



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 07:55 PM JST

PDB ID : 7VXU
EMDB ID : EMD-32188
Title : Matrix arm of deactive state CI from Q10 dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-13
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

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.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

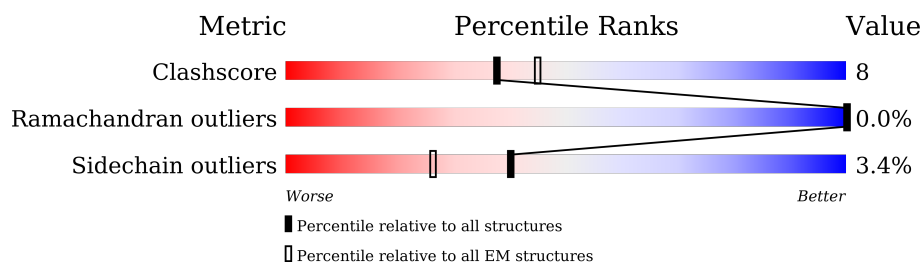
1 Overall quality at a glance

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 ≥ 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	458	
2	B	212	
3	C	196	
4	E	128	
5	F	99	
6	G	156	
7	H	116	
8	I	113	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	376	
10	K	110	
11	L	175	
12	M	718	
13	N	145	
14	O	249	
15	P	264	
16	Q	473	
17	T	123	
18	W	144	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 27965 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	431	Total	C	N	O	S	0	0
			3318	2095	591	612	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 Complex I-20kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1244	792	227	211	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
			691	434	129	126	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
			678	438	102	133	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	297	Total	C	N	O	S	0	0
			2356	1513	421	414	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	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	379	Total	C	N	O	S	0	0
			3044	1945	522	554	23		

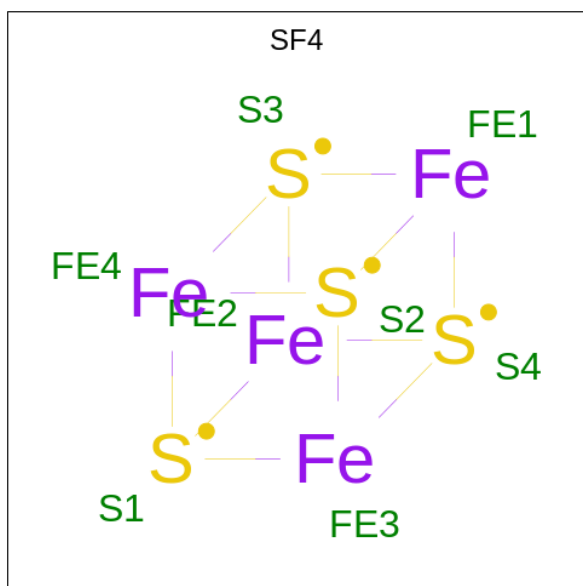
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

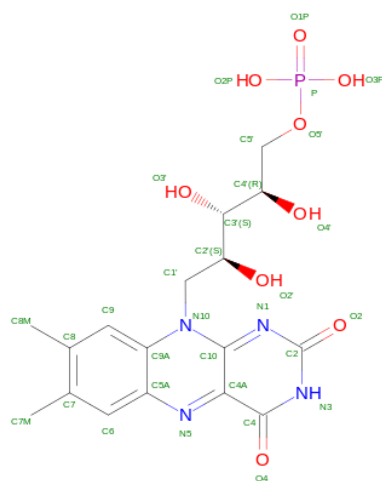
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			218	138	40	39	1		

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



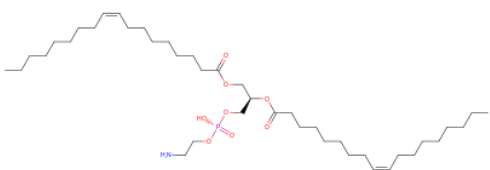
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			16	8	8	
19	B	1	Total	Fe	S	0
			16	8	8	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			16	8	8	
19	M	1	Total	Fe	S	0
			16	8	8	

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

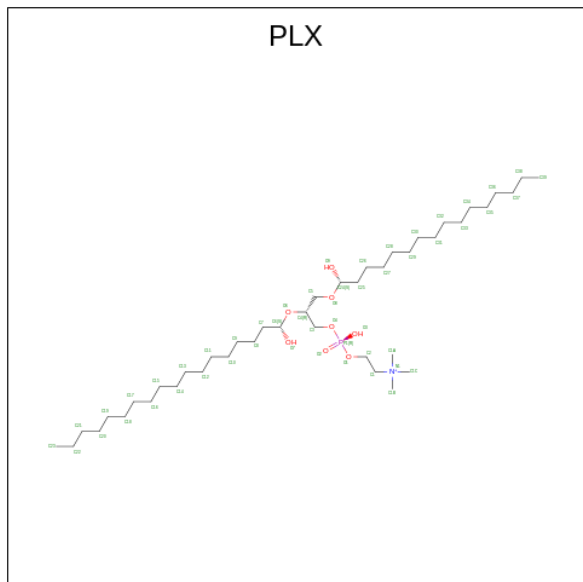
- Molecule 21 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

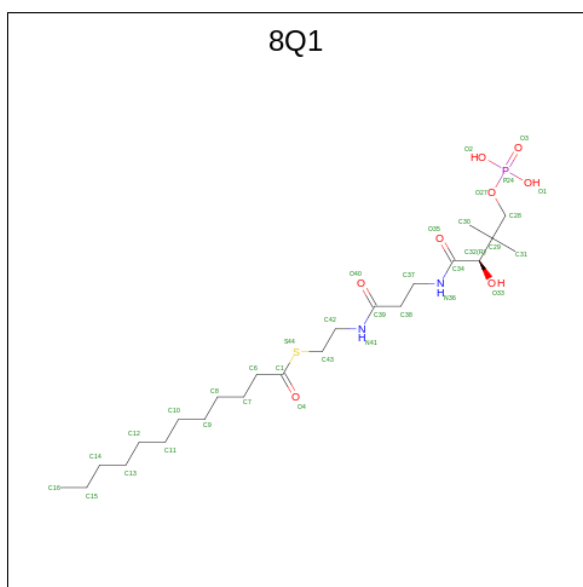
- Molecule 22 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSA

NE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



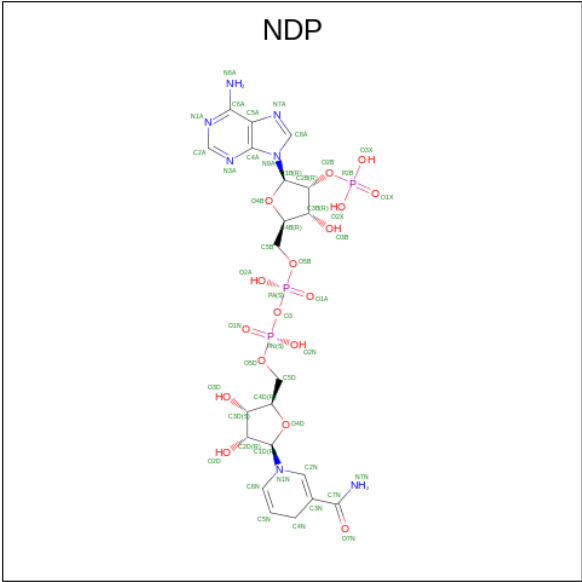
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



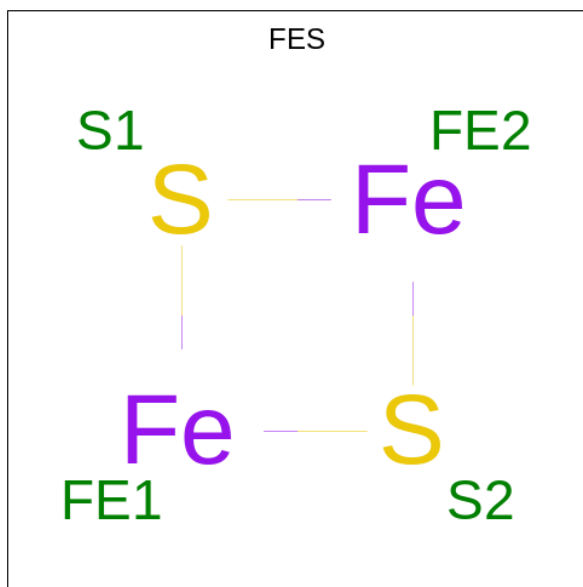
Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total	C	N	O	P	S
			35	23	2	8	1	1

- Molecule 24 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 25 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

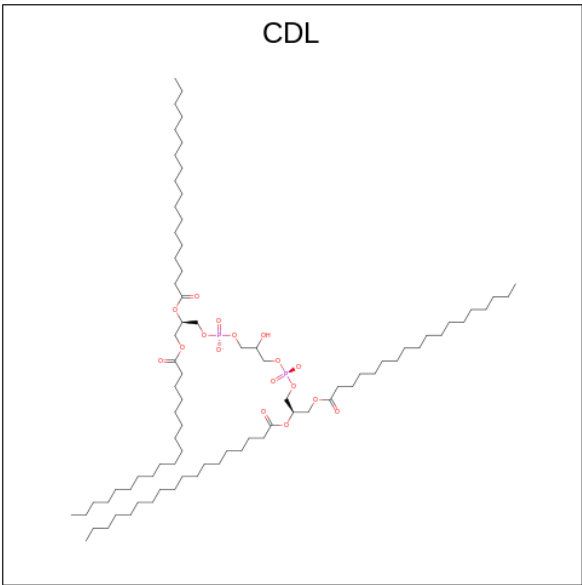


Mol	Chain	Residues	Atoms			AltConf
25	M	1	Total	Fe	S	0
			4	2	2	
25	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

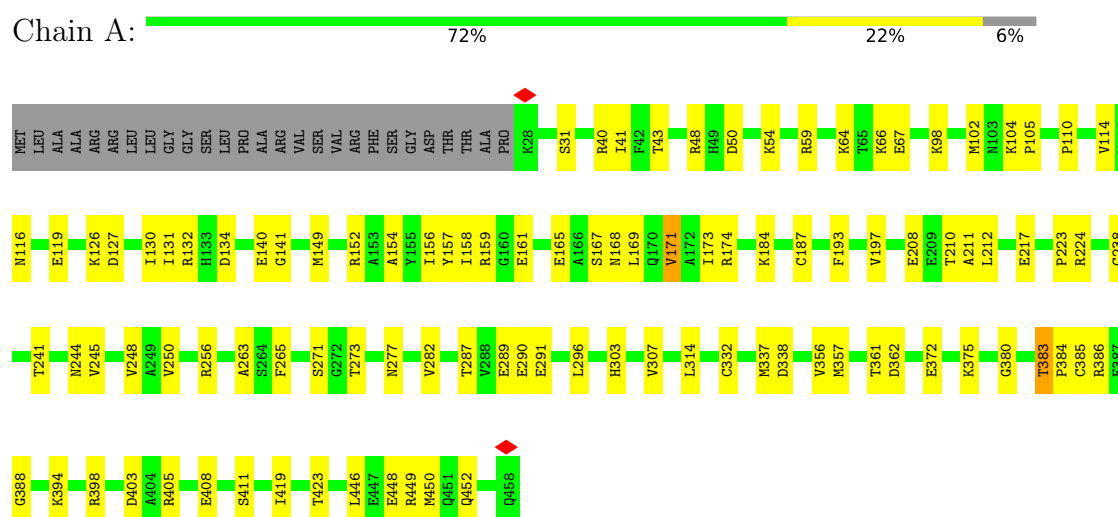
- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

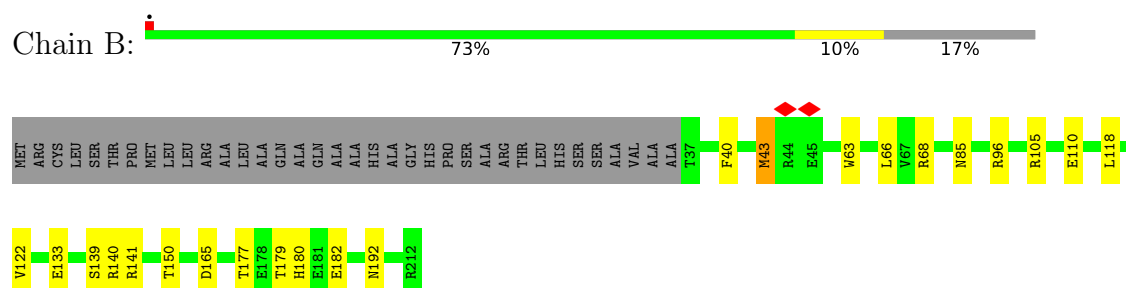
3 Residue-property plots

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.

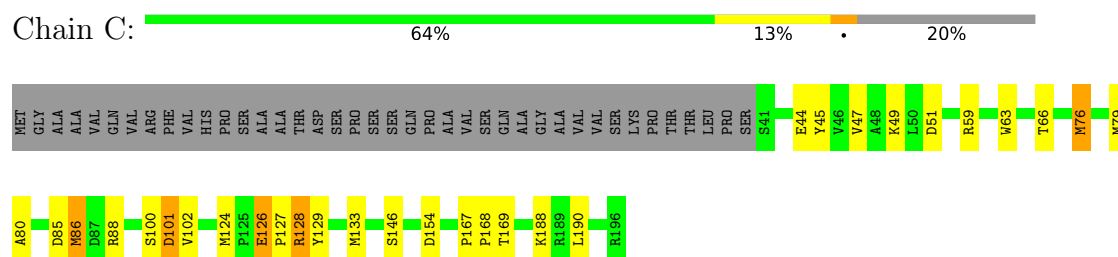
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

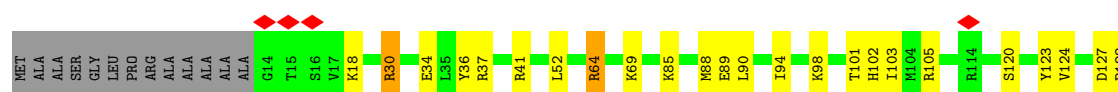


- Molecule 3: Complex I-20kD



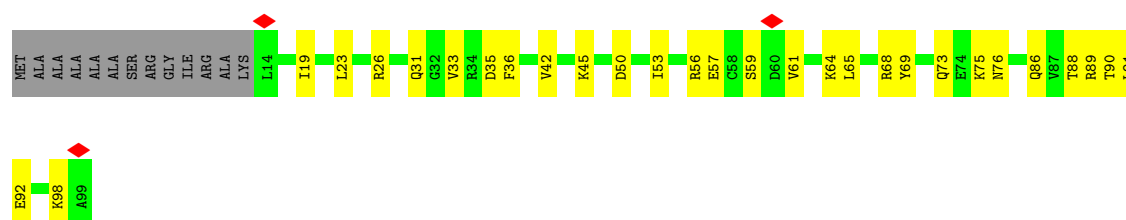
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 

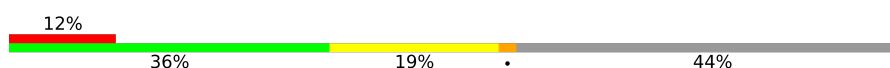


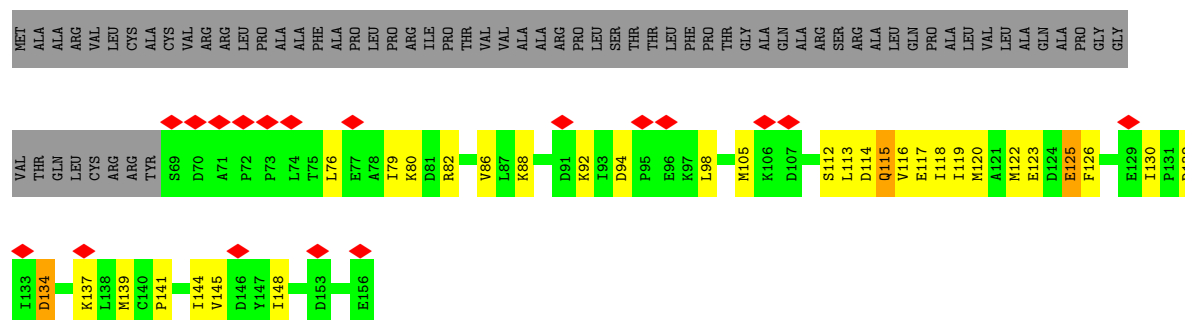
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 




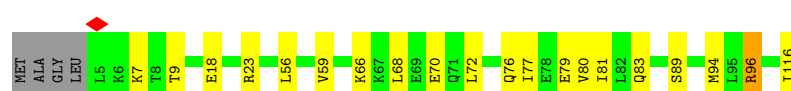
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 



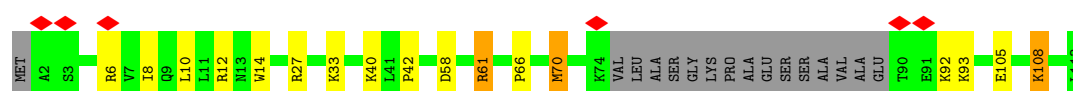
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H: 



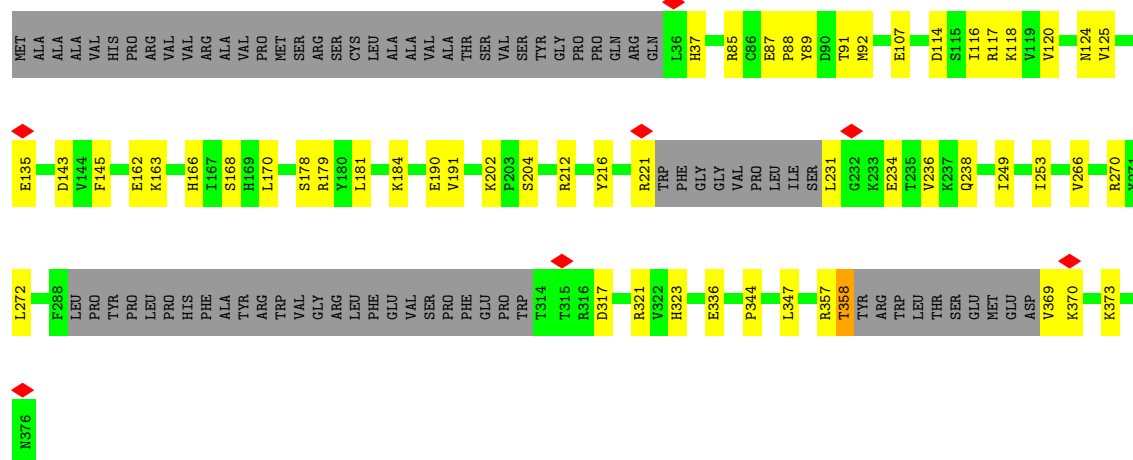
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 



