



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 04:42 pm BST

PDB ID : 7O71 / pdb_00007o71
EMDB ID : EMD-12742
Title : Cryo-EM structure of a respiratory complex I
Authors : Parey, K.; Vonck, J.
Deposited on : 2021-04-12
Resolution : 2.40 Å(reported)
Based on initial model : 6RFR

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

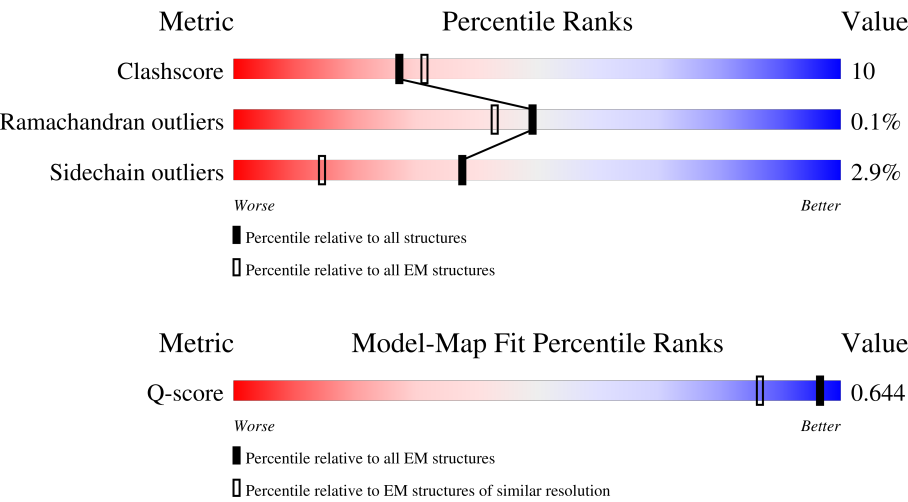
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	25% 74% 20% • 5%
2	B	488	66% 59% 33% • 7%
3	C	466	11% 73% 19% • 6%
4	G	281	7% 70% 15% 15%

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Mol	Chain	Length	Quality of chain
5	H	243	
6	I	229	
7	K	210	
8	L	89	
9	S	249	
10	j	93	
11	1	341	
12	2	469	
13	3	128	
14	4	486	
15	5	655	
16	6	185	
17	g	78	
18	D	87	
19	E	375	
20	F	144	
21	J	198	
22	M	136	
23	O	109	
24	P	124	
25	Q	132	
26	R	109	
27	U	172	
28	W	123	
29	X	169	

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Mol	Chain	Length	Quality of chain
30	Y	161	
31	Z	182	
32	a	149	
33	b	74	
34	c	60	
35	d	92	
36	e	67	
37	f	87	
38	h	138	
39	i	90	
40	n	120	
41	8	99	
42	9	89	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 67428 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called NADH-ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	693	Total	C	N	O	S	0	0
			5269	3272	927	1041	29		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	455	Total	C	N	O	S	0	0
			3517	2223	617	653	24		

- Molecule 3 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	437	Total	C	N	O	S	1	0
			3470	2205	595	648	22		

- Molecule 4 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 6 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 7 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	177	Total	C	N	O	S	0	0
			1395	885	246	249	15		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	89	Total	C	N	O	S	0	0
			693	465	109	116	3		

- Molecule 9 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	182	Total	C	N	O	S	0	0
			1492	961	255	274	2		

- Molecule 10 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	90	Total	C	N	O	S	0	0
			724	465	132	127			

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	340	Total	C	N	O	S	0	0
			2716	1850	393	466	7		

- Molecule 12 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	469	Total	C	N	O	S	0	0
			3776	2558	550	656	12		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	128	Total	C	N	O	S	0	0
			1027	701	151	172	3		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	481	Total	C	N	O	S	0	0
			3815	2573	581	647	14		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	184	Total	C	N	O	S	0	0
			1453	985	208	251	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	1	FME	-	insertion	UNP S5U3X7

- Molecule 17 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	76	Total	C	N	O	0	0
			622	408	113	101		

- Molecule 18 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 40 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	350	Total	C	N	O	S	0	0
			2806	1782	490	524	10		

- Molecule 20 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	120	Total	C	N	O	S	0	0
			981	624	164	191	2		

- Molecule 21 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	178	Total	C	N	O	S	0	0
			1319	838	238	238	5		

- Molecule 22 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 23 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
23	O	71	Total	C	N	O	0	0
			543	344	83	116		

- Molecule 24 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 25 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 26 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 27 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 28 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 29 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	164	Total	C	N	O	S	0	0
			1275	828	217	226	4		

- Molecule 30 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

- Molecule 31 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	181	Total	C	N	O	S	0	0
			1389	893	240	255	1		

- Molecule 32 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 33 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 34 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
34	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 35 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	89	Total	C	N	O	S	0	0
			751	467	136	145	3		

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 37 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	82	Total	C	N	O	S	0	0
			642	403	121	117	1		

- Molecule 38 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 39 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 40 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	114	Total	C	N	O	S	0	0
			913	587	154	171	1		

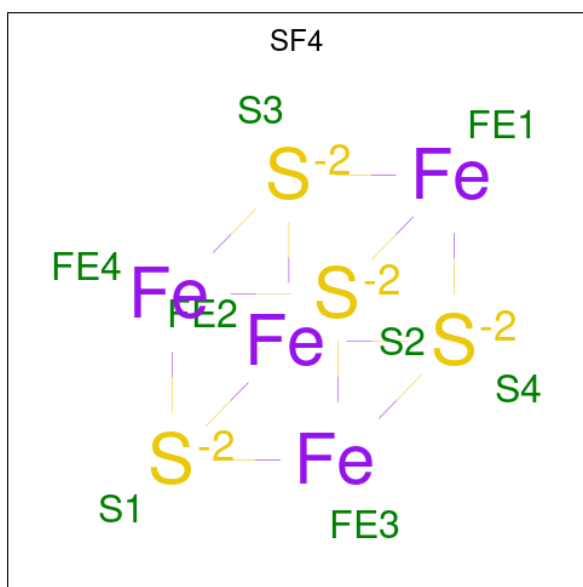
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	71	Total	C	N	O	S	0	0
			594	375	109	102	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

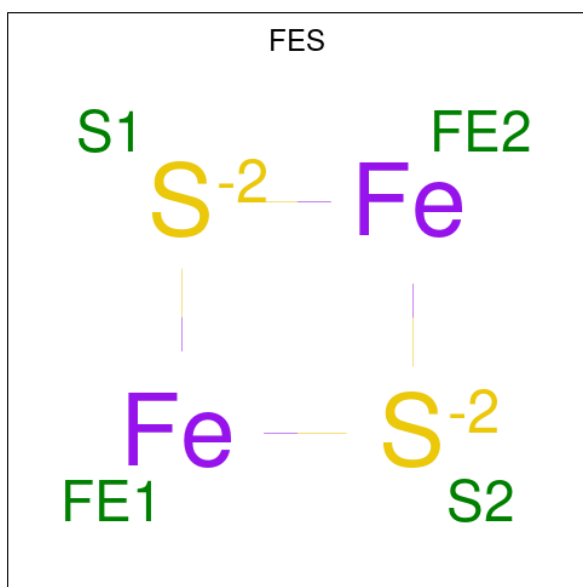
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



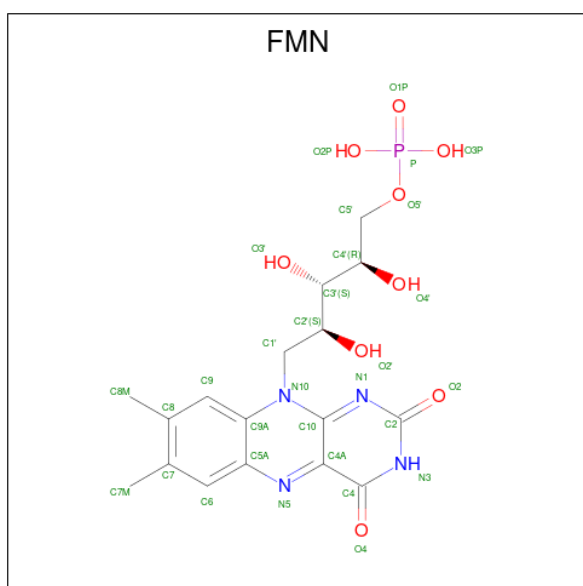
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

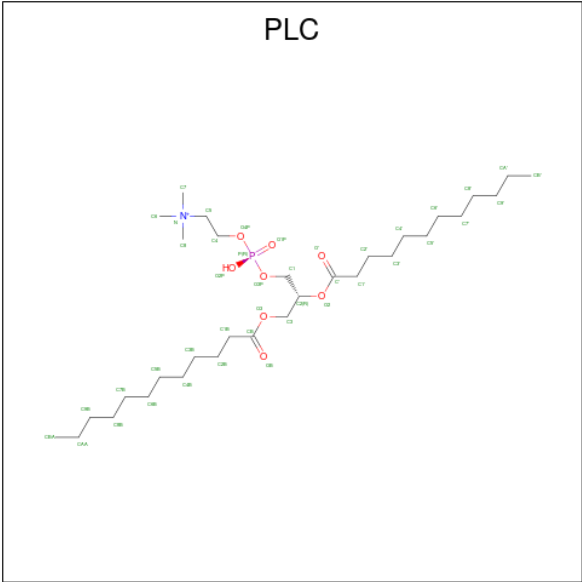
- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

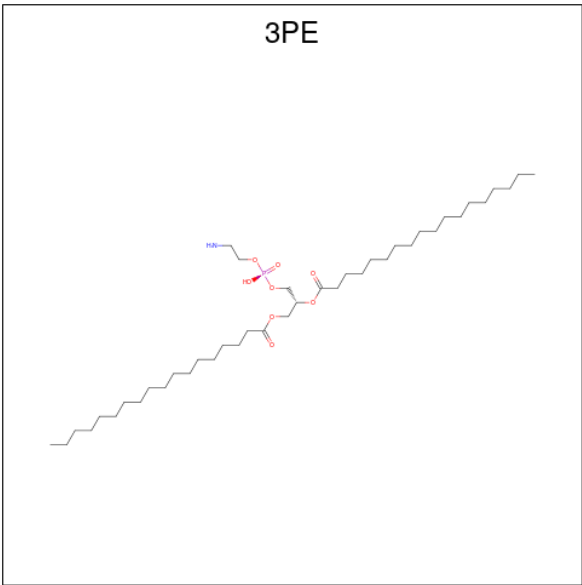
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).





Mol	Chain	Residues	Atoms					AltConf
46	K	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	W	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



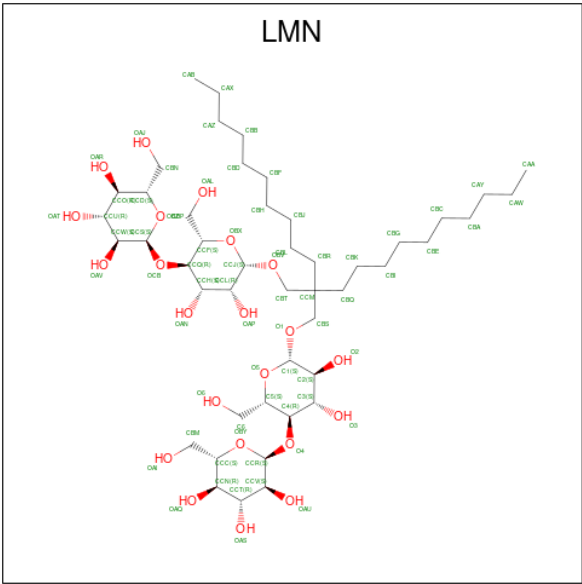
Mol	Chain	Residues	Atoms					AltConf
47	S	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	1	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	4	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	6	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	6	1	Total	C	N	O	P	0
			48	38	1	8	1	
47	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	E	1	Total	C	N	O	P	0
			36	26	1	8	1	

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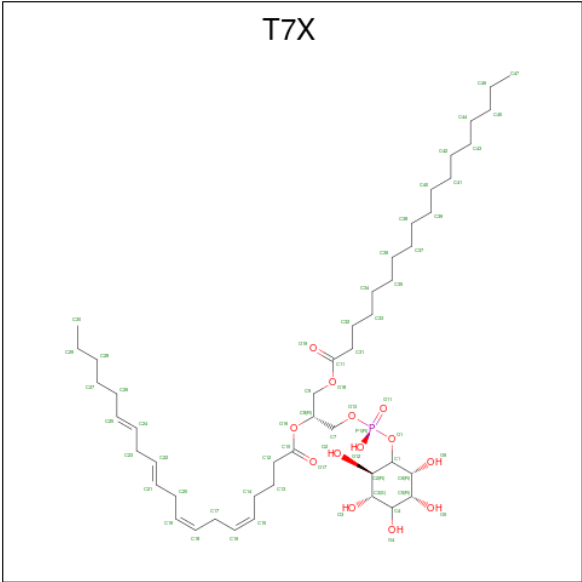
Mol	Chain	Residues	Atoms					AltConf
47	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	J	1	Total	C	N	O	P	0
			34	24	1	8	1	
47	b	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 48 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



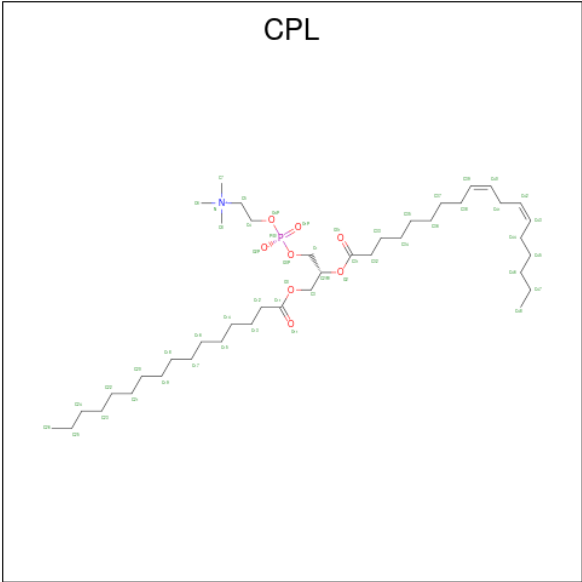
Mol	Chain	Residues	Atoms			AltConf
48	j	1	Total	C	O	0
			65	43	22	
48	J	1	Total	C	O	0
			69	47	22	

- Molecule 49 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



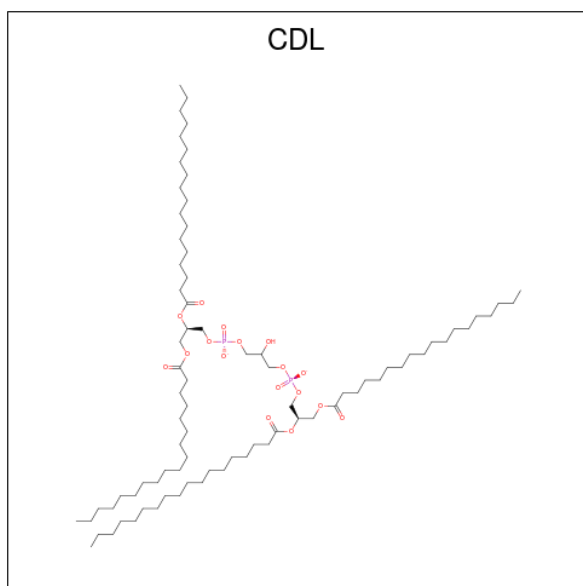
Mol	Chain	Residues	Atoms				AltConf
49	2	1	Total	C	O	P	0
			48	34	13	1	
49	2	1	Total	C	O	P	0
			52	38	13	1	
49	3	1	Total	C	O	P	0
			49	35	13	1	

- Molecule 50 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: C₄₂H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
50	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	g	1	Total	C	O	P	0
			83	64	17	2	
51	E	1	Total	C	O	P	0
			72	53	17	2	
51	W	1	Total	C	O	P	0
			54	35	17	2	
51	X	1	Total	C	O	P	0
			86	67	17	2	
51	Z	1	Total	C	O	P	0
			76	57	17	2	
51	n	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
52	E	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	M	1	Total Zn 1 1	0

- Molecule 54 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl]-}\beta\text{-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
54	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
54	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
55	A	135	Total	O	0
			135	135	
55	B	11	Total	O	0
			11	11	
55	C	168	Total	O	0
			168	168	
55	G	114	Total	O	0
			114	114	
55	H	2	Total	O	0
			2	2	
55	I	95	Total	O	0
			95	95	
55	K	78	Total	O	0
			78	78	
55	L	18	Total	O	0
			18	18	
55	S	4	Total	O	0
			4	4	
55	j	15	Total	O	0
			15	15	
55	1	67	Total	O	0
			67	67	
55	2	158	Total	O	0
			158	158	
55	3	10	Total	O	0
			10	10	
55	4	139	Total	O	0
			139	139	
55	5	57	Total	O	0
			57	57	
55	6	24	Total	O	0
			24	24	
55	g	2	Total	O	0
			2	2	
55	D	17	Total	O	0
			17	17	

Continued on next page...

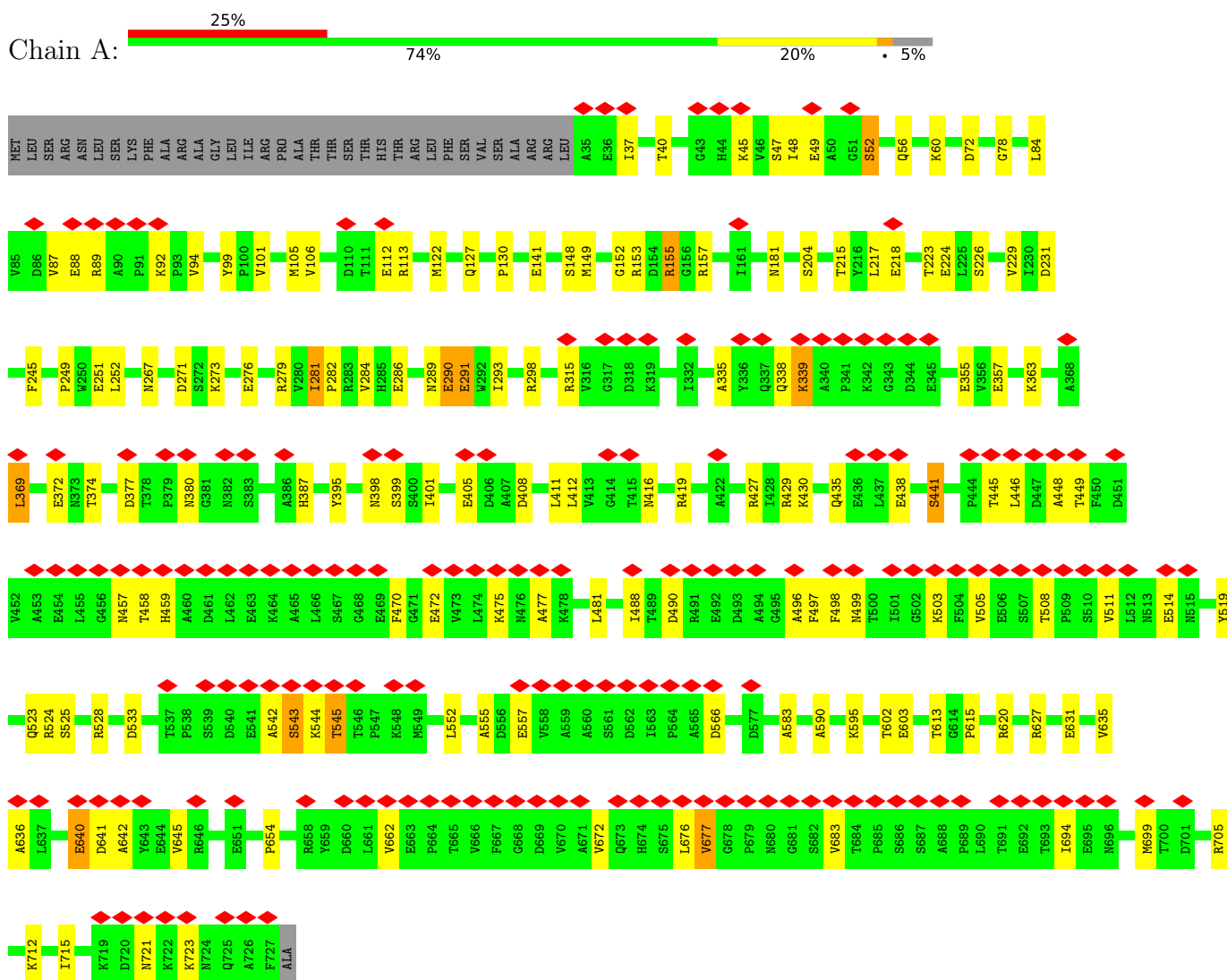
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
55	E	79	Total 79	O 79	0
55	F	15	Total 15	O 15	0
55	J	14	Total 14	O 14	0
55	M	45	Total 45	O 45	0
55	P	15	Total 15	O 15	0
55	R	11	Total 11	O 11	0
55	U	39	Total 39	O 39	0
55	W	23	Total 23	O 23	0
55	X	39	Total 39	O 39	0
55	Y	53	Total 53	O 53	0
55	Z	52	Total 52	O 52	0
55	a	11	Total 11	O 11	0
55	b	6	Total 6	O 6	0
55	d	8	Total 8	O 8	0
55	h	61	Total 61	O 61	0
55	i	3	Total 3	O 3	0
55	n	12	Total 12	O 12	0
55	9	16	Total 16	O 16	0

3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

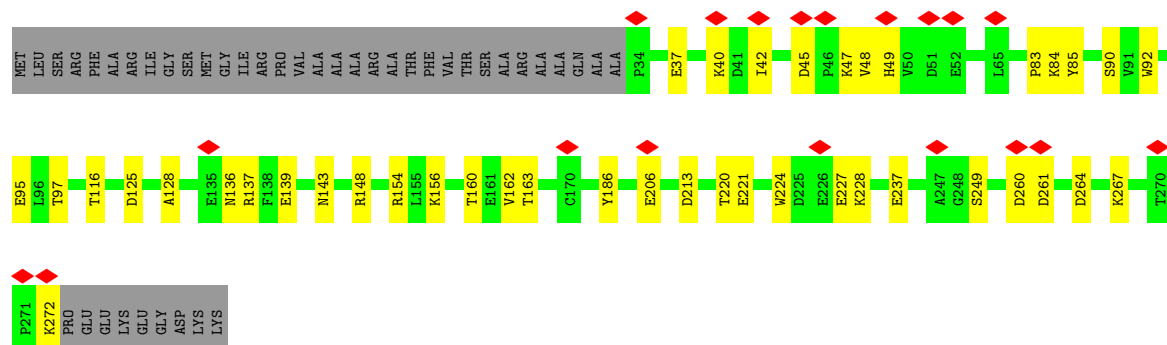
• Molecule 1: NADH-ubiquinone oxidoreductase 78 kDa subunit



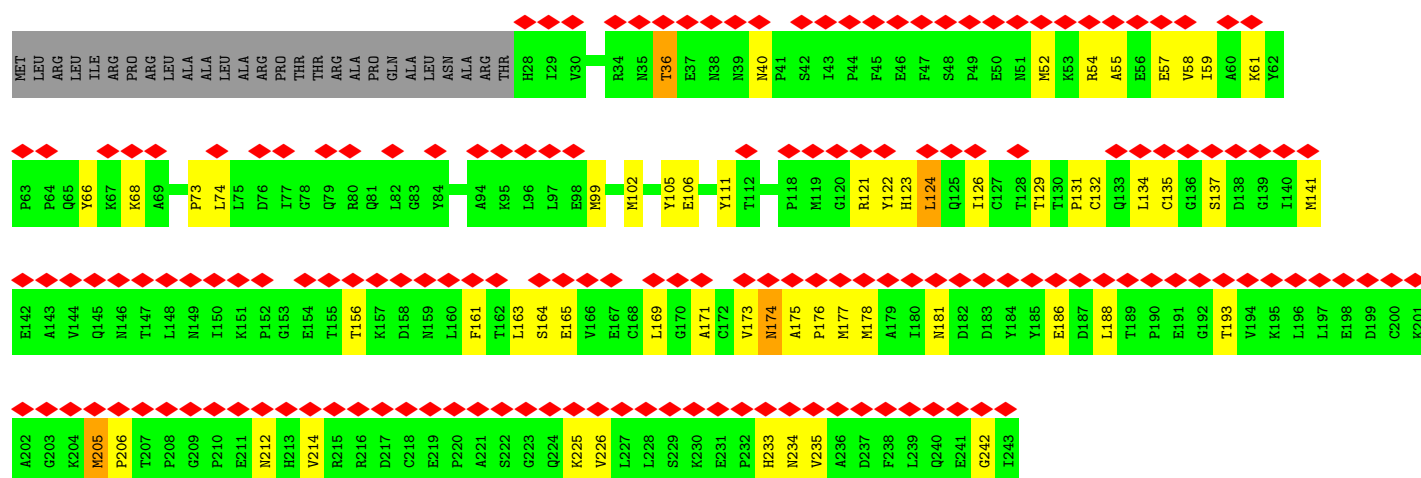
• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



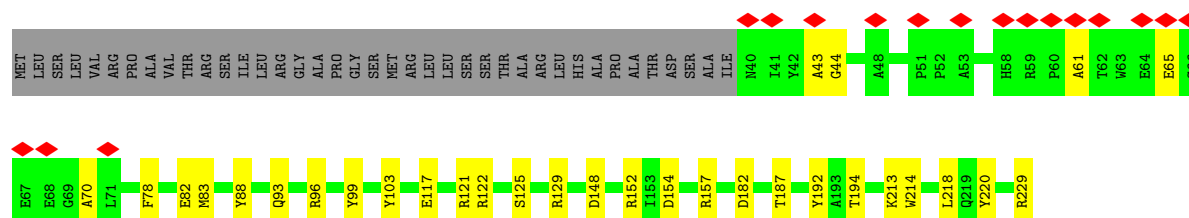




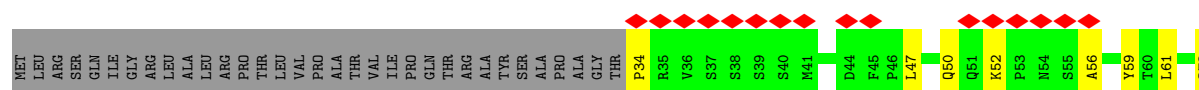
• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

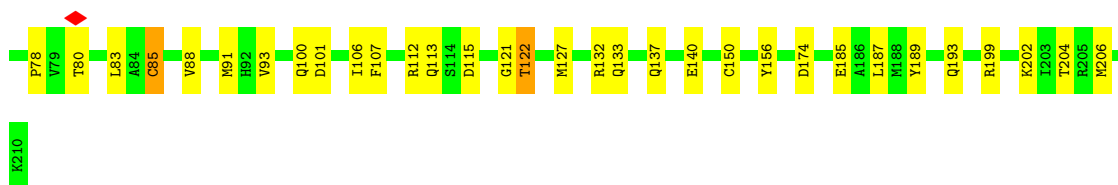


• Molecule 6: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

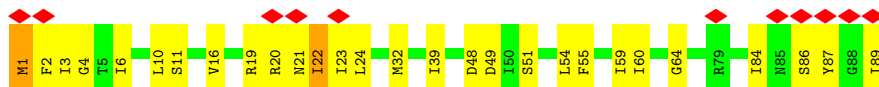


• Molecule 7: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

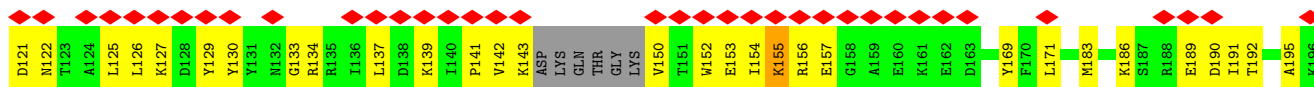
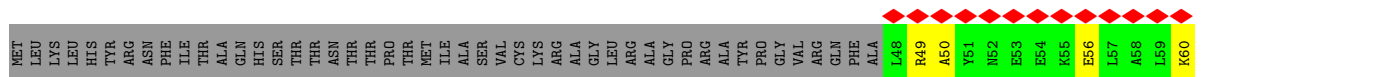




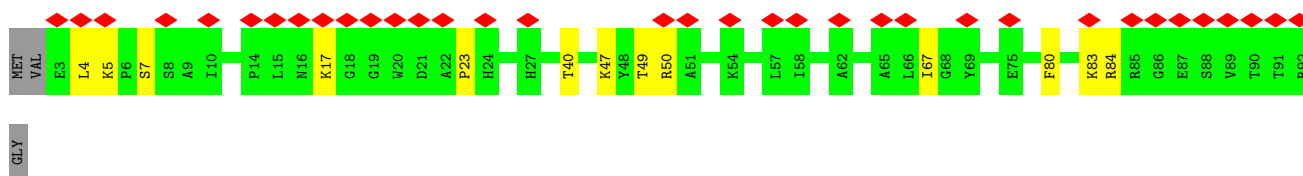
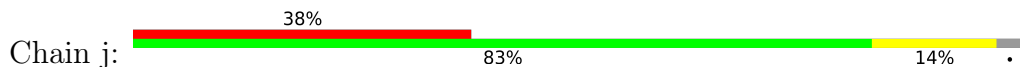
- Molecule 8: NADH-ubiquinone oxidoreductase chain 4L



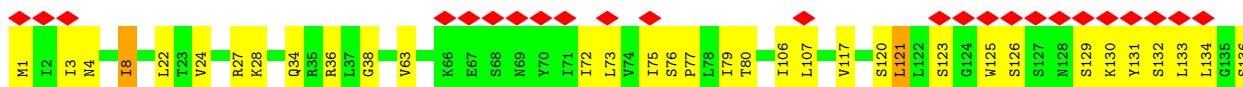
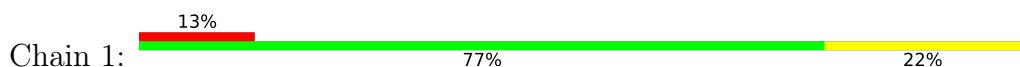
- Molecule 9: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

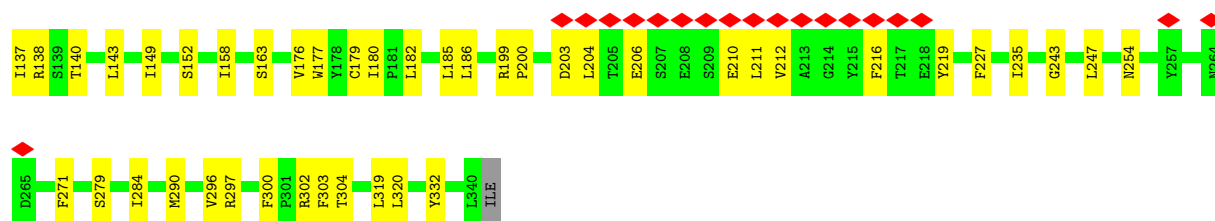


- Molecule 10: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

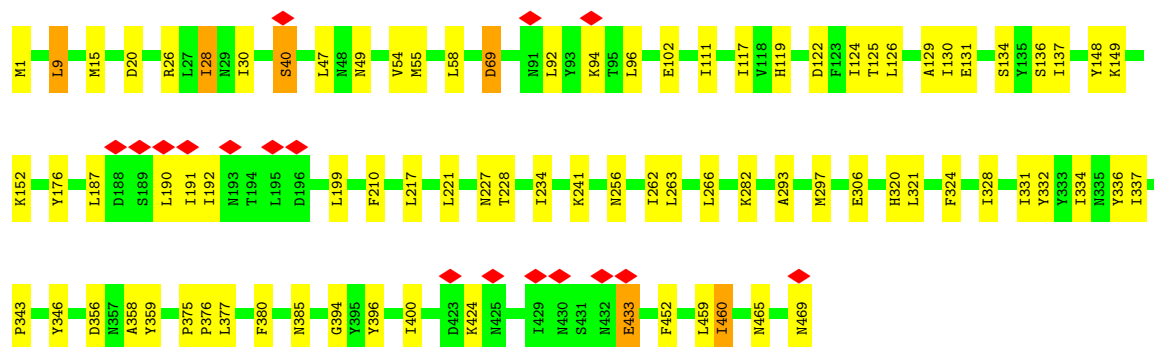
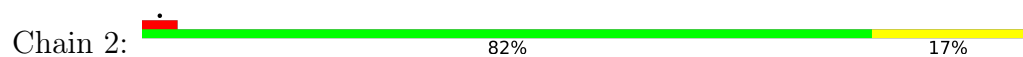


- Molecule 11: NADH-ubiquinone oxidoreductase chain 1

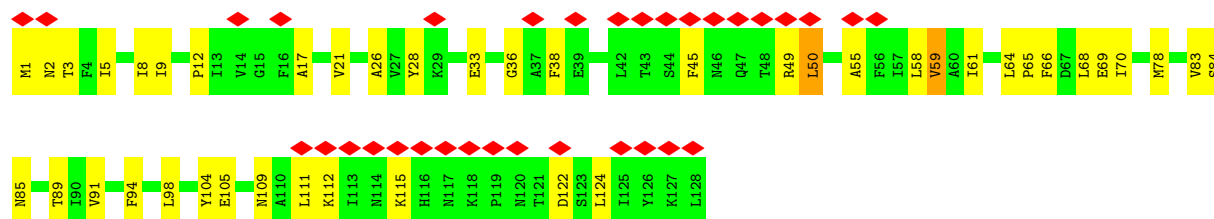




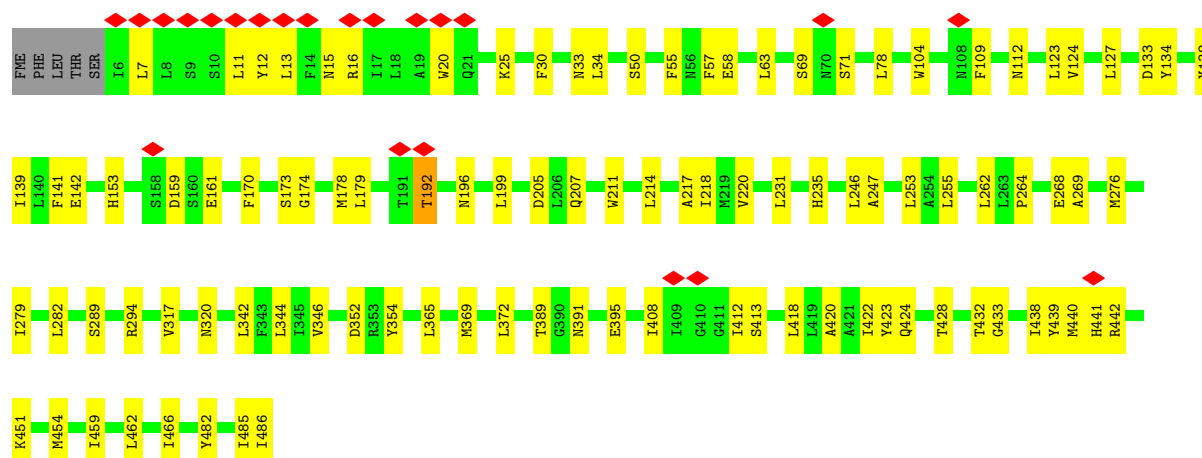
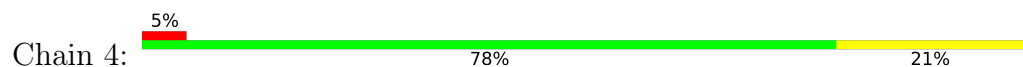
• Molecule 12: NADH dehydrogenase subunit 2



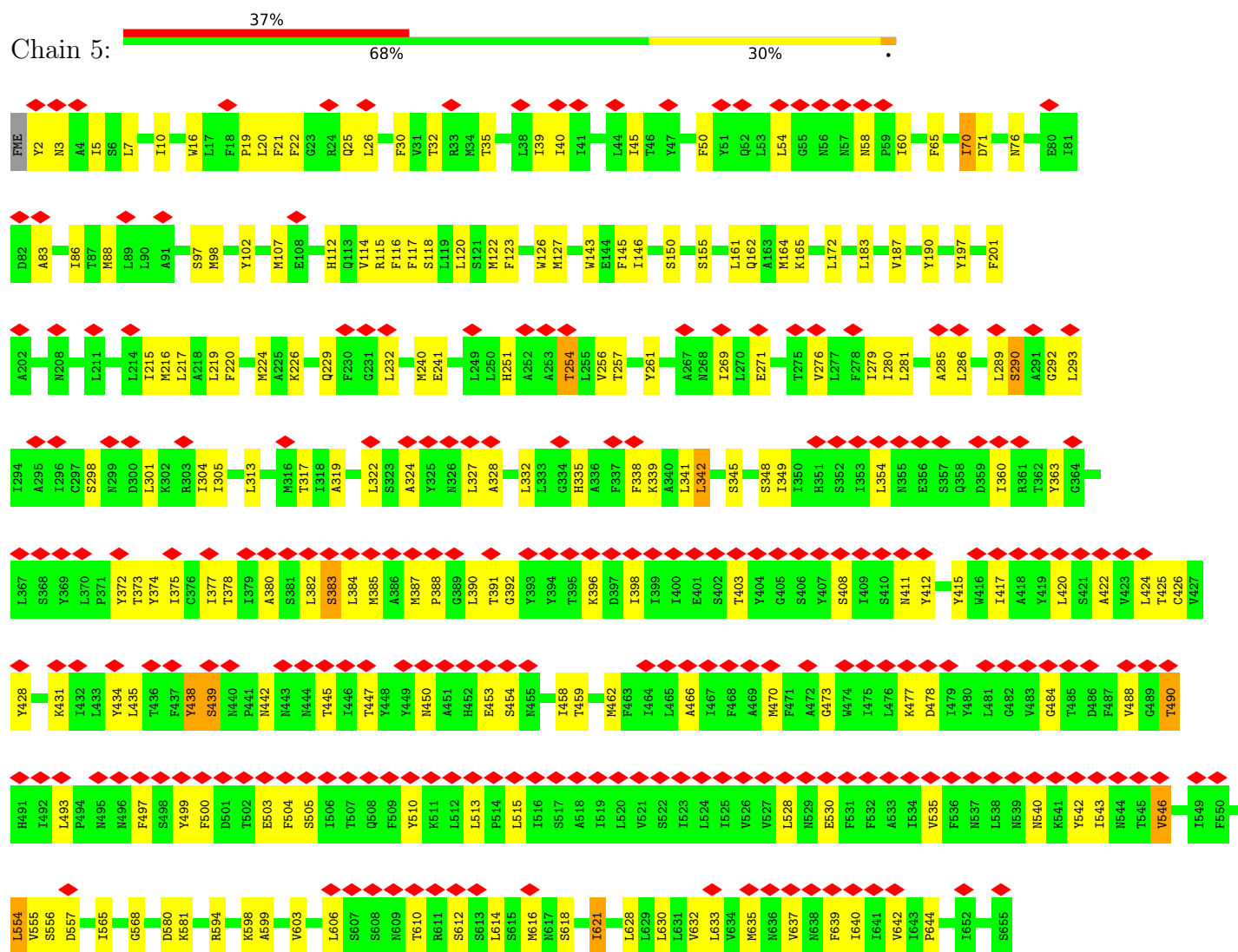
• Molecule 13: NADH-ubiquinone oxidoreductase chain 3



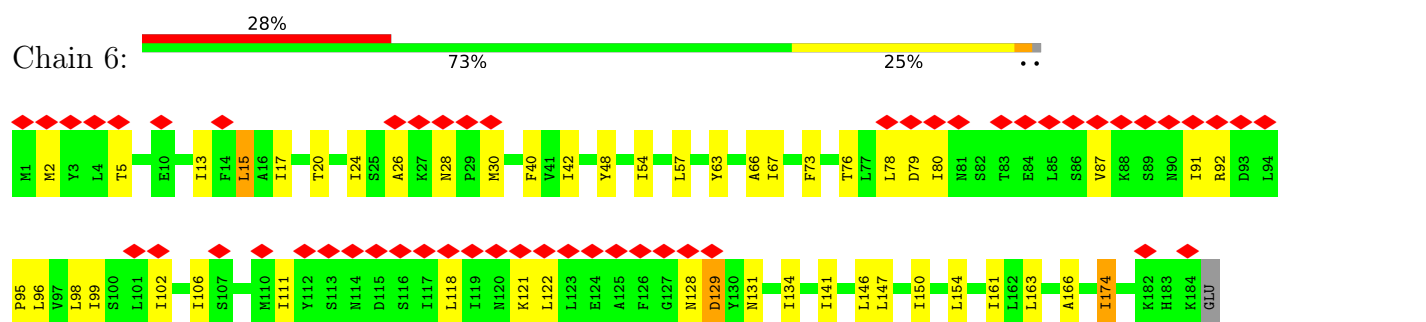
• Molecule 14: NADH-ubiquinone oxidoreductase chain 4



- Molecule 15: NADH-ubiquinone oxidoreductase chain 5



- Molecule 16: NADH-ubiquinone oxidoreductase chain 6

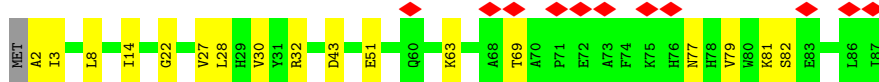
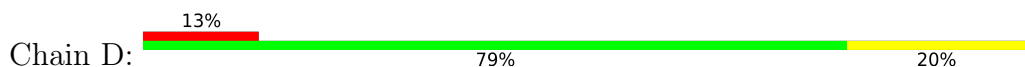


- Molecule 17: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

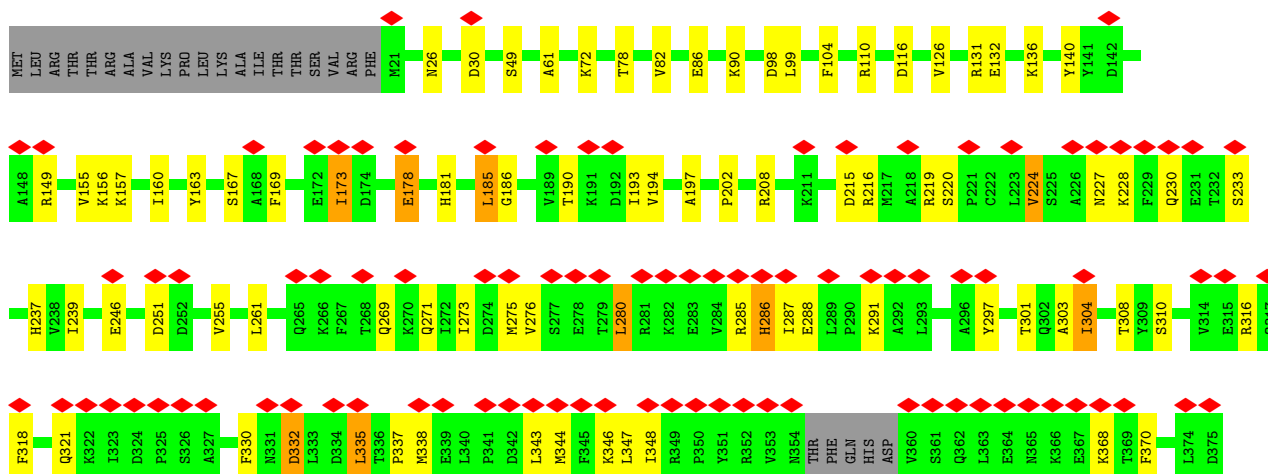




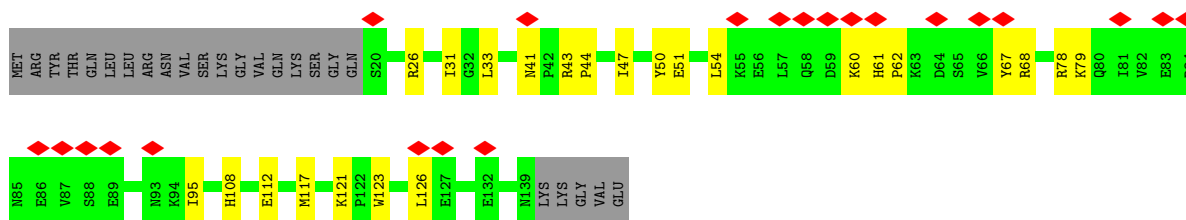
- Molecule 18: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)



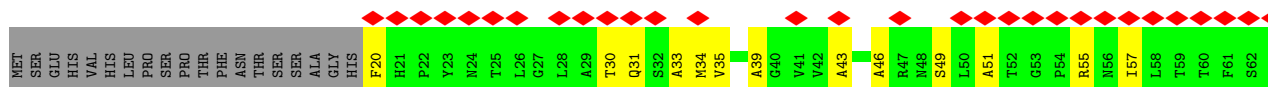
- Molecule 19: NADH-ubiquinone oxidoreductase 40 kDa subunit

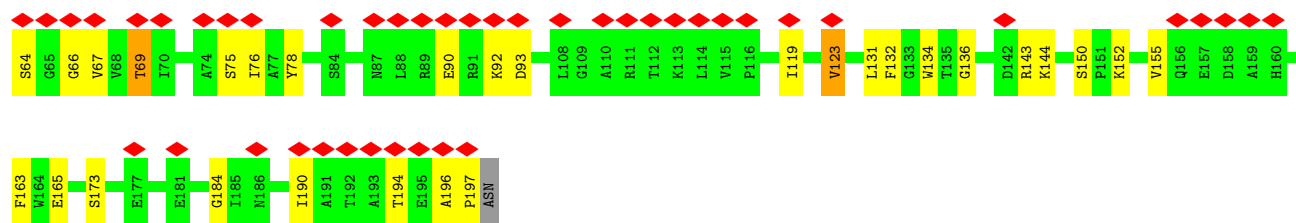


- Molecule 20: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

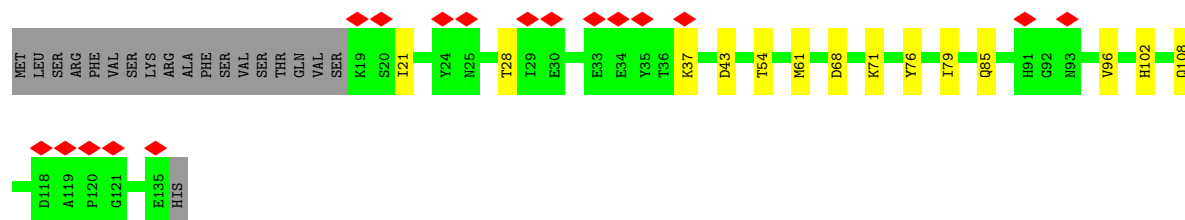
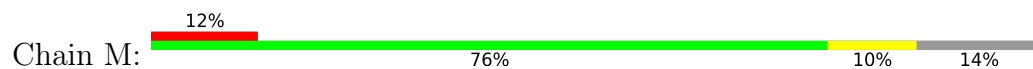


- Molecule 21: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

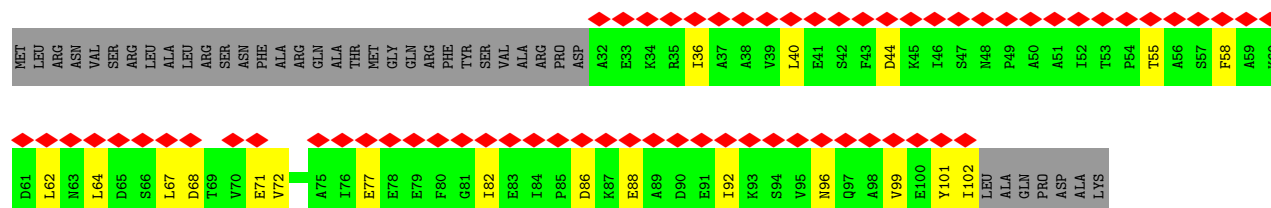




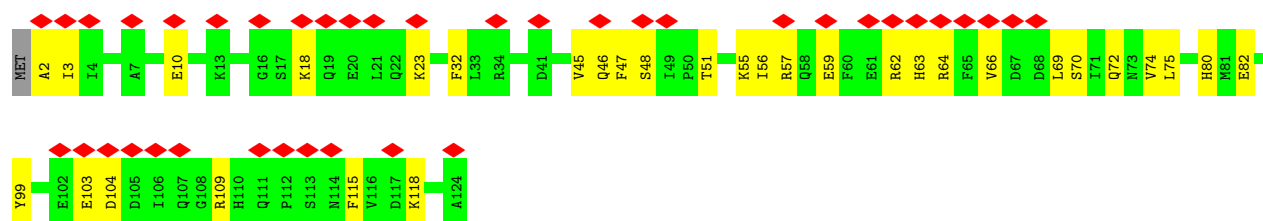
- Molecule 22: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



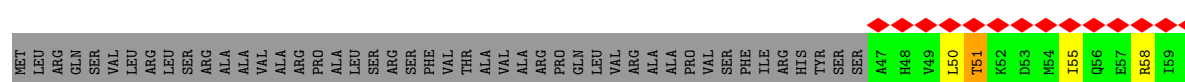
- Molecule 23: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

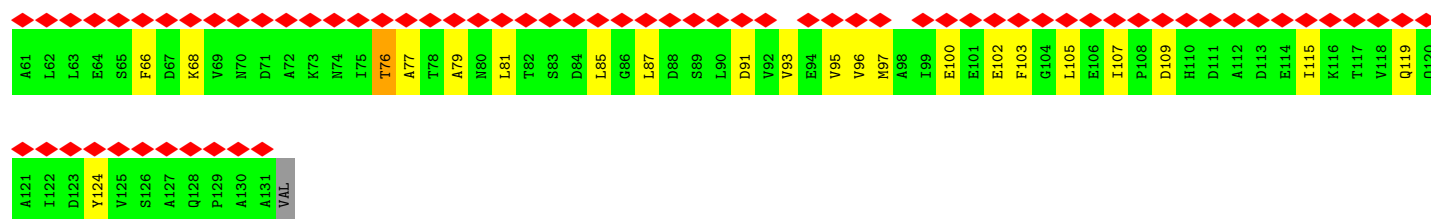


- Molecule 24: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

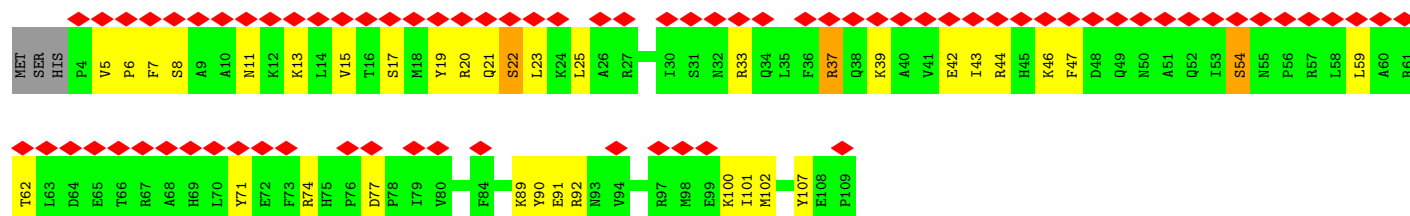


- Molecule 25: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

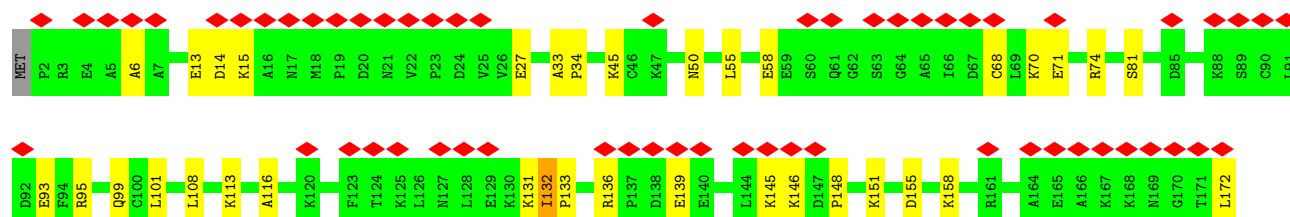
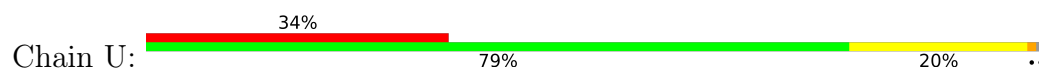




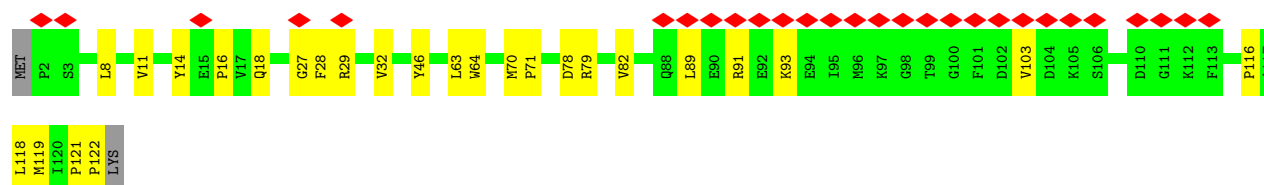
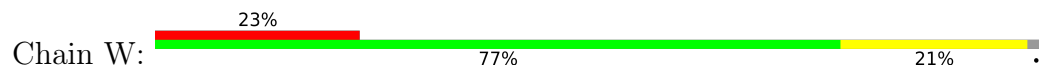
• Molecule 26: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)



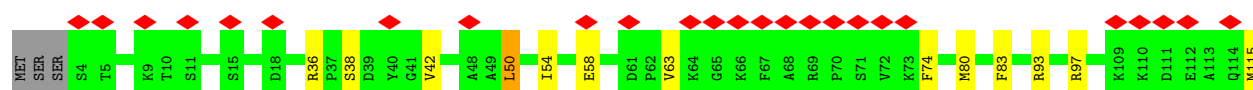
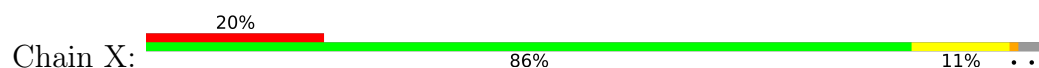
• Molecule 27: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

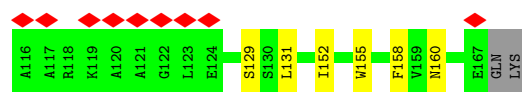


• Molecule 28: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

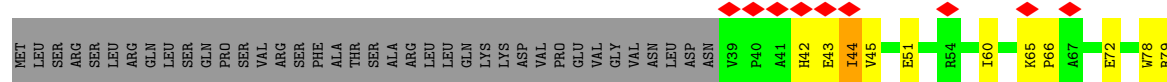


• Molecule 29: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

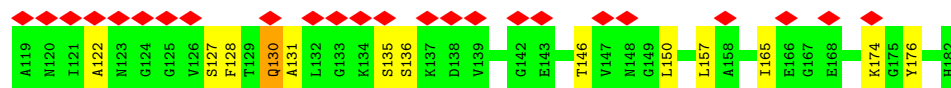
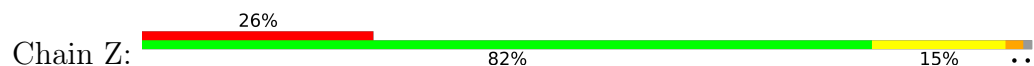




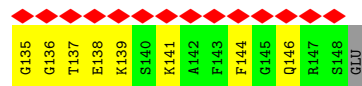
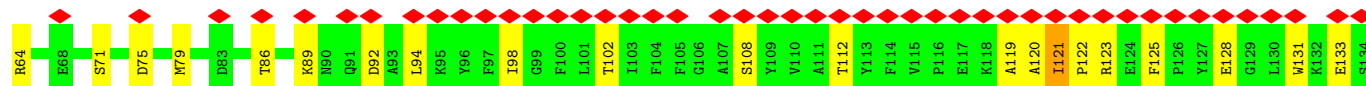
- Molecule 30: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



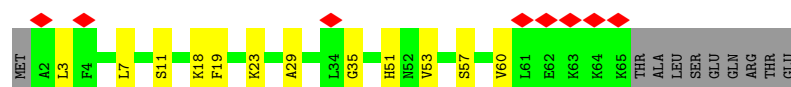
- Molecule 31: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



