



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 08:12 PM JST

PDB ID : 7VYF  
EMDB ID : EMD-32203  
Title : Matrix arm of active state CI from Rotenone dataset  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-14  
Resolution : 2.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

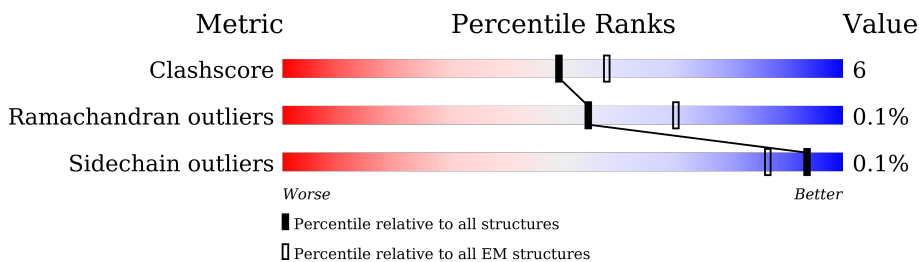
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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.





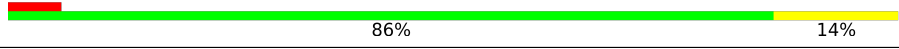



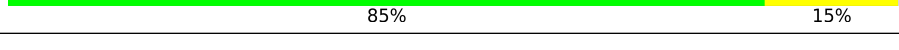
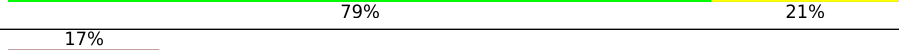
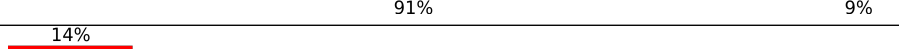
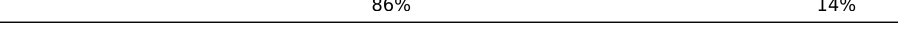
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	 83% 17%
2	B	176	 87% 13%
3	C	156	 86% 14%
4	E	115	 7% 91% 9%
5	F	86	 10% 77% 23%
6	G	88	 32% 78% 22%
7	H	112	 83% 17%
8	I	112	 6% 77% 10% 13%

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Mol	Chain	Length	Quality of chain
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	-
19	SF4	C	301	-	-	X	-

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 28456 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
			1667	1063	281	313	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		

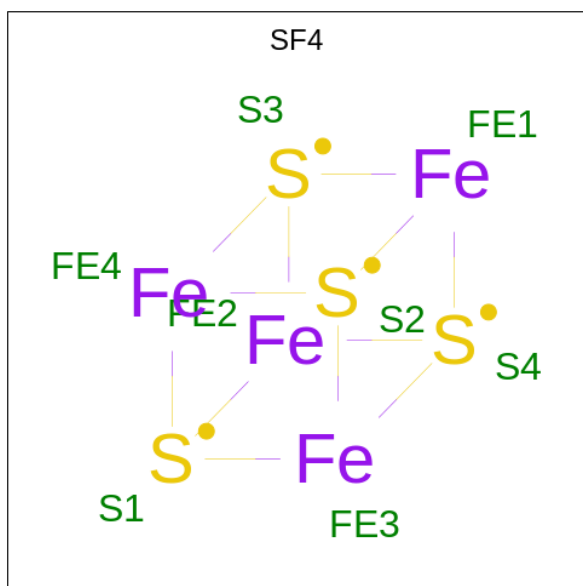
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

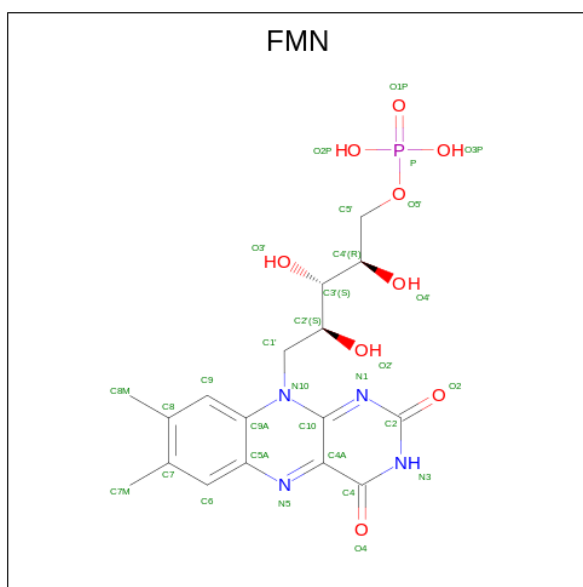
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			218	138	40	39	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



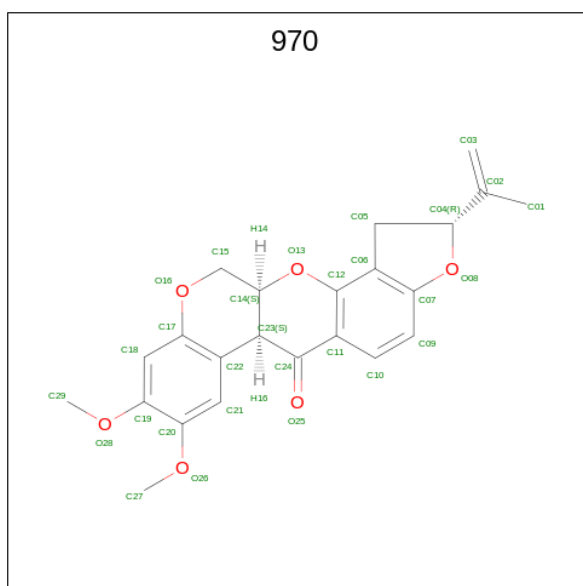
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			16	8	8	
19	B	1	Total	Fe	S	0
			16	8	8	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			16	8	8	
19	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



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

- Molecule 21 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 (three-letter code: 970) (formula:  $C_{23}H_{22}O_6$ ) (labeled as "Ligand of Interest" by depositor).

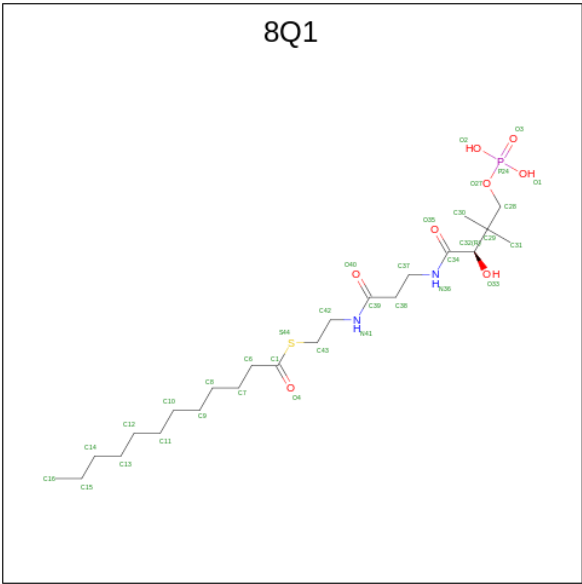


Mol	Chain	Residues	Atoms			AltConf
21	C	1	Total	C	O	0
			29	23	6	

- Molecule 22 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta

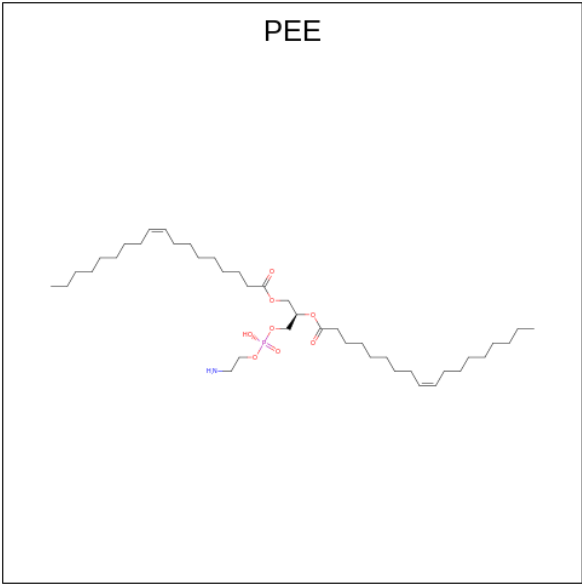


-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



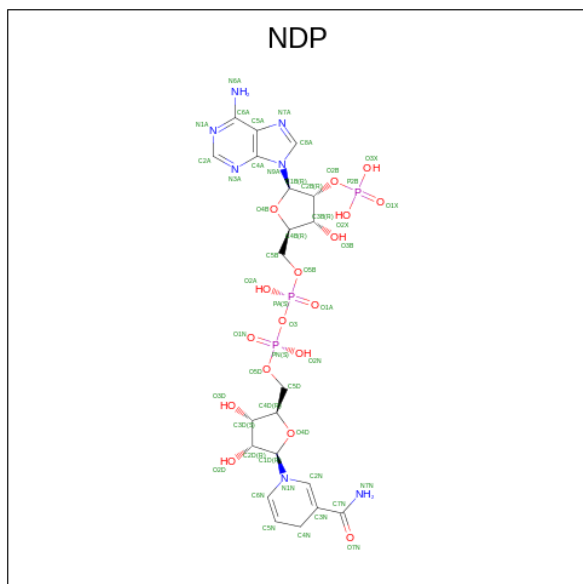
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	G	1	35	23	2	8	1	0

- Molecule 23 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



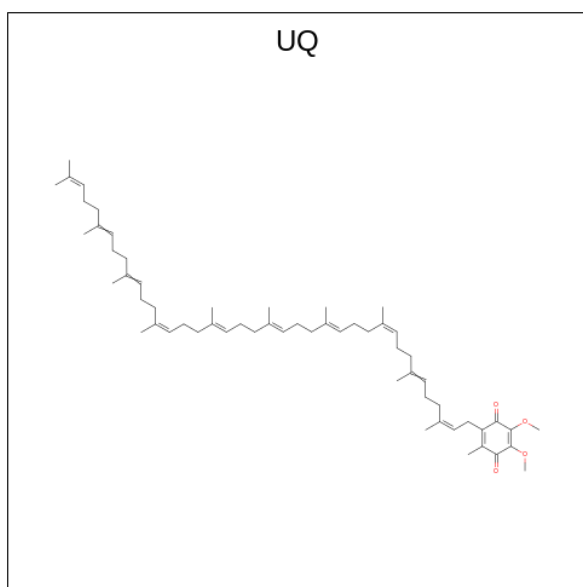
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	J	1	47	37	1	8	1	0

- Molecule 24 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



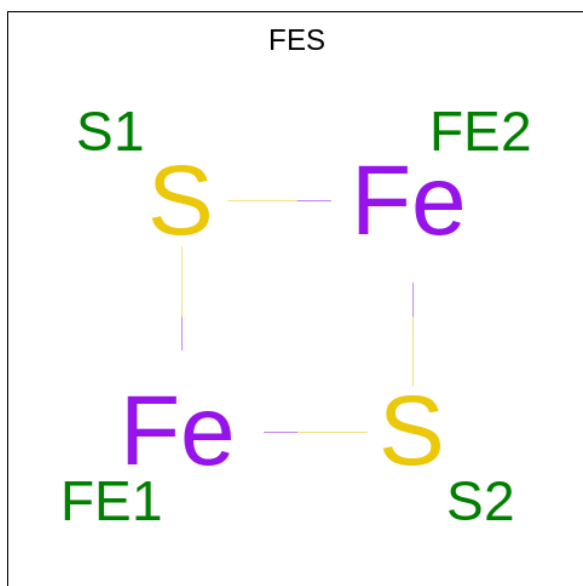
Mol	Chain	Residues	Atoms					AltConf
24	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 25 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

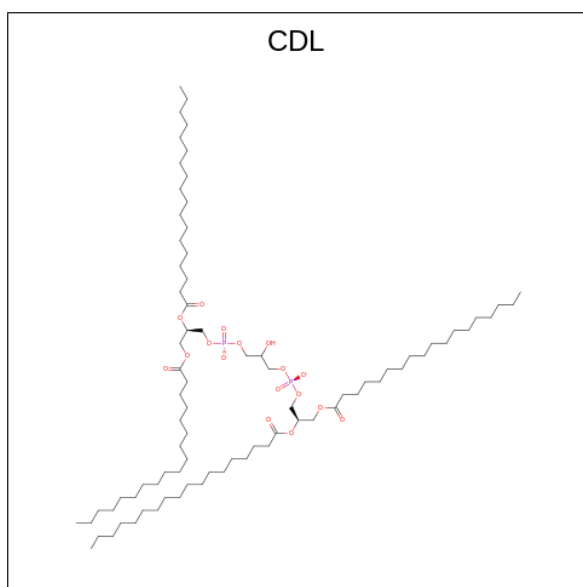


Mol	Chain	Residues	Atoms			AltConf
26	M	1	Total	Fe	S	0
			4	2	2	
26	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 28 is CARDIOLIPIN (three-letter code: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

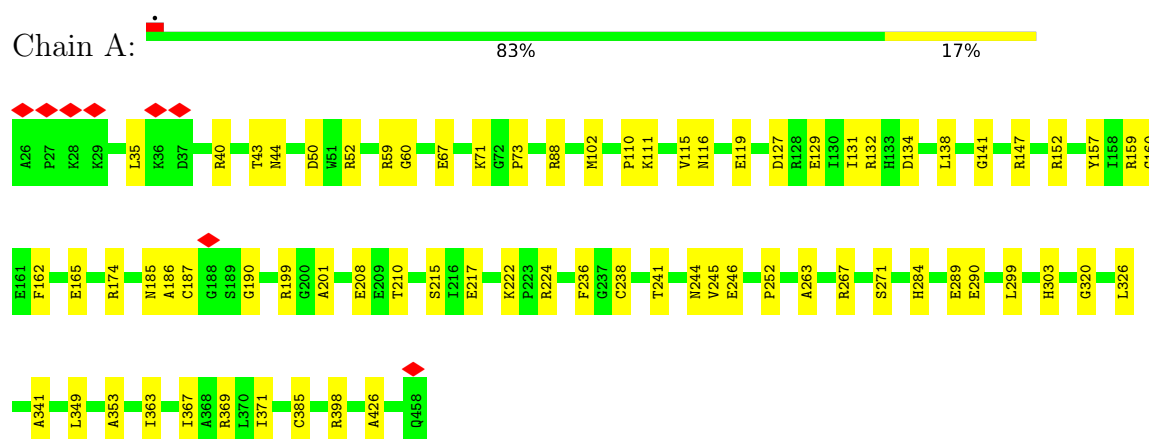
- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

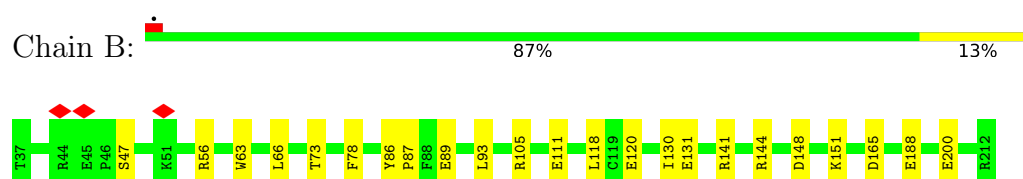
### 3 Residue-property plots

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.

