



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 7VYA / pdb_00007vya
EMDB ID : EMD-32198
Title : Matrix arm of deactive state CI from Q10-NADH 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:

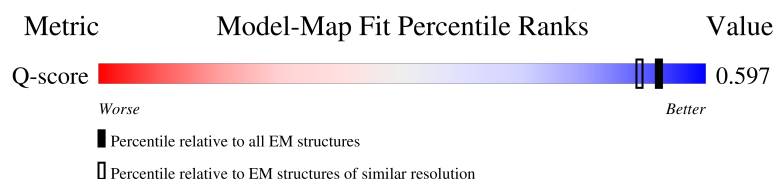
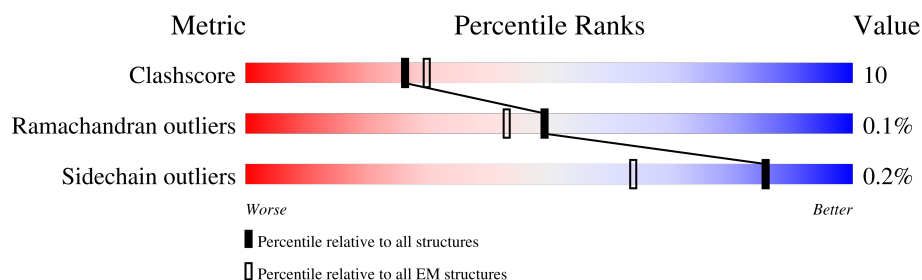
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	431	
2	B	176	
3	C	156	
4	E	115	

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
7	H	112	
8	I	112	
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	385	
17	T	96	
18	W	29	

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

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

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 28031 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 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
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein.

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	297	Total	C	N	O	S	0	0
			2359	1514	421	416	8		

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

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.

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		

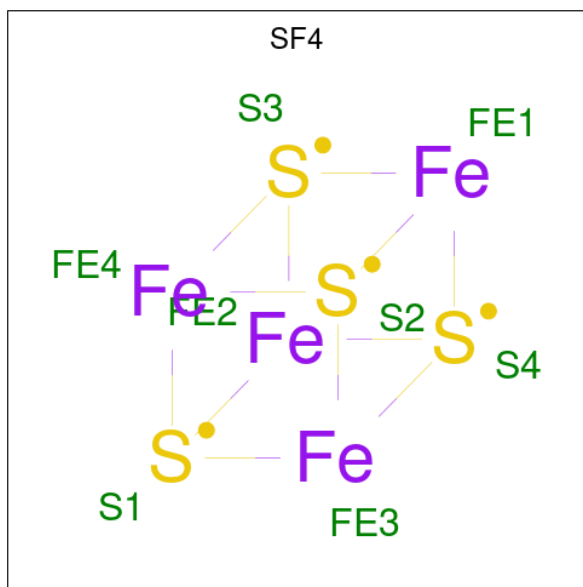
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

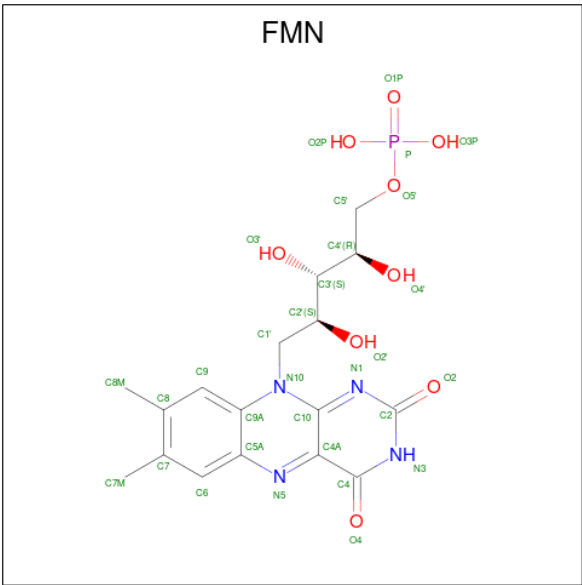
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			218	138	40	39	1		

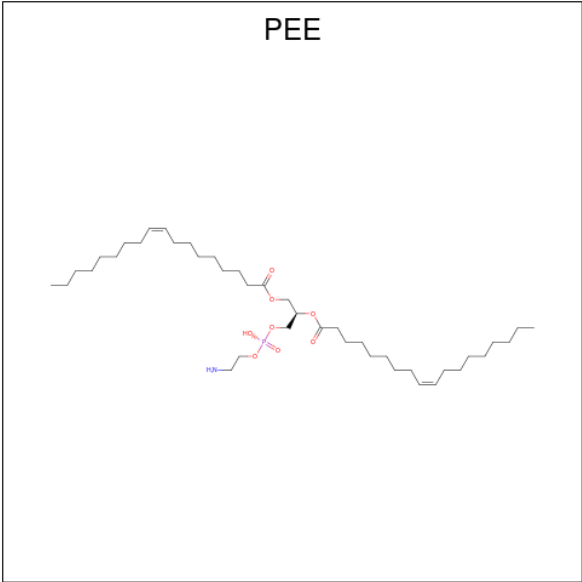
- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

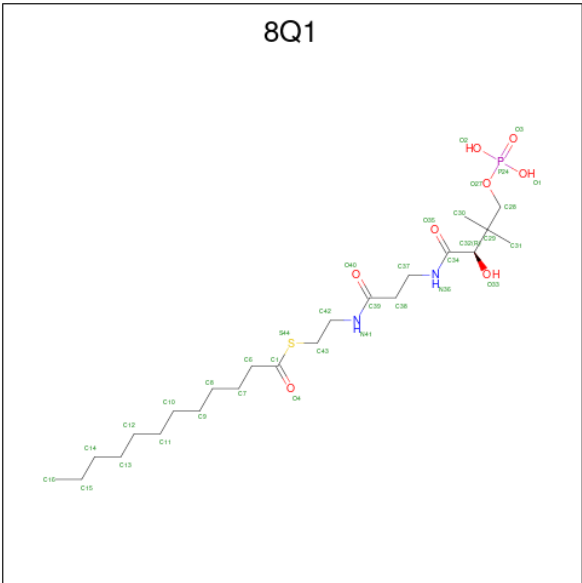
- Molecule 20 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 23 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as
"Ligand of Interest" by depositor).

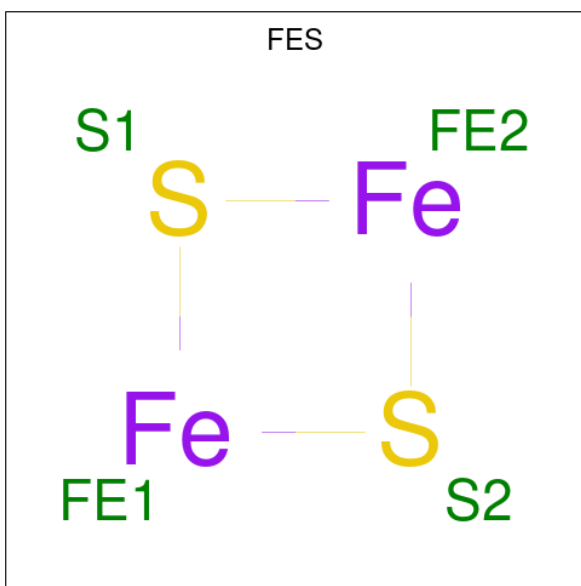


Mol	Chain	Residues	Atoms						AltConf
23	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 24 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

NDP

- Molecule 25 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

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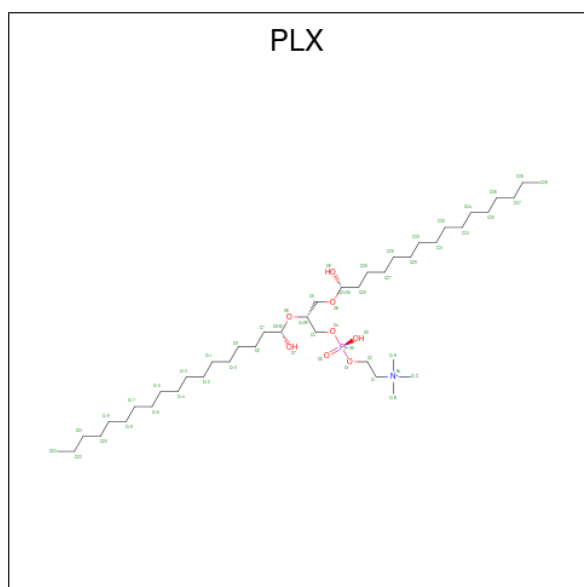
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Mol	Chain	Residues	Atoms			AltConf
25	O	1	Total	Fe	S	0
			4	2	2	

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

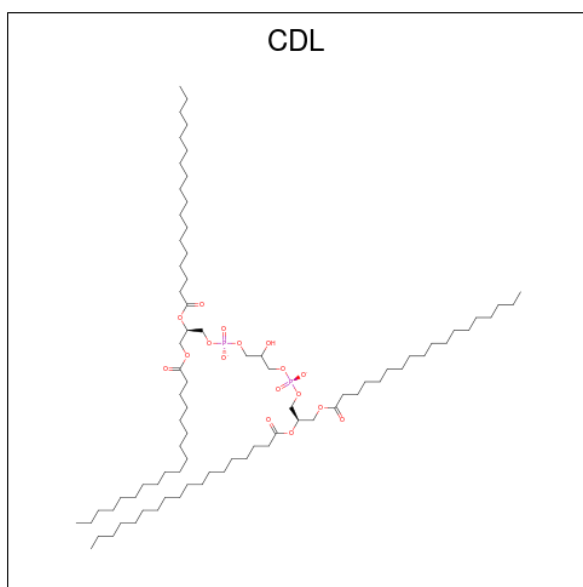
Mol	Chain	Residues	Atoms		AltConf
26	M	1	Total	Mg	0
			1	1	