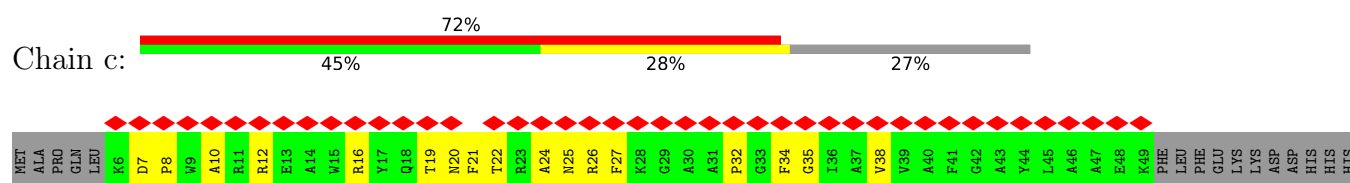
- Molecule 32: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



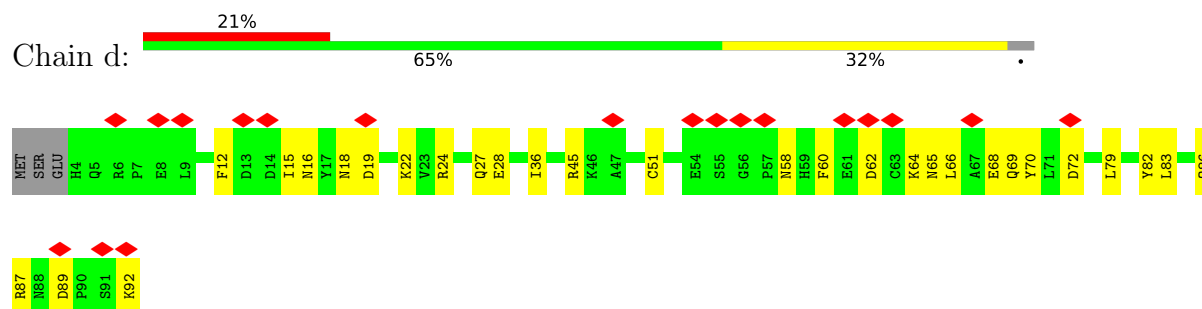
- Molecule 33: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



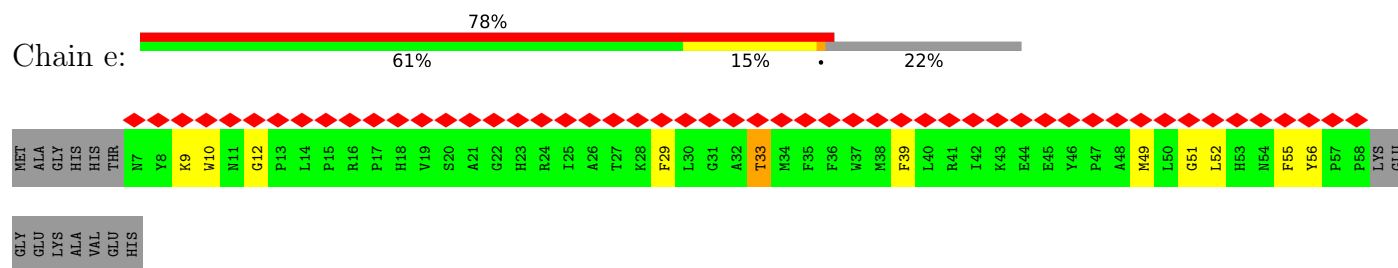
- Molecule 34: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



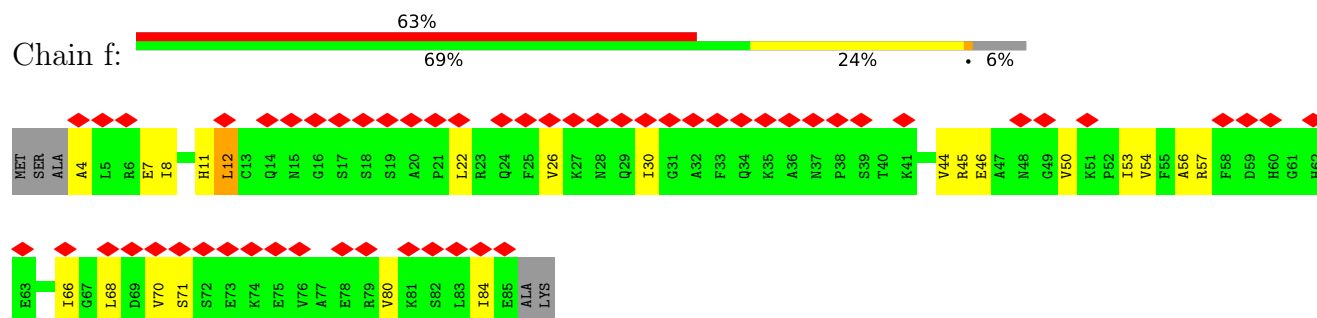
• Molecule 35: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



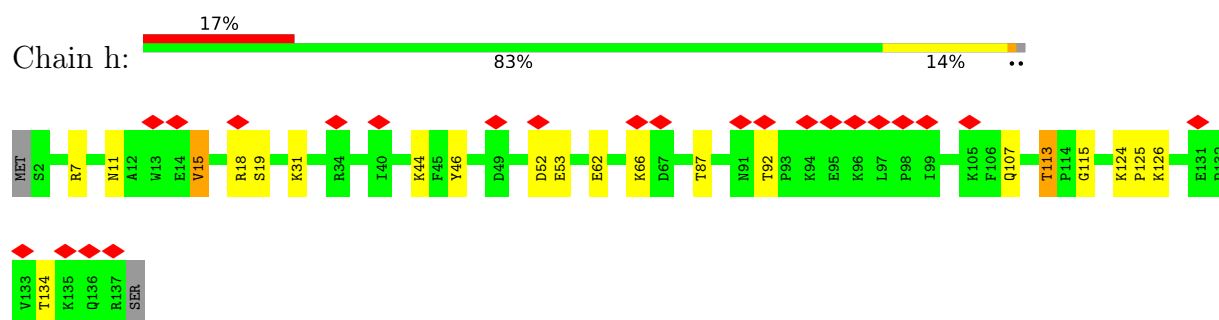
• Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



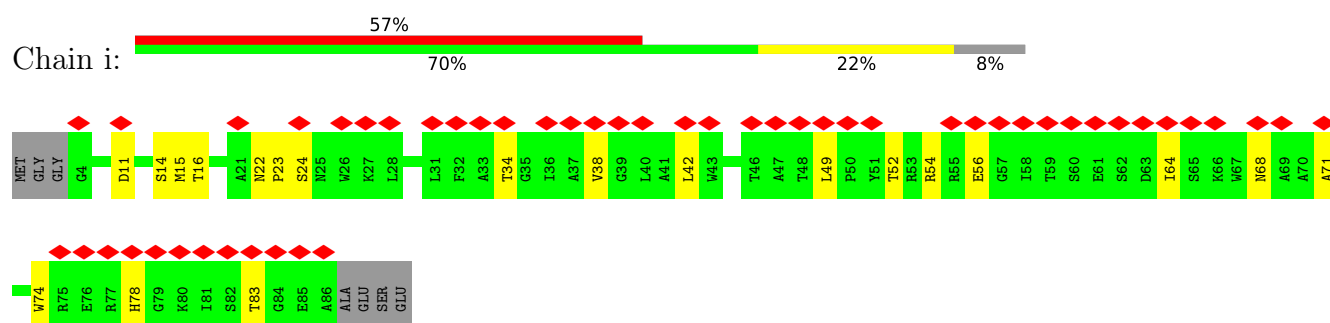
• Molecule 37: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



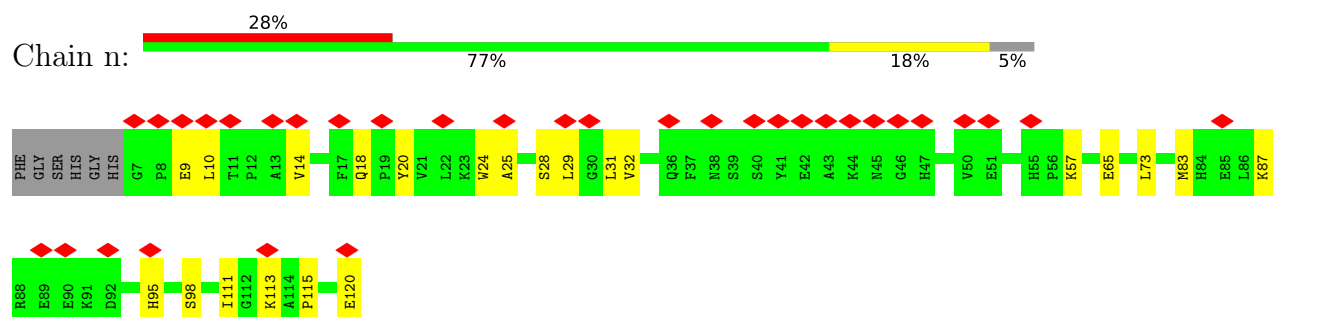
• Molecule 38: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



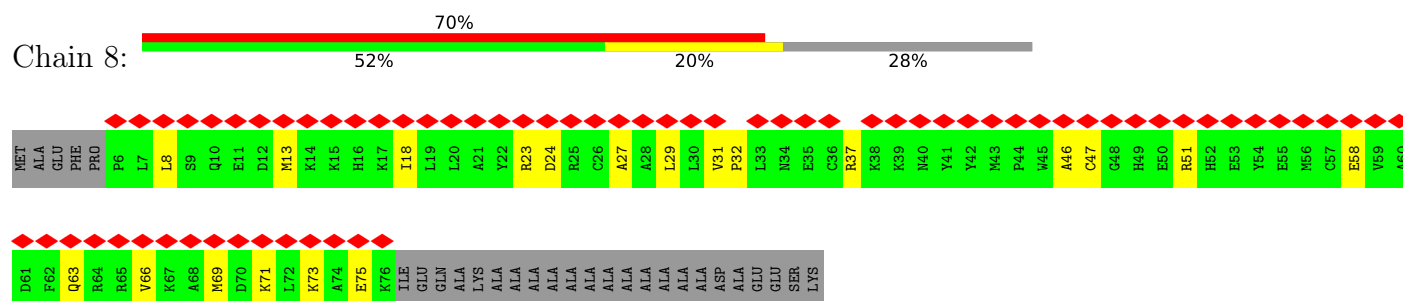
• Molecule 39: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



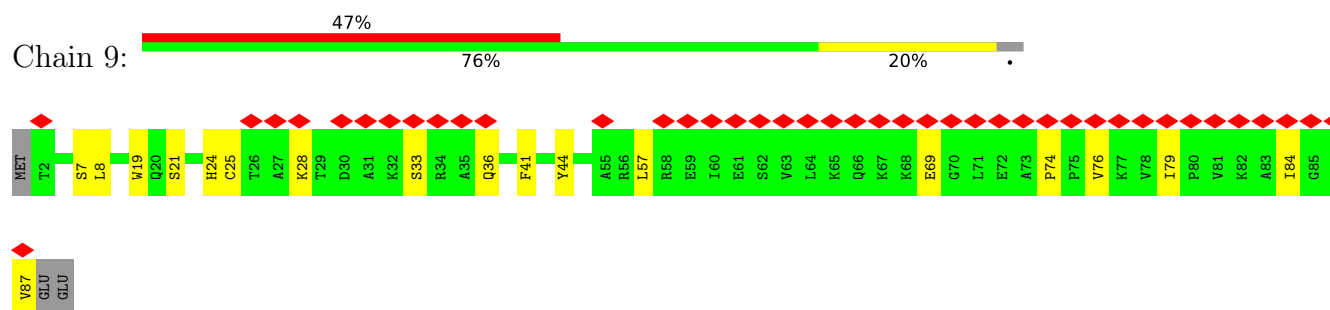
- Molecule 40: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178960	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	96899	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.516, 0.516, 0.516	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, T7X, LMN, FMN, CPL, FME, SF4, FES, 2MR, NDP, ZMP, ZN, PLC

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	A	0.25	0/5363	0.49	2/7278 (0.0%)
2	B	0.25	0/3594	0.48	0/4851
3	C	0.28	0/3541	0.51	0/4799
4	G	0.26	0/2040	0.52	2/2781 (0.1%)
5	H	0.24	0/1725	0.57	1/2343 (0.0%)
6	I	0.27	0/1557	0.44	0/2110
7	K	0.27	0/1434	0.47	0/1950
8	L	0.29	0/692	0.46	0/937
9	S	0.21	0/1517	0.48	0/2046
10	j	0.21	0/745	0.41	0/1006
11	1	0.27	0/2781	0.47	0/3798
12	2	0.26	0/3846	0.43	0/5242
13	3	0.25	0/1041	0.49	0/1420
14	4	0.25	0/3908	0.44	0/5337
15	5	0.25	0/5327	0.49	0/7273
16	6	0.25	0/1468	0.44	0/2003
17	g	0.33	0/648	0.50	0/887
18	D	0.23	0/697	0.41	0/940
19	E	0.27	0/2866	0.50	0/3881
20	F	0.24	0/1002	0.47	0/1359
21	J	0.21	0/1351	0.43	0/1840
22	M	0.24	0/935	0.42	0/1268
23	O	0.19	0/549	0.39	0/746
24	P	0.23	0/1061	0.41	0/1427
25	Q	0.18	0/654	0.38	0/890
26	R	0.23	0/909	0.46	0/1229
27	U	0.25	0/1374	0.48	0/1856
28	W	0.24	0/998	0.45	0/1346
29	X	0.24	0/1314	0.40	0/1783
30	Y	0.26	0/1051	0.44	0/1420
31	Z	0.25	0/1430	0.48	0/1955
32	a	0.23	0/1064	0.42	0/1439

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.20	0/503	0.31	0/679
34	c	0.20	0/364	0.48	0/491
35	d	0.25	0/767	0.41	0/1031
36	e	0.17	0/456	0.38	0/619
37	f	0.23	0/652	0.53	0/874
38	h	0.24	0/1168	0.47	0/1589
39	i	0.21	0/666	0.39	0/907
40	n	0.28	0/941	0.41	0/1276
41	8	0.20	0/606	0.42	0/808
42	9	0.22	0/684	0.39	0/918
All	All	0.25	0/65289	0.47	5/88632 (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
1	A	0	1
3	C	0	1
5	H	0	1
7	K	0	1
13	3	0	1
15	5	0	3
27	U	0	1
28	W	0	1
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	92	TRP	CA-C-N	5.80	132.62	121.54
4	G	92	TRP	C-N-CA	5.80	132.62	121.54
1	A	289	ASN	CA-C-N	5.74	132.50	121.54
1	A	289	ASN	C-N-CA	5.74	132.50	121.54
5	H	205	MET	CB-CG-SD	5.51	129.22	112.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	3	83	VAL	Peptide
15	5	438	TYR	Peptide
15	5	554	LEU	Peptide
15	5	70	ILE	Peptide
1	A	290	GLU	Peptide
3	C	311	TYR	Peptide
5	H	174	ASN	Peptide
7	K	34	PRO	Peptide
27	U	6	ALA	Peptide
28	W	116	PRO	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	A	5269	0	5168	95	0
2	B	3517	0	3476	117	0
3	C	3470	0	3403	76	0
4	G	1978	0	1908	32	0
5	H	1688	0	1660	38	0
6	I	1519	0	1460	28	0
7	K	1395	0	1375	30	0
8	L	693	0	753	27	0
9	S	1492	0	1536	42	0
10	j	724	0	706	13	0
11	1	2716	0	2812	65	0
12	2	3776	0	4004	69	0
13	3	1027	0	1091	33	0
14	4	3815	0	4010	73	0
15	5	5197	0	5353	149	0
16	6	1453	0	1576	53	0
17	g	622	0	602	13	0
18	D	681	0	671	14	0
19	E	2806	0	2792	65	0
20	F	981	0	969	22	0
21	J	1319	0	1304	33	0
22	M	912	0	869	8	0
23	O	543	0	537	14	0
24	P	1036	0	1018	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Q	648	0	636	26	0
26	R	884	0	891	27	0
27	U	1345	0	1327	26	0
28	W	974	0	987	25	0
29	X	1275	0	1250	17	0
30	Y	1021	0	984	25	0
31	Z	1389	0	1395	21	0
32	a	1030	0	967	28	0
33	b	490	0	509	8	0
34	c	353	0	343	17	0
35	d	751	0	715	23	0
36	e	436	0	426	9	0
37	f	642	0	656	19	0
38	h	1130	0	1084	17	0
39	i	646	0	630	22	0
40	n	913	0	879	19	0
41	8	594	0	599	16	0
42	9	672	0	683	12	0
43	A	16	0	0	0	0
43	B	8	0	0	0	0
43	I	16	0	0	0	0
43	K	8	0	0	1	0
44	A	4	0	0	1	0
44	H	4	0	0	0	0
45	B	31	0	19	2	0
46	1	77	0	108	4	0
46	4	35	0	44	1	0
46	5	42	0	64	1	0
46	K	39	0	55	3	0
46	W	41	0	59	1	0
47	1	128	0	184	14	0
47	4	136	0	203	14	0
47	5	126	0	177	15	0
47	6	84	0	117	6	0
47	E	36	0	46	0	0
47	J	119	0	160	12	0
47	S	42	0	61	2	0
47	b	42	0	58	7	0
47	g	43	0	63	4	0
48	J	69	0	88	9	0
48	j	65	0	77	5	0
49	2	100	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	3	49	0	0	1	0
50	2	52	0	80	3	0
51	E	72	0	88	9	0
51	W	54	0	52	3	0
51	X	86	0	119	10	0
51	Z	76	0	96	5	0
51	g	83	0	116	7	0
51	n	92	0	137	13	0
52	E	48	0	26	1	0
53	M	1	0	0	0	0
54	O	33	0	38	3	0
54	Q	33	0	38	3	0
55	1	67	0	0	1	0
55	2	158	0	0	5	0
55	3	10	0	0	0	0
55	4	139	0	0	5	0
55	5	57	0	0	1	0
55	6	24	0	0	1	0
55	9	16	0	0	0	0
55	A	135	0	0	2	0
55	B	11	0	0	0	0
55	C	168	0	0	7	0
55	D	17	0	0	1	0
55	E	79	0	0	1	0
55	F	15	0	0	0	0
55	G	114	0	0	3	0
55	H	2	0	0	0	0
55	I	95	0	0	1	0
55	J	14	0	0	0	0
55	K	78	0	0	2	0
55	L	18	0	0	1	0
55	M	45	0	0	0	0
55	P	15	0	0	1	0
55	R	11	0	0	0	0
55	S	4	0	0	0	0
55	U	39	0	0	1	0
55	W	23	0	0	0	0
55	X	39	0	0	1	0
55	Y	53	0	0	0	0
55	Z	52	0	0	3	0
55	a	11	0	0	0	0
55	b	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	d	8	0	0	5	0
55	g	2	0	0	0	0
55	h	61	0	0	4	0
55	i	3	0	0	0	0
55	j	15	0	0	0	0
55	n	12	0	0	0	0
All	All	67428	0	66387	1299	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 10.

