Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 10:19 AM JST

PDB ID	:	7VBZ / pdb_00007vbz
EMDB ID	:	EMD-31886
Title	:	Matrix arm of active state CI from Rotenone-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-09-01
Resolution	:	2.40 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

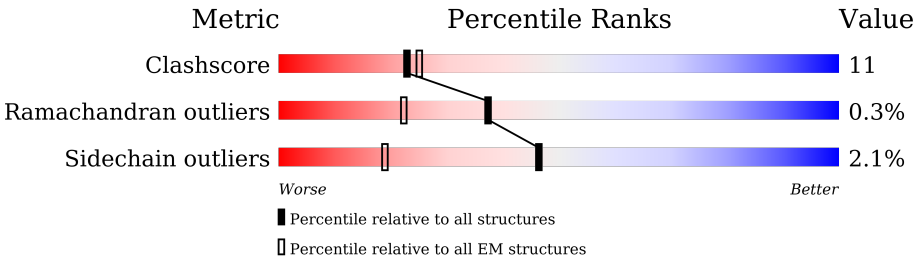
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB 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

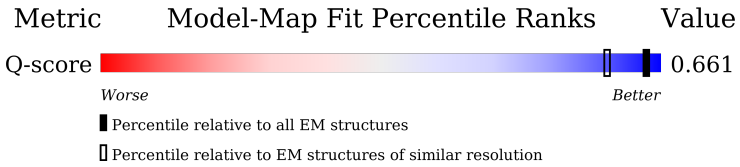
1 Overall quality at a glance (i)

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 <=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	433	75% 24%
2	B	176	82% 18%
3	C	156	81% 18%
4	E	115	8% 88% 10%

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Mol	Chain	Length	Quality of chain
5	F	86	9% 69% 29% •
6	G	88	39% 63% 33% 5%
7	H	112	• 82% 18%
8	I	112	14% 58% 23% 5% 13%
9	J	342	• 82% 18%
10	K	43	12% 56% 42% •
11	L	125	6% 80% 20%
12	M	690	• 77% 22% •
13	N	144	12% 71% 28% •
14	O	217	8% 74% 25% •
15	P	208	78% 20% •
16	Q	386	80% 19% •
17	T	96	11% 88% 11% •
18	W	29	24% 90% 10%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 29292 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	687	432	129	124	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	112	910	588	154	165	3	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	97	780	491	147	139	3	0	0

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	342	2751	1783	481	478	9	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	43	366	228	68	69	1	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	125	1016	642	181	190	3	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5296	3320	923	1014	39	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	144	1204	770	218	212	4	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1671	1065	281	315	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1738	1124	298	314	2	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	386	3096	1976	534	563	23	0	0

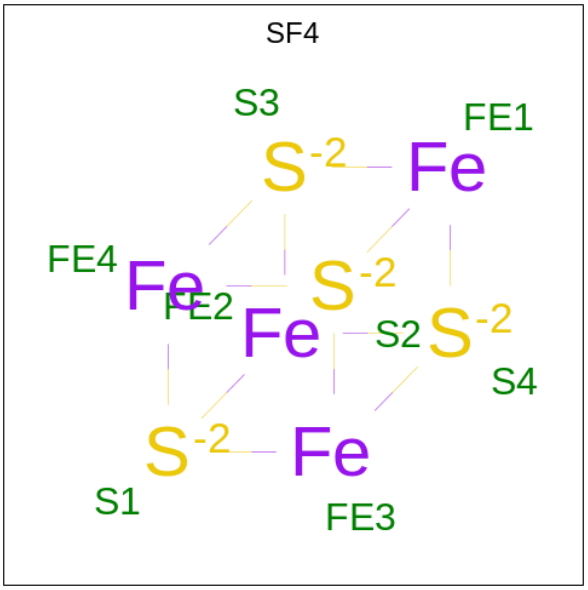
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	96	741	452	140	146	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

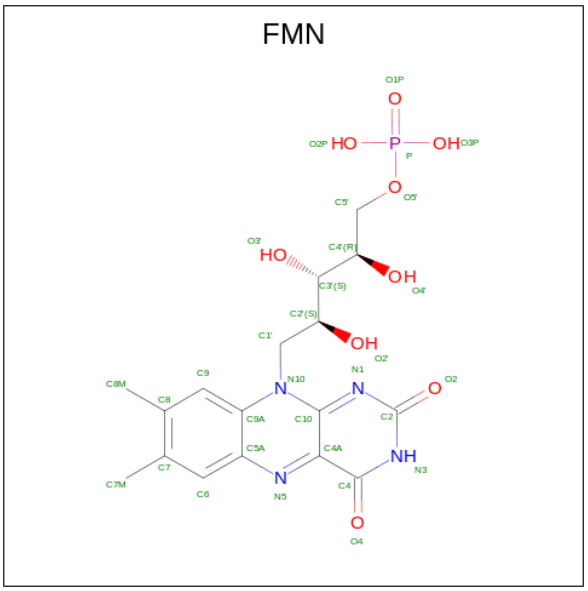
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	29	224	141	43	39	1	0	0

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



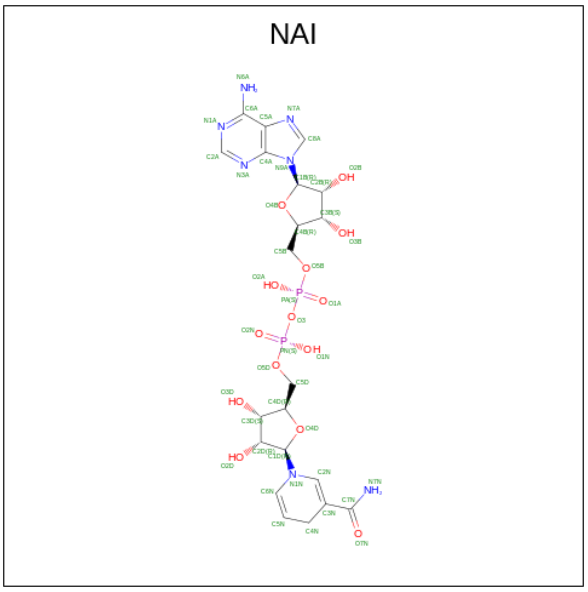
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	A	1	8	4	4	0
19	B	1	8	4	4	0
19	B	1	8	4	4	0
19	C	1	8	4	4	0
19	M	1	8	4	4	0
19	M	1	8	4	4	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



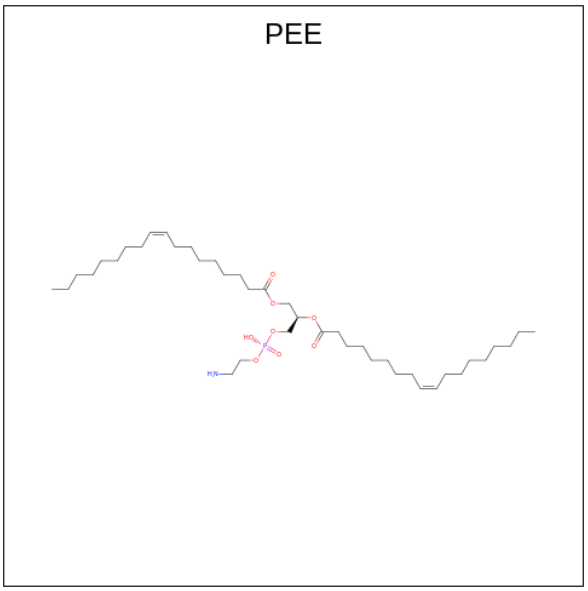
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	A	1	31	17	4	9	1	0

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



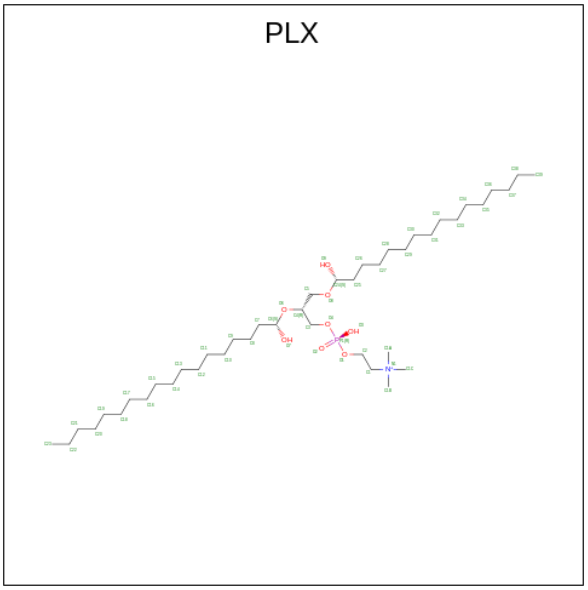
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
21	A	1	44	21	7	14	2	0

- Molecule 22 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



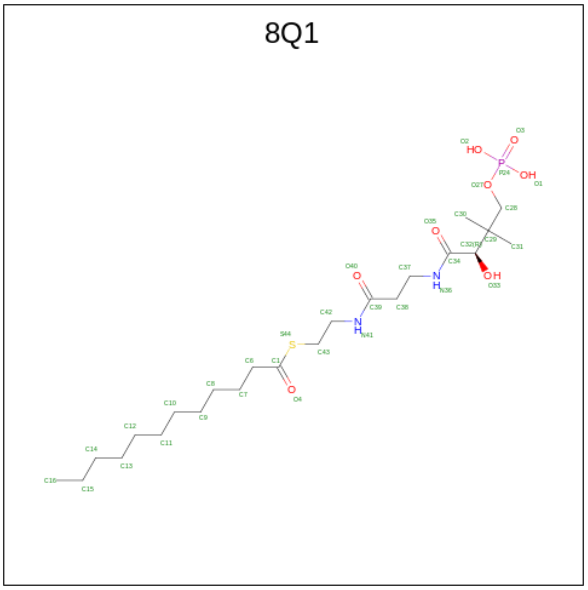
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	C	1	47	37	1	8	1	0

- Molecule 23 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



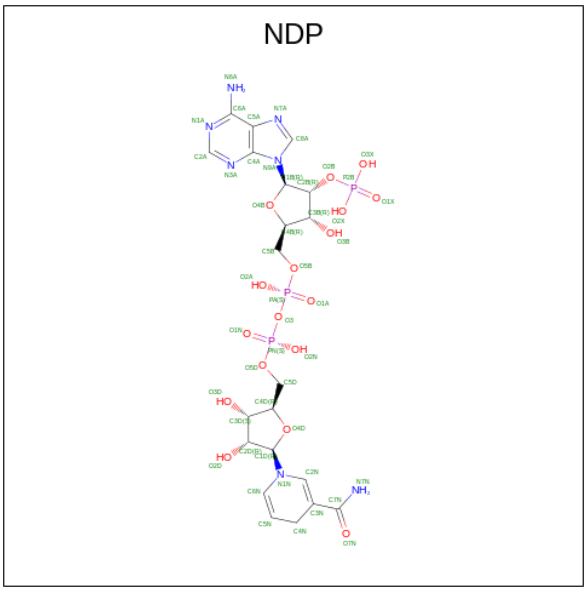
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	C	1	52	42	1	8	1	0

- Molecule 24 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



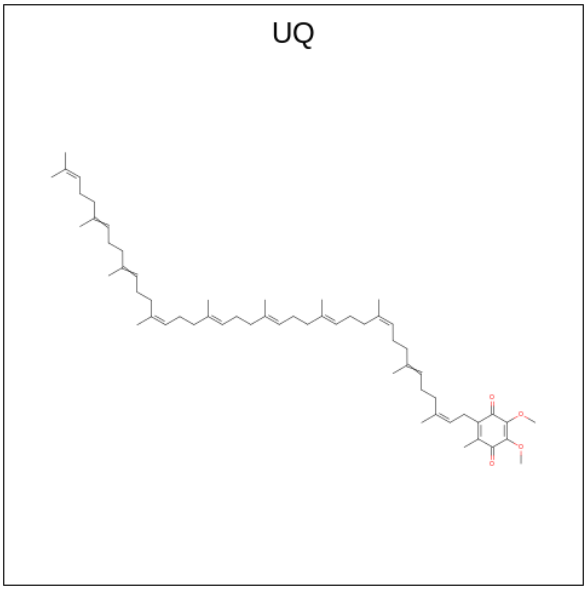
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
24	G	1	35	23	2	8	1	1	0

- Molecule 25 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



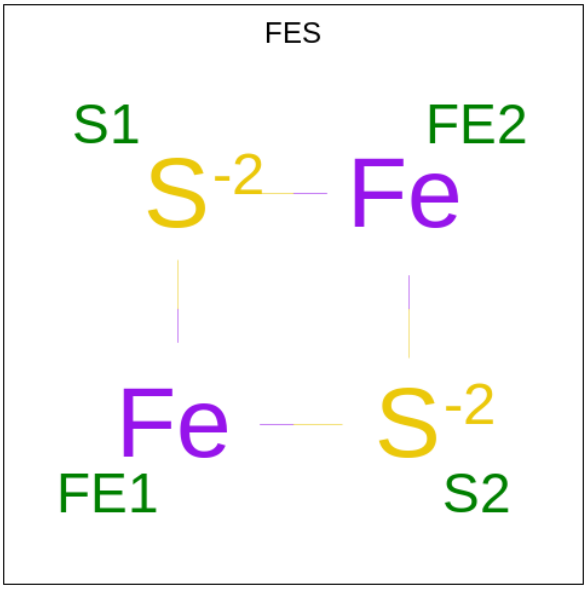
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	J	1	48	21	7	17	3	0

- Molecule 26 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	J	1	33	29	4	0

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

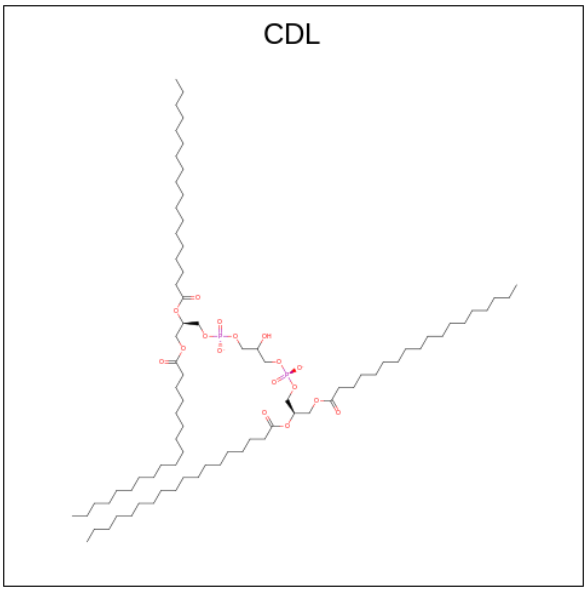


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	M	1	4	2	2	0
			Total	Fe	S	
27	O	1	4	2	2	0

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

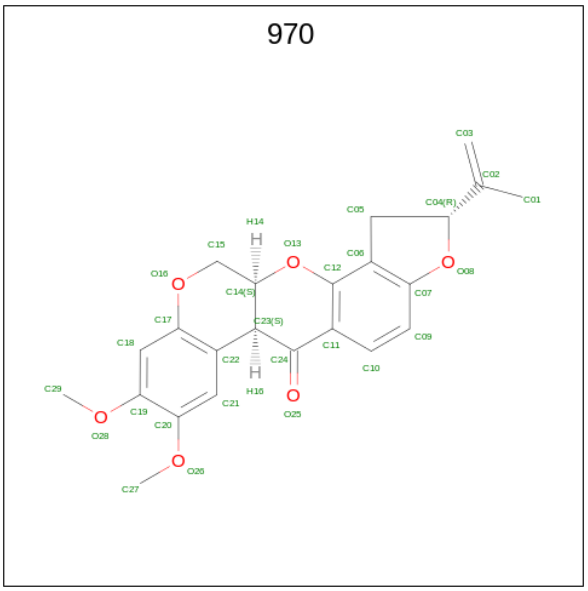
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
28	M	1	1	1	0

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
29	N	1	51	32	17	2	0

- Molecule 30 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2', 3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: $C_{23}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	Q	1	29	23	6	0

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
31	T	1	1	1	0

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
32	A	56	56	56	0
32	B	82	82	82	0
32	C	56	56	56	0
32	E	3	3	3	0
32	F	1	1	1	0
32	H	4	4	4	0
32	I	18	18	18	0

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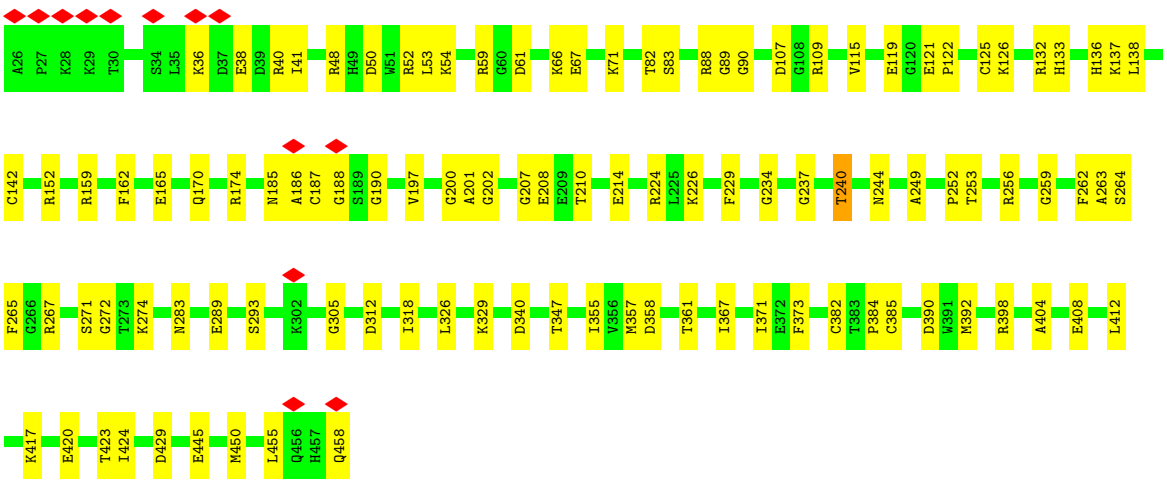
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
32	J	7	7	7	0
			Total	O	
32	K	5	5	5	0
			Total	O	
32	L	24	24	24	0
			Total	O	
32	M	186	186	186	0
			Total	O	
32	N	7	7	7	0
			Total	O	
32	O	15	15	15	0
			Total	O	
32	P	79	79	79	0
			Total	O	
32	Q	179	179	179	0
			Total	O	
32	T	6	6	6	0
			Total	O	
32	W	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

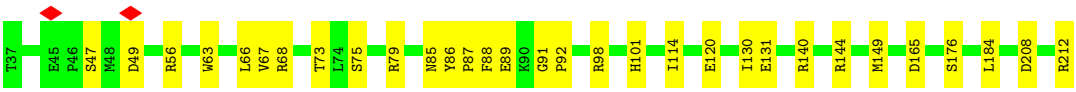
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A: 75% 24%



• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B: 82% 18%

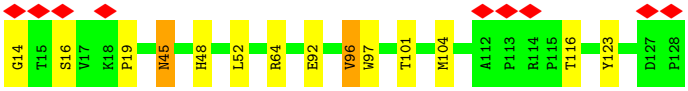


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C: 81% 18%

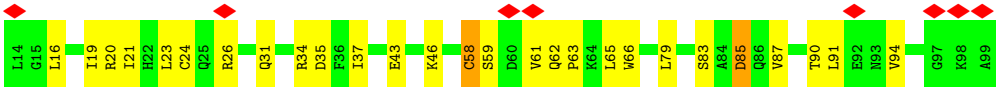
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 8% 88% 10%



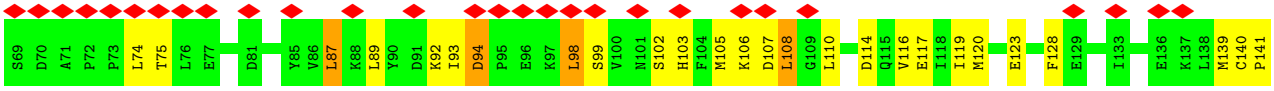
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

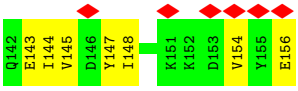
Chain F:



• Molecule 6: Acyl carrier protein, mitochondrial

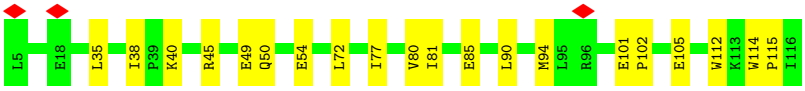
Chain G:





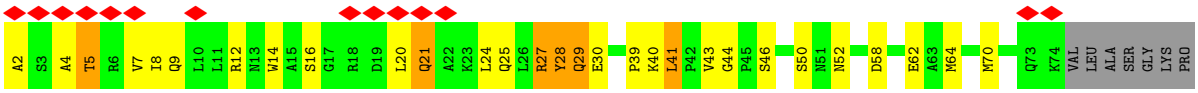
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

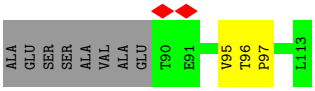
Chain H:



• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

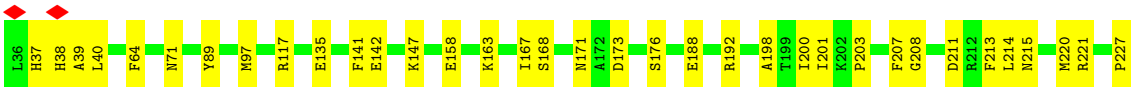
Chain I:

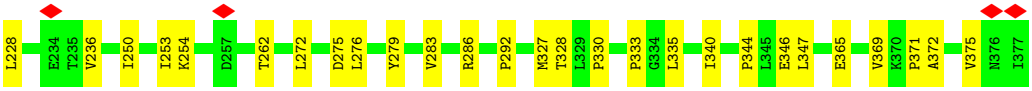




• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

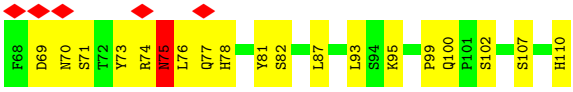
Chain J:





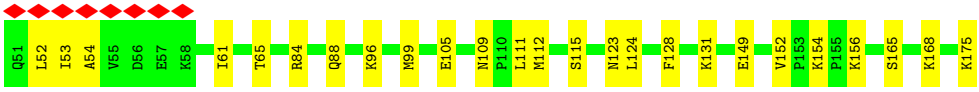
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:



