	2.36	0.46
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.32	0.46
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.34	0.46
32:1a:1400:5MC:N3	53:1y:63:ALA:HA	2.31	0.46
34:1c:29:TYR:OH	45:1n:54:PRO:O	2.34	0.46
36:1e:137:GLU:OE1	36:1e:140:ARG:NH1	2.48	0.46
42:1k:91:ARG:NH1	42:1k:110:ASP:OD2	2.49	0.46
50:1s:3:ARG:HH21	50:1s:7:LYS:HE2	1.80	0.46
1:2A:192:C:O2'	1:2A:802:A:N3	2.47	0.46
1:2A:2206:G:H5"	1:2A:2207:G:C8	2.51	0.46
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.33	0.46
2:2B:8:U:OP1	14:2S:15:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.46
29:27:48:LYS:HB2	29:27:48:LYS:HE2	1.77	0.46
32:2a:53:A:OP2	61:2a:3216:HOH:O	2.21	0.46
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.49	0.46
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.80	0.46
34:2c:71:ALA:HA	34:2c:106:VAL:HB	1.98	0.46
39:2h:19:VAL:HG23	39:2h:21:LYS:HD3	1.97	0.46
41:2j:38:ILE:HD11	41:2j:71:LEU:HD13	1.98	0.46
51:2t:50:GLU:HB2	51:2t:99:LEU:HD12	1.97	0.46
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.51	0.46
1:1A:1175:U:H1'	1:1A:1176:G:OP1	2.16	0.46
1:1A:1773:A:N6	61:1A:4487:HOH:O	2.46	0.46
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.46
32:1a:262:A:H2'	32:1a:263:A:C8	2.51	0.46
32:1a:1216:G:OP1	45:1n:2:ALA:HA	2.15	0.46
33:1b:97:TRP:HH2	33:1b:176:GLU:CD	2.23	0.46
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.51	0.46
1:2A:118:A:H3'	1:2A:119:A:H5"	1.98	0.46
1:2A:2118:U:O2'	1:2A:2119:A:H5"	2.16	0.46
1:2A:2751:G:H3'	1:2A:2752:C:C6	2.50	0.46
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.15	0.46
1:2A:2805:G:C6	1:2A:2807:G:C6	3.04	0.46
8:2I:69:LYS:HB2	8:2I:138:ILE:HG12	1.97	0.46
32:2a:384:G:H2'	32:2a:385:C:C6	2.51	0.46
32:2a:601:C:H2'	32:2a:602:A:C8	2.50	0.46
32:2a:1026:G:N3	32:2a:1026:G:H2'	2.30	0.46
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.97	0.46
40:2i:24:GLY:H	40:2i:60:ASP:HB3	1.80	0.46
40:2i:99:LEU:HB3	40:2i:101:PHE:CE1	2.51	0.46
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.52	0.45
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	1.98	0.45
6:1G:21:ARG:C	6:1G:21:ARG:HD3	2.42	0.45
32:1a:189(A):C:H42	32:1a:189(J):G:H1	1.64	0.45
32:1a:1249:C:O4'	40:1i:70:LYS:HE3	2.15	0.45
50:1s:10:PHE:CE2	50:1s:37:ARG:HD3	2.51	0.45
1:2A:271(K):U:O2	8:2I:50:ARG:HD2	2.16	0.45
1:2A:2341:G:H2'	1:2A:2342:C:C6	2.51	0.45
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.97	0.45
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.98	0.45
32:2a:1505:G:H4'	32:2a:1506:U:H5"	1.98	0.45
33:2b:187:LEU:HD12	33:2b:201:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:83:ARG:O	34:2c:87:LEU:N	2.47	0.45
36:2e:12:LEU:O	36:2e:30:ALA:HA	2.16	0.45
47:2p:42:ARG:HB2	47:2p:44:THR:HG22	1.97	0.45
53:2y:24:LEU:HD23	53:2y:24:LEU:HA	1.78	0.45
53:2y:26:LYS:HG2	53:2y:82:GLU:OE2	2.15	0.45
1:1A:218:A:C2	1:1A:235:U:H4'	2.51	0.45
1:1A:1315:C:O2'	1:1A:1392:A:N3	2.47	0.45
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.52	0.45
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.51	0.45
8:1I:77:LEU:HD22	8:1I:101:LEU:HG	1.98	0.45
13:1R:96:ARG:NH1	13:1R:115:GLU:OE2	2.47	0.45
32:1a:944:G:H1'	32:1a:1339:A:H61	1.79	0.45
32:1a:1026:G:H3'	32:1a:1027:C:C6	2.51	0.45
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.17	0.45
33:1b:160:ASP:OD1	33:1b:160:ASP:N	2.50	0.45
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.48	0.45
1:2A:630:G:N2	1:2A:633:A:OP2	2.36	0.45
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.51	0.45
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.98	0.45
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.51	0.45
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.98	0.45
30:28:32:LEU:O	30:28:36:LYS:HE3	2.15	0.45
32:2a:181:G:N2	32:2a:182:U:O4	2.46	0.45
32:2a:449:C:H2'	32:2a:450:G:O4'	2.16	0.45
32:2a:1121:U:H2'	32:2a:1122:U:O4'	2.16	0.45
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.49	0.45
38:2g:32:ARG:O	38:2g:34:GLY:N	2.49	0.45
1:1A:26:G:H1'	1:1A:515:A:H61	1.81	0.45
1:1A:1094:U:H1'	1:1A:1097:U:C5	2.51	0.45
1:1A:2137:C:N3	1:1A:2154:G:C2	2.84	0.45
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.43	0.45
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.50	0.45
38:1g:74:GLU:OE2	38:1g:95:ARG:NE	2.48	0.45
47:1p:3:LYS:HE2	47:1p:3:LYS:HB3	1.77	0.45
50:1s:52:TYR:HB2	50:1s:57:HIS:CE1	2.51	0.45
1:2A:7:G:H2'	1:2A:8:A:C8	2.51	0.45
1:2A:927:G:H2'	1:2A:928:G:O4'	2.16	0.45
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.51	0.45
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.77	0.45
9:2N:75:TYR:CE2	9:2N:77:GLY:HA2	2.52	0.45
26:24:44:THR:O	26:24:46:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:748:C:H4'	32:2a:749:C:O5'	2.17	0.45
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.32	0.45
42:2k:117:ASN:OD1	42:2k:117:ASN:N	2.49	0.45
1:1A:1179:C:H2'	1:1A:1180:C:C6	2.52	0.45
1:1A:1227:G:OP2	16:1U:16:LYS:NZ	2.44	0.45
6:1G:77:ILE:HG21	6:1G:80:PHE:CD2	2.52	0.45
8:1I:72:LEU:O	8:1I:73:GLU:HB2	2.15	0.45
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.48	0.45
32:1a:22:G:H2'	32:1a:23:C:C6	2.52	0.45
32:1a:171:A:H2'	32:1a:172:A:C8	2.51	0.45
34:1c:123:GLN:HE22	34:1c:140:ARG:HH22	1.64	0.45
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.57	0.45
1:2A:190:A:OP2	23:21:39:LYS:HE3	2.16	0.45
1:2A:1062:G:HO2'	1:2A:1063:G:H8	1.65	0.45
1:2A:1069:A:C4	1:2A:1095:A:H4'	2.51	0.45
1:2A:1576:U:H2'	1:2A:1577:C:H6	1.81	0.45
1:2A:2108:C:H5'	1:2A:2109:U:OP2	2.16	0.45
3:2D:206:LEU:HD23	3:2D:206:LEU:HA	1.73	0.45
21:2Z:22:GLY:O	21:2Z:41:LEU:HB3	2.15	0.45
32:2a:1025:U:O2'	32:2a:1026:G:N7	2.49	0.45
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.51	0.45
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.15	0.45
33:2b:72:GLY:HA2	33:2b:165:VAL:HG11	1.98	0.45
40:2i:53:VAL:C	40:2i:55:ALA:H	2.17	0.45
49:2r:47:THR:HG23	49:2r:49:LYS:HG3	1.98	0.45
50:2s:66:MET:HB3	50:2s:74:PHE:HZ	1.82	0.45
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.51	0.45
1:1A:795:C:H2'	1:1A:796:C:C6	2.52	0.45
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.15	0.45
1:1A:1062:G:H1'	1:1A:1088:A:N7	2.32	0.45
1:1A:1314:C:OP1	61:1A:4111:HOH:O	2.21	0.45
1:1A:1824:G:O3'	3:1D:249:PRO:HD3	2.16	0.45
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.30	0.45
9:1N:110:GLY:O	9:1N:114:ARG:HG3	2.16	0.45
32:1a:59:A:H3'	32:1a:331:G:H22	1.81	0.45
32:1a:555:C:H2'	32:1a:556:C:C6	2.51	0.45
1:2A:218:A:C2	1:2A:235:U:H4'	2.51	0.45
1:2A:2117:A:H5'	1:2A:2147:G:O2'	2.15	0.45
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.57	0.45
32:2a:1349:A:H3'	32:2a:1350:A:H8	1.80	0.45
36:2e:135:THR:O	36:2e:139:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:115:ARG:HD2	38:2g:115:ARG:H	1.82	0.45
1:1A:534:U:H2'	1:1A:535:C:C6	2.51	0.45
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.17	0.45
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.52	0.45
6:1G:104:GLU:O	6:1G:108:ASN:ND2	2.49	0.45
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.56	0.45
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.99	0.45
32:1a:814:A:N7	32:1a:816:A:C4	2.84	0.45
32:1a:909:A:H2'	32:1a:910:C:O4'	2.16	0.45
51:1t:30:LYS:HE3	51:1t:30:LYS:HB2	1.72	0.45
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.52	0.45
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.17	0.45
40:2i:40:LEU:HD11	40:2i:70:LYS:HG2	1.99	0.45
1:1A:189:G:O6	1:1A:205:G:O2'	2.34	0.45
1:1A:359:A:H2'	1:1A:360:G:O4'	2.17	0.45
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.51	0.45
21:1Z:31:ARG:HG3	21:1Z:32:HIS:CE1	2.52	0.45
32:1a:44:G:H2'	32:1a:45:U:O4'	2.17	0.45
43:1l:97:ARG:HB2	43:1l:98:TYR:CE2	2.52	0.45
46:1o:31:LEU:HD23	46:1o:31:LEU:HA	1.85	0.45
48:1q:62:SER:HB3	48:1q:72:ARG:NH1	2.31	0.45
1:2A:1053:C:H4'	1:2A:1054:A:OP1	2.16	0.45
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.52	0.45
1:2A:2128:C:N4	1:2A:2160:G:H1	2.14	0.45
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.45
2:2B:24:G:H4'	2:2B:25:A:C8	2.51	0.45
5:2F:6:VAL:N	5:2F:22:ALA:O	2.50	0.45
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.50	0.45
18:2W:18:ARG:HG3	18:2W:76:VAL:HB	1.98	0.45
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.98	0.45
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.82	0.45
33:2b:83:MET:HE1	33:2b:234:PRO:O	2.17	0.45
44:2m:5:ALA:HB2	44:2m:61:GLU:HG2	1.97	0.45
53:2y:9:GLN:HE21	53:2y:9:GLN:HB2	1.55	0.45
1:1A:264:C:O2'	1:1A:265:A:H2'	2.17	0.45
1:1A:982:C:OP2	61:1A:4159:HOH:O	2.21	0.45
1:1A:2540:C:OP2	61:1A:4158:HOH:O	2.21	0.45
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.42	0.45
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.99	0.45
18:1W:37:ARG:NH1	27:15:48:GLU:OE2	2.50	0.45
20:1Y:34:LYS:O	20:1Y:34:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:50:ARG:HG2	23:11:59:THR:CG2	2.45	0.45
29:17:1:MET:HE2	29:17:1:MET:HB3	1.82	0.45
32:1a:580:U:H2'	32:1a:581:G:O4'	2.17	0.45
32:1a:607:A:H2'	32:1a:608:A:C8	2.52	0.45
32:1a:745:C:H2'	32:1a:746:A:C8	2.52	0.45
1:2A:323:G:H1'	1:2A:1205:U:O2	2.17	0.45
1:2A:582:G:H2'	1:2A:583:G:C8	2.52	0.45
1:2A:746:A:H2'	1:2A:2612:C:H5"	1.99	0.45
1:2A:1062:G:O2'	1:2A:1063:G:H8	2.00	0.45
1:2A:1079:C:C6	1:2A:1088:A:N1	2.85	0.45
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.51	0.45
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.98	0.45
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.45
21:2Z:67:LEU:HD23	21:2Z:67:LEU:HA	1.80	0.45
26:24:40:HIS:O	26:24:44:THR:HG22	2.17	0.45
28:26:35:GLU:HG2	28:26:50:ARG:HG3	1.99	0.45
32:2a:978:A:O2'	32:2a:1322:C:N3	2.48	0.45
32:2a:1151:A:O4'	41:2j:39:PRO:HB2	2.17	0.45
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.82	0.45
42:2k:50:TYR:HE1	42:2k:54:ARG:HH21	1.64	0.45
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.16	0.45
1:1A:307:G:H21	1:1A:330:A:H62	1.64	0.45
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.17	0.45
1:1A:1176:G:H21	1:1A:1178:C:P	2.37	0.45
1:1A:2319:G:H4'	1:1A:2320:A:OP1	2.17	0.45
6:1G:111:LEU:HA	6:1G:114:ILE:HG13	1.98	0.45
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.14	0.45
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.50	0.45
9:1N:60:ILE:HG13	9:1N:61:ARG:H	1.81	0.45
10:1O:64:ARG:HD2	10:1O:81:ASP:OD1	2.16	0.45
21:1Z:31:ARG:NH1	21:1Z:94:GLU:OE2	2.50	0.45
22:10:23:VAL:HG22	22:10:38:VAL:HG22	1.99	0.45
32:1a:266:G:H2'	32:1a:266:G:N3	2.32	0.45
38:1g:77:SER:OG	38:1g:86:GLN:NE2	2.42	0.45
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.32	0.45
42:1k:79:SER:HA	42:1k:104:GLN:HB3	1.98	0.45
1:2A:185:U:H2'	1:2A:186:G:C8	2.52	0.45
1:2A:985:C:H2'	1:2A:986:C:H6	1.82	0.45
1:2A:1084:A:H3'	1:2A:1085:A:C4'	2.44	0.45
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.49	0.45
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.45
12:2Q:18:LYS:O	12:2Q:98:LYS:HE3	2.17	0.45
20:2Y:23:ARG:HG3	20:2Y:42:VAL:HG22	1.99	0.45
31:29:17:ILE:HD13	31:29:17:ILE:HA	1.82	0.45
32:2a:154:C:H2'	32:2a:155:C:C6	2.52	0.45
32:2a:646:U:H2'	32:2a:647:C:C6	2.52	0.45
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.52	0.45
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.82	0.45
36:2e:72:GLN:NE2	36:2e:77:PRO:HB3	2.31	0.45
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.98	0.45
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.98	0.45
47:2p:40:ASP:OD2	47:2p:44:THR:HG23	2.17	0.45
1:1A:1548:C:H2'	1:1A:1549:C:H6	1.82	0.45
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.16	0.45
1:1A:2896:C:H2'	1:1A:2897:U:H6	1.82	0.45
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.17	0.45
5:1F:30:PRO:HB3	11:1P:1:MET:HE1	1.99	0.45
5:1F:191:ARG:NH2	61:1F:409:HOH:O	2.50	0.45
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.99	0.45
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.98	0.45
22:10:53:MET:HG3	22:10:59:LEU:HD23	1.99	0.45
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.50	0.45
31:19:24:TYR:CE1	31:19:35:ARG:HG3	2.52	0.45
32:1a:194:C:C2'	32:1a:195:A:H5"	2.45	0.45
33:1b:15:VAL:HG12	33:1b:16:HIS:HD2	1.82	0.45
1:2A:2262:U:H4'	1:2A:2328:A:H2	1.82	0.45
17:2V:25:LEU:H	17:2V:92:THR:HG1	1.62	0.45
17:2V:82:ARG:HH11	17:2V:82:ARG:HG3	1.82	0.45
21:2Z:42:VAL:O	21:2Z:46:LYS:HG2	2.17	0.45
28:26:9:LEU:HD13	28:26:51:GLU:HG3	1.99	0.45
32:2a:585:G:N3	32:2a:879:C:H4'	2.32	0.45
32:2a:1028:C:C2	32:2a:1033:G:N1	2.82	0.45
32:2a:1111:A:H2'	32:2a:1112:C:C6	2.51	0.45
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.51	0.45
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.65	0.45
41:2j:26:ALA:HB1	41:2j:84:GLN:CD	2.42	0.45
1:1A:330:A:H2	1:1A:1210:A:C2'	2.30	0.44
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.15	0.44
31:19:17:ILE:HG12	31:19:26:ILE:HG12	1.98	0.44
32:1a:38:G:N2	32:1a:397:A:H5'	2.32	0.44
32:1a:1298:C:P	38:1g:114:ARG:HH22	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.74	0.44
40:1i:25:LYS:HB3	40:1i:25:LYS:HE3	1.76	0.44
40:1i:26:VAL:HA	40:1i:61:ALA:HB3	1.99	0.44
40:1i:100:GLY:O	40:1i:103:THR:HG23	2.17	0.44
1:2A:858:U:O2	1:2A:2268:A:H2'	2.17	0.44
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.17	0.44
1:2A:2130:U:H3'	1:2A:2130:U:H6	1.81	0.44
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.39	0.44
2:2B:58:A:OP2	61:2B:304:HOH:O	2.20	0.44
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	1.98	0.44
32:2a:970:C:OP2	61:2a:3217:HOH:O	2.21	0.44
32:2a:979:C:O2	45:2n:19:ARG:NE	2.34	0.44
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.81	0.44
35:2d:108:LEU:HD13	35:2d:183:GLY:HA3	1.98	0.44
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.52	0.44
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.50	0.44
1:1A:645:C:H5'	1:1A:646:A:OP2	2.17	0.44
1:1A:820:A:N3	1:1A:943:U:O2'	2.46	0.44
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.53	0.44
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.17	0.44
1:1A:2287:A:O2'	1:1A:2288:A:H3'	2.17	0.44
7:1H:109:PHE:C	7:1H:111:HIS:H	2.26	0.44
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.32	0.44
32:1a:1425:U:H2'	32:1a:1426:C:C6	2.51	0.44
40:1i:82:ALA:O	40:1i:86:VAL:HG23	2.17	0.44
43:1l:88:GLY:O	43:1l:99:HIS:HD2	2.00	0.44
45:1n:42:ILE:O	45:1n:46:GLU:HG3	2.16	0.44
48:1q:45:HIS:CD2	48:1q:47:PRO:HG3	2.52	0.44
50:1s:31:ILE:HB	50:1s:49:ILE:HG13	1.98	0.44
1:2A:171:G:H2'	1:2A:172:C:C6	2.52	0.44
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.52	0.44
1:2A:1044:G:O2'	1:2A:1048:A:H1'	2.17	0.44
1:2A:1050:A:H2	1:2A:2751:G:C4	2.34	0.44
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.42	0.44
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.52	0.44
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.40	0.44
55:2A:3730:HGR:H3	55:2A:3730:HGR:C16	2.47	0.44
17:2V:52:VAL:CG2	17:2V:55:ALA:HB3	2.47	0.44
19:2X:44:GLU:HG3	19:2X:51:VAL:HG23	1.98	0.44
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.98	0.44
32:2a:256:U:H2'	32:2a:257:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1009:G:C2	32:2a:1010:G:C8	3.05	0.44
34:2c:115:LEU:HD12	34:2c:115:LEU:HA	1.83	0.44
35:2d:92:VAL:O	35:2d:96:LEU:HD13	2.17	0.44
36:2e:71:LEU:HD21	36:2e:115:VAL:HG22	1.98	0.44
45:2n:37:PHE:HB3	45:2n:39:LEU:HD12	1.98	0.44
1:1A:288:C:H2'	1:1A:289:A:H8	1.82	0.44
1:1A:443:A:N7	5:1F:45:ARG:HG2	2.32	0.44
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.32	0.44
1:1A:2604:U:O3'	61:1A:4162:HOH:O	2.21	0.44
2:1B:6:C:H2'	2:1B:7:G:H5"	1.99	0.44
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.37	0.44
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.44
8:1I:72:LEU:HD23	8:1I:75:LEU:HD21	1.99	0.44
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.44
32:1a:448:A:C4	32:1a:487:A:C2	3.05	0.44
32:1a:457:C:H2'	32:1a:458:C:H6	1.82	0.44
32:1a:826:C:O2	39:1h:15:ASN:ND2	2.50	0.44
33:1b:98:LEU:HG	33:1b:101:MET:HE3	1.98	0.44
33:1b:219:VAL:HG12	33:1b:222:ILE:HD12	1.99	0.44
35:1d:155:LEU:HD22	35:1d:157:LEU:H	1.80	0.44
1:2A:861:A:H2'	1:2A:862:G:O4'	2.17	0.44
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.17	0.44
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.17	0.44
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.17	0.44
1:2A:2106:G:C4	1:2A:2107:C:H1'	2.52	0.44
1:2A:2335:A:C8	1:2A:2337:G:C5	3.05	0.44
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.17	0.44
7:2H:90:LYS:HD2	7:2H:159:GLU:HG2	1.98	0.44
21:2Z:39:VAL:HG21	21:2Z:44:PHE:HD1	1.82	0.44
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.53	0.44
32:2a:399:G:H2'	32:2a:400:C:C6	2.53	0.44
32:2a:473:G:OP2	47:2p:75:ARG:HD3	2.16	0.44
32:2a:1122:U:C4	32:2a:1123:A:N7	2.86	0.44
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.34	0.44
33:2b:7:VAL:HA	33:2b:8:LYS:HE3	1.99	0.44
35:2d:196:LEU:H	35:2d:196:LEU:HD12	1.82	0.44
1:1A:568:U:O5'	1:1A:945:A:N6	2.50	0.44
1:1A:578:A:OP1	1:1A:1255:U:O2'	2.30	0.44
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.32	0.44
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.52	0.44
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:108:LYS:HD3	5:1F:112:MET:HE3	1.99	0.44
6:1G:50:ALA:C	6:1G:52:ILE:H	2.25	0.44
8:1I:9:LEU:HD23	8:1I:12:LEU:HD23	1.99	0.44
15:1T:51:ARG:NH1	61:1T:303:HOH:O	2.45	0.44
32:1a:266:G:C5'	32:1a:268:C:H41	2.31	0.44
1:2A:185:U:H2'	1:2A:186:G:H8	1.81	0.44
1:2A:1203:G:C6	1:2A:1204:A:N6	2.85	0.44
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.18	0.44
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.31	0.44
1:2A:2125:G:N2	1:2A:2172:U:H3'	2.28	0.44
1:2A:2136:C:OP2	1:2A:2136:C:C6	2.70	0.44
1:2A:2186:G:C2	1:2A:2187:G:C5	3.05	0.44
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.48	0.44
5:2F:149:ASP:OD1	5:2F:150:GLY:N	2.51	0.44
8:2I:62:LYS:HG2	8:2I:133:HIS:CE1	2.53	0.44
8:2I:130:TYR:CE2	8:2I:132:PRO:HB3	2.52	0.44
12:2Q:55:VAL:HG22	21:2Z:183:LEU:HD11	1.99	0.44
13:2R:36:THR:O	13:2R:112:ALA:N	2.47	0.44
19:2X:66:LEU:HD12	19:2X:66:LEU:HA	1.77	0.44
21:2Z:35:ARG:HD2	21:2Z:35:ARG:HA	1.70	0.44
24:22:35:LEU:HD11	24:22:49:LYS:HB3	2.00	0.44
32:2a:685:G:C2	32:2a:686:U:C4	3.05	0.44
33:2b:102:LEU:HB3	33:2b:180:LEU:HD12	1.99	0.44
34:2c:186:PHE:CZ	34:2c:188:LEU:HD13	2.52	0.44
36:2e:102:ALA:O	36:2e:107:ARG:NH1	2.50	0.44
36:2e:110:LEU:HD13	36:2e:118:ILE:HG12	1.99	0.44
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	2.00	0.44
40:2i:9:ARG:O	40:2i:104:ARG:HG3	2.17	0.44
43:2l:47:LYS:HB2	43:2l:47:LYS:HE3	1.74	0.44
50:2s:66:MET:HB3	50:2s:74:PHE:CZ	2.53	0.44
1:1A:194:G:N3	61:1A:4297:HOH:O	2.36	0.44
1:1A:375:C:H2'	1:1A:376:C:C6	2.53	0.44
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.35	0.44
1:1A:2187:G:C6	1:1A:2188:C:C2	3.05	0.44
14:1S:74:ALA:HA	14:1S:110:LEU:HD22	2.00	0.44
20:1Y:19:LYS:HB3	20:1Y:19:LYS:HE2	1.70	0.44
32:1a:189(G):G:H4'	32:1a:189(H):G:OP2	2.16	0.44
32:1a:971:G:OP1	32:1a:972:C:H5"	2.16	0.44
34:1c:22:TRP:CD1	34:1c:59:ARG:HD2	2.52	0.44
38:1g:57:GLU:O	38:1g:61:VAL:HG23	2.18	0.44
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1096:A:C8	1:2A:1097:U:C5	3.05	0.44
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.52	0.44
1:2A:2639:A:H2'	1:2A:2640:G:O4'	2.18	0.44
2:2B:43:C:H5"	26:24:1:MET:HG3	2.00	0.44
6:2G:42:GLY:HA2	6:2G:89:GLY:HA3	1.98	0.44
9:2N:91:LEU:O	9:2N:95:PRO:HB3	2.18	0.44
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.81	0.44
14:2S:5:THR:HG23	14:2S:8:GLU:OE1	2.16	0.44
21:2Z:3:TYR:CD2	21:2Z:51:ALA:HB2	2.52	0.44
32:2a:114:U:H2'	32:2a:115:G:C8	2.53	0.44
32:2a:598:U:H4'	39:2h:94:TYR:CD2	2.52	0.44
32:2a:1338:G:C6	32:2a:1339:A:C6	3.06	0.44
32:2a:1410:G:H2'	32:2a:1411:C:C6	2.53	0.44
39:2h:14:ARG:O	39:2h:18:ARG:HG3	2.17	0.44
1:1A:305:U:H2'	1:1A:306:U:C6	2.53	0.44
1:1A:802:A:OP1	61:1A:4161:HOH:O	2.21	0.44
15:1T:96:ARG:NH2	61:1T:301:HOH:O	2.44	0.44
21:1Z:40:ASP:OD2	21:1Z:43:GLU:N	2.38	0.44
26:14:69:LYS:HA	50:1s:20:LEU:HD13	1.99	0.44
32:1a:262:A:C6	32:1a:263:A:C6	3.06	0.44
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.50	0.44
32:1a:1394:A:N1	32:1a:1500:A:O2'	2.46	0.44
32:1a:1479:C:H2'	32:1a:1480:G:C8	2.53	0.44
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	2.00	0.44
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	2.00	0.44
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.53	0.44
1:2A:2153:G:H2'	1:2A:2154:G:C8	2.52	0.44
1:2A:2298:A:N6	1:2A:2318:G:C8	2.85	0.44
6:2G:3:LEU:HG	6:2G:97:ASP:OD2	2.17	0.44
6:2G:68:PRO:HA	6:2G:92:VAL:HB	2.00	0.44
22:20:68:GLU:HG3	22:20:82:ARG:HE	1.82	0.44
26:24:57:GLU:HA	26:24:58:ARG:HA	1.67	0.44
32:2a:731:G:H5'	32:2a:766:A:H4'	1.98	0.44
32:2a:838:G:H3'	32:2a:840:C:H41	1.82	0.44
32:2a:932:C:H2'	32:2a:933:G:C8	2.52	0.44
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.52	0.44
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.52	0.44
38:2g:50:ILE:HG22	38:2g:125:MET:HG3	1.99	0.44
44:2m:60:VAL:HG23	44:2m:64:TRP:HZ3	1.82	0.44
48:2q:67:LYS:C	48:2q:69:LYS:H	2.23	0.44
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:161:THR:CG2	6:1G:163:ALA:H	2.23	0.44
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.50	0.44
15:1T:11:GLU:HG2	15:1T:57:PHE:CD2	2.53	0.44
17:1V:49:THR:HG22	17:1V:49:THR:O	2.17	0.44
18:1W:20:VAL:O	18:1W:23:LEU:HB2	2.17	0.44
20:1Y:43:ASN:HD22	20:1Y:43:ASN:HA	1.59	0.44
32:1a:472:A:O3'	47:1p:81:ARG:HA	2.17	0.44
32:1a:1479:C:H2'	32:1a:1480:G:H8	1.82	0.44
34:1c:26:LYS:HB3	34:1c:26:LYS:HE2	1.77	0.44
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.53	0.44
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.50	0.44
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.33	0.44
50:1s:15:LEU:O	50:1s:19:VAL:HG23	2.17	0.44
50:1s:22:LEU:O	50:1s:27:GLU:N	2.51	0.44
1:2A:1087:G:N7	1:2A:1089:G:C8	2.85	0.44
1:2A:1987:G:H2'	1:2A:1988:C:C6	2.52	0.44
1:2A:2473:U:O2	1:2A:2473:U:H2'	2.17	0.44
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.99	0.44
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.35	0.44
6:2G:111:LEU:HB2	6:2G:112:PRO:HD3	2.00	0.44
10:2O:9:GLU:O	10:2O:83:ALA:HA	2.18	0.44
15:2T:17:THR:O	15:2T:17:THR:OG1	2.34	0.44
32:2a:110:C:H2'	32:2a:111:G:O4'	2.18	0.44
32:2a:358:U:H2'	32:2a:359:U:C6	2.53	0.44
38:2g:113:GLU:H	38:2g:113:GLU:HG2	1.40	0.44
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.57	0.44
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.65	0.44
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.44
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.27	0.44
5:1F:132:VAL:HG22	5:1F:163:VAL:HG22	2.00	0.44
6:1G:135:LEU:O	6:1G:154:GLY:HA3	2.18	0.44
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	2.00	0.44
32:1a:1187:G:H4'	40:1i:111:ARG:NH1	2.33	0.44
32:1a:1518:MA6:O5'	32:1a:1518:MA6:H8	2.18	0.44
33:1b:150:SER:OG	33:1b:151:GLY:N	2.49	0.44
33:1b:208:ILE:HA	33:1b:211:ILE:HD12	1.99	0.44
42:1k:62:GLN:O	42:1k:66:LEU:HG	2.17	0.44
45:1n:26:ARG:HH12	45:1n:46:GLU:HB2	1.82	0.44
1:2A:1073:A:H2'	1:2A:1074:G:H8	1.83	0.44
1:2A:1364:G:OP1	23:21:2:SER:HA	2.18	0.44
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.18	0.44
6:2G:82:LEU:HA	6:2G:86:MET:SD	2.57	0.44
21:2Z:157:LEU:H	21:2Z:157:LEU:HD12	1.82	0.44
32:2a:282:A:OP2	32:2a:283:C:N4	2.39	0.44
32:2a:1053:G:N7	32:2a:1200:C:H5"	2.33	0.44
32:2a:1391:U:H2'	32:2a:1392:G:H8	1.82	0.44
34:2c:187:ALA:HB3	34:2c:198:VAL:HB	1.98	0.44
47:2p:5:ARG:HH21	47:2p:24:ALA:HA	1.83	0.44
1:1A:1173:G:C2	1:1A:1175:U:H4'	2.53	0.44
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.32	0.44
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.18	0.44
3:1D:16:MET:HG2	3:1D:211:ARG:HH21	1.82	0.44
8:1I:9:LEU:HD11	8:1I:35:LEU:HD13	1.99	0.44
17:1V:21:ARG:HD3	17:1V:91:TYR:CE1	2.53	0.44
30:18:30:ARG:HD3	61:18:223:HOH:O	2.18	0.44
32:1a:254:G:OP2	61:1a:1914:HOH:O	2.21	0.44
32:1a:833:U:H2'	32:1a:834:C:C6	2.53	0.44
35:1d:155:LEU:HB3	35:1d:158:ILE:HG12	2.00	0.44
40:1i:3:GLN:HE21	40:1i:20:ARG:HH21	1.66	0.44
1:2A:1076:C:H1'	1:2A:1077:A:H5'	2.00	0.44
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.44
8:2I:65:ALA:O	8:2I:69:LYS:HB3	2.18	0.44
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.17	0.44
32:2a:439:A:C5	32:2a:441:A:H1'	2.53	0.44
32:2a:582:U:C2	32:2a:760:G:C6	3.06	0.44
32:2a:1285:A:H4'	32:2a:1286:A:O5'	2.18	0.44
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.82	0.44
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.99	0.44
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.33	0.44
45:2n:9:LYS:HA	45:2n:12:ARG:HB3	1.99	0.44
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.17	0.44
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.18	0.43
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.17	0.43
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.18	0.43
1:1A:2113:U:O4	1:1A:2168:G:H4'	2.18	0.43
1:1A:2531:A:H5"	7:1H:157:TYR:CZ	2.54	0.43
7:1H:25:LYS:HG3	7:1H:34:GLU:HG2	2.00	0.43
9:1N:48:MET:O	9:1N:48:MET:HE3	2.18	0.43
10:1O:115:VAL:O	57:1a:1882:MPD:H13	2.18	0.43
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	2.00	0.43
32:1a:277:C:H5"	48:1q:68:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:741:G:H2'	32:1a:742:G:O4'	2.18	0.43
36:1e:90:VAL:O	36:1e:120:THR:HA	2.18	0.43
1:2A:248:G:H5"	1:2A:386:G:N2	2.33	0.43
1:2A:1448:G:O2'	1:2A:1528(A):A:N1	2.49	0.43
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.00	0.43
1:2A:2136:C:C2	1:2A:2155:G:N2	2.86	0.43
2:2B:3:C:H2'	2:2B:4:C:C6	2.52	0.43
3:2D:92:ILE:HD12	3:2D:104:TYR:CD1	2.53	0.43
4:2E:1:MET:O	4:2E:84:PHE:HB2	2.17	0.43
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.18	0.43
6:2G:12:TYR:HA	6:2G:16:ARG:CG	2.48	0.43
6:2G:72:ARG:HG2	6:2G:87:PRO:HA	2.00	0.43
15:2T:16:ARG:NH2	15:2T:83:ILE:O	2.50	0.43
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	2.00	0.43
26:24:1:MET:HE2	26:24:6:HIS:CG	2.52	0.43
31:29:7:VAL:HG12	31:29:34:GLN:HB3	2.00	0.43
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.53	0.43
32:2a:984:C:H2'	32:2a:985:C:C6	2.53	0.43
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.18	0.43
15:1T:64:ARG:HB2	15:1T:73:GLU:HG2	2.00	0.43
21:1Z:96:VAL:O	21:1Z:127:LYS:HA	2.19	0.43
27:15:9:LYS:O	61:15:201:HOH:O	2.21	0.43
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.49	0.43
32:1a:93:G:H2'	32:1a:96:U:O4'	2.18	0.43
32:1a:408:A:H2'	32:1a:409:G:O4'	2.18	0.43
32:1a:743:U:H2'	32:1a:744:C:C6	2.53	0.43
32:1a:1002:G:H3'	32:1a:1003:G:C8	2.53	0.43
32:1a:1292:U:H2'	32:1a:1293:G:C8	2.53	0.43
32:1a:1299:A:N3	32:1a:1299:A:H5"	2.32	0.43
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	2.01	0.43
48:1q:83:ASP:N	48:1q:83:ASP:OD1	2.51	0.43
1:2A:1087:G:H22	1:2A:1102:C:H42	1.65	0.43
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.43
1:2A:2138:C:H2'	1:2A:2139:C:H6	1.83	0.43
1:2A:2390:U:O2'	1:2A:2391:G:H5'	2.18	0.43
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.99	0.43
7:2H:5:GLY:HA3	7:2H:65:HIS:CD2	2.50	0.43
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.50	0.43
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.18	0.43
32:2a:390:C:H2'	32:2a:391:G:C8	2.53	0.43
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:119:GLU:HG3	33:2b:153:ARG:HH22	1.83	0.43
33:2b:208:ILE:HA	33:2b:211:ILE:HB	2.00	0.43
34:2c:20:SER:HB2	34:2c:40:ARG:HH21	1.82	0.43
40:2i:25:LYS:O	40:2i:60:ASP:HB2	2.18	0.43
51:2t:72:LEU:HD23	51:2t:72:LEU:HA	1.88	0.43
1:1A:876:C:H2'	1:1A:877:U:O4'	2.18	0.43
1:1A:1067:A:H2'	1:1A:1067:A:N3	2.33	0.43
1:1A:1359:A:N1	1:1A:1372:U:C4	2.87	0.43
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.52	0.43
2:1B:14:U:OP2	2:1B:70:C:O2'	2.34	0.43
15:1T:33:LYS:HG2	15:1T:82:LEU:HD23	2.00	0.43
32:1a:437:U:O2	35:1d:119:GLN:NE2	2.52	0.43
32:1a:901:A:O2'	32:1a:1513:A:OP1	2.28	0.43
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.18	0.43
1:2A:108:U:H2'	1:2A:109:G:C8	2.53	0.43
1:2A:118:A:N3	1:2A:178:G:H1'	2.33	0.43
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.18	0.43
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.53	0.43
1:2A:2129:C:N3	1:2A:2159:G:O6	2.50	0.43
1:2A:2462:U:H2'	1:2A:2463:C:C6	2.53	0.43
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.18	0.43
6:2G:9:ARG:O	6:2G:13:GLU:HB2	2.18	0.43
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.99	0.43
7:2H:136:ILE:H	7:2H:136:ILE:HG13	1.54	0.43
32:2a:270:A:H2'	32:2a:271:C:C6	2.54	0.43
32:2a:757:U:H2'	32:2a:758:G:O4'	2.18	0.43
32:2a:1003:G:H2'	32:2a:1004:A:C4'	2.34	0.43
32:2a:1125:U:HO2'	32:2a:1126:U:P	2.40	0.43
33:2b:74:LYS:NZ	33:2b:166:ASP:HB2	2.33	0.43
37:2f:22:GLU:OE2	37:2f:82:ARG:NE	2.52	0.43
40:2i:92:TYR:O	40:2i:96:LEU:HB2	2.18	0.43
41:2j:21:GLN:O	41:2j:25:GLU:HG2	2.18	0.43
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.82	0.43
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.53	0.43
1:1A:2824:C:H5	61:1A:5736:HOH:O	2.00	0.43
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.18	0.43
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.25	0.43
32:1a:176:C:H2'	32:1a:177:C:C6	2.53	0.43
32:1a:868:C:H2'	32:1a:869:G:O4'	2.19	0.43
32:1a:1497:G:H1'	32:1a:1518:MA6:H2	2.00	0.43
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:124:ILE:HD12	34:1c:130:VAL:HG22	2.01	0.43
35:1d:173:TRP:CG	35:1d:189:PRO:HB3	2.53	0.43
39:1h:49:GLU:OE2	39:1h:62:TYR:OH	2.32	0.43
40:1i:19:LEU:HD12	40:1i:84:ALA:HB3	2.00	0.43
1:2A:889:C:O2'	1:2A:890:A:H8	2.01	0.43
1:2A:1000:A:H62	1:2A:1154:G:H2'	1.82	0.43
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.54	0.43
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.49	0.43
6:2G:71:THR:N	6:2G:89:GLY:O	2.40	0.43
6:2G:108:ASN:HA	26:24:37:SER:HB3	2.00	0.43
7:2H:149:ARG:HG3	7:2H:162:ILE:O	2.18	0.43
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.34	0.43
26:24:59:PHE:HE2	50:2s:64:GLU:HB2	1.82	0.43
32:2a:409:G:H2'	32:2a:410:G:O4'	2.17	0.43
32:2a:472:A:H4'	47:2p:80:PHE:O	2.18	0.43
32:2a:520:A:N1	32:2a:536:C:H1'	2.34	0.43
32:2a:531:U:O3'	32:2a:532:A:H4'	2.17	0.43
32:2a:660:G:H1	32:2a:745:C:N4	2.14	0.43
32:2a:683:G:H2'	32:2a:684:A:C8	2.54	0.43
32:2a:1112:C:O2	34:2c:179:ARG:N	2.50	0.43
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	2.00	0.43
40:2i:32:ASP:HB3	40:2i:35:GLU:HB3	2.00	0.43
50:2s:22:LEU:HD12	50:2s:31:ILE:HD11	2.00	0.43
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.53	0.43
1:1A:531:C:H4'	1:1A:532:A:H5"	1.99	0.43
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.54	0.43
1:1A:1639:U:O2'	1:1A:1640:C:H5'	2.18	0.43
32:1a:638:G:H2'	32:1a:639:G:O4'	2.18	0.43
33:1b:150:SER:O	33:1b:153:ARG:HG2	2.18	0.43
33:1b:184:VAL:N	33:1b:198:ASP:OD2	2.49	0.43
35:1d:107:ARG:NH2	35:1d:114:ARG:HH22	2.15	0.43
40:1i:10:ARG:O	40:1i:11:LYS:C	2.62	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.53	0.43
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.83	0.43
1:2A:2186:G:N2	1:2A:2187:G:C4	2.87	0.43
3:2D:61:LEU:O	3:2D:63:ARG:NH1	2.50	0.43
5:2F:152:GLU:HA	5:2F:190:GLU:OE1	2.19	0.43
6:2G:66:GLN:OE1	6:2G:98:ARG:NE	2.50	0.43
10:2O:54:GLU:OE1	61:2O:301:HOH:O	2.21	0.43
15:2T:53:ARG:HB3	15:2T:53:ARG:NH1	2.32	0.43
23:21:50:ARG:NH1	23:21:57:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:353:A:H5'	32:2a:353:A:H8	1.84	0.43
33:2b:8:LYS:O	33:2b:9:GLU:HB2	2.17	0.43
33:2b:24:TRP:HB3	33:2b:40:HIS:CE1	2.54	0.43
39:2h:87:SER:HA	39:2h:93:VAL:HG23	2.00	0.43
44:2m:48:LEU:HD12	44:2m:53:VAL:HG22	2.00	0.43
1:1A:2137:C:N4	1:1A:2154:G:N1	2.31	0.43
5:1F:195:ASP:HB2	5:1F:198:ALA:H	1.83	0.43
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.83	0.43
10:1O:108:GLU:H	10:1O:108:GLU:HG3	1.68	0.43
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.75	0.43
32:1a:60:A:OP1	32:1a:111:G:N2	2.51	0.43
32:1a:1168:A:H2'	32:1a:1169:A:C8	2.54	0.43
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.19	0.43
32:1a:1498:UR3:H4'	32:1a:1519:MA6:H2	2.00	0.43
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.37	0.43
33:1b:47:THR:HG22	33:1b:51:LEU:HD12	2.00	0.43
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.88	0.43
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	2.00	0.43
1:2A:287:C:H2'	1:2A:288:C:C6	2.53	0.43
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.19	0.43
1:2A:1180:C:H2'	1:2A:1181:C:C6	2.53	0.43
1:2A:1204:A:H8	1:2A:1204:A:OP1	2.02	0.43
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.54	0.43
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.53	0.43
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.32	0.43
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	2.01	0.43
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.01	0.43
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.39	0.43
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.19	0.43
40:2i:32:ASP:O	40:2i:36:TYR:N	2.50	0.43
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	2.01	0.43
49:2r:45:SER:OG	49:2r:47:THR:HG22	2.19	0.43
1:1A:256:A:OP2	61:1A:4167:HOH:O	2.22	0.43
1:1A:478:A:C6	1:1A:480:A:C6	3.07	0.43
1:1A:515:A:H2	1:1A:1260:G:N3	2.17	0.43
1:1A:2513:G:O2'	61:1A:4120:HOH:O	2.09	0.43
33:1b:96:ARG:HG2	33:1b:98:LEU:HD23	2.01	0.43
40:1i:10:ARG:HG2	40:1i:75:ASP:HB2	2.00	0.43
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	2.01	0.43
1:2A:297:C:OP1	20:2Y:95:LYS:NZ	2.44	0.43
1:2A:566:U:H2'	1:2A:567:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:690:G:H2'	1:2A:691:C:C6	2.53	0.43
1:2A:1063:G:H1	1:2A:1075:C:H42	1.64	0.43
1:2A:2391:G:O6	1:2A:2425:A:H8	2.01	0.43
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.00	0.43
30:28:34:TRP:CE2	30:28:35:GLN:HB3	2.54	0.43
32:2a:1326:C:OP1	52:2u:12:LYS:NZ	2.49	0.43
34:2c:60:ALA:HB3	34:2c:63:ASN:HD21	1.82	0.43
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	2.00	0.43
1:1A:222:A:H3'	1:1A:421:U:H5'	2.01	0.43
1:1A:330:A:H2	1:1A:1210:A:H2'	1.83	0.43
1:1A:606:U:O2'	61:1A:4165:HOH:O	2.21	0.43
1:1A:1089:G:N2	1:1A:1090:U:O4	2.36	0.43
3:1D:123:ALA:HB3	3:1D:131:LEU:HG	2.01	0.43
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE1	2.34	0.43
30:18:47:LYS:NZ	57:18:103:MPD:H51	2.34	0.43
32:1a:765:G:C6	32:1a:812:C:C2	3.06	0.43
32:1a:1003:G:N2	32:1a:1004:A:N3	2.67	0.43
32:1a:1318:A:H5"	50:1s:3:ARG:HH12	1.83	0.43
32:1a:1431:C:H2'	32:1a:1432:G:O4'	2.19	0.43
32:1a:1447:A:H5"	32:1a:1452:C:OP2	2.19	0.43
34:1c:69:HIS:CD2	34:1c:104:GLN:HG2	2.53	0.43
46:1o:57:LEU:HD23	46:1o:57:LEU:HA	1.89	0.43
1:2A:8:A:H2'	1:2A:9:U:H6	1.83	0.43
1:2A:751:A:C6	1:2A:789:A:C5	3.07	0.43
1:2A:1631(A):A:N6	61:2A:3847:HOH:O	2.19	0.43
1:2A:2144:U:H1'	1:2A:2147:G:O6	2.19	0.43
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.53	0.43
8:2I:23:PRO:O	8:2I:27:ARG:HB2	2.18	0.43
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.18	0.43
12:2Q:68:ILE:HD13	12:2Q:103:MET:HG2	2.00	0.43
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.83	0.43
23:21:51:VAL:HG13	23:21:53:VAL:HG23	2.00	0.43
26:24:61:ARG:HD3	50:2s:67:VAL:HG12	2.01	0.43
30:28:23:VAL:HG13	30:28:47:LYS:HB3	2.01	0.43
32:2a:652:U:H1'	32:2a:653:A:H2	1.83	0.43
32:2a:1134:G:H2'	32:2a:1135:U:H5'	2.01	0.43
36:2e:81:GLU:HG2	36:2e:90:VAL:HG13	2.01	0.43
50:2s:20:LEU:HA	50:2s:23:ASN:ND2	2.30	0.43
1:1A:666:G:H1'	30:18:4:MET:HE3	2.00	0.43
1:1A:888:C:H6	1:1A:888:C:H2'	1.55	0.43
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.42	0.43
32:1a:1061:G:H1'	41:1j:56:HIS:CE1	2.54	0.43
32:1a:1304:G:C6	32:1a:1305:G:N1	2.87	0.43
34:1c:16:ARG:HH21	34:1c:54:ARG:HH21	1.66	0.43
41:1j:43:ARG:O	41:1j:67:THR:HG23	2.18	0.43
41:1j:64:GLU:CD	41:1j:66:ARG:HD3	2.43	0.43
44:1m:40:ASN:HD21	44:1m:42:ALA:HB3	1.82	0.43
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.82	0.43
1:2A:620:G:N3	1:2A:620:G:H5'	2.34	0.43
1:2A:878:A:N6	1:2A:899:A:O2'	2.51	0.43
1:2A:1096:A:H2'	1:2A:1097:U:H6	1.84	0.43
1:2A:1843:C:H5'	3:2D:253:GLN:HE22	1.83	0.43
1:2A:2114:A:N6	1:2A:2119:A:OP2	2.52	0.43
1:2A:2319:G:H22	14:2S:3:ARG:CD	2.31	0.43
1:2A:2619:C:H4'	4:2E:151:TYR:O	2.19	0.43
12:2Q:103:MET:HE1	12:2Q:125:LEU:HD13	2.00	0.43
13:2R:36:THR:HG22	13:2R:37:THR:H	1.84	0.43
21:2Z:18:LEU:HD21	21:2Z:38:TYR:CG	2.53	0.43
32:2a:41:G:H2'	32:2a:42:G:C8	2.53	0.43
32:2a:451:A:N6	32:2a:480:U:H2'	2.34	0.43
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.54	0.43
32:2a:1090:U:H2'	32:2a:1091:U:H6	1.83	0.43
32:2a:1187:G:H5'	40:2i:113:LYS:HE2	2.01	0.43
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.18	0.43
33:2b:93:VAL:HG21	33:2b:97:TRP:CD1	2.54	0.43
33:2b:131:PRO:O	33:2b:135:GLN:HG3	2.19	0.43
39:2h:4:ASP:OD1	39:2h:7:ALA:N	2.36	0.43
40:2i:41:VAL:C	40:2i:43:ALA:H	2.26	0.43
53:2y:60:VAL:HG22	53:2y:62:VAL:HG23	2.01	0.43
1:1A:330:A:HO2'	1:1A:331:A:H8	1.66	0.43
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.53	0.43
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.32	0.43
27:15:37:LYS:HA	27:15:37:LYS:HD3	1.91	0.43
32:1a:73:G:H2'	32:1a:76:C:C6	2.54	0.43
32:1a:189(B):C:H2'	32:1a:189(C):C:C6	2.54	0.43
32:1a:1499:A:H1'	32:1a:1520:G:H5'	2.01	0.43
35:1d:167:GLY:H	35:1d:168:ARG:HH12	1.67	0.43
1:2A:372:G:H8	23:21:65:SER:O	2.02	0.43
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.37	0.43
2:2B:57:A:H4'	6:2G:30:GLU:HG3	2.00	0.43
16:2U:13:LYS:HE2	16:2U:13:LYS:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:5:TYR:HB3	24:22:33:MET:HB2	2.01	0.43
26:24:1:MET:HE2	26:24:6:HIS:CE1	2.54	0.43
32:2a:625:G:H2'	32:2a:626:U:H6	1.84	0.43
32:2a:1067:A:H8	32:2a:1067:A:O5'	2.01	0.43
33:2b:9:GLU:OE1	33:2b:10:LEU:N	2.36	0.43
34:2c:6:HIS:HE1	34:2c:184:TYR:CD2	2.37	0.43
34:2c:17:ASP:OD1	34:2c:21:ARG:HD3	2.19	0.43
36:2e:43:LEU:H	36:2e:65:ASN:ND2	2.17	0.43
47:2p:37:GLY:HA3	47:2p:50:LYS:O	2.19	0.43
48:2q:63:ARG:HG2	48:2q:64:PRO:HD2	2.01	0.43
1:1A:2875:C:OP1	15:1T:3:ARG:NH1	2.31	0.42
2:1B:106:G:H5'	21:1Z:31:ARG:HB3	2.01	0.42
4:1E:18:ASP:HB3	15:1T:82:LEU:HD21	2.01	0.42
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.52	0.42
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.18	0.42
32:1a:302:G:O2'	32:1a:556:C:H5"	2.19	0.42
32:1a:407:G:OP1	35:1d:115:ARG:HD3	2.19	0.42
32:1a:457:C:N4	32:1a:474:G:H1	2.17	0.42
32:1a:820:U:H4'	32:1a:821:G:OP2	2.19	0.42
32:1a:1492:A:H4'	32:1a:1493:A:C6	2.54	0.42
33:1b:207:ALA:O	33:1b:211:ILE:HG13	2.19	0.42
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.35	0.42
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.42
1:2A:388:G:O2'	1:2A:389:G:N7	2.47	0.42
1:2A:882:G:H1	1:2A:894:C:H42	1.65	0.42
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.54	0.42
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.30	0.42
1:2A:2134:A:H1'	1:2A:2159:G:H1'	2.00	0.42
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.17	0.42
1:2A:2611:U:H3'	1:2A:2611:U:OP2	2.19	0.42
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.52	0.42
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	2.01	0.42
7:2H:103:LEU:O	7:2H:114:VAL:HA	2.19	0.42
19:2X:53:LYS:NZ	19:2X:55:ASN:OD1	2.37	0.42
21:2Z:18:LEU:HD12	21:2Z:18:LEU:HA	1.82	0.42
32:2a:250:A:H4'	32:2a:251:G:O5'	2.18	0.42
32:2a:557:G:C6	32:2a:558:G:C6	3.07	0.42
32:2a:615:C:H2'	32:2a:616:G:O4'	2.19	0.42
33:2b:22:LYS:H	33:2b:22:LYS:HG3	1.66	0.42
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	2.01	0.42
35:2d:25:ARG:NH1	35:2d:30:LYS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:49:ALA:HB1	49:2r:80:PRO:HB3	2.01	0.42
40:2i:33:PHE:C	40:2i:33:PHE:CD2	2.97	0.42
44:2m:20:THR:HA	44:2m:25:ILE:O	2.18	0.42
1:1A:1175:U:HO2'	1:1A:1176:G:P	2.42	0.42
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	2.01	0.42
6:1G:138:GLN:NE2	6:1G:153:ARG:HH21	2.17	0.42
26:14:59:PHE:CE1	50:1s:67:VAL:HG21	2.54	0.42
32:1a:495:A:H4'	32:1a:496:A:OP1	2.18	0.42
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	2.01	0.42
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.19	0.42
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.33	0.42
48:1q:76:LEU:HD21	48:1q:79:SER:OG	2.20	0.42
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.42	0.42
1:2A:1445(A):C:H2'	1:2A:1446:C:H6	1.84	0.42
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.34	0.42
1:2A:2116:G:H3'	1:2A:2117:A:C8	2.54	0.42
1:2A:2541:A:N7	61:2A:3953:HOH:O	2.37	0.42
1:2A:2641:G:P	9:2N:74:ARG:HH21	2.41	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	2.00	0.42
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	2.00	0.42
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.34	0.42
6:2G:131:TYR:HE2	6:2G:133:LEU:HD22	1.84	0.42
9:2N:73:THR:HA	9:2N:83:LYS:O	2.19	0.42
21:2Z:3:TYR:O	21:2Z:57:ILE:HA	2.19	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
26:24:37:SER:O	26:24:43:TYR:HD2	2.03	0.42
32:2a:8:A:C5	35:2d:209:ARG:HA	2.54	0.42
32:2a:931:C:H42	32:2a:1386:G:H1	1.66	0.42
32:2a:1279:A:H8	32:2a:1282:C:N3	2.17	0.42
34:2c:139:GLN:O	34:2c:143:GLU:HB2	2.19	0.42
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	2.01	0.42
41:2j:26:ALA:HB1	41:2j:84:GLN:NE2	2.34	0.42
53:2y:29:LYS:HG2	53:2y:30:TRP:CE3	2.54	0.42
1:1A:796:C:H2'	1:1A:797:C:C6	2.55	0.42
1:1A:884:C:H2'	1:1A:885:C:O4'	2.18	0.42
1:1A:1175:U:H3'	1:1A:1177:A:OP2	2.18	0.42
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.51	0.42
1:1A:1762:A:H2'	61:1A:7278:HOH:O	2.18	0.42
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.19	0.42
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:70:ALA:O	4:1E:72:VAL:N	2.52	0.42
6:1G:120:LEU:O	6:1G:181:ARG:HG2	2.20	0.42
20:1Y:23:ARG:NH2	61:1Y:302:HOH:O	2.50	0.42
32:1a:1003:G:H2'	32:1a:1004:A:C4'	2.44	0.42
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.54	0.42
40:1i:84:ALA:O	40:1i:87:GLN:HG2	2.19	0.42
41:1j:7:LYS:HE3	41:1j:9:ARG:HH12	1.85	0.42
44:1m:49:THR:HG23	44:1m:52:GLU:OE1	2.19	0.42
46:1o:47:LYS:HB2	46:1o:47:LYS:HE3	1.78	0.42
1:2A:11:G:N3	1:2A:11:G:H2'	2.33	0.42
1:2A:985:C:H2'	1:2A:986:C:C6	2.54	0.42
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.37	0.42
2:2B:42:C:C4	2:2B:43:C:C4	3.08	0.42
3:2D:164:GLN:OE1	3:2D:176:ARG:NH2	2.28	0.42
3:2D:267:SER:C	3:2D:269:PHE:H	2.26	0.42