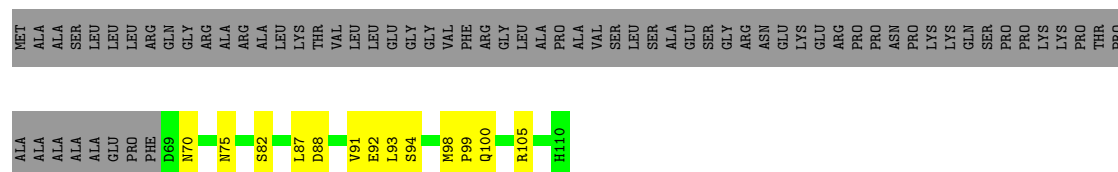
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

Chain J: 



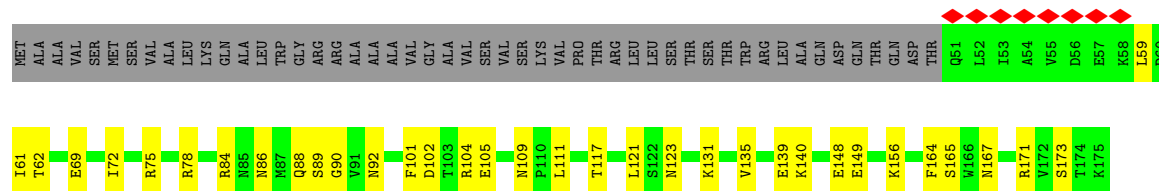
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 




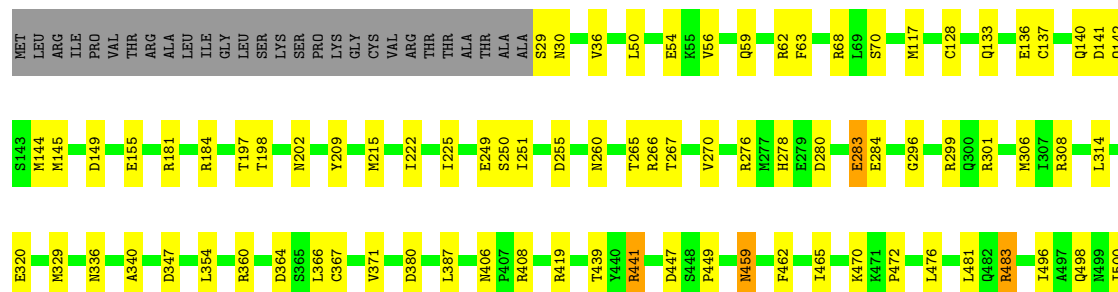
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

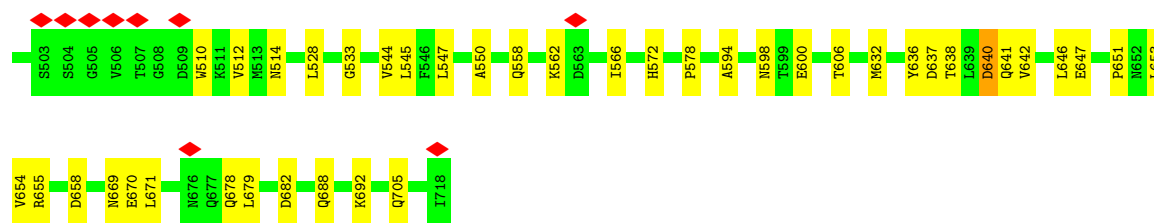
Chain L: 



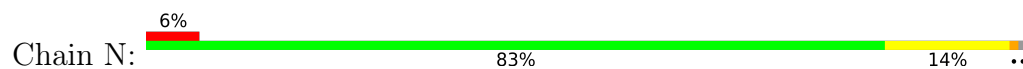
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 

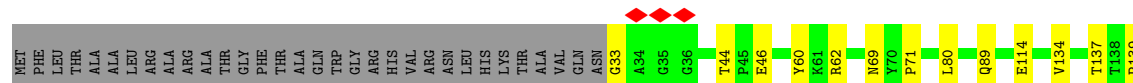




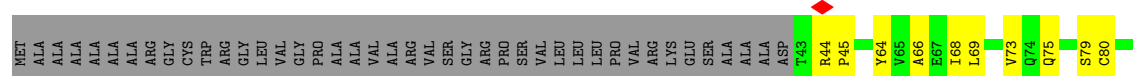
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

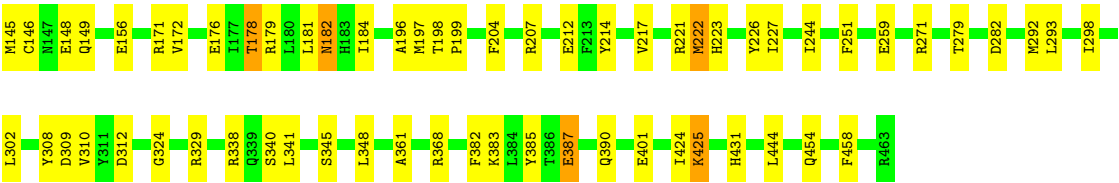


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

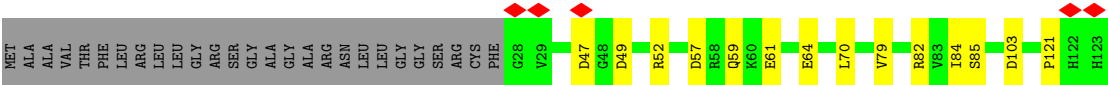


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

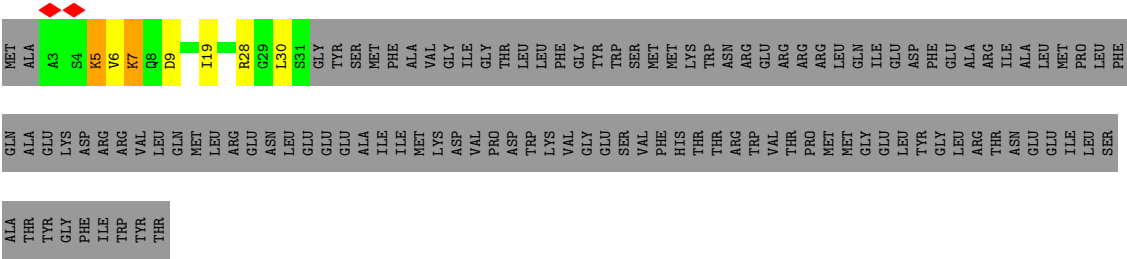




- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193234	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	0.230	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0236	Depositor
Map size (\AA)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3393	0.48	0/4584
2	B	0.25	0/1443	0.50	0/1952
3	C	0.27	0/1275	0.52	0/1725
4	E	0.25	0/995	0.51	0/1340
5	F	0.26	0/702	0.56	0/945
6	G	0.26	0/689	0.53	0/935
7	H	0.25	0/929	0.44	0/1258
8	I	0.25	0/798	0.53	0/1079
9	J	0.25	0/2408	0.49	0/3250
10	K	0.25	0/365	0.52	0/493
11	L	0.25	0/1039	0.50	0/1403
12	M	0.25	0/5384	0.50	0/7295
13	N	0.24	0/1245	0.49	0/1694
14	O	0.25	0/1711	0.46	0/2328
15	P	0.26	0/1789	0.50	0/2436
16	Q	0.26	0/3101	0.49	0/4189
17	T	0.26	0/755	0.51	0/1018
18	W	0.30	0/224	0.56	0/302
All	All	0.25	0/28245	0.50	0/38226

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

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	3318	0	3280	79	0
2	B	1412	0	1363	14	0
3	C	1244	0	1250	25	0
4	E	971	0	975	17	0
5	F	691	0	704	26	0
6	G	678	0	655	42	0
7	H	910	0	950	12	0
8	I	780	0	808	13	0
9	J	2356	0	2400	32	0
10	K	355	0	329	12	0
11	L	1016	0	1016	24	0
12	M	5296	0	5326	87	0
13	N	1204	0	1162	12	0
14	O	1671	0	1673	24	0
15	P	1738	0	1693	30	0
16	Q	3044	0	3018	57	0
17	T	741	0	702	10	0
18	W	218	0	219	7	0
19	A	8	0	0	1	0
19	B	16	0	0	0	0
19	C	8	0	0	1	0
19	M	16	0	0	0	0
20	A	31	0	19	3	0
21	C	47	0	71	0	0
22	C	52	0	88	3	0
23	G	35	0	0	5	0
24	J	48	0	25	2	0
25	M	4	0	0	0	0
25	O	4	0	0	0	0
26	M	1	0	0	0	0
27	N	51	0	46	0	0
28	T	1	0	0	0	0
All	All	27965	0	27772	451	0