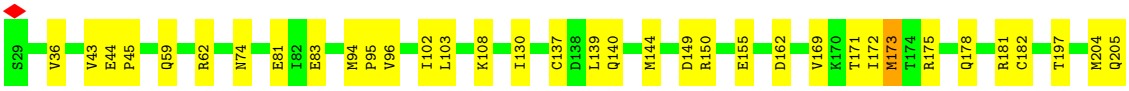
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

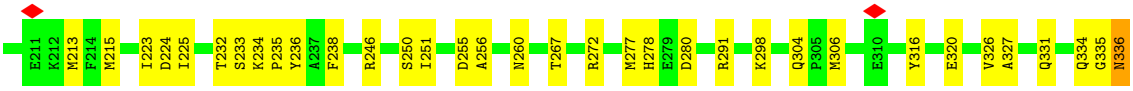
Chain L:

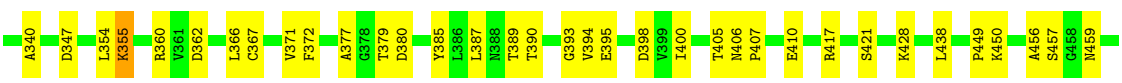


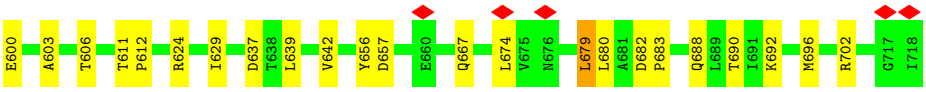
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



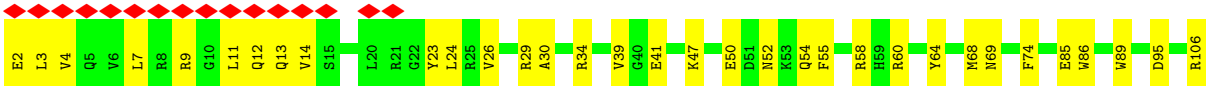


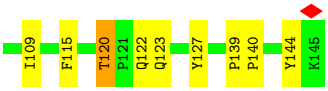




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

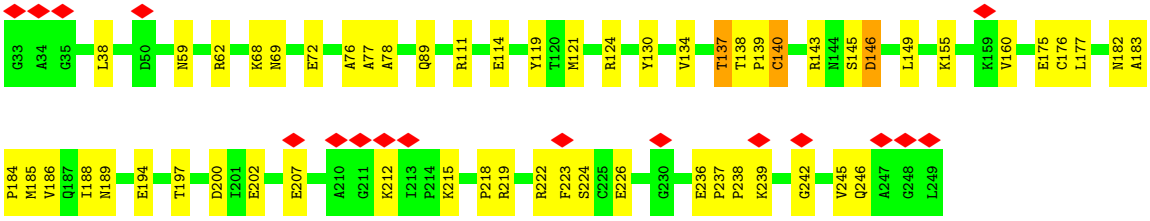
Chain N:





• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:



• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

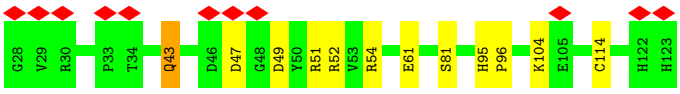
Chain P:

• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:

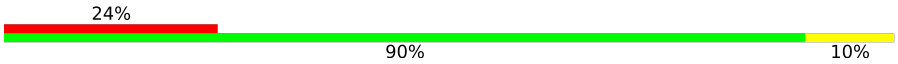
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

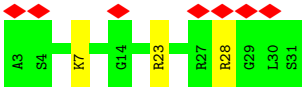
Chain T:



• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:




A3
S4
K7
G14
R23
R27
R28
G29
L30
S31

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0152	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 8Q1, FES, MG, FMN, NAI, 2MR, SF4, UQ, ZN, PEE, PLX, NDP, 970

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	0.24	0/3406	0.46	0/4603
2	B	0.24	0/1443	0.40	0/1952
3	C	0.27	0/1279	0.42	0/1730
4	E	0.22	0/995	0.44	1/1340 (0.1%)
5	F	0.20	0/698	0.37	0/940
6	G	0.21	0/705	0.55	1/956 (0.1%)
7	H	0.23	0/929	0.53	0/1258
8	I	0.27	0/798	0.67	1/1079 (0.1%)
9	J	0.22	0/2828	0.41	0/3834
10	K	0.28	0/377	0.55	1/509 (0.2%)
11	L	0.23	0/1039	0.38	0/1403
12	M	0.29	0/5384	0.61	7/7295 (0.1%)
13	N	0.20	0/1245	0.38	0/1694
14	O	0.22	0/1711	0.50	0/2328
15	P	0.30	0/1789	0.61	2/2436 (0.1%)
16	Q	0.39	3/3157 (0.1%)	0.56	6/4268 (0.1%)
17	T	0.23	0/755	0.42	0/1018
18	W	0.23	0/230	0.65	0/309
All	All	0.27	3/28768 (0.0%)	0.51	19/38952 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	193	ASP	C-N	8.60	1.44	1.33
16	Q	141	TYR	C-N	-7.95	1.25	1.33
16	Q	140	ASP	C-N	6.66	1.45	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	74	ASN	N-CA-C	9.80	122.05	111.36
8	I	28	TYR	N-CA-C	9.47	121.69	111.36
16	Q	193	ASP	O-C-N	7.12	129.78	122.09
6	G	106	LYS	N-CA-C	7.01	118.71	111.14
12	M	173	MET	N-CA-C	6.67	120.52	112.38
16	Q	224	ALA	N-CA-C	6.61	118.14	111.07
16	Q	141	TYR	CA-C-N	-6.11	115.36	122.14
16	Q	141	TYR	C-N-CA	-6.11	115.36	122.14
4	E	97	TRP	N-CA-C	-6.06	104.76	111.36
16	Q	102	SER	N-CA-C	-5.70	97.89	107.99
15	P	196	HIS	CA-C-N	5.66	125.33	119.05
15	P	196	HIS	C-N-CA	5.66	125.33	119.05
12	M	406	ASN	CA-C-N	5.64	125.31	119.05
12	M	406	ASN	C-N-CA	5.64	125.31	119.05
12	M	371	VAL	N-CA-C	5.43	116.06	108.89
10	K	75	ASN	N-CA-C	5.31	122.11	110.80
12	M	612	PRO	CA-C-N	5.13	125.03	119.85
12	M	612	PRO	C-N-CA	5.13	125.03	119.85
16	Q	217	VAL	N-CA-C	5.12	115.89	110.72

There are no chirality outliers.

There are no planarity outliers.

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	3330	0	3292	80	0
2	B	1412	0	1363	26	0
3	C	1248	0	1254	26	0
4	E	971	0	975	16	0
5	F	687	0	700	21	0
6	G	693	0	671	35	0
7	H	910	0	950	15	0
8	I	780	0	808	36	0
9	J	2751	0	2773	47	0
10	K	366	0	338	20	0
11	L	1016	0	1016	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	5296	0	5328	118	0
13	N	1204	0	1162	35	0
14	O	1671	0	1674	44	0
15	P	1738	0	1693	50	0
16	Q	3096	0	3063	68	0
17	T	741	0	702	8	0
18	W	224	0	230	6	0
19	A	8	0	0	1	0
19	B	16	0	0	0	0
19	C	8	0	0	1	0
19	M	16	0	0	1	0
20	A	31	0	19	4	0
21	A	44	0	27	5	0
22	C	47	0	71	7	0
23	C	52	0	88	13	0
24	G	35	0	0	0	0
25	J	48	0	23	3	0
26	J	33	0	39	7	0
27	M	4	0	0	0	0
27	O	4	0	0	0	0
28	M	1	0	0	0	0
29	N	51	0	46	18	0
30	Q	29	0	0	1	0
31	T	1	0	0	0	0
32	A	56	0	0	7	0
32	B	82	0	0	2	0
32	C	56	0	0	2	0
32	E	3	0	0	0	0
32	F	1	0	0	0	0
32	H	4	0	0	0	0
32	I	18	0	0	4	0
32	J	7	0	0	0	0
32	K	5	0	0	3	0
32	L	24	0	0	0	0
32	M	186	0	0	10	0
32	N	7	0	0	2	0
32	O	15	0	0	1	0
32	P	79	0	0	3	0
32	Q	179	0	0	22	0
32	T	6	0	0	0	0
32	W	2	0	0	0	0
All	All	29292	0	28305	632	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 11.