26:24:62:ARG:HB3	26:24:63:TYR:H	1.68	0.42
32:2a:457:C:H2'	32:2a:458:C:H6	1.83	0.42
32:2a:666:G:H5'	32:2a:726:C:H1'	2.01	0.42
32:2a:973:G:H3'	32:2a:974:A:H5"	2.02	0.42
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.47	0.42
33:2b:31:TYR:O	33:2b:42:ILE:HG23	2.20	0.42
40:2i:5:TYR:OH	40:2i:16:ARG:HG2	2.19	0.42
48:2q:62:SER:HB3	48:2q:72:ARG:HH11	1.83	0.42
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.19	0.42
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.29	0.42
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.19	0.42
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	2.02	0.42
2:1B:12:C:O2'	22:10:74:ARG:HG2	2.19	0.42
6:1G:77:ILE:H	6:1G:82:LEU:HB3	1.83	0.42
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.34	0.42
20:1Y:107:ASP:OD1	20:1Y:107:ASP:N	2.49	0.42
32:1a:1125:U:O2	32:1a:1126:U:O2'	2.30	0.42
33:1b:84:GLU:O	33:1b:87:ARG:HB2	2.19	0.42
34:1c:113:ALA:N	34:1c:183:ASP:OD2	2.42	0.42
34:1c:150:LYS:HB2	34:1c:150:LYS:HE3	1.90	0.42
53:1y:55:ASN:OD1	53:1y:60:VAL:HG12	2.19	0.42
1:2A:71:A:H5"	1:2A:73:A:C8	2.55	0.42
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.19	0.42
1:2A:644:A:H4'	1:2A:645:C:C5	2.53	0.42
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.19	0.42
1:2A:2061:G:H5"	1:2A:2503:2MA:C2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2168:G:O2'	1:2A:2170:A:N6	2.47	0.42
56:2A:3731:ZIT:H191	56:2A:3731:ZIT:H8	1.89	0.42
6:2G:125:PHE:CZ	6:2G:173:LEU:HD12	2.55	0.42
14:2S:19:LYS:H	14:2S:19:LYS:HG2	1.58	0.42
32:2a:965:A:O2'	53:2y:40:ILE:HG21	2.19	0.42
32:2a:983:A:H1'	32:2a:1049:U:O2	2.20	0.42
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.85	0.42
51:2t:74:LYS:HE2	51:2t:74:LYS:HB3	1.93	0.42
53:2y:40:ILE:HB	53:2y:51:ASP:HB2	2.00	0.42
1:1A:1045:A:O2'	1:1A:1047:G:C4	2.68	0.42
1:1A:1074:G:C2	1:1A:1075:C:H1'	2.54	0.42
1:1A:1301:A:C8	1:1A:1303:G:C8	3.07	0.42
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.30	0.42
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.46	0.42
1:1A:2168:G:C2	1:1A:2171:A:H8	2.37	0.42
6:1G:2:PRO:HA	6:1G:97:ASP:OD2	2.20	0.42
32:1a:113:G:H2'	32:1a:114:U:C6	2.54	0.42
32:1a:186:C:H2'	32:1a:187:C:C6	2.54	0.42
32:1a:299:G:H2'	32:1a:300:A:C8	2.55	0.42
32:1a:568:G:O2'	32:1a:574:A:N1	2.44	0.42
32:1a:731:G:H5'	32:1a:766:A:H4'	2.01	0.42
33:1b:61:LEU:HD23	33:1b:68:ILE:HD11	2.01	0.42
35:1d:168:ARG:HD3	35:1d:168:ARG:HA	1.23	0.42
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	2.01	0.42
40:1i:89:ASN:HB3	40:1i:92:TYR:CD2	2.55	0.42
1:2A:311:A:C6	1:2A:328:U:C4	3.08	0.42
1:2A:1045:A:H5'	1:2A:1047:G:O4'	2.18	0.42
1:2A:1102:C:H2'	1:2A:1103:A:H8	1.84	0.42
1:2A:2080:G:OP1	23:21:35:THR:HG21	2.19	0.42
3:2D:8:PRO:HB3	3:2D:14:ARG:HG3	2.02	0.42
12:2Q:137:TYR:HB3	21:2Z:76:LEU:HD21	2.01	0.42
21:2Z:5:LEU:HD23	21:2Z:47:VAL:HG21	2.00	0.42
22:20:43:THR:OG1	22:20:46:LYS:HG2	2.20	0.42
28:26:47:THR:HG22	28:26:48:VAL:N	2.34	0.42
32:2a:341:C:H2'	32:2a:342:C:C6	2.55	0.42
32:2a:513:C:H2'	32:2a:514:C:C6	2.54	0.42
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.54	0.42
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	2.00	0.42
1:1A:764:A:H5'	3:1D:210:GLY:HA2	2.00	0.42
1:1A:821:A:H2'	1:1A:946:G:H5"	2.01	0.42
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1809:A:H2'	1:1A:1810:A:C8	2.55	0.42
1:1A:2033:A:O2'	1:1A:2035:G:OP2	2.32	0.42
1:1A:2135:A:H62	1:1A:2156:G:N2	2.15	0.42
5:1F:23:ASP:OD1	5:1F:23:ASP:N	2.53	0.42
57:1T:204:MPD:H11	57:1T:204:MPD:H4	1.69	0.42
32:1a:425:G:O3'	35:1d:45:GLN:NE2	2.52	0.42
32:1a:457:C:H2'	32:1a:458:C:C6	2.54	0.42
32:1a:473:G:H2'	32:1a:474:G:C8	2.54	0.42
32:1a:690:G:C6	32:1a:691:G:C6	3.08	0.42
32:1a:790:A:H2'	32:1a:791:G:C8	2.55	0.42
33:1b:27:LYS:HD2	33:1b:193:ASP:OD1	2.20	0.42
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.84	0.42
36:1e:66:MET:HE3	36:1e:66:MET:HB3	1.94	0.42
36:1e:148:VAL:HG13	36:1e:152:ARG:CZ	2.49	0.42
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.43	0.42
51:1t:58:LYS:HA	51:1t:58:LYS:HD2	1.85	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
1:2A:2892:A:N6	1:2A:2893:G:O6	2.53	0.42
2:2B:66:A:N6	2:2B:108:U:H3'	2.34	0.42
6:2G:36:LYS:HG3	6:2G:38:VAL:HG23	2.02	0.42
6:2G:64:THR:HB	6:2G:94:LEU:HD21	2.01	0.42
6:2G:83:ARG:H	6:2G:86:MET:CE	2.33	0.42
9:2N:67:LEU:HD12	9:2N:67:LEU:HA	1.78	0.42
10:2O:22:ILE:HG12	10:2O:40:VAL:O	2.20	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.67	0.42
25:23:7:LYS:HG3	25:23:34:GLU:HG2	2.00	0.42
34:2c:157:ILE:HG21	34:2c:164:ARG:HH21	1.85	0.42
35:2d:50:ARG:HH12	36:2e:10:MET:HE3	1.85	0.42
40:2i:43:ALA:O	40:2i:45:ALA:N	2.52	0.42
48:2q:45:HIS:CD2	48:2q:65:ILE:HG12	2.55	0.42
51:2t:86:ARG:HH21	51:2t:90:GLN:HE22	1.66	0.42
1:1A:27:G:C2	1:1A:512:G:N3	2.88	0.42
1:1A:251:A:C5	1:1A:252:G:H1'	2.54	0.42
1:1A:1083:U:H1'	1:1A:1086:A:N6	2.34	0.42
1:1A:2124:G:H2'	1:1A:2125:G:H5'	2.01	0.42
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.55	0.42
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.32	0.42
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.35	0.42
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.19	0.42
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	2.01	0.42
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.53	0.42
32:1a:184:G:H2'	32:1a:185:A:C8	2.53	0.42
37:1f:75:LEU:O	37:1f:79:LEU:HG	2.19	0.42
42:1k:59:TYR:CZ	42:1k:63:LEU:HD11	2.55	0.42
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.59	0.42
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.54	0.42
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.55	0.42
1:2A:2134:A:H8	1:2A:2156:G:N2	2.14	0.42
2:2B:94:C:H2'	2:2B:95:C:C6	2.55	0.42
3:2D:70:TRP:HB3	3:2D:190:TYR:CE2	2.55	0.42
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.84	0.42
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.35	0.42
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.35	0.42
32:2a:1493:A:H2'	32:2a:1494:G:H5'	2.01	0.42
33:2b:110:GLN:HA	33:2b:113:HIS:CD2	2.54	0.42
34:2c:124:ILE:HD12	34:2c:196:LEU:HD12	2.00	0.42
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	2.01	0.42
35:2d:73:ARG:HD2	35:2d:73:ARG:HA	1.81	0.42
46:2o:5:LYS:H	46:2o:5:LYS:HG2	1.64	0.42
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.19	0.42
50:2s:18:LYS:H	50:2s:18:LYS:HG3	1.60	0.42
1:1A:747:U:O2	1:1A:2014:A:H1'	2.19	0.42
1:1A:1271:G:H2'	61:1A:4520:HOH:O	2.19	0.42
1:1A:1877:A:H5'	1:1A:1878:G:OP2	2.19	0.42
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.49	0.42
1:1A:2824:C:N4	61:1A:4220:HOH:O	2.29	0.42
8:1I:27:ARG:HD2	23:11:71:TYR:CZ	2.54	0.42
32:1a:1065:U:H1'	32:1a:1066:C:OP2	2.19	0.42
33:1b:10:LEU:HA	33:1b:48:MET:HE1	2.02	0.42
36:1e:79:GLU:H	36:1e:79:GLU:CD	2.27	0.42
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	2.02	0.42
48:1q:22:LEU:HD13	48:1q:41:LYS:HG2	2.01	0.42
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.51	0.42
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.54	0.42
1:2A:2136:C:H2'	1:2A:2137:C:H6	1.85	0.42
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.84	0.42
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.19	0.42
8:2I:102:SER:HB2	8:2I:108:THR:HG22	2.01	0.42
16:2U:5:LYS:NZ	61:2U:301:HOH:O	2.52	0.42
32:2a:977:A:O2'	32:2a:979:C:OP2	2.30	0.42
32:2a:1306:A:H1'	32:2a:1332:A:C2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:184:TYR:HA	34:2c:200:ALA:O	2.20	0.42
42:2k:89:ALA:O	42:2k:91:ARG:N	2.46	0.42
44:2m:74:VAL:O	44:2m:78:ILE:HG12	2.19	0.42
51:2t:53:LEU:O	51:2t:57:ARG:HG3	2.19	0.42
1:1A:118:A:C8	1:1A:119:A:C8	3.08	0.42
1:1A:271(M):G:O2'	1:1A:271(N):U:H5"	2.20	0.42
2:1B:91:C:OP1	12:1Q:16:ARG:NH1	2.52	0.42
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.01	0.42
6:1G:61:ALA:O	26:14:7:PRO:HG2	2.20	0.42
6:1G:161:THR:HG22	6:1G:163:ALA:N	2.24	0.42
10:1O:34:THR:OG1	10:1O:69:ILE:HD11	2.20	0.42
32:1a:114:U:H1'	32:1a:353:A:H1'	2.02	0.42
32:1a:177:C:OP1	51:1t:65:LYS:NZ	2.41	0.42
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.54	0.42
32:1a:1109:C:OP2	34:1c:176:HIS:ND1	2.53	0.42
32:1a:1148:U:O3'	40:1i:14:VAL:HG11	2.20	0.42
32:1a:1412:C:H2'	32:1a:1413:A:H8	1.83	0.42
36:1e:99:GLY:O	36:1e:117:ASP:HA	2.20	0.42
39:1h:6:ILE:O	39:1h:10:LEU:HG	2.19	0.42
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.35	0.42
42:1k:97:ALA:O	42:1k:101:SER:HB3	2.20	0.42
1:2A:391:G:H1'	1:2A:411:G:O4'	2.20	0.42
1:2A:531:C:H4'	1:2A:532:A:H5"	2.02	0.42
1:2A:724:U:H2'	1:2A:725:G:O4'	2.19	0.42
1:2A:889:C:O2'	1:2A:890:A:O5'	2.35	0.42
1:2A:996:A:C2	1:2A:997:G:C8	3.07	0.42
1:2A:1087:G:H1	1:2A:1102:C:H42	1.67	0.42
1:2A:2122:U:O2	1:2A:2176:A:N1	2.53	0.42
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.85	0.42
1:2A:2768:C:H2'	1:2A:2769:C:O4'	2.20	0.42
4:2E:70:ALA:O	4:2E:72:VAL:N	2.53	0.42
6:2G:139:LEU:H	6:2G:139:LEU:HG	1.59	0.42
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.55	0.42
32:2a:551:U:H2'	32:2a:552:U:C6	2.55	0.42
32:2a:1053:G:O2'	32:2a:1199:U:H5	2.03	0.42
32:2a:1124:G:H4'	32:2a:1125:U:OP1	2.20	0.42
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	2.01	0.42
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	2.02	0.42
44:2m:3:ARG:HD3	44:2m:9:ILE:H	1.85	0.42
51:2t:57:ARG:HH12	51:2t:100:ILE:HB	1.85	0.42
1:1A:829:A:N7	1:1A:2248:C:H5'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.53	0.42
6:1G:155:MET:HE2	6:1G:155:MET:HB3	1.86	0.42
7:1H:41:MET:HE2	7:1H:65:HIS:HA	2.02	0.42
8:1I:87:LYS:H	8:1I:87:LYS:CD	2.32	0.42
11:1P:94:GLU:HG3	11:1P:124:LYS:HD3	2.02	0.42
28:16:14:THR:HG21	28:16:48:VAL:HG13	2.02	0.42
32:1a:69:G:H2'	32:1a:70:G:C8	2.55	0.42
32:1a:77:G:C2'	32:1a:78:G:H5'	2.50	0.42
32:1a:181:G:H4'	32:1a:182:U:H5'	2.01	0.42
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.02	0.42
36:1e:80:ILE:HG13	36:1e:81:GLU:N	2.35	0.42
39:1h:87:SER:HB2	39:1h:93:VAL:HB	2.02	0.42
40:1i:111:ARG:HG2	40:1i:112:LYS:N	2.34	0.42
1:2A:784:A:C8	1:2A:792:G:C5	3.08	0.42
1:2A:886:C:H1'	1:2A:890:A:H61	1.85	0.42
1:2A:919:G:N2	1:2A:2269:A:OP2	2.53	0.42
1:2A:1195:G:O2'	1:2A:1226:A:N1	2.46	0.42
1:2A:2107:C:H5'	1:2A:2108:C:OP2	2.20	0.42
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.01	0.42
9:2N:131:GLN:C	9:2N:133:GLN:H	2.27	0.42
24:22:51:ARG:O	24:22:55:ARG:HD2	2.20	0.42
32:2a:118:U:H3'	32:2a:288:A:H61	1.85	0.42
32:2a:1130:A:H5'	40:2i:18:PHE:CE2	2.54	0.42
32:2a:1307:U:H2'	32:2a:1308:U:C6	2.55	0.42
35:2d:79:PHE:CE1	35:2d:204:ILE:HD13	2.55	0.42
37:2f:68:PRO:HG2	37:2f:71:ARG:NH1	2.35	0.42
1:1A:191:A:H2'	1:1A:192:C:C6	2.55	0.41
1:1A:226:G:N2	1:1A:228:A:H62	2.18	0.41
1:1A:278:A:H2'	1:1A:279:C:C6	2.55	0.41
1:1A:1020:A:N1	1:1A:1141:U:O2'	2.48	0.41
1:1A:1055:G:N1	1:1A:1104:C:C2	2.89	0.41
1:1A:2056:G:OP1	61:1A:4155:HOH:O	2.20	0.41
1:1A:2155:G:H2'	1:1A:2156:G:O4'	2.19	0.41
7:1H:126:PRO:HB2	7:1H:130:ARG:HH21	1.84	0.41
13:1R:33:ARG:NH1	13:1R:115:GLU:OE1	2.40	0.41
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.19	0.41
32:1a:1024:G:H2'	32:1a:1024:G:N3	2.34	0.41
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	2.01	0.41
1:2A:1049:C:O2	1:2A:1113:U:H4'	2.20	0.41
1:2A:1057:A:N3	1:2A:1057:A:H2'	2.35	0.41
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.81	0.41
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.34	0.41
24:22:35:LEU:HD21	24:22:49:LYS:HE3	2.02	0.41
32:2a:56:U:H2'	32:2a:57:G:C8	2.55	0.41
32:2a:57:G:H2'	32:2a:58:C:C6	2.55	0.41
32:2a:109:A:H2'	32:2a:326:G:N2	2.35	0.41
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.19	0.41
32:2a:1309:G:OP1	44:2m:88:ARG:HD3	2.20	0.41
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.35	0.41
32:2a:1499:A:H1'	32:2a:1520:G:OP1	2.20	0.41
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.84	0.41
34:2c:6:HIS:CE1	34:2c:184:TYR:CD2	3.08	0.41
47:2p:58:TYR:O	47:2p:61:SER:OG	2.30	0.41
48:2q:3:LYS:HD3	48:2q:61:GLU:O	2.20	0.41
1:1A:35:G:H2'	1:1A:36:G:O4'	2.21	0.41
1:1A:900:A:C4	1:1A:901:A:C8	3.08	0.41
1:1A:1057:A:N1	1:1A:1081:U:O4	2.53	0.41
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.31	0.41
1:1A:1656:C:O5'	1:1A:1656:C:H6	2.03	0.41
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.02	0.41
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.31	0.41
15:1T:23:ARG:HD2	15:1T:120:ARG:CZ	2.50	0.41
24:12:41:ILE:HG13	24:12:43:GLN:HG3	2.02	0.41
26:14:68:ARG:HA	26:14:68:ARG:NH2	2.35	0.41
32:1a:22:G:H2'	32:1a:23:C:H6	1.84	0.41
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.20	0.41
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.53	0.41
39:1h:4:ASP:OD1	39:1h:85:ARG:NH1	2.48	0.41
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.19	0.41
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.55	0.41
1:2A:1056:G:H4'	1:2A:1057:A:H8	1.85	0.41
1:2A:1056:G:N2	1:2A:1103:A:H62	2.18	0.41
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.35	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.55	0.41
5:2F:197:ASP:O	5:2F:201:VAL:HG13	2.20	0.41
6:2G:41:GLN:O	6:2G:43:LEU:HD22	2.19	0.41
6:2G:51:ARG:HD3	6:2G:87:PRO:HD2	2.01	0.41
12:2Q:19:GLY:O	12:2Q:98:LYS:HG2	2.21	0.41
32:2a:189:G:C6	32:2a:189(A):C:C4	3.08	0.41
32:2a:222:U:H2'	32:2a:223:U:H6	1.84	0.41
32:2a:352:C:H4'	32:2a:354:G:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:395:C:C2’	32:2a:396:G:H5’	2.50	0.41
32:2a:1003:G:H3’	32:2a:1003:G:N3	2.35	0.41
32:2a:1016:A:O2’	32:2a:1217:C:O2’	2.32	0.41
32:2a:1227:A:OP1	50:2s:80:TYR:OH	2.24	0.41
32:2a:1273:G:H3’	32:2a:1274:G:H8	1.84	0.41
33:2b:71:VAL:HG12	33:2b:93:VAL:CG2	2.50	0.41
34:2c:181:ASN:ND2	34:2c:204:LEU:HD13	2.34	0.41
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.93	0.41
53:2y:33:HIS:ND1	53:2y:35:ILE:HG12	2.34	0.41
1:1A:271(P):C:H2’	1:1A:271(Q):G:O4’	2.20	0.41
1:1A:644:A:H4’	1:1A:645:C:H5	1.84	0.41
1:1A:2094:G:P	8:1I:22:LYS:HD2	2.60	0.41
1:1A:2185:C:H2’	1:1A:2186:G:O4’	2.19	0.41
13:1R:79:LEU:HA	13:1R:83:ILE:HB	2.03	0.41
32:1a:865:A:C2	32:1a:918:A:H4’	2.56	0.41
32:1a:942:G:N2	40:1i:124:GLN:OE1	2.34	0.41
32:1a:1001:A:H2’	32:1a:1001(A):G:H8	1.83	0.41
32:1a:1005:A:H5”	32:1a:1006:C:OP2	2.19	0.41
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.32	0.41
32:1a:1513:A:H2’	32:1a:1514:C:C6	2.55	0.41
34:1c:134:ILE:HG23	34:1c:151:VAL:HB	2.03	0.41
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	2.01	0.41
39:1h:73:ASP:OD1	39:1h:75:ARG:HG3	2.21	0.41
40:1i:29:ASN:OD1	40:1i:65:VAL:N	2.53	0.41
43:1l:28:LYS:HG3	43:1l:62:SER:HB2	2.01	0.41
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	2.03	0.41
50:1s:3:ARG:NH2	50:1s:7:LYS:HE2	2.35	0.41
1:2A:740:U:H2’	1:2A:741:G:C8	2.55	0.41
1:2A:1050:A:H2’	1:2A:1051:G:H8	1.84	0.41
1:2A:1072:C:H5”	1:2A:1073:A:O5’	2.20	0.41
1:2A:2028:U:H2’	1:2A:2029:G:O4’	2.21	0.41
2:2B:95:C:H2’	2:2B:96:U:C6	2.54	0.41
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.35	0.41
6:2G:83:ARG:O	6:2G:86:MET:HB2	2.20	0.41
7:2H:88:LEU:HD22	7:2H:165:ALA:HA	2.01	0.41
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.55	0.41
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	2.03	0.41
32:2a:41:G:H2’	32:2a:42:G:H8	1.84	0.41
32:2a:1110:A:N6	32:2a:1111:A:N1	2.68	0.41
35:2d:50:ARG:HA	35:2d:51:PRO:HD3	1.87	0.41
50:2s:81:ARG:HH11	50:2s:81:ARG:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2y:41:LEU:HD23	53:2y:41:LEU:HA	1.82	0.41
1:1A:383:U:O2'	61:1A:4168:HOH:O	2.22	0.41
1:1A:1912:A:O2'	32:1a:1494:G:O2'	2.33	0.41
1:1A:2115:G:N3	1:1A:2117:A:N6	2.63	0.41
1:1A:2168:G:C2	1:1A:2171:A:C8	3.08	0.41
1:1A:2292:C:H2'	1:1A:2293:C:C6	2.55	0.41
2:1B:11:C:H3'	2:1B:12:C:C6	2.56	0.41
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.89	0.41
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.53	0.41
32:1a:1136:U:H5"	32:1a:1137:C:C2	2.56	0.41
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.02	0.41
34:1c:135:LYS:HE2	36:1e:53:LEU:HD11	2.03	0.41
43:1l:8:ASN:O	43:1l:12:ARG:HG3	2.20	0.41
43:1l:82:VAL:O	43:1l:106:ASP:HB2	2.20	0.41
43:1l:101:VAL:O	43:1l:104:VAL:HG22	2.20	0.41
53:1y:70:MET:HE2	53:1y:70:MET:HB3	1.98	0.41
1:2A:622:G:OP2	11:2P:108:LYS:NZ	2.30	0.41
1:2A:990:A:OP2	61:2A:3810:HOH:O	2.22	0.41
1:2A:1062:G:H1	1:2A:1088:A:H8	1.64	0.41
1:2A:2811:G:OP1	4:2E:60:ASN:HB2	2.20	0.41
3:2D:34:VAL:HA	3:2D:62:TYR:O	2.20	0.41
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	2.03	0.41
18:2W:41:LYS:HE3	27:25:25:LEU:HD11	2.02	0.41
32:2a:130:A:C8	48:2q:63:ARG:HG3	2.55	0.41
32:2a:786:G:C2	32:2a:797:C:C2	3.09	0.41
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.86	0.41
32:2a:1289:A:N1	32:2a:1371:G:O2'	2.47	0.41
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	2.02	0.41
44:2m:103:THR:O	44:2m:103:THR:OG1	2.34	0.41
46:2o:65:ARG:HG2	46:2o:68:ARG:HH21	1.84	0.41
1:1A:335:C:H2'	1:1A:336:C:H6	1.86	0.41
1:1A:2096:U:H2'	1:1A:2097:C:H6	1.83	0.41
12:1Q:98:LYS:NZ	61:1Q:303:HOH:O	2.49	0.41
12:1Q:111:GLU:OE1	12:1Q:133:ARG:NH2	2.53	0.41
14:1S:47:THR:N	61:1S:7006:HOH:O	2.54	0.41
32:1a:17:U:H1'	32:1a:1080:A:N3	2.35	0.41
32:1a:616:G:O2'	32:1a:617:G:H5'	2.20	0.41
32:1a:981:U:H2'	32:1a:982:U:C5	2.55	0.41
32:1a:1003:G:C2	32:1a:1004:A:N3	2.89	0.41
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.01	0.41
32:1a:1227:A:C8	44:1m:117:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.56	0.41
40:1i:29:ASN:ND2	40:1i:65:VAL:HG12	2.35	0.41
42:1k:109:VAL:HG22	49:1r:86:VAL:HG22	2.01	0.41
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.54	0.41
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.85	0.41
1:2A:1359:A:N1	1:2A:1372:U:O4	2.53	0.41
1:2A:2098:U:H2'	1:2A:2099:U:O4'	2.20	0.41
1:2A:2134:A:O2'	1:2A:2159:G:H1'	2.21	0.41
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.21	0.41
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	2.02	0.41
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.35	0.41
26:24:13:ARG:NH1	26:24:23:GLU:HG2	2.31	0.41
26:24:45:GLY:C	26:24:47:GLN:H	2.29	0.41
29:27:24:THR:HG22	29:27:27:GLY:N	2.18	0.41
32:2a:413:G:N7	35:2d:35:ARG:NH1	2.68	0.41
32:2a:663:A:H5"	49:2r:61:LYS:HE3	2.03	0.41
32:2a:869:G:H4'	32:2a:872:A:C8	2.56	0.41
32:2a:979:C:H2'	32:2a:980:C:H5'	2.03	0.41
34:2c:155:GLY:HA3	34:2c:196:LEU:HD22	2.03	0.41
39:2h:51:VAL:HG21	39:2h:60:ARG:HH11	1.86	0.41
40:2i:54:ASP:C	40:2i:56:LEU:H	2.28	0.41
41:2j:81:THR:O	41:2j:85:LEU:HG	2.21	0.41
1:1A:271(L):U:P	8:1I:50:ARG:HH22	2.42	0.41
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.86	0.41
1:1A:1098:A:H2'	1:1A:1099:G:O4'	2.20	0.41
1:1A:1371:G:H2'	1:1A:1372:U:C5	2.53	0.41
1:1A:2177:C:H2'	1:1A:2178:C:O4'	2.21	0.41
1:1A:2365:G:N7	30:18:39:LYS:NZ	2.49	0.41
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	2.02	0.41
5:1F:27:GLU:O	5:1F:112:MET:HE2	2.19	0.41
8:1I:5:LEU:HD12	8:1I:36:ALA:HB2	2.02	0.41
32:1a:973:G:OP1	41:1j:57:LYS:NZ	2.52	0.41
32:1a:1025:U:H2'	32:1a:1026:G:H5"	2.03	0.41
35:1d:162:LEU:HD22	35:1d:178:VAL:HG13	2.02	0.41
38:1g:104:LEU:HD13	38:1g:104:LEU:HA	1.86	0.41
40:1i:50:LEU:HD22	40:1i:55:ALA:O	2.21	0.41
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	2.01	0.41
46:1o:84:LYS:O	46:1o:84:LYS:HG3	2.21	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.41
1:2A:200:U:O2	1:2A:386:G:N2	2.54	0.41
1:2A:2115:G:N2	1:2A:2119:A:H5'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2186:G:N2	1:2A:2187:G:C5	2.88	0.41
1:2A:2751:G:H3'	1:2A:2752:C:H6	1.86	0.41
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.20	0.41
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.48	0.41
26:24:1:MET:HG2	26:24:6:HIS:NE2	2.35	0.41
32:2a:448:A:P	32:2a:485:G:H22	2.43	0.41
32:2a:971:G:N2	32:2a:1363(A):A:OP2	2.47	0.41
32:2a:1317:C:OP1	45:2n:17:LYS:HG2	2.21	0.41
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.21	0.41
38:2g:26:PHE:O	38:2g:30:ILE:HG13	2.21	0.41
44:2m:60:VAL:HG23	44:2m:64:TRP:CZ3	2.55	0.41
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.60	0.41
47:2p:1:MET:HE2	47:2p:1:MET:H3	1.85	0.41
53:2y:48:PHE:CG	53:2y:70:MET:HB3	2.55	0.41
1:1A:824:A:H1'	1:1A:2358:G:N7	2.35	0.41
1:1A:1166:C:H2'	1:1A:1167:U:H6	1.84	0.41
1:1A:1328:G:O2'	1:1A:1329:U:H2'	2.21	0.41
1:1A:2287:A:C8	1:1A:2289:G:C8	3.08	0.41
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.20	0.41
1:1A:2584:U:H2'	1:1A:2585:U:H2'	2.02	0.41
2:1B:23:G:O6	61:1B:305:HOH:O	2.21	0.41
2:1B:66:A:N6	2:1B:108:U:H2'	2.36	0.41
5:1F:41:LEU:O	5:1F:44:ARG:HG2	2.21	0.41
8:1I:77:LEU:HA	8:1I:77:LEU:HD12	1.78	0.41
11:1P:2:LYS:HE3	11:1P:2:LYS:HB2	1.95	0.41
12:1Q:17:LEU:HA	12:1Q:17:LEU:HD23	1.82	0.41
20:1Y:81:LYS:HE2	20:1Y:81:LYS:HB3	1.83	0.41
30:18:50:LEU:HD23	30:18:50:LEU:HA	1.85	0.41
32:1a:123:C:O2'	32:1a:290:C:O2	2.35	0.41
32:1a:461:A:O2'	32:1a:470:C:H5'	2.21	0.41
33:1b:187:LEU:HD12	33:1b:201:ILE:O	2.21	0.41
46:1o:24:SER:O	46:1o:28:GLN:HG3	2.20	0.41
53:1y:61:LEU:HD11	53:1y:85:LEU:HD13	2.03	0.41
1:2A:851:U:H5'	25:23:49:LYS:HD2	2.02	0.41
1:2A:1007:C:OP1	9:2N:37:LYS:NZ	2.51	0.41
1:2A:1139:G:H5"	9:2N:70:LYS:NZ	2.36	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.08	0.41
1:2A:1772:G:O6	57:2A:3732:MPD:H32	2.21	0.41
1:2A:2187:G:N7	1:2A:2188:C:C4	2.89	0.41
1:2A:2544:G:H2'	1:2A:2545:G:O4'	2.20	0.41
1:2A:2601:C:H5"	1:2A:2602:A:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.55	0.41
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.35	0.41
9:2N:47:ALA:HB2	9:2N:112:LEU:HD11	2.01	0.41
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.20	0.41
19:2X:35:THR:HG22	19:2X:37:THR:H	1.86	0.41
32:2a:131:C:H2'	32:2a:132:C:C6	2.55	0.41
32:2a:187:C:H2'	32:2a:188:C:C6	2.55	0.41
32:2a:782:A:O3'	32:2a:1515:C:H4'	2.21	0.41
32:2a:1058:G:H2'	32:2a:1059:C:O4'	2.20	0.41
33:2b:97:TRP:CH2	33:2b:173:ALA:HA	2.56	0.41
38:2g:78:ARG:HE	38:2g:80:VAL:HG21	1.86	0.41
38:2g:137:LYS:O	38:2g:141:VAL:HG23	2.21	0.41
42:2k:116:HIS:N	42:2k:117:ASN:HA	2.36	0.41
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.21	0.41
53:2y:53:THR:HA	53:2y:61:LEU:O	2.20	0.41
1:1A:13:A:N1	1:1A:525:U:H2'	2.36	0.41
1:1A:2206:G:H2'	1:1A:2207:G:C2	2.55	0.41
1:1A:2791:C:OP2	1:1A:2791:C:H6	2.03	0.41
1:1A:2864:G:H2'	1:1A:2865:U:C6	2.56	0.41
4:1E:1:MET:HE1	4:1E:200:GLU:O	2.20	0.41
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.02	0.41
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.92	0.41
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.20	0.41
24:12:36:ARG:HD3	61:12:106:HOH:O	2.21	0.41
24:12:48:HIS:CE1	24:12:49:LYS:HG3	2.56	0.41
32:1a:865:A:H2'	32:1a:866:C:C6	2.56	0.41
33:1b:160:ASP:O	33:1b:183:PRO:HD2	2.20	0.41
38:1g:68:ASN:O	38:1g:138:LYS:HD2	2.20	0.41
40:1i:4:TYR:O	40:1i:19:LEU:N	2.52	0.41
51:1t:101:GLY:HA2	51:1t:102:GLY:HA2	1.90	0.41
1:2A:185:U:H4'	1:2A:218:A:H4'	2.03	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.36	0.41
1:2A:578:A:OP1	1:2A:1255:U:O2'	2.35	0.41
1:2A:1073:A:C8	1:2A:1073:A:H3'	2.56	0.41
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.02	0.41
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.03	0.41
1:2A:2395:C:O2'	23:21:30:VAL:HG23	2.21	0.41
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.47	0.41
1:2A:2660:A:H2'	1:2A:2661:G:O4'	2.20	0.41
2:2B:80:U:H2'	2:2B:81:G:C8	2.55	0.41
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:56:PRO:C	4:2E:58:ARG:H	2.28	0.41
6:2G:5:VAL:HG22	6:2G:8:LYS:H	1.85	0.41
7:2H:83:TYR:O	7:2H:134:SER:HA	2.19	0.41
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	2.02	0.41
20:2Y:55:TYR:CZ	20:2Y:61:ILE:HG21	2.55	0.41
25:23:3:ARG:HE	25:23:3:ARG:HB2	1.67	0.41
30:28:50:LEU:HD23	30:28:50:LEU:HA	1.70	0.41
32:2a:685:G:O2'	32:2a:686:U:H5'	2.21	0.41
53:2y:76:GLU:HA	53:2y:79:ASN:ND2	2.36	0.41
1:1A:181:A:H5"	29:17:36:GLN:NE2	2.36	0.41
1:1A:536:A:H2'	1:1A:537:C:C6	2.56	0.41
1:1A:879:G:H2'	1:1A:880:G:O4'	2.21	0.41
1:1A:1064:C:N4	1:1A:1065:U:C2	2.89	0.41
1:1A:1358:G:O2'	1:1A:1359:A:H5"	2.20	0.41
1:1A:1578:U:C2'	1:1A:1579:A:H5'	2.50	0.41
1:1A:1652:A:O2'	1:1A:1653:G:H5'	2.21	0.41
1:1A:1904:G:O2'	1:1A:1928:A:N1	2.52	0.41
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.56	0.41
1:1A:2682:U:O2'	15:1T:58:ASN:ND2	2.54	0.41
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.19	0.41
2:1B:30:C:H2'	2:1B:31:C:H5'	2.02	0.41
4:1E:52:LEU:HD12	4:1E:77:ILE:HD11	2.02	0.41
5:1F:12:LEU:HD12	5:1F:12:LEU:HA	1.83	0.41
6:1G:83:ARG:H	6:1G:86:MET:CE	2.31	0.41
7:1H:7:LEU:HD12	7:1H:8:PRO:CD	2.50	0.41
12:1Q:55:VAL:HG12	12:1Q:64:ILE:HD12	2.03	0.41
12:1Q:97:VAL:HG11	12:1Q:103:MET:HE3	2.03	0.41
13:1R:28:LEU:HD23	13:1R:48:VAL:HG11	2.03	0.41
16:1U:11:ARG:O	16:1U:15:LYS:HG3	2.21	0.41
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.21	0.41
20:1Y:87:LYS:HB3	20:1Y:95:LYS:HD2	2.03	0.41
21:1Z:183:LEU:HD23	21:1Z:183:LEU:HA	1.90	0.41
26:14:56:VAL:HB	26:14:60:GLN:NE2	2.34	0.41
27:15:33:CYS:HB2	27:15:40:LYS:HD3	2.03	0.41
30:18:11:LYS:O	61:18:201:HOH:O	2.22	0.41
32:1a:265:G:H5'	48:1q:64:PRO:O	2.20	0.41
32:1a:412:A:OP2	35:1d:35:ARG:NH2	2.50	0.41
32:1a:509:A:O2'	32:1a:510:A:OP1	2.36	0.41
32:1a:615:C:C2	32:1a:616:G:C8	3.09	0.41
32:1a:972:C:OP1	61:1a:1913:HOH:O	2.21	0.41
32:1a:1003:G:O2'	32:1a:1004:A:H4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.86	0.41
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.52	0.41
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.21	0.41
32:1a:1343:G:O2'	40:1i:121:ARG:HD2	2.20	0.41
32:1a:1376:U:P	38:1g:94:ARG:HH12	2.44	0.41
36:1e:121:LYS:HA	36:1e:121:LYS:HD2	1.91	0.41
40:1i:22:GLY:HA3	40:1i:60:ASP:OD2	2.20	0.41
43:1l:47:LYS:HA	43:1l:48:PRO:HA	1.82	0.41
48:1q:10:VAL:HG13	48:1q:19:VAL:HB	2.03	0.41
53:1y:85:LEU:O	53:1y:89:GLN:HG2	2.21	0.41
1:2A:195:A:H2'	1:2A:198:C:N4	2.35	0.41
1:2A:491:G:H2'	1:2A:492:A:C8	2.56	0.41
1:2A:554:U:C4	1:2A:555:U:C4	3.09	0.41
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.35	0.41
1:2A:882:G:H1	1:2A:894:C:N4	2.19	0.41
1:2A:1024:G:O2'	1:2A:1144:G:O2'	2.37	0.41
1:2A:2063:C:OP1	61:2A:3860:HOH:O	2.22	0.41
1:2A:2352:A:OP2	61:2A:3857:HOH:O	2.21	0.41
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.56	0.41
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	2.03	0.41
56:2A:3731:ZIT:H8	56:2A:3731:ZIT:H213	1.84	0.41
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.56	0.41
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.26	0.41
4:2E:108:SER:O	4:2E:162:ALA:HA	2.21	0.41
5:2F:178:PRO:HG2	5:2F:179:GLU:OE2	2.21	0.41
7:2H:126:PRO:HB2	7:2H:127:GLU:H	1.76	0.41
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.21	0.41
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.21	0.41
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.21	0.41
17:2V:1:MET:HE1	17:2V:44:LYS:H	1.85	0.41
21:2Z:3:TYR:CG	21:2Z:51:ALA:HB2	2.56	0.41
21:2Z:91:LEU:HA	21:2Z:91:LEU:HD12	1.81	0.41
26:24:1:MET:HE2	26:24:6:HIS:ND1	2.36	0.41
26:24:50:VAL:HG12	44:2m:65:LYS:HD3	2.03	0.41
32:2a:137:C:H2'	32:2a:138:G:C8	2.56	0.41
32:2a:662:G:O2'	32:2a:836:G:OP1	2.39	0.41
32:2a:689:C:H2'	32:2a:690:G:O4'	2.20	0.41
32:2a:826:C:H4'	39:2h:12:ARG:HG2	2.03	0.41
32:2a:838:G:C2	32:2a:849:C:C2	3.09	0.41
32:2a:980:C:H3'	32:2a:981:U:C6	2.56	0.41
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.44	0.41
33:2b:70:PHE:CD1	33:2b:163:PHE:HB3	2.56	0.41
34:2c:21:ARG:HE	34:2c:21:ARG:HB2	1.62	0.41
35:2d:11:LEU:HD23	35:2d:66:ARG:HG2	2.03	0.41
36:2e:76:ILE:HD12	36:2e:142:LEU:HD21	2.03	0.41
38:2g:33:ASP:OD1	38:2g:33:ASP:N	2.54	0.41
42:2k:20:TYR:CE1	42:2k:83:ILE:HD12	2.56	0.41
46:2o:35:ARG:NH2	46:2o:59:MET:HE2	2.35	0.41
1:1A:566:U:H5"	11:1P:29:LYS:HE3	2.03	0.41
1:1A:582:G:H2'	1:1A:583:G:C8	2.56	0.41
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.36	0.41
1:1A:883:G:C6	1:1A:884:C:C4	3.08	0.41
1:1A:2030:A:H4'	1:1A:2031:A:C8	2.56	0.41
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.21	0.41
6:1G:43:LEU:O	6:1G:45:GLU:HG2	2.20	0.41
11:1P:71:VAL:HG22	11:1P:72:PRO:HA	2.02	0.41
17:1V:101:GLY:HA3	61:1V:331:HOH:O	2.21	0.41
32:1a:691:G:H2'	32:1a:692:U:C6	2.56	0.41
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.21	0.41
1:2A:1341:U:OP1	1:2A:1397:U:N3	2.45	0.41
1:2A:2126:A:N1	1:2A:2162:G:O2'	2.50	0.41
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.21	0.41
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.38	0.41
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.46	0.41
6:2G:55:LYS:HA	6:2G:58:GLN:HB3	2.03	0.41
17:2V:74:LYS:HB2	17:2V:83:ARG:HB2	2.03	0.41
23:21:51:VAL:N	23:21:58:ILE:O	2.46	0.41
27:25:16:ARG:HG2	27:25:16:ARG:HH11	1.84	0.41
32:2a:471:G:H2'	32:2a:472:A:H8	1.86	0.41
32:2a:573:A:OP2	61:2a:3207:HOH:O	2.21	0.41
32:2a:841:U:H6	32:2a:841:U:P	2.43	0.41
32:2a:978:A:OP1	32:2a:1361:G:N2	2.51	0.41
32:2a:1009:G:H2'	32:2a:1009:G:N3	2.36	0.41
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.53	0.41
38:2g:108:ALA:O	38:2g:119:ARG:HD2	2.20	0.41
38:2g:114:ARG:HB2	38:2g:115:ARG:CZ	2.51	0.41
42:2k:99:GLN:HE21	42:2k:105:VAL:HG21	1.86	0.41
44:2m:23:TYR:CE2	44:2m:70:LEU:HD22	2.56	0.41
1:1A:45:C:OP2	1:1A:215:G:H2'	2.21	0.40
1:1A:569:U:C4	1:1A:570:G:C6	3.09	0.40
1:1A:839:U:H2'	1:1A:840:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1176:G:H4'	1:1A:1177:A:OP1	2.21	0.40
1:1A:1501:C:O4'	3:1D:100:GLY:HA2	2.21	0.40
1:1A:2704:C:H2'	1:1A:2705:A:O4'	2.21	0.40
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.21	0.40
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.56	0.40
26:14:24:THR:OG1	26:14:25:TYR:N	2.54	0.40
32:1a:115:G:H4'	32:1a:116:A:O5'	2.21	0.40
32:1a:737:A:H5'	37:1f:90:VAL:O	2.20	0.40
32:1a:926:G:O6	53:1y:87:LYS:HE2	2.21	0.40
32:1a:1026:G:H5'	32:1a:1027:C:C5	2.43	0.40
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.36	0.40
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.20	0.40
47:1p:40:ASP:HB3	47:1p:48:TRP:CB	2.50	0.40
50:1s:12:ASP:HB3	50:1s:14:HIS:CD2	2.56	0.40
1:2A:208:C:H2'	1:2A:209:C:C6	2.56	0.40
1:2A:975(A):G:H1'	1:2A:990:A:C2	2.55	0.40
1:2A:1027:A:C6	1:2A:1126:A:C4	3.10	0.40
1:2A:1063:G:O2'	1:2A:1064:C:H5"	2.21	0.40
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.57	0.40
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.20	0.40
1:2A:2102:U:OP2	61:2A:3862:HOH:O	2.22	0.40
1:2A:2119:A:C2	1:2A:2171:A:H5'	2.56	0.40
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.46	0.40
1:2A:2544:G:H1'	1:2A:2646:C:H4'	2.03	0.40
4:2E:16:ARG:O	4:2E:19:ARG:HB2	2.21	0.40
4:2E:28:ALA:HB3	4:2E:93:VAL:CG1	2.51	0.40
5:2F:32:LEU:HB3	5:2F:112:MET:HE1	2.02	0.40
8:2I:21:VAL:HG21	8:2I:26:ALA:HB2	2.03	0.40
11:2P:59:LEU:HD22	11:2P:60:MET:HE2	2.03	0.40
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.54	0.40
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	2.03	0.40
21:2Z:73:GLN:H	21:2Z:87:ASP:HB2	1.85	0.40
32:2a:309:G:H2'	32:2a:310:G:H8	1.87	0.40
32:2a:396:G:O2'	32:2a:398:C:OP1	2.35	0.40
32:2a:1103:C:H5'	33:2b:98:LEU:HD22	2.03	0.40
32:2a:1267:C:O2	52:2u:20:LYS:HD3	2.20	0.40
32:2a:1329:A:P	44:2m:28:ALA:HB3	2.61	0.40
33:2b:83:MET:HE2	33:2b:83:MET:HB3	1.70	0.40
33:2b:178:ARG:HA	33:2b:178:ARG:HD2	1.77	0.40
34:2c:77:ILE:HG23	34:2c:103:VAL:HG21	2.03	0.40
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:6:PHE:HB2	36:2e:63:ARG:HH12	1.86	0.40
36:2e:143:ARG:HD2	39:2h:77:GLU:OE2	2.22	0.40
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.51	0.40
1:1A:414:C:H4'	1:1A:1879:C:O2	2.21	0.40
1:1A:649:G:H2'	1:1A:650:C:C6	2.55	0.40
1:1A:708:C:H2'	1:1A:709:U:C6	2.56	0.40
1:1A:875:G:H2'	1:1A:876:C:O4'	2.21	0.40
1:1A:2106:G:C4	1:1A:2107:C:H1'	2.55	0.40
1:1A:2186:G:C2	1:1A:2187:G:C8	3.09	0.40
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.36	0.40
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	2.03	0.40
14:1S:58:LEU:HA	14:1S:58:LEU:HD23	1.65	0.40
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.86	0.40
32:1a:603:U:H2'	32:1a:604:G:C8	2.56	0.40
32:1a:1002:G:C6	32:1a:1003:G:C2	3.09	0.40
32:1a:1071:C:H2'	32:1a:1072:G:C8	2.56	0.40
36:1e:94:ALA:HB3	36:1e:117:ASP:C	2.46	0.40
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.21	0.40
51:1t:74:LYS:HB3	51:1t:74:LYS:HE2	1.96	0.40
1:2A:127:A:H5"	1:2A:128:C:C6	2.56	0.40
1:2A:827:U:O2'	1:2A:2068:U:C2	2.69	0.40
1:2A:1741:A:H2'	1:2A:1742:G:O4'	2.21	0.40
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.21	0.40
1:2A:2839:G:C5'	13:2R:46:GLY:HA2	2.51	0.40
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	2.04	0.40
12:2Q:39:PRO:HA	12:2Q:97:VAL:O	2.21	0.40
17:2V:14:VAL:HB	17:2V:96:ILE:HG13	2.03	0.40
17:2V:40:LEU:HB2	17:2V:46:VAL:CG1	2.51	0.40
26:24:13:ARG:HA	26:24:22:ILE:O	2.21	0.40
26:24:14:ILE:HB	26:24:22:ILE:HB	2.03	0.40
32:2a:580:U:H5"	46:2o:58:MET:HG2	2.03	0.40
32:2a:1049:U:OP1	45:2n:3:ARG:HB2	2.21	0.40
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.55	0.40
45:2n:13:THR:HG22	45:2n:14:PRO:HD2	2.02	0.40
50:2s:22:LEU:HD13	50:2s:28:LYS:N	2.33	0.40
51:2t:33:ILE:O	51:2t:37:SER:OG	2.28	0.40
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.21	0.40
11:1P:6:LEU:HD23	11:1P:6:LEU:HA	1.81	0.40
26:14:63:TYR:HA	26:14:64:GLY:HA2	1.83	0.40
29:17:35:ARG:NH1	61:17:202:HOH:O	2.54	0.40
32:1a:335:C:H2'	32:1a:336:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:764:C:H2'	32:1a:765:G:O4'	2.21	0.40
32:1a:1015:A:O3'	45:1n:15:LYS:NZ	2.54	0.40
32:1a:1227:A:OP1	50:1s:80:TYR:OH	2.20	0.40
32:1a:1457:G:H2'	32:1a:1458:G:C8	2.57	0.40
1:2A:30:G:H2'	1:2A:31:C:C6	2.55	0.40
1:2A:249:C:O2	30:28:12:LYS:NZ	2.38	0.40
1:2A:855:G:C5	1:2A:856:C:C4	3.09	0.40
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.36	0.40
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.56	0.40
1:2A:1569:A:H2'	1:2A:1570:A:C8	2.57	0.40
1:2A:1588:C:H2'	1:2A:1589:C:C6	2.57	0.40
1:2A:2019:A:O4'	16:2U:34:LYS:HE2	2.22	0.40
1:2A:2021:C:OP1	27:25:12:SER:OG	2.34	0.40
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.22	0.40
1:2A:2131:G:H5'	1:2A:2133:G:O5'	2.22	0.40
6:2G:165:THR:OG1	6:2G:168:GLU:HG3	2.21	0.40
16:2U:27:LEU:HB3	16:2U:31:SER:HB3	2.03	0.40
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.57	0.40
24:22:62:THR:O	24:22:66:GLU:HG3	2.21	0.40
32:2a:828:A:N6	32:2a:858:G:O2'	2.53	0.40
32:2a:986:A:H1'	50:2s:54:GLY:O	2.21	0.40
32:2a:1002:G:N2	32:2a:1039:C:C2	2.90	0.40
32:2a:1029:C:N4	32:2a:1030:C:H41	2.20	0.40
32:2a:1096:C:H2'	32:2a:1097:C:H6	1.86	0.40
32:2a:1310:G:H2'	32:2a:1311:G:O4'	2.21	0.40
43:2l:113:ARG:HA	43:2l:113:ARG:HD2	1.96	0.40
44:2m:37:THR:HG21	44:2m:56:LEU:HA	2.03	0.40
1:1A:300:A:P	20:1Y:86:ARG:HH22	2.44	0.40
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.04	0.40
1:1A:922:U:H2'	1:1A:923:C:C6	2.56	0.40
1:1A:2017:U:O2	27:15:10:LYS:HB2	2.21	0.40
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.21	0.40
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.56	0.40
4:1E:28:ALA:HB3	4:1E:93:VAL:HG13	2.03	0.40
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.22	0.40
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	2.03	0.40
32:1a:260:G:H2'	32:1a:261:U:C6	2.56	0.40
32:1a:325:A:H2'	32:1a:326:G:O4'	2.22	0.40
32:1a:438:G:H5'	35:1d:123:HIS:HD2	1.85	0.40
32:1a:1328:C:OP1	52:1u:21:TYR:OH	2.38	0.40
33:1b:231:GLU:HG3	33:1b:232:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.22	0.40
51:1t:67:ALA:HA	51:1t:72:LEU:O	2.21	0.40
1:2A:11:G:H2'	1:2A:12:U:H5'	2.02	0.40
1:2A:35:G:H2'	1:2A:36:G:O4'	2.22	0.40
1:2A:272:G:N7	1:2A:421:U:H2'	2.36	0.40
1:2A:422:A:H2'	1:2A:423:A:C8	2.56	0.40
1:2A:1607:C:H4'	1:2A:1608:A:O5'	2.21	0.40
1:2A:1861:G:C2	1:2A:1862:G:C8	3.09	0.40
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.22	0.40
1:2A:2570:G:H2'	1:2A:2571:C:O4'	2.21	0.40
2:2B:53:A:H2'	2:2B:54:G:O4'	2.21	0.40
7:2H:51:ARG:NH1	7:2H:51:ARG:HB2	2.36	0.40
11:2P:148:LEU:HD23	11:2P:148:LEU:HA	1.98	0.40
32:2a:513:C:H2'	32:2a:514:C:H6	1.86	0.40
32:2a:938:A:C6	32:2a:939:G:C5	3.09	0.40
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.56	0.40
32:2a:1125:U:H6	32:2a:1126:U:H2'	1.87	0.40
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.22	0.40
33:2b:51:LEU:HA	33:2b:54:THR:HB	2.03	0.40
33:2b:69:LEU:HD12	33:2b:69:LEU:HA	1.77	0.40
33:2b:215:LEU:O	33:2b:219:VAL:HG23	2.22	0.40
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	2.02	0.40
44:2m:14:ARG:HB2	44:2m:17:VAL:HG23	2.03	0.40
1:1A:559:G:H22	16:1U:49:HIS:CE1	2.40	0.40
1:1A:2142:C:O2	1:1A:2149:G:C2	2.75	0.40
2:1B:12:C:H2'	22:10:73:GLY:HA3	2.03	0.40
6:1G:110:ALA:HB1	6:1G:140:ILE:HG22	2.03	0.40
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	2.03	0.40
32:1a:7:G:O2'	36:1e:120:THR:O	2.39	0.40
32:1a:37:U:O2'	32:1a:547:A:N1	2.53	0.40
32:1a:814:A:H2'	32:1a:816:A:H5"	2.03	0.40
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.51	0.40
33:1b:172:ILE:H	33:1b:172:ILE:HG13	1.66	0.40
35:1d:32:ALA:HB3	60:1d:305:SF4:S2	2.62	0.40
35:1d:107:ARG:CZ	35:1d:194:LEU:HD21	2.51	0.40
44:1m:91:ARG:HA	44:1m:91:ARG:HD2	1.95	0.40
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.77	0.40
48:1q:67:LYS:C	48:1q:69:LYS:H	2.30	0.40
1:2A:537:C:OP1	1:2A:995:C:N4	2.53	0.40
1:2A:875:G:H5"	21:2Z:149:SER:CB	2.52	0.40
1:2A:2138:C:O2	1:2A:2153:G:N1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.64	0.40
3:2D:68:LYS:O	3:2D:69:ARG:HB2	2.21	0.40
4:2E:1:MET:HE1	4:2E:200:GLU:O	2.22	0.40
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.52	0.40
7:2H:27:LYS:HG2	7:2H:32:GLU:HB3	2.03	0.40
10:2O:19:ILE:HB	10:2O:41:ALA:HB1	2.04	0.40
26:24:53:GLU:CD	26:24:54:GLY:H	2.29	0.40
29:27:13:ALA:HB2	29:27:46:VAL:HG21	2.04	0.40
32:2a:130:A:H1'	32:2a:263:A:O2'	2.21	0.40
32:2a:671:G:H2'	32:2a:672:U:O4'	2.22	0.40
32:2a:814:A:N7	32:2a:816:A:C4	2.90	0.40
32:2a:1184:G:H2'	32:2a:1185:G:H8	1.85	0.40
33:2b:63:MET:HE2	33:2b:63:MET:HB3	2.03	0.40
40:2i:100:GLY:O	40:2i:103:THR:HG22	2.22	0.40
43:2l:32:PHE:CB	43:2l:84:LEU:HD11	2.48	0.40
47:2p:20:VAL:HG23	47:2p:34:GLU:O	2.21	0.40
53:2y:70:MET:HE3	53:2y:70:MET:HB2	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100 100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
4	1E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12 24
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12 24
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24 43
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24 43
6	1G	179/182 (98%)	165 (92%)	9 (5%)	5 (3%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	2G	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	7 13
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100 100
7	2H	171/180 (95%)	155 (91%)	15 (9%)	1 (1%)	21 38
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	18 34
8	2I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	18 34
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
10	2O	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18 34
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9 17
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100 100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100 100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100 100
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	14 27
15	1T	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	7 14
15	2T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16 31
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	94 (95%)	5 (5%)	0	100 100
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12 24
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	11 22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11 22
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100 100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
21	1Z	201/206 (98%)	189 (94%)	10 (5%)	2 (1%)	12 24
21	2Z	199/206 (97%)	179 (90%)	19 (10%)	1 (0%)	24 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100 100
22	20	75/85 (88%)	70 (93%)	5 (7%)	0	100 100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11 22
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100 100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	54 (81%)	7 (10%)	6 (9%)	0 0
26	24	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1 1
27	15	57/60 (95%)	57 (100%)	0	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
33	1b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	3 5
33	2b	229/256 (90%)	197 (86%)	23 (10%)	9 (4%)	2 3
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100 100
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12 24
35	1d	206/209 (99%)	199 (97%)	7 (3%)	0	100 100
35	2d	206/209 (99%)	192 (93%)	14 (7%)	0	100 100
36	1e	146/162 (90%)	139 (95%)	4 (3%)	3 (2%)	5 9
36	2e	146/162 (90%)	135 (92%)	9 (6%)	2 (1%)	9 17
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
38	1g	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	18 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	6 10
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16 31
40	2i	124/128 (97%)	105 (85%)	15 (12%)	4 (3%)	3 4
41	1j	95/105 (90%)	82 (86%)	8 (8%)	5 (5%)	1 1
41	2j	94/105 (90%)	76 (81%)	13 (14%)	5 (5%)	1 1
42	1k	112/129 (87%)	99 (88%)	13 (12%)	0	100 100
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6 12
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100 100
44	1m	114/126 (90%)	100 (88%)	10 (9%)	4 (4%)	3 4
44	2m	112/126 (89%)	100 (89%)	10 (9%)	2 (2%)	6 12
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5 8
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10 20
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12 24
48	2q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
49	1r	66/88 (75%)	65 (98%)	0	1 (2%)	8 16
49	2r	66/88 (75%)	58 (88%)	8 (12%)	0	100 100
50	1s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	10 20
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100 100
51	1t	94/106 (89%)	85 (90%)	9 (10%)	0	100 100
51	2t	96/106 (91%)	87 (91%)	6 (6%)	3 (3%)	3 5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100 100
53	2y	94/113 (83%)	89 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11629/12354 (94%)	10840 (93%)	689 (6%)	100 (1%)	14 27