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

All (451) 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)
6:G:112:SER:CB	23:G:201:8Q1:O1	1.70	1.38
3:C:126:GLU:CB	3:C:127:PRO:CD	2.19	1.18
24:J:401:NDP:O4D	24:J:401:NDP:C4D	1.68	1.18
6:G:86:VAL:HG21	6:G:122:MET:HE1	1.25	1.12
6:G:114:ASP:O	6:G:118:ILE:HD12	1.51	1.09
3:C:126:GLU:CB	3:C:127:PRO:HD3	1.83	1.09
6:G:86:VAL:HG21	6:G:122:MET:CE	1.82	1.07
6:G:86:VAL:CG2	6:G:122:MET:HE3	1.93	0.98
6:G:86:VAL:CG2	6:G:122:MET:CE	2.41	0.97
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.03	0.94
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.53	0.90
6:G:86:VAL:HG23	6:G:122:MET:HE3	1.50	0.90
16:Q:172:VAL:HG21	16:Q:310:VAL:CG2	2.02	0.89
3:C:126:GLU:CB	3:C:127:PRO:HD2	2.06	0.86
1:A:184:LYS:HB2	10:K:98:MET:CE	2.07	0.85
19:C:301:SF4:S4	16:Q:223:HIS:CD2	2.70	0.84
6:G:114:ASP:O	6:G:118:ILE:CD1	2.26	0.83
6:G:82:ARG:HD2	6:G:125:GLU:OE2	1.79	0.82
3:C:128:ARG:H	3:C:128:ARG:HD3	1.46	0.81
16:Q:217:VAL:HG22	16:Q:226:TYR:CE1	2.18	0.78
3:C:127:PRO:HA	9:J:89:TYR:OH	1.83	0.77
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.66	0.77
1:A:154:ALA:HB2	1:A:193:PHE:HZ	1.51	0.76
18:W:5:LYS:HE2	18:W:5:LYS:HA	1.67	0.75
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.70	0.74
6:G:112:SER:CB	23:G:201:8Q1:P24	2.76	0.73
11:L:156:LYS:HE2	12:M:68:ARG:NH1	2.03	0.72
1:A:167:SER:O	1:A:171:VAL:HG12	1.91	0.70
6:G:112:SER:CA	23:G:201:8Q1:O1	2.39	0.70
14:O:137:THR:HG22	14:O:139:PRO:HD2	1.74	0.69
6:G:122:MET:HE2	6:G:122:MET:HA	1.75	0.69
1:A:383:THR:HG23	1:A:384:PRO:HD3	1.75	0.69
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.73	0.69
6:G:144:ILE:O	6:G:148:ILE:HD12	1.93	0.69
1:A:168:ASN:O	1:A:171:VAL:HG13	1.93	0.69
1:A:184:LYS:HB2	10:K:98:MET:HE1	1.73	0.69
16:Q:172:VAL:CG2	16:Q:310:VAL:HG22	2.23	0.69
17:T:47:ASP:O	17:T:52:ARG:NH2	2.26	0.68
5:F:57:GLU:O	12:M:651:PRO:HB2	1.93	0.68
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.76	0.68
12:M:558:GLN:N	12:M:558:GLN:OE1	2.27	0.68
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:134:VAL:HG21	14:O:149:LEU:HD13	1.74	0.67
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.75	0.67
1:A:296:LEU:HD23	1:A:332:CYS:HB2	1.76	0.67
4:E:64:ARG:NH2	6:G:114:ASP:OD1	2.28	0.67
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.77	0.67
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.76	0.67
1:A:446:LEU:O	1:A:450:MET:HG3	1.94	0.66
6:G:112:SER:N	23:G:201:8Q1:O1	2.28	0.66
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.78	0.66
1:A:362:ASP:OD1	1:A:449:ARG:NH2	2.29	0.65
6:G:126:PHE:CD2	6:G:148:ILE:HG21	2.30	0.65
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.78	0.65
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.29	0.65
12:M:498:GLN:HB2	12:M:669:ASN:HD21	1.62	0.64
4:E:127:ASP:OD1	11:L:104:ARG:NH1	2.31	0.64
1:A:154:ALA:HB2	1:A:193:PHE:CZ	2.32	0.64
12:M:462:PHE:HA	12:M:465:ILE:HG22	1.80	0.64
16:Q:101:LEU:HD11	16:Q:444:LEU:HD13	1.80	0.63
3:C:80:ALA:HA	3:C:86:MET:HG2	1.80	0.63
12:M:406:ASN:ND2	12:M:688:GLN:O	2.28	0.63
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.80	0.63
3:C:128:ARG:HD3	3:C:128:ARG:N	2.13	0.63
12:M:472:PRO:O	12:M:510:TRP:NE1	2.23	0.63
6:G:122:MET:HE2	6:G:122:MET:CA	2.28	0.63
16:Q:176:GLU:OE1	16:Q:176:GLU:HA	1.97	0.63
6:G:82:ARG:CD	6:G:125:GLU:OE2	2.47	0.62
1:A:50:ASP:O	1:A:59:ARG:NH2	2.31	0.62
1:A:159:ARG:HD3	1:A:161:GLU:HB2	1.82	0.62
1:A:277:ASN:ND2	1:A:287:THR:OG1	2.33	0.62
16:Q:172:VAL:HG21	16:Q:310:VAL:HG23	1.82	0.62
5:F:19:ILE:HG13	5:F:53:ILE:HG23	1.82	0.61
1:A:104:LYS:HB3	1:A:105:PRO:HD2	1.82	0.61
5:F:31:GLN:NE2	5:F:35:ASP:OD2	2.33	0.61
11:L:84:ARG:NH1	11:L:88:GLN:O	2.32	0.61
12:M:266:ARG:HD2	12:M:267:THR:HG23	1.82	0.61
7:H:116:ILE:HG13	15:P:121:THR:HG21	1.83	0.61
9:J:190:GLU:OE1	9:J:190:GLU:HA	2.00	0.61
16:Q:387:GLU:OE1	16:Q:390:GLN:NE2	2.34	0.60
1:A:132:ARG:HB3	1:A:165:GLU:HB3	1.83	0.60
1:A:357:MET:HB3	1:A:361:THR:HG21	1.83	0.60
7:H:59:VAL:HG23	7:H:68:LEU:HD21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:VAL:HG23	3:C:129:TYR:O	2.00	0.60
12:M:647:GLU:HB2	12:M:654:VAL:CG1	2.32	0.60
11:L:109:ASN:ND2	11:L:111:LEU:O	2.35	0.59
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.34	0.59
1:A:174:ARG:HD2	10:K:92:GLU:OE2	2.02	0.59
5:F:33:VAL:O	5:F:36:PHE:HB3	2.03	0.59
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.35	0.59
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.83	0.59
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.35	0.59
1:A:40:ARG:NH1	1:A:289:GLU:O	2.36	0.59
3:C:66:THR:HG21	3:C:76:MET:HG3	1.83	0.59
6:G:122:MET:CE	6:G:122:MET:HA	2.32	0.59
15:P:66:ALA:HA	15:P:73:VAL:HG11	1.83	0.59
1:A:110:PRO:O	1:A:238:CYS:HB3	2.03	0.58
4:E:88:MET:HE1	15:P:171:TRP:HE1	1.68	0.58
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.35	0.58
16:Q:217:VAL:CG2	16:Q:226:TYR:CE1	2.86	0.58
1:A:290:GLU:OE1	1:A:303:HIS:NE2	2.34	0.58
12:M:496:ILE:O	12:M:500:ILE:HG13	2.03	0.58
3:C:59:ARG:NH1	22:C:303:PLX:O3	2.29	0.58
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.29	0.58
16:Q:217:VAL:CG2	16:Q:226:TYR:CZ	2.87	0.58
4:E:37:ARG:NH1	6:G:132:ASP:OD2	2.37	0.58
6:G:105:MET:SD	6:G:105:MET:N	2.77	0.58
12:M:308:ARG:NH2	12:M:578:PRO:O	2.37	0.58
5:F:56:ARG:HB3	12:M:651:PRO:HD2	1.85	0.57
3:C:124:MET:HE3	3:C:128:ARG:HG3	1.87	0.57
13:N:107:LYS:HE2	17:T:70:LEU:HD22	1.84	0.57
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.38	0.57
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.38	0.57
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.77	0.57
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.44	0.57
9:J:249:ILE:O	9:J:253:ILE:HG12	2.05	0.57
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.87	0.57
14:O:134:VAL:HG12	14:O:186:VAL:HG22	1.86	0.56
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.88	0.56
2:B:140:ARG:O	2:B:141:ARG:NH1	2.37	0.56
4:E:128:PRO:HD2	11:L:104:ARG:HH12	1.70	0.56
20:A:502:FMN:O4'	20:A:502:FMN:O2'	2.23	0.56
5:F:56:ARG:CB	12:M:651:PRO:HD2	2.35	0.56
6:G:141:PRO:O	6:G:145:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:347:ASP:OD1	12:M:347:ASP:N	2.36	0.56
16:Q:217:VAL:HG21	16:Q:226:TYR:CZ	2.41	0.56
6:G:86:VAL:CG2	6:G:122:MET:HE1	2.10	0.56
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.05	0.56
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.39	0.56
1:A:184:LYS:HB2	10:K:98:MET:SD	2.46	0.55
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.39	0.55
1:A:152:ARG:NH2	10:K:99:PRO:O	2.39	0.55
6:G:86:VAL:HG23	6:G:122:MET:CE	2.22	0.55
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.87	0.55
15:P:69:LEU:O	15:P:73:VAL:HG12	2.07	0.55
2:B:192:ASN:ND2	17:T:61:GLU:OE2	2.40	0.55
5:F:64:LYS:NZ	5:F:76:ASN:OD1	2.21	0.55
9:J:234:GLU:OE2	9:J:234:GLU:N	2.40	0.55
1:A:64:LYS:HG2	1:A:67:GLU:HB2	1.88	0.55
12:M:598:ASN:ND2	12:M:600:GLU:OE2	2.40	0.55
9:J:204:SER:OG	9:J:238:GLN:O	2.25	0.54
1:A:210:THR:HB	1:A:224:ARG:HG2	1.89	0.54
4:E:101:THR:O	4:E:105:ARG:HG3	2.07	0.54
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.90	0.54
12:M:498:GLN:HB2	12:M:669:ASN:ND2	2.22	0.54
1:A:168:ASN:O	1:A:171:VAL:CG1	2.56	0.54
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.73	0.54
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.90	0.54
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.39	0.54
5:F:69:TYR:HE2	5:F:75:LYS:HG3	1.72	0.54
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.89	0.54
4:E:90:LEU:O	4:E:94:ILE:HG12	2.08	0.53
15:P:190:ASP:OD1	15:P:191:TYR:N	2.41	0.53
1:A:263:ALA:HA	1:A:271:SER:HB3	1.90	0.53
7:H:83:GLN:NE2	7:H:83:GLN:HA	2.24	0.53
16:Q:179:ARG:HD2	16:Q:340:SER:OG	2.09	0.53
7:H:77:ILE:O	7:H:81:ILE:HD12	2.07	0.53
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.23	0.53
1:A:375:LYS:NZ	14:O:33:GLY:O	2.41	0.53
5:F:53:ILE:O	12:M:380:ASP:HB3	2.08	0.53
14:O:198:PRO:O	14:O:202:GLU:HG3	2.09	0.53
15:P:44:ARG:HB3	15:P:45:PRO:HD2	1.90	0.53
4:E:36:TYR:OH	6:G:117:GLU:OE2	2.24	0.53
9:J:184:LYS:NZ	24:J:401:NDP:O2D	2.29	0.53
1:A:244:ASN:N	20:A:502:FMN:O1P	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:87:LEU:HB3	14:O:62:ARG:HG2	1.92	0.52
1:A:131:ILE:HD13	1:A:158:ILE:HD13	1.92	0.52
7:H:9:THR:O	7:H:76:GLN:NE2	2.43	0.52
11:L:69:GLU:H	11:L:69:GLU:CD	2.12	0.52
3:C:85:ASP:O	3:C:88:ARG:HG2	2.10	0.52
12:M:545:LEU:HB3	12:M:566:ILE:HD13	1.92	0.51
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.92	0.51
3:C:154:ASP:OD1	3:C:154:ASP:N	2.35	0.51
1:A:307:VAL:HG21	1:A:314:LEU:HD12	1.92	0.51
1:A:448:GLU:O	1:A:452:GLN:HG2	2.10	0.51
11:L:165:SER:O	11:L:171:ARG:NH1	2.43	0.51
1:A:130:ILE:HD11	1:A:245:VAL:HG12	1.93	0.51
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.42	0.51
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.43	0.51
1:A:43:THR:HG21	14:O:238:PRO:HB3	1.92	0.50
5:F:88:THR:O	5:F:92:GLU:HG2	2.11	0.50
16:Q:324:GLY:O	16:Q:329:ARG:NH2	2.44	0.50
12:M:70:SER:O	12:M:184:ARG:NH1	2.44	0.50
9:J:238:GLN:OE1	9:J:270:ARG:NH1	2.44	0.50
9:J:87:GLU:OE1	9:J:88:PRO:HD2	2.12	0.50
1:A:168:ASN:HA	1:A:171:VAL:CG1	2.41	0.50
6:G:115:GLN:O	6:G:119:ILE:HG12	2.11	0.50
12:M:512:VAL:O	12:M:514:ASN:ND2	2.44	0.50
5:F:42:VAL:HG23	12:M:671:LEU:HG	1.94	0.50
5:F:73:GLN:N	5:F:73:GLN:OE1	2.45	0.50
6:G:123:GLU:HG2	6:G:130:ILE:HG13	1.94	0.50
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.47	0.50
12:M:408:ARG:HD2	12:M:439:THR:HG23	1.93	0.50
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.94	0.49
9:J:162:GLU:HG3	9:J:163:LYS:HG3	1.94	0.49
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.93	0.49
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.94	0.49
12:M:29:SER:OG	12:M:30:ASN:N	2.42	0.49
1:A:394:LYS:HB3	12:M:155:GLU:HG2	1.95	0.49
5:F:42:VAL:HG21	12:M:670:GLU:HG2	1.94	0.49
8:I:58:ASP:OD2	8:I:61:ARG:HB2	2.12	0.49
12:M:250:SER:OG	12:M:251:ILE:N	2.45	0.49
17:T:84:ILE:HD12	17:T:85:SER:H	1.77	0.49
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.48	0.49
5:F:50:ASP:OD1	5:F:50:ASP:N	2.45	0.49
5:F:56:ARG:HB3	12:M:651:PRO:CG	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:86:GLN:O	5:F:90:THR:HG22	2.12	0.49
1:A:102:MET:HE3	1:A:149:MET:HB3	1.95	0.49
14:O:159:LYS:HB2	14:O:162:GLU:HG3	1.94	0.49
4:E:37:ARG:HD2	6:G:120:MET:SD	2.51	0.49
10:K:105:ARG:NH1	11:L:167:ASN:O	2.45	0.49
7:H:76:GLN:O	7:H:79:GLU:HG2	2.13	0.49
12:M:449:PRO:HB2	12:M:679:LEU:HD13	1.95	0.49
13:N:14:VAL:HG23	13:N:23:TYR:CG	2.48	0.49
6:G:118:ILE:O	6:G:122:MET:HG2	2.13	0.49
11:L:135:VAL:O	11:L:139:GLU:HG3	2.11	0.49
12:M:299:ARG:HD2	12:M:705:GLN:HE21	1.76	0.49
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.39	0.48
5:F:57:GLU:O	12:M:651:PRO:CB	2.61	0.48
9:J:87:GLU:HG3	9:J:89:TYR:H	1.78	0.48
1:A:296:LEU:HD13	1:A:337:MET:HE3	1.95	0.48
1:A:98:LYS:NZ	20:A:502:FMN:O3P	2.33	0.48
2:B:96:ARG:NH1	16:Q:217:VAL:O	2.44	0.48
6:G:137:LYS:HB2	6:G:137:LYS:NZ	2.28	0.48
22:C:303:PLX:H31	13:N:75:TRP:CD2	2.48	0.48
5:F:89:ARG:NH1	5:F:89:ARG:HB2	2.28	0.48
12:M:678:GLN:OE1	12:M:678:GLN:N	2.41	0.48
1:A:102:MET:CE	1:A:149:MET:HB3	2.43	0.48
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	1.95	0.48
1:A:48:ARG:NH1	10:K:70:ASN:O	2.36	0.48
7:H:83:GLN:HA	7:H:83:GLN:HE21	1.77	0.48
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.95	0.48
4:E:30:ARG:O	4:E:34:GLU:HG3	2.14	0.48
12:M:655:ARG:HD2	12:M:658:ASP:OD2	2.14	0.48
4:E:69:LYS:HB2	4:E:69:LYS:NZ	2.29	0.48
11:L:75:ARG:HD2	11:L:104:ARG:HH21	1.78	0.48
16:Q:146:CYS:SG	16:Q:178:THR:CG2	3.02	0.48
8:I:40:LYS:HB3	18:W:7:LYS:H	1.79	0.47
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.96	0.47
15:P:155:SER:OG	15:P:167:GLU:OE2	2.30	0.47
11:L:117:THR:HG21	15:P:229:GLU:HG3	1.95	0.47
12:M:62:ARG:H	12:M:142:GLN:HE22	1.62	0.47
12:M:63:PHE:O	12:M:181:ARG:NH2	2.45	0.47
1:A:408:GLU:O	1:A:411:SER:HB3	2.14	0.47
8:I:6:ARG:O	8:I:10:LEU:HG	2.14	0.47
14:O:44:THR:HG22	14:O:46:GLU:H	1.80	0.47
9:J:212:ARG:O	9:J:216:TYR:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:125:VAL:HG11	9:J:253:ILE:HD12	1.95	0.47
9:J:163:LYS:NZ	9:J:253:ILE:O	2.45	0.47
1:A:372:GLU:OE2	14:O:33:GLY:N	2.48	0.47
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.50	0.47
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.97	0.47
1:A:116:ASN:HD22	1:A:212:LEU:HD13	1.79	0.47
6:G:126:PHE:HE2	6:G:148:ILE:HG21	1.75	0.47
11:L:61:ILE:HG12	11:L:140:LYS:HG2	1.96	0.47
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.97	0.47
5:F:56:ARG:HB3	12:M:651:PRO:CD	2.44	0.46
9:J:170:LEU:HA	9:J:202:LYS:HB3	1.96	0.46
14:O:226:GLU:OE1	14:O:226:GLU:N	2.43	0.46
1:A:104:LYS:HB2	1:A:104:LYS:HE3	1.72	0.46
1:A:126:LYS:O	1:A:130:ILE:HG23	2.16	0.46
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.97	0.46
6:G:115:GLN:HG3	6:G:139:MET:HE1	1.97	0.46
1:A:244:ASN:OD1	1:A:245:VAL:N	2.45	0.46
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.48	0.46
16:Q:144:MET:SD	16:Q:222:MET:HG3	2.55	0.46
9:J:118:LYS:HE3	17:T:57:ASP:OD1	2.15	0.46
16:Q:148:GLU:HB3	16:Q:227:ILE:HB	1.97	0.46
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.96	0.46
1:A:66:LYS:HD3	1:A:187:CYS:O	2.16	0.46
3:C:79:MET:HE2	3:C:86:MET:HB3	1.98	0.46
12:M:371:VAL:HG12	12:M:533:GLY:HA2	1.97	0.46
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.98	0.46
17:T:82:ARG:NH1	17:T:103:ASP:OD1	2.49	0.46
12:M:141:ASP:O	12:M:145:MET:HG2	2.14	0.46
12:M:360:ARG:HG2	12:M:360:ARG:HH11	1.80	0.46
14:O:206:ASP:OD1	14:O:207:GLU:N	2.49	0.46
15:P:172:ASP:OD2	15:P:187:ILE:N	2.38	0.46
2:B:177:THR:HG22	2:B:179:THR:H	1.79	0.46
7:H:96:ARG:HG3	7:H:96:ARG:HH11	1.81	0.46
13:N:78:ASP:OD1	13:N:78:ASP:N	2.47	0.46
12:M:459:ASN:N	12:M:459:ASN:OD1	2.49	0.46
1:A:174:ARG:CA	10:K:93:LEU:HD21	2.46	0.45
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.98	0.45
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.98	0.45
6:G:79:ILE:HG22	6:G:145:VAL:HG13	1.97	0.45
9:J:37:HIS:CE1	17:T:49:ASP:HA	2.51	0.45
12:M:296:GLY:O	12:M:572:HIS:NE2	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.69	0.45
6:G:137:LYS:HB2	6:G:137:LYS:HZ3	1.82	0.45
12:M:133:GLN:O	12:M:137:CYS:HB2	2.17	0.45
12:M:251:ILE:HB	12:M:606:THR:HG22	1.99	0.45
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.48	0.45
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.46	0.45
12:M:419:ARG:NH1	12:M:439:THR:O	2.49	0.45
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.45
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.98	0.45
4:E:52:LEU:HD11	4:E:103:ILE:HG21	1.99	0.45
4:E:102:HIS:NE2	15:P:190:ASP:OD1	2.46	0.45
1:A:338:ASP:OD1	1:A:338:ASP:N	2.49	0.45
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.99	0.45
3:C:128:ARG:N	3:C:128:ARG:CD	2.80	0.45
4:E:120:SER:O	4:E:124:VAL:HG22	2.17	0.45
5:F:57:GLU:O	12:M:651:PRO:CG	2.65	0.45
10:K:88:ASP:O	10:K:91:VAL:HG12	2.17	0.45
1:A:54:LYS:HE3	1:A:54:LYS:HB3	1.64	0.45
3:C:167:PRO:HG3	16:Q:222:MET:HE3	1.98	0.45
16:Q:105:MET:SD	16:Q:105:MET:N	2.89	0.45
3:C:124:MET:HE1	3:C:128:ARG:HB2	1.99	0.44
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.82	0.44
11:L:123:ASN:ND2	15:P:230:PHE:HB3	2.32	0.44
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.98	0.44
6:G:122:MET:HE2	6:G:122:MET:N	2.33	0.44
7:H:18:GLU:OE1	7:H:18:GLU:N	2.38	0.44
12:M:640:ASP:OD1	12:M:640:ASP:N	2.50	0.44
1:A:64:LYS:HD2	14:O:249:LEU:HD23	1.98	0.44
5:F:56:ARG:CB	12:M:651:PRO:CD	2.94	0.44
12:M:470:LYS:HD2	12:M:470:LYS:HA	1.69	0.44
1:A:116:ASN:ND2	1:A:212:LEU:HD13	2.32	0.44
9:J:231:LEU:HD23	9:J:323:HIS:HE2	1.81	0.44
12:M:260:ASN:HD21	12:M:278:HIS:CD2	2.36	0.44
16:Q:292:MET:H	16:Q:292:MET:HG2	1.65	0.44
11:L:101:PHE:CE2	11:L:121:LEU:HD13	2.52	0.44
1:A:141:GLY:HA3	1:A:248:VAL:O	2.18	0.44
1:A:296:LEU:HD13	1:A:337:MET:CE	2.48	0.44
3:C:146:SER:OG	16:Q:118:2MR:O	2.26	0.44
9:J:124:ASN:ND2	9:J:125:VAL:HG23	2.32	0.44
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.35	0.44
5:F:23:LEU:O	5:F:57:GLU:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:222:ILE:HA	12:M:225:ILE:HG12	2.00	0.43
1:A:156:ILE:HB	1:A:197:VAL:HG22	2.00	0.43
7:H:23:ARG:HA	7:H:23:ARG:HD2	1.82	0.43
6:G:134:ASP:HB2	6:G:137:LYS:HZ1	1.83	0.43
9:J:168:SER:O	9:J:202:LYS:HA	2.18	0.43
11:L:89:SER:O	12:M:59:GLN:NE2	2.50	0.43
14:O:140:CYS:O	14:O:145:SER:HB2	2.17	0.43
6:G:80:LYS:HE3	6:G:80:LYS:HB3	1.85	0.43
8:I:42:PRO:HD3	18:W:6:VAL:HG13	2.01	0.43
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.66	0.43
12:M:340:ALA:HB1	12:M:354:LEU:HD21	2.00	0.43
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.35	0.43
12:M:255:ASP:N	12:M:255:ASP:OD1	2.51	0.43
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.53	0.43
3:C:51:ASP:HB2	3:C:190:LEU:HB2	2.01	0.43
12:M:50:LEU:O	12:M:54:GLU:HG3	2.19	0.43
14:O:234:LEU:HD13	14:O:234:LEU:HA	1.93	0.43
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.53	0.43
6:G:88:LYS:HE2	6:G:98:LEU:HD21	2.01	0.43
8:I:33:LYS:H	8:I:33:LYS:HG2	1.68	0.43
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.83	0.43
7:H:56:LEU:HA	7:H:59:VAL:HG12	2.00	0.43
12:M:340:ALA:HB3	12:M:366:LEU:HD23	2.01	0.43
1:A:157:TYR:HB3	1:A:212:LEU:HD11	2.00	0.43
22:C:303:PLX:H212	22:C:303:PLX:H181	1.65	0.43
2:B:40:PHE:HB3	2:B:43:MET:HB2	2.01	0.43
6:G:113:LEU:O	6:G:116:VAL:HG22	2.19	0.43
8:I:108:LYS:HB3	8:I:108:LYS:HE3	1.74	0.43
12:M:265:THR:HG22	12:M:270:VAL:HA	2.01	0.43
12:M:283:GLU:HB3	12:M:284:GLU:H	1.69	0.43
12:M:646:LEU:HD22	12:M:653:LEU:CD1	2.49	0.43
15:P:167:GLU:HG2	15:P:178:PHE:CG	2.54	0.43
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.43
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.41	0.43
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.50	0.42
16:Q:431:HIS:HB3	16:Q:454:GLN:HG2	2.01	0.42
1:A:119:GLU:CG	1:A:127:ASP:HB2	2.49	0.42
6:G:82:ARG:HB3	6:G:125:GLU:OE2	2.19	0.42
14:O:169:PHE:HE2	14:O:209:LYS:HD3	1.84	0.42
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	2.00	0.42
16:Q:182:ASN:ND2	16:Q:182:ASN:C	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:66:PRO:HB3	15:P:79:SER:HA	2.00	0.42
9:J:166:HIS:CD2	9:J:191:VAL:HG21	2.54	0.42
16:Q:83:ASN:OD1	16:Q:83:ASN:N	2.52	0.42
18:W:30:LEU:HD12	18:W:30:LEU:HA	1.93	0.42
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.54	0.42
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.00	0.42
1:A:211:ALA:HB2	1:A:223:PRO:HG3	2.01	0.42
11:L:117:THR:O	11:L:117:THR:HG23	2.18	0.42
9:J:178:SER:OG	9:J:317:ASP:OD1	2.29	0.42
12:M:441:ARG:HE	12:M:441:ARG:HB2	1.69	0.42
17:T:64:GLU:OE2	17:T:64:GLU:HA	2.20	0.42
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.02	0.42
3:C:44:GLU:HA	3:C:47:VAL:HG22	2.02	0.42
12:M:367:CYS:HB3	12:M:533:GLY:O	2.20	0.42
15:P:87:PHE:HE2	15:P:144:LYS:HE3	1.83	0.42
15:P:112:ALA:O	16:Q:425:LYS:NZ	2.40	0.42
1:A:169:LEU:O	1:A:173:ILE:HG13	2.20	0.42
9:J:116:ILE:O	9:J:120:VAL:HG22	2.20	0.42
9:J:181:LEU:HD11	9:J:321:ARG:HG2	2.01	0.42
12:M:547:LEU:HD22	12:M:550:ALA:HB3	2.01	0.42
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.02	0.42
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.20	0.42
16:Q:279:THR:OG1	16:Q:282:ASP:OD1	2.38	0.42
8:I:8:ILE:O	8:I:12:ARG:HG3	2.20	0.41
9:J:88:PRO:O	9:J:91:THR:HG22	2.20	0.41
12:M:528:LEU:CD1	12:M:653:LEU:HD11	2.50	0.41
5:F:45:LYS:HB3	12:M:671:LEU:HD21	2.02	0.41
14:O:231:LEU:HD13	14:O:231:LEU:HA	1.97	0.41
18:W:5:LYS:HD3	18:W:6:VAL:H	1.84	0.41
1:A:380:GLY:O	1:A:386:ARG:NH1	2.44	0.41
16:Q:102:SER:O	16:Q:102:SER:OG	2.33	0.41
1:A:102:MET:HG3	1:A:241:THR:OG1	2.21	0.41
1:A:114:VAL:HG11	1:A:212:LEU:HD22	2.03	0.41
14:O:152:ILE:HG21	14:O:171:LEU:HD13	2.02	0.41
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.83	0.41
6:G:112:SER:O	6:G:116:VAL:HG13	2.20	0.41
9:J:145:PHE:CE1	9:J:184:LYS:HE2	2.55	0.41
9:J:236:VAL:HG12	9:J:272:LEU:HD22	2.02	0.41
12:M:306:MET:HB3	12:M:314:LEU:HD22	2.02	0.41
17:T:79:VAL:O	17:T:121:PRO:HD3	2.21	0.41
1:A:131:ILE:HD11	1:A:169:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLU:OE2	13:N:131:ARG:NH2	2.53	0.41
3:C:133:MET:HG3	3:C:168:PRO:HG2	2.03	0.41
8:I:92:LYS:HD2	8:I:92:LYS:HA	1.91	0.41
14:O:69:ASN:HD22	14:O:69:ASN:HA	1.68	0.41
9:J:212:ARG:O	9:J:216:TYR:CB	2.68	0.41
23:G:201:8Q1:O40	23:G:201:8Q1:N36	2.52	0.41
8:I:14:TRP:O	18:W:28:ARG:NH2	2.53	0.41
8:I:105:GLU:OE2	8:I:105:GLU:HA	2.21	0.41
12:M:197:THR:O	14:O:114:GLU:HG2	2.20	0.41
1:A:386:ARG:HG3	12:M:202:ASN:HA	2.02	0.41
3:C:45:TYR:HE1	3:C:49:LYS:HZ3	1.66	0.41
8:I:70:MET:HG3	15:P:66:ALA:HB1	2.01	0.41
12:M:249:GLU:HG2	12:M:276:ARG:HD3	2.03	0.41
14:O:222:ARG:HD2	14:O:226:GLU:O	2.21	0.41
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.56	0.41
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.56	0.41
4:E:41:ARG:HG3	4:E:41:ARG:HH11	1.86	0.41
11:L:59:LEU:HD22	11:L:140:LYS:HG3	2.02	0.41
12:M:476:LEU:HD21	12:M:481:LEU:HD11	2.03	0.41
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.85	0.41
1:A:273:THR:OG1	1:A:289:GLU:OE1	2.26	0.40
3:C:169:THR:HG22	16:Q:221:ARG:HD3	2.03	0.40
5:F:59:SER:O	5:F:61:VAL:HG23	2.21	0.40
13:N:21:ARG:HD2	13:N:21:ARG:HA	1.87	0.40
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.56	0.40
3:C:63:TRP:H	3:C:101:ASP:HB2	1.86	0.40
9:J:358:THR:O	9:J:358:THR:OG1	2.37	0.40
12:M:198:THR:HG21	12:M:209:TYR:HB2	2.03	0.40
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.03	0.40
1:A:265:PHE:HB3	1:A:291:GLU:HG3	2.04	0.40
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.03	0.40
1:A:140:GLU:OE2	1:A:256:ARG:NH2	2.54	0.40
2:B:85:ASN:OD1	3:C:88:ARG:NH2	2.54	0.40
11:L:102:ASP:N	11:L:102:ASP:OD1	2.55	0.40
12:M:483:ARG:HH22	12:M:682:ASP:HB2	1.87	0.40
13:N:122:GLN:HA	17:T:59:GLN:HG2	2.04	0.40
16:Q:345:SER:HB2	18:W:19:ILE:HD12	2.03	0.40
1:A:244:ASN:O	1:A:248:VAL:HG22	2.21	0.40
12:M:117:MET:HE1	12:M:142:GLN:HB3	2.03	0.40
12:M:637:ASP:N	12:M:641:GLN:OE1	2.52	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	429/458 (94%)	422 (98%)	7 (2%)	0	100	100
2	B	174/212 (82%)	172 (99%)	2 (1%)	0	100	100
3	C	154/196 (79%)	149 (97%)	4 (3%)	1 (1%)	25	56
4	E	113/128 (88%)	110 (97%)	3 (3%)	0	100	100
5	F	84/99 (85%)	80 (95%)	4 (5%)	0	100	100
6	G	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
7	H	110/116 (95%)	103 (94%)	7 (6%)	0	100	100
8	I	93/113 (82%)	83 (89%)	10 (11%)	0	100	100
9	J	289/376 (77%)	280 (97%)	9 (3%)	0	100	100
10	K	40/110 (36%)	40 (100%)	0	0	100	100
11	L	123/175 (70%)	120 (98%)	3 (2%)	0	100	100
12	M	688/718 (96%)	669 (97%)	19 (3%)	0	100	100
13	N	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
14	O	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
15	P	206/264 (78%)	195 (95%)	11 (5%)	0	100	100
16	Q	374/473 (79%)	360 (96%)	14 (4%)	0	100	100
17	T	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
18	W	27/144 (19%)	26 (96%)	1 (4%)	0	100	100
All	All	3441/4255 (81%)	3330 (97%)	110 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	126	GLU