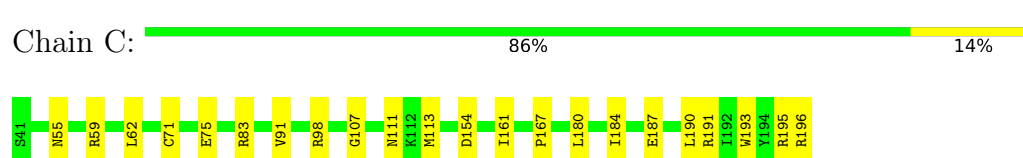
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



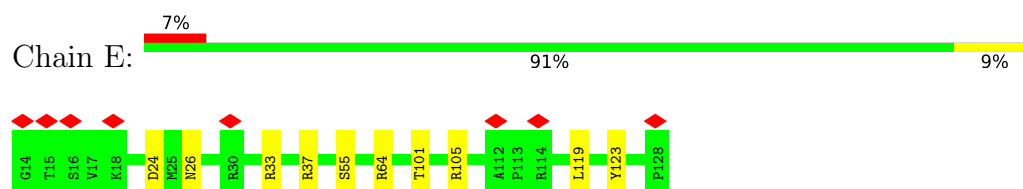
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



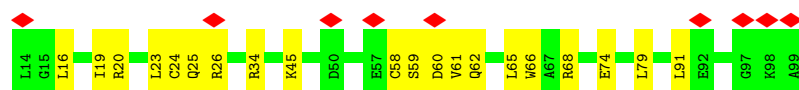
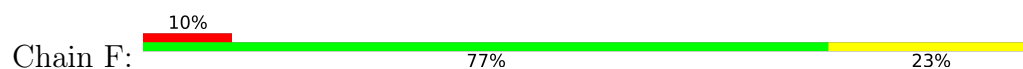
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



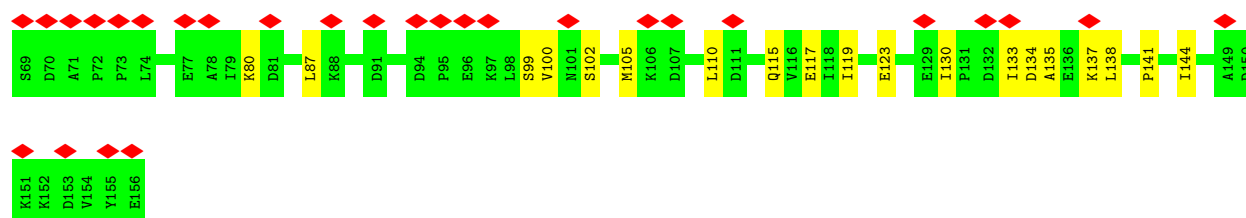
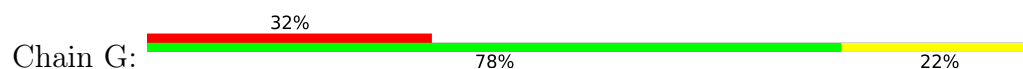
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



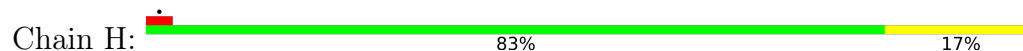
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



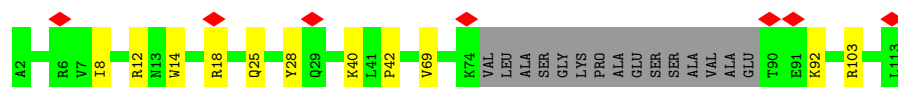
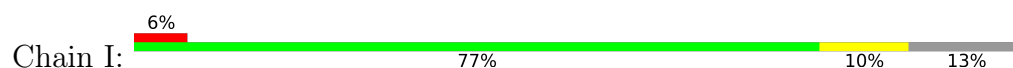
- Molecule 6: Acyl carrier protein, mitochondrial



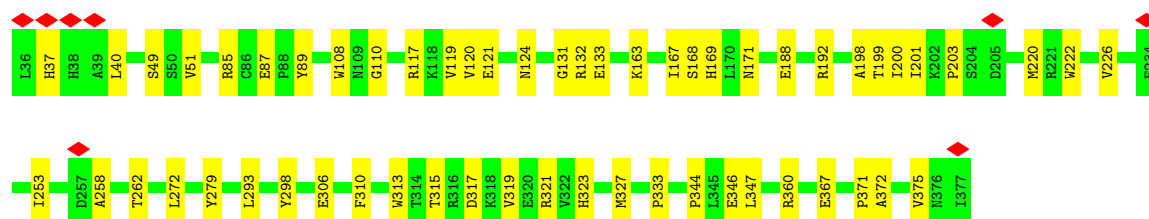
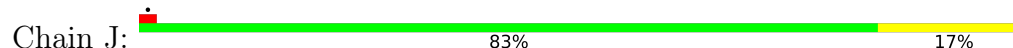
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



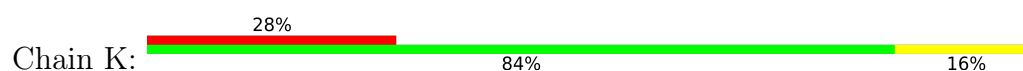
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

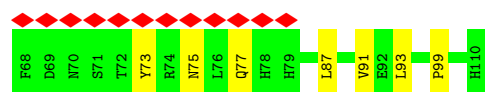


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

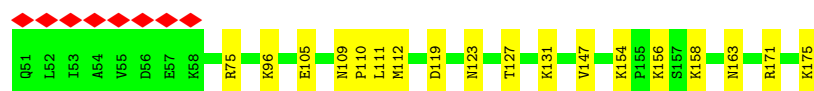
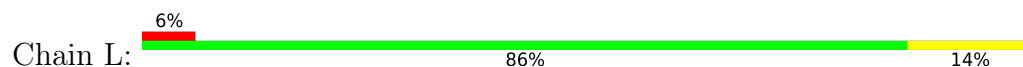


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

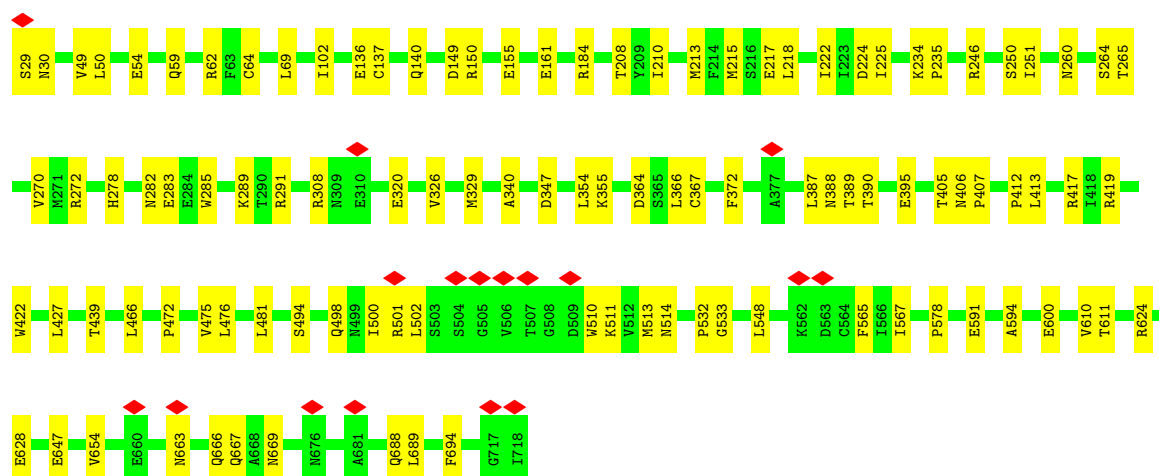
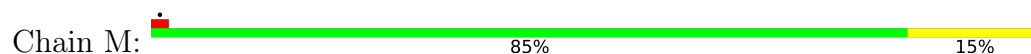




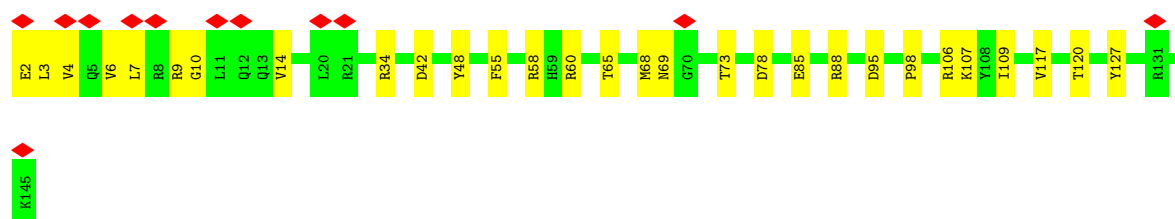
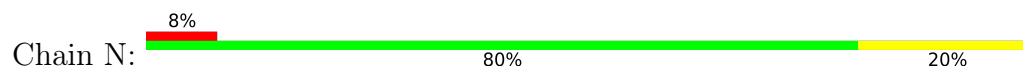
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



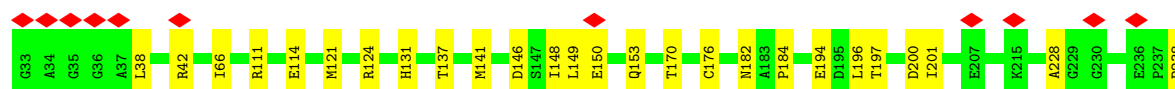
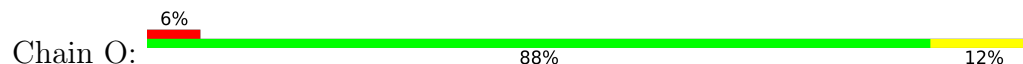
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

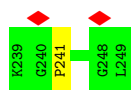


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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





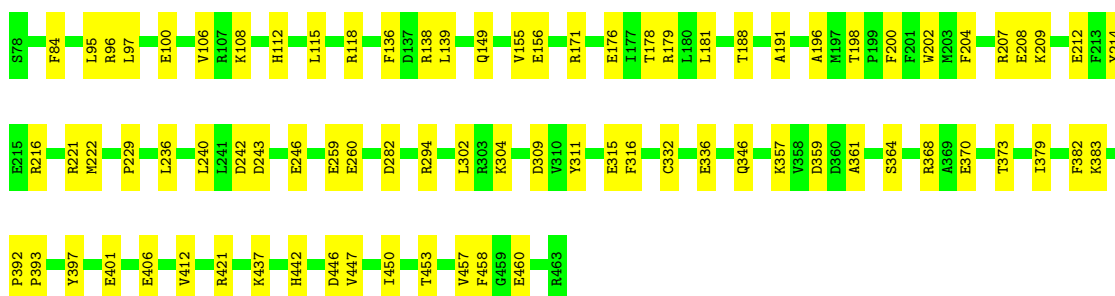
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 85% 15%



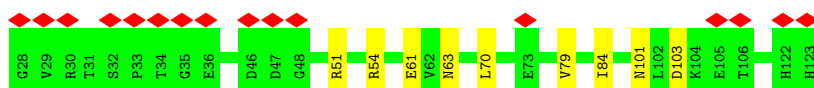
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q: 79% 21%



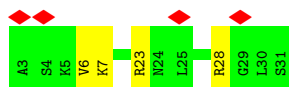
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 17% 91% 9%



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

Chain W: 14% 86% 14%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111024	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	0.200	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0309	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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: ZN, MG, FMN, 8Q1, UQ, PEE, FES, SF4, CDL, 970, NDP, 2MR

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	0.27	0/3406	0.49	0/4603
2	B	0.28	0/1443	0.51	0/1952
3	C	0.30	0/1279	0.51	0/1730
4	E	0.26	0/995	0.54	0/1340
5	F	0.32	0/698	0.58	0/940
6	G	0.26	0/705	0.48	0/956
7	H	0.26	0/929	0.45	0/1258
8	I	0.26	0/798	0.50	0/1079
9	J	0.27	0/2828	0.49	0/3834
10	K	0.25	0/377	0.51	0/509
11	L	0.26	0/1039	0.49	0/1403
12	M	0.26	0/5384	0.51	0/7295
13	N	0.26	0/1245	0.52	0/1694
14	O	0.28	0/1707	0.49	0/2323
15	P	0.28	0/1789	0.52	0/2436
16	Q	0.28	0/3157	0.51	0/4268
17	T	0.25	0/755	0.51	0/1018
18	W	0.28	0/224	0.53	0/302
All	All	0.27	0/28758	0.50	0/38940

There are no bond length outliers.

There are no bond angle outliers.