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
6	1G	47	LYS
6	1G	50	ALA
21	1Z	53	ILE
26	14	55	ARG
33	1b	8	LYS
33	1b	22	LYS
33	1b	126	GLU
44	1m	67	GLU
44	1m	107	ALA
5	2F	130	ALA
26	24	62	ARG
33	2b	9	GLU
33	2b	17	PHE
40	2i	54	ASP
41	2j	56	HIS
51	2t	100	ILE
5	1F	130	ALA
15	1T	128	GLU
26	14	45	GLY
26	14	49	PHE
33	1b	127	ILE
40	1i	11	LYS
41	1j	55	LYS
44	1m	3	ARG
50	1s	27	GLU
4	2E	71	GLY
6	2G	124	SER
7	2H	126	PRO
8	2I	117	GLU
15	2T	127	ALA
17	2V	79	VAL
19	2X	94	GLY
26	24	49	PHE
33	2b	16	HIS
34	2c	95	THR
36	2e	97	GLY

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Mol	Chain	Res	Type
40	2i	43	ALA
41	2j	79	ARG
42	2k	89	ALA
4	1E	52	LEU
6	1G	43	LEU
19	1X	94	GLY
26	14	39	CYS
33	1b	129	GLU
36	1e	38	GLN
41	1j	77	PRO
44	1m	12	ASN
46	1o	87	ILE
11	2P	29	LYS
26	24	53	GLU
33	2b	22	LYS
34	2c	98	ASN
41	2j	29	ARG
51	2t	95	ALA
6	1G	51	ARG
23	11	3	LYS
33	1b	124	SER
41	1j	78	ASN
4	2E	52	LEU
6	2G	81	LYS
21	2Z	52	SER
26	24	45	GLY
33	2b	20	GLU
33	2b	95	GLN
33	2b	126	GLU
36	2e	96	PRO
38	2g	33	ASP
38	2g	109	ASN
41	2j	78	ASN
11	1P	29	LYS
15	1T	126	ALA
26	14	57	GLU
26	14	61	ARG
33	1b	231	GLU
38	1g	55	GLY
49	1r	27	GLY
6	2G	117	PHE
33	2b	204	ASN

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Mol	Chain	Res	Type
38	2g	53	LYS
40	2i	11	LYS
40	2i	44	VAL
44	2m	21	TYR
21	1Z	52	SER
41	1j	26	ALA
44	2m	106	ASN
46	2o	87	ILE
36	1e	77	PRO
51	2t	102	GLY
6	1G	24	GLY
48	1q	33	GLY
11	2P	122	PRO
41	2j	37	PRO
41	1j	91	PRO
33	2b	125	PRO
8	1I	71	ILE
36	1e	22	GLY
46	1o	19	PRO
14	2S	35	ILE
42	2k	90	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	199 (93%)	15 (7%)	14 29
3	2D	215/218 (99%)	197 (92%)	18 (8%)	10 22
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22 45
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22 45
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5 11
5	2F	159/166 (96%)	139 (87%)	20 (13%)	4 9
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10 22
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22 45
7	2H	143/148 (97%)	127 (89%)	16 (11%)	6 12
8	1I	111/124 (90%)	100 (90%)	11 (10%)	7 16
8	2I	108/124 (87%)	94 (87%)	14 (13%)	4 8
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 13
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12 26
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22 44
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17 36
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21 42
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26 51
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11 23
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16 34
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 20
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14 30
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8 19
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5 11
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21 42
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16 34
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15 32
16	2U	93/94 (99%)	91 (98%)	2 (2%)	45 73
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10 21
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5 12
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25 50
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45 73
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28 55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 68
20	1Y	86/91 (94%)	75 (87%)	11 (13%)	4 9
20	2Y	86/91 (94%)	80 (93%)	6 (7%)	14 29
21	1Z	169/179 (94%)	157 (93%)	12 (7%)	13 29
21	2Z	165/179 (92%)	158 (96%)	7 (4%)	26 52
22	10	61/67 (91%)	61 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	20	61/67 (91%)	58 (95%)	3 (5%)	22 45
23	11	79/83 (95%)	72 (91%)	7 (9%)	9 20
23	21	81/83 (98%)	72 (89%)	9 (11%)	6 12
24	12	65/67 (97%)	62 (95%)	3 (5%)	24 48
24	22	66/67 (98%)	56 (85%)	10 (15%)	3 5
25	13	51/52 (98%)	47 (92%)	4 (8%)	11 24
25	23	50/52 (96%)	46 (92%)	4 (8%)	11 24
26	14	58/63 (92%)	52 (90%)	6 (10%)	7 14
26	24	54/63 (86%)	48 (89%)	6 (11%)	6 12
27	15	51/52 (98%)	46 (90%)	5 (10%)	7 16
27	25	50/52 (96%)	48 (96%)	2 (4%)	28 54
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 11
28	26	50/52 (96%)	47 (94%)	3 (6%)	17 36
29	17	41/42 (98%)	35 (85%)	6 (15%)	3 6
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 10
30	18	54/55 (98%)	53 (98%)	1 (2%)	50 76
30	28	54/55 (98%)	53 (98%)	1 (2%)	50 76
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18 37
33	1b	191/220 (87%)	175 (92%)	16 (8%)	10 22
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3 6
34	1c	144/188 (77%)	134 (93%)	10 (7%)	14 30
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8 18
35	1d	171/181 (94%)	157 (92%)	14 (8%)	10 23
35	2d	172/181 (95%)	155 (90%)	17 (10%)	7 16
36	1e	114/123 (93%)	101 (89%)	13 (11%)	5 12
36	2e	114/123 (93%)	105 (92%)	9 (8%)	11 24
37	1f	85/90 (94%)	74 (87%)	11 (13%)	4 9
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6 14
38	1g	120/127 (94%)	112 (93%)	8 (7%)	15 31
38	2g	119/127 (94%)	110 (92%)	9 (8%)	12 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	1h	116/119 (98%)	107 (92%)	9 (8%)	11 24
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8 17
40	1i	91/99 (92%)	80 (88%)	11 (12%)	5 10
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5 12
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18 37
41	2j	68/92 (74%)	62 (91%)	6 (9%)	9 20
42	1k	83/99 (84%)	81 (98%)	2 (2%)	43 70
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13 28
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16 34
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13 27
44	1m	90/101 (89%)	83 (92%)	7 (8%)	11 24
44	2m	87/101 (86%)	81 (93%)	6 (7%)	14 30
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 15
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3 6
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12 25
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12 25
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3 6
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 11
48	1q	94/97 (97%)	91 (97%)	3 (3%)	34 62
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26 51
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21 43
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21 43
50	1s	68/80 (85%)	65 (96%)	3 (4%)	25 50
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5 11
51	1t	71/82 (87%)	68 (96%)	3 (4%)	26 52
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18 39
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	79 (96%)	3 (4%)	30 57
53	2y	79/98 (81%)	68 (86%)	11 (14%)	3 7
All	All	9524/10260 (93%)	8766 (92%)	758 (8%)	11 24

All (758) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	88	ARG
3	1D	94	LEU
3	1D	111	LEU
3	1D	113	VAL
3	1D	131	LEU
3	1D	140	THR
3	1D	141	VAL
3	1D	155	LEU
3	1D	173	VAL
3	1D	183	ARG
3	1D	193	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	275	LYS
4	1E	7	VAL
4	1E	9	VAL
4	1E	12	THR
4	1E	77	ILE
4	1E	89	ASP
4	1E	93	VAL
4	1E	94	GLU
4	1E	116	VAL
5	1F	12	LEU
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	110	LEU
5	1F	125	LEU
5	1F	126	VAL
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL

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Mol	Chain	Res	Type
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	79	ASN
6	1G	82	LEU
6	1G	105	LYS
6	1G	145	THR
6	1G	153	ARG
6	1G	175	LEU
7	1H	24	VAL
7	1H	71	LEU
7	1H	89	ILE
7	1H	105	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
8	1I	5	LEU
8	1I	9	LEU
8	1I	35	LEU
8	1I	38	LEU
8	1I	41	GLU
8	1I	44	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	109	ILE
8	1I	120	ILE
8	1I	127	VAL
9	1N	1	MET
9	1N	5	VAL
9	1N	14	VAL
9	1N	33	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	121	LYS

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Mol	Chain	Res	Type
9	1N	133	GLN
10	1O	8	LEU
10	1O	24	VAL
10	1O	69	ILE
10	1O	92	GLU
10	1O	108	GLU
11	1P	3	LEU
11	1P	59	LEU
11	1P	75	ILE
11	1P	95	VAL
11	1P	99	LEU
11	1P	135	LEU
12	1Q	2	LEU
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	129	THR
12	1Q	130	LYS
13	1R	6	SER
13	1R	15	SER
13	1R	33	ARG
13	1R	36	THR
13	1R	67	LEU
13	1R	75	LEU
13	1R	78	LYS
13	1R	100	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	43	GLU
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	76	LYS
14	1S	80	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	53	ARG

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Mol	Chain	Res	Type
15	1T	96	ARG
15	1T	118	ARG
16	1U	5	LYS
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	108	GLU
16	1U	117	GLN
17	1V	32	THR
17	1V	44	LYS
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	23	LEU
18	1W	67	ASP
18	1W	96	ILE
19	1X	38	GLU
19	1X	65	ARG
19	1X	72	LYS
20	1Y	9	LYS
20	1Y	11	ASP
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	73	ARG
20	1Y	86	ARG
20	1Y	92	ASN
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	61	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	119	GLU
21	1Z	126	VAL
21	1Z	155	LEU

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Mol	Chain	Res	Type
21	1Z	161	VAL
21	1Z	171	ILE
21	1Z	191	VAL
23	11	30	VAL
23	11	46	LEU
23	11	51	VAL
23	11	57	GLU
23	11	59	THR
23	11	74	VAL
23	11	91	LYS
24	12	53	LEU
24	12	55	ARG
24	12	70	GLN
25	13	23	LEU
25	13	31	LEU
25	13	37	LEU
25	13	54	VAL
26	14	10	VAL
26	14	14	ILE
26	14	49	PHE
26	14	50	VAL
26	14	60	GLN
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	40	LYS
27	15	58	LEU
27	15	60	VAL
28	16	19	ARG
28	16	44	ARG
28	16	45	LYS
28	16	47	THR
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	24	THR
29	17	43	THR
29	17	46	VAL
29	17	47	ARG
29	17	48	LYS
30	18	23	VAL
31	19	33	LYS

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Mol	Chain	Res	Type
33	1b	10	LEU
33	1b	15	VAL
33	1b	23	ARG
33	1b	39	ILE
33	1b	51	LEU
33	1b	71	VAL
33	1b	96	ARG
33	1b	111	ARG
33	1b	112	VAL
33	1b	119	GLU
33	1b	128	GLU
33	1b	154	LEU
33	1b	158	LEU
33	1b	160	ASP
33	1b	185	ILE
33	1b	230	VAL
34	1c	3	ASN
34	1c	16	ARG
34	1c	36	ASP
34	1c	55	VAL
34	1c	70	VAL
34	1c	102	ASN
34	1c	104	GLN
34	1c	105	GLU
34	1c	115	LEU
34	1c	144	SER
35	1d	8	VAL
35	1d	17	VAL
35	1d	26	CYS
35	1d	58	LEU
35	1d	67	ILE
35	1d	76	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	157	LEU
35	1d	168	ARG
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	10	MET
36	1e	11	ILE

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Mol	Chain	Res	Type
36	1e	33	VAL
36	1e	34	VAL
36	1e	64	ARG
36	1e	67	VAL
36	1e	68	GLU
36	1e	69	VAL
36	1e	79	GLU
36	1e	80	ILE
36	1e	112	LEU
36	1e	126	ARG
36	1e	148	VAL
37	1f	10	LEU
37	1f	17	SER
37	1f	40	VAL
37	1f	45	LEU
37	1f	48	LEU
37	1f	54	LYS
37	1f	64	GLN
37	1f	69	GLU
37	1f	72	VAL
37	1f	73	ASN
37	1f	86	ARG
38	1g	6	ARG
38	1g	13	GLN
38	1g	16	LEU
38	1g	52	GLU
38	1g	104	LEU
38	1g	106	GLN
38	1g	113	GLU
38	1g	138	LYS
39	1h	25	ASP
39	1h	26	VAL
39	1h	38	ILE
39	1h	51	VAL
39	1h	54	ASP
39	1h	63	LEU
39	1h	102	ARG
39	1h	105	ARG
39	1h	133	LEU
40	1i	14	VAL
40	1i	17	VAL
40	1i	50	LEU

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Mol	Chain	Res	Type
40	1i	54	ASP
40	1i	56	LEU
40	1i	64	THR
40	1i	65	VAL
40	1i	81	ILE
40	1i	103	THR
40	1i	104	ARG
40	1i	125	TYR
41	1j	38	ILE
41	1j	55	LYS
41	1j	67	THR
41	1j	100	THR
42	1k	16	SER
42	1k	114	VAL
43	1l	18	VAL
43	1l	24	VAL
43	1l	41	ARG
43	1l	46	LYS
43	1l	60	LEU
43	1l	83	VAL
44	1m	3	ARG
44	1m	8	GLU
44	1m	19	LEU
44	1m	70	LEU
44	1m	86	CYS
44	1m	98	VAL
44	1m	106	ASN
45	1n	13	THR
45	1n	18	VAL
45	1n	29	ARG
45	1n	33	VAL
45	1n	44	LEU
46	1o	39	LEU
46	1o	47	LYS
46	1o	60	VAL
46	1o	76	GLU
46	1o	84	LYS
46	1o	88	ARG
47	1p	2	VAL
47	1p	8	ARG
47	1p	20	VAL
47	1p	21	VAL

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Mol	Chain	Res	Type
47	1p	34	GLU
47	1p	42	ARG
47	1p	53	VAL
47	1p	62	VAL
47	1p	67	THR
47	1p	74	LEU
48	1q	78	GLU
48	1q	85	VAL
48	1q	97	SER
49	1r	25	THR
49	1r	31	LEU
49	1r	85	LEU
50	1s	5	LEU
50	1s	28	LYS
50	1s	35	SER
51	1t	30	LYS
51	1t	37	SER
51	1t	70	SER
53	1y	42	SER
53	1y	46	GLN
53	1y	53	THR
3	2D	3	VAL
3	2D	61	LEU
3	2D	64	ILE
3	2D	73	VAL
3	2D	103	ARG
3	2D	113	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	147	LEU
3	2D	155	LEU
3	2D	162	SER
3	2D	173	VAL
3	2D	183	ARG
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	274	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR

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Mol	Chain	Res	Type
4	2E	89	ASP
4	2E	116	VAL
4	2E	163	GLU
4	2E	188	VAL
4	2E	195	LEU
5	2F	15	SER
5	2F	20	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	38	ARG
5	2F	53	THR
5	2F	57	VAL
5	2F	60	SER
5	2F	74	ARG
5	2F	120	GLU
5	2F	126	VAL
5	2F	132	VAL
5	2F	140	LEU
5	2F	158	THR
5	2F	161	GLU
5	2F	170	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	26	GLN
6	2G	28	VAL
6	2G	31	VAL
6	2G	39	ILE
6	2G	43	LEU
6	2G	49	ASP
6	2G	67	LYS
6	2G	88	ILE
6	2G	92	VAL
6	2G	106	LEU
6	2G	113	ARG
6	2G	116	ASP
6	2G	133	LEU
6	2G	139	LEU
6	2G	149	VAL

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Mol	Chain	Res	Type
6	2G	157	ILE
6	2G	159	VAL
6	2G	165	THR
7	2H	4	ILE
7	2H	25	LYS
7	2H	33	LEU
7	2H	37	VAL
7	2H	43	VAL
7	2H	45	VAL
7	2H	47	GLU
7	2H	81	GLU
7	2H	86	GLU
7	2H	88	LEU
7	2H	95	ARG
7	2H	122	THR
7	2H	133	VAL
7	2H	134	SER
7	2H	136	ILE
7	2H	148	ILE
8	2I	31	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	50	ARG
8	2I	51	ILE
8	2I	57	ARG
8	2I	68	LEU
8	2I	69	LYS
8	2I	76	THR
8	2I	92	VAL
8	2I	102	SER
8	2I	117	GLU
8	2I	140	LEU
8	2I	142	VAL
9	2N	28	THR
9	2N	34	LEU
9	2N	38	HIS
9	2N	48	MET
9	2N	65	LYS
9	2N	67	LEU
9	2N	83	LYS
9	2N	99	LEU
9	2N	115	ARG

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Mol	Chain	Res	Type
10	2O	8	LEU
10	2O	20	MET
10	2O	24	VAL
10	2O	53	LYS
10	2O	98	VAL
10	2O	108	GLU
11	2P	3	LEU
11	2P	99	LEU
11	2P	106	LEU
11	2P	135	LEU
11	2P	149	GLU
12	2Q	7	MET
12	2Q	22	LYS
12	2Q	55	VAL
12	2Q	75	THR
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	111	GLU
13	2R	33	ARG
13	2R	36	THR
13	2R	86	ARG
13	2R	100	LEU
13	2R	113	LEU
13	2R	114	VAL
13	2R	117	VAL
14	2S	5	THR
14	2S	12	PHE
14	2S	23	ARG
14	2S	25	ARG
14	2S	27	SER
14	2S	36	TYR
14	2S	44	LYS
14	2S	48	LEU
14	2S	52	SER
14	2S	69	VAL
15	2T	17	THR
15	2T	28	VAL
15	2T	34	VAL
15	2T	39	ARG
15	2T	40	THR
15	2T	72	VAL
15	2T	89	VAL

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Mol	Chain	Res	Type
16	2U	70	ARG
16	2U	74	LEU
17	2V	12	TYR
17	2V	18	LEU
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	79	VAL
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	63	ASP
19	2X	45	THR
19	2X	50	LYS
20	2Y	2	ARG
20	2Y	3	VAL
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	41	LEU
21	2Z	107	THR
21	2Z	121	HIS
21	2Z	128	VAL
21	2Z	155	LEU
21	2Z	170	THR
21	2Z	185	GLU
22	20	11	ARG
22	20	36	ILE
22	20	68	GLU
23	21	11	ARG
23	21	21	ARG
23	21	26	ARG
23	21	30	VAL
23	21	40	ARG
23	21	51	VAL
23	21	59	THR
23	21	80	LEU
23	21	85	LEU
24	22	1	MET
24	22	2	LYS

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Mol	Chain	Res	Type
24	22	25	VAL
24	22	27	GLU
24	22	32	LEU
24	22	40	SER
24	22	53	LEU
24	22	62	THR
24	22	63	VAL
24	22	70	GLN
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	21	VAL
26	24	37	SER
26	24	53	GLU
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
27	25	6	VAL
27	25	40	LYS
28	26	14	THR
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	24	THR
29	27	43	THR
29	27	46	VAL
29	27	48	LYS
30	28	23	VAL
31	29	6	SER
31	29	17	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	44	LEU
33	2b	45	GLN
33	2b	52	GLU
33	2b	56	ARG
33	2b	67	THR
33	2b	68	ILE
33	2b	76	GLN
33	2b	80	ILE

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Mol	Chain	Res	Type
33	2b	81	VAL
33	2b	83	MET
33	2b	90	MET
33	2b	96	ARG
33	2b	111	ARG
33	2b	118	LEU
33	2b	127	ILE
33	2b	154	LEU
33	2b	157	ARG
33	2b	160	ASP
33	2b	187	LEU
33	2b	189	ASP
33	2b	197	VAL
33	2b	200	ILE
33	2b	208	ILE
33	2b	229	VAL
34	2c	3	ASN
34	2c	15	THR
34	2c	32	LEU
34	2c	33	LEU
34	2c	52	LEU
34	2c	105	GLU
34	2c	115	LEU
34	2c	127	ARG
34	2c	143	GLU
34	2c	152	ILE
34	2c	157	ILE
34	2c	206	GLU
34	2c	207	VAL
35	2d	3	ARG
35	2d	5	ILE
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	53	ASP
35	2d	59	ARG
35	2d	80	GLU
35	2d	83	SER
35	2d	96	LEU
35	2d	135	LEU
35	2d	157	LEU
35	2d	158	ILE

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Mol	Chain	Res	Type
35	2d	166	LYS
35	2d	170	VAL
35	2d	175	SER
35	2d	190	ASP
36	2e	31	LEU
36	2e	34	VAL
36	2e	38	GLN
36	2e	65	ASN
36	2e	75	THR
36	2e	112	LEU
36	2e	118	ILE
36	2e	143	ARG
36	2e	150	ARG
37	2f	10	LEU
37	2f	22	GLU
37	2f	61	LEU
37	2f	69	GLU
37	2f	72	VAL
37	2f	73	ASN
37	2f	75	LEU
37	2f	81	ILE
37	2f	91	VAL
38	2g	9	VAL
38	2g	27	ILE
38	2g	51	GLN
38	2g	57	GLU
38	2g	75	VAL
38	2g	113	GLU
38	2g	131	LYS
38	2g	153	HIS
38	2g	155	ARG
39	2h	10	LEU
39	2h	25	ASP
39	2h	29	SER
39	2h	37	ARG
39	2h	63	LEU
39	2h	85	ARG
39	2h	91	ARG
39	2h	97	VAL
39	2h	109	ILE
39	2h	112	LEU
39	2h	133	LEU

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Mol	Chain	Res	Type
40	2i	7	THR
40	2i	27	THR
40	2i	28	VAL
40	2i	40	LEU
40	2i	75	ASP
40	2i	81	ILE
40	2i	102	LEU
40	2i	108	VAL
40	2i	109	VAL
40	2i	125	TYR
41	2j	16	LEU
41	2j	29	ARG
41	2j	30	SER
41	2j	34	VAL
41	2j	95	GLU
41	2j	98	ILE
42	2k	18	ARG
42	2k	41	THR
42	2k	79	SER
42	2k	84	VAL
42	2k	116	HIS
42	2k	117	ASN
43	2l	18	VAL
43	2l	36	VAL
43	2l	41	ARG
43	2l	43	VAL
43	2l	55	VAL
43	2l	83	VAL
43	2l	100	ILE
44	2m	15	VAL
44	2m	17	VAL
44	2m	19	LEU
44	2m	65	LYS
44	2m	90	LEU
44	2m	106	ASN
45	2n	3	ARG
45	2n	7	ILE
45	2n	13	THR
45	2n	18	VAL
45	2n	33	VAL
45	2n	42	ILE
45	2n	57	ARG

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Mol	Chain	Res	Type
46	2o	3	ILE
46	2o	39	LEU
46	2o	76	GLU
46	2o	84	LYS
46	2o	87	ILE
46	2o	88	ARG
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	21	VAL
47	2p	44	THR
47	2p	45	THR
47	2p	49	LEU
47	2p	67	THR
48	2q	16	GLN
48	2q	60	ILE
48	2q	70	ARG
48	2q	78	GLU
49	2r	21	LYS
49	2r	31	LEU
49	2r	37	VAL
50	2s	5	LEU
50	2s	32	LYS
50	2s	41	VAL
50	2s	48	THR
50	2s	63	THR
50	2s	66	MET
50	2s	77	THR
50	2s	81	ARG
51	2t	20	LEU
51	2t	24	LEU
51	2t	62	LEU
51	2t	84	LEU
53	2y	3	MET
53	2y	5	ILE
53	2y	8	LYS
53	2y	9	GLN
53	2y	10	MET
53	2y	11	GLU
53	2y	13	THR
53	2y	16	ILE
53	2y	24	LEU

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Mol	Chain	Res	Type
53	2y	32	THR
53	2y	46	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	253	GLN
4	1E	55	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	40	ASN
6	1G	108	ASN
8	1I	74	ASN
9	1N	69	GLN
9	1N	94	HIS
9	1N	131	GLN
9	1N	133	GLN
11	1P	84	ASN
13	1R	31	HIS
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN
15	1T	104	ASN
15	1T	123	GLN
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	32	HIS
21	1Z	73	GLN
22	10	35	ASN
23	11	19	GLN
23	11	56	GLN
25	13	32	GLN
26	14	60	GLN
29	17	36	GLN
33	1b	212	GLN

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Mol	Chain	Res	Type
34	1c	6	HIS
34	1c	28	GLN
34	1c	69	HIS
34	1c	102	ASN
34	1c	104	GLN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	129	ASN
36	1e	56	GLN
36	1e	141	GLN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
40	1i	3	GLN
40	1i	87	GLN
42	1k	93	GLN
43	1l	99	HIS
44	1m	40	ASN
44	1m	106	ASN
46	1o	28	GLN
47	1p	16	HIS
48	1q	45	HIS
50	1s	14	HIS
50	1s	56	GLN
50	1s	83	HIS
51	1t	75	ASN
51	1t	90	GLN
53	1y	38	HIS
3	2D	253	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
5	2F	203	GLN
6	2G	79	ASN
7	2H	143	GLN
7	2H	147	ASN
8	2I	11	ASN
8	2I	43	ASN
8	2I	104	GLN

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Mol	Chain	Res	Type
8	2I	139	GLN
9	2N	133	GLN
10	2O	3	GLN
11	2P	27	HIS
12	2Q	89	ASN
12	2Q	123	HIS
12	2Q	141	GLN
13	2R	71	GLN
14	2S	68	GLN
16	2U	94	ASN
17	2V	64	HIS
23	21	56	GLN
24	22	9	GLN
24	22	56	GLN
24	22	70	GLN
25	23	32	GLN
26	24	40	HIS
28	26	20	ASN
30	28	35	GLN
33	2b	113	HIS
34	2c	6	HIS
34	2c	37	GLN
34	2c	63	ASN
34	2c	69	HIS
34	2c	136	GLN
34	2c	176	HIS
35	2d	42	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	161	ASN
36	2e	20	GLN
36	2e	65	ASN
37	2f	64	GLN
38	2g	11	GLN
38	2g	13	GLN
38	2g	109	ASN
39	2h	81	HIS
40	2i	58	HIS
41	2j	21	GLN
41	2j	62	HIS
41	2j	68	HIS

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Mol	Chain	Res	Type
41	2j	84	GLN
42	2k	93	GLN
42	2k	99	GLN
43	2l	99	HIS
44	2m	12	ASN
44	2m	77	ASN
46	2o	9	GLN
46	2o	28	GLN
47	2p	13	HIS
50	2s	23	ASN
50	2s	83	HIS
51	2t	90	GLN
53	2y	9	GLN
53	2y	38	HIS
53	2y	46	GLN
53	2y	79	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	399 (13%)	31 (1%)
1	2A	2858/2915 (98%)	463 (16%)	38 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	239 (15%)	0
All	All	8959/9114 (98%)	1372 (15%)	69 (0%)

All (1372) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G

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Mol	Chain	Res	Type
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	311	A
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	422	A
1	1A	428	A
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C

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Mol	Chain	Res	Type
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	652(V)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	805	G

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Mol	Chain	Res	Type
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	882	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1053	C
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G

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Mol	Chain	Res	Type
1	1A	1065	U
1	1A	1066	U
1	1A	1068	G
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1104	C
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1128	A
1	1A	1129	A
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1300	U

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Mol	Chain	Res	Type
1	1A	1301	A
1	1A	1303	G
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1505	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1539	G
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C

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Mol	Chain	Res	Type
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1756	G
1	1A	1757	U
1	1A	1758	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A

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Mol	Chain	Res	Type
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2111	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2138	C
1	1A	2139	C
1	1A	2142	C
1	1A	2146	C
1	1A	2148	G
1	1A	2154	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2162	G
1	1A	2172	U

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Mol	Chain	Res	Type
1	1A	2173	A
1	1A	2176	A
1	1A	2178	C
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2279	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2326	C
1	1A	2327	A
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A

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Mol	Chain	Res	Type
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2555	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2662	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G

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Mol	Chain	Res	Type
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	30	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	6	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	53	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	96	U
32	1a	101	A
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	143	A

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Mol	Chain	Res	Type
32	1a	144	G
32	1a	156	G
32	1a	163	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	253	U
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G

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Mol	Chain	Res	Type
32	1a	427	U
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	456	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	480	U
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	514	C
32	1a	518	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	633	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G

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Mol	Chain	Res	Type
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	870	U
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001	A

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Mol	Chain	Res	Type
32	1a	1001(A)	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1130	A
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1144	G
32	1a	1146	A
32	1a	1150	U
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C

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Mol	Chain	Res	Type
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C

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Mol	Chain	Res	Type
32	1a	1456	G
32	1a	1492	A
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	104	U
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A

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Mol	Chain	Res	Type
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	312	G
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	429	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	702	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	877	U

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Mol	Chain	Res	Type
1	2A	880	G
1	2A	883	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	968	G
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1042	G
1	2A	1044	G
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U

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Mol	Chain	Res	Type
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1096	A
1	2A	1097	U
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A

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Mol	Chain	Res	Type
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1537	G

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Mol	Chain	Res	Type
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1817	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G

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Mol	Chain	Res	Type
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2096	U
1	2A	2099	U
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A

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Mol	Chain	Res	Type
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2180	U
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G

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Mol	Chain	Res	Type
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2293	C
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2310	A
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2326	C
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2407	G
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G

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Mol	Chain	Res	Type
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2491	U
1	2A	2492	U
1	2A	2498	C
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2543	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2752	C
1	2A	2757	A
1	2A	2764	A
1	2A	2765	A

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Mol	Chain	Res	Type
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2803	C
1	2A	2811	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	22	U
2	2B	33	G
2	2B	35	U
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	90	A
2	2B	94	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	29	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G

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Mol	Chain	Res	Type
32	2a	66	G
32	2a	89	C
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	396	G
32	2a	397	A
32	2a	398	C

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Mol	Chain	Res	Type
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	482	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	685	G
32	2a	687	A
32	2a	688	G

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Mol	Chain	Res	Type
32	2a	695	A
32	2a	705	U
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	735	C
32	2a	749	C
32	2a	755	G
32	2a	763	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	785	G
32	2a	793	U
32	2a	794	A
32	2a	802	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A

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Mol	Chain	Res	Type
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1041	A
32	2a	1044	A
32	2a	1047	G
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1100	C
32	2a	1101	A
32	2a	1104	G
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A

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Mol	Chain	Res	Type
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1162	C
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1248	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1317	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1349	A
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A

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Mol	Chain	Res	Type
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1460	A
32	2a	1477	C
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	839	U
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1379	A
1	1A	1442	G

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Mol	Chain	Res	Type
1	1A	1608	A
1	1A	1653	G
1	1A	2116	G
1	1A	2126	A
1	1A	2288	A
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2602	A
1	1A	2611	U
1	1A	2689	U
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	974	G
1	2A	993	G
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1493	C
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U

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Mol	Chain	Res	Type
1	2A	2321	G
1	2A	2406	U
1	2A	2439	A
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.14	2 (7%)
1	5MU	1A	1939	54,1	19,22,23	1.41	4 (21%)	27,32,35	2.13	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.05	10 (30%)
1	OMG	2A	2251	54,1	23,26,27	1.21	2 (8%)	32,38,41	1.90	5 (15%)
32	PSU	2a	516	32,54	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.96	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.00	5 (23%)
32	2MG	2a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.12	5 (15%)
1	5MC	1A	1942	54,1	19,22,23	1.62	3 (15%)	26,32,35	1.07	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.88	9 (27%)
32	UR3	2a	1498	32,54	19,22,23	1.02	2 (10%)	26,32,35	1.62	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.87	1 (4%)
32	5MC	1a	967	32	19,22,23	1.56	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
1	5MC	1A	1962	54,1	19,22,23	1.69	3 (15%)	26,32,35	1.09	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.70	3 (15%)	26,32,35	1.15	4 (15%)
1	5MU	2A	1939	54,1	19,22,23	1.39	5 (26%)	27,32,35	2.28	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	2605	1	18,21,22	1.38	4 (22%)	21,30,33	2.11	4 (19%)
1	2MU	2A	2552	54,1	19,22,24	1.33	4 (21%)	25,31,36	1.72	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.25	2 (8%)	33,38,41	2.38	10 (30%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	3 (11%)
32	PSU	1a	516	32,54	18,21,22	1.41	2 (11%)	21,30,33	1.95	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.85	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.43	4 (21%)	27,32,35	2.22	8 (29%)
32	M2G	2a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.84	5 (15%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.99	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	1.94	9 (27%)
1	PSU	1A	2605	1	18,21,22	1.47	3 (16%)	21,30,33	2.04	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.35	3 (16%)	21,30,33	2.09	3 (14%)
1	5MC	2A	1942	54,1	19,22,23	1.75	3 (15%)	26,32,35	1.21	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.91	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	2 (10%)	26,32,35	1.13	2 (7%)
1	2MU	1A	2552	54,1	19,22,24	1.24	3 (15%)	25,31,36	1.97	6 (24%)
1	PSU	1A	1917	54,1	18,21,22	1.33	2 (11%)	21,30,33	1.97	3 (14%)
1	2MA	1A	2503	54,1	22,25,26	1.45	5 (22%)	32,37,40	2.27	7 (21%)
32	G7M	2a	527	32,54	23,26,27	2.35	5 (21%)	34,39,42	3.01	10 (29%)
1	5MU	1A	1915	54,1	19,22,23	1.48	5 (26%)	27,32,35	2.29	9 (33%)
43	0TD	2l	92	43	8,9,10	4.64	1 (12%)	6,11,13	7.26	2 (33%)
1	OMG	1A	2251	54,1	23,26,27	1.25	3 (13%)	32,38,41	2.06	6 (18%)
43	0TD	1l	92	43	8,9,10	4.59	2 (25%)	6,11,13	7.05	3 (50%)
32	5MC	2a	967	32	19,22,23	1.76	2 (10%)	26,32,35	1.03	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.12	10 (30%)
1	2MA	2A	2503	54,1	22,25,26	1.49	4 (18%)	32,37,40	2.44	8 (25%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
1	5MC	2A	1962	54,1	19,22,23	1.66	3 (15%)	26,32,35	1.20	2 (7%)
32	G7M	1a	527	32,54	23,26,27	2.38	5 (21%)	34,39,42	2.94	10 (29%)
32	5MC	2a	1400	32	19,22,23	1.59	3 (15%)	26,32,35	1.19	2 (7%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.83	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	54,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	54,1	-	1/9/27/28	0/2/2/2
1	PSU	1A	1917	54,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	2/7/25/26	0/3/3/3
32	G7M	2a	527	32,54	-	2/7/25/26	0/3/3/3
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	2MA	2A	2503	54,1	-	0/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.64	1.69	1.82
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
32	2a	527	G7M	C8-N7	7.57	1.46	1.33
32	1a	527	G7M	C8-N7	7.42	1.45	1.33
32	2a	1404	5MC	C5-C4	7.21	1.49	1.44
32	2a	967	5MC	C5-C4	6.53	1.49	1.44
1	2A	1942	5MC	C5-C4	6.41	1.49	1.44
32	1a	1407	5MC	C5-C4	6.27	1.48	1.44
32	1a	1400	5MC	C5-C4	6.22	1.48	1.44
1	1A	1962	5MC	C5-C4	6.06	1.48	1.44
32	1a	1404	5MC	C5-C4	6.04	1.48	1.44
1	2A	1962	5MC	C5-C4	5.95	1.48	1.44
32	2a	1407	5MC	C5-C4	5.95	1.48	1.44
1	1A	1942	5MC	C5-C4	5.80	1.48	1.44
32	2a	1400	5MC	C5-C4	5.66	1.48	1.44
32	1a	967	5MC	C5-C4	5.49	1.48	1.44
32	1a	527	G7M	C5-N7	-5.00	1.33	1.39
32	2a	527	G7M	C5-N7	-4.43	1.34	1.39
1	2A	2503	2MA	C5-C4	4.42	1.47	1.39
32	1a	527	G7M	C8-N9	4.31	1.47	1.35
32	2a	527	G7M	C8-N9	4.30	1.47	1.35
1	1A	2503	2MA	C5-C4	4.05	1.46	1.39
32	1a	527	G7M	C5-C4	3.82	1.47	1.38
1	1A	2605	PSU	C6-C5	3.81	1.39	1.35
32	2a	527	G7M	C5-C4	3.79	1.47	1.38
32	1a	516	PSU	C6-C5	3.72	1.39	1.35
1	1A	1911	PSU	C6-C5	3.55	1.39	1.35
1	2A	1911	PSU	C6-C5	3.55	1.39	1.35
1	1A	1917	PSU	C6-C5	3.49	1.39	1.35
32	2a	966	M2G	C5-C4	3.37	1.48	1.38
32	2a	1207	2MG	C5-C4	3.29	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	516	PSU	C6-C5	3.27	1.38	1.35
1	2A	2251	OMG	C5-C4	3.26	1.47	1.38
32	1a	966	M2G	C5-C4	3.24	1.47	1.38
1	1A	2251	OMG	C5-C4	3.21	1.47	1.38
1	1A	1939	5MU	C6-C5	3.19	1.39	1.34
32	1a	1400	5MC	C6-C5	3.15	1.39	1.34
1	1A	1915	5MU	C2-N1	3.12	1.43	1.38
1	2A	1917	PSU	C6-C5	3.10	1.38	1.35
1	1A	2503	2MA	C5-N7	-3.07	1.33	1.39
1	1A	2605	PSU	C4-N3	-3.03	1.33	1.38
32	1a	1207	2MG	C5-C4	3.02	1.47	1.38
32	1a	1404	5MC	C6-C5	2.98	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.96	1.33	1.38
1	1A	1942	5MC	C6-C5	2.95	1.39	1.34
1	2A	1915	5MU	C2-N1	2.95	1.43	1.38
1	2A	2605	PSU	C6-C5	2.94	1.38	1.35
32	2a	1407	5MC	C6-C5	2.91	1.39	1.34
32	2a	1404	5MC	C6-C5	2.90	1.39	1.34
32	2a	967	5MC	C6-C5	2.90	1.39	1.34
1	2A	1915	5MU	C6-C5	2.89	1.39	1.34
32	2a	1400	5MC	C6-C5	2.81	1.39	1.34
1	2A	1942	5MC	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.76	1.33	1.38
1	2A	1962	5MC	C6-C5	2.76	1.39	1.34
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.75	1.33	1.38
32	1a	1407	5MC	C6-C5	2.74	1.39	1.34
1	1A	1962	5MC	C6-C5	2.73	1.39	1.34
32	1a	967	5MC	C6-C5	2.72	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
32	2a	966	M2G	C2-N2	2.70	1.40	1.35
1	2A	1939	5MU	C6-C5	2.69	1.39	1.34
1	1A	1962	5MC	C6-N1	-2.69	1.33	1.38
32	1a	966	M2G	C2-N2	2.66	1.40	1.35
1	2A	2251	OMG	C6-N1	-2.62	1.33	1.38
32	1a	966	M2G	C6-N1	-2.61	1.34	1.38
1	1A	1939	5MU	C4-N3	-2.59	1.34	1.38
43	1l	92	0TD	CB-CA	2.58	1.55	1.54
1	2A	1939	5MU	C4-C5	2.56	1.49	1.44
1	2A	2503	2MA	C5-C6	2.53	1.48	1.41
32	1a	1207	2MG	C6-N1	-2.53	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.50	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C6-N1	-2.48	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.48	1.34	1.38
1	1A	2552	2MU	C4-N3	-2.48	1.34	1.38
1	1A	1939	5MU	C4-C5	2.48	1.48	1.44
32	2a	966	M2G	C6-N1	-2.47	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.46	1.34	1.38
32	2a	516	PSU	C4-N3	-2.46	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.43	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.42	1.34	1.38
1	2A	2503	2MA	C8-N7	2.38	1.36	1.31
1	2A	2552	2MU	C2-N3	-2.37	1.33	1.38
1	2A	2503	2MA	C5-N7	-2.34	1.34	1.39
1	1A	1917	PSU	C4-N3	-2.33	1.34	1.38
1	1A	1915	5MU	C4-C5	2.33	1.48	1.44
32	1a	1498	UR3	C2-N1	2.32	1.41	1.38
1	2A	1942	5MC	C6-N1	-2.31	1.34	1.38
32	2a	527	G7M	C6-N1	-2.29	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.29	1.34	1.38
1	2A	2605	PSU	C2-N1	-2.28	1.33	1.36
1	2A	1915	5MU	C4-C5	2.26	1.48	1.44
1	1A	1939	5MU	C2-N3	-2.26	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.24	1.34	1.38
1	2A	2552	2MU	C5-C4	2.24	1.48	1.43
32	2a	1400	5MC	C6-N1	-2.24	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.23	1.34	1.38
32	1a	527	G7M	C6-N1	-2.22	1.34	1.38
32	1a	516	PSU	C4-N3	-2.19	1.34	1.38
1	1A	2552	2MU	C5-C4	2.18	1.48	1.43
1	2A	2552	2MU	C2-N1	2.17	1.41	1.38
32	2a	1498	UR3	C2-N1	2.16	1.41	1.38
32	1a	966	M2G	C5-N7	-2.15	1.34	1.39
1	1A	2251	OMG	C5-N7	-2.14	1.34	1.39
32	1a	967	5MC	C6-N1	-2.14	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.13	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.13	1.33	1.37
1	1A	1942	5MC	C6-N1	-2.12	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.12	1.34	1.37
32	2a	1498	UR3	C6-C5	2.11	1.40	1.35
32	2a	1404	5MC	C6-N1	-2.10	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.09	1.34	1.37
32	1a	1498	UR3	C6-C5	2.09	1.39	1.35
32	2a	1207	2MG	C2-N3	2.09	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2503	2MA	C5-C6	2.08	1.46	1.41
32	2a	1407	5MC	C6-N1	-2.08	1.34	1.38
1	2A	1911	PSU	C2-N3	-2.07	1.34	1.37
32	1a	1407	5MC	C6-N1	-2.05	1.34	1.38
1	2A	1939	5MU	C2-N1	2.04	1.41	1.38
1	1A	2503	2MA	C8-N7	2.04	1.35	1.31
1	1A	2552	2MU	C2-N3	-2.04	1.34	1.38
1	2A	1917	PSU	C2-N1	-2.03	1.34	1.36
32	2a	1207	2MG	C5-N7	-2.02	1.35	1.39