- Molecule 27 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

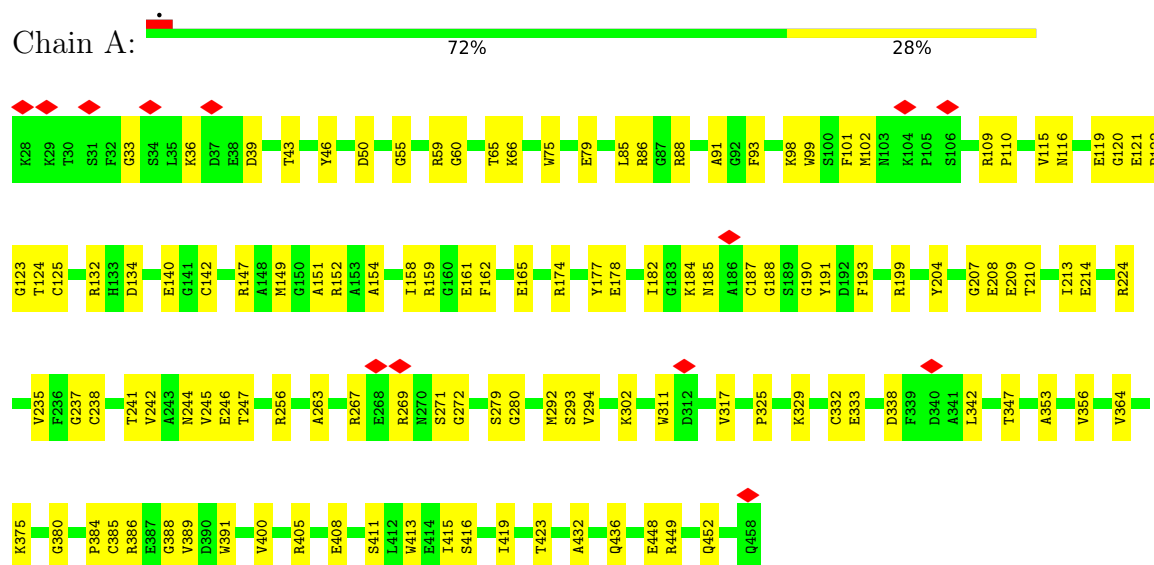
- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

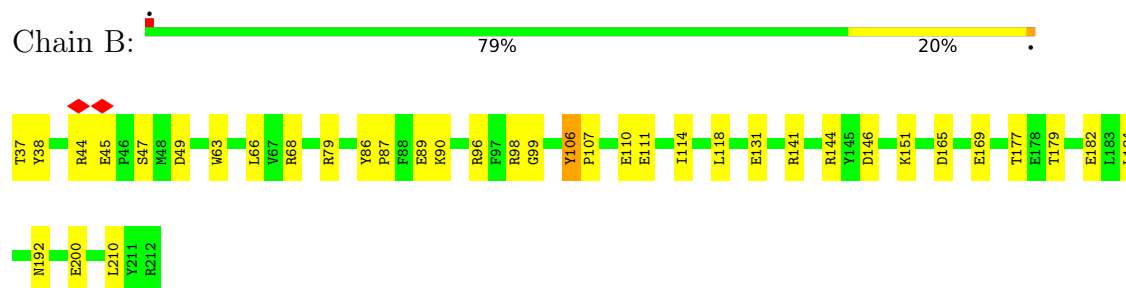
3 Residue-property plots

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.

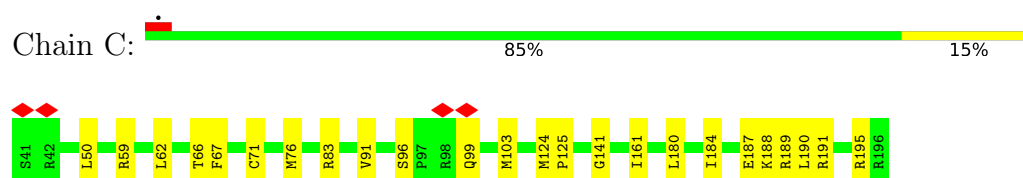
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



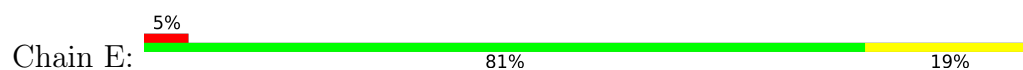
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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



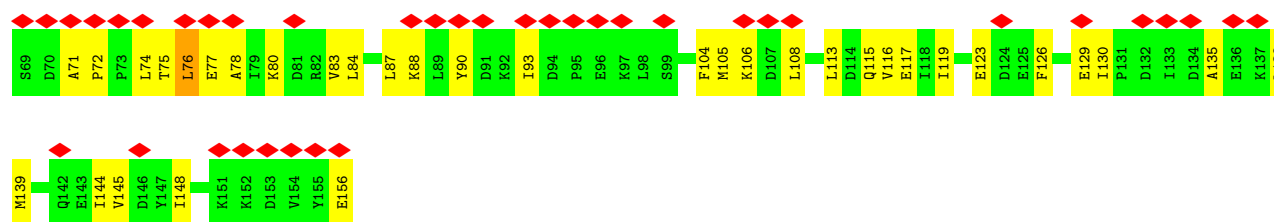
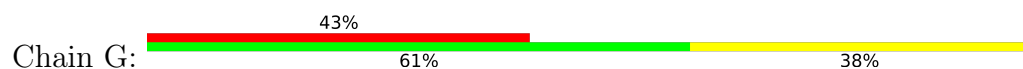
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



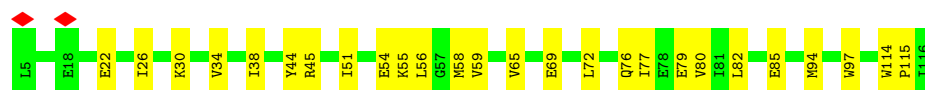
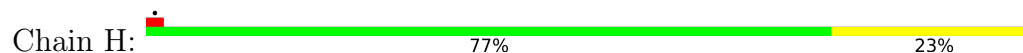
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



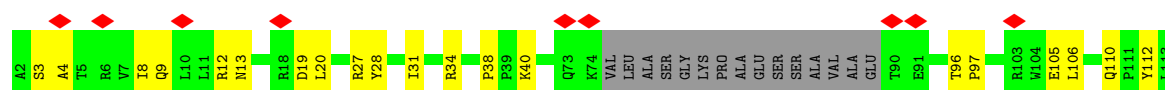
- Molecule 6: Acyl carrier protein



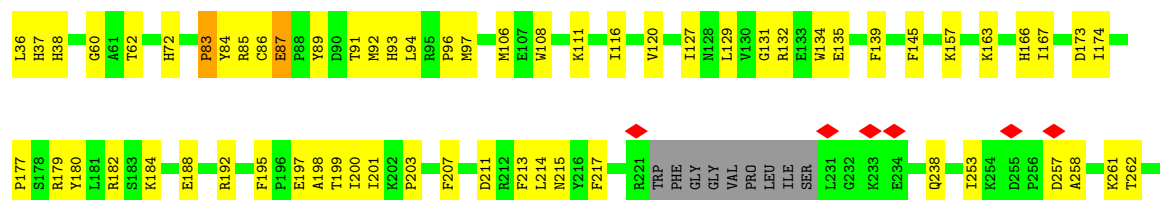
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

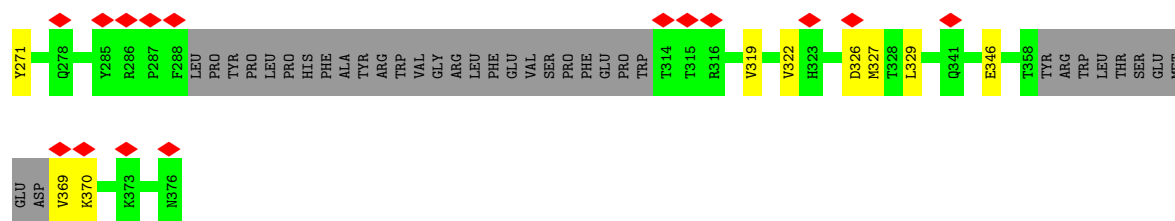


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

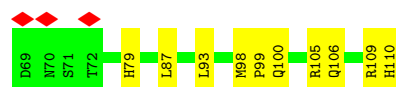
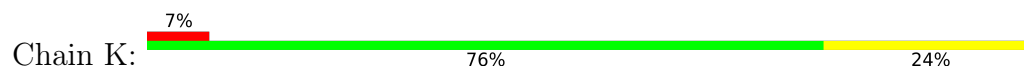


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

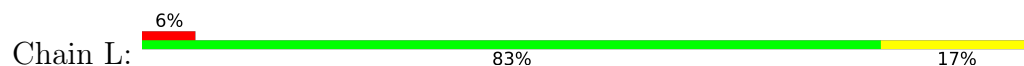




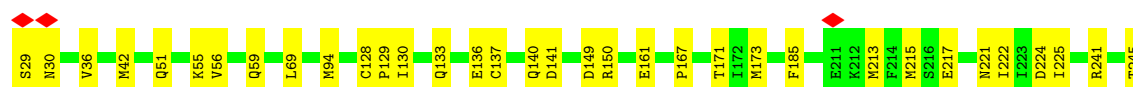
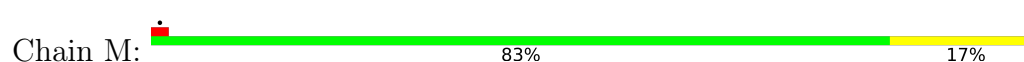
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3



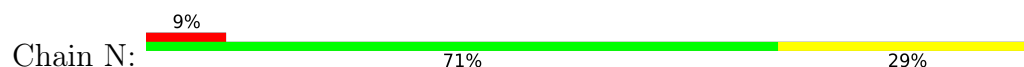
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

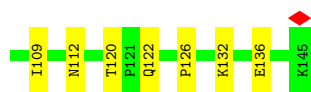


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

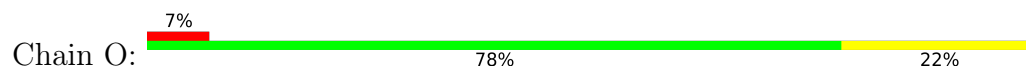


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

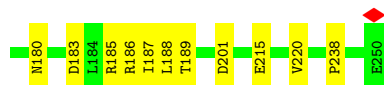
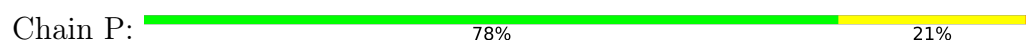