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	53	0
2	B	1412	0	1363	16	0
3	C	1248	0	1254	18	0
4	E	971	0	975	8	0
5	F	687	0	700	15	0
6	G	693	0	671	13	0
7	H	910	0	950	14	0
8	I	780	0	808	11	0
9	J	2751	0	2773	41	0
10	K	366	0	338	6	0
11	L	1016	0	1016	15	0
12	M	5296	0	5326	66	0
13	N	1204	0	1162	20	0
14	O	1667	0	1669	19	0
15	P	1738	0	1693	20	0
16	Q	3096	0	3063	50	0
17	T	741	0	702	7	0
18	W	218	0	219	4	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	3	0
19	M	16	0	0	0	0
20	A	31	0	19	6	0
21	C	29	0	0	0	0
22	G	35	0	0	0	0
23	J	47	0	71	3	0
24	J	48	0	24	3	0
25	J	33	0	39	6	0
26	M	4	0	0	0	0
26	O	4	0	0	1	0
27	M	1	0	0	0	0
28	N	51	0	46	1	0
29	T	1	0	0	0	0
All	All	28456	0	28173	345	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 (345) 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:J:402:NDP:C4D	24:J:402:NDP:O4D	1.68	1.20
20:A:502:FMN:N1	20:A:502:FMN:O3'	2.08	0.87
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.64	0.79
1:A:152:ARG:NH2	10:K:99:PRO:O	2.21	0.74
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.71	0.73
2:B:47:SER:O	2:B:56:ARG:NH2	2.23	0.72
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.72	0.71
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.29	0.71
17:T:79:VAL:HG11	17:T:84:ILE:HD13	1.72	0.71
1:A:244:ASN:N	20:A:502:FMN:O1P	2.23	0.71
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.24	0.70
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.73	0.70
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.69
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.74	0.68
1:A:43:THR:HG21	14:O:238:PRO:HB3	1.75	0.68
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.68
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.76	0.67
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.77	0.67
11:L:105:GLU:HA	12:M:611:THR:HG21	1.77	0.66
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.66
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.77	0.66
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.29	0.66
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.28	0.66
4:E:101:THR:O	4:E:105:ARG:HG3	1.95	0.65
3:C:55:ASN:O	3:C:59:ARG:HG2	1.97	0.65
12:M:308:ARG:NH2	12:M:578:PRO:O	2.30	0.65
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.29	0.65
12:M:161:GLU:OE2	14:O:42:ARG:NH2	2.30	0.64
1:A:52:ARG:HH21	10:K:77:GLN:HG2	1.62	0.64
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.78	0.64
7:H:70:GLU:OE2	8:I:103:ARG:NH2	2.31	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.78	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.79	0.62
12:M:406:ASN:ND2	12:M:688:GLN:O	2.30	0.62
20:A:502:FMN:HO3'	20:A:502:FMN:C2	2.07	0.62
12:M:472:PRO:O	12:M:510:TRP:NE1	2.29	0.62
1:A:40:ARG:NH1	1:A:289:GLU:O	2.33	0.62
14:O:38:LEU:O	14:O:124:ARG:NH2	2.33	0.62
13:N:2:GLU:HG3	13:N:4:VAL:HG12	1.80	0.62
1:A:127:ASP:O	1:A:131:ILE:HG12	2.00	0.62
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.82	0.61
1:A:222:LYS:O	11:L:175:LYS:NZ	2.31	0.61
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.83	0.61
2:B:111:GLU:O	2:B:141:ARG:NH1	2.35	0.60
12:M:224:ASP:OD2	12:M:291:ARG:NH1	2.35	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.60
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.83	0.60
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.29	0.60
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.34	0.60
13:N:68:MET:HG3	13:N:69:ASN:H	1.66	0.60
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.48	0.59
28:N:201:CDL:H512	28:N:201:CDL:H722	1.83	0.59
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.36	0.59
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.85	0.59
3:C:191:ARG:HB3	3:C:195:ARG:NH1	2.18	0.59
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.28	0.58
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.85	0.58
9:J:199:THR:OG1	9:J:258:ALA:O	2.22	0.58
3:C:191:ARG:HB3	3:C:195:ARG:HH12	1.69	0.58
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.86	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.86	0.57
13:N:117:VAL:O	13:N:120:THR:OG1	2.23	0.57
7:H:9:THR:O	7:H:76:GLN:NE2	2.31	0.57
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.38	0.57
9:J:49:SER:OG	15:P:225:GLU:HB3	2.05	0.57
12:M:388:ASN:ND2	12:M:513:MET:O	2.38	0.57
1:A:50:ASP:O	1:A:59:ARG:NH2	2.37	0.56
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.87	0.56
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.87	0.56
9:J:310:PHE:HE1	23:J:401:PEE:H15	1.71	0.56
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.86	0.56
2:B:148:ASP:HB3	2:B:151:LYS:HB2	1.86	0.56
5:F:65:LEU:HD11	5:F:91:LEU:HD21	1.88	0.56
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.86	0.56
16:Q:242:ASP:O	16:Q:246:GLU:HG2	2.06	0.56
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.88	0.56
3:C:190:LEU:HD22	23:J:401:PEE:H13	1.88	0.55
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.36	0.55
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.86	0.55
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	1.88	0.55
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:133:GLU:OE1	9:J:321:ARG:NH2	2.39	0.55
1:A:263:ALA:HA	1:A:271:SER:HB3	1.87	0.55
14:O:150:GLU:OE2	14:O:150:GLU:N	2.38	0.55
12:M:390:THR:HA	12:M:600:GLU:HG2	1.87	0.55
1:A:116:ASN:O	1:A:245:VAL:HG23	2.06	0.54
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.54
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.38	0.54
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.88	0.54
13:N:127:TYR:OH	17:T:61:GLU:O	2.22	0.54
1:A:67:GLU:O	1:A:71:LYS:HG2	2.08	0.54
9:J:323:HIS:O	9:J:323:HIS:CG	2.60	0.54
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.40	0.54
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.89	0.54
1:A:185:ASN:OD1	1:A:190:GLY:N	2.35	0.54
11:L:75:ARG:NH1	11:L:119:ASP:OD1	2.35	0.54
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.41	0.54
12:M:285:TRP:HB2	12:M:413:LEU:HD11	1.90	0.53
12:M:282:ASN:O	12:M:283:GLU:HG2	2.08	0.53
8:I:40:LYS:HB3	18:W:7:LYS:H	1.73	0.53
9:J:272:LEU:HD11	9:J:375:VAL:HG11	1.90	0.53
12:M:250:SER:OG	12:M:251:ILE:N	2.42	0.53
16:Q:179:ARG:NH2	16:Q:401:GLU:O	2.36	0.53
3:C:71:CYS:HB3	19:C:301:SF4:S4	2.46	0.53
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.91	0.52
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.39	0.52
12:M:367:CYS:HB2	12:M:533:GLY:O	2.09	0.52
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.91	0.52
12:M:264:SER:HB2	12:M:272:ARG:HG2	1.92	0.52
11:L:109:ASN:ND2	11:L:111:LEU:O	2.41	0.52
3:C:184:ILE:O	3:C:187:GLU:HG2	2.10	0.52
6:G:141:PRO:HA	6:G:144:ILE:HD12	1.92	0.52
9:J:222:TRP:HB3	25:J:403:UQ:H152	1.92	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.44	0.51
10:K:87:LEU:O	10:K:91:VAL:HG23	2.10	0.51
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.92	0.51
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.41	0.51
17:T:51:ARG:HG2	17:T:54:ARG:HH21	1.76	0.51
5:F:61:VAL:HG23	5:F:62:GLN:H	1.76	0.51
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.45	0.51
15:P:43:THR:HA	15:P:47:ILE:HD12	1.93	0.51
12:M:388:ASN:HB3	12:M:511:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:51:ARG:HG2	17:T:54:ARG:NH2	2.26	0.50
1:A:267:ARG:HH12	1:A:341:ALA:HB2	1.76	0.50
4:E:24:ASP:OD2	4:E:26:ASN:ND2	2.43	0.50
1:A:129:GLU:HA	1:A:132:ARG:HG2	1.93	0.50
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.45	0.50
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.94	0.50
1:A:44:ASN:HB3	1:A:134:ASP:OD1	2.12	0.49
19:C:301:SF4:S2	16:Q:138:ARG:HG2	2.51	0.49
5:F:58:CYS:SG	5:F:59:SER:N	2.85	0.49
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.93	0.49
9:J:37:HIS:CD2	9:J:40:LEU:HD12	2.46	0.49
12:M:64:CYS:O	12:M:184:ARG:NH2	2.28	0.49
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.92	0.49
1:A:320:GLY:HA2	1:A:353:ALA:H	1.77	0.49
6:G:99:SER:OG	6:G:102:SER:OG	2.24	0.49
1:A:185:ASN:C	1:A:187:CYS:H	2.16	0.49
1:A:217:GLU:CD	11:L:171:ARG:NH2	2.66	0.49
1:A:210:THR:HB	1:A:224:ARG:H	1.76	0.49
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.52	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.48	0.49
5:F:25:GLN:HG2	5:F:26:ARG:HD3	1.94	0.49
7:H:116:ILE:HD12	11:L:127:THR:HG22	1.95	0.49
9:J:222:TRP:CD1	25:J:403:UQ:H101	2.48	0.49
16:Q:259:GLU:OE1	18:W:23:ARG:NH1	2.39	0.49
12:M:265:THR:HG22	12:M:270:VAL:HA	1.95	0.49
9:J:293:LEU:HD23	9:J:298:TYR:HB2	1.94	0.49
17:T:101:ASN:ND2	17:T:103:ASP:OD2	2.45	0.49
1:A:157:TYR:HH	1:A:215:SER:HG	1.59	0.48
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.93	0.48
5:F:61:VAL:HG23	5:F:62:GLN:N	2.27	0.48
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.25	0.48
1:A:35:LEU:HD21	1:A:290:GLU:HA	1.95	0.48
8:I:69:VAL:O	15:P:76:VAL:HB	2.14	0.48
2:B:105:ARG:NH2	17:T:63:ASN:OD1	2.46	0.48
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.95	0.48
14:O:149:LEU:O	14:O:153:GLN:HG2	2.13	0.48
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.49	0.48
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.27	0.48
1:A:398:ARG:NE	12:M:155:GLU:OE2	2.46	0.48
8:I:42:PRO:HB3	18:W:6:VAL:HG21	1.96	0.48
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.94	0.48
13:N:3:LEU:O	13:N:7:LEU:HG	2.13	0.48
4:E:55:SER:HB2	9:J:367:GLU:OE2	2.13	0.48
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.48	0.48
9:J:168:SER:OG	9:J:169:HIS:N	2.46	0.48
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.78	0.48
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.95	0.48
12:M:419:ARG:NH1	12:M:439:THR:O	2.46	0.48
9:J:132:ARG:NH2	24:J:402:NDP:O2X	2.47	0.47
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.96	0.47
15:P:65:VAL:HG11	15:P:86:ILE:HD13	1.96	0.47
11:L:158:LYS:NZ	12:M:69:LEU:O	2.35	0.47
13:N:34:ARG:HH12	13:N:58:ARG:HB3	1.80	0.47
14:O:137:THR:O	14:O:141:MET:N	2.44	0.47
12:M:389:THR:O	12:M:390:THR:OG1	2.21	0.47
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.97	0.47
7:H:35:LEU:HD11	7:H:48:THR:HG22	1.97	0.47
8:I:18:ARG:HH22	16:Q:260:GLU:HG3	1.79	0.47
12:M:501:ARG:HH12	12:M:666:GLN:HB3	1.79	0.47
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.97	0.47
1:A:102:MET:O	1:A:111:LYS:NZ	2.42	0.47
1:A:102:MET:SD	1:A:241:THR:OG1	2.56	0.47
2:B:188:GLU:HG3	13:N:127:TYR:OH	2.15	0.47
3:C:107:GLY:HA2	19:C:301:SF4:S1	2.55	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.96	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.96	0.46
13:N:107:LYS:HE3	17:T:70:LEU:HD22	1.97	0.46
5:F:59:SER:OG	5:F:60:ASP:N	2.48	0.46
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.77	0.46
12:M:213:MET:HB3	12:M:215:MET:HG2	1.97	0.46
16:Q:136:PHE:HA	16:Q:139:LEU:HD12	1.97	0.46
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.98	0.46
3:C:196:ARG:HB2	9:J:85:ARG:HH12	1.80	0.46
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.97	0.46
3:C:113:MET:SD	16:Q:115:LEU:HD23	2.56	0.46
9:J:313:TRP:CD2	25:J:403:UQ:H72	2.50	0.46
9:J:87:GLU:HG3	9:J:89:TYR:H	1.81	0.46
25:J:403:UQ:HM51	25:J:403:UQ:H71	1.61	0.46
13:N:55:PHE:CE1	13:N:58:ARG:HG3	2.51	0.46
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.46
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:O	1:A:199:ARG:NH2	2.49	0.46
1:A:426:ALA:HB3	20:A:502:FMN:HM81	1.97	0.46
16:Q:100:GLU:OE1	16:Q:108:LYS:HB3	2.16	0.46
6:G:133:ILE:O	6:G:134:ASP:OD1	2.34	0.45
16:Q:450:ILE:HA	16:Q:453:THR:HG22	1.98	0.45
5:F:20:ARG:NH2	5:F:74:GLU:OE2	2.49	0.45
9:J:375:VAL:HG23	9:J:375:VAL:O	2.16	0.45
1:A:320:GLY:HA3	1:A:349:LEU:O	2.17	0.45
3:C:75:GLU:OE2	16:Q:221:ARG:NH1	2.49	0.45
11:L:163:ASN:O	11:L:171:ARG:HA	2.17	0.45
12:M:29:SER:OG	12:M:30:ASN:N	2.50	0.45
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.98	0.45
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	1.99	0.45
3:C:62:LEU:O	3:C:91:VAL:HA	2.17	0.45
12:M:260:ASN:ND2	12:M:278:HIS:HD2	2.15	0.45
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.48	0.45
12:M:494:SER:OG	12:M:669:ASN:ND2	2.47	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.17	0.45
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.99	0.44
13:N:78:ASP:OD1	13:N:78:ASP:N	2.50	0.44
16:Q:370:GLU:HA	16:Q:373:THR:HG22	1.99	0.44
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.78	0.44
8:I:14:TRP:O	18:W:28:ARG:NH2	2.50	0.44
14:O:148:ILE:HD12	14:O:184:PRO:HB2	1.99	0.44
5:F:45:LYS:HA	5:F:45:LYS:HD2	1.78	0.44
9:J:40:LEU:HD13	9:J:124:ASN:ND2	2.32	0.44
9:J:51:VAL:HG22	11:L:110:PRO:HG3	2.00	0.44
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.99	0.44
6:G:105:MET:HG3	6:G:110:LEU:O	2.18	0.44
1:A:157:TYR:OH	1:A:215:SER:OG	2.34	0.44
2:B:78:PHE:HB2	8:I:12:ARG:HG2	2.00	0.44
2:B:144:ARG:NH1	11:L:112:MET:O	2.30	0.44
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.44
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.82	0.44
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.32	0.44
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.49	0.44
7:H:116:ILE:HG21	11:L:96:LYS:HD2	2.00	0.44
25:J:403:UQ:H171	25:J:403:UQ:H151	1.59	0.44
8:I:8:ILE:O	8:I:12:ARG:HG3	2.18	0.43
9:J:298:TYR:CE2	9:J:319:VAL:HG22	2.53	0.43
12:M:59:GLN:NE2	12:M:62:ARG:HH12	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:208:THR:OG1	12:M:210:ILE:O	2.32	0.43
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.99	0.43
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.00	0.43
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.33	0.43
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.57	0.43
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.51	0.43
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.99	0.43
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.01	0.43
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.35	0.43
9:J:163:LYS:NZ	9:J:253:ILE:O	2.35	0.43
14:O:146:ASP:O	14:O:150:GLU:OE2	2.37	0.43
15:P:197:PRO:HA	15:P:202:PHE:CG	2.54	0.43
7:H:47:TYR:HE1	8:I:92:LYS:O	2.01	0.43
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.01	0.43
15:P:62:GLY:HA3	15:P:76:VAL:HG11	2.00	0.43
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.43
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.30	0.43
9:J:37:HIS:CD2	9:J:40:LEU:HB2	2.54	0.42
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.26	0.42
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.02	0.42
9:J:108:TRP:HZ3	9:J:110:GLY:HA2	1.84	0.42
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.84	0.42
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.42
1:A:119:GLU:O	1:A:159:ARG:NH1	2.52	0.42
12:M:329:MET:HG2	12:M:565:PHE:CG	2.54	0.42
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.20	0.42
3:C:111:ASN:CG	15:P:210:LEU:HD13	2.39	0.42
3:C:154:ASP:OD1	3:C:154:ASP:N	2.53	0.42
5:F:16:LEU:HD11	5:F:19:ILE:HD11	2.00	0.42
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.54	0.42
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.01	0.42
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.20	0.42
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.35	0.42
1:A:244:ASN:OD1	20:A:502:FMN:O2	2.38	0.42
25:J:403:UQ:H202	25:J:403:UQ:H172	1.82	0.42
13:N:10:GLY:O	13:N:14:VAL:HG23	2.20	0.42
13:N:65:THR:O	13:N:73:THR:OG1	2.32	0.42
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.55	0.42
3:C:193:TRP:HA	3:C:196:ARG:HG2	2.01	0.42
12:M:326:VAL:HG13	12:M:567:ILE:HD13	2.02	0.42
12:M:666:GLN:HG3	12:M:667:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.42
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.55	0.42
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.54	0.42
9:J:117:ARG:O	9:J:121:GLU:HG3	2.19	0.42
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.37	0.42
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.49	0.42
16:Q:383:LYS:HB3	16:Q:383:LYS:HE3	1.92	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41
12:M:647:GLU:HB2	12:M:654:VAL:HG11	2.02	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.41
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.00	0.41
5:F:23:LEU:HD12	5:F:34:ARG:HG2	2.02	0.41
6:G:134:ASP:HA	6:G:137:LYS:NZ	2.35	0.41
4:E:33:ARG:O	4:E:37:ARG:HG3	2.21	0.41
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.02	0.41
12:M:50:LEU:O	12:M:54:GLU:HG2	2.20	0.41
12:M:498:GLN:HG3	12:M:502:LEU:HD23	2.02	0.41
12:M:689:LEU:HD23	12:M:689:LEU:HA	1.92	0.41
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.35	0.41
12:M:289:LYS:HE2	12:M:694:PHE:O	2.21	0.41
1:A:201:ALA:HA	14:O:121:MET:HE3	2.02	0.41
6:G:87:LEU:HD23	6:G:87:LEU:HA	1.91	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.02	0.41
12:M:591:GLU:HG3	12:M:610:VAL:HG23	2.03	0.41
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	1.97	0.41
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.02	0.41
9:J:171:ASN:OD1	9:J:327:MET:HG3	2.21	0.41
8:I:28:TYR:HA	13:N:55:PHE:HA	2.03	0.41
23:J:401:PEE:H82	23:J:401:PEE:H74	1.88	0.41
12:M:475:VAL:HG22	12:M:514:ASN:HB2	2.03	0.41
12:M:511:LYS:HE2	12:M:663:ASN:HB2	2.02	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
7:H:38:ILE:O	7:H:45:ARG:NH1	2.46	0.41
11:L:154:LYS:O	11:L:156:LYS:NZ	2.51	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.41
12:M:405:THR:HG23	12:M:407:PRO:HD3	2.02	0.41
1:A:369:ARG:HD2	1:A:369:ARG:HA	1.88	0.41
9:J:262:THR:O	9:J:333:PRO:HD2	2.21	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.41
12:M:422:TRP:HA	12:M:427:LEU:HB3	2.02	0.41
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:131:GLY:O	24:J:402:NDP:H51A	2.22	0.40
14:O:131:HIS:CD2	14:O:170:THR:HG23	2.56	0.40
15:P:170:ILE:HG22	15:P:176:VAL:HB	2.04	0.40
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.02	0.40
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.56	0.40
3:C:98:ARG:H	3:C:98:ARG:HG2	1.74	0.40
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.79	0.40
15:P:148:ASP:OD1	15:P:148:ASP:N	2.54	0.40
7:H:55:LYS:HE3	15:P:104:THR:HG21	2.02	0.40
9:J:220:MET:HE3	9:J:226:VAL:HG13	2.03	0.40
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.04	0.40
14:O:137:THR:HB	26:O:301:FES:S2	2.61	0.40
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	2.02	0.40
1:A:217:GLU:OE1	1:A:236:PHE:N	2.47	0.40
6:G:115:GLN:O	6:G:119:ILE:HG12	2.21	0.40
9:J:344:PRO:HB2	9:J:346:GLU:OE1	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%)	419 (97%)	11 (3%)	1 (0%)	47	78
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	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%)	17	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	660 (96%)	28 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	201 (94%)	14 (6%)	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%)	3364 (96%)	138 (4%)	2 (0%)	54	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
7	H	77	ILE

### 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%)	346 (100%)	0	100	100
2	B	151/151 (100%)	150 (99%)	1 (1%)	84	95
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	295 (100%)	1 (0%)	92	98
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	580 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	182/183 (100%)	182 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	332/332 (100%)	332 (100%)	0	100	100
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	23/24 (96%)	23 (100%)	0	100	100
All	All	3040/3058 (99%)	3038 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	THR
9	J	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
9	J	37	HIS
12	M	260	ASN
12	M	278	HIS
12	M	604	GLN
14	O	41	HIS

