



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:02 AM JST

PDB ID : 7VYN / pdb_00007vyn
EMDB ID : EMD-32210
Title : Matrix arm of active state CI from Q1-NADH dataset
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-14
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

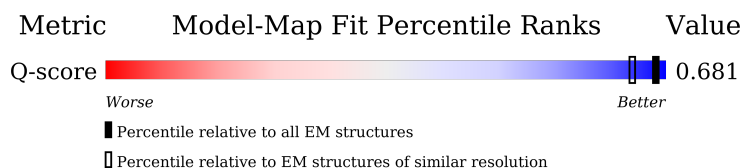
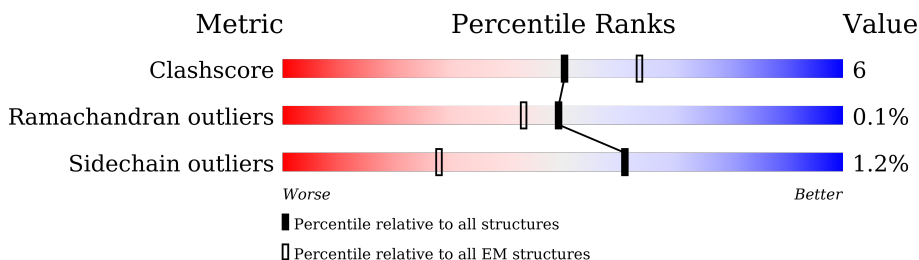
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	386	
17	T	96	
18	W	29	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	A	501	-	-	X	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 29298 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
1	A	433	Total	C	N	O	S	0	0
			3330	2103	593	614	20		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

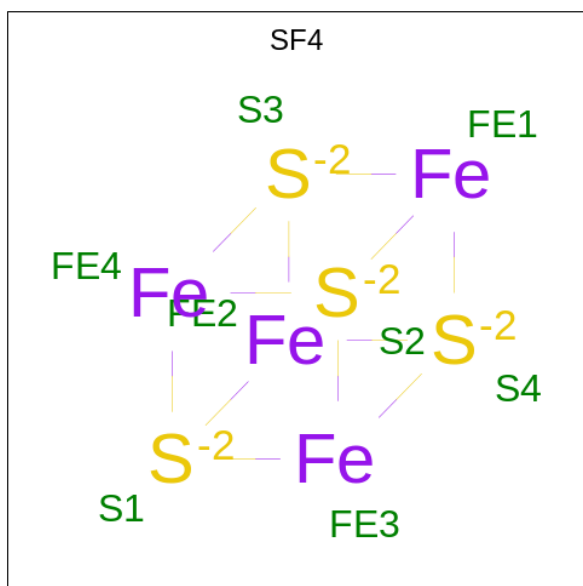
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

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

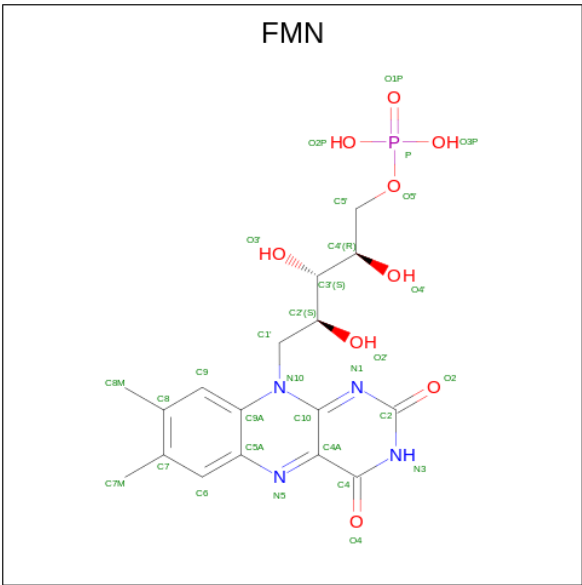
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			218	138	40	39	1		

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



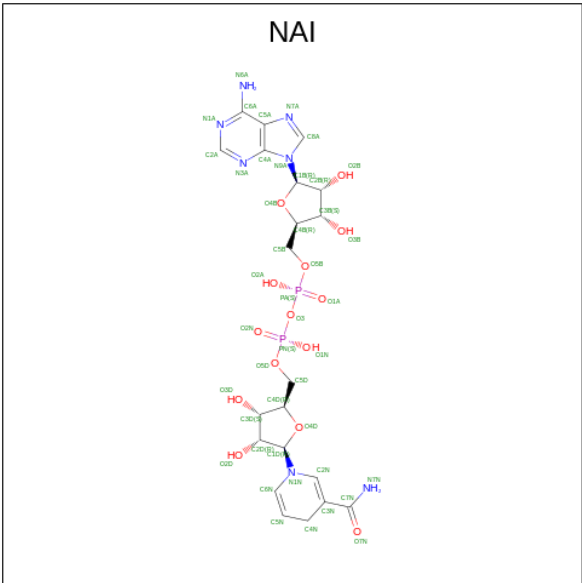
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			8	4	4	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



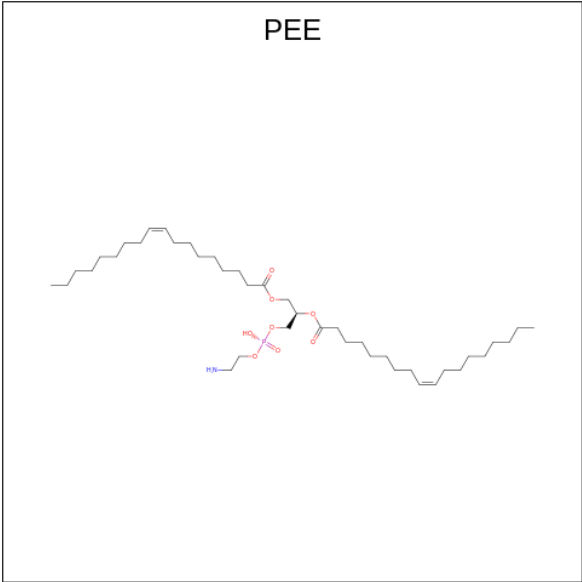
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



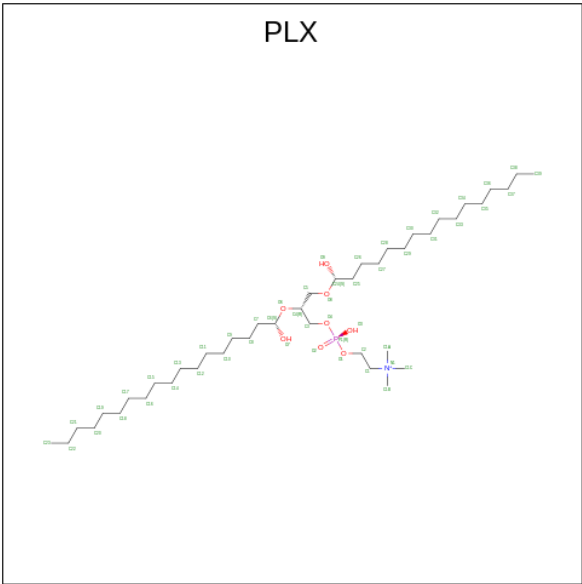
Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 22 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



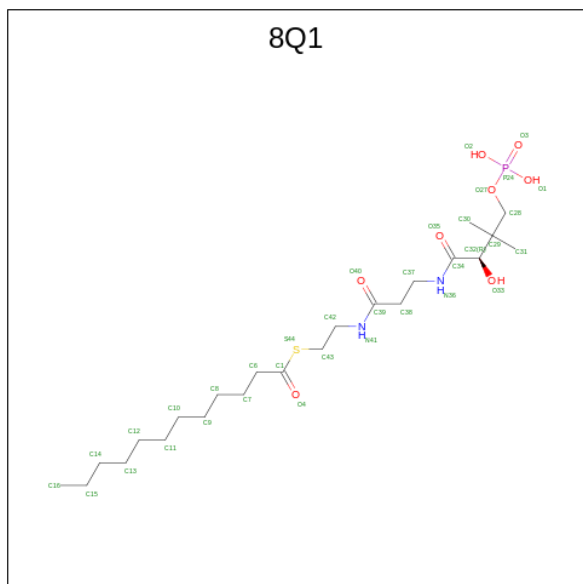
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	C	1	47	37	1	8	1	0

- 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: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



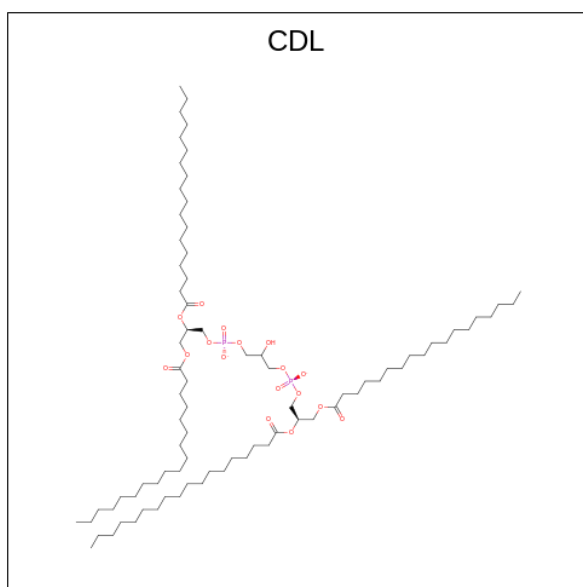
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	C	1	52	42	1	8	1	0

- 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).



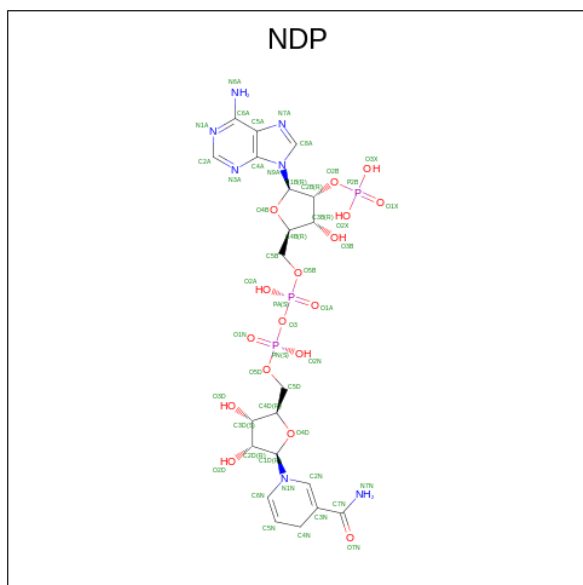
Mol	Chain	Residues	Atoms						AltConf
24	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



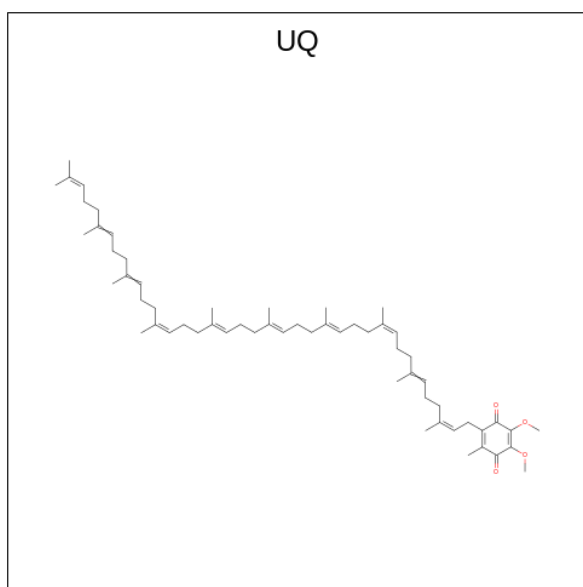
Mol	Chain	Residues	Atoms				AltConf
25	I	1	Total	C	O	P	0
			51	32	17	2	

- Molecule 26 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).



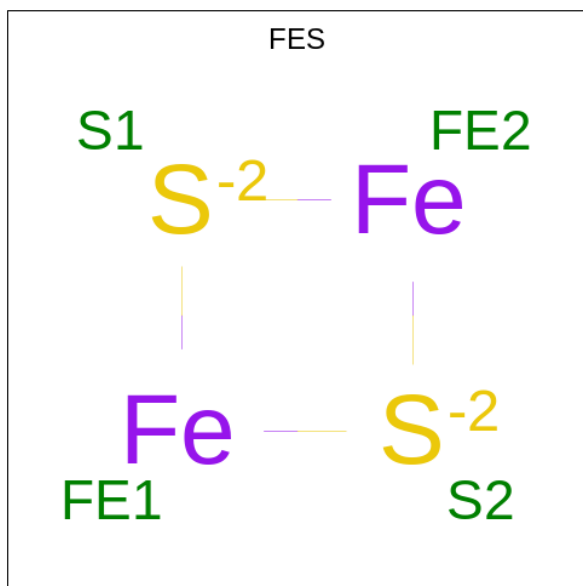
Mol	Chain	Residues	Atoms					AltConf
26	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 27 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
27	J	1	Total	C	O	0
			33	29	4	

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

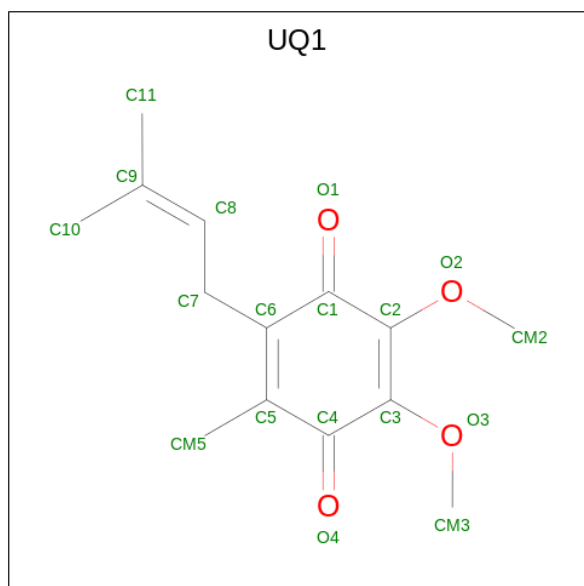


Mol	Chain	Residues	Atoms			AltConf
28	M	1	Total	Fe	S	0
			4	2	2	
28	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 30 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	Q	1	Total	C	O	0
			18	14	4	
30	Q	1	Total	C	O	0
			18	14	4	

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

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

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	50	Total	O	0
			50	50	

Continued on next page...

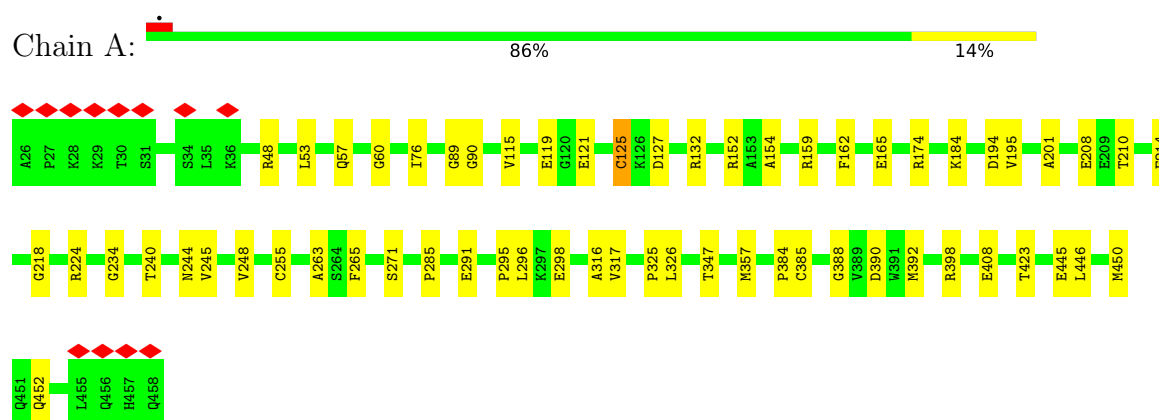
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
32	B	76	Total 76	O 76	0
32	C	54	Total 54	O 54	0
32	E	3	Total 3	O 3	0
32	F	1	Total 1	O 1	0
32	H	6	Total 6	O 6	0
32	I	14	Total 14	O 14	0
32	J	7	Total 7	O 7	0
32	K	6	Total 6	O 6	0
32	L	24	Total 24	O 24	0
32	M	196	Total 196	O 196	0
32	N	8	Total 8	O 8	0
32	O	14	Total 14	O 14	0
32	P	74	Total 74	O 74	0
32	Q	191	Total 191	O 191	0
32	T	9	Total 9	O 9	0
32	W	2	Total 2	O 2	0

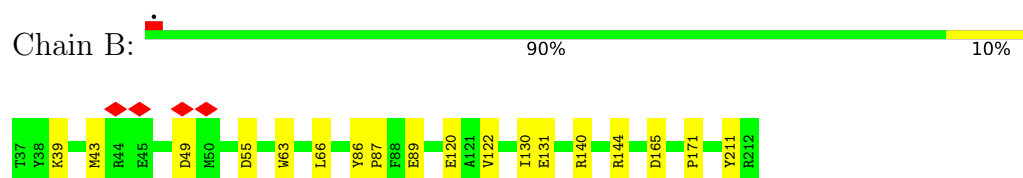
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

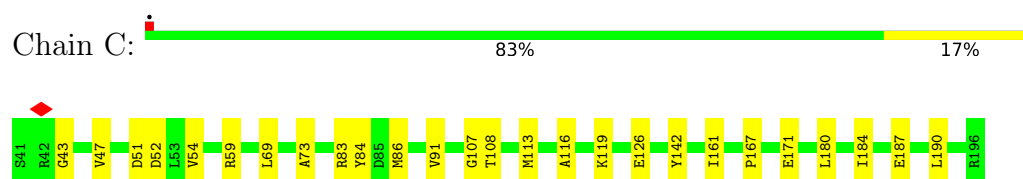
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



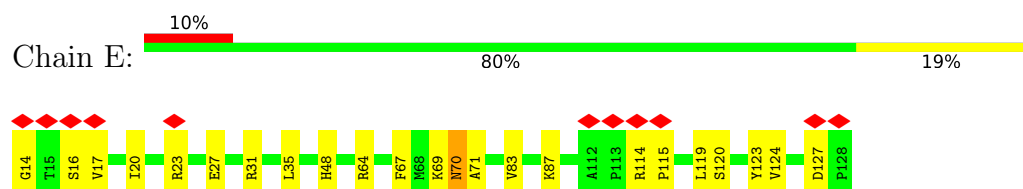
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



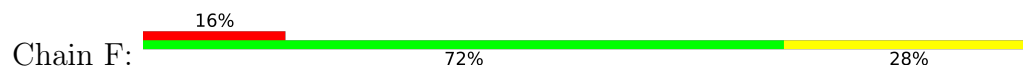
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



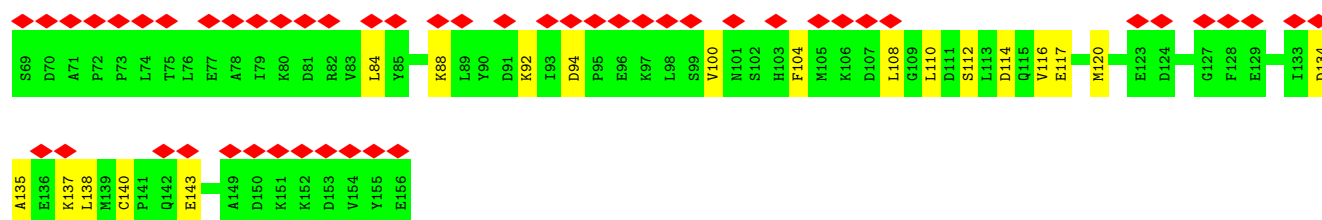
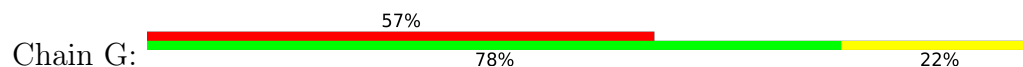
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