All (1299) 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)
19:E:173:ILE:O	19:E:181:HIS:ND1	2.06	0.88
1:A:47:SER:O	1:A:60:LYS:NZ	2.07	0.86
15:5:354:LEU:HD21	15:5:450:ASN:HB2	1.59	0.83
9:S:56:GLU:HB3	9:S:118:LEU:HD21	1.61	0.83
2:B:64:THR:HA	2:B:67:LEU:HD12	1.60	0.82
1:A:218:GLU:HG2	1:A:723:LYS:HE2	1.60	0.82
48:J:202:LMN:HBP	48:J:202:LMN:HCS	1.60	0.82
14:4:442:ARG:HH22	39:i:11:ASP:HB2	1.45	0.81
5:H:141:MET:HE3	5:H:165:GLU:HG2	1.59	0.81
19:E:297:TYR:HB2	51:E:402:CDL:H382	1.63	0.80
17:g:64:LEU:HD12	17:g:65:PRO:HD2	1.63	0.80
14:4:124:VAL:HG22	47:4:503:3PE:H2I3	1.64	0.79
2:B:333:ILE:HD13	2:B:347:VAL:HG21	1.64	0.79
7:K:101:ASP:OD2	11:1:36:ARG:NH1	2.14	0.79
1:A:112:GLU:OE1	55:A:901:HOH:O	2.01	0.79
2:B:454:LYS:O	2:B:458:GLU:HB2	1.82	0.79
15:5:568:GLY:HA3	47:5:702:3PE:H292	1.65	0.78
15:5:630:LEU:HB3	47:J:203:3PE:H3A1	1.65	0.77
54:O:201:ZMP:H4	24:P:59:GLU:HG2	1.66	0.77
14:4:276:MET:HA	14:4:279:ILE:HD12	1.66	0.77
21:J:136:GLY:HA2	48:J:202:LMN:H3	1.66	0.77
12:2:94:LYS:NZ	55:2:602:HOH:O	2.14	0.77
2:B:34:LEU:HB3	2:B:39:ARG:HE	1.49	0.76
27:U:145:LYS:HE2	27:U:148:PRO:HA	1.65	0.76
35:d:89:ASP:OD1	55:d:101:HOH:O	2.02	0.76
15:5:58:ASN:HB3	39:i:54:ARG:HH11	1.50	0.76
12:2:69:ASP:OD2	55:2:601:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:60:ILE:HG23	16:6:63:TYR:HE1	1.50	0.76
1:A:339:LYS:NZ	1:A:566:ASP:O	2.19	0.75
26:R:37:ARG:HE	26:R:37:ARG:HA	1.51	0.75
3:C:443:ARG:NH2	24:P:2:ALA:O	2.16	0.75
17:g:56:SER:OG	27:U:139:GLU:OE1	2.04	0.75
15:5:484:GLY:H	41:8:37:ARG:HH12	1.34	0.75
13:3:124:LEU:HD13	20:F:26:ARG:HH12	1.50	0.74
15:5:528:LEU:HD23	15:5:535:VAL:HG11	1.69	0.74
14:4:395:GLU:OE2	55:4:601:HOH:O	2.05	0.74
25:Q:91:ASP:OD1	26:R:44:ARG:NH1	2.21	0.74
15:5:391:THR:HG22	15:5:473:GLY:H	1.53	0.74
19:E:251:ASP:OD2	24:P:109:ARG:NH2	2.20	0.74
5:H:174:ASN:HB3	5:H:186:GLU:HB3	1.70	0.73
38:h:44:LYS:NZ	38:h:46:TYR:OH	2.19	0.73
1:A:88:GLU:HG3	1:A:106:VAL:HB	1.69	0.73
11:1:125:TRP:HZ2	16:6:28:ASN:HD21	1.37	0.73
35:d:92:LYS:N	55:d:101:HOH:O	2.15	0.73
15:5:554:LEU:O	15:5:556:SER:N	2.21	0.73
16:6:129:ASP:N	16:6:129:ASP:OD1	2.22	0.73
16:6:163:LEU:HD13	51:X:201:CDL:H421	1.71	0.73
34:c:7:ASP:HB3	34:c:10:ALA:HB2	1.70	0.73
3:C:208:GLU:HG3	6:I:99:TYR:CD2	2.24	0.73
1:A:429:ARG:NH1	1:A:449:THR:O	2.21	0.72
15:5:345:SER:HB2	15:5:377:ILE:HD13	1.70	0.72
15:5:644:PRO:HG3	21:J:78:TYR:HB3	1.71	0.72
14:4:12:TYR:CZ	14:4:16:ARG:HD2	2.25	0.72
2:B:142:GLU:OE2	2:B:258:ARG:NH1	2.23	0.72
5:H:205:MET:HE3	5:H:206:PRO:HD2	1.71	0.71
35:d:62:ASP:OD1	55:d:102:HOH:O	2.07	0.71
2:B:290:VAL:HG21	2:B:305:HIS:CE1	2.25	0.71
3:C:118:LEU:HD22	7:K:127:MET:HG2	1.73	0.71
7:K:83:LEU:HB2	7:K:121:GLY:HA3	1.71	0.71
11:1:177:TRP:CD2	47:1:504:3PE:H322	2.25	0.71
19:E:136:LYS:NZ	55:E:501:HOH:O	2.07	0.70
4:G:125:ASP:OD1	4:G:143:ASN:HB2	1.91	0.70
46:1:505:PLC:H2'2	46:1:505:PLC:H1A1	1.73	0.70
14:4:58:GLU:HG3	14:4:78:LEU:HD23	1.72	0.70
14:4:352:ASP:OD2	55:4:602:HOH:O	2.08	0.70
9:S:121:ASP:O	9:S:125:LEU:HD12	1.92	0.70
48:j:101:LMN:HAYA	47:J:204:3PE:H352	1.73	0.70
14:4:294:ARG:NE	32:a:75:ASP:OD2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:610:THR:HG21	15:5:616:MET:HG3	1.73	0.70
16:6:42:ILE:HD11	47:6:202:3PE:H3F2	1.73	0.69
2:B:315:ASN:HA	2:B:361:LYS:HD2	1.75	0.69
15:5:632:VAL:HA	15:5:635:MET:HG3	1.74	0.69
37:f:70:VAL:HG12	37:f:71:SER:H	1.58	0.69
26:R:39:LYS:O	26:R:43:ILE:HG12	1.91	0.69
3:C:197:VAL:HG21	3:C:271:TRP:HZ3	1.57	0.68
15:5:58:ASN:HD21	39:i:56:GLU:HB3	1.57	0.68
23:O:68:ASP:HA	23:O:71:GLU:HG3	1.75	0.68
15:5:215:ILE:HG22	15:5:216:MET:HE2	1.76	0.68
4:G:206:GLU:OE2	55:G:301:HOH:O	2.11	0.68
39:i:22:ASN:ND2	40:n:9:GLU:O	2.23	0.67
8:L:87:TYR:HB3	15:5:612:SER:HB3	1.74	0.67
3:C:312:ASP:OD1	55:C:501:HOH:O	2.11	0.67
15:5:88:MET:HE2	15:5:261:TYR:HB2	1.75	0.67
51:g:201:CDL:H241	51:X:201:CDL:H672	1.75	0.67
9:S:67:PRO:O	9:S:129:TYR:OH	2.11	0.67
31:Z:100:LEU:HG	31:Z:108:ILE:HD12	1.77	0.67
31:Z:14:THR:HG21	31:Z:37:GLY:H	1.58	0.67
1:A:290:GLU:OE1	1:A:430:LYS:NZ	2.27	0.67
47:b:201:3PE:H322	47:b:201:3PE:H221	1.76	0.67
2:B:102:ASN:OD1	2:B:152:ASN:ND2	2.28	0.66
11:1:132:SER:HA	11:1:211:LEU:HD11	1.75	0.66
18:D:51:GLU:OE1	55:D:101:HOH:O	2.14	0.66
26:R:42:GLU:O	26:R:46:LYS:HG2	1.95	0.66
2:B:147:ALA:HB1	2:B:151:MET:HE1	1.78	0.66
12:2:465:ASN:HB3	40:n:83:MET:HE2	1.77	0.66
6:I:152:ARG:HD3	22:M:79:ILE:HD12	1.78	0.66
15:5:360:ILE:HG23	15:5:435:LEU:HD23	1.77	0.66
1:A:335:ALA:O	1:A:339:LYS:HB2	1.95	0.66
3:C:267:ASP:OD1	55:C:502:HOH:O	2.13	0.66
7:K:93:VAL:HG12	7:K:100:GLN:HB3	1.78	0.65
10:j:84:ARG:NH2	35:d:72:ASP:OD1	2.27	0.65
19:E:271:GLN:O	19:E:275:MET:HG3	1.95	0.65
14:4:424:GLN:O	14:4:428:THR:HG23	1.96	0.65
1:A:363:LYS:HG3	1:A:374:THR:HG21	1.78	0.65
19:E:301:THR:HA	51:E:402:CDL:H172	1.77	0.65
5:H:126:ILE:HD11	5:H:178:MET:HE3	1.79	0.65
8:L:86:SER:O	55:L:101:HOH:O	2.14	0.65
13:3:89:THR:HG21	51:X:201:CDL:H311	1.79	0.65
15:5:342:LEU:HD22	15:5:380:ALA:HB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:175:ALA:HB3	5:H:176:PRO:HD3	1.79	0.65
12:2:377:LEU:HD11	47:4:501:3PE:H2F2	1.78	0.64
20:F:47:ILE:O	20:F:51:GLU:HG2	1.96	0.64
19:E:163:TYR:HD2	19:E:194:VAL:HG21	1.62	0.64
15:5:341:LEU:HD22	15:5:380:ALA:HB2	1.79	0.64
15:5:530:GLU:OE2	34:c:26:ARG:NH1	2.29	0.64
15:5:425:THR:HA	15:5:428:TYR:CE2	2.31	0.64
33:b:18:LYS:HE3	33:b:35:GLY:HA3	1.79	0.64
27:U:113:LYS:NZ	27:U:155:ASP:OD2	2.30	0.64
32:a:36:MET:HE3	32:a:36:MET:HA	1.80	0.64
11:1:279:SER:OG	18:D:22:GLY:HA3	1.98	0.64
15:5:25:GLN:HE21	40:n:18:GLN:HG2	1.63	0.64
15:5:554:LEU:C	15:5:556:SER:H	2.05	0.64
7:K:56:ALA:HA	7:K:59:TYR:HB2	1.80	0.64
8:L:89:ILE:HD13	15:5:614:LEU:HD22	1.79	0.63
14:4:174:GLY:HA3	14:4:220:VAL:HG21	1.78	0.63
15:5:415:TYR:CZ	15:5:510:TYR:HD1	2.16	0.63
46:W:401:PLC:HTA1	51:Z:201:CDL:H592	1.80	0.63
2:B:173:THR:O	2:B:177:GLU:HG2	1.97	0.63
8:L:2:PHE:O	8:L:6:ILE:HD12	1.99	0.63
14:4:30:PHE:CE1	14:4:34:LEU:HD11	2.33	0.63
22:M:21:ILE:HG12	22:M:54:THR:HG23	1.79	0.63
1:A:543:SER:OG	1:A:544:LYS:NZ	2.32	0.63
15:5:20:LEU:HB3	47:5:701:3PE:H352	1.81	0.63
25:Q:96:VAL:HG22	25:Q:115:ILE:HD11	1.81	0.63
28:W:91:ARG:NH2	42:9:74:PRO:O	2.31	0.63
3:C:124:GLU:HG2	3:C:425:CYS:O	1.99	0.63
28:W:93:LYS:HA	28:W:103:VAL:HG21	1.80	0.63
1:A:282:PRO:HG3	1:A:293:ILE:HG12	1.80	0.62
2:B:276:LYS:HB2	2:B:294:MET:HE1	1.81	0.62
8:L:23:ILE:HD11	16:6:80:ILE:HG13	1.81	0.62
39:i:24:SER:HA	40:n:10:LEU:HD22	1.81	0.62
2:B:212:THR:HG21	2:B:226:ARG:HB2	1.81	0.62
20:F:61:HIS:O	20:F:68:ARG:NH1	2.28	0.62
2:B:288:CYS:SG	2:B:289:THR:N	2.72	0.62
15:5:143:TRP:CE2	15:5:226:LYS:HE2	2.35	0.62
11:1:72:ILE:HD11	47:6:202:3PE:H31	1.82	0.62
37:f:4:ALA:HB2	37:f:56:ALA:HB1	1.82	0.62
15:5:488:VAL:HG12	15:5:490:THR:HG22	1.82	0.62
11:1:177:TRP:CG	47:1:504:3PE:H322	2.34	0.62
15:5:58:ASN:ND2	39:i:56:GLU:HB3	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:VAL:HG11	2:B:305:HIS:CD2	2.35	0.61
32:a:37:LEU:HD12	32:a:40:TYR:O	2.00	0.61
23:O:58:PHE:HB3	23:O:64:LEU:HD12	1.81	0.61
11:1:129:SER:O	11:1:132:SER:OG	2.18	0.61
14:4:420:ALA:HA	14:4:423:TYR:CE2	2.35	0.61
39:i:49:LEU:O	39:i:52:THR:OG1	2.18	0.61
14:4:451:LYS:NZ	51:n:200:CDL:OA4	2.29	0.61
15:5:71:ASP:HB2	35:d:79:LEU:HD12	1.81	0.61
27:U:58:GLU:OE1	40:n:115:PRO:HA	2.00	0.61
11:1:76:SER:O	11:1:80:THR:HG23	2.00	0.61
9:S:93:GLU:HG3	9:S:150:VAL:HB	1.83	0.61
12:2:96:LEU:HD22	12:2:343:PRO:HG3	1.82	0.61
24:P:82:GLU:OE2	55:P:201:HOH:O	2.16	0.61
47:b:201:3PE:H341	47:b:201:3PE:H241	1.81	0.61
41:8:31:VAL:HB	41:8:32:PRO:HD3	1.83	0.61
9:S:208:PRO:O	9:S:211:ASN:HB2	2.01	0.61
14:4:12:TYR:O	14:4:16:ARG:HG2	2.00	0.61
21:J:190:ILE:O	21:J:194:THR:HG23	2.01	0.61
1:A:149:MET:SD	3:C:365:LYS:HG2	2.41	0.60
20:F:51:GLU:CD	20:F:79:LYS:HZ3	2.08	0.60
1:A:552:LEU:HB3	1:A:555:ALA:HB3	1.81	0.60
8:L:3:ILE:HB	16:6:13:ILE:HG12	1.83	0.60
11:1:200:PRO:HG2	11:1:297:ARG:HD2	1.81	0.60
15:5:162:GLN:HB3	15:5:241:GLU:OE1	2.01	0.60
5:H:171:ALA:HB3	5:H:177:MET:HG2	1.81	0.60
9:S:183:MET:HE1	51:n:200:CDL:H622	1.84	0.60
24:P:75:LEU:HD11	30:Y:44:ILE:HD11	1.84	0.60
30:Y:65:LYS:HE3	30:Y:72:GLU:HG3	1.82	0.60
31:Z:165:ILE:O	55:Z:301:HOH:O	2.16	0.60
11:1:254:ASN:OD1	55:1:601:HOH:O	2.16	0.60
15:5:466:ALA:O	15:5:470:MET:HG3	2.01	0.60
24:P:66:VAL:O	24:P:72:GLN:NE2	2.34	0.60
24:P:48:SER:O	24:P:51:THR:OG1	2.18	0.60
16:6:54:ILE:HD11	16:6:147:LEU:HD22	1.84	0.60
31:Z:127:SER:OG	31:Z:130:GLN:HG3	2.02	0.60
12:2:15:MET:HE1	51:g:201:CDL:HA62	1.83	0.60
12:2:228:THR:O	12:2:282:LYS:NZ	2.35	0.60
14:4:133:ASP:HB2	14:4:192:THR:HG22	1.83	0.60
1:A:411:LEU:HB2	1:A:470:PHE:HE1	1.67	0.60
17:g:39:ALA:O	17:g:43:LEU:HB2	2.02	0.60
41:8:69:MET:HE3	41:8:73:LYS:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLU:CD	1:A:427:ARG:HD2	2.27	0.59
6:I:117:GLU:HB2	6:I:192:TYR:CZ	2.37	0.59
11:1:131:TYR:HD2	11:1:210:GLU:HB3	1.67	0.59
1:A:284:VAL:HG22	1:A:291:GLU:HB3	1.84	0.59
2:B:37:GLN:O	2:B:259:ARG:NH2	2.30	0.59
47:1:504:3PE:H111	27:U:151:LYS:HZ1	1.67	0.59
14:4:389:THR:HG22	14:4:391:ASN:H	1.67	0.59
15:5:500:PHE:CD1	41:8:58:GLU:HG2	2.37	0.59
1:A:204:SER:O	55:A:902:HOH:O	2.16	0.59
2:B:92:PHE:CG	2:B:93:PRO:HD2	2.37	0.59
12:2:49:ASN:O	55:2:603:HOH:O	2.17	0.59
15:5:322:LEU:HD11	15:5:403:THR:HG22	1.84	0.59
1:A:377:ASP:HB3	1:A:528:ARG:HH12	1.67	0.59
54:O:201:ZMP:H15	24:P:63:HIS:O	2.03	0.59
54:O:201:ZMP:O6	24:P:64:ARG:NH1	2.30	0.59
14:4:141:PHE:HE1	14:4:253:LEU:HB3	1.67	0.59
12:2:149:LYS:HB3	12:2:227:ASN:HB3	1.83	0.59
14:4:231:LEU:HG	14:4:235:HIS:HD2	1.67	0.59
25:Q:50:LEU:HD13	25:Q:55:ILE:HD11	1.84	0.59
2:B:213:SER:HB2	2:B:225:PRO:HG3	1.85	0.59
19:E:216:ARG:HG3	51:E:402:CDL:HA22	1.84	0.59
29:X:115:MET:HE2	29:X:115:MET:HA	1.85	0.59
2:B:329:LEU:HD13	2:B:333:ILE:HD11	1.85	0.59
27:U:93:GLU:CD	27:U:93:GLU:H	2.11	0.59
4:G:162:VAL:HB	24:P:70:SER:HB2	1.85	0.58
9:S:50:ALA:HB3	9:S:103:VAL:HA	1.84	0.58
26:R:19:TYR:CZ	26:R:23:LEU:HD11	2.38	0.58
1:A:615:PRO:HD3	30:Y:86:ASP:OD1	2.02	0.58
18:D:3:ILE:HD12	51:Z:201:CDL:HA4	1.85	0.58
13:3:64:LEU:HD13	16:6:66:ALA:HB1	1.85	0.58
23:O:44:ASP:OD1	23:O:44:ASP:N	2.33	0.58
9:S:133:GLY:HA3	9:S:152:TRP:CH2	2.38	0.58
12:2:58:LEU:HD22	12:2:124:ILE:HD11	1.84	0.58
15:5:107:MET:HE2	15:5:116:PHE:CG	2.38	0.58
7:K:100:GLN:HE22	7:K:107:PHE:HD2	1.51	0.58
14:4:438:ILE:HD13	32:a:59:ASP:HB2	1.86	0.58
36:e:29:PHE:O	36:e:33:THR:OG1	2.18	0.58
11:1:199:ARG:HD3	11:1:235:ILE:HD11	1.85	0.58
12:2:55:MET:HE1	29:X:155:TRP:CD2	2.39	0.58
19:E:285:ARG:HG3	19:E:285:ARG:HH11	1.67	0.58
35:d:51:CYS:HA	39:i:64:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1:FME:HG3	8:L:39:ILE:HA	1.84	0.58
37:f:22:LEU:HD13	37:f:68:LEU:HD23	1.85	0.58
7:K:88:VAL:HA	7:K:91:MET:HE3	1.85	0.58
8:L:20:ARG:NH1	16:6:26:ALA:O	2.37	0.58
48:j:101:LMN:HAW	21:J:119:ILE:HG21	1.84	0.58
2:B:61:TRP:CD2	2:B:183:LEU:HD13	2.39	0.58
3:C:281:VAL:HG22	3:C:441:ILE:HG12	1.85	0.58
15:5:70:ILE:HG22	15:5:71:ASP:H	1.68	0.58
19:E:132:GLU:OE2	19:E:316:ARG:NH1	2.29	0.58
19:E:194:VAL:HG23	19:E:197:ALA:HB2	1.86	0.58
24:P:18:LYS:HG2	24:P:69:LEU:HD13	1.86	0.58
37:f:26:VAL:O	37:f:30:ILE:HB	2.03	0.58
2:B:321:PRO:O	2:B:326:VAL:HG21	2.04	0.57
9:S:92:ALA:HB2	9:S:152:TRP:CD1	2.39	0.57
12:2:376:PRO:HG3	47:4:503:3PE:H3G1	1.86	0.57
21:J:150:SER:O	21:J:152:LYS:NZ	2.35	0.57
9:S:169:TYR:OH	51:n:200:CDL:OB3	2.21	0.57
15:5:387:MET:HB2	15:5:390:LEU:HD12	1.86	0.57
16:6:92:ARG:HG3	16:6:92:ARG:HH11	1.69	0.57
19:E:304:ILE:HB	51:E:402:CDL:H171	1.85	0.57
46:1:505:PLC:H1'2	28:W:46:TYR:HA	1.85	0.57
40:n:120:GLU:HA	42:9:24:HIS:CD2	2.39	0.57
3:C:144:TYR:HB2	7:K:85:CYS:HB3	1.87	0.57
1:A:380:ASN:ND2	1:A:490:ASP:O	2.34	0.57
3:C:205:TRP:CZ2	6:I:93:GLN:HG3	2.39	0.57
8:L:54:LEU:HD11	16:6:154:LEU:HD13	1.86	0.57
7:K:101:ASP:OD1	11:1:38:GLY:HA2	2.04	0.57
4:G:84:LYS:HD3	4:G:85:TYR:CZ	2.40	0.57
37:f:54:VAL:HG12	37:f:68:LEU:HD11	1.86	0.57
1:A:446:LEU:HD13	1:A:448:ALA:HB2	1.87	0.57
23:O:58:PHE:HA	23:O:62:LEU:HD23	1.86	0.57
6:I:129:ARG:NH1	22:M:108:GLN:O	2.37	0.57
14:4:57:PHE:HB3	47:4:503:3PE:H32	1.85	0.57
1:A:641:ASP:OD1	1:A:642:ALA:N	2.37	0.57
2:B:439:GLY:HA2	2:B:442:ARG:HH12	1.70	0.57
6:I:121:ARG:NH2	55:I:404:HOH:O	2.37	0.56
30:Y:60:ILE:HB	30:Y:131:ILE:HD13	1.86	0.56
11:1:206:GLU:HG2	11:1:216:PHE:HE1	1.70	0.56
13:3:59:VAL:HG13	13:3:111:LEU:HD22	1.87	0.56
15:5:183:LEU:O	15:5:187:VAL:HG23	2.04	0.56
33:b:3:LEU:HD13	33:b:51:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:9:25:CYS:HA	42:9:28:LYS:HE2	1.88	0.56
3:C:249:MET:HE2	4:G:42:ILE:HD11	1.86	0.56
9:S:143:LYS:C	9:S:150:VAL:HA	2.30	0.56
12:2:102:GLU:OE2	13:3:104:TYR:OH	2.17	0.56
12:2:148:TYR:CE2	19:E:368:LYS:HD3	2.41	0.56
15:5:384:LEU:O	15:5:396:LYS:NZ	2.36	0.56
38:h:15:VAL:HG13	38:h:19:SER:HB3	1.85	0.56
2:B:345:LYS:NZ	2:B:345:LYS:HB3	2.21	0.56
37:f:11:HIS:HB2	37:f:53:ILE:CG2	2.36	0.56
3:C:191:CYS:HB3	3:C:203:PHE:HA	1.88	0.56
15:5:240:MET:HE3	15:5:251:HIS:CE1	2.41	0.56
24:P:55:LYS:NZ	24:P:99:TYR:O	2.34	0.56
25:Q:107:ILE:O	26:R:20:ARG:NH2	2.36	0.56
4:G:227:GLU:OE1	19:E:72:LYS:NZ	2.39	0.56
31:Z:21:TRP:CD1	51:Z:201:CDL:H1O1	2.24	0.56
32:a:123:ARG:NH1	41:8:24:ASP:OD2	2.39	0.56
19:E:227:ASN:HA	19:E:228:LYS:NZ	2.20	0.56
1:A:315:ARG:NH1	38:h:134:THR:HB	2.20	0.56
12:2:124:ILE:HD12	12:2:125:THR:N	2.21	0.55
24:P:32:PHE:HB3	24:P:56:ILE:HD13	1.88	0.55
24:P:62:ARG:HH21	24:P:62:ARG:HG3	1.71	0.55
30:Y:43:GLU:HG3	30:Y:125:GLN:O	2.05	0.55
2:B:34:LEU:HD21	2:B:275:THR:HG21	1.87	0.55
2:B:64:THR:O	2:B:68:ILE:HG13	2.05	0.55
2:B:309:ILE:HG12	2:B:316:LEU:HG	1.88	0.55
10:j:40:THR:O	15:5:581:LYS:NZ	2.39	0.55
47:1:503:3PE:H361	51:E:402:CDL:H592	1.88	0.55
19:E:131:ARG:NH1	52:E:400:NDP:O1A	2.40	0.55
19:E:275:MET:HB2	19:E:344:MET:HE1	1.87	0.55
32:a:37:LEU:H	32:a:37:LEU:HD23	1.71	0.55
27:U:101:LEU:HD21	27:U:108:LEU:HD23	1.89	0.55
15:5:285:ALA:HB1	15:5:417:ILE:HG21	1.89	0.55
19:E:276:VAL:O	19:E:280:LEU:HB2	2.06	0.55
23:O:40:LEU:HD13	23:O:72:VAL:HG21	1.89	0.55
1:A:99:TYR:HE2	1:A:105:MET:HE1	1.71	0.55
14:4:196:ASN:HB2	14:4:199:LEU:HD12	1.86	0.55
19:E:330:PHE:CD2	19:E:337:PRO:HG3	2.42	0.55
26:R:100:LYS:HE3	26:R:101:ILE:O	2.06	0.55
1:A:355:GLU:OE2	1:A:357:GLU:HB2	2.07	0.55
13:3:66:PHE:O	13:3:70:ILE:HG12	2.06	0.55
20:F:31:ILE:HD12	20:F:33:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:237:GLU:HG2	19:E:49:SER:HB3	1.89	0.55
2:B:136:ASP:HB3	2:B:139:LYS:HD3	1.88	0.55
11:1:180:ILE:HD11	47:1:504:3PE:H362	1.88	0.55
15:5:161:LEU:CD1	15:5:165:LYS:HD2	2.37	0.55
21:J:33:ALA:HB2	21:J:76:ILE:HD11	1.88	0.55
38:h:11:ASN:O	38:h:15:VAL:HB	2.07	0.55
4:G:125:ASP:OD1	4:G:125:ASP:N	2.38	0.55
38:h:7:ARG:NH2	38:h:53:GLU:OE1	2.39	0.55
11:1:130:LYS:HE3	13:3:49:ARG:HG2	1.87	0.54
1:A:204:SER:O	5:H:106:GLU:HG2	2.08	0.54
1:A:286:GLU:HG3	30:Y:138:LYS:H	1.72	0.54
2:B:269:ARG:HG3	2:B:295:SER:OG	2.07	0.54
15:5:599:ALA:O	15:5:603:VAL:HG13	2.07	0.54
22:M:68:ASP:OD1	22:M:71:LYS:HG2	2.07	0.54
15:5:161:LEU:HD13	15:5:165:LYS:HD2	1.88	0.54
2:B:117:VAL:HB	2:B:158:ILE:HG13	1.89	0.54
41:8:8:LEU:HB2	41:8:13:MET:HE2	1.88	0.54
2:B:103:PRO:HD2	2:B:106:TRP:HB3	1.88	0.54
2:B:334:CYS:HA	2:B:337:VAL:HG12	1.90	0.54
15:5:286:LEU:O	15:5:290:SER:OG	2.25	0.54
15:5:565:ILE:HG23	47:5:702:3PE:H252	1.90	0.54
8:L:23:ILE:HD12	16:6:80:ILE:HG21	1.88	0.54
11:1:290:MET:HE1	18:D:14:ILE:HD13	1.88	0.54
15:5:22:PHE:HA	15:5:25:GLN:OE1	2.07	0.54
15:5:594:ARG:HD3	47:5:703:3PE:H111	1.88	0.54
19:E:98:ASP:OD1	19:E:99:LEU:N	2.41	0.54
41:8:46:ALA:O	41:8:51:ARG:NH1	2.41	0.54
2:B:405:GLN:NE2	2:B:466:GLY:O	2.35	0.54
3:C:197:VAL:HG21	3:C:271:TRP:CZ3	2.40	0.54
3:C:371:ARG:NH2	6:I:182:ASP:OD1	2.34	0.54
9:S:134:ARG:HG3	9:S:156:ARG:HH11	1.72	0.54
19:E:220:SER:OG	51:E:402:CDL:OA4	2.17	0.54
21:J:93:ASP:HA	48:J:202:LMN:H6	1.90	0.54
6:I:213:LYS:HG2	6:I:214:TRP:CD1	2.43	0.54
11:1:216:PHE:HA	11:1:219:TYR:HD2	1.71	0.54
15:5:127:MET:SD	15:5:254:THR:OG1	2.53	0.54
37:f:70:VAL:HG12	37:f:71:SER:N	2.22	0.54
1:A:279:ARG:HD2	1:A:281:ILE:HD11	1.90	0.53
9:S:134:ARG:HG3	9:S:156:ARG:NH1	2.23	0.53
9:S:218:ARG:O	9:S:222:ILE:HD12	2.09	0.53
15:5:435:LEU:HA	15:5:439:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:89:ASN:O	30:Y:90:ARG:NH1	2.37	0.53
35:d:58:ASN:HB2	55:d:102:HOH:O	2.07	0.53
40:n:24:TRP:CE2	51:n:200:CDL:H122	2.43	0.53
15:5:19:PRO:HB2	15:5:118:SER:HB3	1.90	0.53
25:Q:76:THR:HG23	25:Q:79:ALA:HB2	1.91	0.53
34:c:21:PHE:HA	34:c:26:ARG:HG3	1.88	0.53
2:B:445:ARG:O	2:B:449:GLU:HG2	2.09	0.53
1:A:87:VAL:HG12	1:A:89:ARG:HG3	1.90	0.53
1:A:411:LEU:HB2	1:A:470:PHE:CE1	2.42	0.53
15:5:363:TYR:O	15:5:442:ASN:HB2	2.08	0.53
47:5:701:3PE:H3B1	51:n:200:CDL:H431	1.90	0.53
5:H:58:VAL:HG11	5:H:73:PRO:HB2	1.90	0.53
47:4:503:3PE:H2I1	47:4:503:3PE:H3H2	1.90	0.53
1:A:525:SER:HB2	1:A:528:ARG:HG2	1.89	0.53
8:L:1:FME:HG2	8:L:39:ILE:HG12	1.89	0.53
9:S:209:GLU:H	9:S:209:GLU:CD	2.16	0.53
12:2:191:ILE:HD12	42:9:41:PHE:CE1	2.44	0.53
15:5:98:MET:HE2	15:5:98:MET:HA	1.89	0.53
15:5:412:TYR:OH	15:5:510:TYR:OH	2.10	0.53
15:5:477:LYS:C	15:5:477:LYS:HD2	2.34	0.53
16:6:48:TYR:CZ	47:6:201:3PE:H232	2.44	0.53
1:A:429:ARG:HD2	1:A:449:THR:HB	1.91	0.53
2:B:439:GLY:HA2	2:B:442:ARG:NH1	2.23	0.53
6:I:117:GLU:HB2	6:I:192:TYR:CE1	2.44	0.53
28:W:18:GLN:HB2	31:Z:7:VAL:HG13	1.89	0.53
28:W:28:PHE:CZ	51:W:402:CDL:H512	2.44	0.53
4:G:136:ASN:HA	4:G:160:THR:HG22	1.90	0.53
12:2:26:ARG:CZ	29:X:63:VAL:HG22	2.39	0.53
15:5:7:LEU:HA	15:5:10:ILE:HG22	1.90	0.53
29:X:58:GLU:OE2	29:X:63:VAL:HG23	2.09	0.53
3:C:98:LEU:HB2	3:C:461:PHE:CZ	2.44	0.53
14:4:441:HIS:CD2	26:R:102:MET:HE3	2.44	0.53
6:I:152:ARG:HD2	6:I:154:ASP:OD1	2.08	0.53
16:6:146:LEU:HD11	42:9:8:LEU:HD22	1.91	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.74	0.52
15:5:165:LYS:NZ	47:5:702:3PE:O14	2.42	0.52
15:5:458:ILE:O	15:5:462:MET:HG3	2.09	0.52
38:h:46:TYR:CE1	38:h:62:GLU:HG3	2.44	0.52
15:5:16:TRP:CE2	15:5:122:MET:HG3	2.45	0.52
16:6:106:ILE:HG23	16:6:122:LEU:HD13	1.90	0.52
1:A:496:ALA:H	1:A:683:VAL:HG11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:HG	2:B:100:PHE:CZ	2.44	0.52
2:B:432:ALA:O	2:B:436:PRO:HD3	2.10	0.52
5:H:234:ASN:OD1	5:H:235:VAL:N	2.42	0.52
15:5:116:PHE:O	15:5:120:LEU:HD23	2.09	0.52
25:Q:87:LEU:HD12	25:Q:91:ASP:HB3	1.92	0.52
1:A:408:ASP:OD2	1:A:477:ALA:HB1	2.09	0.52
3:C:185:ASN:OD1	3:C:407:LYS:NZ	2.42	0.52
15:5:388:PRO:HB3	36:e:49:MET:HE3	1.92	0.52
10:j:23:PRO:HB2	26:R:102:MET:SD	2.49	0.52
11:1:319:LEU:HD22	17:g:29:ALA:HB2	1.91	0.52
12:2:234:ILE:HD11	12:2:321:LEU:HD23	1.90	0.52
14:4:127:LEU:HD21	47:4:503:3PE:H3B2	1.90	0.52
15:5:375:ILE:HD13	34:c:32:PRO:HG2	1.91	0.52
16:6:54:ILE:HD13	16:6:147:LEU:HB2	1.91	0.52
20:F:117:MET:HE3	20:F:117:MET:HA	1.89	0.52
26:R:6:PRO:HB3	26:R:54:SER:HA	1.92	0.52
34:c:19:THR:HG23	34:c:20:ASN:N	2.25	0.52
3:C:45:ASP:HA	12:2:336:TYR:CE2	2.44	0.52
11:1:303:PHE:HZ	47:1:501:3PE:H242	1.73	0.52
51:g:201:CDL:H231	29:X:83:PHE:HE2	1.74	0.52
41:8:63:GLN:O	41:8:66:VAL:HG12	2.10	0.52
1:A:252:LEU:HD13	1:A:271:ASP:HB3	1.92	0.52
11:1:243:GLY:HA2	11:1:247:LEU:HB2	1.92	0.52
15:5:3:ASN:HD21	15:5:5:ILE:HG22	1.75	0.52
19:E:330:PHE:HD2	19:E:337:PRO:HG3	1.75	0.52
25:Q:93:VAL:O	25:Q:97:MET:HG3	2.09	0.52
30:Y:133:GLU:OE1	30:Y:134:PRO:HD2	2.09	0.52
20:F:54:LEU:HD12	20:F:79:LYS:NZ	2.24	0.52
1:A:245:PHE:CG	6:I:157:ARG:HG3	2.44	0.52
5:H:54:ARG:O	5:H:58:VAL:HG23	2.10	0.52
47:1:504:3PE:H332	47:1:504:3PE:H251	1.92	0.52
13:3:49:ARG:HE	16:6:79:ASP:HA	1.75	0.52
1:A:377:ASP:OD2	1:A:557:GLU:HB2	2.09	0.52
1:A:387:HIS:CE1	1:A:395:TYR:HB3	2.45	0.52
11:1:117:VAL:HG12	11:1:143:LEU:HB3	1.92	0.52
21:J:39:ALA:HB2	47:J:203:3PE:H392	1.92	0.52
6:I:88:TYR:HD2	31:Z:30:ILE:HG12	1.75	0.51
19:E:61:ALA:HB3	19:E:82:VAL:HG13	1.91	0.51
3:C:248:TYR:CE1	28:W:14:TYR:HB3	2.45	0.51
11:1:133:LEU:HD22	16:6:76:THR:HG23	1.91	0.51
12:2:119:HIS:CE1	29:X:152:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:40:ILE:HD13	15:5:97:SER:HB2	1.92	0.51
15:5:335:HIS:HA	15:5:338:PHE:CZ	2.45	0.51
17:g:19:SER:OG	47:g:202:3PE:H222	2.10	0.51
1:A:315:ARG:NH2	1:A:583:ALA:O	2.42	0.51
5:H:66:TYR:HH	30:Y:151:SER:H	1.58	0.51
8:L:49:ASP:OD2	12:2:176:TYR:OH	2.27	0.51
9:S:66:LEU:HD11	9:S:94:ILE:HD12	1.91	0.51
10:j:47:LYS:HB2	32:a:36:MET:HE1	1.92	0.51
21:J:66:GLY:O	21:J:69:THR:OG1	2.24	0.51
21:J:143:ARG:HH21	21:J:143:ARG:HB3	1.73	0.51
23:O:82:ILE:HD12	23:O:82:ILE:O	2.10	0.51
23:O:86:ASP:N	23:O:86:ASP:OD1	2.44	0.51
28:W:29:ARG:HG3	28:W:32:VAL:HG23	1.93	0.51
6:I:70:ALA:HB2	17:g:21:HIS:CD2	2.45	0.51
10:j:49:THR:HB	48:j:101:LMN:H5	1.92	0.51
12:2:124:ILE:HD13	16:6:161:ILE:HG13	1.92	0.51
19:E:228:LYS:HG3	19:E:288:GLU:OE2	2.11	0.51
38:h:52:ASP:OD2	55:h:201:HOH:O	2.19	0.51
1:A:398:ASN:ND2	1:A:519:TYR:O	2.42	0.51
2:B:71:GLY:O	2:B:75:ILE:HD12	2.11	0.51
14:4:15:ASN:HD22	14:4:16:ARG:HE	1.59	0.51
15:5:58:ASN:HB3	39:i:54:ARG:NH1	2.23	0.51
9:S:207:HIS:CE1	9:S:225:ARG:HE	2.29	0.51
14:4:159:ASP:OD1	55:4:604:HOH:O	2.18	0.51
14:4:408:ILE:O	14:4:412:ILE:HG13	2.10	0.51
16:6:2:MET:HA	16:6:5:THR:HG22	1.91	0.51
25:Q:97:MET:O	25:Q:100:GLU:HG2	2.10	0.51
12:2:256:ASN:O	49:2:503:T7X:O6	2.29	0.51
47:5:701:3PE:H111	47:5:701:3PE:H11	1.93	0.51
2:B:461:ALA:O	2:B:468:MET:HG2	2.11	0.51
15:5:598:LYS:HZ2	47:5:703:3PE:H12	1.76	0.51
40:n:28:SER:O	40:n:32:VAL:HG23	2.11	0.51
3:C:445:HIS:HB3	3:C:449:ASP:HB2	1.92	0.51
14:4:134:TYR:H	14:4:192:THR:HG23	1.76	0.51
31:Z:44:TYR:OH	55:Z:302:HOH:O	2.19	0.51
32:a:98:ILE:O	32:a:102:THR:OG1	2.25	0.51
5:H:102:MET:HE3	5:H:105:TYR:HB2	1.93	0.50
12:2:187:LEU:HD13	12:2:192:ILE:HD11	1.93	0.50
14:4:55:PHE:HB3	47:4:503:3PE:O22	2.11	0.50
15:5:372:TYR:HB3	15:5:453:GLU:OE1	2.12	0.50
1:A:699:MET:HG2	1:A:705:ARG:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:GLU:OE2	11:1:138:ARG:NH2	2.41	0.50
15:5:639:PHE:O	15:5:642:VAL:HG12	2.12	0.50
20:F:108:HIS:O	20:F:112:GLU:HG3	2.11	0.50
7:K:174:ASP:OD2	55:K:401:HOH:O	2.19	0.50
13:3:94:PHE:CD1	16:6:166:ALA:HB2	2.47	0.50
18:D:82:SER:OG	28:W:119:MET:SD	2.66	0.50
7:K:122:THR:HA	7:K:150:CYS:HB3	1.93	0.50
15:5:292:GLY:HA3	15:5:424:LEU:HD23	1.93	0.50
14:4:344:LEU:HD23	14:4:454:MET:HG3	1.93	0.50
15:5:372:TYR:CE2	15:5:459:THR:HG23	2.47	0.50
47:5:703:3PE:H3I2	21:J:132:PHE:CD2	2.46	0.50
2:B:61:TRP:CZ3	2:B:142:GLU:HG3	2.47	0.50
2:B:290:VAL:HG22	2:B:291:GLU:H	1.77	0.50
2:B:400:ARG:HH22	2:B:410:GLU:CD	2.20	0.50
1:A:499:ASN:O	1:A:503:LYS:HG2	2.12	0.50
2:B:299:ARG:HD2	2:B:313:TRP:CE3	2.47	0.50
3:C:453:ILE:O	3:C:456:THR:HG22	2.12	0.50
4:G:84:LYS:HA	20:F:126:LEU:HA	1.93	0.50
17:g:34:ILE:HD11	47:g:202:3PE:H2F2	1.93	0.50
1:A:475:LYS:HD3	1:A:508:THR:HG23	1.94	0.50
2:B:400:ARG:HG2	2:B:484:PRO:HG2	1.94	0.50
2:B:401:PHE:CE2	2:B:414:LEU:HD22	2.46	0.50
3:C:332:ARG:HH21	3:C:456:THR:HG21	1.77	0.50
8:L:64:GLY:HA3	13:3:68:LEU:HD11	1.93	0.50
26:R:17:SER:O	26:R:21:GLN:HG3	2.12	0.50
1:A:620:ARG:HH22	19:E:30:ASP:CG	2.20	0.50
2:B:128:LYS:O	2:B:132:ILE:HG13	2.12	0.50
9:S:127:LYS:HE2	26:R:107:TYR:CE1	2.47	0.50
11:1:332:TYR:CZ	51:X:201:CDL:H122	2.47	0.50
21:J:30:THR:O	21:J:34:MET:HG3	2.12	0.50
12:2:210:PHE:CG	12:2:217:LEU:HD12	2.47	0.49
25:Q:85:LEU:HB3	25:Q:87:LEU:HD23	1.94	0.49
14:4:418:LEU:O	14:4:422:ILE:HG13	2.12	0.49
16:6:146:LEU:O	16:6:150:ILE:HD12	2.13	0.49
27:U:116:ALA:HB1	27:U:172:LEU:HD11	1.93	0.49
16:6:40:PHE:CZ	16:6:63:TYR:CD2	3.00	0.49
19:E:233:SER:HA	19:E:321:GLN:HB2	1.95	0.49
48:J:202:LMN:HCS	48:J:202:LMN:CBP	2.37	0.49
27:U:45:LYS:NZ	27:U:81:SER:OG	2.30	0.49
27:U:70:LYS:HD3	27:U:74:ARG:HH11	1.77	0.49
9:S:171:LEU:HG	14:4:33:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:95:PRO:HD3	21:J:57:ILE:HG13	1.94	0.49
1:A:37:ILE:HD11	1:A:101:VAL:HG23	1.94	0.49
2:B:140:LEU:HD23	2:B:171:LEU:HD11	1.93	0.49
7:K:112:ARG:NH2	13:3:36:GLY:O	2.46	0.49
12:2:266:LEU:HD22	47:J:203:3PE:H2A1	1.94	0.49
13:3:122:ASP:O	20:F:26:ARG:HD2	2.13	0.49
15:5:197:TYR:HB3	15:5:201:PHE:CE2	2.48	0.49
2:B:39:ARG:HH12	5:H:226:VAL:HB	1.77	0.49
2:B:122:GLY:H	2:B:161:ARG:NH2	2.11	0.49
9:S:195:ALA:HB1	35:d:36:ILE:HD13	1.94	0.49
19:E:155:VAL:HG13	19:E:160:ILE:HB	1.95	0.49
20:F:50:TYR:CB	20:F:79:LYS:HE3	2.42	0.49
1:A:141:GLU:OE2	1:A:249:PRO:HB3	2.12	0.49
2:B:275:THR:HG22	2:B:293:GLU:HA	1.95	0.49
8:L:6:ILE:HG21	16:6:17:ILE:HG12	1.93	0.49
13:3:26:ALA:O	49:3:201:T7X:O2	2.30	0.49
18:D:2:ALA:N	51:Z:201:CDL:HB31	2.27	0.49
32:a:128:GLU:HB2	32:a:131:TRP:CD1	2.47	0.49
1:A:654:PRO:HB3	37:f:50:VAL:HG11	1.94	0.49
4:G:264:ASP:OD1	4:G:267:LYS:NZ	2.46	0.49
6:I:194:THR:HG22	55:h:208:HOH:O	2.12	0.49
12:2:400:ILE:HD12	21:J:131:LEU:HD11	1.95	0.49
14:4:354:TYR:CE1	14:4:440:MET:HB2	2.47	0.49
16:6:98:LEU:O	16:6:102:ILE:HG12	2.13	0.49
32:a:62:ASP:HA	32:a:79:MET:HG3	1.95	0.49
3:C:305:ILE:HB	3:C:404:GLU:HB2	1.94	0.49
11:1:149:ILE:HG23	11:1:320:LEU:HD11	1.94	0.49
25:Q:102:GLU:OE1	34:c:12:ARG:NH2	2.45	0.49
31:Z:78:ASP:OD2	31:Z:81:ARG:NH2	2.44	0.49
1:A:712:LYS:O	1:A:715:ILE:HG13	2.13	0.49
5:H:58:VAL:O	5:H:61:LYS:HG3	2.12	0.49
15:5:16:TRP:CD1	15:5:122:MET:HB2	2.48	0.49
15:5:454:SER:HB3	15:5:458:ILE:HD12	1.94	0.49
16:6:118:LEU:HD13	16:6:121:LYS:HD2	1.95	0.49
2:B:101:MET:HE2	2:B:151:MET:HB3	1.94	0.48
3:C:348:GLU:OE2	28:W:16:PRO:HA	2.13	0.48
9:S:141:PRO:HB3	9:S:152:TRP:CH2	2.48	0.48
14:4:459:ILE:HG21	51:n:200:CDL:H551	1.95	0.48
23:O:68:ASP:OD1	24:P:57:ARG:NH2	2.46	0.48
2:B:249:THR:HG21	45:B:502:FMN:O3P	2.12	0.48
13:3:112:LYS:HD3	13:3:112:LYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:4:231:LEU:HG	14:4:235:HIS:CD2	2.47	0.48
15:5:102:TYR:CE1	15:5:458:ILE:HG23	2.47	0.48
17:g:61:SER:HB3	40:n:111:ILE:O	2.13	0.48
26:R:90:TYR:CD2	26:R:91:GLU:HG3	2.47	0.48
2:B:128:LYS:HE3	2:B:353:THR:HB	1.96	0.48
5:H:121:ARG:HB3	5:H:122:TYR:CD1	2.48	0.48
11:1:107:LEU:HB3	16:6:57:LEU:HD13	1.94	0.48
14:4:207:GLN:HB3	14:4:269:ALA:HB2	1.94	0.48
15:5:58:ASN:O	39:i:54:ARG:NH1	2.45	0.48
20:F:50:TYR:HB3	20:F:79:LYS:HE3	1.95	0.48
32:a:108:SER:O	32:a:112:THR:HG23	2.13	0.48
1:A:152:GLY:O	3:C:365:LYS:NZ	2.47	0.48
2:B:298:LEU:O	2:B:302:LEU:HG	2.14	0.48
2:B:472:ARG:HD2	22:M:102:HIS:CE1	2.48	0.48
4:G:128:ALA:HB3	4:G:186:TYR:CD2	2.47	0.48
47:6:202:3PE:H3I3	47:6:202:3PE:H3F1	1.65	0.48
19:E:269:GLN:O	19:E:273:ILE:HG13	2.13	0.48
37:f:7:GLU:HB3	37:f:57:ARG:HB3	1.95	0.48
37:f:26:VAL:HG22	37:f:30:ILE:HD13	1.96	0.48
2:B:62:TYR:CD2	2:B:63:LYS:HG2	2.49	0.48
5:H:52:MET:O	5:H:55:ALA:N	2.46	0.48
5:H:124:LEU:HD12	5:H:178:MET:HE2	1.95	0.48
11:1:125:TRP:CD1	16:6:30:MET:SD	3.07	0.48
15:5:499:TYR:O	15:5:503:GLU:HG3	2.12	0.48
26:R:25:LEU:HD11	26:R:74:ARG:HA	1.95	0.48
33:b:19:PHE:CD2	47:b:201:3PE:H351	2.48	0.48
1:A:122:MET:HE2	1:A:148:SER:HA	1.95	0.48
2:B:92:PHE:CD2	2:B:93:PRO:HD2	2.48	0.48
7:K:73:GLN:CD	46:K:302:PLC:H51	2.39	0.48
25:Q:115:ILE:HG13	25:Q:115:ILE:O	2.12	0.48
37:f:4:ALA:N	37:f:8:ILE:HD11	2.28	0.48
38:h:113:THR:HG22	38:h:115:GLY:H	1.77	0.48
38:h:115:GLY:O	55:h:202:HOH:O	2.20	0.48
2:B:264:PHE:CZ	2:B:274:GLY:HA3	2.48	0.48
2:B:270:GLU:OE1	2:B:271:ARG:NE	2.46	0.48
3:C:447:LEU:HB3	3:C:448:PRO:HD3	1.96	0.48
8:L:55:PHE:O	8:L:59:ILE:HG12	2.14	0.48
9:S:190:ASP:OD1	9:S:191:ILE:N	2.47	0.48
11:1:134:LEU:HD22	13:3:50:LEU:HD22	1.95	0.48
12:2:148:TYR:CZ	19:E:368:LYS:HD3	2.48	0.48
15:5:505:SER:O	36:e:56:TYR:OH	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:303:ALA:HB3	51:E:402:CDL:H181	1.95	0.48
20:F:41:ASN:OD1	20:F:44:PRO:HG2	2.13	0.48
21:J:43:ALA:HB2	47:J:203:3PE:H332	1.95	0.48
26:R:39:LYS:HD2	26:R:43:ILE:HD11	1.96	0.48
35:d:65:ASN:HB3	39:i:71:ALA:HB3	1.96	0.48
2:B:127:CYS:SG	5:H:173:VAL:HG23	2.54	0.48
6:I:220:TYR:OH	38:h:92:THR:HG21	2.13	0.48
10:j:17:LYS:HD3	14:4:109:PHE:CD2	2.49	0.48
29:X:36:ARG:HD2	29:X:97:ARG:CZ	2.43	0.48
32:a:136:GLY:HA2	32:a:144:PHE:HD2	1.78	0.48
2:B:61:TRP:CE3	2:B:142:GLU:HG3	2.49	0.48
12:2:28:ILE:HD13	12:2:28:ILE:HA	1.73	0.48
14:4:138:TYR:O	14:4:142:GLU:HG2	2.13	0.48
21:J:31:GLN:O	21:J:35:VAL:HG23	2.14	0.48
31:Z:95:THR:O	31:Z:99:GLU:HG2	2.13	0.48
37:f:68:LEU:C	37:f:70:VAL:HG23	2.38	0.48
8:L:55:PHE:CD1	12:2:124:ILE:HG22	2.49	0.48
10:j:80:PHE:HB2	15:5:190:TYR:CE2	2.49	0.48
15:5:378:THR:O	15:5:382:LEU:HG	2.14	0.48
1:A:153:ARG:NH2	1:A:157:ARG:HG3	2.29	0.47
3:C:77:ASN:HA	19:E:370:PHE:O	2.14	0.47
7:K:61:LEU:HD22	7:K:204:THR:HB	1.96	0.47
9:S:137:LEU:HB2	9:S:139:LYS:HG2	1.94	0.47
25:Q:81:LEU:HD23	25:Q:85:LEU:HD23	1.96	0.47
32:a:94:LEU:O	32:a:98:ILE:HG12	2.14	0.47
15:5:2:TYR:OH	15:5:45:ILE:HG12	2.14	0.47
15:5:542:TYR:O	15:5:546:VAL:HG12	2.14	0.47
19:E:186:GLY:O	19:E:190:THR:OG1	2.25	0.47
19:E:194:VAL:HG23	19:E:194:VAL:O	2.15	0.47
30:Y:43:GLU:HG3	30:Y:125:GLN:C	2.39	0.47
35:d:83:LEU:O	35:d:87:ARG:HG3	2.14	0.47
37:f:80:VAL:O	37:f:84:ILE:HG12	2.13	0.47
3:C:49:GLN:HB2	3:C:71:ILE:HD11	1.95	0.47
10:j:47:LYS:N	32:a:36:MET:HE2	2.29	0.47
23:O:88:GLU:OE1	23:O:101:TYR:OH	2.22	0.47
51:X:201:CDL:H542	51:X:201:CDL:H571	1.38	0.47
2:B:290:VAL:HG22	2:B:291:GLU:N	2.29	0.47
15:5:301:LEU:O	15:5:305:ILE:HG12	2.15	0.47
51:g:201:CDL:H412	29:X:80:MET:HG2	1.96	0.47
34:c:34:PHE:O	34:c:38:VAL:HG13	2.14	0.47
2:B:44:LEU:HG	2:B:291:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:37:GLU:HA	4:G:37:GLU:OE1	2.14	0.47
9:S:186:LYS:O	9:S:189:GLU:HG2	2.15	0.47
46:1:502:PLC:H42	46:1:502:PLC:H72	1.67	0.47
12:2:241:LYS:HE2	12:2:293:ALA:HB2	1.96	0.47
14:4:235:HIS:CE1	14:4:247:ALA:HB2	2.49	0.47
15:5:76:ASN:N	55:5:803:HOH:O	2.43	0.47
16:6:131:ASN:O	28:W:118:LEU:HA	2.14	0.47
54:Q:201:ZMP:H4	26:R:22:SER:HB3	1.96	0.47
51:X:201:CDL:H672	51:X:201:CDL:H641	1.69	0.47
12:2:385:ASN:ND2	55:2:609:HOH:O	2.43	0.47
15:5:224:MET:HG2	15:5:229:GLN:HB2	1.97	0.47
15:5:256:VAL:HB	15:5:313:LEU:HD11	1.96	0.47
51:g:201:CDL:H792	51:X:201:CDL:H241	1.96	0.47
19:E:291:LYS:HG3	19:E:318:PHE:HE2	1.80	0.47
2:B:85:ARG:NH1	2:B:271:ARG:O	2.36	0.47
14:4:205:ASP:HB3	21:J:163:PHE:HE1	1.79	0.47
15:5:554:LEU:C	15:5:556:SER:N	2.72	0.47
16:6:54:ILE:CD1	16:6:147:LEU:HB2	2.45	0.47
24:P:74:VAL:HG11	30:Y:45:VAL:CG2	2.44	0.47
1:A:45:LYS:HD2	1:A:45:LYS:HA	1.57	0.47
1:A:87:VAL:HG11	1:A:105:MET:HE2	1.96	0.47
2:B:411:ILE:HG12	2:B:448:MET:HE2	1.95	0.47
3:C:429:ALA:HB1	3:C:463:GLU:HG2	1.97	0.47
5:H:68:LYS:HB2	5:H:99:MET:HE3	1.96	0.47
2:B:39:ARG:HH22	5:H:226:VAL:HG11	1.80	0.47
9:S:137:LEU:CB	9:S:139:LYS:HG2	2.45	0.47
13:3:28:TYR:CD2	51:E:402:CDL:H512	2.50	0.47
14:4:369:MET:HE3	14:4:372:LEU:HD23	1.97	0.47
20:F:78:ARG:HG2	20:F:95:ILE:HD12	1.96	0.47
54:Q:201:ZMP:H14	26:R:59:LEU:HD11	1.96	0.47
31:Z:92:LYS:NZ	31:Z:122:ALA:O	2.36	0.47
1:A:627:ARG:HH21	1:A:640:GLU:HG2	1.80	0.47
2:B:374:ALA:HA	2:B:395:LEU:HD22	1.96	0.47
3:C:82:ALA:HB2	3:C:110:ILE:HD11	1.96	0.47
5:H:163:LEU:HD12	5:H:164:SER:H	1.79	0.47
9:S:62:ARG:HG2	9:S:94:ILE:HD11	1.96	0.47
10:j:67:ILE:HD13	14:4:282:LEU:HD23	1.96	0.47
11:1:182:LEU:HB3	11:1:185:LEU:HD12	1.97	0.47
25:Q:102:GLU:HB2	34:c:12:ARG:NH2	2.30	0.47
26:R:33:ARG:HE	34:c:16:ARG:NE	2.13	0.47
41:8:71:LYS:O	41:8:75:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:NZ	5:H:242:GLY:O	2.48	0.46
5:H:212:ASN:O	5:H:214:VAL:N	2.49	0.46
7:K:140:GLU:HG2	55:K:427:HOH:O	2.14	0.46
13:3:55:ALA:O	13:3:59:VAL:HG22	2.14	0.46
19:E:237:HIS:NE2	19:E:239:ILE:HG12	2.30	0.46
23:O:99:VAL:O	23:O:102:ILE:HG22	2.14	0.46
30:Y:116:GLU:H	30:Y:116:GLU:CD	2.23	0.46
1:A:590:ALA:HB3	1:A:595:LYS:HD3	1.96	0.46
13:3:2:ASN:OD1	13:3:5:ILE:HG22	2.15	0.46
14:4:320:ASN:O	55:4:605:HOH:O	2.20	0.46
15:5:319:ALA:HB3	15:5:328:ALA:HB2	1.97	0.46
21:J:20:PHE:CE1	21:J:90:GLU:HA	2.50	0.46
1:A:72:ASP:O	30:Y:142:LYS:HE2	2.15	0.46
1:A:99:TYR:CE2	1:A:105:MET:HE1	2.49	0.46
1:A:224:GLU:CD	1:A:224:GLU:H	2.22	0.46
1:A:226:SER:O	1:A:229:VAL:HG22	2.15	0.46
2:B:272:ASN:N	2:B:272:ASN:ND2	2.63	0.46
8:L:11:SER:HB3	8:L:32:MET:HG3	1.97	0.46
12:2:262:ILE:HG23	47:J:203:3PE:H2E1	1.96	0.46
15:5:50:PHE:CZ	15:5:54:LEU:HD11	2.49	0.46
24:P:74:VAL:HG11	30:Y:45:VAL:HG23	1.96	0.46
32:a:135:GLY:N	35:d:60:PHE:HB3	2.29	0.46
9:S:117:ARG:HG3	9:S:120:ARG:HH11	1.80	0.46
15:5:324:ALA:HB1	15:5:327:LEU:HD23	1.98	0.46
19:E:346:LYS:HB2	24:P:46:GLN:HG2	1.97	0.46
26:R:71:TYR:O	26:R:74:ARG:HD3	2.16	0.46
37:f:11:HIS:HB2	37:f:53:ILE:HG22	1.97	0.46
51:n:200:CDL:H422	51:n:200:CDL:H452	1.68	0.46
5:H:123:HIS:N	5:H:181:ASN:OD1	2.46	0.46
11:1:3:ILE:HG23	18:D:28:LEU:HD22	1.97	0.46
14:4:123:LEU:HB3	47:4:503:3PE:H2E2	1.97	0.46
47:4:501:3PE:H321	47:4:501:3PE:H352	1.71	0.46
16:6:134:ILE:HB	18:D:81:LYS:HB2	1.96	0.46
16:6:141:ILE:HD12	28:W:63:LEU:HD22	1.97	0.46
1:A:372:GLU:OE2	37:f:57:ARG:NH1	2.48	0.46
6:I:125:SER:HB3	22:M:85:GLN:NE2	2.30	0.46
15:5:276:VAL:HA	15:5:279:ILE:HD12	1.98	0.46
15:5:385:MET:HG2	15:5:426:CYS:SG	2.56	0.46
16:6:15:LEU:HB3	16:6:42:ILE:HD13	1.98	0.46
32:a:89:LYS:HB2	32:a:92:ASP:OD2	2.16	0.46
42:9:25:CYS:O	42:9:28:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:VAL:HG13	1:A:676:LEU:HD12	1.97	0.46
2:B:453:LYS:HE3	2:B:453:LYS:HB3	1.75	0.46
2:B:477:LYS:HD3	2:B:477:LYS:N	2.31	0.46
4:G:137:ARG:NH2	4:G:213:ASP:OD1	2.43	0.46
11:1:125:TRP:HZ2	16:6:28:ASN:ND2	2.10	0.46
12:2:9:LEU:HD22	12:2:9:LEU:HA	1.76	0.46
17:g:41:LEU:HG	51:X:201:CDL:H152	1.98	0.46
48:J:202:LMN:HBI	48:J:202:LMN:HBC	1.49	0.46
26:R:5:VAL:HG12	26:R:7:PHE:H	1.81	0.46
12:2:234:ILE:HD13	12:2:324:PHE:HB2	1.97	0.46
14:4:235:HIS:HE1	14:4:247:ALA:HB2	1.80	0.46
15:5:372:TYR:O	15:5:375:ILE:HG22	2.16	0.46
19:E:332:ASP:OD1	19:E:332:ASP:N	2.48	0.46
29:X:38:SER:OG	29:X:93:ARG:NH2	2.49	0.46
37:f:12:LEU:O	37:f:46:GLU:HA	2.15	0.46
39:i:15:MET:HE1	40:n:20:TYR:CE1	2.51	0.46
40:n:113:LYS:HB2	40:n:113:LYS:HE3	1.69	0.46
7:K:199:ARG:NH2	46:K:302:PLC:H73	2.31	0.46
15:5:271:GLU:OE2	15:5:493:LEU:N	2.45	0.46
15:5:540:ASN:HB2	15:5:543:ILE:HD12	1.98	0.46
19:E:228:LYS:HB2	19:E:230:GLN:HG2	1.98	0.46
32:a:27:ALA:HB3	32:a:30:ASP:OD2	2.16	0.46
37:f:53:ILE:HD12	37:f:66:ILE:C	2.41	0.46
1:A:92:LYS:HA	1:A:113:ARG:HH12	1.80	0.45
4:G:47:LYS:O	4:G:49:HIS:NE2	2.49	0.45
7:K:133:GLN:HG3	7:K:137:GLN:OE1	2.16	0.45
41:8:13:MET:HG3	41:8:18:ILE:HD12	1.98	0.45
1:A:401:ILE:N	1:A:603:GLU:OE2	2.42	0.45
4:G:272:LYS:HB3	4:G:272:LYS:HE3	1.55	0.45
26:R:13:LYS:HE3	26:R:13:LYS:HB2	1.70	0.45
28:W:27:GLY:HA2	51:W:402:CDL:HA61	1.96	0.45
30:Y:91:TRP:CE2	30:Y:100:SER:HB2	2.51	0.45
2:B:468:MET:HE3	2:B:468:MET:HB2	1.65	0.45
14:4:153:HIS:NE2	14:4:161:GLU:HG3	2.32	0.45
19:E:149:ARG:HG2	19:E:193:ILE:HD11	1.97	0.45
19:E:224:VAL:HA	19:E:287:ILE:O	2.17	0.45
31:Z:128:PHE:O	31:Z:131:ALA:HB3	2.15	0.45
35:d:92:LYS:HG3	55:d:101:HOH:O	2.17	0.45
51:n:200:CDL:H772	51:n:200:CDL:H741	1.51	0.45
6:I:43:ALA:O	20:F:78:ARG:NH1	2.50	0.45
9:S:63:LEU:HD13	9:S:125:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:33:GLU:OE1	19:E:208:ARG:NH1	2.48	0.45
19:E:156:LYS:HB2	19:E:194:VAL:HG12	1.97	0.45
1:A:155:ARG:HE	1:A:155:ARG:HB3	1.65	0.45
2:B:61:TRP:CZ3	2:B:183:LEU:HB3	2.52	0.45
2:B:137:PRO:O	2:B:141:VAL:HG23	2.17	0.45
3:C:179:GLU:OE2	3:C:343:SER:OG	2.26	0.45
14:4:7:LEU:O	14:4:11:LEU:HD23	2.17	0.45
14:4:58:GLU:HB3	14:4:69:SER:HB3	1.99	0.45
15:5:383:SER:O	15:5:392:GLY:HA3	2.16	0.45
18:D:77:ASN:HA	27:U:13:GLU:OE1	2.17	0.45
29:X:158:PHE:CD2	51:X:201:CDL:H532	2.51	0.45
31:Z:146:THR:HG23	31:Z:150:LEU:O	2.17	0.45
37:f:44:VAL:O	37:f:45:ARG:HD2	2.16	0.45
1:A:130:PRO:HG3	1:A:181:ASN:HB3	1.98	0.45
1:A:267:ASN:N	1:A:267:ASN:HD22	2.15	0.45
2:B:468:MET:HE1	2:B:482:PRO:HD2	1.98	0.45
4:G:83:PRO:O	20:F:126:LEU:HB3	2.16	0.45
7:K:78:PRO:HB2	7:K:107:PHE:CE1	2.52	0.45
11:1:4:ASN:OD1	18:D:32:ARG:NH2	2.45	0.45
15:5:35:THR:O	15:5:39:ILE:HG12	2.17	0.45
15:5:500:PHE:HD2	32:a:123:ARG:HH22	1.64	0.45
31:Z:17:SER:OG	31:Z:22:GLU:OE2	2.30	0.45
39:i:38:VAL:O	39:i:42:LEU:HD13	2.17	0.45
1:A:523:GLN:H	1:A:602:THR:HG22	1.82	0.45
3:C:307:LYS:HD3	3:C:319:PHE:CZ	2.52	0.45
15:5:65:PHE:HB3	46:5:704:PLC:H32	1.99	0.45
20:F:121:LYS:HD3	20:F:123:TRP:CZ2	2.51	0.45
27:U:50:ASN:HB3	28:W:71:PRO:HG2	1.98	0.45
1:A:412:LEU:HB2	1:A:441:SER:HB2	1.99	0.45
2:B:87:ARG:HG3	2:B:248:GLU:CD	2.42	0.45
2:B:164:PHE:HB3	2:B:167:GLU:HB2	1.99	0.45
3:C:103:GLU:O	3:C:110:ILE:HG12	2.17	0.45
7:K:189:TYR:O	7:K:193:GLN:HG2	2.17	0.45
16:6:91:ILE:HD12	16:6:91:ILE:HA	1.84	0.45
19:E:228:LYS:HA	19:E:288:GLU:CD	2.41	0.45
27:U:14:ASP:C	27:U:15:LYS:HE2	2.42	0.45
29:X:129:SER:HB2	29:X:160:ASN:O	2.15	0.45
3:C:440:HIS:HD1	24:P:2:ALA:N	2.14	0.45
4:G:48:VAL:HG12	28:W:11:VAL:HA	1.98	0.45
4:G:260:ASP:HB3	31:Z:85:GLN:OE1	2.16	0.45
7:K:93:VAL:HG21	7:K:187:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:8:ILE:HD11	13:3:3:THR:O	2.17	0.45
11:1:73:LEU:O	11:1:219:TYR:HE1	2.00	0.45
16:6:48:TYR:OH	47:6:201:3PE:H232	2.16	0.45
27:U:68:CYS:HA	27:U:71:GLU:OE2	2.16	0.45
34:c:19:THR:O	34:c:25:ASN:ND2	2.48	0.45
2:B:298:LEU:HD13	2:B:339:MET:SD	2.57	0.45
4:G:97:THR:HG21	4:G:156:LYS:HE3	1.99	0.45
11:1:107:LEU:HD12	11:1:107:LEU:HA	1.80	0.45
12:2:126:LEU:HG	12:2:130:ILE:HD12	1.99	0.45
15:5:633:LEU:O	15:5:637:VAL:HG23	2.17	0.45
48:J:202:LMN:HBLA	48:J:202:LMN:HBSA	1.66	0.45
26:R:77:ASP:OD1	26:R:77:ASP:N	2.50	0.45
11:1:152:SER:HB2	11:1:320:LEU:HD13	1.99	0.44
12:2:131:GLU:OE1	12:2:131:GLU:HA	2.17	0.44
14:4:432:THR:OG1	55:4:603:HOH:O	2.17	0.44
15:5:25:GLN:NE2	40:n:18:GLN:HG2	2.30	0.44
15:5:354:LEU:HD23	15:5:447:THR:HA	1.98	0.44
15:5:477:LYS:HD2	15:5:478:ASP:N	2.32	0.44
2:B:359:ILE:HG12	5:H:134:LEU:HD11	1.99	0.44
6:I:122:ARG:NH2	22:M:76:TYR:O	2.34	0.44
9:S:108:ILE:HG22	14:4:20:TRP:CD2	2.52	0.44
11:1:121:LEU:HD22	11:1:140:THR:HG21	1.99	0.44
12:2:234:ILE:HD12	12:2:320:HIS:NE2	2.32	0.44
12:2:375:PRO:HB2	14:4:139:ILE:HG23	1.98	0.44
14:4:25:LYS:HE3	14:4:104:TRP:CE2	2.52	0.44
14:4:112:ASN:HB3	47:4:501:3PE:H11	1.99	0.44
15:5:280:ILE:HG23	15:5:317:THR:HG23	1.98	0.44
27:U:133:PRO:HG2	28:W:64:TRP:CD2	2.52	0.44
32:a:137:THR:HG22	32:a:139:LYS:H	1.81	0.44
2:B:290:VAL:HG11	2:B:305:HIS:NE2	2.31	0.44
3:C:365:LYS:HE3	3:C:383:HIS:NE2	2.32	0.44
12:2:47:LEU:HD11	33:b:60:VAL:HG11	2.00	0.44
50:2:502:CPL:HC51	33:b:53:VAL:HG21	1.99	0.44
19:E:338:MET:HE2	19:E:343:LEU:HD11	1.99	0.44
23:O:77:GLU:HB2	23:O:82:ILE:O	2.17	0.44
51:X:201:CDL:H561	51:X:201:CDL:H591	1.89	0.44
2:B:113:ARG:HD3	2:B:152:ASN:O	2.17	0.44
2:B:163:GLU:OE1	2:B:163:GLU:N	2.48	0.44
2:B:400:ARG:NH2	2:B:410:GLU:OE2	2.51	0.44
4:G:228:LYS:HD3	24:P:104:ASP:OD1	2.18	0.44
12:2:20:ASP:HB3	29:X:74:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:134:SER:O	12:2:137:ILE:HG22	2.18	0.44
14:4:439:TYR:OH	32:a:64:ARG:NH1	2.50	0.44
15:5:107:MET:HE2	15:5:116:PHE:CD2	2.52	0.44
32:a:138:GLU:HA	32:a:141:LYS:HE2	1.99	0.44
3:C:71:ILE:HD12	3:C:71:ILE:C	2.42	0.44
8:L:10:LEU:HB3	16:6:20:THR:HG21	1.98	0.44
47:6:202:3PE:H3G2	47:6:202:3PE:H3D1	1.37	0.44
28:W:89:LEU:HD23	28:W:89:LEU:HA	1.84	0.44
38:h:113:THR:CG2	38:h:115:GLY:H	2.30	0.44
2:B:68:ILE:HD11	2:B:145:LEU:HD21	2.00	0.44
2:B:72:ASP:OD1	2:B:73:THR:N	2.51	0.44
2:B:78:GLU:OE2	2:B:257:LEU:HA	2.18	0.44
2:B:203:MET:O	5:H:111:TYR:HB3	2.18	0.44
2:B:235:VAL:HG13	2:B:239:GLY:HA2	1.99	0.44
2:B:369:ILE:HG13	2:B:440:LEU:HB2	2.00	0.44
3:C:50:ASP:CG	3:C:51:LEU:H	2.24	0.44
4:G:221:GLU:OE2	4:G:237:GLU:N	2.45	0.44
19:E:286:HIS:N	19:E:286:HIS:CD2	2.86	0.44
21:J:163:PHE:HB2	48:J:202:LMN:HCW	1.99	0.44
1:A:89:ARG:HH22	1:A:105:MET:HA	1.83	0.44
1:A:99:TYR:HE2	1:A:105:MET:CE	2.31	0.44
2:B:34:LEU:HB3	2:B:39:ARG:NE	2.25	0.44
2:B:61:TRP:HA	2:B:64:THR:OG1	2.18	0.44
47:S:501:3PE:N	47:b:201:3PE:H112	2.33	0.44
15:5:422:ALA:O	15:5:425:THR:HB	2.18	0.44
16:6:63:TYR:HA	16:6:67:ILE:HD12	1.99	0.44
18:D:8:LEU:HB3	51:Z:201:CDL:H201	1.99	0.44
19:E:335:LEU:HD12	19:E:335:LEU:HA	1.84	0.44
26:R:11:ASN:O	26:R:15:VAL:HG23	2.17	0.44
1:A:631:GLU:HA	1:A:636:ALA:HB2	1.99	0.44
2:B:224:LYS:HB2	30:Y:161:LYS:HE3	1.99	0.44
2:B:408:GLU:H	2:B:408:GLU:CD	2.25	0.44
3:C:34:SER:HB2	3:C:38:GLY:HA2	2.00	0.44
3:C:365:LYS:HG3	3:C:383:HIS:CD2	2.52	0.44
6:I:103:TYR:CD1	7:K:185:GLU:HG2	2.52	0.44
6:I:187:THR:HG22	6:I:218:LEU:HD21	2.00	0.44
11:1:76:SER:O	11:1:79:ILE:HG13	2.17	0.44
25:Q:103:PHE:HB2	25:Q:105:LEU:CD2	2.47	0.44
25:Q:109:ASP:OD1	25:Q:109:ASP:N	2.49	0.44
35:d:16:ASN:OD1	35:d:18:ASN:HB2	2.17	0.44
36:e:51:GLY:O	36:e:52:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:48:VAL:HG22	28:W:8:LEU:HB3	2.00	0.44
4:G:224:TRP:CZ3	7:K:132:ARG:HG2	2.53	0.44
47:1:501:3PE:H2A2	47:1:501:3PE:H272	1.27	0.44
12:2:152:LYS:HB3	12:2:152:LYS:HE3	1.75	0.44
19:E:167:SER:O	19:E:202:PRO:HD2	2.18	0.44
25:Q:76:THR:OG1	25:Q:79:ALA:N	2.50	0.44
31:Z:176:TYR:HA	55:Z:345:HOH:O	2.17	0.44
2:B:357:ILE:HD13	5:H:131:PRO:HG3	1.98	0.43
9:S:219:ASP:HA	9:S:222:ILE:HD12	2.00	0.43
35:d:64:LYS:NZ	35:d:68:GLU:OE1	2.51	0.43
2:B:114:TYR:CG	2:B:237:LEU:HD23	2.53	0.43
3:C:267:ASP:O	6:I:82:GLU:HG3	2.18	0.43
3:C:439:ASP:OD2	24:P:3:ILE:HA	2.17	0.43
4:G:85:TYR:O	55:G:302:HOH:O	2.21	0.43
5:H:225:LYS:HE3	5:H:225:LYS:HB3	1.80	0.43
9:S:141:PRO:HB3	9:S:152:TRP:CZ3	2.53	0.43
12:2:375:PRO:HB3	12:2:380:PHE:CD2	2.53	0.43
13:3:9:ILE:O	13:3:12:PRO:HD2	2.18	0.43
15:5:123:PHE:HE1	15:5:254:THR:OG1	2.01	0.43
19:E:163:TYR:CD2	19:E:194:VAL:HG21	2.49	0.43
20:F:62:PRO:O	20:F:68:ARG:HD3	2.17	0.43
23:O:88:GLU:O	23:O:92:ILE:HG13	2.18	0.43
30:Y:78:TRP:CZ3	30:Y:115:LYS:HG3	2.53	0.43
35:d:27:GLN:HG2	35:d:82:TYR:CD1	2.53	0.43
3:C:45:ASP:O	3:C:47:SER:N	2.51	0.43
7:K:47:LEU:H	7:K:50:GLN:NE2	2.15	0.43
12:2:55:MET:HE1	29:X:155:TRP:CE2	2.53	0.43
12:2:199:LEU:HD21	16:6:111:ILE:HG22	2.00	0.43
15:5:126:TRP:CG	15:5:145:PHE:HB3	2.53	0.43
17:g:65:PRO:HB2	17:g:67:ARG:HG2	1.99	0.43
35:d:69:GLN:HG3	39:i:74:TRP:CE3	2.53	0.43
1:A:40:THR:HB	1:A:45:LYS:HZ2	1.83	0.43
4:G:95:GLU:OE1	4:G:154:ARG:NH2	2.32	0.43
5:H:132:CYS:HB3	5:H:137:SER:HB2	1.99	0.43
12:2:459:LEU:HD23	12:2:460:ILE:HD13	2.00	0.43
14:4:211:TRP:NE1	14:4:262:LEU:HD21	2.34	0.43
15:5:408:SER:HB3	15:5:411:ASN:ND2	2.32	0.43
19:E:216:ARG:NE	51:E:402:CDL:OA3	2.44	0.43
24:P:10:GLU:HB3	24:P:80:HIS:CE1	2.53	0.43
32:a:125:PHE:CD2	32:a:146:GLN:HB3	2.53	0.43
34:c:35:GLY:O	34:c:38:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:57:LYS:NZ	40:n:65:GLU:OE2	2.47	0.43
42:9:33:SER:O	42:9:36:GLN:HB3	2.18	0.43
3:C:97:VAL:O	3:C:118:LEU:HD12	2.19	0.43
3:C:170:GLY:O	3:C:174:ARG:HG3	2.19	0.43
8:L:22:ILE:HG21	8:L:84:ILE:HG21	2.00	0.43
47:S:501:3PE:H251	47:b:201:3PE:H352	2.00	0.43
11:1:106:ILE:HG21	11:1:158:ILE:HD11	1.99	0.43
47:1:504:3PE:H32	47:1:504:3PE:H321	1.69	0.43
12:2:122:ASP:OD1	12:2:124:ILE:HG13	2.18	0.43
15:5:115:ARG:HB2	39:i:16:THR:HG21	1.99	0.43
18:D:79:VAL:HG21	42:9:84:ILE:HD13	2.00	0.43
19:E:90:LYS:HD3	19:E:104:PHE:CE1	2.53	0.43
25:Q:51:THR:O	25:Q:55:ILE:HG13	2.19	0.43
54:Q:201:ZMP:H8	26:R:47:PHE:CE1	2.53	0.43
28:W:70:MET:HB3	28:W:71:PRO:HD3	2.01	0.43
31:Z:72:ASN:OD1	31:Z:72:ASN:N	2.50	0.43
42:9:19:TRP:HB2	42:9:44:TYR:CE1	2.54	0.43
1:A:459:HIS:HB2	1:A:497:PHE:CZ	2.54	0.43
7:K:52:LYS:HB2	7:K:52:LYS:NZ	2.34	0.43
7:K:106:ILE:HD11	11:1:27:ARG:CZ	2.49	0.43
47:4:501:3PE:H2H1	47:4:501:3PE:H2E2	1.80	0.43
15:5:220:PHE:CD1	15:5:280:ILE:HG12	2.53	0.43
15:5:374:TYR:O	15:5:378:THR:OG1	2.31	0.43
19:E:194:VAL:CG2	19:E:197:ALA:HB2	2.47	0.43
21:J:64:SER:OG	21:J:67:VAL:HG12	2.19	0.43
35:d:19:ASP:OD2	35:d:22:LYS:HG2	2.18	0.43
35:d:66:LEU:CD1	39:i:68:ASN:HA	2.48	0.43
37:f:44:VAL:C	37:f:45:ARG:HD2	2.44	0.43
51:n:200:CDL:H311	51:n:200:CDL:HA62	1.78	0.43
8:L:4:GLY:HA3	8:L:39:ILE:HG13	2.00	0.43
12:2:263:LEU:HD23	12:2:263:LEU:HA	1.86	0.43
15:5:628:LEU:O	15:5:632:VAL:HG23	2.18	0.43
25:Q:77:ALA:O	25:Q:119:GLN:N	2.52	0.43
28:W:78:ASP:O	28:W:82:VAL:HG23	2.18	0.43
51:n:200:CDL:H602	51:n:200:CDL:H631	1.29	0.43
1:A:672:VAL:O	1:A:677:VAL:HG13	2.18	0.43
11:1:77:PRO:HB3	11:1:227:PHE:CE2	2.54	0.43
47:1:503:3PE:H221	47:1:503:3PE:H252	1.74	0.43
12:2:469:ASN:ND2	40:n:87:LYS:HB2	2.34	0.43
15:5:114:VAL:HB	39:i:16:THR:HG22	2.00	0.43
47:5:703:3PE:H122	47:J:204:3PE:O11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:92:ARG:HE	21:J:55:ARG:HB2	1.84	0.43
19:E:297:TYR:O	19:E:301:THR:HG23	2.19	0.43
20:F:43:ARG:HB2	20:F:44:PRO:HD3	2.01	0.43
27:U:131:LYS:HD2	27:U:132:ILE:N	2.33	0.43
2:B:333:ILE:HG13	2:B:334:CYS:N	2.34	0.43
5:H:124:LEU:HD21	5:H:161:PHE:CD1	2.53	0.43
6:I:83:MET:HE2	11:1:300:PHE:CE1	2.53	0.43
8:L:19:ARG:HH12	16:6:92:ARG:NH1	2.17	0.43
12:2:40:SER:OG	50:2:502:CPL:HC81	2.18	0.43
15:5:112:HIS:CE1	47:5:701:3PE:H112	2.52	0.43
15:5:377:ILE:HD12	15:5:377:ILE:HA	1.84	0.43
19:E:185:LEU:HD12	19:E:185:LEU:HA	1.81	0.43
27:U:158:LYS:HB3	27:U:158:LYS:HE2	1.86	0.43
3:C:363:ASP:OD2	3:C:366:ILE:HG12	2.19	0.43
5:H:36:THR:O	5:H:40:ASN:HB2	2.19	0.43
11:1:22:LEU:HD13	11:1:290:MET:CE	2.49	0.43
13:3:65:PRO:O	13:3:69:GLU:HG3	2.19	0.43
14:4:138:TYR:CE1	14:4:179:LEU:HD13	2.53	0.43
47:5:701:3PE:H3A2	51:n:200:CDL:H412	2.01	0.43
19:E:347:LEU:HD23	19:E:347:LEU:HA	1.84	0.43
21:J:93:ASP:HB2	47:J:201:3PE:O14	2.19	0.43
21:J:134:TRP:CH2	47:J:201:3PE:H222	2.54	0.43
30:Y:65:LYS:HD3	30:Y:66:PRO:HD2	2.00	0.43
3:C:454:ILE:HD13	3:C:454:ILE:HA	1.92	0.42
11:1:284:ILE:HD12	11:1:284:ILE:HA	1.79	0.42
12:2:199:LEU:CD2	16:6:111:ILE:HG22	2.48	0.42
15:5:515:LEU:HD22	36:e:49:MET:HE2	2.00	0.42
51:g:201:CDL:H172	29:X:80:MET:HB3	2.00	0.42
47:g:202:3PE:H2F1	47:g:202:3PE:H2C1	1.77	0.42
19:E:261:LEU:HD22	19:E:330:PHE:CE1	2.54	0.42
25:Q:102:GLU:HB2	34:c:12:ARG:HH22	1.83	0.42
26:R:89:LYS:HG2	26:R:92:ARG:CZ	2.49	0.42
1:A:505:VAL:HG13	1:A:511:VAL:HG12	2.00	0.42
25:Q:66:PHE:CE1	34:c:8:PRO:HB2	2.54	0.42
25:Q:107:ILE:HD12	25:Q:124:TYR:HE2	1.83	0.42
30:Y:79:ARG:HD2	30:Y:109:GLN:OE1	2.19	0.42
38:h:31:LYS:HE3	38:h:31:LYS:HB3	1.74	0.42
40:n:25:ALA:O	40:n:29:LEU:HD12	2.18	0.42
8:L:21:ASN:HD21	8:L:24:LEU:HD23	1.84	0.42
9:S:203:VAL:HG11	9:S:222:ILE:HG23	2.00	0.42
14:4:486:ILE:HD13	14:4:486:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:32:THR:HG22	15:5:117:PHE:CE1	2.54	0.42
47:g:202:3PE:H2F1	47:g:202:3PE:H2I3	1.86	0.42
48:J:202:LMN:HBR	48:J:202:LMN:HBKA	1.86	0.42
1:A:276:GLU:OE2	38:h:126:LYS:HD2	2.20	0.42
1:A:498:PHE:HE1	1:A:519:TYR:OH	2.03	0.42
2:B:97:LYS:HA	2:B:100:PHE:CD1	2.54	0.42
3:C:377:ASP:OD1	55:C:503:HOH:O	2.22	0.42
3:C:458:ASP:HB3	55:C:530:HOH:O	2.18	0.42
48:j:101:LMN:HBQA	48:j:101:LMN:HBL	1.84	0.42
12:2:92:LEU:HD11	12:2:337:ILE:HD13	2.02	0.42
12:2:452:PHE:CE1	47:4:502:3PE:H3E2	2.55	0.42
14:4:63:LEU:HD12	14:4:71:SER:HB2	2.01	0.42
14:4:264:PRO:HG3	14:4:482:TYR:CE1	2.54	0.42
47:4:501:3PE:H372	47:4:501:3PE:H341	1.84	0.42
28:W:29:ARG:HG2	51:W:402:CDL:OB3	2.20	0.42
33:b:3:LEU:O	33:b:7:LEU:HG	2.19	0.42
35:d:12:PHE:CE1	35:d:86:GLN:HB2	2.54	0.42
38:h:66:LYS:HE3	38:h:66:LYS:HA	2.01	0.42
41:8:27:ALA:O	41:8:31:VAL:HG23	2.20	0.42
1:A:56:GLN:NE2	30:Y:140:ARG:O	2.43	0.42
1:A:84:LEU:HA	1:A:94:VAL:O	2.19	0.42
2:B:120:ASP:O	2:B:161:ARG:HD2	2.20	0.42
7:K:206:MET:HG2	19:E:86:GLU:HB2	2.00	0.42
9:S:122:ASN:O	9:S:126:LEU:HG	2.19	0.42
11:1:131:TYR:CD2	11:1:210:GLU:HB3	2.50	0.42
16:6:87:VAL:HG13	16:6:91:ILE:HB	2.01	0.42
21:J:196:ALA:HB3	21:J:197:PRO:HD3	2.02	0.42
25:Q:81:LEU:HA	25:Q:85:LEU:HD23	2.02	0.42
28:W:121:PRO:HA	28:W:122:PRO:HD3	1.82	0.42
9:S:130:TYR:CD2	9:S:141:PRO:HG2	2.54	0.42
12:2:331:ILE:O	12:2:334:ILE:HG12	2.19	0.42
55:6:305:HOH:O	18:D:43:ASP:HB2	2.18	0.42
19:E:26:ASN:HB3	19:E:246:GLU:OE2	2.19	0.42
20:F:67:TYR:CZ	20:F:117:MET:HG2	2.55	0.42
21:J:92:LYS:HB3	48:J:202:LMN:OAQ	2.19	0.42
21:J:119:ILE:O	21:J:123:VAL:HG13	2.20	0.42
26:R:19:TYR:CE2	26:R:23:LEU:HD11	2.54	0.42
1:A:231:ASP:OD2	1:A:298:ARG:NH2	2.49	0.42
1:A:457:ASN:OD1	1:A:458:THR:HG23	2.20	0.42
3:C:46:GLU:HG3	12:2:336:TYR:CE1	2.55	0.42
3:C:49:GLN:CB	3:C:71:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:160:THR:OG1	4:G:163:THR:HG23	2.20	0.42
7:K:121:GLY:HA2	43:K:301:SF4:S3	2.60	0.42
17:g:74:GLY:O	27:U:74:ARG:HD3	2.20	0.42
20:F:54:LEU:HD12	20:F:79:LYS:HZ1	1.85	0.42
27:U:27:GLU:OE2	28:W:79:ARG:NH2	2.53	0.42
1:A:416:ASN:OD1	1:A:419:ARG:HG3	2.19	0.42
5:H:126:ILE:HB	5:H:141:MET:HE2	2.02	0.42
12:2:332:TYR:OH	12:2:433:GLU:HG3	2.20	0.42
15:5:60:ILE:HD11	39:i:54:ARG:CZ	2.50	0.42
15:5:257:THR:HB	15:5:332:LEU:HD11	2.02	0.42
15:5:281:LEU:HD21	15:5:411:ASN:OD1	2.19	0.42
55:U:207:HOH:O	28:W:79:ARG:HD3	2.20	0.42
1:A:387:HIS:HB3	1:A:498:PHE:CZ	2.55	0.42
1:A:542:ALA:O	1:A:545:THR:HG23	2.19	0.42
2:B:327:PRO:HD2	2:B:349:SER:HA	2.02	0.42
4:G:90:SER:HA	31:Z:87:ALA:O	2.19	0.42
6:I:93:GLN:OE1	6:I:96:ARG:NH1	2.53	0.42
10:j:83:LYS:HD3	10:j:83:LYS:HA	1.87	0.42
11:1:176:VAL:HA	47:1:504:3PE:O31	2.19	0.42
11:1:212:VAL:HG21	13:3:38:PHE:HE2	1.83	0.42
11:1:271:PHE:CD2	18:D:30:VAL:HG11	2.55	0.42
14:4:170:PHE:CZ	46:4:504:PLC:H2'2	2.55	0.42
15:5:349:ILE:HG13	15:5:373:THR:HG21	2.01	0.42
17:g:9:TRP:CD1	51:g:201:CDL:HA31	2.55	0.42
27:U:136:ARG:HB2	27:U:139:GLU:HG3	2.01	0.42
34:c:22:THR:HG22	34:c:24:ALA:H	1.85	0.42
2:B:377:LYS:HD2	2:B:395:LEU:HD23	2.02	0.42
3:C:107:GLU:CD	11:1:138:ARG:HH12	2.27	0.42
11:1:131:TYR:HB3	11:1:210:GLU:HB3	2.01	0.42
11:1:203:ASP:OD1	11:1:203:ASP:N	2.53	0.42
12:2:30:ILE:HG22	29:X:50:LEU:HD13	2.02	0.42
12:2:54:VAL:HG13	55:X:313:HOH:O	2.20	0.42
12:2:356:ASP:OD2	12:2:424:LYS:NZ	2.53	0.42
50:2:502:CPL:HC62	50:2:502:CPL:HC42	1.66	0.42
13:3:85:ASN:HB2	29:X:131:LEU:HD21	2.02	0.42
13:3:109:ASN:HA	13:3:112:LYS:HE2	2.02	0.42
27:U:33:ALA:HB3	27:U:34:PRO:HD3	2.02	0.42
30:Y:82:TRP:CZ2	30:Y:105:MET:HE2	2.54	0.42
32:a:120:ALA:HA	41:8:66:VAL:HA	2.01	0.42
41:8:29:LEU:O	41:8:32:PRO:HD2	2.20	0.42
1:A:641:ASP:O	1:A:645:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:SER:OG	3:C:439:ASP:HA	2.21	0.41
12:2:190:LEU:HD22	12:2:191:ILE:HD13	2.02	0.41
15:5:21:PHE:CD1	51:n:200:CDL:H152	2.55	0.41
15:5:598:LYS:NZ	47:5:703:3PE:H12	2.35	0.41
47:5:703:3PE:H3G2	21:J:132:PHE:HB2	2.02	0.41
19:E:116:ASP:OD2	19:E:157:LYS:NZ	2.43	0.41
3:C:311:TYR:O	55:C:504:HOH:O	2.22	0.41
12:2:117:ILE:HG13	12:2:129:ALA:HB1	2.01	0.41
55:2:726:HOH:O	40:n:95:HIS:HB3	2.21	0.41
14:4:178:MET:HB2	14:4:217:ALA:HB2	2.02	0.41
27:U:131:LYS:HZ2	27:U:133:PRO:HG3	1.84	0.41
29:X:38:SER:O	29:X:42:VAL:HG23	2.20	0.41
32:a:34:GLU:HA	32:a:37:LEU:HD21	2.02	0.41
32:a:119:ALA:O	41:8:66:VAL:HG23	2.20	0.41
40:n:24:TRP:HA	51:n:200:CDL:OB9	2.20	0.41
2:B:289:THR:OG1	5:H:173:VAL:HG21	2.20	0.41
2:B:367:ARG:HG3	2:B:402:ARG:NH2	2.35	0.41
2:B:440:LEU:HD12	2:B:444:PHE:HD2	1.85	0.41
3:C:50:ASP:HB3	3:C:53:PHE:HD2	1.85	0.41
3:C:424:LYS:NZ	3:C:426:LYS:HB2	2.35	0.41
10:j:84:ARG:HD2	39:i:83:THR:OG1	2.21	0.41
15:5:26:LEU:HD13	15:5:30:PHE:CD2	2.55	0.41
15:5:434:TYR:HA	15:5:438:TYR:CD2	2.55	0.41
15:5:497:PHE:CZ	15:5:499:TYR:HB3	2.55	0.41
27:U:133:PRO:HD2	28:W:64:TRP:CD1	2.54	0.41
2:B:323:GLY:O	2:B:326:VAL:HG22	2.19	0.41
3:C:48:HIS:ND1	3:C:64:THR:HG21	2.36	0.41
9:S:207:HIS:HB3	9:S:209:GLU:OE2	2.21	0.41
10:j:4:LEU:O	10:j:5:LYS:HD3	2.20	0.41
11:1:123:SER:O	11:1:126:SER:HB2	2.20	0.41
11:1:163:SER:HA	13:3:78:MET:HE1	2.02	0.41
47:1:504:3PE:H271	47:1:504:3PE:H241	1.82	0.41
15:5:598:LYS:HZ2	47:5:703:3PE:C1	2.33	0.41
20:F:126:LEU:HD23	20:F:126:LEU:H	1.85	0.41
24:P:115:PHE:HA	24:P:118:LYS:NZ	2.35	0.41
3:C:118:LEU:HD13	7:K:127:MET:HE2	2.01	0.41
13:3:61:ILE:O	13:3:65:PRO:HD2	2.19	0.41
14:4:433:GLY:HA3	15:5:164:MET:HE2	2.02	0.41
15:5:293:LEU:HD23	15:5:424:LEU:HD21	2.03	0.41
15:5:327:LEU:HD11	15:5:398:ILE:HG13	2.02	0.41
25:Q:66:PHE:HE1	34:c:8:PRO:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:W:118:LEU:O	42:9:57:LEU:HD11	2.20	0.41
32:a:121:ILE:HG23	32:a:122:PRO:O	2.21	0.41
1:A:49:GLU:O	1:A:52:SER:OG	2.32	0.41
2:B:37:GLN:HA	5:H:233:HIS:CD2	2.55	0.41
2:B:478:VAL:HG11	2:B:483:LEU:HD21	2.03	0.41
3:C:61:ASP:OD2	3:C:61:ASP:N	2.53	0.41
3:C:107:GLU:HG3	3:C:446:PHE:CD1	2.56	0.41
3:C:449:ASP:OD2	13:3:115:LYS:NZ	2.50	0.41
6:I:78:PHE:CD2	47:1:501:3PE:H3G2	2.55	0.41
6:I:88:TYR:CD2	31:Z:30:ILE:HG12	2.55	0.41
12:2:221:LEU:HD23	12:2:221:LEU:HA	1.85	0.41
13:3:105:GLU:OE2	13:3:111:LEU:HG	2.21	0.41
14:4:78:LEU:HD11	40:n:73:LEU:HD11	2.01	0.41
14:4:462:LEU:HD23	14:4:462:LEU:HA	1.93	0.41
15:5:217:LEU:HD12	15:5:217:LEU:HA	1.91	0.41
15:5:220:PHE:CE1	15:5:280:ILE:HG12	2.55	0.41
15:5:289:LEU:HD12	15:5:289:LEU:HA	1.94	0.41
15:5:298:SER:HB2	15:5:304:ILE:HG12	2.02	0.41
16:6:96:LEU:HD22	21:J:46:ALA:HA	2.02	0.41
21:J:123:VAL:HG21	47:J:204:3PE:H372	2.01	0.41
21:J:155:VAL:HG12	21:J:165:GLU:HB3	2.02	0.41
23:O:55:THR:HA	23:O:96:ASN:HB2	2.03	0.41
23:O:67:LEU:HD12	24:P:64:ARG:HH21	1.86	0.41
24:P:23:LYS:HB2	24:P:23:LYS:HE3	1.67	0.41
39:i:34:THR:O	39:i:38:VAL:HG23	2.21	0.41
2:B:116:VAL:HG11	2:B:214:LEU:HD22	2.03	0.41
2:B:382:GLY:O	2:B:388:ARG:HD3	2.20	0.41
3:C:87:PHE:CZ	3:C:93:ALA:HB3	2.56	0.41
3:C:104:LEU:HA	3:C:108:GLU:O	2.21	0.41
5:H:169:LEU:HD12	5:H:177:MET:HE1	2.03	0.41
7:K:113:GLN:NE2	11:1:219:TYR:O	2.52	0.41
8:L:1:FME:CG	8:L:39:ILE:HA	2.48	0.41
9:S:225:ARG:HA	9:S:225:ARG:HD2	1.66	0.41
11:1:75:ILE:O	11:1:79:ILE:HG23	2.21	0.41
15:5:83:ALA:O	15:5:86:ILE:HG22	2.20	0.41
19:E:215:ASP:O	19:E:219:ARG:HG2	2.21	0.41
27:U:95:ARG:HG2	27:U:99:GLN:NE2	2.36	0.41
30:Y:116:GLU:CD	30:Y:116:GLU:N	2.78	0.41
35:d:24:ARG:O	35:d:28:GLU:HG3	2.21	0.41
1:A:279:ARG:CD	1:A:281:ILE:HD11	2.51	0.41
2:B:51:ASP:OD1	2:B:52:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLY:HA3	45:B:502:FMN:N5	2.35	0.41
3:C:292:SER:HB2	55:C:650:HOH:O	2.19	0.41
4:G:40:LYS:NZ	4:G:45:ASP:OD2	2.48	0.41
12:2:394:GLY:HA2	12:2:396:TYR:CZ	2.56	0.41
15:5:339:LYS:HD3	15:5:339:LYS:HA	1.80	0.41
19:E:169:PHE:CD2	19:E:321:GLN:HG3	2.55	0.41
24:P:62:ARG:HG3	24:P:62:ARG:NH2	2.36	0.41
25:Q:91:ASP:O	25:Q:95:VAL:HG23	2.20	0.41
32:a:133:GLU:O	35:d:60:PHE:HB2	2.20	0.41
33:b:29:ALA:HB2	47:b:201:3PE:O14	2.20	0.41
35:d:45:ARG:HD3	35:d:70:TYR:CE1	2.56	0.41
1:A:338:GLN:OE1	1:A:339:LYS:HD3	2.19	0.41
2:B:52:LEU:HB2	2:B:138:HIS:NE2	2.35	0.41
3:C:40:LYS:HD2	3:C:41:VAL:N	2.36	0.41
3:C:44:VAL:HG11	12:2:346:TYR:CD2	2.55	0.41
3:C:208:GLU:HG3	6:I:99:TYR:CG	2.55	0.41
3:C:272:LYS:HZ2	3:C:272:LYS:HG2	1.76	0.41
3:C:458:ASP:HA	55:C:653:HOH:O	2.21	0.41
5:H:59:ILE:HD11	5:H:74:LEU:HD11	2.02	0.41
8:L:10:LEU:CB	16:6:20:THR:HG21	2.51	0.41
8:L:48:ASP:O	42:9:7:SER:HA	2.20	0.41
8:L:49:ASP:OD2	8:L:51:SER:HB2	2.21	0.41
10:j:50:ARG:H	48:j:101:LMN:H1	1.86	0.41
46:1:505:PLC:H2	46:1:505:PLC:H1'1	1.57	0.41
14:4:134:TYR:N	14:4:192:THR:HG23	2.36	0.41
15:5:220:PHE:CZ	15:5:224:MET:HG3	2.56	0.41
15:5:618:SER:HA	15:5:621:ILE:HG22	2.03	0.41
16:6:20:THR:O	16:6:24:ILE:HD12	2.20	0.41
16:6:92:ARG:NH2	21:J:51:ALA:O	2.54	0.41
25:Q:68:LYS:HA	25:Q:68:LYS:HD2	1.83	0.41
30:Y:90:ARG:HA	30:Y:100:SER:O	2.20	0.41
1:A:490:ASP:OD2	1:A:524:ARG:NH1	2.54	0.41
1:A:721:ASN:OD1	1:A:723:LYS:HB2	2.20	0.41
2:B:304:LYS:HZ1	2:B:305:HIS:CD2	2.39	0.41
7:K:112:ARG:NH1	11:1:63:VAL:HG11	2.36	0.41
46:K:302:PLC:H7'1	46:K:302:PLC:H2A2	2.02	0.41
11:1:179:CYS:HB2	11:1:186:LEU:HD22	2.03	0.41
12:2:359:TYR:CG	33:b:23:LYS:HB3	2.56	0.41
14:4:268:GLU:OE1	14:4:268:GLU:N	2.48	0.41
14:4:365:LEU:HD22	14:4:369:MET:CE	2.51	0.41
15:5:155:SER:HB2	15:5:164:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:47:PHE:CD2	24:P:103:GLU:HG3	2.56	0.41
30:Y:42:HIS:HA	30:Y:45:VAL:HG12	2.03	0.41
32:a:139:LYS:HB3	32:a:139:LYS:HE2	1.85	0.41
35:d:15:ILE:HG21	35:d:22:LYS:HB3	2.02	0.41
36:e:9:LYS:HD2	36:e:12:GLY:HA3	2.03	0.41
38:h:15:VAL:HG13	38:h:19:SER:CB	2.50	0.41
38:h:107:GLN:HB2	55:h:257:HOH:O	2.20	0.41
1:A:78:GLY:HA2	44:A:803:FES:S1	2.61	0.40
2:B:213:SER:OG	2:B:223:GLY:O	2.34	0.40
3:C:43:HIS:O	3:C:48:HIS:NE2	2.54	0.40
3:C:269:ARG:NH2	47:1:501:3PE:O32	2.49	0.40
5:H:135:CYS:SG	5:H:175:ALA:HB1	2.61	0.40
9:S:155:LYS:NZ	9:S:157:GLU:O	2.54	0.40
11:1:24:VAL:O	11:1:28:LYS:HG2	2.21	0.40
12:2:306:GLU:H	12:2:306:GLU:CD	2.29	0.40
12:2:358:ALA:HB1	47:4:501:3PE:H232	2.03	0.40
13:3:78:MET:HG3	16:6:147:LEU:HD23	2.02	0.40
14:4:178:MET:HB2	14:4:217:ALA:CB	2.51	0.40
14:4:342:LEU:O	14:4:346:VAL:HG22	2.21	0.40
15:5:146:ILE:HD11	15:5:226:LYS:HE3	2.03	0.40
15:5:216:MET:HE3	15:5:269:ILE:HG21	2.02	0.40
19:E:227:ASN:HA	19:E:228:LYS:HZ3	1.85	0.40
30:Y:79:ARG:CD	30:Y:111:LYS:HZ2	2.34	0.40
41:8:13:MET:SD	41:8:23:ARG:HB3	2.61	0.40
1:A:251:GLU:HG3	1:A:273:LYS:HE2	2.02	0.40
1:A:369:LEU:HD13	1:A:635:VAL:HG11	2.01	0.40
2:B:145:LEU:HD23	2:B:146:LEU:HD22	2.04	0.40
3:C:198:GLY:HA3	11:1:302:ARG:HG3	2.03	0.40
5:H:188:LEU:HD13	5:H:193:THR:HG22	2.02	0.40
9:S:154:ILE:O	9:S:156:ARG:N	2.54	0.40
9:S:203:VAL:HG21	9:S:226:ILE:HG13	2.03	0.40
9:S:230:ASP:OD2	39:i:78:HIS:NE2	2.51	0.40
12:2:234:ILE:HD13	12:2:324:PHE:CB	2.51	0.40
13:3:104:TYR:CD2	16:6:174:ILE:HD13	2.57	0.40
14:4:134:TYR:HB2	14:4:192:THR:HG23	2.03	0.40
15:5:504:PHE:HD1	36:e:55:PHE:CG	2.39	0.40
15:5:530:GLU:OE2	34:c:27:PHE:HE2	2.05	0.40
17:g:65:PRO:HG2	27:U:55:LEU:HD11	2.03	0.40
19:E:140:TYR:CD2	19:E:178:GLU:HB3	2.56	0.40
47:J:201:3PE:H252	47:J:201:3PE:H221	1.75	0.40
47:J:204:3PE:H322	47:J:204:3PE:H31	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:37:LYS:NZ	22:M:43:ASP:OD1	2.46	0.40
26:R:5:VAL:HG11	26:R:8:SER:HB3	2.03	0.40
27:U:13:GLU:OE2	42:9:79:ILE:HG21	2.22	0.40
41:8:47:CYS:HB2	41:8:51:ARG:NH2	2.36	0.40
3:C:150:ASN:O	3:C:153:VAL:HG12	2.21	0.40
4:G:116:THR:HG22	6:I:44:GLY:HA3	2.03	0.40
4:G:148:ARG:NH2	55:G:318:HOH:O	2.52	0.40
9:S:49:ARG:HB2	9:S:106:LEU:HB3	2.02	0.40
11:1:120:SER:O	11:1:136:SER:HB2	2.21	0.40
14:4:15:ASN:ND2	14:4:16:ARG:HH21	2.19	0.40
16:6:95:PRO:O	16:6:99:ILE:HD12	2.21	0.40
19:E:348:ILE:HA	19:E:348:ILE:HD13	1.82	0.40
25:Q:58:ARG:HG3	36:e:10:TRP:CH2	2.57	0.40
34:c:34:PHE:CE1	36:e:39:PHE:HZ	2.38	0.40
39:i:23:PRO:HB3	40:n:14:VAL:HG22	2.03	0.40
1:A:215:THR:C	1:A:217:LEU:H	2.30	0.40
1:A:472:GLU:OE2	1:A:472:GLU:HA	2.21	0.40
2:B:113:ARG:HB2	2:B:153:ALA:HA	2.04	0.40
2:B:259:ARG:HD2	2:B:263:TRP:CH2	2.56	0.40
2:B:333:ILE:HD12	2:B:337:VAL:HB	2.04	0.40
3:C:262:GLU:OE2	3:C:341:ARG:NH2	2.50	0.40
3:C:283:ALA:HB1	3:C:301:ILE:HD11	2.03	0.40
4:G:261:ASP:OD2	31:Z:84:PRO:HB3	2.21	0.40
6:I:61:ALA:HB1	6:I:65:GLU:HG3	2.03	0.40
14:4:214:LEU:O	14:4:218:ILE:HG12	2.22	0.40
14:4:485:ILE:HD13	21:J:184:GLY:HA3	2.03	0.40
15:5:86:ILE:HD12	15:5:86:ILE:HA	1.95	0.40
15:5:431:LYS:O	15:5:435:LEU:HB2	2.21	0.40
19:E:275:MET:HG3	19:E:275:MET:H	1.74	0.40
21:J:144:LYS:HB3	21:J:144:LYS:HE3	1.85	0.40
31:Z:174:LYS:HB3	31:Z:174:LYS:HE3	1.69	0.40
2:B:87:ARG:HD3	2:B:87:ARG:HA	1.72	0.40
3:C:204:LEU:HG	11:1:34:GLN:HB3	2.04	0.40
9:S:60:LYS:HE2	9:S:60:LYS:HB2	1.78	0.40
11:1:137:ILE:HG23	16:6:73:PHE:CZ	2.56	0.40
11:1:204:LEU:HD21	11:1:304:THR:C	2.45	0.40
13:3:17:ALA:O	13:3:21:VAL:HG23	2.22	0.40
13:3:94:PHE:CZ	13:3:98:LEU:HD11	2.57	0.40
14:4:15:ASN:OD1	47:b:201:3PE:H32	2.21	0.40
15:5:172:LEU:HD23	15:5:172:LEU:HA	1.89	0.40
15:5:450:ASN:OD1	15:5:450:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:124:LYS:HB2	38:h:125:PRO:HD2	2.04	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 PDB entries followed by that with respect to all EM entries.