### 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	6.06	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	5.67	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	12.42	130.87	119.48
16	Q	118	2MR	CD-NE-CZ	4.20	131.27	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.02	130.53	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	SF4	A	501	1	0,12,12	-	-	-		
21	970	C	302	-	33,33,33	4.79	15 (45%)	48,50,50	2.87	22 (45%)
25	UQ	J	403	-	33,33,63	3.46	10 (30%)	40,43,79	2.81	14 (35%)
20	FMN	A	502	-	33,33,33	1.41	6 (18%)	48,50,50	1.25	7 (14%)
23	PEE	J	401	-	46,46,50	1.21	6 (13%)	49,51,55	0.99	2 (4%)
28	CDL	N	201	-	50,50,99	1.40	9 (18%)	56,62,111	1.18	4 (7%)
26	FES	M	803	12	0,4,4	-	-	-		
22	8Q1	G	201	-	31,34,34	1.68	6 (19%)	40,43,43	1.65	5 (12%)
19	SF4	B	301	2	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		
26	FES	O	301	14	0,4,4	-	-	-		
24	NDP	J	402	-	45,52,52	4.55	20 (44%)	53,80,80	1.99	7 (13%)
19	SF4	M	801	12	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
21	970	C	302	-	-	4/8/41/41	0/5/5/5
19	SF4	A	501	1	-	-	0/6/5/5
25	UQ	J	403	-	-	12/27/51/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FMN	A	502	-	-	9/18/18/18	0/3/3/3
28	CDL	N	201	-	-	34/61/61/110	-
26	FES	M	803	12	-	-	0/1/1/1
22	8Q1	G	201	-	-	17/41/41/41	-
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	B	301	2	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
19	SF4	C	301	3	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5
26	FES	O	301	14	-	-	0/1/1/1
24	NDP	J	402	-	-	10/30/77/77	0/4/5/5
23	PEE	J	401	-	-	24/50/50/54	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	302	970	O16-C17	17.88	1.57	1.37
24	J	402	NDP	C3B-C2B	-12.90	1.24	1.52
24	J	402	NDP	C6N-C5N	12.31	1.55	1.33
21	C	302	970	O25-C24	10.74	1.37	1.22
24	J	402	NDP	O4D-C4D	10.69	1.68	1.45
24	J	402	NDP	C3D-C4D	-9.89	1.27	1.53
25	J	403	UQ	C18-C19	9.62	1.56	1.33
25	J	403	UQ	C13-C14	9.30	1.55	1.33
25	J	403	UQ	C8-C9	8.80	1.54	1.33
21	C	302	970	C23-C24	8.67	1.61	1.52
24	J	402	NDP	O4B-C1B	8.31	1.52	1.41
24	J	402	NDP	O4B-C4B	-7.91	1.27	1.45
25	J	403	UQ	C23-C24	7.86	1.55	1.32
21	C	302	970	C14-C23	-7.39	1.45	1.52
24	J	402	NDP	C2N-C3N	7.35	1.55	1.34
21	C	302	970	O08-C07	6.39	1.47	1.37
24	J	402	NDP	P2B-O2B	5.48	1.69	1.59
24	J	402	NDP	C3B-C4B	5.34	1.66	1.53
22	G	201	8Q1	C34-N36	5.30	1.45	1.33
22	G	201	8Q1	C39-N41	5.28	1.45	1.33
21	C	302	970	C05-C04	-5.16	1.46	1.54
21	C	302	970	O13-C12	4.97	1.45	1.37
24	J	402	NDP	O4D-C1D	-4.95	1.30	1.42
24	J	402	NDP	C6N-N1N	4.90	1.49	1.37
21	C	302	970	C03-C02	4.73	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	502	FMN	C9A-C5A	4.71	1.49	1.41
24	J	402	NDP	O2D-C2D	-4.27	1.32	1.43
24	J	402	NDP	C7N-N7N	4.15	1.44	1.33
24	J	402	NDP	C6A-N6A	4.02	1.48	1.34
23	J	401	PEE	C18-C19	3.75	1.53	1.31
23	J	401	PEE	C39-C38	3.65	1.52	1.31
21	C	302	970	C15-C14	3.50	1.57	1.51
28	N	201	CDL	OA8-CA7	3.41	1.43	1.33
20	A	502	FMN	C8-C7	3.24	1.49	1.40
21	C	302	970	C11-C24	3.20	1.54	1.48
21	C	302	970	O16-C15	3.15	1.52	1.44
28	N	201	CDL	OA6-CA5	3.14	1.43	1.34
28	N	201	CDL	OB8-CB7	3.08	1.42	1.33
24	J	402	NDP	O3D-C3D	3.01	1.50	1.43
28	N	201	CDL	OB6-CB5	2.95	1.42	1.34
25	J	403	UQ	C6-C1	2.91	1.54	1.46
24	J	402	NDP	C7N-C3N	2.83	1.54	1.48
20	A	502	FMN	C4-N3	-2.74	1.33	1.38
21	C	302	970	C09-C07	2.62	1.45	1.39
21	C	302	970	C12-C06	2.60	1.43	1.39
25	J	403	UQ	C7-C8	2.45	1.54	1.50
23	J	401	PEE	O3-C30	2.45	1.40	1.33
23	J	401	PEE	O2-C2	-2.43	1.40	1.46
22	G	201	8Q1	C1-S44	2.40	1.81	1.76
22	G	201	8Q1	O35-C34	-2.34	1.18	1.23
24	J	402	NDP	O2B-C2B	2.32	1.52	1.44
22	G	201	8Q1	O40-C39	-2.31	1.18	1.23
20	A	502	FMN	C5A-N5	-2.24	1.35	1.39
23	J	401	PEE	O2-C10	2.24	1.40	1.34
20	A	502	FMN	C4A-N5	2.22	1.35	1.30
22	G	201	8Q1	C6-C1	2.20	1.53	1.50
28	N	201	CDL	OB6-CB4	-2.20	1.41	1.46
24	J	402	NDP	O7N-C7N	-2.20	1.19	1.24
28	N	201	CDL	PB2-OB5	2.19	1.68	1.59
24	J	402	NDP	C2D-C3D	2.18	1.59	1.53
25	J	403	UQ	O4-C4	-2.18	1.18	1.23
28	N	201	CDL	PB2-OB2	2.14	1.68	1.59
24	J	402	NDP	PA-O5B	2.10	1.67	1.59
28	N	201	CDL	OA6-CA4	-2.10	1.41	1.46
23	J	401	PEE	O3-C3	-2.10	1.40	1.45
21	C	302	970	O26-C20	2.06	1.40	1.37
28	N	201	CDL	C11-CA5	2.03	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	302	970	O28-C19	2.02	1.40	1.37
25	J	403	UQ	O3-CM3	-2.02	1.40	1.45
20	A	502	FMN	C2-N3	-2.01	1.34	1.39
25	J	403	UQ	C21-C19	2.01	1.55	1.51
25	J	403	UQ	O1-C1	-2.00	1.19	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	302	970	O25-C24-C23	-8.61	108.62	121.00
21	C	302	970	O25-C24-C11	-8.20	108.83	121.98
25	J	403	UQ	C7-C8-C9	-8.15	113.23	126.79
24	J	402	NDP	C3N-C2N-N1N	-7.99	111.70	123.10
24	J	402	NDP	C1D-N1N-C2N	-7.21	109.11	121.11
21	C	302	970	O08-C07-C06	-7.11	108.66	113.00
22	G	201	8Q1	C6-C1-S44	6.66	121.21	113.46
25	J	403	UQ	C12-C13-C14	-5.88	113.51	127.66
25	J	403	UQ	C17-C18-C19	-5.85	113.58	127.66
24	J	402	NDP	C1D-N1N-C6N	-5.50	108.98	120.83
21	C	302	970	C06-C05-C04	5.49	106.38	101.45
25	J	403	UQ	C10-C9-C8	-4.72	111.56	123.68
25	J	403	UQ	C22-C23-C24	-4.34	112.90	127.75
28	N	201	CDL	OA6-CA5-C11	4.28	120.73	111.50
28	N	201	CDL	OB6-CB5-C51	4.16	120.47	111.50
25	J	403	UQ	C11-C9-C8	-4.12	112.77	121.12
21	C	302	970	C01-C02-C03	-4.04	111.66	121.38
25	J	403	UQ	C16-C14-C13	-4.03	112.95	121.12
25	J	403	UQ	C21-C19-C18	-4.02	112.99	121.12
24	J	402	NDP	N3A-C2A-N1A	-4.00	122.42	128.68
25	J	403	UQ	C15-C14-C13	-3.94	113.58	123.68
23	J	401	PEE	O2-C10-C11	3.87	119.85	111.50
21	C	302	970	O08-C07-C09	3.86	131.72	123.89
25	J	403	UQ	C20-C19-C18	-3.78	113.98	123.68
22	G	201	8Q1	O4-C1-C6	-3.74	119.58	123.99
21	C	302	970	C04-C02-C03	-3.55	112.30	120.31
21	C	302	970	C22-C23-C14	3.36	114.26	109.56
21	C	302	970	C09-C07-C06	-3.35	119.61	123.20
25	J	403	UQ	C25-C24-C23	-3.34	113.00	122.65
25	J	403	UQ	C7-C6-C1	3.31	122.46	118.48
21	C	302	970	C05-C04-C02	-3.26	110.85	115.62
25	J	403	UQ	C26-C24-C23	-3.20	113.40	122.65
21	C	302	970	O28-C19-C20	2.99	119.58	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	302	970	O26-C20-C19	2.94	119.51	115.41
21	C	302	970	O13-C14-C23	2.92	115.35	112.40
25	J	403	UQ	CM5-C5-C6	-2.74	119.92	124.40
28	N	201	CDL	OA8-CA7-C31	2.70	120.39	111.91
20	A	502	FMN	C4A-C10-N1	-2.68	118.52	124.73
23	J	401	PEE	O3-C30-C31	2.67	120.29	111.91
28	N	201	CDL	OB8-CB7-C71	2.64	120.19	111.91
22	G	201	8Q1	O4-C1-S44	-2.62	119.21	122.61
20	A	502	FMN	C4-C4A-N5	2.56	121.88	118.23
22	G	201	8Q1	C38-C39-N41	2.56	120.72	116.42
24	J	402	NDP	C2B-C3B-C4B	2.45	107.32	101.99
20	A	502	FMN	O4-C4-C4A	-2.42	120.18	126.60
21	C	302	970	C21-C22-C17	2.38	120.44	117.06
24	J	402	NDP	C4A-C5A-N7A	-2.35	106.95	109.40
24	J	402	NDP	PN-O3-PA	-2.34	124.80	132.83
21	C	302	970	O28-C19-C18	-2.31	120.14	124.12
22	G	201	8Q1	C37-C38-C39	2.26	116.12	112.36
21	C	302	970	C11-C12-C06	-2.22	119.57	123.16
20	A	502	FMN	O2-C2-N1	-2.21	118.16	121.83
20	A	502	FMN	C10-N1-C2	2.20	121.31	116.90
21	C	302	970	O16-C17-C22	-2.18	120.40	122.84
21	C	302	970	C01-C02-C04	-2.13	111.51	116.47
20	A	502	FMN	C4A-C4-N3	2.13	118.61	113.19
21	C	302	970	C21-C22-C23	-2.11	117.15	121.17
21	C	302	970	C07-C06-C12	2.04	120.74	118.74
21	C	302	970	C29-O28-C19	-2.04	114.45	117.53
21	C	302	970	O26-C20-C21	-2.02	120.65	124.12
20	A	502	FMN	C4-N3-C2	-2.01	121.92	125.64

There are no chirality outliers.

All (110) 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
20	A	502	FMN	C5'-O5'-P-O2P
20	A	502	FMN	C5'-O5'-P-O3P
21	C	302	970	C03-C02-C04-C05
21	C	302	970	C03-C02-C04-O08

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Mol	Chain	Res	Type	Atoms
22	G	201	8Q1	C28-C29-C32-C34
22	G	201	8Q1	C30-C29-C32-C34
22	G	201	8Q1	C30-C29-C32-O33
22	G	201	8Q1	C31-C29-C32-C34
22	G	201	8Q1	O33-C32-C34-N36
22	G	201	8Q1	C42-C43-S44-C1
24	J	402	NDP	C5B-O5B-PA-O1A
24	J	402	NDP	O4B-C4B-C5B-O5B
24	J	402	NDP	C2N-C3N-C7N-N7N
25	J	403	UQ	C1-C6-C7-C8
25	J	403	UQ	C5-C6-C7-C8
25	J	403	UQ	C7-C8-C9-C10
25	J	403	UQ	C12-C13-C14-C16
25	J	403	UQ	C14-C16-C17-C18
28	N	201	CDL	O1-C1-CB2-OB2
28	N	201	CDL	C11-CA5-OA6-CA4
28	N	201	CDL	CB2-OB2-PB2-OB3
28	N	201	CDL	CB3-OB5-PB2-OB3
23	J	401	PEE	O4-C10-O2-C2
28	N	201	CDL	OA7-CA5-OA6-CA4
23	J	401	PEE	C11-C10-O2-C2
28	N	201	CDL	O1-C1-CA2-OA2
25	J	403	UQ	C22-C23-C24-C26
25	J	403	UQ	C13-C14-C16-C17
28	N	201	CDL	CA2-C1-CB2-OB2
28	N	201	CDL	CB7-C71-C72-C73
28	N	201	CDL	CA7-C31-C32-C33
23	J	401	PEE	C30-C31-C32-C33
28	N	201	CDL	CA2-OA2-PA1-OA5
24	J	402	NDP	C2D-C1D-N1N-C6N
28	N	201	CDL	CB2-C1-CA2-OA2
23	J	401	PEE	C42-C43-C44-C45
28	N	201	CDL	C71-C72-C73-C74
23	J	401	PEE	C32-C33-C34-C35
23	J	401	PEE	C33-C34-C35-C36
28	N	201	CDL	C11-C12-C13-C14
23	J	401	PEE	C34-C35-C36-C37
23	J	401	PEE	C19-C20-C21-C22
28	N	201	CDL	C51-C52-C53-C54
23	J	401	PEE	C13-C14-C15-C16
24	J	402	NDP	O4D-C4D-C5D-O5D
28	N	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
28	N	201	CDL	OA5-CA3-CA4-CA6
23	J	401	PEE	C1-C2-C3-O3
22	G	201	8Q1	O33-C32-C34-O35
23	J	401	PEE	C11-C12-C13-C14
22	G	201	8Q1	O27-C28-C29-C30
22	G	201	8Q1	O27-C28-C29-C31
28	N	201	CDL	CA6-CA4-OA6-CA5
22	G	201	8Q1	C31-C29-C32-O33
22	G	201	8Q1	C29-C32-C34-O35
28	N	201	CDL	C31-CA7-OA8-CA6
28	N	201	CDL	OB6-CB4-CB6-OB8
28	N	201	CDL	C31-C32-C33-C34
28	N	201	CDL	OB5-CB3-CB4-CB6
22	G	201	8Q1	C6-C7-C8-C9
24	J	402	NDP	O4D-C1D-N1N-C6N
23	J	401	PEE	O2-C2-C3-O3
23	J	401	PEE	C15-C16-C17-C18
28	N	201	CDL	OA9-CA7-OA8-CA6
22	G	201	8Q1	C13-C14-C15-C16
28	N	201	CDL	CB2-OB2-PB2-OB5
23	J	401	PEE	C1-O3P-P-O2P
28	N	201	CDL	CA2-OA2-PA1-OA4
28	N	201	CDL	CB2-OB2-PB2-OB4
28	N	201	CDL	CB3-OB5-PB2-OB4
23	J	401	PEE	C12-C13-C14-C15
24	J	402	NDP	C3D-C4D-C5D-O5D
28	N	201	CDL	OA5-CA3-CA4-OA6
23	J	401	PEE	C43-C44-C45-C46
22	G	201	8Q1	O27-C28-C29-C32
22	G	201	8Q1	C28-C29-C32-O33
24	J	402	NDP	C2N-C3N-C7N-O7N
25	J	403	UQ	C15-C14-C16-C17
28	N	201	CDL	CA3-OA5-PA1-OA2
28	N	201	CDL	CB3-CB4-CB6-OB8
23	J	401	PEE	C31-C30-O3-C3
21	C	302	970	C20-C19-O28-C29
23	J	401	PEE	O5-C30-O3-C3
28	N	201	CDL	C52-C53-C54-C55
20	A	502	FMN	C2'-C1'-N10-C10
22	G	201	8Q1	C29-C32-C34-N36
28	N	201	CDL	OB5-CB3-CB4-OB6
28	N	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	J	401	PEE	C37-C38-C39-C40
23	J	401	PEE	C38-C39-C40-C41
23	J	401	PEE	C36-C37-C38-C39
25	J	403	UQ	C12-C11-C9-C10
23	J	401	PEE	O3-C30-C31-C32
28	N	201	CDL	C72-C71-CB7-OB8
22	G	201	8Q1	N36-C37-C38-C39
24	J	402	NDP	C5B-O5B-PA-O3
25	J	403	UQ	C22-C23-C24-C25
23	J	401	PEE	O5-C30-C31-C32
24	J	402	NDP	C3B-C4B-C5B-O5B
23	J	401	PEE	C44-C45-C46-C47
28	N	201	CDL	C72-C71-CB7-OB9
20	A	502	FMN	C1'-C2'-C3'-O3'
25	J	403	UQ	C7-C8-C9-C11
21	C	302	970	C18-C19-O28-C29
25	J	403	UQ	C11-C12-C13-C14

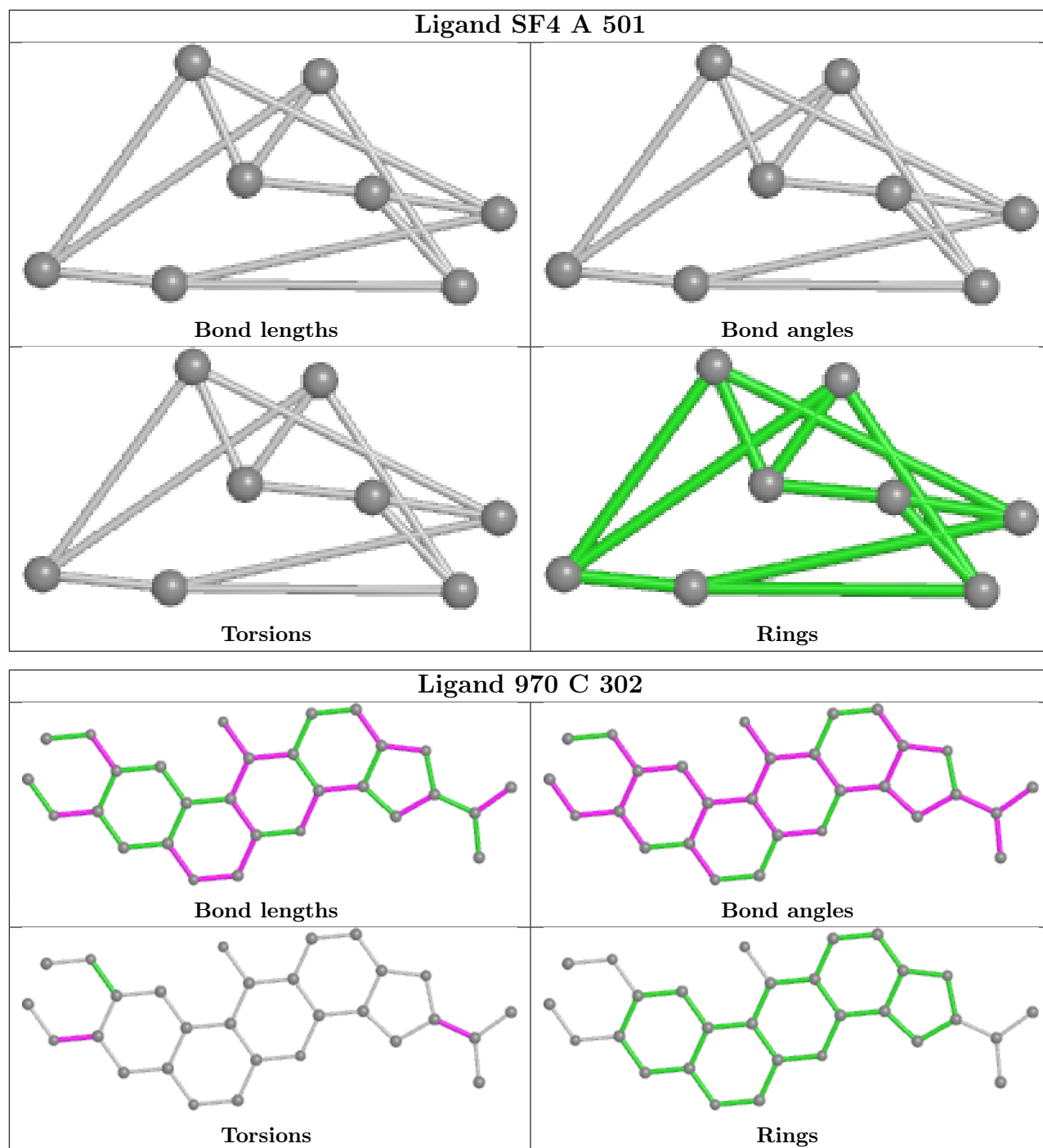
There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	501	SF4	2	0
25	J	403	UQ	6	0
20	A	502	FMN	6	0
23	J	401	PEE	3	0
28	N	201	CDL	1	0
19	C	301	SF4	3	0
26	O	301	FES	1	0
24	J	402	NDP	3	0