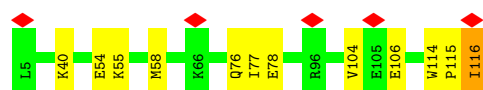
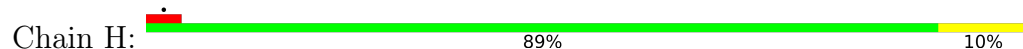
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



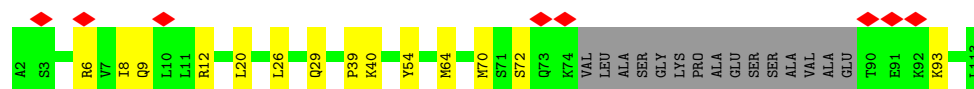
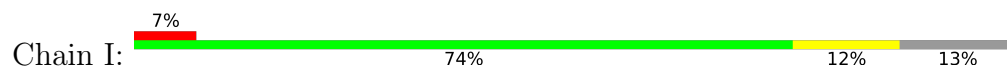
- Molecule 6: Acyl carrier protein, mitochondrial



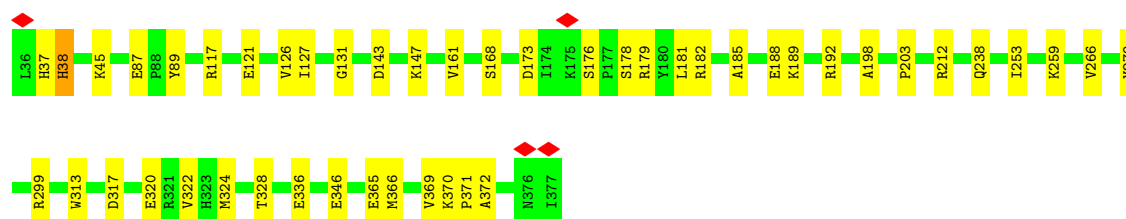
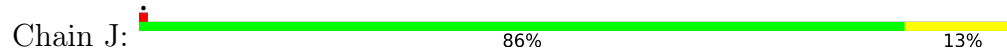
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



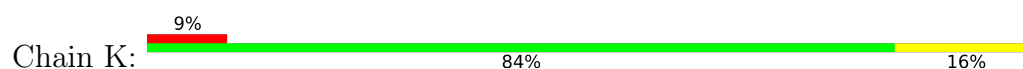
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

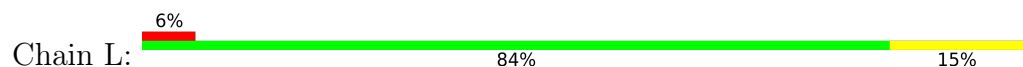


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

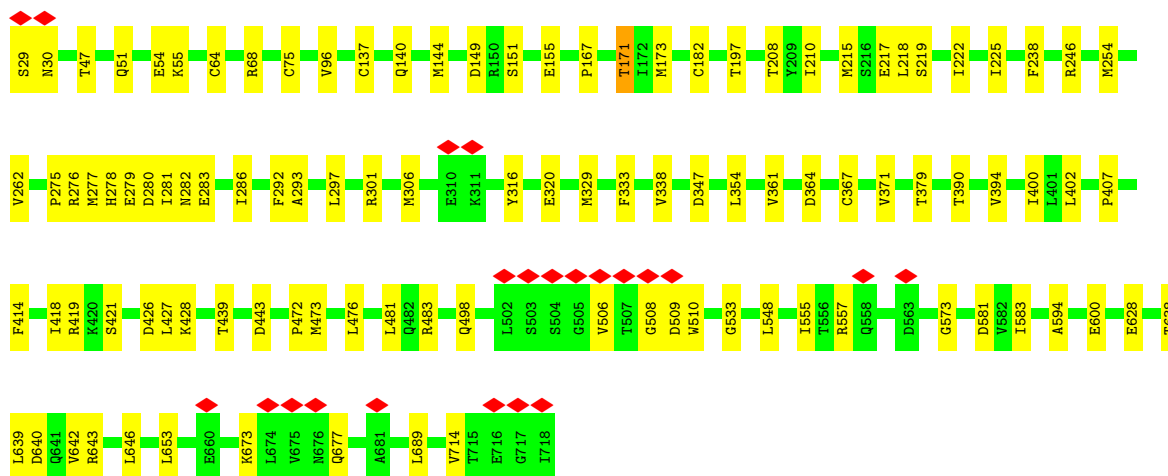
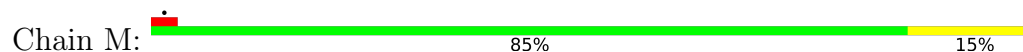




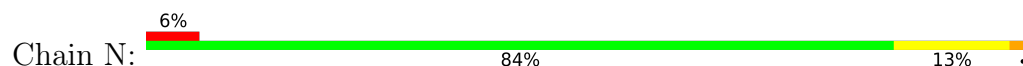
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



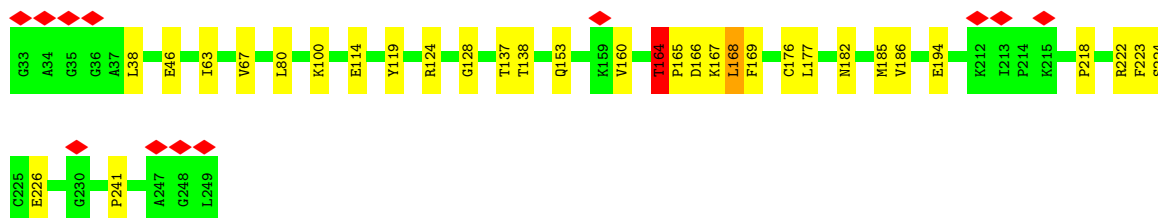
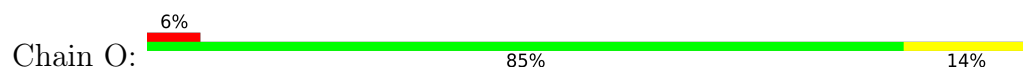
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



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



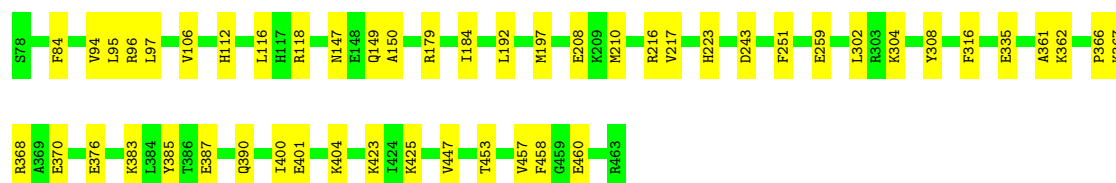
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P:  87% 13%



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

Chain Q:  87% 13%



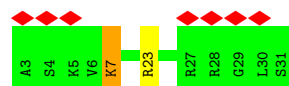
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  7% 92% 8%



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

Chain W:  24% 93% 2%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.127	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0162	Depositor
Map size (Å)	263.496, 263.496, 263.496	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.54895, 0.54895, 0.54895	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, ZN, SF4, PLX, MG, 8Q1, 2MR, UQ1, FMN, CDL, UQ, PEE, FES, NAI

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	0.13	0/3406	0.31	0/4603
2	B	0.13	0/1443	0.33	0/1952
3	C	0.14	0/1279	0.34	0/1730
4	E	0.20	0/995	0.45	0/1340
5	F	0.13	0/698	0.37	0/940
6	G	0.11	0/705	0.32	0/956
7	H	0.15	0/929	0.37	0/1258
8	I	0.16	0/798	0.41	0/1079
9	J	0.15	0/2828	0.38	0/3834
10	K	0.11	0/377	0.33	0/509
11	L	0.16	0/1039	0.42	1/1403 (0.1%)
12	M	0.15	0/5384	0.39	1/7295 (0.0%)
13	N	0.15	0/1245	0.39	2/1694 (0.1%)
14	O	0.17	0/1711	0.48	3/2328 (0.1%)
15	P	0.15	0/1789	0.37	1/2436 (0.0%)
16	Q	0.16	0/3157	0.38	2/4268 (0.0%)
17	T	0.11	0/755	0.30	0/1018
18	W	0.13	0/224	0.29	0/302
All	All	0.15	0/28762	0.38	10/38945 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	111	LEU	N-CA-C	7.54	119.28	111.14
14	O	164	THR	CA-C-N	6.62	126.40	119.05
14	O	164	THR	C-N-CA	6.62	126.40	119.05
13	N	120	THR	CA-C-N	6.17	125.89	119.05
13	N	120	THR	C-N-CA	6.17	125.89	119.05
15	P	102	ASP	N-CA-C	5.44	120.07	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	169	PHE	N-CA-C	5.32	117.63	109.07
12	M	292	PHE	N-CA-C	5.29	119.71	112.88
16	Q	425	LYS	CA-C-N	5.20	129.94	121.83
16	Q	425	LYS	C-N-CA	5.20	129.94	121.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	45	0
2	B	1412	0	1363	14	0
3	C	1248	0	1254	18	0
4	E	971	0	975	19	0
5	F	687	0	700	14	0
6	G	693	0	671	14	0
7	H	910	0	950	7	0
8	I	780	0	808	13	0
9	J	2751	0	2773	32	0
10	K	366	0	338	7	0
11	L	1016	0	1016	15	0
12	M	5296	0	5326	70	0
13	N	1204	0	1162	20	0
14	O	1671	0	1673	23	0
15	P	1738	0	1693	18	0
16	Q	3096	0	3063	32	0
17	T	741	0	702	5	0
18	W	218	0	219	2	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	1	0
19	M	16	0	0	0	0
20	A	31	0	19	4	0
21	A	44	0	27	5	0
22	C	47	0	71	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	52	0	88	3	0
24	E	35	0	0	4	0
25	I	51	0	46	1	0
26	J	48	0	25	2	0
27	J	33	0	39	2	0
28	M	4	0	0	0	0
28	O	4	0	0	0	0
29	M	1	0	0	0	0
30	Q	36	0	36	2	0
31	T	1	0	0	0	0
32	A	50	0	0	1	0
32	B	76	0	0	0	0
32	C	54	0	0	0	0
32	E	3	0	0	0	0
32	F	1	0	0	0	0
32	H	6	0	0	0	0
32	I	14	0	0	0	0
32	J	7	0	0	0	0
32	K	6	0	0	0	0
32	L	24	0	0	0	0
32	M	196	0	0	1	0
32	N	8	0	0	0	0
32	O	14	0	0	0	0
32	P	74	0	0	0	0
32	Q	191	0	0	5	0
32	T	9	0	0	0	0
32	W	2	0	0	0	0
All	All	29298	0	28329	318	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 6.