All (632) 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)
9:J:220:MET:CE	9:J:227:PRO:HD2	1.58	1.33
12:M:379:THR:HG21	32:M:1006:HOH:O	1.28	1.29
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.24
6:G:105:MET:HG2	6:G:139:MET:CE	1.68	1.23
25:J:401:NDP:O4D	25:J:401:NDP:C4D	1.69	1.22
1:A:66:LYS:HE3	1:A:188:GLY:O	1.41	1.19
6:G:105:MET:HE2	6:G:139:MET:SD	1.88	1.12
8:I:4:ALA:HA	29:N:201:CDL:HA22	1.28	1.11
9:J:220:MET:HE3	9:J:227:PRO:HD2	1.34	1.03
6:G:105:MET:HG2	6:G:139:MET:HE1	1.36	1.03
8:I:4:ALA:HA	29:N:201:CDL:CA2	1.95	0.97
9:J:208:GLY:H	9:J:211:ASP:CG	1.73	0.97
12:M:485:ASP:OD1	12:M:680:LEU:HD12	1.65	0.97
9:J:207:PHE:HA	9:J:211:ASP:OD2	1.65	0.96
6:G:105:MET:CG	6:G:139:MET:CE	2.42	0.96
8:I:2:ALA:HB2	8:I:24:LEU:CD1	1.97	0.94
23:C:303:PLX:H393	23:C:303:PLX:H211	1.50	0.94
6:G:105:MET:HG2	6:G:139:MET:HE2	1.49	0.92
15:P:127:GLU:OE1	15:P:144:LYS:NZ	2.04	0.90
8:I:2:ALA:HB2	8:I:24:LEU:HD13	1.54	0.89
8:I:5:THR:CG2	8:I:7:VAL:HG12	2.04	0.88
6:G:105:MET:CG	6:G:139:MET:HE1	2.02	0.87
1:A:48:ARG:NH1	10:K:70:ASN:O	2.07	0.86
16:Q:137:ASP:OD1	16:Q:148:GLU:OE2	1.94	0.86
29:N:201:CDL:H742	29:N:201:CDL:C55	2.05	0.86
3:C:51:ASP:OD2	3:C:188:LYS:HA	1.75	0.85
1:A:244:ASN:ND2	20:A:502:FMN:O2	2.08	0.84
2:B:79:ARG:HH11	8:I:25:GLN:HE22	1.24	0.84
8:I:5:THR:HG21	8:I:7:VAL:HG12	1.58	0.84
1:A:82:THR:HG23	1:A:259:GLY:HA3	1.59	0.84
9:J:220:MET:HE2	9:J:227:PRO:HD2	1.59	0.84
6:G:105:MET:CG	6:G:139:MET:HE2	2.04	0.84
29:N:201:CDL:HA62	29:N:201:CDL:C12	2.08	0.84
16:Q:333:ARG:NH1	32:Q:601:HOH:O	2.02	0.83
32:B:437:HOH:O	17:T:114:CYS:SG	2.18	0.83
6:G:105:MET:HE2	6:G:139:MET:CE	2.09	0.83
12:M:44:GLU:OE1	12:M:45:PRO:HD2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N:201:CDL:HA62	29:N:201:CDL:H122	1.61	0.82
15:P:125:ARG:NH2	15:P:199:ARG:HG2	1.95	0.82
15:P:161:LYS:HE3	16:Q:285:ASN:OD1	1.80	0.81
23:C:303:PLX:H211	23:C:303:PLX:C39	2.11	0.80
16:Q:92:HIS:CD2	32:Q:643:HOH:O	2.33	0.80
10:K:87:LEU:CD2	32:K:202:HOH:O	2.30	0.80
1:A:252:PRO:HG2	32:A:630:HOH:O	1.81	0.80
9:J:208:GLY:N	9:J:211:ASP:OD2	2.15	0.79
10:K:100:GLN:NE2	14:O:69:ASN:O	2.15	0.79
8:I:40:LYS:HB3	18:W:7:LYS:H	1.48	0.78
3:C:56:TRP:CE2	23:C:303:PLX:H112	2.18	0.78
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.17	0.78
9:J:207:PHE:CA	9:J:211:ASP:OD2	2.31	0.78
11:L:109:ASN:ND2	11:L:111:LEU:O	2.15	0.78
26:J:402:UQ:H101	26:J:402:UQ:H152	1.66	0.77
12:M:336:ASN:ND2	12:M:540:ASN:CB	2.48	0.77
8:I:96:THR:HB	8:I:97:PRO:HD2	1.64	0.77
30:Q:501:970:C15	32:Q:643:HOH:O	2.33	0.77
12:M:336:ASN:ND2	12:M:540:ASN:HB3	1.99	0.77
15:P:85:GLU:OE2	15:P:144:LYS:HE2	1.83	0.77
5:F:43:GLU:HA	5:F:46:LYS:HG3	1.65	0.77
1:A:50:ASP:O	1:A:59:ARG:NH2	2.17	0.76
10:K:87:LEU:HD22	32:K:202:HOH:O	1.83	0.76
1:A:252:PRO:CG	32:A:630:HOH:O	2.32	0.76
12:M:83:GLU:OE1	32:M:902:HOH:O	2.03	0.75
14:O:207:GLU:HG3	14:O:212:LYS:HE2	1.67	0.74
9:J:208:GLY:O	9:J:211:ASP:OD1	2.04	0.74
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.68	0.74
2:B:79:ARG:HH11	8:I:25:GLN:NE2	1.84	0.74
29:N:201:CDL:H122	29:N:201:CDL:CA6	2.18	0.74
6:G:105:MET:CE	6:G:139:MET:SD	2.75	0.73
13:N:120:THR:HG22	13:N:122:GLN:H	1.53	0.73
14:O:143:ARG:O	14:O:184:PRO:HG3	1.89	0.73
16:Q:236:LEU:O	32:Q:602:HOH:O	2.07	0.73
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.21	0.73
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.22	0.72
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.72
10:K:78:HIS:HA	10:K:81:TYR:CD2	2.24	0.72
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.71	0.72
6:G:108:LEU:HD12	6:G:108:LEU:N	2.04	0.72
12:M:327:ALA:O	12:M:331:GLN:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:336:ASN:HD21	12:M:540:ASN:CB	2.03	0.72
9:J:135:GLU:OE2	9:J:141:PHE:N	2.18	0.71
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.71	0.71
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.71	0.71
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.72	0.71
16:Q:360:ASP:OD2	32:Q:603:HOH:O	2.09	0.71
9:J:220:MET:CE	9:J:227:PRO:CD	2.55	0.71
15:P:207:TYR:C	15:P:224:VAL:HG23	2.16	0.71
14:O:222:ARG:NH1	14:O:226:GLU:O	2.23	0.71
29:N:201:CDL:OA3	29:N:201:CDL:O1	2.06	0.71
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.25	0.70
12:M:377:ALA:O	12:M:380:ASP:HB2	1.91	0.70
12:M:298:LYS:HG3	32:M:901:HOH:O	1.92	0.70
9:J:215:ASN:HD22	26:J:402:UQ:HM31	1.57	0.69
12:M:400:ILE:HD12	12:M:473:MET:HE3	1.74	0.69
1:A:390:ASP:OD1	32:A:601:HOH:O	2.11	0.69
13:N:68:MET:HG3	13:N:69:ASN:H	1.56	0.69
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.74	0.69
12:M:483:ARG:NH2	12:M:682:ASP:HB2	2.08	0.69
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.26	0.68
16:Q:193:ASP:HB2	32:Q:608:HOH:O	1.93	0.68
12:M:336:ASN:HD21	12:M:540:ASN:ND2	1.91	0.68
15:P:173:MET:HE1	15:P:189:THR:HG23	1.74	0.68
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.76	0.68
23:C:303:PLX:H393	23:C:303:PLX:C21	2.23	0.68
8:I:2:ALA:HB2	8:I:24:LEU:HD11	1.76	0.67
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.77	0.67
12:M:255:ASP:OD1	32:M:903:HOH:O	2.12	0.67
15:P:113:ASP:HB3	16:Q:425:LYS:HG3	1.75	0.67
12:M:534:VAL:HG21	12:M:555:ILE:CG1	2.24	0.67
2:B:68:ARG:HH12	18:W:28:ARG:HB3	1.59	0.67
16:Q:92:HIS:CG	32:Q:643:HOH:O	2.48	0.67
2:B:47:SER:OG	2:B:49:ASP:OD1	2.13	0.67
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.67
14:O:197:THR:OG1	14:O:200:ASP:OD1	2.10	0.67
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.77	0.66
3:C:66:THR:O	32:C:401:HOH:O	2.13	0.66
1:A:89:GLY:O	21:A:503:NAI:H2N	1.95	0.66
12:M:534:VAL:HG21	12:M:555:ILE:HG12	1.78	0.66
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.77	0.66
5:F:31:GLN:NE2	5:F:35:ASP:OD1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.29	0.66
6:G:105:MET:HE2	6:G:139:MET:HE1	1.78	0.66
4:E:64:ARG:NH2	6:G:117:GLU:OE1	2.25	0.66
12:M:81:GLU:HG3	12:M:108:LYS:HD2	1.76	0.66
16:Q:456:ILE:O	32:Q:605:HOH:O	2.14	0.66
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.77	0.66
5:F:85:ASP:OD1	5:F:85:ASP:N	2.20	0.66
1:A:59:ARG:O	14:O:239:LYS:O	2.13	0.65
6:G:105:MET:SD	6:G:139:MET:HE1	2.36	0.65
12:M:367:CYS:HB3	12:M:533:GLY:O	1.96	0.65
16:Q:162:GLN:O	32:Q:604:HOH:O	2.13	0.65
2:B:47:SER:O	2:B:56:ARG:NH2	2.30	0.65
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.77	0.65
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.79	0.65
3:C:56:TRP:CZ2	23:C:303:PLX:H112	2.32	0.65
9:J:117:ARG:HH22	9:J:158:GLU:HG2	1.61	0.65
5:F:83:SER:OG	5:F:85:ASP:OD1	2.11	0.65
6:G:87:LEU:HD23	6:G:98:LEU:HD11	1.80	0.64
1:A:90:GLY:HA3	21:A:503:NAI:H1D	1.78	0.64
1:A:36:LYS:H	1:A:36:LYS:HD3	1.62	0.64
1:A:357:MET:HB3	1:A:361:THR:HG21	1.80	0.64
9:J:220:MET:HE1	9:J:227:PRO:HD2	1.75	0.64
13:N:9:ARG:NH1	29:N:201:CDL:OB2	2.31	0.64
1:A:159:ARG:NH2	14:O:176:CYS:O	2.29	0.64
8:I:2:ALA:CB	8:I:24:LEU:HD11	2.28	0.63
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.32	0.63
1:A:109:ARG:NH1	1:A:237:GLY:O	2.32	0.63
10:K:73:TYR:HB2	14:O:223:PHE:CD1	2.34	0.63
12:M:456:ALA:O	12:M:499:ASN:ND2	2.31	0.63
1:A:263:ALA:HA	1:A:271:SER:HB3	1.81	0.63
13:N:140:PRO:O	32:N:301:HOH:O	2.15	0.63
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.06	0.63
12:M:43:VAL:HG21	12:M:96:VAL:HG21	1.81	0.63
14:O:177:LEU:HD12	14:O:185:MET:SD	2.39	0.63
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.38	0.62
4:E:96:VAL:HG12	4:E:96:VAL:O	1.99	0.62
13:N:29:ARG:NH2	13:N:64:TYR:O	2.31	0.62
15:P:147:THR:HB	15:P:153:ILE:HD11	1.81	0.62
23:C:303:PLX:C26	23:C:303:PLX:H102	2.29	0.62
12:M:336:ASN:HD22	12:M:540:ASN:HB3	1.64	0.62
4:E:92:GLU:OE1	15:P:191:TYR:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:162:ASP:O	17:T:104:LYS:NZ	2.31	0.62
8:I:27:ARG:NH2	16:Q:212:GLU:OE1	2.33	0.61
16:Q:193:ASP:CB	32:Q:608:HOH:O	2.48	0.61
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.33	0.61
9:J:171:ASN:HA	9:J:327:MET:HE3	1.81	0.61
11:L:165:SER:OG	11:L:168:LYS:HB2	2.00	0.61
16:Q:92:HIS:HE1	16:Q:189:THR:HB	1.66	0.61
11:L:105:GLU:HA	12:M:611:THR:HG21	1.81	0.61
15:P:86:ILE:HD12	15:P:141:ILE:HD11	1.82	0.60
6:G:105:MET:CE	6:G:139:MET:CE	2.78	0.60
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.82	0.60
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.84	0.60
8:I:5:THR:O	8:I:9:GLN:HG3	2.01	0.60
15:P:43:THR:HA	15:P:47:ILE:HD12	1.83	0.60
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.83	0.60
16:Q:402:ALA:O	32:Q:606:HOH:O	2.16	0.60
1:A:40:ARG:NH1	1:A:289:GLU:O	2.34	0.60
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.37	0.60
10:K:87:LEU:HD23	32:K:202:HOH:O	2.00	0.60
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.02	0.59
12:M:566:ILE:HD13	12:M:579:MET:HE3	1.83	0.59
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.83	0.59
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.34	0.59
3:C:196:ARG:NH2	25:J:401:NDP:O2X	2.34	0.59
3:C:56:TRP:CD2	23:C:303:PLX:H112	2.37	0.59
8:I:2:ALA:CB	8:I:24:LEU:CD1	2.77	0.59
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.36	0.59
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.36	0.59
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.02	0.59
9:J:64:PHE:CE2	9:J:211:ASP:HB3	2.38	0.59
26:J:402:UQ:H161	26:J:402:UQ:H203	1.84	0.59
12:M:335:GLY:HA2	12:M:362:ASP:O	2.03	0.59
12:M:182:CYS:HG	19:M:802:SF4:FE3	1.20	0.59
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.84	0.58
26:J:402:UQ:HM23	26:J:402:UQ:O1	2.02	0.58
8:I:5:THR:HG22	8:I:7:VAL:HG12	1.85	0.58
11:L:84:ARG:NH1	11:L:88:GLN:O	2.35	0.58
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.85	0.58
12:M:336:ASN:HD21	12:M:540:ASN:HD22	1.49	0.58
1:A:88:ARG:O	1:A:126:LYS:NZ	2.35	0.58
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.37	0.58
1:A:326:LEU:HD22	32:A:647:HOH:O	2.03	0.57
7:H:81:ILE:O	7:H:85:GLU:HG3	2.04	0.57
16:Q:94:VAL:O	16:Q:94:VAL:HG23	2.04	0.57
6:G:105:MET:HG3	6:G:139:MET:HE2	1.85	0.57
2:B:63:TRP:O	2:B:67:VAL:HG23	2.04	0.57
15:P:85:GLU:OE2	32:P:301:HOH:O	2.18	0.57
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.40	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.84	0.57
9:J:220:MET:HE3	9:J:227:PRO:CD	2.21	0.57
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.86	0.57
8:I:30:GLU:CD	8:I:30:GLU:H	2.12	0.57
14:O:242:GLY:HA2	14:O:245:VAL:HG13	1.87	0.57
1:A:382:CYS:HB3	1:A:424:ILE:HD12	1.87	0.56
5:F:46:LYS:HE3	12:M:674:LEU:HD11	1.88	0.56
6:G:105:MET:CE	6:G:139:MET:HE1	2.35	0.56
1:A:152:ARG:NH2	10:K:99:PRO:O	2.38	0.56
6:G:156:GLU:OE1	6:G:156:GLU:N	2.36	0.56
32:I:217:HOH:O	15:P:80:CYS:CB	2.53	0.56
9:J:208:GLY:N	9:J:211:ASP:CG	2.56	0.56
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.70	0.56
15:P:87:PHE:N	15:P:87:PHE:CD1	2.73	0.56
15:P:201:ASP:OD1	15:P:201:ASP:N	2.37	0.56
1:A:36:LYS:HG2	1:A:38:GLU:HG2	1.88	0.56
1:A:170:GLN:HE21	1:A:197:VAL:HB	1.71	0.56
9:J:192:ARG:NH1	9:J:198:ALA:O	2.39	0.56
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.70	0.56
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.86	0.56
11:L:165:SER:CB	11:L:168:LYS:HB2	2.35	0.56
7:H:105:GLU:HA	7:H:105:GLU:OE1	2.06	0.56
1:A:283:ASN:ND2	1:A:305:GLY:O	2.37	0.56
5:F:59:SER:O	5:F:61:VAL:N	2.39	0.56
12:M:83:GLU:HG3	12:M:103:LEU:HD11	1.87	0.56
12:M:696:MET:HE2	12:M:702:ARG:HA	1.86	0.55
10:K:77:GLN:OE1	10:K:77:GLN:N	2.39	0.55
12:M:395:GLU:OE1	12:M:417:ARG:NH1	2.38	0.55
2:B:79:ARG:NH1	8:I:25:GLN:HE22	2.01	0.55
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.06	0.55
11:L:168:LYS:HE2	11:L:168:LYS:HA	1.88	0.55
13:N:3:LEU:HD11	29:N:201:CDL:H312	1.88	0.54
4:E:52:LEU:HD22	4:E:104:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:598:ASN:C	12:M:598:ASN:HD22	2.15	0.54
22:C:302:PEE:H26	22:C:302:PEE:H58	1.90	0.54
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.90	0.54
1:A:185:ASN:O	1:A:187:CYS:N	2.41	0.54
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.90	0.54
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.47	0.54
6:G:93:ILE:HD13	6:G:108:LEU:CD2	2.38	0.54
17:T:47:ASP:O	17:T:52:ARG:NH2	2.40	0.54
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.89	0.53
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.38	0.53
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.89	0.53
1:A:263:ALA:C	1:A:265:PHE:H	2.16	0.53
6:G:141:PRO:O	6:G:145:VAL:HG23	2.08	0.53
17:T:49:ASP:OD2	17:T:51:ARG:NH2	2.35	0.53
7:H:94:MET:HE2	15:P:99:PHE:HD2	1.73	0.53
2:B:68:ARG:NH1	18:W:28:ARG:HB3	2.24	0.53
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.73	0.53
9:J:283:VAL:HG22	9:J:369:VAL:HG11	1.90	0.53
1:A:132:ARG:HG3	1:A:133:HIS:CD2	2.44	0.53
1:A:455:LEU:O	1:A:458:GLN:NE2	2.42	0.53
1:A:119:GLU:O	1:A:159:ARG:NH1	2.43	0.52
12:M:457:SER:OG	12:M:459:ASN:OD1	2.26	0.52
1:A:358:ASP:O	1:A:361:THR:HG22	2.10	0.52
4:E:92:GLU:OE1	15:P:191:TYR:CB	2.57	0.52
8:I:5:THR:HG22	8:I:7:VAL:H	1.74	0.52
9:J:168:SER:O	9:J:203:PRO:HD2	2.08	0.52
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.45	0.52
12:M:407:PRO:HD2	12:M:438:LEU:HD21	1.90	0.52
20:A:502:FMN:N5	21:A:503:NAI:H4N	2.24	0.52
4:E:16:SER:HA	11:L:52:LEU:HD23	1.90	0.52
9:J:71:ASN:HA	9:J:97:MET:HG2	1.92	0.52
15:P:115:THR:HB	16:Q:423:LYS:HE3	1.90	0.52
15:P:181:HIS:O	32:P:302:HOH:O	2.19	0.52
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.91	0.52
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.90	0.52
3:C:193:TRP:CD2	22:C:302:PEE:H13	2.44	0.52
4:E:19:PRO:HB3	11:L:53:ILE:HD13	1.92	0.52
4:E:92:GLU:OE1	15:P:191:TYR:HD1	1.93	0.52
6:G:119:ILE:O	6:G:123:GLU:HG3	2.09	0.52
9:J:335:LEU:HB3	9:J:340:ILE:HB	1.92	0.52
15:P:154:GLU:OE2	15:P:180:ASN:OD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:J:402:UQ:O1	26:J:402:UQ:H8	2.09	0.51
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.43	0.51
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.92	0.51
8:I:46:SER:O	8:I:52:ASN:ND2	2.41	0.51
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.93	0.51
23:C:303:PLX:H1C3	23:C:303:PLX:O1	2.10	0.51
6:G:144:ILE:O	6:G:148:ILE:HG13	2.09	0.51
12:M:336:ASN:HD21	12:M:540:ASN:CG	2.19	0.51
12:M:379:THR:O	12:M:379:THR:HG22	2.10	0.51
14:O:215:LYS:O	14:O:219:ARG:NH1	2.43	0.51
10:K:100:GLN:HG3	14:O:68:LYS:O	2.11	0.51
29:N:201:CDL:C55	29:N:201:CDL:C74	2.86	0.51
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.93	0.51
32:I:217:HOH:O	15:P:80:CYS:HB3	2.10	0.51
10:K:102:SER:HB2	14:O:72:GLU:OE1	2.09	0.51
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.76	0.51
1:A:263:ALA:O	1:A:265:PHE:N	2.44	0.51
1:A:404:ALA:HB3	1:A:450:MET:HE2	1.93	0.50
6:G:92:LYS:HE2	6:G:114:ASP:OD1	2.10	0.50
6:G:94:ASP:OD1	6:G:94:ASP:N	2.34	0.50
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.46	0.50
12:M:355:LYS:HG2	12:M:366:LEU:HD13	1.93	0.50
12:M:405:THR:HB	12:M:477:GLY:HA3	1.94	0.50
12:M:449:PRO:HB2	12:M:679:LEU:HD22	1.92	0.50
1:A:185:ASN:OD1	1:A:190:GLY:N	2.33	0.50
12:M:255:ASP:HB2	32:M:949:HOH:O	2.11	0.50
12:M:603:ALA:O	12:M:656:TYR:HA	2.11	0.50
22:C:302:PEE:O4	22:C:302:PEE:H7	2.08	0.50
12:M:400:ILE:CD1	12:M:473:MET:HE3	2.41	0.50
14:O:182:ASN:HB3	14:O:194:GLU:CB	2.38	0.50
16:Q:92:HIS:CE1	16:Q:189:THR:HB	2.44	0.50
5:F:61:VAL:HG13	5:F:62:GLN:H	1.76	0.50
10:K:69:ASP:OD1	10:K:71:SER:OG	2.22	0.50
8:I:12:ARG:HD2	8:I:20:LEU:HD12	1.93	0.50
11:L:165:SER:OG	11:L:168:LYS:CB	2.59	0.50
12:M:389:THR:HG21	12:M:473:MET:SD	2.52	0.50
1:A:67:GLU:O	1:A:71:LYS:HG2	2.11	0.50
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.94	0.50
12:M:256:ALA:O	12:M:598:ASN:HB2	2.11	0.50
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.47	0.49
16:Q:426:ALA:O	32:Q:607:HOH:O	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.45	0.49
12:M:178:GLN:HG2	12:M:204:MET:CE	2.42	0.49
12:M:407:PRO:HD2	12:M:438:LEU:CD2	2.42	0.49
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.94	0.49
16:Q:145:MET:HG3	16:Q:214:TYR:OH	2.12	0.49
6:G:128:PHE:HE2	6:G:147:TYR:HE1	1.61	0.49
12:M:558:GLN:N	12:M:558:GLN:OE1	2.46	0.49
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	1.95	0.49
16:Q:144:MET:SD	16:Q:144:MET:N	2.83	0.49
13:N:29:ARG:HD2	13:N:74:PHE:O	2.13	0.49
10:K:78:HIS:HA	10:K:81:TYR:CE2	2.48	0.48
11:L:154:LYS:O	11:L:156:LYS:NZ	2.46	0.48
12:M:360:ARG:HG2	12:M:360:ARG:HH11	1.77	0.48
13:N:3:LEU:O	13:N:7:LEU:HG	2.13	0.48
3:C:80:ALA:HA	3:C:86:MET:HG2	1.96	0.48
12:M:181:ARG:HB3	12:M:225:ILE:HD12	1.95	0.48
13:N:39:VAL:HG23	13:N:50:GLU:HG2	1.95	0.48
14:O:155:LYS:HD3	14:O:202:GLU:HG2	1.95	0.48
14:O:188:ILE:O	14:O:189:ASN:C	2.55	0.48
3:C:64:PRO:HD2	3:C:92:VAL:O	2.13	0.48
3:C:193:TRP:CE2	22:C:302:PEE:H13	2.47	0.48
8:I:5:THR:HG22	8:I:7:VAL:N	2.29	0.48
12:M:272:ARG:NH1	32:M:913:HOH:O	2.35	0.48
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.95	0.48
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.95	0.48
6:G:108:LEU:N	6:G:108:LEU:CD1	2.73	0.48
9:J:375:VAL:HG23	9:J:375:VAL:O	2.13	0.48
12:M:390:THR:HB	12:M:600:GLU:OE2	2.14	0.48
10:K:74:ARG:O	10:K:76:LEU:N	2.47	0.48
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.48	0.48
15:P:87:PHE:HD1	15:P:87:PHE:H	1.60	0.48
1:A:249:ALA:O	1:A:252:PRO:HD2	2.13	0.48
8:I:64:MET:HE2	15:P:80:CYS:SG	2.53	0.48
12:M:355:LYS:CE	12:M:528:LEU:O	2.62	0.48
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.23	0.48
1:A:202:GLY:N	32:A:610:HOH:O	2.47	0.48
13:N:127:TYR:OH	17:T:61:GLU:O	2.26	0.48
2:B:208:ASP:OD2	2:B:212:ARG:NE	2.47	0.48
3:C:108:THR:HA	3:C:136:CYS:HB3	1.95	0.48
9:J:208:GLY:O	9:J:211:ASP:CG	2.57	0.48
1:A:200:GLY:O	32:A:602:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:48:HIS:NE2	9:J:365:GLU:OE1	2.44	0.48
8:I:2:ALA:HA	8:I:28:TYR:CZ	2.49	0.48
9:J:215:ASN:HD22	26:J:402:UQ:CM3	2.26	0.47
12:M:398:ASP:OD1	12:M:398:ASP:N	2.46	0.47
14:O:137:THR:HG22	14:O:138:THR:H	1.77	0.47
15:P:86:ILE:CD1	15:P:141:ILE:HD11	2.42	0.47
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.96	0.47
16:Q:270:ASN:CB	32:Q:759:HOH:O	2.62	0.47
1:A:122:PRO:HA	14:O:176:CYS:SG	2.55	0.47
12:M:232:THR:HG22	32:M:1036:HOH:O	2.14	0.47
12:M:484:SER:OG	12:M:680:LEU:HD11	2.14	0.47
14:O:121:MET:HB3	32:O:413:HOH:O	2.14	0.47
15:P:68:ILE:HG21	15:P:99:PHE:CE2	2.50	0.47
4:E:14:GLY:O	11:L:54:ALA:HA	2.15	0.47
12:M:493:VAL:HG12	12:M:513:MET:HE1	1.96	0.47
13:N:34:ARG:NH1	13:N:54:GLN:OE1	2.37	0.47
12:M:372:PHE:CZ	12:M:385:TYR:HB3	2.49	0.47
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.15	0.47
1:A:61:ASP:OD1	1:A:137:LYS:HG2	2.14	0.47
1:A:185:ASN:C	1:A:187:CYS:H	2.22	0.47
4:E:92:GLU:OE1	15:P:191:TYR:CD1	2.67	0.47
8:I:27:ARG:HD3	32:I:216:HOH:O	2.15	0.47
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.95	0.47
13:N:3:LEU:HD12	29:N:201:CDL:H121	1.96	0.47
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.95	0.47
3:C:107:GLY:HA2	19:C:301:SF4:S1	2.55	0.47
23:C:303:PLX:H102	23:C:303:PLX:H262	1.95	0.47
1:A:367:ILE:O	1:A:371:ILE:HG12	2.14	0.47
1:A:48:ARG:HH21	14:O:226:GLU:CD	2.22	0.47
3:C:59:ARG:NH2	32:C:404:HOH:O	2.45	0.47
9:J:64:PHE:CZ	9:J:211:ASP:HB3	2.50	0.46
14:O:140:CYS:HA	14:O:183:ALA:HB1	1.97	0.46
16:Q:401:GLU:OE2	32:Q:606:HOH:O	2.20	0.46
12:M:483:ARG:HH22	12:M:682:ASP:HB2	1.76	0.46
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.97	0.46
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.51	0.46
12:M:534:VAL:HG21	12:M:555:ILE:HG13	1.95	0.46
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.50	0.46
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.30	0.46
3:C:84:TYR:OH	3:C:171:GLU:OE2	2.33	0.46
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.98	0.46
1:A:53:LEU:HB2	1:A:136:HIS:NE2	2.30	0.46
1:A:252:PRO:HG3	32:A:630:HOH:O	2.06	0.46
1:A:256:ARG:O	14:O:246:GLN:HG2	2.15	0.46
22:C:302:PEE:H63	22:C:302:PEE:H68	1.60	0.46
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.32	0.46
1:A:267:ARG:HG3	1:A:293:SER:OG	2.16	0.46
26:J:402:UQ:HM53	26:J:402:UQ:H71	1.78	0.46
1:A:201:ALA:O	14:O:119:TYR:HB3	2.15	0.46
1:A:373:PHE:HD1	14:O:175:GLU:HB3	1.80	0.46
12:M:298:LYS:NZ	32:M:901:HOH:O	1.91	0.46
13:N:9:ARG:HH12	29:N:201:CDL:HB21	1.80	0.46
14:O:146:ASP:OD1	14:O:146:ASP:N	2.49	0.46
12:M:598:ASN:C	12:M:598:ASN:ND2	2.73	0.46
13:N:9:ARG:O	13:N:12:GLN:HG3	2.16	0.46
22:C:302:PEE:O5	22:C:302:PEE:H52	2.16	0.45
11:L:115:SER:HB2	12:M:267:THR:HB	1.97	0.45
12:M:169:VAL:HG22	12:M:223:ILE:HD11	1.97	0.45
12:M:197:THR:HA	12:M:205:GLN:O	2.16	0.45
14:O:76:ALA:C	14:O:78:ALA:N	2.74	0.45
1:A:83:SER:HB3	1:A:259:GLY:HA2	1.97	0.45
1:A:234:GLY:HA3	1:A:240:THR:OG1	2.16	0.45
4:E:101:THR:OG1	15:P:219:VAL:O	2.22	0.45
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.99	0.45
3:C:63:TRP:CD1	3:C:92:VAL:HG22	2.52	0.45
8:I:2:ALA:HB3	8:I:21:GLN:OE1	2.16	0.45
9:J:37:HIS:O	9:J:39:ALA:N	2.50	0.45
9:J:221:ARG:HD2	9:J:286:ARG:HD2	1.98	0.45
12:M:395:GLU:HA	12:M:421:SER:OG	2.16	0.45
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.98	0.45
16:Q:92:HIS:HA	32:Q:643:HOH:O	2.16	0.45
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.52	0.45
5:F:61:VAL:HG13	5:F:62:GLN:N	2.31	0.45
11:L:99:MET:HE3	11:L:128:PHE:CE1	2.51	0.45
7:H:50:GLN:O	7:H:54:GLU:HG3	2.16	0.45
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.52	0.45
12:M:393:GLY:O	12:M:394:VAL:C	2.58	0.45
13:N:7:LEU:O	13:N:11:LEU:HD23	2.17	0.45
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.52	0.45
15:P:125:ARG:CZ	15:P:199:ARG:HG2	2.46	0.45
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:144:TYR:HD1	13:N:144:TYR:H	1.65	0.45
3:C:154:ASP:HA	3:C:157:VAL:O	2.17	0.45
14:O:224:SER:HB2	14:O:226:GLU:HG2	1.99	0.45
16:Q:193:ASP:OD2	32:Q:608:HOH:O	2.21	0.45
1:A:445:GLU:OE1	1:A:445:GLU:N	2.49	0.44
5:F:90:THR:O	5:F:94:VAL:HG12	2.18	0.44
9:J:236:VAL:HG22	9:J:272:LEU:HD23	1.99	0.44
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.17	0.44
4:E:104:MET:HE2	4:E:104:MET:HA	1.99	0.44
13:N:4:VAL:HA	13:N:7:LEU:HD12	1.99	0.44
5:F:26:ARG:HB3	5:F:26:ARG:NH1	2.33	0.44
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.47	0.44
12:M:639:LEU:O	12:M:642:VAL:HG12	2.17	0.44
15:P:122:ARG:NH1	15:P:127:GLU:OE2	2.50	0.44
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.99	0.44
1:A:263:ALA:C	1:A:265:PHE:N	2.75	0.44
3:C:49:LYS:HA	3:C:49:LYS:HD3	1.71	0.44
7:H:35:LEU:HD13	7:H:49:GLU:HG3	2.00	0.44
8:I:70:MET:O	8:I:70:MET:SD	2.75	0.44
9:J:173:ASP:HB3	9:J:176:SER:HB3	1.99	0.44
11:L:105:GLU:HA	12:M:611:THR:CG2	2.47	0.44
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.51	0.44
15:P:50:ARG:NH2	15:P:80:CYS:SG	2.90	0.44
16:Q:80:LEU:HD22	16:Q:101:LEU:HD12	1.99	0.44
16:Q:97:LEU:HG	16:Q:99:MET:HG3	2.00	0.44
5:F:16:LEU:HD21	5:F:19:ILE:HD11	1.99	0.44
9:J:163:LYS:NZ	9:J:253:ILE:O	2.40	0.44
3:C:173:LEU:O	3:C:177:ILE:HG12	2.18	0.44
6:G:89:LEU:HD12	6:G:89:LEU:HA	1.81	0.44
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.52	0.44
12:M:213:MET:HB3	12:M:215:MET:HG2	2.00	0.44
11:L:165:SER:OG	11:L:168:LYS:CG	2.65	0.44
12:M:59:GLN:HG3	12:M:62:ARG:NH2	2.32	0.44
13:N:9:ARG:HH12	29:N:201:CDL:CB2	2.31	0.44
17:T:43:GLN:C	17:T:43:GLN:CD	2.85	0.44
22:C:302:PEE:H21	22:C:302:PEE:H28	1.45	0.44
7:H:112:TRP:CD2	15:P:87:PHE:HD2	2.36	0.44
10:K:95:LYS:HE2	10:K:95:LYS:HB3	1.77	0.44
12:M:44:GLU:OE1	12:M:45:PRO:CD	2.60	0.44
16:Q:92:HIS:CA	32:Q:643:HOH:O	2.65	0.44
1:A:41:ILE:HG12	1:A:253:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HD13	14:O:139:PRO:HG3	2.00	0.43
1:A:392:MET:HG2	1:A:412:LEU:HD11	2.00	0.43
2:B:88:PHE:CZ	13:N:30:ALA:HA	2.53	0.43
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.52	0.43
13:N:123:GLN:NE2	32:N:302:HOH:O	2.51	0.43
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.48	0.43
15:P:101:ARG:O	15:P:101:ARG:HG2	2.17	0.43
16:Q:365:PRO:HG3	32:Q:773:HOH:O	2.17	0.43
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.51	0.43
5:F:83:SER:O	5:F:87:VAL:HG23	2.18	0.43
8:I:44:GLY:HA3	16:Q:359:ASP:OD2	2.18	0.43
16:Q:99:MET:HE1	16:Q:444:LEU:HD11	1.99	0.43
1:A:107:ASP:OD1	1:A:107:ASP:N	2.48	0.43
12:M:94:MET:HA	12:M:95:PRO:HD3	1.88	0.43
15:P:125:ARG:NH1	15:P:199:ARG:HD3	2.33	0.43
7:H:38:ILE:O	7:H:45:ARG:NH1	2.52	0.43
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.99	0.43
9:J:262:THR:O	9:J:333:PRO:HD2	2.19	0.43
12:M:306:MET:HE1	13:N:139:PRO:HG3	2.01	0.43
8:I:14:TRP:O	18:W:28:ARG:NH2	2.38	0.43
12:M:172:ILE:HD12	12:M:175:ARG:NH1	2.33	0.43
8:I:96:THR:HB	8:I:97:PRO:CD	2.41	0.43
12:M:137:CYS:SG	12:M:139:LEU:HB3	2.58	0.43
12:M:233:SER:HB3	12:M:236:TYR:HB3	2.00	0.43
29:N:201:CDL:OA9	29:N:201:CDL:H531	2.18	0.43
16:Q:259:GLU:OE1	18:W:23:ARG:NH1	2.45	0.43
1:A:340:ASP:OD1	1:A:340:ASP:N	2.51	0.43
16:Q:193:ASP:CG	32:Q:608:HOH:O	2.62	0.43
17:T:95:HIS:ND1	17:T:96:PRO:O	2.44	0.43
1:A:88:ARG:HD2	1:A:274:LYS:HE2	2.02	0.42
2:B:85:ASN:HB3	32:B:444:HOH:O	2.19	0.42
3:C:196:ARG:NH2	25:J:401:NDP:P2B	2.92	0.42
9:J:214:LEU:HD23	9:J:214:LEU:HA	1.84	0.42
12:M:674:LEU:HD23	12:M:674:LEU:HA	1.88	0.42
13:N:60:ARG:NH1	13:N:89:TRP:O	2.51	0.42
7:H:105:GLU:HB3	15:P:89:HIS:NE2	2.34	0.42
16:Q:228:ARG:O	16:Q:230:GLY:N	2.51	0.42
3:C:56:TRP:CH2	23:C:303:PLX:H112	2.55	0.42
12:M:667:GLN:OE1	12:M:667:GLN:N	2.49	0.42
16:Q:270:ASN:HB3	32:Q:759:HOH:O	2.20	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:93:ILE:HD11	6:G:110:LEU:HD11	2.02	0.42
29:N:201:CDL:H721	29:N:201:CDL:H542	2.01	0.42
2:B:75:SER:OG	8:I:16:SER:HB3	2.20	0.42
7:H:90:LEU:O	7:H:94:MET:HG2	2.19	0.42
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.79	0.42
12:M:534:VAL:HG22	12:M:537:ILE:HB	2.02	0.42
29:N:201:CDL:H122	29:N:201:CDL:HA61	1.98	0.42
6:G:107:ASP:HB2	6:G:108:LEU:HD12	2.02	0.42
13:N:11:LEU:HA	13:N:14:VAL:HG12	2.01	0.42
16:Q:228:ARG:C	16:Q:230:GLY:H	2.28	0.42
1:A:226:LYS:HD2	1:A:229:PHE:CD2	2.55	0.42
8:I:58:ASP:O	8:I:62:GLU:HG3	2.20	0.42
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	2.01	0.42
8:I:8:ILE:HD11	29:N:201:CDL:H141	2.00	0.42
9:J:142:GLU:OE1	9:J:147:LYS:HE3	2.20	0.42
14:O:149:LEU:HD11	14:O:160:VAL:HG12	2.02	0.42
6:G:74:LEU:HD23	6:G:154:VAL:HG21	2.01	0.42
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.55	0.42
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.01	0.42
16:Q:270:ASN:HB2	32:Q:759:HOH:O	2.19	0.42
16:Q:274:ASP:CG	16:Q:323:ARG:HH12	2.28	0.42
16:Q:356:ILE:HG12	32:Q:723:HOH:O	2.19	0.42
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.89	0.41
5:F:23:LEU:HD13	5:F:37:ILE:HD12	2.02	0.41
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.35	0.41
12:M:36:VAL:HG22	12:M:102:ILE:HD12	2.01	0.41
14:O:242:GLY:HA2	14:O:245:VAL:CG1	2.50	0.41
1:A:373:PHE:CD1	14:O:175:GLU:HB3	2.55	0.41
23:C:303:PLX:H251	23:C:303:PLX:H282	1.68	0.41
8:I:28:TYR:O	8:I:29:GLN:OE1	2.37	0.41
12:M:509:ASP:OD1	12:M:509:ASP:N	2.48	0.41
12:M:682:ASP:HA	12:M:683:PRO:HD3	1.87	0.41
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.45	0.41
15:P:207:TYR:O	15:P:224:VAL:HG23	2.20	0.41
15:P:208:VAL:N	15:P:224:VAL:HG23	2.35	0.41
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.20	0.41
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.55	0.41
7:H:72:LEU:HD13	7:H:80:VAL:HG11	2.02	0.41
12:M:277:MET:HE3	12:M:277:MET:HB3	1.93	0.41
12:M:355:LYS:HE2	12:M:528:LEU:O	2.21	0.41
12:M:449:PRO:CB	12:M:679:LEU:HD22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:383:LYS:HA	16:Q:383:LYS:HD2	1.90	0.41
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.71	0.41
6:G:93:ILE:HG12	6:G:108:LEU:HD23	2.01	0.41
12:M:260:ASN:ND2	12:M:278:HIS:HD2	2.19	0.41
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.41
12:M:593:SER:HA	12:M:606:THR:O	2.21	0.41
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.60	0.41
7:H:101:GLU:HB3	7:H:102:PRO:HD2	2.02	0.41
10:K:73:TYR:CE2	10:K:75:ASN:HB3	2.55	0.41
14:O:76:ALA:O	14:O:78:ALA:N	2.54	0.41
6:G:147:TYR:CD1	6:G:147:TYR:C	2.97	0.41
9:J:228:LEU:O	9:J:292:PRO:HA	2.20	0.41
13:N:85:GLU:HG2	13:N:86:TRP:H	1.86	0.41
1:A:318:ILE:HG13	1:A:357:MET:HE2	2.03	0.41
2:B:176:SER:HB2	3:C:179:GLN:OE1	2.20	0.41
13:N:2:GLU:HG2	13:N:3:LEU:H	1.86	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
11:L:61:ILE:O	11:L:65:THR:HG23	2.19	0.41
12:M:468:GLU:H	12:M:468:GLU:HG2	1.73	0.41
29:N:201:CDL:H712	29:N:201:CDL:H512	2.03	0.41
14:O:185:MET:SD	14:O:185:MET:C	3.04	0.41
3:C:47:VAL:O	3:C:51:ASP:HB2	2.20	0.41
3:C:64:PRO:HA	3:C:102:VAL:O	2.21	0.41
23:C:303:PLX:H1A2	23:C:303:PLX:H21	1.82	0.41
6:G:103:HIS:CE1	6:G:139:MET:HE2	2.56	0.41
32:I:203:HOH:O	15:P:80:CYS:HB2	2.20	0.41
12:M:81:GLU:OE2	12:M:103:LEU:HD12	2.20	0.41
12:M:236:TYR:HB2	32:M:988:HOH:O	2.21	0.41
12:M:250:SER:OG	12:M:251:ILE:N	2.54	0.41
12:M:410:GLU:OE1	32:M:904:HOH:O	2.22	0.41
12:M:450:LYS:HE3	12:M:450:LYS:HB3	1.91	0.41
12:M:629:ILE:HD13	12:M:629:ILE:HA	1.83	0.41
13:N:3:LEU:HD23	13:N:7:LEU:HD11	2.02	0.41
13:N:68:MET:HG2	13:N:115:PHE:HD2	1.85	0.41
14:O:177:LEU:HD13	14:O:185:MET:HE1	2.03	0.41
14:O:237:PRO:HA	14:O:238:PRO:HD3	1.90	0.41
16:Q:319:PRO:HG3	16:Q:335:GLU:HG3	2.03	0.41
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.51	0.40
4:E:45:ASN:OD1	4:E:45:ASN:N	2.54	0.40
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.44	0.40
15:P:99:PHE:CD1	15:P:99:PHE:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:303:PLX:H102	23:C:303:PLX:H261	2.00	0.40
12:M:428:LYS:HE2	12:M:465:ILE:HD13	2.02	0.40
5:F:24:CYS:O	5:F:34:ARG:NH1	2.54	0.40
5:F:62:GLN:HG3	5:F:63:PRO:HD2	2.03	0.40
7:H:40:LYS:HA	7:H:45:ARG:HD3	2.03	0.40
10:K:87:LEU:HB3	14:O:62:ARG:HD3	2.02	0.40
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.04	0.40
13:N:41:GLU:HG3	13:N:47:LYS:HG2	2.03	0.40
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.03	0.40
15:P:149:GLU:OE1	32:P:303:HOH:O	2.22	0.40
1:A:207:GLY:HA3	20:A:502:FMN:N5	2.36	0.40
1:A:384:PRO:HB2	1:A:423:THR:CG2	2.45	0.40
2:B:114:ILE:HD12	12:M:130:ILE:HG23	2.04	0.40
5:F:23:LEU:C	5:F:58:CYS:HB3	2.46	0.40
9:J:250:ILE:O	9:J:254:LYS:HG3	2.21	0.40
17:T:51:ARG:HG2	17:T:54:ARG:HH21	1.86	0.40
2:B:91:GLY:HA2	2:B:92:PRO:HD3	1.97	0.40
7:H:114:TRP:CG	7:H:115:PRO:HA	2.57	0.40
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.92	0.40
14:O:76:ALA:C	14:O:78:ALA:H	2.30	0.40
16:Q:259:GLU:OE2	18:W:23:ARG:HD3	2.22	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	431/433 (100%)	412 (96%)	17 (4%)	2 (0%)	24 37
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100 100
3	C	154/156 (99%)	145 (94%)	9 (6%)	0	100 100
4	E	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	22
8	I	93/112 (83%)	83 (89%)	8 (9%)	2 (2%)	5	6
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	50
10	K	41/43 (95%)	39 (95%)	1 (2%)	1 (2%)	4	5
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	37
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	383/386 (99%)	371 (97%)	11 (3%)	1 (0%)	36	50
17	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
18	W	27/29 (93%)	23 (85%)	4 (15%)	0	100	100
All	All	3504/3558 (98%)	3364 (96%)	130 (4%)	10 (0%)	37	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	K	75	ASN
1	A	264	SER
8	I	29	GLN
9	J	38	HIS
7	H	77	ILE
14	O	77	ALA
16	Q	229	PRO
8	I	41	LEU
1	A	186	ALA
4	E	96	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	346/346 (100%)	341 (99%)	5 (1%)	59	79
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	88
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	77
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	71
5	F	75/76 (99%)	73 (97%)	2 (3%)	39	62
6	G	76/81 (94%)	69 (91%)	7 (9%)	8	14
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	81 (93%)	6 (7%)	14	24
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	93
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	65
11	L	113/113 (100%)	110 (97%)	3 (3%)	39	62
12	M	580/580 (100%)	570 (98%)	10 (2%)	53	74
13	N	130/130 (100%)	125 (96%)	5 (4%)	29	49
14	O	183/183 (100%)	177 (97%)	6 (3%)	33	55
15	P	190/190 (100%)	184 (97%)	6 (3%)	34	56
16	Q	332/332 (100%)	328 (99%)	4 (1%)	63	81
17	T	79/79 (100%)	77 (98%)	2 (2%)	42	64
18	W	24/24 (100%)	24 (100%)	0	100	100
All	All	3042/3058 (100%)	2979 (98%)	63 (2%)	46	69