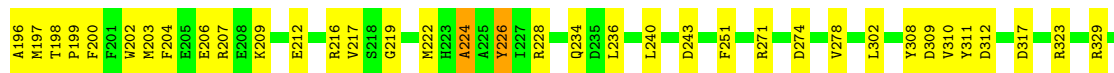
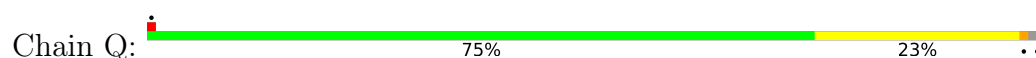
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



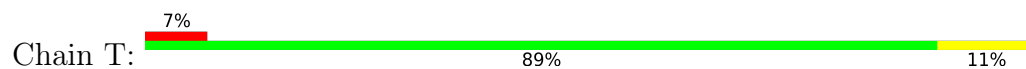
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3



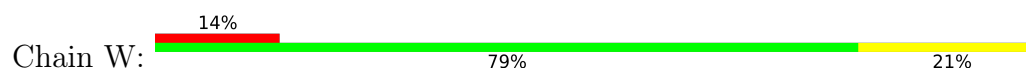
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

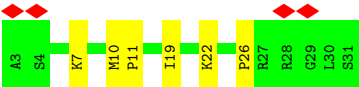


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- 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	104881	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	0.192	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0301	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: NDP, FES, MG, ZN, PLX, SF4, 2MR, CDL, FMN, NAI, PEE, 8Q1

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	0.21	0/3393	0.48	3/4584 (0.1%)
2	B	0.26	0/1443	0.44	2/1952 (0.1%)
3	C	0.24	0/1279	0.40	0/1730
4	E	0.20	0/995	0.40	0/1340
5	F	0.16	0/702	0.37	0/945
6	G	0.19	0/705	0.51	0/956
7	H	0.18	0/929	0.40	0/1258
8	I	0.21	0/798	0.47	0/1079
9	J	0.20	0/2411	0.48	2/3254 (0.1%)
10	K	0.13	0/365	0.27	0/493
11	L	0.20	0/1039	0.35	0/1403
12	M	0.19	0/5384	0.34	0/7295
13	N	0.18	0/1245	0.39	0/1694
14	O	0.17	0/1711	0.42	0/2328
15	P	0.25	0/1789	0.48	2/2436 (0.1%)
16	Q	0.25	0/3101	0.46	4/4189 (0.1%)
17	T	0.16	0/755	0.30	0/1018
18	W	0.20	0/224	0.30	0/302
All	All	0.21	0/28268	0.42	13/38256 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLY	N-CA-C	8.10	122.45	112.73
1	A	405	ARG	CA-C-N	7.12	126.96	119.05
1	A	405	ARG	C-N-CA	7.12	126.96	119.05
2	B	106	TYR	CA-C-N	6.95	126.77	119.05
2	B	106	TYR	C-N-CA	6.95	126.77	119.05
16	Q	217	VAL	N-CA-C	6.04	116.82	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	142	VAL	N-CA-C	-6.00	107.65	113.53
15	P	101	ARG	N-CA-C	5.71	117.59	111.36
16	Q	224	ALA	N-CA-C	5.42	117.19	111.28
9	J	87	GLU	CA-C-N	5.30	125.11	119.28
9	J	87	GLU	C-N-CA	5.30	125.11	119.28
15	P	82	ASN	N-CA-C	5.30	118.89	111.74
16	Q	226	TYR	N-CA-C	5.24	117.07	111.36