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-17.39	71.10	102.36
43	1l	92	0TD	CSB-SB-CB	-16.65	72.44	102.36
1	2A	2503	2MA	C5-C4-N3	-8.74	117.98	127.18
32	2a	527	G7M	CN7-N7-C8	-8.43	112.02	124.79
1	1A	2503	2MA	C5-C4-N3	-7.75	119.02	127.18
32	1a	527	G7M	CN7-N7-C8	-7.72	113.09	124.79
32	1a	1498	UR3	C4-N3-C2	-7.34	118.67	124.58
32	1a	1207	2MG	C2-N3-C4	7.17	120.97	112.00
1	2A	2503	2MA	N3-C4-N9	6.91	135.76	126.99
32	2a	527	G7M	N9-C8-N7	-6.87	95.79	112.48
32	2a	1207	2MG	C2-N3-C4	6.81	120.52	112.00
1	1A	2605	PSU	N1-C2-N3	6.62	122.15	115.17
32	1a	527	G7M	N9-C8-N7	-6.62	96.42	112.48
32	2a	527	G7M	C8-N7-C5	6.53	115.95	107.78
1	2A	2605	PSU	N1-C2-N3	6.49	122.01	115.17
32	2a	1498	UR3	C4-N3-C2	-6.48	119.37	124.58
1	1A	1911	PSU	N1-C2-N3	6.45	121.97	115.17
1	2A	1911	PSU	N1-C2-N3	6.40	121.92	115.17
1	1A	2251	OMG	C5-C4-N3	-6.35	118.29	128.39
32	2a	516	PSU	N1-C2-N3	6.33	121.85	115.17
1	2A	1917	PSU	N1-C2-N3	6.28	121.79	115.17
32	1a	527	G7M	N9-C4-N3	6.22	138.40	125.95
32	1a	527	G7M	C8-N7-C5	6.22	115.55	107.78
32	2a	966	M2G	C5-C4-N3	-6.21	118.51	128.39
1	1A	2503	2MA	N3-C4-N9	6.21	134.87	126.99
32	2a	527	G7M	N9-C4-N3	6.03	138.02	125.95
32	1a	966	M2G	C5-C4-N3	-6.03	118.79	128.39
1	1A	1917	PSU	N1-C2-N3	6.01	121.51	115.17
32	1a	1207	2MG	C5-C4-N3	-6.01	118.83	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1207	2MG	C5-C4-N3	-6.00	118.84	128.39
1	2A	2251	OMG	C5-C4-N3	-5.92	118.98	128.39
32	1a	516	PSU	N1-C2-N3	5.74	121.23	115.17
1	2A	1939	5MU	C4-N3-C2	-5.65	119.93	127.34
1	2A	1939	5MU	N3-C2-N1	5.60	122.18	114.89
1	1A	2251	OMG	C2-N3-C4	5.44	121.67	112.30
32	1a	527	G7M	C5-C4-N3	-5.33	118.08	128.15
1	1A	1939	5MU	N3-C2-N1	5.10	121.54	114.89
1	1A	1939	5MU	C4-N3-C2	-5.08	120.68	127.34
1	2A	1915	5MU	N3-C2-N1	5.07	121.49	114.89
1	1A	2552	2MU	N3-C2-N1	5.03	121.44	114.89
32	2a	527	G7M	C5-C4-N3	-5.03	118.65	128.15
1	1A	1915	5MU	N3-C2-N1	4.99	121.39	114.89
32	2a	1518	MA6	N1-C2-N3	-4.94	121.11	128.58
32	2a	1519	MA6	N1-C2-N3	-4.93	121.12	128.58
1	2A	2251	OMG	C2-N3-C4	4.93	120.79	112.30
32	1a	1519	MA6	C5-C4-N3	-4.88	120.00	126.72
1	2A	2552	2MU	N3-C2-N1	4.85	121.20	114.89
32	1a	1519	MA6	N1-C2-N3	-4.68	121.50	128.58
1	2A	1915	5MU	C4-N3-C2	-4.68	121.21	127.34
1	2A	1917	PSU	O2-C2-N1	-4.65	118.00	122.79
1	1A	1915	5MU	C1'-N1-C2	4.58	125.81	117.59
1	1A	1939	5MU	C5-C4-N3	4.57	119.29	115.32
1	2A	1939	5MU	C5-C4-N3	4.54	119.27	115.32
32	2a	966	M2G	N9-C4-N3	4.52	134.99	125.95
1	1A	1915	5MU	C4-N3-C2	-4.52	121.42	127.34
1	1A	2552	2MU	C4-N3-C2	-4.46	121.08	126.61
32	2a	1519	MA6	C5-C4-N3	-4.44	120.60	126.72
32	1a	966	M2G	N9-C4-N3	4.43	134.81	125.95
32	2a	527	G7M	C8-N9-C4	4.41	118.01	107.09
1	1A	1915	5MU	C5-C4-N3	4.38	119.13	115.32
1	2A	2552	2MU	C4-N3-C2	-4.38	121.18	126.61
1	1A	2503	2MA	N6-C6-N1	4.36	122.91	117.03
32	1a	1518	MA6	N1-C2-N3	-4.34	122.02	128.58
32	2a	1207	2MG	N9-C4-N3	4.32	134.60	125.95
32	2a	966	M2G	C2-N3-C4	4.32	120.50	112.51
1	2A	2251	OMG	N9-C4-N3	4.31	134.57	125.95
32	1a	966	M2G	C2-N3-C4	4.31	120.48	112.51
32	1a	527	G7M	C2-N3-C4	4.24	119.60	112.30
1	2A	2605	PSU	C4-N3-C2	-4.24	120.54	126.37
32	2a	516	PSU	C4-N3-C2	-4.23	120.54	126.37
32	2a	527	G7M	CN7-N7-C5	4.20	132.03	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2251	OMG	N9-C4-N3	4.20	134.34	125.95
1	2A	1939	5MU	O4-C4-C5	-4.18	120.13	124.92
32	2a	1519	MA6	C4-C5-N7	-4.17	105.81	110.58
32	2a	527	G7M	C2-N3-C4	4.16	119.46	112.30
32	1a	527	G7M	C8-N9-C4	4.13	117.32	107.09
32	2a	516	PSU	O2-C2-N1	-4.11	118.55	122.79
32	2a	1518	MA6	C2-N1-C6	4.11	121.86	111.83
32	2a	1518	MA6	C5-C4-N3	-4.08	121.09	126.72
1	2A	1917	PSU	C4-N3-C2	-4.08	120.75	126.37
32	1a	1518	MA6	C5-C4-N3	-4.08	121.10	126.72
1	2A	1911	PSU	C4-N3-C2	-4.07	120.77	126.37
32	2a	1519	MA6	C5-N7-C8	4.04	109.80	103.45
1	2A	1915	5MU	C1'-N1-C2	4.03	124.83	117.59
1	2A	1915	5MU	C5-C4-N3	4.01	118.81	115.32
32	2a	1519	MA6	C2-N1-C6	3.99	121.58	111.83
1	1A	1917	PSU	C4-N3-C2	-3.98	120.88	126.37
1	1A	1911	PSU	O2-C2-N1	-3.95	118.71	122.79
1	1A	1939	5MU	C5-C6-N1	-3.95	119.02	123.31
1	1A	2605	PSU	C4-N3-C2	-3.95	120.93	126.37
1	2A	1915	5MU	O4-C4-C5	-3.92	120.43	124.92
32	1a	1519	MA6	C2-N1-C6	3.88	121.30	111.83
1	2A	2605	PSU	O2-C2-N1	-3.86	118.81	122.79
32	1a	1518	MA6	C2-N1-C6	3.84	121.22	111.83
32	1a	1207	2MG	C6-C5-N7	3.84	137.27	130.29
32	1a	1207	2MG	N9-C4-N3	3.83	133.60	125.95
32	1a	516	PSU	C4-N3-C2	-3.82	121.11	126.37
32	1a	1400	5MC	C5-C6-N1	-3.79	119.20	123.31
1	2A	1942	5MC	C5-C6-N1	-3.79	119.20	123.31
32	1a	1519	MA6	C4-C5-N7	-3.77	106.27	110.58
1	1A	1939	5MU	O4-C4-C5	-3.77	120.61	124.92
1	2A	2503	2MA	C4-C5-N7	-3.74	106.31	110.58
32	2a	1400	5MC	C5-C6-N1	-3.70	119.29	123.31
1	1A	1911	PSU	C4-N3-C2	-3.70	121.27	126.37
1	1A	2251	OMG	C6-C5-N7	3.70	137.02	130.29
1	1A	1915	5MU	O4-C4-C5	-3.69	120.69	124.92
1	1A	2552	2MU	C2'-C1'-N1	-3.69	107.24	114.24
1	1A	1915	5MU	C1'-N1-C6	-3.69	115.07	121.15
32	1a	527	G7M	C1'-N9-C8	-3.68	114.31	126.74
32	1a	527	G7M	CN7-N7-C5	3.65	131.35	126.80
1	1A	1942	5MC	C5-C6-N1	-3.64	119.36	123.31
32	1a	516	PSU	O2-C2-N1	-3.61	119.07	122.79
1	1A	1939	5MU	O2-C2-N1	-3.61	118.10	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	O2-C2-N1	-3.59	119.08	122.79
32	1a	1404	5MC	C5-C6-N1	-3.59	119.41	123.31
32	2a	1518	MA6	C5-N7-C8	3.57	109.06	103.45
32	1a	1519	MA6	C5-N7-C8	3.53	109.00	103.45
32	2a	527	G7M	C1'-N9-C8	-3.52	114.84	126.74
32	1a	1519	MA6	C2-N3-C4	3.50	120.37	111.83
32	1a	1518	MA6	C5-N7-C8	3.49	108.93	103.45
32	2a	1519	MA6	C2-N3-C4	3.46	120.29	111.83
1	2A	1962	5MC	C5-C6-N1	-3.46	119.55	123.31
43	1l	92	0TD	OD2-CG-CB	3.43	120.56	113.15
32	2a	1519	MA6	N9-C8-N7	-3.43	109.08	113.94
1	2A	1939	5MU	O2-C2-N1	-3.43	118.34	122.80
32	2a	1518	MA6	C2-N3-C4	3.34	119.99	111.83
32	1a	1518	MA6	C4-C5-N7	-3.34	106.76	110.58
32	2a	967	5MC	C5-C6-N1	-3.34	119.69	123.31
1	2A	1915	5MU	C1'-N1-C6	-3.29	115.74	121.15
1	2A	2251	OMG	C6-C5-N7	3.26	136.22	130.29
32	2a	1207	2MG	C6-C5-N7	3.25	136.21	130.29
32	1a	1498	UR3	C5-C4-N3	3.25	119.32	115.04
32	2a	1404	5MC	C5-C6-N1	-3.24	119.79	123.31
32	2a	1404	5MC	C5-C4-N3	-3.22	118.46	121.75
1	1A	1962	5MC	C5-C6-N1	-3.20	119.84	123.31
32	2a	1518	MA6	C4-C5-N7	-3.19	106.93	110.58
32	1a	1207	2MG	C4-C5-N7	-3.16	105.67	110.67
1	2A	2552	2MU	C5-C4-N3	3.15	119.20	114.80
32	1a	1518	MA6	N9-C8-N7	-3.13	109.50	113.94
32	1a	967	5MC	C5-C6-N1	-3.11	119.94	123.31
32	2a	1407	5MC	C5-C4-N3	-3.08	118.60	121.75
32	1a	966	M2G	C6-C5-N7	3.07	135.87	130.29
1	1A	2503	2MA	C4-C5-N7	-3.06	107.08	110.58
32	1a	1407	5MC	C5-C6-N1	-3.05	120.00	123.31
1	2A	1939	5MU	C5-C6-N1	-3.05	120.01	123.31
1	1A	2251	OMG	C4-C5-N7	-3.04	105.85	110.67
32	1a	1518	MA6	C2-N3-C4	3.04	119.25	111.83
32	2a	966	M2G	C6-C5-N7	3.03	135.81	130.29
32	1a	1207	2MG	N1-C2-N2	3.02	119.64	116.56
1	1A	1915	5MU	O2-C2-N3	-3.01	115.94	121.49
32	2a	1498	UR3	C5-C4-N3	3.00	119.00	115.04
32	2a	1518	MA6	N9-C8-N7	-2.98	109.70	113.94
1	2A	2503	2MA	C4-N9-C8	2.95	108.83	105.74
32	1a	1519	MA6	C4-C5-C6	2.93	118.94	115.91
1	2A	2503	2MA	C5-N7-C8	2.91	108.03	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1407	5MC	C5-C6-N1	-2.90	120.16	123.31
32	1a	527	G7M	O6-C6-C5	-2.88	121.57	128.01
43	2l	92	0TD	OD2-CG-CB	2.88	119.37	113.15
32	1a	1400	5MC	C5-C4-N3	-2.82	118.86	121.75
1	2A	2503	2MA	N6-C6-N1	2.80	120.81	117.03
32	1a	967	5MC	C5-C4-N3	-2.79	118.89	121.75
32	1a	1519	MA6	N3-C4-N9	2.79	131.92	127.17
32	2a	1518	MA6	N3-C4-N9	2.79	131.91	127.17
32	1a	1498	UR3	C3U-N3-C2	2.79	122.19	117.33
1	1A	2552	2MU	O4-C4-C5	-2.78	120.37	125.16
32	1a	1519	MA6	N9-C8-N7	-2.78	109.99	113.94
1	2A	1942	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	1407	5MC	C5-C4-N3	-2.72	118.97	121.75
32	2a	1207	2MG	C4-C5-N7	-2.72	106.36	110.67
1	1A	2552	2MU	O2-C2-N1	-2.69	119.29	122.80
32	2a	966	M2G	C4-C5-N7	-2.67	106.44	110.67
1	1A	2552	2MU	C5-C4-N3	2.67	118.53	114.80
32	1a	1402	4OC	C6-C5-C4	2.64	120.19	117.00
1	2A	1962	5MC	C5-C4-N3	-2.64	119.05	121.75
1	1A	1920	OMC	O2-C2-N3	-2.63	118.18	122.33
32	2a	1400	5MC	C5-C4-N3	-2.63	119.06	121.75
32	1a	1518	MA6	N3-C4-N9	2.61	131.61	127.17
32	1a	1207	2MG	N2-C2-N3	-2.60	117.20	120.51
1	2A	1915	5MU	C5-C6-N1	-2.56	120.53	123.31
1	1A	2503	2MA	C4-N9-C8	2.55	108.42	105.74
1	2A	2503	2MA	C2-N1-C6	2.55	122.03	118.10
32	1a	1404	5MC	C5-C4-N3	-2.55	119.14	121.75
1	1A	2503	2MA	C2-N1-C6	2.55	122.02	118.10
1	2A	1911	PSU	O2-C2-N1	-2.54	120.17	122.79
1	1A	2605	PSU	O2-C2-N1	-2.54	120.17	122.79
32	1a	1498	UR3	C6-N1-C2	-2.47	119.78	121.80
32	2a	1519	MA6	N3-C4-N9	2.47	131.36	127.17
1	2A	2251	OMG	C4-C5-N7	-2.46	106.76	110.67
1	1A	2503	2MA	C5-N7-C8	2.44	107.28	103.45
32	1a	966	M2G	C4-C5-N7	-2.43	106.82	110.67
32	2a	1407	5MC	O2-C2-N3	-2.42	118.52	122.33
32	2a	527	G7M	O6-C6-C5	-2.41	122.62	128.01
1	2A	2503	2MA	N9-C8-N7	-2.37	110.57	113.94
1	2A	2552	2MU	O4-C4-C5	-2.36	121.09	125.16
1	1A	2605	PSU	O2-C2-N3	-2.36	117.68	121.86
32	2a	516	PSU	O4'-C1'-C2'	2.35	108.41	105.15
32	1a	1518	MA6	C4-C5-C6	2.34	118.33	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	967	5MC	C5-C4-N3	-2.34	119.36	121.75
1	1A	1962	5MC	C5-C4-N3	-2.34	119.36	121.75
32	1a	1207	2MG	O3'-C3'-C2'	2.33	119.28	111.82
32	2a	1518	MA6	C4-C5-C6	2.32	118.31	115.91
1	2A	1939	5MU	C5M-C5-C4	2.32	121.25	118.78
32	2a	1402	4OC	C6-C5-C4	2.31	119.79	117.00
32	1a	516	PSU	C6-C5-C4	-2.30	116.62	118.17
32	2a	1519	MA6	C4-C5-C6	2.29	118.28	115.91
1	2A	1911	PSU	C5-C6-N1	-2.28	118.97	122.14
43	1l	92	0TD	OD1-CG-CB	-2.26	117.70	122.44
1	2A	1915	5MU	O2-C2-N3	-2.26	117.31	121.49
32	2a	516	PSU	C5-C6-N1	-2.26	119.00	122.14
1	2A	1911	PSU	O2-C2-N3	-2.22	117.92	121.86
32	2a	1404	5MC	CM5-C5-C6	-2.21	119.86	122.85
1	1A	1915	5MU	C6-N1-C2	-2.20	119.11	121.30
1	2A	2605	PSU	C5-C6-N1	-2.19	119.10	122.14
1	2A	1920	OMC	O2-C2-N3	-2.16	118.92	122.33
32	1a	966	M2G	O6-C6-C5	-2.16	120.84	126.53
1	1A	1942	5MC	C5-C4-N3	-2.14	119.56	121.75
1	1A	1911	PSU	O4'-C1'-C2'	2.13	108.09	105.15
1	1A	1962	5MC	CM5-C5-C6	-2.12	119.97	122.85
1	1A	1915	5MU	C5-C6-N1	-2.12	121.01	123.31
32	1a	1407	5MC	CM5-C5-C6	-2.11	120.00	122.85
1	1A	2605	PSU	C5-C6-N1	-2.08	119.25	122.14
32	1a	1407	5MC	O2-C2-N3	-2.08	119.05	122.33
32	1a	1519	MA6	C5-C4-N9	2.08	108.08	105.81
32	2a	1519	MA6	C5-C4-N9	2.04	108.03	105.81
32	1a	1207	2MG	C8-N7-C5	2.03	107.88	104.26
1	1A	2251	OMG	C8-N7-C5	2.02	107.87	104.26
32	1a	1207	2MG	C2-N1-C6	-2.02	122.11	124.55

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	1207	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
32	2a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	1911	PSU	O4'-C1'-C5-C4
32	2a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	1911	PSU	O4'-C1'-C5-C6
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1920	OMC	C3'-C2'-O2'-CM2
1	1A	2552	2MU	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

19 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1400	5MC	2	0
1	1A	1939	5MU	1	0
32	1a	1519	MA6	2	0
1	2A	2251	OMG	2	0
32	1a	1402	4OC	1	0
32	2a	1207	2MG	1	0
32	1a	1518	MA6	3	0
1	2A	1920	OMC	1	0
1	2A	1939	5MU	3	0
1	2A	2552	2MU	1	0
32	1a	1498	UR3	1	0
1	2A	1915	5MU	1	0
1	1A	1920	OMC	1	0
32	2a	1518	MA6	2	0
32	2a	1404	5MC	1	0
32	2a	1519	MA6	2	0
1	2A	2503	2MA	1	0
32	2a	1402	4OC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1400	5MC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2525 ligands modelled in this entry, 2510 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.52	0
57	MPD	2B	217	-	7,7,7	0.32	0	9,10,10	0.30	0
58	ARG	1B	230	-	10,11,11	0.76	1 (10%)	9,13,13	1.10	1 (11%)
57	MPD	1a	1882	32	7,7,7	0.41	0	9,10,10	0.64	0
58	ARG	1F	318	54	10,11,11	0.73	1 (10%)	9,13,13	0.94	1 (11%)
60	SF4	2d	501	35	0,12,12	-	-	-		
55	HGR	1A	4022	-	39,39,39	2.48	11 (28%)	48,58,58	1.72	13 (27%)
57	MPD	2A	3733	-	7,7,7	0.30	0	9,10,10	0.36	0
57	MPD	1A	4024	-	7,7,7	0.38	0	9,10,10	0.37	0
56	ZIT	1A	4023	-	54,54,54	0.88	2 (3%)	82,83,83	1.35	11 (13%)
57	MPD	1T	204	-	7,7,7	0.30	0	9,10,10	0.34	0
55	HGR	2A	3730	-	39,39,39	2.42	10 (25%)	48,58,58	1.64	12 (25%)
60	SF4	1d	305	35	0,12,12	-	-	-		
56	ZIT	2A	3731	-	54,54,54	0.89	2 (3%)	82,83,83	1.44	12 (14%)
57	MPD	2A	3732	-	7,7,7	0.33	0	9,10,10	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	18	103	-	-	3/5/5/5	-
57	MPD	2B	217	-	-	3/5/5/5	-
58	ARG	1B	230	-	-	2/11/11/11	-
57	MPD	1a	1882	32	-	3/5/5/5	-
58	ARG	1F	318	54	-	1/11/11/11	-
60	SF4	2d	501	35	-	-	0/6/5/5
55	HGR	1A	4022	-	-	6/20/79/79	0/4/4/4
57	MPD	2A	3733	-	-	4/5/5/5	-
57	MPD	1A	4024	-	-	1/5/5/5	-
56	ZIT	1A	4023	-	-	6/72/107/107	0/3/3/3
57	MPD	1T	204	-	-	3/5/5/5	-
55	HGR	2A	3730	-	-	9/20/79/79	0/4/4/4
60	SF4	1d	305	35	-	-	0/6/5/5
56	ZIT	2A	3731	-	-	8/72/107/107	0/3/3/3
57	MPD	2A	3732	-	-	0/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4022	HGR	C12-C14	9.19	1.55	1.33
55	2A	3730	HGR	C12-C14	8.94	1.54	1.33
55	2A	3730	HGR	C5-C4	-5.53	1.39	1.49
55	1A	4022	HGR	C5-C4	-5.46	1.39	1.49
55	2A	3730	HGR	C5-C6	-5.32	1.39	1.50
55	1A	4022	HGR	C5-C6	-5.27	1.39	1.50
56	2A	3731	ZIT	O14-C1	4.94	1.45	1.34
55	2A	3730	HGR	C3-C2	-4.90	1.39	1.48
56	1A	4023	ZIT	O14-C1	4.76	1.45	1.34
55	1A	4022	HGR	C3-C2	-4.69	1.39	1.48
55	1A	4022	HGR	O4-C2	4.38	1.36	1.24
55	2A	3730	HGR	O4-C2	4.26	1.35	1.24
55	1A	4022	HGR	O1-C10	2.85	1.46	1.41
55	1A	4022	HGR	O8-C23	2.65	1.45	1.41
55	2A	3730	HGR	O1-C10	2.54	1.46	1.41
55	2A	3730	HGR	O9-C23	2.44	1.45	1.41
56	1A	4023	ZIT	O14-C14	-2.39	1.42	1.46
55	2A	3730	HGR	O8-C23	2.36	1.45	1.41
56	2A	3731	ZIT	O14-C14	-2.26	1.42	1.46
58	1B	230	ARG	OXT-C	-2.22	1.23	1.30
55	1A	4022	HGR	O9-C23	2.18	1.44	1.41
55	1A	4022	HGR	C8-C7	-2.11	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3730	HGR	C1-C2	-2.06	1.39	1.44
58	1F	318	ARG	OXT-C	-2.06	1.24	1.30
55	2A	3730	HGR	C17-N1	2.06	1.49	1.45
55	1A	4022	HGR	C1-C6	2.05	1.39	1.36
55	1A	4022	HGR	C1-C2	-2.03	1.39	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4022	HGR	C4-C5-C6	4.33	121.60	112.35
56	2A	3731	ZIT	O3B-C3B-C4B	4.20	109.94	103.86
55	2A	3730	HGR	C4-C5-C6	4.17	121.25	112.35
56	1A	4023	ZIT	O3B-C3B-C4B	3.95	109.58	103.86
56	2A	3731	ZIT	C6-C5-C4	-3.74	108.46	113.89
55	1A	4022	HGR	C4-C3-C2	-3.63	118.68	121.81
56	2A	3731	ZIT	O14-C1-C2	3.39	118.77	111.53
56	2A	3731	ZIT	O3B-C3B-C2B	-3.39	107.73	112.95
55	2A	3730	HGR	O8-C18-C22	-3.37	98.91	106.03
56	1A	4023	ZIT	C6-C5-C4	-3.26	109.17	113.89
55	2A	3730	HGR	C4-C3-C2	-3.22	119.03	121.81
55	1A	4022	HGR	O9-C22-C18	-3.20	99.27	106.03
58	1B	230	ARG	OXT-C-O	-3.16	116.92	124.08
56	1A	4023	ZIT	C14-O14-C1	-3.14	112.72	118.20
56	1A	4023	ZIT	O1A-C5-C6	3.03	110.01	106.40
55	2A	3730	HGR	O1-C10-C9	-3.02	101.14	104.98
55	2A	3730	HGR	O3-C10-C9	2.98	111.53	106.69
55	2A	3730	HGR	C9-C8-C7	-2.98	98.18	101.69
56	1A	4023	ZIT	C8B-O3B-C3B	2.97	123.55	117.51
55	1A	4022	HGR	O1-C10-C9	-2.96	101.22	104.98
55	1A	4022	HGR	C23-O9-C22	-2.92	101.86	106.31
55	1A	4022	HGR	O3-C10-C9	2.90	111.40	106.69
55	2A	3730	HGR	O4-C2-C3	-2.88	116.95	121.28
55	2A	3730	HGR	C12-C6-C1	-2.80	116.23	119.35
55	2A	3730	HGR	C10-C9-C8	-2.79	98.82	102.29
58	1F	318	ARG	OXT-C-O	-2.77	117.80	124.08
56	1A	4023	ZIT	O14-C1-C2	2.75	117.41	111.53
56	1A	4023	ZIT	C9-N10-C11	-2.73	107.52	112.06
55	1A	4022	HGR	O3-C3-C2	2.73	117.46	112.51
56	2A	3731	ZIT	C8B-O3B-C3B	2.71	123.03	117.51
56	1A	4023	ZIT	O14-C1-O1	-2.71	119.06	123.95
55	1A	4022	HGR	O4-C2-C3	-2.66	117.28	121.28
55	1A	4022	HGR	C19-C17-N1	2.63	115.46	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4022	HGR	C1-C2-C3	2.61	120.96	116.06
56	2A	3731	ZIT	O14-C1-O1	-2.57	119.31	123.95
56	2A	3731	ZIT	O5B-C5B-C4B	2.54	114.41	110.04
56	2A	3731	ZIT	C14-O14-C1	-2.54	113.77	118.20
55	2A	3730	HGR	C1-C2-C3	2.52	120.80	116.06
55	1A	4022	HGR	C12-C6-C1	-2.48	116.58	119.35
56	2A	3731	ZIT	C22-C11-C12	-2.46	110.52	113.79
55	2A	3730	HGR	O3-C3-C2	2.45	116.96	112.51
55	1A	4022	HGR	O8-C18-C22	-2.42	100.92	106.03
55	1A	4022	HGR	C10-C9-C8	-2.35	99.36	102.29
56	2A	3731	ZIT	C15-C14-C13	-2.32	110.95	115.20
56	1A	4023	ZIT	O1A-C5-C4	-2.30	108.25	111.58
56	2A	3731	ZIT	C8-C9-N10	-2.22	109.54	113.95
56	2A	3731	ZIT	C3B-C2B-C1B	-2.08	111.48	114.99
56	1A	4023	ZIT	C3B-C2B-C1B	-2.07	111.49	114.99
55	2A	3730	HGR	C10-O3-C3	-2.05	110.97	115.41
56	1A	4023	ZIT	O3B-C3B-C2B	-2.04	109.80	112.95

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3730	HGR	C2-C3-O3-C10
55	2A	3730	HGR	C14-C12-C6-C1
56	1A	4023	ZIT	C12-C11-N10-C9
56	1A	4023	ZIT	C22-C11-N10-C9
56	1A	4023	ZIT	C12-C11-N10-C21
56	1A	4023	ZIT	C22-C11-N10-C21
56	1A	4023	ZIT	C4B-C3B-O3B-C8B
56	2A	3731	ZIT	C7-C8-C9-N10
56	2A	3731	ZIT	C20-C8-C9-N10
56	2A	3731	ZIT	C22-C11-N10-C9
56	2A	3731	ZIT	C22-C11-N10-C21
56	2A	3731	ZIT	C2B-C3B-O3B-C8B
56	2A	3731	ZIT	C4B-C3B-O3B-C8B
56	2A	3731	ZIT	C7B-C3B-O3B-C8B
57	18	103	MPD	C2-C3-C4-O4
57	18	103	MPD	C2-C3-C4-C5
57	1a	1882	MPD	C2-C3-C4-O4
57	1a	1882	MPD	C2-C3-C4-C5
57	2A	3733	MPD	C2-C3-C4-O4
57	2A	3733	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
58	1B	230	ARG	NE-CD-CG-CB
55	1A	4022	HGR	C14-C12-C6-C1
58	1B	230	ARG	CA-CB-CG-CD
55	1A	4022	HGR	C12-C14-C15-O7
55	2A	3730	HGR	C12-C14-C15-O7
55	2A	3730	HGR	C12-C14-C15-N1
56	2A	3731	ZIT	C8-C9-N10-C11
55	1A	4022	HGR	C2-C3-O3-C10
57	1T	204	MPD	C1-C2-C3-C4
57	2A	3733	MPD	C1-C2-C3-C4
57	2B	217	MPD	C2-C3-C4-C5
55	1A	4022	HGR	C12-C14-C15-N1
55	1A	4022	HGR	C16-C14-C15-O7
55	2A	3730	HGR	C16-C14-C15-O7
55	2A	3730	HGR	C16-C14-C15-N1
55	2A	3730	HGR	O1-C10-O3-C3
57	1A	4024	MPD	O2-C2-C3-C4
57	2B	217	MPD	O2-C2-C3-C4
55	2A	3730	HGR	O6-C11-C7-O1
57	1T	204	MPD	C2-C3-C4-O4
57	2B	217	MPD	C2-C3-C4-O4
57	1T	204	MPD	CM-C2-C3-C4
57	18	103	MPD	C1-C2-C3-C4
57	1a	1882	MPD	CM-C2-C3-C4
57	2A	3733	MPD	CM-C2-C3-C4
56	1A	4023	ZIT	C2B-C3B-O3B-C8B
58	1F	318	ARG	OXT-C-CA-N
55	2A	3730	HGR	C19-C17-N1-C15
55	1A	4022	HGR	C16-C14-C15-N1

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	18	103	MPD	1	0
58	1B	230	ARG	2	0
57	1a	1882	MPD	5	0
58	1F	318	ARG	2	0
55	1A	4022	HGR	1	0
57	1T	204	MPD	1	0
55	2A	3730	HGR	2	0
60	1d	305	SF4	2	0

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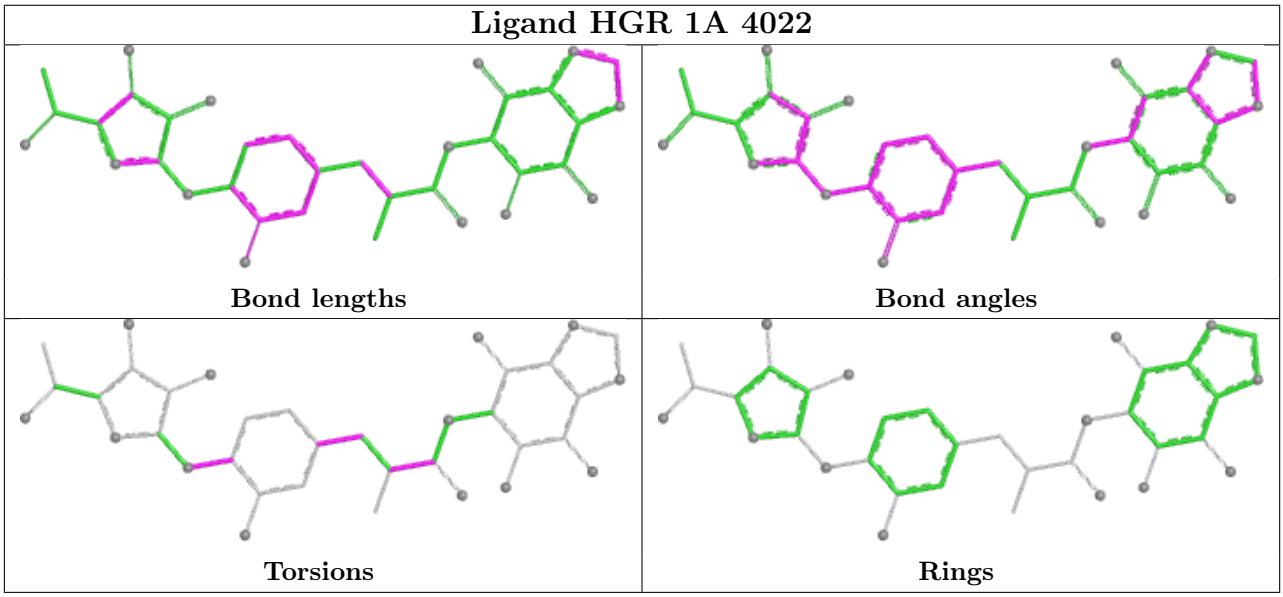
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2A	3731	ZIT	2	0
57	2A	3732	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

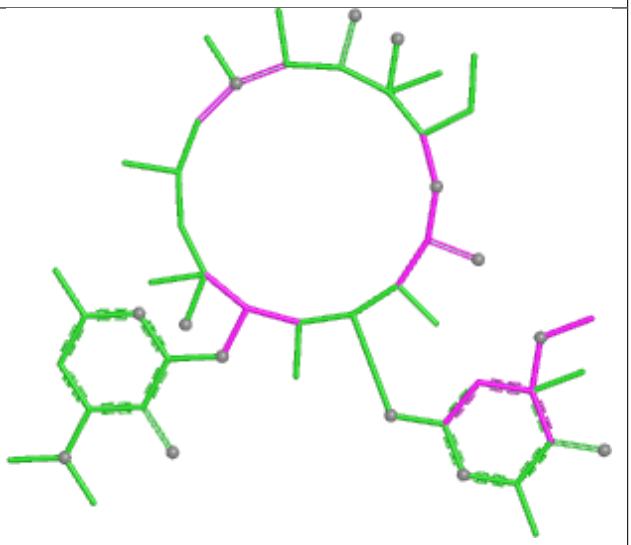
Ligand HGR 1A 4022



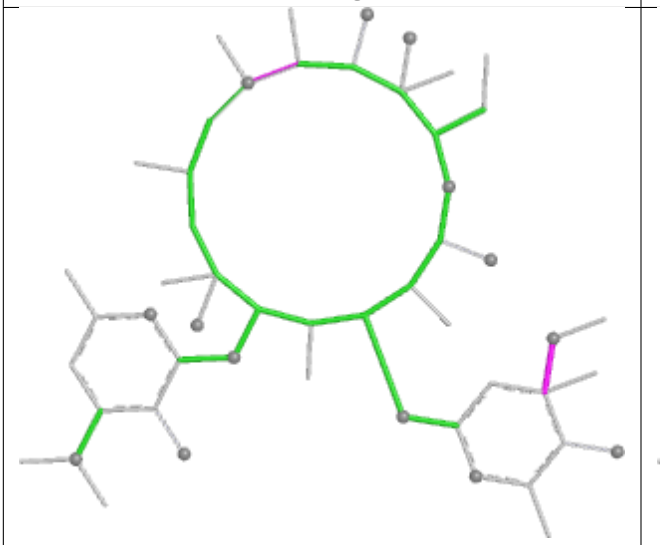
Ligand ZIT 1A 4023



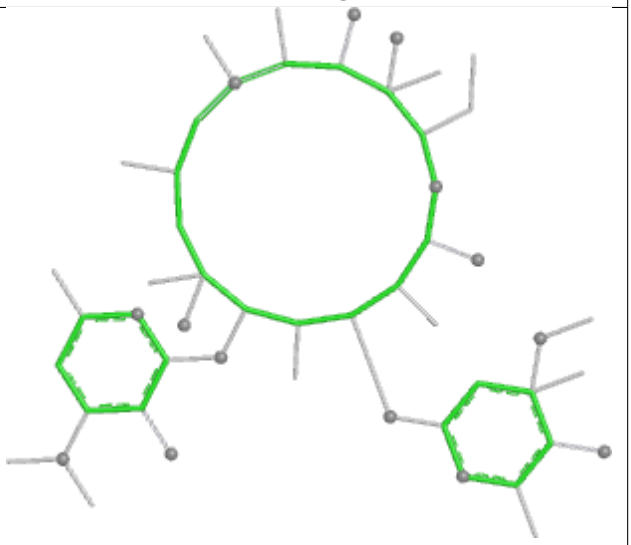
Bond lengths



Bond angles

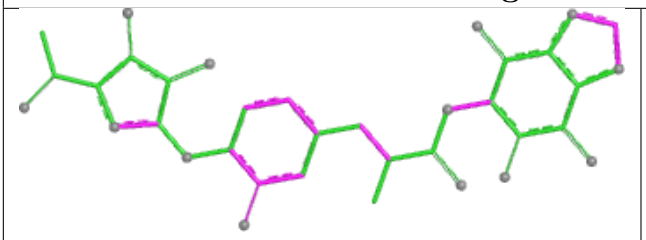


Torsions

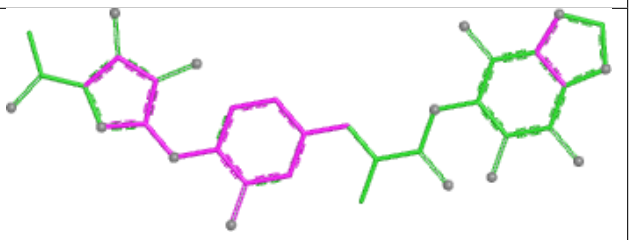


Rings

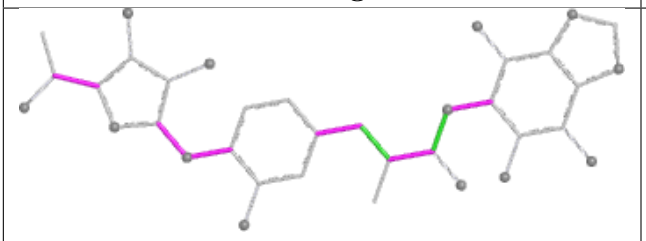
Ligand HGR 2A 3730



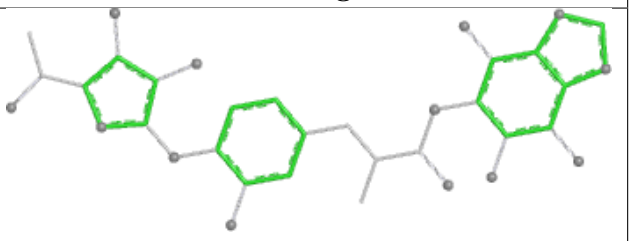
Bond lengths



Bond angles

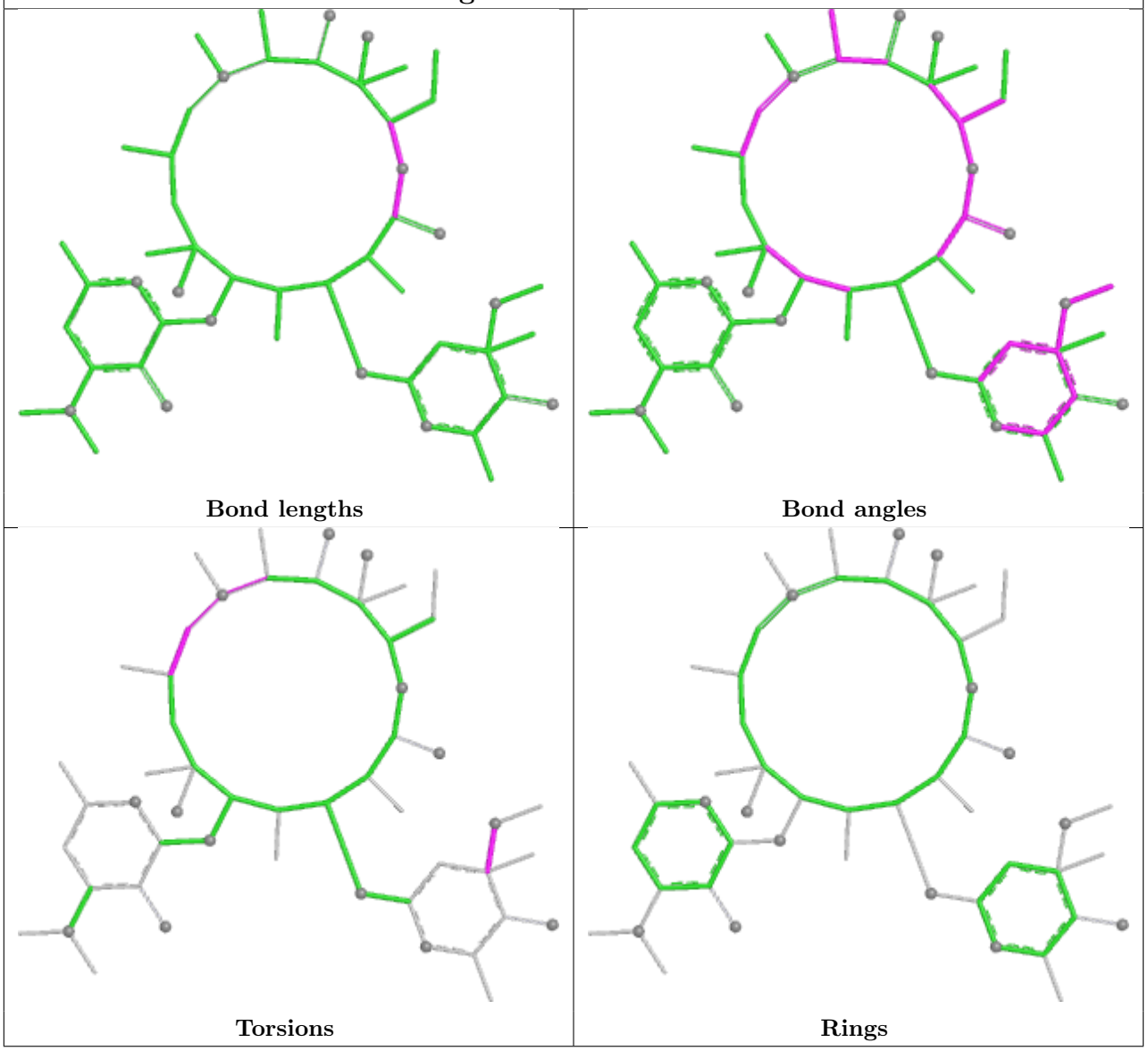


Torsions



Rings

Ligand ZIT 2A 3731



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2861/2915 (98%)	-0.58	109 (3%) 44 39	26, 41, 95, 108	0
1	2A	2856/2915 (97%)	-0.21	127 (4%) 39 34	37, 59, 98, 107	0
2	1B	120/121 (99%)	-0.49	1 (0%) 82 80	36, 54, 69, 84	0
2	2B	120/121 (99%)	0.30	2 (1%) 69 65	61, 78, 86, 90	0
3	1D	275/276 (99%)	-0.08	1 (0%) 88 86	28, 43, 56, 75	0
3	2D	275/276 (99%)	0.17	1 (0%) 88 86	36, 54, 64, 79	0
4	1E	204/206 (99%)	-0.07	2 (0%) 79 76	26, 45, 65, 80	0
4	2E	204/206 (99%)	0.17	2 (0%) 79 76	37, 59, 73, 88	0
5	1F	203/210 (96%)	-0.10	1 (0%) 87 85	25, 46, 71, 86	0
5	2F	203/210 (96%)	0.42	2 (0%) 79 76	36, 67, 80, 87	0
6	1G	181/182 (99%)	0.47	6 (3%) 49 45	52, 67, 81, 86	0
6	2G	181/182 (99%)	1.33	31 (17%) 4 3	74, 82, 89, 93	0
7	1H	174/180 (96%)	0.15	1 (0%) 85 83	41, 56, 69, 74	0
7	2H	173/180 (96%)	1.08	15 (8%) 16 14	70, 81, 89, 92	0
8	1I	147/148 (99%)	0.71	3 (2%) 65 61	48, 73, 82, 87	0
8	2I	146/148 (98%)	1.12	19 (13%) 7 6	60, 75, 85, 90	0
9	1N	140/140 (100%)	-0.13	0 100 100	30, 43, 62, 77	0
9	2N	140/140 (100%)	0.40	1 (0%) 84 81	49, 64, 77, 79	0
10	1O	122/122 (100%)	-0.07	0 100 100	34, 45, 60, 66	0
10	2O	122/122 (100%)	0.39	2 (1%) 70 67	46, 57, 72, 76	0
11	1P	149/150 (99%)	0.03	0 100 100	26, 50, 68, 84	0
11	2P	149/150 (99%)	0.50	1 (0%) 84 81	43, 67, 81, 86	0
12	1Q	141/141 (100%)	-0.16	0 100 100	31, 44, 56, 72	0
12	2Q	141/141 (100%)	0.72	4 (2%) 55 50	47, 65, 74, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.25	0 100 100	31, 40, 51, 62	0
13	2R	118/118 (100%)	0.15	1 (0%) 82 80	41, 54, 64, 71	0
14	1S	110/112 (98%)	0.21	1 (0%) 81 78	44, 53, 65, 71	0
14	2S	110/112 (98%)	1.05	9 (8%) 17 15	65, 74, 79, 85	0
15	1T	131/146 (89%)	0.05	4 (3%) 51 47	38, 48, 70, 86	0
15	2T	131/146 (89%)	0.38	2 (1%) 72 68	51, 61, 79, 85	0
16	1U	116/118 (98%)	-0.33	0 100 100	27, 36, 49, 63	0
16	2U	116/118 (98%)	0.33	1 (0%) 81 78	42, 60, 72, 77	0
17	1V	101/101 (100%)	-0.22	0 100 100	28, 45, 61, 68	0
17	2V	101/101 (100%)	0.49	1 (0%) 79 76	42, 70, 78, 83	0
18	1W	112/113 (99%)	-0.21	1 (0%) 81 78	29, 37, 57, 81	0
18	2W	112/113 (99%)	0.14	1 (0%) 81 78	40, 51, 69, 87	0
19	1X	95/96 (98%)	0.08	3 (3%) 50 46	33, 41, 64, 76	0
19	2X	95/96 (98%)	0.42	3 (3%) 50 46	48, 62, 73, 81	0
20	1Y	107/110 (97%)	0.18	1 (0%) 81 78	40, 52, 65, 74	0
20	2Y	107/110 (97%)	0.80	4 (3%) 45 40	61, 70, 80, 85	0
21	1Z	203/206 (98%)	0.36	3 (1%) 72 68	41, 61, 75, 84	0
21	2Z	201/206 (97%)	1.00	12 (5%) 27 24	67, 78, 86, 89	0
22	10	77/85 (90%)	-0.04	1 (1%) 75 71	34, 42, 59, 66	0
22	20	77/85 (90%)	0.97	9 (11%) 9 7	50, 64, 72, 84	0
23	11	97/98 (98%)	0.09	1 (1%) 79 76	34, 48, 69, 74	0
23	21	97/98 (98%)	0.58	4 (4%) 41 37	43, 59, 75, 78	0
24	12	70/72 (97%)	0.25	2 (2%) 53 49	41, 53, 62, 79	0
24	22	70/72 (97%)	0.64	2 (2%) 53 49	60, 71, 78, 80	0
25	13	59/60 (98%)	-0.06	1 (1%) 69 65	28, 41, 66, 74	0
25	23	59/60 (98%)	0.34	0 100 100	53, 62, 74, 84	0
26	14	69/71 (97%)	0.90	11 (15%) 5 4	61, 79, 92, 93	0
26	24	69/71 (97%)	1.71	22 (31%) 1 1	82, 89, 94, 95	0
27	15	59/60 (98%)	-0.26	0 100 100	26, 39, 53, 63	0
27	25	59/60 (98%)	0.04	0 100 100	36, 52, 66, 75	0
28	16	53/54 (98%)	-0.11	0 100 100	38, 47, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.51	3 (5%) 29 26	54, 63, 71, 76	0
29	17	48/49 (97%)	-0.18	2 (4%) 40 36	27, 34, 58, 67	0
29	27	48/49 (97%)	0.10	2 (4%) 40 36	38, 46, 66, 76	0
30	18	64/65 (98%)	-0.27	0 100 100	33, 39, 45, 55	0
30	28	64/65 (98%)	0.54	1 (1%) 70 67	49, 56, 63, 70	0
31	19	37/37 (100%)	0.02	0 100 100	36, 46, 60, 64	0
31	29	37/37 (100%)	0.89	1 (2%) 56 51	58, 66, 73, 76	0
32	1a	1488/1521 (97%)	0.04	26 (1%) 69 65	42, 71, 94, 109	0
32	2a	1492/1521 (98%)	0.30	35 (2%) 61 57	51, 78, 96, 107	0
33	1b	231/256 (90%)	1.07	30 (12%) 7 6	68, 80, 89, 95	0
33	2b	231/256 (90%)	1.53	60 (25%) 1 1	75, 85, 91, 95	0
34	1c	206/239 (86%)	0.83	13 (6%) 26 23	61, 74, 84, 90	0
34	2c	206/239 (86%)	1.37	42 (20%) 3 2	78, 84, 89, 91	0
35	1d	208/209 (99%)	0.97	20 (9%) 13 11	58, 72, 81, 89	0
35	2d	208/209 (99%)	0.85	7 (3%) 48 43	64, 74, 80, 83	0
36	1e	148/162 (91%)	0.45	0 100 100	57, 68, 76, 86	0
36	2e	148/162 (91%)	0.93	5 (3%) 48 43	63, 74, 82, 87	0
37	1f	100/101 (99%)	0.33	1 (1%) 79 76	59, 69, 78, 84	0
37	2f	100/101 (99%)	0.46	0 100 100	60, 71, 78, 86	0
38	1g	155/156 (99%)	0.62	6 (3%) 43 38	68, 75, 82, 86	0
38	2g	155/156 (99%)	1.14	20 (12%) 7 6	74, 82, 87, 91	0
39	1h	137/138 (99%)	0.52	4 (2%) 53 49	59, 70, 76, 81	0
39	2h	137/138 (99%)	0.77	3 (2%) 62 58	66, 75, 80, 83	0
40	1i	127/128 (99%)	1.26	18 (14%) 6 5	67, 79, 85, 87	0
40	2i	126/128 (98%)	1.97	58 (46%) 0 0	78, 86, 90, 93	0
41	1j	97/105 (92%)	1.53	29 (29%) 1 1	62, 79, 89, 91	0
41	2j	96/105 (91%)	1.80	35 (36%) 1 1	77, 86, 91, 94	0
42	1k	114/129 (88%)	0.54	3 (2%) 57 52	50, 68, 77, 85	0
42	2k	114/129 (88%)	0.82	5 (4%) 39 34	61, 75, 82, 86	0
43	1l	121/132 (91%)	0.53	4 (3%) 49 45	54, 62, 72, 75	0
43	2l	121/132 (91%)	0.71	4 (3%) 49 45	61, 69, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.92	8 (6%) 23 20	62, 77, 82, 86	0
44	2m	114/126 (90%)	1.73	40 (35%) 1 1	77, 84, 89, 92	0
45	1n	60/61 (98%)	0.90	2 (3%) 49 45	65, 72, 79, 82	0
45	2n	60/61 (98%)	1.66	22 (36%) 1 1	77, 84, 89, 94	0
46	1o	88/89 (98%)	0.64	2 (2%) 61 57	53, 67, 78, 83	0
46	2o	88/89 (98%)	0.81	3 (3%) 48 43	62, 73, 81, 87	0
47	1p	82/88 (93%)	1.21	9 (10%) 10 8	62, 73, 82, 85	0
47	2p	82/88 (93%)	1.09	6 (7%) 21 19	64, 72, 80, 85	0
48	1q	99/105 (94%)	0.88	3 (3%) 52 48	59, 71, 78, 81	0
48	2q	99/105 (94%)	0.80	3 (3%) 52 48	59, 72, 79, 85	0
49	1r	68/88 (77%)	0.57	3 (4%) 39 34	61, 68, 80, 88	0
49	2r	68/88 (77%)	0.43	1 (1%) 72 68	65, 75, 83, 86	0
50	1s	83/93 (89%)	1.05	7 (8%) 17 15	70, 77, 83, 87	0
50	2s	83/93 (89%)	1.65	29 (34%) 1 1	79, 87, 91, 92	0
51	1t	96/106 (90%)	1.02	9 (9%) 14 12	64, 72, 80, 84	0
51	2t	98/106 (92%)	0.85	10 (10%) 12 10	60, 71, 81, 85	0
52	1u	23/27 (85%)	1.40	6 (26%) 1 1	71, 76, 78, 82	0
52	2u	23/27 (85%)	2.09	10 (43%) 0 0	79, 82, 85, 89	0
53	1y	97/113 (85%)	0.88	11 (11%) 10 8	59, 68, 77, 81	0
53	2y	96/113 (84%)	1.86	38 (39%) 1 0	73, 82, 89, 91	0
All	All	20766/21468 (96%)	0.26	1090 (5%) 33 29	25, 66, 89, 109	0