All (318) 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)
24:E:201:8Q1:O1	6:G:112:SER:CB	1.86	1.23
26:J:401:NDP:O4D	26:J:401:NDP:C4D	1.69	1.16
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.16
14:O:164:THR:HG22	14:O:165:PRO:HD2	1.29	1.09
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.59	0.83
14:O:164:THR:HG22	14:O:165:PRO:CD	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:164:THR:CG2	14:O:165:PRO:HD2	2.08	0.80
12:M:51:GLN:O	12:M:54:GLU:HG2	1.81	0.80
8:I:40:LYS:HB3	18:W:7:LYS:H	1.46	0.80
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.66	0.78
12:M:379:THR:HG21	32:M:954:HOH:O	1.85	0.75
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.69	0.74
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.69	0.73
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.72	0.72
4:E:119:LEU:HG	12:M:628:GLU:OE2	1.89	0.72
1:A:285:PRO:O	14:O:222:ARG:NH2	2.22	0.72
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.71	0.71
9:J:192:ARG:NH1	9:J:198:ALA:O	2.24	0.71
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.24	0.70
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.74	0.69
1:A:445:GLU:OE1	1:A:445:GLU:N	2.26	0.68
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.74	0.68
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.26	0.68
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.76	0.68
14:O:128:GLY:HA2	14:O:167:LYS:O	1.93	0.67
7:H:40:LYS:H	7:H:40:LYS:HD2	1.58	0.67
9:J:181:LEU:HD12	9:J:324:MET:HE1	1.75	0.67
6:G:92:LYS:NZ	6:G:114:ASP:OD1	2.25	0.66
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.77	0.66
11:L:78:ARG:NH1	11:L:148:GLU:OE1	2.29	0.66
16:Q:147:ASN:ND2	32:Q:612:HOH:O	2.28	0.65
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.27	0.65
4:E:71:ALA:HB1	24:E:201:8Q1:O33	1.97	0.64
12:M:498:GLN:OE1	12:M:673:LYS:NZ	2.31	0.63
1:A:184:LYS:HB2	10:K:98:MET:HE1	1.82	0.62
5:F:61:VAL:HG23	5:F:62:GLN:H	1.65	0.61
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.39	0.61
1:A:89:GLY:O	21:A:503:NAI:H2N	2.01	0.61
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.83	0.61
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.26	0.61
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.34	0.60
4:E:48:HIS:NE2	9:J:365:GLU:OE1	2.34	0.60
24:E:201:8Q1:P24	6:G:112:SER:CB	2.88	0.60
9:J:336:GLU:H	9:J:336:GLU:CD	2.08	0.60
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.84	0.59
11:L:112:MET:SD	13:N:126:PRO:HB2	2.42	0.59
12:M:306:MET:HB2	12:M:583:ILE:HB	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.36	0.59
12:M:51:GLN:CA	12:M:54:GLU:HG2	2.32	0.58
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.37	0.58
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.36	0.58
14:O:38:LEU:O	14:O:124:ARG:NH2	2.36	0.58
9:J:178:SER:OG	9:J:317:ASP:OD1	2.20	0.57
11:L:76:LYS:NZ	12:M:640:ASP:OD2	2.36	0.57
5:F:24:CYS:N	5:F:58:CYS:SG	2.78	0.57
12:M:379:THR:O	12:M:379:THR:HG22	2.03	0.57
6:G:134:ASP:HA	6:G:137:LYS:HE2	1.87	0.57
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.86	0.56
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.88	0.56
4:E:67:PHE:O	4:E:70:ASN:ND2	2.39	0.56
12:M:51:GLN:C	12:M:54:GLU:HG2	2.29	0.56
14:O:164:THR:CG2	14:O:165:PRO:CD	2.76	0.56
9:J:313:TRP:CD1	27:J:402:UQ:H8	2.41	0.56
5:F:90:THR:O	5:F:94:VAL:HG23	2.06	0.56
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.87	0.56
15:P:147:THR:HB	15:P:153:ILE:HD11	1.86	0.56
1:A:263:ALA:HA	1:A:271:SER:HB3	1.87	0.55
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.87	0.55
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.39	0.55
1:A:174:ARG:NH1	10:K:92:GLU:OE1	2.40	0.55
1:A:210:THR:HB	1:A:224:ARG:HG2	1.89	0.55
4:E:127:ASP:OD1	11:L:104:ARG:NH1	2.40	0.55
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.55
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.88	0.55
4:E:64:ARG:NH2	6:G:117:GLU:OE1	2.40	0.55
9:J:143:ASP:OD1	9:J:147:LYS:NZ	2.39	0.55
13:N:121:PRO:O	17:T:58:ARG:HA	2.07	0.55
15:P:43:THR:HA	15:P:47:ILE:HD12	1.89	0.54
3:C:190:LEU:HD22	22:C:302:PEE:H14	1.90	0.54
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.90	0.54
4:E:120:SER:O	4:E:124:VAL:HG22	2.08	0.54
14:O:166:ASP:HB3	14:O:168:LEU:HD21	1.88	0.54
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	1.90	0.53
4:E:70:ASN:ND2	4:E:70:ASN:H	2.07	0.53
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.43	0.53
16:Q:179:ARG:NH1	32:Q:624:HOH:O	2.41	0.53
14:O:128:GLY:CA	14:O:167:LYS:O	2.55	0.53
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:120:THR:HB	13:N:121:PRO:HD2	1.91	0.53
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.30	0.53
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.39	0.53
3:C:84:TYR:OH	3:C:171:GLU:OE2	2.20	0.53
2:B:171:PRO:HB3	13:N:93:MET:HE1	1.91	0.52
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.91	0.52
12:M:197:THR:O	14:O:114:GLU:HG2	2.08	0.52
12:M:509:ASP:N	12:M:509:ASP:OD1	2.40	0.52
16:Q:259:GLU:OE2	18:W:23:ARG:NH1	2.36	0.52
12:M:419:ARG:NH1	12:M:439:THR:O	2.42	0.52
7:H:106:GLU:OE2	8:I:72:SER:OG	2.21	0.52
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.92	0.52
2:B:43:MET:HA	2:B:43:MET:HE2	1.91	0.52
12:M:51:GLN:O	12:M:54:GLU:CG	2.55	0.52
15:P:201:ASP:OD1	15:P:201:ASP:N	2.41	0.52
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.92	0.52
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.91	0.51
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.44	0.51
9:J:126:VAL:HG23	9:J:161:VAL:HG11	1.93	0.51
9:J:185:ALA:O	9:J:188:GLU:HG2	2.11	0.51
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.50	0.51
17:T:32:SER:OG	17:T:36:GLU:O	2.25	0.51
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.45	0.51
14:O:153:GLN:HE21	14:O:160:VAL:HG13	1.76	0.51
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.11	0.51
7:H:54:GLU:O	7:H:58:MET:HG3	2.10	0.51
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.93	0.51
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.93	0.51
6:G:94:ASP:OD1	6:G:94:ASP:N	2.41	0.51
12:M:277:MET:HE3	12:M:279:GLU:HG2	1.93	0.50
2:B:49:ASP:OD1	2:B:49:ASP:N	2.45	0.50
13:N:8:ARG:HA	13:N:11:LEU:HD12	1.93	0.50
3:C:73:ALA:HB1	30:Q:501:UQ1:H112	1.92	0.50
3:C:59:ARG:NH1	23:C:303:PLX:O2	2.45	0.50
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.76	0.50
1:A:446:LEU:O	1:A:450:MET:HG3	2.12	0.50
4:E:70:ASN:OD1	24:E:201:8Q1:O4	2.29	0.49
4:E:127:ASP:OD2	9:J:45:LYS:NZ	2.44	0.49
12:M:639:LEU:O	12:M:643:ARG:HG3	2.12	0.49
3:C:52:ASP:HB3	23:C:303:PLX:H251	1.94	0.49
12:M:400:ILE:HG22	12:M:427:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:329:MET:HE1	12:M:333:PHE:HE2	1.78	0.49
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.94	0.49
9:J:87:GLU:HG3	9:J:89:TYR:H	1.77	0.49
1:A:325:PRO:O	1:A:347:THR:OG1	2.26	0.49
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.48	0.49
8:I:64:MET:HE2	15:P:80:CYS:SG	2.53	0.48
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.95	0.48
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.95	0.48
4:E:23:ARG:HH22	11:L:51:GLN:HB2	1.78	0.48
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.95	0.48
22:C:302:PEE:H66	22:C:302:PEE:H32	1.96	0.48
12:M:29:SER:OG	12:M:30:ASN:N	2.47	0.48
1:A:90:GLY:HA3	21:A:503:NAI:H1D	1.96	0.48
14:O:63:ILE:O	14:O:67:VAL:HG23	2.14	0.48
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.95	0.48
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.96	0.48
1:A:194:ASP:OD2	10:K:98:MET:HG2	2.12	0.48
12:M:171:THR:HG23	12:M:173:MET:SD	2.54	0.48
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.96	0.48
12:M:390:THR:HA	12:M:600:GLU:HG2	1.96	0.48
5:F:69:TYR:CE1	5:F:75:LYS:HE2	2.48	0.47
3:C:54:VAL:HG21	22:C:302:PEE:H55	1.95	0.47
11:L:131:LYS:HD3	11:L:147:VAL:HG11	1.95	0.47
12:M:557:ARG:NH2	12:M:581:ASP:OD1	2.47	0.47
13:N:4:VAL:HA	13:N:7:LEU:HD12	1.94	0.47
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.49	0.47
1:A:154:ALA:HB3	1:A:195:VAL:HG12	1.96	0.47
11:L:168:LYS:HA	11:L:168:LYS:HD3	1.64	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.95	0.47
11:L:109:ASN:N	11:L:114:TRP:O	2.38	0.47
20:A:502:FMN:N1	20:A:502:FMN:O3'	2.32	0.47
9:J:369:VAL:HG12	9:J:369:VAL:O	2.14	0.47
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.96	0.47
12:M:167:PRO:HD2	12:M:215:MET:HE1	1.97	0.47
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.33	0.47
12:M:208:THR:OG1	12:M:210:ILE:O	2.29	0.46
12:M:219:SER:O	12:M:222:ILE:HG12	2.15	0.46
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.80	0.46
12:M:421:SER:HB3	12:M:427:LEU:HD22	1.97	0.46
11:L:119:ASP:OD1	11:L:122:SER:HB3	2.16	0.46
7:H:76:GLN:O	7:H:78:GLU:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:137:THR:HG22	14:O:138:THR:H	1.80	0.46
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.46	0.46
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.50	0.46
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.98	0.46
12:M:68:ARG:NH1	12:M:283:GLU:OE2	2.49	0.46
12:M:646:LEU:HD22	12:M:653:LEU:HD13	1.98	0.46
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.98	0.46
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.98	0.46
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.31	0.46
1:A:195:VAL:O	10:K:97:ARG:NH1	2.47	0.45
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.98	0.45
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.51	0.45
9:J:131:GLY:O	26:J:401:NDP:H51A	2.17	0.45
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.45
16:Q:401:GLU:OE2	32:Q:602:HOH:O	2.21	0.45
1:A:115:VAL:HG22	1:A:248:VAL:HG21	1.98	0.45
1:A:119:GLU:OE2	1:A:125:CYS:HA	2.17	0.45
4:E:83:VAL:HG12	4:E:87:LYS:HD2	1.98	0.45
16:Q:367:LYS:HB2	16:Q:370:GLU:HG3	1.98	0.45
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.17	0.45
5:F:44:LEU:HD23	5:F:53:ILE:HD13	1.99	0.45
12:M:394:VAL:HA	12:M:473:MET:HE1	1.99	0.45
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.99	0.45
13:N:85:GLU:HG2	13:N:86:TRP:H	1.82	0.45
4:E:27:GLU:O	4:E:31:ARG:HG3	2.17	0.45
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.99	0.45
3:C:119:LYS:HB2	3:C:119:LYS:HE3	1.73	0.45
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.52	0.44
8:I:93:LYS:HA	8:I:93:LYS:HD3	1.55	0.44
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.97	0.44
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.44
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.98	0.44
17:T:52:ARG:HG2	17:T:52:ARG:HH11	1.82	0.44
12:M:506:VAL:HG12	12:M:508:GLY:H	1.83	0.44
14:O:100:LYS:HB2	14:O:100:LYS:HE2	1.66	0.44
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.98	0.44
1:A:388:GLY:O	1:A:392:MET:HG3	2.17	0.44
3:C:107:GLY:HA2	19:C:301:SF4:S1	2.58	0.44
22:C:302:PEE:H82	22:C:302:PEE:H74	1.84	0.44
1:A:53:LEU:O	1:A:57:GLN:HG3	2.16	0.44
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.53	0.44
1:A:357:MET:HE3	1:A:357:MET:HB2	1.87	0.44
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.17	0.44
1:A:159:ARG:NH2	14:O:176:CYS:O	2.43	0.44
9:J:369:VAL:O	9:J:369:VAL:CG1	2.65	0.44
6:G:88:LYS:HB3	6:G:88:LYS:HE2	1.80	0.44
8:I:6:ARG:HG2	13:N:2:GLU:OE2	2.18	0.44
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.99	0.44
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.99	0.44
27:J:402:UQ:H111	27:J:402:UQ:H71	1.78	0.44
9:J:369:VAL:C	9:J:370:LYS:HG3	2.43	0.43
3:C:83:ARG:NE	16:Q:208:GLU:HG2	2.33	0.43
3:C:184:ILE:O	3:C:187:GLU:HG2	2.17	0.43
9:J:189:LYS:HB2	9:J:189:LYS:HE3	1.77	0.43
12:M:215:MET:HG2	12:M:714:VAL:HG12	2.00	0.43
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.65	0.43
6:G:84:LEU:O	6:G:88:LYS:HG2	2.19	0.43
9:J:299:ARG:HH21	9:J:320:GLU:HG3	1.84	0.43
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.53	0.43
12:M:371:VAL:HG22	12:M:533:GLY:HA2	2.01	0.43
12:M:402:LEU:HD13	12:M:407:PRO:HG2	2.01	0.43
5:F:61:VAL:HG23	5:F:62:GLN:N	2.31	0.43
16:Q:149:GLN:OE1	32:Q:601:HOH:O	2.21	0.43
17:T:107:LYS:HG2	17:T:108:THR:N	2.33	0.43
1:A:244:ASN:ND2	20:A:502:FMN:O2	2.44	0.43
1:A:265:PHE:HB3	1:A:291:GLU:HG3	2.01	0.43
3:C:86:MET:HG3	3:C:91:VAL:HB	2.01	0.43
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.54	0.43
13:N:120:THR:HB	13:N:121:PRO:CD	2.49	0.43
12:M:47:THR:O	12:M:96:VAL:HG22	2.19	0.43
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.43
12:M:428:LYS:NZ	12:M:443:ASP:OD2	2.47	0.43
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.54	0.42
3:C:59:ARG:HH12	23:C:303:PLX:P1	2.42	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.88	0.42
16:Q:192:LEU:HD23	16:Q:197:MET:HA	2.02	0.42
5:F:87:VAL:HA	5:F:90:THR:HG22	2.00	0.42
9:J:179:ARG:HD3	9:J:182:ARG:HH21	1.84	0.42
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.42
6:G:135:ALA:HA	6:G:138:LEU:HG	2.01	0.42
8:I:70:MET:O	8:I:70:MET:SD	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:35:LEU:HD13	4:E:87:LYS:HG3	2.02	0.42
9:J:37:HIS:CE1	17:T:49:ASP:HA	2.55	0.42
12:M:278:HIS:CD2	12:M:281:ILE:HD12	2.55	0.42
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.01	0.42
16:Q:404:LYS:HE2	16:Q:457:VAL:HG12	2.01	0.42
4:E:114:ARG:HA	4:E:115:PRO:HD3	1.90	0.42
9:J:212:ARG:HG2	9:J:212:ARG:HH11	1.85	0.42
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.49	0.42
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.59	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.00	0.42
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.02	0.42
15:P:167:GLU:HG2	15:P:178:PHE:CE2	2.54	0.42
20:A:502:FMN:N5	21:A:503:NAI:H4N	2.35	0.41
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.55	0.41
15:P:154:GLU:OE1	15:P:180:ASN:ND2	2.53	0.41
16:Q:366:PRO:O	32:Q:603:HOH:O	2.22	0.41
3:C:43:GLY:O	3:C:47:VAL:HG22	2.20	0.41
8:I:8:ILE:HD11	25:I:201:CDL:H111	2.01	0.41
9:J:117:ARG:O	9:J:121:GLU:HG3	2.20	0.41
12:M:282:ASN:O	12:M:283:GLU:HG2	2.20	0.41
12:M:297:LEU:O	12:M:301:ARG:HD3	2.21	0.41
15:P:85:GLU:HG2	15:P:142:ARG:HD2	2.02	0.41
1:A:390:ASP:OD1	32:A:601:HOH:O	2.21	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.28	0.41
9:J:366:MET:HB2	9:J:366:MET:HE2	1.83	0.41
12:M:254:MET:HE2	12:M:293:ALA:CB	2.50	0.41
15:P:214:ASP:O	15:P:217:LYS:NZ	2.51	0.41
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.53	0.41
7:H:116:ILE:HD13	11:L:96:LYS:HD2	2.01	0.41
6:G:110:LEU:HB3	6:G:114:ASP:HB2	2.01	0.41
9:J:168:SER:O	9:J:203:PRO:HD2	2.21	0.41
10:K:105:ARG:HH22	12:M:426:ASP:CG	2.28	0.41
15:P:115:THR:HB	16:Q:423:LYS:HE3	2.02	0.41
8:I:6:ARG:HA	8:I:9:GLN:HG3	2.03	0.41
4:E:69:LYS:HE3	4:E:69:LYS:HB2	1.89	0.41
9:J:192:ARG:HA	9:J:192:ARG:HD3	1.86	0.41
12:M:55:LYS:HB2	12:M:55:LYS:HE3	1.74	0.41
12:M:306:MET:HE1	13:N:139:PRO:HG3	2.03	0.41
12:M:367:CYS:HB3	12:M:533:GLY:O	2.20	0.41
15:P:161:LYS:HD3	15:P:161:LYS:HA	1.88	0.41
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:MET:HE3	3:C:116:ALA:HB3	2.02	0.41
5:F:23:LEU:O	5:F:57:GLU:HA	2.21	0.41
5:F:30:SER:OG	5:F:63:PRO:HG3	2.21	0.41
12:M:151:SER:HB2	16:Q:376:GLU:OE1	2.20	0.41
13:N:101:LYS:HB2	13:N:101:LYS:HE2	1.71	0.41
30:Q:502:UQ1:H113	30:Q:502:UQ1:H72	1.83	0.41
8:I:26:LEU:HD13	13:N:55:PHE:CD2	2.56	0.41
11:L:66:GLY:HA2	15:P:194:GLU:OE1	2.21	0.41
11:L:109:ASN:O	11:L:113:GLY:HA2	2.21	0.41
12:M:182:CYS:HA	12:M:225:ILE:HD11	2.03	0.41
14:O:224:SER:OG	14:O:226:GLU:OE2	2.31	0.41
6:G:117:GLU:HA	6:G:120:MET:HE3	2.02	0.40
5:F:83:SER:O	5:F:87:VAL:HG13	2.21	0.40
9:J:38:HIS:CE1	13:N:132:LYS:HD3	2.57	0.40
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.90	0.40
12:M:338:VAL:HG21	12:M:361:VAL:HG11	2.03	0.40
14:O:177:LEU:HD12	14:O:185:MET:SD	2.62	0.40
1:A:218:GLY:HA2	14:O:80:LEU:HD23	2.03	0.40
4:E:17:VAL:HG21	11:L:55:VAL:HG22	2.03	0.40
12:M:414:PHE:CE2	12:M:418:ILE:HD11	2.56	0.40
13:N:68:MET:O	13:N:69:ASN:C	2.64	0.40
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.61	0.40
1:A:316:ALA:HB1	1:A:326:LEU:HD12	2.02	0.40
12:M:673:LYS:HB3	12:M:673:LYS:HE3	1.87	0.40
16:Q:184:ILE:HD12	16:Q:210:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	420 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	14	22
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	50
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	23 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	383/386 (99%)	372 (97%)	11 (3%)	0	100	100
17	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
18	W	27/29 (93%)	24 (89%)	3 (11%)	0	100	100
All	All	3504/3558 (98%)	3381 (96%)	121 (4%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	77	ILE
9	J	38	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	343 (99%)	3 (1%)	70	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	88
3	C	132/132 (100%)	129 (98%)	3 (2%)	44	66
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%)	75 (99%)	1 (1%)	61	80
7	H	99/99 (100%)	97 (98%)	2 (2%)	48	70
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	82
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	88
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	65
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	85
12	M	580/580 (100%)	576 (99%)	4 (1%)	76	88
13	N	130/130 (100%)	127 (98%)	3 (2%)	44	66
14	O	183/183 (100%)	179 (98%)	4 (2%)	45	67
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	332/332 (100%)	329 (99%)	3 (1%)	70	85
17	T	79/79 (100%)	78 (99%)	1 (1%)	61	80
18	W	23/24 (96%)	22 (96%)	1 (4%)	26	44
All	All	3041/3058 (99%)	3006 (99%)	35 (1%)	61	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	CYS
1	A	245	VAL
1	A	452	GLN
2	B	55	ASP
3	C	51	ASP
3	C	108	THR
3	C	142	TYR
4	E	20	ILE
4	E	70	ASN
5	F	27	SER
5	F	37	ILE
6	G	100	VAL
7	H	104	VAL
7	H	116	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	29	GLN
9	J	322	VAL
9	J	328	THR
10	K	85	THR
11	L	119	ASP
12	M	171	THR
12	M	483	ARG
12	M	555	ILE
12	M	677	GLN
13	N	4	VAL
13	N	68	MET
13	N	132	LYS
14	O	46	GLU
14	O	164	THR
14	O	168	LEU
14	O	186	VAL
16	Q	217	VAL
16	Q	308	TYR
16	Q	453	THR
17	T	114	CYS
18	W	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	281	HIS
1	A	381	GLN
2	B	204	ASN
3	C	123	GLN
3	C	181	GLN
4	E	70	ASN
4	E	126	HIS
5	F	86	GLN
7	H	50	GLN
9	J	43	HIS
11	L	71	HIS
11	L	86	ASN
11	L	109	ASN
12	M	39	GLN
12	M	178	GLN
12	M	331	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	425	ASN
12	M	663	ASN
12	M	669	ASN
12	M	676	ASN
12	M	677	GLN
13	N	12	GLN
13	N	112	ASN
14	O	90	ASN
14	O	131	HIS
14	O	133	GLN
14	O	153	GLN
14	O	246	GLN
15	P	77	GLN
15	P	196	HIS
15	P	228	GLN
16	Q	162	GLN
17	T	120	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1 (10%)	5,13,15	5.92	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.02	130.50	119.48
16	Q	118	2MR	CD-NE-CZ	3.77	130.47	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.57	131.76	123.86

There are no chirality outliers.

All (2) 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

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	1.10	2 (6%)	48,50,50	1.28	9 (18%)
21	NAI	A	503	-	45,48,48	3.90	19 (42%)	60,73,73	1.80	13 (21%)
19	SF4	A	501	1	0,12,12	-	-	-	-	-
25	CDL	I	201	-	50,50,99	1.40	8 (16%)	56,62,111	1.13	4 (7%)
28	FES	O	301	14	0,4,4	-	-	-	-	-
27	UQ	J	402	-	33,33,63	3.45	10 (30%)	40,43,79	2.72	14 (35%)
19	SF4	M	801	12	0,12,12	-	-	-	-	-
24	8Q1	E	201	-	31,34,34	1.70	6 (19%)	40,43,43	1.61	6 (15%)
28	FES	M	803	12	0,4,4	-	-	-	-	-
30	UQ1	Q	502	-	18,18,18	2.33	6 (33%)	22,25,25	1.59	4 (18%)
19	SF4	B	301	2	0,12,12	-	-	-	-	-
19	SF4	M	802	12	0,12,12	-	-	-	-	-
30	UQ1	Q	501	-	18,18,18	2.38	5 (27%)	22,25,25	1.95	6 (27%)
23	PLX	C	303	-	51,51,51	1.12	3 (5%)	55,59,59	0.59	1 (1%)
19	SF4	B	302	2	0,12,12	-	-	-	-	-
26	NDP	J	401	-	49,52,52	4.38	23 (46%)	66,80,80	2.15	13 (19%)
22	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.95	2 (4%)
19	SF4	C	301	3	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	-	-	9/18/18/18	0/3/3/3
21	NAI	A	503	-	-	6/29/72/72	0/5/5/5
25	CDL	I	201	-	-	30/61/61/110	-
19	SF4	A	501	1	-	-	0/6/5/5
28	FES	O	301	14	-	-	0/1/1/1
27	UQ	J	402	-	-	13/27/51/87	0/1/1/1
19	SF4	M	801	12	-	-	0/6/5/5
24	8Q1	E	201	-	-	12/41/41/41	-
30	UQ1	Q	502	-	-	2/9/33/33	0/1/1/1
28	FES	M	803	12	-	-	0/1/1/1
19	SF4	B	301	2	-	-	0/6/5/5
30	UQ1	Q	501	-	-	4/9/33/33	0/1/1/1
19	SF4	M	802	12	-	-	0/6/5/5
23	PLX	C	303	-	-	25/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	SF4	B	302	2	-	-	0/6/5/5
26	NDP	J	401	-	-	10/34/77/77	0/4/5/5
22	PEE	C	302	-	-	25/50/50/54	-
19	SF4	C	301	3	-	-	0/6/5/5