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	
1	A	691/728 (95%)	666 (96%)	24 (4%)	1 (0%)	48	64
2	B	453/488 (93%)	426 (94%)	26 (6%)	1 (0%)	43	58
3	C	435/466 (93%)	416 (96%)	19 (4%)	0	100	100
4	G	237/281 (84%)	230 (97%)	7 (3%)	0	100	100
5	H	214/243 (88%)	194 (91%)	20 (9%)	0	100	100
6	I	188/229 (82%)	184 (98%)	4 (2%)	0	100	100
7	K	175/210 (83%)	168 (96%)	7 (4%)	0	100	100
8	L	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
9	S	176/249 (71%)	173 (98%)	3 (2%)	0	100	100
10	j	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
11	1	338/341 (99%)	328 (97%)	10 (3%)	0	100	100
12	2	467/469 (100%)	462 (99%)	5 (1%)	0	100	100
13	3	126/128 (98%)	124 (98%)	1 (1%)	1 (1%)	16	25
14	4	479/486 (99%)	466 (97%)	13 (3%)	0	100	100
15	5	652/655 (100%)	624 (96%)	26 (4%)	2 (0%)	36	50
16	6	182/185 (98%)	179 (98%)	3 (2%)	0	100	100
17	g	74/78 (95%)	68 (92%)	6 (8%)	0	100	100
18	D	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
19	E	346/375 (92%)	336 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	F	118/144 (82%)	114 (97%)	4 (3%)	0	100	100
21	J	176/198 (89%)	170 (97%)	6 (3%)	0	100	100
22	M	115/136 (85%)	115 (100%)	0	0	100	100
23	O	69/109 (63%)	69 (100%)	0	0	100	100
24	P	121/124 (98%)	121 (100%)	0	0	100	100
25	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
26	R	104/109 (95%)	102 (98%)	2 (2%)	0	100	100
27	U	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
28	W	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
29	X	162/169 (96%)	160 (99%)	2 (1%)	0	100	100
30	Y	121/161 (75%)	119 (98%)	2 (2%)	0	100	100
31	Z	179/182 (98%)	174 (97%)	5 (3%)	0	100	100
32	a	122/149 (82%)	117 (96%)	5 (4%)	0	100	100
33	b	62/74 (84%)	62 (100%)	0	0	100	100
34	c	42/60 (70%)	40 (95%)	2 (5%)	0	100	100
35	d	87/92 (95%)	85 (98%)	2 (2%)	0	100	100
36	e	50/67 (75%)	46 (92%)	4 (8%)	0	100	100
37	f	80/87 (92%)	77 (96%)	3 (4%)	0	100	100
38	h	134/138 (97%)	130 (97%)	4 (3%)	0	100	100
39	i	81/90 (90%)	79 (98%)	2 (2%)	0	100	100
40	n	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
41	8	69/99 (70%)	69 (100%)	0	0	100	100
42	9	84/89 (94%)	84 (100%)	0	0	100	100
All	All	7951/8704 (91%)	7702 (97%)	244 (3%)	5 (0%)	49	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	5	555	VAL
13	3	84	SER
1	A	291	GLU
2	B	121	GLU
15	5	439	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	566/595 (95%)	542 (96%)	24 (4%)	26	45
2	B	363/389 (93%)	341 (94%)	22 (6%)	17	30
3	C	373/393 (95%)	366 (98%)	7 (2%)	50	71
4	G	216/245 (88%)	213 (99%)	3 (1%)	59	79
5	H	191/212 (90%)	186 (97%)	5 (3%)	40	63
6	I	156/187 (83%)	154 (99%)	2 (1%)	61	80
7	K	154/180 (86%)	148 (96%)	6 (4%)	28	48
8	L	76/76 (100%)	74 (97%)	2 (3%)	40	63
9	S	157/211 (74%)	152 (97%)	5 (3%)	34	56
10	j	71/73 (97%)	70 (99%)	1 (1%)	59	79
11	1	300/301 (100%)	297 (99%)	3 (1%)	68	84
12	2	432/432 (100%)	422 (98%)	10 (2%)	44	66
13	3	113/113 (100%)	107 (95%)	6 (5%)	20	36
14	4	429/433 (99%)	419 (98%)	10 (2%)	44	66
15	5	579/579 (100%)	561 (97%)	18 (3%)	35	57
16	6	165/166 (99%)	160 (97%)	5 (3%)	36	58
17	g	63/65 (97%)	61 (97%)	2 (3%)	34	56
18	D	68/69 (99%)	65 (96%)	3 (4%)	25	43
19	E	306/329 (93%)	291 (95%)	15 (5%)	22	39
20	F	108/129 (84%)	107 (99%)	1 (1%)	70	85
21	J	129/147 (88%)	124 (96%)	5 (4%)	28	48
22	M	97/115 (84%)	94 (97%)	3 (3%)	35	57
23	O	60/91 (66%)	59 (98%)	1 (2%)	53	74
24	P	109/110 (99%)	108 (99%)	1 (1%)	70	85
25	Q	72/111 (65%)	70 (97%)	2 (3%)	38	60
26	R	97/100 (97%)	93 (96%)	4 (4%)	27	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	U	147/148 (99%)	145 (99%)	2 (1%)	59	79
28	W	100/102 (98%)	100 (100%)	0	100	100
29	X	128/133 (96%)	126 (98%)	2 (2%)	55	76
30	Y	105/140 (75%)	102 (97%)	3 (3%)	37	60
31	Z	147/148 (99%)	140 (95%)	7 (5%)	23	40
32	a	108/129 (84%)	102 (94%)	6 (6%)	19	33
33	b	50/59 (85%)	48 (96%)	2 (4%)	28	47
34	c	30/45 (67%)	30 (100%)	0	100	100
35	d	82/85 (96%)	82 (100%)	0	100	100
36	e	44/55 (80%)	43 (98%)	1 (2%)	44	66
37	f	70/73 (96%)	69 (99%)	1 (1%)	59	79
38	h	121/123 (98%)	117 (97%)	4 (3%)	33	55
39	i	64/68 (94%)	63 (98%)	1 (2%)	55	76
40	n	98/102 (96%)	96 (98%)	2 (2%)	48	70
41	8	63/76 (83%)	63 (100%)	0	100	100
42	9	73/76 (96%)	69 (94%)	4 (6%)	19	34
All	All	6880/7413 (93%)	6679 (97%)	201 (3%)	38	60

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	52	SER
1	A	127	GLN
1	A	155	ARG
1	A	223	THR
1	A	281	ILE
1	A	339	LYS
1	A	369	LEU
1	A	399	SER
1	A	435	GLN
1	A	438	GLU
1	A	441	SER
1	A	445	THR
1	A	481	LEU
1	A	488	ILE

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Mol	Chain	Res	Type
1	A	514	GLU
1	A	533	ASP
1	A	543	SER
1	A	545	THR
1	A	613	THR
1	A	640	GLU
1	A	662	VAL
1	A	677	VAL
1	A	694	ILE
2	B	76	ILE
2	B	77	ASP
2	B	85	ARG
2	B	121	GLU
2	B	127	CYS
2	B	189	CYS
2	B	247	VAL
2	B	272	ASN
2	B	273	SER
2	B	289	THR
2	B	291	GLU
2	B	316	LEU
2	B	317	LEU
2	B	328	ILE
2	B	333	ILE
2	B	338	LEU
2	B	358	VAL
2	B	370	GLN
2	B	385	THR
2	B	417	LEU
2	B	463	SER
2	B	477	LYS
3	C	32	ILE
3	C	34	SER
3	C	44	VAL
3	C	51	LEU
3	C	97	VAL
3	C	372	ASN
3	C	447	LEU
4	G	139	GLU
4	G	220	THR
4	G	249	SER
5	H	36	THR

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Mol	Chain	Res	Type
5	H	57	GLU
5	H	124	LEU
5	H	129	THR
5	H	156	THR
6	I	148	ASP
6	I	229	ARG
7	K	80	THR
7	K	85	CYS
7	K	115	ASP
7	K	122	THR
7	K	156	TYR
7	K	202	LYS
8	L	16	VAL
8	L	22	ILE
9	S	118	LEU
9	S	142	VAL
9	S	153	GLU
9	S	155	LYS
9	S	192	THR
10	j	7	SER
11	1	8	ILE
11	1	121	LEU
11	1	296	VAL
12	2	9	LEU
12	2	28	ILE
12	2	40	SER
12	2	69	ASP
12	2	111	ILE
12	2	136	SER
12	2	297	MET
12	2	328	ILE
12	2	433	GLU
12	2	460	ILE
13	3	8	ILE
13	3	45	PHE
13	3	50	LEU
13	3	58	LEU
13	3	59	VAL
13	3	91	VAL
14	4	13	LEU
14	4	50	SER
14	4	173	SER

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Mol	Chain	Res	Type
14	4	192	THR
14	4	246	LEU
14	4	255	LEU
14	4	289	SER
14	4	317	VAL
14	4	413	SER
14	4	466	ILE
15	5	150	SER
15	5	219	LEU
15	5	232	LEU
15	5	254	THR
15	5	290	SER
15	5	342	LEU
15	5	348	SER
15	5	383	SER
15	5	420	LEU
15	5	445	THR
15	5	490	THR
15	5	513	LEU
15	5	546	VAL
15	5	557	ASP
15	5	580	ASP
15	5	606	LEU
15	5	621	ILE
15	5	640	ILE
16	6	15	LEU
16	6	78	LEU
16	6	128	ASN
16	6	129	ASP
16	6	174	ILE
17	g	72	LEU
17	g	73	THR
18	D	27	VAL
18	D	63	LYS
18	D	69	THR
19	E	78	THR
19	E	110	ARG
19	E	126	VAL
19	E	173	ILE
19	E	178	GLU
19	E	185	LEU
19	E	224	VAL

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Mol	Chain	Res	Type
19	E	255	VAL
19	E	280	LEU
19	E	286	HIS
19	E	304	ILE
19	E	308	THR
19	E	310	SER
19	E	332	ASP
19	E	335	LEU
20	F	60	LYS
21	J	49	SER
21	J	69	THR
21	J	75	SER
21	J	123	VAL
21	J	173	SER
22	M	28	THR
22	M	61	MET
22	M	96	VAL
23	O	36	ILE
24	P	45	VAL
25	Q	51	THR
25	Q	76	THR
26	R	22	SER
26	R	37	ARG
26	R	54	SER
26	R	62	THR
27	U	132	ILE
27	U	146	LYS
29	X	50	LEU
29	X	54	ILE
30	Y	44	ILE
30	Y	51	GLU
30	Y	120	LYS
31	Z	7	VAL
31	Z	30	ILE
31	Z	100	LEU
31	Z	130	GLN
31	Z	135	SER
31	Z	136	SER
31	Z	157	LEU
32	a	37	LEU
32	a	43	ILE
32	a	50	LEU

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Mol	Chain	Res	Type
32	a	71	SER
32	a	86	THR
32	a	121	ILE
33	b	11	SER
33	b	57	SER
36	e	33	THR
37	f	12	LEU
38	h	15	VAL
38	h	18	ARG
38	h	87	THR
38	h	113	THR
39	i	14	SER
40	n	31	LEU
40	n	98	SER
42	9	21	SER
42	9	69	GLU
42	9	76	VAL
42	9	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	222	ASN
1	A	479	ASN
2	B	118	ASN
2	B	152	ASN
2	B	315	ASN
2	B	362	GLN
2	B	383	GLN
3	C	72	ASN
3	C	77	ASN
3	C	284	GLN
4	G	73	GLN
4	G	99	HIS
4	G	208	HIS
6	I	219	GLN
7	K	200	ASN
11	1	242	ASN
12	2	110	ASN
12	2	173	ASN
12	2	180	ASN

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Mol	Chain	Res	Type
12	2	198	ASN
12	2	252	ASN
12	2	335	ASN
12	2	392	ASN
14	4	15	ASN
14	4	45	ASN
14	4	51	ASN
14	4	108	ASN
14	4	190	ASN
14	4	383	ASN
14	4	481	ASN
15	5	3	ASN
15	5	25	GLN
15	5	229	GLN
15	5	299	ASN
15	5	537	ASN
15	5	539	ASN
15	5	551	ASN
15	5	636	ASN
16	6	158	ASN
17	g	22	ASN
18	D	64	GLN
19	E	137	ASN
19	E	188	GLN
19	E	257	GLN
19	E	365	ASN
20	F	24	GLN
20	F	61	HIS
21	J	160	HIS
22	M	126	GLN
24	P	80	HIS
24	P	111	GLN
26	R	93	ASN
26	R	103	GLN
27	U	61	GLN
28	W	22	ASN
30	Y	55	ASN
30	Y	62	GLN
31	Z	38	ASN
31	Z	79	HIS
31	Z	161	GLN
31	Z	182	HIS

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Mol	Chain	Res	Type
33	b	51	HIS
35	d	20	HIS
36	e	23	HIS
38	h	55	HIS
40	n	71	GLN
41	8	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
12	FME	2	1	12	8,9,10	0.92	0	7,9,11	1.04	1 (14%)
3	2MR	C	121	3	10,12,13	1.76	1 (10%)	5,13,15	2.51	2 (40%)
16	FME	6	1	16	8,9,10	0.96	0	7,9,11	0.95	0
13	FME	3	1	13	8,9,10	0.84	0	7,9,11	1.33	1 (14%)
11	FME	1	1	11	8,9,10	0.95	0	7,9,11	1.05	1 (14%)
8	FME	L	1	8	8,9,10	0.44	0	7,9,11	1.36	1 (14%)

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
12	FME	2	1	12	-	4/7/9/11	-
3	2MR	C	121	3	-	4/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	FME	6	1	16	-	4/7/9/11	-
13	FME	3	1	13	-	3/7/9/11	-
11	FME	1	1	11	-	0/7/9/11	-
8	FME	L	1	8	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	121	2MR	CZ-NE	4.83	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	121	2MR	NE-CZ-NH2	4.81	123.89	119.48
3	C	121	2MR	CD-NE-CZ	2.73	128.53	123.41
13	3	1	FME	C-CA-N	2.69	114.58	109.73
8	L	1	FME	C-CA-N	2.58	114.38	109.73
12	2	1	FME	C-CA-N	2.34	113.95	109.73
11	1	1	FME	C-CA-N	2.12	113.56	109.73

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	121	2MR	C-CA-CB-CG
8	L	1	FME	N-CA-CB-CG
12	2	1	FME	C-CA-CB-CG
16	6	1	FME	O1-CN-N-CA
16	6	1	FME	N-CA-CB-CG
16	6	1	FME	C-CA-CB-CG
16	6	1	FME	CA-CB-CG-SD
12	2	1	FME	CA-CB-CG-SD
12	2	1	FME	CB-CG-SD-CE
13	3	1	FME	CB-CG-SD-CE
3	C	121	2MR	CA-CB-CG-CD
8	L	1	FME	C-CA-CB-CG
12	2	1	FME	N-CA-CB-CG
13	3	1	FME	C-CA-CB-CG
13	3	1	FME	CA-CB-CG-SD
3	C	121	2MR	NE-CD-CG-CB
3	C	121	2MR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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	$\# Z > 2$
47	3PE	E	401	-	35,35,50	1.01	4 (11%)	38,40,55	1.18	2 (5%)
44	FES	H	301	5	0,4,4	-	-	-	-	-
47	3PE	5	701	-	41,41,50	0.96	4 (9%)	44,46,55	1.17	2 (4%)
46	PLC	4	504	-	34,34,41	1.42	6 (17%)	40,42,49	1.23	2 (5%)
51	CDL	W	402	-	53,53,99	1.18	7 (13%)	59,65,111	1.20	4 (6%)
47	3PE	5	702	-	40,40,50	0.96	3 (7%)	43,45,55	1.21	3 (6%)
43	SF4	K	301	7	0,12,12	-	-	-	-	-
47	3PE	1	504	11	40,40,50	0.92	2 (5%)	43,45,55	1.06	1 (2%)
51	CDL	E	402	-	71,71,99	1.03	7 (9%)	77,83,111	1.15	5 (6%)
46	PLC	1	502	-	34,34,41	1.40	5 (14%)	40,42,49	1.09	3 (7%)
46	PLC	5	704	-	41,41,41	1.30	5 (12%)	47,49,49	1.08	2 (4%)
47	3PE	5	703	-	42,42,50	0.99	3 (7%)	45,47,55	1.07	2 (4%)
47	3PE	6	201	-	35,35,50	1.02	4 (11%)	38,40,55	1.25	2 (5%)
45	FMN	B	502	-	33,33,33	3.00	14 (42%)	48,50,50	1.48	11 (22%)
47	3PE	4	501	-	42,42,50	0.94	4 (9%)	45,47,55	1.16	2 (4%)
48	LMN	J	202	-	72,72,72	1.50	9 (12%)	96,98,98	1.48	11 (11%)
48	LMN	j	101	-	68,68,72	1.58	10 (14%)	92,94,98	1.20	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	3PE	g	202	-	42,42,50	0.95	4 (9%)	45,47,55	1.07	2 (4%)
50	CPL	2	502	-	51,51,51	0.98	4 (7%)	57,59,59	1.07	2 (3%)
46	PLC	W	401	-	40,40,41	1.33	5 (12%)	46,48,49	1.19	3 (6%)
47	3PE	1	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.13	2 (5%)
43	SF4	B	501	2	0,12,12	-	-	-	-	-
51	CDL	g	201	-	82,82,99	0.97	7 (8%)	88,94,111	1.17	5 (5%)
54	ZMP	O	201	23	26,32,36	1.81	5 (19%)	31,39,45	1.99	9 (29%)
47	3PE	6	202	-	46,46,50	0.91	4 (8%)	49,51,55	1.07	2 (4%)
51	CDL	X	201	-	85,85,99	0.94	8 (9%)	91,97,111	1.16	4 (4%)
47	3PE	4	502	-	41,41,50	0.95	4 (9%)	44,46,55	1.11	2 (4%)
44	FES	A	803	1	0,4,4	-	-	-	-	-
47	3PE	4	503	-	50,50,50	0.85	3 (6%)	53,55,55	1.21	3 (5%)
43	SF4	A	801	1	0,12,12	-	-	-	-	-
43	SF4	A	802	1	0,12,12	-	-	-	-	-
43	SF4	I	302	6	0,12,12	-	-	-	-	-
43	SF4	I	301	6	0,12,12	-	-	-	-	-
47	3PE	J	204	-	33,33,50	1.06	3 (9%)	36,38,55	1.16	2 (5%)
46	PLC	K	302	-	38,38,41	1.37	4 (10%)	44,46,49	1.05	2 (4%)
49	T7X	3	201	-	49,49,61	0.94	3 (6%)	59,61,73	1.17	6 (10%)
49	T7X	2	503	-	52,52,61	0.92	5 (9%)	62,64,73	1.35	7 (11%)
52	NDP	E	400	-	49,52,52	3.64	19 (38%)	66,80,80	2.16	15 (22%)
54	ZMP	Q	201	26,25	26,32,36	1.83	5 (19%)	31,39,45	1.71	6 (19%)
47	3PE	J	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.14	2 (4%)
46	PLC	1	505	-	41,41,41	1.30	5 (12%)	47,49,49	1.11	2 (4%)
47	3PE	J	203	21	43,43,50	0.92	4 (9%)	46,48,55	1.19	3 (6%)
51	CDL	Z	201	-	75,75,99	1.03	7 (9%)	81,87,111	1.16	6 (7%)
47	3PE	1	501	-	50,50,50	0.86	3 (6%)	53,55,55	1.12	4 (7%)
49	T7X	2	501	-	48,48,61	0.92	4 (8%)	57,60,73	1.24	6 (10%)
51	CDL	n	200	-	91,91,99	0.91	8 (8%)	97,103,111	1.18	4 (4%)
47	3PE	b	201	-	41,41,50	0.96	4 (9%)	44,46,55	1.07	2 (4%)
47	3PE	S	501	-	41,41,50	0.95	3 (7%)	44,46,55	1.11	2 (4%)

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
47	3PE	E	401	-	-	14/39/39/54	-
44	FES	H	301	5	-	-	0/1/1/1
47	3PE	5	701	-	-	15/45/45/54	-
46	PLC	4	504	-	-	21/38/38/45	-
51	CDL	W	402	-	-	31/64/64/110	-
47	3PE	5	702	-	-	21/44/44/54	-
47	3PE	1	504	11	-	15/44/44/54	-
43	SF4	K	301	7	-	-	0/6/5/5
51	CDL	E	402	-	-	34/82/82/110	-
46	PLC	1	502	-	-	16/38/38/45	-
46	PLC	5	704	-	-	17/45/45/45	-
47	3PE	5	703	-	-	25/46/46/54	-
47	3PE	6	201	-	-	23/39/39/54	-
45	FMN	B	502	-	-	9/18/18/18	0/3/3/3
47	3PE	4	501	-	-	19/46/46/54	-
48	LMN	J	202	-	-	34/50/130/130	0/4/4/4
48	LMN	j	101	-	-	21/46/126/130	0/4/4/4
47	3PE	g	202	-	-	23/46/46/54	-
50	CPL	2	502	-	-	20/55/55/55	-
46	PLC	W	401	-	-	21/44/44/45	-
47	3PE	1	503	-	-	21/39/39/54	-
43	SF4	B	501	2	-	-	0/6/5/5
51	CDL	g	201	-	-	36/93/93/110	-
54	ZMP	O	201	23	-	17/37/39/43	-
47	3PE	6	202	-	-	23/50/50/54	-
51	CDL	X	201	-	-	35/96/96/110	-
47	3PE	4	502	-	-	22/45/45/54	-
44	FES	A	803	1	-	-	0/1/1/1
47	3PE	4	503	-	-	22/54/54/54	-
43	SF4	A	801	1	-	-	0/6/5/5
43	SF4	A	802	1	-	-	0/6/5/5
43	SF4	I	302	6	-	-	0/6/5/5
43	SF4	I	301	6	-	-	0/6/5/5
47	3PE	J	204	-	-	17/37/37/54	-
46	PLC	K	302	-	-	18/42/42/45	-
49	T7X	3	201	-	-	15/44/68/80	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	T7X	2	503	-	-	27/47/71/80	0/1/1/1
52	NDP	E	400	-	-	5/34/77/77	0/5/5/5
54	ZMP	Q	201	26,25	-	8/37/39/43	-
47	3PE	J	201	-	-	17/44/44/54	-
46	PLC	1	505	-	-	28/45/45/45	-
47	3PE	J	203	21	-	27/47/47/54	-
51	CDL	Z	201	-	-	40/86/86/110	-
47	3PE	1	501	-	-	29/54/54/54	-
49	T7X	2	501	-	-	14/43/67/80	0/1/1/1
51	CDL	n	200	-	-	44/102/102/110	-
47	3PE	b	201	-	-	23/45/45/54	-
47	3PE	S	501	-	-	18/45/45/54	-

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	E	400	NDP	C6N-C5N	12.27	1.55	1.33
45	B	502	FMN	C4A-N5	7.75	1.45	1.30
52	E	400	NDP	C2B-C1B	-7.58	1.33	1.53
52	E	400	NDP	O4D-C1D	7.52	1.59	1.42
52	E	400	NDP	O4B-C1B	7.40	1.59	1.42
52	E	400	NDP	C2D-C1D	-7.21	1.30	1.53
45	B	502	FMN	C10-N1	7.01	1.47	1.33
52	E	400	NDP	O4D-C4D	-6.91	1.29	1.45
52	E	400	NDP	O4B-C4B	-6.60	1.30	1.45
54	O	201	ZMP	C16-N2	5.85	1.46	1.33
54	Q	201	ZMP	C16-N2	5.56	1.45	1.33
45	B	502	FMN	C9A-N10	5.45	1.50	1.41
54	Q	201	ZMP	C13-N1	5.40	1.45	1.33
45	B	502	FMN	C5A-N5	5.30	1.49	1.39
52	E	400	NDP	C2N-C3N	5.23	1.49	1.34
48	J	202	LMN	O1-C1	-5.20	1.31	1.40
45	B	502	FMN	C2-N1	5.17	1.49	1.36
48	j	101	LMN	O1-C1	-5.16	1.31	1.40
48	j	101	LMN	O5-C1	5.16	1.55	1.41
48	J	202	LMN	O5-C1	5.11	1.54	1.41
54	O	201	ZMP	C13-N1	5.04	1.44	1.33
52	E	400	NDP	C6A-N6A	4.48	1.45	1.34
45	B	502	FMN	C10-N10	4.41	1.47	1.37
45	B	502	FMN	C2-N3	4.28	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	E	400	NDP	O2D-C2D	4.23	1.52	1.43
52	E	400	NDP	C4N-C3N	4.11	1.58	1.49
52	E	400	NDP	P2B-O2B	4.05	1.67	1.59
45	B	502	FMN	C4-N3	3.77	1.45	1.38
46	K	302	PLC	O2-C'	3.62	1.44	1.34
47	5	703	3PE	O21-C2	-3.52	1.37	1.46
46	K	302	PLC	O3-CB	3.36	1.43	1.33
46	5	704	PLC	O3-CB	3.35	1.43	1.33
46	4	504	PLC	O2-C'	3.32	1.43	1.34
46	W	401	PLC	O2-C'	3.31	1.43	1.34
46	1	502	PLC	O3-CB	3.30	1.43	1.33
46	1	505	PLC	O3-CB	3.29	1.43	1.33
46	W	401	PLC	O3-CB	3.25	1.42	1.33
52	E	400	NDP	C7N-N7N	3.22	1.42	1.33
46	5	704	PLC	O2-C'	3.21	1.43	1.34
46	1	505	PLC	O2-C'	3.18	1.43	1.34
46	1	502	PLC	O2-C'	3.17	1.43	1.34
48	j	101	LMN	CBT-CCM	3.13	1.60	1.53
46	4	504	PLC	O3-CB	3.04	1.42	1.33
52	E	400	NDP	C6N-N1N	3.01	1.44	1.37
48	J	202	LMN	CBT-CCM	2.97	1.60	1.53
45	B	502	FMN	O2-C2	-2.95	1.18	1.24
51	Z	201	CDL	OB6-CB4	-2.87	1.39	1.46
51	g	201	CDL	OA6-CA4	-2.86	1.39	1.46
47	E	401	3PE	O21-C2	-2.81	1.39	1.46
48	J	202	LMN	CBS-CCM	2.80	1.59	1.53
51	X	201	CDL	OB6-CB4	-2.80	1.39	1.46
51	Z	201	CDL	OA6-CA4	-2.78	1.39	1.46
52	E	400	NDP	C5A-C4A	-2.73	1.33	1.39
47	5	702	3PE	O21-C2	-2.72	1.39	1.46
52	E	400	NDP	C4N-C5N	2.72	1.56	1.48
47	J	204	3PE	O21-C2	-2.70	1.39	1.46
48	j	101	LMN	OBY-CCR	2.69	1.48	1.41
47	b	201	3PE	O21-C2	-2.67	1.39	1.46
47	4	503	3PE	O21-C2	-2.67	1.39	1.46
51	Z	201	CDL	OB8-CB7	2.65	1.41	1.33
47	4	502	3PE	O21-C2	-2.65	1.40	1.46
47	6	202	3PE	O21-C2	-2.65	1.40	1.46
51	E	402	CDL	OB6-CB4	-2.63	1.40	1.46
49	3	201	T7X	O16-C8	-2.62	1.40	1.46
52	E	400	NDP	C5D-C4D	2.62	1.59	1.51
48	j	101	LMN	CBS-CCM	2.62	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	E	402	CDL	OA8-CA7	2.61	1.41	1.33
48	J	202	LMN	O4-C4	2.61	1.50	1.43
47	1	501	3PE	O21-C2	-2.57	1.40	1.46
47	5	702	3PE	O31-C3	-2.56	1.39	1.45
46	1	505	PLC	O2-C2	-2.56	1.40	1.46
48	j	101	LMN	OBZ-CCS	2.56	1.48	1.41
47	J	201	3PE	O21-C2	-2.55	1.40	1.46
47	1	503	3PE	O21-C2	-2.55	1.40	1.46
47	S	501	3PE	O31-C31	2.54	1.40	1.33
51	W	402	CDL	OB8-CB7	2.53	1.40	1.33
51	X	201	CDL	OA8-CA7	2.52	1.40	1.33
51	Z	201	CDL	OA8-CA7	2.52	1.40	1.33
52	E	400	NDP	C5A-N7A	-2.51	1.34	1.39
47	5	703	3PE	O31-C3	-2.51	1.39	1.45
51	E	402	CDL	OB8-CB7	2.51	1.40	1.33
47	4	501	3PE	O21-C2	-2.50	1.40	1.46
47	J	203	3PE	O21-C2	-2.50	1.40	1.46
45	B	502	FMN	O4-C4	-2.50	1.18	1.23
47	g	202	3PE	O31-C31	2.50	1.40	1.33
47	1	504	3PE	O31-C31	2.49	1.40	1.33
51	g	201	CDL	OB6-CB4	-2.49	1.40	1.46
48	j	101	LMN	O4-C4	2.48	1.50	1.43
46	1	502	PLC	O2-C2	-2.47	1.40	1.46
47	g	202	3PE	O21-C2	-2.46	1.40	1.46
51	n	200	CDL	OA6-CA4	-2.46	1.40	1.46
50	2	502	CPL	O2-C2	-2.46	1.40	1.46
47	1	501	3PE	O31-C3	-2.45	1.39	1.45
51	X	201	CDL	OB8-CB7	2.45	1.40	1.33
51	E	402	CDL	OA6-CA4	-2.44	1.40	1.46
48	j	101	LMN	CBR-CCM	2.44	1.58	1.54
51	W	402	CDL	OA6-CA4	-2.43	1.40	1.46
47	5	701	3PE	O21-C2	-2.43	1.40	1.46
47	J	204	3PE	O31-C3	-2.42	1.39	1.45
47	E	401	3PE	O31-C3	-2.42	1.39	1.45
47	4	502	3PE	O31-C31	2.42	1.40	1.33
51	g	201	CDL	OA8-CA7	2.42	1.40	1.33
47	6	202	3PE	O31-C31	2.42	1.40	1.33
46	W	401	PLC	P-O3P	2.41	1.69	1.59
51	n	200	CDL	OA8-CA7	2.41	1.40	1.33
47	S	501	3PE	O21-C2	-2.41	1.40	1.46
54	O	201	ZMP	O2-C13	-2.41	1.18	1.23
51	n	200	CDL	OB8-CB7	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	J	203	3PE	O31-C3	-2.40	1.39	1.45
47	6	201	3PE	O31-C3	-2.39	1.39	1.45
47	6	201	3PE	O31-C31	2.39	1.40	1.33
47	5	701	3PE	O31-C3	-2.38	1.39	1.45
51	W	402	CDL	OB6-CB5	2.38	1.41	1.34
51	W	402	CDL	OA6-CA5	2.38	1.41	1.34
48	J	202	LMN	OBZ-CCR	2.38	1.47	1.41
51	n	200	CDL	OB6-CB4	-2.38	1.40	1.46
50	2	502	CPL	O3-C3	-2.37	1.39	1.45
48	j	101	LMN	CBQ-CCM	2.37	1.58	1.54
46	K	302	PLC	P-O3P	2.37	1.68	1.59
49	2	503	T7X	O18-C9	-2.37	1.39	1.45
47	b	201	3PE	O31-C31	2.36	1.40	1.33
50	2	502	CPL	O2-C31	2.36	1.41	1.34
46	5	704	PLC	O2-C2	-2.36	1.40	1.46
54	Q	201	ZMP	C10-S1	2.36	1.81	1.76
49	3	201	T7X	O18-C11	2.36	1.40	1.33
47	1	503	3PE	O31-C31	2.35	1.40	1.33
48	J	202	LMN	OBZ-CCS	2.34	1.47	1.41
51	W	402	CDL	OA8-CA7	2.34	1.40	1.33
46	W	401	PLC	P-O4P	2.32	1.68	1.59
47	J	201	3PE	O31-C31	2.31	1.40	1.33
49	2	503	T7X	O16-C10	2.31	1.40	1.34
51	g	201	CDL	OA8-CA6	-2.31	1.39	1.45
54	O	201	ZMP	C10-S1	2.30	1.81	1.76
50	2	502	CPL	O3-C11	2.30	1.40	1.33
45	B	502	FMN	C7M-C7	2.30	1.55	1.51
49	2	503	T7X	O16-C8	-2.30	1.40	1.46
47	4	503	3PE	O31-C3	-2.29	1.39	1.45
47	b	201	3PE	O31-C3	-2.28	1.39	1.45
51	W	402	CDL	OA8-CA6	-2.28	1.39	1.45
47	1	504	3PE	O21-C21	2.28	1.40	1.34
45	B	502	FMN	P-O5'	2.28	1.67	1.60
51	n	200	CDL	OB8-CB6	-2.27	1.40	1.45
48	J	202	LMN	CBQ-CCM	2.27	1.58	1.54
47	J	204	3PE	O31-C31	2.27	1.40	1.33
51	W	402	CDL	OB6-CB4	-2.27	1.40	1.46
47	6	201	3PE	O21-C21	2.27	1.40	1.34
47	4	501	3PE	O31-C31	2.26	1.39	1.33
46	4	504	PLC	O2-C2	-2.26	1.40	1.46
47	6	201	3PE	O21-C2	-2.26	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.25	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	4	501	3PE	O21-C21	2.25	1.40	1.34
51	g	201	CDL	OB8-CB7	2.25	1.39	1.33
48	j	101	LMN	OBX-CCJ	2.24	1.47	1.41
46	4	504	PLC	P-O4P	2.24	1.68	1.59
49	2	501	T7X	O18-C9	-2.24	1.40	1.45
49	2	503	T7X	O18-C11	2.24	1.39	1.33
47	J	203	3PE	O21-C21	2.24	1.40	1.34
46	4	504	PLC	P-O3P	2.23	1.68	1.59
54	Q	201	ZMP	O2-C13	-2.23	1.18	1.23
47	g	202	3PE	O21-C21	2.23	1.40	1.34
47	J	201	3PE	O31-C3	-2.23	1.40	1.45
45	B	502	FMN	C4A-C4	2.23	1.52	1.44
51	X	201	CDL	OA8-CA6	-2.23	1.40	1.45
48	J	202	LMN	CBR-CCM	2.22	1.58	1.54
47	5	701	3PE	O21-C21	2.22	1.40	1.34
46	K	302	PLC	P-O4P	2.21	1.68	1.59
54	O	201	ZMP	O3-C16	-2.21	1.19	1.23
49	3	201	T7X	O18-C9	-2.21	1.40	1.45
46	1	505	PLC	P-O4P	2.21	1.68	1.59
46	W	401	PLC	O2-C2	-2.20	1.41	1.46
52	E	400	NDP	C8A-N9A	-2.20	1.33	1.37
47	J	203	3PE	O31-C31	2.19	1.39	1.33
47	5	703	3PE	O31-C31	2.19	1.39	1.33
49	2	503	T7X	P1-O1	2.19	1.66	1.60
51	E	402	CDL	OA6-CA5	2.18	1.40	1.34
54	Q	201	ZMP	C9-C10	2.18	1.53	1.50
51	g	201	CDL	OA6-CA5	2.17	1.40	1.34
51	X	201	CDL	OB8-CB6	-2.17	1.40	1.45
47	4	501	3PE	O31-C3	-2.17	1.40	1.45
47	1	501	3PE	O21-C21	2.16	1.40	1.34
47	5	702	3PE	O31-C31	2.16	1.39	1.33
46	1	505	PLC	P-O3P	2.15	1.68	1.59
47	S	501	3PE	O21-C21	2.15	1.40	1.34
47	g	202	3PE	O31-C3	-2.15	1.40	1.45
51	g	201	CDL	OB6-CB5	2.15	1.40	1.34
47	6	202	3PE	O31-C3	-2.15	1.40	1.45
47	4	502	3PE	O31-C3	-2.14	1.40	1.45
51	E	402	CDL	OB8-CB6	-2.14	1.40	1.45
49	2	501	T7X	O18-C11	2.14	1.39	1.33
49	2	501	T7X	O16-C10	2.14	1.40	1.34
49	2	501	T7X	O16-C8	-2.13	1.41	1.46
47	4	502	3PE	O21-C21	2.13	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	1	503	3PE	O21-C21	2.12	1.40	1.34
46	1	502	PLC	P-O4P	2.12	1.67	1.59
51	n	200	CDL	OA6-CA5	2.11	1.40	1.34
47	4	503	3PE	O31-C31	2.10	1.39	1.33
51	X	201	CDL	OA6-CA5	2.09	1.40	1.34
47	1	503	3PE	O31-C3	-2.09	1.40	1.45
51	Z	201	CDL	OA6-CA5	2.09	1.40	1.34
45	B	502	FMN	C8M-C8	2.09	1.55	1.51
47	5	701	3PE	O31-C31	2.08	1.39	1.33
46	5	704	PLC	P-O3P	2.08	1.67	1.59
46	1	502	PLC	P-O3P	2.07	1.67	1.59
51	n	200	CDL	OB6-CB5	2.07	1.40	1.34
51	E	402	CDL	OB6-CB5	2.06	1.40	1.34
47	J	201	3PE	O21-C21	2.05	1.40	1.34
47	b	201	3PE	O21-C21	2.05	1.40	1.34
51	Z	201	CDL	OA8-CA6	-2.05	1.40	1.45
51	n	200	CDL	OA8-CA6	-2.05	1.40	1.45
47	E	401	3PE	O21-C21	2.05	1.40	1.34
46	5	704	PLC	P-O4P	2.04	1.67	1.59
47	6	202	3PE	O21-C21	2.04	1.40	1.34
51	X	201	CDL	OB6-CB5	2.03	1.40	1.34
47	E	401	3PE	O31-C31	2.02	1.39	1.33
46	4	504	PLC	C8-N	-2.02	1.44	1.50
51	Z	201	CDL	OB8-CB6	-2.01	1.40	1.45