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	54	LYS
1	A	125	CYS
1	A	240	THR
1	A	347	THR
2	B	73	THR
3	C	76	MET
3	C	188	LYS
4	E	45	ASN
4	E	116	THR
5	F	58	CYS
5	F	85	ASP

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Mol	Chain	Res	Type
6	G	75	THR
6	G	87	LEU
6	G	94	ASP
6	G	98	LEU
6	G	99	SER
6	G	102	SER
6	G	108	LEU
8	I	5	THR
8	I	21	GLN
8	I	27	ARG
8	I	43	VAL
8	I	50	SER
8	I	95	VAL
9	J	275	ASP
10	K	82	SER
11	L	124	LEU
11	L	152	VAL
11	L	175	LYS
12	M	171	THR
12	M	173	MET
12	M	334	GLN
12	M	336	ASN
12	M	355	LYS
12	M	470	LYS
12	M	598	ASN
12	M	657	ASP
12	M	679	LEU
12	M	688	GLN
13	N	13	GLN
13	N	24	LEU
13	N	26	VAL
13	N	52	ASN
13	N	120	THR
14	O	137	THR
14	O	140	CYS
14	O	145	SER
14	O	146	ASP
14	O	186	VAL
14	O	236	GLU
15	P	56	LYS
15	P	87	PHE
15	P	101	ARG

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Mol	Chain	Res	Type
15	P	110	SER
15	P	199	ARG
15	P	201	ASP
16	Q	217	VAL
16	Q	281	GLU
16	Q	336	GLU
16	Q	453	THR
17	T	43	GLN
17	T	81	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
4	E	126	HIS
5	F	48	ASN
5	F	93	ASN
6	G	142	GLN
7	H	37	GLN
8	I	21	GLN
8	I	25	GLN
8	I	29	GLN
9	J	43	HIS
9	J	215	ASN
10	K	79	HIS
12	M	133	GLN
12	M	278	HIS
12	M	300	GLN
12	M	304	GLN
12	M	336	ASN
12	M	406	ASN
12	M	424	HIS
12	M	425	ASN
12	M	453	GLN
12	M	540	ASN
12	M	598	ASN
12	M	604	GLN
13	N	52	ASN
13	N	123	GLN
14	O	131	HIS
14	O	133	GLN
15	P	82	ASN

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Mol	Chain	Res	Type
15	P	181	HIS
15	P	228	GLN
16	Q	149	GLN
16	Q	183	HIS
16	Q	454	GLN
17	T	43	GLN
17	T	123	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.01	2 (20%)	5,13,15	6.12	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.57	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.03	1.42	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.43	130.87	119.48
16	Q	118	2MR	CD-NE-CZ	4.43	131.70	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.23	131.00	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
20	FMN	A	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.27	9 (18%)
29	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.27	6 (10%)
19	SF4	B	301	2	0,12,12	-	-	-		
27	FES	M	803	12	0,4,4	-	-	-		
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	M	801	12	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	970	Q	501	-	33,33,33	4.84	14 (42%)	48,50,50	2.42	21 (43%)
27	FES	O	301	14	0,4,4	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		
26	UQ	J	402	-	33,33,63	3.42	8 (24%)	40,43,79	2.87	13 (32%)
25	NDP	J	401	-	49,52,52	4.37	23 (46%)	66,80,80	2.14	12 (18%)
21	NAI	A	503	-	45,48,48	3.90	19 (42%)	60,73,73	1.77	12 (20%)
19	SF4	B	302	2	0,12,12	-	-	-		
24	8Q1	G	201	6	31,34,34	2.12	6 (19%)	40,43,43	1.81	12 (30%)
22	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	0.99	2 (4%)
23	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.74	0
19	SF4	A	501	1	0,12,12	-	-	-		

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
20	FMN	A	502	-	-	7/18/18/18	0/3/3/3
19	SF4	B	301	2	-	-	0/6/5/5
27	FES	M	803	12	-	-	0/1/1/1
19	SF4	C	301	3	-	-	0/6/5/5
19	SF4	M	801	12	-	-	0/6/5/5
30	970	Q	501	-	-	6/8/41/41	0/5/5/5
27	FES	O	301	14	-	-	0/1/1/1
19	SF4	B	302	2	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5
26	UQ	J	402	-	-	14/27/51/87	0/1/1/1
25	NDP	J	401	-	-	8/34/77/77	0/4/5/5
21	NAI	A	503	-	-	8/29/72/72	0/5/5/5
29	CDL	N	201	-	-	37/61/61/110	-
24	8Q1	G	201	6	-	17/41/41/41	-
22	PEE	C	302	-	-	36/50/50/54	-
23	PLX	C	303	-	-	13/55/55/55	-
19	SF4	A	501	1	-	-	0/6/5/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	501	970	O16-C17	19.02	1.58	1.37
25	J	401	NDP	C6N-C5N	12.40	1.55	1.33
25	J	401	NDP	C3B-C2B	-12.39	1.25	1.52
30	Q	501	970	C14-C23	-11.89	1.41	1.52
25	J	401	NDP	O4D-C4D	10.79	1.69	1.45
21	A	503	NAI	C3D-C4D	-10.27	1.26	1.53
25	J	401	NDP	C3D-C4D	-9.91	1.27	1.53
26	J	402	UQ	C18-C19	9.52	1.55	1.33
21	A	503	NAI	O4B-C1B	9.23	1.63	1.42
26	J	402	UQ	C13-C14	9.17	1.55	1.33
26	J	402	UQ	C8-C9	8.93	1.54	1.33
30	Q	501	970	O13-C12	8.27	1.50	1.37
21	A	503	NAI	O4B-C4B	-8.14	1.26	1.45
25	J	401	NDP	O4B-C4B	-7.94	1.27	1.45
26	J	402	UQ	C23-C24	7.83	1.54	1.32
21	A	503	NAI	C2D-C1D	-7.58	1.29	1.53
24	G	201	8Q1	P24-O27	7.58	1.84	1.60
25	J	401	NDP	C2N-C3N	7.42	1.55	1.34
21	A	503	NAI	C2B-C1B	-7.19	1.30	1.53
21	A	503	NAI	O4D-C4D	6.86	1.60	1.45
30	Q	501	970	O08-C07	6.73	1.47	1.37
21	A	503	NAI	C2D-C3D	5.94	1.69	1.53
25	J	401	NDP	C6A-N6A	5.92	1.49	1.34
21	A	503	NAI	C7N-N7N	5.73	1.48	1.33
30	Q	501	970	C23-C24	-5.55	1.46	1.52
25	J	401	NDP	C3B-C4B	5.47	1.67	1.53
21	A	503	NAI	O4D-C1D	5.46	1.54	1.42
25	J	401	NDP	P2B-O2B	5.45	1.69	1.59
30	Q	501	970	C22-C23	-5.36	1.43	1.51
21	A	503	NAI	C6A-N6A	5.19	1.47	1.34
21	A	503	NAI	C4N-C3N	-4.99	1.40	1.49
25	J	401	NDP	C6N-N1N	4.88	1.49	1.37
25	J	401	NDP	O4D-C1D	-4.85	1.30	1.42
25	J	401	NDP	O4B-C1B	4.60	1.52	1.42
21	A	503	NAI	O2B-C2B	4.54	1.53	1.43
25	J	401	NDP	C1B-N9A	-4.45	1.33	1.46
25	J	401	NDP	O2D-C2D	-4.26	1.32	1.43
29	N	201	CDL	OA8-CA7	4.26	1.45	1.33
29	N	201	CDL	OB8-CB7	4.24	1.45	1.33
25	J	401	NDP	C7N-N7N	4.13	1.44	1.33
29	N	201	CDL	OA6-CA5	4.10	1.45	1.34
29	N	201	CDL	OB6-CB5	4.08	1.45	1.34
21	A	503	NAI	C6N-C5N	4.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	201	8Q1	C1-S44	3.97	1.85	1.76
24	G	201	8Q1	C6-C1	3.84	1.54	1.50
30	Q	501	970	C05-C04	-3.82	1.48	1.54
22	C	302	PEE	C18-C19	3.73	1.53	1.31
22	C	302	PEE	C39-C38	3.66	1.53	1.31
20	A	502	FMN	C4A-N5	3.57	1.37	1.30
30	Q	501	970	O13-C14	3.57	1.49	1.45
21	A	503	NAI	C7N-C3N	3.56	1.56	1.48
24	G	201	8Q1	C34-N36	3.48	1.41	1.33
24	G	201	8Q1	O27-C28	-3.39	1.32	1.43
30	Q	501	970	O16-C15	3.33	1.52	1.44
21	A	503	NAI	C4N-C5N	-3.29	1.40	1.48
25	J	401	NDP	C7N-C3N	3.07	1.55	1.48
25	J	401	NDP	C8A-N9A	-3.06	1.32	1.37
25	J	401	NDP	O3D-C3D	3.05	1.50	1.43
24	G	201	8Q1	C39-N41	2.95	1.40	1.33
25	J	401	NDP	C5A-N7A	-2.90	1.33	1.39
30	Q	501	970	O25-C24	-2.78	1.18	1.22
30	Q	501	970	C10-C11	2.73	1.44	1.39
26	J	402	UQ	C6-C1	2.66	1.54	1.46
30	Q	501	970	C12-C06	2.60	1.43	1.39
25	J	401	NDP	O2B-C2B	2.57	1.53	1.44
21	A	503	NAI	C8A-N9A	-2.51	1.33	1.37
21	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
22	C	302	PEE	O2-C2	-2.47	1.40	1.46
21	A	503	NAI	PN-O5D	2.43	1.69	1.59
22	C	302	PEE	O3-C30	2.33	1.40	1.33
21	A	503	NAI	C5B-C4B	2.30	1.58	1.51
26	J	402	UQ	C7-C8	2.30	1.54	1.50
20	A	502	FMN	C10-N1	2.27	1.37	1.33
30	Q	501	970	C05-C06	-2.24	1.48	1.51
25	J	401	NDP	C2D-C3D	2.23	1.59	1.53
22	C	302	PEE	O3-C3	-2.20	1.40	1.45
26	J	402	UQ	O4-C4	-2.19	1.18	1.23
22	C	302	PEE	O2-C10	2.19	1.40	1.34
25	J	401	NDP	O7N-C7N	-2.16	1.19	1.24
25	J	401	NDP	PA-O5B	2.06	1.67	1.59
30	Q	501	970	C04-C02	2.05	1.52	1.50
26	J	402	UQ	O1-C1	-2.01	1.19	1.23