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	93	0
2	B	1412	0	1363	38	0
3	C	1248	0	1254	31	0
4	E	971	0	975	22	0
5	F	691	0	704	19	0
6	G	693	0	671	24	0
7	H	910	0	950	24	0
8	I	780	0	808	22	0
9	J	2359	0	2402	56	0
10	K	355	0	329	14	0
11	L	1016	0	1016	22	0
12	M	5296	0	5326	89	0
13	N	1204	0	1162	33	0
14	O	1671	0	1673	36	0
15	P	1738	0	1693	39	0
16	Q	3044	0	3018	58	0
17	T	741	0	702	9	0
18	W	218	0	219	5	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	0	0
19	M	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	31	0	19	4	0
21	A	44	0	27	5	0
22	C	47	0	71	14	0
23	G	35	0	0	1	0
24	J	48	0	25	6	0
25	M	4	0	0	0	0
25	O	4	0	0	0	0
26	M	1	0	0	0	0
27	N	52	0	88	2	0
28	N	51	0	46	12	0
29	T	1	0	0	0	0
All	All	28031	0	27821	561	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (561) 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)
7:H:97:TRP:CH2	15:P:98:THR:HG21	1.46	1.51
3:C:50:LEU:CD2	22:C:302:PEE:H25	1.53	1.39
24:J:401:NDP:O4D	24:J:401:NDP:C4D	1.68	1.21
3:C:50:LEU:CD2	22:C:302:PEE:C17	2.20	1.18
3:C:50:LEU:HD21	22:C:302:PEE:C17	1.79	1.11
3:C:50:LEU:HD22	22:C:302:PEE:H25	1.30	1.07
7:H:97:TRP:CH2	15:P:98:THR:CG2	2.37	1.06
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.36	1.02
28:N:202:CDL:H312	28:N:202:CDL:H522	1.44	0.98
28:N:202:CDL:H541	28:N:202:CDL:H321	1.47	0.96
7:H:97:TRP:CZ3	15:P:98:THR:HG21	2.10	0.87
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.59	0.84
7:H:94:MET:HE1	15:P:99:PHE:HD1	1.43	0.83
28:N:202:CDL:H541	28:N:202:CDL:C32	2.08	0.83
9:J:83:PRO:HA	9:J:106:MET:O	1.79	0.82
3:C:50:LEU:HD11	22:C:302:PEE:H59	1.62	0.81
15:P:83:GLU:HG2	15:P:142:ARG:NH2	1.97	0.79
8:I:8:ILE:HG13	28:N:202:CDL:HA32	1.66	0.78
18:W:10:MET:HE3	18:W:11:PRO:HD2	1.64	0.78
6:G:74:LEU:H	6:G:74:LEU:HD23	1.49	0.78
1:A:204:TYR:OH	21:A:503:NAI:H5N	1.84	0.77
7:H:97:TRP:HH2	15:P:98:THR:HG21	0.90	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.67	0.76
2:B:111:GLU:O	2:B:141:ARG:NH1	2.19	0.76
9:J:145:PHE:CE1	9:J:184:LYS:HE2	2.21	0.76
12:M:213:MET:HG3	12:M:215:MET:HG2	1.68	0.76
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.69	0.74
7:H:97:TRP:CZ3	15:P:98:THR:CG2	2.69	0.74
15:P:83:GLU:HG2	15:P:142:ARG:HH22	1.52	0.74
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.21	0.73
1:A:60:GLY:O	1:A:256:ARG:NH1	2.22	0.73
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.21	0.73
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.24	0.72
9:J:180:TYR:O	9:J:184:LYS:HG2	1.89	0.72
11:L:112:MET:HE3	13:N:126:PRO:HB2	1.71	0.72
3:C:50:LEU:CD2	22:C:302:PEE:H26	2.15	0.72
22:C:302:PEE:H58	22:C:302:PEE:H27	1.71	0.72
1:A:121:GLU:HB2	21:A:503:NAI:C4N	2.20	0.71
10:K:105:ARG:NH1	11:L:167:ASN:O	2.23	0.70
3:C:59:ARG:NH1	27:N:201:PLX:O3	2.23	0.70
9:J:177:PRO:O	9:J:182:ARG:NH2	2.24	0.70
1:A:86:ARG:NH2	1:A:269:ARG:O	2.25	0.70
1:A:33:GLY:O	1:A:302:LYS:NZ	2.25	0.69
12:M:472:PRO:O	12:M:510:TRP:NE1	2.22	0.69
3:C:50:LEU:HD21	22:C:302:PEE:C18	2.23	0.69
9:J:85:ARG:NH2	24:J:401:NDP:O2X	2.23	0.69
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.23	0.69
16:Q:308:TYR:CE2	16:Q:311:TYR:HE2	2.10	0.69
16:Q:79:ASN:HA	16:Q:101:LEU:O	1.94	0.67
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.28	0.67
11:L:109:ASN:ND2	11:L:111:LEU:O	2.27	0.67
6:G:119:ILE:HG21	6:G:135:ALA:HB1	1.77	0.66
1:A:121:GLU:HG3	1:A:122:PRO:HD2	1.77	0.66
2:B:192:ASN:ND2	17:T:61:GLU:OE2	2.26	0.66
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.60	0.66
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.66
1:A:185:ASN:OD1	1:A:190:GLY:N	2.21	0.66
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.28	0.66
1:A:152:ARG:NH2	10:K:99:PRO:O	2.29	0.65
15:P:94:ILE:HB	15:P:95:PRO:HD3	1.77	0.65
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.78	0.65
5:F:57:GLU:O	12:M:655:ARG:NH2	2.30	0.65
16:Q:308:TYR:CE2	16:Q:311:TYR:CE2	2.85	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.78	0.64
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.24	0.64
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.78	0.64
3:C:50:LEU:HD23	22:C:302:PEE:C17	2.24	0.63
6:G:105:MET:HE2	6:G:139:MET:HE1	1.79	0.63
6:G:138:LEU:HD23	6:G:144:ILE:HG12	1.80	0.63
3:C:50:LEU:HD21	22:C:302:PEE:H26	1.73	0.63
9:J:213:PHE:HD1	9:J:214:LEU:HD12	1.62	0.63
9:J:135:GLU:OE1	9:J:179:ARG:NH1	2.31	0.63
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.33	0.62
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.81	0.62
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.82	0.62
9:J:132:ARG:NH2	24:J:401:NDP:O2X	2.33	0.62
9:J:327:MET:HE2	9:J:329:LEU:HD11	1.79	0.62
11:L:131:LYS:HE3	11:L:147:VAL:HG11	1.82	0.62
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.82	0.61
15:P:169:GLU:OE2	16:Q:463:ARG:NH2	2.33	0.61
14:O:149:LEU:O	14:O:153:GLN:HG2	2.01	0.61
2:B:177:THR:HG22	2:B:179:THR:H	1.65	0.61
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.34	0.61
14:O:60:TYR:O	14:O:64:GLU:HG3	2.01	0.61
15:P:76:VAL:HG22	15:P:86:ILE:HG12	1.83	0.61
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.27	0.61
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.25	0.61
12:M:636:TYR:CD1	12:M:642:VAL:HG22	2.36	0.61
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.83	0.61
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.34	0.60
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.30	0.60
9:J:174:ILE:O	9:J:182:ARG:HG3	2.01	0.60
1:A:214:GLU:OE2	1:A:224:ARG:NE	2.29	0.60
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.82	0.60
1:A:88:ARG:HG3	1:A:246:GLU:CG	2.31	0.60
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.35	0.60
13:N:5:GLN:OE1	13:N:9:ARG:NH1	2.34	0.60
1:A:177:TYR:HD2	10:K:93:LEU:HD22	1.66	0.60
7:H:94:MET:HE1	15:P:99:PHE:CD1	2.31	0.60
14:O:70:TYR:HB3	14:O:71:PRO:HD2	1.83	0.60
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.83	0.59
6:G:115:GLN:O	6:G:119:ILE:HG12	2.01	0.59
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.83	0.59
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:22:GLU:O	7:H:26:ILE:HG12	2.02	0.59
12:M:299:ARG:HG2	12:M:300:GLN:HG2	1.84	0.58
12:M:308:ARG:NH2	12:M:578:PRO:O	2.36	0.58
5:F:69:TYR:HE2	5:F:75:LYS:HG3	1.68	0.58
9:J:60:GLY:HA2	24:J:401:NDP:O3B	2.04	0.58
12:M:390:THR:HA	12:M:600:GLU:HG2	1.84	0.58
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.86	0.58
12:M:260:ASN:HD22	12:M:278:HIS:HB2	1.67	0.58
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.85	0.58
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.42	0.58
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.39	0.58
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.86	0.58
12:M:336:ASN:O	12:M:336:ASN:ND2	2.37	0.58
13:N:13:GLN:NE2	13:N:33:VAL:HG23	2.19	0.58
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.36	0.58
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.86	0.58
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.86	0.58
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.86	0.58
12:M:647:GLU:HB2	12:M:654:VAL:HG21	1.86	0.58
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.33	0.57
1:A:391:TRP:HD1	1:A:391:TRP:O	1.87	0.57
2:B:106:TYR:HB3	2:B:107:PRO:HD2	1.85	0.57
4:E:100:ARG:HB3	4:E:100:ARG:NH1	2.19	0.57
2:B:110:GLU:OE2	17:T:114:CYS:O	2.21	0.57
12:M:370:GLU:OE2	12:M:518:ARG:NH2	2.38	0.57
1:A:33:GLY:HA2	1:A:294:VAL:HG22	1.86	0.57
8:I:3:SER:O	28:N:202:CDL:HA22	2.05	0.57
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.38	0.57
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.86	0.57
16:Q:99:MET:HG2	16:Q:109:CYS:HA	1.86	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.88	0.56
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.88	0.56
15:P:147:THR:HB	15:P:153:ILE:HD11	1.86	0.56
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.87	0.56
14:O:198:PRO:O	14:O:202:GLU:HG2	2.06	0.56
1:A:43:THR:HA	14:O:234:LEU:HD11	1.87	0.56
3:C:191:ARG:O	3:C:195:ARG:HG3	2.06	0.56
7:H:97:TRP:HH2	15:P:98:THR:CG2	1.86	0.56
13:N:7:LEU:O	13:N:11:LEU:HG	2.06	0.56
1:A:380:GLY:O	1:A:386:ARG:NH1	2.39	0.56
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:302:PEE:H27	22:C:302:PEE:C36	2.36	0.55
4:E:78:VAL:O	4:E:82:LEU:HG	2.06	0.55
1:A:375:LYS:NZ	14:O:33:GLY:O	2.40	0.55
11:L:163:ASN:O	11:L:171:ARG:HA	2.07	0.55
1:A:66:LYS:NZ	1:A:188:GLY:O	2.39	0.55
14:O:59:ASN:O	14:O:63:ILE:HG12	2.06	0.55
4:E:110:THR:HG21	15:P:220:VAL:HG11	1.88	0.55
12:M:51:GLN:O	12:M:55:LYS:HG2	2.06	0.55
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.39	0.55
1:A:93:PHE:CD1	1:A:98:LYS:HG3	2.41	0.55
9:J:145:PHE:CD1	9:J:184:LYS:HE2	2.42	0.55
17:T:119:ARG:HD3	17:T:122:HIS:CD2	2.42	0.55
6:G:75:THR:O	6:G:78:ALA:N	2.39	0.55
14:O:54:ASP:OD1	14:O:55:PHE:N	2.40	0.55
1:A:244:ASN:N	20:A:502:FMN:O1P	2.38	0.55
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.88	0.55
9:J:238:GLN:N	9:J:326:ASP:OD2	2.36	0.55
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.89	0.54
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.89	0.54
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.89	0.54
9:J:211:ASP:O	9:J:215:ASN:ND2	2.40	0.54
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.89	0.54
1:A:50:ASP:O	1:A:59:ARG:NH2	2.36	0.54
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	1.90	0.54
17:T:119:ARG:HD3	17:T:122:HIS:HD2	1.71	0.54
3:C:50:LEU:HD21	22:C:302:PEE:H27	1.90	0.54
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.23	0.54
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.72	0.54
2:B:68:ARG:NH2	18:W:26:PRO:O	2.41	0.54
13:N:4:VAL:HA	13:N:7:LEU:HD12	1.88	0.54
6:G:83:VAL:O	6:G:87:LEU:HD23	2.08	0.54
4:E:118:PHE:CD1	4:E:118:PHE:C	2.86	0.54
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.38	0.54
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.56	0.53
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.89	0.53
14:O:38:LEU:O	14:O:124:ARG:NH2	2.41	0.53
1:A:119:GLU:O	1:A:119:GLU:HG3	2.09	0.53
16:Q:274:ASP:OD1	16:Q:323:ARG:NH1	2.41	0.53
16:Q:102:SER:OG	16:Q:107:ARG:NH1	2.42	0.53
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.90	0.53
7:H:51:ILE:HG22	7:H:55:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:487:THR:OG1	12:M:677:GLN:OE1	2.21	0.53
3:C:188:LYS:O	9:J:87:GLU:OE2	2.26	0.53
13:N:68:MET:CG	13:N:69:ASN:H	2.22	0.53
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.41	0.53
2:B:99:GLY:O	2:B:169:GLU:HG3	2.09	0.53
12:M:389:THR:O	12:M:390:THR:OG1	2.24	0.53
9:J:257:ASP:O	9:J:261:LYS:NZ	2.40	0.52
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.35	0.52
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.42	0.52
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.90	0.52
12:M:638:THR:O	12:M:642:VAL:HG23	2.10	0.52
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.91	0.52
8:I:13:ASN:HD22	8:I:19:ASP:HA	1.74	0.52
11:L:89:SER:O	12:M:59:GLN:NE2	2.41	0.52
12:M:406:ASN:ND2	12:M:688:GLN:O	2.35	0.52
1:A:93:PHE:CE1	1:A:98:LYS:HG3	2.45	0.52
14:O:171:LEU:O	14:O:172:ILE:HD13	2.10	0.52
1:A:185:ASN:C	1:A:187:CYS:H	2.18	0.52
1:A:391:TRP:CD1	1:A:391:TRP:C	2.88	0.52
1:A:102:MET:HG2	1:A:149:MET:HE2	1.91	0.52
6:G:75:THR:O	6:G:76:LEU:C	2.53	0.52
10:K:109:ARG:HH11	10:K:109:ARG:HG3	1.75	0.52
11:L:112:MET:HA	11:L:112:MET:HE2	1.92	0.52
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.51
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.51
4:E:100:ARG:NH1	4:E:100:ARG:CB	2.73	0.51
6:G:90:TYR:OH	6:G:117:GLU:OE1	2.25	0.51
9:J:94:LEU:HA	9:J:97:MET:HG3	1.92	0.51
1:A:213:ILE:HG12	1:A:235:VAL:HG13	1.92	0.51
9:J:173:ASP:OD1	9:J:173:ASP:N	2.41	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.43	0.51
2:B:99:GLY:H	2:B:169:GLU:HG2	1.75	0.51
7:H:30:LYS:O	7:H:34:VAL:HG23	2.11	0.51
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.93	0.51
14:O:236:GLU:HG2	14:O:237:PRO:HD2	1.93	0.51
8:I:8:ILE:HD11	28:N:202:CDL:H142	1.93	0.51
10:K:98:MET:SD	10:K:98:MET:N	2.83	0.51
8:I:40:LYS:HB3	18:W:7:LYS:H	1.76	0.51
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.23	0.51
9:J:192:ARG:NH1	9:J:198:ALA:O	2.44	0.51
9:J:93:HIS:O	9:J:96:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:39:VAL:CG2	13:N:50:GLU:HG2	2.42	0.50
3:C:188:LYS:N	9:J:87:GLU:OE2	2.42	0.50
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.92	0.50
12:M:538:ARG:HG2	12:M:538:ARG:HH11	1.77	0.50
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.94	0.50
5:F:44:LEU:HD22	5:F:91:LEU:HD21	1.93	0.50
8:I:8:ILE:CG1	28:N:202:CDL:HA32	2.38	0.50
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.50
14:O:110:MET:O	14:O:114:GLU:HG3	2.12	0.50
1:A:210:THR:HB	1:A:224:ARG:HG2	1.93	0.50
3:C:187:GLU:OE2	3:C:189:ARG:NH1	2.45	0.50
14:O:179:ALA:HB3	14:O:185:MET:SD	2.52	0.50
8:I:3:SER:O	28:N:202:CDL:CA2	2.59	0.49
28:N:202:CDL:C34	28:N:202:CDL:CA7	2.89	0.49
14:O:206:ASP:OD1	14:O:207:GLU:N	2.45	0.49
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.20	0.49
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.44	0.49
13:N:73:THR:HG22	13:N:73:THR:O	2.11	0.49
1:A:364:VAL:HG12	1:A:400:VAL:HG22	1.94	0.49
2:B:44:ARG:HH21	8:I:112:TYR:HB3	1.77	0.49
16:Q:431:HIS:O	16:Q:454:GLN:NE2	2.45	0.49
2:B:96:ARG:O	16:Q:219:GLY:HA3	2.13	0.49
12:M:149:ASP:OD2	12:M:150:ARG:NH1	2.46	0.49
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.35	0.49
1:A:400:VAL:O	1:A:449:ARG:HD3	2.13	0.49
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.94	0.49
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.95	0.49
7:H:69:GLU:HG2	7:H:77:ILE:HG12	1.95	0.48
1:A:182:ILE:HD11	1:A:193:PHE:HD2	1.78	0.48
5:F:37:ILE:HD12	5:F:37:ILE:H	1.78	0.48
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.95	0.48
12:M:171:THR:HG23	12:M:173:MET:SD	2.52	0.48
15:P:50:ARG:HH12	15:P:80:CYS:HB2	1.78	0.48
14:O:100:LYS:O	14:O:104:ILE:HG12	2.13	0.48
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.53	0.48
3:C:67:PHE:HE2	3:C:103:MET:HE2	1.79	0.48
4:E:100:ARG:CB	4:E:100:ARG:HH11	2.27	0.48
11:L:174:THR:HG23	14:O:111:ARG:HD2	1.94	0.48
13:N:120:THR:HG22	13:N:122:GLN:H	1.78	0.48
16:Q:84:PHE:HE2	16:Q:444:LEU:HD11	1.78	0.48
2:B:47:SER:OG	2:B:49:ASP:OD1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:158:LYS:NZ	12:M:69:LEU:O	2.30	0.48
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.43	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.79	0.48
15:P:186:ARG:NH1	15:P:189:THR:OG1	2.39	0.48
6:G:75:THR:HB	6:G:156:GLU:OE1	2.14	0.48