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	J	202	LMN	CBR-CBL-CBJ	6.36	132.13	113.19
52	E	400	NDP	N6A-C6A-N1A	-6.15	104.88	118.35
52	E	400	NDP	C4A-N9A-C1B	-6.01	112.28	126.59
54	O	201	ZMP	C9-C10-S1	5.98	120.42	113.46
48	j	101	LMN	CBR-CBL-CBJ	5.82	130.53	113.19
52	E	400	NDP	N3A-C2A-N1A	-5.51	119.98	128.60
52	E	400	NDP	C5A-C6A-N6A	5.47	135.33	123.43
52	E	400	NDP	C1B-N9A-C8A	5.44	139.41	127.14
54	Q	201	ZMP	C9-C10-S1	5.30	119.63	113.46
52	E	400	NDP	C5A-C4A-N3A	-5.30	119.84	126.75
47	6	201	3PE	O21-C21-C22	5.06	122.40	111.50
46	4	504	PLC	O2-C'-C1'	4.92	122.11	111.50
49	2	503	T7X	C6-C1-C2	4.66	117.58	110.85
47	4	503	3PE	O21-C21-C22	4.54	121.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	2	503	T7X	O16-C10-C12	4.48	121.15	111.50
51	E	402	CDL	OA6-CA5-C11	4.40	120.99	111.50
52	E	400	NDP	N9A-C8A-N7A	-4.38	107.93	113.91
47	5	701	3PE	O21-C21-C22	4.36	120.89	111.50
51	X	201	CDL	OB6-CB5-C51	4.31	120.79	111.50
50	2	502	CPL	O2-C31-C32	4.31	120.79	111.50
51	n	200	CDL	OA6-CA5-C11	4.26	120.68	111.50
51	W	402	CDL	OB6-CB5-C51	4.25	120.66	111.50
47	4	501	3PE	O21-C21-C22	4.25	120.65	111.50
51	X	201	CDL	OA6-CA5-C11	4.16	120.48	111.50
47	5	702	3PE	O21-C21-C22	4.16	120.47	111.50
51	n	200	CDL	OB6-CB5-C51	4.15	120.44	111.50
47	1	501	3PE	O21-C21-C22	4.14	120.43	111.50
46	W	401	PLC	O2-C'-C1'	4.13	120.41	111.50
51	W	402	CDL	OA6-CA5-C11	4.09	120.31	111.50
47	S	501	3PE	O21-C21-C22	4.06	120.24	111.50
51	Z	201	CDL	OA6-CA5-C11	4.04	120.21	111.50
49	3	201	T7X	O16-C10-C12	4.02	120.17	111.50
46	1	505	PLC	O2-C'-C1'	4.00	120.11	111.50
46	5	704	PLC	O2-C'-C1'	3.99	120.09	111.50
47	J	203	3PE	O21-C21-C22	3.98	120.09	111.50
45	B	502	FMN	C7M-C7-C6	-3.98	112.13	119.49
49	2	501	T7X	O16-C10-C12	3.96	120.04	111.50
51	g	201	CDL	OB6-CB5-C51	3.95	120.01	111.50
47	J	204	3PE	O21-C21-C22	3.94	119.99	111.50
47	1	503	3PE	O21-C21-C22	3.92	119.95	111.50
48	J	202	LMN	CCT-CCN-CCC	3.92	117.22	110.24
47	g	202	3PE	O21-C21-C22	3.91	119.93	111.50
47	E	401	3PE	O21-C21-C22	3.88	119.87	111.50
47	6	202	3PE	O21-C21-C22	3.86	119.82	111.50
47	1	504	3PE	O21-C21-C22	3.80	119.70	111.50
47	J	201	3PE	O21-C21-C22	3.75	119.58	111.50
51	g	201	CDL	OA6-CA5-C11	3.72	119.51	111.50
54	O	201	ZMP	O1-C10-C9	-3.64	119.69	123.99
51	Z	201	CDL	OB6-CB5-C51	3.63	119.32	111.50
47	b	201	3PE	O21-C21-C22	3.62	119.31	111.50
51	E	402	CDL	OB6-CB5-C51	3.62	119.30	111.50
47	4	502	3PE	O21-C21-C22	3.60	119.25	111.50
46	K	302	PLC	O2-C'-C1'	3.59	119.24	111.50
52	E	400	NDP	C2A-N3A-C4A	3.57	120.19	111.75
49	2	501	T7X	C6-C1-C2	3.56	115.99	110.85
48	J	202	LMN	OBY-CCC-CCN	3.56	116.16	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B	502	FMN	C4-N3-C2	-3.45	119.27	125.64
45	B	502	FMN	C7M-C7-C8	3.38	127.67	120.74
52	E	400	NDP	N3A-C4A-N9A	3.34	132.58	127.08
46	1	502	PLC	O2-C'-C1'	3.28	118.57	111.50
54	O	201	ZMP	C15-N2-C16	3.27	128.43	122.59
49	3	201	T7X	O1-C1-C6	3.26	116.24	108.66
52	E	400	NDP	C5A-N7A-C8A	3.25	108.13	103.51
48	J	202	LMN	CCL-CCH-CCQ	3.25	117.10	109.68
54	O	201	ZMP	C14-C15-N2	3.25	118.45	111.90
48	J	202	LMN	OCB-CCS-CCW	3.18	116.34	108.10
46	W	401	PLC	O3-CB-C1B	3.12	121.70	111.91
54	Q	201	ZMP	O1-C10-C9	-3.12	120.30	123.99
51	Z	201	CDL	OB8-CB7-C71	3.10	121.63	111.91
47	J	201	3PE	O31-C31-C32	3.09	121.60	111.91
49	2	501	T7X	C5-C6-C1	3.06	116.67	109.68
51	n	200	CDL	OB8-CB7-C71	3.01	121.35	111.91
54	O	201	ZMP	C12-N1-C13	-3.00	117.26	122.84
49	2	501	T7X	C12-C13-C14	-2.99	107.90	113.23
52	E	400	NDP	C2B-C1B-N9A	-2.96	108.55	113.53
48	J	202	LMN	OCB-CCQ-CCF	2.95	117.53	109.45
54	Q	201	ZMP	C11-S1-C10	2.94	111.02	101.87
54	O	201	ZMP	C19-C18-C17	2.94	113.91	108.82
51	g	201	CDL	OB8-CB7-C71	2.92	121.09	111.91
47	4	501	3PE	O31-C31-C32	2.91	121.03	111.91
49	2	503	T7X	O18-C11-C31	2.89	120.97	111.91
49	3	201	T7X	O18-C11-C31	2.85	120.85	111.91
47	J	203	3PE	O31-C31-C32	2.84	120.83	111.91
54	O	201	ZMP	C14-C13-N1	2.84	121.21	116.42
48	J	202	LMN	O5-C5-C4	2.83	115.73	109.75
49	2	503	T7X	C3-C2-C1	2.83	116.15	109.68
47	5	703	3PE	O21-C21-C22	2.82	117.57	111.50
47	S	501	3PE	O31-C31-C32	2.80	120.69	111.91
54	Q	201	ZMP	C15-C14-C13	-2.79	107.71	112.36
46	1	502	PLC	O3-CB-C1B	2.78	120.63	111.91
46	4	504	PLC	O3-CB-C1B	2.75	120.53	111.91
47	5	701	3PE	O31-C31-C32	2.74	120.52	111.91
51	E	402	CDL	OB8-CB7-C71	2.71	120.42	111.91
46	1	505	PLC	O3-CB-C1B	2.69	120.36	111.91
46	5	704	PLC	O3-CB-C1B	2.69	120.35	111.91
50	2	502	CPL	O3-C11-C12	2.65	120.24	111.91
46	K	302	PLC	O3-CB-C1B	2.65	120.22	111.91
51	Z	201	CDL	OA8-CA7-C31	2.64	120.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B	502	FMN	C4A-C4-N3	2.63	119.88	113.19
51	W	402	CDL	OB8-CB7-C71	2.62	120.14	111.91
51	X	201	CDL	OB8-CB7-C71	2.61	120.11	111.91
47	5	703	3PE	O31-C31-C32	2.61	120.11	111.91
51	g	201	CDL	OA8-CA7-C31	2.60	120.07	111.91
47	4	502	3PE	O31-C31-C32	2.59	120.05	111.91
47	6	202	3PE	O31-C31-C32	2.59	120.04	111.91
47	1	501	3PE	O31-C31-C32	2.59	120.03	111.91
47	g	202	3PE	O31-C31-C32	2.55	119.92	111.91
47	1	503	3PE	O31-C31-C32	2.54	119.89	111.91
54	Q	201	ZMP	C14-C15-N2	-2.53	106.78	111.90
49	2	501	T7X	O18-C11-C31	2.53	119.86	111.91
51	n	200	CDL	OA8-CA7-C31	2.51	119.78	111.91
48	j	101	LMN	CCR-O4-C4	-2.51	111.76	117.96
47	5	702	3PE	O31-C31-C32	2.50	119.75	111.91
47	b	201	3PE	O31-C31-C32	2.49	119.72	111.91
49	2	503	T7X	P1-O1-C1	2.47	128.40	119.41
46	1	502	PLC	C2-O2-C'	-2.45	111.77	117.79
45	B	502	FMN	C4A-C10-N1	-2.44	119.06	124.73
48	J	202	LMN	O5-C1-C2	-2.44	105.19	110.35
51	X	201	CDL	OA8-CA7-C31	2.43	119.54	111.91
54	Q	201	ZMP	C14-C13-N1	2.42	120.49	116.42
49	3	201	T7X	O1-C1-C2	2.41	114.28	108.66
51	E	402	CDL	OA8-CA7-C31	2.40	119.44	111.91
48	J	202	LMN	O3-C3-C2	-2.39	104.83	110.35
48	j	101	LMN	C2-C3-C4	2.38	115.11	109.68
52	E	400	NDP	C4A-N9A-C8A	2.38	108.31	105.73
48	J	202	LMN	CCS-OBZ-CCD	-2.38	109.02	113.69
45	B	502	FMN	C4-C4A-C10	2.36	120.76	116.79
45	B	502	FMN	C4A-C10-N10	2.34	119.90	116.48
47	J	204	3PE	O31-C31-C32	2.34	119.24	111.91
45	B	502	FMN	O4-C4-C4A	-2.32	120.45	126.60
47	5	702	3PE	C2-O21-C21	-2.31	112.10	117.79
47	4	503	3PE	O31-C31-C32	2.31	119.16	111.91
48	J	202	LMN	O4-C4-C3	2.29	113.36	107.28
47	6	201	3PE	O31-C31-C32	2.28	119.05	111.91
51	E	402	CDL	CA4-OA6-CA5	-2.26	112.22	117.79
47	E	401	3PE	O31-C31-C32	2.25	118.98	111.91
51	W	402	CDL	OA8-CA7-C31	2.22	118.88	111.91
45	B	502	FMN	C10-C4A-N5	-2.22	120.16	124.86
47	J	203	3PE	C3-C2-C1	-2.21	106.56	111.79
49	2	503	T7X	O12-P1-O1	2.20	115.46	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	Z	201	CDL	CB4-OB6-CB5	-2.20	112.38	117.79
47	4	503	3PE	C3-C2-C1	-2.19	106.61	111.79
49	3	201	T7X	C8-O16-C10	-2.19	112.41	117.79
48	j	101	LMN	CBL-CBR-CCM	-2.18	110.16	117.16
46	W	401	PLC	C3-C2-C1	-2.17	106.65	111.79
49	3	201	T7X	P1-O1-C1	2.17	127.29	119.41
49	2	503	T7X	C5-C6-C1	2.12	114.52	109.68
49	2	501	T7X	C3-C2-C1	2.11	114.51	109.68
47	1	501	3PE	C3-C2-C1	-2.11	106.80	111.79
51	g	201	CDL	CA6-CA4-CA3	-2.11	106.81	111.79
54	O	201	ZMP	O1-C10-S1	-2.10	119.88	122.61
52	E	400	NDP	C4A-C5A-N7A	-2.10	108.06	110.62
45	B	502	FMN	C9A-C5A-N5	-2.10	120.15	122.43
52	E	400	NDP	PN-O3-PA	-2.10	125.63	132.83
52	E	400	NDP	C6A-C5A-C4A	2.07	119.96	117.18
51	Z	201	CDL	C52-C51-CB5	-2.07	106.11	113.62
48	j	101	LMN	CCL-CCH-CCQ	2.07	114.40	109.68
54	O	201	ZMP	O2-C13-N1	-2.02	119.20	123.01
47	1	501	3PE	O21-C21-O22	-2.01	118.84	123.70
45	B	502	FMN	C10-N1-C2	2.01	120.92	116.90

There are no chirality outliers.

All (885) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	C3'-C4'-C5'-O5'
45	B	502	FMN	O4'-C4'-C5'-O5'
45	B	502	FMN	C4'-C5'-O5'-P
45	B	502	FMN	C5'-O5'-P-O1P
45	B	502	FMN	C5'-O5'-P-O2P
45	B	502	FMN	C5'-O5'-P-O3P
46	K	302	PLC	C1-O3P-P-O1P
46	K	302	PLC	C4-O4P-P-O3P
46	1	502	PLC	O4P-C4-C5-N
46	1	502	PLC	O'-C'-O2-C2
46	1	505	PLC	O4P-C4-C5-N
46	1	505	PLC	C1'-C'-O2-C2
46	1	505	PLC	O'-C'-O2-C2
46	1	505	PLC	C1-O3P-P-O2P
46	1	505	PLC	C4-O4P-P-O1P
46	1	505	PLC	C4-O4P-P-O2P
46	1	505	PLC	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
46	4	504	PLC	C1-O3P-P-O1P
46	4	504	PLC	C4-O4P-P-O1P
46	4	504	PLC	C4-O4P-P-O2P
46	4	504	PLC	C4-O4P-P-O3P
46	5	704	PLC	C1-O3P-P-O2P
46	5	704	PLC	C1-O3P-P-O4P
46	W	401	PLC	C4-O4P-P-O2P
47	S	501	3PE	C1-O11-P-O12
47	S	501	3PE	C1-O11-P-O13
47	S	501	3PE	C1-O11-P-O14
47	S	501	3PE	O13-C11-C12-N
47	1	501	3PE	C11-O13-P-O12
47	1	501	3PE	C22-C21-O21-C2
47	1	503	3PE	C1-O11-P-O12
47	1	503	3PE	C1-O11-P-O14
47	1	503	3PE	O13-C11-C12-N
47	1	503	3PE	O22-C21-O21-C2
47	1	504	3PE	O13-C11-C12-N
47	1	504	3PE	O32-C31-O31-C3
47	1	504	3PE	C32-C31-O31-C3
47	4	501	3PE	C11-O13-P-O11
47	4	501	3PE	C11-O13-P-O14
47	4	502	3PE	C1-O11-P-O12
47	4	502	3PE	C1-O11-P-O14
47	5	701	3PE	O13-C11-C12-N
47	5	701	3PE	C22-C21-O21-C2
47	5	702	3PE	O13-C11-C12-N
47	5	703	3PE	C11-O13-P-O14
47	6	201	3PE	C1-O11-P-O12
47	6	201	3PE	C1-O11-P-O13
47	6	201	3PE	C1-O11-P-O14
47	6	201	3PE	C11-O13-P-O14
47	6	202	3PE	C1-O11-P-O12
47	g	202	3PE	C1-O11-P-O12
47	g	202	3PE	C1-O11-P-O13
47	g	202	3PE	C1-O11-P-O14
47	g	202	3PE	C11-O13-P-O14
47	g	202	3PE	O13-C11-C12-N
47	E	401	3PE	C1-O11-P-O12
47	E	401	3PE	C1-O11-P-O13
47	E	401	3PE	C1-O11-P-O14
47	E	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
47	E	401	3PE	C11-O13-P-O12
47	E	401	3PE	O13-C11-C12-N
47	J	201	3PE	C1-O11-P-O12
47	J	201	3PE	C1-O11-P-O13
47	J	201	3PE	C1-O11-P-O14
47	J	201	3PE	C11-O13-P-O12
47	J	201	3PE	C11-O13-P-O14
47	J	201	3PE	O13-C11-C12-N
47	J	203	3PE	C1-O11-P-O12
47	J	203	3PE	C1-O11-P-O13
47	J	203	3PE	C1-O11-P-O14
47	J	203	3PE	C22-C21-O21-C2
47	J	204	3PE	O13-C11-C12-N
47	b	201	3PE	C1-O11-P-O14
48	j	101	LMN	C2-C1-O1-CBS
48	j	101	LMN	O5-C1-O1-CBS
48	j	101	LMN	CBK-CBQ-CCM-CBR
48	j	101	LMN	CBK-CBQ-CCM-CBS
48	j	101	LMN	CBK-CBQ-CCM-CBT
48	j	101	LMN	OBX-CCJ-OBV-CBT
48	j	101	LMN	CCL-CCJ-OBV-CBT
48	J	202	LMN	C2-C1-O1-CBS
48	J	202	LMN	O5-C1-O1-CBS
48	J	202	LMN	OBV-CBT-CCM-CBQ
48	J	202	LMN	OBV-CBT-CCM-CBR
49	2	501	T7X	C12-C10-O16-C8
49	2	503	T7X	C6-C1-O1-P1
49	2	503	T7X	C1-O1-P1-O12
49	2	503	T7X	C7-O13-P1-O1
49	2	503	T7X	C9-C8-O16-C10
49	2	503	T7X	C12-C10-O16-C8
49	2	503	T7X	O19-C11-O18-C9
49	2	503	T7X	C31-C11-O18-C9
49	2	503	T7X	C19-C20-C21-C22
49	3	201	T7X	C2-C1-O1-P1
49	3	201	T7X	C6-C1-O1-P1
49	3	201	T7X	C7-O13-P1-O1
49	3	201	T7X	C15-C16-C17-C18
50	2	502	CPL	C1-O3P-P-O1P
50	2	502	CPL	C1-O3P-P-O2P
51	E	402	CDL	CB2-C1-CA2-OA2
51	E	402	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	E	402	CDL	CB2-OB2-PB2-OB4
51	W	402	CDL	O1-C1-CA2-OA2
51	X	201	CDL	CA2-OA2-PA1-OA3
51	X	201	CDL	CA2-OA2-PA1-OA4
51	X	201	CDL	CA2-OA2-PA1-OA5
51	X	201	CDL	C11-CA5-OA6-CA4
51	X	201	CDL	OB7-CB5-OB6-CB4
51	X	201	CDL	C51-CB5-OB6-CB4
51	Z	201	CDL	CA3-OA5-PA1-OA4
51	Z	201	CDL	C11-CA5-OA6-CA4
51	Z	201	CDL	CB3-OB5-PB2-OB4
51	n	200	CDL	C1-CA2-OA2-PA1
51	n	200	CDL	CA3-OA5-PA1-OA2
51	n	200	CDL	CA3-OA5-PA1-OA3
51	n	200	CDL	CB3-OB5-PB2-OB3
51	n	200	CDL	CB3-OB5-PB2-OB4
51	n	200	CDL	OB7-CB5-OB6-CB4
52	E	400	NDP	C2B-O2B-P2B-O3X
52	E	400	NDP	O4D-C4D-C5D-O5D
54	O	201	ZMP	O4-C17-C18-C21
54	O	201	ZMP	C16-C17-C18-C21
54	O	201	ZMP	O4-C17-C18-C19
54	O	201	ZMP	C16-C17-C18-C19
54	O	201	ZMP	O4-C17-C18-C20
54	O	201	ZMP	C16-C17-C18-C20
54	O	201	ZMP	C13-C14-C15-N2
54	O	201	ZMP	C12-C11-S1-C10
54	O	201	ZMP	C7-C8-C9-C10
54	Q	201	ZMP	C20-C18-C21-O5
54	Q	201	ZMP	C17-C18-C21-O5
54	Q	201	ZMP	C12-C11-S1-C10
54	Q	201	ZMP	C7-C8-C9-C10
48	j	101	LMN	OBY-CCR-O4-C4
47	S	501	3PE	O32-C31-O31-C3
51	Z	201	CDL	OB9-CB7-OB8-CB6
51	n	200	CDL	OA9-CA7-OA8-CA6
47	S	501	3PE	C32-C31-O31-C3
51	n	200	CDL	C31-CA7-OA8-CA6
47	1	503	3PE	O32-C31-O31-C3
47	4	501	3PE	O32-C31-O31-C3
47	J	204	3PE	O32-C31-O31-C3
49	3	201	T7X	O19-C11-O18-C9

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Mol	Chain	Res	Type	Atoms
51	Z	201	CDL	OA9-CA7-OA8-CA6
51	n	200	CDL	OB9-CB7-OB8-CB6
54	O	201	ZMP	C14-C15-N2-C16
47	1	501	3PE	O22-C21-O21-C2
47	5	701	3PE	O22-C21-O21-C2
47	b	201	3PE	O22-C21-O21-C2
49	2	501	T7X	O17-C10-O16-C8
49	2	503	T7X	O17-C10-O16-C8
51	g	201	CDL	OA7-CA5-OA6-CA4
51	X	201	CDL	OA7-CA5-OA6-CA4
51	Z	201	CDL	OA7-CA5-OA6-CA4
51	n	200	CDL	OA7-CA5-OA6-CA4
47	4	501	3PE	C32-C31-O31-C3
47	J	204	3PE	C32-C31-O31-C3
49	3	201	T7X	C31-C11-O18-C9
51	Z	201	CDL	C31-CA7-OA8-CA6
51	Z	201	CDL	C71-CB7-OB8-CB6
46	1	502	PLC	C1'-C'-O2-C2
47	1	503	3PE	C22-C21-O21-C2
47	b	201	3PE	C22-C21-O21-C2
51	n	200	CDL	C51-CB5-OB6-CB4
46	1	505	PLC	OB-CB-O3-C3
48	J	202	LMN	OAL-CBP-CCF-OBX
46	1	505	PLC	C1B-CB-O3-C3
47	1	503	3PE	C32-C31-O31-C3
51	n	200	CDL	C71-CB7-OB8-CB6
47	J	203	3PE	O22-C21-O21-C2
51	W	402	CDL	OA7-CA5-OA6-CA4
51	E	402	CDL	O1-C1-CB2-OB2
47	4	503	3PE	C22-C21-O21-C2
47	5	702	3PE	C22-C21-O21-C2
47	5	703	3PE	C22-C21-O21-C2
47	g	202	3PE	C22-C21-O21-C2
47	J	201	3PE	C22-C21-O21-C2
51	g	201	CDL	C11-CA5-OA6-CA4
51	W	402	CDL	C11-CA5-OA6-CA4
51	n	200	CDL	C11-CA5-OA6-CA4
48	J	202	LMN	OAI-CBM-CCC-OBY
46	5	704	PLC	C2B-C3B-C4B-C5B
51	X	201	CDL	C71-C72-C73-C74
48	J	202	LMN	CCW-CCS-OCB-CCQ
47	1	501	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
47	6	202	3PE	C3D-C3E-C3F-C3G
48	J	202	LMN	OAI-CBM-CCC-CCN
47	J	201	3PE	O22-C21-O21-C2
48	J	202	LMN	OAL-CBP-CCF-CCQ
47	5	702	3PE	O22-C21-O21-C2
47	g	202	3PE	O22-C21-O21-C2
46	W	401	PLC	C4-C5-N-C8
46	K	302	PLC	C1B-CB-O3-C3
47	b	201	3PE	C32-C31-O31-C3
47	4	503	3PE	C29-C2A-C2B-C2C
47	4	503	3PE	O22-C21-O21-C2
46	1	502	PLC	CB-C1B-C2B-C3B
47	4	501	3PE	C21-C22-C23-C24
47	5	701	3PE	C21-C22-C23-C24
51	n	200	CDL	CB5-C51-C52-C53
46	K	302	PLC	OB-CB-O3-C3
51	X	201	CDL	C54-C55-C56-C57
48	j	101	LMN	OAI-CBM-CCC-OBY
48	J	202	LMN	CBC-CBE-CBG-CBI
47	4	502	3PE	C21-C22-C23-C24
47	E	401	3PE	C21-C22-C23-C24
48	J	202	LMN	OBZ-CCS-OCB-CCQ
51	Z	201	CDL	C72-C73-C74-C75
51	n	200	CDL	C60-C61-C62-C63
46	K	302	PLC	CB-C1B-C2B-C3B
46	1	502	PLC	C'-C1'-C2'-C3'
46	1	505	PLC	CB-C1B-C2B-C3B
46	4	504	PLC	CB-C1B-C2B-C3B
47	5	702	3PE	C21-C22-C23-C24
47	J	203	3PE	C31-C32-C33-C34
47	J	203	3PE	C21-C22-C23-C24
49	2	501	T7X	C10-C12-C13-C14
49	2	503	T7X	C10-C12-C13-C14
49	3	201	T7X	C10-C12-C13-C14
51	g	201	CDL	CA5-C11-C12-C13
51	X	201	CDL	CA7-C31-C32-C33
47	5	702	3PE	C2A-C2B-C2C-C2D
52	E	400	NDP	C3D-C4D-C5D-O5D
46	W	401	PLC	C4-C5-N-C7
47	1	503	3PE	C31-C32-C33-C34
47	1	504	3PE	C22-C21-O21-C2
47	b	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
51	E	402	CDL	O1-C1-CA2-OA2
47	1	504	3PE	O22-C21-O21-C2
47	5	703	3PE	O22-C21-O21-C2
46	K	302	PLC	C1-O3P-P-O4P
46	1	505	PLC	C1-O3P-P-O4P
46	W	401	PLC	C4-O4P-P-O3P
47	1	501	3PE	C1-O11-P-O13
47	1	501	3PE	C11-O13-P-O11
47	1	503	3PE	C1-O11-P-O13
47	4	502	3PE	C1-O11-P-O13
47	6	202	3PE	C1-O11-P-O13
47	g	202	3PE	C11-O13-P-O11
47	J	201	3PE	C11-O13-P-O11
47	b	201	3PE	C1-O11-P-O13
50	2	502	CPL	C1-O3P-P-O4P
51	W	402	CDL	CB3-OB5-PB2-OB2
51	Z	201	CDL	CA3-OA5-PA1-OA2
51	n	200	CDL	CB2-OB2-PB2-OB5
51	n	200	CDL	CB3-OB5-PB2-OB2
47	E	401	3PE	C31-C32-C33-C34
47	5	703	3PE	C32-C31-O31-C3
51	W	402	CDL	CB2-C1-CA2-OA2
48	J	202	LMN	OAJ-CBN-CCD-OBZ
47	5	703	3PE	C33-C34-C35-C36
47	6	202	3PE	C37-C38-C39-C3A
49	3	201	T7X	C12-C10-O16-C8
46	K	302	PLC	C6B-C7B-C8B-C9B
47	4	502	3PE	C32-C33-C34-C35
47	4	502	3PE	C36-C37-C38-C39
47	4	503	3PE	C36-C37-C38-C39
47	J	203	3PE	C36-C37-C38-C39
50	2	502	CPL	C20-C21-C22-C23
50	2	502	CPL	C33-C34-C35-C36
51	X	201	CDL	C31-C32-C33-C34
54	Q	201	ZMP	C19-C18-C21-O5
46	1	505	PLC	C1B-C2B-C3B-C4B
46	W	401	PLC	C2'-C3'-C4'-C5'
51	n	200	CDL	C14-C15-C16-C17
49	3	201	T7X	O17-C10-O16-C8
46	1	505	PLC	C2B-C3B-C4B-C5B
47	5	701	3PE	C34-C35-C36-C37
47	6	202	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
47	g	202	3PE	C34-C35-C36-C37
47	E	401	3PE	C32-C33-C34-C35
47	b	201	3PE	C25-C26-C27-C28
51	X	201	CDL	C58-C59-C60-C61
51	X	201	CDL	C60-C61-C62-C63
51	n	200	CDL	C54-C55-C56-C57
51	X	201	CDL	O1-C1-CA2-OA2
51	Z	201	CDL	O1-C1-CB2-OB2
47	1	504	3PE	C34-C35-C36-C37
47	4	503	3PE	C37-C38-C39-C3A
47	g	202	3PE	C2B-C2C-C2D-C2E
48	j	101	LMN	CCH-CCQ-OCB-CCS
51	E	402	CDL	C31-CA7-OA8-CA6
47	1	501	3PE	C38-C39-C3A-C3B
47	4	503	3PE	C33-C34-C35-C36
47	6	202	3PE	C32-C33-C34-C35
47	J	203	3PE	C23-C24-C25-C26
51	n	200	CDL	C33-C34-C35-C36
47	J	203	3PE	C38-C39-C3A-C3B
51	X	201	CDL	C32-C33-C34-C35
51	X	201	CDL	C51-C52-C53-C54
51	n	200	CDL	C59-C60-C61-C62
46	1	502	PLC	C2B-C3B-C4B-C5B
47	4	501	3PE	C2D-C2E-C2F-C2G
48	J	202	LMN	CBA-CBC-CBE-CBG
51	g	201	CDL	C51-C52-C53-C54
51	Z	201	CDL	C32-C33-C34-C35
46	W	401	PLC	C5B-C6B-C7B-C8B
47	E	401	3PE	C37-C38-C39-C3A
51	W	402	CDL	OB7-CB5-OB6-CB4
47	4	501	3PE	C22-C21-O21-C2
51	W	402	CDL	C51-CB5-OB6-CB4
47	1	501	3PE	C22-C23-C24-C25
47	g	202	3PE	C24-C25-C26-C27
48	j	101	LMN	CAY-CBA-CBC-CBE
51	n	200	CDL	C16-C17-C18-C19
46	W	401	PLC	C'-C1'-C2'-C3'
51	g	201	CDL	CA7-C31-C32-C33
47	1	501	3PE	C3C-C3D-C3E-C3F
47	1	501	3PE	C2E-C2F-C2G-C2H
47	4	501	3PE	C29-C2A-C2B-C2C
47	4	502	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
47	5	703	3PE	C32-C33-C34-C35
47	5	703	3PE	C3D-C3E-C3F-C3G
47	b	201	3PE	C2A-C2B-C2C-C2D
49	2	503	T7X	C36-C37-C38-C39
51	n	200	CDL	C74-C75-C76-C77
50	2	502	CPL	C44-C45-C46-C47
51	g	201	CDL	C38-C39-C40-C41
51	Z	201	CDL	C37-C38-C39-C40
47	4	502	3PE	O13-C11-C12-N
47	5	702	3PE	C33-C34-C35-C36
47	6	201	3PE	C26-C27-C28-C29
50	2	502	CPL	C32-C33-C34-C35
51	g	201	CDL	C22-C23-C24-C25
47	5	703	3PE	C21-C22-C23-C24
47	J	204	3PE	C21-C22-C23-C24
47	1	501	3PE	C2D-C2E-C2F-C2G
47	5	702	3PE	C32-C33-C34-C35
47	b	201	3PE	C23-C24-C25-C26
48	J	202	LMN	CBB-CBD-CBF-CBH
51	n	200	CDL	C37-C38-C39-C40
49	2	503	T7X	C34-C35-C36-C37
47	6	201	3PE	C34-C35-C36-C37
51	g	201	CDL	C14-C15-C16-C17
51	E	402	CDL	C11-C12-C13-C14
51	Z	201	CDL	CB3-CB4-CB6-OB8
47	J	203	3PE	C2B-C2C-C2D-C2E
47	g	202	3PE	C31-C32-C33-C34
47	5	703	3PE	C36-C37-C38-C39
48	J	202	LMN	C5-C4-O4-CCR
51	n	200	CDL	C72-C73-C74-C75
47	5	703	3PE	O32-C31-O31-C3
47	1	501	3PE	C28-C29-C2A-C2B
50	2	502	CPL	C18-C19-C20-C21
51	W	402	CDL	C31-CA7-OA8-CA6
47	5	701	3PE	C31-C32-C33-C34
46	1	502	PLC	C3'-C4'-C5'-C6'
47	4	501	3PE	O22-C21-O21-C2
48	J	202	LMN	OBV-CBT-CCM-CBS
54	O	201	ZMP	C2-C3-C4-C5
51	E	402	CDL	OA9-CA7-OA8-CA6
47	5	703	3PE	C22-C23-C24-C25
47	J	203	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
48	j	101	LMN	CCF-CCQ-OCB-CCS
48	J	202	LMN	C3-C4-O4-CCR
48	J	202	LMN	CCH-CCQ-OCB-CCS
51	E	402	CDL	C31-C32-C33-C34
46	W	401	PLC	C4-C5-N-C6
49	2	503	T7X	C31-C32-C33-C34
54	Q	201	ZMP	C1-C2-C3-C4
46	4	504	PLC	C1'-C'-O2-C2
46	5	704	PLC	C1'-C'-O2-C2
47	6	201	3PE	C28-C29-C2A-C2B
51	Z	201	CDL	C51-C52-C53-C54
46	4	504	PLC	C'-C1'-C2'-C3'
47	J	201	3PE	C31-C32-C33-C34
47	6	202	3PE	C3C-C3D-C3E-C3F
47	6	201	3PE	C35-C36-C37-C38
46	4	504	PLC	O'-C'-O2-C2
47	g	202	3PE	C27-C28-C29-C2A
47	b	201	3PE	C33-C34-C35-C36
46	1	505	PLC	C1'-C2'-C3'-C4'
51	X	201	CDL	C35-C36-C37-C38
51	X	201	CDL	C11-C12-C13-C14
51	W	402	CDL	OA9-CA7-OA8-CA6
47	4	503	3PE	C24-C25-C26-C27
47	6	202	3PE	C3E-C3F-C3G-C3H
48	J	202	LMN	CAY-CBA-CBC-CBE
51	E	402	CDL	C51-C52-C53-C54
46	W	401	PLC	C1'-C'-O2-C2
47	4	502	3PE	C26-C27-C28-C29
47	J	203	3PE	C24-C25-C26-C27
46	W	401	PLC	O'-C'-O2-C2
51	g	201	CDL	C15-C16-C17-C18
47	g	202	3PE	O21-C2-C3-O31
47	J	203	3PE	C32-C33-C34-C35
51	Z	201	CDL	C11-C12-C13-C14
47	S	501	3PE	C33-C34-C35-C36
47	1	503	3PE	C23-C24-C25-C26
47	4	503	3PE	C3D-C3E-C3F-C3G
48	j	101	LMN	CBJ-CBL-CBR-CCM
46	4	504	PLC	C6B-C7B-C8B-C9B
54	Q	201	ZMP	C5-C6-C7-C8
47	1	501	3PE	C26-C27-C28-C29
46	5	704	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
47	J	204	3PE	C22-C21-O21-C2
46	4	504	PLC	C3B-C4B-C5B-C6B
47	4	501	3PE	C26-C27-C28-C29
48	J	202	LMN	CAZ-CBB-CBD-CBF
47	5	703	3PE	C11-O13-P-O11
51	W	402	CDL	CA3-OA5-PA1-OA2
51	Z	201	CDL	CB3-OB5-PB2-OB2
47	4	503	3PE	C32-C31-O31-C3
47	5	702	3PE	O11-C1-C2-C3
47	5	703	3PE	O11-C1-C2-C3
51	Z	201	CDL	OB5-CB3-CB4-CB6
47	4	502	3PE	C22-C23-C24-C25
47	6	202	3PE	C31-C32-C33-C34
46	W	401	PLC	C1B-C2B-C3B-C4B
51	n	200	CDL	C41-C42-C43-C44
51	Z	201	CDL	C14-C15-C16-C17
49	2	503	T7X	C12-C13-C14-C15
49	2	503	T7X	C32-C33-C34-C35
51	g	201	CDL	CB2-C1-CA2-OA2
51	g	201	CDL	C16-C17-C18-C19
51	g	201	CDL	C78-C79-C80-C81
48	J	202	LMN	OBY-CCR-O4-C4
47	S	501	3PE	C32-C33-C34-C35
47	S	501	3PE	C3A-C3B-C3C-C3D
47	1	503	3PE	C24-C25-C26-C27
46	1	505	PLC	C1-C2-C3-O3
47	1	501	3PE	C1-C2-C3-O31
47	5	701	3PE	C28-C29-C2A-C2B
47	5	702	3PE	C1-C2-C3-O31
47	6	201	3PE	C1-C2-C3-O31
51	E	402	CDL	CA3-CA4-CA6-OA8
51	W	402	CDL	CA3-CA4-CA6-OA8
51	g	201	CDL	C74-C75-C76-C77
46	1	502	PLC	C1'-C2'-C3'-C4'
47	4	503	3PE	C38-C39-C3A-C3B
47	b	201	3PE	C29-C2A-C2B-C2C
46	1	505	PLC	C4'-C5'-C6'-C7'
46	4	504	PLC	C2'-C3'-C4'-C5'
47	1	504	3PE	C26-C27-C28-C29
47	5	701	3PE	C37-C38-C39-C3A
51	W	402	CDL	C32-C31-CA7-OA8
47	4	502	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	CB5-C51-C52-C53
54	O	201	ZMP	O3-C16-C17-O4
47	J	201	3PE	C3C-C3D-C3E-C3F
49	2	503	T7X	C1-O1-P1-O13
47	S	501	3PE	C26-C27-C28-C29
48	J	202	LMN	CCF-CCQ-OCB-CCS
51	W	402	CDL	CA5-C11-C12-C13
47	6	201	3PE	O21-C21-C22-C23
48	j	101	LMN	OAL-CBP-CCF-CCQ
47	1	501	3PE	C3B-C3C-C3D-C3E
51	n	200	CDL	C57-C58-C59-C60
47	5	703	3PE	C3F-C3G-C3H-C3I
51	g	201	CDL	C79-C80-C81-C82
51	Z	201	CDL	C13-C14-C15-C16
47	4	503	3PE	C2F-C2G-C2H-C2I
50	2	502	CPL	C34-C35-C36-C37
47	4	501	3PE	O11-C1-C2-O21
51	g	201	CDL	OA5-CA3-CA4-OA6
47	4	503	3PE	C31-C32-C33-C34
51	W	402	CDL	C54-C55-C56-C57
51	g	201	CDL	O1-C1-CA2-OA2
47	6	202	3PE	C3B-C3C-C3D-C3E
47	4	503	3PE	C32-C33-C34-C35
48	J	202	LMN	CBH-CBJ-CBL-CBR
51	g	201	CDL	C72-C71-CB7-OB8
47	4	502	3PE	O21-C2-C3-O31
47	5	702	3PE	O21-C2-C3-O31
47	6	201	3PE	O21-C2-C3-O31
49	2	501	T7X	O16-C8-C9-O18
47	4	503	3PE	O32-C31-O31-C3
46	4	504	PLC	C1'-C2'-C3'-C4'
47	5	702	3PE	C27-C28-C29-C2A
48	J	202	LMN	CAX-CAZ-CBB-CBD
46	5	704	PLC	C4'-C5'-C6'-C7'
47	5	703	3PE	C24-C25-C26-C27
46	5	704	PLC	C1B-CB-O3-C3
46	W	401	PLC	C6B-C7B-C8B-C9B
47	b	201	3PE	C32-C33-C34-C35
47	E	401	3PE	C33-C34-C35-C36
47	6	201	3PE	C24-C25-C26-C27
47	5	702	3PE	C32-C31-O31-C3
47	g	202	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	4	501	3PE	C34-C35-C36-C37
47	J	203	3PE	C39-C3A-C3B-C3C
51	n	200	CDL	C34-C35-C36-C37
48	J	202	LMN	CBJ-CBL-CBR-CCM
47	4	502	3PE	C3B-C3C-C3D-C3E
47	4	501	3PE	O11-C1-C2-C3
47	6	202	3PE	O11-C1-C2-C3
47	g	202	3PE	O11-C1-C2-C3
47	b	201	3PE	O11-C1-C2-C3
49	2	503	T7X	O13-C7-C8-C9
51	E	402	CDL	OA5-CA3-CA4-CA6
51	Z	201	CDL	OA5-CA3-CA4-CA6
47	4	501	3PE	C24-C25-C26-C27
47	J	204	3PE	O22-C21-O21-C2
46	1	502	PLC	C1B-C2B-C3B-C4B
47	1	501	3PE	C36-C37-C38-C39
50	2	502	CPL	C17-C18-C19-C20
51	Z	201	CDL	C56-C57-C58-C59
47	J	204	3PE	C2-C1-O11-P
51	g	201	CDL	C1-CB2-OB2-PB2
51	X	201	CDL	CA4-CA3-OA5-PA1
46	W	401	PLC	C6'-C7'-C8'-C9'
47	S	501	3PE	C36-C37-C38-C39
47	b	201	3PE	C35-C36-C37-C38
47	b	201	3PE	C38-C39-C3A-C3B
49	3	201	T7X	C31-C32-C33-C34
51	n	200	CDL	C76-C77-C78-C79
46	4	504	PLC	C1-C2-C3-O3
47	5	703	3PE	C1-C2-C3-O31
47	g	202	3PE	C1-C2-C3-O31
47	E	401	3PE	C1-C2-C3-O31
51	X	201	CDL	CA3-CA4-CA6-OA8
47	4	501	3PE	C28-C29-C2A-C2B
51	Z	201	CDL	CA5-C11-C12-C13
47	1	501	3PE	C2F-C2G-C2H-C2I
47	4	502	3PE	C37-C38-C39-C3A
49	2	503	T7X	C1-O1-P1-O11
47	1	503	3PE	C22-C23-C24-C25
47	1	503	3PE	C25-C26-C27-C28
47	6	201	3PE	C32-C33-C34-C35
51	g	201	CDL	C72-C73-C74-C75
54	O	201	ZMP	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
50	2	502	CPL	C39-C40-C41-C42
51	E	402	CDL	CB2-OB2-PB2-OB5
47	1	503	3PE	C35-C36-C37-C38
47	4	503	3PE	C39-C3A-C3B-C3C
48	J	202	LMN	C4-C5-C6-O6
46	4	504	PLC	C2B-C3B-C4B-C5B
49	2	503	T7X	C33-C34-C35-C36
47	5	702	3PE	O11-C1-C2-O21
47	b	201	3PE	O11-C1-C2-O21
51	X	201	CDL	OA5-CA3-CA4-OA6
51	Z	201	CDL	OA5-CA3-CA4-OA6
51	n	200	CDL	OA5-CA3-CA4-OA6
49	3	201	T7X	C32-C33-C34-C35
46	1	505	PLC	O2-C2-C3-O3
46	4	504	PLC	O2-C2-C3-O3
47	6	202	3PE	O21-C2-C3-O31
47	E	401	3PE	O21-C2-C3-O31
47	J	204	3PE	O21-C2-C3-O31
51	E	402	CDL	CA2-C1-CB2-OB2
47	1	501	3PE	C29-C2A-C2B-C2C
47	1	504	3PE	C38-C39-C3A-C3B
51	g	201	CDL	C44-C45-C46-C47
47	b	201	3PE	C2D-C2E-C2F-C2G
51	n	200	CDL	C64-C65-C66-C67
47	1	503	3PE	C2-C1-O11-P
47	g	202	3PE	C2-C1-O11-P
46	5	704	PLC	OB-CB-O3-C3
51	E	402	CDL	C12-C13-C14-C15
54	O	201	ZMP	O1-C10-S1-C11
47	g	202	3PE	C21-C22-C23-C24
51	Z	201	CDL	C15-C16-C17-C18
51	E	402	CDL	C13-C14-C15-C16
47	1	501	3PE	C3D-C3E-C3F-C3G
50	2	502	CPL	C21-C22-C23-C24
47	g	202	3PE	O32-C31-O31-C3
51	g	201	CDL	OA5-CA3-CA4-CA6
51	W	402	CDL	C32-C33-C34-C35
48	j	101	LMN	OAI-CBM-CCC-CCN
47	1	503	3PE	C28-C29-C2A-C2B
52	E	400	NDP	O4D-C1D-N1N-C6N
47	b	201	3PE	C37-C38-C39-C3A
51	Z	201	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
47	5	702	3PE	O32-C31-O31-C3
48	j	101	LMN	CBH-CBJ-CBL-CBR
46	K	302	PLC	C1'-C'-O2-C2
51	X	201	CDL	C52-C53-C54-C55
54	O	201	ZMP	N2-C16-C17-O4
47	5	703	3PE	C37-C38-C39-C3A
50	2	502	CPL	C12-C13-C14-C15
51	Z	201	CDL	C38-C39-C40-C41
47	1	503	3PE	C34-C35-C36-C37
51	Z	201	CDL	C33-C34-C35-C36
49	2	501	T7X	C7-C8-O16-C10
51	W	402	CDL	CA6-CA4-OA6-CA5
51	X	201	CDL	CA6-CA4-OA6-CA5
54	O	201	ZMP	C9-C10-S1-C11
46	K	302	PLC	O'-C'-O2-C2
47	6	201	3PE	C21-C22-C23-C24
47	4	503	3PE	C3C-C3D-C3E-C3F
50	2	502	CPL	C12-C11-O3-C3
45	B	502	FMN	O2'-C2'-C3'-C4'
48	J	202	LMN	OBX-CCJ-OBV-CBT
46	1	502	PLC	C1-C2-C3-O3
46	W	401	PLC	C1-C2-C3-O3
47	5	701	3PE	C1-C2-C3-O31
47	6	202	3PE	C1-C2-C3-O31
51	Z	201	CDL	CA4-CA3-OA5-PA1
51	n	200	CDL	C61-C62-C63-C64
47	6	202	3PE	O11-C1-C2-O21
49	2	503	T7X	O13-C7-C8-O16
51	E	402	CDL	OA5-CA3-CA4-OA6
51	Z	201	CDL	OB5-CB3-CB4-OB6
47	J	201	3PE	C23-C24-C25-C26
47	6	202	3PE	C3F-C3G-C3H-C3I
51	X	201	CDL	C14-C15-C16-C17
51	Z	201	CDL	CB2-C1-CA2-OA2
51	n	200	CDL	CB2-C1-CA2-OA2
46	K	302	PLC	O2-C2-C3-O3
46	1	502	PLC	O2-C2-C3-O3
47	1	501	3PE	O21-C2-C3-O31
51	W	402	CDL	OA6-CA4-CA6-OA8
51	X	201	CDL	OA6-CA4-CA6-OA8
48	J	202	LMN	O1-CBS-CCM-CBQ
46	W	401	PLC	C8B-C9B-CAA-CBA

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Mol	Chain	Res	Type	Atoms
50	2	502	CPL	C43-C44-C45-C46
46	1	502	PLC	C3B-C4B-C5B-C6B
47	S	501	3PE	C23-C24-C25-C26
47	4	501	3PE	C2E-C2F-C2G-C2H
47	J	203	3PE	C25-C26-C27-C28
49	3	201	T7X	C11-C31-C32-C33
51	n	200	CDL	C75-C76-C77-C78
47	5	702	3PE	C26-C27-C28-C29
47	J	203	3PE	C3A-C3B-C3C-C3D
47	5	701	3PE	C38-C39-C3A-C3B
46	4	504	PLC	C1-O3P-P-O4P
47	6	201	3PE	C11-O13-P-O11
51	E	402	CDL	CA2-OA2-PA1-OA5
47	1	504	3PE	C29-C2A-C2B-C2C
47	g	202	3PE	C25-C26-C27-C28
47	5	702	3PE	C34-C35-C36-C37
46	K	302	PLC	C1-O3P-P-O2P
46	1	502	PLC	C1-O3P-P-O2P
46	1	505	PLC	C1-O3P-P-O1P
46	5	704	PLC	C1-O3P-P-O1P
46	W	401	PLC	C4-O4P-P-O1P
47	1	501	3PE	C1-O11-P-O12
47	1	501	3PE	C1-O11-P-O14
47	1	504	3PE	C1-O11-P-O12
47	4	503	3PE	C1-O11-P-O12
47	5	703	3PE	C11-O13-P-O12
47	6	202	3PE	C1-O11-P-O14
47	E	401	3PE	C11-O13-P-O14
51	E	402	CDL	CB2-OB2-PB2-OB3
51	W	402	CDL	CA2-OA2-PA1-OA3
51	W	402	CDL	CA3-OA5-PA1-OA3
51	W	402	CDL	CB3-OB5-PB2-OB3
51	W	402	CDL	CB3-OB5-PB2-OB4
51	X	201	CDL	CB2-OB2-PB2-OB4
51	Z	201	CDL	CB3-OB5-PB2-OB3
51	n	200	CDL	CB2-OB2-PB2-OB4
46	4	504	PLC	O3P-C1-C2-C3
46	5	704	PLC	O3P-C1-C2-C3
47	J	203	3PE	O11-C1-C2-C3
51	n	200	CDL	OA5-CA3-CA4-CA6
51	E	402	CDL	C37-C38-C39-C40
47	1	501	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
48	j	101	LMN	OAL-CBP-CCF-OBX
47	J	204	3PE	C33-C34-C35-C36
46	4	504	PLC	O3P-C1-C2-O2
46	5	704	PLC	O3P-C1-C2-O2
47	5	703	3PE	O11-C1-C2-O21
47	g	202	3PE	O11-C1-C2-O21
47	J	203	3PE	O11-C1-C2-O21
51	E	402	CDL	CA5-C11-C12-C13
47	5	703	3PE	C26-C27-C28-C29
50	2	502	CPL	O11-C11-O3-C3
46	W	401	PLC	O2-C'-C1'-C2'
47	5	701	3PE	C26-C27-C28-C29
51	n	200	CDL	C39-C40-C41-C42
46	K	302	PLC	C1-C2-C3-O3
46	K	302	PLC	O4P-C4-C5-N
47	J	204	3PE	C1-C2-C3-O31
51	g	201	CDL	C33-C34-C35-C36
47	5	701	3PE	O21-C2-C3-O31
47	5	703	3PE	O21-C2-C3-O31
51	Z	201	CDL	OB6-CB4-CB6-OB8
51	n	200	CDL	C1-CB2-OB2-PB2
51	g	201	CDL	C43-C44-C45-C46
51	Z	201	CDL	C73-C74-C75-C76
47	6	201	3PE	C33-C34-C35-C36
49	2	501	T7X	C11-C31-C32-C33
48	j	101	LMN	C4-C5-C6-O6
47	5	703	3PE	C3E-C3F-C3G-C3H
49	2	501	T7X	C32-C33-C34-C35
51	g	201	CDL	C37-C38-C39-C40
47	6	201	3PE	C25-C26-C27-C28
46	1	505	PLC	C2'-C3'-C4'-C5'
48	j	101	LMN	OAJ-CBN-CCD-OBZ
46	K	302	PLC	C3-C2-O2-C'
51	X	201	CDL	CB2-C1-CA2-OA2
47	6	201	3PE	C2A-C2B-C2C-C2D
49	2	503	T7X	C8-C7-O13-P1
47	4	502	3PE	C35-C36-C37-C38
47	J	204	3PE	C23-C24-C25-C26
47	4	503	3PE	O31-C31-C32-C33
51	E	402	CDL	C51-CB5-OB6-CB4
51	E	402	CDL	C38-C39-C40-C41
51	E	402	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
51	Z	201	CDL	OA6-CA4-CA6-OA8
46	W	401	PLC	C1-O3P-P-O4P
47	5	702	3PE	C11-O13-P-O11
47	6	202	3PE	C11-O13-P-O11
47	J	204	3PE	C1-O11-P-O13
51	g	201	CDL	CB2-OB2-PB2-OB5
47	b	201	3PE	C21-C22-C23-C24
46	1	502	PLC	C5'-C6'-C7'-C8'
51	X	201	CDL	C41-C42-C43-C44
47	4	502	3PE	C1-C2-C3-O31
49	2	501	T7X	C7-C8-C9-O18
51	Z	201	CDL	CA3-CA4-CA6-OA8
51	X	201	CDL	C57-C58-C59-C60
47	4	501	3PE	C32-C33-C34-C35
47	5	702	3PE	C22-C23-C24-C25
46	K	302	PLC	C3'-C4'-C5'-C6'
51	W	402	CDL	C32-C31-CA7-OA9
47	6	202	3PE	O21-C21-C22-C23
51	Z	201	CDL	O1-C1-CA2-OA2
46	4	504	PLC	C2-C1-O3P-P
51	W	402	CDL	CB4-CB3-OB5-PB2
51	g	201	CDL	C31-C32-C33-C34
47	g	202	3PE	C2C-C2D-C2E-C2F
47	S	501	3PE	C3D-C3E-C3F-C3G
47	1	501	3PE	C24-C25-C26-C27
47	6	202	3PE	C38-C39-C3A-C3B
47	J	201	3PE	C3A-C3B-C3C-C3D
49	2	503	T7X	C25-C26-C27-C28
51	X	201	CDL	C53-C54-C55-C56
48	J	202	LMN	CCV-CCR-O4-C4
47	5	703	3PE	C23-C24-C25-C26
51	E	402	CDL	OB7-CB5-OB6-CB4
45	B	502	FMN	C2'-C1'-N10-C10
51	n	200	CDL	C63-C64-C65-C66
50	2	502	CPL	C45-C46-C47-C48
46	W	401	PLC	C4'-C5'-C6'-C7'
46	1	505	PLC	C5B-C6B-C7B-C8B
47	6	201	3PE	O22-C21-C22-C23
51	g	201	CDL	C72-C71-CB7-OB9
46	5	704	PLC	C1'-C2'-C3'-C4'
47	1	501	3PE	C1-C2-O21-C21
47	1	504	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
48	J	202	LMN	CBF-CBH-CBJ-CBL
50	2	502	CPL	C42-C43-C44-C45
47	5	702	3PE	C28-C29-C2A-C2B
46	1	502	PLC	C1-O3P-P-O4P
47	4	503	3PE	C1-O11-P-O13
49	2	501	T7X	C16-C17-C18-C19
49	2	503	T7X	C15-C16-C17-C18
49	3	201	T7X	C18-C19-C20-C21
50	2	502	CPL	C40-C41-C42-C43
51	W	402	CDL	CA2-OA2-PA1-OA5
46	K	302	PLC	C5B-C6B-C7B-C8B
46	4	504	PLC	C4B-C5B-C6B-C7B
49	2	501	T7X	C34-C35-C36-C37
51	W	402	CDL	C1-CA2-OA2-PA1
47	J	203	3PE	C27-C28-C29-C2A
47	4	502	3PE	O11-C1-C2-O21
47	6	201	3PE	O11-C1-C2-C3
50	2	502	CPL	O3P-C1-C2-C3
48	J	202	LMN	OAJ-CBN-CCD-CCO
47	S	501	3PE	C24-C25-C26-C27
51	n	200	CDL	OB6-CB4-CB6-OB8
51	W	402	CDL	C12-C13-C14-C15
51	g	201	CDL	CB5-C51-C52-C53
47	5	702	3PE	C24-C25-C26-C27
51	E	402	CDL	C33-C34-C35-C36
46	1	505	PLC	C7B-C8B-C9B-CAA
51	g	201	CDL	C32-C33-C34-C35
51	g	201	CDL	C13-C14-C15-C16
47	4	501	3PE	C23-C24-C25-C26
47	J	201	3PE	O31-C31-C32-C33
47	4	501	3PE	C2C-C2D-C2E-C2F
46	1	505	PLC	C4B-C5B-C6B-C7B
47	b	201	3PE	C27-C28-C29-C2A
47	6	201	3PE	O11-C1-C2-O21
51	E	402	CDL	OB5-CB3-CB4-OB6
47	S	501	3PE	C39-C3A-C3B-C3C
47	6	202	3PE	C39-C3A-C3B-C3C
54	O	201	ZMP	O2-C13-C14-C15
46	4	504	PLC	C5B-C6B-C7B-C8B
47	1	504	3PE	O31-C31-C32-C33
46	1	505	PLC	C6'-C7'-C8'-C9'
51	g	201	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
47	5	701	3PE	C1-O11-P-O13
46	5	704	PLC	C4-C5-N-C7
47	5	701	3PE	C25-C26-C27-C28
47	5	702	3PE	C2C-C2D-C2E-C2F
49	2	501	T7X	C13-C14-C15-C16
47	1	501	3PE	C3-C2-O21-C21
47	J	204	3PE	O21-C21-C22-C23
49	2	501	T7X	O16-C10-C12-C13
45	B	502	FMN	O2'-C2'-C3'-O3'
51	g	201	CDL	C19-C20-C21-C22
49	2	503	T7X	C37-C38-C39-C40
52	E	400	NDP	O4B-C4B-C5B-O5B
47	6	202	3PE	O31-C31-C32-C33
47	J	204	3PE	O31-C31-C32-C33
51	X	201	CDL	C13-C14-C15-C16
47	S	501	3PE	C35-C36-C37-C38
47	J	201	3PE	C22-C23-C24-C25
51	g	201	CDL	C32-C31-CA7-OA8
54	Q	201	ZMP	C4-C5-C6-C7
47	6	201	3PE	O31-C31-C32-C33
47	4	502	3PE	O31-C31-C32-C33
47	4	502	3PE	O21-C21-C22-C23
47	4	503	3PE	O21-C21-C22-C23
48	J	202	LMN	O1-CBS-CCM-CBR
46	1	502	PLC	C4B-C5B-C6B-C7B
48	J	202	LMN	CAW-CAY-CBA-CBC
47	1	503	3PE	C32-C33-C34-C35
47	b	201	3PE	O21-C21-C22-C23
51	W	402	CDL	C72-C71-CB7-OB8
51	W	402	CDL	C52-C53-C54-C55
49	2	503	T7X	C13-C14-C15-C16
47	1	504	3PE	C22-C23-C24-C25
47	5	701	3PE	C23-C24-C25-C26
51	n	200	CDL	C12-C11-CA5-OA6
51	X	201	CDL	C62-C63-C64-C65
47	J	204	3PE	C25-C26-C27-C28
51	g	201	CDL	C32-C31-CA7-OA9
47	1	501	3PE	C32-C31-O31-C3
47	J	204	3PE	O22-C21-C22-C23
47	4	503	3PE	C2E-C2F-C2G-C2H
47	J	203	3PE	C35-C36-C37-C38
46	K	302	PLC	O2-C'-C1'-C2'

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Mol	Chain	Res	Type	Atoms
47	1	503	3PE	C33-C34-C35-C36
47	1	504	3PE	C1-O11-P-O13
46	1	505	PLC	C5'-C6'-C7'-C8'
51	g	201	CDL	C23-C24-C25-C26
47	4	502	3PE	O32-C31-C32-C33
51	E	402	CDL	C73-C74-C75-C76
46	5	704	PLC	C4-C5-N-C8
46	5	704	PLC	C4-O4P-P-O1P
46	W	401	PLC	C1-O3P-P-O1P
47	S	501	3PE	C11-O13-P-O14
47	6	202	3PE	C11-O13-P-O14
49	2	501	T7X	C7-O13-P1-O11
51	g	201	CDL	CB2-OB2-PB2-OB3
51	E	402	CDL	CB3-OB5-PB2-OB3
51	W	402	CDL	CA3-OA5-PA1-OA4
51	Z	201	CDL	CA2-OA2-PA1-OA3
46	W	401	PLC	O2-C2-C3-O3
47	1	504	3PE	O32-C31-C32-C33
49	2	501	T7X	O17-C10-C12-C13
47	4	502	3PE	O11-C1-C2-C3
48	j	101	LMN	CBG-CBI-CBK-CBQ
47	J	203	3PE	O13-C11-C12-N
47	6	202	3PE	O32-C31-C32-C33
47	J	204	3PE	O32-C31-C32-C33
46	1	505	PLC	O2-C'-C1'-C2'
51	E	402	CDL	C52-C51-CB5-OB6
49	3	201	T7X	C33-C34-C35-C36
51	E	402	CDL	C55-C56-C57-C58
51	X	201	CDL	C61-C62-C63-C64
47	1	501	3PE	O31-C31-C32-C33
49	2	503	T7X	O18-C11-C31-C32
51	E	402	CDL	C71-C72-C73-C74
51	X	201	CDL	C64-C65-C66-C67
46	1	505	PLC	C5-C4-O4P-P
47	b	201	3PE	C12-C11-O13-P
47	1	501	3PE	O32-C31-O31-C3
51	W	402	CDL	C31-C32-C33-C34
48	J	202	LMN	CBE-CBG-CBI-CBK
47	1	503	3PE	O31-C31-C32-C33
47	J	203	3PE	O31-C31-C32-C33
47	J	203	3PE	O21-C21-C22-C23
47	S	501	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
48	j	101	LMN	CBA-CBC-CBE-CBG
47	4	502	3PE	O22-C21-C22-C23
46	5	704	PLC	C3B-C4B-C5B-C6B
47	1	503	3PE	O21-C21-C22-C23
47	6	201	3PE	O32-C31-C32-C33
46	1	505	PLC	C2-C1-O3P-P
49	3	201	T7X	C8-C7-O13-P1
47	J	201	3PE	C25-C26-C27-C28
46	K	302	PLC	O'-C'-C1'-C2'
47	4	503	3PE	O22-C21-C22-C23
47	J	203	3PE	O32-C31-C32-C33
47	J	203	3PE	O22-C21-C22-C23
51	W	402	CDL	C72-C71-CB7-OB9
47	5	703	3PE	O31-C31-C32-C33
51	Z	201	CDL	C39-C40-C41-C42
47	5	703	3PE	O32-C31-C32-C33
47	J	201	3PE	O21-C21-C22-C23
51	E	402	CDL	C32-C31-CA7-OA8
47	J	203	3PE	C34-C35-C36-C37
47	b	201	3PE	O22-C21-C22-C23
49	2	503	T7X	O19-C11-C31-C32
51	n	200	CDL	C12-C11-CA5-OA7
51	n	200	CDL	O1-C1-CA2-OA2
46	1	505	PLC	C2B-C1B-CB-O3
51	n	200	CDL	C72-C71-CB7-OB8
51	E	402	CDL	C52-C51-CB5-OB7
46	5	704	PLC	C4-C5-N-C6
51	Z	201	CDL	C35-C36-C37-C38

There are no ring outliers.