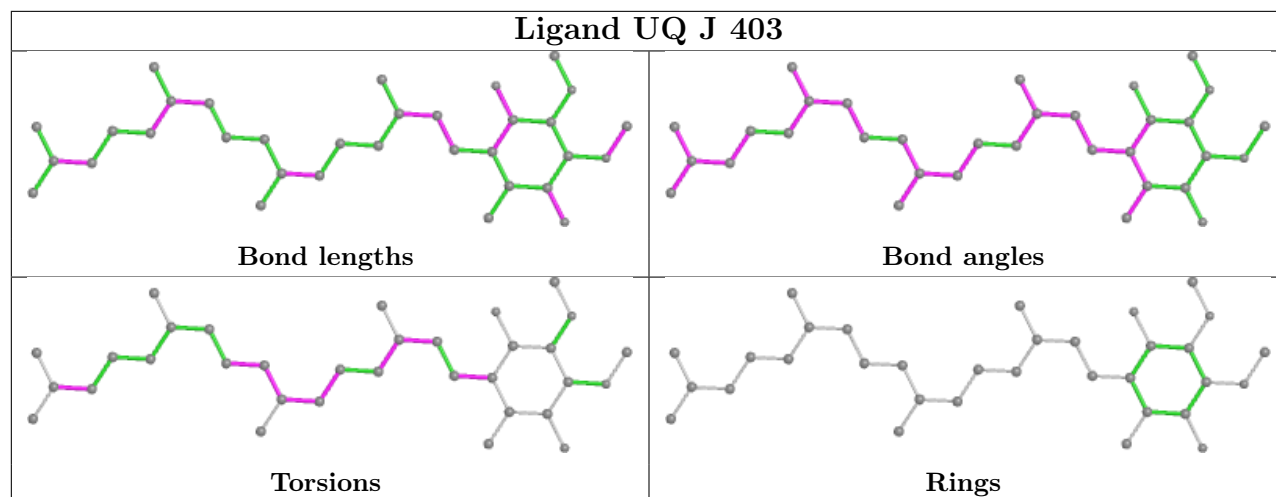
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

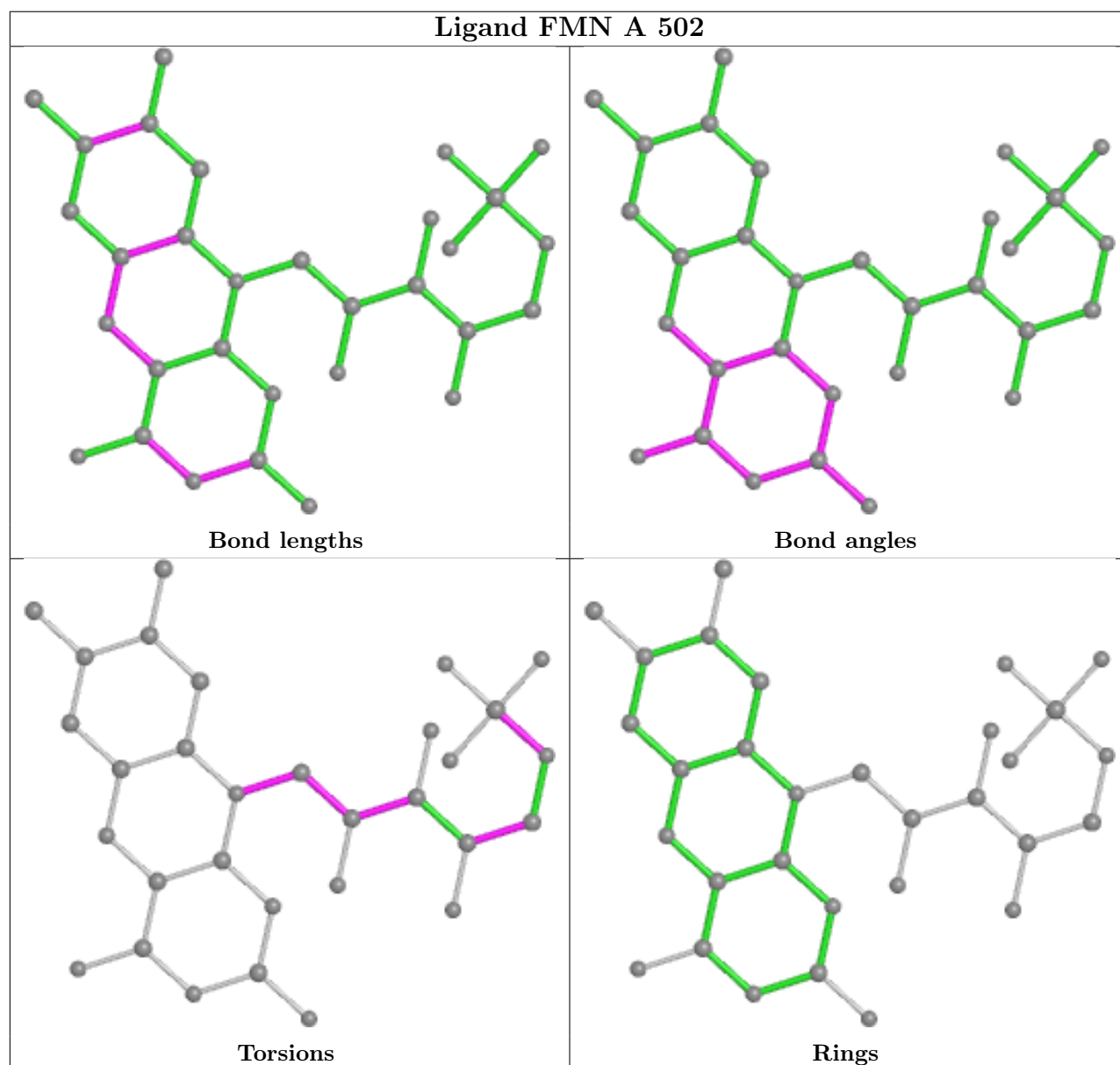


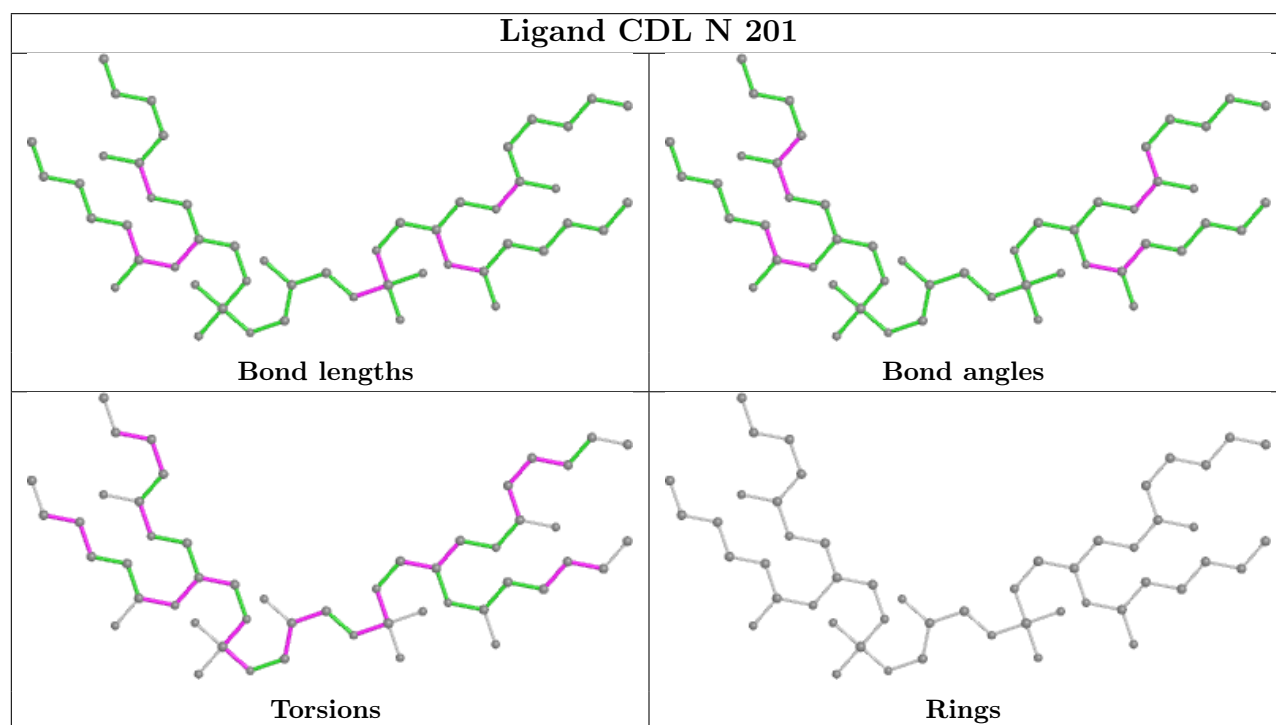
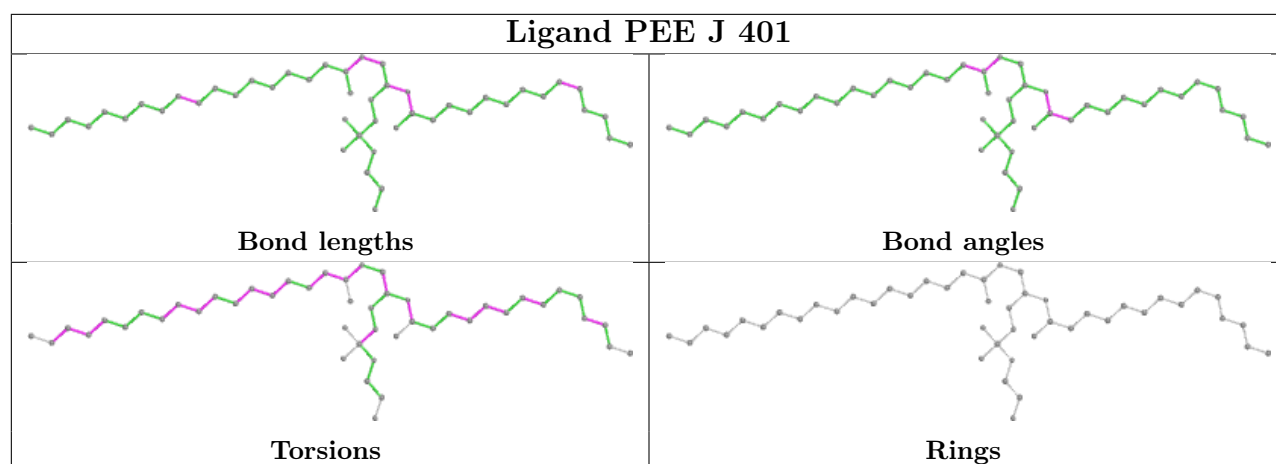


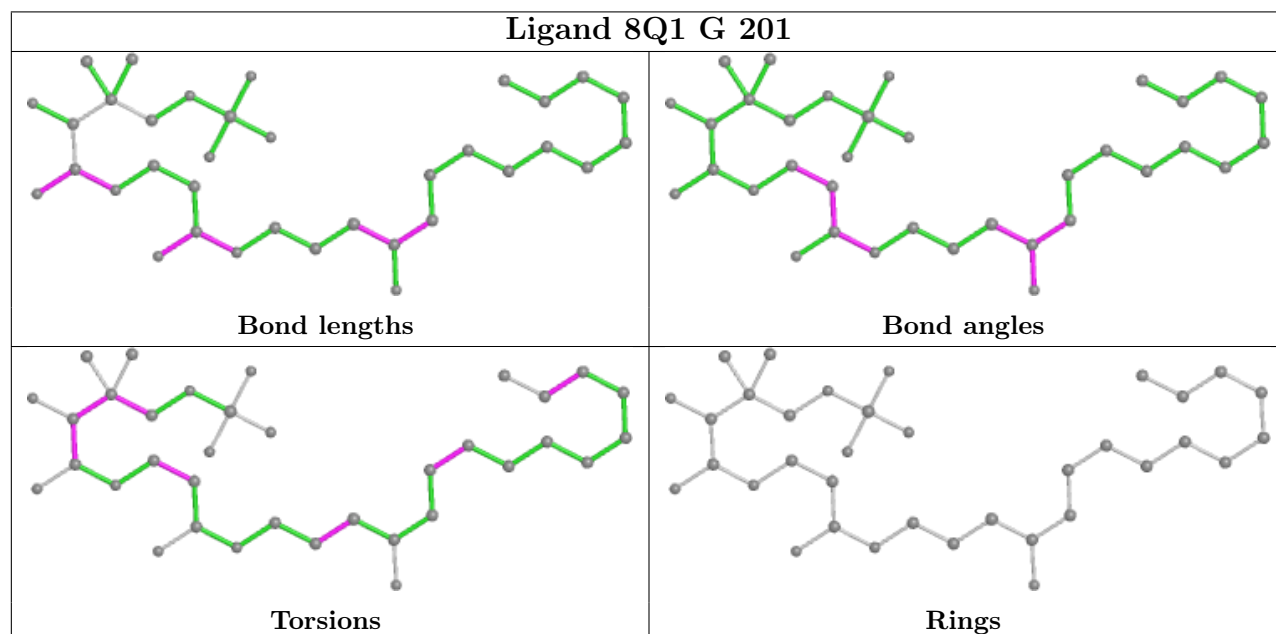
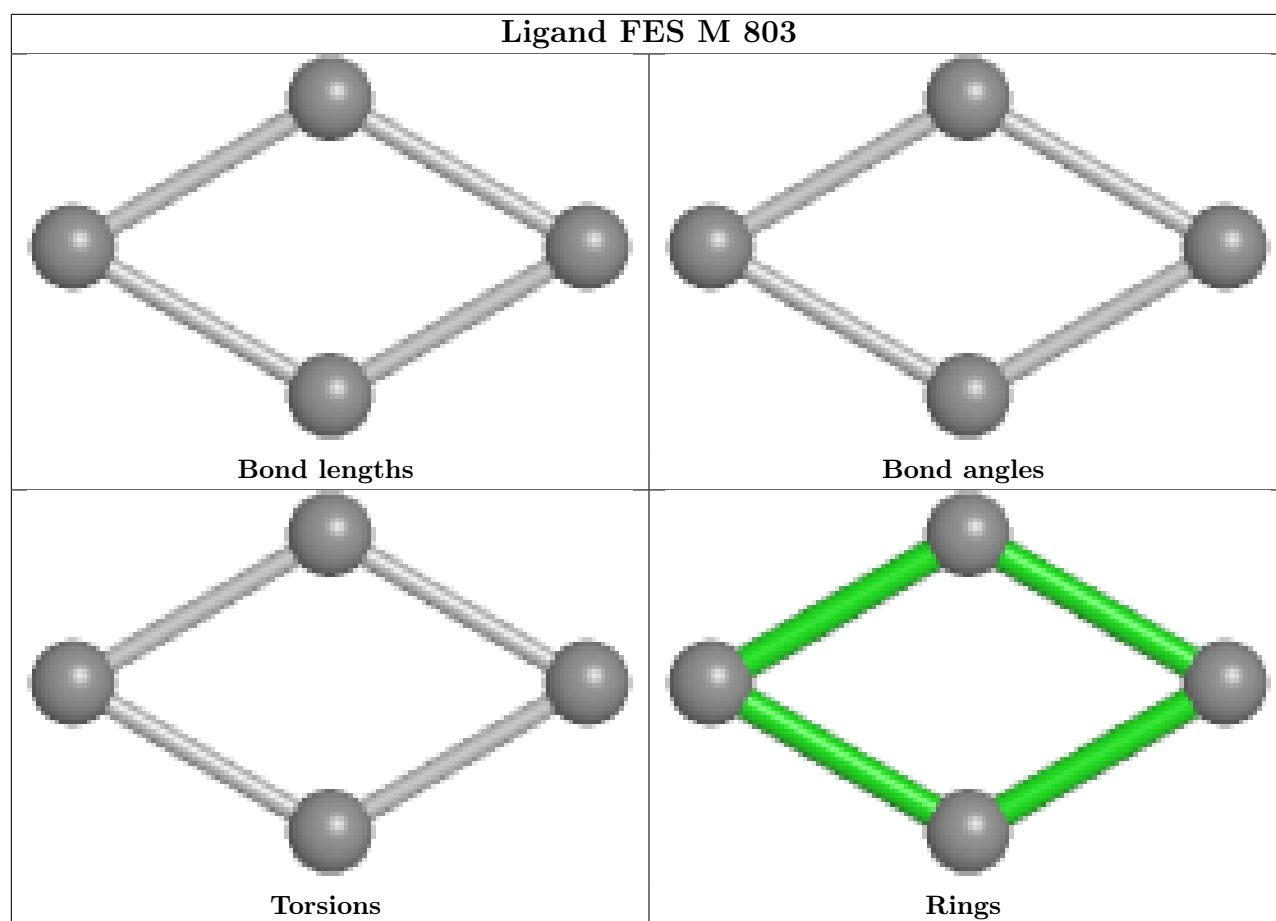
## Ligand UQ J 403