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	C3B-C2B	-12.78	1.24	1.52
26	J	401	NDP	C6N-C5N	12.40	1.55	1.33
26	J	401	NDP	O4D-C4D	10.75	1.69	1.45
21	A	503	NAI	C3D-C4D	-10.30	1.26	1.53
26	J	401	NDP	C3D-C4D	-9.78	1.28	1.53
27	J	402	UQ	C18-C19	9.61	1.56	1.33
27	J	402	UQ	C13-C14	9.14	1.54	1.33
21	A	503	NAI	O4B-C1B	9.11	1.63	1.42
27	J	402	UQ	C8-C9	9.03	1.54	1.33
21	A	503	NAI	O4B-C4B	-8.28	1.26	1.45
26	J	401	NDP	O4B-C4B	-7.85	1.27	1.45
27	J	402	UQ	C23-C24	7.82	1.54	1.32
21	A	503	NAI	C2D-C1D	-7.55	1.29	1.53
26	J	401	NDP	C2N-C3N	7.43	1.55	1.34
30	Q	501	UQ1	C8-C9	7.28	1.53	1.32
30	Q	502	UQ1	C8-C9	7.25	1.53	1.32
21	A	503	NAI	C2B-C1B	-7.18	1.30	1.53
21	A	503	NAI	O4D-C4D	6.91	1.60	1.45
21	A	503	NAI	C2D-C3D	5.96	1.69	1.53
26	J	401	NDP	C6A-N6A	5.88	1.48	1.34
21	A	503	NAI	C7N-N7N	5.75	1.48	1.33
26	J	401	NDP	P2B-O2B	5.61	1.69	1.59
26	J	401	NDP	C3B-C4B	5.48	1.67	1.53
21	A	503	NAI	O4D-C1D	5.42	1.54	1.42
24	E	201	8Q1	C34-N36	5.37	1.45	1.33
24	E	201	8Q1	C39-N41	5.29	1.45	1.33
21	A	503	NAI	C6A-N6A	5.18	1.47	1.34
21	A	503	NAI	C4N-C3N	-5.06	1.40	1.49
26	J	401	NDP	O4D-C1D	-4.87	1.30	1.42
26	J	401	NDP	C6N-N1N	4.83	1.49	1.37
26	J	401	NDP	O4B-C1B	4.57	1.52	1.42
21	A	503	NAI	O2B-C2B	4.56	1.53	1.43
26	J	401	NDP	C1B-N9A	-4.43	1.33	1.46
26	J	401	NDP	O2D-C2D	-4.26	1.32	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	C7N-N7N	4.21	1.44	1.33
21	A	503	NAI	C6N-C5N	4.06	1.40	1.33
20	A	502	FMN	C4A-N5	3.75	1.38	1.30
22	C	302	PEE	C18-C19	3.72	1.53	1.31
22	C	302	PEE	C39-C38	3.65	1.52	1.31
21	A	503	NAI	C7N-C3N	3.57	1.56	1.48
25	I	201	CDL	OA8-CA7	3.43	1.43	1.33
21	A	503	NAI	C4N-C5N	-3.26	1.40	1.48
26	J	401	NDP	O3D-C3D	3.11	1.50	1.43
26	J	401	NDP	C8A-N9A	-3.05	1.32	1.37
25	I	201	CDL	OB8-CB7	3.04	1.42	1.33
26	J	401	NDP	C7N-C3N	2.97	1.55	1.48
26	J	401	NDP	C5A-N7A	-2.93	1.33	1.39
25	I	201	CDL	OB6-CB5	2.91	1.42	1.34
25	I	201	CDL	OA6-CA5	2.91	1.42	1.34
27	J	402	UQ	C6-C1	2.80	1.54	1.46
30	Q	501	UQ1	C6-C1	2.79	1.54	1.46
23	C	303	PLX	O6-C4	-2.58	1.41	1.44
21	A	503	NAI	C8A-N9A	-2.57	1.32	1.37
21	A	503	NAI	O3B-C3B	-2.52	1.37	1.43
22	C	302	PEE	O2-C2	-2.48	1.40	1.46
24	E	201	8Q1	C1-S44	2.47	1.82	1.76
25	I	201	CDL	OA6-CA4	-2.42	1.40	1.46
20	A	502	FMN	C10-N1	2.41	1.38	1.33
22	C	302	PEE	O3-C30	2.41	1.40	1.33
26	J	401	NDP	O2B-C2B	2.39	1.52	1.44
27	J	402	UQ	C7-C8	2.37	1.54	1.50
21	A	503	NAI	PN-O5D	2.35	1.68	1.59
30	Q	502	UQ1	C6-C1	2.34	1.53	1.46
26	J	401	NDP	C2D-C3D	2.32	1.59	1.53
24	E	201	8Q1	O35-C34	-2.32	1.18	1.23
24	E	201	8Q1	O40-C39	-2.30	1.18	1.23
24	E	201	8Q1	C6-C1	2.29	1.53	1.50
23	C	303	PLX	C7-C6	2.25	1.55	1.50
30	Q	501	UQ1	O2-CM2	-2.24	1.40	1.45
22	C	302	PEE	O2-C10	2.23	1.40	1.34
21	A	503	NAI	C5B-C4B	2.23	1.58	1.51
25	I	201	CDL	OB6-CB4	-2.22	1.41	1.46
27	J	402	UQ	O4-C4	-2.18	1.18	1.23
25	I	201	CDL	PB2-OB2	2.17	1.68	1.59
25	I	201	CDL	PB2-OB5	2.17	1.68	1.59
26	J	401	NDP	PA-O5B	2.16	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	O7N-C7N	-2.15	1.19	1.24
22	C	302	PEE	O3-C3	-2.15	1.40	1.45
30	Q	502	UQ1	O3-CM3	-2.14	1.40	1.45
30	Q	501	UQ1	O4-C4	-2.13	1.18	1.23
30	Q	502	UQ1	O2-CM2	-2.13	1.40	1.45
30	Q	501	UQ1	O1-C1	-2.13	1.18	1.23
27	J	402	UQ	C21-C19	2.12	1.55	1.51
30	Q	502	UQ1	O1-C1	-2.11	1.18	1.23
30	Q	502	UQ1	O4-C4	-2.09	1.18	1.23
23	C	303	PLX	P1-O4	2.06	1.67	1.59
27	J	402	UQ	O1-C1	-2.05	1.18	1.23
27	J	402	UQ	O3-CM3	-2.00	1.40	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	401	NDP	C3N-C2N-N1N	-7.99	111.69	123.10
27	J	402	UQ	C7-C8-C9	-7.64	114.07	126.79
26	J	401	NDP	C1D-N1N-C2N	-6.37	110.50	121.11
24	E	201	8Q1	C6-C1-S44	6.35	120.85	113.46
27	J	402	UQ	C12-C13-C14	-6.18	112.78	127.66
26	J	401	NDP	C5A-C4A-N3A	-5.85	119.12	126.75
21	A	503	NAI	C5A-C4A-N3A	-5.80	119.18	126.75
27	J	402	UQ	C17-C18-C19	-5.77	113.77	127.66
26	J	401	NDP	C1D-N1N-C6N	-5.22	109.58	120.83
30	Q	501	UQ1	C7-C6-C1	5.13	124.65	118.48
27	J	402	UQ	C20-C19-C18	-4.52	112.09	123.68
27	J	402	UQ	C22-C23-C24	-4.48	112.43	127.75
27	J	402	UQ	C10-C9-C8	-4.36	112.49	123.68
30	Q	502	UQ1	C7-C8-C9	-4.35	113.64	127.26
21	A	503	NAI	N3A-C2A-N1A	-4.30	121.88	128.60
27	J	402	UQ	C15-C14-C13	-4.14	113.07	123.68
26	J	401	NDP	N3A-C4A-N9A	4.10	133.83	127.08
21	A	503	NAI	N3A-C4A-N9A	4.09	133.83	127.08
27	J	402	UQ	C16-C14-C13	-4.08	112.85	121.12
26	J	401	NDP	N3A-C2A-N1A	-4.08	122.23	128.60
25	I	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
30	Q	501	UQ1	C7-C8-C9	-3.93	114.94	127.26
21	A	503	NAI	C2A-N3A-C4A	3.87	120.89	111.75
27	J	402	UQ	C21-C19-C18	-3.83	113.36	121.12
25	I	201	CDL	OA6-CA5-C11	3.82	119.74	111.50
22	C	302	PEE	O2-C10-C11	3.77	119.62	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	E	201	8Q1	O4-C1-C6	-3.76	119.55	123.99
21	A	503	NAI	C5A-N7A-C8A	3.76	108.84	103.51
26	J	401	NDP	C2A-N3A-C4A	3.75	120.62	111.75
27	J	402	UQ	C11-C9-C8	-3.52	114.00	121.12
21	A	503	NAI	N9A-C8A-N7A	-3.47	109.17	113.91
30	Q	502	UQ1	C10-C9-C8	-3.46	112.64	122.65
26	J	401	NDP	C5A-N7A-C8A	3.35	108.27	103.51
27	J	402	UQ	C26-C24-C23	-3.32	113.06	122.65
30	Q	501	UQ1	C10-C9-C8	-3.29	113.13	122.65
26	J	401	NDP	N9A-C8A-N7A	-3.25	109.47	113.91
20	A	502	FMN	C4-N3-C2	-3.23	119.67	125.64
21	A	503	NAI	C4A-C5A-N7A	-3.23	106.69	110.62
27	J	402	UQ	C25-C24-C23	-3.22	113.34	122.65
30	Q	502	UQ1	C11-C9-C8	-3.21	113.37	122.65
24	E	201	8Q1	C37-C38-C39	3.20	117.68	112.36
21	A	503	NAI	C3D-C2D-C1D	3.10	107.32	101.43
26	J	401	NDP	C4A-C5A-N7A	-3.05	106.91	110.62
21	A	503	NAI	C4D-O4D-C1D	-2.96	102.95	109.47
20	A	502	FMN	C4A-C4-N3	2.80	120.29	113.19
30	Q	501	UQ1	C11-C9-C8	-2.76	114.67	122.65
25	I	201	CDL	OB8-CB7-C71	2.72	120.45	111.91
25	I	201	CDL	OA8-CA7-C31	2.70	120.39	111.91
21	A	503	NAI	C2D-C3D-C4D	2.59	107.68	102.64
20	A	502	FMN	O4-C4-C4A	-2.58	119.75	126.60
27	J	402	UQ	CM5-C5-C6	-2.57	120.21	124.40
22	C	302	PEE	O3-C30-C31	2.52	119.82	111.91
21	A	503	NAI	PN-O3-PA	-2.48	124.32	132.83
26	J	401	NDP	PN-O3-PA	-2.46	124.37	132.83
20	A	502	FMN	C4A-C10-N1	-2.45	119.04	124.73
21	A	503	NAI	C4A-N9A-C8A	2.39	108.31	105.73
26	J	401	NDP	C4A-N9A-C8A	2.38	108.31	105.73
24	E	201	8Q1	C43-S44-C1	2.33	109.12	101.87
24	E	201	8Q1	O4-C1-S44	-2.32	119.60	122.61
20	A	502	FMN	C4A-C10-N10	2.31	119.86	116.48
24	E	201	8Q1	C38-C39-N41	2.30	120.29	116.42
30	Q	501	UQ1	CM5-C5-C6	-2.28	120.68	124.40
20	A	502	FMN	C9A-C5A-N5	-2.28	119.96	122.43
26	J	401	NDP	C2B-C3B-C4B	2.24	106.86	101.99
30	Q	502	UQ1	CM5-C5-C6	-2.19	120.82	124.40
23	C	303	PLX	C1A-N1-C1	2.19	118.87	109.92
20	A	502	FMN	C10-C4A-N5	-2.17	120.26	124.86
20	A	502	FMN	C5A-C9A-N10	2.16	120.19	117.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	501	UQ1	C6-C5-C4	2.15	120.88	119.18
27	J	402	UQ	C7-C6-C1	2.08	120.98	118.48
21	A	503	NAI	C3B-C2B-C1B	2.04	105.31	101.43
20	A	502	FMN	C10-N1-C2	2.02	120.94	116.90

There are no chirality outliers.

All (136) 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'
20	A	502	FMN	C5'-O5'-P-O1P
22	C	302	PEE	C4-O4P-P-O1P
23	C	303	PLX	O7-C6-C7-C8
23	C	303	PLX	O6-C4-C5-O8
23	C	303	PLX	O9-C24-O8-C5
24	E	201	8Q1	O27-C28-C29-C32
24	E	201	8Q1	C28-C29-C32-C34
24	E	201	8Q1	C28-C29-C32-O33
24	E	201	8Q1	C30-C29-C32-C34
24	E	201	8Q1	C30-C29-C32-O33
24	E	201	8Q1	C31-C29-C32-C34
24	E	201	8Q1	C31-C29-C32-O33
24	E	201	8Q1	C28-O27-P24-O3
24	E	201	8Q1	C28-O27-P24-O2
24	E	201	8Q1	C28-O27-P24-O1
25	I	201	CDL	CA2-OA2-PA1-OA4
25	I	201	CDL	CB2-OB2-PB2-OB3
25	I	201	CDL	CB2-OB2-PB2-OB4
25	I	201	CDL	CB3-OB5-PB2-OB3
26	J	401	NDP	C5B-O5B-PA-O1A
26	J	401	NDP	C5B-O5B-PA-O3
26	J	401	NDP	O4B-C4B-C5B-O5B
27	J	402	UQ	C7-C8-C9-C10
27	J	402	UQ	C12-C13-C14-C15
27	J	402	UQ	C15-C14-C16-C17
27	J	402	UQ	C17-C18-C19-C20
27	J	402	UQ	C18-C19-C21-C22
27	J	402	UQ	C20-C19-C21-C22
30	Q	501	UQ1	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	Q	501	UQ1	C5-C6-C7-C8
30	Q	501	UQ1	C7-C8-C9-C10
25	I	201	CDL	O1-C1-CA2-OA2
21	A	503	NAI	C3D-C4D-C5D-O5D
27	J	402	UQ	C22-C23-C24-C26
27	J	402	UQ	C12-C11-C9-C8
23	C	303	PLX	C25-C26-C27-C28
25	I	201	CDL	OA5-CA3-CA4-OA6
25	I	201	CDL	CA7-C31-C32-C33
23	C	303	PLX	C27-C28-C29-C30
30	Q	502	UQ1	C7-C8-C9-C11
22	C	302	PEE	C10-C11-C12-C13
27	J	402	UQ	C14-C16-C17-C18
22	C	302	PEE	C4-O4P-P-O3P
25	I	201	CDL	CA2-OA2-PA1-OA5
25	I	201	CDL	CB2-OB2-PB2-OB5
25	I	201	CDL	CB3-OB5-PB2-OB2
26	J	401	NDP	C2D-C1D-N1N-C6N
25	I	201	CDL	CB2-C1-CA2-OA2
23	C	303	PLX	O6-C6-C7-C8
23	C	303	PLX	C10-C11-C12-C13
22	C	302	PEE	C11-C12-C13-C14
23	C	303	PLX	C28-C29-C30-C31
23	C	303	PLX	C11-C10-C9-C8
23	C	303	PLX	C33-C34-C35-C36
30	Q	502	UQ1	C7-C8-C9-C10
22	C	302	PEE	C34-C35-C36-C37
23	C	303	PLX	C9-C10-C11-C12
22	C	302	PEE	C31-C30-O3-C3
23	C	303	PLX	C11-C12-C13-C14
25	I	201	CDL	C51-CB5-OB6-CB4
22	C	302	PEE	C15-C16-C17-C18
25	I	201	CDL	OB7-CB5-OB6-CB4
22	C	302	PEE	O5-C30-O3-C3
22	C	302	PEE	O4-C10-O2-C2
25	I	201	CDL	C31-CA7-OA8-CA6
22	C	302	PEE	C11-C10-O2-C2
23	C	303	PLX	C16-C17-C18-C19
23	C	303	PLX	C14-C15-C16-C17
21	A	503	NAI	O4D-C4D-C5D-O5D
25	I	201	CDL	OA5-CA3-CA4-CA6
25	I	201	CDL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	C	302	PEE	C1-C2-C3-O3
23	C	303	PLX	C3-C4-C5-O8
27	J	402	UQ	C5-C6-C7-C8
22	C	302	PEE	C12-C13-C14-C15
22	C	302	PEE	C19-C20-C21-C22
25	I	201	CDL	OA9-CA7-OA8-CA6
24	E	201	8Q1	O27-C28-C29-C30
24	E	201	8Q1	O27-C28-C29-C31
27	J	402	UQ	C1-C6-C7-C8
22	C	302	PEE	C42-C43-C44-C45
22	C	302	PEE	C32-C33-C34-C35
23	C	303	PLX	C7-C8-C9-C10
23	C	303	PLX	C31-C32-C33-C34
22	C	302	PEE	C44-C45-C46-C47
22	C	302	PEE	O2-C2-C3-O3
25	I	201	CDL	C51-C52-C53-C54
25	I	201	CDL	OB5-CB3-CB4-CB6
20	A	502	FMN	C5'-O5'-P-O2P
27	J	402	UQ	C12-C11-C9-C10
26	J	401	NDP	PN-O3-PA-O1A
26	J	401	NDP	O4D-C1D-N1N-C6N
22	C	302	PEE	C4-O4P-P-O2P
25	I	201	CDL	CB3-OB5-PB2-OB4
30	Q	501	UQ1	C6-C7-C8-C9
20	A	502	FMN	C1'-C2'-C3'-O3'
23	C	303	PLX	C25-C24-O8-C5
25	I	201	CDL	OB5-CB3-CB4-OB6
23	C	303	PLX	N1-C1-C2-O1
20	A	502	FMN	O2'-C2'-C3'-C4'
23	C	303	PLX	C13-C14-C15-C16
23	C	303	PLX	C26-C27-C28-C29
23	C	303	PLX	C15-C16-C17-C18
23	C	303	PLX	C3-O4-P1-O1
25	I	201	CDL	CA3-CA4-CA6-OA8
21	A	503	NAI	O4D-C1D-N1N-C2N
22	C	302	PEE	C16-C17-C18-C19
21	A	503	NAI	C2D-C1D-N1N-C2N
22	C	302	PEE	C41-C42-C43-C44
25	I	201	CDL	CB7-C71-C72-C73
25	I	201	CDL	C52-C53-C54-C55
22	C	302	PEE	C36-C37-C38-C39
27	J	402	UQ	C17-C18-C19-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	C	302	PEE	C33-C34-C35-C36
26	J	401	NDP	O4D-C4D-C5D-O5D
20	A	502	FMN	O2'-C2'-C3'-O3'
22	C	302	PEE	C13-C14-C15-C16
25	I	201	CDL	C12-C11-CA5-OA6
25	I	201	CDL	C72-C71-CB7-OB8
21	A	503	NAI	C5D-O5D-PN-O3
23	C	303	PLX	O9-C24-C25-C26
26	J	401	NDP	C2B-O2B-P2B-O2X
25	I	201	CDL	C52-C51-CB5-OB6
25	I	201	CDL	C72-C71-CB7-OB9
25	I	201	CDL	C12-C11-CA5-OA7
23	C	303	PLX	C2-O1-P1-O3
26	J	401	NDP	C2N-C3N-C7N-N7N
26	J	401	NDP	C3D-C4D-C5D-O5D
25	I	201	CDL	C52-C51-CB5-OB7
22	C	302	PEE	O3-C30-C31-C32
22	C	302	PEE	O5-C30-C31-C32
21	A	503	NAI	C2D-C1D-N1N-C6N

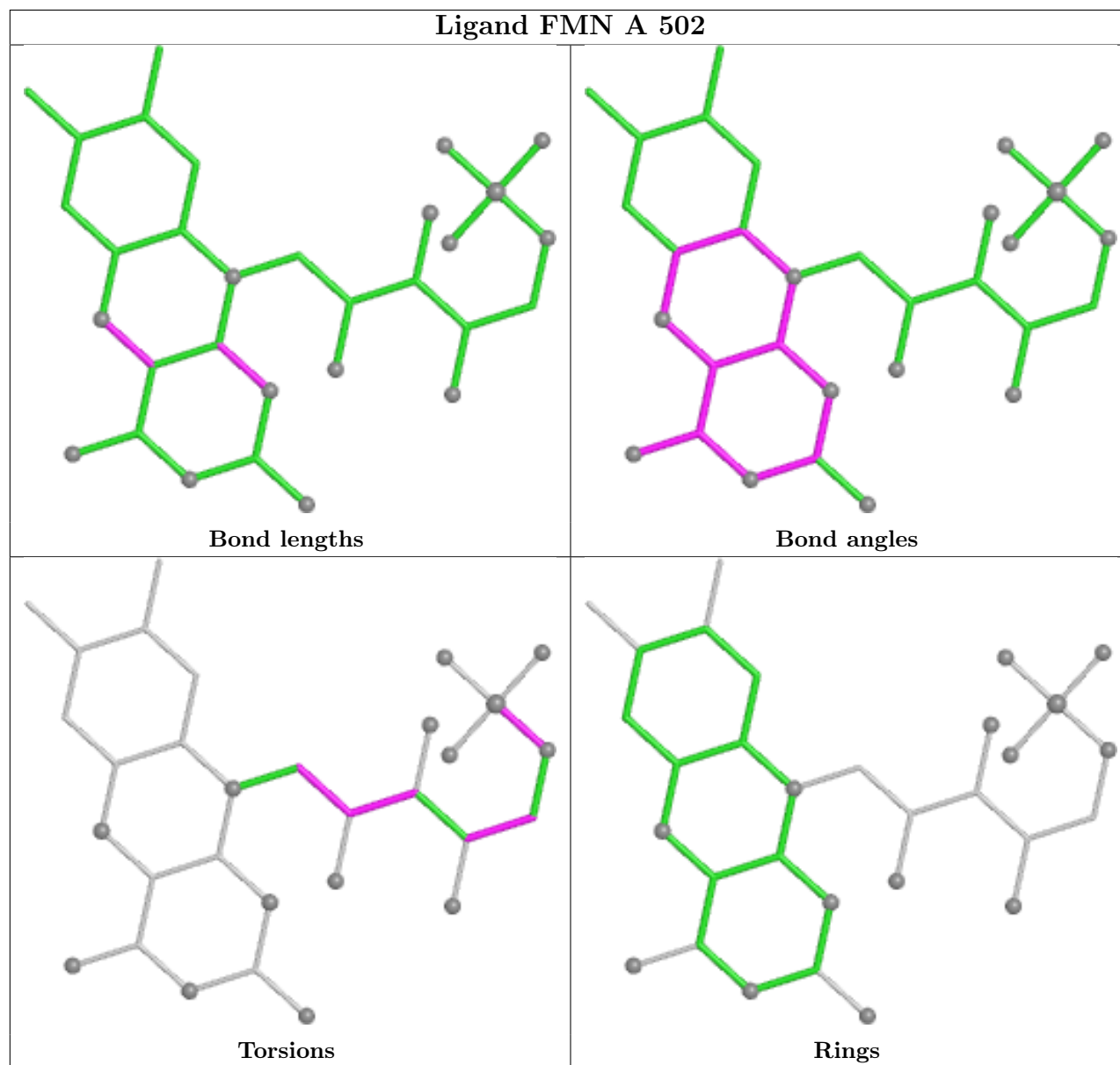
There are no ring outliers.