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	402	UQ	C7-C8-C9	-8.19	113.16	126.79
25	J	401	NDP	C3N-C2N-N1N	-7.90	111.83	123.10
30	Q	501	970	O08-C07-C06	-7.66	108.33	113.00
25	J	401	NDP	C1D-N1N-C2N	-6.75	109.88	121.11
26	J	402	UQ	C12-C13-C14	-6.42	112.20	127.66
26	J	402	UQ	C17-C18-C19	-6.32	112.44	127.66
25	J	401	NDP	C5A-C4A-N3A	-5.87	119.09	126.75
30	Q	501	970	C15-C14-C23	5.85	115.36	110.62
21	A	503	NAI	C5A-C4A-N3A	-5.83	119.14	126.75
24	G	201	8Q1	C6-C1-S44	5.22	119.54	113.46
25	J	401	NDP	C1D-N1N-C6N	-5.12	109.79	120.83
30	Q	501	970	C05-C04-C02	-4.54	108.96	115.62
26	J	402	UQ	C22-C23-C24	-4.43	112.59	127.75
26	J	402	UQ	C20-C19-C18	-4.35	112.52	123.68
26	J	402	UQ	C10-C9-C8	-4.30	112.64	123.68
21	A	503	NAI	N3A-C2A-N1A	-4.29	121.89	128.60
26	J	402	UQ	C11-C9-C8	-4.26	112.50	121.12
26	J	402	UQ	C15-C14-C13	-4.23	112.83	123.68
26	J	402	UQ	C21-C19-C18	-4.22	112.57	121.12
25	J	401	NDP	N3A-C2A-N1A	-4.06	122.25	128.60
21	A	503	NAI	N3A-C4A-N9A	4.04	133.74	127.08
26	J	402	UQ	C16-C14-C13	-4.03	112.96	121.12
25	J	401	NDP	N3A-C4A-N9A	4.03	133.72	127.08
29	N	201	CDL	OA6-CA5-C11	4.01	120.14	111.50
22	C	302	PEE	O2-C10-C11	3.95	120.00	111.50
29	N	201	CDL	OB6-CB5-C51	3.95	120.00	111.50
30	Q	501	970	O08-C07-C09	3.94	131.89	123.89
21	A	503	NAI	C2A-N3A-C4A	3.86	120.86	111.75
25	J	401	NDP	C2A-N3A-C4A	3.78	120.69	111.75
24	G	201	8Q1	C43-S44-C1	3.74	113.52	101.87
21	A	503	NAI	C5A-N7A-C8A	3.71	108.78	103.51
30	Q	501	970	C22-C23-C14	3.67	114.70	109.56
30	Q	501	970	O28-C19-C20	3.58	120.40	115.41
26	J	402	UQ	C26-C24-C23	-3.40	112.82	122.65
26	J	402	UQ	C25-C24-C23	-3.40	112.83	122.65
25	J	401	NDP	C5A-N7A-C8A	3.38	108.32	103.51
21	A	503	NAI	N9A-C8A-N7A	-3.35	109.33	113.91
30	Q	501	970	C06-C05-C04	3.31	104.42	101.45
21	A	503	NAI	C4A-C5A-N7A	-3.26	106.65	110.62
24	G	201	8Q1	O35-C34-N36	-3.25	116.01	122.99
20	A	502	FMN	C4-N3-C2	-3.25	119.64	125.64
21	A	503	NAI	C3D-C2D-C1D	3.21	107.53	101.43
25	J	401	NDP	N9A-C8A-N7A	-3.21	109.52	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Q	501	970	C09-C07-C06	-3.20	119.78	123.20
25	J	401	NDP	C4A-C5A-N7A	-3.18	106.74	110.62
21	A	503	NAI	C4D-O4D-C1D	-3.16	102.50	109.47
30	Q	501	970	C07-C06-C12	2.95	121.63	118.74
24	G	201	8Q1	O2-P24-O27	-2.89	99.04	106.73
24	G	201	8Q1	C37-C38-C39	2.87	117.14	112.36
30	Q	501	970	O26-C20-C19	2.87	119.40	115.41
24	G	201	8Q1	O4-C1-S44	-2.83	118.94	122.61
20	A	502	FMN	C4A-C4-N3	2.75	120.18	113.19
30	Q	501	970	O28-C19-C18	-2.73	119.42	124.12
30	Q	501	970	C29-O28-C19	-2.68	113.49	117.53
29	N	201	CDL	OA8-CA7-C31	2.66	120.25	111.91
29	N	201	CDL	OB8-CB7-C71	2.63	120.16	111.91
21	A	503	NAI	PN-O3-PA	-2.63	123.80	132.83
24	G	201	8Q1	O40-C39-N41	-2.63	118.05	123.01
20	A	502	FMN	O4-C4-C4A	-2.60	119.72	126.60
30	Q	501	970	C11-C24-C23	2.59	119.64	115.92
24	G	201	8Q1	C32-C34-N36	2.58	121.71	116.58
26	J	402	UQ	CM5-C5-C6	-2.57	120.20	124.40
22	C	302	PEE	O3-C30-C31	2.54	119.88	111.91
30	Q	501	970	C11-C12-C06	-2.46	119.19	123.16
20	A	502	FMN	C4A-C10-N1	-2.42	119.12	124.73
29	N	201	CDL	CB4-OB6-CB5	-2.41	111.87	117.79
21	A	503	NAI	C2D-C3D-C4D	2.31	107.13	102.64
25	J	401	NDP	C4A-N9A-C8A	2.30	108.22	105.73
29	N	201	CDL	CA4-OA6-CA5	-2.30	112.13	117.79
24	G	201	8Q1	O1-P24-O2	2.30	116.42	107.64
20	A	502	FMN	C4A-C10-N10	2.29	119.82	116.48
30	Q	501	970	C27-O26-C20	-2.28	114.09	117.53
20	A	502	FMN	C9A-C5A-N5	-2.26	119.98	122.43
30	Q	501	970	C05-C06-C12	-2.26	127.26	131.59
30	Q	501	970	O26-C20-C21	-2.24	120.26	124.12
30	Q	501	970	C15-O16-C17	-2.24	110.63	115.30
30	Q	501	970	C12-O13-C14	-2.22	112.27	116.06
21	A	503	NAI	C4A-N9A-C8A	2.21	108.12	105.73
25	J	401	NDP	PN-O3-PA	-2.19	125.31	132.83
24	G	201	8Q1	C38-C39-N41	2.18	120.09	116.42
30	Q	501	970	C05-C06-C07	2.15	111.11	108.54
24	G	201	8Q1	O27-P24-O3	-2.13	100.49	106.47
20	A	502	FMN	C5A-C9A-N10	2.12	120.15	117.95
30	Q	501	970	O13-C14-C23	2.12	114.55	112.40
20	A	502	FMN	C10-C4A-N5	-2.11	120.38	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	201	8Q1	O4-C1-C6	-2.09	121.53	123.99
20	A	502	FMN	C4-C4A-C10	2.03	120.21	116.79

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	N10-C1'-C2'-O2'
20	A	502	FMN	N10-C1'-C2'-C3'
20	A	502	FMN	C3'-C4'-C5'-O5'
20	A	502	FMN	O4'-C4'-C5'-O5'
21	A	503	NAI	C5B-O5B-PA-O1A
21	A	503	NAI	C5B-O5B-PA-O2A
21	A	503	NAI	C5B-O5B-PA-O3
21	A	503	NAI	C3D-C4D-C5D-O5D
22	C	302	PEE	C17-C18-C19-C20
22	C	302	PEE	C1-O3P-P-O2P
22	C	302	PEE	C1-O3P-P-O1P
22	C	302	PEE	C4-O4P-P-O1P
22	C	302	PEE	O4P-C4-C5-N
23	C	303	PLX	C3-O4-P1-O1
24	G	201	8Q1	C1-C6-C7-C8
24	G	201	8Q1	O27-C28-C29-C32
24	G	201	8Q1	C28-C29-C32-C34
24	G	201	8Q1	C28-C29-C32-O33
24	G	201	8Q1	C30-C29-C32-C34
24	G	201	8Q1	C30-C29-C32-O33
24	G	201	8Q1	C31-C29-C32-C34
24	G	201	8Q1	C31-C29-C32-O33
24	G	201	8Q1	C28-O27-P24-O2
24	G	201	8Q1	C28-O27-P24-O1
25	J	401	NDP	C2N-C3N-C7N-O7N
26	J	402	UQ	C1-C6-C7-C8
26	J	402	UQ	C5-C6-C7-C8
26	J	402	UQ	C7-C8-C9-C11
26	J	402	UQ	C12-C13-C14-C16
29	N	201	CDL	C1-CA2-OA2-PA1
29	N	201	CDL	CA2-OA2-PA1-OA3
29	N	201	CDL	CA2-OA2-PA1-OA4
29	N	201	CDL	CA2-OA2-PA1-OA5
29	N	201	CDL	CA3-OA5-PA1-OA2
29	N	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
29	N	201	CDL	C31-CA7-OA8-CA6
29	N	201	CDL	CB2-OB2-PB2-OB4
30	Q	501	970	C03-C02-C04-C05
30	Q	501	970	C03-C02-C04-O08
29	N	201	CDL	OA9-CA7-OA8-CA6
29	N	201	CDL	OA7-CA5-OA6-CA4
26	J	402	UQ	C22-C23-C24-C26
22	C	302	PEE	C31-C30-O3-C3
26	J	402	UQ	C7-C8-C9-C10
26	J	402	UQ	C17-C18-C19-C21
22	C	302	PEE	O5-C30-O3-C3
29	N	201	CDL	C51-C52-C53-C54
21	A	503	NAI	O4D-C4D-C5D-O5D
26	J	402	UQ	C12-C11-C9-C8
22	C	302	PEE	C42-C43-C44-C45
22	C	302	PEE	C10-C11-C12-C13
25	J	401	NDP	C2D-C1D-N1N-C6N
22	C	302	PEE	C37-C38-C39-C40
26	J	402	UQ	C9-C11-C12-C13
22	C	302	PEE	C15-C16-C17-C18
22	C	302	PEE	C1-O3P-P-O4P
29	N	201	CDL	CB2-OB2-PB2-OB5
29	N	201	CDL	CB3-OB5-PB2-OB2
29	N	201	CDL	C71-CB7-OB8-CB6
22	C	302	PEE	C40-C41-C42-C43
24	G	201	8Q1	C10-C11-C12-C13
22	C	302	PEE	C12-C13-C14-C15
22	C	302	PEE	C32-C33-C34-C35
22	C	302	PEE	C13-C14-C15-C16
22	C	302	PEE	C44-C45-C46-C47
29	N	201	CDL	CA7-C31-C32-C33
22	C	302	PEE	C31-C32-C33-C34
29	N	201	CDL	OB9-CB7-OB8-CB6
24	G	201	8Q1	C12-C13-C14-C15
29	N	201	CDL	C71-C72-C73-C74
29	N	201	CDL	C51-CB5-OB6-CB4
29	N	201	CDL	OB7-CB5-OB6-CB4
22	C	302	PEE	C19-C20-C21-C22
22	C	302	PEE	C39-C40-C41-C42
22	C	302	PEE	O4-C10-O2-C2
30	Q	501	970	C20-C19-O28-C29
22	C	302	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
23	C	303	PLX	C10-C11-C12-C13
22	C	302	PEE	C11-C12-C13-C14
29	N	201	CDL	C72-C73-C74-C75
29	N	201	CDL	CB7-C71-C72-C73
22	C	302	PEE	C20-C21-C22-C23
22	C	302	PEE	C14-C15-C16-C17
24	G	201	8Q1	O27-C28-C29-C30
24	G	201	8Q1	O27-C28-C29-C31
29	N	201	CDL	CA6-CA4-OA6-CA5
20	A	502	FMN	C5'-O5'-P-O1P
24	G	201	8Q1	C28-O27-P24-O3
24	G	201	8Q1	C11-C12-C13-C14
23	C	303	PLX	O4-C3-C4-O6
22	C	302	PEE	C35-C36-C37-C38
26	J	402	UQ	C3-C2-O2-CM2
23	C	303	PLX	O4-C3-C4-C5
22	C	302	PEE	C34-C35-C36-C37
23	C	303	PLX	C11-C12-C13-C14
22	C	302	PEE	C4-O4P-P-O3P
22	C	302	PEE	C38-C39-C40-C41
29	N	201	CDL	CB2-C1-CA2-OA2
24	G	201	8Q1	C13-C14-C15-C16
22	C	302	PEE	C33-C34-C35-C36
30	Q	501	970	C18-C19-O28-C29
22	C	302	PEE	C3-C2-O2-C10
29	N	201	CDL	C31-C32-C33-C34
22	C	302	PEE	O2-C2-C3-O3
26	J	402	UQ	C20-C19-C21-C22
21	A	503	NAI	PN-O3-PA-O2A
23	C	303	PLX	C25-C26-C27-C28
23	C	303	PLX	C15-C16-C17-C18
23	C	303	PLX	C9-C10-C11-C12
23	C	303	PLX	C3-O4-P1-O3
25	J	401	NDP	C2N-C3N-C7N-N7N
29	N	201	CDL	CA3-OA5-PA1-OA4
29	N	201	CDL	CB3-OB5-PB2-OB4
22	C	302	PEE	O3P-C1-C2-C3
20	A	502	FMN	C1'-C2'-C3'-O3'
30	Q	501	970	C01-C02-C04-C05
30	Q	501	970	C01-C02-C04-O08
29	N	201	CDL	O1-C1-CA2-OA2
22	C	302	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	N	201	CDL	OA6-CA4-CA6-OA8
26	J	402	UQ	C4-C3-O3-CM3
23	C	303	PLX	C2-O1-P1-O4
21	A	503	NAI	O4D-C1D-N1N-C2N
29	N	201	CDL	OA5-CA3-CA4-OA6
29	N	201	CDL	C12-C13-C14-C15
23	C	303	PLX	C11-C10-C9-C8
25	J	401	NDP	O4D-C1D-N1N-C6N
29	N	201	CDL	CA2-C1-CB2-OB2
20	A	502	FMN	O2'-C2'-C3'-C4'
29	N	201	CDL	C12-C11-CA5-OA6
26	J	402	UQ	C13-C14-C16-C17
29	N	201	CDL	CA3-CA4-CA6-OA8
29	N	201	CDL	C52-C51-CB5-OB6
23	C	303	PLX	O7-C6-C7-C8
23	C	303	PLX	O9-C24-C25-C26
25	J	401	NDP	C5D-O5D-PN-O3
22	C	302	PEE	C36-C37-C38-C39
26	J	402	UQ	C2-C3-O3-CM3
25	J	401	NDP	O4B-C4B-C5B-O5B
25	J	401	NDP	PN-O3-PA-O1A
29	N	201	CDL	C12-C11-CA5-OA7
25	J	401	NDP	C5D-O5D-PN-O2N
29	N	201	CDL	C52-C51-CB5-OB7
29	N	201	CDL	C1-CB2-OB2-PB2
22	C	302	PEE	O3P-C1-C2-O2
21	A	503	NAI	C2D-C1D-N1N-C2N

There are no ring outliers.

11 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	502	FMN	4	0
29	N	201	CDL	18	0
19	C	301	SF4	1	0
30	Q	501	970	1	0
19	M	802	SF4	1	0
26	J	402	UQ	7	0
25	J	401	NDP	3	0
21	A	503	NAI	5	0
22	C	302	PEE	7	0
23	C	303	PLX	13	0

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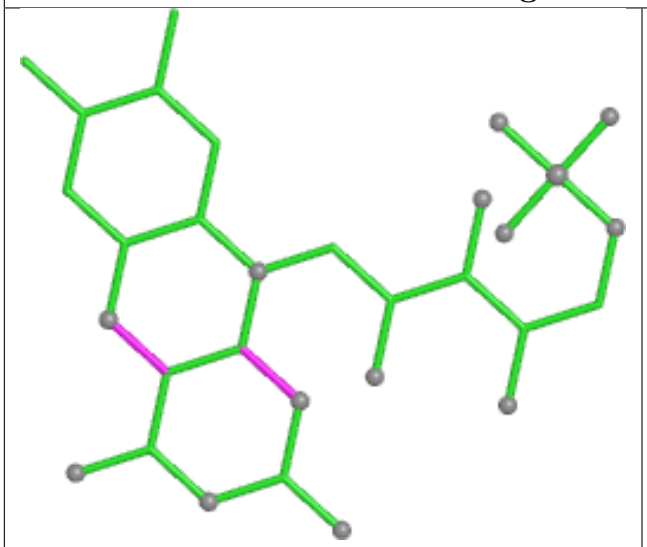
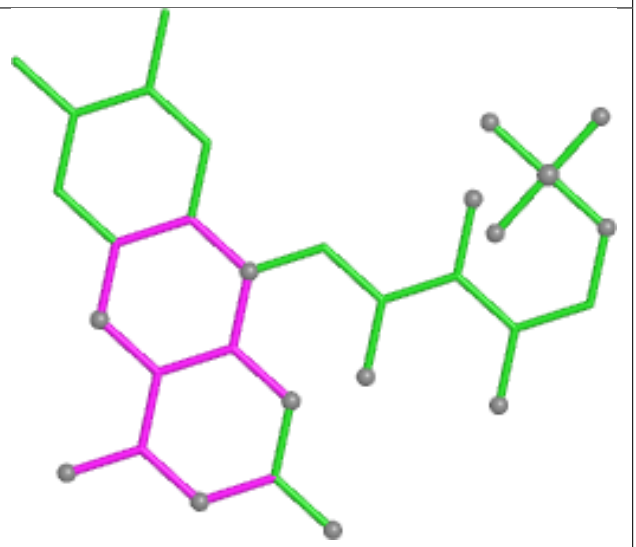
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	501	SF4	1	0

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

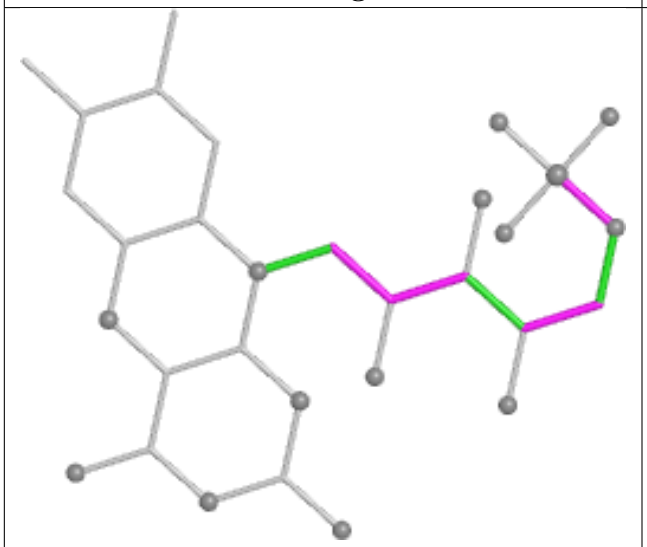
Ligand FMN A 502



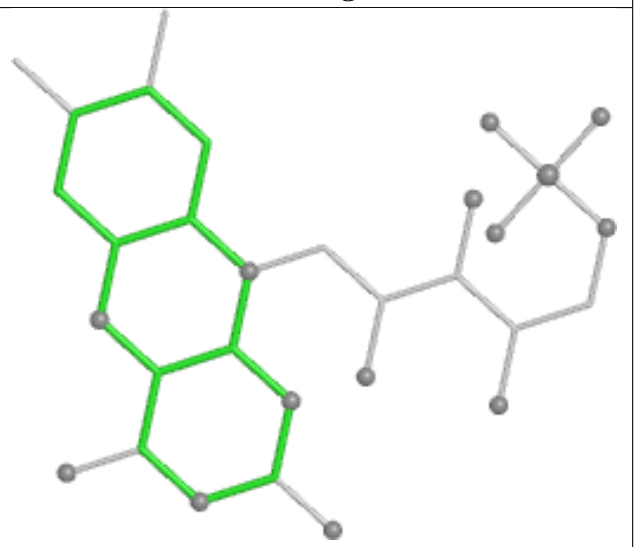
Bond lengths



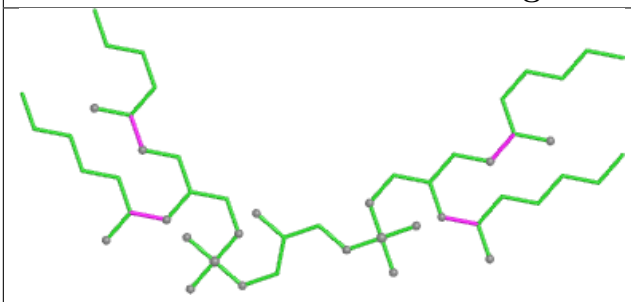
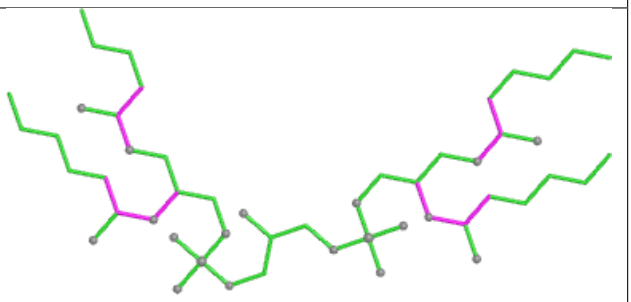
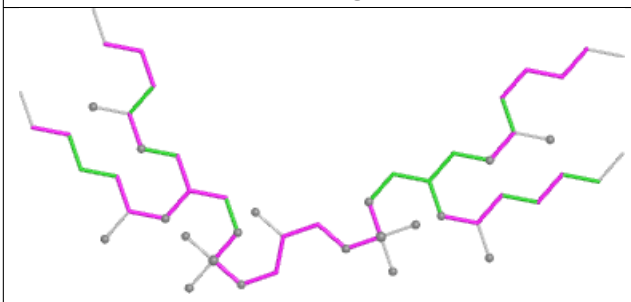
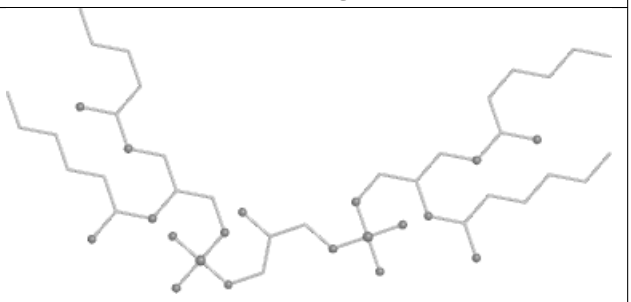
Bond angles

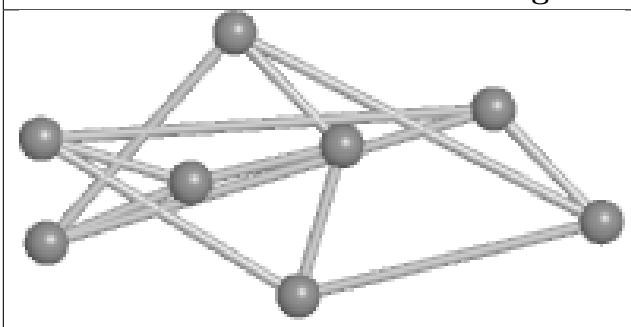
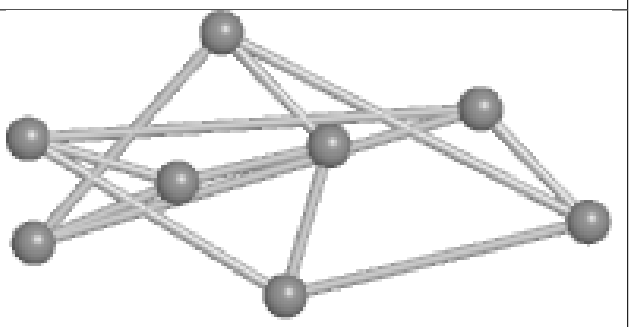
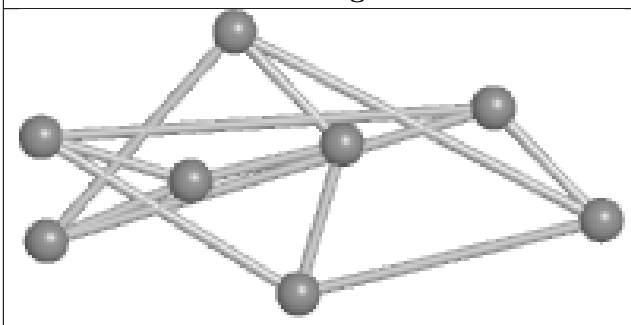
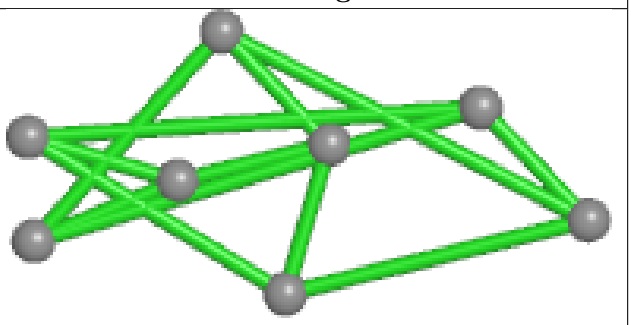