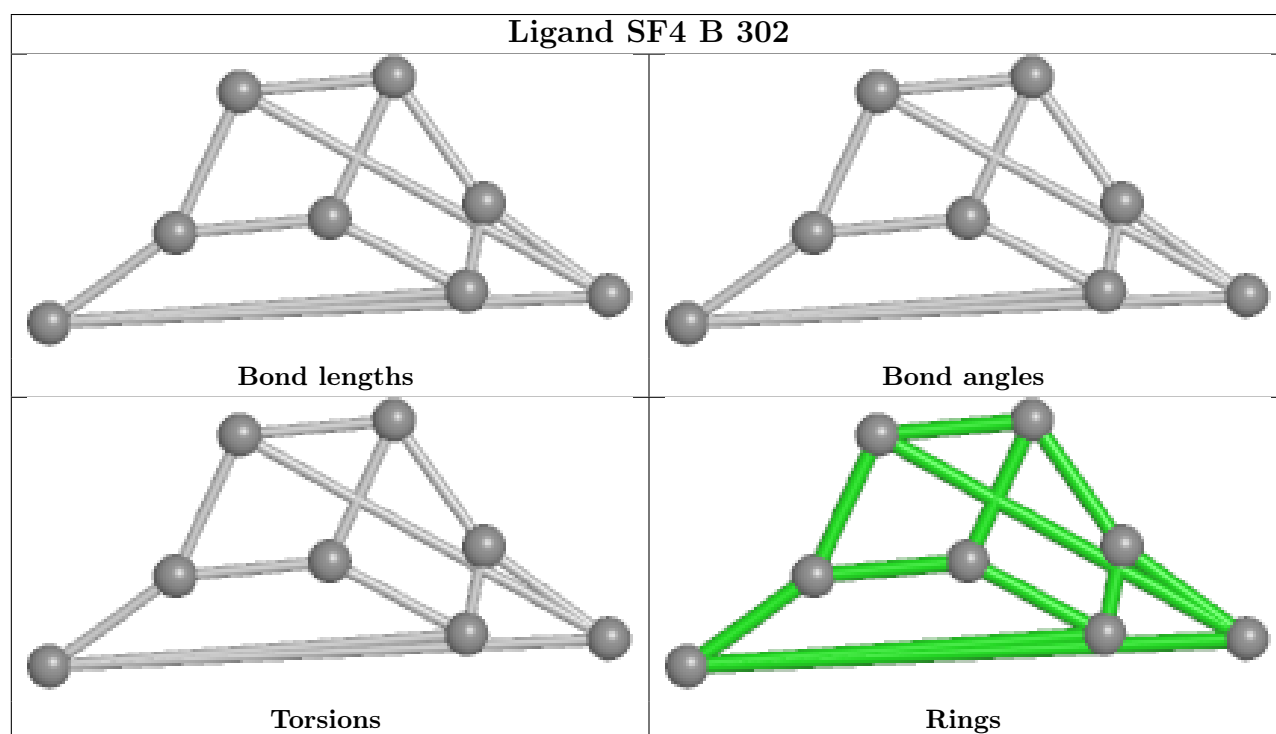
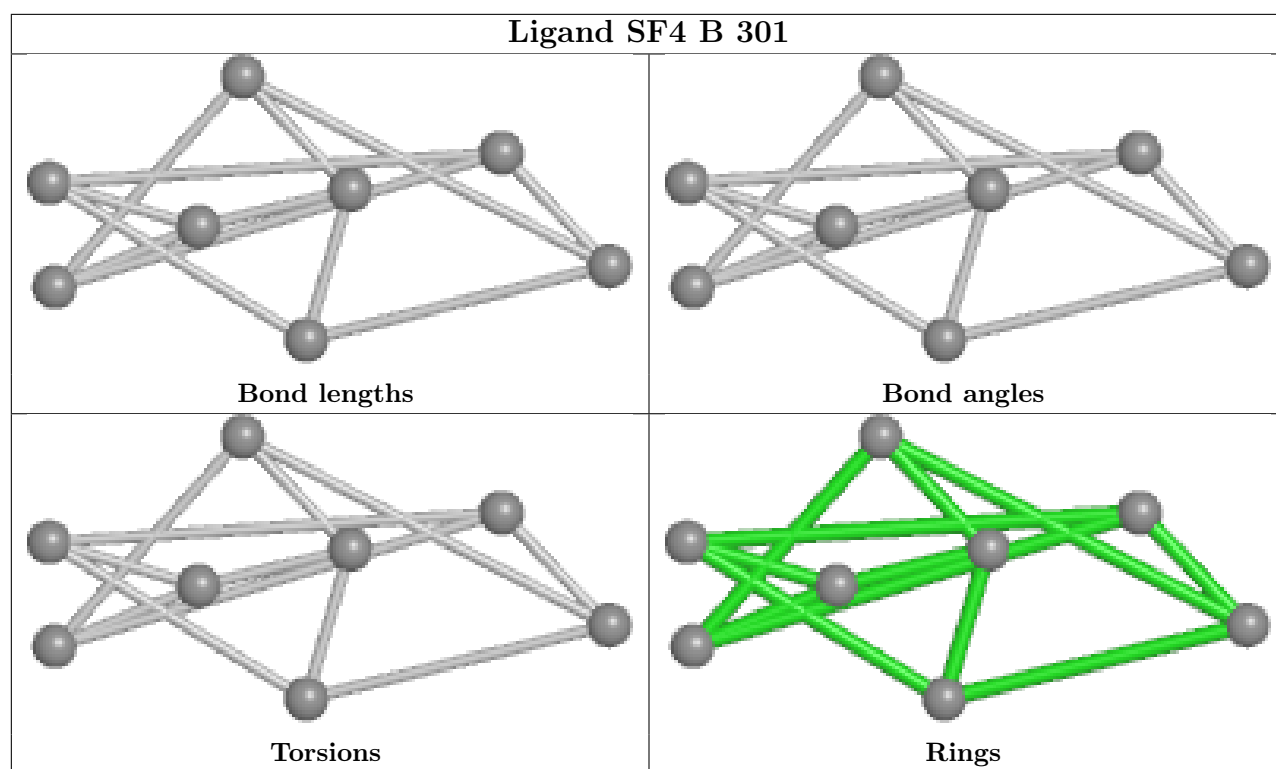


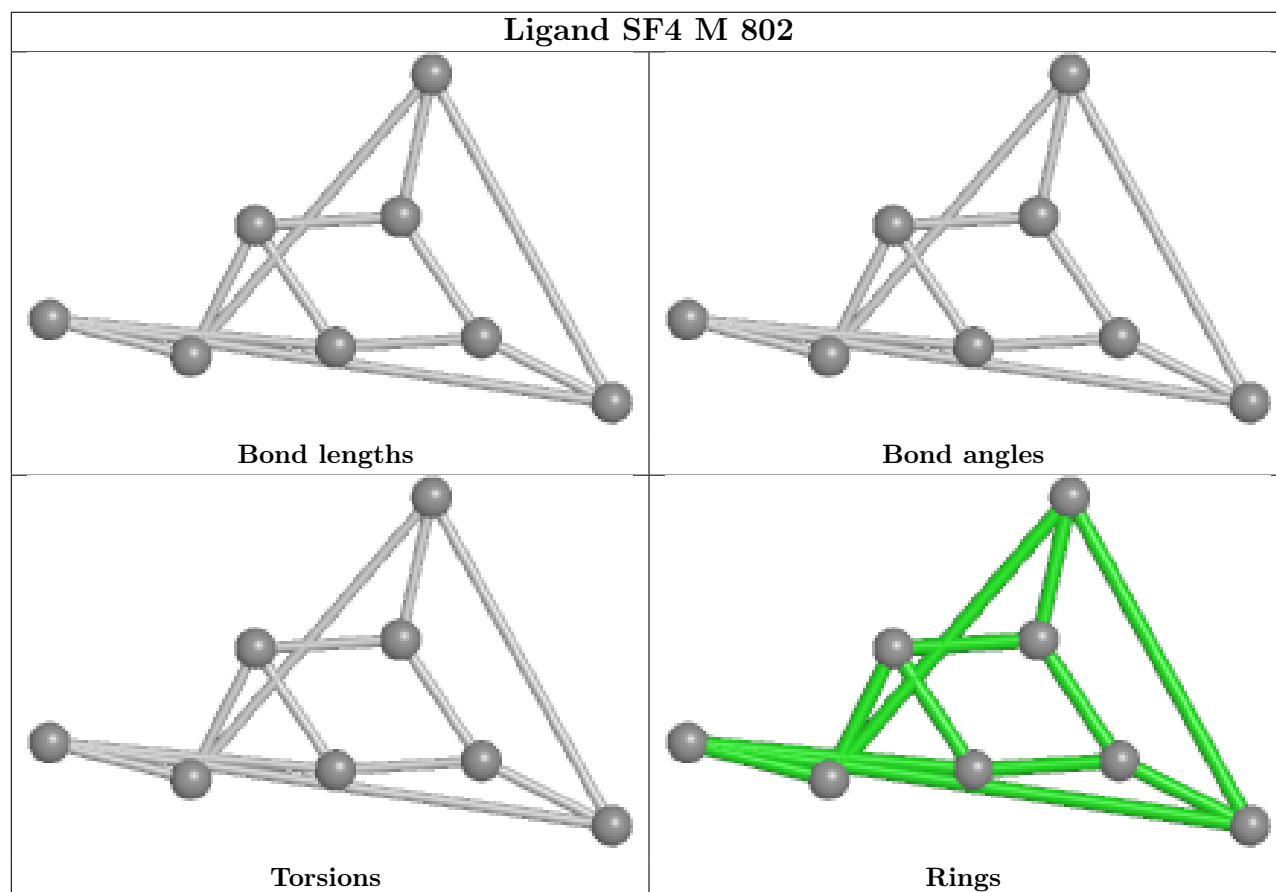
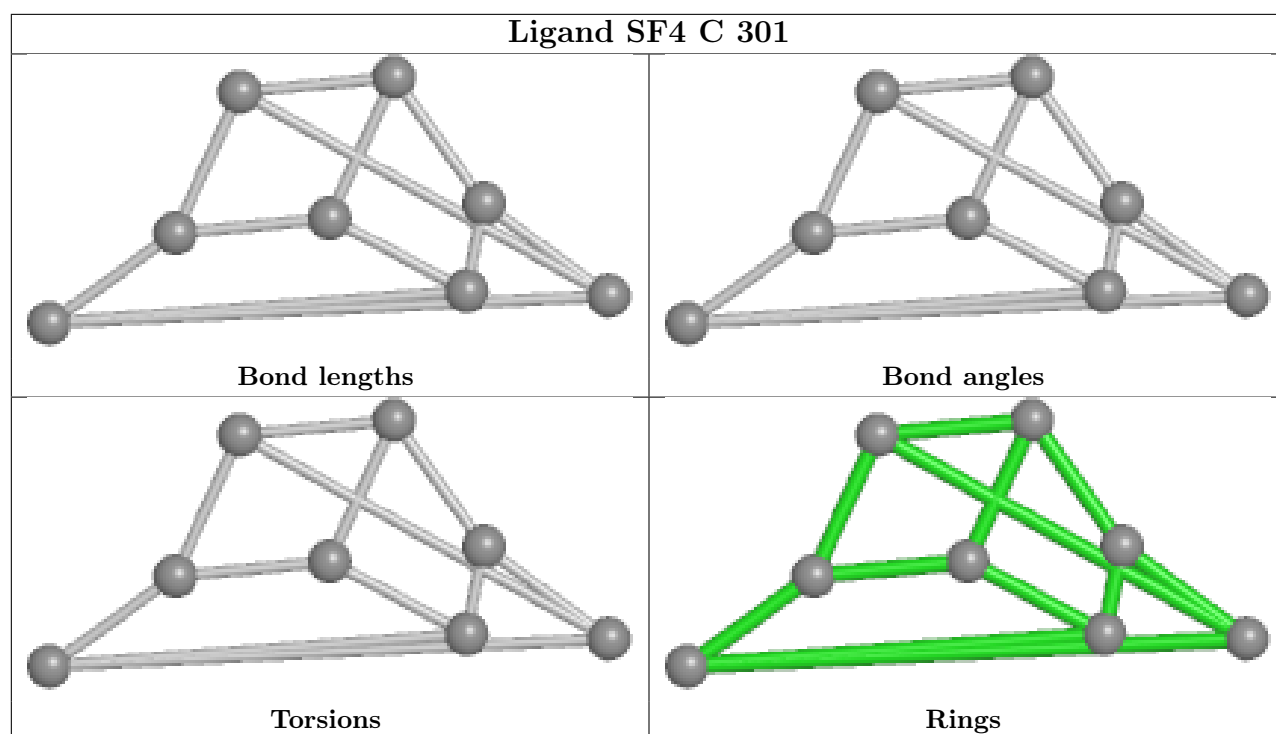
## Ligand FMN A 502