40 monomers are involved in 151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	5	701	3PE	5	0
46	4	504	PLC	1	0
51	W	402	CDL	3	0
47	5	702	3PE	3	0
43	K	301	SF4	1	0
47	1	504	3PE	8	0
51	E	402	CDL	9	0
46	1	502	PLC	1	0
46	5	704	PLC	1	0

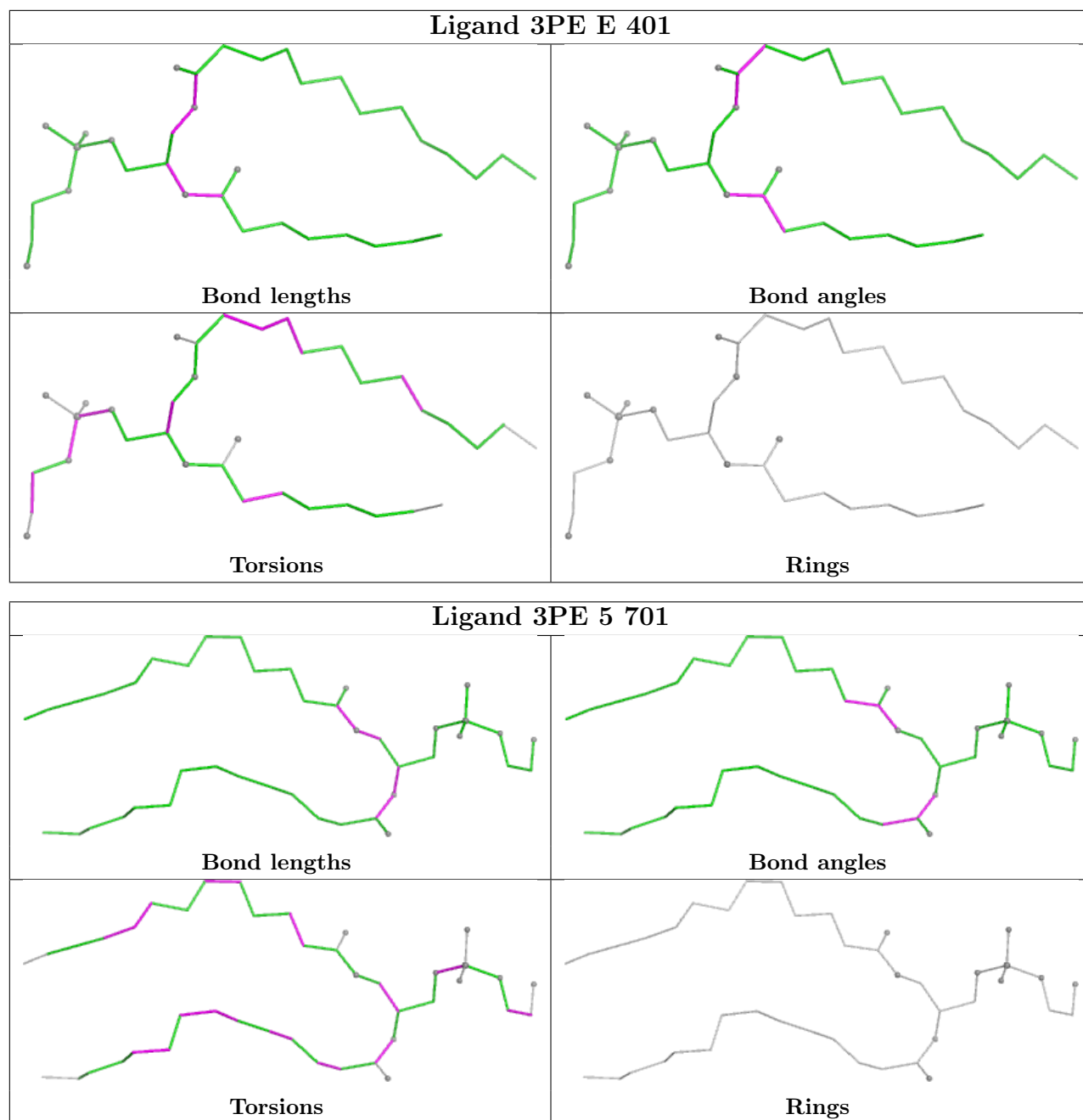
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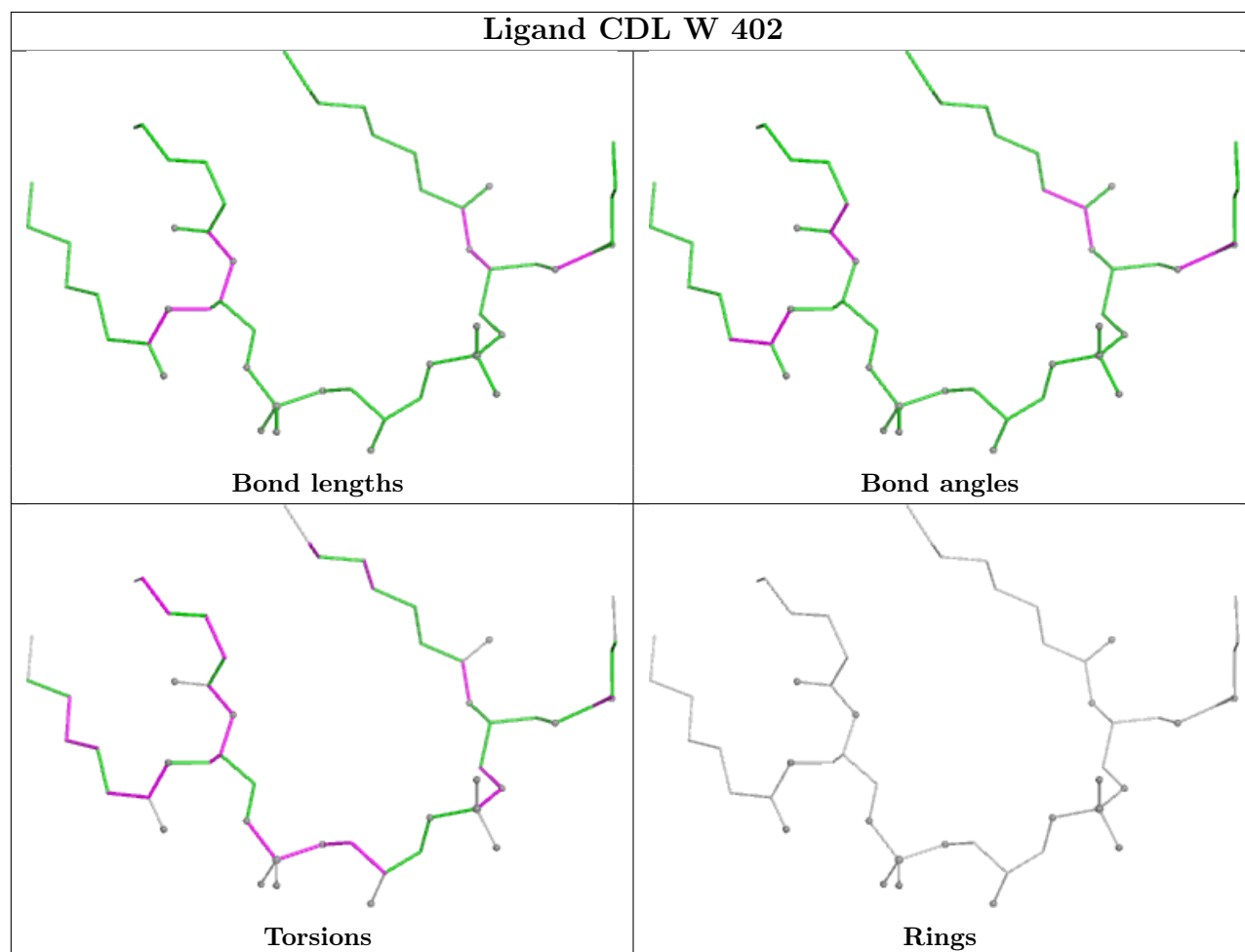
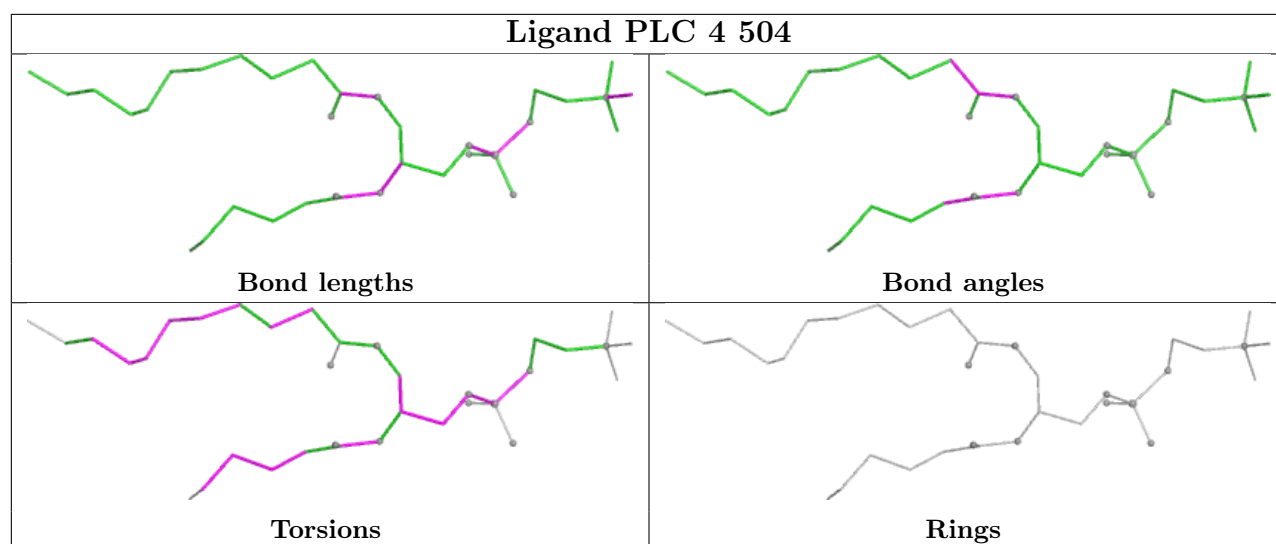
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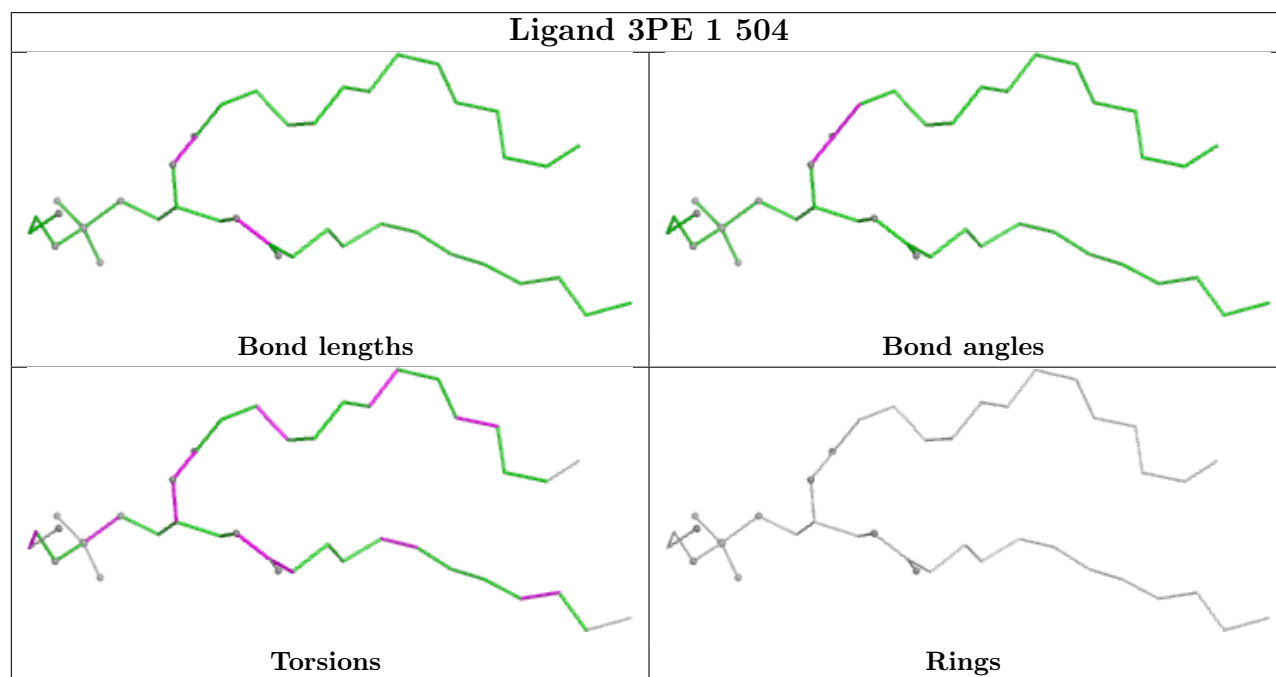
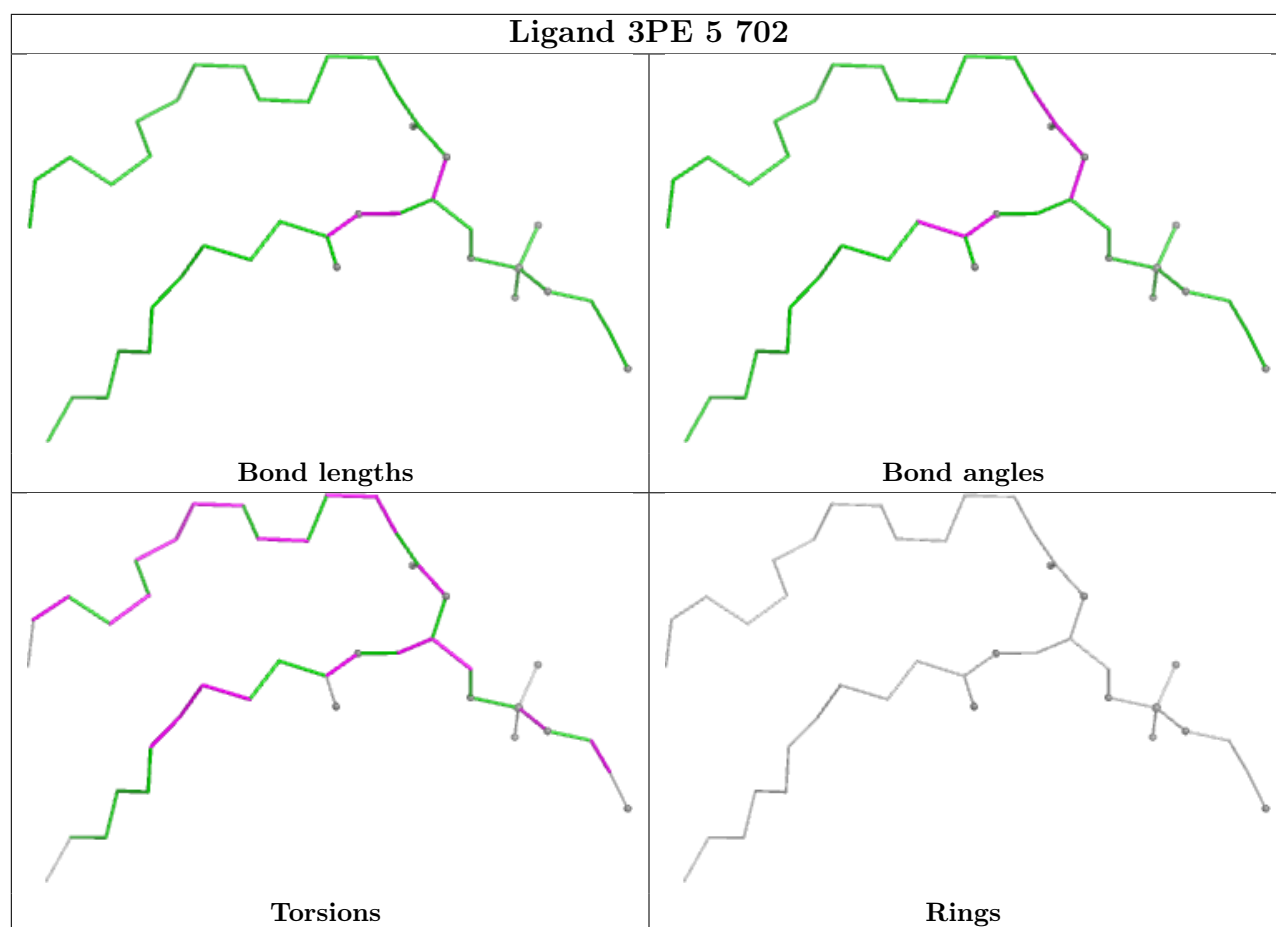
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	5	703	3PE	7	0
47	6	201	3PE	2	0
45	B	502	FMN	2	0
47	4	501	3PE	6	0
48	J	202	LMN	9	0
48	j	101	LMN	5	0
47	g	202	3PE	4	0
50	2	502	CPL	3	0
46	W	401	PLC	1	0
47	1	503	3PE	2	0
51	g	201	CDL	7	0
54	O	201	ZMP	3	0
47	6	202	3PE	4	0
51	X	201	CDL	10	0
47	4	502	3PE	1	0
44	A	803	FES	1	0
47	4	503	3PE	7	0
47	J	204	3PE	4	0
46	K	302	PLC	3	0
49	3	201	T7X	1	0
49	2	503	T7X	1	0
52	E	400	NDP	1	0
54	Q	201	ZMP	3	0
47	J	201	3PE	3	0
46	1	505	PLC	3	0
47	J	203	3PE	5	0
51	Z	201	CDL	5	0
47	1	501	3PE	4	0
51	n	200	CDL	13	0
47	b	201	3PE	7	0
47	S	501	3PE	2	0

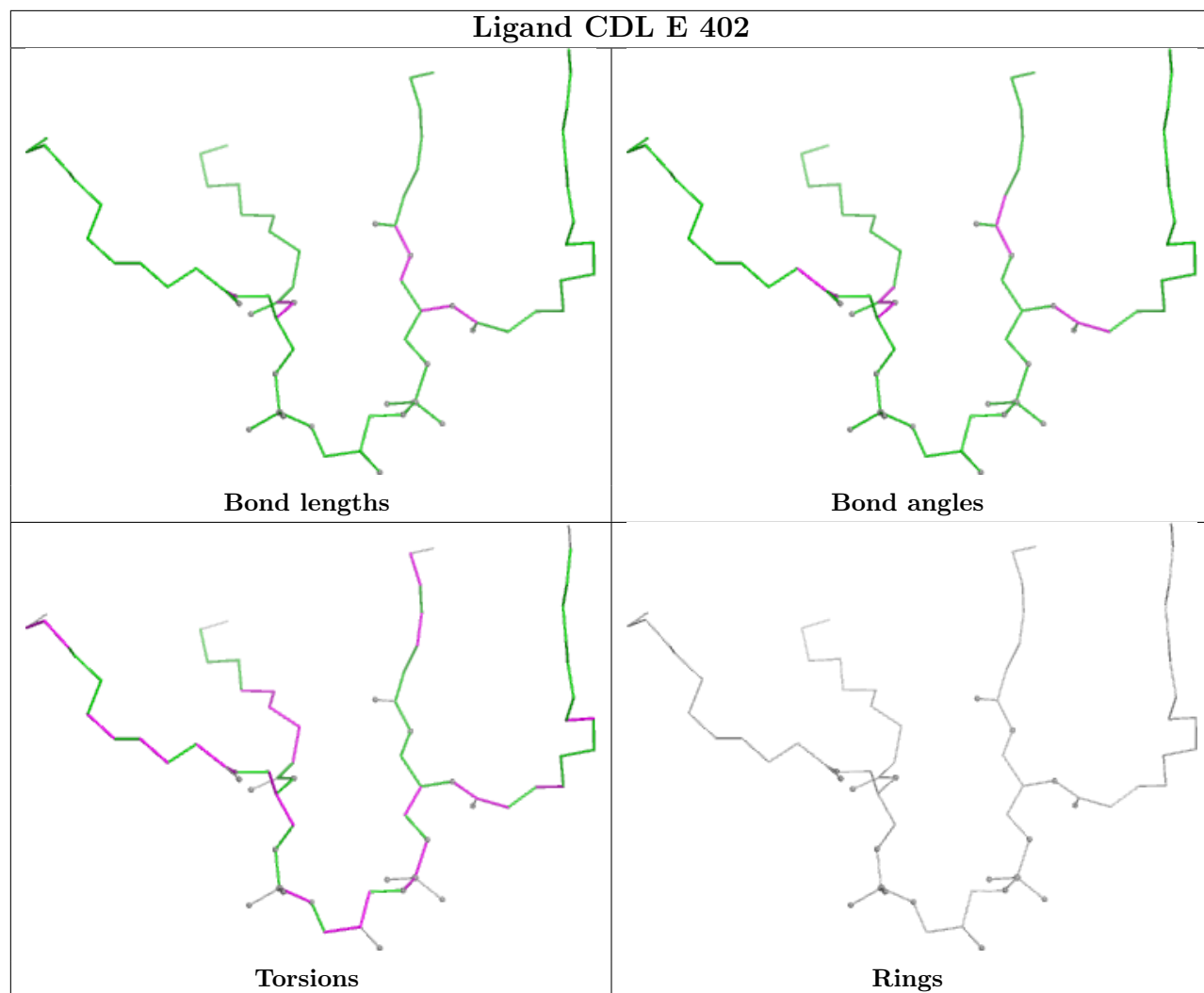
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

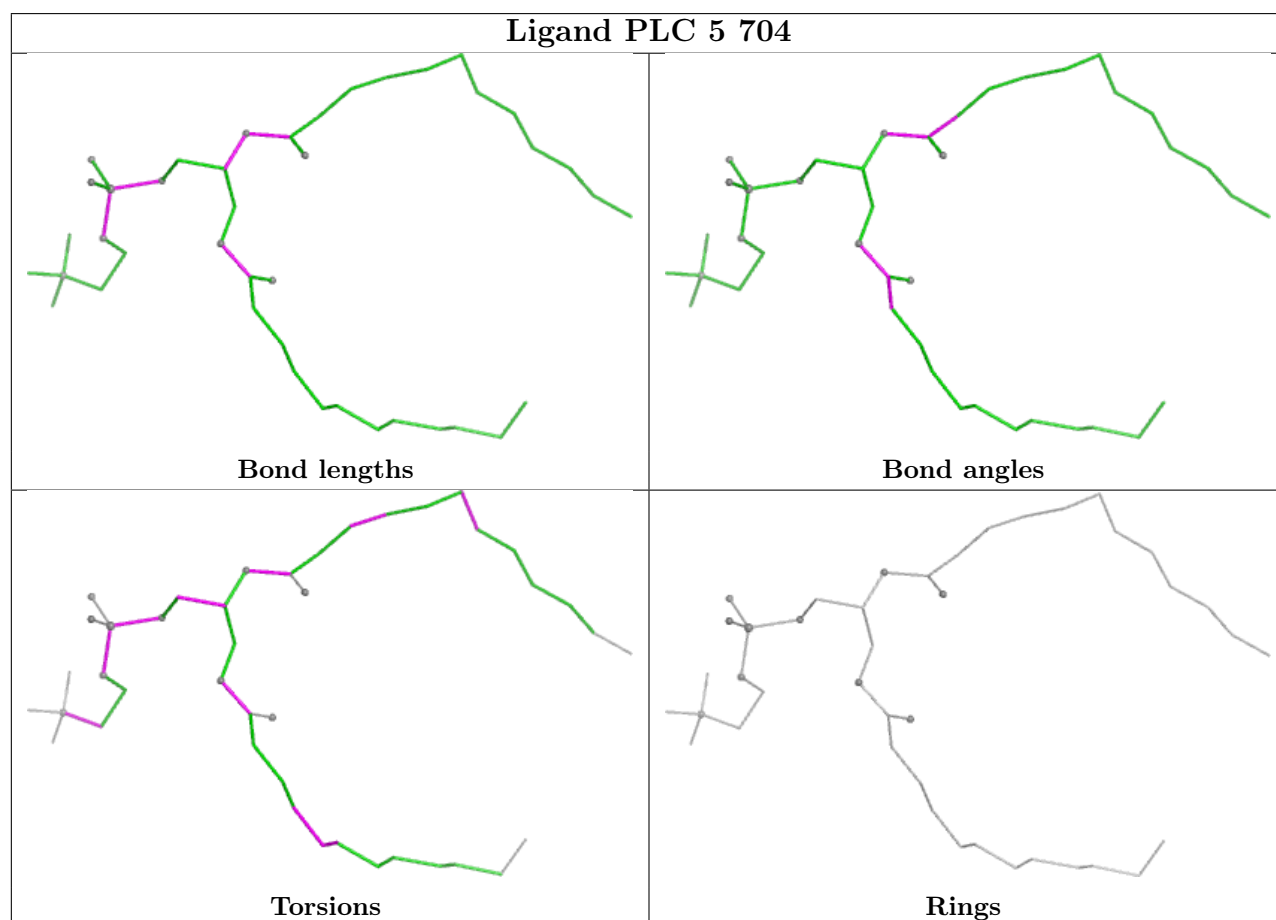
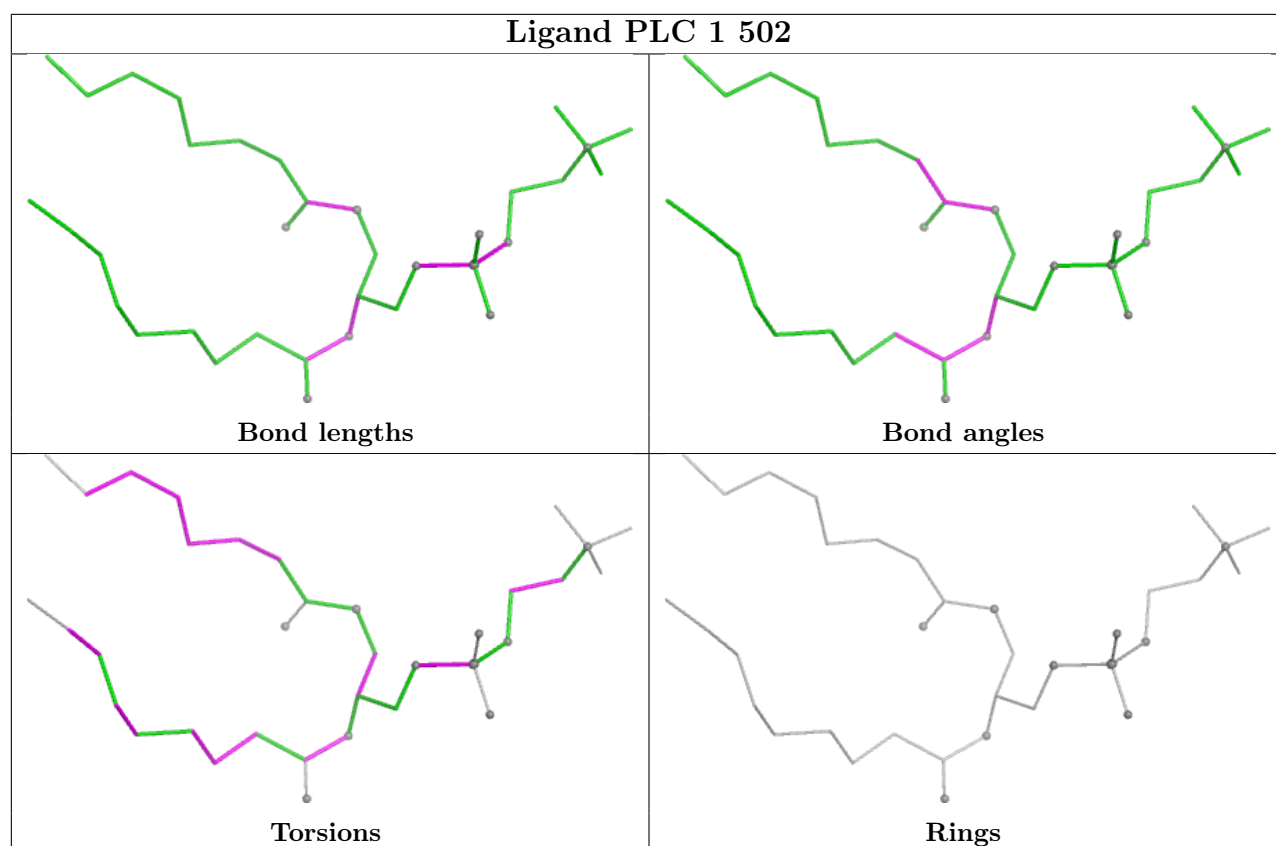
equivalents in the CSD to analyse the geometry.

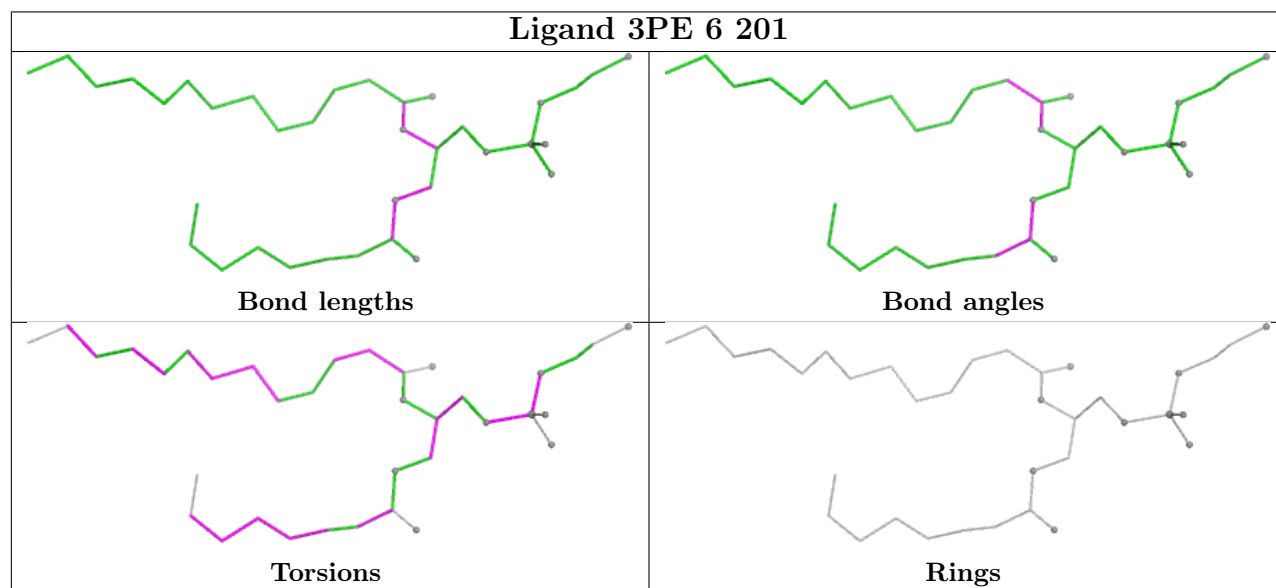
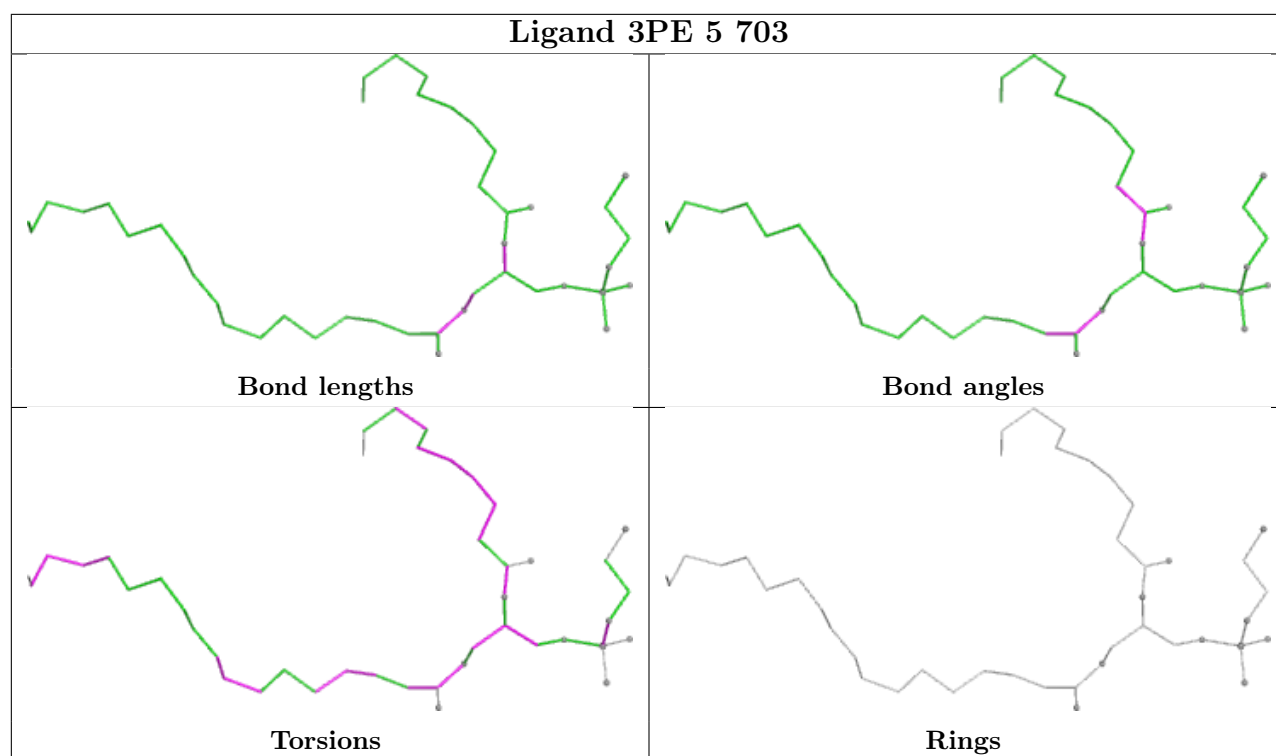


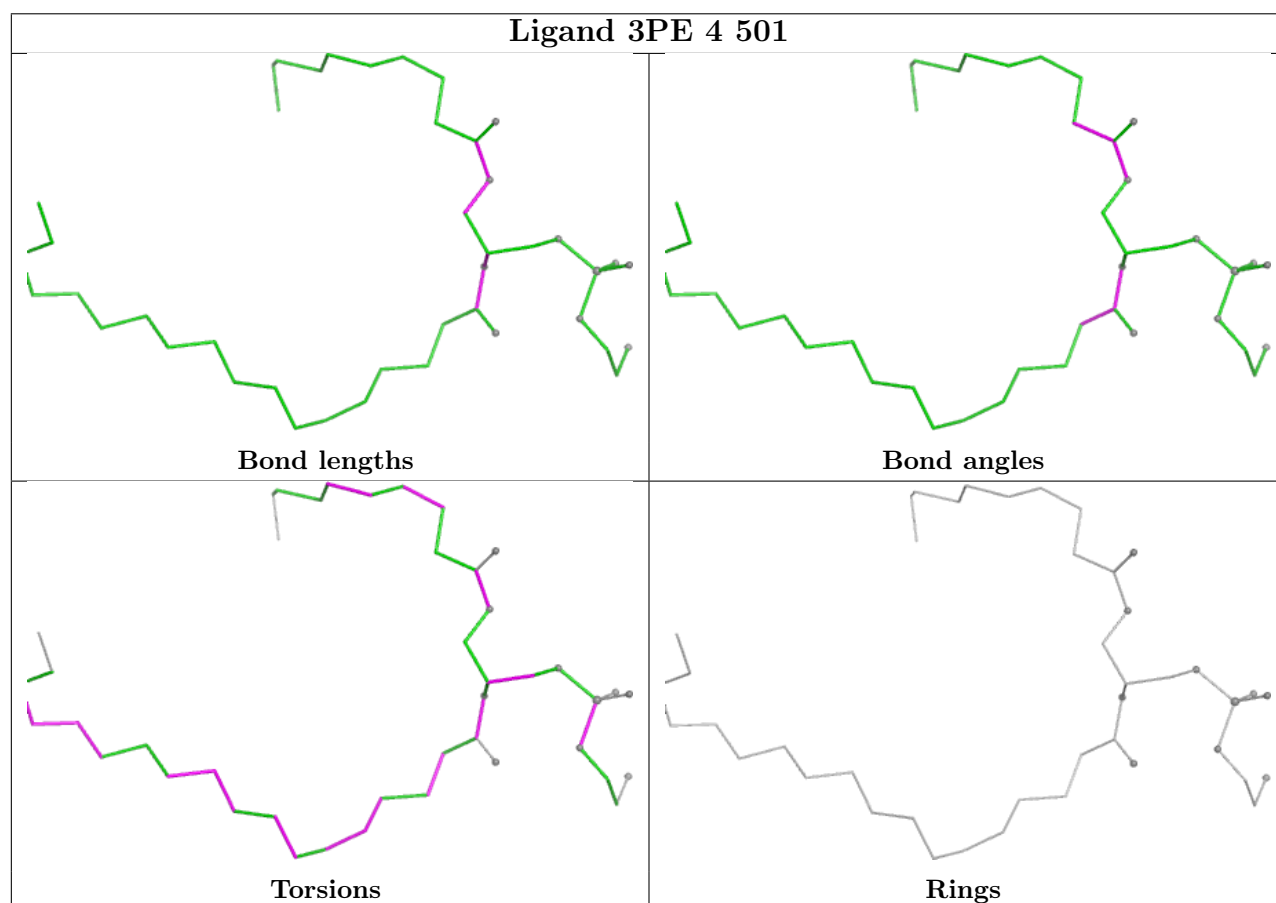
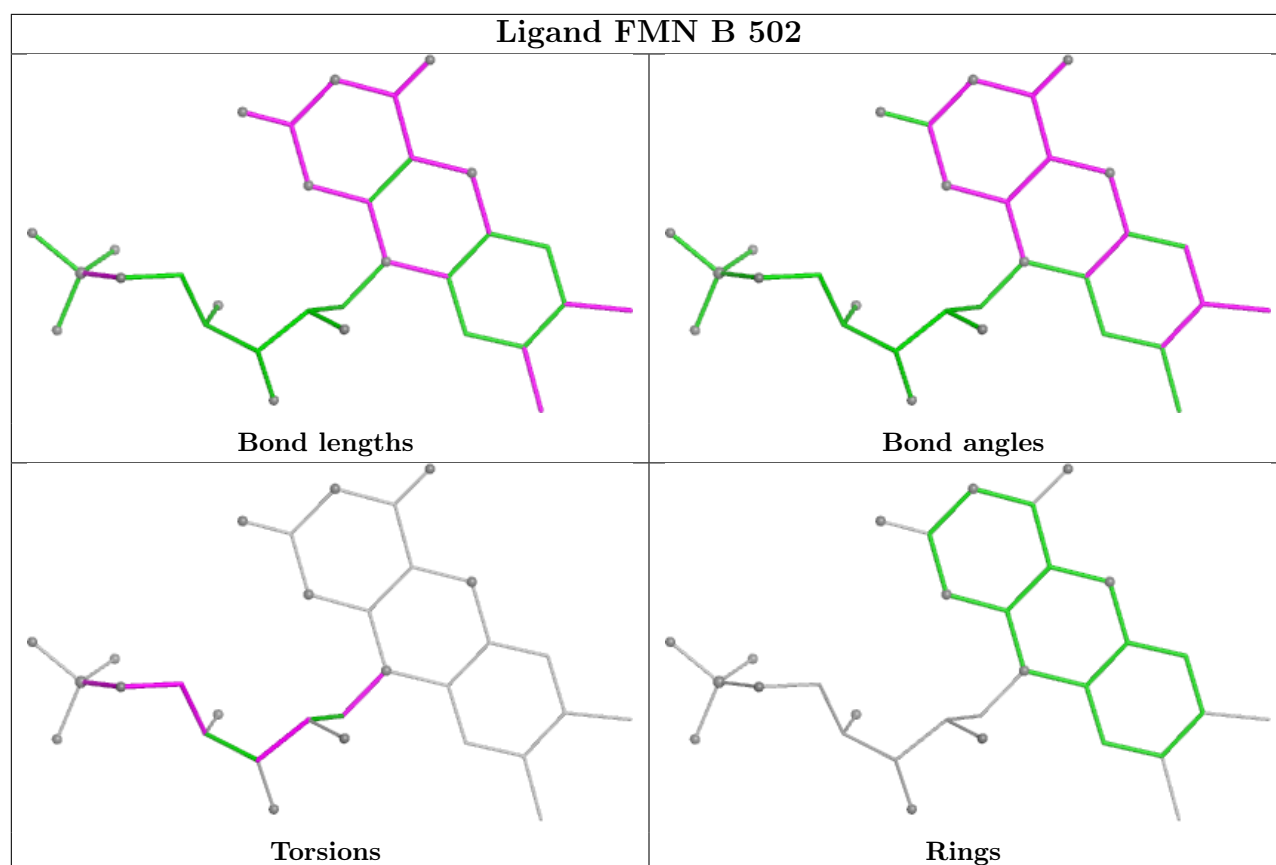


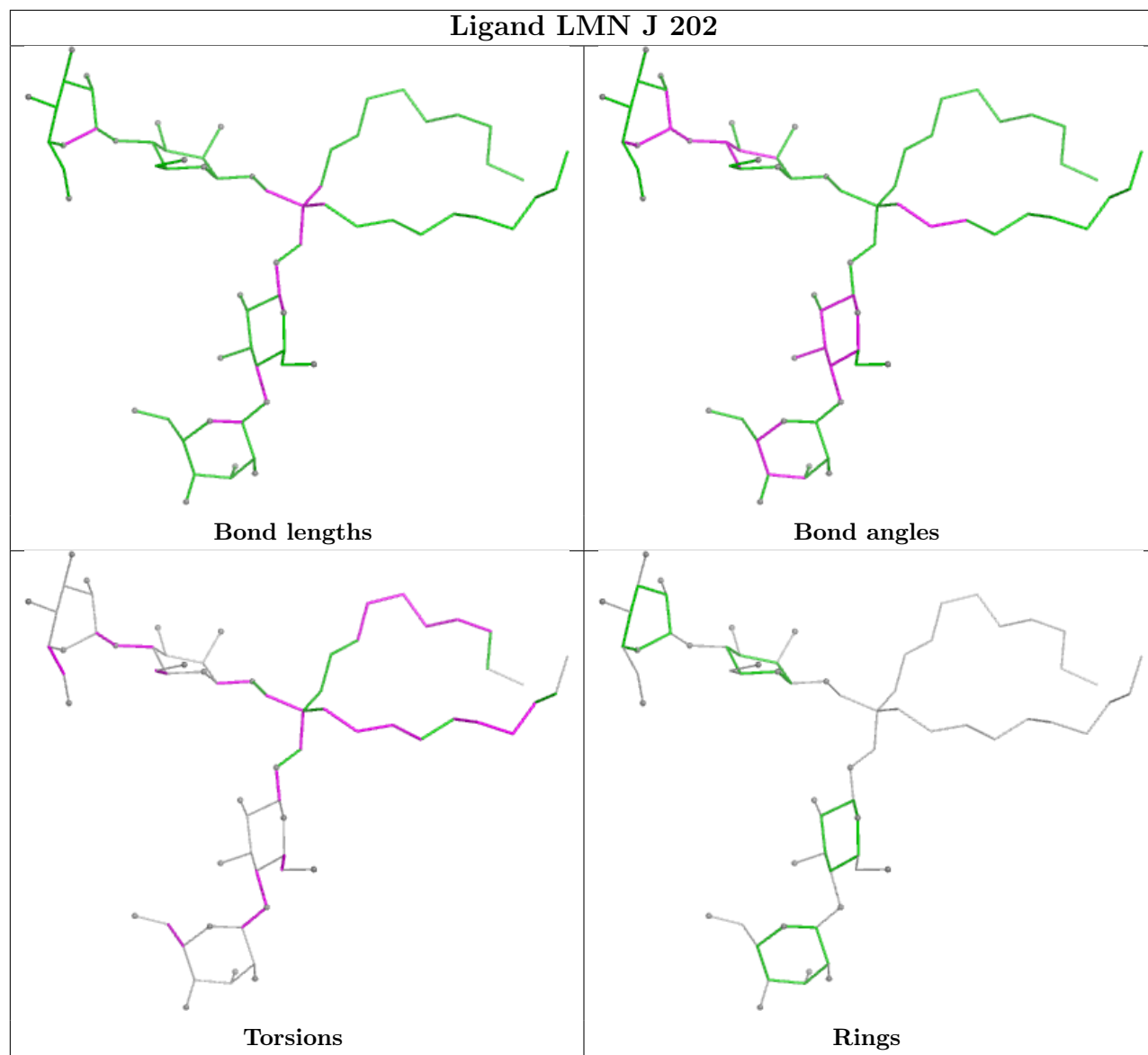




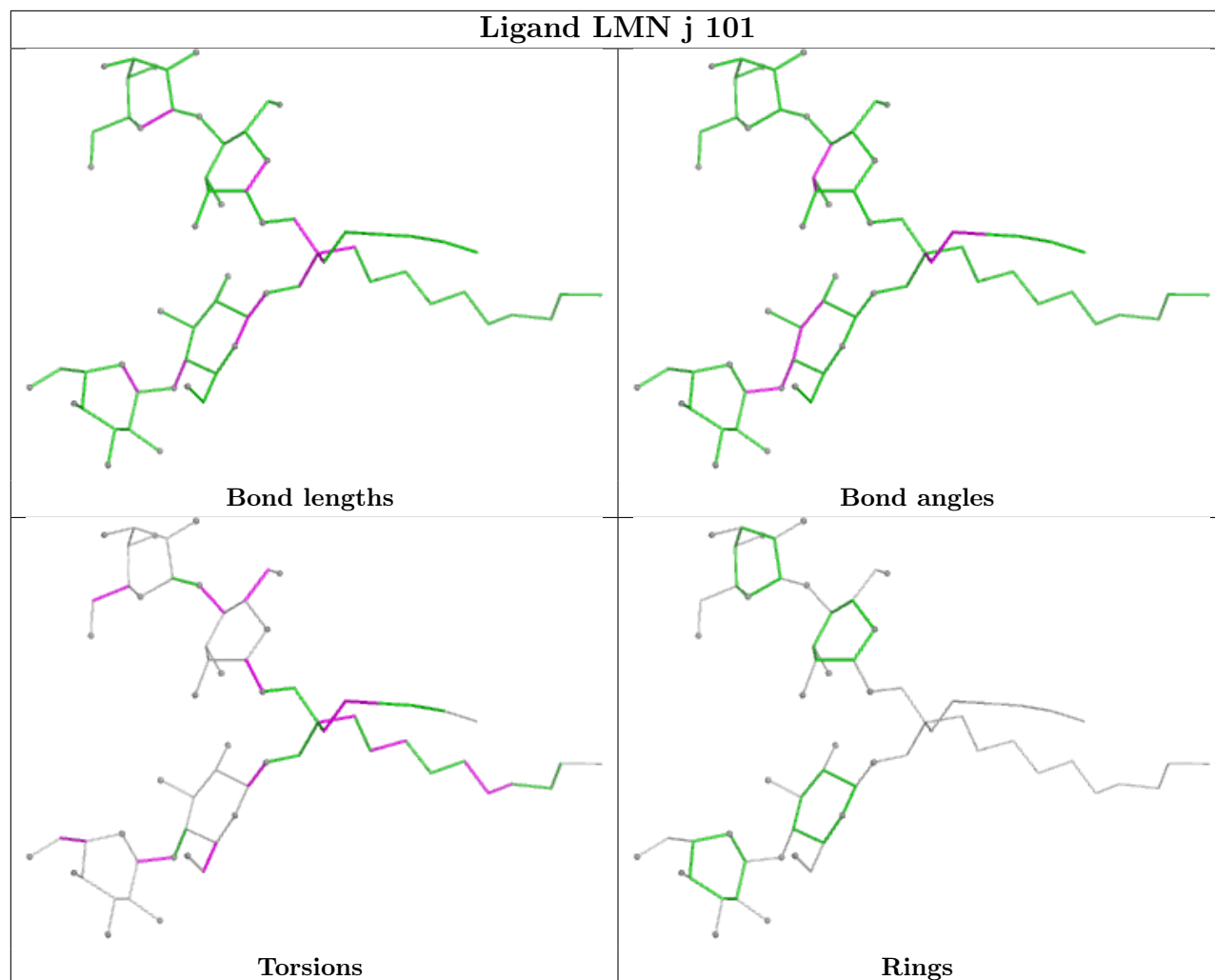




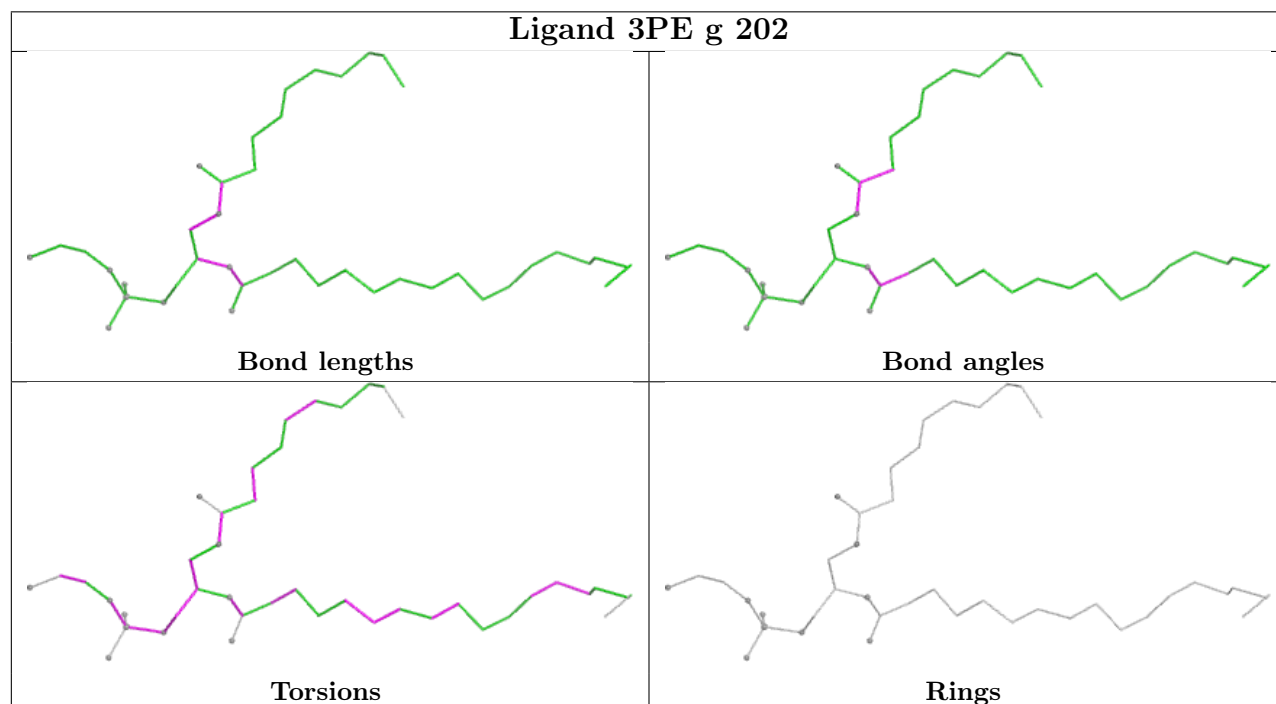


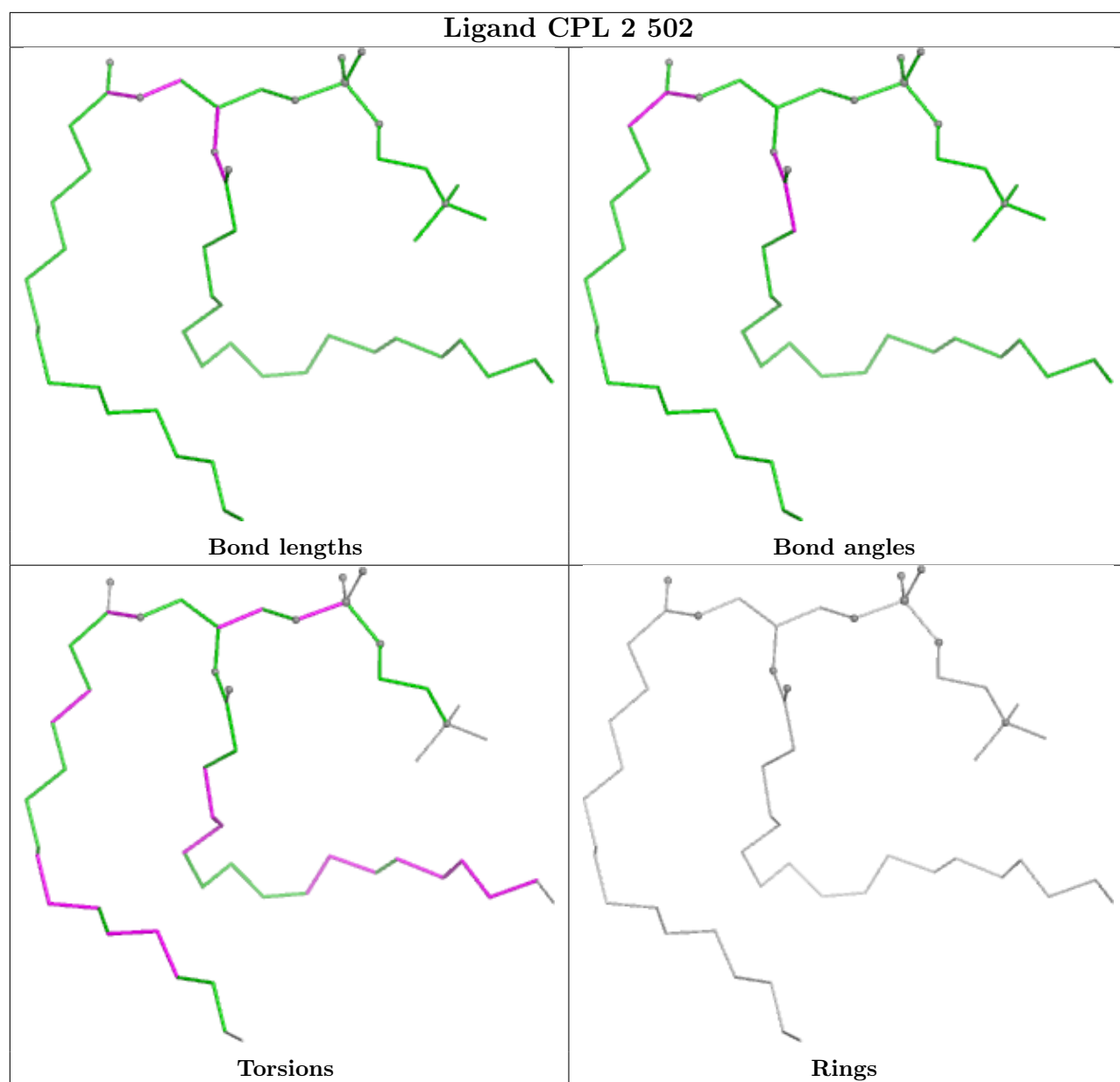


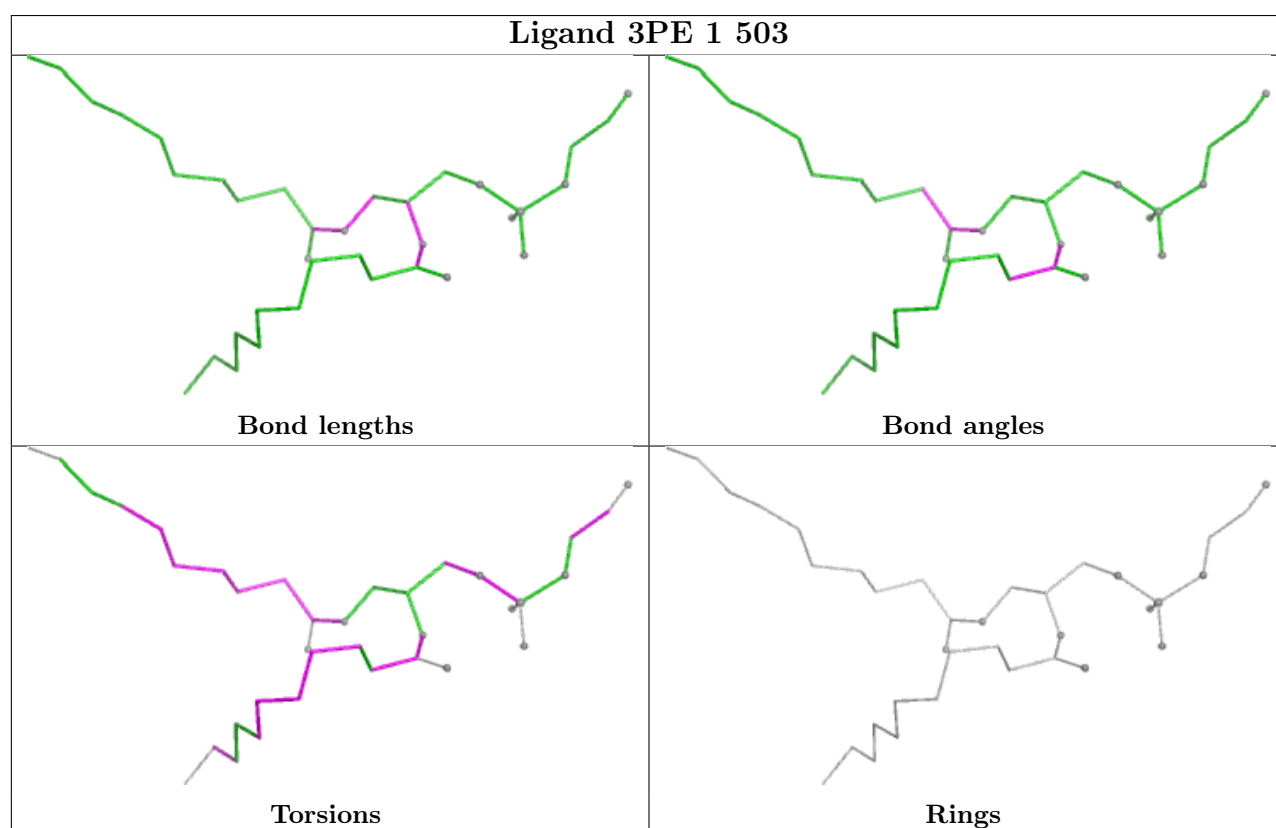
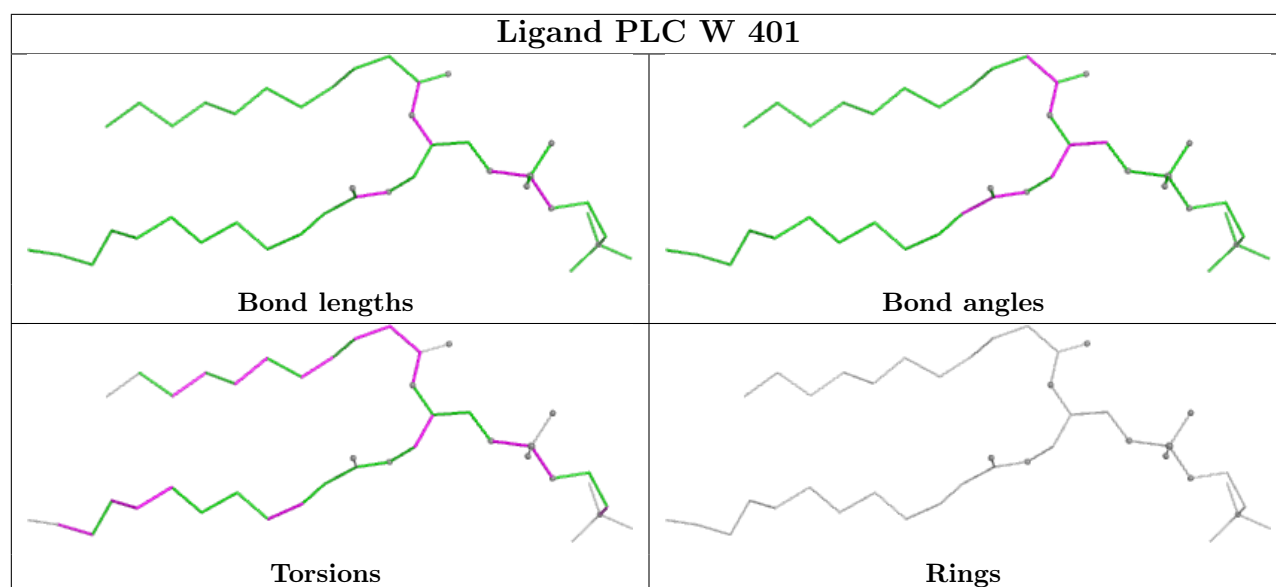
Ligand LMN j 101