Torsions

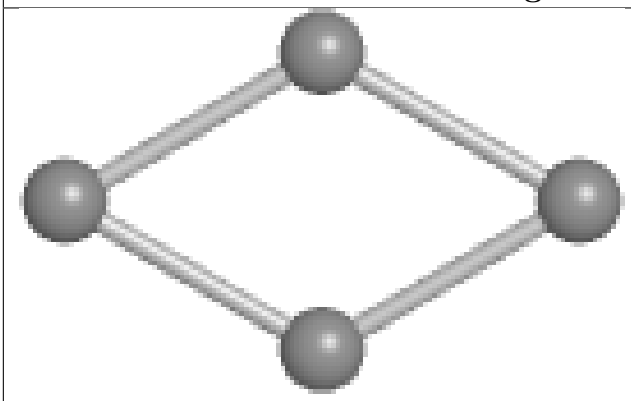


Rings

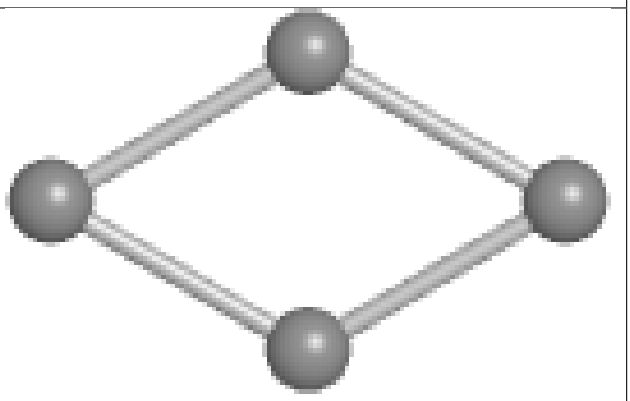
Ligand CDL N 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

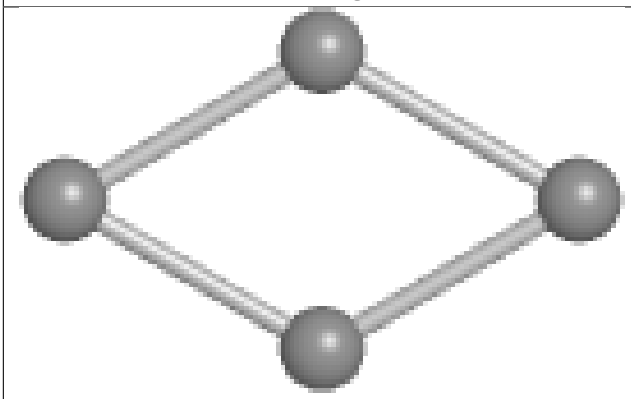
Ligand FES M 803



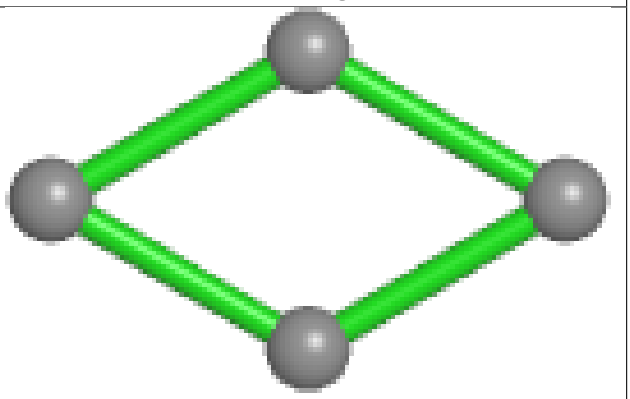
Bond lengths



Bond angles

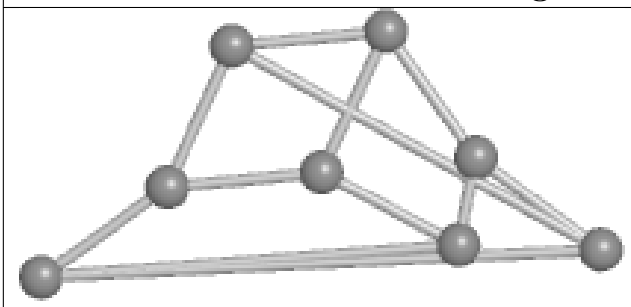


Torsions

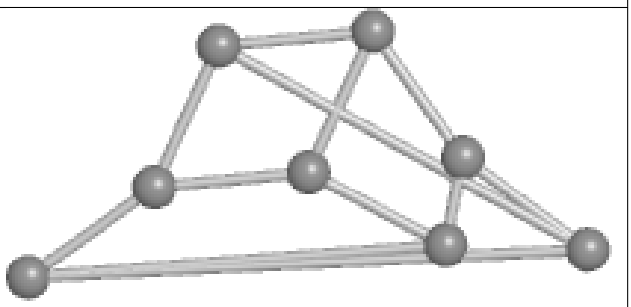


Rings

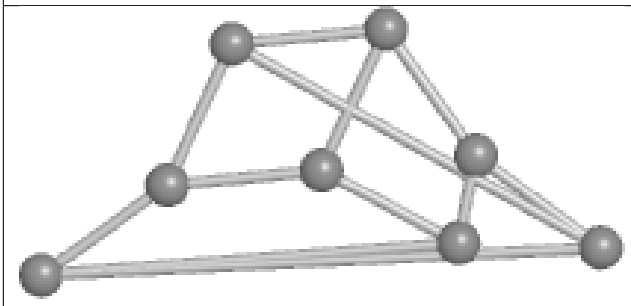
Ligand SF4 C 301



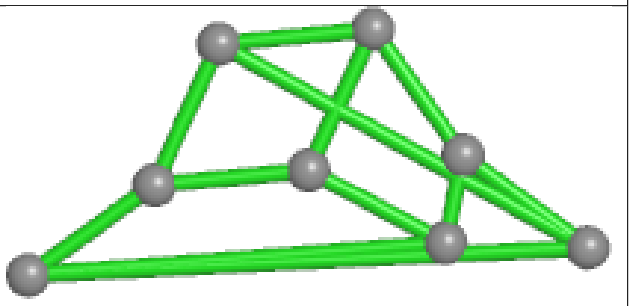
Bond lengths



Bond angles

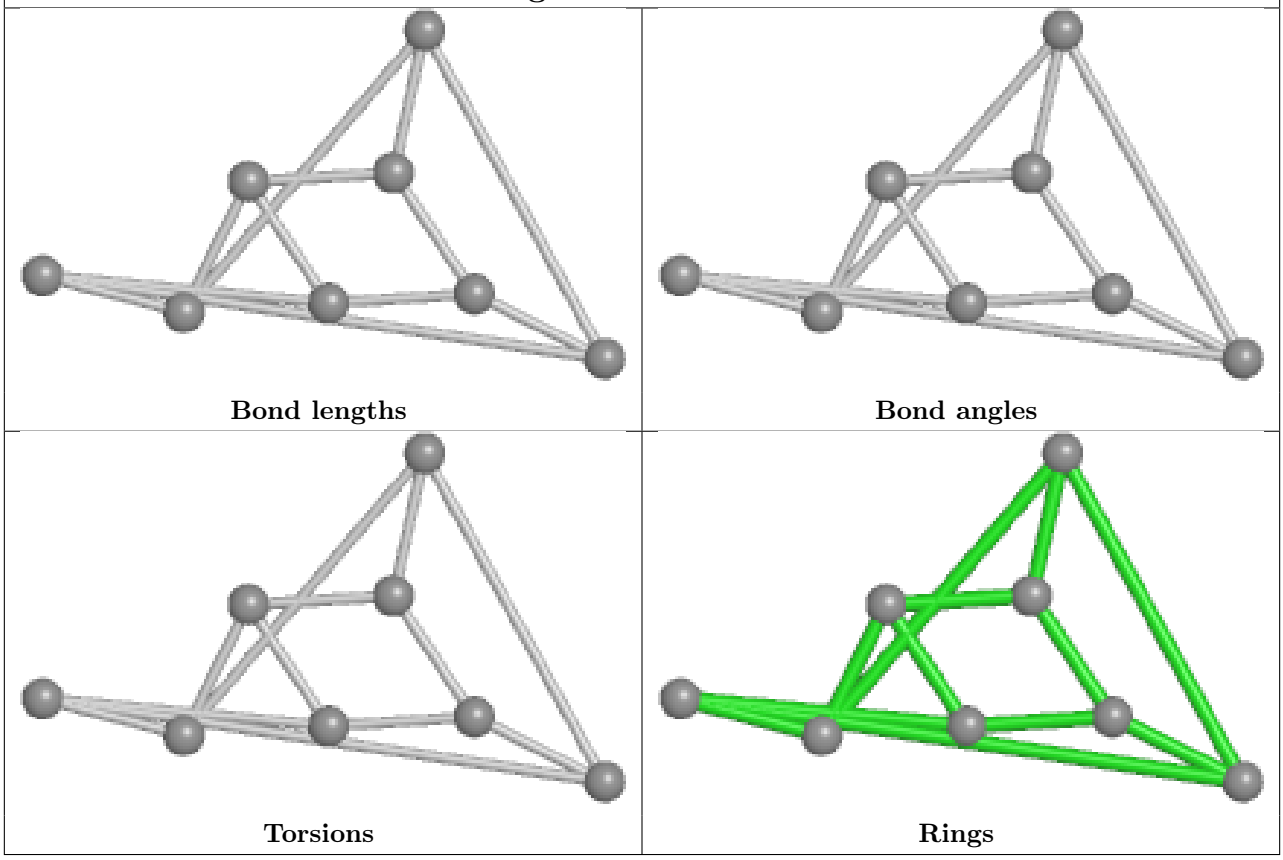


Torsions

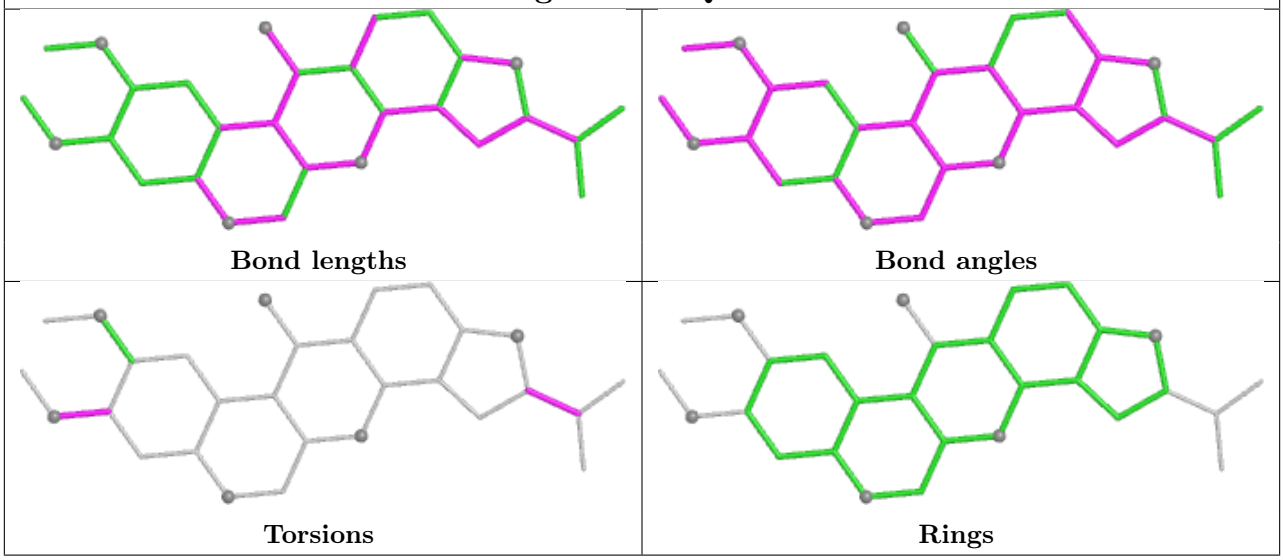


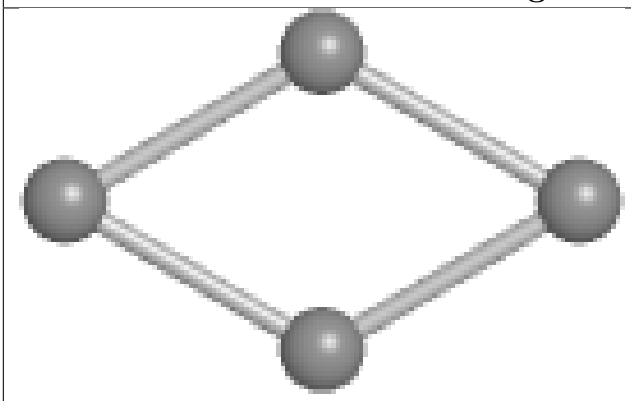
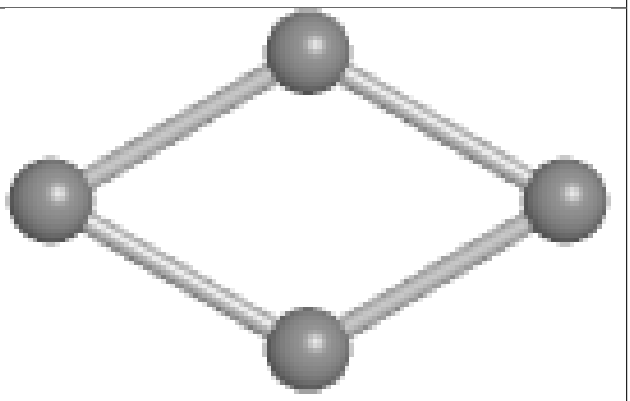
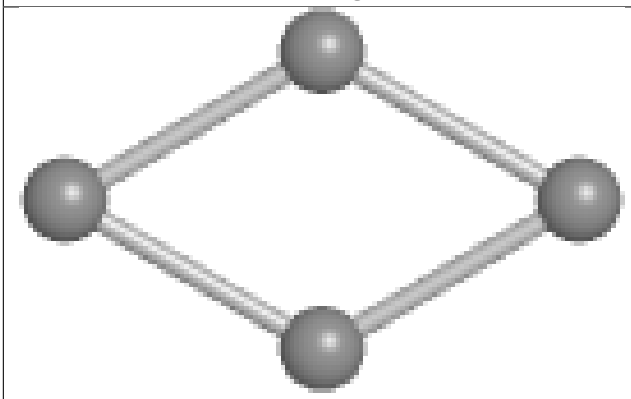
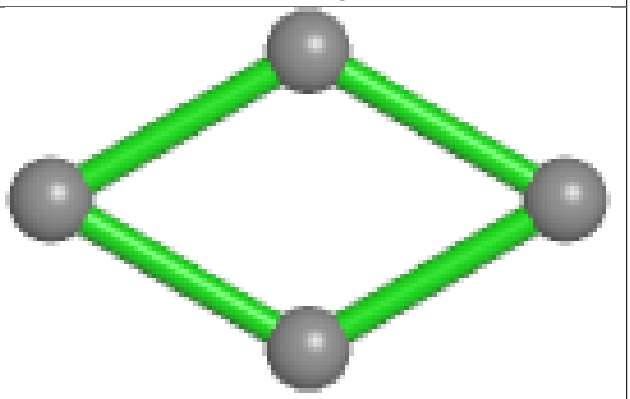
Rings