All (1090) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	12.1
1	1A	1089	G	8.9
1	1A	1090	U	8.2
1	1A	1091	G	7.5
45	2n	2	ALA	7.5
1	1A	1072	C	7.0
1	1A	1077	A	7.0
1	1A	1078	U	6.6
1	1A	1086	A	6.4
26	24	56	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	1A	1102	C	6.2
1	1A	1076	C	6.1
1	1A	1071	G	6.1
1	1A	1103	A	6.0
51	1t	103	GLY	6.0
53	2y	98	ALA	6.0
1	1A	1088	A	5.9
40	2i	102	LEU	5.9
44	2m	102	ARG	5.8
45	1n	2	ALA	5.7
1	2A	2602	A	5.7
1	1A	1092	C	5.7
53	1y	98	ALA	5.6
32	2a	1030(A)	G	5.6
23	11	2	SER	5.6
1	1A	1079	C	5.3
32	2a	1030(B)	C	5.3
1	1A	1075	C	5.2
44	1m	2	ALA	5.2
1	1A	1080	C	5.1
1	1A	1064	C	5.1
41	2j	34	VAL	5.0
12	2Q	104	PHE	5.0
1	1A	1104	C	5.0
33	2b	237	ALA	4.9
51	2t	6	PRO	4.9
41	2j	75	ILE	4.9
1	2A	1536	C	4.8
29	27	48	LYS	4.8
41	1j	4	ILE	4.8
1	2A	1064	C	4.7
1	1A	1057	A	4.7
1	1A	1093	G	4.6
40	2i	2	GLU	4.6
1	1A	1081	U	4.6
1	1A	2804	C	4.6
1	2A	2174	C	4.6
1	1A	1082	U	4.5
26	24	49	PHE	4.5
23	21	2	SER	4.5
26	14	56	VAL	4.5
33	2b	122	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
7	1H	2	SER	4.4
1	1A	1066	U	4.4
8	2I	146	ALA	4.4
51	2t	103	GLY	4.4
1	2A	2803	C	4.4
33	2b	133	LYS	4.4
40	1i	106	ALA	4.4
40	2i	105	ASP	4.3
38	2g	83	ALA	4.3
1	1A	1063	G	4.3
15	1T	130	ALA	4.3
15	1T	131	ALA	4.3
44	2m	106	ASN	4.2
33	2b	236	TYR	4.2
1	1A	2803	C	4.2
35	1d	167	GLY	4.2
41	2j	37	PRO	4.2
26	24	55	ARG	4.2
39	2h	2	LEU	4.2
1	2A	2793	G	4.2
6	2G	20	ILE	4.1
33	1b	7	VAL	4.1
1	2A	2169	A	4.1
1	2A	2147	G	4.1
1	2A	2173	A	4.1
1	2A	2805	G	4.1
53	2y	49	VAL	4.1
12	2Q	59	ARG	4.0
1	1A	1074	G	4.0
1	1A	2805	G	4.0
1	1A	1067	A	4.0
1	1A	2602	A	4.0
22	20	84	LEU	4.0
42	1k	25	TYR	4.0
26	14	59	PHE	4.0
35	1d	2	GLY	4.0
1	2A	2145	C	4.0
1	1A	1065	U	3.9
53	2y	38	HIS	3.9
1	2A	2124	G	3.9
1	2A	2804	C	3.9
8	1I	147	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
8	2I	3	VAL	3.9
32	2a	1030	C	3.9
52	2u	6	ARG	3.9
1	1A	2793	G	3.8
1	2A	2139	C	3.8
53	2y	40	ILE	3.8
35	1d	179	GLU	3.8
43	2l	18	VAL	3.8
1	1A	1085	A	3.8
8	2I	20	ASP	3.8
38	2g	16	LEU	3.8
1	2A	1076	C	3.8
21	2Z	191	VAL	3.7
12	2Q	65	PHE	3.7
1	1A	888	C	3.7
40	2i	7	THR	3.7
1	2A	2125	G	3.7
53	2y	7	SER	3.7
15	2T	130	ALA	3.7
21	2Z	51	ALA	3.7
53	2y	97	ALA	3.7
50	1s	9	VAL	3.7
1	2A	2168	G	3.7
22	20	74	ARG	3.7
41	2j	74	ILE	3.7
40	2i	125	TYR	3.7
33	2b	97	TRP	3.6
1	2A	1075	C	3.6
38	2g	80	VAL	3.6
15	1T	37	GLY	3.6
38	2g	32	ARG	3.6
1	2A	2162	G	3.6
26	24	63	TYR	3.6
50	2s	9	VAL	3.6
1	1A	2117	A	3.6
43	2l	17	LYS	3.6
26	14	63	TYR	3.6
1	1A	1176	G	3.6
1	2A	2146	C	3.5
33	2b	7	VAL	3.5
1	1A	1083	U	3.5
33	2b	136	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
41	1j	87	THR	3.5
40	1i	46	ALA	3.5
1	1A	1058	G	3.5
1	1A	1062	G	3.5
40	1i	66	ARG	3.5
40	1i	128	ARG	3.5
33	2b	230	VAL	3.5
1	1A	1101	U	3.5
1	2A	1090	U	3.5
32	2a	1257	U	3.5
1	2A	1046	A	3.4
50	2s	41	VAL	3.4
3	1D	276	LYS	3.4
21	1Z	192	ALA	3.4
48	1q	99	SER	3.4
1	2A	2153	G	3.4
33	2b	44	LEU	3.4
33	2b	132	LYS	3.4
26	24	54	GLY	3.4
53	1y	94	ALA	3.4
1	1A	34	C	3.4
1	2A	2896	C	3.4
19	1X	95	LEU	3.4
53	2y	45	PRO	3.4
40	2i	62	TYR	3.4
40	2i	18	PHE	3.4
1	1A	1070	A	3.4
26	24	50	VAL	3.4
50	1s	84	GLY	3.4
33	2b	172	ILE	3.4
40	2i	10	ARG	3.4
40	2i	126	SER	3.4
1	2A	2893	G	3.3
1	2A	2894	G	3.3
1	2A	2175	C	3.3
46	2o	75	PRO	3.3
1	2A	2892	A	3.3
41	2j	38	ILE	3.3
1	1A	1056	G	3.3
24	12	70	GLN	3.3
40	2i	9	ARG	3.3
33	1b	40	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
34	1c	159	GLY	3.3
44	2m	9	ILE	3.3
1	1A	1073	A	3.3
1	2A	2119	A	3.3
45	2n	5	ALA	3.3
36	2e	10	MET	3.3
34	1c	193	TYR	3.3
38	2g	154	TYR	3.3
53	2y	27	LEU	3.3
34	2c	79	ARG	3.3
53	2y	8	LYS	3.3
52	2u	23	PRO	3.3
44	2m	116	THR	3.3
41	2j	30	SER	3.2
1	1A	2892	A	3.2
53	2y	9	GLN	3.2
52	2u	24	ARG	3.2
35	1d	155	LEU	3.2
44	1m	117	VAL	3.2
44	2m	54	VAL	3.2
33	1b	228	GLY	3.2
1	1A	2894	G	3.2
32	2a	1031	G	3.2
32	2a	1036	G	3.2
41	2j	72	VAL	3.2
47	1p	19	ILE	3.2
40	2i	43	ALA	3.2
32	2a	1202	G	3.2
47	2p	82	GLN	3.2
14	1S	3	ARG	3.2
52	1u	24	ARG	3.2
1	2A	1085	A	3.2
20	1Y	1	MET	3.2
1	2A	614(A)	U	3.2
1	2A	2172	U	3.2
6	2G	159	VAL	3.2
33	1b	165	VAL	3.2
33	2b	15	VAL	3.2
40	2i	109	VAL	3.2
44	2m	100	GLY	3.2
52	2u	14	TRP	3.2
40	2i	101	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2802	G	3.2
40	2i	6	GLY	3.2
34	1c	107	GLN	3.1
53	1y	95	ARG	3.1
1	1A	1053	C	3.1
1	2A	2138	C	3.1
20	2Y	1	MET	3.1
33	1b	229	VAL	3.1
1	1A	1105	U	3.1
33	1b	131	PRO	3.1
40	2i	56	LEU	3.1
32	2a	1116	C	3.1
53	1y	92	GLY	3.1
32	2a	1033	G	3.1
32	1a	1286	A	3.1
33	1b	236	TYR	3.1
2	1B	1	U	3.1
50	2s	2	PRO	3.1
39	1h	2	LEU	3.1
34	2c	2	GLY	3.1
45	2n	13	THR	3.1
41	2j	33	GLN	3.1
1	2A	1091	G	3.1
1	2A	2106	G	3.1
33	1b	12	GLU	3.1
40	2i	123	PRO	3.1
6	2G	139	LEU	3.1
22	20	76	GLY	3.1
7	2H	45	VAL	3.1
41	1j	34	VAL	3.1
1	2A	2140	C	3.1
1	2A	1097	U	3.0
6	2G	87	PRO	3.0
43	1l	63	GLY	3.0
53	1y	91	LYS	3.0
53	2y	52	ALA	3.0
50	2s	80	TYR	3.0
1	1A	2118	U	3.0
1	2A	2130	U	3.0
52	2u	5	ASP	3.0
1	1A	2116	G	3.0
48	2q	68	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
53	2y	42	SER	3.0
38	1g	84	ASN	3.0
48	2q	65	ILE	3.0
50	2s	67	VAL	3.0
53	2y	46	GLN	3.0
1	2A	1079	C	3.0
1	2A	1096	A	3.0
33	2b	21	ARG	3.0
22	20	69	PHE	3.0
1	2A	2127	G	3.0
32	2a	1224	G	3.0
8	2I	92	VAL	3.0
33	2b	165	VAL	3.0
34	2c	168	ALA	3.0
33	2b	131	PRO	3.0
43	1l	64	TYR	3.0
1	2A	2107	C	3.0
33	1b	11	LEU	3.0
33	2b	121	LEU	3.0
1	2A	2118	U	3.0
1	2A	2144	U	3.0
26	14	49	PHE	3.0
1	2A	2135	A	3.0
32	1a	1001	A	3.0
51	2t	11	SER	3.0
50	2s	82	GLY	3.0
34	2c	207	VAL	2.9
53	2y	35	ILE	2.9
53	2y	54	ILE	2.9
1	1A	2147	G	2.9
1	2A	2131	G	2.9
32	2a	1032	G	2.9
45	2n	30	ALA	2.9
53	2y	33	HIS	2.9
35	1d	194	LEU	2.9
1	2A	2136	C	2.9
26	24	51	ASP	2.9
45	2n	16	PHE	2.9
32	2a	1235	U	2.9
36	2e	85	GLY	2.9
1	2A	2123	G	2.9
1	2A	2154	G	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1036	G	2.9
32	2a	1001(A)	G	2.9
44	2m	31	LYS	2.9
53	2y	61	LEU	2.9
26	24	67	TYR	2.9
40	2i	4	TYR	2.9
33	1b	17	PHE	2.9
1	1A	1026	U	2.9
1	1A	2161	C	2.9
6	2G	76	SER	2.9
1	2A	6	A	2.9
14	2S	35	ILE	2.9
32	1a	1447	A	2.9
26	14	50	VAL	2.9
40	2i	41	VAL	2.9
26	24	58	ARG	2.9
8	2I	134	PRO	2.9
39	1h	133	LEU	2.9
44	2m	59	TYR	2.9
32	1a	1257	U	2.9
1	1A	2794	C	2.9
32	2a	1030(D)	A	2.9
52	2u	15	ARG	2.9
50	2s	71	LEU	2.9
51	1t	18	GLN	2.9
44	2m	89	GLY	2.9
24	12	69	ARG	2.8
26	24	66	SER	2.8
1	2A	1082	U	2.8
1	2A	229	A	2.8
33	2b	168	THR	2.8
15	2T	131	ALA	2.8
33	1b	237	ALA	2.8
41	1j	32	ALA	2.8
33	2b	118	LEU	2.8
40	1i	75	ASP	2.8
23	21	26	ARG	2.8
28	26	54	ILE	2.8
1	2A	1083	U	2.8
4	2E	204	ALA	2.8
32	1a	1030	C	2.8
1	2A	1067	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2176	A	2.8
33	2b	86	GLU	2.8
33	2b	17	PHE	2.8
41	2j	78	ASN	2.8
40	2i	17	VAL	2.8
1	1A	2112	G	2.8
1	2A	171	G	2.8
1	2A	1071	G	2.8
32	2a	1030(C)	G	2.8
10	2O	51	ALA	2.8
22	20	43	THR	2.8
34	2c	52	LEU	2.8
41	2j	32	ALA	2.8
44	2m	75	ALA	2.8
1	1A	887	A	2.8
6	1G	48	GLU	2.8
36	2e	22	GLY	2.8
33	2b	201	ILE	2.8
33	1b	37	ASN	2.8
41	2j	91	PRO	2.8
33	2b	73	THR	2.8
41	2j	67	THR	2.8
1	2A	2152	G	2.8
32	1a	1026	G	2.8
33	2b	130	ARG	2.8
40	2i	66	ARG	2.8
44	2m	65	LYS	2.8
1	1A	2114	A	2.8
1	1A	2158	A	2.8
20	2Y	80	GLY	2.7
50	2s	68	GLY	2.7
53	2y	48	PHE	2.8
7	2H	21	PRO	2.7
42	2k	117	ASN	2.7
53	2y	64	SER	2.7
8	2I	18	VAL	2.7
7	2H	7	LEU	2.7
7	2H	129	THR	2.7
38	2g	116	ALA	2.7
40	2i	127	LYS	2.7
26	24	57	GLU	2.7
53	2y	44	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2792	G	2.7
26	14	45	GLY	2.7
50	2s	19	VAL	2.7
33	1b	10	LEU	2.7
41	1j	27	ALA	2.7
41	1j	100	THR	2.7
43	1l	20	LYS	2.7
14	2S	3	ARG	2.7
40	2i	42	ARG	2.7
44	2m	3	ARG	2.7
2	2B	1	U	2.7
50	1s	13	ASP	2.7
44	2m	85	GLY	2.7
1	1A	1100	C	2.7
1	2A	888	C	2.7
1	2A	2126	A	2.7
1	2A	2143	C	2.7
1	2A	2801(A)	A	2.7
41	1j	76	ASN	2.7
41	2j	76	ASN	2.7
8	1I	3	VAL	2.7
40	1i	126	SER	2.7
40	2i	53	VAL	2.7
21	1Z	1	MET	2.7
44	2m	82	MET	2.7
45	2n	59	ALA	2.7
50	1s	77	THR	2.7
1	2A	2167	U	2.7
1	2A	2808	U	2.7
53	2y	51	ASP	2.7
40	2i	115	GLY	2.7
41	2j	36	GLY	2.7
41	1j	75	ILE	2.7
1	1A	2119	A	2.7
1	2A	2133	G	2.7
1	2A	2159	G	2.7
1	2A	2170	A	2.7
32	1a	1001(A)	G	2.7
14	2S	33	LYS	2.7
34	2c	4	LYS	2.7
6	2G	15	VAL	2.7
22	20	75	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
41	1j	24	VAL	2.7
6	1G	146	TYR	2.7
26	24	53	GLU	2.7
47	2p	38	TYR	2.7
41	2j	100	THR	2.7
53	1y	2	THR	2.7
26	24	46	GLN	2.7
26	24	65	ASP	2.6
40	2i	91	ASP	2.6
26	14	64	GLY	2.6
34	1c	10	PHE	2.6
52	2u	20	LYS	2.6
1	1A	1084	A	2.6
1	2A	1084	A	2.6
33	2b	174	VAL	2.6
44	2m	15	VAL	2.6
53	2y	41	LEU	2.6
1	1A	889	C	2.6
1	2A	1074	G	2.6
1	2A	2116	G	2.6
1	2A	2142	C	2.6
1	2A	2155	G	2.6
32	2a	1003	G	2.6
7	2H	165	ALA	2.6
40	2i	13	ALA	2.6
40	2i	36	TYR	2.6
45	2n	34	TYR	2.6
34	1c	62	ASP	2.6
50	1s	8	GLY	2.6
33	1b	39	ILE	2.6
33	2b	232	PRO	2.6
41	2j	40	LEU	2.6
53	2y	81	LEU	2.6
44	2m	58	GLU	2.6
1	2A	2171	A	2.6
1	1A	2146	C	2.6
40	2i	94	ALA	2.6
44	1m	116	THR	2.6
49	2r	20	ALA	2.6
53	2y	6	THR	2.6
1	2A	2160	G	2.6
1	2A	2807	G	2.6

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Mol	Chain	Res	Type	RSRZ
8	2I	106	GLY	2.6
44	2m	24	GLY	2.6
51	2t	96	GLY	2.6
51	2t	102	GLY	2.6
1	1A	2167	U	2.6
34	2c	77	ILE	2.6
34	2c	152	ILE	2.6
40	2i	104	ARG	2.6
33	2b	48	MET	2.6
33	2b	163	PHE	2.6
8	2I	38	LEU	2.6
40	1i	56	LEU	2.6
41	1j	44	VAL	2.6
1	1A	2173	A	2.6
1	2A	1086	A	2.6
8	2I	129	THR	2.6
32	2a	1236	A	2.6
50	2s	33	THR	2.6
53	2y	66	LYS	2.6
1	1A	1099	G	2.6
1	1A	2792	G	2.6
35	1d	76	ARG	2.6
40	2i	21	PRO	2.6
14	2S	40	ILE	2.6
41	1j	6	ILE	2.6
33	2b	57	PHE	2.6
38	1g	16	LEU	2.6
34	2c	138	VAL	2.6
44	2m	7	VAL	2.6
29	17	45	ALA	2.6
41	1j	26	ALA	2.6
19	1X	69	TYR	2.6
1	1A	2139	C	2.5
1	2A	2105	C	2.5
1	2A	2137	C	2.5
41	2j	5	ARG	2.5
50	2s	34	TRP	2.5
1	1A	2115	G	2.5
1	1A	2148	G	2.5
1	1A	2893	G	2.5
33	2b	152	PHE	2.5
40	2i	99	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
38	1g	11	GLN	2.5
42	1k	117	ASN	2.5
45	2n	18	VAL	2.5
6	1G	50	ALA	2.5
38	2g	25	ALA	2.5
38	2g	128	ALA	2.5
40	2i	106	ALA	2.5
45	2n	17	LYS	2.5
1	2A	2117	A	2.5
12	2Q	1	MET	2.5
34	2c	185	GLY	2.5
40	2i	49	PRO	2.5
41	1j	77	PRO	2.5
1	1A	2129	C	2.5
1	1A	2138	C	2.5
32	1a	1030(B)	C	2.5
6	2G	23	PHE	2.5
1	2A	2165	G	2.5
32	1a	1002	G	2.5
51	1t	10	LEU	2.5
1	2A	2109	U	2.5
26	14	69	LYS	2.5
40	1i	14	VAL	2.5
40	2i	108	VAL	2.5
45	2n	33	VAL	2.5
45	2n	50	LYS	2.5
34	2c	200	ALA	2.5
40	2i	46	ALA	2.5
41	1j	46	ARG	2.5
7	2H	41	MET	2.5
41	1j	86	MET	2.5
6	2G	146	TYR	2.5
42	2k	25	TYR	2.5
47	1p	17	TYR	2.5
1	2A	2320	A	2.5
32	1a	1035	A	2.5
23	21	83	GLU	2.5
34	2c	5	ILE	2.5
32	1a	1027	C	2.5
32	1a	1028	C	2.5
34	1c	52	LEU	2.5
1	2A	2150	U	2.5

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Mol	Chain	Res	Type	RSRZ
6	2G	160	VAL	2.5
33	1b	19	HIS	2.5
1	1A	275	G	2.5
32	1a	1033	G	2.5
32	2a	630	G	2.5
45	1n	3	ARG	2.5
45	2n	12	ARG	2.5
14	2S	53	SER	2.5
6	2G	155	MET	2.5
40	2i	98	PRO	2.5
18	2W	112	GLY	2.5
26	24	30	GLU	2.5
31	29	37	GLY	2.5
52	2u	2	GLY	2.5
40	2i	81	ILE	2.5
41	1j	50	ILE	2.5
44	2m	4	ILE	2.5
1	1A	2790	A	2.5
6	2G	19	LEU	2.5
7	2H	71	LEU	2.5
33	2b	196	LEU	2.5
33	2b	213	LEU	2.5
50	2s	25	LYS	2.5
1	1A	2145	C	2.5
1	2A	2108	C	2.5
41	2j	62	HIS	2.5
9	2N	140	VAL	2.5
34	1c	99	VAL	2.5
41	2j	44	VAL	2.5
33	1b	36	ARG	2.5
45	2n	3	ARG	2.5
21	1Z	51	ALA	2.5
53	2y	50	ALA	2.5
1	1A	2155	G	2.5
8	2I	79	ILE	2.4
36	2e	13	ILE	2.4
41	1j	80	LYS	2.4
45	2n	15	LYS	2.4
47	2p	19	ILE	2.4
19	2X	95	LEU	2.4
34	1c	87	LEU	2.4
50	2s	5	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
50	2s	15	LEU	2.4
1	1A	229	A	2.4
47	1p	82	GLN	2.4
41	1j	66	ARG	2.4
1	1A	2143	C	2.4
32	2a	1037	C	2.4
34	2c	173	VAL	2.4
40	2i	14	VAL	2.4
32	2a	1219	U	2.4
35	1d	195	ALA	2.4
49	1r	24	ALA	2.4
41	2j	77	PRO	2.4
53	2y	68	GLU	2.4
1	1A	2153	G	2.4
2	2B	118	G	2.4
41	1j	74	ILE	2.4
33	2b	92	TYR	2.4
33	2b	95	GLN	2.4
34	2c	47	LEU	2.4
35	1d	138	TYR	2.4
35	1d	157	LEU	2.4
40	2i	88	TYR	2.4
35	1d	153	ARG	2.4
42	2k	125	PHE	2.4
40	2i	29	ASN	2.4
40	2i	86	VAL	2.4
43	1l	18	VAL	2.4
40	2i	122	ALA	2.4
20	2Y	54	LYS	2.4
26	14	57	GLU	2.4
46	1o	19	PRO	2.4
44	2m	27	LYS	2.4
34	2c	80	GLY	2.4
44	2m	6	GLY	2.4
34	2c	124	ILE	2.4
1	2A	614(B)	G	2.4
1	2A	1087	G	2.4
1	2A	2319	G	2.4
32	2a	1002	G	2.4
33	2b	11	LEU	2.4
40	1i	19	LEU	2.4
40	2i	19	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
44	2m	87	TYR	2.4
33	1b	15	VAL	2.4
33	2b	93	VAL	2.4
40	2i	44	VAL	2.4
5	2F	21	ALA	2.4
41	2j	26	ALA	2.4
47	1p	22	THR	2.4
1	2A	886	C	2.4
32	1a	1000	U	2.4
32	1a	1029	C	2.4
32	2a	1029	C	2.4
26	24	45	GLY	2.4
34	1c	2	GLY	2.4
35	1d	124	GLY	2.4
40	2i	8	GLY	2.4
50	2s	31	ILE	2.4
11	2P	99	LEU	2.4
13	2R	68	ARG	2.4
38	2g	5	ARG	2.4
38	2g	76	ARG	2.4
40	1i	91	ASP	2.4
41	2j	79	ARG	2.4
44	2m	90	LEU	2.4
48	2q	98	LEU	2.4
1	2A	1089	G	2.4
14	2S	92	TYR	2.4
24	22	1	MET	2.4
32	1a	1032	G	2.4
40	1i	125	TYR	2.4
33	2b	71	VAL	2.4
34	1c	207	VAL	2.4
41	1j	49	VAL	2.4
33	1b	22	LYS	2.4
1	1A	2801(A)	A	2.4
44	2m	33	ALA	2.4
53	1y	97	ALA	2.4
25	13	2	PRO	2.3
34	2c	7	PRO	2.3
52	1u	23	PRO	2.3
1	2A	1072	C	2.3
34	2c	171	GLY	2.3
30	28	46	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
33	1b	200	ILE	2.3
33	1b	214	ILE	2.3
34	2c	170	GLN	2.3
35	1d	126	ILE	2.3
39	1h	112	LEU	2.3
40	2i	96	LEU	2.3
41	2j	85	LEU	2.3
53	1y	70	MET	2.3
37	1f	97	PHE	2.3
21	2Z	198	LYS	2.3
40	2i	28	VAL	2.3
32	1a	1003	G	2.3
32	1a	1031	G	2.3
32	1a	1034	G	2.3
32	2a	1034	G	2.3
53	2y	79	ASN	2.3
34	2c	146	ALA	2.3
43	2l	56	ALA	2.3
45	2n	14	PRO	2.3
50	2s	42	PRO	2.3
1	1A	2170	A	2.3
1	2A	1073	A	2.3
7	2H	42	ARG	2.3
41	1j	28	ARG	2.3
50	2s	35	SER	2.3
26	14	54	GLY	2.3
51	1t	102	GLY	2.3
8	1I	38	LEU	2.3
28	26	11	LEU	2.3
41	2j	6	ILE	2.3
44	1m	56	LEU	2.3
50	1s	15	LEU	2.3
1	2A	1118	C	2.3
38	2g	33	ASP	2.3
21	2Z	1	MET	2.3
29	17	48	LYS	2.3
40	2i	11	LYS	2.3
14	2S	49	VAL	2.3
33	2b	81	VAL	2.3
42	2k	75	TYR	2.3
21	2Z	145	GLU	2.3
6	2G	163	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
33	1b	188	ALA	2.3
38	2g	147	ALA	2.3
49	1r	20	ALA	2.3
50	2s	24	ALA	2.3
1	1A	2159	G	2.3
32	1a	1023	G	2.3
32	1a	1024	G	2.3
6	1G	89	GLY	2.3
32	2a	1286	A	2.3
33	1b	97	TRP	2.3
33	2b	72	GLY	2.3
40	2i	69	GLY	2.3
45	2n	61	TRP	2.3
51	1t	69	GLY	2.3
52	1u	2	GLY	2.3
6	1G	82	LEU	2.3
6	2G	3	LEU	2.3
6	2G	53	LEU	2.3
7	2H	89	ILE	2.3
33	1b	127	ILE	2.3
34	2c	8	ILE	2.3
41	2j	90	LEU	2.3
1	2A	2113	U	2.3
47	1p	1	MET	2.3
1	2A	1509	C	2.3
32	2a	1028	C	2.3
8	2I	135	GLU	2.3
33	1b	33	TYR	2.3
53	2y	60	VAL	2.3
34	2c	129	ALA	2.3
40	2i	119	ALA	2.3
47	1p	46	PRO	2.3
51	1t	59	ALA	2.3
5	1F	208	GLY	2.3
40	2i	30	GLY	2.3
1	1A	2127	G	2.3
1	1A	2149	G	2.3
1	2A	2110	G	2.3
6	2G	43	LEU	2.3
32	1a	1030(A)	G	2.3
35	1d	101	LEU	2.3
40	1i	102	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
44	2m	46	LYS	2.3
53	1y	87	LYS	2.3
1	1A	2130	U	2.3
1	2A	34	C	2.3
1	2A	1092	C	2.3
49	1r	43	PHE	2.3
33	2b	164	VAL	2.3
15	1T	129	ARG	2.3
44	1m	113	PRO	2.3
52	1u	9	ARG	2.3
35	2d	111	ALA	2.2
47	1p	69	THR	2.2
47	2p	69	THR	2.2
3	2D	106	ILE	2.2
7	2H	136	ILE	2.2
41	1j	98	ILE	2.2
1	1A	548	A	2.2
1	2A	1070	A	2.2
28	26	42	TRP	2.2
34	2c	167	TRP	2.2
42	1k	42	TRP	2.2
1	2A	1533	G	2.2
1	2A	2148	G	2.2
1	2A	2157	G	2.2
1	1A	2150	U	2.2
7	2H	130	ARG	2.2
29	27	47	ARG	2.2
1	2A	645	C	2.2
38	1g	75	VAL	2.2
51	1t	98	PRO	2.2
8	2I	115	ALA	2.2
33	1b	207	ALA	2.2
33	2b	37	ASN	2.2
41	2j	27	ALA	2.2
40	2i	5	TYR	2.2
50	2s	79	THR	2.2
6	2G	42	GLY	2.2
23	21	28	GLY	2.2
50	2s	30	LEU	2.2
41	2j	82	ILE	2.2
40	2i	75	ASP	2.2
38	2g	156	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
6	2G	137	GLU	2.2
32	2a	1004	A	2.2
1	1A	1061	U	2.2
1	1A	1097	U	2.2
1	1A	2132	U	2.2
1	2A	2132	U	2.2
1	2A	2180	U	2.2
32	1a	630	G	2.2
26	24	41	PRO	2.2
33	2b	219	VAL	2.2
34	2c	86	VAL	2.2
39	2h	72	PRO	2.2
21	2Z	192	ALA	2.2
34	2c	50	ALA	2.2
41	1j	78	ASN	2.2
44	2m	107	ALA	2.2
53	2y	73	ALA	2.2
7	2H	175	LYS	2.2
21	2Z	99	TYR	2.2
22	20	78	TYR	2.2
40	1i	78	LYS	2.2
26	24	52	THR	2.2
33	2b	67	THR	2.2
40	2i	27	THR	2.2
41	2j	42	THR	2.2
4	2E	182	LEU	2.2
19	2X	92	LEU	2.2
34	2c	87	LEU	2.2
46	2o	89	GLY	2.2
6	2G	39	ILE	2.2
53	2y	5	ILE	2.2
41	2j	83	GLU	2.2
19	2X	68	ARG	2.2
35	1d	132	ARG	2.2
1	1A	529	A	2.2
1	1A	1098	A	2.2
1	1A	2172	U	2.2
7	2H	37	VAL	2.2
35	1d	170	VAL	2.2
36	2e	67	VAL	2.2
1	1A	1055	G	2.2
1	1A	2162	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	1171	G	2.2
1	2A	2318	G	2.2
34	2c	187	ALA	2.2
35	2d	149	ALA	2.2
51	1t	97	ALA	2.2
51	2t	7	LYS	2.2
33	2b	90	MET	2.2
1	1A	2137	C	2.2
33	2b	10	LEU	2.2
33	2b	69	LEU	2.2
33	2b	149	LEU	2.2
41	1j	88	LEU	2.2
44	1m	87	TYR	2.2
51	2t	10	LEU	2.2
35	2d	70	ILE	2.2
45	2n	7	ILE	2.2
45	2n	60	SER	2.2
41	1j	64	GLU	2.2
44	2m	69	GLU	2.2
6	2G	136	ARG	2.2
4	1E	56	PRO	2.2
53	2y	14	PRO	2.2
1	2A	2897	U	2.2
14	2S	12	PHE	2.2
21	2Z	48	PHE	2.2
21	2Z	199	LYS	2.2
32	1a	841	U	2.2
33	2b	22	LYS	2.2
35	1d	110	PHE	2.2
38	1g	43	PHE	2.2
41	2j	55	LYS	2.2
43	2l	47	LYS	2.2
34	1c	86	VAL	2.1
44	2m	45	VAL	2.1
45	2n	25	VAL	2.1
33	2b	225	ALA	2.1
34	2c	65	ALA	2.1
34	2c	149	ALA	2.1
38	2g	152	ALA	2.1
50	1s	56	GLN	2.1
51	2t	97	ALA	2.1
1	2A	2112	G	2.1