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	345/365 (94%)	340 (99%)	5 (1%)	67	90
2	B	151/176 (86%)	147 (97%)	4 (3%)	46	79
3	C	131/163 (80%)	125 (95%)	6 (5%)	27	60
4	E	107/112 (96%)	102 (95%)	5 (5%)	26	59
5	F	76/82 (93%)	74 (97%)	2 (3%)	46	79
6	G	72/132 (54%)	66 (92%)	6 (8%)	11	32
7	H	99/101 (98%)	93 (94%)	6 (6%)	18	48
8	I	87/98 (89%)	83 (95%)	4 (5%)	27	60
9	J	254/322 (79%)	243 (96%)	11 (4%)	29	62
10	K	41/92 (45%)	38 (93%)	3 (7%)	14	38
11	L	113/152 (74%)	109 (96%)	4 (4%)	36	70
12	M	580/602 (96%)	566 (98%)	14 (2%)	49	81
13	N	130/131 (99%)	122 (94%)	8 (6%)	18	47
14	O	183/207 (88%)	178 (97%)	5 (3%)	44	78
15	P	190/228 (83%)	184 (97%)	6 (3%)	39	73
16	Q	327/401 (82%)	318 (97%)	9 (3%)	43	77
17	T	79/97 (81%)	79 (100%)	0	100	100
18	W	23/124 (18%)	20 (87%)	3 (13%)	4	13
All	All	2988/3585 (83%)	2887 (97%)	101 (3%)	40	71

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	134	ASP
1	A	171	VAL
1	A	383	THR
1	A	405	ARG
2	B	43	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	68	ARG
2	B	110	GLU
2	B	139	SER
3	C	76	MET
3	C	86	MET
3	C	100	SER
3	C	101	ASP
3	C	128	ARG
3	C	188	LYS
4	E	18	LYS
4	E	30	ARG
4	E	64	ARG
4	E	85	LYS
4	E	89	GLU
5	F	26	ARG
5	F	98	LYS
6	G	76	LEU
6	G	92	LYS
6	G	94	ASP
6	G	115	GLN
6	G	125	GLU
6	G	134	ASP
7	H	7	LYS
7	H	66	LYS
7	H	70	GLU
7	H	89	SER
7	H	94	MET
7	H	96	ARG
8	I	61	ARG
8	I	70	MET
8	I	93	LYS
8	I	108	LYS
9	J	85	ARG
9	J	92	MET
9	J	107	GLU
9	J	114	ASP
9	J	117	ARG
9	J	143	ASP
9	J	221	ARG
9	J	336	GLU
9	J	357	ARG
9	J	358	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	J	373	LYS
10	K	75	ASN
10	K	82	SER
10	K	94	SER
11	L	86	ASN
11	L	105	GLU
11	L	164	PHE
11	L	173	SER
12	M	215	MET
12	M	283	GLU
12	M	329	MET
12	M	336	ASN
12	M	441	ARG
12	M	447	ASP
12	M	459	ASN
12	M	483	ARG
12	M	544	VAL
12	M	562	LYS
12	M	632	MET
12	M	636	TYR
12	M	640	ASP
12	M	692	LYS
13	N	8	ARG
13	N	27	LEU
13	N	101	LYS
13	N	107	LYS
13	N	118	SER
13	N	123	GLN
13	N	132	LYS
13	N	133	LYS
14	O	60	TYR
14	O	80	LEU
14	O	89	GLN
14	O	141	MET
14	O	246	GLN
15	P	80	CYS
15	P	85	GLU
15	P	109	LYS
15	P	110	SER
15	P	161	LYS
15	P	231	ARG
16	Q	83	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Q	108	LYS
16	Q	144	MET
16	Q	178	THR
16	Q	182	ASN
16	Q	222	MET
16	Q	308	TYR
16	Q	387	GLU
16	Q	425	LYS
18	W	5	LYS
18	W	7	LYS
18	W	9	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
12	M	260	ASN
12	M	604	GLN
17	T	63	ASN

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	1.95	1 (10%)	5,13,15	6.15	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.60	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	12.59	131.03	119.48
16	Q	118	2MR	CD-NE-CZ	4.52	131.88	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.03	130.56	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
23	8Q1	G	201	-	31,34,34	1.71	6 (19%)	40,43,43	1.63	6 (15%)
19	SF4	B	301	2	0,12,12	-	-	-	-	-
24	NDP	J	401	-	45,52,52	4.57	20 (44%)	53,80,80	1.93	6 (11%)
19	SF4	B	302	2	0,12,12	-	-	-	-	-
19	SF4	M	801	12	0,12,12	-	-	-	-	-
19	SF4	C	301	16,3	0,12,12	-	-	-	-	-
25	FES	O	301	14	0,4,4	-	-	-	-	-
19	SF4	M	802	12	0,12,12	-	-	-	-	-
19	SF4	A	501	1	0,12,12	-	-	-	-	-
27	CDL	N	201	-	50,50,99	1.41	9 (18%)	56,62,111	1.12	4 (7%)
25	FES	M	803	12	0,4,4	-	-	-	-	-
21	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.97	2 (4%)
20	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.20	7 (14%)
22	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)

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
23	8Q1	G	201	-	-	14/41/41/41	-
19	SF4	B	301	2	-	-	0/6/5/5
24	NDP	J	401	-	-	7/30/77/77	0/4/5/5
19	SF4	B	302	2	-	-	0/6/5/5
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	C	301	16,3	-	-	0/6/5/5
25	FES	O	301	14	-	-	0/1/1/1
19	SF4	M	802	12	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5
27	CDL	N	201	-	-	33/61/61/110	-
25	FES	M	803	12	-	-	0/1/1/1
21	PEE	C	302	-	-	21/50/50/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	FMN	A	502	-	-	5/18/18/18	0/3/3/3
22	PLX	C	303	-	-	27/55/55/55	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	401	NDP	C3B-C2B	-12.98	1.24	1.52
24	J	401	NDP	C6N-C5N	12.41	1.55	1.33
24	J	401	NDP	O4D-C4D	10.71	1.68	1.45
24	J	401	NDP	C3D-C4D	-9.84	1.27	1.53
24	J	401	NDP	O4B-C1B	8.57	1.53	1.41
24	J	401	NDP	O4B-C4B	-7.86	1.27	1.45
24	J	401	NDP	C2N-C3N	7.40	1.55	1.34
24	J	401	NDP	P2B-O2B	5.63	1.69	1.59
23	G	201	8Q1	C34-N36	5.45	1.45	1.33
24	J	401	NDP	C3B-C4B	5.33	1.66	1.53
23	G	201	8Q1	C39-N41	5.29	1.45	1.33
24	J	401	NDP	O4D-C1D	-4.88	1.30	1.42
24	J	401	NDP	C6N-N1N	4.86	1.49	1.37
24	J	401	NDP	C7N-N7N	4.22	1.44	1.33
24	J	401	NDP	O2D-C2D	-4.18	1.33	1.43
24	J	401	NDP	C6A-N6A	4.08	1.48	1.34
20	A	502	FMN	C4A-N5	3.83	1.38	1.30
21	C	302	PEE	C18-C19	3.75	1.53	1.31
21	C	302	PEE	C39-C38	3.64	1.52	1.31
27	N	201	CDL	OA8-CA7	3.44	1.43	1.33
24	J	401	NDP	O3D-C3D	3.11	1.50	1.43
27	N	201	CDL	OA6-CA5	3.09	1.43	1.34
27	N	201	CDL	OB6-CB5	3.03	1.42	1.34
27	N	201	CDL	OB8-CB7	3.01	1.42	1.33
24	J	401	NDP	C7N-C3N	3.00	1.55	1.48
22	C	303	PLX	O6-C4	-2.74	1.40	1.44
20	A	502	FMN	C10-N1	2.49	1.38	1.33
21	C	302	PEE	O3-C30	2.49	1.40	1.33
23	G	201	8Q1	C1-S44	2.43	1.82	1.76
23	G	201	8Q1	O40-C39	-2.42	1.18	1.23
21	C	302	PEE	O2-C2	-2.42	1.40	1.46
23	G	201	8Q1	O35-C34	-2.42	1.18	1.23
24	J	401	NDP	O2B-C2B	2.39	1.52	1.44
22	C	303	PLX	C7-C6	2.34	1.55	1.50
24	J	401	NDP	C2D-C3D	2.31	1.59	1.53
21	C	302	PEE	O2-C10	2.27	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	201	CDL	OB6-CB4	-2.19	1.41	1.46
27	N	201	CDL	PB2-OB2	2.16	1.68	1.59
27	N	201	CDL	PB2-OB5	2.16	1.68	1.59
24	J	401	NDP	PA-O5B	2.14	1.68	1.59
24	J	401	NDP	O7N-C7N	-2.13	1.19	1.24
22	C	303	PLX	P1-O4	2.09	1.67	1.59
27	N	201	CDL	OA6-CA4	-2.09	1.41	1.46
23	G	201	8Q1	C6-C1	2.08	1.53	1.50
21	C	302	PEE	O3-C3	-2.07	1.40	1.45
27	N	201	CDL	C11-CA5	2.06	1.56	1.50
22	C	303	PLX	P1-O1	2.04	1.67	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	401	NDP	C3N-C2N-N1N	-7.92	111.80	123.10
24	J	401	NDP	C1D-N1N-C2N	-6.90	109.62	121.11
23	G	201	8Q1	C6-C1-S44	6.15	120.62	113.46
24	J	401	NDP	C1D-N1N-C6N	-5.08	109.89	120.83
24	J	401	NDP	N3A-C2A-N1A	-4.10	122.28	128.68
21	C	302	PEE	O2-C10-C11	3.89	119.89	111.50
27	N	201	CDL	OA6-CA5-C11	3.84	119.79	111.50
27	N	201	CDL	OB6-CB5-C51	3.83	119.75	111.50
23	G	201	8Q1	O4-C1-C6	-3.82	119.47	123.99
20	A	502	FMN	C4-N3-C2	-3.10	119.91	125.64
23	G	201	8Q1	C37-C38-C39	3.01	117.37	112.36
23	G	201	8Q1	C38-C39-N41	3.00	121.48	116.42
24	J	401	NDP	PN-O3-PA	-2.79	123.24	132.83
20	A	502	FMN	C4A-C4-N3	2.67	119.98	113.19
27	N	201	CDL	OB8-CB7-C71	2.66	120.25	111.91
27	N	201	CDL	OA8-CA7-C31	2.63	120.15	111.91
21	C	302	PEE	O3-C30-C31	2.53	119.84	111.91
20	A	502	FMN	O4-C4-C4A	-2.51	119.94	126.60
23	G	201	8Q1	C43-S44-C1	2.39	109.31	101.87
20	A	502	FMN	C4A-C10-N10	2.37	119.95	116.48
24	J	401	NDP	C4A-C5A-N7A	-2.32	106.98	109.40
22	C	303	PLX	C1A-N1-C1	2.26	119.15	109.92
20	A	502	FMN	C10-C4A-N5	-2.20	120.19	124.86
20	A	502	FMN	C4A-C10-N1	-2.15	119.74	124.73
20	A	502	FMN	C9A-C5A-N5	-2.11	120.14	122.43
23	G	201	8Q1	O4-C1-S44	-2.09	119.90	122.61

There are no chirality outliers.