9:J:163:LYS:NZ	9:J:253:ILE:O	2.42	0.48
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.95	0.48
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.95	0.47
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.49	0.47
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.49	0.47
5:F:71:PHE:CD1	12:M:362:ASP:HB2	2.49	0.47
7:H:38:ILE:HB	7:H:45:ARG:HD2	1.94	0.47
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.44	0.47
5:F:23:LEU:O	5:F:57:GLU:HA	2.14	0.47
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.54	0.47
3:C:50:LEU:HD23	22:C:302:PEE:H26	1.92	0.47
5:F:42:VAL:HG23	12:M:671:LEU:CD1	2.44	0.47
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.25	0.47
17:T:47:ASP:O	17:T:52:ARG:NH1	2.47	0.47
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.80	0.47
9:J:37:HIS:CE1	17:T:49:ASP:HA	2.49	0.47
12:M:266:ARG:HB3	12:M:271:MET:HE3	1.96	0.47
28:N:202:CDL:C32	28:N:202:CDL:C54	2.88	0.47
2:B:106:TYR:HB3	2:B:107:PRO:CD	2.44	0.47
1:A:151:ALA:O	1:A:191:TYR:OH	2.25	0.47
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.39	0.47
1:A:134:ASP:N	1:A:134:ASP:OD1	2.47	0.47
5:F:18:GLU:OE1	5:F:68:ARG:NH1	2.48	0.47
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.14	0.47
4:E:16:SER:HA	11:L:54:ALA:HA	1.97	0.46
28:N:202:CDL:H312	28:N:202:CDL:C52	2.31	0.46
1:A:177:TYR:CD2	10:K:93:LEU:HD22	2.49	0.46
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.98	0.46
9:J:213:PHE:CD1	9:J:214:LEU:HD12	2.47	0.46
12:M:251:ILE:HB	12:M:606:THR:HG22	1.96	0.46
2:B:114:ILE:HD12	12:M:130:ILE:HG23	1.97	0.46
12:M:29:SER:OG	12:M:30:ASN:N	2.48	0.46
12:M:445:LEU:HD22	12:M:460:HIS:HE1	1.80	0.46
1:A:65:THR:OG1	1:A:140:GLU:OE1	2.33	0.46
14:O:168:LEU:HB3	14:O:169:PHE:HD1	1.81	0.46
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:62:THR:CG2	9:J:91:THR:HG22	2.45	0.46
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.98	0.46
6:G:74:LEU:HD23	6:G:74:LEU:N	2.24	0.46
8:I:13:ASN:ND2	8:I:20:LEU:H	2.14	0.46
8:I:13:ASN:ND2	8:I:19:ASP:HA	2.30	0.46
13:N:4:VAL:O	13:N:8:ARG:HG3	2.15	0.46
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.50	0.45
5:F:90:THR:HA	5:F:93:ASN:HD22	1.80	0.45
12:M:382:ARG:HE	12:M:527:ASP:CG	2.24	0.45
12:M:445:LEU:HD22	12:M:460:HIS:CE1	2.51	0.45
1:A:116:ASN:O	1:A:245:VAL:HG23	2.16	0.45
8:I:4:ALA:O	8:I:9:GLN:NE2	2.38	0.45
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.97	0.45
1:A:36:LYS:HB2	1:A:39:ASP:HB2	1.99	0.45
1:A:110:PRO:O	1:A:238:CYS:HB3	2.17	0.45
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.99	0.45
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.97	0.45
7:H:76:GLN:O	7:H:79:GLU:N	2.48	0.45
10:K:106:GLN:HB2	10:K:110:HIS:CD2	2.52	0.45
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.97	0.45
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.99	0.45
12:M:129:PRO:O	12:M:241:ARG:NH2	2.50	0.45
14:O:215:LYS:HA	14:O:215:LYS:HD2	1.83	0.45
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.50	0.45
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.99	0.45
17:T:60:LYS:HG2	17:T:62:VAL:HG23	1.99	0.45
5:F:30:SER:OG	5:F:63:PRO:HG3	2.16	0.45
1:A:244:ASN:ND2	20:A:502:FMN:O2	2.49	0.45
8:I:96:THR:HB	8:I:97:PRO:HD2	1.99	0.45
12:M:478:SER:O	12:M:482:GLN:HG2	2.16	0.45
14:O:164:THR:CG2	14:O:169:PHE:H	2.29	0.45
16:Q:397:TYR:OH	16:Q:406:GLU:OE2	2.34	0.45
1:A:184:LYS:HD3	10:K:98:MET:HE1	1.98	0.45
9:J:84:TYR:O	9:J:84:TYR:CG	2.70	0.45
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.52	0.45
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.99	0.45
3:C:188:LYS:HD3	3:C:191:ARG:HD3	1.98	0.45
12:M:341:ILE:HG13	12:M:545:LEU:HD11	1.99	0.45
14:O:198:PRO:O	14:O:201:ILE:HG22	2.17	0.45
16:Q:372:LYS:NZ	17:T:94:GLY:O	2.39	0.45
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLU:HG3	1:A:122:PRO:CD	2.47	0.44
6:G:123:GLU:OE1	6:G:129:GLU:HA	2.16	0.44
9:J:195:PHE:HB3	9:J:198:ALA:HB2	1.99	0.44
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.52	0.44
8:I:110:GLN:NE2	18:W:22:LYS:HD2	2.32	0.44
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.83	0.44
1:A:116:ASN:ND2	1:A:207:GLY:O	2.33	0.44
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.44
16:Q:393:PRO:HA	16:Q:413:SER:O	2.18	0.44
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.98	0.44
9:J:111:LYS:HE3	9:J:139:PHE:CE1	2.52	0.44
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.52	0.44
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.99	0.44
4:E:100:ARG:HB3	4:E:100:ARG:CZ	2.48	0.44
27:N:201:PLX:H281	27:N:201:PLX:H311	1.71	0.44
4:E:24:ASP:OD1	4:E:24:ASP:N	2.51	0.44
9:J:188:GLU:C	9:J:188:GLU:CD	2.85	0.44
10:K:106:GLN:HB2	10:K:110:HIS:HD2	1.82	0.44
13:N:13:GLN:HE21	13:N:33:VAL:C	2.26	0.44
1:A:154:ALA:HB2	1:A:193:PHE:CZ	2.53	0.44
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.53	0.44
10:K:79:HIS:ND1	14:O:215:LYS:HE3	2.31	0.44
13:N:26:VAL:HG13	13:N:33:VAL:HG12	1.99	0.44
1:A:121:GLU:HB2	21:A:503:NAI:C3N	2.48	0.44
1:A:325:PRO:HD2	1:A:347:THR:HA	2.00	0.44
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.34	0.44
5:F:27:SER:O	5:F:34:ARG:NH2	2.51	0.44
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.18	0.44
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.99	0.44
1:A:123:GLY:N	14:O:180:CYS:SG	2.85	0.44
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.44
3:C:66:THR:HG21	3:C:76:MET:HE2	2.00	0.43
8:I:28:TYR:O	8:I:31:ILE:HG12	2.18	0.43
11:L:115:SER:HB2	12:M:267:THR:HB	2.00	0.43
12:M:161:GLU:OE1	14:O:42:ARG:NH2	2.51	0.43
16:Q:271:ARG:HD2	16:Q:271:ARG:HA	1.77	0.43
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.71	0.43
9:J:217:PHE:HZ	9:J:322:VAL:HG21	1.82	0.43
9:J:271:TYR:OH	9:J:346:GLU:OE1	2.30	0.43
4:E:100:ARG:HH11	4:E:100:ARG:HB2	1.83	0.43
9:J:85:ARG:HD2	24:J:401:NDP:C2A	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:116:ILE:O	9:J:120:VAL:HG22	2.18	0.43
13:N:78:ASP:OD2	13:N:80:SER:OG	2.26	0.43
3:C:184:ILE:O	3:C:187:GLU:HG2	2.18	0.43
4:E:17:VAL:O	11:L:53:ILE:HD12	2.18	0.43
10:K:79:HIS:CE1	14:O:215:LYS:HB3	2.53	0.43
10:K:87:LEU:HD11	14:O:66:ILE:HD11	2.00	0.43
12:M:389:THR:HG21	12:M:473:MET:SD	2.59	0.43
3:C:188:LYS:O	3:C:188:LYS:HG3	2.19	0.43
4:E:105:ARG:C	4:E:107:PHE:H	2.26	0.43
6:G:75:THR:O	6:G:77:GLU:N	2.51	0.43
6:G:80:LYS:HG2	6:G:145:VAL:HG21	1.99	0.43
7:H:82:LEU:HA	7:H:85:GLU:OE2	2.18	0.43
14:O:63:ILE:HD12	14:O:82:VAL:HG22	1.99	0.43
16:Q:83:ASN:ND2	16:Q:96:ARG:HH21	2.17	0.43
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.99	0.43
1:A:123:GLY:O	1:A:353:ALA:HB1	2.19	0.43
1:A:149:MET:HE1	1:A:241:THR:CB	2.48	0.43
1:A:210:THR:O	1:A:214:GLU:HG2	2.18	0.43
3:C:96:SER:HB3	3:C:99:GLN:CD	2.44	0.43
9:J:36:LEU:HB3	12:M:304:GLN:OE1	2.19	0.43
12:M:347:ASP:OD1	12:M:347:ASP:N	2.43	0.43
16:Q:278:VAL:HG23	16:Q:437:LYS:NZ	2.33	0.43
1:A:174:ARG:HD2	1:A:178:GLU:OE1	2.17	0.43
3:C:188:LYS:C	9:J:87:GLU:OE2	2.61	0.43
4:E:98:LYS:HE2	4:E:102:HIS:HB3	2.01	0.43
15:P:161:LYS:HA	15:P:161:LYS:HD3	1.87	0.43
16:Q:431:HIS:HB3	16:Q:454:GLN:HG2	2.00	0.43
17:T:37:LYS:HE3	17:T:37:LYS:HB2	1.76	0.43
1:A:177:TYR:CD1	1:A:182:ILE:HG23	2.54	0.43
1:A:432:ALA:O	1:A:436:GLN:HG3	2.19	0.43
12:M:260:ASN:ND2	12:M:278:HIS:HB2	2.34	0.43
15:P:101:ARG:O	15:P:107:GLN:HA	2.18	0.43
1:A:385:CYS:O	1:A:389:VAL:HB	2.19	0.43
1:A:391:TRP:O	1:A:391:TRP:CD1	2.70	0.43
4:E:19:PRO:HA	11:L:53:ILE:HD11	2.01	0.43
4:E:119:LEU:CD1	12:M:628:GLU:OE1	2.67	0.43
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.99	0.43
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.01	0.43
3:C:190:LEU:HD23	3:C:190:LEU:HA	1.86	0.43
7:H:65:VAL:O	7:H:69:GLU:HG3	2.18	0.43
15:P:94:ILE:N	15:P:95:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.54	0.42
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.54	0.42
8:I:105:GLU:OE1	8:I:105:GLU:HA	2.19	0.42
9:J:94:LEU:O	9:J:97:MET:HG3	2.19	0.42
9:J:131:GLY:O	24:J:401:NDP:H52A	2.19	0.42
9:J:319:VAL:HA	9:J:322:VAL:HG12	2.01	0.42
9:J:132:ARG:HD2	9:J:134:TRP:CZ2	2.53	0.42
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.89	0.42
5:F:64:LYS:HD3	5:F:76:ASN:HB2	2.01	0.42
5:F:83:SER:OG	5:F:86:GLN:HG3	2.19	0.42
12:M:173:MET:HE1	19:M:802:SF4:S1	2.60	0.42
12:M:538:ARG:HG2	12:M:538:ARG:NH1	2.33	0.42
13:N:68:MET:SD	13:N:81:MET:HG2	2.59	0.42
16:Q:139:LEU:HD23	16:Q:139:LEU:HA	1.89	0.42
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.99	0.42
1:A:413:TRP:O	1:A:416:SER:OG	2.26	0.42
6:G:139:MET:HA	6:G:139:MET:HE3	2.00	0.42
12:M:361:VAL:HG12	12:M:361:VAL:O	2.20	0.42
20:A:502:FMN:HM71	20:A:502:FMN:HM83	1.84	0.42
12:M:436:VAL:O	12:M:442:TYR:OH	2.33	0.42
1:A:85:LEU:HD21	1:A:247:THR:HG23	2.01	0.42
1:A:161:GLU:N	1:A:161:GLU:OE1	2.52	0.42
11:L:92:ASN:HB3	15:P:238:PRO:HA	2.01	0.42
12:M:391:ILE:N	12:M:600:GLU:OE2	2.40	0.42
12:M:605:GLN:OE1	12:M:643:ARG:NH1	2.46	0.42
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.50	0.42
2:B:63:TRP:HB3	2:B:66:LEU:HD12	2.00	0.42
2:B:99:GLY:N	2:B:169:GLU:HG2	2.34	0.42
3:C:62:LEU:O	3:C:91:VAL:HA	2.19	0.42
4:E:98:LYS:HB3	4:E:102:HIS:HB2	2.01	0.42
6:G:113:LEU:HA	6:G:116:VAL:HG12	2.02	0.42
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	2.02	0.42
13:N:42:ASP:OD2	13:N:44:TYR:HD2	2.02	0.42
1:A:263:ALA:HA	1:A:271:SER:HB3	2.01	0.42
1:A:448:GLU:O	1:A:452:GLN:HG2	2.20	0.42
2:B:200:GLU:HG3	13:N:88:ARG:HD3	2.02	0.42
4:E:105:ARG:C	4:E:107:PHE:N	2.78	0.42
7:H:56:LEU:HA	7:H:59:VAL:HG12	2.01	0.42
16:Q:97:LEU:HD11	16:Q:109:CYS:SG	2.59	0.42
12:M:419:ARG:NH1	12:M:439:THR:O	2.53	0.42
1:A:46:TYR:CD1	14:O:226:GLU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASP:HB3	1:A:55:GLY:HA3	2.02	0.42
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.01	0.42
6:G:71:ALA:HB1	6:G:72:PRO:HD2	2.02	0.42
7:H:26:ILE:O	7:H:30:LYS:HG3	2.19	0.42
13:N:85:GLU:HG2	13:N:86:TRP:N	2.34	0.42
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.95	0.42
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.89	0.42
1:A:109:ARG:NH1	1:A:237:GLY:O	2.53	0.41
3:C:76:MET:HE3	3:C:76:MET:HB3	1.90	0.41
5:F:33:VAL:O	5:F:36:PHE:HB3	2.20	0.41
12:M:260:ASN:HD21	12:M:278:HIS:CD2	2.37	0.41
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.85	0.41
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.35	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.41
1:A:338:ASP:O	1:A:342:LEU:HB2	2.20	0.41
3:C:124:MET:HA	3:C:125:PRO:HD3	1.84	0.41
6:G:106:LYS:H	6:G:106:LYS:HG2	1.73	0.41
9:J:36:LEU:N	12:M:304:GLN:HE22	2.17	0.41
12:M:94:MET:HE2	12:M:94:MET:HB2	1.90	0.41
15:P:108:PHE:O	15:P:160:TYR:OH	2.32	0.41
16:Q:144:MET:HE3	16:Q:222:MET:HB2	2.01	0.41
1:A:329:LYS:HA	1:A:332:CYS:SG	2.61	0.41
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.55	0.41
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.53	0.41
15:P:107:GLN:NE2	15:P:136:ARG:HG2	2.36	0.41
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.30	0.41
1:A:317:VAL:HG23	1:A:356:VAL:HG12	2.02	0.41
2:B:151:LYS:HA	3:C:141:GLY:HA2	2.01	0.41
12:M:42:MET:HE3	12:M:42:MET:HA	2.01	0.41
12:M:698:ASP:N	12:M:698:ASP:OD1	2.53	0.41
15:P:183:ASP:OD1	15:P:185:ARG:NE	2.53	0.41
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.02	0.41
8:I:8:ILE:HG13	28:N:202:CDL:CA3	2.44	0.41
12:M:185:PHE:CZ	12:M:221:ASN:HB2	2.56	0.41
12:M:625:ALA:O	12:M:629:ILE:HG12	2.21	0.41
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.56	0.41
1:A:91:ALA:CB	21:A:503:NAI:H51A	2.51	0.41
1:A:121:GLU:HA	1:A:122:PRO:HD3	1.82	0.41
2:B:99:GLY:O	2:B:169:GLU:CG	2.69	0.41
4:E:52:LEU:HD21	4:E:103:ILE:HG21	2.02	0.41
9:J:72:HIS:NE2	15:P:215:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:154:LYS:HE2	11:L:154:LYS:HB3	1.79	0.41
1:A:99:TRP:N	1:A:99:TRP:CD1	2.87	0.41
22:C:302:PEE:H20	22:C:302:PEE:H28	2.02	0.41
4:E:70:ASN:O	23:G:201:8Q1:O40	2.38	0.41
5:F:56:ARG:HB3	12:M:651:PRO:HD2	2.03	0.41
6:G:130:ILE:HG22	6:G:135:ALA:HB2	2.03	0.41
9:J:89:TYR:CD1	9:J:89:TYR:C	2.98	0.41
12:M:167:PRO:HD2	12:M:215:MET:HE1	2.03	0.41
12:M:372:PHE:H	12:M:532:PRO:HB2	1.86	0.41
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.22	0.41
5:F:89:ARG:O	5:F:93:ASN:ND2	2.54	0.41
7:H:76:GLN:O	7:H:79:GLU:HG2	2.21	0.41
9:J:84:TYR:HD2	9:J:86:CYS:O	2.04	0.41
12:M:245:THR:HA	12:M:265:THR:O	2.21	0.41
12:M:402:LEU:HD23	12:M:475:VAL:HB	2.03	0.41
12:M:624:ARG:HH12	12:M:628:GLU:HG3	1.86	0.41
1:A:75:TRP:CH2	1:A:79:GLU:HG3	2.55	0.40
1:A:122:PRO:HA	14:O:176:CYS:SG	2.60	0.40
1:A:272:GLY:O	1:A:292:MET:HB2	2.20	0.40
2:B:90:LYS:HG3	13:N:91:HIS:CE1	2.56	0.40
7:H:54:GLU:O	7:H:58:MET:HG3	2.21	0.40
1:A:158:ILE:HG23	1:A:199:ARG:HG2	2.04	0.40
1:A:279:SER:OG	1:A:280:GLY:N	2.54	0.40
2:B:177:THR:CG2	2:B:182:GLU:HB2	2.50	0.40
6:G:93:ILE:HG23	6:G:108:LEU:HD22	2.01	0.40
9:J:62:THR:HG22	9:J:91:THR:HG22	2.03	0.40
9:J:89:TYR:HA	9:J:92:MET:HG2	2.04	0.40
9:J:199:THR:OG1	9:J:258:ALA:O	2.39	0.40
11:L:53:ILE:HG22	11:L:55:VAL:HB	2.02	0.40
16:Q:383:LYS:HD2	16:Q:383:LYS:HA	1.92	0.40
1:A:411:SER:O	1:A:415:ILE:HG12	2.21	0.40
4:E:119:LEU:HD23	4:E:119:LEU:HA	1.78	0.40
6:G:84:LEU:HB3	6:G:88:LYS:HZ3	1.86	0.40
8:I:34:ARG:HB2	13:N:95:ASP:OD1	2.22	0.40
12:M:133:GLN:O	12:M:137:CYS:HB2	2.22	0.40
16:Q:345:SER:HB2	18:W:19:ILE:HD12	2.02	0.40
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.90	0.40
1:A:209:GLU:HB2	1:A:242:VAL:HG21	2.02	0.40
1:A:267:ARG:HG3	1:A:293:SER:OG	2.20	0.40
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.57	0.40
2:B:44:ARG:HD3	2:B:45:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:3:LEU:HD23	13:N:7:LEU:HD11	2.02	0.40
14:O:63:ILE:HD12	14:O:82:VAL:HG13	2.04	0.40
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	2.03	0.40
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.37	0.40
9:J:201:ILE:HG22	9:J:203:PRO:HD3	2.02	0.40
14:O:186:VAL:HG22	14:O:196:LEU:HD11	2.03	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	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	84 (98%)	1 (1%)	1 (1%)	10	34
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	289/341 (85%)	273 (94%)	14 (5%)	2 (1%)	18	47
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	662 (96%)	25 (4%)	1 (0%)	48	77
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	374/385 (97%)	365 (98%)	9 (2%)	0	100	100
17	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
18	W	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	3441/3553 (97%)	3312 (96%)	125 (4%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
6	G	76	LEU
12	M	283	GLU
9	J	83	PRO