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Mol	Chain	Res	Type	RSRZ
14	2S	58	LEU	2.1
19	1X	66	LEU	2.1
33	1b	14	GLY	2.1
50	2s	16	LEU	2.1
39	1h	134	ILE	2.1
22	20	77	ARG	2.1
33	2b	134	GLU	2.1
41	2j	35	SER	2.1
48	1q	68	ARG	2.1
53	1y	42	SER	2.1
7	2H	118	PRO	2.1
8	2I	131	LYS	2.1
26	24	69	LYS	2.1
33	1b	132	LYS	2.1
38	2g	93	PRO	2.1
41	2j	63	PHE	2.1
50	2s	74	PHE	2.1
6	2G	109	VAL	2.1
16	2U	90	VAL	2.1
34	2c	130	VAL	2.1
35	2d	8	VAL	2.1
41	1j	72	VAL	2.1
1	1A	2144	U	2.1
1	2A	2122	U	2.1
53	2y	67	HIS	2.1
1	2A	2114	A	2.1
24	22	70	GLN	2.1
8	2I	55	ALA	2.1
34	2c	60	ALA	2.1
34	2c	163	ALA	2.1
35	1d	111	ALA	2.1
38	2g	117	ALA	2.1
53	2y	63	ALA	2.1
6	2G	133	LEU	2.1
10	2O	74	GLY	2.1
22	10	84	LEU	2.1
34	2c	175	LEU	2.1
41	1j	65	LEU	2.1
51	2t	69	GLY	2.1
8	2I	109	ILE	2.1
34	2c	14	ILE	2.1
6	1G	21	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	3	ARG	2.1
20	2Y	55	TYR	2.1
35	2d	50	ARG	2.1
40	1i	107	ARG	2.1
44	2m	29	ARG	2.1
1	1A	2141	G	2.1
1	1A	2166	G	2.1
1	2A	2166	G	2.1
41	2j	58	ASP	2.1
50	2s	12	ASP	2.1
6	2G	182	LYS	2.1
39	2h	56	LYS	2.1
42	2k	124	LYS	2.1
6	2G	80	PHE	2.1
18	1W	111	HIS	2.1
53	2y	3	MET	2.1
6	2G	28	VAL	2.1
21	2Z	90	VAL	2.1
26	24	35	VAL	2.1
44	2m	53	VAL	2.1
44	2m	98	VAL	2.1
50	2s	11	VAL	2.1
5	2F	172	TRP	2.1
32	1a	1446	U	2.1
32	2a	1000	U	2.1
33	1b	13	ALA	2.1
34	2c	189	ALA	2.1
38	2g	2	ALA	2.1
41	1j	18	ALA	2.1
44	1m	51	ALA	2.1
50	2s	53	ASN	2.1
1	2A	1088	A	2.1
32	2a	1001	A	2.1
40	1i	47	LEU	2.1
40	2i	40	LEU	2.1
40	2i	64	THR	2.1
40	2i	103	THR	2.1
47	2p	25	ARG	2.1
26	14	53	GLU	2.1
34	2c	182	ILE	2.1
35	1d	192	GLU	2.1
44	2m	22	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
40	1i	114	TYR	2.1
33	2b	169	LYS	2.1
44	2m	36	LYS	2.1
1	1A	1068	G	2.1
1	2A	2141	G	2.1
1	2A	2149	G	2.1
32	2a	1026	G	2.1
1	1A	2107	C	2.1
1	1A	2142	C	2.1
1	2A	2111	C	2.1
1	2A	2128	C	2.1
1	2A	2179	C	2.1
32	2a	1006	C	2.1
40	2i	90	PRO	2.1
44	2m	41	PRO	2.1
6	2G	41	GLN	2.1
34	2c	70	VAL	2.1
38	2g	118	VAL	2.1
8	2I	65	ALA	2.1
34	2c	71	ALA	2.1
1	2A	12	U	2.1
38	2g	99	LEU	2.1
45	2n	6	LEU	2.1
45	2n	55	GLY	2.1
46	2o	68	ARG	2.1
48	1q	91	ARG	2.1
50	2s	20	LEU	2.1
52	2u	9	ARG	2.1
34	2c	90	GLU	2.1
40	1i	64	THR	2.1
44	2m	37	THR	2.1
50	2s	63	THR	2.1
52	1u	17	THR	2.1
6	2G	52	ILE	2.1
33	2b	208	ILE	2.1
53	2y	12	ILE	2.1
21	2Z	201	LYS	2.1
33	2b	148	TYR	2.1
38	1g	85	TYR	2.1
38	2g	85	TYR	2.1
1	1A	886	C	2.1
1	1A	2802	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	2120	G	2.0
1	2A	2121	G	2.0
1	2A	2161	C	2.1
1	2A	2789	C	2.1
32	2a	1118	C	2.1
33	1b	70	PHE	2.0
33	2b	181	PHE	2.0
34	2c	103	VAL	2.0
34	2c	186	PHE	2.0
35	1d	8	VAL	2.0
6	2G	171	ALA	2.0
33	2b	13	ALA	2.0
51	2t	86	ARG	2.0
41	2j	69	ASN	2.0
47	1p	49	LEU	2.0
53	2y	4	ASN	2.0
53	2y	77	LEU	2.0
6	2G	100	TRP	2.0
17	2V	63	GLY	2.0
33	2b	89	GLY	2.0
35	2d	180	GLY	2.0
41	1j	31	GLY	2.0
50	2s	64	GLU	2.0
21	2Z	170	THR	2.0
32	2a	1025	U	2.0
44	2m	64	TRP	2.0
33	2b	58	ILE	2.0
35	1d	5	ILE	2.0
35	2d	158	ILE	2.0
46	1o	3	ILE	2.0
1	1A	2629	A	2.0
1	2A	887	A	2.0
1	2A	1069	A	2.0
32	2a	994	A	2.0
41	2j	59	SER	2.0
8	2I	136	VAL	2.0
26	24	62	ARG	2.0
34	2c	131	ARG	2.0
44	2m	104	ARG	2.0
47	2p	80	PHE	2.0
51	1t	8	ARG	2.0
1	1A	1173	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	1047	G	2.0
32	2a	1373	G	2.0
8	2I	35	LEU	2.0
33	1b	34	ALA	2.0
34	1c	100	ALA	2.0
40	1i	15	ALA	2.0
44	2m	18	ALA	2.0
44	2m	66	LEU	2.0
45	2n	20	ALA	2.0
4	1E	57	LYS	2.0
8	2I	85	GLU	2.0
33	2b	139	LYS	2.0
34	1c	90	GLU	2.0
6	2G	123	ASN	2.0
44	1m	115	LYS	2.0
52	1u	16	GLY	2.0
53	1y	36	ASN	2.0
6	2G	144	ILE	2.0
6	2G	145	THR	2.0
33	2b	190	THR	2.0
44	2m	78	ILE	2.0
1	1A	2126	A	2.0
22	20	71	ASP	2.0
32	2a	532	A	2.0
47	1p	68	ASP	2.0
26	24	32	TYR	2.0
33	2b	140	HIS	2.0
33	2b	233	SER	2.0
50	2s	14	HIS	2.0
52	2u	18	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.81	0.11	81,88,95,108	0
32	M2G	2a	966	25/26	0.86	0.16	67,77,87,95	0
32	2MG	2a	1207	24/25	0.86	0.13	83,89,95,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	1A	1915	21/22	0.88	0.11	76,81,85,87	0
1	PSU	2A	1911	20/21	0.89	0.09	64,75,83,88	0
1	PSU	2A	1917	20/21	0.90	0.08	72,80,90,94	0
1	PSU	1A	1917	20/21	0.91	0.10	69,74,81,85	0
43	0TD	1l	92	10/11	0.92	0.11	57,62,66,72	0
32	5MC	2a	967	21/22	0.92	0.12	72,78,84,88	0
32	2MG	1a	1207	24/25	0.92	0.10	65,75,77,81	0
43	0TD	2l	92	10/11	0.92	0.11	64,68,70,82	0
1	PSU	1A	1911	20/21	0.94	0.08	63,72,79,83	0
1	OMC	2A	1920	21/22	0.94	0.09	67,71,74,78	0
32	PSU	2a	516	20/21	0.94	0.08	70,78,80,80	0
32	G7M	2a	527	24/25	0.94	0.10	61,68,75,80	0
32	PSU	1a	516	20/21	0.95	0.08	58,66,71,73	0
32	4OC	2a	1402	22/23	0.95	0.09	60,69,74,76	0
32	5MC	2a	1404	21/22	0.95	0.09	60,68,71,75	0
32	5MC	1a	967	21/22	0.95	0.11	65,72,79,85	0
32	5MC	1a	1407	21/22	0.96	0.10	50,60,64,65	0
32	MA6	1a	1518	24/25	0.96	0.10	48,54,59,60	0
32	M2G	1a	966	25/26	0.96	0.10	60,66,70,74	0
1	OMC	1A	1920	21/22	0.96	0.10	46,62,65,65	0
32	G7M	1a	527	24/25	0.96	0.09	54,59,65,68	0
32	5MC	2a	1400	21/22	0.96	0.09	71,75,77,81	0
32	4OC	1a	1402	22/23	0.96	0.10	53,58,62,67	0
32	5MC	1a	1404	21/22	0.96	0.09	49,54,57,62	0
32	5MC	2a	1407	21/22	0.96	0.09	61,69,73,81	0
32	UR3	2a	1498	21/22	0.96	0.08	63,67,70,72	0
32	MA6	2a	1518	24/25	0.96	0.10	62,68,74,75	0
32	MA6	2a	1519	24/25	0.96	0.11	61,68,71,71	0
1	5MC	2A	1942	21/22	0.96	0.08	50,58,64,66	0
32	UR3	1a	1498	21/22	0.97	0.09	52,57,61,66	0
1	5MC	2A	1962	21/22	0.97	0.07	43,50,54,64	0
1	OMG	2A	2251	24/25	0.97	0.08	40,44,47,48	0
1	2MA	2A	2503	23/24	0.97	0.07	33,37,43,49	0
1	2MU	2A	2552	21/23	0.97	0.07	39,45,48,49	0
32	5MC	1a	1400	21/22	0.97	0.10	53,58,63,66	0
32	MA6	1a	1519	24/25	0.97	0.09	46,55,60,61	0
1	PSU	1A	2605	20/21	0.97	0.09	29,34,40,40	0
1	5MU	2A	1939	21/22	0.97	0.08	35,42,47,50	0
1	PSU	2A	2605	20/21	0.98	0.07	34,42,46,48	0
1	5MU	1A	1939	21/22	0.98	0.07	29,33,37,38	0
1	5MC	1A	1942	21/22	0.98	0.06	35,44,49,58	0
1	5MC	1A	1962	21/22	0.98	0.07	35,40,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMG	1A	2251	24/25	0.98	0.07	26,32,35,35	0
1	2MA	1A	2503	23/24	0.98	0.06	21,29,32,34	0
1	2MU	1A	2552	21/23	0.98	0.07	28,36,39,45	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3985	1/1	0.54	0.18	41,41,41,41	0
54	MG	2a	3182	1/1	0.59	0.32	84,84,84,84	0
54	MG	2A	3327	1/1	0.61	0.34	78,78,78,78	0
54	MG	1a	1778	1/1	0.61	0.19	79,79,79,79	0
54	MG	2A	3534	1/1	0.63	0.32	74,74,74,74	0
54	MG	2A	3468	1/1	0.66	0.33	67,67,67,67	0
54	MG	1B	226	1/1	0.68	0.15	81,81,81,81	0
54	MG	2A	3476	1/1	0.68	0.27	65,65,65,65	0
54	MG	1a	1878	1/1	0.69	0.20	88,88,88,88	0
54	MG	1a	1744	1/1	0.69	0.25	86,86,86,86	0
54	MG	1A	3292	1/1	0.69	0.16	84,84,84,84	0
54	MG	2G	201	1/1	0.70	0.22	81,81,81,81	0
54	MG	2A	3501	1/1	0.71	0.22	70,70,70,70	0
54	MG	2A	3463	1/1	0.71	0.39	61,61,61,61	0
54	MG	2A	3265	1/1	0.71	0.27	85,85,85,85	0
54	MG	2A	3193	1/1	0.71	0.30	78,78,78,78	0
54	MG	1a	1805	1/1	0.72	0.16	81,81,81,81	0
54	MG	1A	3989	1/1	0.72	0.21	80,80,80,80	0
54	MG	1a	1786	1/1	0.73	0.25	74,74,74,74	0
54	MG	1A	3533	1/1	0.73	0.16	59,59,59,59	0
54	MG	2A	3713	1/1	0.73	0.17	66,66,66,66	0
54	MG	1A	3186	1/1	0.73	0.19	64,64,64,64	0
54	MG	2O	202	1/1	0.73	0.15	82,82,82,82	0
54	MG	2a	3020	1/1	0.73	0.17	90,90,90,90	0
54	MG	2A	3499	1/1	0.73	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3464	1/1	0.74	0.12	59,59,59,59	0
54	MG	1A	3832	1/1	0.74	0.27	47,47,47,47	0
54	MG	1a	1811	1/1	0.75	0.19	85,85,85,85	0
54	MG	1a	1722	1/1	0.75	0.24	77,77,77,77	0
54	MG	1a	1781	1/1	0.75	0.14	67,67,67,67	0
54	MG	2A	3723	1/1	0.75	0.38	77,77,77,77	0
54	MG	1A	3621	1/1	0.76	0.20	69,69,69,69	0
54	MG	2A	3666	1/1	0.76	0.20	82,82,82,82	0
54	MG	2A	3675	1/1	0.76	0.32	71,71,71,71	0
54	MG	2A	3345	1/1	0.76	0.29	81,81,81,81	0
54	MG	1a	1773	1/1	0.76	0.17	72,72,72,72	0
54	MG	1A	3664	1/1	0.76	0.17	70,70,70,70	0
54	MG	2A	3111	1/1	0.76	0.16	78,78,78,78	0
54	MG	1A	3198	1/1	0.76	0.12	67,67,67,67	0
54	MG	2a	3024	1/1	0.76	0.28	85,85,85,85	0
54	MG	1A	3960	1/1	0.76	0.15	84,84,84,84	0
54	MG	2A	3638	1/1	0.77	0.17	77,77,77,77	0
54	MG	15	106	1/1	0.77	0.18	49,49,49,49	0
54	MG	1a	1670	1/1	0.77	0.26	81,81,81,81	0
54	MG	2A	3230	1/1	0.77	0.25	83,83,83,83	0
54	MG	1a	1685	1/1	0.77	0.34	75,75,75,75	0
54	MG	1A	3649	1/1	0.77	0.23	62,62,62,62	0
54	MG	2A	3519	1/1	0.77	0.19	64,64,64,64	0
54	MG	2A	3080	1/1	0.77	0.22	84,84,84,84	0
54	MG	2A	3554	1/1	0.77	0.20	71,71,71,71	0
54	MG	2a	3046	1/1	0.77	0.26	81,81,81,81	0
54	MG	2A	3614	1/1	0.77	0.20	62,62,62,62	0
54	MG	2j	201	1/1	0.77	0.24	74,74,74,74	0
58	ARG	1F	318	12/12	0.77	0.16	57,65,72,73	0
54	MG	1A	3862	1/1	0.78	0.14	70,70,70,70	0
54	MG	1A	3700	1/1	0.78	0.14	74,74,74,74	0
54	MG	1A	3516	1/1	0.78	0.14	56,56,56,56	0
54	MG	1a	1796	1/1	0.78	0.21	80,80,80,80	0
54	MG	2A	3263	1/1	0.78	0.14	79,79,79,79	0
54	MG	1a	1728	1/1	0.78	0.24	67,67,67,67	0
54	MG	2A	3549	1/1	0.78	0.20	61,61,61,61	0
54	MG	1a	1808	1/1	0.78	0.22	86,86,86,86	0
54	MG	2a	3055	1/1	0.78	0.28	72,72,72,72	0
54	MG	2a	3060	1/1	0.78	0.31	82,82,82,82	0
54	MG	2a	3113	1/1	0.78	0.29	77,77,77,77	0
54	MG	2a	3129	1/1	0.78	0.37	82,82,82,82	0
54	MG	2a	3144	1/1	0.78	0.31	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1641	1/1	0.78	0.25	74,74,74,74	0
54	MG	2a	3188	1/1	0.78	0.18	73,73,73,73	0
54	MG	2A	3411	1/1	0.78	0.15	70,70,70,70	0
54	MG	1a	1651	1/1	0.78	0.12	65,65,65,65	0
54	MG	2B	204	1/1	0.79	0.20	81,81,81,81	0
54	MG	2A	3488	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3489	1/1	0.79	0.17	77,77,77,77	0
54	MG	1a	1853	1/1	0.79	0.15	75,75,75,75	0
54	MG	1A	3462	1/1	0.79	0.20	80,80,80,80	0
54	MG	2A	3290	1/1	0.79	0.26	87,87,87,87	0
54	MG	2A	3291	1/1	0.79	0.14	64,64,64,64	0
54	MG	2A	3326	1/1	0.79	0.24	67,67,67,67	0
54	MG	2a	3067	1/1	0.79	0.22	76,76,76,76	0
54	MG	1d	301	1/1	0.79	0.26	83,83,83,83	0
54	MG	2A	3054	1/1	0.79	0.32	76,76,76,76	0
54	MG	1a	1757	1/1	0.79	0.20	82,82,82,82	0
54	MG	2A	3440	1/1	0.79	0.22	88,88,88,88	0
54	MG	1a	1701	1/1	0.79	0.33	82,82,82,82	0
54	MG	2a	3193	1/1	0.79	0.18	84,84,84,84	0
54	MG	1A	3495	1/1	0.79	0.13	40,40,40,40	0
54	MG	2o	101	1/1	0.79	0.13	70,70,70,70	0
54	MG	1A	3660	1/1	0.79	0.17	72,72,72,72	0
54	MG	1T	202	1/1	0.80	0.19	70,70,70,70	0
54	MG	2A	3205	1/1	0.80	0.32	72,72,72,72	0
54	MG	14	101	1/1	0.80	0.10	65,65,65,65	0
54	MG	2G	202	1/1	0.80	0.21	81,81,81,81	0
54	MG	2A	3253	1/1	0.80	0.16	69,69,69,69	0
54	MG	1A	3477	1/1	0.80	0.23	67,67,67,67	0
54	MG	1A	3502	1/1	0.80	0.12	63,63,63,63	0
54	MG	1a	1873	1/1	0.80	0.20	75,75,75,75	0
54	MG	1a	1876	1/1	0.80	0.12	63,63,63,63	0
54	MG	2A	3541	1/1	0.80	0.14	73,73,73,73	0
54	MG	1A	3597	1/1	0.80	0.14	56,56,56,56	0
54	MG	2a	3111	1/1	0.80	0.35	73,73,73,73	0
54	MG	1A	3835	1/1	0.80	0.14	68,68,68,68	0
54	MG	2A	3053	1/1	0.80	0.40	80,80,80,80	0
54	MG	2A	3629	1/1	0.80	0.13	44,44,44,44	0
54	MG	2A	3633	1/1	0.80	0.34	79,79,79,79	0
54	MG	1A	3842	1/1	0.80	0.11	63,63,63,63	0
54	MG	2A	3433	1/1	0.80	0.17	52,52,52,52	0
54	MG	2A	3669	1/1	0.80	0.22	59,59,59,59	0
54	MG	1a	1698	1/1	0.80	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1D	311	1/1	0.80	0.36	54,54,54,54	0
54	MG	2A	3023	1/1	0.81	0.21	64,64,64,64	0
54	MG	2A	3457	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3036	1/1	0.81	0.26	76,76,76,76	0
54	MG	1A	3851	1/1	0.81	0.13	63,63,63,63	0
54	MG	2A	3469	1/1	0.81	0.18	63,63,63,63	0
54	MG	2A	3273	1/1	0.81	0.45	80,80,80,80	0
54	MG	1a	1813	1/1	0.81	0.15	81,81,81,81	0
54	MG	1A	3580	1/1	0.81	0.21	64,64,64,64	0
54	MG	1A	3088	1/1	0.81	0.18	64,64,64,64	0
54	MG	1A	3657	1/1	0.81	0.27	69,69,69,69	0
54	MG	1a	1761	1/1	0.81	0.24	70,70,70,70	0
54	MG	2a	3187	1/1	0.81	0.20	45,45,45,45	0
54	MG	2A	3399	1/1	0.81	0.15	72,72,72,72	0
54	MG	2A	3216	1/1	0.81	0.27	73,73,73,73	0
54	MG	1a	1714	1/1	0.81	0.33	73,73,73,73	0
54	MG	2T	202	1/1	0.81	0.23	77,77,77,77	0
54	MG	2a	3011	1/1	0.81	0.23	74,74,74,74	0
54	MG	2A	3679	1/1	0.82	0.16	75,75,75,75	0
54	MG	1A	3918	1/1	0.82	0.14	53,53,53,53	0
54	MG	2A	3717	1/1	0.82	0.17	64,64,64,64	0
54	MG	1a	1753	1/1	0.82	0.28	64,64,64,64	0
54	MG	2A	3728	1/1	0.82	0.21	69,69,69,69	0
54	MG	1A	3217	1/1	0.82	0.33	84,84,84,84	0
54	MG	1A	3647	1/1	0.82	0.19	75,75,75,75	0
54	MG	2A	3264	1/1	0.82	0.26	71,71,71,71	0
54	MG	1a	1652	1/1	0.82	0.29	73,73,73,73	0
54	MG	1A	3542	1/1	0.82	0.17	60,60,60,60	0
54	MG	2a	3010	1/1	0.82	0.30	75,75,75,75	0
54	MG	1B	220	1/1	0.82	0.17	57,57,57,57	0
54	MG	2A	3502	1/1	0.82	0.17	70,70,70,70	0
54	MG	1A	3272	1/1	0.82	0.33	79,79,79,79	0
54	MG	2A	3317	1/1	0.82	0.55	77,77,77,77	0
54	MG	2A	3324	1/1	0.82	0.35	69,69,69,69	0
54	MG	1A	3591	1/1	0.82	0.13	44,44,44,44	0
54	MG	1a	1707	1/1	0.82	0.26	71,71,71,71	0
54	MG	2a	3072	1/1	0.82	0.18	70,70,70,70	0
54	MG	2a	3081	1/1	0.82	0.20	80,80,80,80	0
54	MG	2a	3089	1/1	0.82	0.33	81,81,81,81	0
54	MG	2A	3564	1/1	0.82	0.20	74,74,74,74	0
54	MG	2A	3587	1/1	0.82	0.17	48,48,48,48	0
54	MG	2A	3591	1/1	0.82	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3608	1/1	0.82	0.23	68,68,68,68	0
54	MG	2A	3335	1/1	0.82	0.28	70,70,70,70	0
54	MG	1O	201	1/1	0.82	0.23	67,67,67,67	0
54	MG	2A	3128	1/1	0.82	0.29	76,76,76,76	0
54	MG	2A	3189	1/1	0.82	0.32	58,58,58,58	0
54	MG	1A	3483	1/1	0.82	0.14	60,60,60,60	0
54	MG	1A	3886	1/1	0.82	0.12	70,70,70,70	0
54	MG	2A	3208	1/1	0.82	0.17	69,69,69,69	0
54	MG	2A	3699	1/1	0.83	0.20	70,70,70,70	0
54	MG	1A	3894	1/1	0.83	0.12	59,59,59,59	0
54	MG	1A	3453	1/1	0.83	0.22	74,74,74,74	0
54	MG	1A	3942	1/1	0.83	0.19	61,61,61,61	0
54	MG	1A	3189	1/1	0.83	0.12	66,66,66,66	0
54	MG	2B	202	1/1	0.83	0.17	78,78,78,78	0
54	MG	2A	3214	1/1	0.83	0.28	74,74,74,74	0
54	MG	1A	3982	1/1	0.83	0.17	66,66,66,66	0
54	MG	1A	3244	1/1	0.83	0.12	70,70,70,70	0
54	MG	2O	201	1/1	0.83	0.21	63,63,63,63	0
54	MG	2A	3493	1/1	0.83	0.20	56,56,56,56	0
54	MG	2A	3250	1/1	0.83	0.25	70,70,70,70	0
54	MG	1A	3191	1/1	0.83	0.21	82,82,82,82	0
54	MG	1a	1704	1/1	0.83	0.25	76,76,76,76	0
54	MG	1A	3789	1/1	0.83	0.14	36,36,36,36	0
54	MG	2A	3532	1/1	0.83	0.15	73,73,73,73	0
54	MG	2a	3038	1/1	0.83	0.12	82,82,82,82	0
54	MG	1a	1710	1/1	0.83	0.12	72,72,72,72	0
54	MG	2A	3540	1/1	0.83	0.17	41,41,41,41	0
54	MG	1A	3126	1/1	0.83	0.32	66,66,66,66	0
54	MG	2a	3061	1/1	0.83	0.32	75,75,75,75	0
54	MG	2a	3062	1/1	0.83	0.26	76,76,76,76	0
54	MG	1A	3421	1/1	0.83	0.17	61,61,61,61	0
54	MG	1d	302	1/1	0.83	0.23	77,77,77,77	0
54	MG	1D	316	1/1	0.83	0.13	68,68,68,68	0
54	MG	2a	3087	1/1	0.83	0.14	78,78,78,78	0
54	MG	2A	3035	1/1	0.83	0.19	64,64,64,64	0
54	MG	2a	3106	1/1	0.83	0.42	67,67,67,67	0
54	MG	1A	3635	1/1	0.83	0.12	29,29,29,29	0
54	MG	1A	3447	1/1	0.83	0.16	41,41,41,41	0
54	MG	2a	3119	1/1	0.83	0.13	67,67,67,67	0
54	MG	2A	3609	1/1	0.83	0.22	62,62,62,62	0
54	MG	11	104	1/1	0.83	0.13	70,70,70,70	0
54	MG	1A	3449	1/1	0.83	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3094	1/1	0.83	0.26	66,66,66,66	0
54	MG	1A	3652	1/1	0.83	0.36	47,47,47,47	0
54	MG	2A	3421	1/1	0.83	0.21	74,74,74,74	0
54	MG	2A	3123	1/1	0.83	0.25	79,79,79,79	0
54	MG	1a	1640	1/1	0.83	0.21	69,69,69,69	0
57	MPD	2B	217	8/8	0.83	0.26	61,68,76,77	0
54	MG	2A	3444	1/1	0.83	0.15	73,73,73,73	0
54	MG	1A	3816	1/1	0.84	0.11	80,80,80,80	0
54	MG	1l	202	1/1	0.84	0.14	81,81,81,81	0
54	MG	2a	3022	1/1	0.84	0.27	74,74,74,74	0
54	MG	2A	3232	1/1	0.84	0.26	64,64,64,64	0
54	MG	2a	3028	1/1	0.84	0.14	77,77,77,77	0
54	MG	1A	3344	1/1	0.84	0.11	59,59,59,59	0
54	MG	2A	3616	1/1	0.84	0.12	65,65,65,65	0
54	MG	1a	1783	1/1	0.84	0.14	74,74,74,74	0
54	MG	2a	3057	1/1	0.84	0.27	72,72,72,72	0
54	MG	1A	3170	1/1	0.84	0.17	66,66,66,66	0
54	MG	1a	1604	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3641	1/1	0.84	0.13	74,74,74,74	0
54	MG	2a	3063	1/1	0.84	0.28	84,84,84,84	0
54	MG	1A	3926	1/1	0.84	0.12	32,32,32,32	0
54	MG	1B	229	1/1	0.84	0.14	80,80,80,80	0
54	MG	2A	3280	1/1	0.84	0.27	75,75,75,75	0
54	MG	2a	3084	1/1	0.84	0.47	68,68,68,68	0
54	MG	1A	3687	1/1	0.84	0.17	64,64,64,64	0
54	MG	2A	3682	1/1	0.84	0.17	65,65,65,65	0
54	MG	1A	3548	1/1	0.84	0.14	51,51,51,51	0
54	MG	2A	3118	1/1	0.84	0.25	76,76,76,76	0
54	MG	1G	202	1/1	0.84	0.16	63,63,63,63	0
54	MG	2A	3513	1/1	0.84	0.13	55,55,55,55	0
54	MG	1a	1863	1/1	0.84	0.20	72,72,72,72	0
54	MG	1a	1872	1/1	0.84	0.19	84,84,84,84	0
54	MG	2A	3190	1/1	0.84	0.20	61,61,61,61	0
54	MG	1a	1674	1/1	0.84	0.27	69,69,69,69	0
54	MG	2A	3350	1/1	0.84	0.16	59,59,59,59	0
54	MG	2A	3358	1/1	0.84	0.15	60,60,60,60	0
54	MG	1A	3963	1/1	0.84	0.18	70,70,70,70	0
54	MG	1A	3294	1/1	0.84	0.17	74,74,74,74	0
54	MG	2a	3005	1/1	0.84	0.15	66,66,66,66	0
54	MG	1a	1775	1/1	0.84	0.15	76,76,76,76	0
54	MG	1A	3327	1/1	0.85	0.26	61,61,61,61	0
54	MG	1A	3983	1/1	0.85	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1681	1/1	0.85	0.19	88,88,88,88	0
54	MG	1A	3792	1/1	0.85	0.14	45,45,45,45	0
54	MG	2A	3336	1/1	0.85	0.15	41,41,41,41	0
54	MG	2A	3703	1/1	0.85	0.13	68,68,68,68	0
54	MG	2A	3704	1/1	0.85	0.12	79,79,79,79	0
54	MG	1A	3027	1/1	0.85	0.15	71,71,71,71	0
54	MG	1B	210	1/1	0.85	0.31	70,70,70,70	0
54	MG	1A	3450	1/1	0.85	0.20	63,63,63,63	0
54	MG	2A	3362	1/1	0.85	0.21	77,77,77,77	0
54	MG	1B	224	1/1	0.85	0.15	65,65,65,65	0
54	MG	1A	3354	1/1	0.85	0.14	73,73,73,73	0
54	MG	1A	3360	1/1	0.85	0.18	55,55,55,55	0
54	MG	2A	3042	1/1	0.85	0.28	81,81,81,81	0
54	MG	1A	3848	1/1	0.85	0.16	60,60,60,60	0
54	MG	1A	3310	1/1	0.85	0.19	73,73,73,73	0
54	MG	1A	3574	1/1	0.85	0.10	49,49,49,49	0
54	MG	2a	3002	1/1	0.85	0.27	70,70,70,70	0
54	MG	2a	3003	1/1	0.85	0.21	71,71,71,71	0
54	MG	1a	1746	1/1	0.85	0.18	81,81,81,81	0
54	MG	1a	1748	1/1	0.85	0.21	79,79,79,79	0
54	MG	2A	3114	1/1	0.85	0.25	65,65,65,65	0
54	MG	1H	201	1/1	0.85	0.14	64,64,64,64	0
54	MG	1A	3882	1/1	0.85	0.14	55,55,55,55	0
54	MG	1R	208	1/1	0.85	0.21	53,53,53,53	0
54	MG	2A	3162	1/1	0.85	0.35	72,72,72,72	0
54	MG	1A	3468	1/1	0.85	0.14	66,66,66,66	0
54	MG	10	106	1/1	0.85	0.14	66,66,66,66	0
54	MG	10	107	1/1	0.85	0.17	69,69,69,69	0
54	MG	2A	3203	1/1	0.85	0.20	68,68,68,68	0
54	MG	1A	3680	1/1	0.85	0.40	39,39,39,39	0
54	MG	2A	3520	1/1	0.85	0.10	67,67,67,67	0
54	MG	2A	3523	1/1	0.85	0.12	63,63,63,63	0
54	MG	1A	3424	1/1	0.85	0.16	78,78,78,78	0
54	MG	1A	3695	1/1	0.85	0.09	77,77,77,77	0
54	MG	2a	3069	1/1	0.85	0.20	73,73,73,73	0
54	MG	1a	1793	1/1	0.85	0.14	68,68,68,68	0
54	MG	2a	3080	1/1	0.85	0.09	73,73,73,73	0
54	MG	1A	3932	1/1	0.85	0.18	57,57,57,57	0
54	MG	1a	1802	1/1	0.85	0.13	79,79,79,79	0
54	MG	2A	3249	1/1	0.85	0.19	64,64,64,64	0
54	MG	2a	3088	1/1	0.85	0.20	70,70,70,70	0
54	MG	1a	1624	1/1	0.85	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3583	1/1	0.85	0.14	47,47,47,47	0
54	MG	1A	3436	1/1	0.85	0.11	66,66,66,66	0
54	MG	2A	3590	1/1	0.85	0.16	66,66,66,66	0
54	MG	1A	3945	1/1	0.85	0.12	69,69,69,69	0
54	MG	1A	3707	1/1	0.85	0.19	71,71,71,71	0
54	MG	2a	3142	1/1	0.85	0.25	67,67,67,67	0
54	MG	1a	1820	1/1	0.85	0.12	76,76,76,76	0
54	MG	2a	3180	1/1	0.85	0.14	76,76,76,76	0
54	MG	1a	1839	1/1	0.85	0.15	77,77,77,77	0
54	MG	2a	3183	1/1	0.85	0.21	69,69,69,69	0
54	MG	2A	3275	1/1	0.85	0.27	73,73,73,73	0
54	MG	1a	1842	1/1	0.85	0.14	62,62,62,62	0
54	MG	1a	1844	1/1	0.85	0.16	75,75,75,75	0
54	MG	1A	3780	1/1	0.85	0.11	38,38,38,38	0
54	MG	1a	1664	1/1	0.85	0.23	77,77,77,77	0
57	MPD	1a	1882	8/8	0.85	0.14	55,67,72,79	0
54	MG	2A	3655	1/1	0.85	0.23	78,78,78,78	0
54	MG	2A	3323	1/1	0.85	0.25	63,63,63,63	0
54	MG	1a	1881	1/1	0.86	0.23	66,66,66,66	0
54	MG	2A	3640	1/1	0.86	0.27	62,62,62,62	0
54	MG	1A	3861	1/1	0.86	0.15	48,48,48,48	0
54	MG	2A	3643	1/1	0.86	0.10	69,69,69,69	0
54	MG	2A	3296	1/1	0.86	0.28	61,61,61,61	0
54	MG	1A	3196	1/1	0.86	0.14	57,57,57,57	0
54	MG	1h	202	1/1	0.86	0.20	74,74,74,74	0
54	MG	1A	3865	1/1	0.86	0.10	63,63,63,63	0
54	MG	1t	201	1/1	0.86	0.13	69,69,69,69	0
54	MG	1A	4001	1/1	0.86	0.24	60,60,60,60	0
54	MG	2A	3683	1/1	0.86	0.16	62,62,62,62	0
54	MG	2A	3687	1/1	0.86	0.14	55,55,55,55	0
54	MG	2A	3693	1/1	0.86	0.10	46,46,46,46	0
54	MG	2A	3328	1/1	0.86	0.43	67,67,67,67	0
54	MG	2A	3329	1/1	0.86	0.18	66,66,66,66	0
54	MG	2A	3033	1/1	0.86	0.11	68,68,68,68	0
54	MG	1a	1637	1/1	0.86	0.24	60,60,60,60	0
54	MG	1A	3874	1/1	0.86	0.17	68,68,68,68	0
54	MG	2A	3348	1/1	0.86	0.19	63,63,63,63	0
54	MG	1A	3793	1/1	0.86	0.14	42,42,42,42	0
54	MG	1a	1765	1/1	0.86	0.23	70,70,70,70	0
54	MG	1A	3798	1/1	0.86	0.23	65,65,65,65	0
54	MG	2B	208	1/1	0.86	0.20	73,73,73,73	0
54	MG	2B	211	1/1	0.86	0.22	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3368	1/1	0.86	0.17	59,59,59,59	0
54	MG	2A	3068	1/1	0.86	0.28	64,64,64,64	0
54	MG	1A	3893	1/1	0.86	0.18	48,48,48,48	0
54	MG	2A	3088	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3428	1/1	0.86	0.09	40,40,40,40	0
54	MG	2W	203	1/1	0.86	0.18	77,77,77,77	0
54	MG	27	103	1/1	0.86	0.17	68,68,68,68	0
54	MG	2A	3432	1/1	0.86	0.17	56,56,56,56	0
54	MG	1a	1657	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3438	1/1	0.86	0.25	65,65,65,65	0
54	MG	2a	3006	1/1	0.86	0.39	78,78,78,78	0
54	MG	1A	3328	1/1	0.86	0.38	69,69,69,69	0
54	MG	2A	3441	1/1	0.86	0.24	80,80,80,80	0
54	MG	2a	3012	1/1	0.86	0.25	78,78,78,78	0
54	MG	2A	3113	1/1	0.86	0.19	59,59,59,59	0
54	MG	2A	3453	1/1	0.86	0.21	73,73,73,73	0
54	MG	1A	3912	1/1	0.86	0.12	33,33,33,33	0
54	MG	1a	1672	1/1	0.86	0.39	71,71,71,71	0
54	MG	2a	3032	1/1	0.86	0.22	77,77,77,77	0
54	MG	2a	3037	1/1	0.86	0.20	68,68,68,68	0
54	MG	2A	3464	1/1	0.86	0.14	61,61,61,61	0
54	MG	2a	3039	1/1	0.86	0.12	86,86,86,86	0
54	MG	1A	3830	1/1	0.86	0.16	76,76,76,76	0
54	MG	1a	1678	1/1	0.86	0.16	55,55,55,55	0
54	MG	2A	3148	1/1	0.86	0.20	69,69,69,69	0
54	MG	2A	3485	1/1	0.86	0.13	71,71,71,71	0
54	MG	1a	1798	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3163	1/1	0.86	0.25	84,84,84,84	0
54	MG	2A	3184	1/1	0.86	0.14	70,70,70,70	0
54	MG	1A	3601	1/1	0.86	0.13	49,49,49,49	0
54	MG	1a	1684	1/1	0.86	0.23	66,66,66,66	0
54	MG	1A	3479	1/1	0.86	0.12	42,42,42,42	0
54	MG	1a	1686	1/1	0.86	0.19	75,75,75,75	0
54	MG	2A	3516	1/1	0.86	0.11	46,46,46,46	0
54	MG	1A	3838	1/1	0.86	0.15	69,69,69,69	0
54	MG	1P	204	1/1	0.86	0.24	47,47,47,47	0
54	MG	2A	3210	1/1	0.86	0.18	66,66,66,66	0
54	MG	2A	3213	1/1	0.86	0.15	62,62,62,62	0
54	MG	2a	3101	1/1	0.86	0.21	71,71,71,71	0
54	MG	1a	1824	1/1	0.86	0.21	69,69,69,69	0
54	MG	1A	3840	1/1	0.86	0.11	68,68,68,68	0
54	MG	2a	3112	1/1	0.86	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3229	1/1	0.86	0.15	68,68,68,68	0
54	MG	1a	1706	1/1	0.86	0.18	80,80,80,80	0
54	MG	1A	3764	1/1	0.86	0.30	67,67,67,67	0
54	MG	1a	1847	1/1	0.86	0.16	68,68,68,68	0
54	MG	2A	3568	1/1	0.86	0.17	66,66,66,66	0
54	MG	2a	3171	1/1	0.86	0.17	71,71,71,71	0
54	MG	1A	3576	1/1	0.86	0.11	56,56,56,56	0
54	MG	1A	3967	1/1	0.86	0.15	77,77,77,77	0
54	MG	1a	1869	1/1	0.86	0.20	82,82,82,82	0
54	MG	1a	1715	1/1	0.86	0.31	75,75,75,75	0
54	MG	1a	1718	1/1	0.86	0.12	69,69,69,69	0
54	MG	2A	3271	1/1	0.86	0.17	70,70,70,70	0
54	MG	1A	3438	1/1	0.86	0.11	46,46,46,46	0
54	MG	1a	1726	1/1	0.86	0.16	68,68,68,68	0
54	MG	1a	1880	1/1	0.86	0.26	69,69,69,69	0
54	MG	2A	3284	1/1	0.86	0.19	68,68,68,68	0
54	MG	2A	3634	1/1	0.86	0.15	37,37,37,37	0
54	MG	19	102	1/1	0.87	0.14	64,64,64,64	0
54	MG	2B	214	1/1	0.87	0.12	72,72,72,72	0
54	MG	2D	311	1/1	0.87	0.09	36,36,36,36	0
54	MG	1A	3476	1/1	0.87	0.13	51,51,51,51	0
54	MG	2A	3272	1/1	0.87	0.12	65,65,65,65	0
54	MG	2I	201	1/1	0.87	0.13	77,77,77,77	0
54	MG	2A	3047	1/1	0.87	0.20	66,66,66,66	0
54	MG	2A	3510	1/1	0.87	0.09	68,68,68,68	0
54	MG	1A	3446	1/1	0.87	0.19	52,52,52,52	0
54	MG	1a	1636	1/1	0.87	0.34	72,72,72,72	0
54	MG	1A	3098	1/1	0.87	0.12	67,67,67,67	0
54	MG	1A	3389	1/1	0.87	0.16	55,55,55,55	0
54	MG	1A	3490	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3529	1/1	0.87	0.19	60,60,60,60	0
54	MG	2A	3089	1/1	0.87	0.32	72,72,72,72	0
54	MG	2A	3311	1/1	0.87	0.22	60,60,60,60	0
54	MG	2A	3316	1/1	0.87	0.38	71,71,71,71	0
54	MG	1a	1717	1/1	0.87	0.12	72,72,72,72	0
54	MG	1a	1646	1/1	0.87	0.25	70,70,70,70	0
54	MG	2A	3553	1/1	0.87	0.14	71,71,71,71	0
54	MG	1a	1826	1/1	0.87	0.26	85,85,85,85	0
54	MG	2a	3026	1/1	0.87	0.22	79,79,79,79	0
54	MG	1a	1837	1/1	0.87	0.27	68,68,68,68	0
54	MG	1a	1720	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3396	1/1	0.87	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3584	1/1	0.87	0.12	44,44,44,44	0
54	MG	1a	1725	1/1	0.87	0.23	70,70,70,70	0
54	MG	2A	3333	1/1	0.87	0.17	60,60,60,60	0
54	MG	2A	3133	1/1	0.87	0.23	67,67,67,67	0
54	MG	1A	3335	1/1	0.87	0.18	62,62,62,62	0
54	MG	1A	3949	1/1	0.87	0.12	51,51,51,51	0
54	MG	1a	1662	1/1	0.87	0.11	74,74,74,74	0
54	MG	1A	3958	1/1	0.87	0.11	62,62,62,62	0
54	MG	2A	3618	1/1	0.87	0.11	60,60,60,60	0
54	MG	2a	3066	1/1	0.87	0.27	69,69,69,69	0
54	MG	2A	3351	1/1	0.87	0.13	46,46,46,46	0
54	MG	2A	3631	1/1	0.87	0.17	82,82,82,82	0
54	MG	1A	3337	1/1	0.87	0.35	68,68,68,68	0
54	MG	1A	3880	1/1	0.87	0.19	42,42,42,42	0
54	MG	2A	3191	1/1	0.87	0.13	54,54,54,54	0
54	MG	1A	3173	1/1	0.87	0.15	55,55,55,55	0
54	MG	1a	1677	1/1	0.87	0.15	65,65,65,65	0
54	MG	1a	1879	1/1	0.87	0.32	75,75,75,75	0
54	MG	2A	3207	1/1	0.87	0.29	70,70,70,70	0
54	MG	2a	3095	1/1	0.87	0.44	74,74,74,74	0
54	MG	2a	3098	1/1	0.87	0.21	72,72,72,72	0
54	MG	1A	3222	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3888	1/1	0.87	0.09	32,32,32,32	0
54	MG	2a	3108	1/1	0.87	0.30	64,64,64,64	0
54	MG	2A	3671	1/1	0.87	0.13	75,75,75,75	0
54	MG	2A	3212	1/1	0.87	0.31	64,64,64,64	0
54	MG	1A	3891	1/1	0.87	0.17	57,57,57,57	0
54	MG	1a	1777	1/1	0.87	0.14	64,64,64,64	0
54	MG	2a	3126	1/1	0.87	0.14	74,74,74,74	0
54	MG	1d	304	1/1	0.87	0.09	86,86,86,86	0
54	MG	1e	204	1/1	0.87	0.13	77,77,77,77	0
54	MG	1A	3892	1/1	0.87	0.11	56,56,56,56	0
54	MG	2a	3156	1/1	0.87	0.17	80,80,80,80	0
54	MG	2a	3157	1/1	0.87	0.14	70,70,70,70	0
54	MG	2a	3159	1/1	0.87	0.15	76,76,76,76	0
54	MG	2A	3695	1/1	0.87	0.14	69,69,69,69	0
54	MG	2a	3172	1/1	0.87	0.30	76,76,76,76	0
54	MG	2A	3462	1/1	0.87	0.22	77,77,77,77	0
54	MG	1A	3997	1/1	0.87	0.15	76,76,76,76	0
54	MG	2A	3241	1/1	0.87	0.21	60,60,60,60	0
54	MG	2a	3186	1/1	0.87	0.43	72,72,72,72	0
54	MG	2A	3466	1/1	0.87	0.14	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1689	1/1	0.87	0.36	68,68,68,68	0
54	MG	2A	3021	1/1	0.87	0.33	56,56,56,56	0
54	MG	2A	3251	1/1	0.87	0.26	67,67,67,67	0
54	MG	2B	201	1/1	0.87	0.14	74,74,74,74	0
54	MG	1a	1696	1/1	0.87	0.19	73,73,73,73	0
54	MG	1a	1790	1/1	0.87	0.22	74,74,74,74	0
54	MG	1A	3731	1/1	0.87	0.13	52,52,52,52	0
54	MG	2A	3137	1/1	0.88	0.22	69,69,69,69	0
54	MG	1a	1690	1/1	0.88	0.48	76,76,76,76	0
54	MG	1a	1819	1/1	0.88	0.16	73,73,73,73	0
54	MG	1A	3673	1/1	0.88	0.09	35,35,35,35	0
54	MG	2A	3725	1/1	0.88	0.14	69,69,69,69	0
54	MG	2A	3170	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3178	1/1	0.88	0.21	70,70,70,70	0
54	MG	2A	3182	1/1	0.88	0.15	61,61,61,61	0
54	MG	2B	203	1/1	0.88	0.27	74,74,74,74	0
54	MG	1N	204	1/1	0.88	0.24	59,59,59,59	0
54	MG	2A	3186	1/1	0.88	0.19	67,67,67,67	0
54	MG	1A	3594	1/1	0.88	0.20	59,59,59,59	0
54	MG	2B	213	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1827	1/1	0.88	0.17	64,64,64,64	0
54	MG	1A	3947	1/1	0.88	0.08	45,45,45,45	0
54	MG	2A	3192	1/1	0.88	0.27	71,71,71,71	0
54	MG	1a	1705	1/1	0.88	0.50	78,78,78,78	0
54	MG	1a	1840	1/1	0.88	0.19	81,81,81,81	0
54	MG	2A	3467	1/1	0.88	0.15	49,49,49,49	0
54	MG	1A	3595	1/1	0.88	0.30	47,47,47,47	0
54	MG	2P	202	1/1	0.88	0.25	77,77,77,77	0
54	MG	2Q	202	1/1	0.88	0.34	63,63,63,63	0
54	MG	1A	3022	1/1	0.88	0.10	52,52,52,52	0
54	MG	2A	3472	1/1	0.88	0.16	68,68,68,68	0
54	MG	21	101	1/1	0.88	0.28	73,73,73,73	0
54	MG	1a	1845	1/1	0.88	0.26	76,76,76,76	0
54	MG	1A	3546	1/1	0.88	0.10	55,55,55,55	0
54	MG	1a	1711	1/1	0.88	0.30	66,66,66,66	0
54	MG	1A	3547	1/1	0.88	0.15	40,40,40,40	0
54	MG	1A	3964	1/1	0.88	0.13	66,66,66,66	0
54	MG	2A	3494	1/1	0.88	0.24	74,74,74,74	0
54	MG	2A	3215	1/1	0.88	0.16	59,59,59,59	0
54	MG	2A	3500	1/1	0.88	0.23	71,71,71,71	0
54	MG	1a	1716	1/1	0.88	0.26	68,68,68,68	0
54	MG	2A	3224	1/1	0.88	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3716	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3630	1/1	0.88	0.29	66,66,66,66	0
54	MG	1A	3041	1/1	0.88	0.19	58,58,58,58	0
54	MG	1A	3768	1/1	0.88	0.16	65,65,65,65	0
54	MG	1a	1623	1/1	0.88	0.17	63,63,63,63	0
54	MG	1A	3778	1/1	0.88	0.15	76,76,76,76	0
54	MG	1a	1633	1/1	0.88	0.14	66,66,66,66	0
54	MG	1a	1732	1/1	0.88	0.15	75,75,75,75	0
54	MG	2a	3048	1/1	0.88	0.25	75,75,75,75	0
54	MG	1a	1736	1/1	0.88	0.18	79,79,79,79	0
54	MG	1A	3992	1/1	0.88	0.27	60,60,60,60	0
54	MG	1A	3994	1/1	0.88	0.16	47,47,47,47	0
54	MG	2A	3544	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3548	1/1	0.88	0.19	70,70,70,70	0
54	MG	1i	3101	1/1	0.88	0.16	66,66,66,66	0
54	MG	1A	3282	1/1	0.88	0.14	56,56,56,56	0
54	MG	1A	3999	1/1	0.88	0.12	64,64,64,64	0
54	MG	2A	3558	1/1	0.88	0.11	51,51,51,51	0
54	MG	1a	1755	1/1	0.88	0.17	63,63,63,63	0
54	MG	2a	3075	1/1	0.88	0.40	76,76,76,76	0
54	MG	2A	3565	1/1	0.88	0.11	65,65,65,65	0
54	MG	1a	1644	1/1	0.88	0.24	64,64,64,64	0
54	MG	1A	4000	1/1	0.88	0.17	70,70,70,70	0
54	MG	1A	3367	1/1	0.88	0.15	57,57,57,57	0
54	MG	1A	4006	1/1	0.88	0.31	63,63,63,63	0
54	MG	1A	4008	1/1	0.88	0.25	64,64,64,64	0
54	MG	2a	3090	1/1	0.88	0.32	64,64,64,64	0
54	MG	2a	3092	1/1	0.88	0.12	70,70,70,70	0
54	MG	2a	3093	1/1	0.88	0.18	67,67,67,67	0
54	MG	2a	3094	1/1	0.88	0.38	75,75,75,75	0
54	MG	2A	3302	1/1	0.88	0.32	59,59,59,59	0
54	MG	1B	203	1/1	0.88	0.18	61,61,61,61	0
54	MG	1B	206	1/1	0.88	0.21	61,61,61,61	0
54	MG	2a	3102	1/1	0.88	0.37	73,73,73,73	0
54	MG	1a	1665	1/1	0.88	0.10	72,72,72,72	0
54	MG	2A	3321	1/1	0.88	0.12	63,63,63,63	0
54	MG	2a	3109	1/1	0.88	0.42	70,70,70,70	0
54	MG	2A	3062	1/1	0.88	0.17	50,50,50,50	0
54	MG	1A	3578	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3079	1/1	0.88	0.17	61,61,61,61	0
54	MG	2a	3117	1/1	0.88	0.12	78,78,78,78	0
54	MG	1A	3655	1/1	0.88	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3125	1/1	0.88	0.17	89,89,89,89	0
54	MG	1A	3656	1/1	0.88	0.11	69,69,69,69	0
54	MG	2A	3635	1/1	0.88	0.19	55,55,55,55	0
54	MG	2a	3138	1/1	0.88	0.16	80,80,80,80	0
54	MG	1A	3318	1/1	0.88	0.38	72,72,72,72	0
54	MG	1B	228	1/1	0.88	0.08	63,63,63,63	0
54	MG	2a	3153	1/1	0.88	0.21	82,82,82,82	0
54	MG	1A	3658	1/1	0.88	0.15	67,67,67,67	0
54	MG	1a	1801	1/1	0.88	0.11	69,69,69,69	0
54	MG	1A	3831	1/1	0.88	0.12	24,24,24,24	0
54	MG	2a	3164	1/1	0.88	0.12	71,71,71,71	0
54	MG	1a	1804	1/1	0.88	0.18	75,75,75,75	0
54	MG	2A	3668	1/1	0.88	0.14	73,73,73,73	0
54	MG	1A	3588	1/1	0.88	0.17	76,76,76,76	0
54	MG	2A	3126	1/1	0.88	0.15	73,73,73,73	0
54	MG	1E	302	1/1	0.88	0.17	38,38,38,38	0
54	MG	2A	3676	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3359	1/1	0.88	0.16	54,54,54,54	0
54	MG	2A	3131	1/1	0.88	0.33	65,65,65,65	0
54	MG	2a	3189	1/1	0.88	0.28	69,69,69,69	0
54	MG	2a	3192	1/1	0.88	0.21	62,62,62,62	0
54	MG	1A	3455	1/1	0.88	0.20	67,67,67,67	0
54	MG	2A	3394	1/1	0.88	0.13	48,48,48,48	0
54	MG	2A	3396	1/1	0.88	0.15	52,52,52,52	0
54	MG	2A	3135	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3400	1/1	0.88	0.13	54,54,54,54	0
54	MG	2A	3404	1/1	0.88	0.16	56,56,56,56	0
54	MG	1A	3334	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1767	1/1	0.89	0.18	61,61,61,61	0
54	MG	2A	3164	1/1	0.89	0.13	70,70,70,70	0
54	MG	2A	3546	1/1	0.89	0.23	65,65,65,65	0
54	MG	1A	3796	1/1	0.89	0.13	60,60,60,60	0
54	MG	1a	1774	1/1	0.89	0.13	66,66,66,66	0
54	MG	2A	3180	1/1	0.89	0.21	76,76,76,76	0
54	MG	1a	1688	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3205	1/1	0.89	0.19	56,56,56,56	0
54	MG	1A	3156	1/1	0.89	0.24	66,66,66,66	0
54	MG	2a	3014	1/1	0.89	0.26	71,71,71,71	0
54	MG	1a	1692	1/1	0.89	0.22	74,74,74,74	0
54	MG	1e	201	1/1	0.89	0.16	72,72,72,72	0
54	MG	2A	3573	1/1	0.89	0.10	67,67,67,67	0
54	MG	1a	1694	1/1	0.89	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1f	201	1/1	0.89	0.29	75,75,75,75	0
54	MG	1A	3608	1/1	0.89	0.16	67,67,67,67	0
54	MG	1B	201	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3375	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3595	1/1	0.89	0.15	72,72,72,72	0
54	MG	2a	3040	1/1	0.89	0.19	64,64,64,64	0
54	MG	2a	3041	1/1	0.89	0.15	78,78,78,78	0
54	MG	2A	3388	1/1	0.89	0.26	63,63,63,63	0
54	MG	1A	3610	1/1	0.89	0.17	48,48,48,48	0
54	MG	1n	101	1/1	0.89	0.11	63,63,63,63	0
54	MG	1A	3471	1/1	0.89	0.13	57,57,57,57	0
54	MG	1y	202	1/1	0.89	0.13	74,74,74,74	0
54	MG	2A	3621	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3622	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3623	1/1	0.89	0.13	46,46,46,46	0
54	MG	2A	3401	1/1	0.89	0.16	54,54,54,54	0
54	MG	1y	203	1/1	0.89	0.14	83,83,83,83	0
54	MG	2A	3001	1/1	0.89	0.13	57,57,57,57	0
54	MG	1A	3549	1/1	0.89	0.13	57,57,57,57	0
54	MG	2A	3424	1/1	0.89	0.19	63,63,63,63	0
54	MG	2a	3079	1/1	0.89	0.24	70,70,70,70	0
54	MG	1B	211	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3429	1/1	0.89	0.09	43,43,43,43	0
54	MG	1B	216	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3219	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3436	1/1	0.89	0.13	49,49,49,49	0
54	MG	2A	3661	1/1	0.89	0.14	41,41,41,41	0
54	MG	2A	3437	1/1	0.89	0.14	60,60,60,60	0
54	MG	2A	3221	1/1	0.89	0.24	73,73,73,73	0
54	MG	2A	3034	1/1	0.89	0.27	66,66,66,66	0
54	MG	1A	3702	1/1	0.89	0.17	77,77,77,77	0
54	MG	1a	1639	1/1	0.89	0.19	71,71,71,71	0
54	MG	1a	1713	1/1	0.89	0.27	52,52,52,52	0
54	MG	2a	3100	1/1	0.89	0.30	78,78,78,78	0
54	MG	1A	3573	1/1	0.89	0.19	67,67,67,67	0
54	MG	1B	225	1/1	0.89	0.11	49,49,49,49	0
54	MG	1a	1818	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3841	1/1	0.89	0.13	41,41,41,41	0
54	MG	2A	3063	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	3110	1/1	0.89	0.26	67,67,67,67	0
54	MG	1A	3639	1/1	0.89	0.13	67,67,67,67	0
54	MG	1A	3717	1/1	0.89	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3720	1/1	0.89	0.12	58,58,58,58	0
54	MG	2a	3116	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3270	1/1	0.89	0.26	74,74,74,74	0
54	MG	2A	3707	1/1	0.89	0.21	68,68,68,68	0
54	MG	1a	1655	1/1	0.89	0.21	63,63,63,63	0
54	MG	2A	3716	1/1	0.89	0.11	79,79,79,79	0
54	MG	1a	1831	1/1	0.89	0.09	92,92,92,92	0
54	MG	1A	3498	1/1	0.89	0.12	42,42,42,42	0
54	MG	2A	3102	1/1	0.89	0.34	67,67,67,67	0
54	MG	2A	3727	1/1	0.89	0.19	62,62,62,62	0
54	MG	2a	3145	1/1	0.89	0.34	70,70,70,70	0
54	MG	2A	3490	1/1	0.89	0.15	65,65,65,65	0
54	MG	2A	3491	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1658	1/1	0.89	0.26	51,51,51,51	0
54	MG	1A	3746	1/1	0.89	0.11	52,52,52,52	0
54	MG	2a	3160	1/1	0.89	0.13	75,75,75,75	0
54	MG	2A	3496	1/1	0.89	0.14	60,60,60,60	0
54	MG	2A	3288	1/1	0.89	0.26	78,78,78,78	0
54	MG	1F	316	1/1	0.89	0.10	62,62,62,62	0
54	MG	1A	3762	1/1	0.89	0.29	41,41,41,41	0
54	MG	1A	3501	1/1	0.89	0.10	30,30,30,30	0
54	MG	1A	3474	1/1	0.89	0.11	51,51,51,51	0
54	MG	2E	305	1/1	0.89	0.11	41,41,41,41	0
54	MG	2F	302	1/1	0.89	0.13	55,55,55,55	0
54	MG	2F	303	1/1	0.89	0.15	62,62,62,62	0
54	MG	1A	3439	1/1	0.89	0.11	34,34,34,34	0
54	MG	2A	3313	1/1	0.89	0.25	74,74,74,74	0
54	MG	1A	3521	1/1	0.89	0.12	75,75,75,75	0
54	MG	1A	3531	1/1	0.89	0.14	65,65,65,65	0
54	MG	1a	1871	1/1	0.89	0.08	84,84,84,84	0
57	MPD	1T	204	8/8	0.89	0.19	68,72,74,77	0
54	MG	1A	3361	1/1	0.89	0.13	58,58,58,58	0
57	MPD	2A	3732	8/8	0.89	0.23	50,56,61,64	0
54	MG	1Z	301	1/1	0.89	0.13	71,71,71,71	0
54	MG	2A	3325	1/1	0.89	0.24	65,65,65,65	0
54	MG	1a	1743	1/1	0.90	0.11	62,62,62,62	0
54	MG	1A	3382	1/1	0.90	0.19	66,66,66,66	0
54	MG	2A	3459	1/1	0.90	0.21	74,74,74,74	0
54	MG	2A	3461	1/1	0.90	0.24	74,74,74,74	0
54	MG	1A	4003	1/1	0.90	0.25	42,42,42,42	0
54	MG	1A	3387	1/1	0.90	0.21	69,69,69,69	0
54	MG	1a	1643	1/1	0.90	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3696	1/1	0.90	0.11	54,54,54,54	0
54	MG	2D	301	1/1	0.90	0.35	53,53,53,53	0
54	MG	2D	310	1/1	0.90	0.14	52,52,52,52	0
54	MG	1f	202	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3218	1/1	0.90	0.23	71,71,71,71	0
54	MG	1A	4015	1/1	0.90	0.09	46,46,46,46	0
54	MG	1A	3211	1/1	0.90	0.20	61,61,61,61	0
54	MG	1k	201	1/1	0.90	0.20	57,57,57,57	0
54	MG	1B	202	1/1	0.90	0.20	63,63,63,63	0
54	MG	1A	3147	1/1	0.90	0.15	58,58,58,58	0
54	MG	2I	202	1/1	0.90	0.14	70,70,70,70	0
54	MG	1B	205	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3611	1/1	0.90	0.10	64,64,64,64	0
54	MG	2A	3248	1/1	0.90	0.17	62,62,62,62	0
54	MG	1A	3613	1/1	0.90	0.11	52,52,52,52	0
54	MG	1A	3614	1/1	0.90	0.10	50,50,50,50	0
54	MG	2W	202	1/1	0.90	0.20	57,57,57,57	0
54	MG	1A	3620	1/1	0.90	0.35	33,33,33,33	0
54	MG	1A	3723	1/1	0.90	0.17	42,42,42,42	0
54	MG	2A	3259	1/1	0.90	0.17	64,64,64,64	0
54	MG	1a	1782	1/1	0.90	0.13	68,68,68,68	0
54	MG	1A	3724	1/1	0.90	0.14	34,34,34,34	0
54	MG	1A	3470	1/1	0.90	0.10	55,55,55,55	0
54	MG	2A	3267	1/1	0.90	0.26	64,64,64,64	0
54	MG	1A	3125	1/1	0.90	0.17	46,46,46,46	0
54	MG	2A	3037	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3038	1/1	0.90	0.26	69,69,69,69	0
54	MG	1a	1792	1/1	0.90	0.18	70,70,70,70	0
54	MG	2A	3528	1/1	0.90	0.17	68,68,68,68	0
54	MG	2A	3044	1/1	0.90	0.19	59,59,59,59	0
54	MG	2a	3023	1/1	0.90	0.15	58,58,58,58	0
54	MG	2A	3531	1/1	0.90	0.12	71,71,71,71	0
54	MG	2a	3025	1/1	0.90	0.12	71,71,71,71	0
54	MG	2A	3276	1/1	0.90	0.17	70,70,70,70	0
54	MG	2A	3278	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3633	1/1	0.90	0.15	73,73,73,73	0
54	MG	2a	3034	1/1	0.90	0.27	64,64,64,64	0
54	MG	1A	3225	1/1	0.90	0.16	49,49,49,49	0
54	MG	2A	3286	1/1	0.90	0.30	66,66,66,66	0
54	MG	1a	1797	1/1	0.90	0.13	78,78,78,78	0
54	MG	2A	3060	1/1	0.90	0.26	71,71,71,71	0
54	MG	1A	3434	1/1	0.90	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3042	1/1	0.90	0.37	75,75,75,75	0
54	MG	2A	3550	1/1	0.90	0.25	75,75,75,75	0
54	MG	1D	315	1/1	0.90	0.30	51,51,51,51	0
54	MG	2A	3067	1/1	0.90	0.16	63,63,63,63	0
54	MG	2A	3557	1/1	0.90	0.08	40,40,40,40	0
54	MG	2A	3308	1/1	0.90	0.39	68,68,68,68	0
54	MG	1A	3646	1/1	0.90	0.12	32,32,32,32	0
54	MG	1D	318	1/1	0.90	0.16	66,66,66,66	0
54	MG	1A	3166	1/1	0.90	0.17	56,56,56,56	0
54	MG	1a	1806	1/1	0.90	0.10	73,73,73,73	0
54	MG	2A	3580	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3581	1/1	0.90	0.20	66,66,66,66	0
54	MG	1E	304	1/1	0.90	0.09	28,28,28,28	0
54	MG	2a	3073	1/1	0.90	0.19	71,71,71,71	0
54	MG	2A	3322	1/1	0.90	0.31	68,68,68,68	0
54	MG	2A	3092	1/1	0.90	0.27	66,66,66,66	0
54	MG	1A	3788	1/1	0.90	0.11	48,48,48,48	0
54	MG	2A	3095	1/1	0.90	0.27	68,68,68,68	0
54	MG	2A	3096	1/1	0.90	0.09	63,63,63,63	0
54	MG	1A	3557	1/1	0.90	0.08	37,37,37,37	0
54	MG	1A	3790	1/1	0.90	0.19	50,50,50,50	0
54	MG	1A	3195	1/1	0.90	0.13	68,68,68,68	0
54	MG	1A	3342	1/1	0.90	0.12	62,62,62,62	0
54	MG	1P	203	1/1	0.90	0.23	77,77,77,77	0
54	MG	1A	3957	1/1	0.90	0.15	50,50,50,50	0
54	MG	1R	204	1/1	0.90	0.15	43,43,43,43	0
54	MG	1A	3795	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3627	1/1	0.90	0.20	61,61,61,61	0
54	MG	1a	1834	1/1	0.90	0.20	74,74,74,74	0
54	MG	2A	3630	1/1	0.90	0.19	63,63,63,63	0
54	MG	1a	1709	1/1	0.90	0.41	73,73,73,73	0
54	MG	2A	3356	1/1	0.90	0.19	67,67,67,67	0
54	MG	2A	3357	1/1	0.90	0.16	59,59,59,59	0
54	MG	1a	1838	1/1	0.90	0.09	67,67,67,67	0
54	MG	1A	3489	1/1	0.90	0.12	53,53,53,53	0
54	MG	1W	201	1/1	0.90	0.22	50,50,50,50	0
54	MG	2A	3152	1/1	0.90	0.28	64,64,64,64	0
54	MG	2A	3371	1/1	0.90	0.10	39,39,39,39	0
54	MG	2A	3646	1/1	0.90	0.08	58,58,58,58	0
54	MG	2A	3649	1/1	0.90	0.20	67,67,67,67	0
54	MG	2A	3654	1/1	0.90	0.11	54,54,54,54	0
54	MG	2a	3123	1/1	0.90	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3154	1/1	0.90	0.20	63,63,63,63	0
54	MG	2A	3658	1/1	0.90	0.14	60,60,60,60	0
54	MG	2A	3160	1/1	0.90	0.16	50,50,50,50	0
54	MG	2a	3131	1/1	0.90	0.19	64,64,64,64	0
54	MG	1A	3797	1/1	0.90	0.09	38,38,38,38	0
54	MG	1A	3010	1/1	0.90	0.21	56,56,56,56	0
54	MG	2A	3398	1/1	0.90	0.08	42,42,42,42	0
54	MG	1A	3800	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3197	1/1	0.90	0.35	69,69,69,69	0
54	MG	2a	3155	1/1	0.90	0.18	70,70,70,70	0
54	MG	1a	1852	1/1	0.90	0.13	75,75,75,75	0
54	MG	1A	3817	1/1	0.90	0.19	33,33,33,33	0
54	MG	2A	3680	1/1	0.90	0.13	65,65,65,65	0
54	MG	2A	3681	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3181	1/1	0.90	0.16	69,69,69,69	0
54	MG	1a	1854	1/1	0.90	0.16	76,76,76,76	0
54	MG	1A	3172	1/1	0.90	0.14	62,62,62,62	0
54	MG	2A	3425	1/1	0.90	0.21	64,64,64,64	0
54	MG	2A	3694	1/1	0.90	0.13	58,58,58,58	0
54	MG	1A	3986	1/1	0.90	0.10	52,52,52,52	0
54	MG	1A	3661	1/1	0.90	0.14	48,48,48,48	0
54	MG	2A	3700	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3298	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3672	1/1	0.90	0.09	44,44,44,44	0
54	MG	1A	3129	1/1	0.90	0.25	63,63,63,63	0
54	MG	1a	1729	1/1	0.90	0.23	70,70,70,70	0
54	MG	2A	3201	1/1	0.90	0.11	58,58,58,58	0
54	MG	2A	3439	1/1	0.90	0.16	50,50,50,50	0
54	MG	1A	3679	1/1	0.90	0.19	64,64,64,64	0
54	MG	1A	3509	1/1	0.90	0.14	44,44,44,44	0
54	MG	2A	3726	1/1	0.90	0.29	71,71,71,71	0
54	MG	1a	1741	1/1	0.90	0.15	75,75,75,75	0
54	MG	2A	3446	1/1	0.90	0.09	40,40,40,40	0
54	MG	1a	1612	1/1	0.91	0.27	67,67,67,67	0
54	MG	1a	1742	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3194	1/1	0.91	0.34	68,68,68,68	0
54	MG	2A	3195	1/1	0.91	0.34	68,68,68,68	0
54	MG	2A	3196	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3159	1/1	0.91	0.08	49,49,49,49	0
54	MG	1A	3615	1/1	0.91	0.09	50,50,50,50	0
54	MG	1a	1631	1/1	0.91	0.28	55,55,55,55	0
54	MG	1A	3403	1/1	0.91	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3449	1/1	0.91	0.11	41,41,41,41	0
54	MG	1a	1750	1/1	0.91	0.14	68,68,68,68	0
54	MG	2B	206	1/1	0.91	0.17	73,73,73,73	0
54	MG	1A	3412	1/1	0.91	0.07	44,44,44,44	0
54	MG	2A	3211	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3708	1/1	0.91	0.08	45,45,45,45	0
54	MG	1A	3711	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3165	1/1	0.91	0.32	66,66,66,66	0
54	MG	1A	3853	1/1	0.91	0.08	57,57,57,57	0
54	MG	1a	1766	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3856	1/1	0.91	0.14	58,58,58,58	0
54	MG	1o	101	1/1	0.91	0.32	77,77,77,77	0
54	MG	1A	3554	1/1	0.91	0.08	58,58,58,58	0
54	MG	1A	4016	1/1	0.91	0.12	61,61,61,61	0
54	MG	1A	3047	1/1	0.91	0.28	68,68,68,68	0