All (107) 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'
22	C	303	PLX	O7-C6-O6-C4
22	C	303	PLX	C3-C4-O6-C6
22	C	303	PLX	N1-C1-C2-O1
23	G	201	8Q1	O27-C28-C29-C32
23	G	201	8Q1	N36-C37-C38-C39
23	G	201	8Q1	N41-C42-C43-S44
23	G	201	8Q1	C28-O27-P24-O3
23	G	201	8Q1	C28-O27-P24-O2
23	G	201	8Q1	C28-O27-P24-O1
24	J	401	NDP	C2N-C3N-C7N-O7N
27	N	201	CDL	O1-C1-CB2-OB2
27	N	201	CDL	CA2-C1-CB2-OB2
27	N	201	CDL	CA2-OA2-PA1-OA3
27	N	201	CDL	CA2-OA2-PA1-OA4
27	N	201	CDL	CA3-OA5-PA1-OA4
27	N	201	CDL	C11-CA5-OA6-CA4
27	N	201	CDL	CB2-OB2-PB2-OB3
27	N	201	CDL	CB2-OB2-PB2-OB4
27	N	201	CDL	CB2-OB2-PB2-OB5
27	N	201	CDL	CB3-OB5-PB2-OB2
27	N	201	CDL	CB3-OB5-PB2-OB3
27	N	201	CDL	CB3-OB5-PB2-OB4
27	N	201	CDL	OA7-CA5-OA6-CA4
27	N	201	CDL	C11-C12-C13-C14
24	J	401	NDP	C2D-C1D-N1N-C6N
22	C	303	PLX	C3-O4-P1-O1
27	N	201	CDL	CA2-OA2-PA1-OA5
27	N	201	CDL	CA3-OA5-PA1-OA2
22	C	303	PLX	C9-C10-C11-C12
23	G	201	8Q1	O27-C28-C29-C30
23	G	201	8Q1	O27-C28-C29-C31
27	N	201	CDL	CA6-CA4-OA6-CA5
22	C	303	PLX	C25-C26-C27-C28
22	C	303	PLX	C14-C15-C16-C17
27	N	201	CDL	C51-C52-C53-C54
22	C	303	PLX	C16-C17-C18-C19
22	C	303	PLX	C27-C28-C29-C30
27	N	201	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	C	303	PLX	O9-C24-C25-C26
22	C	303	PLX	C13-C14-C15-C16
21	C	302	PEE	C42-C43-C44-C45
21	C	302	PEE	C32-C33-C34-C35
27	N	201	CDL	CA7-C31-C32-C33
21	C	302	PEE	C11-C10-O2-C2
27	N	201	CDL	OA9-CA7-OA8-CA6
22	C	303	PLX	C18-C19-C20-C21
22	C	303	PLX	C15-C16-C17-C18
21	C	302	PEE	O4-C10-O2-C2
22	C	303	PLX	C7-C8-C9-C10
22	C	303	PLX	C33-C34-C35-C36
22	C	303	PLX	C26-C27-C28-C29
27	N	201	CDL	CA3-CA4-CA6-OA8
22	C	303	PLX	C31-C32-C33-C34
21	C	302	PEE	C19-C20-C21-C22
23	G	201	8Q1	C9-C10-C11-C12
22	C	303	PLX	O4-C3-C4-O6
27	N	201	CDL	OB5-CB3-CB4-OB6
22	C	303	PLX	C11-C12-C13-C14
27	N	201	CDL	OB5-CB3-CB4-CB6
21	C	302	PEE	C31-C30-O3-C3
22	C	303	PLX	C17-C18-C19-C20
24	J	401	NDP	O4D-C1D-N1N-C6N
21	C	302	PEE	C33-C34-C35-C36
21	C	302	PEE	C1-C2-C3-O3
22	C	303	PLX	C11-C10-C9-C8
23	G	201	8Q1	C42-C43-S44-C1
21	C	302	PEE	O2-C2-C3-O3
27	N	201	CDL	C31-C32-C33-C34
23	G	201	8Q1	O4-C1-S44-C43
22	C	303	PLX	O4-C3-C4-C5
24	J	401	NDP	O4D-C4D-C5D-O5D
23	G	201	8Q1	C6-C1-S44-C43
21	C	302	PEE	O5-C30-O3-C3
27	N	201	CDL	OA6-CA4-CA6-OA8
21	C	302	PEE	C39-C40-C41-C42
20	A	502	FMN	C3'-C4'-C5'-O5'
21	C	302	PEE	C1-O3P-P-O2P
22	C	303	PLX	C3-O4-P1-O3
24	J	401	NDP	C2N-C3N-C7N-N7N
21	C	302	PEE	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	C1'-C2'-C3'-O3'
27	N	201	CDL	CB7-C71-C72-C73
20	A	502	FMN	O2'-C2'-C3'-C4'
22	C	303	PLX	C30-C31-C32-C33
21	C	302	PEE	C18-C19-C20-C21
27	N	201	CDL	OB9-CB7-OB8-CB6
21	C	302	PEE	C13-C14-C15-C16
27	N	201	CDL	C71-CB7-OB8-CB6
23	G	201	8Q1	C11-C12-C13-C14
21	C	302	PEE	C16-C17-C18-C19
21	C	302	PEE	C38-C39-C40-C41
23	G	201	8Q1	C6-C7-C8-C9
27	N	201	CDL	OB7-CB5-OB6-CB4
22	C	303	PLX	C28-C29-C30-C31
21	C	302	PEE	C14-C15-C16-C17
22	C	303	PLX	O8-C24-C25-C26
21	C	302	PEE	O4P-C4-C5-N
24	J	401	NDP	C3D-C4D-C5D-O5D
27	N	201	CDL	C72-C71-CB7-OB8
27	N	201	CDL	C51-CB5-OB6-CB4
24	J	401	NDP	O4B-C4B-C5B-O5B
27	N	201	CDL	C72-C71-CB7-OB9
22	C	303	PLX	C36-C37-C38-C39
21	C	302	PEE	O3-C30-C31-C32
21	C	302	PEE	O5-C30-C31-C32

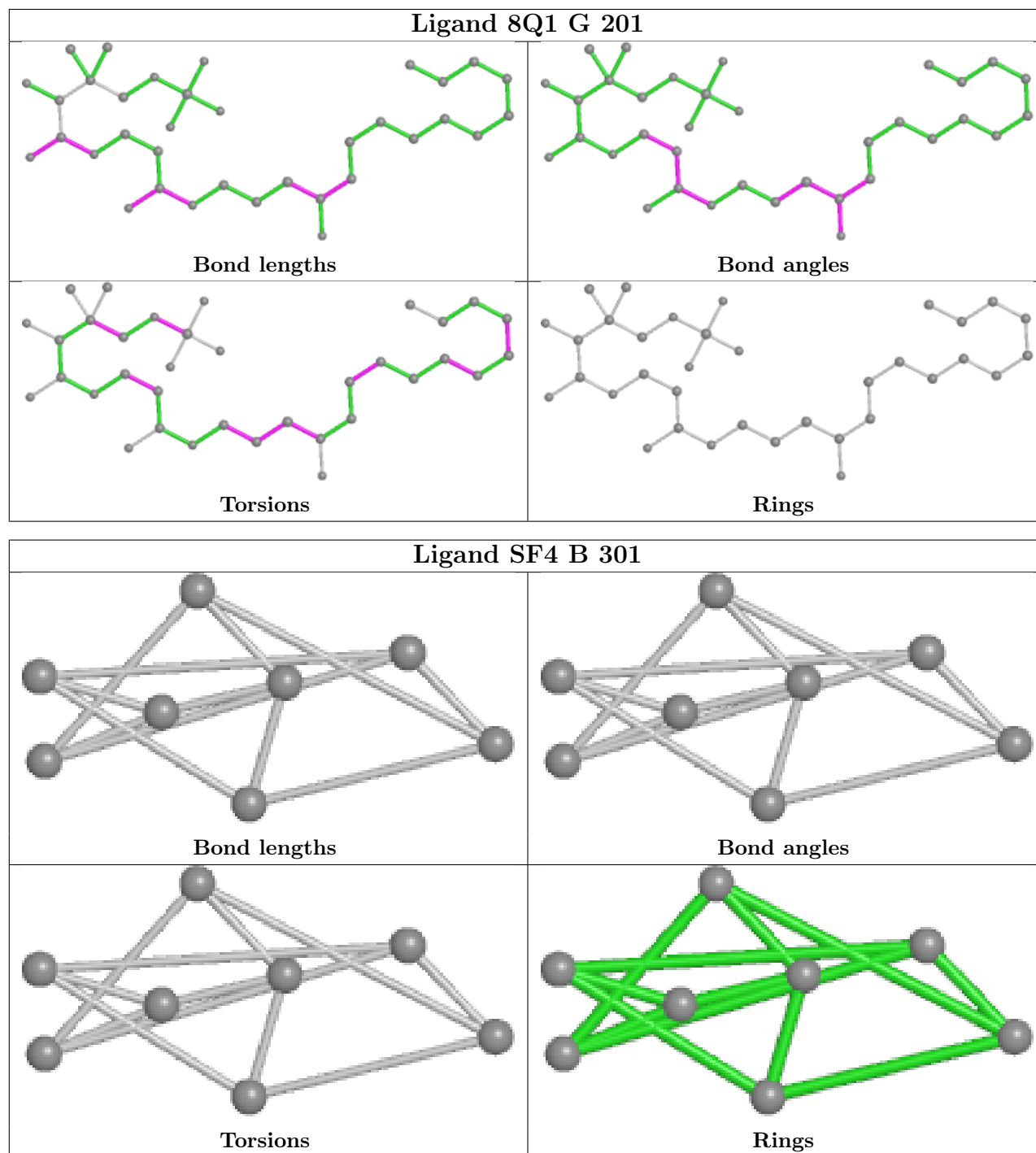
There are no ring outliers.

6 monomers are involved in 15 short contacts:

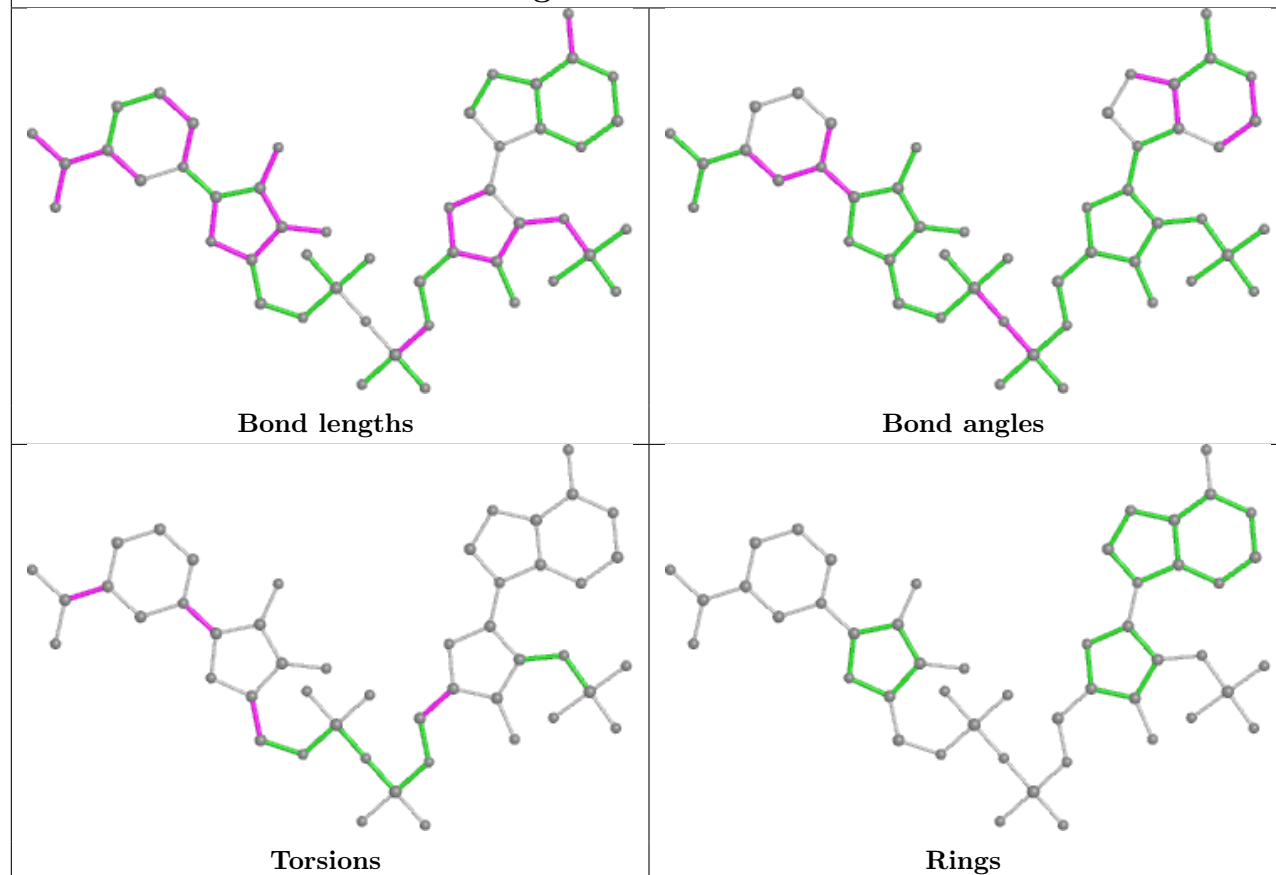
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	201	8Q1	5	0
24	J	401	NDP	2	0
19	C	301	SF4	1	0
19	A	501	SF4	1	0
20	A	502	FMN	3	0
22	C	303	PLX	3	0

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.

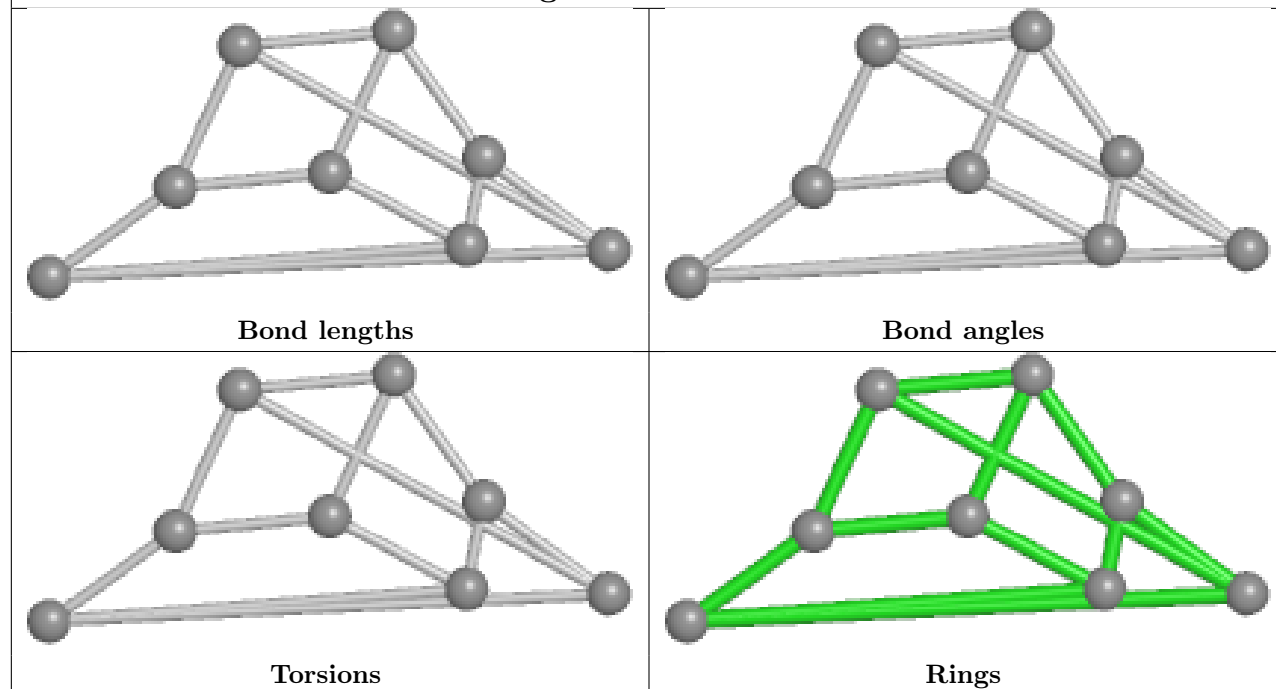
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