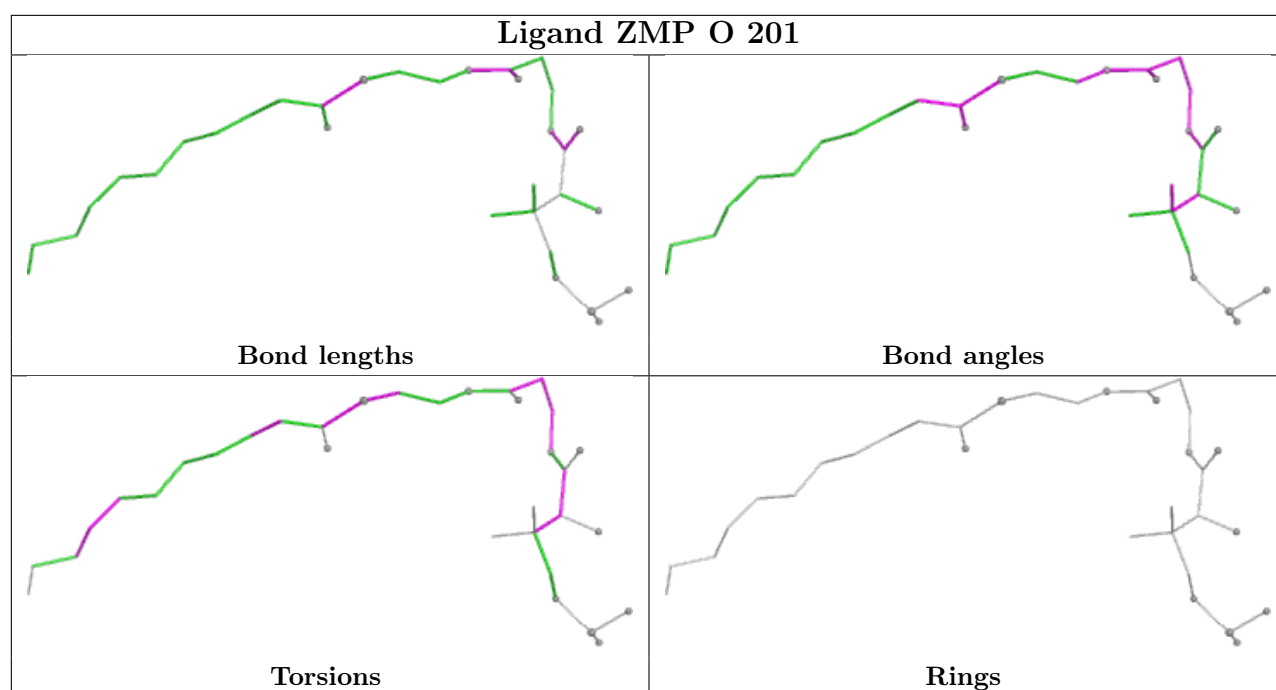
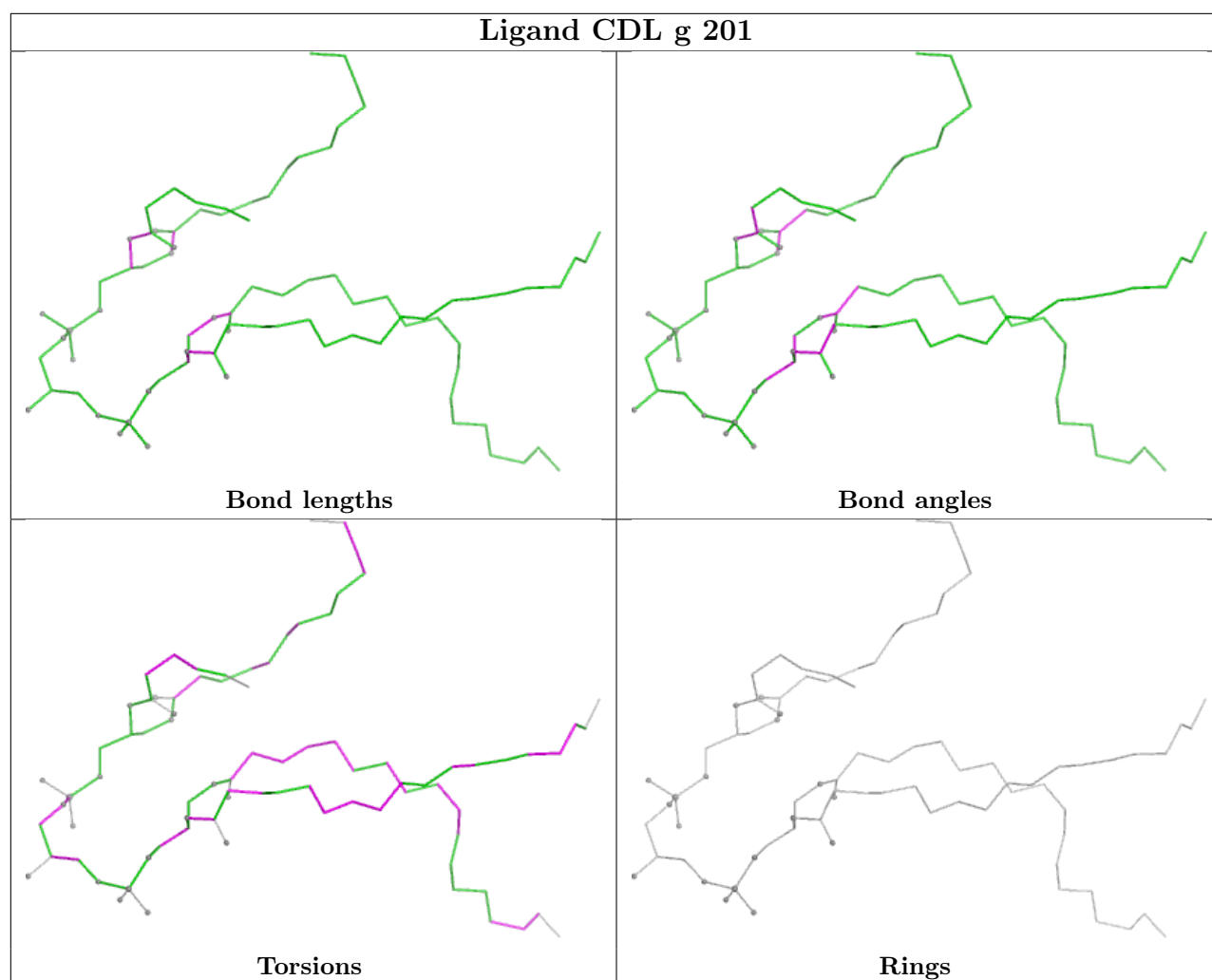


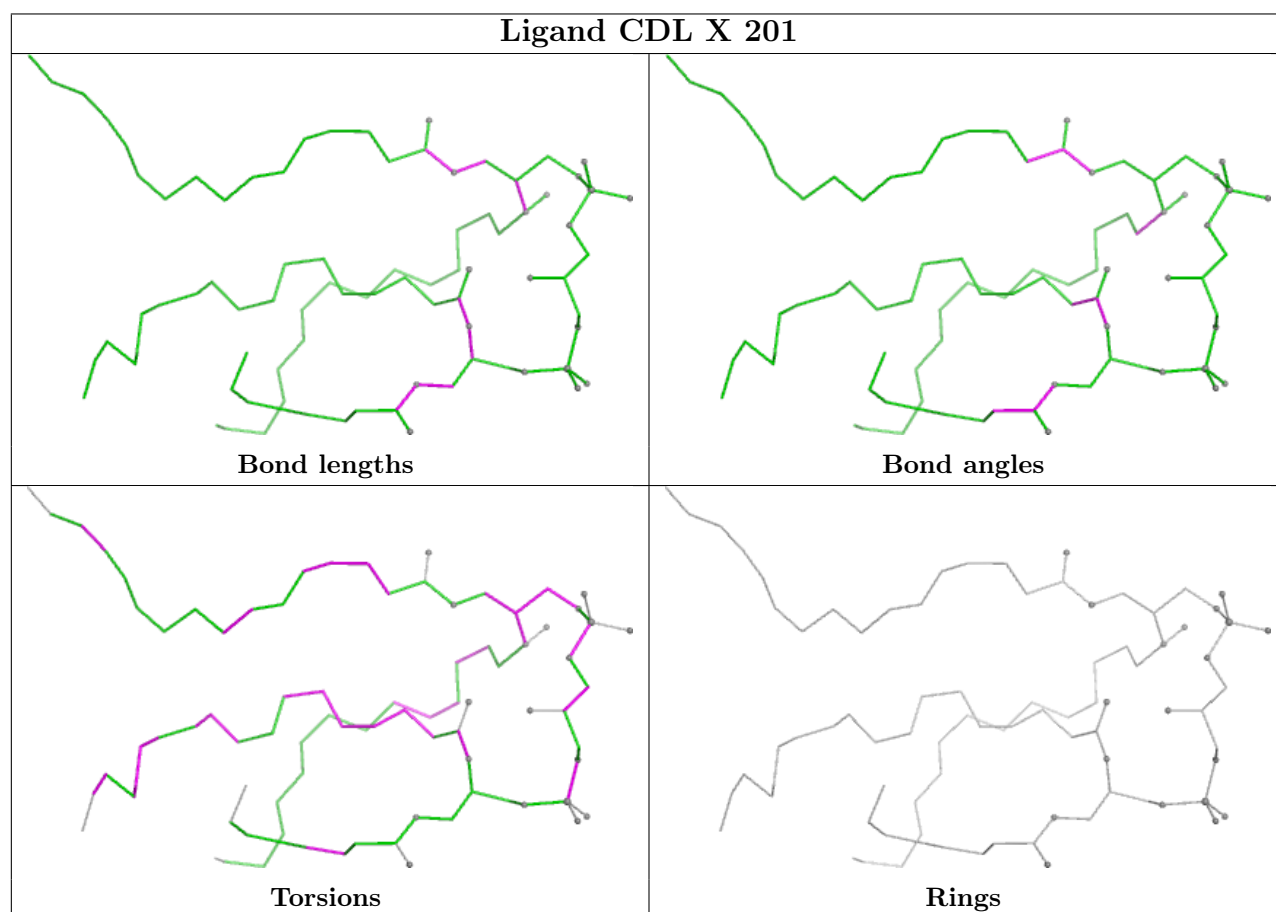
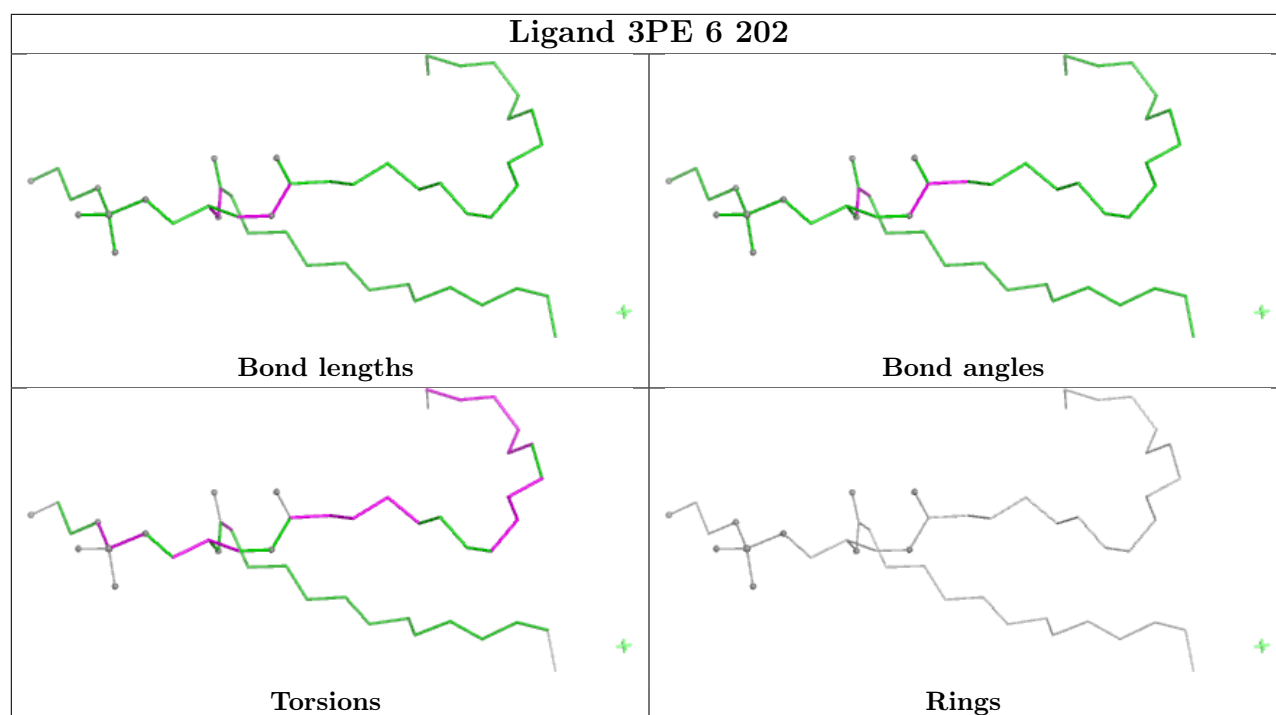
Ligand 3PE g 202

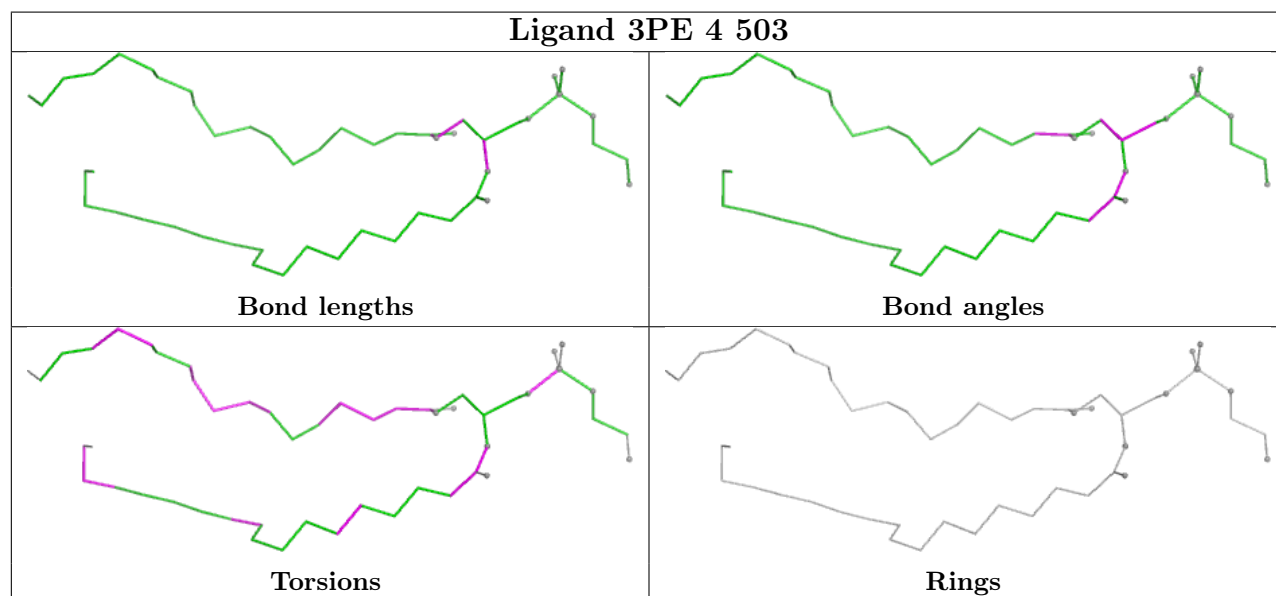
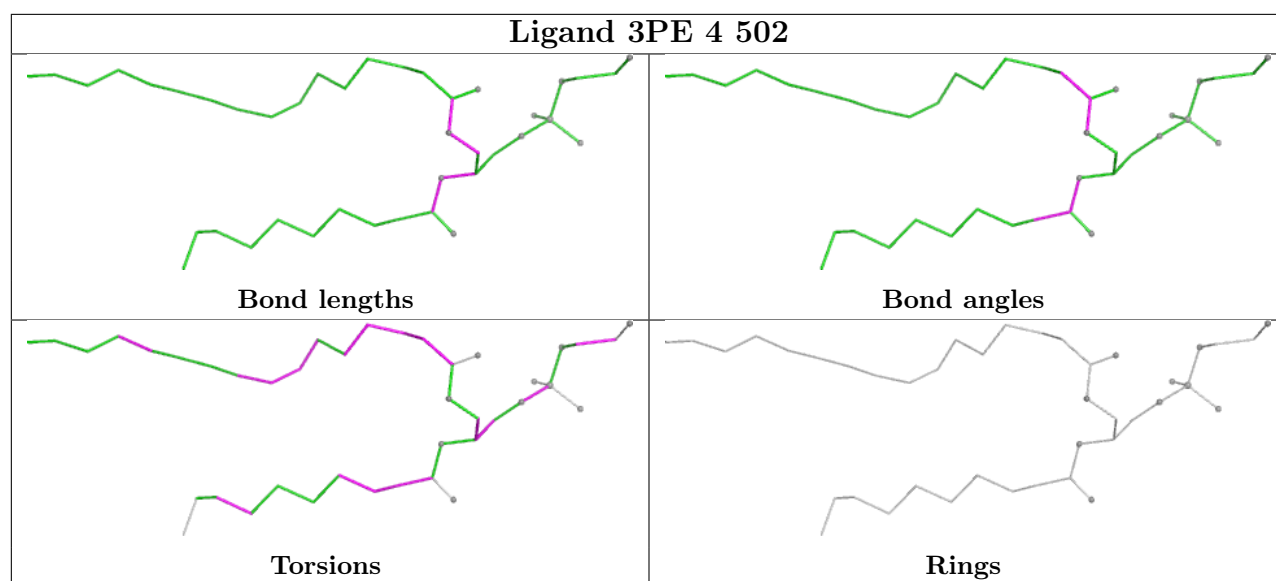




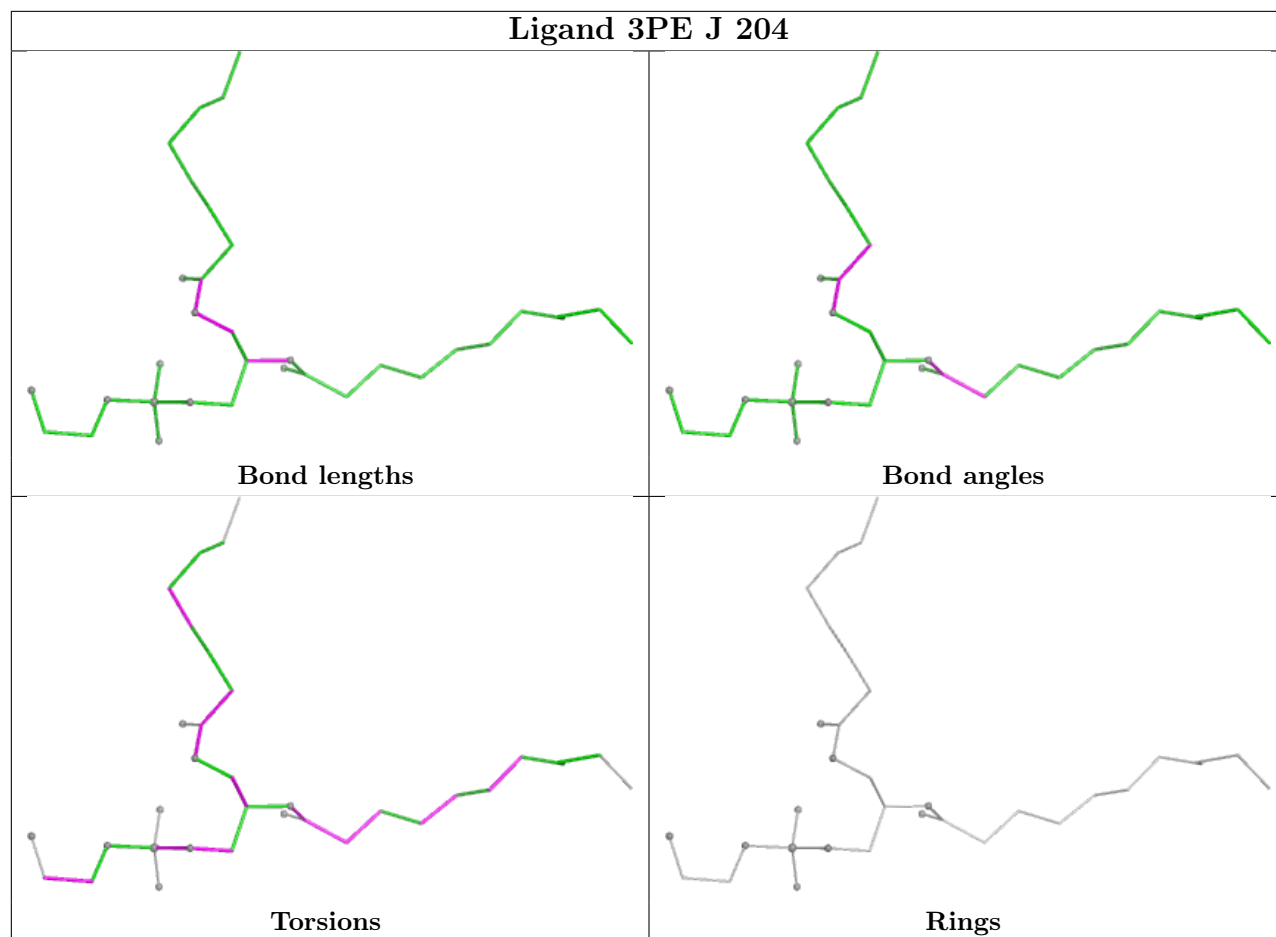




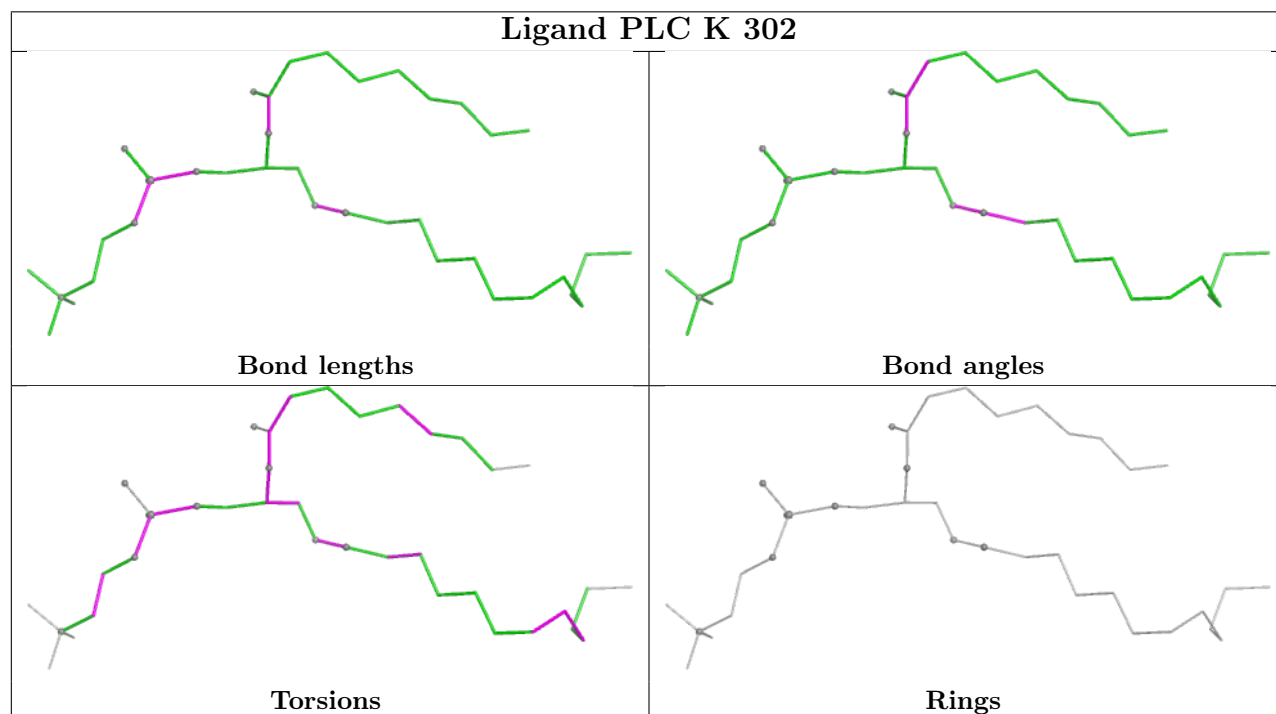




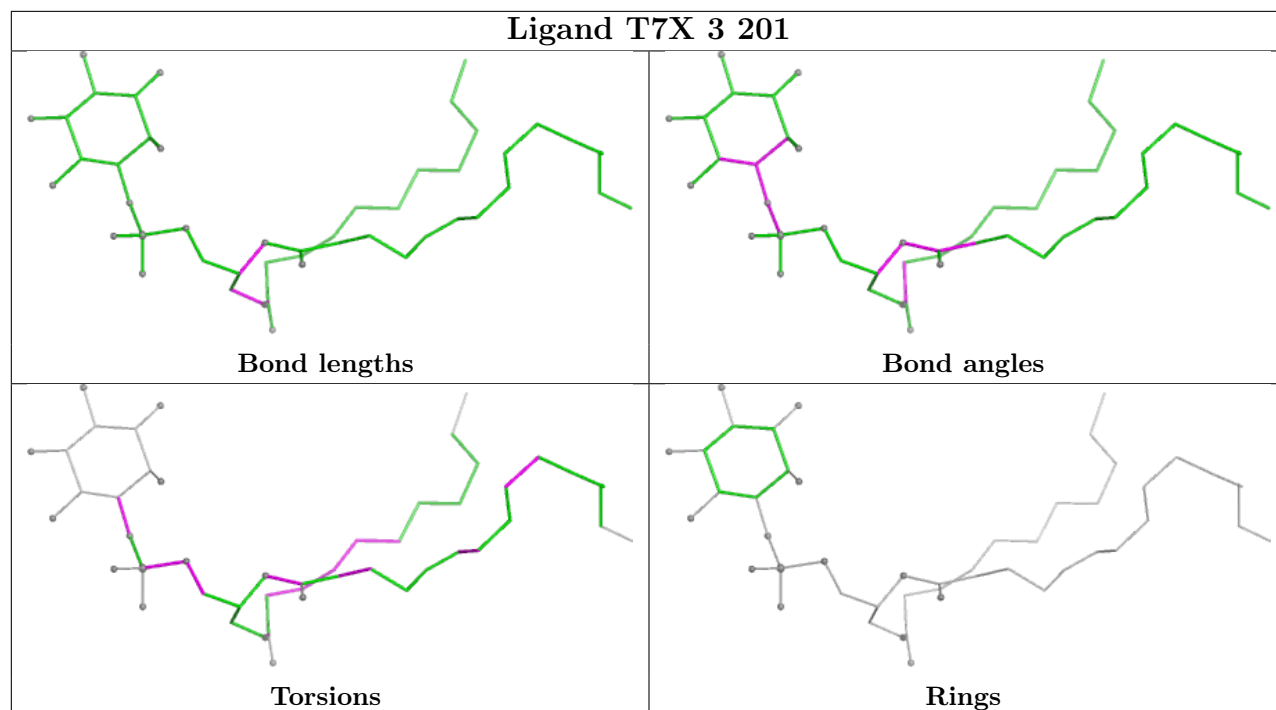
Ligand 3PE J 204



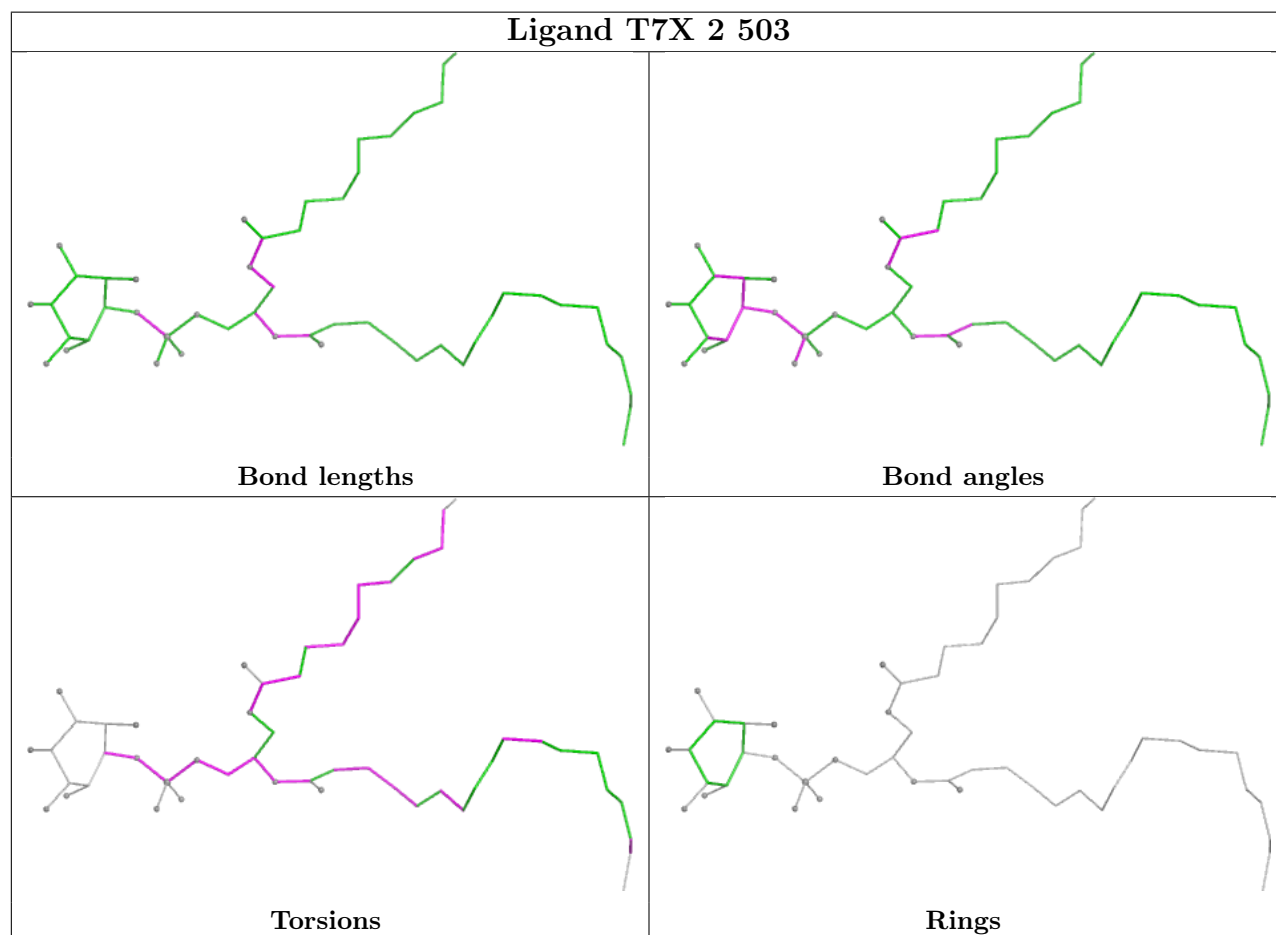
Ligand PLC K 302

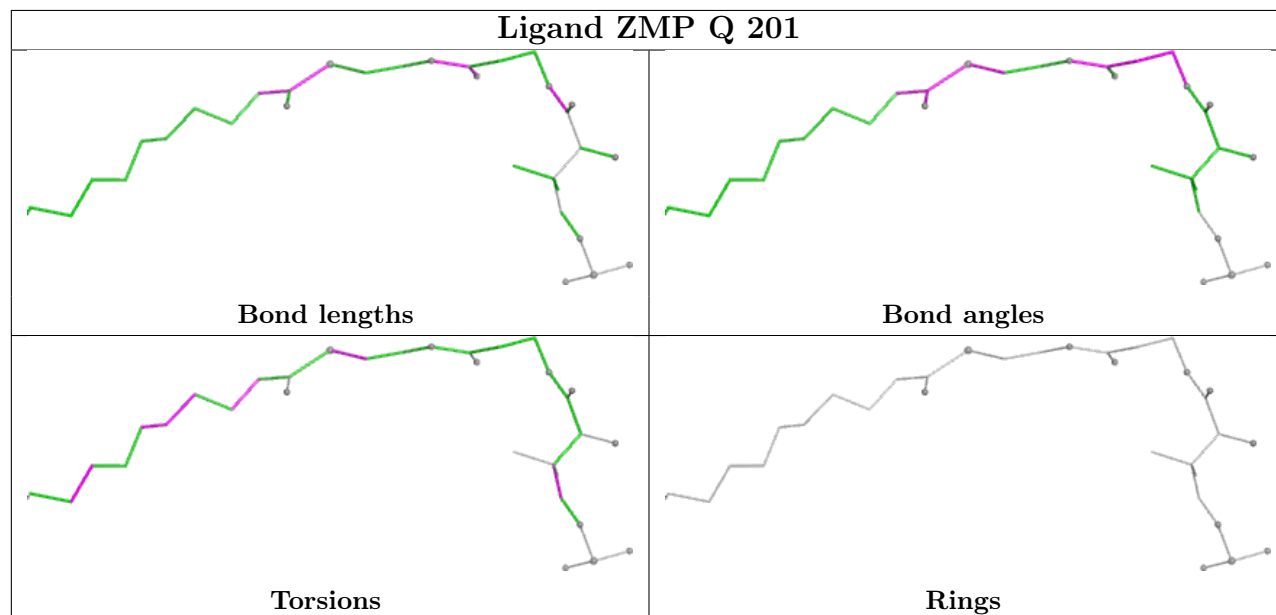
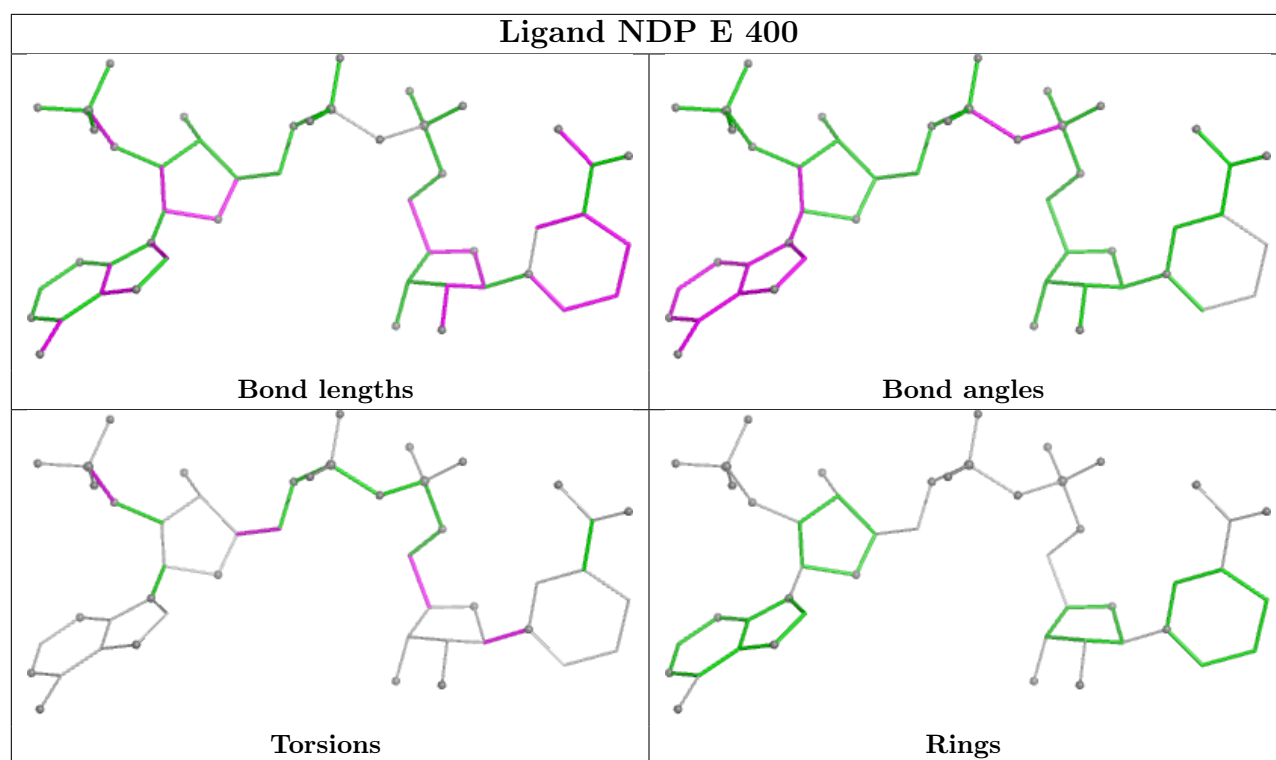


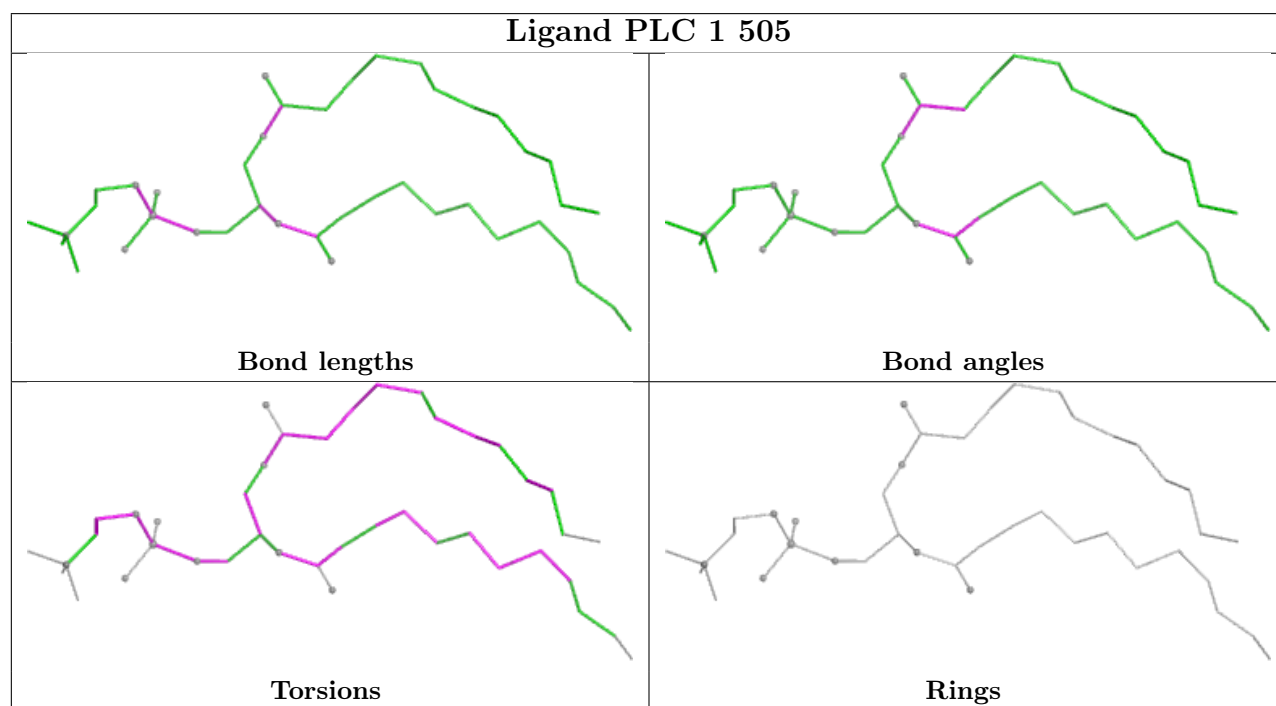
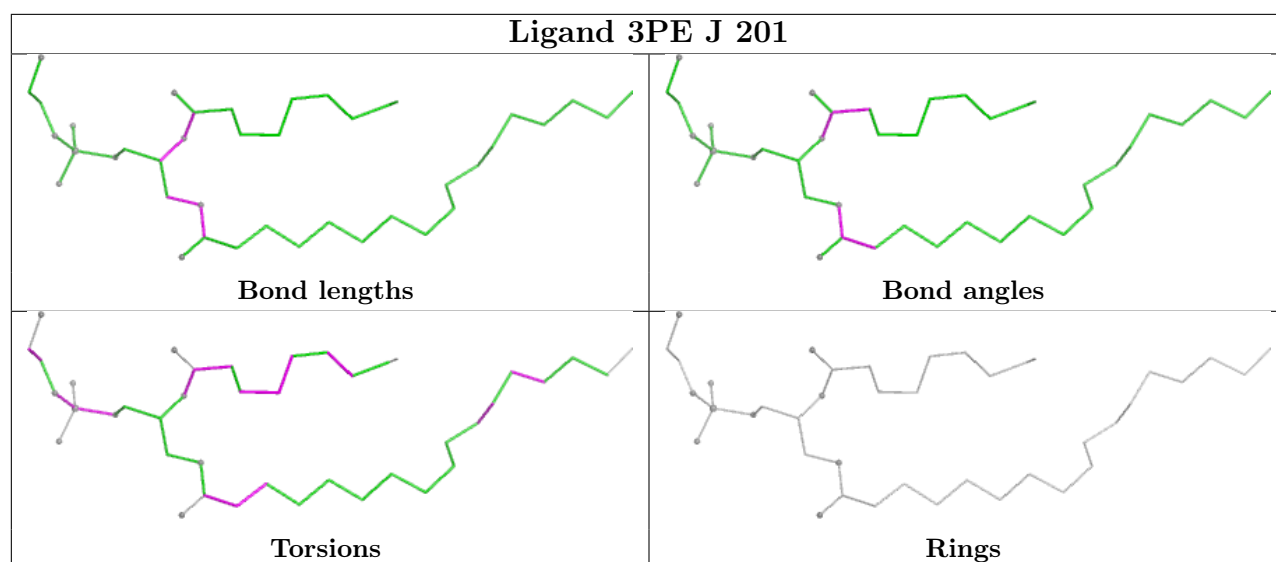
Ligand T7X 3 201

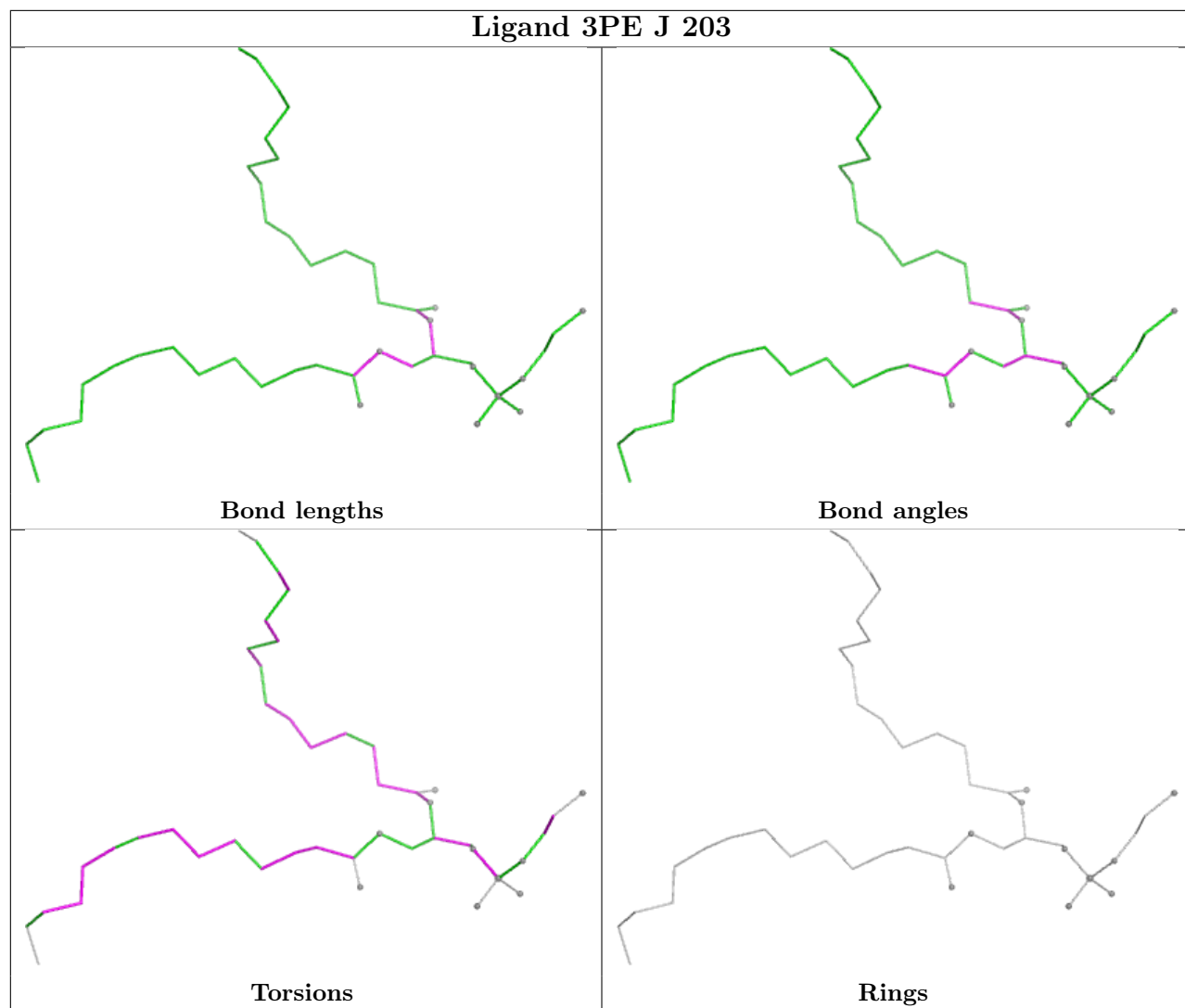


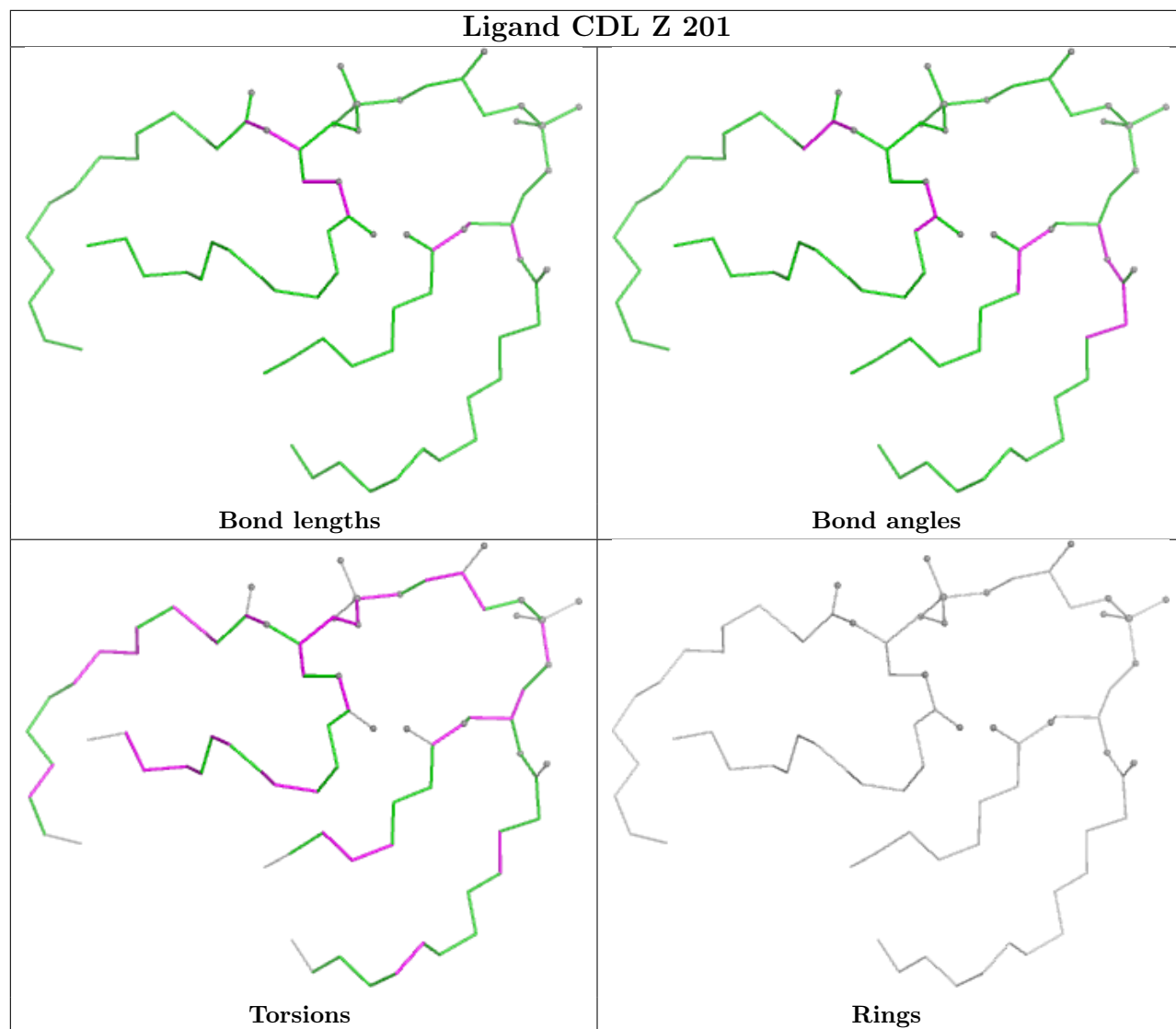
Ligand T7X 2 503

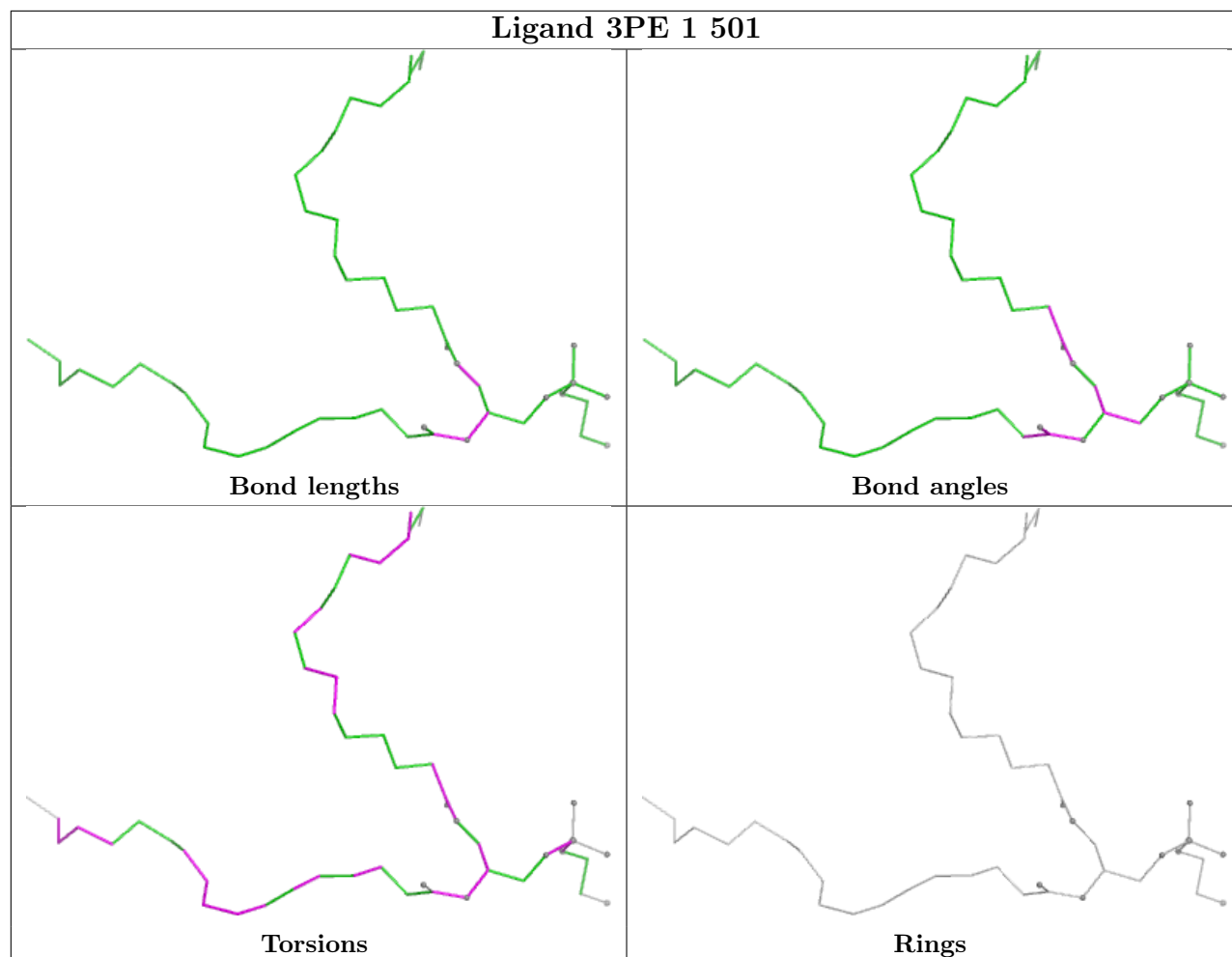
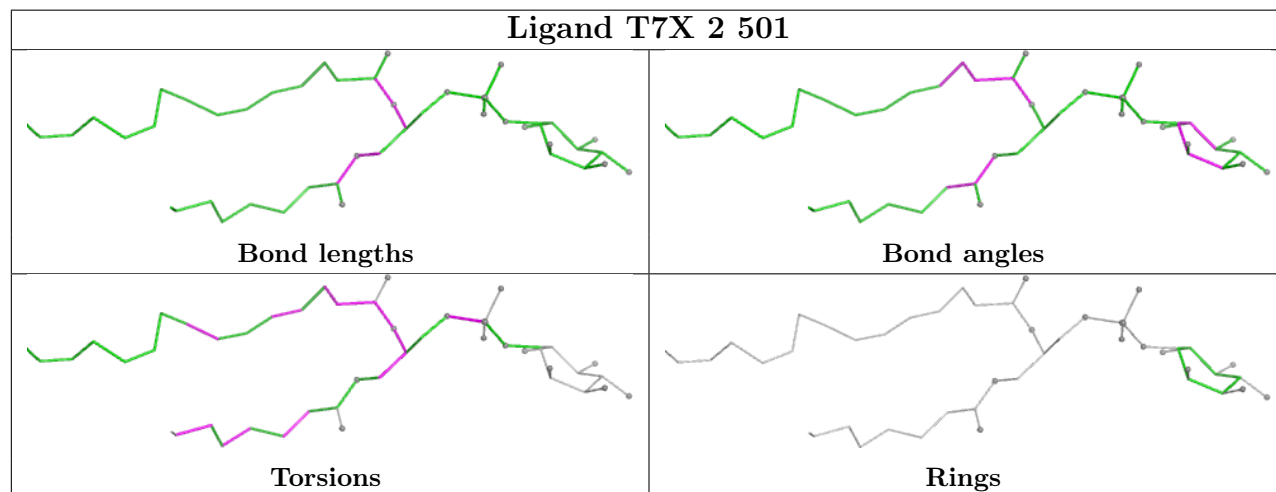