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	345/345 (100%)	342 (99%)	3 (1%)	70	89
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	106 (99%)	1 (1%)	70	89
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	255/295 (86%)	255 (100%)	0	100	100
10	K	41/41 (100%)	41 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	87
16	Q	327/331 (99%)	326 (100%)	1 (0%)	86	95
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	23/24 (96%)	23 (100%)	0	100	100
All	All	2994/3054 (98%)	2987 (100%)	7 (0%)	85	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	125	CYS
1	A	408	GLU
4	E	101	THR
15	P	83	GLU
15	P	85	GLU
16	Q	312	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	283	ASN
1	A	457	HIS
3	C	123	GLN
4	E	58	GLN
5	F	81	ASN
6	G	142	GLN
7	H	21	HIS
7	H	76	GLN
8	I	13	ASN
8	I	110	GLN
9	J	122	HIS
9	J	376	ASN
12	M	123	ASN
12	M	260	ASN
12	M	300	GLN
12	M	388	ASN
12	M	498	GLN

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Mol	Chain	Res	Type
12	M	604	GLN
12	M	663	ASN
13	N	13	GLN
13	N	135	GLN
14	O	69	ASN
14	O	133	GLN
15	P	63	GLN
15	P	107	GLN
15	P	131	ASN
15	P	181	HIS
16	Q	183	HIS
16	Q	234	GLN
16	Q	250	ASN
16	Q	306	GLN
16	Q	454	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	6.21	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	5.58	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	12.76	131.18	119.48
16	Q	118	2MR	CD-NE-CZ	4.41	131.65	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.08	130.26	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
28	CDL	N	202	-	50,50,99	1.27	4 (8%)	56,62,111	1.32	7 (12%)
19	SF4	M	802	12	0,12,12	-	-	-	-	-
21	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.68	12 (18%)
19	SF4	B	301	2	0,12,12	-	-	-	-	-
20	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.28	8 (16%)
24	NDP	J	401	-	51,52,52	4.25	25 (49%)	71,80,80	2.21	14 (19%)
27	PLX	N	201	-	51,51,51	1.19	3 (5%)	53,59,59	0.63	1 (1%)
19	SF4	M	801	12	0,12,12	-	-	-	-	-
19	SF4	A	501	1	0,12,12	-	-	-	-	-
19	SF4	B	302	2	0,12,12	-	-	-	-	-
25	FES	O	301	14	0,4,4	-	-	-	-	-
23	8Q1	G	201	6	32,34,34	2.24	7 (21%)	39,43,43	1.69	11 (28%)
19	SF4	C	301	3	0,12,12	-	-	-	-	-
25	FES	M	803	12	0,4,4	-	-	-	-	-
22	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	0.97	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CDL	N	202	-	-	22/61/61/110	-
19	SF4	M	802	12	-	-	0/6/5/5
21	NAI	A	503	-	-	5/29/72/72	0/5/5/5
19	SF4	B	301	2	-	-	0/6/5/5
20	FMN	A	502	-	-	6/18/18/18	0/3/3/3
24	NDP	J	401	-	-	12/34/77/77	0/5/5/5
27	PLX	N	201	-	-	34/55/55/55	-
19	SF4	C	301	3	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
25	FES	O	301	14	-	-	0/1/1/1
23	8Q1	G	201	6	-	19/41/41/41	-
25	FES	M	803	12	-	-	0/1/1/1
22	PEE	C	302	-	-	24/50/50/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	401	NDP	C3B-C2B	-13.06	1.24	1.53
24	J	401	NDP	O4D-C4D	10.66	1.68	1.45
21	A	503	NAI	C3D-C4D	-10.38	1.26	1.53
24	J	401	NDP	C3D-C4D	-10.03	1.27	1.53
21	A	503	NAI	O4B-C1B	9.27	1.63	1.42
21	A	503	NAI	O4B-C4B	-8.35	1.26	1.45
24	J	401	NDP	O4B-C4B	-7.96	1.27	1.45
23	G	201	8Q1	P24-O27	7.86	1.85	1.60
21	A	503	NAI	C2D-C1D	-7.74	1.29	1.53
21	A	503	NAI	C2B-C1B	-7.43	1.30	1.53
24	J	401	NDP	C2N-C3N	7.40	1.55	1.35
24	J	401	NDP	C6N-C5N	7.26	1.55	1.33
21	A	503	NAI	O4D-C4D	6.90	1.60	1.45
24	J	401	NDP	PN-O3	6.20	1.66	1.59
21	A	503	NAI	PA-O3	6.18	1.66	1.59
21	A	503	NAI	C2D-C3D	5.96	1.69	1.53
24	J	401	NDP	C6A-N6A	5.77	1.48	1.34
24	J	401	NDP	P2B-O2B	5.66	1.69	1.59
21	A	503	NAI	O4D-C1D	5.65	1.55	1.42
23	G	201	8Q1	C28-C29	5.48	1.61	1.52
21	A	503	NAI	PN-O3	5.40	1.65	1.59
21	A	503	NAI	C7N-N7N	5.32	1.48	1.33
21	A	503	NAI	C4N-C3N	-5.31	1.40	1.50
24	J	401	NDP	PA-O3	5.21	1.65	1.59
24	J	401	NDP	C3B-C4B	5.17	1.66	1.53
24	J	401	NDP	O4D-C1D	-5.09	1.30	1.42
21	A	503	NAI	C6A-N6A	5.06	1.47	1.34
24	J	401	NDP	C6N-N1N	5.01	1.49	1.37
24	J	401	NDP	O4B-C1B	4.77	1.53	1.42
24	J	401	NDP	C1B-N9A	-4.64	1.33	1.46
21	A	503	NAI	O2B-C2B	4.36	1.53	1.43
28	N	202	CDL	OB8-CB7	4.28	1.45	1.33
28	N	202	CDL	OA8-CA7	4.20	1.45	1.33
28	N	202	CDL	OA6-CA5	4.13	1.46	1.34
28	N	202	CDL	OB6-CB5	3.97	1.45	1.34
24	J	401	NDP	O2D-C2D	-3.90	1.33	1.43
24	J	401	NDP	C7N-N7N	3.83	1.44	1.33
22	C	302	PEE	C18-C19	3.83	1.53	1.31
23	G	201	8Q1	C1-S44	3.82	1.85	1.76
22	C	302	PEE	C39-C38	3.75	1.53	1.31
21	A	503	NAI	C7N-C3N	3.50	1.56	1.48
21	A	503	NAI	C4N-C5N	-3.42	1.40	1.49
23	G	201	8Q1	O27-C28	-3.31	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	401	NDP	C8A-N9A	-3.31	1.31	1.37
20	A	502	FMN	C4A-N5	3.29	1.37	1.30
23	G	201	8Q1	C34-N36	3.28	1.41	1.33
24	J	401	NDP	C5A-N7A	-3.20	1.33	1.39
24	J	401	NDP	O3D-C3D	2.95	1.50	1.43
27	N	201	PLX	O6-C4	-2.93	1.40	1.44
24	J	401	NDP	C7N-C3N	2.87	1.54	1.48
23	G	201	8Q1	C6-C1	2.82	1.53	1.50
21	A	503	NAI	C8A-N9A	-2.72	1.32	1.37
24	J	401	NDP	O2B-C2B	2.66	1.53	1.44
23	G	201	8Q1	C39-N41	2.59	1.39	1.33
22	C	302	PEE	O2-C2	-2.54	1.40	1.46
22	C	302	PEE	O3-C30	2.53	1.40	1.33
24	J	401	NDP	C2D-C3D	2.52	1.60	1.53
21	A	503	NAI	C6N-C5N	2.45	1.40	1.33
21	A	503	NAI	PN-O5D	2.41	1.68	1.59
21	A	503	NAI	C5B-C4B	2.36	1.58	1.51
21	A	503	NAI	O3B-C3B	-2.36	1.37	1.43
22	C	302	PEE	O2-C10	2.30	1.40	1.34
20	A	502	FMN	C10-N1	2.27	1.37	1.33
24	J	401	NDP	O7N-C7N	-2.22	1.19	1.24
27	N	201	PLX	C7-C6	2.16	1.55	1.50
21	A	503	NAI	C5A-N7A	-2.12	1.35	1.39
22	C	302	PEE	O3-C3	-2.09	1.40	1.45
27	N	201	PLX	P1-O4	2.09	1.67	1.59
24	J	401	NDP	PA-O5B	2.03	1.67	1.59