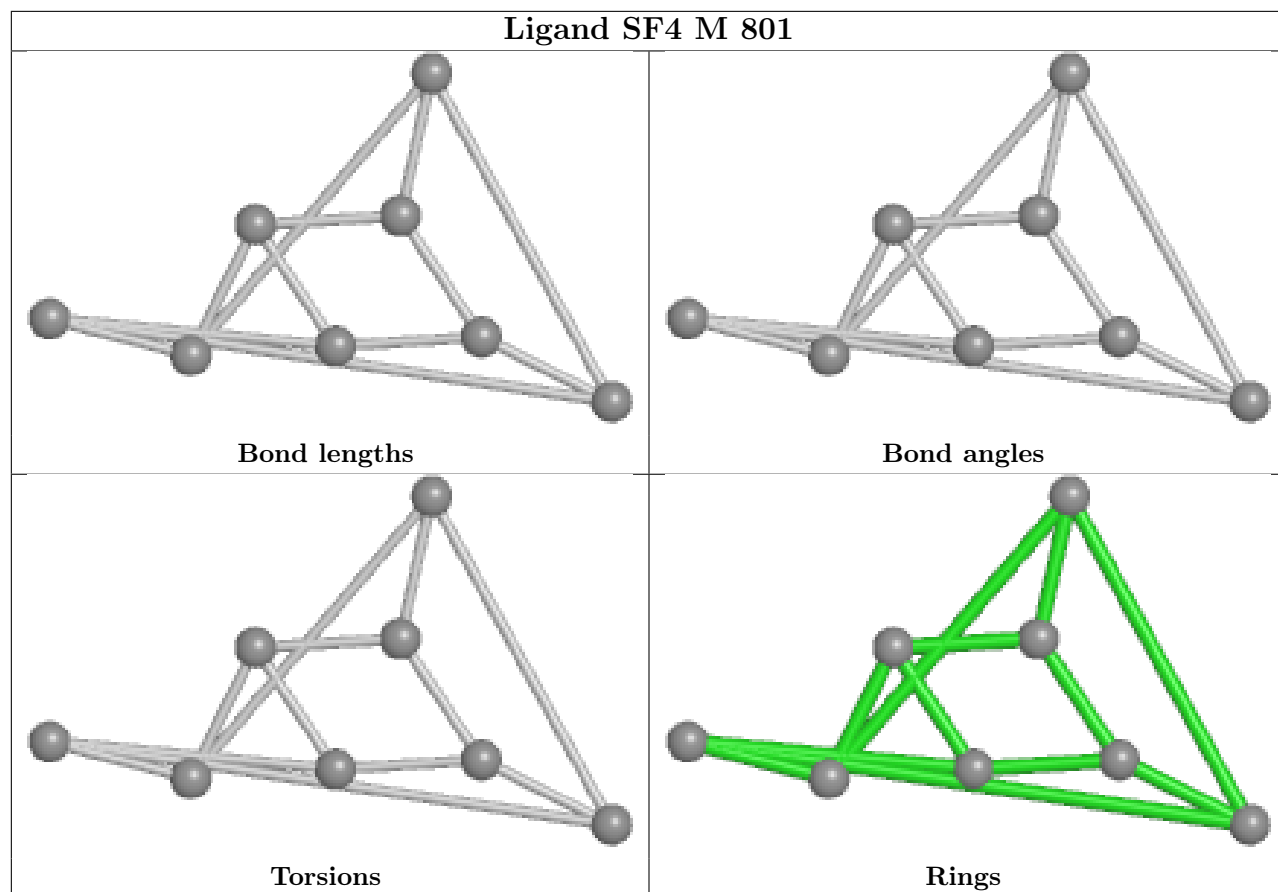
Ligand NDP J 401



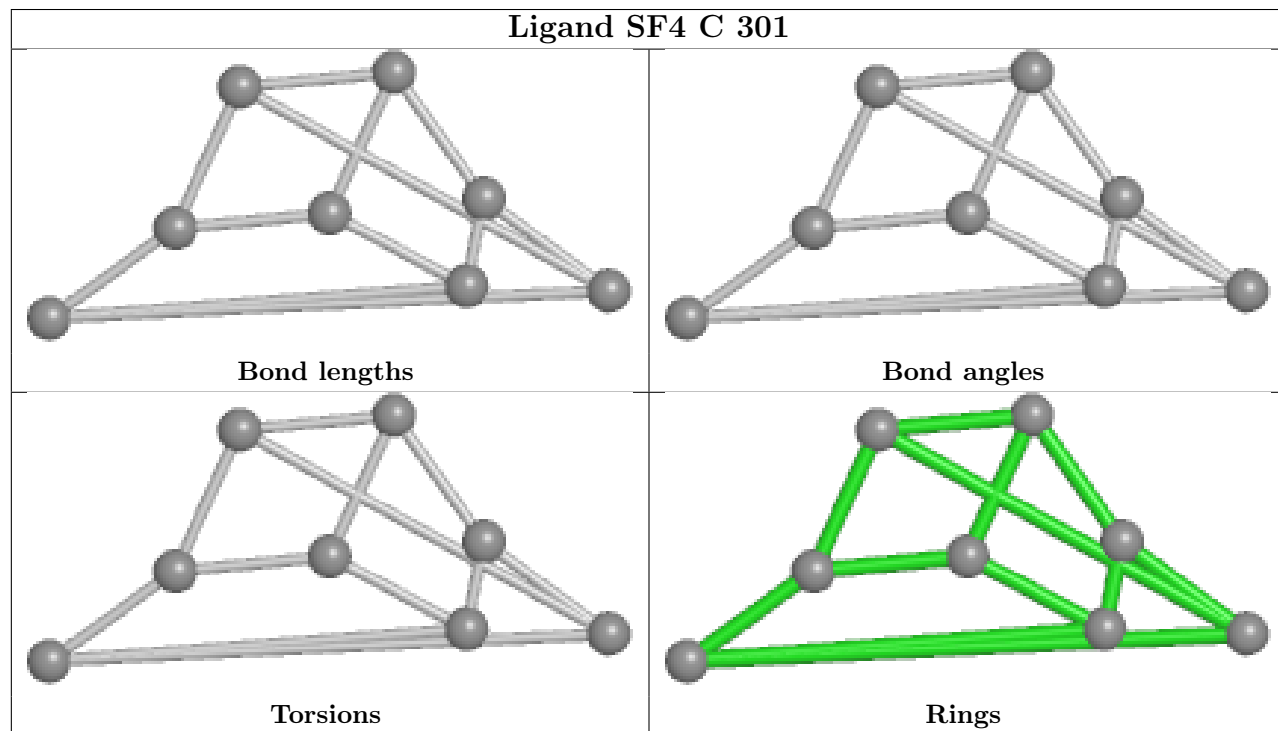
Ligand SF4 B 302

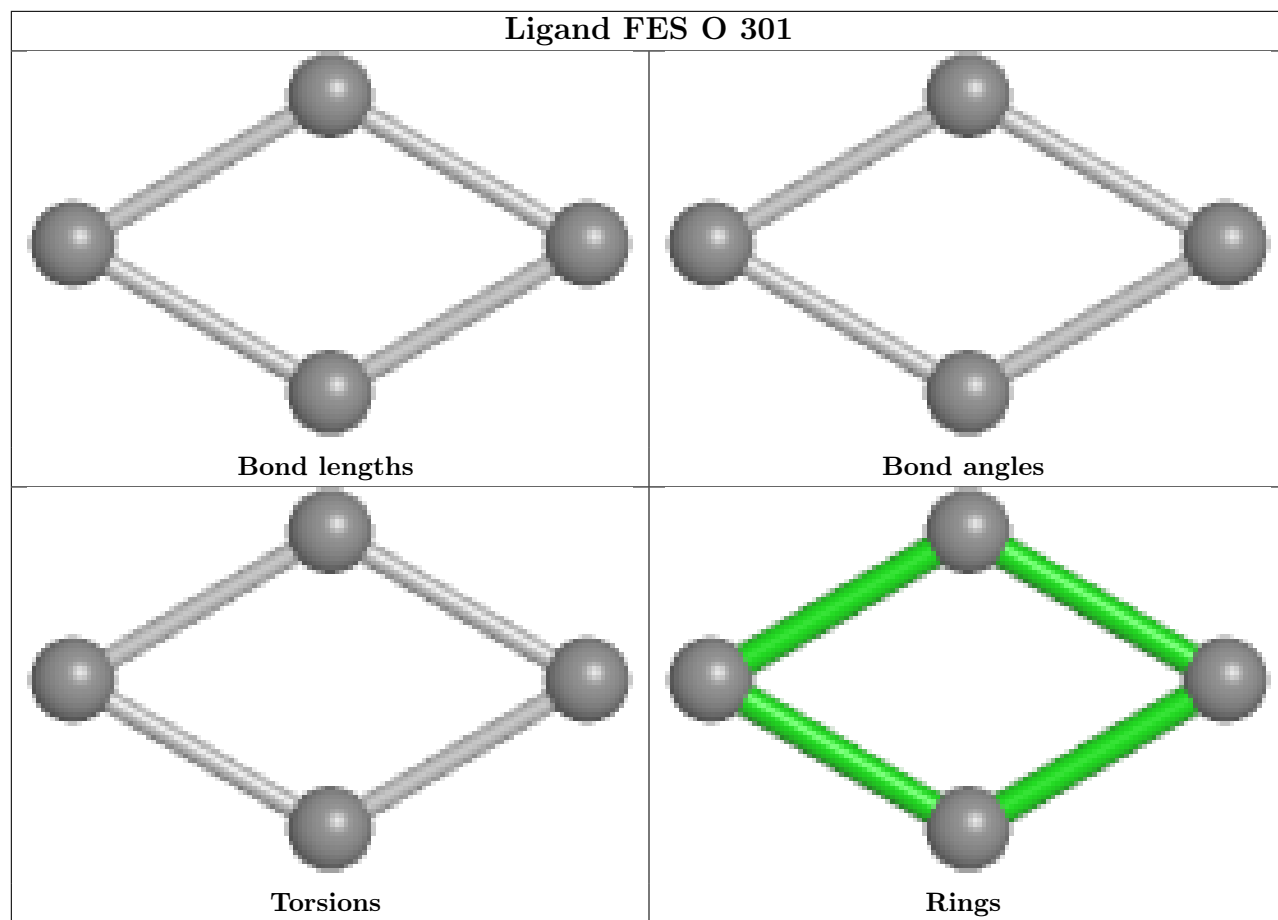


Ligand SF4 M 801

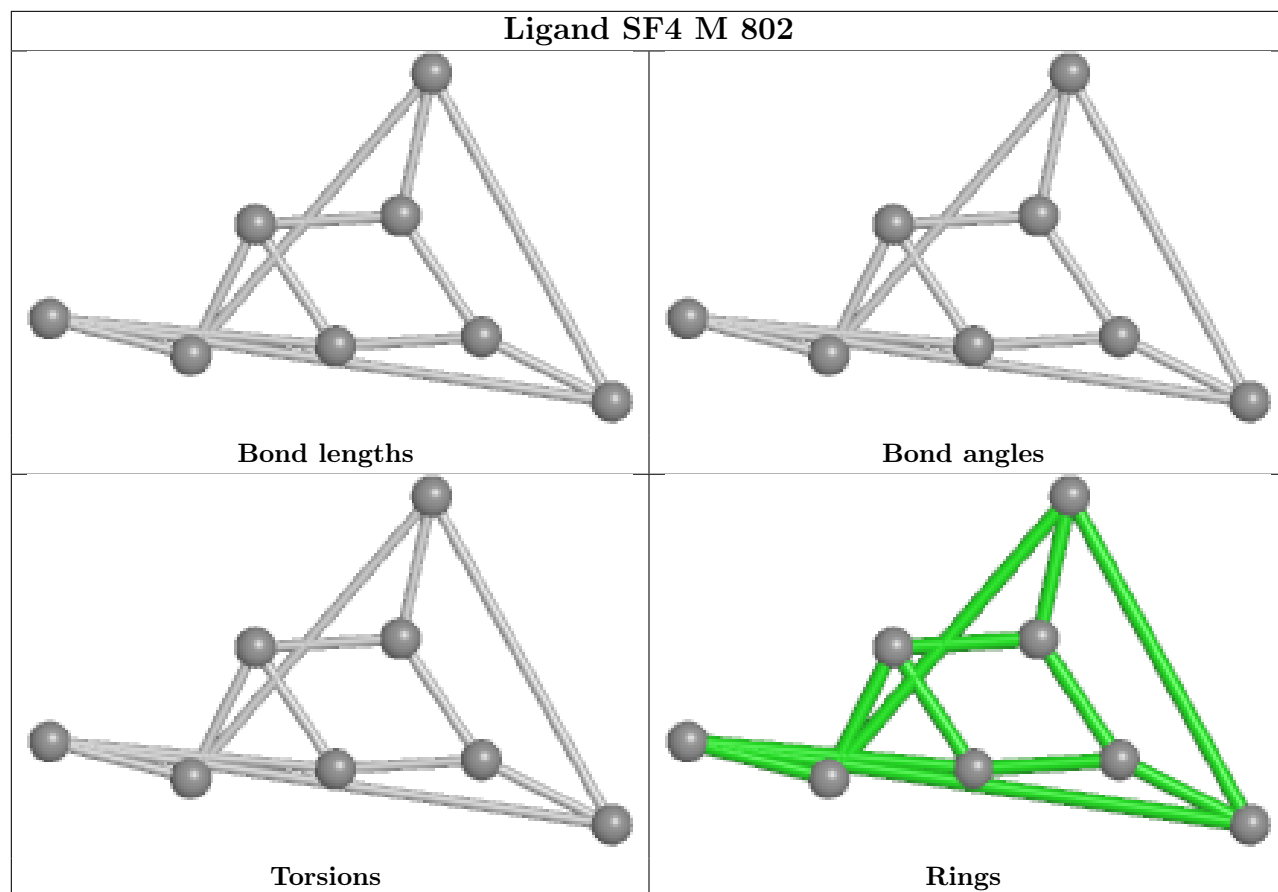


Ligand SF4 C 301

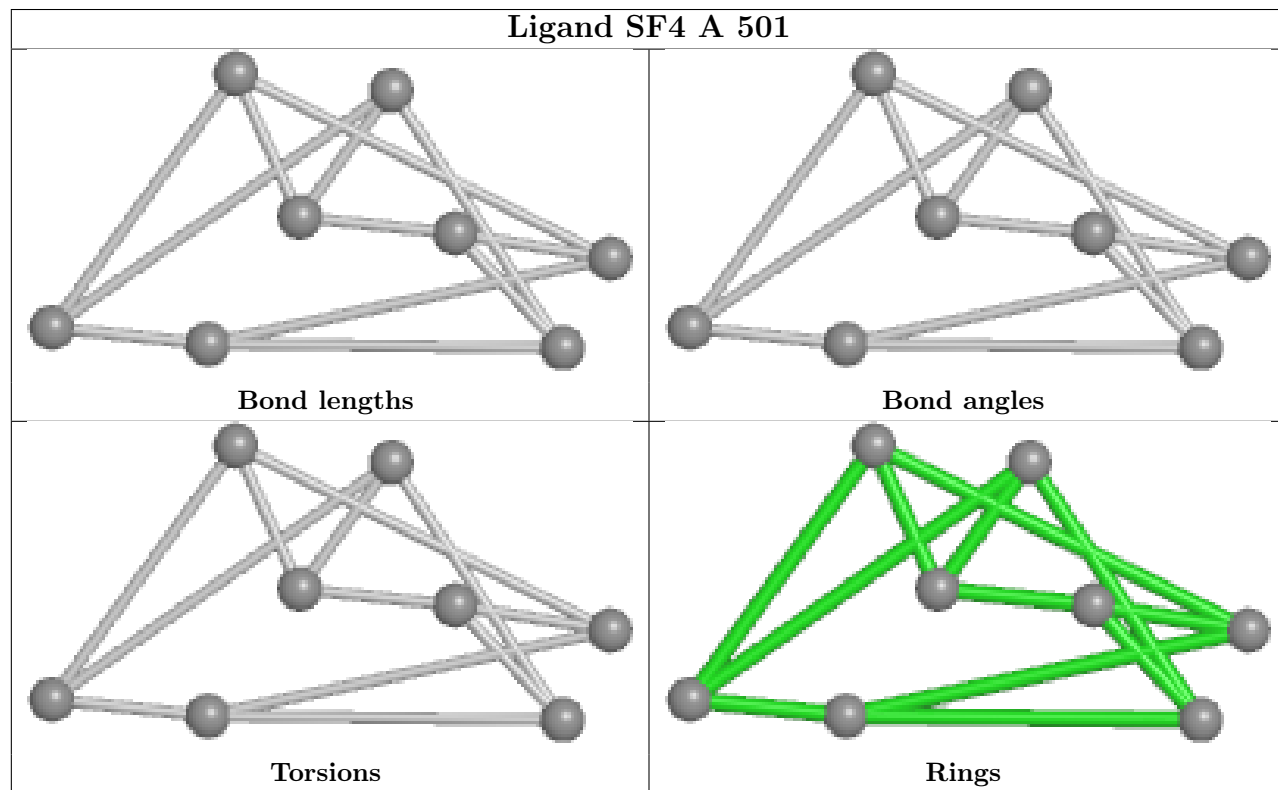


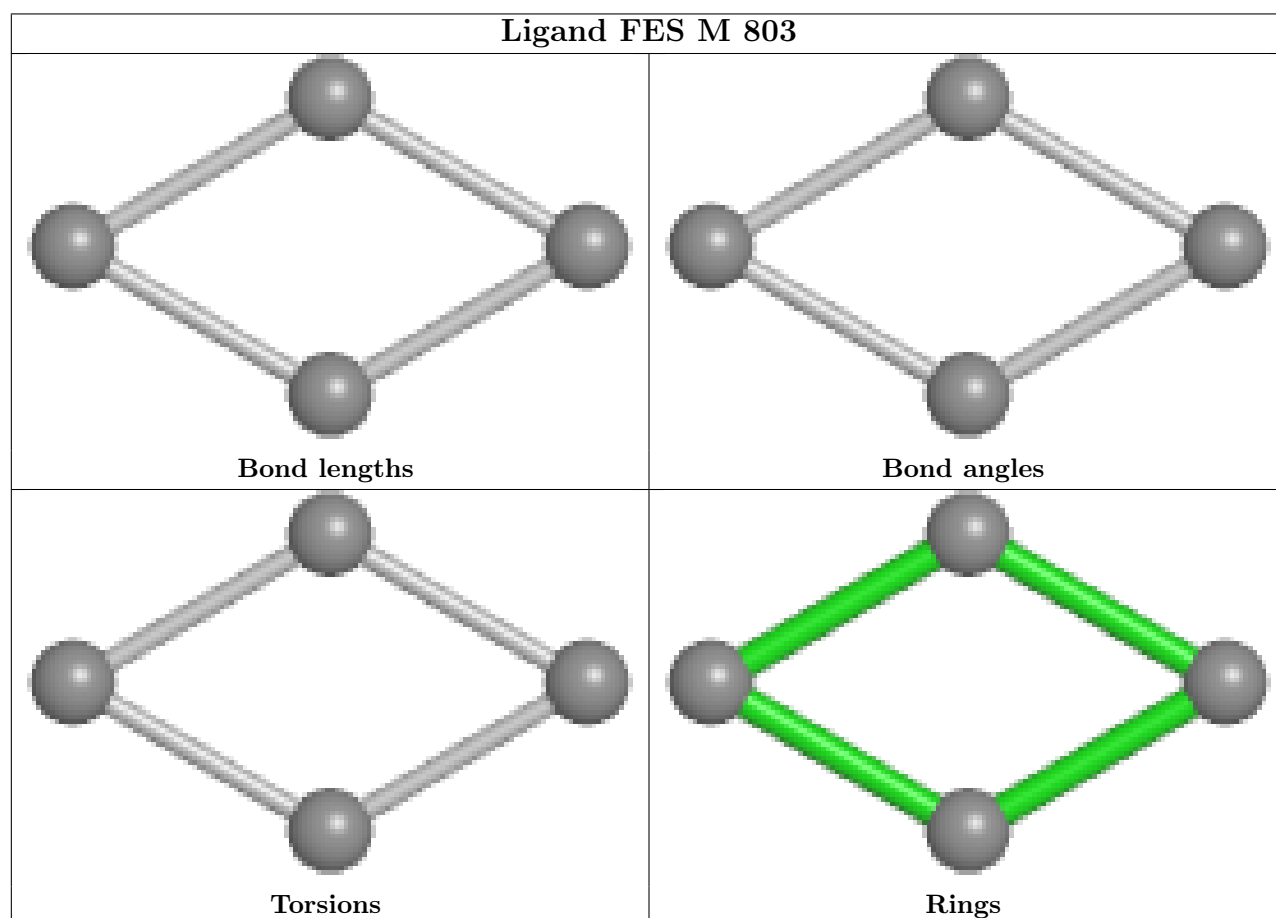
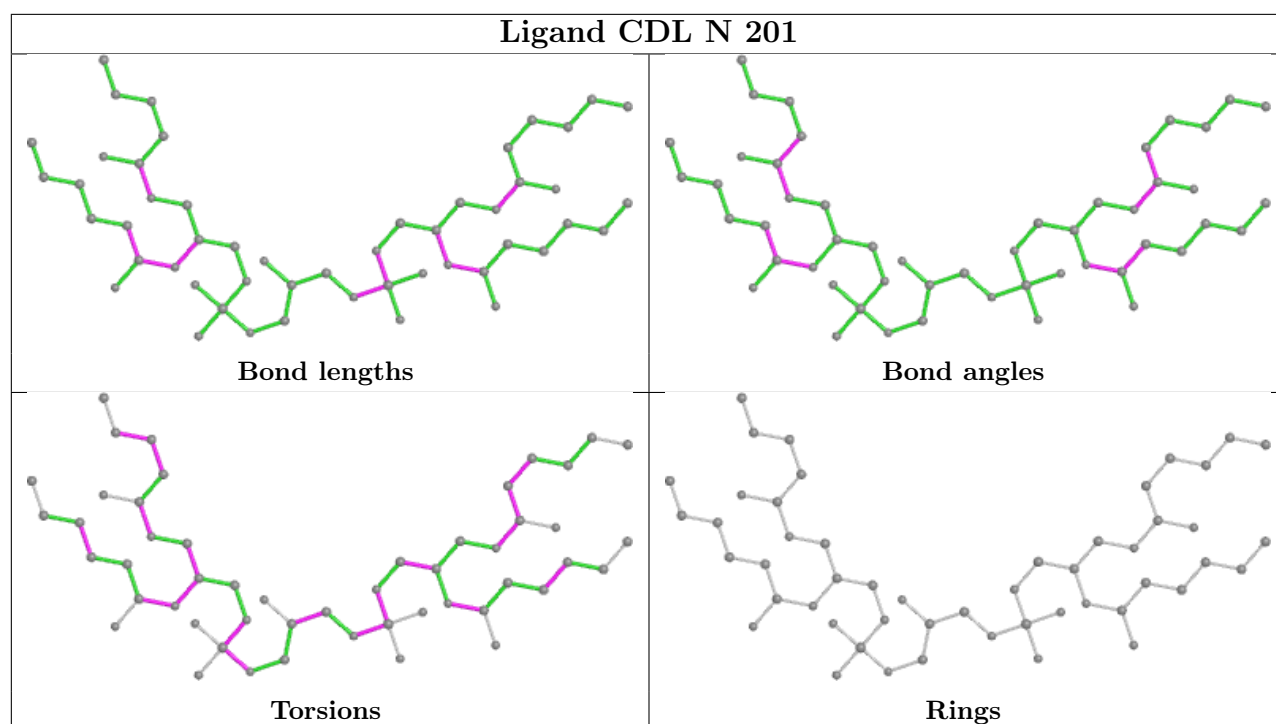