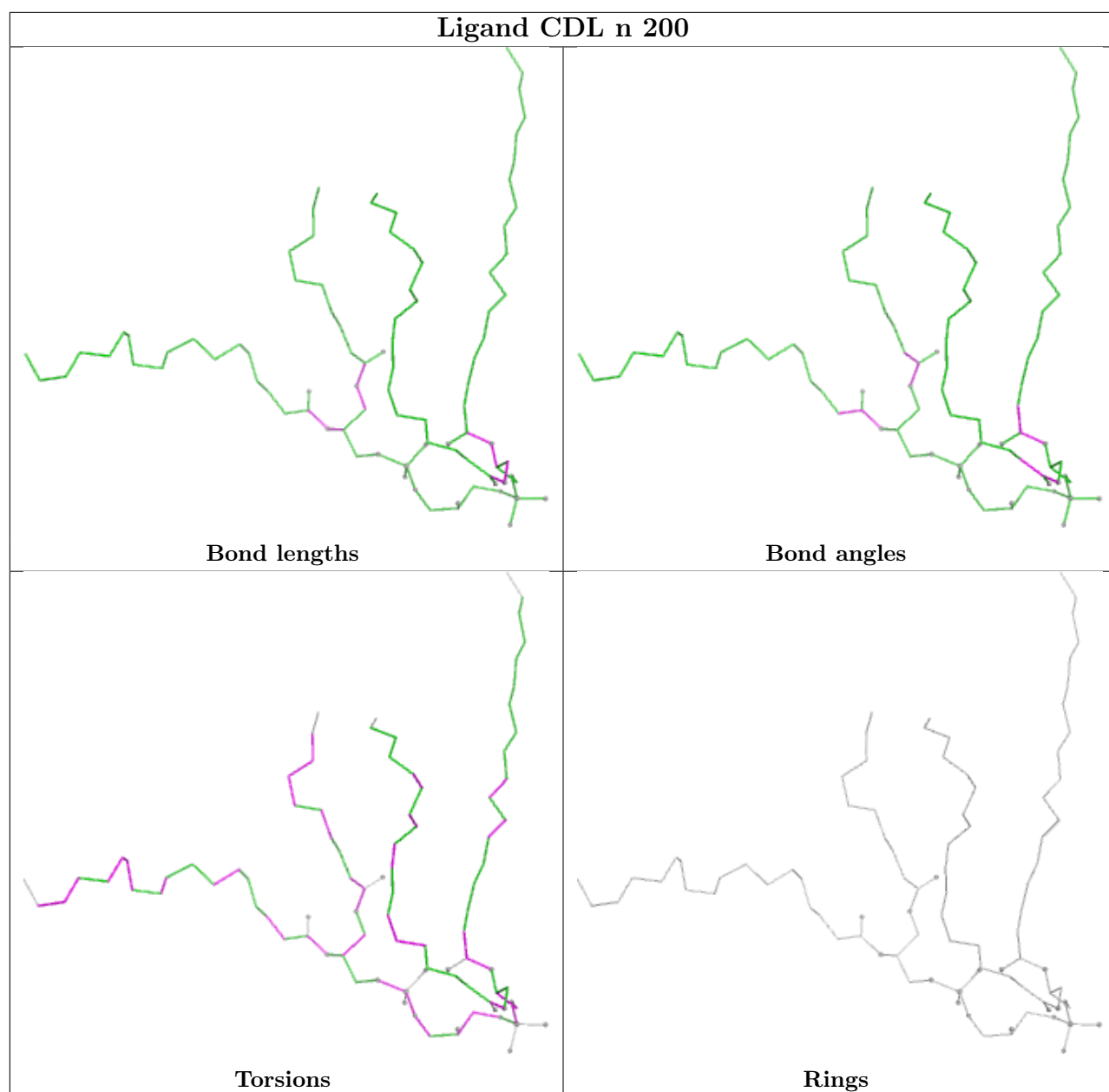


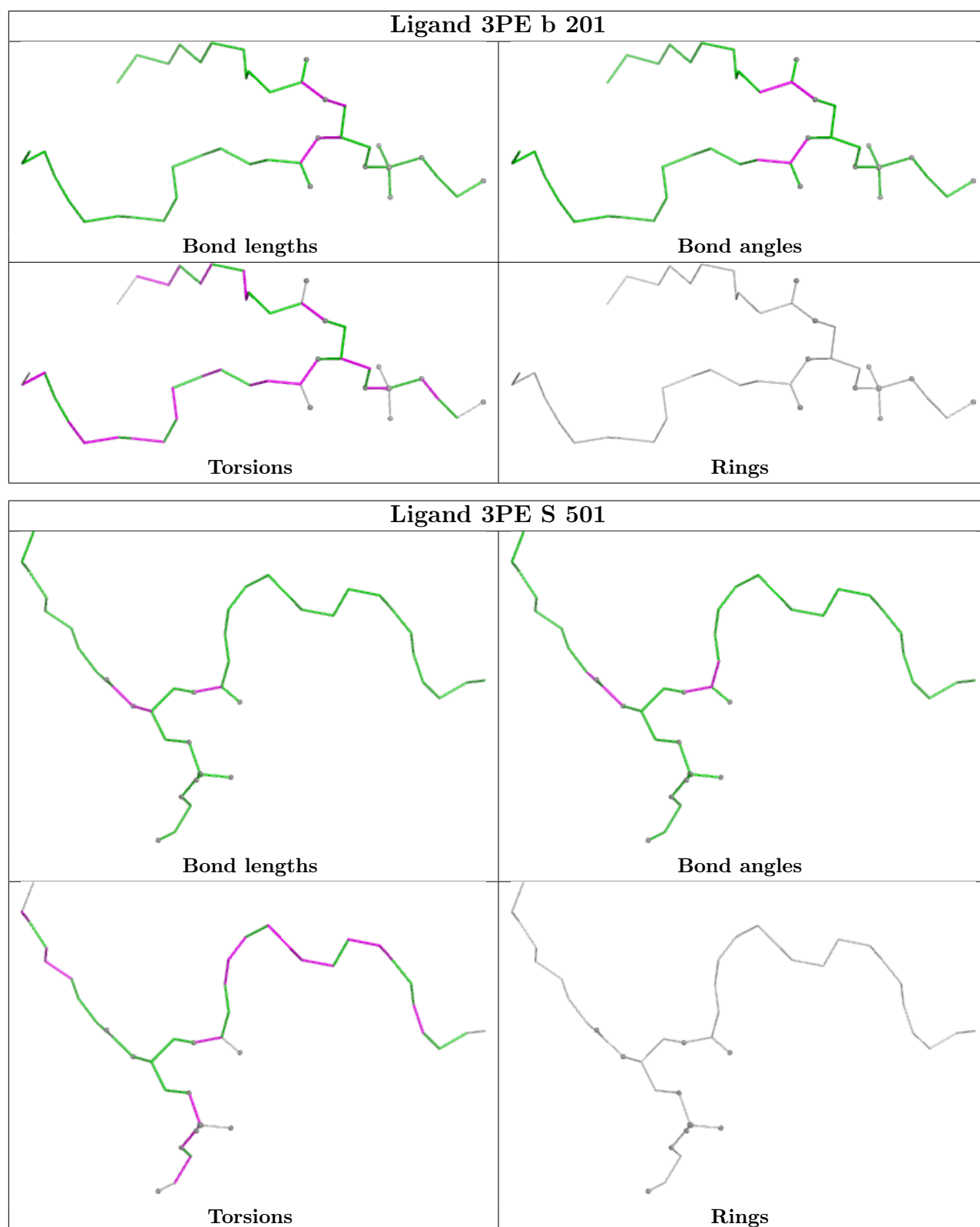






Ligand 3PE 1 501**Ligand T7X 2 501**





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

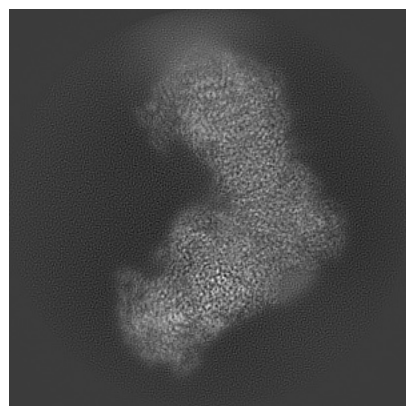
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12742. These allow visual inspection of the internal detail of the map and identification of artifacts.

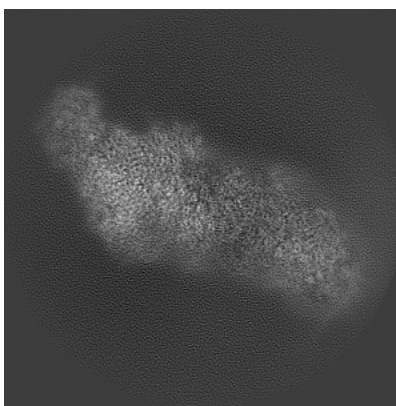
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

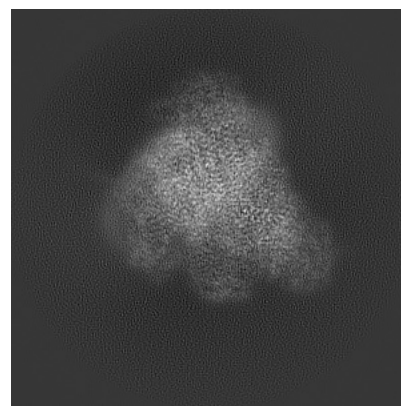
6.1.1 Primary map



X

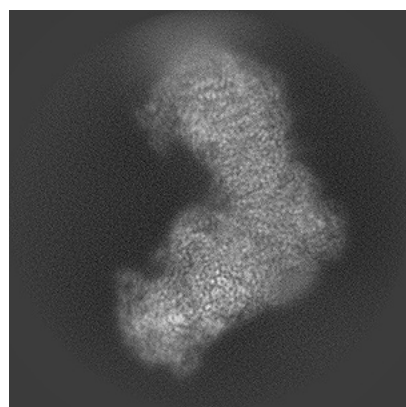


Y

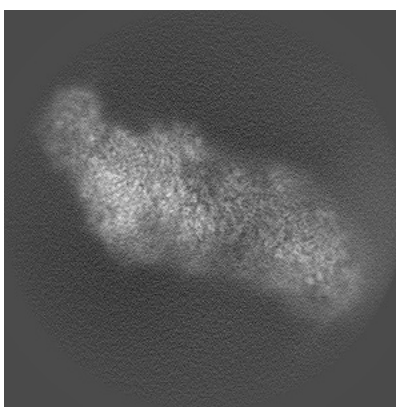


Z

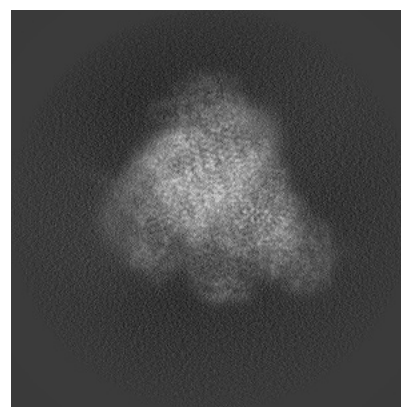
6.1.2 Raw map



X



Y

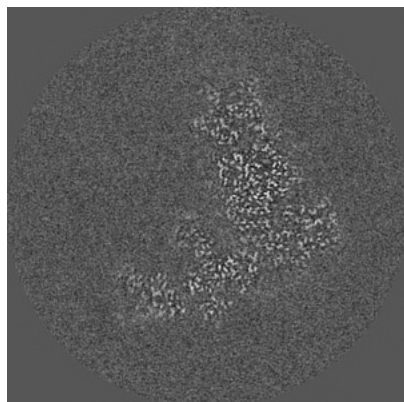


Z

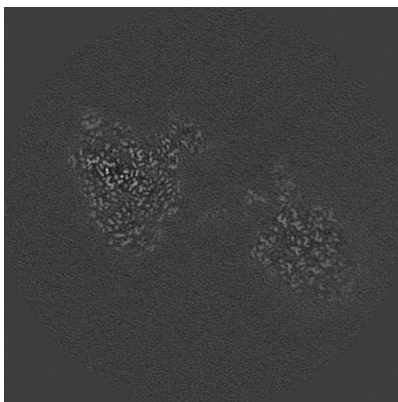
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

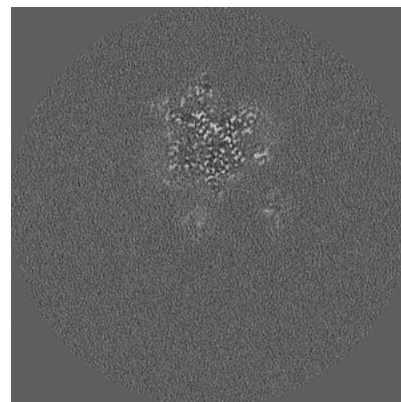
6.2.1 Primary map



X Index: 300

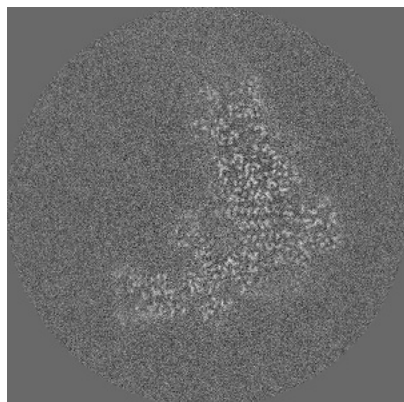


Y Index: 300

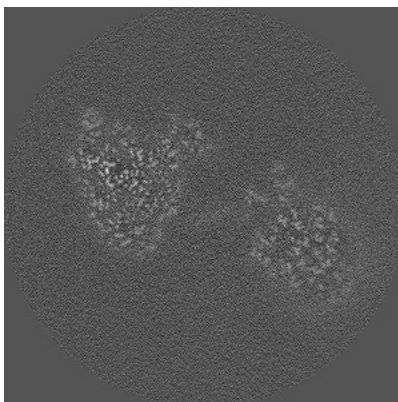


Z Index: 300

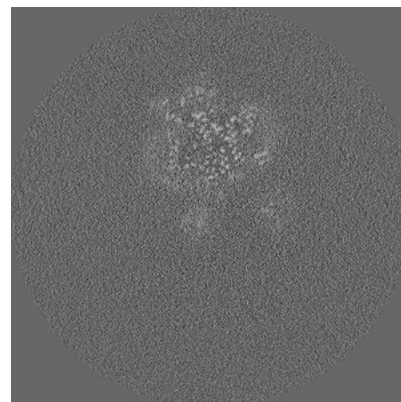
6.2.2 Raw map



X Index: 300



Y Index: 300

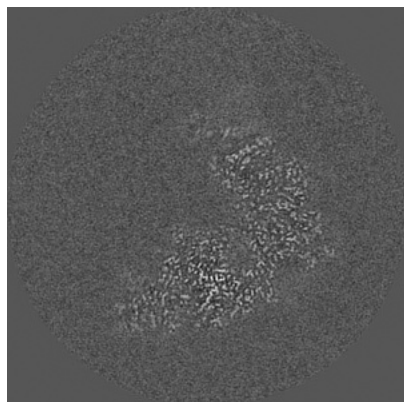


Z Index: 300

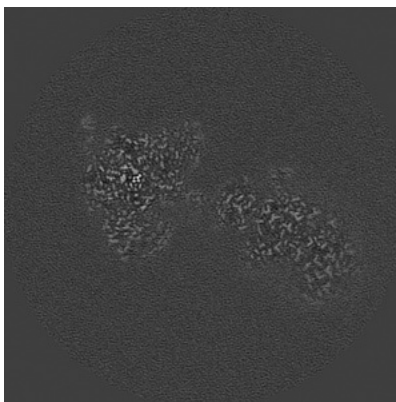
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

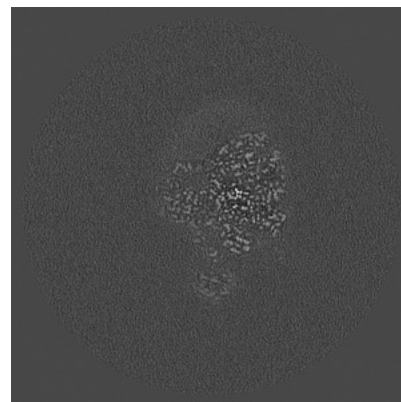
6.3.1 Primary map



X Index: 332

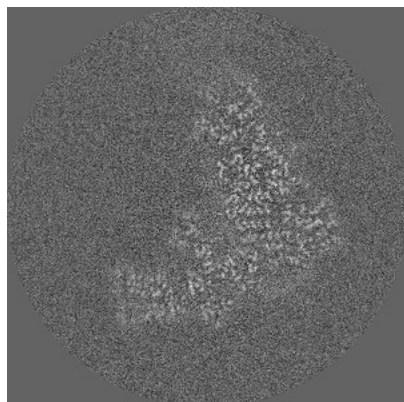


Y Index: 319

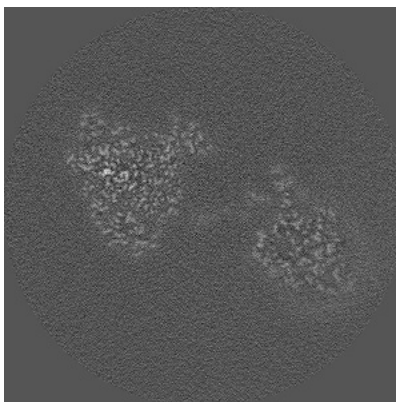


Z Index: 197

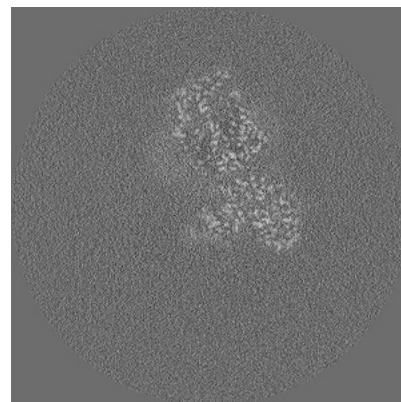
6.3.2 Raw map



X Index: 301



Y Index: 298

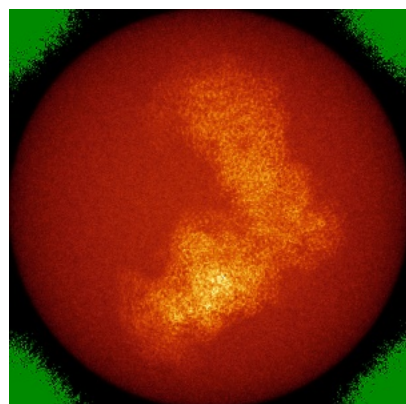


Z Index: 261

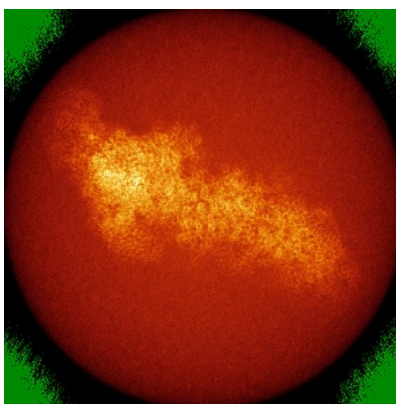
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

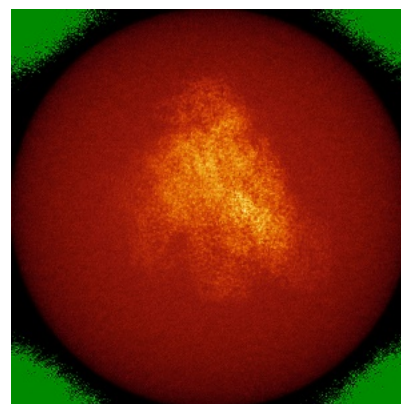
6.4.1 Primary map



X

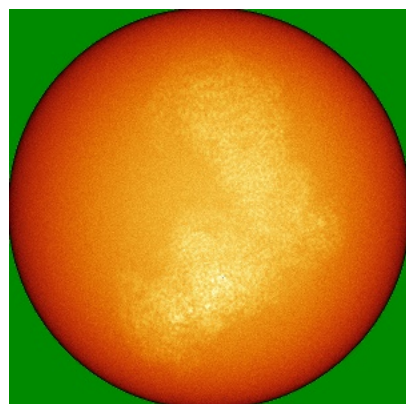


Y

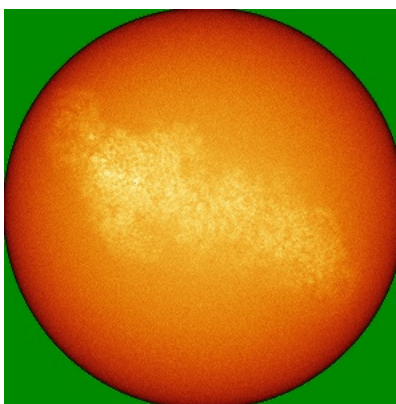


Z

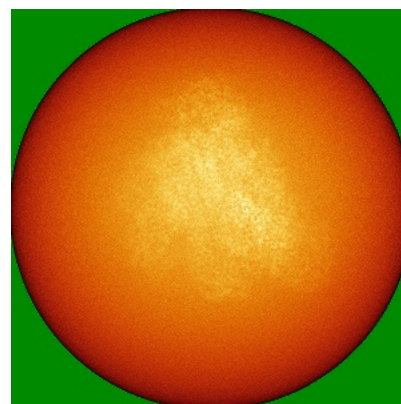
6.4.2 Raw map



X



Y

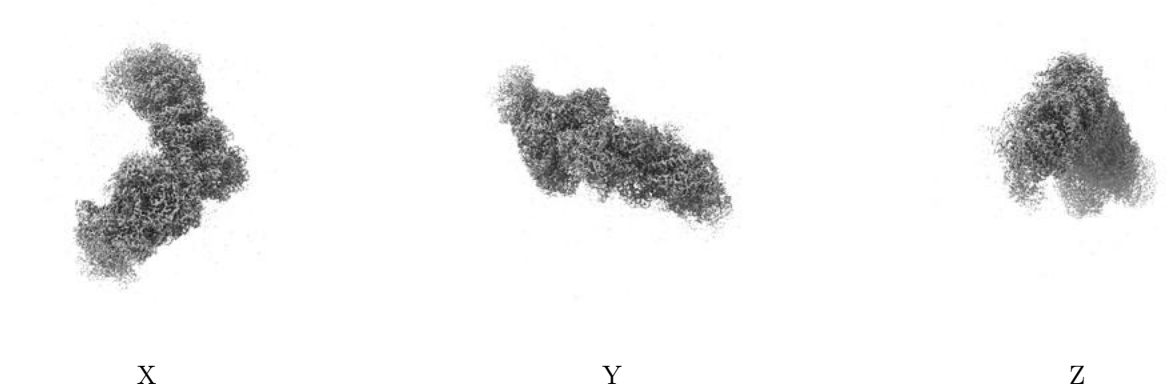


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

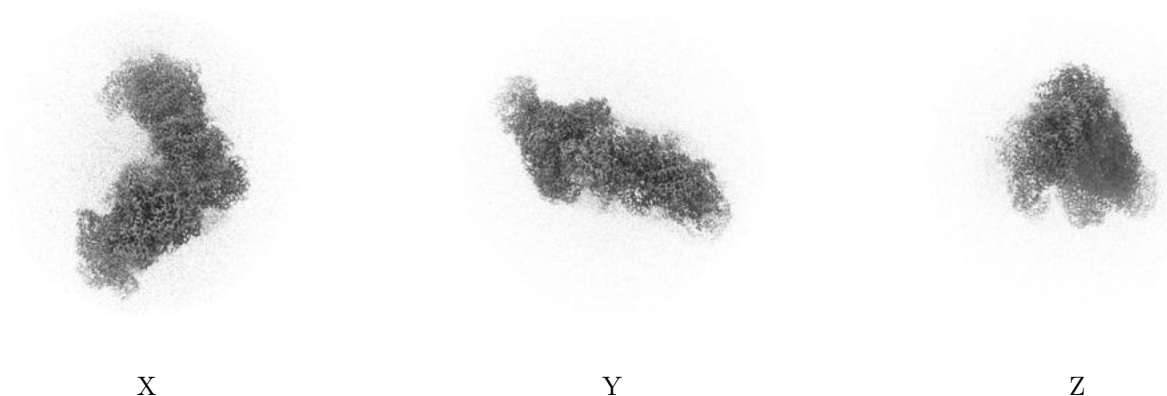
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

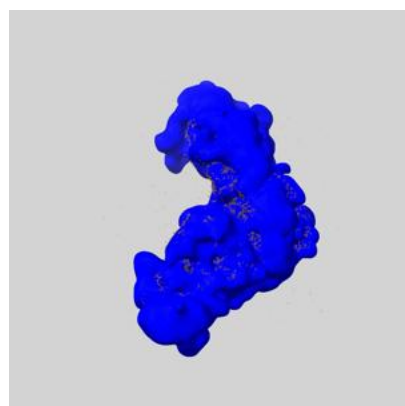
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

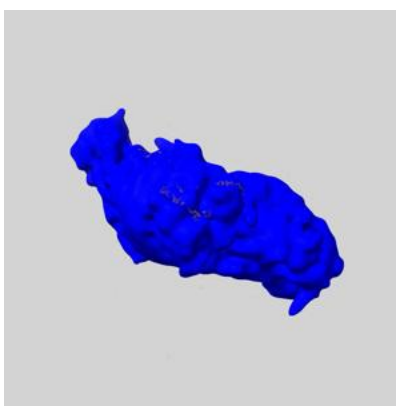
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

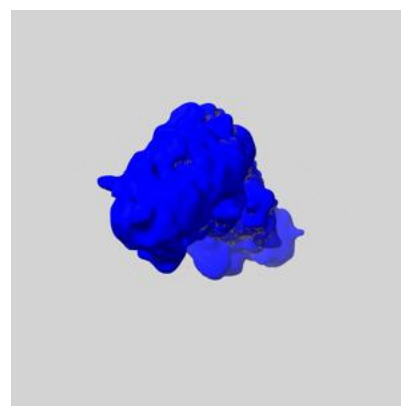
6.6.1 emd_12742_msk_1.map [i](#)



X



Y

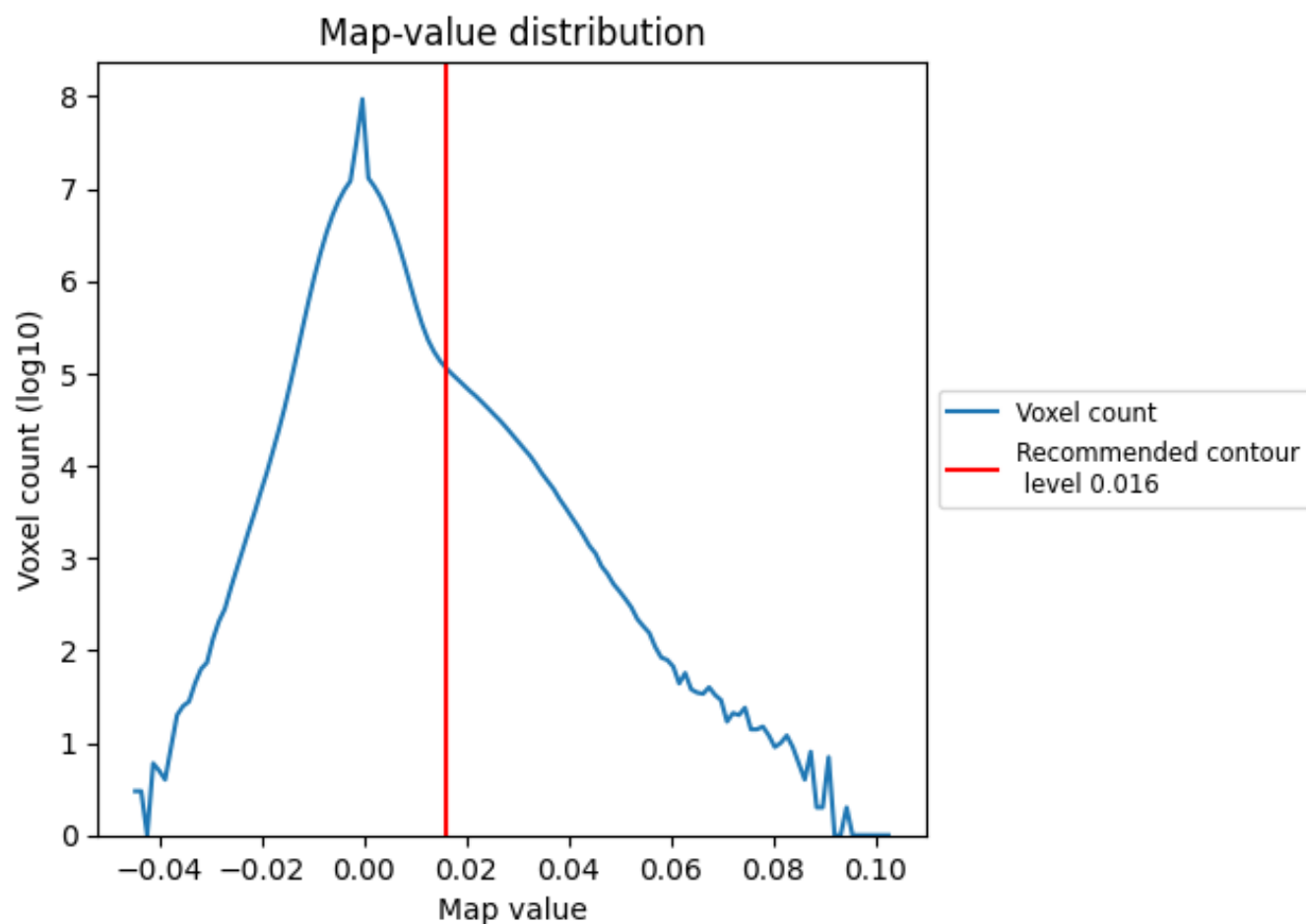


Z

7 Map analysis [i](#)

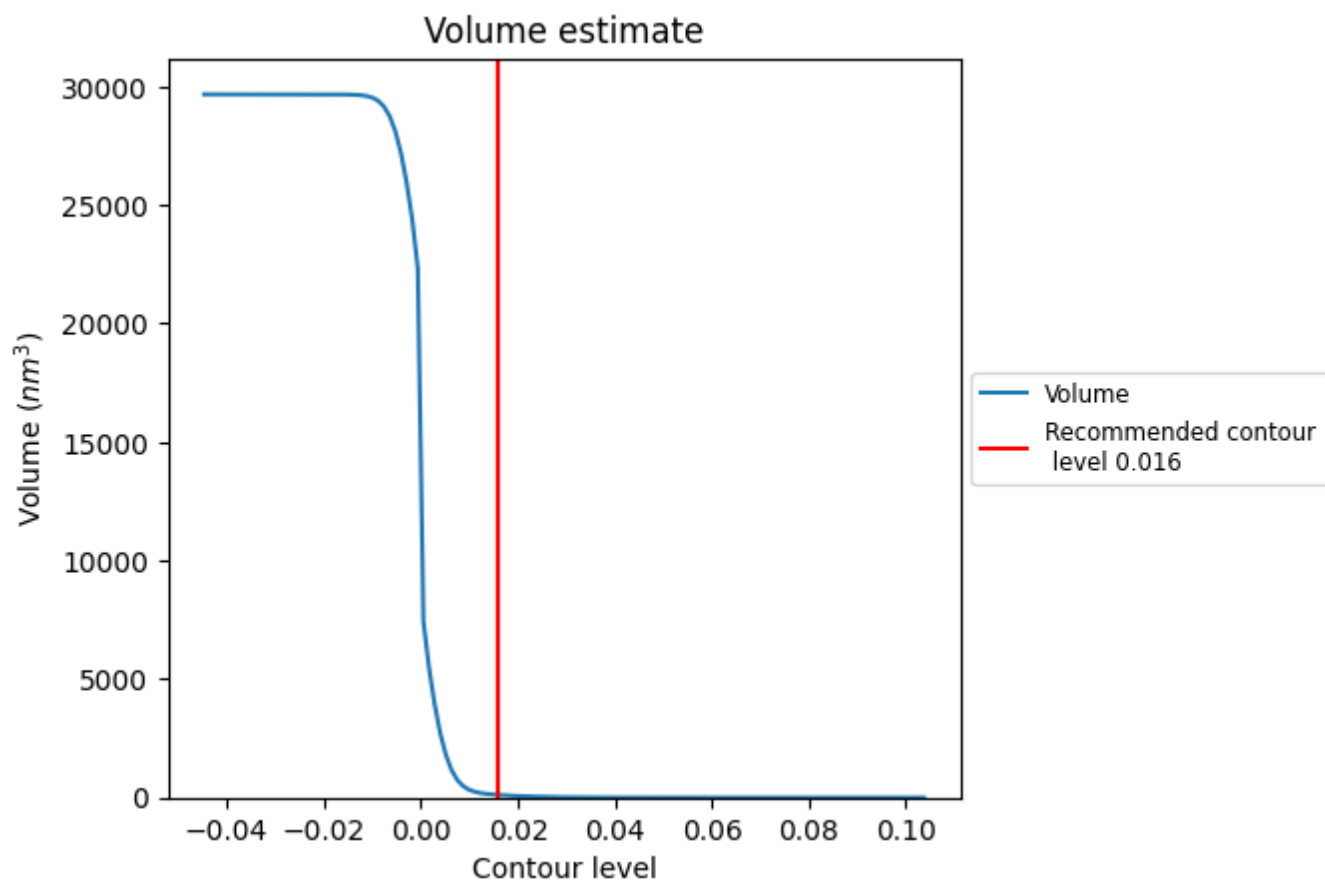
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

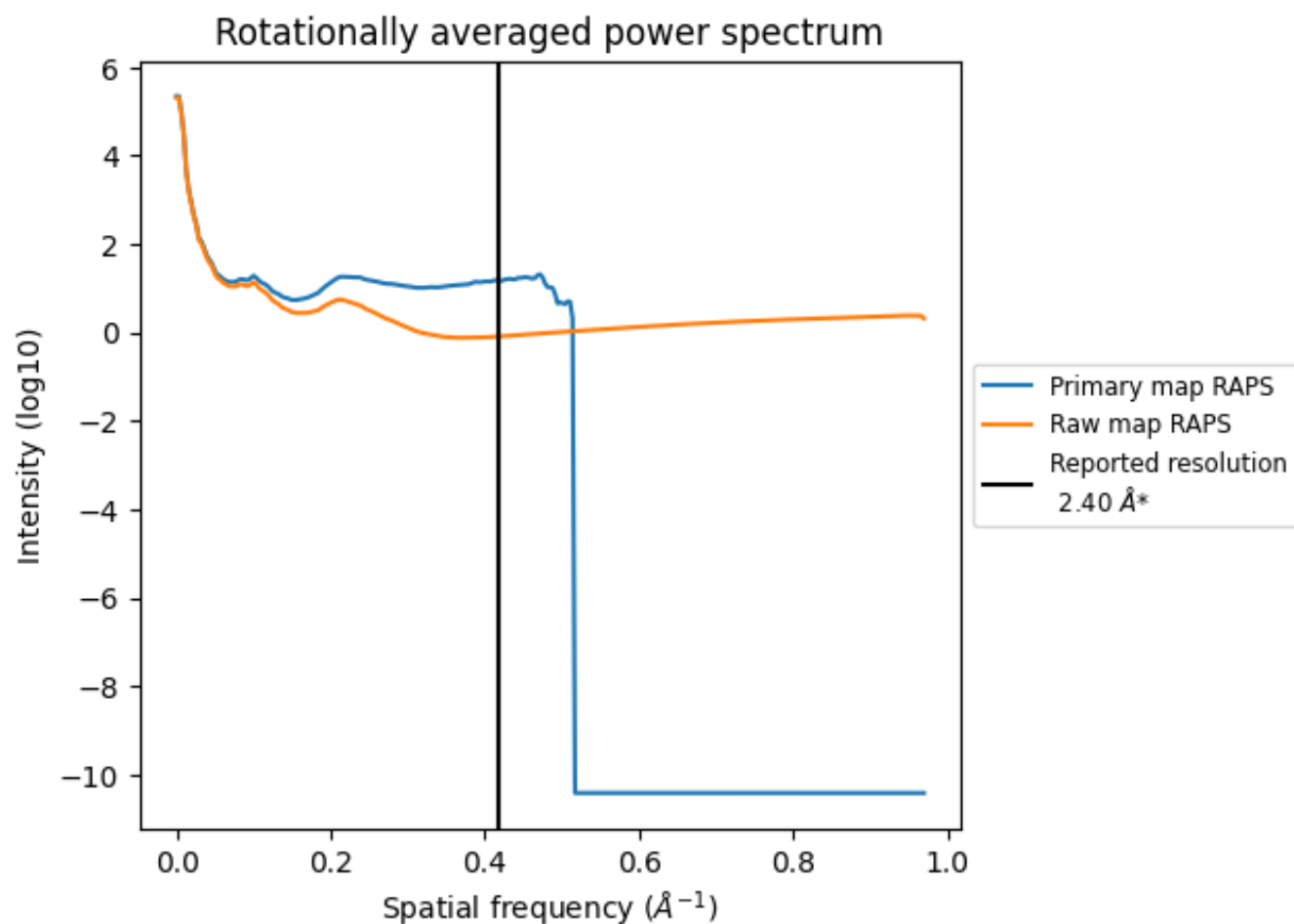
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 101 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

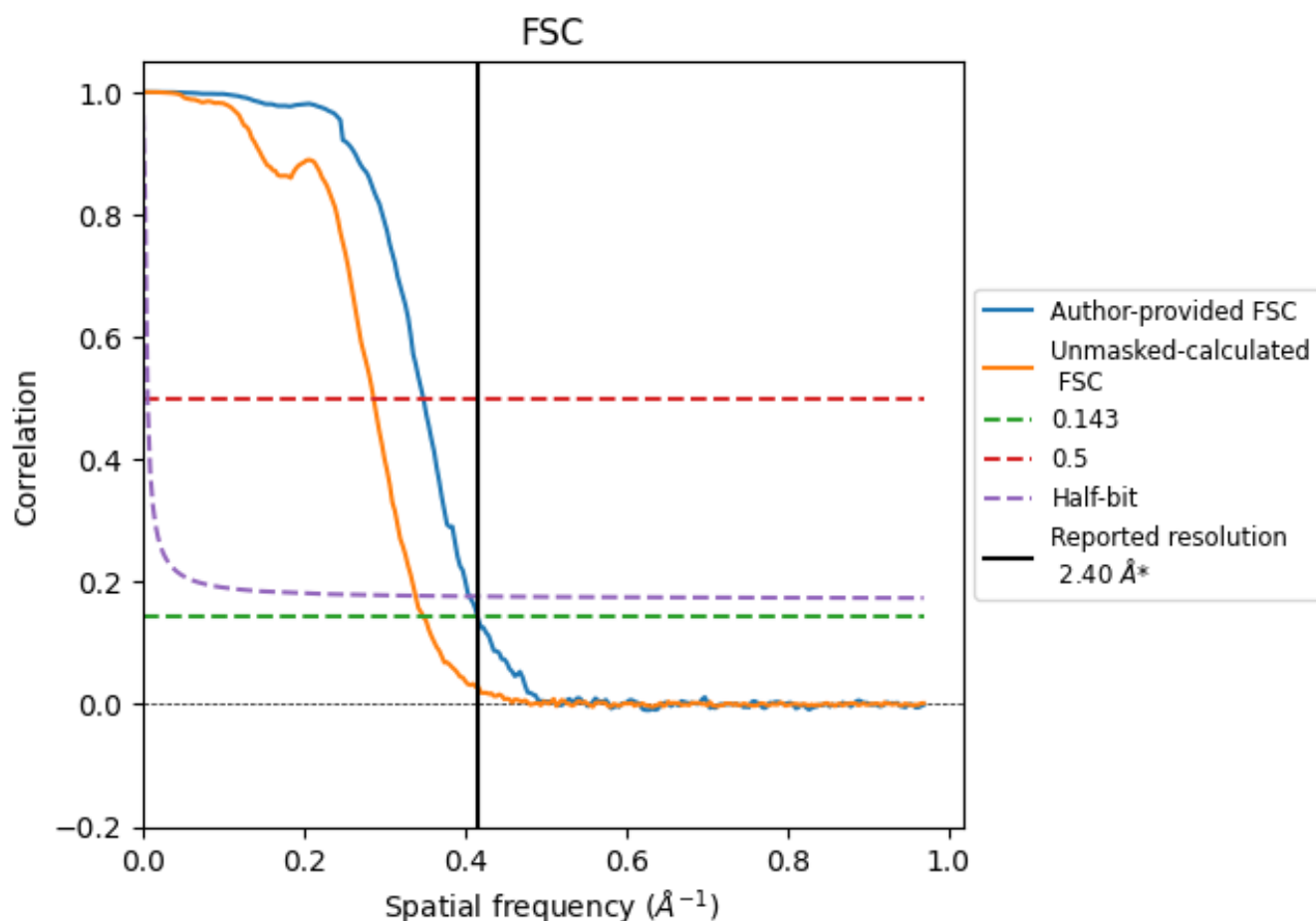


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

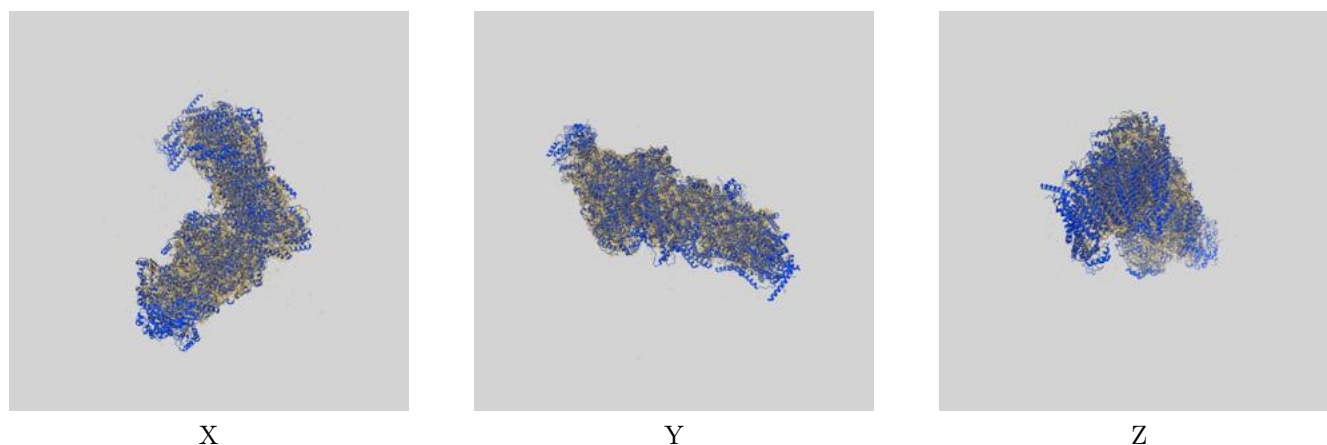
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.41	2.87	2.46
Unmasked-calculated*	2.87	3.49	2.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.87 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

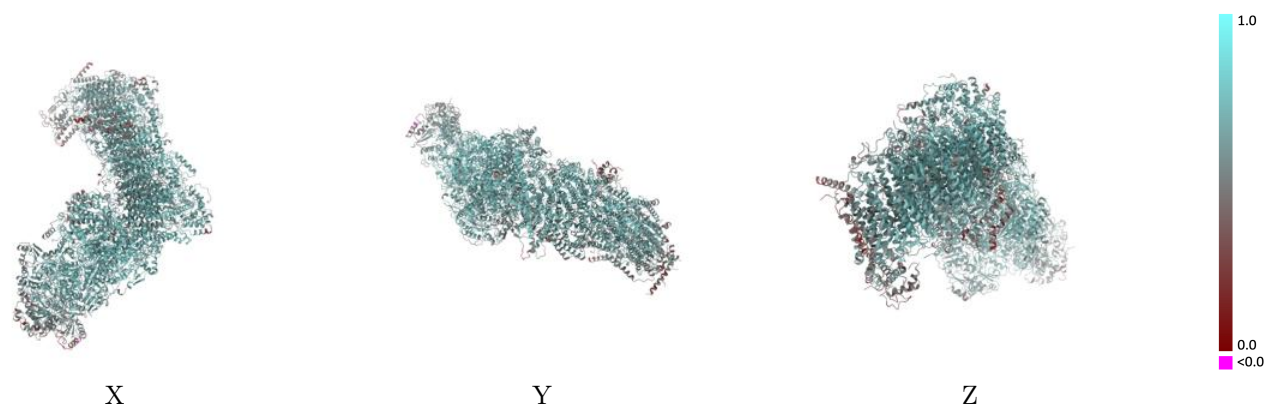
This section contains information regarding the fit between EMDB map EMD-12742 and PDB model 7O71. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



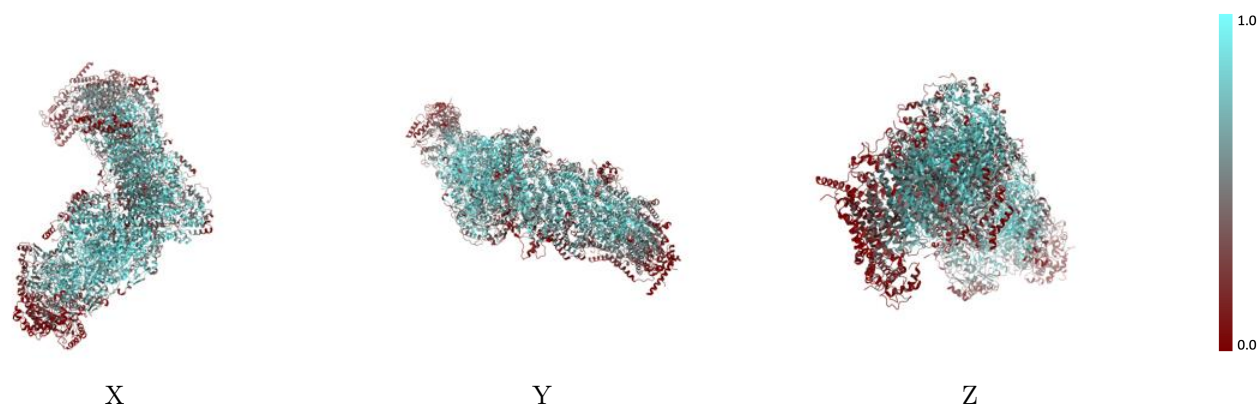
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



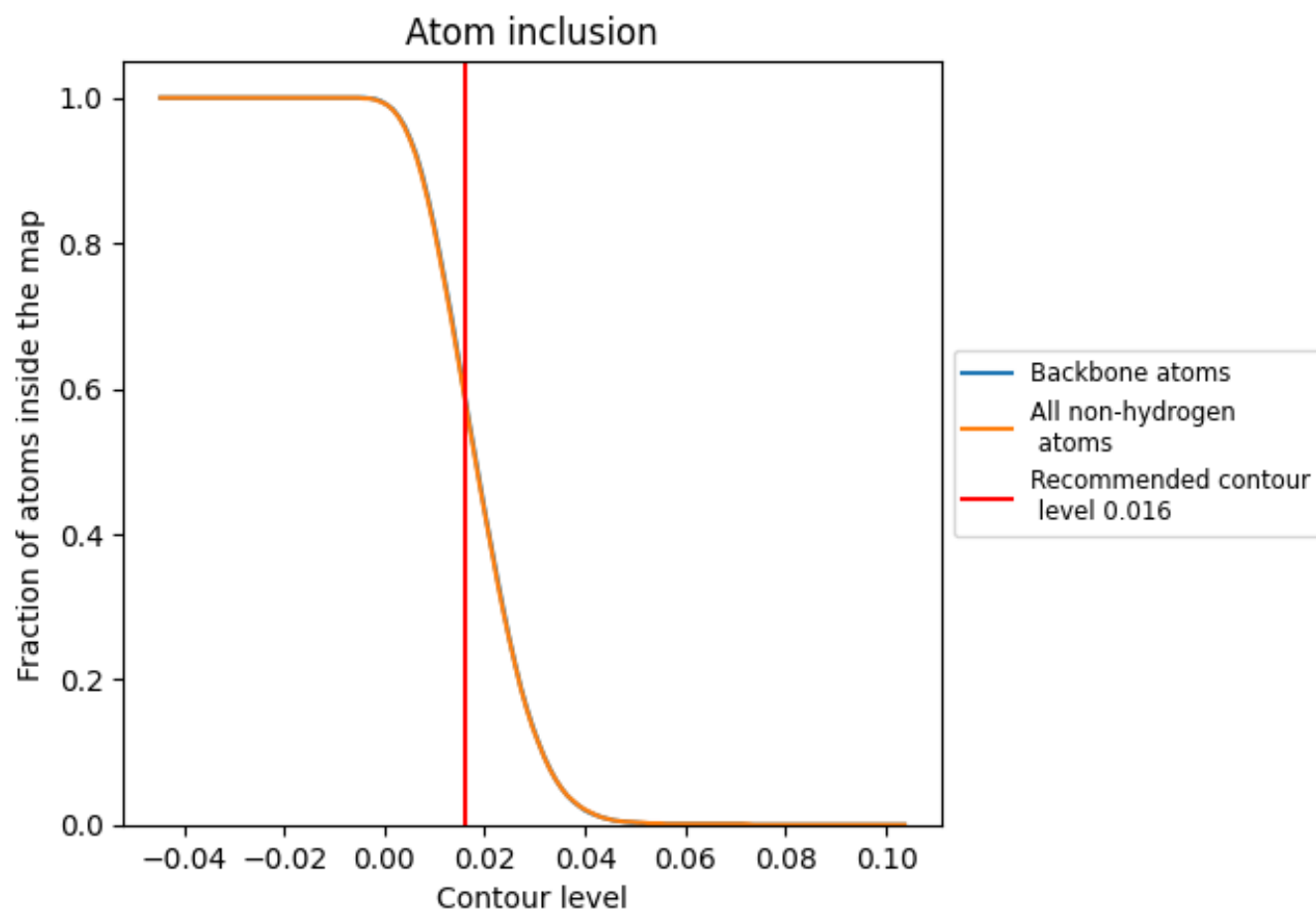
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5880	 0.6440
1	 0.7260	 0.6880
2	 0.8590	 0.7290
3	 0.5810	 0.6340
4	 0.7920	 0.7060
5	 0.5100	 0.6360
6	 0.5600	 0.6440
8	 0.1180	 0.4910
9	 0.4610	 0.5950
A	 0.6350	 0.6650
B	 0.3000	 0.5630
C	 0.8160	 0.7170
D	 0.7120	 0.6900
E	 0.5920	 0.6440
F	 0.6100	 0.6600
G	 0.8290	 0.7160
H	 0.2400	 0.5030
I	 0.8610	 0.7310
J	 0.4410	 0.5980
K	 0.8220	 0.7180
L	 0.7590	 0.7020
M	 0.7430	 0.6940
O	 0.0860	 0.3970
P	 0.5850	 0.6400
Q	 0.0900	 0.4420
R	 0.2720	 0.5240
S	 0.2550	 0.4720
U	 0.5590	 0.6450
W	 0.6160	 0.6560
X	 0.6650	 0.6740
Y	 0.7270	 0.6820
Z	 0.6250	 0.6560
a	 0.3340	 0.5810
b	 0.6560	 0.6750
c	 0.1180	 0.4570



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.6180	 0.6570
e	 0.1010	 0.4670
f	 0.3030	 0.5590
g	 0.4910	 0.6220
h	 0.7380	 0.6880
i	 0.3720	 0.5910
j	 0.4910	 0.6040
n	 0.5060	 0.6310