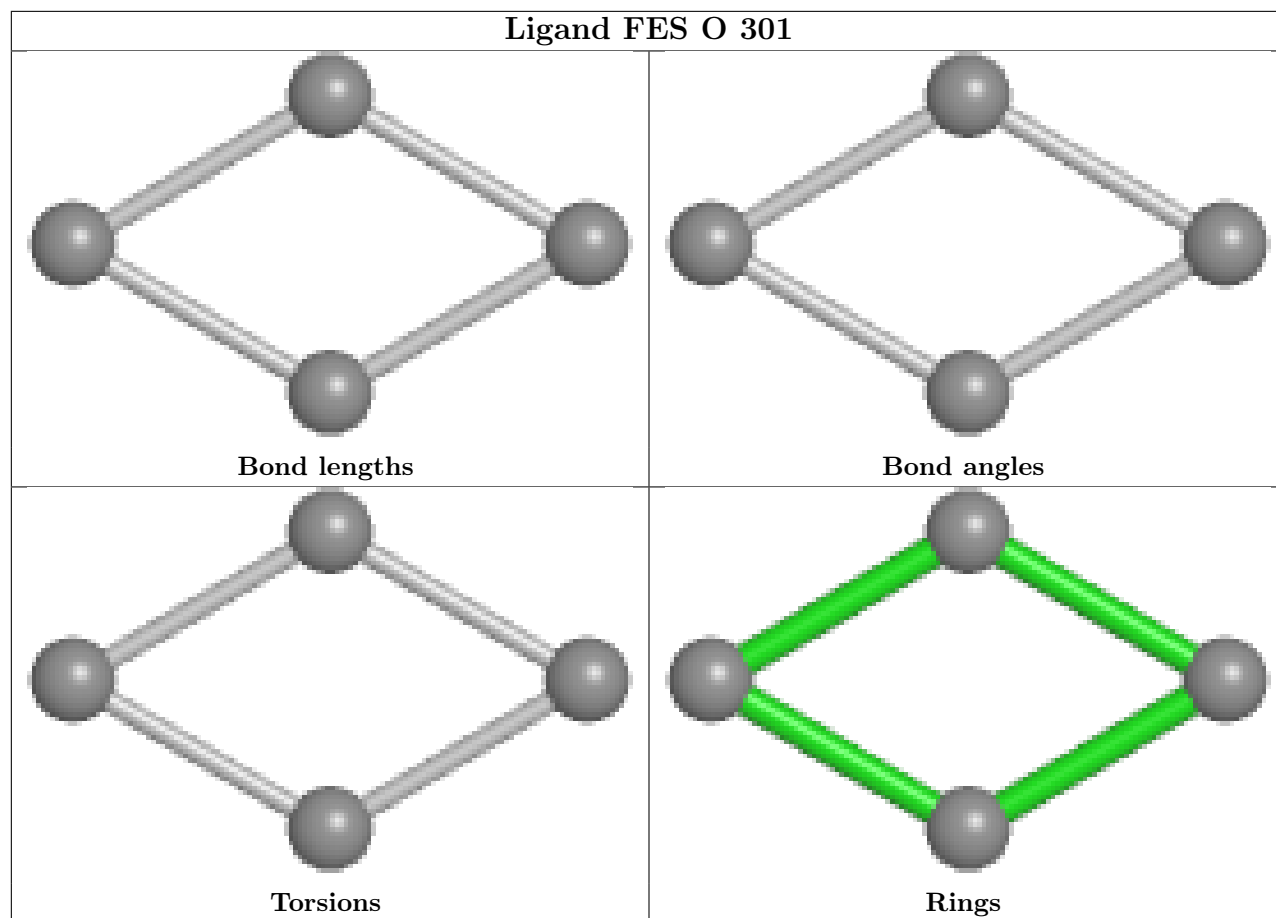


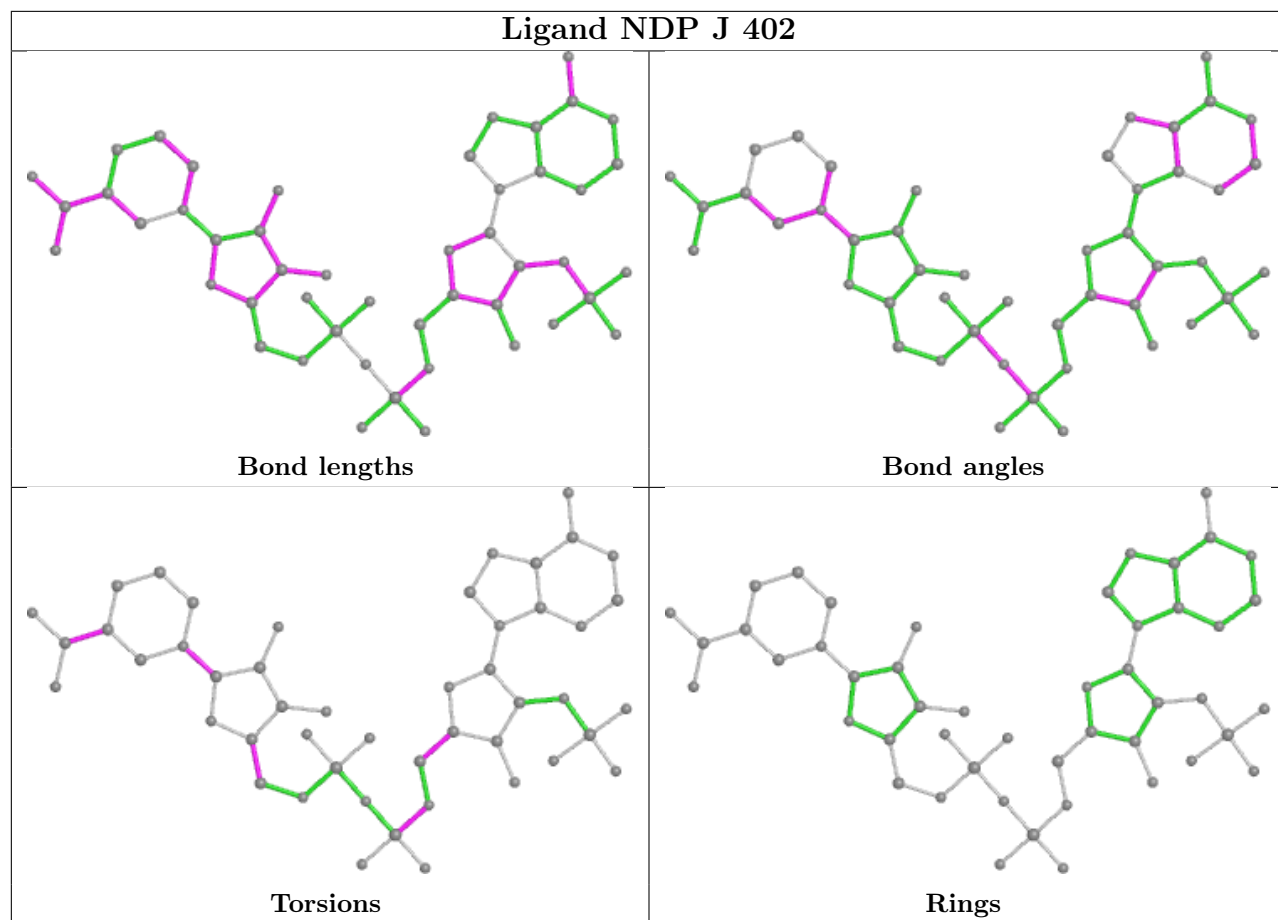


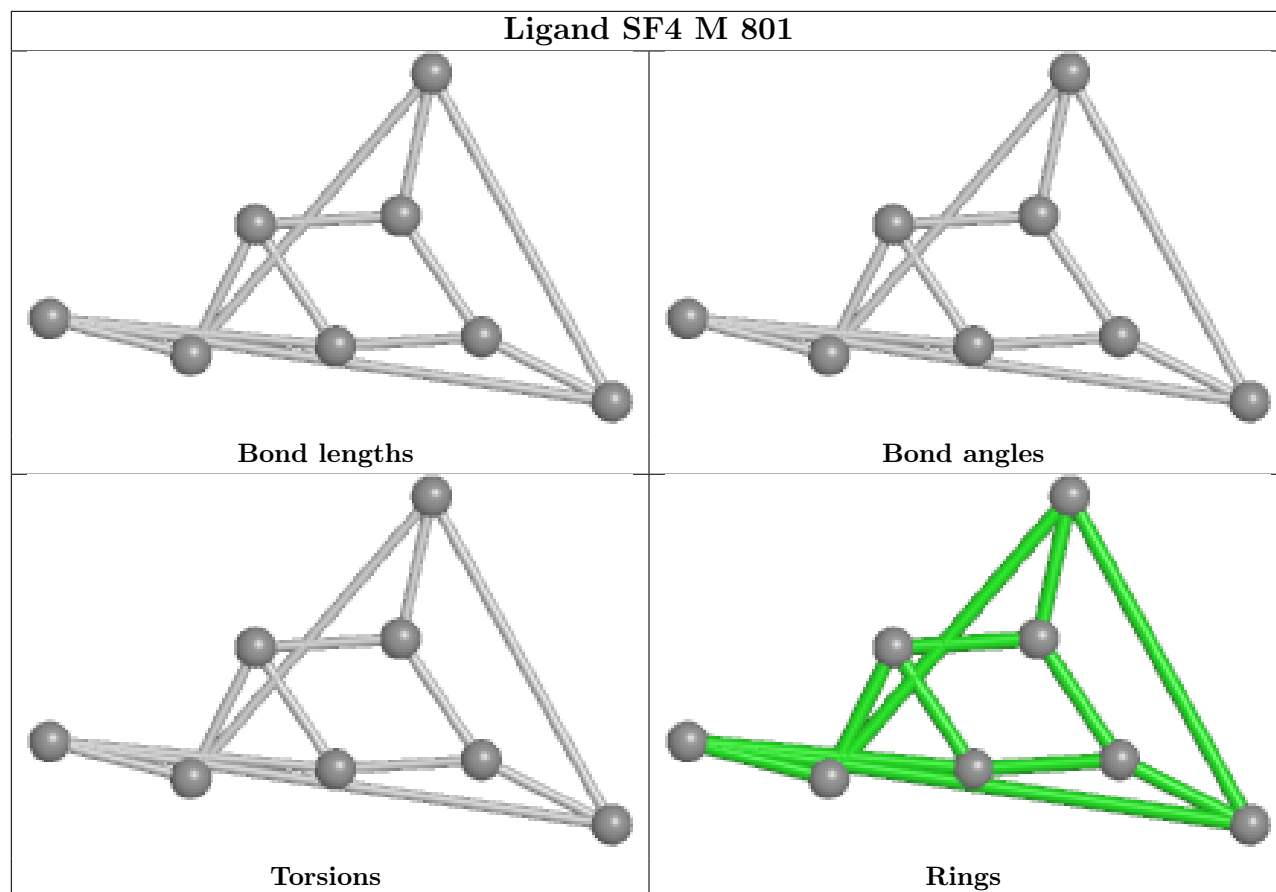












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



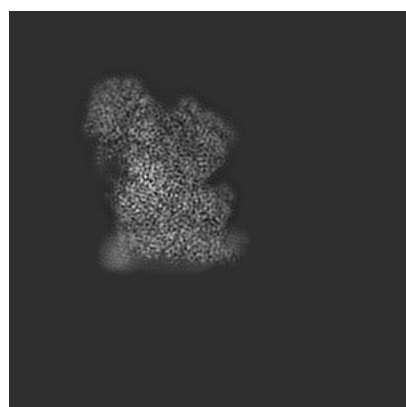
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32203. These allow visual inspection of the internal detail of the map and identification of artifacts.

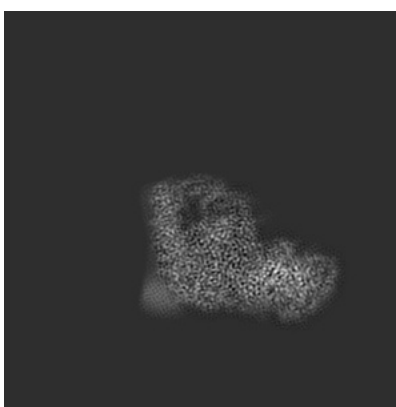
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

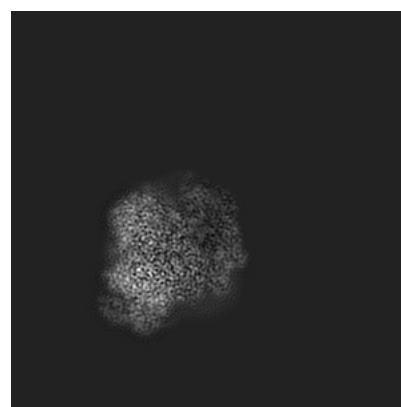
#### 6.1.1 Primary map



X



Y

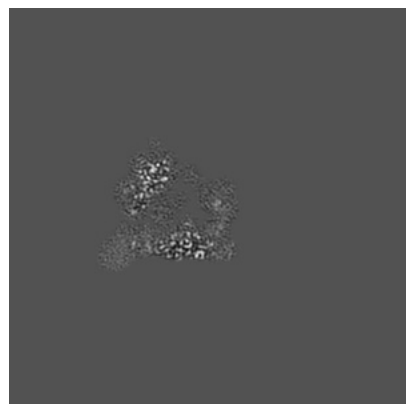


Z

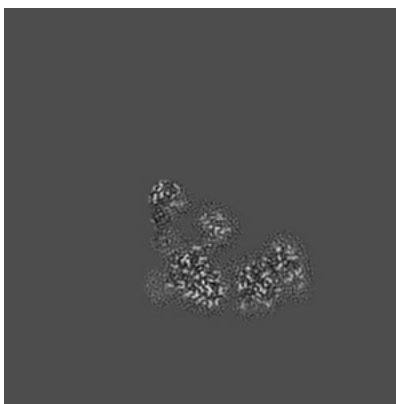
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

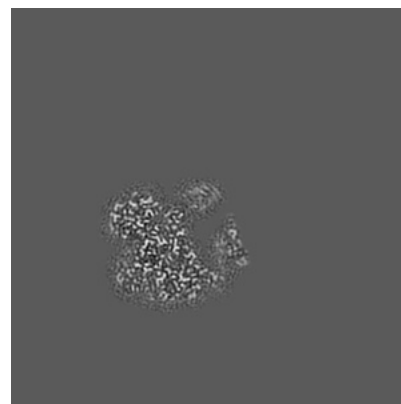
#### 6.2.1 Primary map



X Index: 155



Y Index: 155

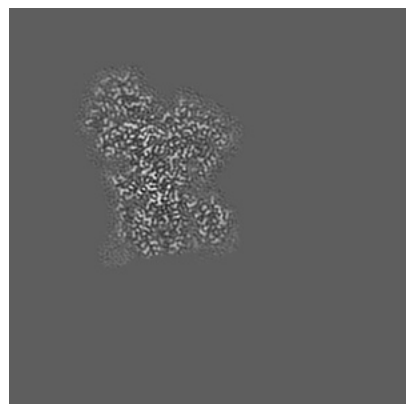


Z Index: 155

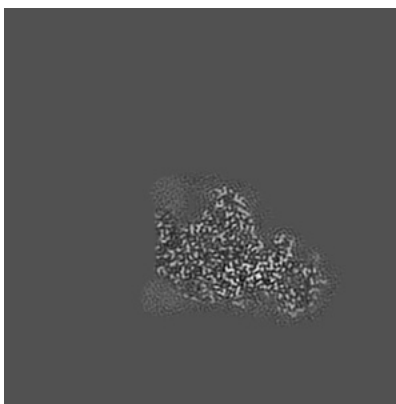
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

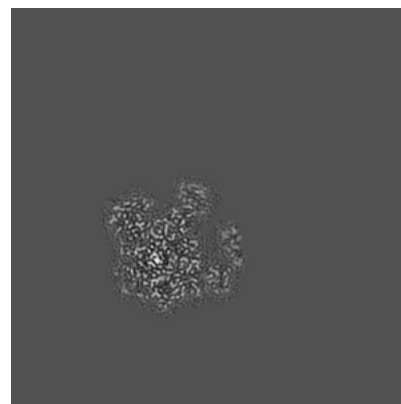
### 6.3.1 Primary map



X Index: 108



Y Index: 106

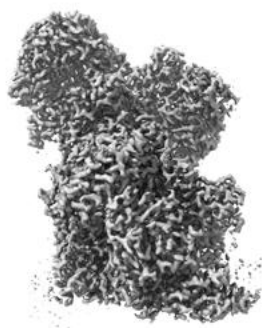


Z Index: 164

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0309. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

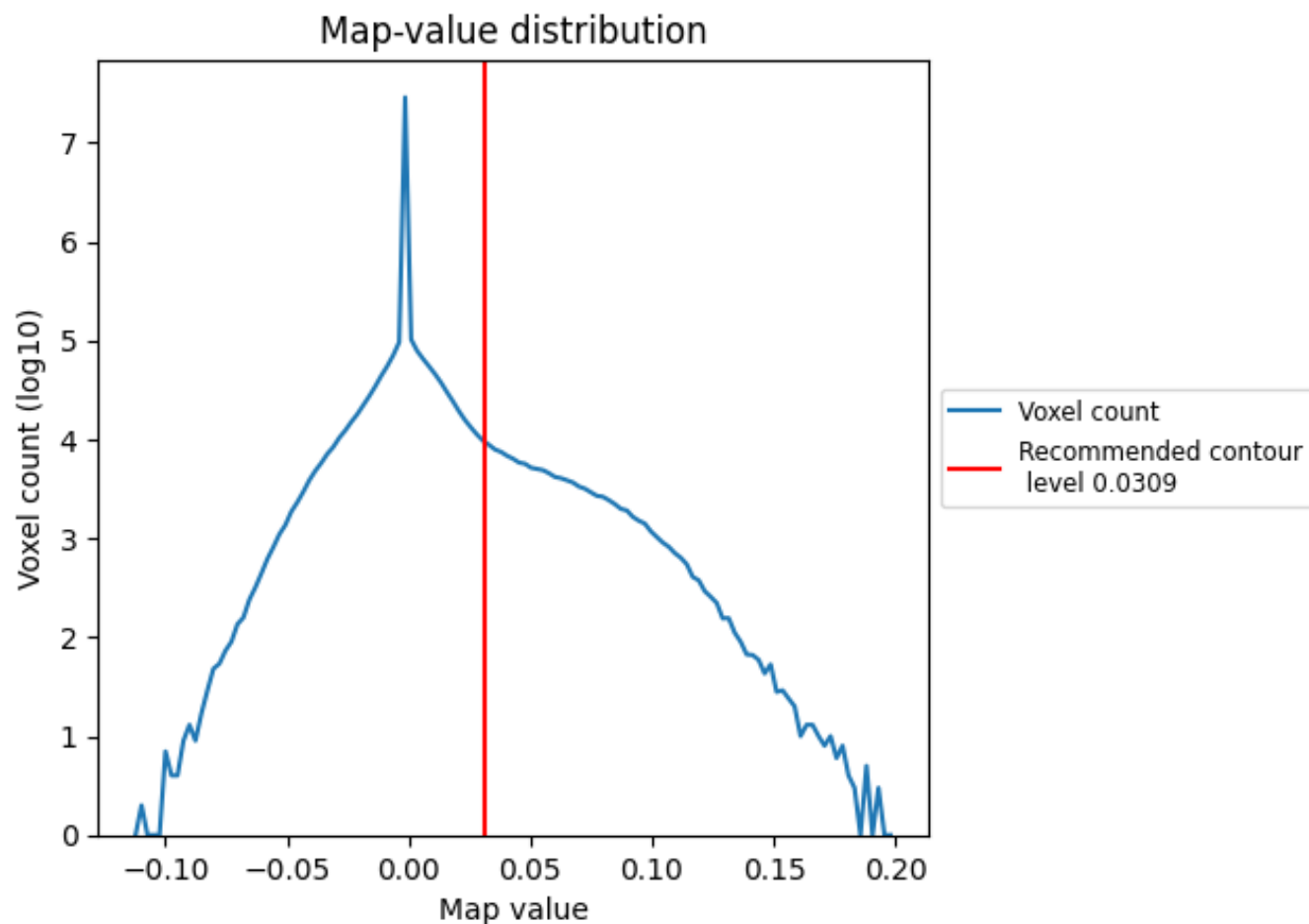
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