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	401	NDP	C3N-C2N-N1N	-7.68	111.92	123.20
24	J	401	NDP	C1D-N1N-C2N	-6.92	109.73	121.14
24	J	401	NDP	C6N-N1N-C2N	-6.71	112.14	119.32
24	J	401	NDP	C5A-C4A-N3A	-5.58	119.03	126.72
21	A	503	NAI	C5A-C4A-N3A	-5.43	119.25	126.72
24	J	401	NDP	C1D-N1N-C6N	-5.30	109.56	120.77
21	A	503	NAI	N3A-C2A-N1A	-4.44	121.86	128.58
23	G	201	8Q1	C6-C1-S44	4.37	118.60	113.40
24	J	401	NDP	N3A-C2A-N1A	-4.12	122.34	128.58
28	N	202	CDL	OB6-CB5-C51	4.09	120.34	111.48
28	N	202	CDL	OA6-CA5-C11	4.00	120.13	111.48
24	J	401	NDP	N3A-C4A-N9A	3.97	133.92	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	302	PEE	O2-C10-C11	3.86	119.84	111.48
21	A	503	NAI	N3A-C4A-N9A	3.86	133.73	127.17
21	A	503	NAI	C2A-N3A-C4A	3.68	120.82	111.83
24	J	401	NDP	C2A-N3A-C4A	3.62	120.66	111.83
20	A	502	FMN	C4-N3-C2	-3.45	119.52	125.64
23	G	201	8Q1	O35-C34-N36	-3.41	115.76	122.98
21	A	503	NAI	C4A-C5A-N7A	-3.34	106.76	110.58
23	G	201	8Q1	C43-S44-C1	3.34	111.71	101.84
21	A	503	NAI	C5A-N7A-C8A	3.31	108.65	103.45
21	A	503	NAI	N9A-C8A-N7A	-3.20	109.39	113.94
24	J	401	NDP	C4A-C5A-N7A	-3.20	106.93	110.58
24	J	401	NDP	N9A-C8A-N7A	-3.16	109.45	113.94
21	A	503	NAI	C4D-O4D-C1D	-3.15	102.51	109.47
24	J	401	NDP	C5A-N7A-C8A	3.09	108.31	103.45
21	A	503	NAI	C3D-C2D-C1D	3.04	107.22	101.46
28	N	202	CDL	OA8-CA7-C31	2.95	120.82	111.83
28	N	202	CDL	OB8-CB7-C71	2.73	120.16	111.83
20	A	502	FMN	C5A-C9A-N10	2.68	120.39	117.97
22	C	302	PEE	O3-C30-C31	2.60	119.76	111.83
20	A	502	FMN	C4A-C4-N3	2.60	119.86	113.25
20	A	502	FMN	C4A-C10-N10	2.59	120.19	116.48
23	G	201	8Q1	O2-P24-O27	-2.58	99.94	106.67
21	A	503	NAI	C2D-C3D-C4D	2.57	107.58	102.61
23	G	201	8Q1	O40-C39-N41	-2.56	118.00	123.03
28	N	202	CDL	CB4-OB6-CB5	-2.54	111.71	117.80
23	G	201	8Q1	C37-C38-C39	2.44	116.45	112.39
20	A	502	FMN	O4-C4-C4A	-2.43	120.13	126.53
23	G	201	8Q1	C32-C34-N36	2.42	121.08	116.48
24	J	401	NDP	C4A-N9A-C8A	2.40	108.26	105.74
23	G	201	8Q1	O1-P24-O2	2.36	116.67	107.80
21	A	503	NAI	C4A-N9A-C8A	2.32	108.17	105.74
23	G	201	8Q1	O4-C1-S44	-2.29	119.77	122.68
23	G	201	8Q1	O27-P24-O3	-2.26	100.32	106.44
20	A	502	FMN	C9A-C5A-N5	-2.24	120.08	122.45
24	J	401	NDP	O4B-C1B-C2B	-2.22	102.76	106.59
27	N	201	PLX	C1A-N1-C1	2.22	118.74	109.91
24	J	401	NDP	C2D-C3D-C4D	2.18	106.82	102.61
20	A	502	FMN	C10-C4A-N5	-2.17	120.37	124.81
28	N	202	CDL	OB6-CB5-OB7	-2.12	118.76	123.70
21	A	503	NAI	C6N-N1N-C2N	2.09	121.56	119.32
20	A	502	FMN	C4A-C10-N1	-2.07	119.50	124.59
23	G	201	8Q1	O4-C1-C6	-2.04	121.62	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	202	CDL	OA8-CA7-OA9	-2.01	118.61	123.63