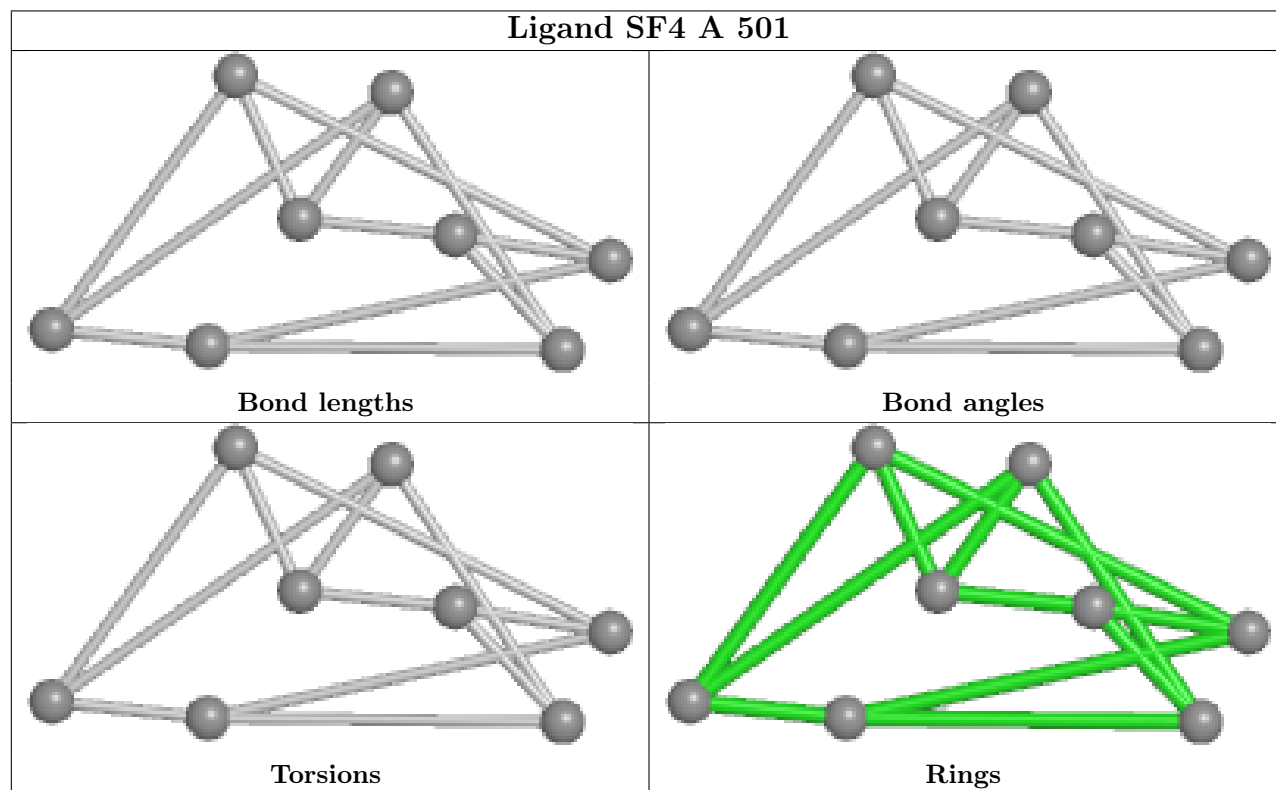
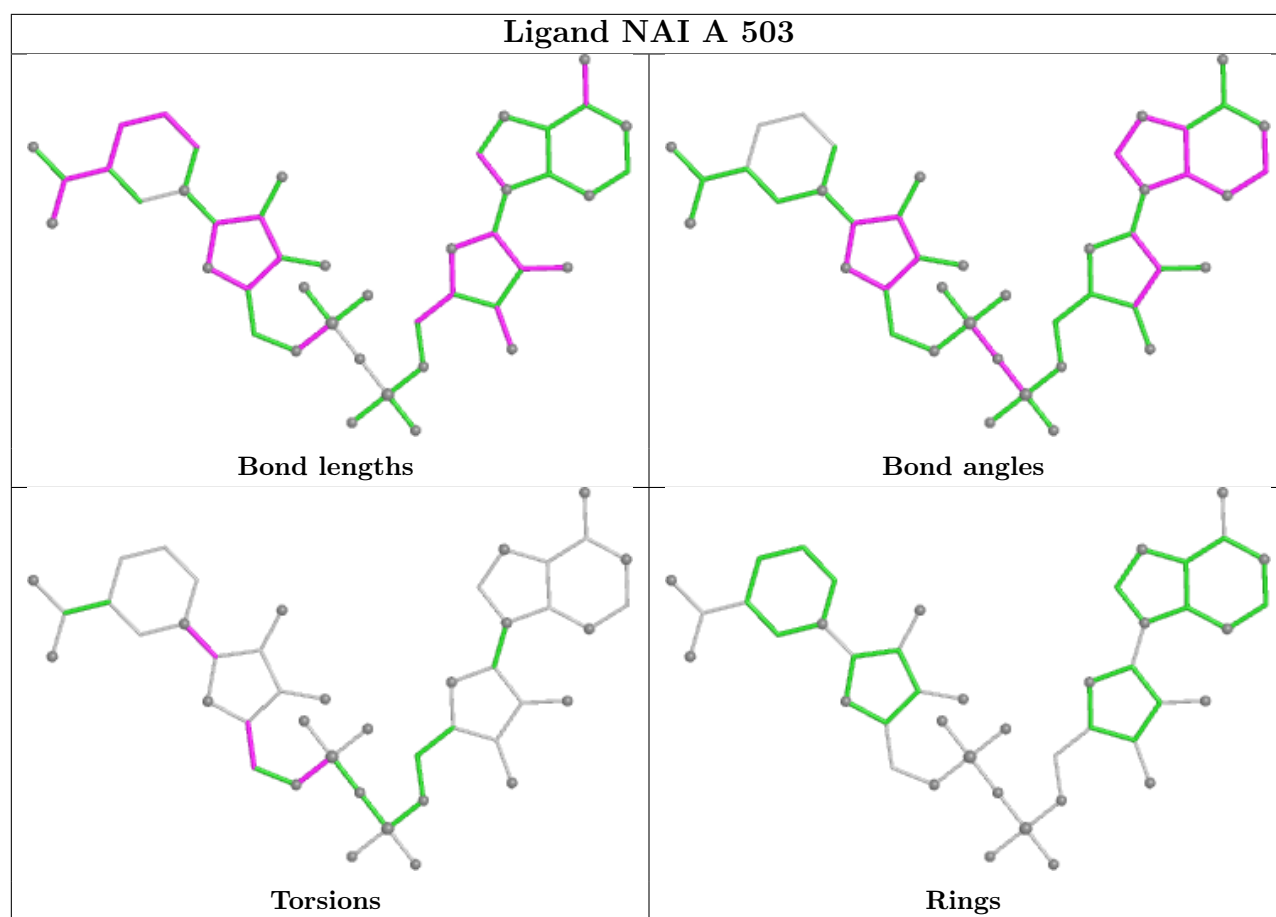
12 monomers are involved in 29 short contacts:

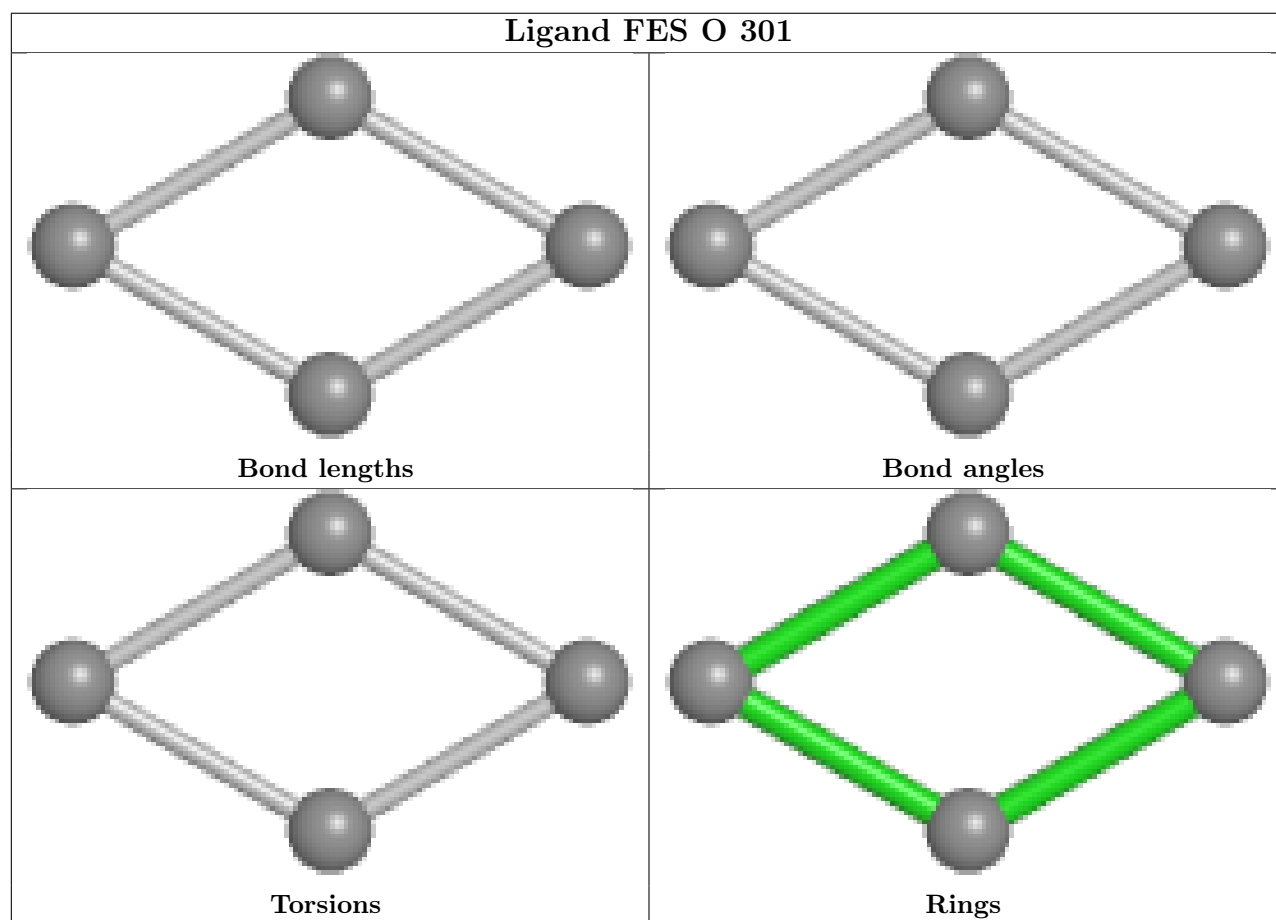
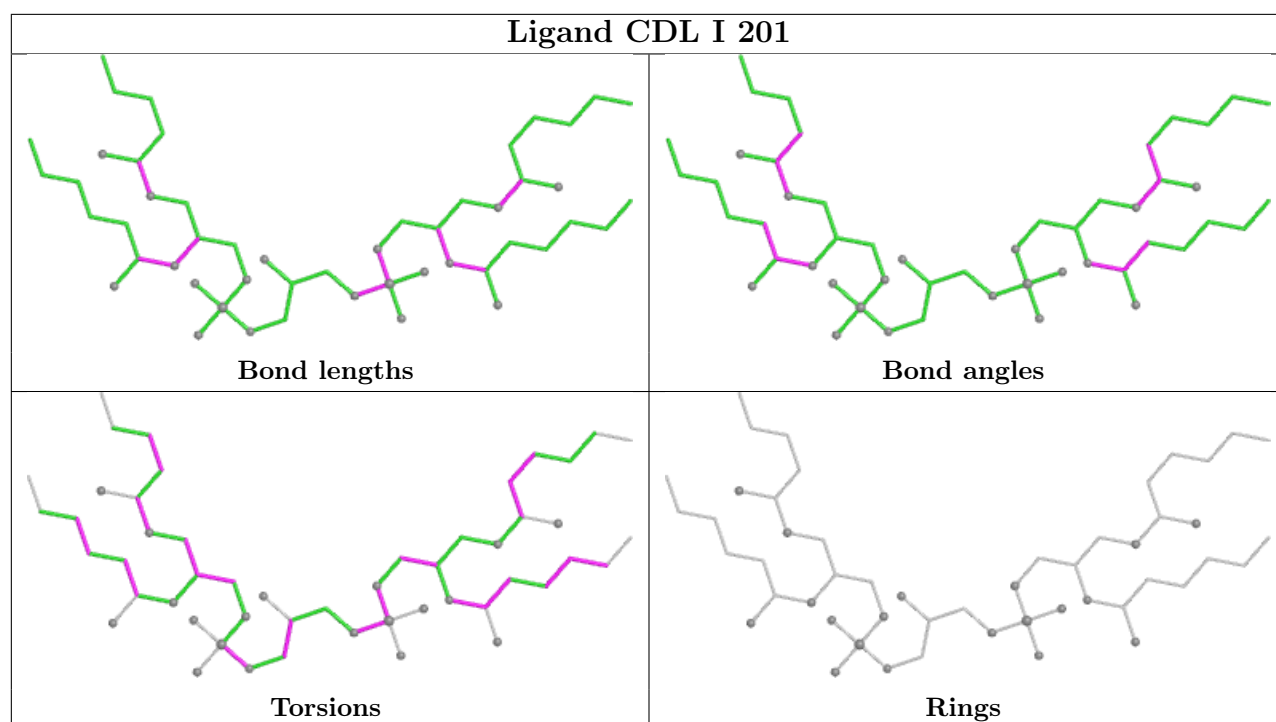
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	502	FMN	4	0
21	A	503	NAI	5	0
19	A	501	SF4	2	0
25	I	201	CDL	1	0
27	J	402	UQ	2	0
24	E	201	8Q1	4	0
30	Q	502	UQ1	1	0
30	Q	501	UQ1	1	0
23	C	303	PLX	3	0
26	J	401	NDP	2	0
22	C	302	PEE	4	0
19	C	301	SF4	1	0

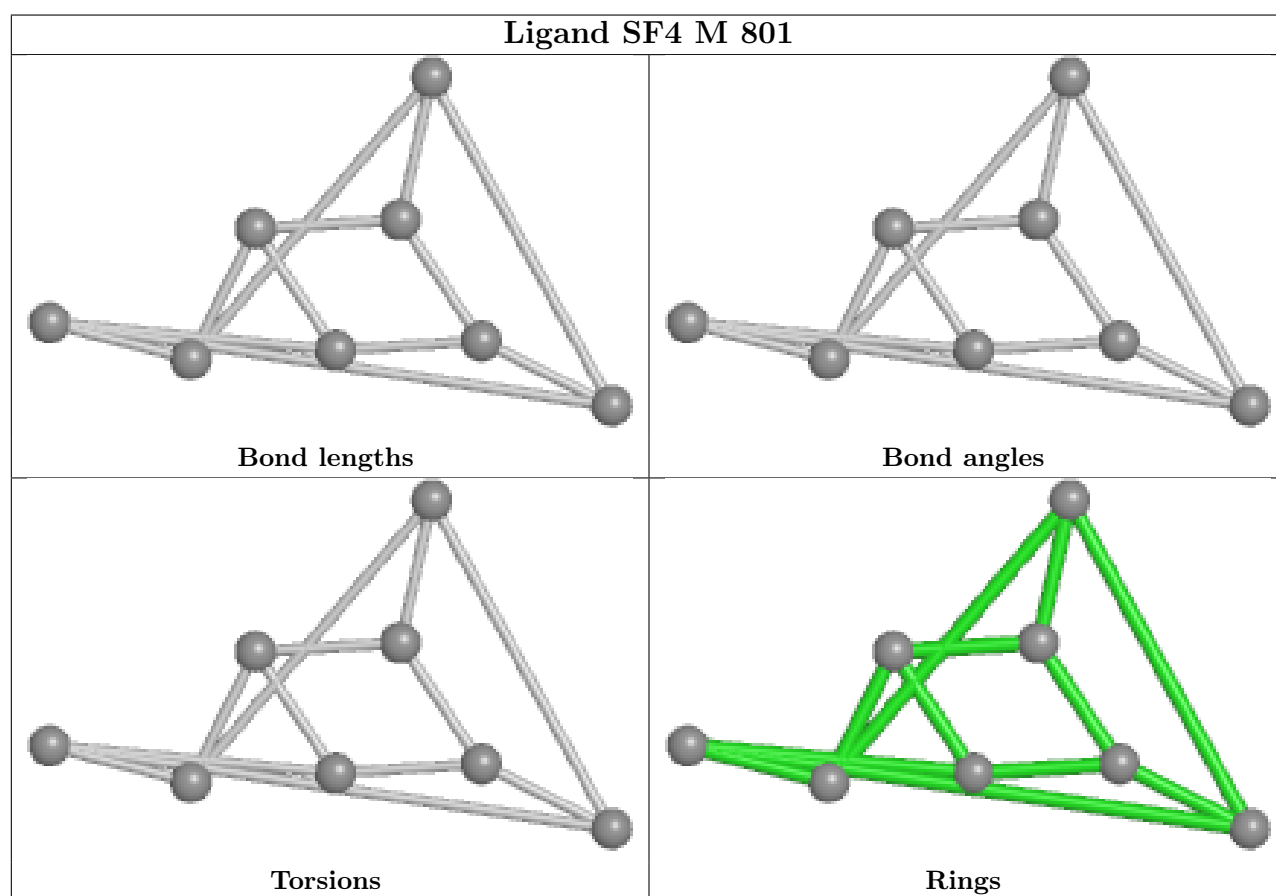
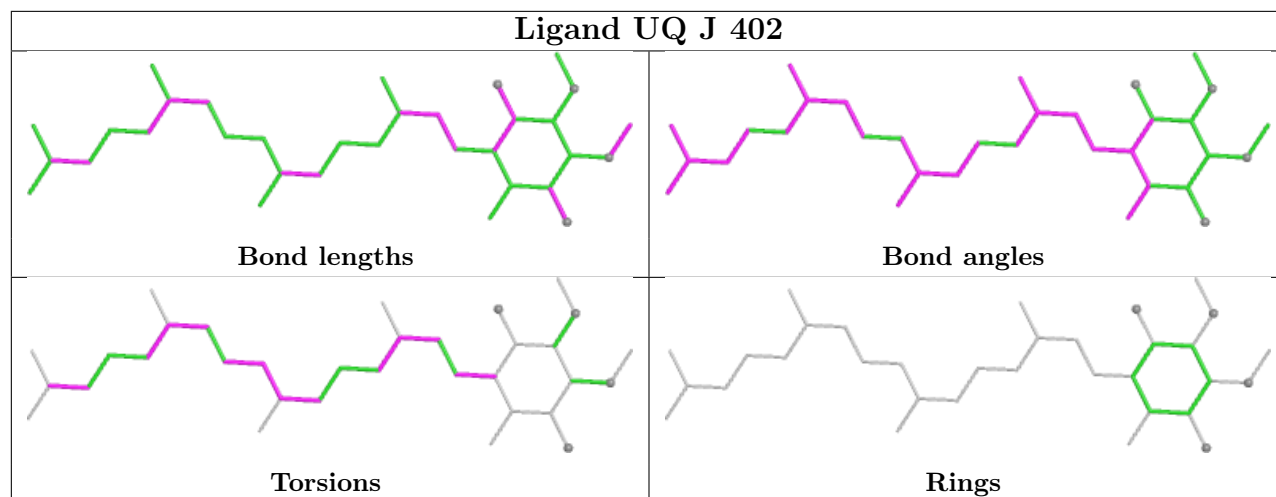
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