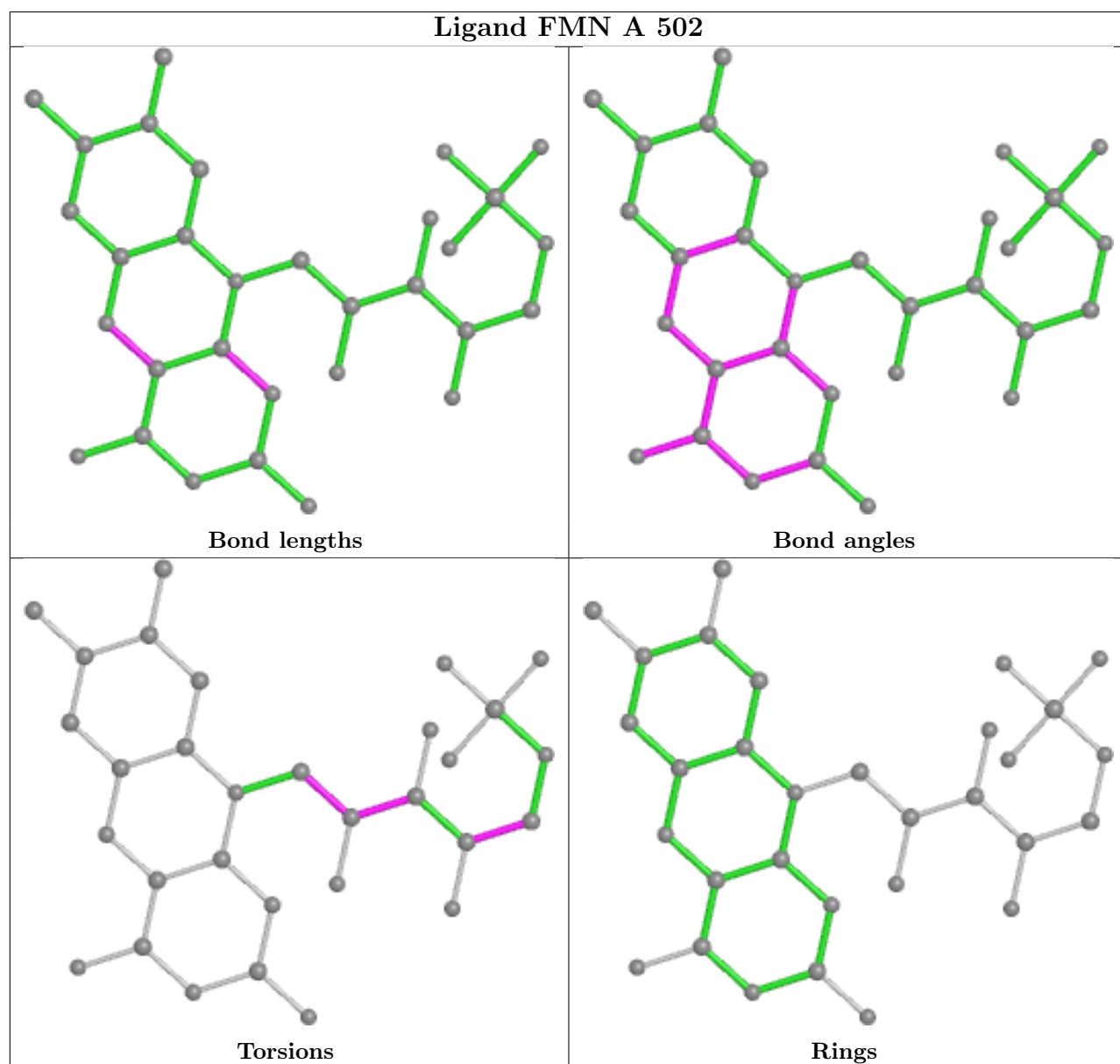
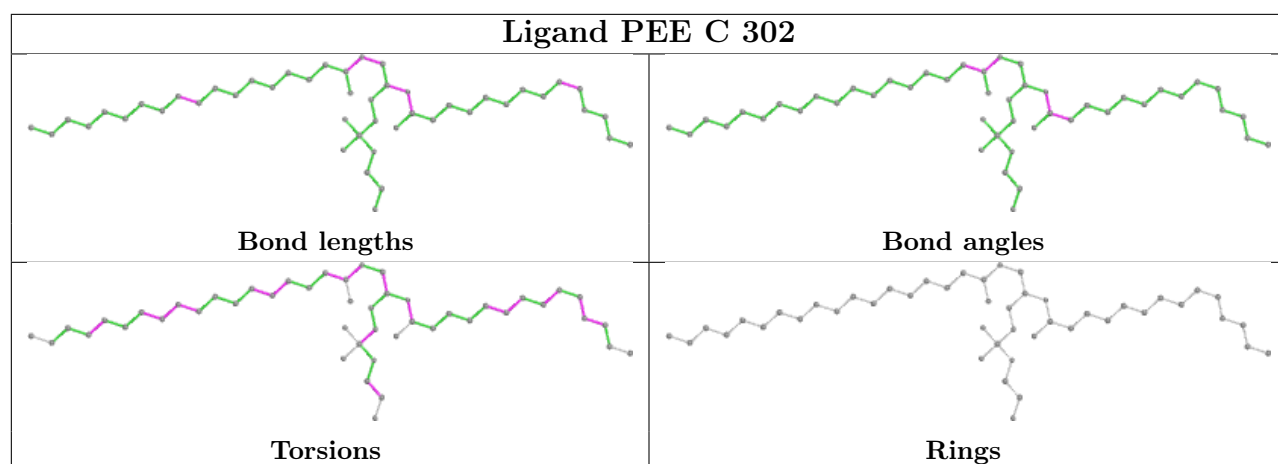
Ligand SF4 M 802

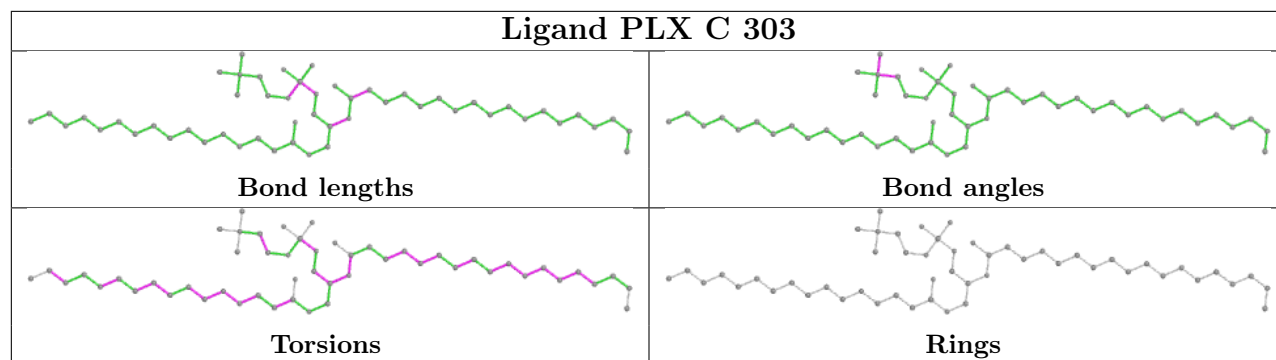


Ligand SF4 A 501









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.

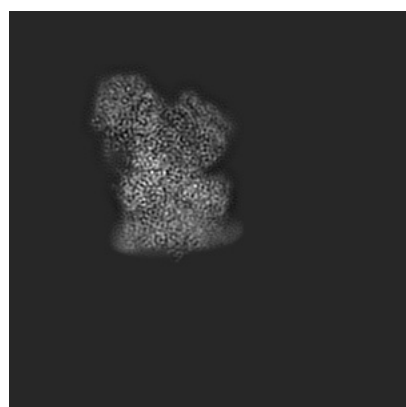
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32188. These allow visual inspection of the internal detail of the map and identification of artifacts.

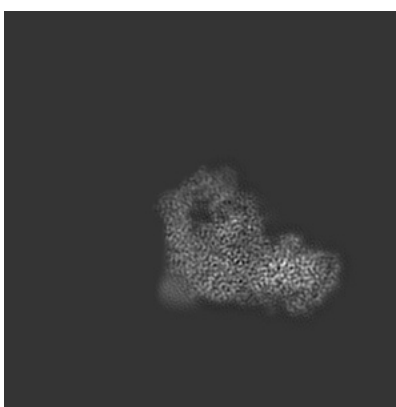
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

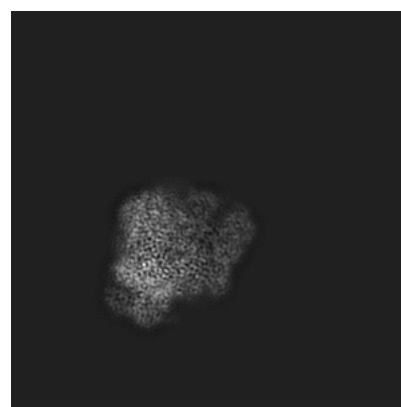
6.1.1 Primary map



X



Y

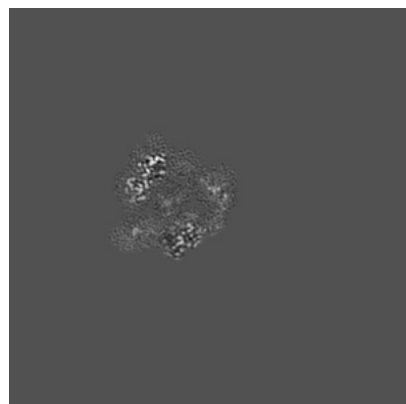


Z

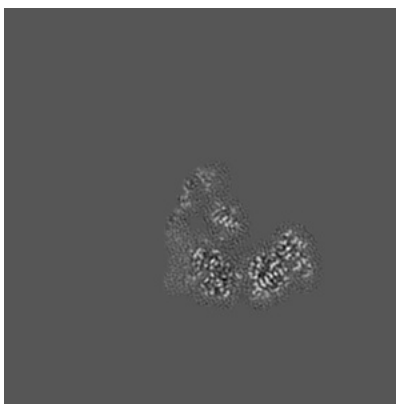
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

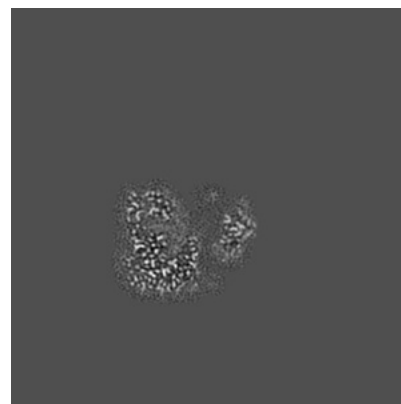
6.2.1 Primary map



X Index: 165



Y Index: 165



Z Index: 165

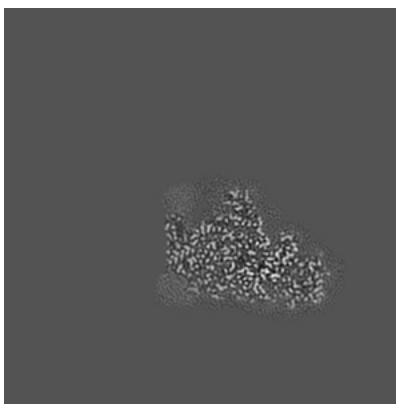
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 117



Y Index: 115

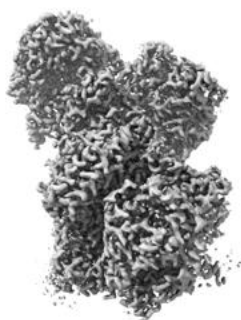


Z Index: 183

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

6.4 Orthogonal surface views [i](#)

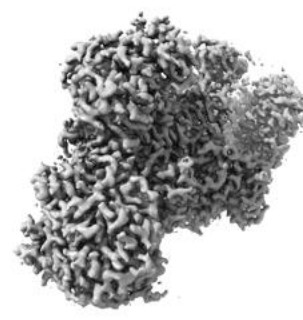
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0236. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