Ligand SF4 M 801

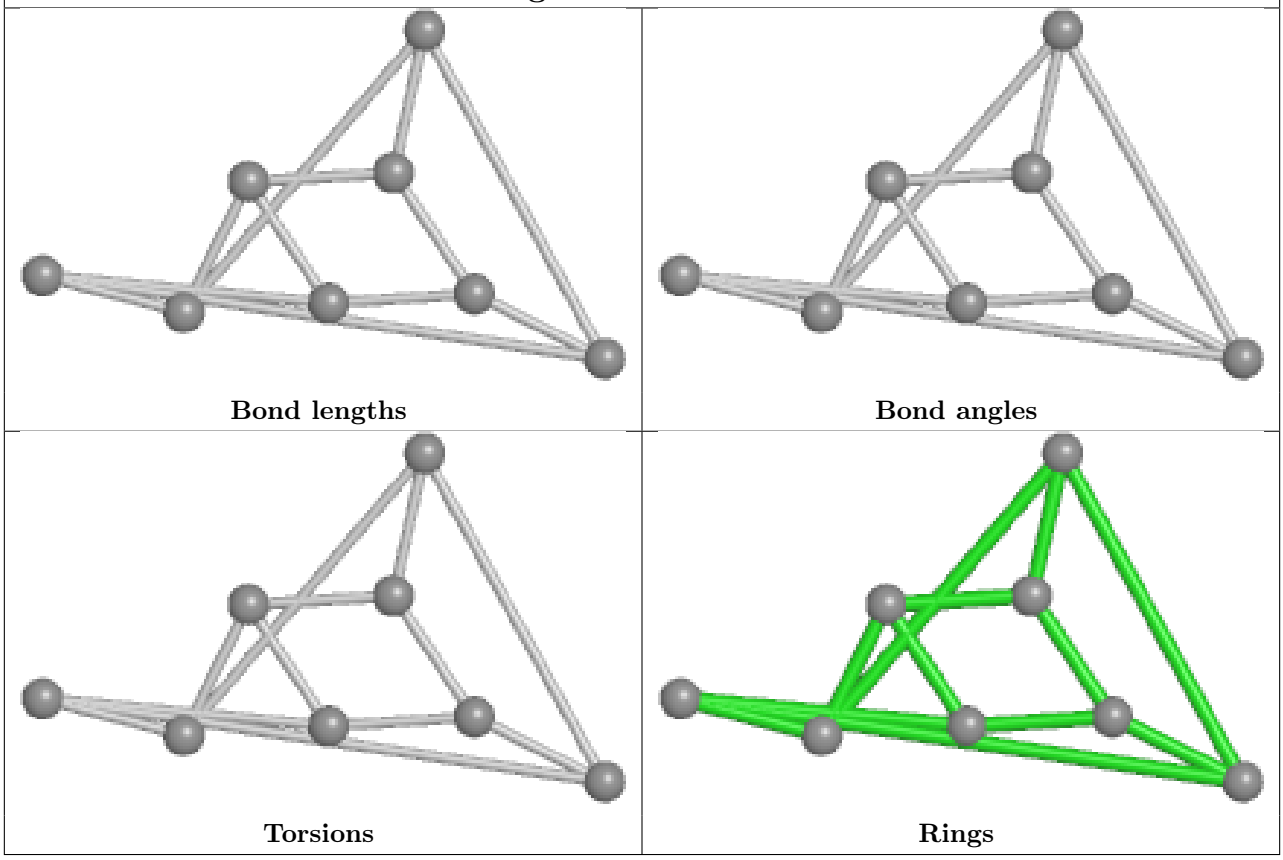


Ligand 970 Q 501

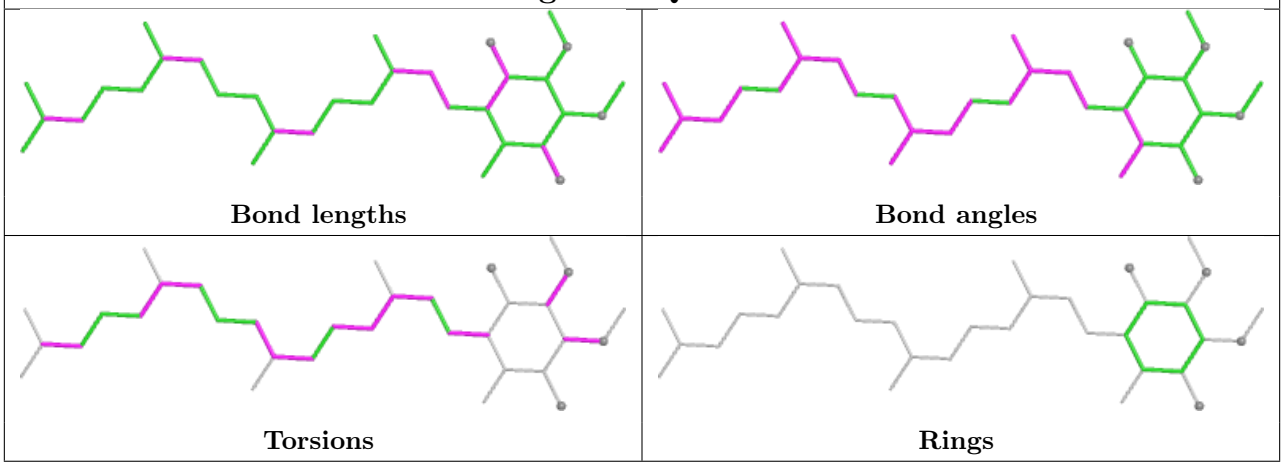


Ligand FES O 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

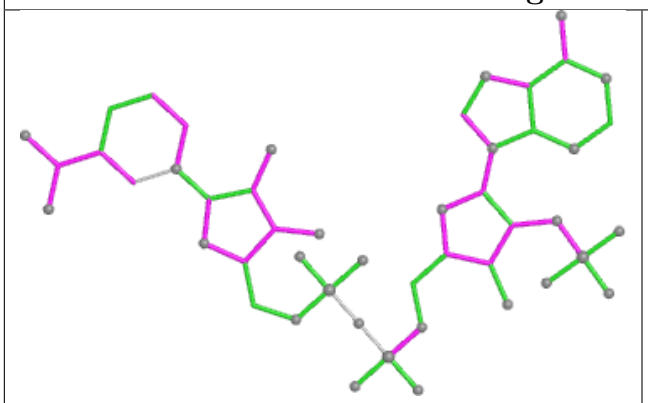
Ligand SF4 M 802



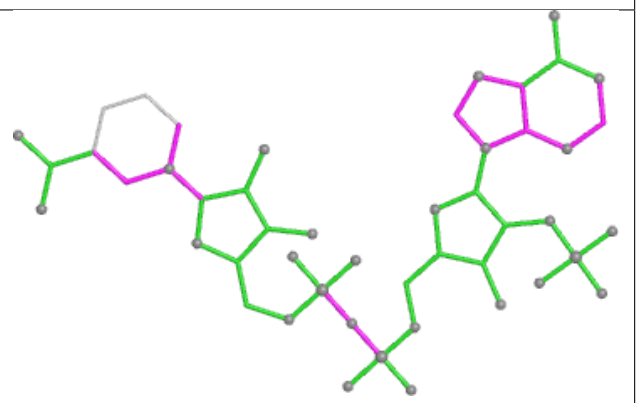
Ligand UQ J 402



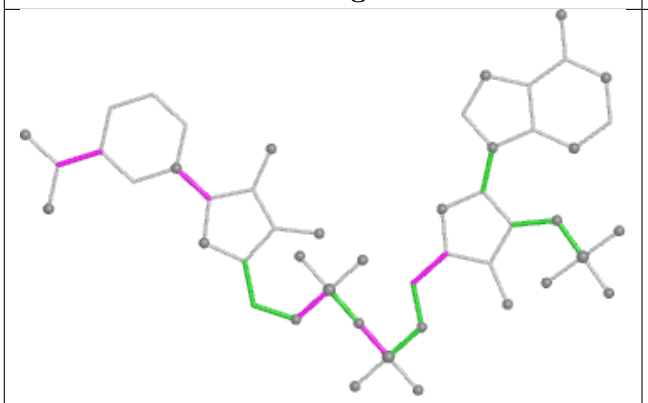
Ligand NDP J 401



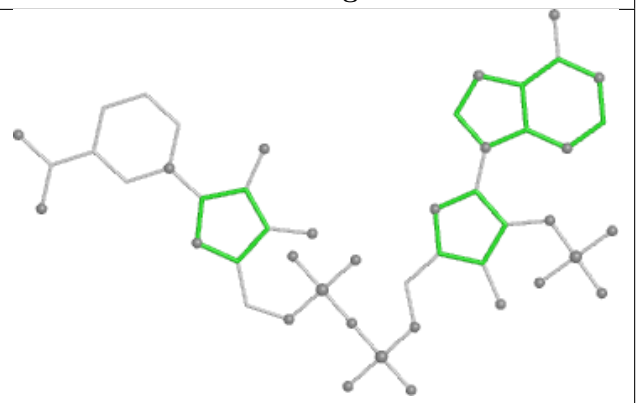
Bond lengths



Bond angles

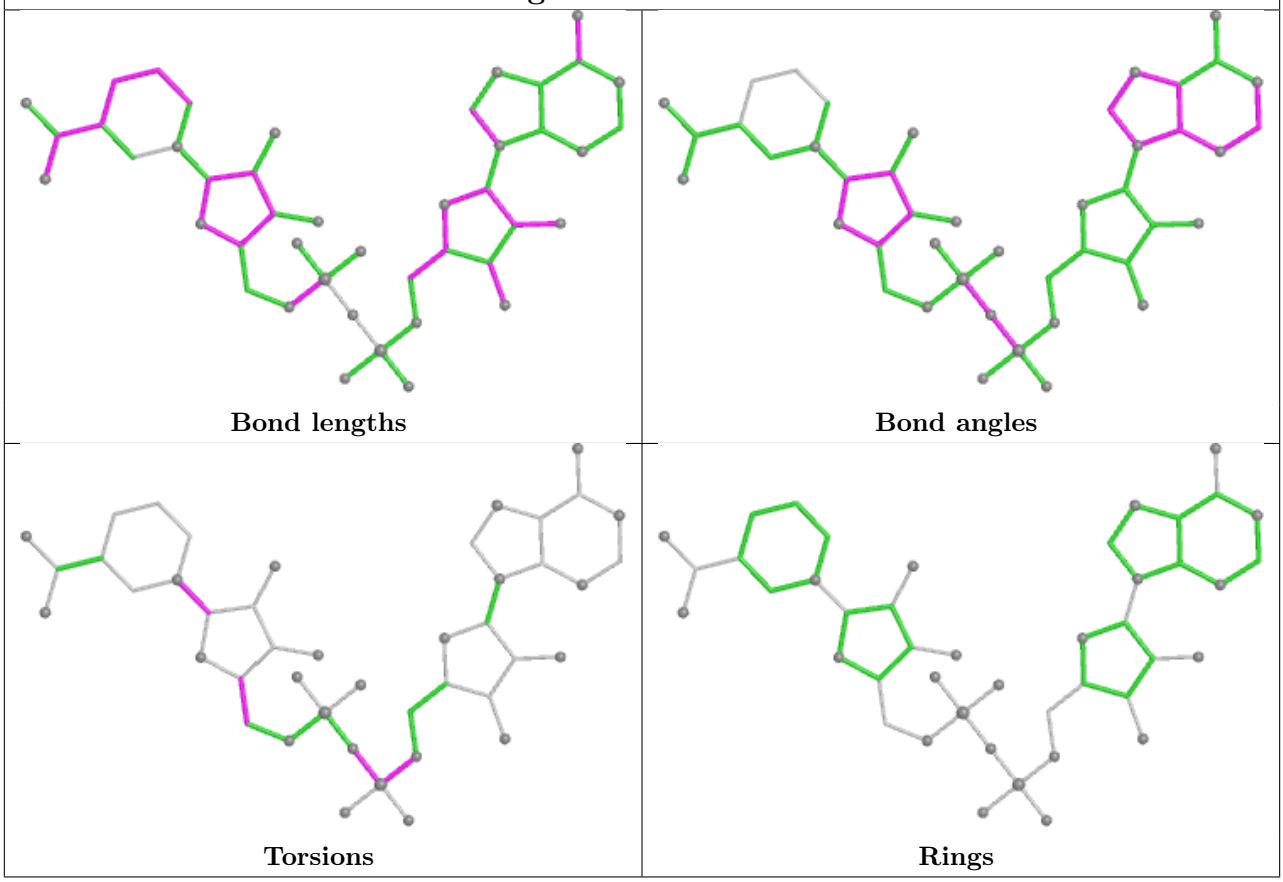


Torsions

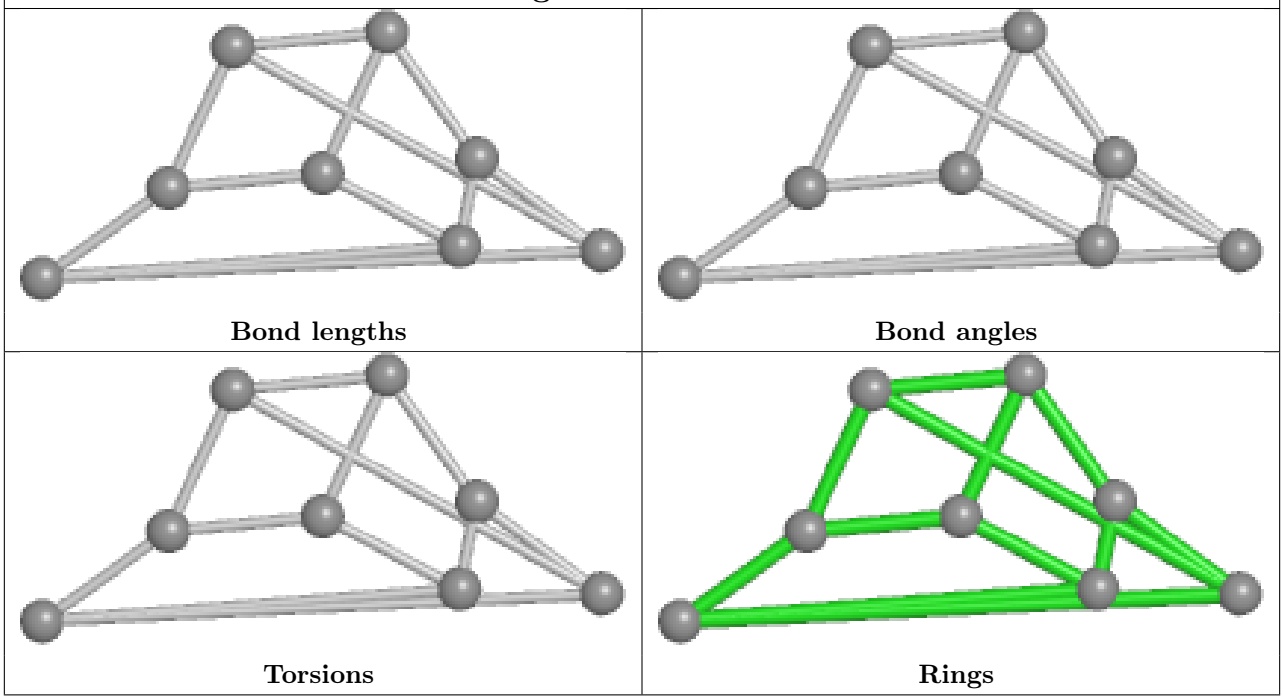


Rings

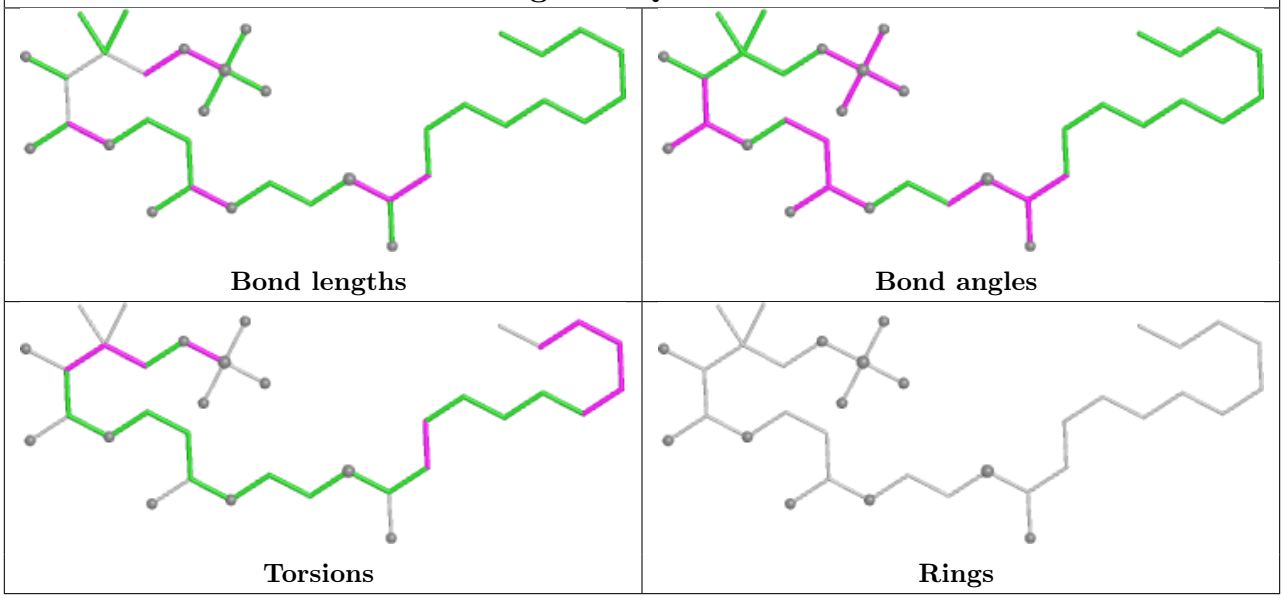
Ligand NAI A 503



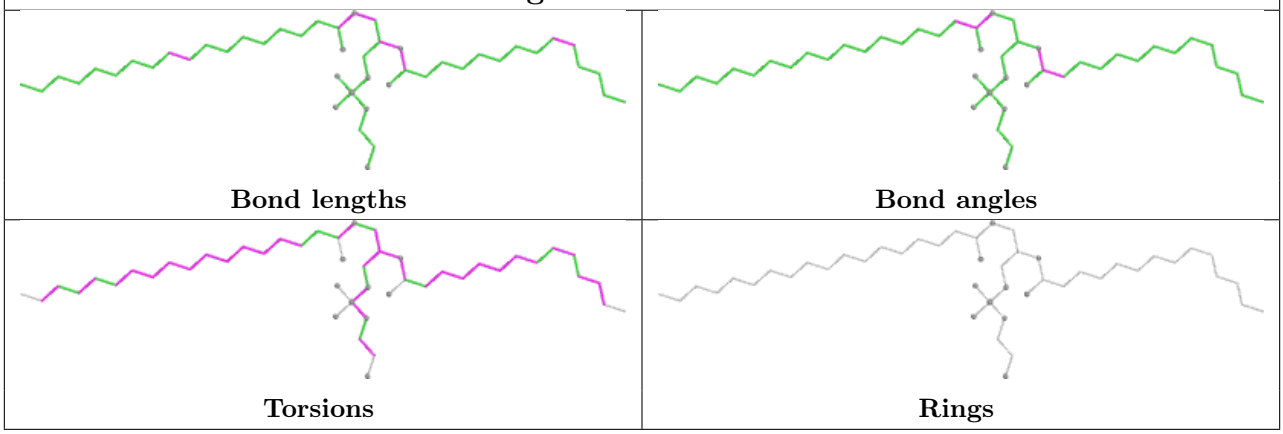
Ligand SF4 B 302



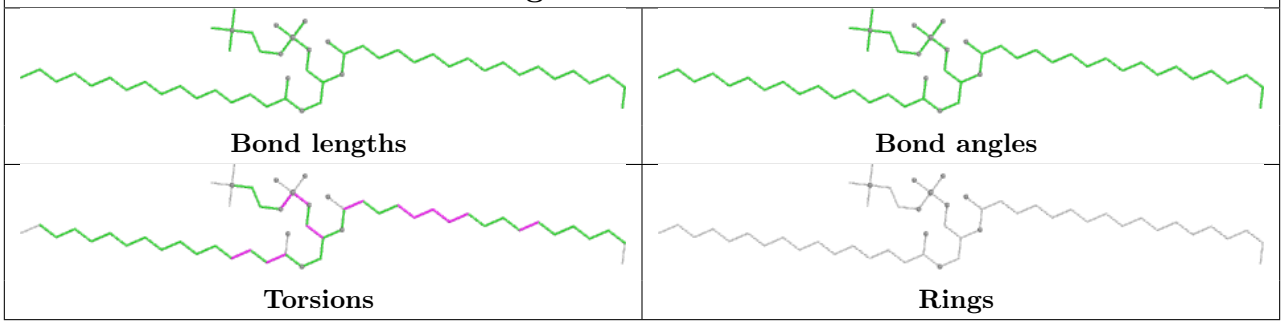
Ligand 8Q1 G 201

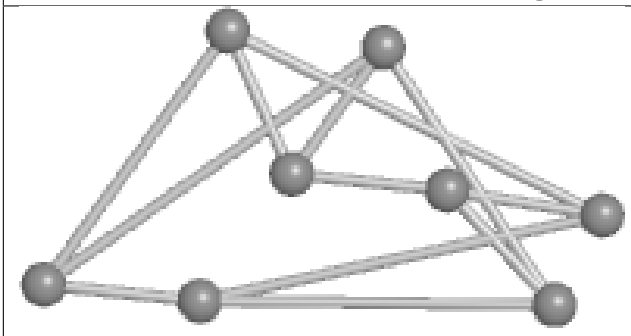
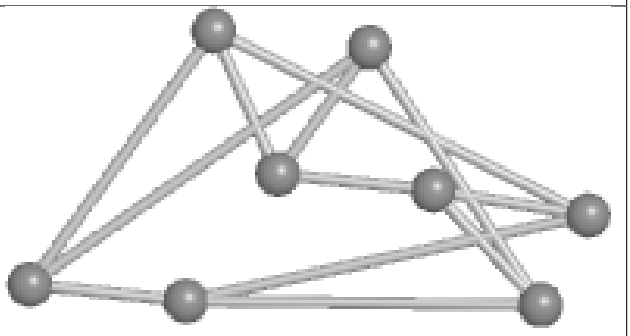
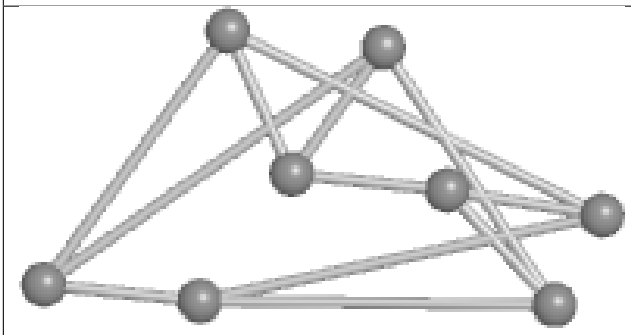
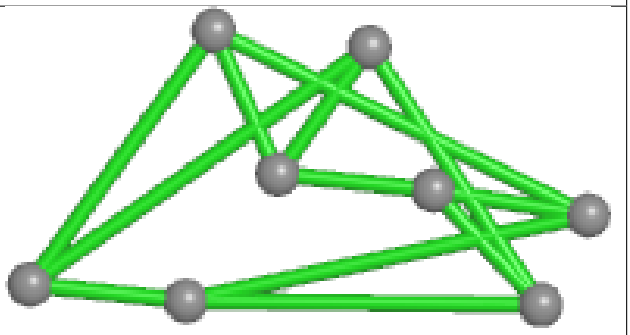


Ligand PEE C 302



Ligand PLX C 303



Ligand SF4 A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

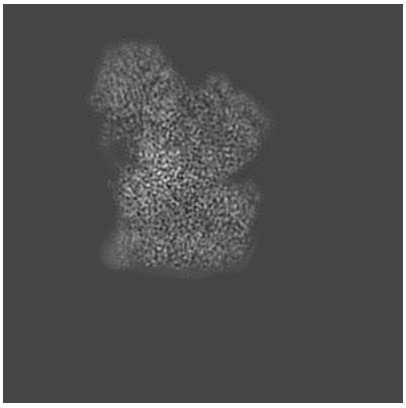
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31886. These allow visual inspection of the internal detail of the map and identification of artifacts.

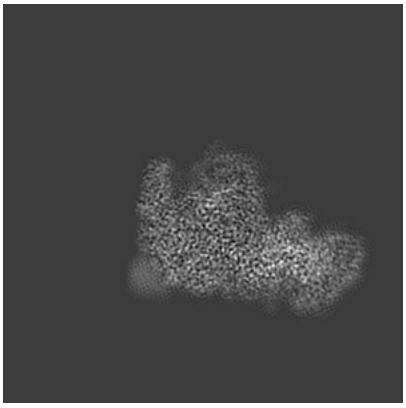
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

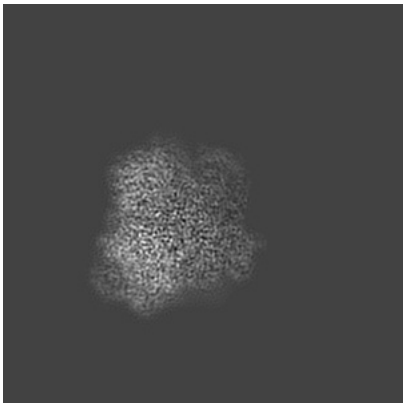
6.1.1 Primary map



X



Y

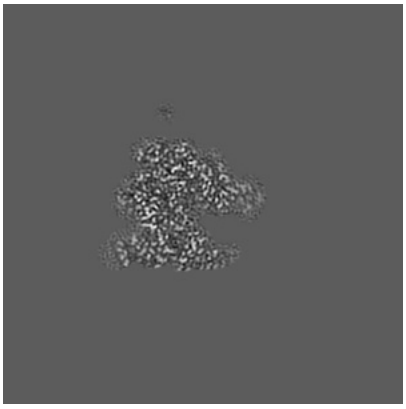


Z

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

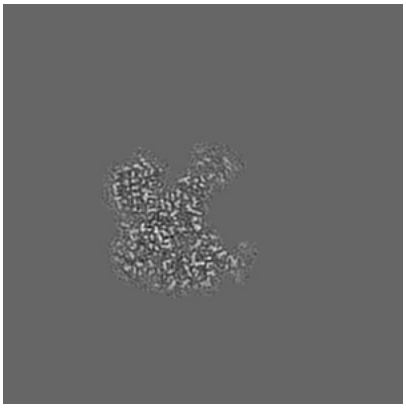
6.2 Central slices (i)

6.2.1 Primary map



X Index: 256

Y Index: 256

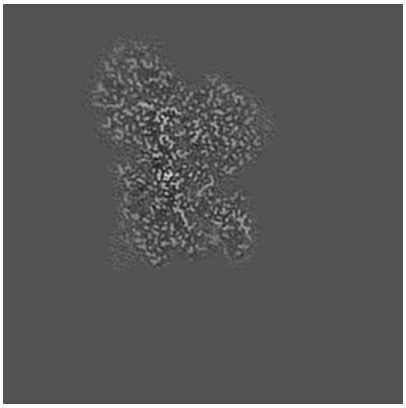


Z Index: 256

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: 194

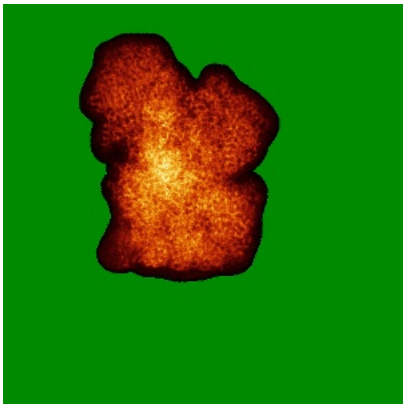
Y Index: 206

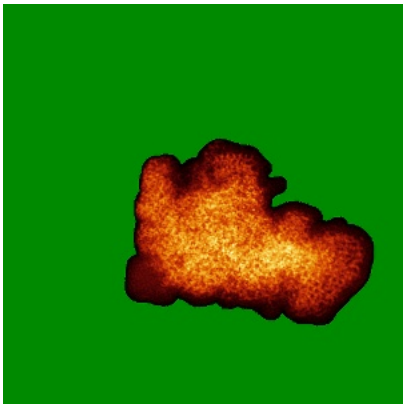
Z Index: 293

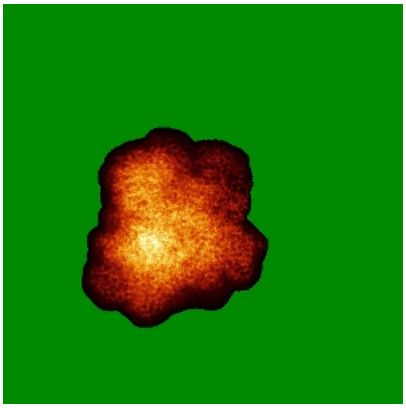
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