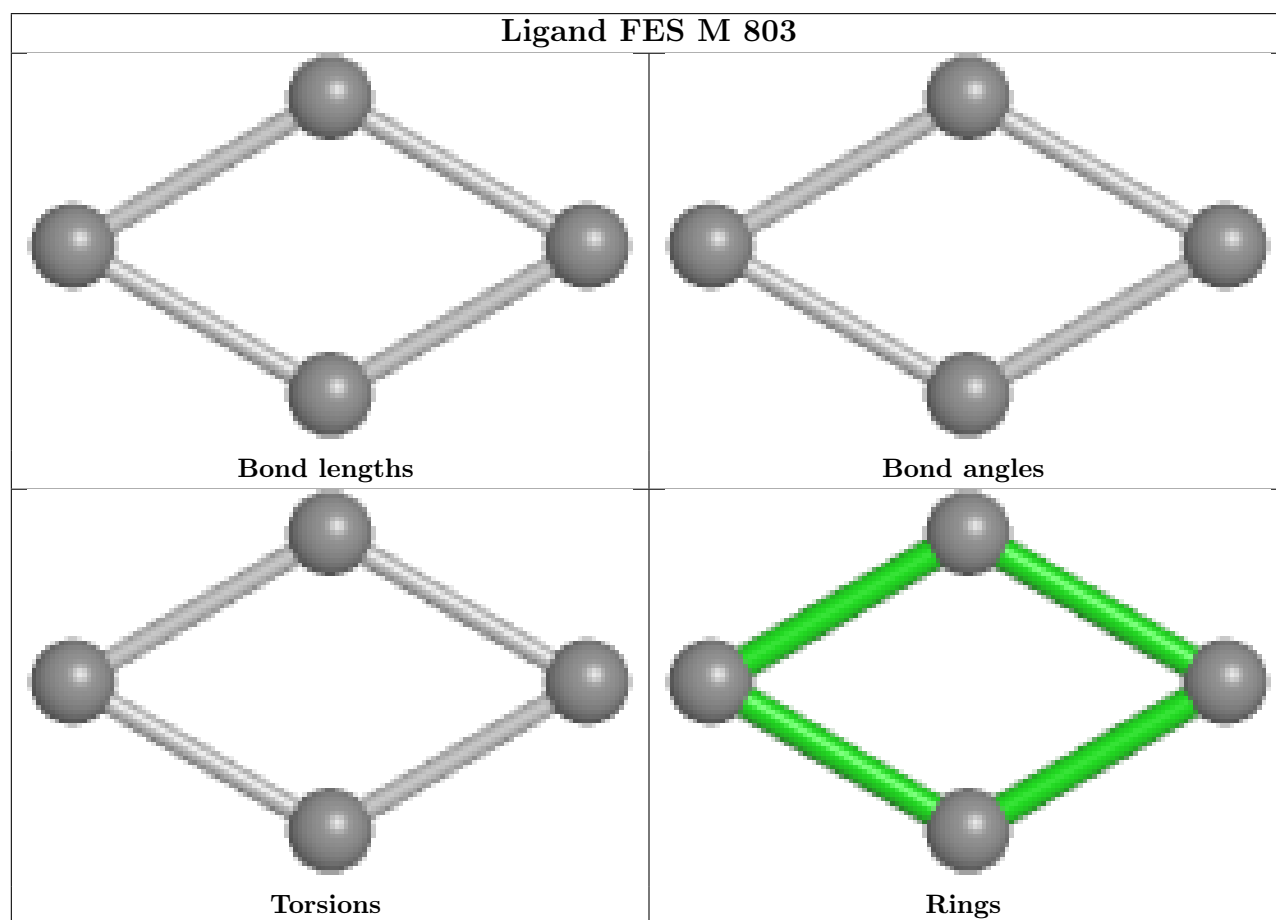
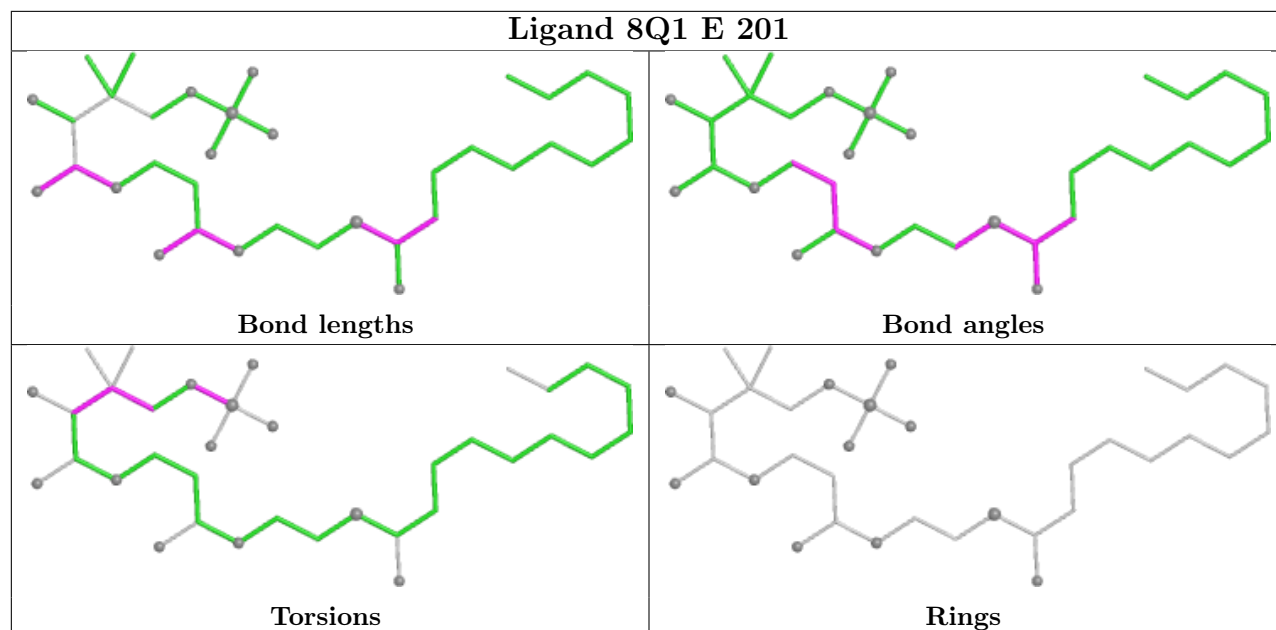
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

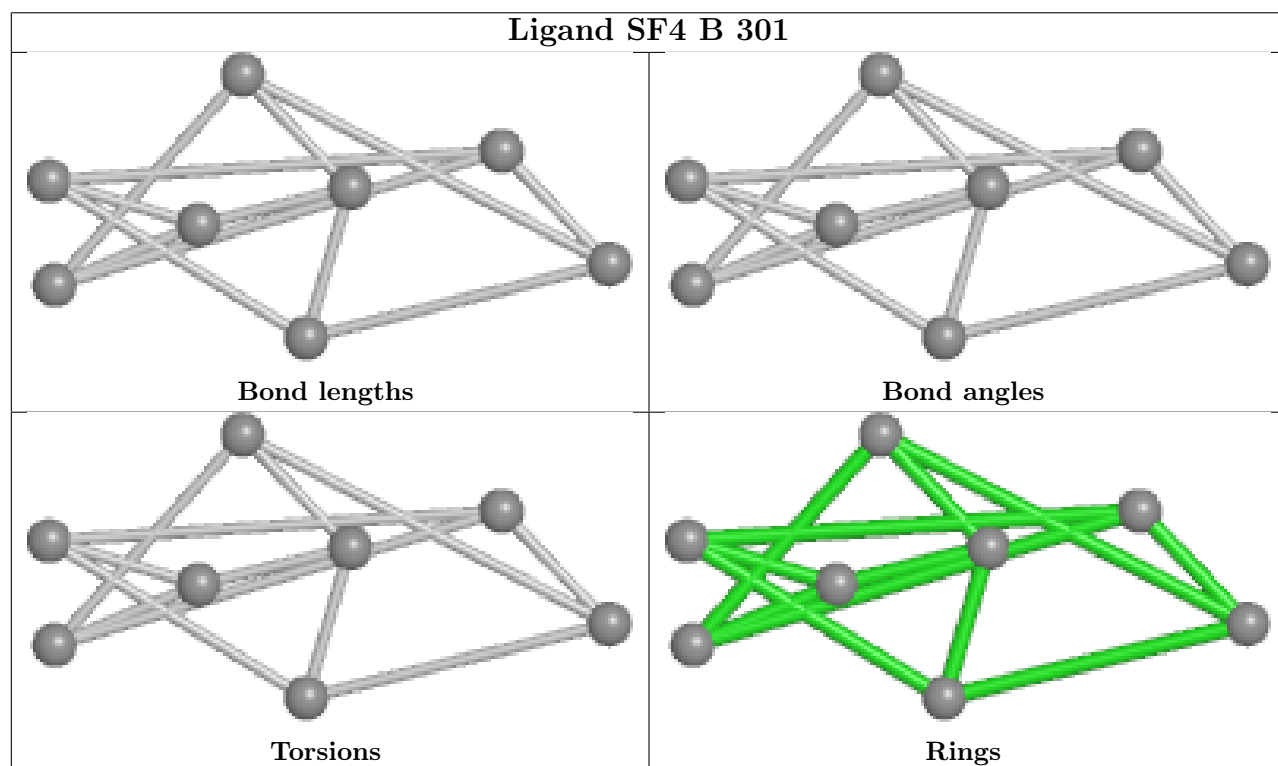
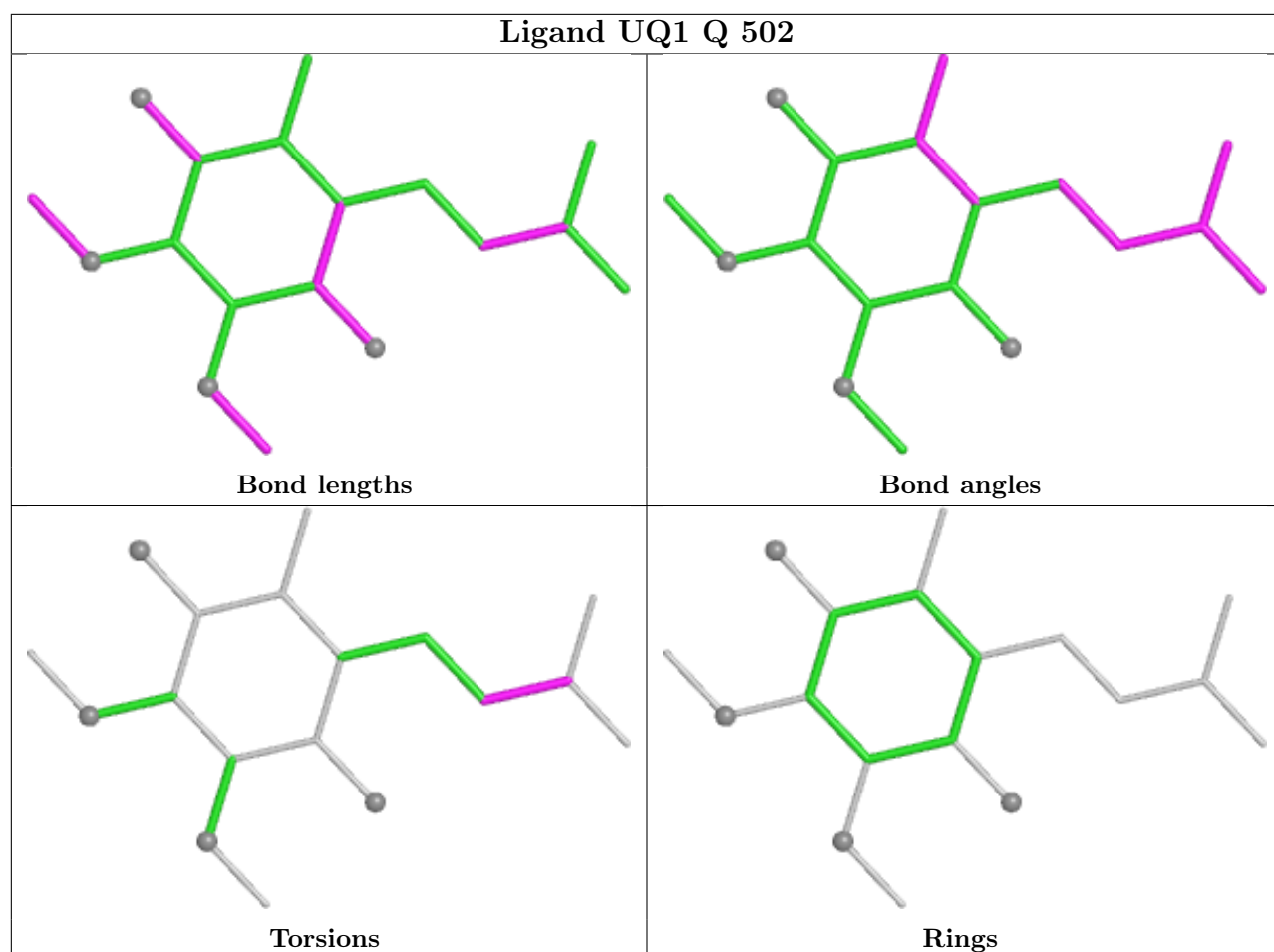