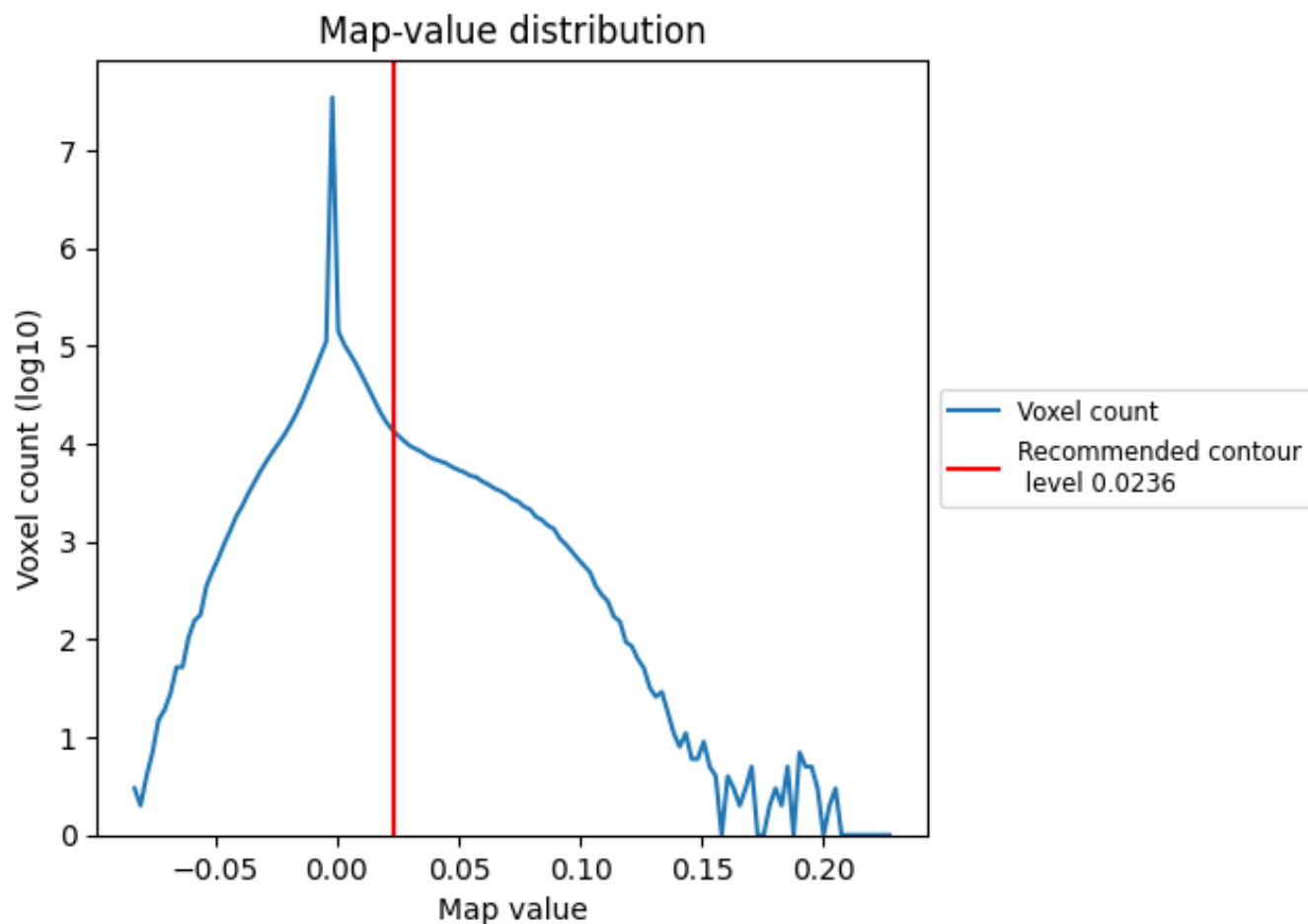
6.5 Mask visualisation

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

7 Map analysis [i](#)

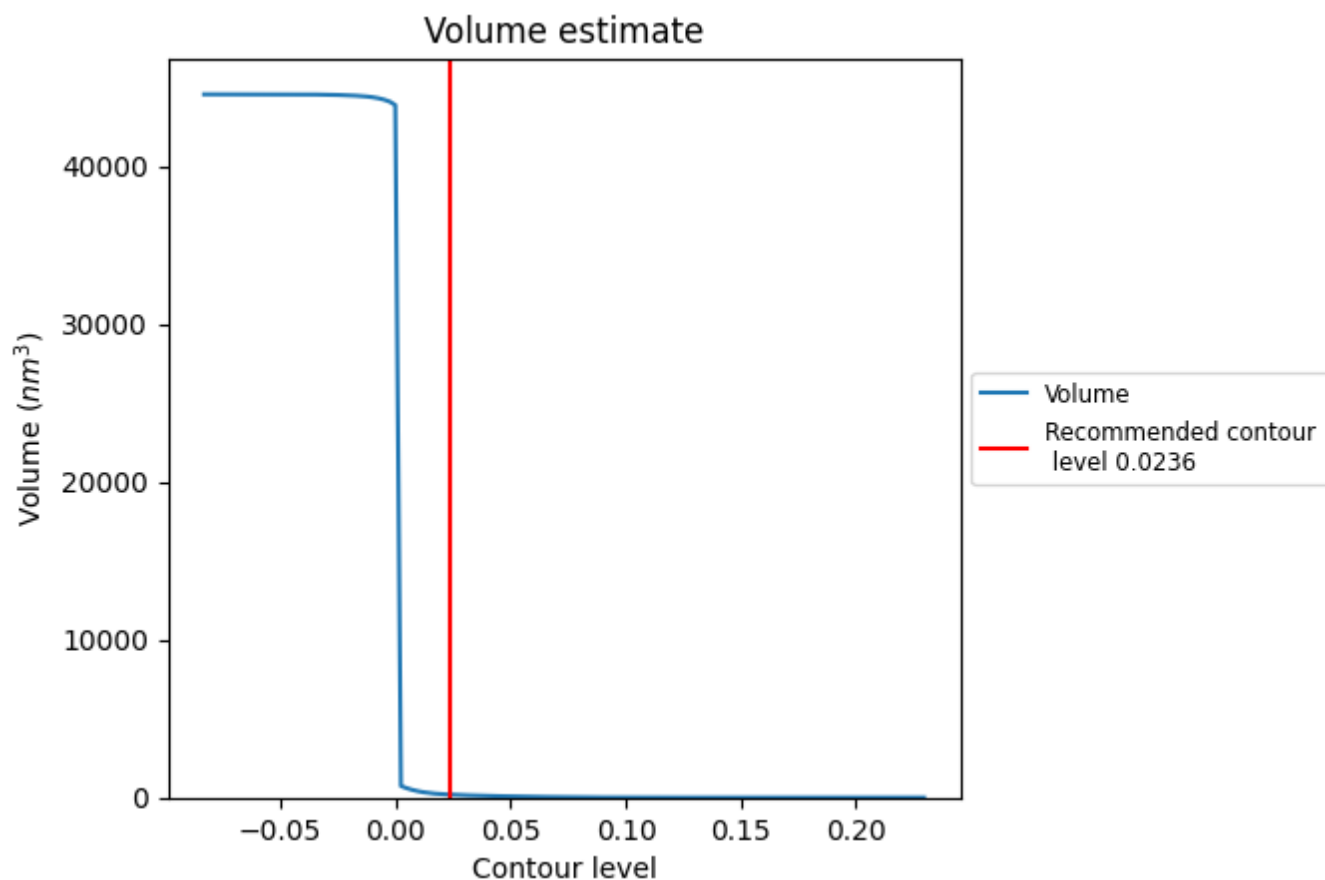
This section contains the results of statistical analysis of the map.

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.

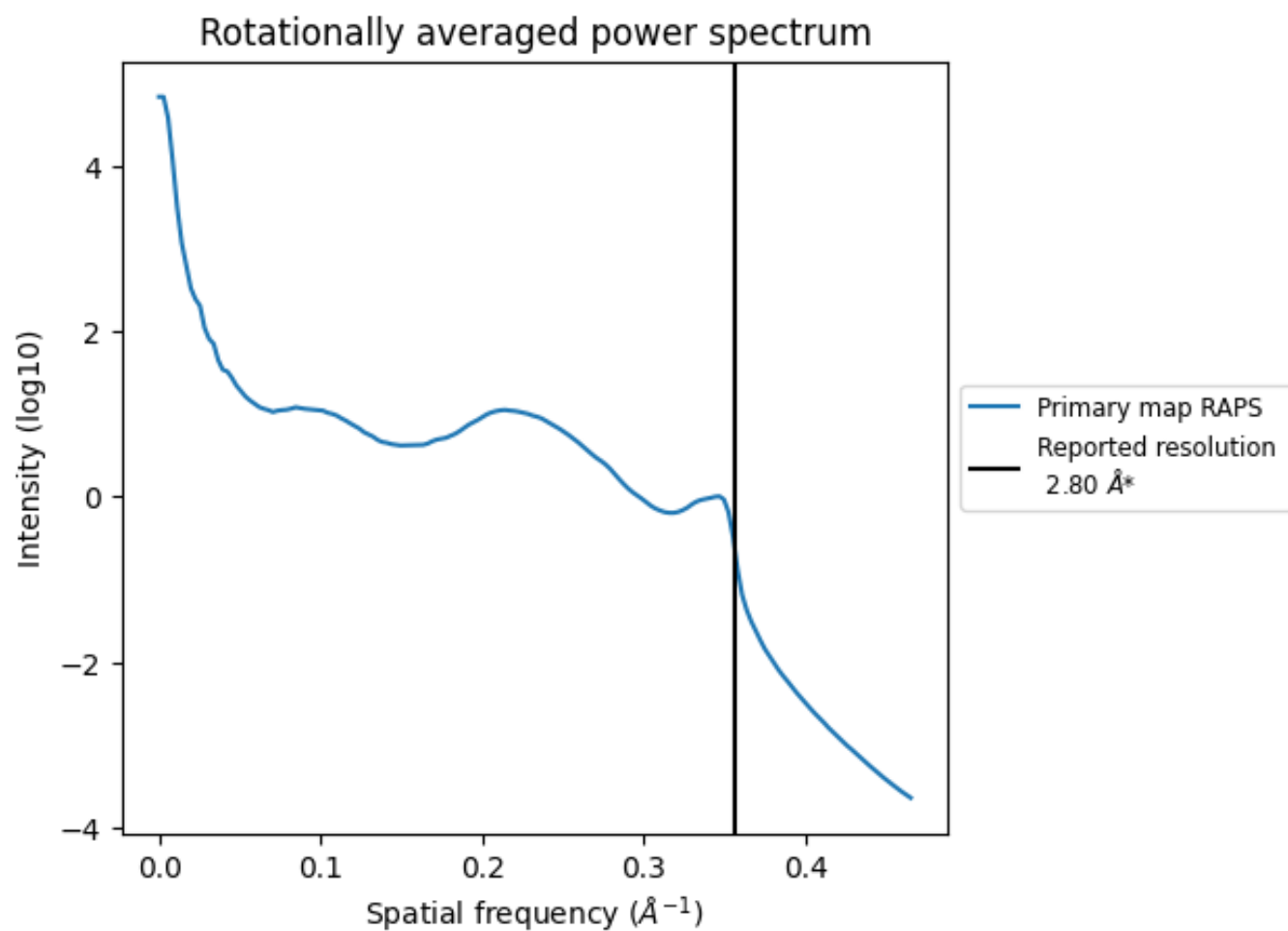
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm³; this corresponds to an approximate mass of 169 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 Å⁻¹

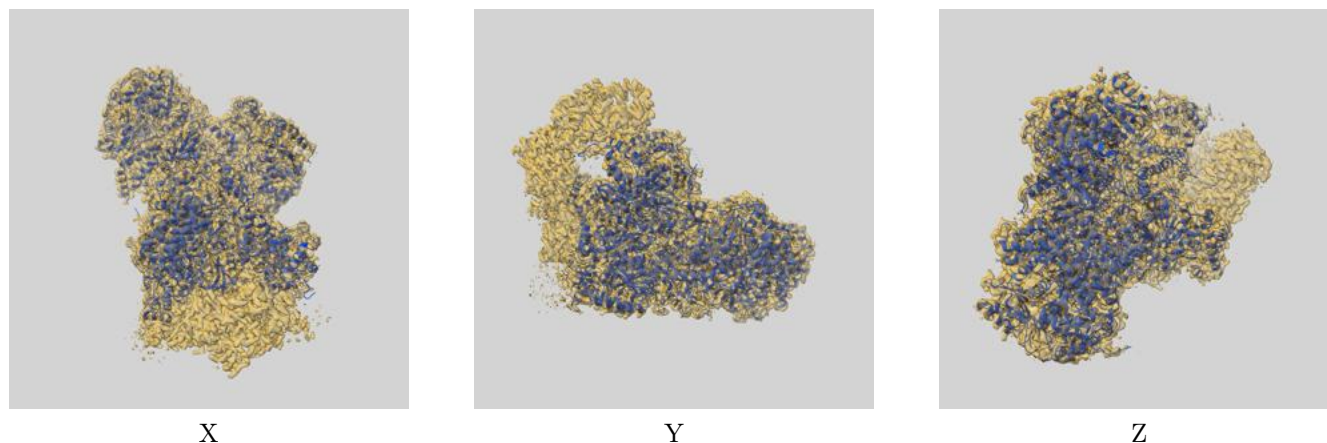
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

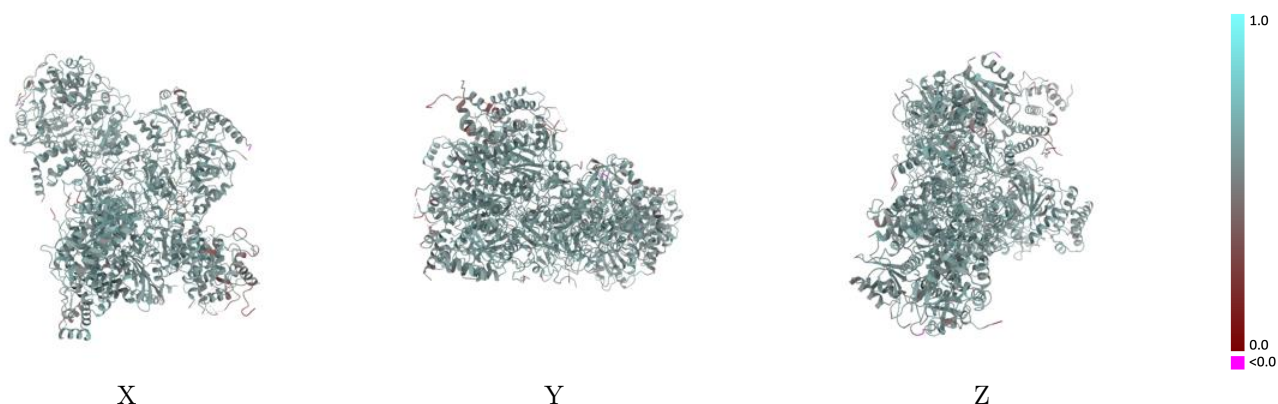
This section contains information regarding the fit between EMDB map EMD-32188 and PDB model 7VXU. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



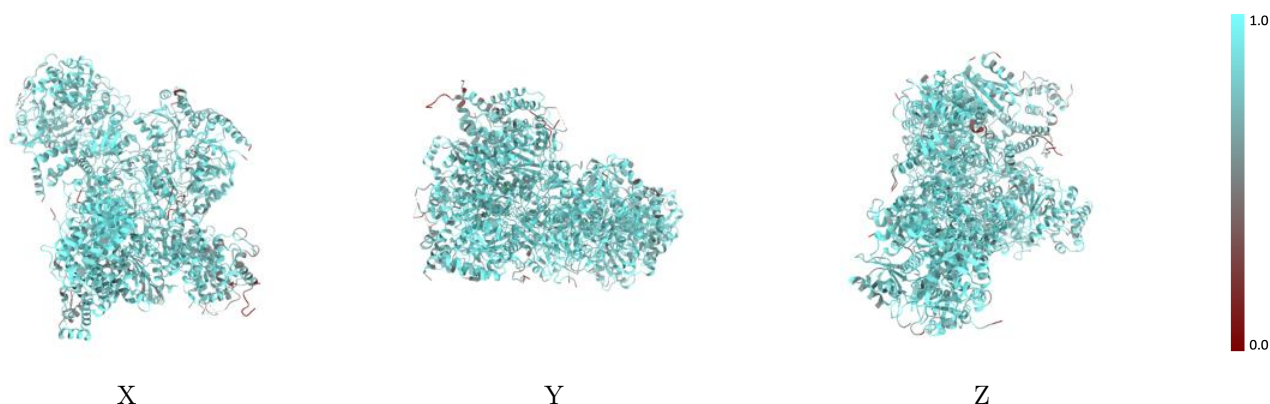
The images above show the 3D surface view of the map at the recommended contour level 0.0236 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



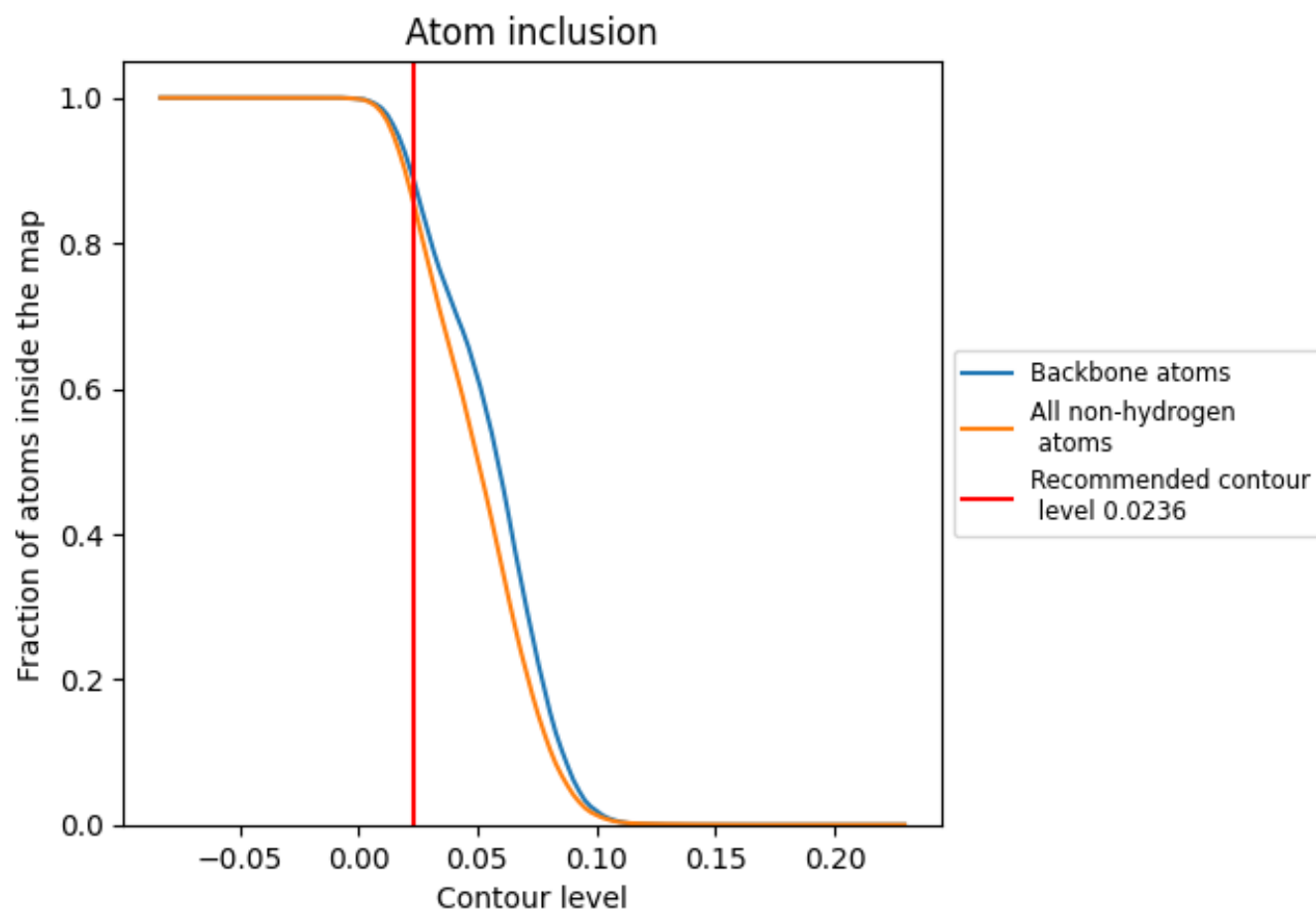
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0236).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.0236) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8507	 0.5820
A	 0.8624	 0.5800
B	 0.9179	 0.6070
C	 0.8657	 0.5940
E	 0.8291	 0.5790
F	 0.7976	 0.5530
G	 0.6469	 0.4840
H	 0.8335	 0.5650
I	 0.7963	 0.5570
J	 0.8309	 0.5710
K	 0.8401	 0.5710
L	 0.8451	 0.5900
M	 0.8714	 0.5910
N	 0.7780	 0.5680
O	 0.8206	 0.5590
P	 0.9072	 0.6110
Q	 0.8902	 0.6030
T	 0.8283	 0.5920
W	 0.8302	 0.5490