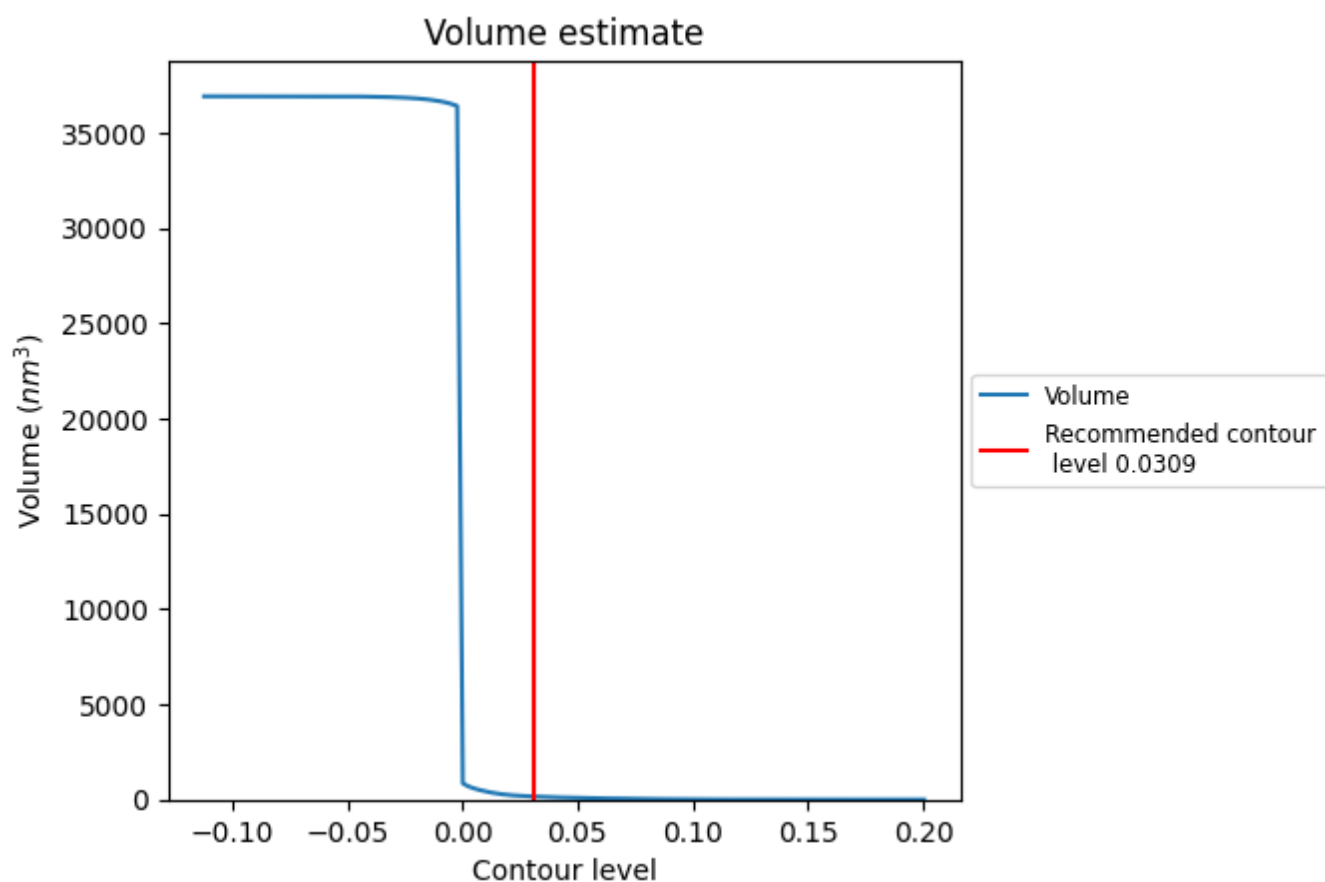
This section contains the results of statistical analysis of the map.

### 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.

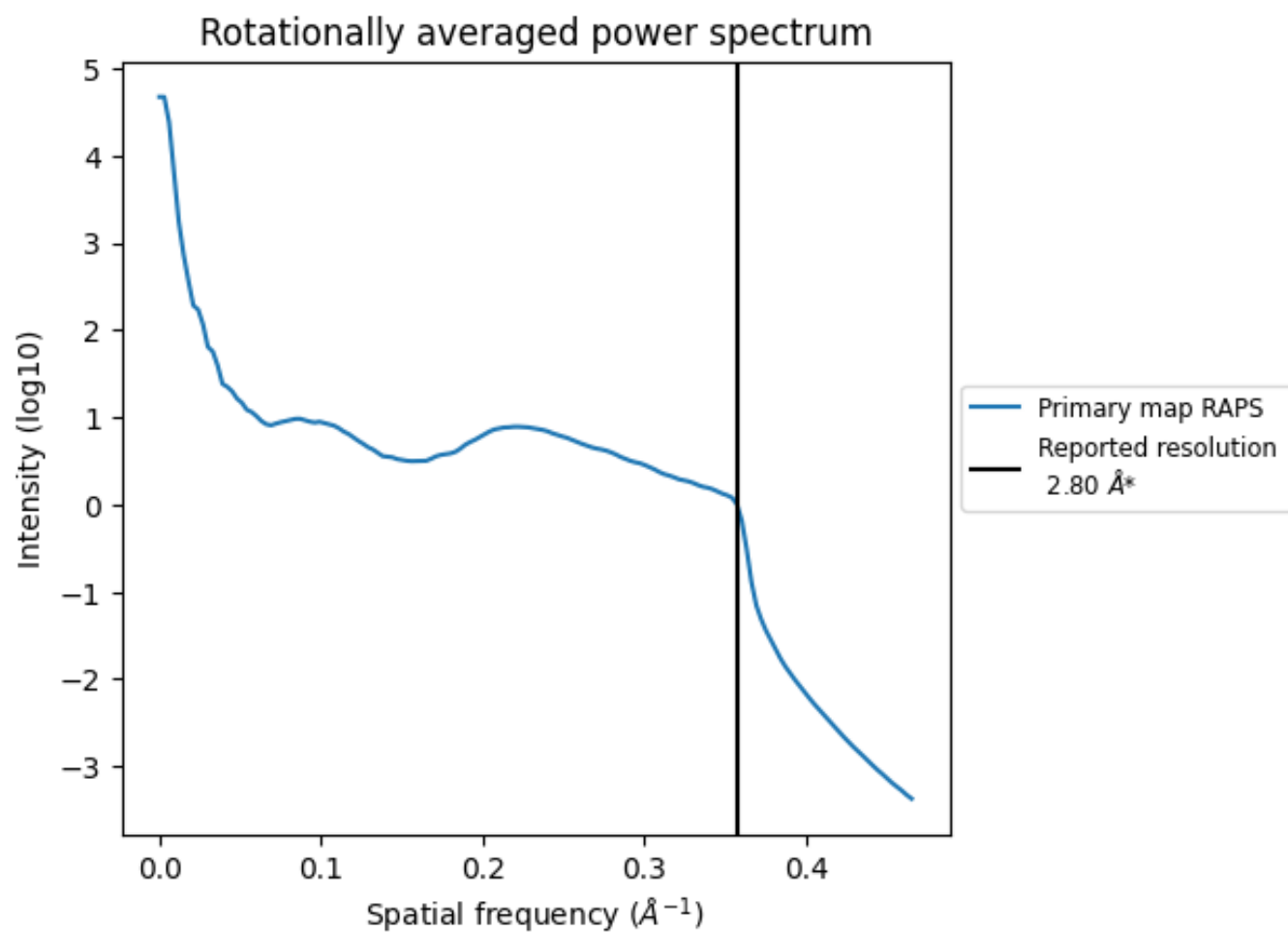
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160  $\text{nm}^3$ ; this corresponds to an approximate mass of 144 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 0.357  $\text{\AA}^{-1}$

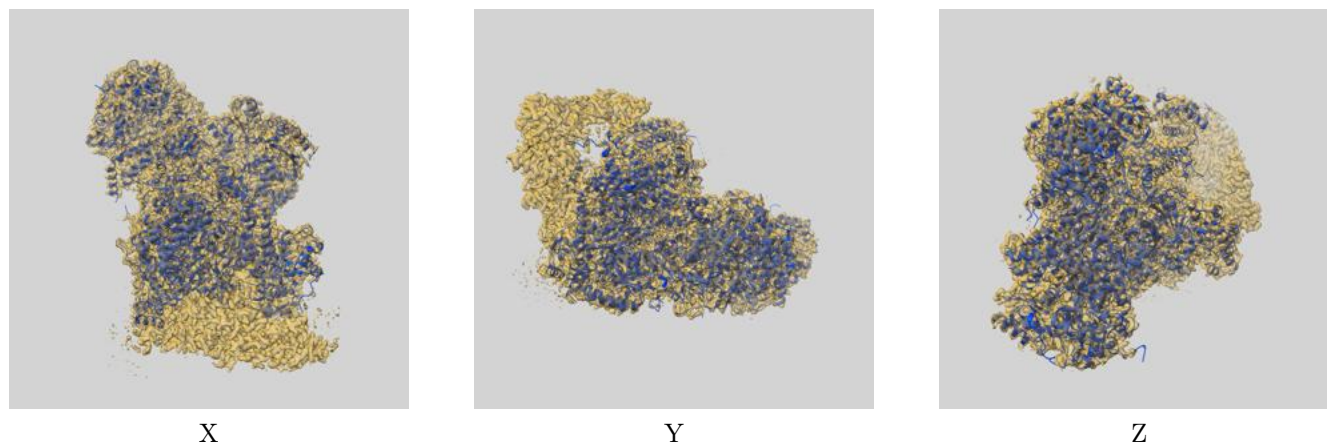
## 8 Fourier-Shell correlation

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-32203 and PDB model 7VYF. Per-residue inclusion information can be found in section [3](#) on page [13](#).

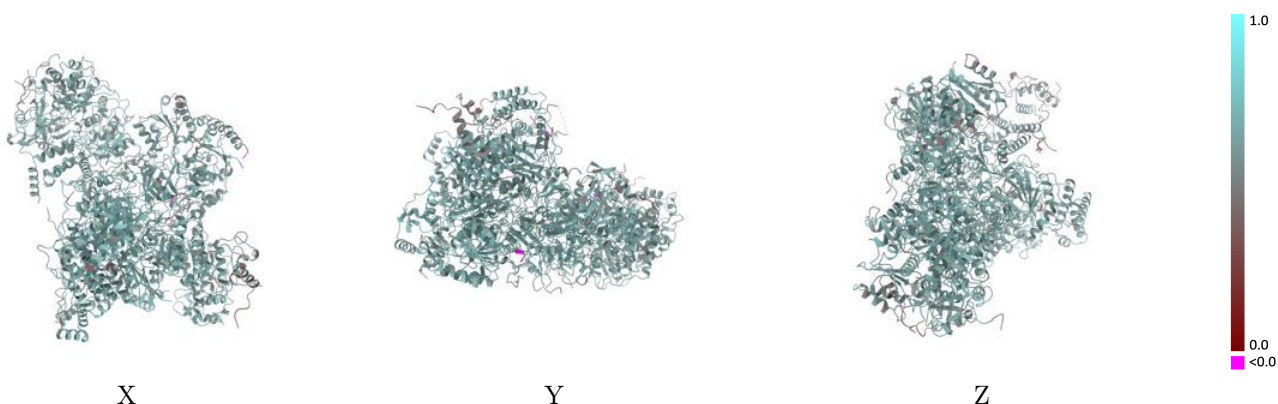
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0309 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.

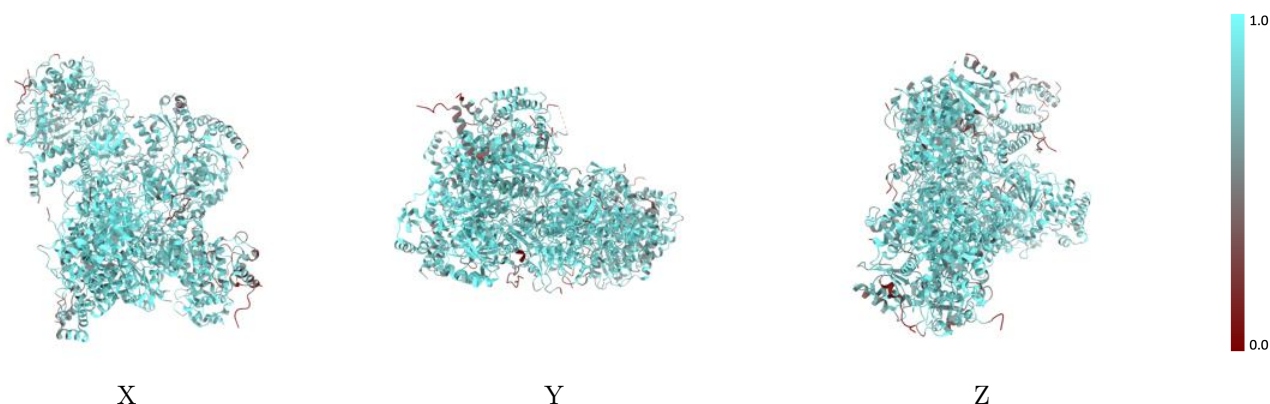


## 9.2 Q-score mapped to coordinate model [i](#)



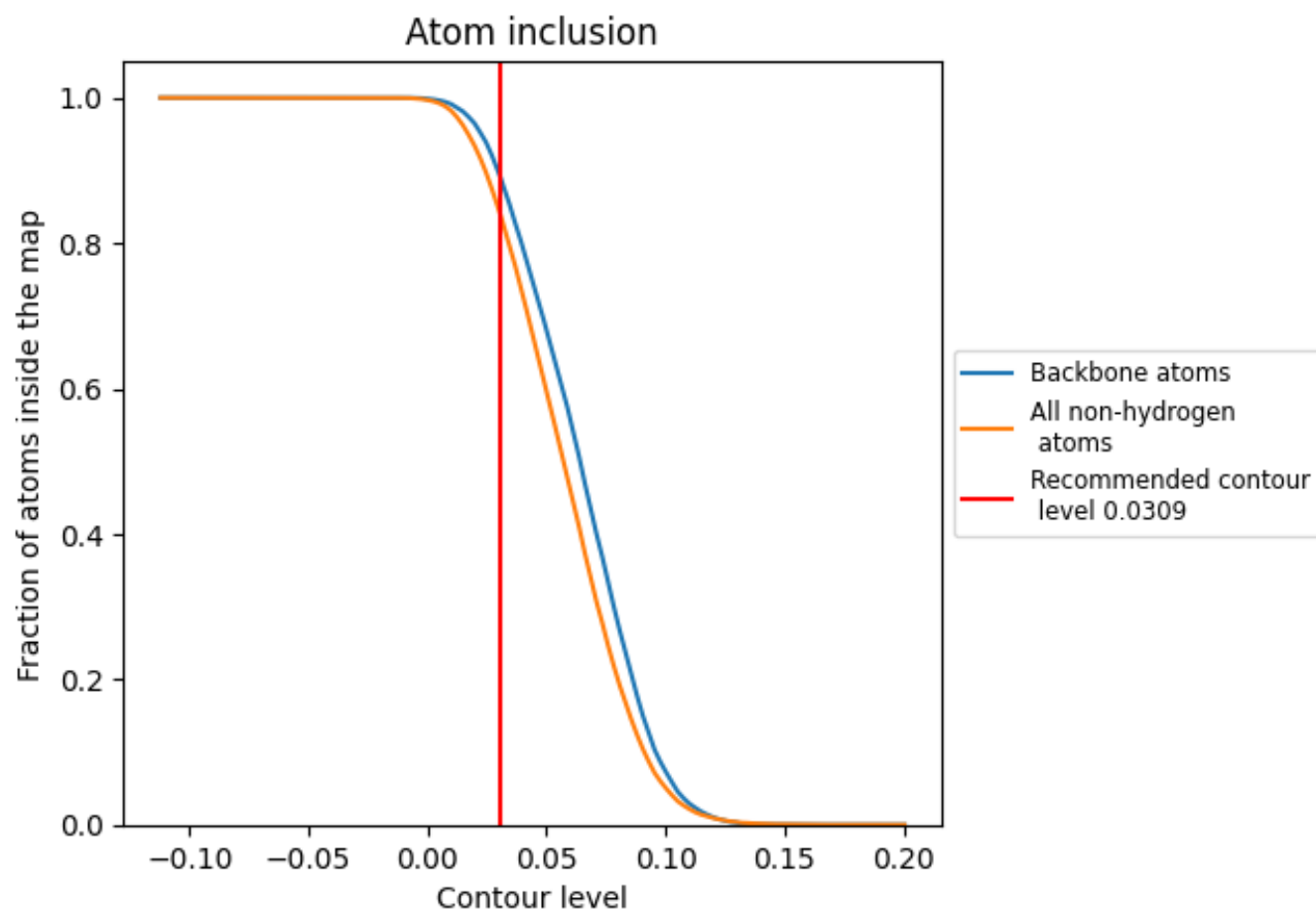
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0309).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.0309) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8365	 0.6180
A	 0.8289	 0.6110
B	 0.9158	 0.6470
C	 0.9353	 0.6470
E	 0.8047	 0.6080
F	 0.7320	 0.5650
G	 0.5734	 0.5100
H	 0.8067	 0.6000
I	 0.7540	 0.5940
J	 0.8483	 0.6210
K	 0.5972	 0.5420
L	 0.8410	 0.6250
M	 0.8641	 0.6250
N	 0.7360	 0.6050
O	 0.7728	 0.5920
P	 0.9273	 0.6480
Q	 0.9226	 0.6500
T	 0.7091	 0.5960
W	 0.7500	 0.5770