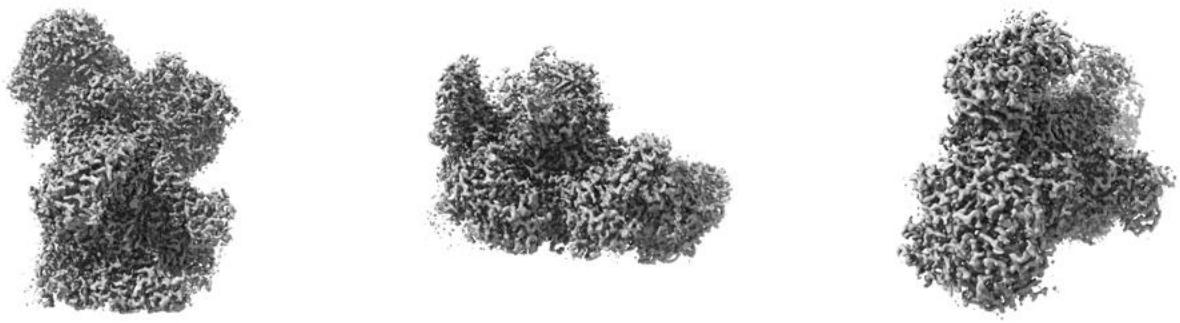

Y


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

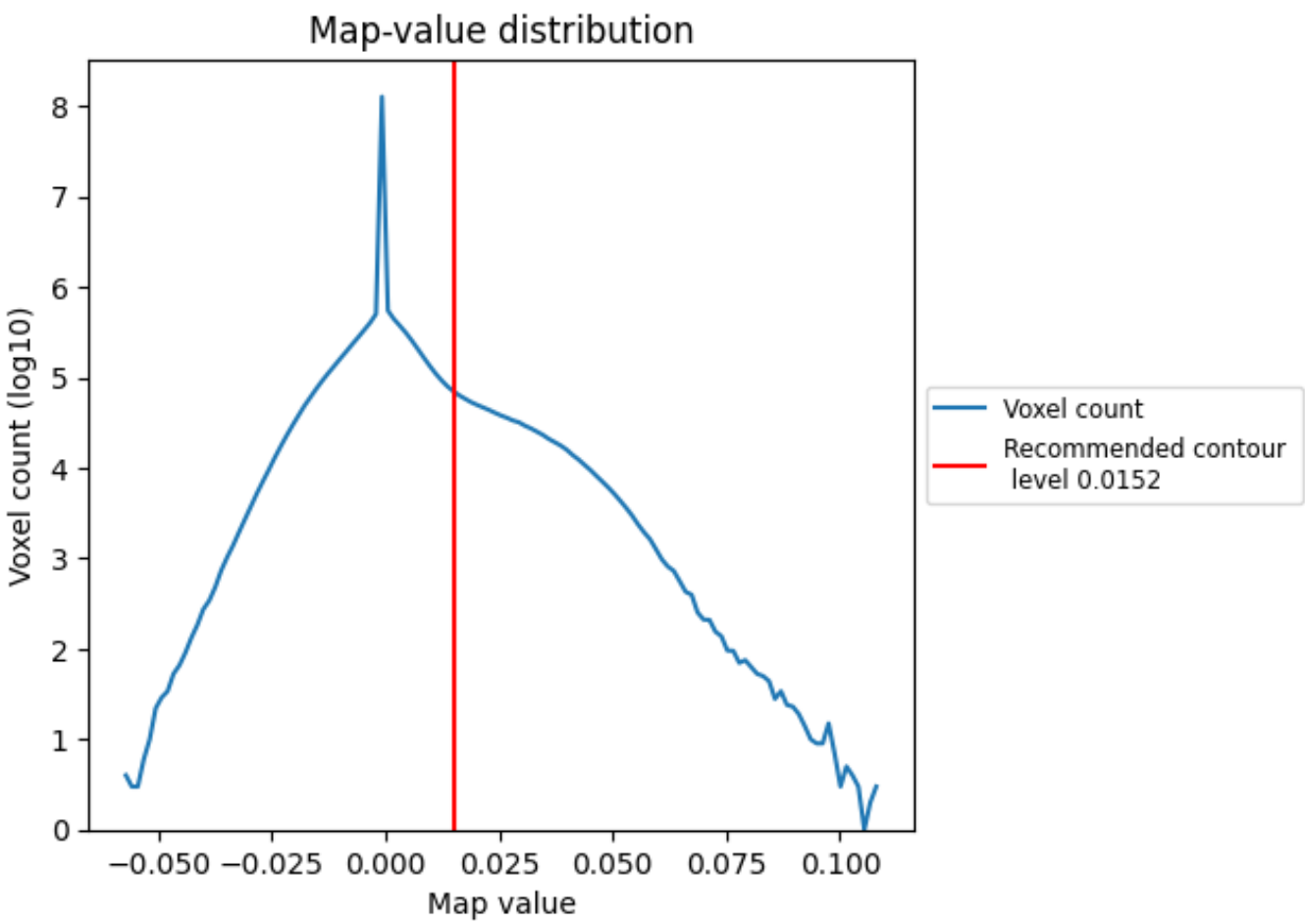
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

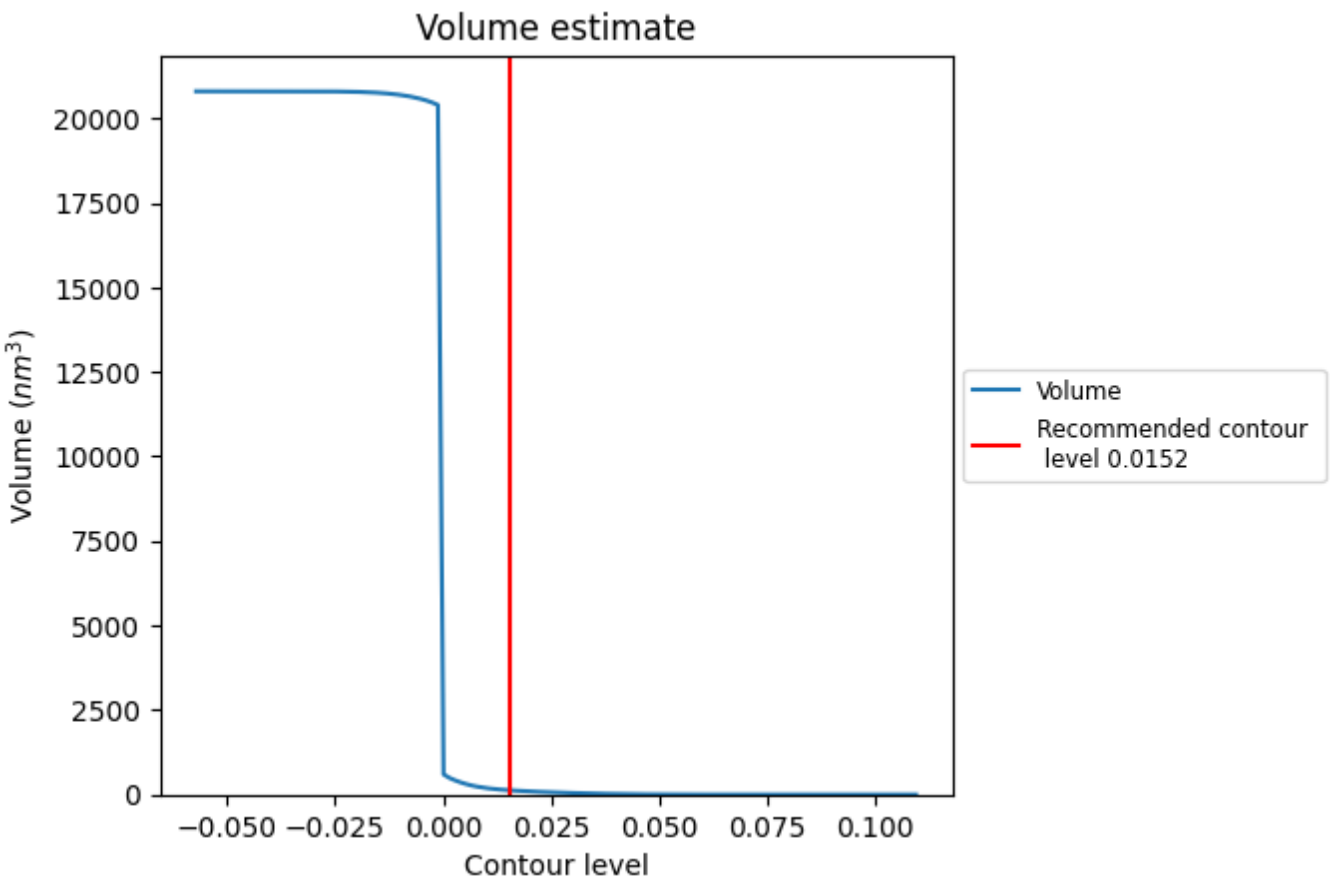
This section contains the results of statistical analysis of the map.

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.

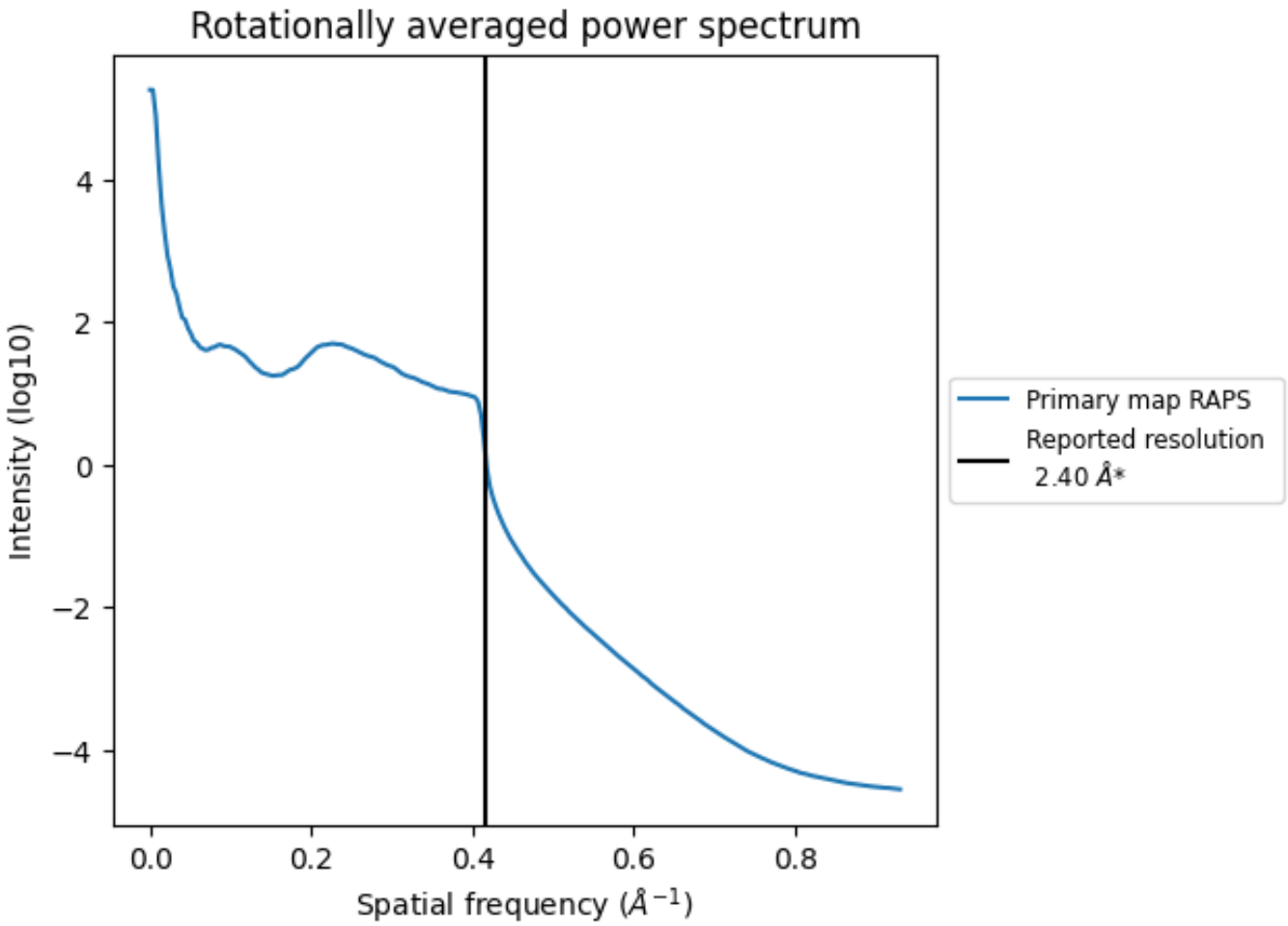
7.2 Volume estimate (i)



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 116 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 (i)



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

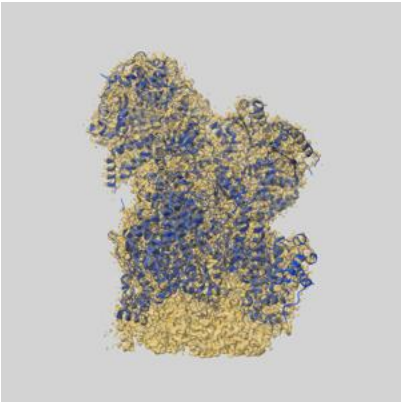
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

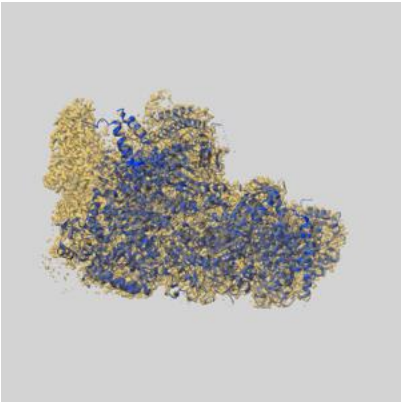
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31886 and PDB model 7VBZ. Per-residue inclusion information can be found in section 3 on page 15.

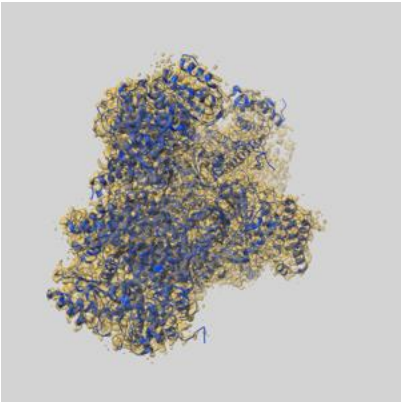
9.1 Map-model overlay (i)



X



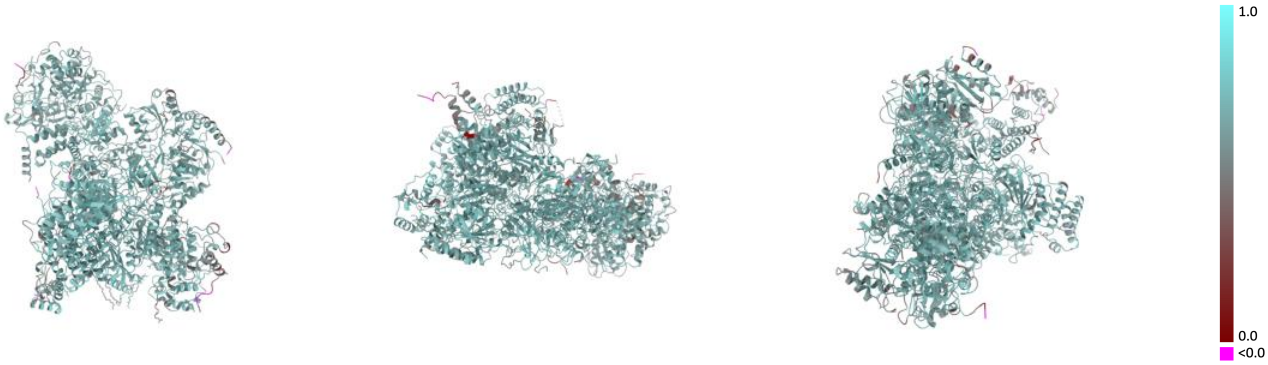
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0152 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.

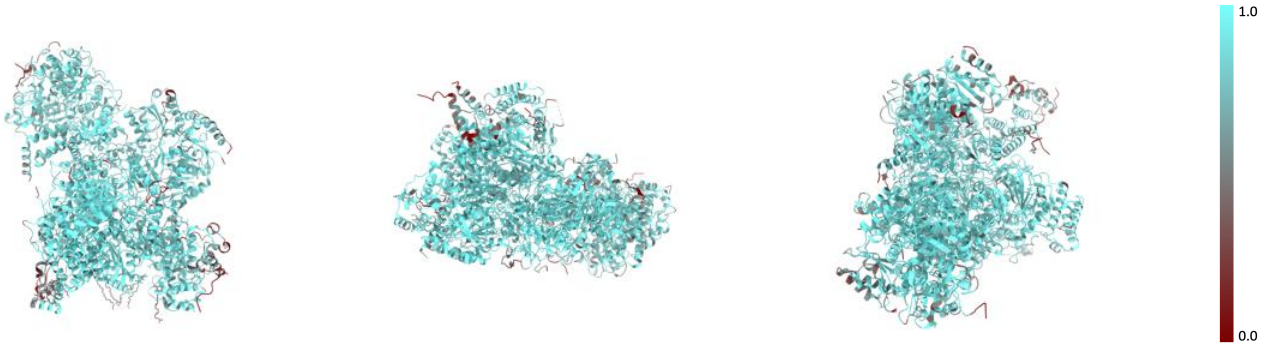
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

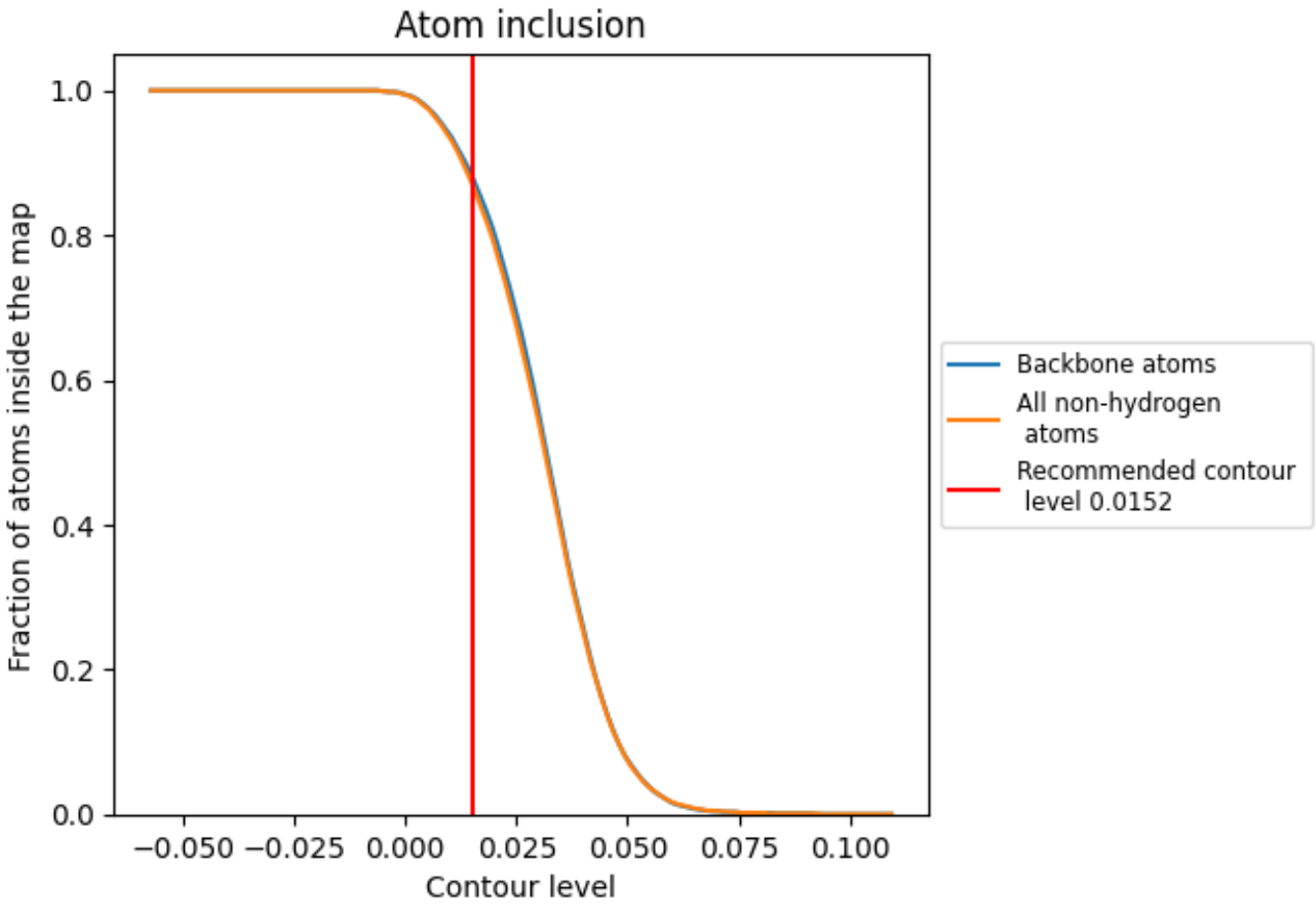
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0152).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.6610
A	0.8720	0.6490
B	0.9440	0.7040
C	0.9300	0.6970
E	0.8610	0.6610
F	0.7500	0.5880
G	0.5350	0.4970
H	0.8640	0.6450
I	0.7210	0.6070
J	0.8940	0.6670
K	0.7070	0.5830
L	0.8750	0.6740
M	0.9000	0.6740
N	0.7660	0.6360
O	0.7980	0.6170
P	0.9500	0.7060
Q	0.9680	0.7090
T	0.8170	0.6510
W	0.7270	0.5830