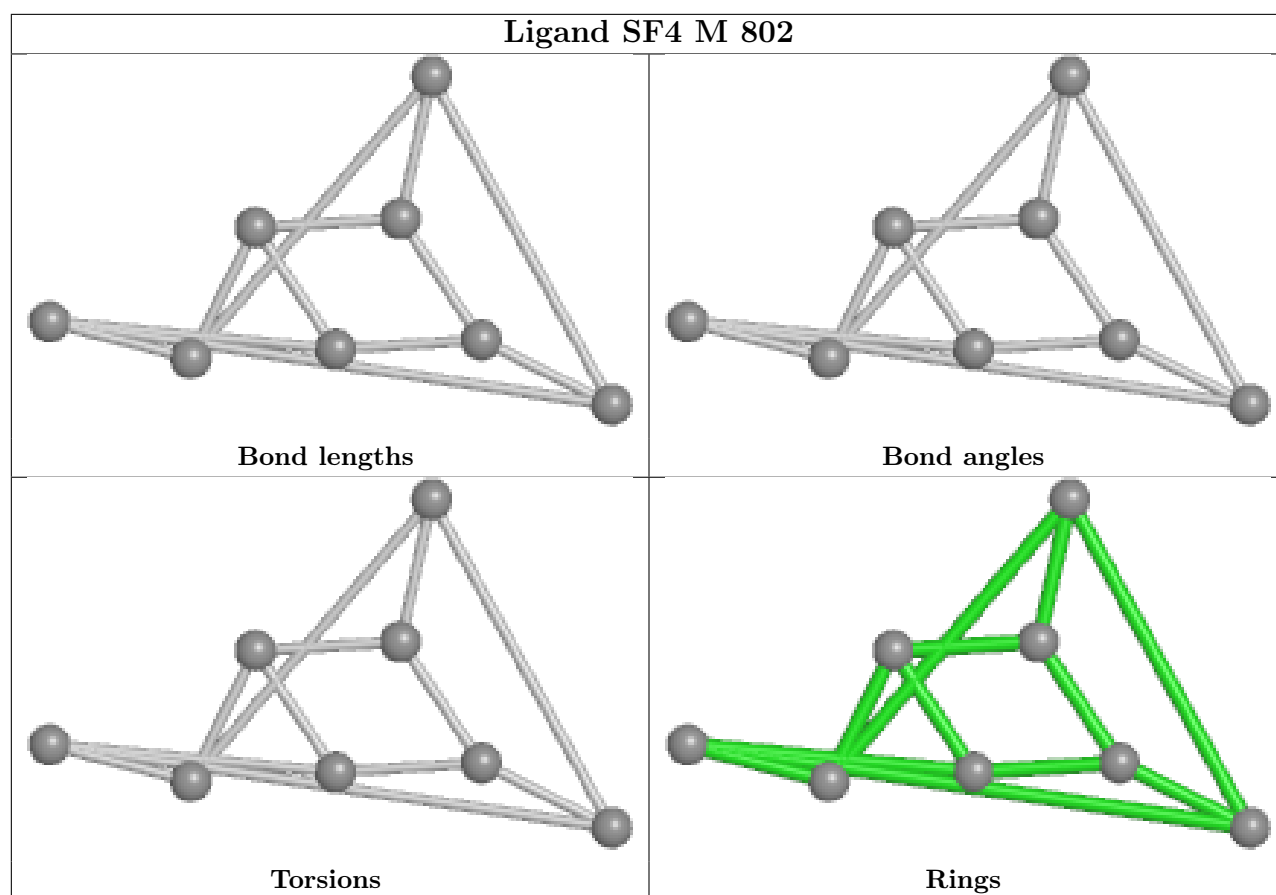


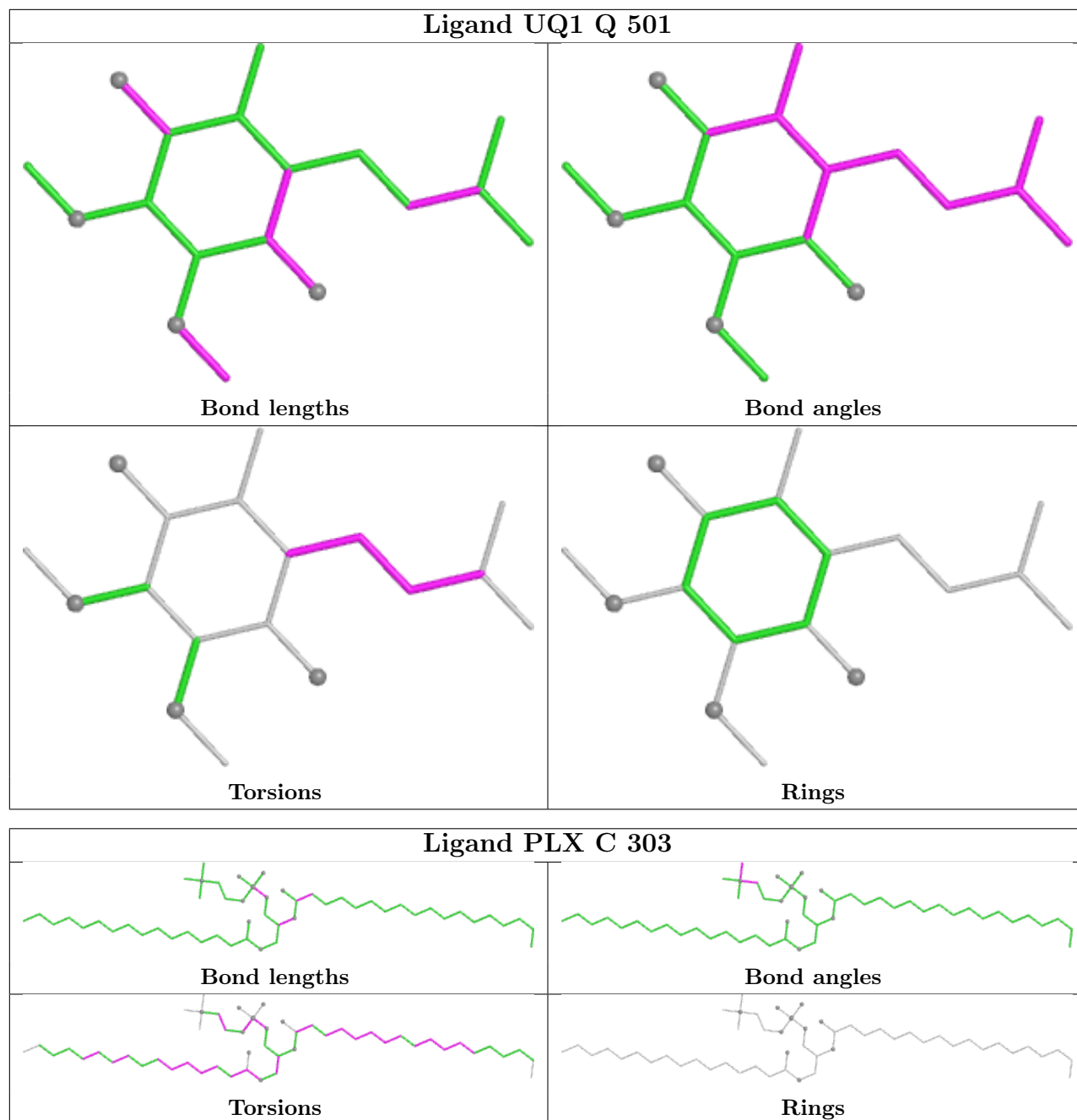


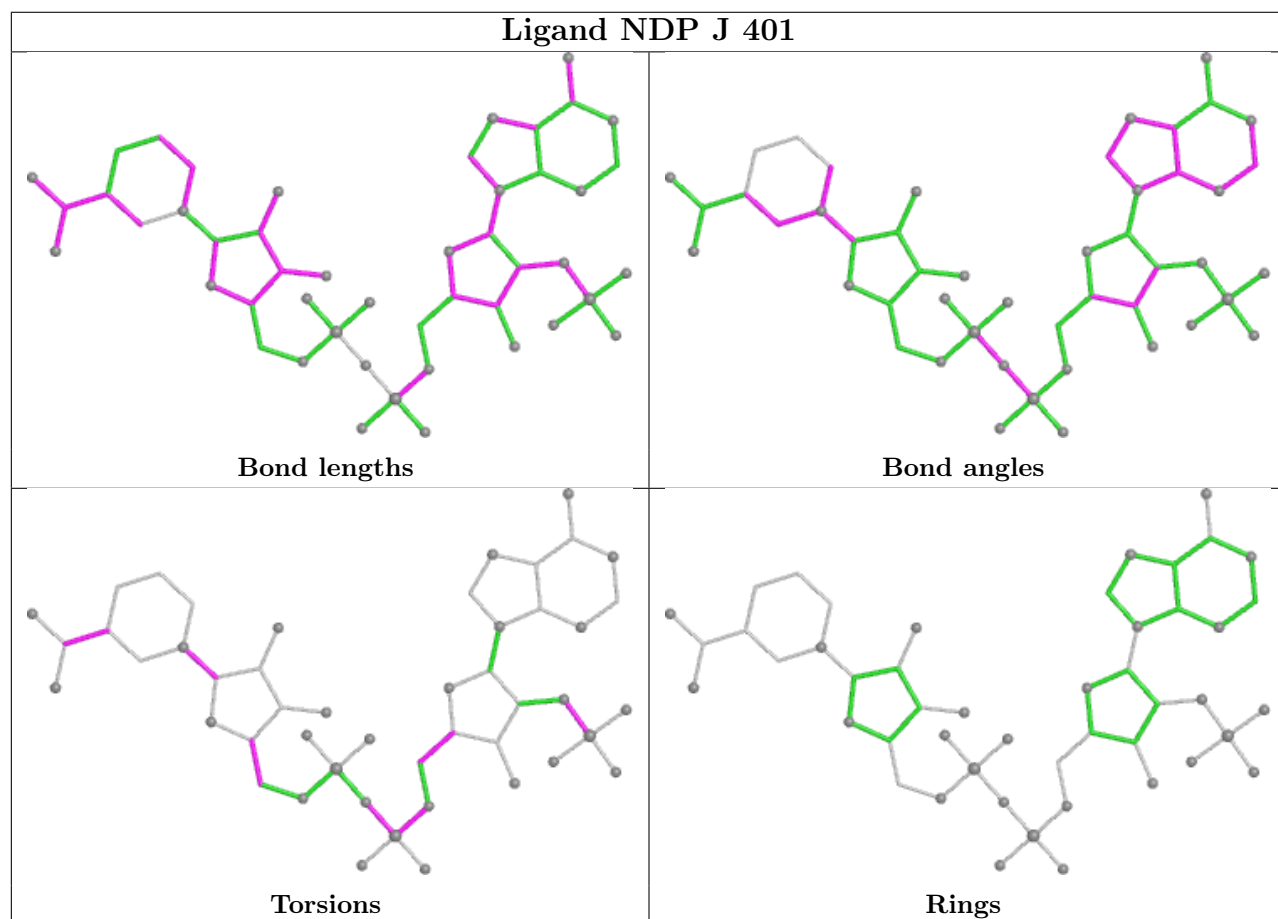
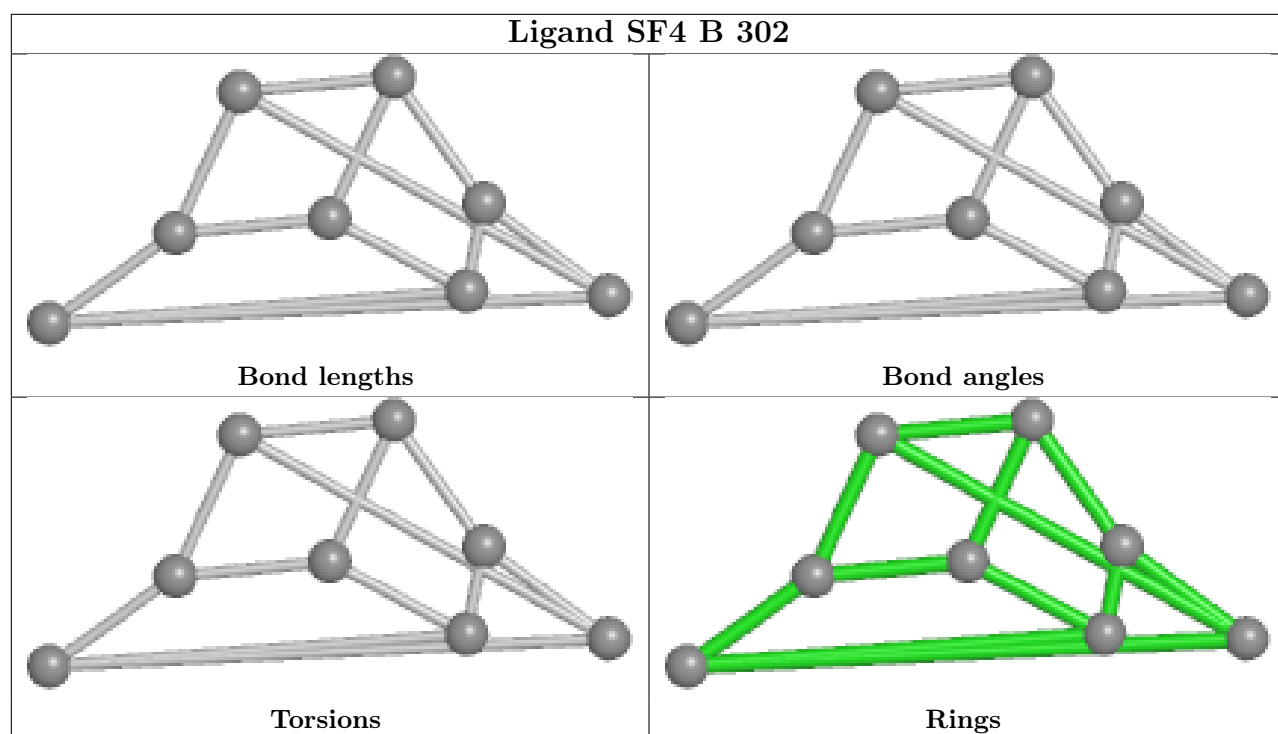


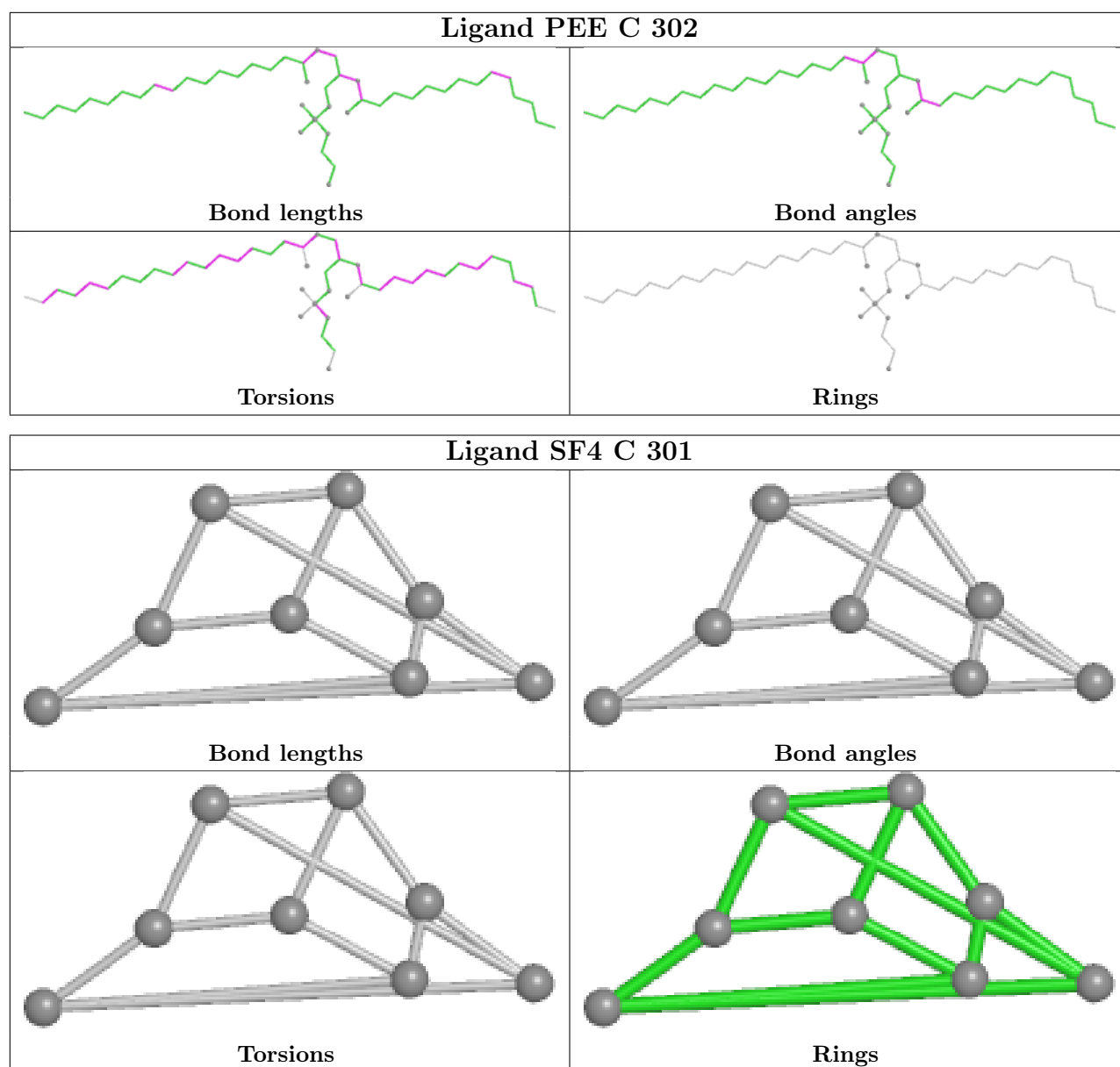












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

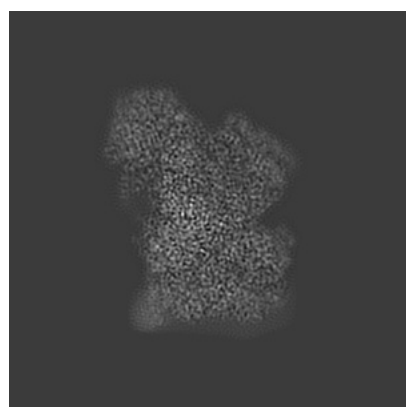
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32210. These allow visual inspection of the internal detail of the map and identification of artifacts.

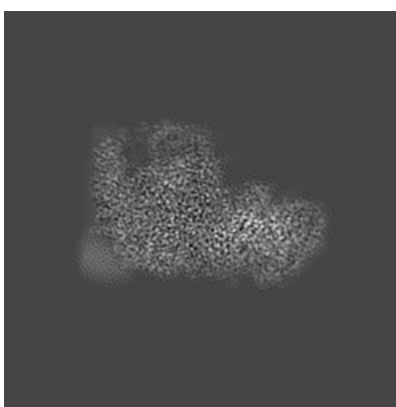
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

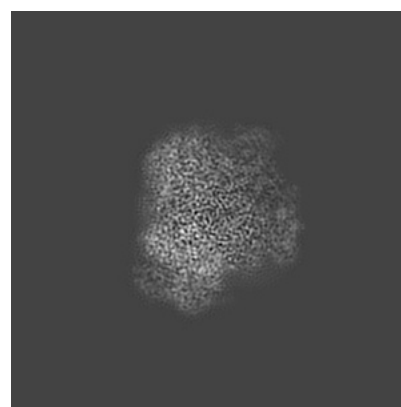
6.1.1 Primary map



X



Y

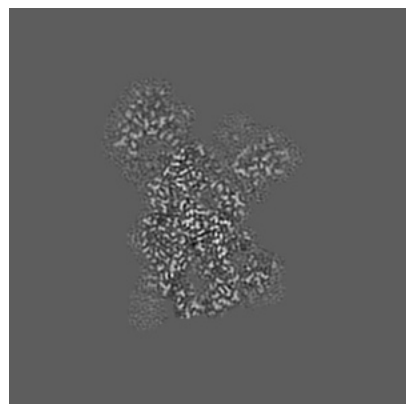


Z

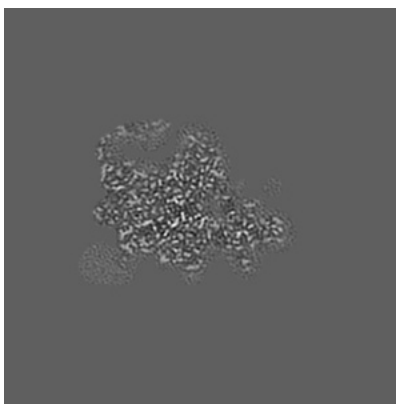
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

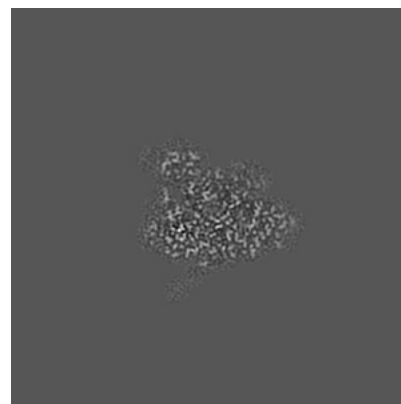
6.2.1 Primary map



X Index: 240



Y Index: 240

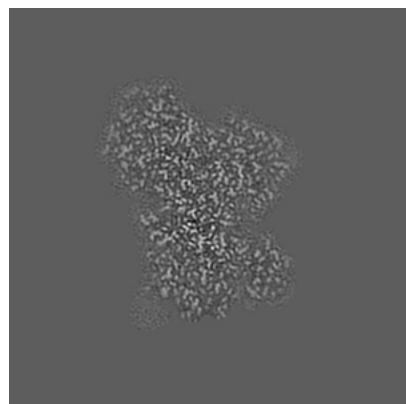


Z Index: 240

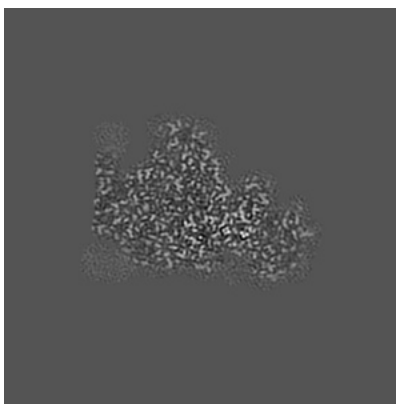
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

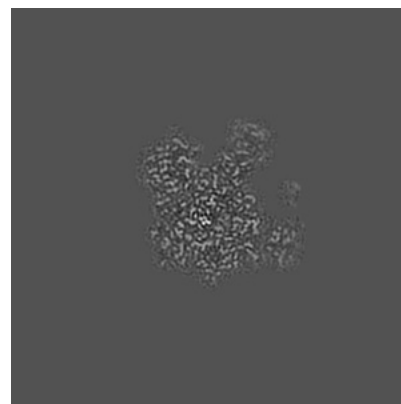
6.3.1 Primary map



X Index: 222



Y Index: 210

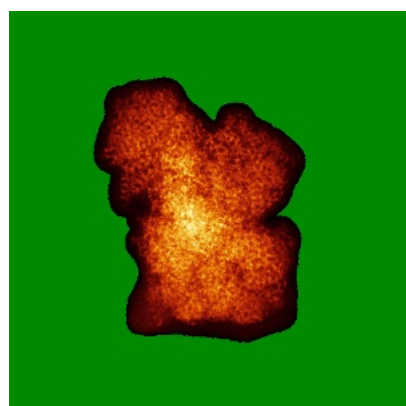


Z Index: 200

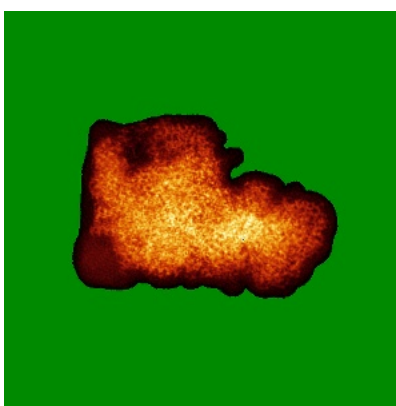
The images above show the largest variance slices of the map in three orthogonal directions.

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

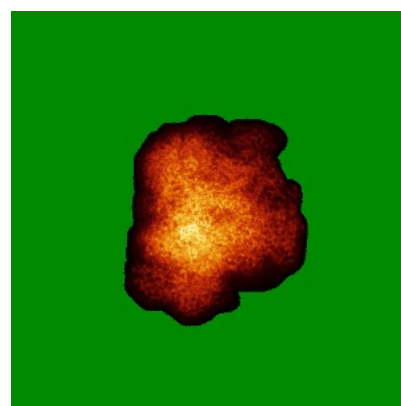
6.4.1 Primary map



X



Y

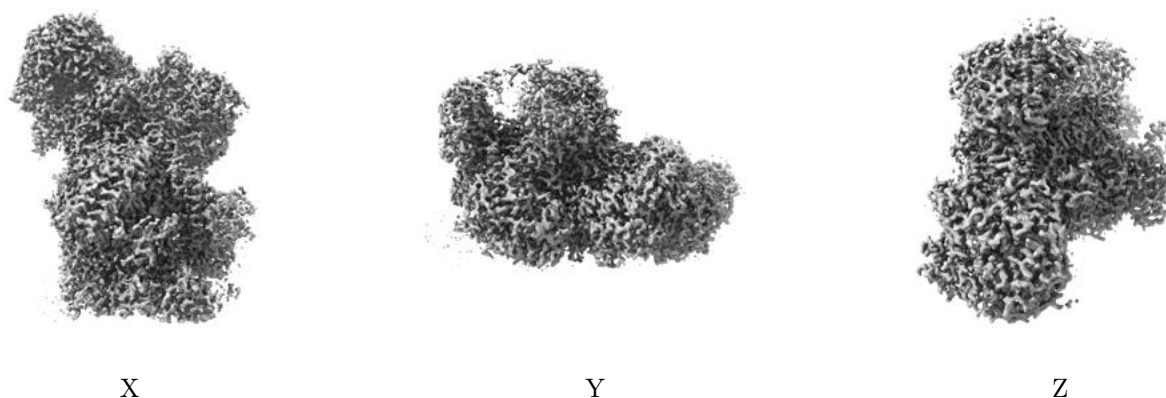


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0162. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