54	MG	2A	3483	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3262	1/1	0.91	0.17	53,53,53,53	0
54	MG	2A	3231	1/1	0.91	0.24	62,62,62,62	0
54	MG	2A	3007	1/1	0.91	0.11	45,45,45,45	0
54	MG	2A	3236	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	3057	1/1	0.91	0.14	49,49,49,49	0
54	MG	2A	3243	1/1	0.91	0.33	56,56,56,56	0
54	MG	1A	3729	1/1	0.91	0.11	50,50,50,50	0
54	MG	2A	3495	1/1	0.91	0.13	64,64,64,64	0
54	MG	2A	3030	1/1	0.91	0.14	69,69,69,69	0
54	MG	1A	3280	1/1	0.91	0.16	69,69,69,69	0
54	MG	28	102	1/1	0.91	0.21	64,64,64,64	0
54	MG	1A	3066	1/1	0.91	0.10	56,56,56,56	0
54	MG	1A	3748	1/1	0.91	0.10	38,38,38,38	0
54	MG	1B	214	1/1	0.91	0.09	58,58,58,58	0
54	MG	2A	3509	1/1	0.91	0.13	69,69,69,69	0
54	MG	2a	3007	1/1	0.91	0.11	64,64,64,64	0
54	MG	1a	1791	1/1	0.91	0.07	76,76,76,76	0
54	MG	2A	3512	1/1	0.91	0.14	64,64,64,64	0
54	MG	1A	3757	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3440	1/1	0.91	0.14	43,43,43,43	0
54	MG	1A	3654	1/1	0.91	0.27	39,39,39,39	0
54	MG	1A	3585	1/1	0.91	0.21	50,50,50,50	0
54	MG	2A	3048	1/1	0.91	0.20	58,58,58,58	0
54	MG	2A	3052	1/1	0.91	0.16	54,54,54,54	0
54	MG	1A	3895	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3530	1/1	0.91	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3027	1/1	0.91	0.34	72,72,72,72	0
54	MG	1a	1799	1/1	0.91	0.22	81,81,81,81	0
54	MG	2A	3057	1/1	0.91	0.18	52,52,52,52	0
54	MG	2A	3277	1/1	0.91	0.22	61,61,61,61	0
54	MG	1A	3771	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3586	1/1	0.91	0.10	43,43,43,43	0
54	MG	2A	3542	1/1	0.91	0.11	66,66,66,66	0
54	MG	2A	3281	1/1	0.91	0.28	74,74,74,74	0
54	MG	1A	3920	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3291	1/1	0.91	0.11	72,72,72,72	0
54	MG	2a	3043	1/1	0.91	0.23	66,66,66,66	0
54	MG	2A	3287	1/1	0.91	0.21	65,65,65,65	0
54	MG	2a	3047	1/1	0.91	0.32	68,68,68,68	0
54	MG	1A	3589	1/1	0.91	0.09	61,61,61,61	0
54	MG	2a	3051	1/1	0.91	0.31	73,73,73,73	0
54	MG	2a	3052	1/1	0.91	0.37	67,67,67,67	0
54	MG	2a	3054	1/1	0.91	0.25	72,72,72,72	0
54	MG	2A	3076	1/1	0.91	0.19	55,55,55,55	0
54	MG	1a	1807	1/1	0.91	0.17	61,61,61,61	0
54	MG	1A	3201	1/1	0.91	0.35	48,48,48,48	0
54	MG	2A	3297	1/1	0.91	0.28	61,61,61,61	0
54	MG	2A	3561	1/1	0.91	0.09	58,58,58,58	0
54	MG	2A	3562	1/1	0.91	0.16	58,58,58,58	0
54	MG	2a	3065	1/1	0.91	0.18	70,70,70,70	0
54	MG	2A	3300	1/1	0.91	0.30	69,69,69,69	0
54	MG	2A	3083	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3305	1/1	0.91	0.19	66,66,66,66	0
54	MG	2A	3086	1/1	0.91	0.11	52,52,52,52	0
54	MG	2A	3579	1/1	0.91	0.17	67,67,67,67	0
54	MG	1a	1809	1/1	0.91	0.14	74,74,74,74	0
54	MG	2a	3076	1/1	0.91	0.32	57,57,57,57	0
54	MG	1a	1810	1/1	0.91	0.11	65,65,65,65	0
54	MG	1A	3943	1/1	0.91	0.08	51,51,51,51	0
54	MG	2A	3093	1/1	0.91	0.15	70,70,70,70	0
54	MG	2A	3318	1/1	0.91	0.15	63,63,63,63	0
54	MG	2a	3086	1/1	0.91	0.35	64,64,64,64	0
54	MG	1A	3004	1/1	0.91	0.15	53,53,53,53	0
54	MG	1F	315	1/1	0.91	0.24	50,50,50,50	0
54	MG	1A	3152	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3599	1/1	0.91	0.20	62,62,62,62	0
54	MG	2A	3101	1/1	0.91	0.20	57,57,57,57	0
54	MG	1A	3451	1/1	0.91	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3103	1/1	0.91	0.31	66,66,66,66	0
54	MG	1A	3308	1/1	0.91	0.10	47,47,47,47	0
54	MG	1H	202	1/1	0.91	0.08	56,56,56,56	0
54	MG	1N	203	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3676	1/1	0.91	0.16	68,68,68,68	0
54	MG	1A	3677	1/1	0.91	0.11	30,30,30,30	0
54	MG	1A	3961	1/1	0.91	0.10	48,48,48,48	0
54	MG	2A	3342	1/1	0.91	0.10	44,44,44,44	0
54	MG	1A	3008	1/1	0.91	0.12	48,48,48,48	0
54	MG	1A	3458	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3965	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3681	1/1	0.91	0.16	64,64,64,64	0
54	MG	1A	3978	1/1	0.91	0.13	61,61,61,61	0
54	MG	2A	3141	1/1	0.91	0.15	58,58,58,58	0
54	MG	1A	3219	1/1	0.91	0.11	46,46,46,46	0
54	MG	2A	3151	1/1	0.91	0.34	58,58,58,58	0
54	MG	1a	1846	1/1	0.91	0.10	69,69,69,69	0
54	MG	2a	3124	1/1	0.91	0.10	76,76,76,76	0
54	MG	2A	3644	1/1	0.91	0.16	71,71,71,71	0
54	MG	1A	3821	1/1	0.91	0.09	48,48,48,48	0
54	MG	2A	3158	1/1	0.91	0.11	70,70,70,70	0
54	MG	2A	3372	1/1	0.91	0.09	51,51,51,51	0
54	MG	1a	1848	1/1	0.91	0.11	74,74,74,74	0
54	MG	2A	3377	1/1	0.91	0.09	47,47,47,47	0
54	MG	2A	3387	1/1	0.91	0.14	66,66,66,66	0
54	MG	2A	3662	1/1	0.91	0.14	44,44,44,44	0
54	MG	2a	3152	1/1	0.91	0.19	72,72,72,72	0
54	MG	1A	3692	1/1	0.91	0.09	71,71,71,71	0
54	MG	1A	3694	1/1	0.91	0.07	79,79,79,79	0
54	MG	2A	3395	1/1	0.91	0.22	78,78,78,78	0
54	MG	1A	3987	1/1	0.91	0.08	74,74,74,74	0
54	MG	2A	3674	1/1	0.91	0.18	52,52,52,52	0
54	MG	2A	3397	1/1	0.91	0.11	45,45,45,45	0
54	MG	2A	3165	1/1	0.91	0.18	67,67,67,67	0
54	MG	2a	3169	1/1	0.91	0.08	68,68,68,68	0
54	MG	2a	3170	1/1	0.91	0.19	63,63,63,63	0
54	MG	1A	3988	1/1	0.91	0.11	49,49,49,49	0
54	MG	2A	3172	1/1	0.91	0.14	60,60,60,60	0
54	MG	2a	3177	1/1	0.91	0.20	76,76,76,76	0
54	MG	1a	1867	1/1	0.91	0.09	59,59,59,59	0
54	MG	19	101	1/1	0.91	0.14	57,57,57,57	0
54	MG	2A	3406	1/1	0.91	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3184	1/1	0.91	0.33	66,66,66,66	0
54	MG	1a	1870	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3689	1/1	0.91	0.20	57,57,57,57	0
54	MG	2A	3690	1/1	0.91	0.08	66,66,66,66	0
54	MG	2A	3414	1/1	0.91	0.10	67,67,67,67	0
54	MG	2a	3190	1/1	0.91	0.27	77,77,77,77	0
54	MG	1A	3395	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3423	1/1	0.91	0.26	80,80,80,80	0
54	MG	1A	3991	1/1	0.91	0.08	25,25,25,25	0
54	MG	1a	1608	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1609	1/1	0.91	0.12	69,69,69,69	0
54	MG	1a	1739	1/1	0.91	0.12	74,74,74,74	0
54	MG	2A	3706	1/1	0.91	0.10	68,68,68,68	0
54	MG	2A	3430	1/1	0.91	0.12	62,62,62,62	0
54	MG	1a	1740	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3256	1/1	0.92	0.23	60,60,60,60	0
54	MG	1A	3825	1/1	0.92	0.15	69,69,69,69	0
54	MG	1a	1785	1/1	0.92	0.22	62,62,62,62	0
54	MG	2D	302	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3567	1/1	0.92	0.17	61,61,61,61	0
54	MG	1A	3995	1/1	0.92	0.11	61,61,61,61	0
54	MG	2D	312	1/1	0.92	0.19	63,63,63,63	0
54	MG	1A	3034	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3452	1/1	0.92	0.07	59,59,59,59	0
54	MG	2A	3498	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3058	1/1	0.92	0.11	59,59,59,59	0
54	MG	1A	3365	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	3836	1/1	0.92	0.11	58,58,58,58	0
54	MG	1A	3071	1/1	0.92	0.36	40,40,40,40	0
54	MG	2A	3504	1/1	0.92	0.35	63,63,63,63	0
54	MG	2A	3505	1/1	0.92	0.14	74,74,74,74	0
54	MG	1A	3371	1/1	0.92	0.07	48,48,48,48	0
54	MG	2Q	201	1/1	0.92	0.17	60,60,60,60	0
54	MG	1A	3583	1/1	0.92	0.07	22,22,22,22	0
54	MG	2A	3072	1/1	0.92	0.20	59,59,59,59	0
54	MG	1A	4010	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	4011	1/1	0.92	0.16	62,62,62,62	0
54	MG	20	103	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3517	1/1	0.92	0.16	69,69,69,69	0
54	MG	25	101	1/1	0.92	0.45	48,48,48,48	0
54	MG	1a	1803	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3081	1/1	0.92	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	28	103	1/1	0.92	0.20	60,60,60,60	0
54	MG	1a	1656	1/1	0.92	0.11	74,74,74,74	0
54	MG	1A	3376	1/1	0.92	0.09	51,51,51,51	0
54	MG	2A	3087	1/1	0.92	0.07	42,42,42,42	0
54	MG	1A	3463	1/1	0.92	0.08	57,57,57,57	0
54	MG	2A	3295	1/1	0.92	0.30	67,67,67,67	0
54	MG	2a	3008	1/1	0.92	0.25	60,60,60,60	0
54	MG	1a	1659	1/1	0.92	0.26	71,71,71,71	0
54	MG	1a	1661	1/1	0.92	0.18	66,66,66,66	0
54	MG	2A	3536	1/1	0.92	0.14	65,65,65,65	0
54	MG	2A	3537	1/1	0.92	0.08	68,68,68,68	0
54	MG	2a	3017	1/1	0.92	0.09	67,67,67,67	0
54	MG	1A	4017	1/1	0.92	0.17	53,53,53,53	0
54	MG	1A	3377	1/1	0.92	0.08	38,38,38,38	0
54	MG	2A	3303	1/1	0.92	0.24	58,58,58,58	0
54	MG	1A	3380	1/1	0.92	0.10	29,29,29,29	0
54	MG	2A	3545	1/1	0.92	0.13	65,65,65,65	0
54	MG	1A	3228	1/1	0.92	0.17	45,45,45,45	0
54	MG	2A	3098	1/1	0.92	0.11	52,52,52,52	0
54	MG	1a	1814	1/1	0.92	0.07	62,62,62,62	0
54	MG	2a	3030	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3315	1/1	0.92	0.28	73,73,73,73	0
54	MG	1A	3858	1/1	0.92	0.12	45,45,45,45	0
54	MG	2a	3035	1/1	0.92	0.39	76,76,76,76	0
54	MG	1A	3386	1/1	0.92	0.09	37,37,37,37	0
54	MG	1B	207	1/1	0.92	0.30	63,63,63,63	0
54	MG	2A	3319	1/1	0.92	0.36	66,66,66,66	0
54	MG	1B	209	1/1	0.92	0.12	56,56,56,56	0
54	MG	1A	3073	1/1	0.92	0.12	50,50,50,50	0
54	MG	1A	3316	1/1	0.92	0.39	53,53,53,53	0
54	MG	1A	3598	1/1	0.92	0.09	48,48,48,48	0
54	MG	2a	3044	1/1	0.92	0.19	74,74,74,74	0
54	MG	2a	3045	1/1	0.92	0.16	74,74,74,74	0
54	MG	2A	3566	1/1	0.92	0.09	74,74,74,74	0
54	MG	1B	215	1/1	0.92	0.14	51,51,51,51	0
54	MG	2A	3571	1/1	0.92	0.25	64,64,64,64	0
54	MG	1a	1835	1/1	0.92	0.12	72,72,72,72	0
54	MG	2A	3129	1/1	0.92	0.18	61,61,61,61	0
54	MG	1A	3391	1/1	0.92	0.10	44,44,44,44	0
54	MG	1A	3603	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3393	1/1	0.92	0.10	59,59,59,59	0
54	MG	2a	3059	1/1	0.92	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1691	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3251	1/1	0.92	0.13	51,51,51,51	0
54	MG	2A	3337	1/1	0.92	0.21	67,67,67,67	0
54	MG	2A	3147	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3593	1/1	0.92	0.26	56,56,56,56	0
54	MG	1A	3890	1/1	0.92	0.08	33,33,33,33	0
54	MG	2A	3596	1/1	0.92	0.09	52,52,52,52	0
54	MG	1A	3321	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3402	1/1	0.92	0.08	29,29,29,29	0
54	MG	1A	3325	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3406	1/1	0.92	0.08	47,47,47,47	0
54	MG	1a	1851	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3257	1/1	0.92	0.13	44,44,44,44	0
54	MG	1A	3897	1/1	0.92	0.23	47,47,47,47	0
54	MG	1A	3898	1/1	0.92	0.12	63,63,63,63	0
54	MG	2a	3082	1/1	0.92	0.11	65,65,65,65	0
54	MG	2a	3083	1/1	0.92	0.26	70,70,70,70	0
54	MG	1A	3416	1/1	0.92	0.06	22,22,22,22	0
54	MG	1A	3751	1/1	0.92	0.08	47,47,47,47	0
54	MG	1A	3629	1/1	0.92	0.17	58,58,58,58	0
54	MG	2A	3173	1/1	0.92	0.09	71,71,71,71	0
54	MG	1A	3758	1/1	0.92	0.14	60,60,60,60	0
54	MG	2A	3179	1/1	0.92	0.25	70,70,70,70	0
54	MG	2a	3091	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3503	1/1	0.92	0.08	31,31,31,31	0
54	MG	1A	3077	1/1	0.92	0.24	56,56,56,56	0
54	MG	1N	202	1/1	0.92	0.19	51,51,51,51	0
54	MG	1a	1874	1/1	0.92	0.15	83,83,83,83	0
54	MG	2a	3096	1/1	0.92	0.25	76,76,76,76	0
54	MG	1A	3131	1/1	0.92	0.13	40,40,40,40	0
54	MG	2A	3188	1/1	0.92	0.22	73,73,73,73	0
54	MG	1A	3517	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3776	1/1	0.92	0.14	57,57,57,57	0
54	MG	2a	3104	1/1	0.92	0.28	60,60,60,60	0
54	MG	1A	3641	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3432	1/1	0.92	0.13	32,32,32,32	0
54	MG	2A	3405	1/1	0.92	0.12	73,73,73,73	0
54	MG	1A	3783	1/1	0.92	0.08	33,33,33,33	0
54	MG	1A	3277	1/1	0.92	0.26	59,59,59,59	0
54	MG	1A	3139	1/1	0.92	0.08	50,50,50,50	0
54	MG	1U	202	1/1	0.92	0.41	45,45,45,45	0
54	MG	2a	3114	1/1	0.92	0.31	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3667	1/1	0.92	0.10	53,53,53,53	0
54	MG	2A	3197	1/1	0.92	0.11	51,51,51,51	0
54	MG	1V	205	1/1	0.92	0.13	67,67,67,67	0
54	MG	1A	3650	1/1	0.92	0.14	54,54,54,54	0
54	MG	1Y	201	1/1	0.92	0.17	56,56,56,56	0
54	MG	1A	3538	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3340	1/1	0.92	0.14	49,49,49,49	0
54	MG	1A	3084	1/1	0.92	0.14	59,59,59,59	0
54	MG	11	102	1/1	0.92	0.19	59,59,59,59	0
54	MG	2A	3435	1/1	0.92	0.24	50,50,50,50	0
54	MG	2a	3140	1/1	0.92	0.21	71,71,71,71	0
54	MG	1A	3968	1/1	0.92	0.16	57,57,57,57	0
54	MG	2a	3143	1/1	0.92	0.12	70,70,70,70	0
54	MG	1n	102	1/1	0.92	0.15	68,68,68,68	0
54	MG	1A	3975	1/1	0.92	0.11	56,56,56,56	0
54	MG	2a	3150	1/1	0.92	0.19	78,78,78,78	0
54	MG	1A	3289	1/1	0.92	0.19	64,64,64,64	0
54	MG	18	102	1/1	0.92	0.15	46,46,46,46	0
54	MG	1A	3981	1/1	0.92	0.09	80,80,80,80	0
54	MG	1A	3345	1/1	0.92	0.09	29,29,29,29	0
54	MG	2A	3220	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3698	1/1	0.92	0.13	67,67,67,67	0
54	MG	2A	3448	1/1	0.92	0.10	57,57,57,57	0
54	MG	2a	3162	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3002	1/1	0.92	0.09	48,48,48,48	0
54	MG	2a	3165	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3452	1/1	0.92	0.08	39,39,39,39	0
54	MG	2A	3015	1/1	0.92	0.29	76,76,76,76	0
54	MG	1A	3659	1/1	0.92	0.11	40,40,40,40	0
54	MG	2A	3022	1/1	0.92	0.16	67,67,67,67	0
54	MG	2a	3173	1/1	0.92	0.15	69,69,69,69	0
54	MG	2A	3711	1/1	0.92	0.14	66,66,66,66	0
54	MG	1A	3803	1/1	0.92	0.13	59,59,59,59	0
54	MG	2a	3181	1/1	0.92	0.16	77,77,77,77	0
54	MG	1A	3357	1/1	0.92	0.08	44,44,44,44	0
54	MG	2A	3233	1/1	0.92	0.16	66,66,66,66	0
54	MG	2A	3718	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3234	1/1	0.92	0.14	58,58,58,58	0
54	MG	1a	1617	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3238	1/1	0.92	0.07	60,60,60,60	0
54	MG	1a	1618	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	1621	1/1	0.92	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3729	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3097	1/1	0.92	0.18	57,57,57,57	0
54	MG	1A	3820	1/1	0.92	0.12	65,65,65,65	0
54	MG	2A	3481	1/1	0.92	0.14	60,60,60,60	0
55	HGR	2A	3730	36/36	0.92	0.13	35,49,57,66	0
57	MPD	1A	4024	8/8	0.92	0.20	50,57,60,63	0
54	MG	1a	1780	1/1	0.92	0.13	60,60,60,60	0
54	MG	2B	205	1/1	0.92	0.22	73,73,73,73	0
54	MG	1a	1628	1/1	0.92	0.10	74,74,74,74	0
57	MPD	2A	3733	8/8	0.92	0.17	54,63,65,65	0
54	MG	2A	3487	1/1	0.92	0.11	60,60,60,60	0
54	MG	1A	3563	1/1	0.92	0.09	63,63,63,63	0
54	MG	1A	3605	1/1	0.93	0.17	61,61,61,61	0
54	MG	2B	212	1/1	0.93	0.22	69,69,69,69	0
54	MG	1A	3526	1/1	0.93	0.11	31,31,31,31	0
54	MG	2A	3474	1/1	0.93	0.09	42,42,42,42	0
54	MG	2B	215	1/1	0.93	0.08	80,80,80,80	0
54	MG	2A	3032	1/1	0.93	0.24	60,60,60,60	0
54	MG	2A	3477	1/1	0.93	0.12	50,50,50,50	0
54	MG	1A	3528	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3482	1/1	0.93	0.12	63,63,63,63	0
54	MG	1a	1616	1/1	0.93	0.19	79,79,79,79	0
54	MG	2E	304	1/1	0.93	0.27	51,51,51,51	0
54	MG	1A	3107	1/1	0.93	0.18	41,41,41,41	0
54	MG	2E	307	1/1	0.93	0.21	68,68,68,68	0
54	MG	2A	3486	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3067	1/1	0.93	0.14	58,58,58,58	0
54	MG	2A	3245	1/1	0.93	0.17	64,64,64,64	0
54	MG	1a	1776	1/1	0.93	0.16	65,65,65,65	0
54	MG	1a	1620	1/1	0.93	0.07	68,68,68,68	0
54	MG	1A	3837	1/1	0.93	0.10	59,59,59,59	0
54	MG	2A	3043	1/1	0.93	0.17	54,54,54,54	0
54	MG	1a	1779	1/1	0.93	0.20	71,71,71,71	0
54	MG	2P	201	1/1	0.93	0.22	64,64,64,64	0
54	MG	1A	3534	1/1	0.93	0.07	24,24,24,24	0
54	MG	1A	3224	1/1	0.93	0.22	41,41,41,41	0
54	MG	1A	3068	1/1	0.93	0.12	46,46,46,46	0
54	MG	2R	201	1/1	0.93	0.28	48,48,48,48	0
54	MG	2R	202	1/1	0.93	0.14	53,53,53,53	0
54	MG	1a	1629	1/1	0.93	0.24	65,65,65,65	0
54	MG	2T	204	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3710	1/1	0.93	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3347	1/1	0.93	0.21	55,55,55,55	0
54	MG	20	101	1/1	0.93	0.10	55,55,55,55	0
54	MG	1a	1787	1/1	0.93	0.14	71,71,71,71	0
54	MG	1a	1789	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	4013	1/1	0.93	0.24	42,42,42,42	0
54	MG	1A	3713	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3064	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3511	1/1	0.93	0.24	68,68,68,68	0
54	MG	2A	3065	1/1	0.93	0.08	56,56,56,56	0
54	MG	1A	3627	1/1	0.93	0.16	49,49,49,49	0
54	MG	1A	3628	1/1	0.93	0.15	39,39,39,39	0
54	MG	1a	1795	1/1	0.93	0.07	74,74,74,74	0
54	MG	2A	3073	1/1	0.93	0.24	67,67,67,67	0
54	MG	2A	3074	1/1	0.93	0.20	54,54,54,54	0
54	MG	1A	4019	1/1	0.93	0.21	84,84,84,84	0
54	MG	2A	3077	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	4020	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3719	1/1	0.93	0.09	70,70,70,70	0
54	MG	2a	3016	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3405	1/1	0.93	0.08	41,41,41,41	0
54	MG	2a	3019	1/1	0.93	0.22	60,60,60,60	0
54	MG	2A	3292	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3293	1/1	0.93	0.39	79,79,79,79	0
54	MG	1A	3070	1/1	0.93	0.29	45,45,45,45	0
54	MG	1A	3407	1/1	0.93	0.07	40,40,40,40	0
54	MG	1A	3726	1/1	0.93	0.08	66,66,66,66	0
54	MG	2A	3299	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3727	1/1	0.93	0.23	43,43,43,43	0
54	MG	1A	3550	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3638	1/1	0.93	0.11	35,35,35,35	0
54	MG	2A	3304	1/1	0.93	0.25	61,61,61,61	0
54	MG	2a	3033	1/1	0.93	0.17	71,71,71,71	0
54	MG	2A	3547	1/1	0.93	0.18	57,57,57,57	0
54	MG	1A	3738	1/1	0.93	0.12	70,70,70,70	0
54	MG	1A	3234	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3310	1/1	0.93	0.35	65,65,65,65	0
54	MG	2A	3552	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	3747	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	3300	1/1	0.93	0.13	59,59,59,59	0
54	MG	2A	3555	1/1	0.93	0.10	63,63,63,63	0
54	MG	2A	3556	1/1	0.93	0.20	66,66,66,66	0
54	MG	2A	3314	1/1	0.93	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1B	218	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3645	1/1	0.93	0.08	43,43,43,43	0
54	MG	1B	221	1/1	0.93	0.11	61,61,61,61	0
54	MG	1a	1815	1/1	0.93	0.12	69,69,69,69	0
54	MG	2a	3049	1/1	0.93	0.26	59,59,59,59	0
54	MG	2a	3050	1/1	0.93	0.19	76,76,76,76	0
54	MG	2A	3104	1/1	0.93	0.15	66,66,66,66	0
54	MG	2A	3107	1/1	0.93	0.11	57,57,57,57	0
54	MG	2a	3053	1/1	0.93	0.23	61,61,61,61	0
54	MG	2A	3108	1/1	0.93	0.14	67,67,67,67	0
54	MG	1A	3754	1/1	0.93	0.16	48,48,48,48	0
54	MG	1A	3092	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3199	1/1	0.93	0.27	67,67,67,67	0
54	MG	2A	3115	1/1	0.93	0.21	72,72,72,72	0
54	MG	2A	3117	1/1	0.93	0.20	58,58,58,58	0
54	MG	1A	3761	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3902	1/1	0.93	0.11	58,58,58,58	0
54	MG	2a	3064	1/1	0.93	0.35	75,75,75,75	0
54	MG	2A	3586	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3570	1/1	0.93	0.17	58,58,58,58	0
54	MG	1a	1829	1/1	0.93	0.07	72,72,72,72	0
54	MG	1A	3427	1/1	0.93	0.18	52,52,52,52	0
54	MG	2A	3130	1/1	0.93	0.19	66,66,66,66	0
54	MG	2A	3341	1/1	0.93	0.15	59,59,59,59	0
54	MG	1a	1833	1/1	0.93	0.24	73,73,73,73	0
54	MG	1A	3256	1/1	0.93	0.21	51,51,51,51	0
54	MG	2a	3078	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3653	1/1	0.93	0.18	66,66,66,66	0
54	MG	2A	3349	1/1	0.93	0.13	54,54,54,54	0
54	MG	1D	320	1/1	0.93	0.08	52,52,52,52	0
54	MG	1A	3773	1/1	0.93	0.13	45,45,45,45	0
54	MG	2A	3352	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3353	1/1	0.93	0.07	49,49,49,49	0
54	MG	1A	3368	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1693	1/1	0.93	0.10	74,74,74,74	0
54	MG	1E	306	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3628	1/1	0.93	0.16	63,63,63,63	0
54	MG	1E	308	1/1	0.93	0.08	33,33,33,33	0
54	MG	1F	313	1/1	0.93	0.09	49,49,49,49	0
54	MG	2A	3367	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3155	1/1	0.93	0.27	60,60,60,60	0
54	MG	2A	3156	1/1	0.93	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1699	1/1	0.93	0.25	66,66,66,66	0
54	MG	1a	1700	1/1	0.93	0.36	67,67,67,67	0
54	MG	2A	3639	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3777	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3382	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3385	1/1	0.93	0.08	36,36,36,36	0
54	MG	1a	1849	1/1	0.93	0.23	63,63,63,63	0
54	MG	2A	3645	1/1	0.93	0.21	61,61,61,61	0
54	MG	1A	3944	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3132	1/1	0.93	0.14	53,53,53,53	0
54	MG	2A	3652	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3579	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3492	1/1	0.93	0.06	26,26,26,26	0
54	MG	2A	3657	1/1	0.93	0.11	61,61,61,61	0
54	MG	1A	3950	1/1	0.93	0.14	70,70,70,70	0
54	MG	1A	3261	1/1	0.93	0.32	71,71,71,71	0
54	MG	1A	3014	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3265	1/1	0.93	0.07	76,76,76,76	0
54	MG	2a	3121	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3791	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3208	1/1	0.93	0.30	67,67,67,67	0
54	MG	1A	3663	1/1	0.93	0.07	54,54,54,54	0
54	MG	1R	207	1/1	0.93	0.14	57,57,57,57	0
54	MG	2a	3127	1/1	0.93	0.19	58,58,58,58	0
54	MG	2a	3128	1/1	0.93	0.10	67,67,67,67	0
54	MG	2A	3673	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3409	1/1	0.93	0.14	69,69,69,69	0
54	MG	2a	3136	1/1	0.93	0.11	72,72,72,72	0
54	MG	1A	3329	1/1	0.93	0.10	44,44,44,44	0
54	MG	1a	1877	1/1	0.93	0.10	58,58,58,58	0
54	MG	2a	3141	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3416	1/1	0.93	0.25	63,63,63,63	0
54	MG	2A	3419	1/1	0.93	0.07	44,44,44,44	0
54	MG	1A	3665	1/1	0.93	0.07	39,39,39,39	0
54	MG	2A	3422	1/1	0.93	0.10	52,52,52,52	0
54	MG	1a	1721	1/1	0.93	0.33	82,82,82,82	0
54	MG	2a	3151	1/1	0.93	0.12	80,80,80,80	0
54	MG	2A	3686	1/1	0.93	0.12	69,69,69,69	0
54	MG	1A	3505	1/1	0.93	0.07	44,44,44,44	0
54	MG	1a	1723	1/1	0.93	0.10	51,51,51,51	0
54	MG	1b	301	1/1	0.93	0.11	78,78,78,78	0
54	MG	2A	3691	1/1	0.93	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1V	204	1/1	0.93	0.12	57,57,57,57	0
54	MG	1A	3035	1/1	0.93	0.10	45,45,45,45	0
54	MG	2a	3161	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3511	1/1	0.93	0.15	59,59,59,59	0
54	MG	2A	3199	1/1	0.93	0.15	62,62,62,62	0
54	MG	2A	3434	1/1	0.93	0.07	44,44,44,44	0
54	MG	2a	3166	1/1	0.93	0.16	72,72,72,72	0
54	MG	1A	3106	1/1	0.93	0.11	42,42,42,42	0
54	MG	2A	3701	1/1	0.93	0.08	55,55,55,55	0
54	MG	1a	1730	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3804	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3206	1/1	0.93	0.28	64,64,64,64	0
54	MG	2a	3174	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3806	1/1	0.93	0.07	55,55,55,55	0
54	MG	2A	3710	1/1	0.93	0.07	46,46,46,46	0
54	MG	1A	3814	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3281	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3599	1/1	0.93	0.15	66,66,66,66	0
54	MG	13	102	1/1	0.93	0.25	61,61,61,61	0
54	MG	2a	3185	1/1	0.93	0.23	71,71,71,71	0
54	MG	2A	3447	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3520	1/1	0.93	0.09	27,27,27,27	0
54	MG	2A	3724	1/1	0.93	0.21	63,63,63,63	0
54	MG	1A	3392	1/1	0.93	0.11	75,75,75,75	0
54	MG	1a	1745	1/1	0.93	0.12	78,78,78,78	0
54	MG	15	107	1/1	0.93	0.08	57,57,57,57	0
54	MG	17	105	1/1	0.93	0.21	64,64,64,64	0
54	MG	2e	201	1/1	0.93	0.35	72,72,72,72	0
54	MG	1A	3990	1/1	0.93	0.07	55,55,55,55	0
54	MG	1A	3689	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3827	1/1	0.93	0.15	42,42,42,42	0
54	MG	1A	3993	1/1	0.93	0.12	40,40,40,40	0
54	MG	2A	3226	1/1	0.93	0.18	42,42,42,42	0
54	MG	2A	3018	1/1	0.93	0.34	54,54,54,54	0
54	MG	1a	1758	1/1	0.93	0.20	49,49,49,49	0
54	MG	2B	207	1/1	0.93	0.18	72,72,72,72	0
54	MG	1a	1605	1/1	0.93	0.23	72,72,72,72	0
58	ARG	1B	230	12/12	0.93	0.10	34,54,66,69	0
54	MG	2B	209	1/1	0.93	0.10	69,69,69,69	0
54	MG	2A	3150	1/1	0.94	0.20	72,72,72,72	0
54	MG	1a	1630	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3535	1/1	0.94	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3153	1/1	0.94	0.11	46,46,46,46	0
54	MG	1a	1632	1/1	0.94	0.23	59,59,59,59	0
54	MG	1A	3017	1/1	0.94	0.23	36,36,36,36	0
54	MG	1a	1635	1/1	0.94	0.12	57,57,57,57	0
54	MG	1a	1816	1/1	0.94	0.13	68,68,68,68	0
54	MG	1A	3541	1/1	0.94	0.33	39,39,39,39	0
54	MG	2A	3161	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3108	1/1	0.94	0.07	43,43,43,43	0
54	MG	1a	1638	1/1	0.94	0.17	51,51,51,51	0
54	MG	1a	1822	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3349	1/1	0.94	0.08	29,29,29,29	0
54	MG	2A	3169	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3441	1/1	0.94	0.11	27,27,27,27	0
54	MG	1A	3200	1/1	0.94	0.28	44,44,44,44	0
54	MG	1A	3998	1/1	0.94	0.06	57,57,57,57	0
54	MG	2A	3176	1/1	0.94	0.12	60,60,60,60	0
54	MG	2B	216	1/1	0.94	0.09	59,59,59,59	0
54	MG	1A	3268	1/1	0.94	0.30	40,40,40,40	0
54	MG	1a	1832	1/1	0.94	0.11	70,70,70,70	0
54	MG	2D	304	1/1	0.94	0.17	57,57,57,57	0
54	MG	2D	307	1/1	0.94	0.28	44,44,44,44	0
54	MG	1a	1645	1/1	0.94	0.22	62,62,62,62	0
54	MG	1A	3805	1/1	0.94	0.20	64,64,64,64	0
54	MG	1A	3110	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	4002	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3809	1/1	0.94	0.09	63,63,63,63	0
54	MG	2A	3187	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	4005	1/1	0.94	0.13	69,69,69,69	0
54	MG	1A	3811	1/1	0.94	0.23	41,41,41,41	0
54	MG	1A	3812	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	4009	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3465	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3552	1/1	0.94	0.18	68,68,68,68	0
54	MG	1A	3202	1/1	0.94	0.09	50,50,50,50	0
54	MG	1a	1663	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3204	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	4014	1/1	0.94	0.08	52,52,52,52	0
54	MG	2A	3473	1/1	0.94	0.19	62,62,62,62	0
54	MG	1a	1850	1/1	0.94	0.11	75,75,75,75	0
54	MG	2Q	203	1/1	0.94	0.18	64,64,64,64	0
54	MG	2A	3198	1/1	0.94	0.16	65,65,65,65	0
54	MG	1a	1668	1/1	0.94	0.33	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3479	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3480	1/1	0.94	0.10	62,62,62,62	0
54	MG	2U	201	1/1	0.94	0.05	65,65,65,65	0
54	MG	1a	1669	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3202	1/1	0.94	0.22	48,48,48,48	0
54	MG	2Y	201	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3560	1/1	0.94	0.13	52,52,52,52	0
54	MG	1a	1671	1/1	0.94	0.14	66,66,66,66	0
54	MG	1a	1858	1/1	0.94	0.10	72,72,72,72	0
54	MG	1A	3666	1/1	0.94	0.18	61,61,61,61	0
54	MG	25	103	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1673	1/1	0.94	0.19	62,62,62,62	0
54	MG	1A	3822	1/1	0.94	0.05	40,40,40,40	0
54	MG	1A	4018	1/1	0.94	0.10	52,52,52,52	0
54	MG	2a	3001	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3116	1/1	0.94	0.09	46,46,46,46	0
54	MG	2A	3492	1/1	0.94	0.10	49,49,49,49	0
54	MG	2a	3004	1/1	0.94	0.09	58,58,58,58	0
54	MG	1a	1679	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3087	1/1	0.94	0.43	41,41,41,41	0
54	MG	1a	1682	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3674	1/1	0.94	0.12	68,68,68,68	0
54	MG	2a	3009	1/1	0.94	0.07	76,76,76,76	0
54	MG	2A	3217	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3675	1/1	0.94	0.06	19,19,19,19	0
54	MG	1A	3210	1/1	0.94	0.22	52,52,52,52	0
54	MG	1a	1687	1/1	0.94	0.15	60,60,60,60	0
54	MG	2a	3015	1/1	0.94	0.16	62,62,62,62	0
54	MG	1A	3571	1/1	0.94	0.08	42,42,42,42	0
54	MG	2A	3503	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3572	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3225	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3168	1/1	0.94	0.12	49,49,49,49	0
54	MG	1A	3460	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3216	1/1	0.94	0.39	45,45,45,45	0
54	MG	1d	303	1/1	0.94	0.21	71,71,71,71	0
54	MG	1A	3577	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3691	1/1	0.94	0.10	55,55,55,55	0
54	MG	1a	1695	1/1	0.94	0.07	68,68,68,68	0
54	MG	1A	3843	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3169	1/1	0.94	0.09	32,32,32,32	0
54	MG	1h	201	1/1	0.94	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3526	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3242	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3218	1/1	0.94	0.40	42,42,42,42	0
54	MG	2A	3244	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3060	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3128	1/1	0.94	0.15	53,53,53,53	0
54	MG	1a	1702	1/1	0.94	0.37	66,66,66,66	0
54	MG	2A	3535	1/1	0.94	0.07	63,63,63,63	0
54	MG	1m	201	1/1	0.94	0.07	74,74,74,74	0
54	MG	1A	3309	1/1	0.94	0.22	63,63,63,63	0
54	MG	2A	3252	1/1	0.94	0.18	61,61,61,61	0
54	MG	1A	3701	1/1	0.94	0.15	66,66,66,66	0
54	MG	1A	3223	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3475	1/1	0.94	0.08	29,29,29,29	0
54	MG	1a	1708	1/1	0.94	0.24	62,62,62,62	0
54	MG	1A	3868	1/1	0.94	0.11	49,49,49,49	0
54	MG	1D	307	1/1	0.94	0.19	48,48,48,48	0
54	MG	2A	3004	1/1	0.94	0.10	67,67,67,67	0
54	MG	2A	3268	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3062	1/1	0.94	0.18	42,42,42,42	0
54	MG	2A	3009	1/1	0.94	0.15	58,58,58,58	0
54	MG	2a	3056	1/1	0.94	0.16	71,71,71,71	0
54	MG	1a	1712	1/1	0.94	0.38	73,73,73,73	0
54	MG	1D	313	1/1	0.94	0.18	40,40,40,40	0
54	MG	1A	3875	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3877	1/1	0.94	0.11	60,60,60,60	0
54	MG	1D	317	1/1	0.94	0.11	68,68,68,68	0
54	MG	2A	3024	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3027	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3878	1/1	0.94	0.08	33,33,33,33	0
54	MG	2A	3282	1/1	0.94	0.34	70,70,70,70	0
54	MG	2A	3031	1/1	0.94	0.13	52,52,52,52	0
54	MG	2a	3068	1/1	0.94	0.07	81,81,81,81	0
54	MG	1A	3590	1/1	0.94	0.08	26,26,26,26	0
54	MG	2a	3071	1/1	0.94	0.10	67,67,67,67	0
54	MG	1a	1719	1/1	0.94	0.26	70,70,70,70	0
54	MG	2A	3569	1/1	0.94	0.17	70,70,70,70	0
54	MG	2A	3570	1/1	0.94	0.11	53,53,53,53	0
54	MG	1A	3181	1/1	0.94	0.14	53,53,53,53	0
54	MG	2a	3077	1/1	0.94	0.17	72,72,72,72	0
54	MG	2A	3572	1/1	0.94	0.09	63,63,63,63	0
54	MG	1A	3319	1/1	0.94	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3481	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3596	1/1	0.94	0.30	60,60,60,60	0
54	MG	1F	312	1/1	0.94	0.37	51,51,51,51	0
54	MG	2A	3040	1/1	0.94	0.15	52,52,52,52	0
54	MG	1A	3227	1/1	0.94	0.13	46,46,46,46	0
54	MG	1a	1727	1/1	0.94	0.19	72,72,72,72	0
54	MG	2A	3298	1/1	0.94	0.38	66,66,66,66	0
54	MG	1A	3487	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3721	1/1	0.94	0.11	47,47,47,47	0
54	MG	2A	3301	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3594	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3398	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3049	1/1	0.94	0.26	66,66,66,66	0
54	MG	2A	3597	1/1	0.94	0.07	49,49,49,49	0
54	MG	1G	204	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3603	1/1	0.94	0.08	62,62,62,62	0
54	MG	2A	3607	1/1	0.94	0.05	70,70,70,70	0
54	MG	2a	3099	1/1	0.94	0.26	64,64,64,64	0
54	MG	1A	3399	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3896	1/1	0.94	0.16	40,40,40,40	0
54	MG	2A	3612	1/1	0.94	0.09	69,69,69,69	0
54	MG	2A	3309	1/1	0.94	0.42	53,53,53,53	0
54	MG	2A	3055	1/1	0.94	0.24	65,65,65,65	0
54	MG	2a	3107	1/1	0.94	0.31	53,53,53,53	0
54	MG	2A	3617	1/1	0.94	0.07	65,65,65,65	0
54	MG	1A	3725	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3620	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3322	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	3493	1/1	0.94	0.07	31,31,31,31	0
54	MG	1A	3910	1/1	0.94	0.13	38,38,38,38	0
54	MG	2A	3625	1/1	0.94	0.08	56,56,56,56	0
54	MG	1P	201	1/1	0.94	0.27	39,39,39,39	0
54	MG	1A	3038	1/1	0.94	0.24	58,58,58,58	0
54	MG	1A	3496	1/1	0.94	0.11	39,39,39,39	0
54	MG	2a	3120	1/1	0.94	0.11	65,65,65,65	0
54	MG	1R	203	1/1	0.94	0.21	53,53,53,53	0
54	MG	1A	3737	1/1	0.94	0.12	48,48,48,48	0
54	MG	1R	205	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3232	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3743	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3636	1/1	0.94	0.11	56,56,56,56	0
54	MG	2A	3075	1/1	0.94	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3937	1/1	0.94	0.11	68,68,68,68	0
54	MG	2a	3130	1/1	0.94	0.10	79,79,79,79	0
54	MG	1T	203	1/1	0.94	0.06	70,70,70,70	0
54	MG	1A	3612	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3642	1/1	0.94	0.09	74,74,74,74	0
54	MG	1A	3499	1/1	0.94	0.08	29,29,29,29	0
54	MG	1A	3051	1/1	0.94	0.29	56,56,56,56	0
54	MG	2A	3082	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3101	1/1	0.94	0.23	42,42,42,42	0
54	MG	1A	3411	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3339	1/1	0.94	0.08	50,50,50,50	0
54	MG	2a	3148	1/1	0.94	0.13	78,78,78,78	0
54	MG	1A	3948	1/1	0.94	0.07	30,30,30,30	0
54	MG	1A	3756	1/1	0.94	0.19	67,67,67,67	0
54	MG	1A	3504	1/1	0.94	0.06	31,31,31,31	0
54	MG	2A	3091	1/1	0.94	0.14	60,60,60,60	0
54	MG	10	108	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3954	1/1	0.94	0.07	29,29,29,29	0
54	MG	1A	3956	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3623	1/1	0.94	0.15	33,33,33,33	0
54	MG	1A	3330	1/1	0.94	0.08	52,52,52,52	0
54	MG	2A	3355	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3959	1/1	0.94	0.07	71,71,71,71	0
54	MG	1A	3331	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3763	1/1	0.94	0.11	46,46,46,46	0
54	MG	17	106	1/1	0.94	0.08	50,50,50,50	0
54	MG	2a	3168	1/1	0.94	0.14	66,66,66,66	0
54	MG	2A	3360	1/1	0.94	0.10	45,45,45,45	0
54	MG	1a	1788	1/1	0.94	0.12	74,74,74,74	0
54	MG	1A	3417	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3420	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3109	1/1	0.94	0.11	59,59,59,59	0
54	MG	2A	3110	1/1	0.94	0.08	69,69,69,69	0
54	MG	1A	3143	1/1	0.94	0.05	30,30,30,30	0
54	MG	1a	1602	1/1	0.94	0.10	79,79,79,79	0
54	MG	1A	3519	1/1	0.94	0.06	46,46,46,46	0
54	MG	2A	3383	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3253	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3116	1/1	0.94	0.09	57,57,57,57	0
54	MG	1A	3970	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3425	1/1	0.94	0.08	31,31,31,31	0
54	MG	2A	3697	1/1	0.94	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3078	1/1	0.94	0.35	42,42,42,42	0
54	MG	1a	1615	1/1	0.94	0.09	63,63,63,63	0
54	MG	1a	1800	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3980	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3643	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3527	1/1	0.94	0.11	27,27,27,27	0
54	MG	2A	3705	1/1	0.94	0.09	79,79,79,79	0
54	MG	1A	3787	1/1	0.94	0.10	60,60,60,60	0
54	MG	2t	201	1/1	0.94	0.19	53,53,53,53	0
54	MG	1A	3150	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3433	1/1	0.94	0.13	27,27,27,27	0
54	MG	1A	3648	1/1	0.94	0.07	39,39,39,39	0
54	MG	2A	3143	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3144	1/1	0.94	0.13	65,65,65,65	0
54	MG	2A	3146	1/1	0.94	0.14	43,43,43,43	0
54	MG	1A	3258	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3417	1/1	0.94	0.13	57,57,57,57	0
54	MG	1A	3260	1/1	0.94	0.24	65,65,65,65	0
54	MG	1Q	203	1/1	0.95	0.08	50,50,50,50	0
54	MG	2A	3454	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3556	1/1	0.95	0.06	39,39,39,39	0
54	MG	2A	3458	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3775	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3465	1/1	0.95	0.10	52,52,52,52	0
54	MG	1R	206	1/1	0.95	0.11	34,34,34,34	0
54	MG	1A	3235	1/1	0.95	0.12	36,36,36,36	0
54	MG	1A	3952	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3469	1/1	0.95	0.07	63,63,63,63	0
54	MG	1A	3955	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3779	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	3565	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3237	1/1	0.95	0.23	41,41,41,41	0
54	MG	2A	3005	1/1	0.95	0.09	60,60,60,60	0
54	MG	2D	305	1/1	0.95	0.41	50,50,50,50	0
54	MG	2D	306	1/1	0.95	0.10	61,61,61,61	0
54	MG	2A	3222	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3223	1/1	0.95	0.10	69,69,69,69	0
54	MG	1V	206	1/1	0.95	0.09	54,54,54,54	0
54	MG	1A	3568	1/1	0.95	0.11	59,59,59,59	0
54	MG	2A	3478	1/1	0.95	0.08	64,64,64,64	0
54	MG	2A	3011	1/1	0.95	0.15	69,69,69,69	0
54	MG	2A	3227	1/1	0.95	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1731	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3569	1/1	0.95	0.09	54,54,54,54	0
54	MG	1A	3149	1/1	0.95	0.32	35,35,35,35	0
54	MG	2A	3484	1/1	0.95	0.16	65,65,65,65	0
54	MG	1a	1738	1/1	0.95	0.08	46,46,46,46	0
54	MG	10	102	1/1	0.95	0.15	49,49,49,49	0
54	MG	10	103	1/1	0.95	0.10	62,62,62,62	0
54	MG	2A	3235	1/1	0.95	0.13	59,59,59,59	0
54	MG	1A	3962	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3394	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3239	1/1	0.95	0.31	48,48,48,48	0
54	MG	1A	3320	1/1	0.95	0.07	34,34,34,34	0
54	MG	11	101	1/1	0.95	0.13	51,51,51,51	0
54	MG	1A	3245	1/1	0.95	0.28	64,64,64,64	0
54	MG	1A	3397	1/1	0.95	0.08	50,50,50,50	0
54	MG	2T	201	1/1	0.95	0.11	53,53,53,53	0
54	MG	11	105	1/1	0.95	0.08	44,44,44,44	0
54	MG	2T	203	1/1	0.95	0.14	71,71,71,71	0
54	MG	2A	3247	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3246	1/1	0.95	0.33	59,59,59,59	0
54	MG	1a	1751	1/1	0.95	0.09	62,62,62,62	0
54	MG	1a	1752	1/1	0.95	0.12	65,65,65,65	0
54	MG	2A	3039	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3969	1/1	0.95	0.11	52,52,52,52	0
54	MG	20	102	1/1	0.95	0.40	61,61,61,61	0
54	MG	2A	3041	1/1	0.95	0.06	26,26,26,26	0
54	MG	15	105	1/1	0.95	0.24	32,32,32,32	0
54	MG	23	101	1/1	0.95	0.16	61,61,61,61	0
54	MG	2A	3507	1/1	0.95	0.08	69,69,69,69	0
54	MG	25	102	1/1	0.95	0.11	61,61,61,61	0
54	MG	2A	3508	1/1	0.95	0.09	33,33,33,33	0
54	MG	27	101	1/1	0.95	0.21	49,49,49,49	0
54	MG	27	102	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3249	1/1	0.95	0.22	54,54,54,54	0
54	MG	2A	3262	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3971	1/1	0.95	0.15	53,53,53,53	0
54	MG	2A	3045	1/1	0.95	0.21	65,65,65,65	0
54	MG	1A	3973	1/1	0.95	0.07	43,43,43,43	0
54	MG	1a	1762	1/1	0.95	0.21	56,56,56,56	0
54	MG	1a	1764	1/1	0.95	0.15	67,67,67,67	0
54	MG	1A	3974	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3011	1/1	0.95	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3521	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3667	1/1	0.95	0.14	55,55,55,55	0
54	MG	1a	1770	1/1	0.95	0.14	61,61,61,61	0
54	MG	2A	3527	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3056	1/1	0.95	0.08	37,37,37,37	0
54	MG	1a	1771	1/1	0.95	0.16	67,67,67,67	0
54	MG	1a	1772	1/1	0.95	0.18	59,59,59,59	0
54	MG	1A	3799	1/1	0.95	0.12	65,65,65,65	0
54	MG	2A	3061	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3670	1/1	0.95	0.38	52,52,52,52	0
54	MG	1A	3802	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3113	1/1	0.95	0.08	44,44,44,44	0
54	MG	2a	3021	1/1	0.95	0.07	63,63,63,63	0
54	MG	1a	1606	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3538	1/1	0.95	0.16	56,56,56,56	0
54	MG	1a	1607	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	3153	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3289	1/1	0.95	0.15	50,50,50,50	0
54	MG	2A	3543	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3581	1/1	0.95	0.07	53,53,53,53	0
54	MG	2a	3029	1/1	0.95	0.15	66,66,66,66	0
54	MG	1a	1610	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3582	1/1	0.95	0.21	49,49,49,49	0
54	MG	1a	1613	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3294	1/1	0.95	0.23	65,65,65,65	0
54	MG	1A	3807	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3808	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3551	1/1	0.95	0.16	60,60,60,60	0
54	MG	2A	3078	1/1	0.95	0.11	64,64,64,64	0
54	MG	1A	3114	1/1	0.95	0.18	47,47,47,47	0
54	MG	1A	3025	1/1	0.95	0.21	45,45,45,45	0
54	MG	1A	3259	1/1	0.95	0.21	55,55,55,55	0
54	MG	1A	3160	1/1	0.95	0.20	37,37,37,37	0
54	MG	1A	3815	1/1	0.95	0.22	52,52,52,52	0
54	MG	1A	3413	1/1	0.95	0.06	54,54,54,54	0
54	MG	1A	3683	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3819	1/1	0.95	0.08	33,33,33,33	0
54	MG	2A	3563	1/1	0.95	0.19	70,70,70,70	0
54	MG	1A	3686	1/1	0.95	0.10	46,46,46,46	0
54	MG	2A	3090	1/1	0.95	0.13	51,51,51,51	0
54	MG	1A	3054	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3093	1/1	0.95	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3312	1/1	0.95	0.28	65,65,65,65	0
54	MG	1A	3592	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3593	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3829	1/1	0.95	0.24	44,44,44,44	0
54	MG	1A	3419	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3574	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3575	1/1	0.95	0.09	59,59,59,59	0
54	MG	1A	3056	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3036	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3834	1/1	0.95	0.06	27,27,27,27	0
54	MG	1A	3697	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3422	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3585	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3212	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3273	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3099	1/1	0.95	0.08	41,41,41,41	0
54	MG	2a	3070	1/1	0.95	0.15	72,72,72,72	0
54	MG	1a	1648	1/1	0.95	0.20	46,46,46,46	0
54	MG	1A	3512	1/1	0.95	0.16	37,37,37,37	0
54	MG	1A	3604	1/1	0.95	0.09	58,58,58,58	0
54	MG	1a	1654	1/1	0.95	0.17	62,62,62,62	0
54	MG	2A	3330	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3332	1/1	0.95	0.11	65,65,65,65	0
54	MG	2A	3598	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3430	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3600	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3601	1/1	0.95	0.15	50,50,50,50	0
54	MG	1a	1817	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3353	1/1	0.95	0.13	38,38,38,38	0
54	MG	1A	3714	1/1	0.95	0.21	56,56,56,56	0
54	MG	2A	3120	1/1	0.95	0.12	50,50,50,50	0
54	MG	2A	3340	1/1	0.95	0.09	22,22,22,22	0
54	MG	1A	3012	1/1	0.95	0.18	43,43,43,43	0
54	MG	2A	3124	1/1	0.95	0.21	48,48,48,48	0
54	MG	2A	3343	1/1	0.95	0.06	44,44,44,44	0
54	MG	1A	3356	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3619	1/1	0.95	0.10	49,49,49,49	0
54	MG	2A	3347	1/1	0.95	0.12	59,59,59,59	0
54	MG	1B	204	1/1	0.95	0.07	54,54,54,54	0
54	MG	1A	3133	1/1	0.95	0.22	51,51,51,51	0
54	MG	1A	3358	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3179	1/1	0.95	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1830	1/1	0.95	0.06	72,72,72,72	0
54	MG	1B	208	1/1	0.95	0.06	46,46,46,46	0
54	MG	2A	3354	1/1	0.95	0.08	37,37,37,37	0
54	MG	2A	3136	1/1	0.95	0.07	47,47,47,47	0
54	MG	2a	3103	1/1	0.95	0.30	53,53,53,53	0
54	MG	1A	3864	1/1	0.95	0.08	53,53,53,53	0
54	MG	2a	3105	1/1	0.95	0.40	67,67,67,67	0
54	MG	2A	3632	1/1	0.95	0.14	58,58,58,58	0
54	MG	2A	3139	1/1	0.95	0.12	65,65,65,65	0
54	MG	1A	3180	1/1	0.95	0.20	36,36,36,36	0
54	MG	1A	3616	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3870	1/1	0.95	0.06	66,66,66,66	0
54	MG	2A	3145	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3364	1/1	0.95	0.17	45,45,45,45	0
54	MG	2A	3365	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3366	1/1	0.95	0.12	56,56,56,56	0
54	MG	2a	3115	1/1	0.95	0.51	69,69,69,69	0
54	MG	1A	3617	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3619	1/1	0.95	0.08	39,39,39,39	0
54	MG	2a	3118	1/1	0.95	0.12	74,74,74,74	0
54	MG	2A	3369	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3876	1/1	0.95	0.05	35,35,35,35	0
54	MG	1a	1676	1/1	0.95	0.21	59,59,59,59	0
54	MG	2a	3122	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3374	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3651	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3529	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3376	1/1	0.95	0.10	64,64,64,64	0
54	MG	1a	1843	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3656	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3728	1/1	0.95	0.24	47,47,47,47	0
54	MG	1A	3134	1/1	0.95	0.16	44,44,44,44	0
54	MG	2A	3659	1/1	0.95	0.15	55,55,55,55	0
54	MG	2a	3135	1/1	0.95	0.10	73,73,73,73	0
54	MG	2A	3384	1/1	0.95	0.09	46,46,46,46	0
54	MG	2a	3137	1/1	0.95	0.08	69,69,69,69	0
54	MG	1a	1680	1/1	0.95	0.19	65,65,65,65	0
54	MG	2A	3663	1/1	0.95	0.06	47,47,47,47	0
54	MG	1A	3730	1/1	0.95	0.05	32,32,32,32	0
54	MG	2A	3157	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3885	1/1	0.95	0.08	33,33,33,33	0
54	MG	1a	1683	1/1	0.95	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3030	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3626	1/1	0.95	0.21	36,36,36,36	0
54	MG	1A	3141	1/1	0.95	0.28	48,48,48,48	0
54	MG	1A	3369	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3744	1/1	0.95	0.06	59,59,59,59	0
54	MG	1A	3536	1/1	0.95	0.13	61,61,61,61	0
54	MG	1a	1860	1/1	0.95	0.07	59,59,59,59	0
54	MG	1a	1861	1/1	0.95	0.08	58,58,58,58	0
54	MG	1a	1862	1/1	0.95	0.09	62,62,62,62	0
54	MG	2a	3158	1/1	0.95	0.09	69,69,69,69	0
54	MG	1A	3190	1/1	0.95	0.08	54,54,54,54	0
54	MG	2A	3684	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3685	1/1	0.95	0.08	67,67,67,67	0
54	MG	1a	1865	1/1	0.95	0.16	76,76,76,76	0
54	MG	1A	3632	1/1	0.95	0.10	34,34,34,34	0
54	MG	2A	3415	1/1	0.95	0.13	55,55,55,55	0
54	MG	1A	3375	1/1	0.95	0.07	49,49,49,49	0
54	MG	2a	3167	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3142	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3636	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3420	1/1	0.95	0.09	70,70,70,70	0
54	MG	2A	3183	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3301	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3185	1/1	0.95	0.12	63,63,63,63	0
54	MG	1A	3909	1/1	0.95	0.07	58,58,58,58	0
54	MG	1A	3379	1/1	0.95	0.07	52,52,52,52	0
54	MG	2a	3178	1/1	0.95	0.14	63,63,63,63	0
54	MG	2a	3179	1/1	0.95	0.11	78,78,78,78	0
54	MG	2A	3427	1/1	0.95	0.08	65,65,65,65	0
54	MG	1A	3911	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	3307	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3230	1/1	0.95	0.21	50,50,50,50	0
54	MG	2A	3431	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3919	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3709	1/1	0.95	0.09	46,46,46,46	0
54	MG	1a	1703	1/1	0.95	0.28	58,58,58,58	0
54	MG	1G	201	1/1	0.95	0.05	69,69,69,69	0
54	MG	1A	3080	1/1	0.95	0.15	50,50,50,50	0
54	MG	2A	3715	1/1	0.95	0.10	66,66,66,66	0
54	MG	2a	3191	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3045	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3931	1/1	0.95	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3765	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3721	1/1	0.95	0.06	55,55,55,55	0
54	MG	2A	3722	1/1	0.95	0.16	57,57,57,57	0
54	MG	1A	3936	1/1	0.95	0.09	59,59,59,59	0
54	MG	1A	3312	1/1	0.95	0.31	45,45,45,45	0
54	MG	2A	3200	1/1	0.95	0.07	50,50,50,50	0
54	MG	1e	202	1/1	0.95	0.26	59,59,59,59	0
57	MPD	18	103	8/8	0.95	0.13	31,44,47,48	0
54	MG	1A	3940	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3769	1/1	0.95	0.08	41,41,41,41	0
54	MG	1A	3770	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3555	1/1	0.95	0.05	30,30,30,30	0
54	MG	2A	3450	1/1	0.95	0.10	53,53,53,53	0
54	MG	1A	3772	1/1	0.95	0.17	58,58,58,58	0
54	MG	2D	309	1/1	0.96	0.15	55,55,55,55	0
54	MG	1A	3324	1/1	0.96	0.21	49,49,49,49	0
54	MG	13	103	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3587	1/1	0.96	0.09	47,47,47,47	0
54	MG	2E	302	1/1	0.96	0.11	52,52,52,52	0
54	MG	2A	3254	1/1	0.96	0.25	49,49,49,49	0
54	MG	2A	3255	1/1	0.96	0.05	40,40,40,40	0
54	MG	2E	306	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3488	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3258	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3046	1/1	0.96	0.11	64,64,64,64	0
54	MG	2A	3261	1/1	0.96	0.20	50,50,50,50	0
54	MG	1a	1759	1/1	0.96	0.11	60,60,60,60	0
54	MG	1a	1760	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3684	1/1	0.96	0.16	52,52,52,52	0
54	MG	2A	3050	1/1	0.96	0.12	49,49,49,49	0
54	MG	2A	3266	1/1	0.96	0.20	55,55,55,55	0
54	MG	2A	3506	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3039	1/1	0.96	0.10	54,54,54,54	0
54	MG	15	108	1/1	0.96	0.18	66,66,66,66	0
54	MG	2A	3269	1/1	0.96	0.17	61,61,61,61	0
54	MG	17	102	1/1	0.96	0.13	42,42,42,42	0
54	MG	17	104	1/1	0.96	0.15	33,33,33,33	0
54	MG	1A	3400	1/1	0.96	0.12	36,36,36,36	0
54	MG	1A	3688	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3515	1/1	0.96	0.07	60,60,60,60	0
54	MG	18	101	1/1	0.96	0.12	49,49,49,49	0
54	MG	1A	3074	1/1	0.96	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3214	1/1	0.96	0.08	46,46,46,46	0
54	MG	2V	201	1/1	0.96	0.10	65,65,65,65	0
54	MG	2V	203	1/1	0.96	0.11	61,61,61,61	0
54	MG	1A	3404	1/1	0.96	0.05	33,33,33,33	0
54	MG	1a	1601	1/1	0.96	0.07	46,46,46,46	0
54	MG	2X	101	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3984	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3524	1/1	0.96	0.11	58,58,58,58	0
54	MG	1A	3052	1/1	0.96	0.21	51,51,51,51	0
54	MG	2A	3283	1/1	0.96	0.14	37,37,37,37	0
54	MG	1A	3497	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3177	1/1	0.96	0.15	34,34,34,34	0
54	MG	2A	3069	1/1	0.96	0.16	44,44,44,44	0
54	MG	2A	3070	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3267	1/1	0.96	0.12	58,58,58,58	0
54	MG	2A	3533	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3698	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3408	1/1	0.96	0.06	37,37,37,37	0
54	MG	28	101	1/1	0.96	0.36	68,68,68,68	0
54	MG	1A	3826	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3104	1/1	0.96	0.26	39,39,39,39	0
54	MG	1A	3270	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3703	1/1	0.96	0.10	50,50,50,50	0
54	MG	1A	3705	1/1	0.96	0.05	53,53,53,53	0
54	MG	1A	3706	1/1	0.96	0.19	49,49,49,49	0
54	MG	1A	3602	1/1	0.96	0.08	50,50,50,50	0
54	MG	1a	1619	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3064	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3085	1/1	0.96	0.33	53,53,53,53	0
54	MG	1A	3709	1/1	0.96	0.42	42,42,42,42	0
54	MG	1A	3065	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3341	1/1	0.96	0.09	52,52,52,52	0
54	MG	1a	1626	1/1	0.96	0.09	65,65,65,65	0
54	MG	2a	3013	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3306	1/1	0.96	0.06	42,42,42,42	0
54	MG	1a	1627	1/1	0.96	0.05	55,55,55,55	0
54	MG	1A	3607	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3274	1/1	0.96	0.20	38,38,38,38	0
54	MG	2a	3018	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3276	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3185	1/1	0.96	0.27	41,41,41,41	0
54	MG	1A	3844	1/1	0.96	0.05	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3845	1/1	0.96	0.09	50,50,50,50	0
54	MG	2A	3559	1/1	0.96	0.12	38,38,38,38	0
54	MG	2A	3560	1/1	0.96	0.15	41,41,41,41	0
54	MG	1A	3846	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3099	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3847	1/1	0.96	0.25	56,56,56,56	0
54	MG	1A	3346	1/1	0.96	0.12	32,32,32,32	0
54	MG	1A	3850	1/1	0.96	0.11	53,53,53,53	0
54	MG	1A	3423	1/1	0.96	0.09	35,35,35,35	0
54	MG	2A	3105	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3278	1/1	0.96	0.23	47,47,47,47	0
54	MG	1A	3083	1/1	0.96	0.24	41,41,41,41	0
54	MG	1a	1642	1/1	0.96	0.09	65,65,65,65	0
54	MG	2a	3036	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3857	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3350	1/1	0.96	0.05	32,32,32,32	0
54	MG	2A	3112	1/1	0.96	0.26	65,65,65,65	0
54	MG	1A	3859	1/1	0.96	0.08	69,69,69,69	0
54	MG	2A	3577	1/1	0.96	0.15	59,59,59,59	0
54	MG	1A	3351	1/1	0.96	0.10	16,16,16,16	0
54	MG	1a	1647	1/1	0.96	0.20	61,61,61,61	0
54	MG	1A	3618	1/1	0.96	0.07	56,56,56,56	0
54	MG	2A	3582	1/1	0.96	0.07	64,64,64,64	0
54	MG	1a	1650	1/1	0.96	0.22	59,59,59,59	0
54	MG	1A	3431	1/1	0.96	0.06	28,28,28,28	0
54	MG	2A	3119	1/1	0.96	0.11	54,54,54,54	0
54	MG	2A	3338	1/1	0.96	0.05	38,38,38,38	0
54	MG	1a	1823	1/1	0.96	0.07	78,78,78,78	0
54	MG	2A	3588	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3589	1/1	0.96	0.10	41,41,41,41	0
54	MG	1A	3023	1/1	0.96	0.16	36,36,36,36	0
54	MG	1a	1825	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3866	1/1	0.96	0.06	49,49,49,49	0
54	MG	1A	3530	1/1	0.96	0.09	25,25,25,25	0
54	MG	2A	3344	1/1	0.96	0.12	55,55,55,55	0
54	MG	2a	3058	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3869	1/1	0.96	0.18	40,40,40,40	0
54	MG	1A	3622	1/1	0.96	0.12	63,63,63,63	0
54	MG	1A	3148	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3132	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3732	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3735	1/1	0.96	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3736	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3532	1/1	0.96	0.05	58,58,58,58	0
54	MG	2A	3138	1/1	0.96	0.07	44,44,44,44	0
54	MG	1a	1836	1/1	0.96	0.08	71,71,71,71	0
54	MG	2A	3140	1/1	0.96	0.07	50,50,50,50	0
54	MG	1B	217	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3615	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3285	1/1	0.96	0.18	54,54,54,54	0
54	MG	1a	1666	1/1	0.96	0.06	74,74,74,74	0
54	MG	2a	3074	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	1667	1/1	0.96	0.18	64,64,64,64	0
54	MG	1A	3739	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3884	1/1	0.96	0.10	38,38,38,38	0
54	MG	1B	222	1/1	0.96	0.06	59,59,59,59	0
54	MG	1A	3085	1/1	0.96	0.26	41,41,41,41	0
54	MG	1A	3437	1/1	0.96	0.08	30,30,30,30	0
54	MG	1A	3290	1/1	0.96	0.12	54,54,54,54	0
54	MG	1B	227	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3631	1/1	0.96	0.23	52,52,52,52	0
54	MG	1A	3359	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3373	1/1	0.96	0.13	49,49,49,49	0
54	MG	1D	301	1/1	0.96	0.29	39,39,39,39	0
54	MG	1D	303	1/1	0.96	0.14	43,43,43,43	0
54	MG	1D	305	1/1	0.96	0.11	58,58,58,58	0
54	MG	2A	3159	1/1	0.96	0.13	49,49,49,49	0
54	MG	2A	3379	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3749	1/1	0.96	0.09	49,49,49,49	0
54	MG	1a	1857	1/1	0.96	0.05	60,60,60,60	0
54	MG	1A	3192	1/1	0.96	0.16	40,40,40,40	0
54	MG	1a	1859	1/1	0.96	0.08	67,67,67,67	0
54	MG	1A	3752	1/1	0.96	0.12	53,53,53,53	0
54	MG	2a	3097	1/1	0.96	0.23	56,56,56,56	0
54	MG	1A	3634	1/1	0.96	0.06	52,52,52,52	0
54	MG	2A	3389	1/1	0.96	0.07	41,41,41,41	0
54	MG	2A	3391	1/1	0.96	0.06	47,47,47,47	0
54	MG	2A	3392	1/1	0.96	0.16	65,65,65,65	0
54	MG	2A	3168	1/1	0.96	0.06	54,54,54,54	0
54	MG	1A	3086	1/1	0.96	0.23	46,46,46,46	0
54	MG	1A	3442	1/1	0.96	0.10	32,32,32,32	0
54	MG	1A	3362	1/1	0.96	0.10	54,54,54,54	0
54	MG	1a	1866	1/1	0.96	0.07	44,44,44,44	0
54	MG	2A	3174	1/1	0.96	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3175	1/1	0.96	0.17	48,48,48,48	0
54	MG	1D	319	1/1	0.96	0.14	61,61,61,61	0
54	MG	2A	3402	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3177	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3364	1/1	0.96	0.06	52,52,52,52	0
54	MG	1A	3907	1/1	0.96	0.08	63,63,63,63	0
54	MG	2A	3407	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3293	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3642	1/1	0.96	0.09	63,63,63,63	0
54	MG	1A	3366	1/1	0.96	0.10	37,37,37,37	0
54	MG	1F	303	1/1	0.96	0.17	36,36,36,36	0
54	MG	2A	3670	1/1	0.96	0.15	70,70,70,70	0
54	MG	1F	306	1/1	0.96	0.12	31,31,31,31	0
54	MG	2A	3672	1/1	0.96	0.10	57,57,57,57	0
54	MG	1F	310	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3418	1/1	0.96	0.16	66,66,66,66	0
54	MG	1F	311	1/1	0.96	0.24	53,53,53,53	0
54	MG	1A	3151	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3678	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3913	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3915	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3916	1/1	0.96	0.05	34,34,34,34	0
54	MG	1A	3766	1/1	0.96	0.05	57,57,57,57	0
54	MG	1A	3553	1/1	0.96	0.34	38,38,38,38	0
54	MG	2a	3134	1/1	0.96	0.20	67,67,67,67	0
54	MG	1G	203	1/1	0.96	0.07	60,60,60,60	0
54	MG	1A	3295	1/1	0.96	0.12	64,64,64,64	0
54	MG	1A	3049	1/1	0.96	0.16	60,60,60,60	0
54	MG	1A	3927	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3454	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3123	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3935	1/1	0.96	0.07	37,37,37,37	0
54	MG	2A	3692	1/1	0.96	0.11	51,51,51,51	0
54	MG	1g	201	1/1	0.96	0.31	75,75,75,75	0
54	MG	1A	3651	1/1	0.96	0.16	51,51,51,51	0
54	MG	2a	3146	1/1	0.96	0.13	65,65,65,65	0
54	MG	2a	3147	1/1	0.96	0.05	68,68,68,68	0
54	MG	1A	3558	1/1	0.96	0.07	39,39,39,39	0
54	MG	2a	3149	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3696	1/1	0.96	0.07	57,57,57,57	0
54	MG	1P	202	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3456	1/1	0.96	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3372	1/1	0.96	0.08	29,29,29,29	0
54	MG	1Q	202	1/1	0.96	0.04	34,34,34,34	0
54	MG	1A	3241	1/1	0.96	0.12	39,39,39,39	0
54	MG	2A	3209	1/1	0.96	0.24	54,54,54,54	0
54	MG	2A	3445	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3566	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3302	1/1	0.96	0.10	37,37,37,37	0
54	MG	1A	3303	1/1	0.96	0.09	51,51,51,51	0
54	MG	1y	201	1/1	0.96	0.09	70,70,70,70	0
54	MG	2a	3163	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3785	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3786	1/1	0.96	0.06	30,30,30,30	0
54	MG	2A	3712	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3242	1/1	0.96	0.28	38,38,38,38	0
54	MG	2A	3714	1/1	0.96	0.06	65,65,65,65	0
54	MG	2A	3002	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3456	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3951	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3124	1/1	0.96	0.06	37,37,37,37	0
54	MG	2A	3720	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3953	1/1	0.96	0.06	70,70,70,70	0
54	MG	1U	205	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3050	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3014	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3090	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3016	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3127	1/1	0.96	0.06	48,48,48,48	0
54	MG	1a	1733	1/1	0.96	0.08	52,52,52,52	0
54	MG	1a	1734	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3313	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3470	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3471	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1737	1/1	0.96	0.06	60,60,60,60	0
54	MG	2A	3025	1/1	0.96	0.15	58,58,58,58	0
54	MG	2A	3026	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3069	1/1	0.96	0.10	40,40,40,40	0
54	MG	2A	3028	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3317	1/1	0.96	0.26	36,36,36,36	0
54	MG	1A	3252	1/1	0.96	0.33	44,44,44,44	0
54	MG	2f	201	1/1	0.96	0.05	54,54,54,54	0
54	MG	1A	3167	1/1	0.96	0.06	41,41,41,41	0
54	MG	2k	201	1/1	0.96	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3240	1/1	0.96	0.27	41,41,41,41	0
54	MG	10	104	1/1	0.96	0.13	58,58,58,58	0
55	HGR	1A	4022	36/36	0.96	0.08	23,32,37,43	0
54	MG	1A	3207	1/1	0.96	0.09	56,56,56,56	0
56	ZIT	2A	3731	52/52	0.96	0.10	33,45,64,67	0
54	MG	1A	3480	1/1	0.96	0.09	60,60,60,60	0
54	MG	1A	3058	1/1	0.96	0.15	54,54,54,54	0
54	MG	1A	3801	1/1	0.96	0.07	31,31,31,31	0
54	MG	2D	303	1/1	0.96	0.38	49,49,49,49	0
54	MG	1A	3059	1/1	0.96	0.14	27,27,27,27	0
54	MG	1A	3584	1/1	0.96	0.06	52,52,52,52	0
54	MG	1A	3486	1/1	0.96	0.06	33,33,33,33	0
54	MG	13	101	1/1	0.96	0.13	42,42,42,42	0
54	MG	2D	308	1/1	0.96	0.06	45,45,45,45	0
59	ZN	14	102	1/1	0.96	0.09	113,113,113,113	0
54	MG	2A	3167	1/1	0.97	0.14	46,46,46,46	0
54	MG	1U	201	1/1	0.97	0.16	44,44,44,44	0
54	MG	2A	3361	1/1	0.97	0.05	31,31,31,31	0
54	MG	1A	3824	1/1	0.97	0.05	47,47,47,47	0
54	MG	2A	3363	1/1	0.97	0.08	65,65,65,65	0
54	MG	1e	203	1/1	0.97	0.06	61,61,61,61	0
54	MG	1U	203	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3513	1/1	0.97	0.04	63,63,63,63	0
54	MG	1V	201	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3606	1/1	0.97	0.06	25,25,25,25	0
54	MG	1A	3515	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3370	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3828	1/1	0.97	0.36	38,38,38,38	0
54	MG	1A	3003	1/1	0.97	0.04	31,31,31,31	0
54	MG	1W	203	1/1	0.97	0.07	40,40,40,40	0
54	MG	1l	201	1/1	0.97	0.18	67,67,67,67	0
54	MG	1A	3429	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3592	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3979	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3215	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3016	1/1	0.97	0.28	38,38,38,38	0
54	MG	1A	3833	1/1	0.97	0.08	36,36,36,36	0
54	MG	1o	102	1/1	0.97	0.16	60,60,60,60	0
54	MG	10	105	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3053	1/1	0.97	0.17	38,38,38,38	0
54	MG	1A	3522	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3523	1/1	0.97	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3602	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3718	1/1	0.97	0.07	38,38,38,38	0
54	MG	2A	3604	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3606	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3091	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3024	1/1	0.97	0.03	22,22,22,22	0
54	MG	1A	3435	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3611	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3283	1/1	0.97	0.15	46,46,46,46	0
54	MG	2A	3613	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3284	1/1	0.97	0.05	44,44,44,44	0
54	MG	2a	3031	1/1	0.97	0.13	65,65,65,65	0
54	MG	2A	3010	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3171	1/1	0.97	0.23	41,41,41,41	0
54	MG	2A	3013	1/1	0.97	0.07	57,57,57,57	0
54	MG	1A	3288	1/1	0.97	0.23	44,44,44,44	0
54	MG	15	102	1/1	0.97	0.12	47,47,47,47	0
54	MG	15	104	1/1	0.97	0.24	39,39,39,39	0
54	MG	2A	3403	1/1	0.97	0.09	38,38,38,38	0
54	MG	2A	3017	1/1	0.97	0.30	41,41,41,41	0
54	MG	2A	3204	1/1	0.97	0.19	60,60,60,60	0
54	MG	2A	3624	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3037	1/1	0.97	0.09	54,54,54,54	0
54	MG	2A	3626	1/1	0.97	0.05	28,28,28,28	0
54	MG	2A	3019	1/1	0.97	0.15	47,47,47,47	0
54	MG	1A	3625	1/1	0.97	0.34	47,47,47,47	0
54	MG	1A	3996	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3094	1/1	0.97	0.28	35,35,35,35	0
54	MG	1A	3363	1/1	0.97	0.07	28,28,28,28	0
54	MG	17	103	1/1	0.97	0.25	40,40,40,40	0
54	MG	1a	1754	1/1	0.97	0.05	57,57,57,57	0
54	MG	1A	3443	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3537	1/1	0.97	0.06	28,28,28,28	0
54	MG	2A	3029	1/1	0.97	0.13	32,32,32,32	0
54	MG	2A	3637	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3854	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3855	1/1	0.97	0.11	43,43,43,43	0
54	MG	1A	3444	1/1	0.97	0.05	19,19,19,19	0
54	MG	1A	4004	1/1	0.97	0.08	18,18,18,18	0
54	MG	1A	3540	1/1	0.97	0.04	35,35,35,35	0
54	MG	1a	1763	1/1	0.97	0.04	49,49,49,49	0
54	MG	1A	3176	1/1	0.97	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4007	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3072	1/1	0.97	0.21	38,38,38,38	0
54	MG	1A	3543	1/1	0.97	0.09	48,48,48,48	0
54	MG	1a	1769	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3740	1/1	0.97	0.07	55,55,55,55	0
54	MG	2A	3228	1/1	0.97	0.31	45,45,45,45	0
54	MG	1A	3863	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3545	1/1	0.97	0.05	50,50,50,50	0
54	MG	1A	3007	1/1	0.97	0.05	38,38,38,38	0
54	MG	1A	3026	1/1	0.97	0.19	40,40,40,40	0
54	MG	1a	1611	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3135	1/1	0.97	0.24	43,43,43,43	0
54	MG	1A	3640	1/1	0.97	0.13	56,56,56,56	0
54	MG	2A	3443	1/1	0.97	0.08	44,44,44,44	0
54	MG	2A	3664	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3665	1/1	0.97	0.04	28,28,28,28	0
54	MG	1a	1614	1/1	0.97	0.12	58,58,58,58	0
54	MG	2A	3237	1/1	0.97	0.18	52,52,52,52	0
54	MG	1A	3233	1/1	0.97	0.26	40,40,40,40	0
54	MG	1A	3872	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3873	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3182	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	3551	1/1	0.97	0.09	61,61,61,61	0
54	MG	2A	3451	1/1	0.97	0.19	65,65,65,65	0
54	MG	1A	3753	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3644	1/1	0.97	0.08	34,34,34,34	0
54	MG	1A	3136	1/1	0.97	0.06	53,53,53,53	0
54	MG	2A	3246	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3236	1/1	0.97	0.23	37,37,37,37	0
54	MG	1a	1625	1/1	0.97	0.15	54,54,54,54	0
54	MG	1A	3137	1/1	0.97	0.31	36,36,36,36	0
54	MG	1A	3457	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3304	1/1	0.97	0.22	52,52,52,52	0
54	MG	1A	3306	1/1	0.97	0.11	35,35,35,35	0
54	MG	1a	1794	1/1	0.97	0.07	62,62,62,62	0
54	MG	1A	3461	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3239	1/1	0.97	0.29	47,47,47,47	0
54	MG	2A	3688	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3561	1/1	0.97	0.04	40,40,40,40	0
54	MG	2A	3071	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3767	1/1	0.97	0.08	50,50,50,50	0
54	MG	2A	3260	1/1	0.97	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1634	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3562	1/1	0.97	0.19	47,47,47,47	0
54	MG	1A	3240	1/1	0.97	0.16	48,48,48,48	0
54	MG	1B	219	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3475	1/1	0.97	0.12	64,64,64,64	0
54	MG	1A	3564	1/1	0.97	0.25	57,57,57,57	0
54	MG	1A	3384	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3188	1/1	0.97	0.28	45,45,45,45	0
54	MG	1B	223	1/1	0.97	0.06	65,65,65,65	0
54	MG	2A	3702	1/1	0.97	0.10	62,62,62,62	0
54	MG	1A	3467	1/1	0.97	0.05	28,28,28,28	0
54	MG	1A	3774	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3906	1/1	0.97	0.05	62,62,62,62	0
54	MG	2A	3084	1/1	0.97	0.10	49,49,49,49	0
54	MG	1A	3076	1/1	0.97	0.10	35,35,35,35	0
54	MG	2A	3708	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3311	1/1	0.97	0.08	52,52,52,52	0
54	MG	1a	1812	1/1	0.97	0.15	72,72,72,72	0
54	MG	1A	3040	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3105	1/1	0.97	0.28	40,40,40,40	0
54	MG	2A	3279	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3472	1/1	0.97	0.07	54,54,54,54	0
54	MG	1D	304	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3020	1/1	0.97	0.29	41,41,41,41	0
54	MG	1a	1653	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3914	1/1	0.97	0.04	54,54,54,54	0
54	MG	1D	309	1/1	0.97	0.04	47,47,47,47	0
54	MG	2a	3132	1/1	0.97	0.12	60,60,60,60	0
54	MG	1D	310	1/1	0.97	0.11	33,33,33,33	0
54	MG	2A	3497	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3097	1/1	0.97	0.04	56,56,56,56	0
54	MG	1A	3781	1/1	0.97	0.06	50,50,50,50	0
54	MG	1D	312	1/1	0.97	0.08	45,45,45,45	0
54	MG	2a	3139	1/1	0.97	0.12	73,73,73,73	0
54	MG	2A	3100	1/1	0.97	0.16	50,50,50,50	0
54	MG	1A	3193	1/1	0.97	0.19	45,45,45,45	0
54	MG	1a	1660	1/1	0.97	0.08	68,68,68,68	0
54	MG	1A	3917	1/1	0.97	0.08	24,24,24,24	0
54	MG	1a	1828	1/1	0.97	0.05	70,70,70,70	0
54	MG	1A	3668	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3669	1/1	0.97	0.08	60,60,60,60	0
54	MG	1A	3194	1/1	0.97	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3921	1/1	0.97	0.04	21,21,21,21	0
54	MG	1A	3923	1/1	0.97	0.17	41,41,41,41	0
54	MG	1A	3925	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3671	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3061	1/1	0.97	0.08	52,52,52,52	0
54	MG	1E	307	1/1	0.97	0.10	26,26,26,26	0
54	MG	1A	3929	1/1	0.97	0.08	55,55,55,55	0
54	MG	1E	309	1/1	0.97	0.06	54,54,54,54	0
54	MG	1E	310	1/1	0.97	0.08	56,56,56,56	0
54	MG	1F	302	1/1	0.97	0.21	38,38,38,38	0
54	MG	1a	1675	1/1	0.97	0.11	70,70,70,70	0
54	MG	1A	3930	1/1	0.97	0.06	64,64,64,64	0
54	MG	2A	3122	1/1	0.97	0.15	54,54,54,54	0
54	MG	1F	305	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3478	1/1	0.97	0.09	50,50,50,50	0
54	MG	1F	308	1/1	0.97	0.21	60,60,60,60	0
54	MG	2A	3127	1/1	0.97	0.23	53,53,53,53	0
54	MG	1F	309	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3081	1/1	0.97	0.18	38,38,38,38	0
54	MG	1A	3082	1/1	0.97	0.06	42,42,42,42	0
54	MG	2A	3320	1/1	0.97	0.22	49,49,49,49	0
54	MG	1A	3112	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3021	1/1	0.97	0.15	40,40,40,40	0
54	MG	1F	314	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3134	1/1	0.97	0.12	77,77,77,77	0
54	MG	1A	3401	1/1	0.97	0.07	33,33,33,33	0
54	MG	2a	3175	1/1	0.97	0.05	67,67,67,67	0
54	MG	2A	3539	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3031	1/1	0.97	0.10	20,20,20,20	0
54	MG	1A	3032	1/1	0.97	0.23	65,65,65,65	0
54	MG	1A	3682	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3154	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3155	1/1	0.97	0.10	36,36,36,36	0
54	MG	2A	3331	1/1	0.97	0.05	67,67,67,67	0
54	MG	1A	3264	1/1	0.97	0.05	47,47,47,47	0
54	MG	2A	3142	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3334	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3117	1/1	0.97	0.23	40,40,40,40	0
54	MG	1a	1864	1/1	0.97	0.05	60,60,60,60	0
54	MG	1A	3332	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3266	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3118	1/1	0.97	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3336	1/1	0.97	0.40	47,47,47,47	0
54	MG	1A	3120	1/1	0.97	0.31	38,38,38,38	0
54	MG	1A	3269	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3810	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3162	1/1	0.97	0.27	41,41,41,41	0
54	MG	1P	205	1/1	0.97	0.07	38,38,38,38	0
54	MG	1Q	201	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3271	1/1	0.97	0.06	50,50,50,50	0
54	MG	2V	202	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3813	1/1	0.97	0.06	46,46,46,46	0
56	ZIT	1A	4023	52/52	0.97	0.09	20,37,57,63	0
54	MG	2W	201	1/1	0.97	0.26	49,49,49,49	0
54	MG	1A	3343	1/1	0.97	0.11	29,29,29,29	0
54	MG	1A	3699	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3163	1/1	0.97	0.07	46,46,46,46	0
54	MG	1A	3033	1/1	0.97	0.13	44,44,44,44	0
54	MG	2A	3567	1/1	0.97	0.08	59,59,59,59	0
54	MG	1A	3510	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3213	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3704	1/1	0.97	0.08	61,61,61,61	0
54	MG	1A	3275	1/1	0.97	0.38	37,37,37,37	0
54	MG	2A	3166	1/1	0.97	0.11	52,52,52,52	0
54	MG	2A	3650	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3125	1/1	0.98	0.15	40,40,40,40	0
54	MG	1a	1724	1/1	0.98	0.07	68,68,68,68	0
54	MG	2A	3653	1/1	0.98	0.10	63,63,63,63	0
54	MG	1A	3255	1/1	0.98	0.10	35,35,35,35	0
54	MG	1A	4021	1/1	0.98	0.06	58,58,58,58	0
54	MG	1A	3784	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3144	1/1	0.98	0.12	41,41,41,41	0
54	MG	1A	3175	1/1	0.98	0.12	35,35,35,35	0
54	MG	1A	3690	1/1	0.98	0.10	60,60,60,60	0
54	MG	2A	3660	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3145	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3905	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3524	1/1	0.98	0.04	26,26,26,26	0
54	MG	1A	3693	1/1	0.98	0.04	67,67,67,67	0
54	MG	1a	1735	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3370	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3146	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3178	1/1	0.98	0.15	33,33,33,33	0
54	MG	1B	212	1/1	0.98	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3373	1/1	0.98	0.09	32,32,32,32	0
54	MG	2A	3307	1/1	0.98	0.18	55,55,55,55	0
54	MG	1A	3121	1/1	0.98	0.07	25,25,25,25	0
54	MG	1g	202	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3314	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3448	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3315	1/1	0.98	0.13	40,40,40,40	0
54	MG	2A	3677	1/1	0.98	0.07	41,41,41,41	0
54	MG	1a	1603	1/1	0.98	0.09	51,51,51,51	0
54	MG	2A	3149	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3100	1/1	0.98	0.12	52,52,52,52	0
54	MG	1a	1747	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3046	1/1	0.98	0.07	16,16,16,16	0
54	MG	1A	3381	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3102	1/1	0.98	0.29	35,35,35,35	0
54	MG	1A	3383	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3183	1/1	0.98	0.10	34,34,34,34	0
54	MG	1A	3924	1/1	0.98	0.04	48,48,48,48	0
54	MG	1A	3385	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3220	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3624	1/1	0.98	0.21	38,38,38,38	0
54	MG	1A	3928	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3221	1/1	0.98	0.16	28,28,28,28	0
54	MG	2A	3003	1/1	0.98	0.05	42,42,42,42	0
54	MG	1D	302	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3712	1/1	0.98	0.12	43,43,43,43	0
54	MG	2A	3006	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3544	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3008	1/1	0.98	0.05	46,46,46,46	0
54	MG	1A	3388	1/1	0.98	0.08	52,52,52,52	0
54	MG	1D	306	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3171	1/1	0.98	0.05	47,47,47,47	0
54	MG	2A	3518	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3934	1/1	0.98	0.10	60,60,60,60	0
54	MG	2A	3012	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3715	1/1	0.98	0.04	38,38,38,38	0
54	MG	2A	3522	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3184	1/1	0.98	0.08	35,35,35,35	0
54	MG	2a	3085	1/1	0.98	0.25	60,60,60,60	0
54	MG	1A	3323	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3938	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3939	1/1	0.98	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1D	314	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3103	1/1	0.98	0.05	56,56,56,56	0
54	MG	2A	3020	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3941	1/1	0.98	0.08	67,67,67,67	0
54	MG	1A	3013	1/1	0.98	0.06	20,20,20,20	0
54	MG	1A	3818	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3187	1/1	0.98	0.16	43,43,43,43	0
54	MG	1A	3226	1/1	0.98	0.12	43,43,43,43	0
54	MG	2A	3719	1/1	0.98	0.11	47,47,47,47	0
54	MG	1E	301	1/1	0.98	0.18	38,38,38,38	0
54	MG	1A	3722	1/1	0.98	0.04	44,44,44,44	0
54	MG	1E	303	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3001	1/1	0.98	0.04	38,38,38,38	0
54	MG	1a	1784	1/1	0.98	0.17	64,64,64,64	0
54	MG	1E	305	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3823	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3019	1/1	0.98	0.23	32,32,32,32	0
54	MG	1A	3229	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3130	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3028	1/1	0.98	0.25	40,40,40,40	0
54	MG	1A	3279	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3157	1/1	0.98	0.23	44,44,44,44	0
54	MG	1F	304	1/1	0.98	0.25	40,40,40,40	0
54	MG	1A	3559	1/1	0.98	0.08	40,40,40,40	0
54	MG	1a	1649	1/1	0.98	0.15	61,61,61,61	0
54	MG	1A	3158	1/1	0.98	0.36	46,46,46,46	0
54	MG	1F	307	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3338	1/1	0.98	0.08	33,33,33,33	0
54	MG	2B	210	1/1	0.98	0.36	57,57,57,57	0
54	MG	1A	3733	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3734	1/1	0.98	0.06	75,75,75,75	0
54	MG	1A	3339	1/1	0.98	0.03	34,34,34,34	0
54	MG	1A	3075	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3109	1/1	0.98	0.13	48,48,48,48	0
54	MG	1A	3063	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3378	1/1	0.98	0.05	50,50,50,50	0
54	MG	2A	3051	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3380	1/1	0.98	0.09	37,37,37,37	0
54	MG	2A	3381	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3482	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3409	1/1	0.98	0.06	26,26,26,26	0
54	MG	1F	317	1/1	0.98	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3741	1/1	0.98	0.06	30,30,30,30	0
54	MG	2A	3386	1/1	0.98	0.06	41,41,41,41	0
54	MG	2a	3133	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3742	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3484	1/1	0.98	0.04	54,54,54,54	0
54	MG	1A	3410	1/1	0.98	0.06	27,27,27,27	0
54	MG	2E	301	1/1	0.98	0.07	60,60,60,60	0
54	MG	2A	3059	1/1	0.98	0.04	46,46,46,46	0
54	MG	1A	3972	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3745	1/1	0.98	0.19	38,38,38,38	0
54	MG	1N	201	1/1	0.98	0.10	48,48,48,48	0
54	MG	2A	3578	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3238	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3286	1/1	0.98	0.06	34,34,34,34	0
54	MG	2F	304	1/1	0.98	0.17	49,49,49,49	0
54	MG	1A	3976	1/1	0.98	0.03	27,27,27,27	0
54	MG	2A	3066	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3287	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3415	1/1	0.98	0.10	31,31,31,31	0
54	MG	1A	3750	1/1	0.98	0.05	25,25,25,25	0
54	MG	1a	1821	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3029	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3164	1/1	0.98	0.16	38,38,38,38	0
54	MG	1A	3418	1/1	0.98	0.06	29,29,29,29	0
54	MG	1A	3042	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3755	1/1	0.98	0.06	64,64,64,64	0
54	MG	2A	3410	1/1	0.98	0.08	51,51,51,51	0
54	MG	1A	3043	1/1	0.98	0.12	26,26,26,26	0
54	MG	1Q	204	1/1	0.98	0.06	42,42,42,42	0
54	MG	1Q	205	1/1	0.98	0.09	50,50,50,50	0
54	MG	1A	3860	1/1	0.98	0.10	37,37,37,37	0
54	MG	1A	3662	1/1	0.98	0.09	34,34,34,34	0
54	MG	1A	3243	1/1	0.98	0.17	32,32,32,32	0
54	MG	1A	3759	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3760	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3138	1/1	0.98	0.26	36,36,36,36	0
54	MG	1A	3500	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3867	1/1	0.98	0.09	57,57,57,57	0
54	MG	1A	3096	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3355	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3203	1/1	0.98	0.06	54,54,54,54	0
54	MG	1a	1841	1/1	0.98	0.05	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1U	204	1/1	0.98	0.19	32,32,32,32	0
54	MG	2A	3610	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3871	1/1	0.98	0.07	35,35,35,35	0
54	MG	1U	206	1/1	0.98	0.15	37,37,37,37	0
54	MG	1a	1697	1/1	0.98	0.13	52,52,52,52	0
54	MG	1A	3426	1/1	0.98	0.04	43,43,43,43	0
54	MG	2A	3257	1/1	0.98	0.14	28,28,28,28	0
54	MG	1V	203	1/1	0.98	0.17	48,48,48,48	0
54	MG	1A	3297	1/1	0.98	0.07	20,20,20,20	0
54	MG	1A	3506	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3507	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3428	1/1	0.98	0.03	34,34,34,34	0
54	MG	1W	202	1/1	0.98	0.21	48,48,48,48	0
54	MG	1A	3247	1/1	0.98	0.34	39,39,39,39	0
54	MG	2A	3442	1/1	0.98	0.07	42,42,42,42	0
54	MG	1W	204	1/1	0.98	0.08	53,53,53,53	0
54	MG	1a	1856	1/1	0.98	0.04	56,56,56,56	0
54	MG	1A	3299	1/1	0.98	0.09	35,35,35,35	0
54	MG	2A	3106	1/1	0.98	0.10	37,37,37,37	0
54	MG	1A	3248	1/1	0.98	0.13	38,38,38,38	0
54	MG	10	101	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3140	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3883	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3514	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3274	1/1	0.98	0.06	45,45,45,45	0
54	MG	1A	3055	1/1	0.98	0.25	41,41,41,41	0
54	MG	1A	3044	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	4012	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3887	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3015	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3889	1/1	0.98	0.06	60,60,60,60	0
54	MG	11	103	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3518	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3600	1/1	0.98	0.05	53,53,53,53	0
54	MG	2A	3121	1/1	0.98	0.05	43,43,43,43	0
54	MG	2A	3285	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3254	1/1	0.98	0.52	48,48,48,48	0
54	MG	1A	3782	1/1	0.98	0.04	49,49,49,49	0
54	MG	1a	1875	1/1	0.98	0.04	56,56,56,56	0
59	ZN	2Y	202	1/1	0.98	0.04	92,92,92,92	0
59	ZN	24	501	1/1	0.98	0.10	128,128,128,128	0
59	ZN	29	501	1/1	0.98	0.04	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	2n	501	1/1	0.98	0.05	95,95,95,95	0
60	SF4	2d	501	8/8	0.98	0.05	72,83,85,87	0
54	MG	1R	201	1/1	0.99	0.10	41,41,41,41	0
54	MG	1R	202	1/1	0.99	0.14	43,43,43,43	0
54	MG	1A	3263	1/1	0.99	0.08	32,32,32,32	0
54	MG	1A	3119	1/1	0.99	0.14	34,34,34,34	0
54	MG	1A	3348	1/1	0.99	0.09	28,28,28,28	0
54	MG	2A	3408	1/1	0.99	0.08	51,51,51,51	0
54	MG	1A	3374	1/1	0.99	0.03	22,22,22,22	0
54	MG	1A	3459	1/1	0.99	0.03	33,33,33,33	0
54	MG	1A	3966	1/1	0.99	0.06	50,50,50,50	0
54	MG	2A	3413	1/1	0.99	0.04	43,43,43,43	0
54	MG	1a	1855	1/1	0.99	0.03	52,52,52,52	0
54	MG	1T	201	1/1	0.99	0.04	63,63,63,63	0
54	MG	1A	3494	1/1	0.99	0.03	32,32,32,32	0
54	MG	1A	3005	1/1	0.99	0.14	28,28,28,28	0
54	MG	2A	3346	1/1	0.99	0.10	42,42,42,42	0
54	MG	1A	3326	1/1	0.99	0.04	28,28,28,28	0
54	MG	2a	3154	1/1	0.99	0.05	54,54,54,54	0
54	MG	2A	3648	1/1	0.99	0.03	34,34,34,34	0
54	MG	1A	3305	1/1	0.99	0.11	43,43,43,43	0
54	MG	1A	3378	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3006	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3678	1/1	0.99	0.03	45,45,45,45	0
54	MG	1A	3922	1/1	0.99	0.07	47,47,47,47	0
54	MG	1A	3231	1/1	0.99	0.19	39,39,39,39	0
54	MG	2A	3426	1/1	0.99	0.03	66,66,66,66	0
54	MG	1V	202	1/1	0.99	0.19	39,39,39,39	0
54	MG	1F	301	1/1	0.99	0.06	37,37,37,37	0
54	MG	1a	1868	1/1	0.99	0.04	54,54,54,54	0
54	MG	1A	3794	1/1	0.99	0.06	33,33,33,33	0
54	MG	1A	3466	1/1	0.99	0.05	29,29,29,29	0
54	MG	1A	3122	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3250	1/1	0.99	0.12	36,36,36,36	0
54	MG	1A	3879	1/1	0.99	0.03	51,51,51,51	0
54	MG	1a	1622	1/1	0.99	0.04	56,56,56,56	0
54	MG	1A	3609	1/1	0.99	0.05	51,51,51,51	0
54	MG	1A	3881	1/1	0.99	0.06	35,35,35,35	0
54	MG	1A	3111	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	3685	1/1	0.99	0.11	38,38,38,38	0
54	MG	2a	3176	1/1	0.99	0.14	56,56,56,56	0
54	MG	1a	1749	1/1	0.99	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3575	1/1	0.99	0.06	36,36,36,36	0
54	MG	1A	3333	1/1	0.99	0.07	24,24,24,24	0
54	MG	1A	3095	1/1	0.99	0.05	47,47,47,47	0
54	MG	1A	3174	1/1	0.99	0.06	50,50,50,50	0
54	MG	1A	3508	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3473	1/1	0.99	0.03	55,55,55,55	0
54	MG	1a	1756	1/1	0.99	0.08	59,59,59,59	0
54	MG	1A	3414	1/1	0.99	0.07	20,20,20,20	0
54	MG	1A	3161	1/1	0.99	0.14	41,41,41,41	0
54	MG	2A	3525	1/1	0.99	0.04	65,65,65,65	0
54	MG	1A	3018	1/1	0.99	0.21	27,27,27,27	0
54	MG	1A	3445	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3852	1/1	0.99	0.06	41,41,41,41	0
54	MG	2E	303	1/1	0.99	0.04	55,55,55,55	0
54	MG	2A	3605	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3089	1/1	0.99	0.07	45,45,45,45	0
54	MG	1A	3946	1/1	0.99	0.05	62,62,62,62	0
54	MG	2A	3455	1/1	0.99	0.03	40,40,40,40	0
54	MG	2F	301	1/1	0.99	0.17	43,43,43,43	0
54	MG	1A	3390	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3206	1/1	0.99	0.13	38,38,38,38	0
54	MG	1A	3296	1/1	0.99	0.10	23,23,23,23	0
54	MG	1A	3899	1/1	0.99	0.03	37,37,37,37	0
54	MG	2A	3460	1/1	0.99	0.04	56,56,56,56	0
54	MG	1a	1768	1/1	0.99	0.04	52,52,52,52	0
54	MG	15	101	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3900	1/1	0.99	0.03	51,51,51,51	0
54	MG	15	103	1/1	0.99	0.18	34,34,34,34	0
54	MG	2A	3390	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3901	1/1	0.99	0.09	46,46,46,46	0
54	MG	1A	3115	1/1	0.99	0.12	37,37,37,37	0
54	MG	2A	3393	1/1	0.99	0.08	45,45,45,45	0
54	MG	1D	308	1/1	0.99	0.03	23,23,23,23	0
54	MG	1A	3903	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3904	1/1	0.99	0.04	35,35,35,35	0
54	MG	17	101	1/1	0.99	0.05	38,38,38,38	0
59	ZN	15	109	1/1	0.99	0.05	48,48,48,48	0
59	ZN	16	501	1/1	0.99	0.05	45,45,45,45	0
59	ZN	19	103	1/1	0.99	0.03	46,46,46,46	0
59	ZN	1n	103	1/1	0.99	0.03	67,67,67,67	0
54	MG	1A	3009	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3209	1/1	0.99	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	26	501	1/1	0.99	0.03	66,66,66,66	0
54	MG	1A	3048	1/1	0.99	0.02	29,29,29,29	0
54	MG	1A	3908	1/1	0.99	0.06	55,55,55,55	0
60	SF4	1d	305	8/8	0.99	0.04	63,70,75,78	0
54	MG	1A	3079	1/1	0.99	0.12	36,36,36,36	0
54	MG	2A	3412	1/1	1.00	0.04	38,38,38,38	0
54	MG	1B	213	1/1	1.00	0.03	48,48,48,48	0
54	MG	1A	3849	1/1	1.00	0.03	26,26,26,26	0
59	ZN	1Y	202	1/1	1.00	0.03	63,63,63,63	0
54	MG	2A	3576	1/1	1.00	0.02	27,27,27,27	0
54	MG	2A	3647	1/1	1.00	0.06	36,36,36,36	0
54	MG	1A	3637	1/1	1.00	0.09	34,34,34,34	0
54	MG	1A	3525	1/1	1.00	0.02	23,23,23,23	0
54	MG	1A	3977	1/1	1.00	0.03	36,36,36,36	0
54	MG	2A	3514	1/1	1.00	0.04	43,43,43,43	0
54	MG	1A	3485	1/1	1.00	0.03	35,35,35,35	0
59	ZN	25	104	1/1	1.00	0.03	54,54,54,54	0
54	MG	1A	3933	1/1	1.00	0.02	53,53,53,53	0
54	MG	1A	3539	1/1	1.00	0.02	45,45,45,45	0
54	MG	1A	3839	1/1	1.00	0.05	49,49,49,49	0
54	MG	1A	3352	1/1	1.00	0.07	38,38,38,38	0
54	MG	1A	3491	1/1	1.00	0.08	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.