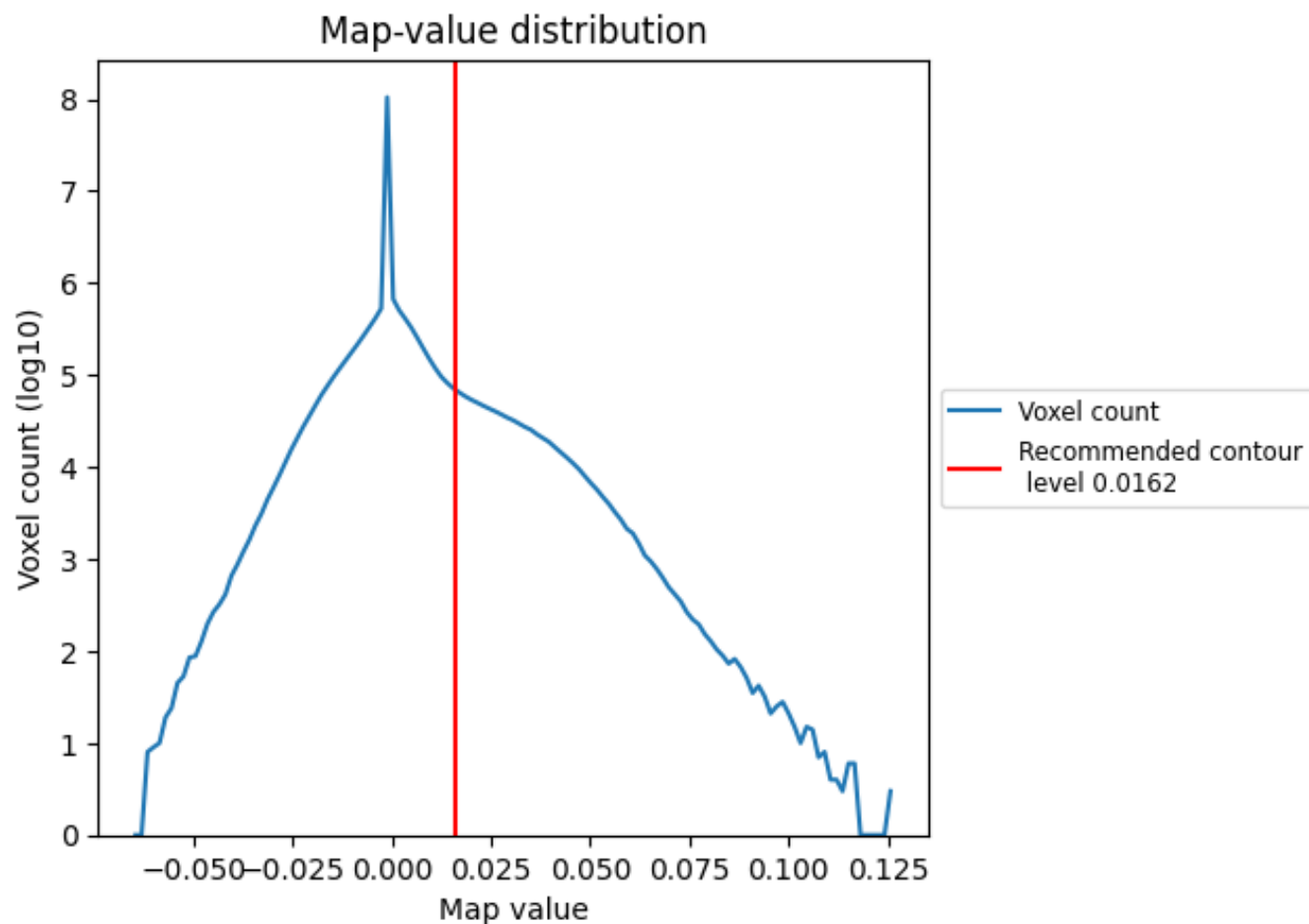
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

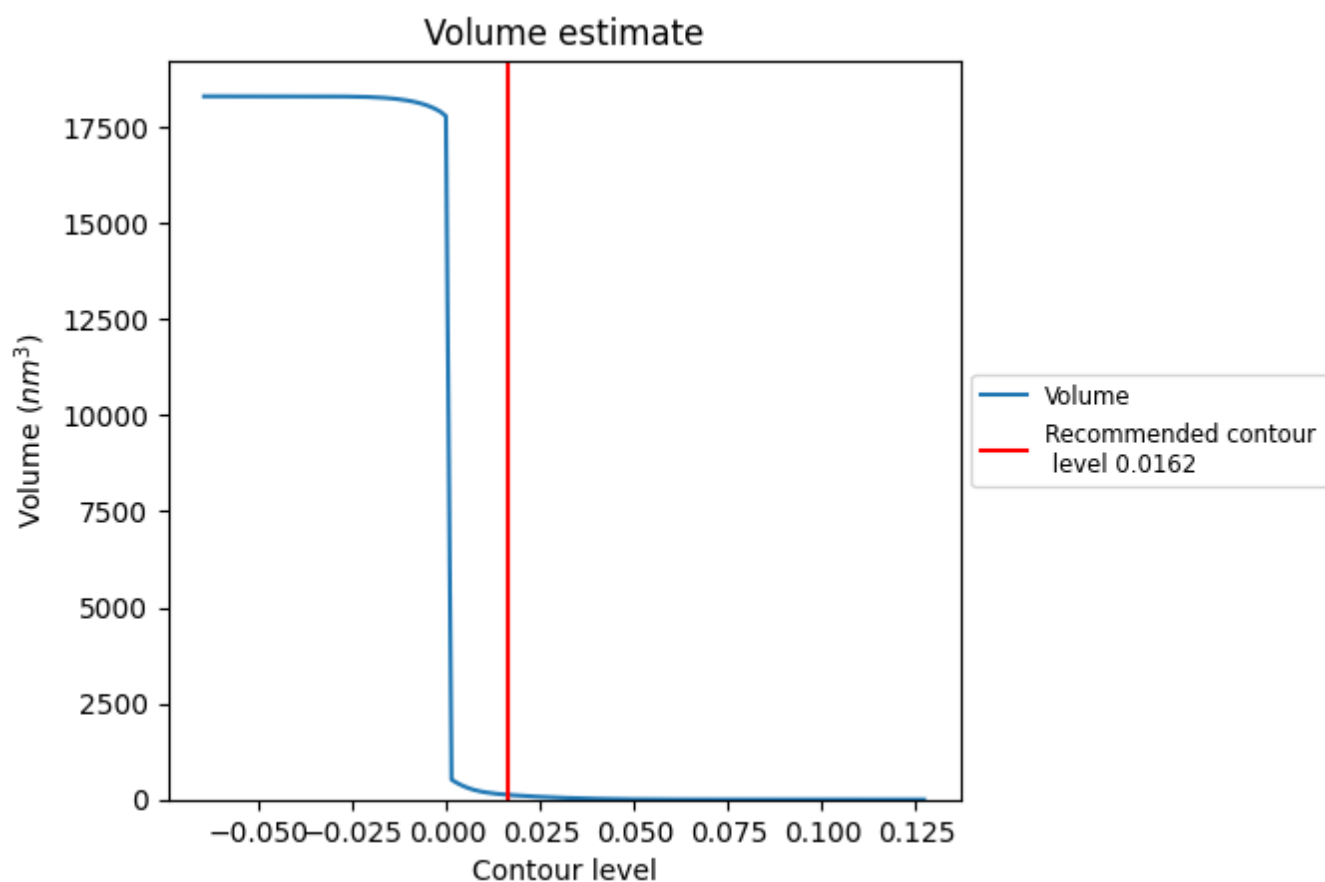
This section contains the results of statistical analysis of the map.

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.

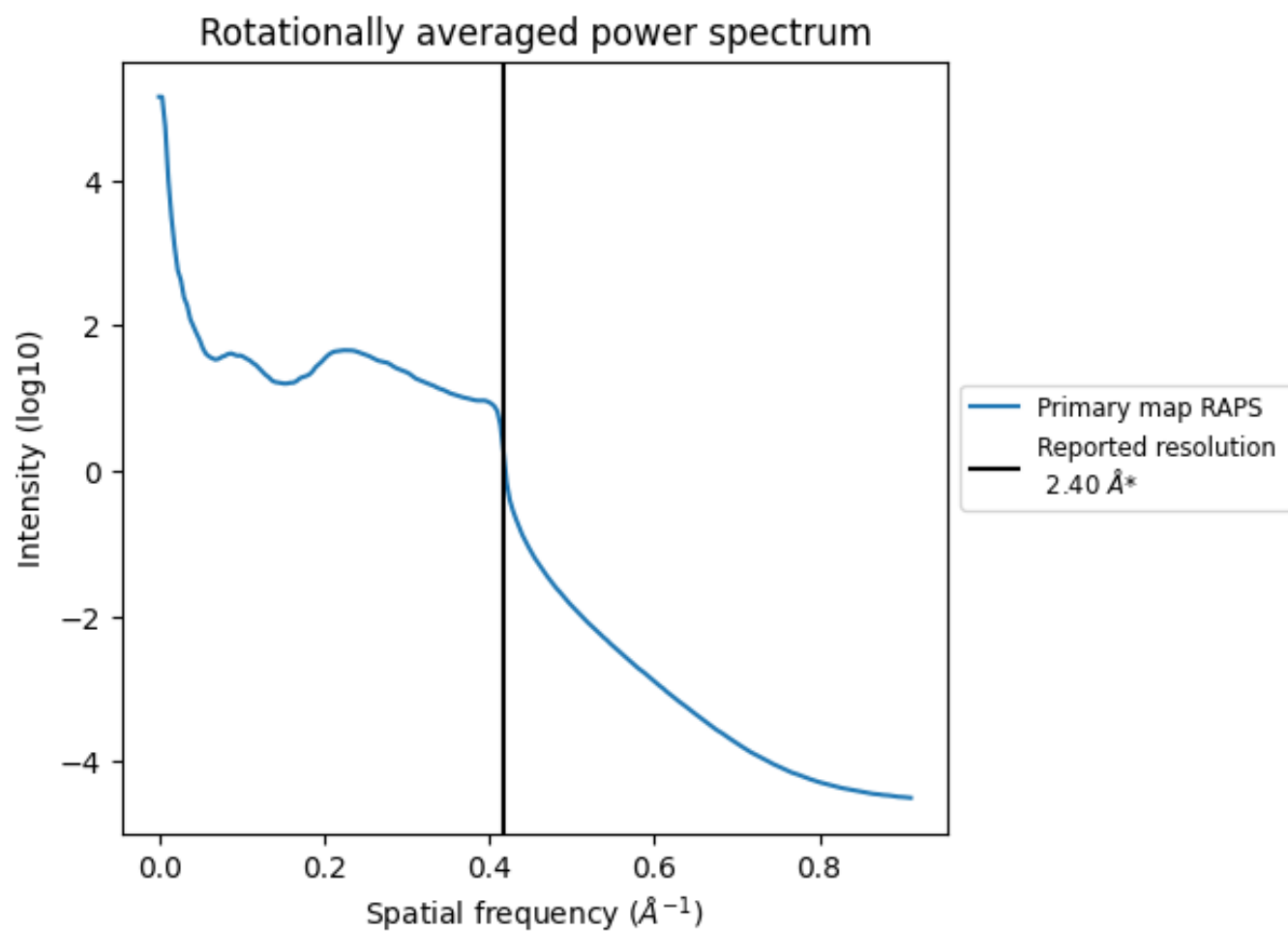
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

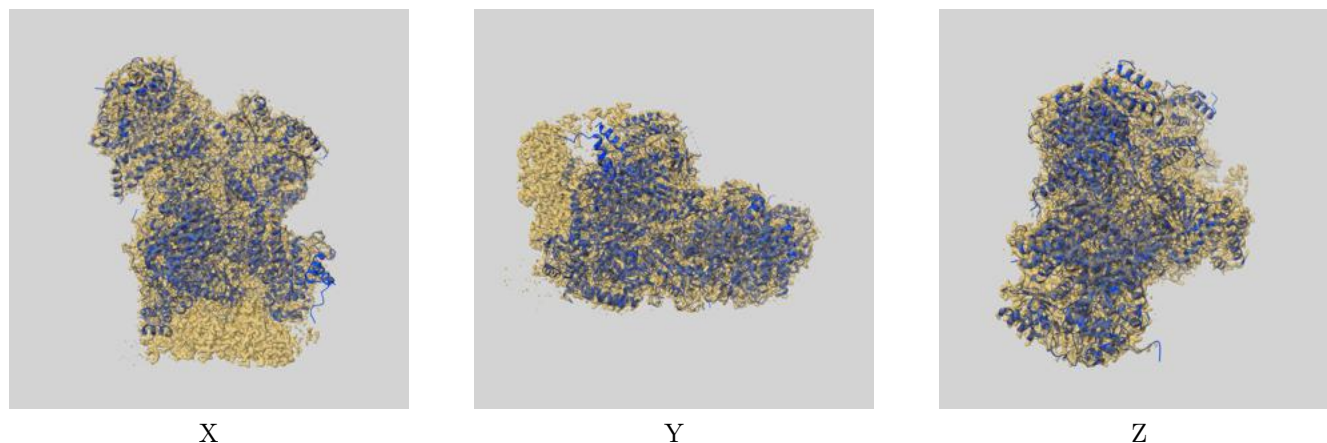
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

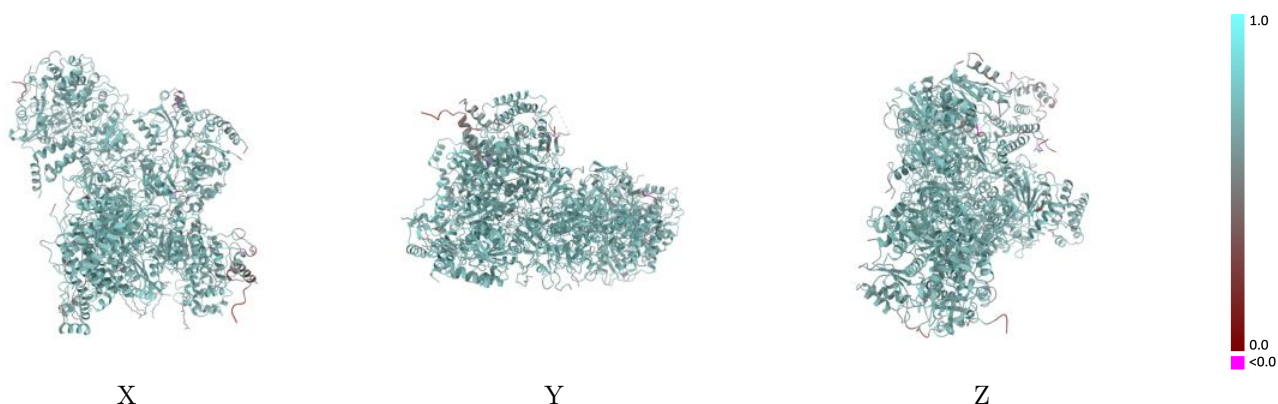
This section contains information regarding the fit between EMDB map EMD-32210 and PDB model 7VYN. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



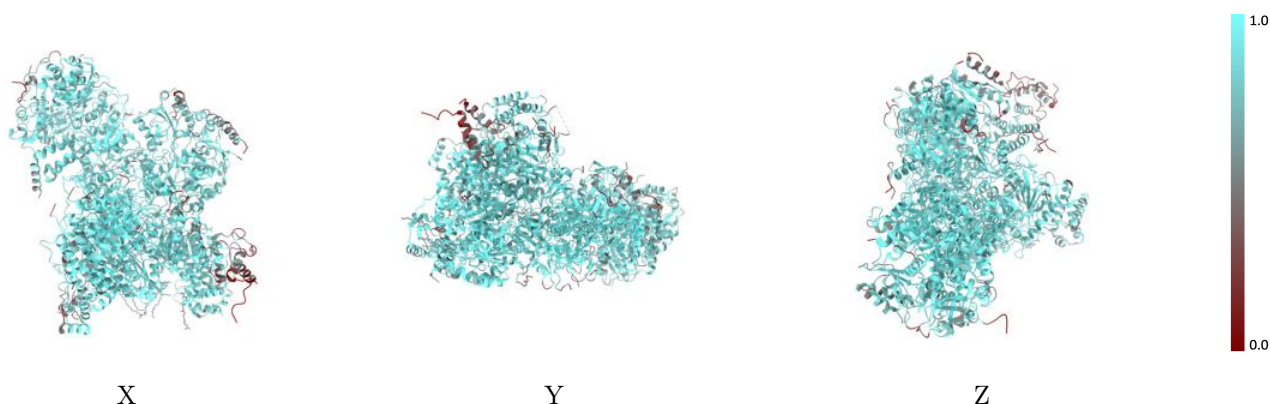
The images above show the 3D surface view of the map at the recommended contour level 0.0162 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



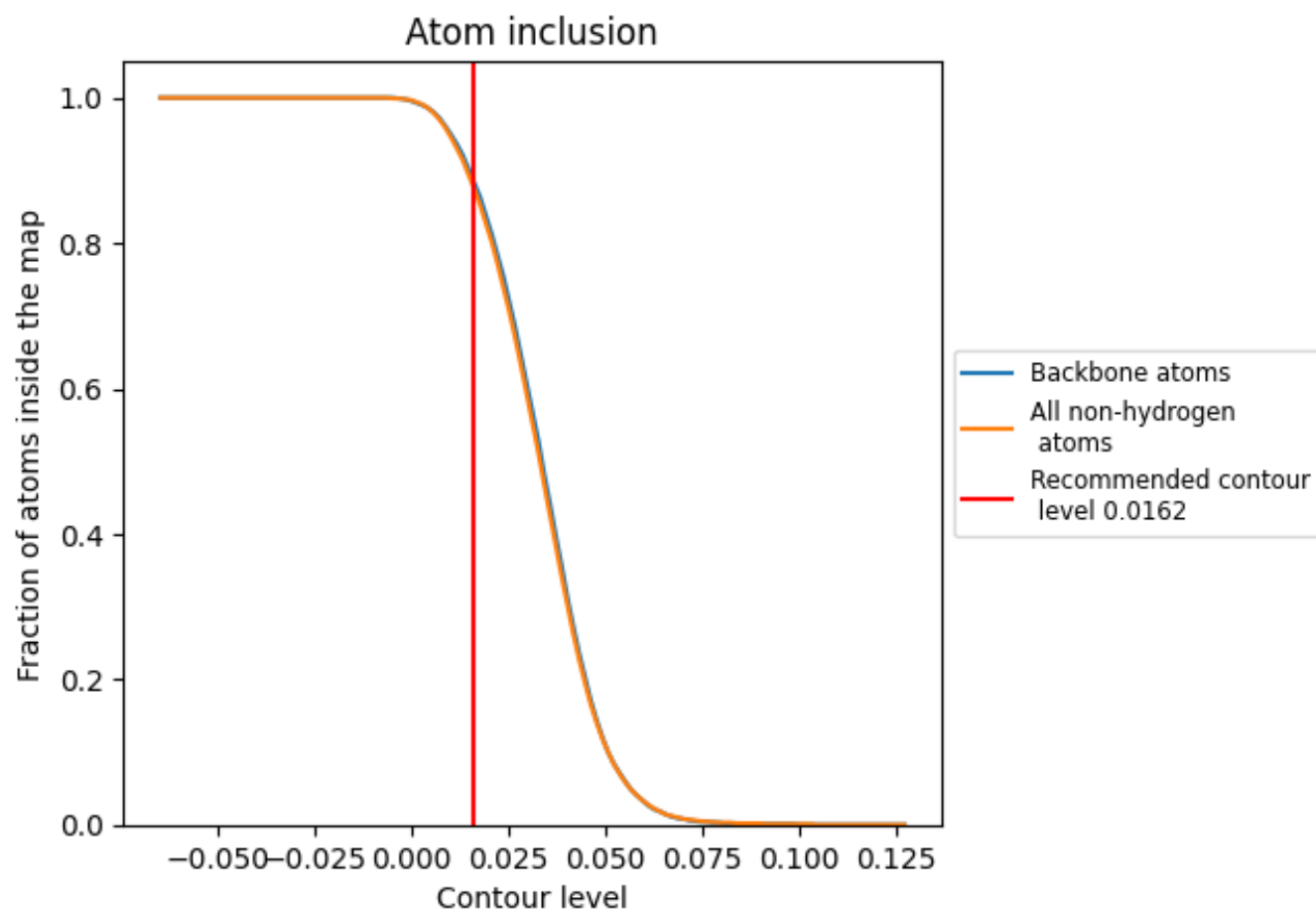
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0162).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0162) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.6810
A	 0.8880	 0.6720
B	 0.9520	 0.7140
C	 0.9370	 0.7090
E	 0.8390	 0.6730
F	 0.6930	 0.6130
G	 0.3800	 0.4880
H	 0.8110	 0.6490
I	 0.7830	 0.6440
J	 0.8960	 0.6870
K	 0.7910	 0.6380
L	 0.8870	 0.6940
M	 0.9030	 0.6910
N	 0.8660	 0.6840
O	 0.8240	 0.6510
P	 0.9550	 0.7130
Q	 0.9660	 0.7170
T	 0.8530	 0.6800
W	 0.7410	 0.6330