There are no chirality outliers.

All (122) 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	C1'-C2'-C3'-O3'
20	A	502	FMN	C1'-C2'-C3'-C4'
22	C	302	PEE	O4P-C4-C5-N
23	G	201	8Q1	O4-C1-S44-C43
23	G	201	8Q1	C6-C1-S44-C43
23	G	201	8Q1	O27-C28-C29-C30
23	G	201	8Q1	O27-C28-C29-C31
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	C42-C43-S44-C1
23	G	201	8Q1	C28-O27-P24-O2
23	G	201	8Q1	C28-O27-P24-O1
24	J	401	NDP	O4D-C4D-C5D-O5D
24	J	401	NDP	C2N-C3N-C7N-N7N
27	N	201	PLX	O7-C6-C7-C8
27	N	201	PLX	O4-C3-C4-O6
27	N	201	PLX	C3-O4-P1-O1
27	N	201	PLX	C3-O4-P1-O2
27	N	201	PLX	C3-O4-P1-O3
27	N	201	PLX	C2-O1-P1-O2
27	N	201	PLX	O9-C24-O8-C5
28	N	202	CDL	CA2-OA2-PA1-OA4
28	N	202	CDL	CA2-OA2-PA1-OA5
28	N	202	CDL	CA3-OA5-PA1-OA2
28	N	202	CDL	CA3-OA5-PA1-OA4
28	N	202	CDL	C11-CA5-OA6-CA4
28	N	202	CDL	CB2-OB2-PB2-OB3
28	N	202	CDL	CB2-OB2-PB2-OB4
28	N	202	CDL	CB2-OB2-PB2-OB5
28	N	202	CDL	OA7-CA5-OA6-CA4
28	N	202	CDL	O1-C1-CB2-OB2
22	C	302	PEE	C11-C10-O2-C2
28	N	202	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
22	C	302	PEE	O4-C10-O2-C2
27	N	201	PLX	C28-C29-C30-C31
24	J	401	NDP	C2D-C1D-N1N-C6N
28	N	202	CDL	OB7-CB5-OB6-CB4
20	A	502	FMN	O2'-C2'-C3'-C4'
22	C	302	PEE	C14-C15-C16-C17
28	N	202	CDL	CB5-C51-C52-C53
24	J	401	NDP	C3D-C4D-C5D-O5D
27	N	201	PLX	O6-C6-C7-C8
28	N	202	CDL	CA6-CA4-OA6-CA5
27	N	201	PLX	C17-C18-C19-C20
27	N	201	PLX	C33-C34-C35-C36
27	N	201	PLX	O9-C24-C25-C26
22	C	302	PEE	C42-C43-C44-C45
21	A	503	NAI	C3D-C4D-C5D-O5D
20	A	502	FMN	O2'-C2'-C3'-O3'
27	N	201	PLX	C16-C17-C18-C19
27	N	201	PLX	C13-C14-C15-C16
27	N	201	PLX	C7-C8-C9-C10
27	N	201	PLX	C11-C12-C13-C14
22	C	302	PEE	C37-C38-C39-C40
23	G	201	8Q1	C10-C11-C12-C13
22	C	302	PEE	C39-C40-C41-C42
27	N	201	PLX	O4-C3-C4-C5
22	C	302	PEE	C1-C2-C3-O3
22	C	302	PEE	C15-C16-C17-C18
27	N	201	PLX	C30-C31-C32-C33
27	N	201	PLX	C31-C32-C33-C34
23	G	201	8Q1	C11-C12-C13-C14
23	G	201	8Q1	C28-O27-P24-O3
27	N	201	PLX	C25-C26-C27-C28
23	G	201	8Q1	C29-C32-C34-N36
22	C	302	PEE	C43-C44-C45-C46
27	N	201	PLX	C36-C37-C38-C39
27	N	201	PLX	O6-C4-C5-O8
27	N	201	PLX	O8-C24-C25-C26
21	A	503	NAI	PN-O3-PA-O5B
28	N	202	CDL	CA2-C1-CB2-OB2
23	G	201	8Q1	C6-C7-C8-C9
27	N	201	PLX	C14-C15-C16-C17
22	C	302	PEE	C13-C14-C15-C16
22	C	302	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	C	302	PEE	O2-C2-C3-O3
27	N	201	PLX	C9-C10-C11-C12
22	C	302	PEE	C10-C11-C12-C13
27	N	201	PLX	N1-C1-C2-O1
22	C	302	PEE	C33-C34-C35-C36
28	N	202	CDL	OA5-CA3-CA4-CA6
24	J	401	NDP	C2N-C3N-C7N-O7N
22	C	302	PEE	C18-C19-C20-C21
27	N	201	PLX	C3-C4-C5-O8
21	A	503	NAI	O4D-C4D-C5D-O5D
22	C	302	PEE	C4-O4P-P-O2P
24	J	401	NDP	C5D-O5D-PN-O3
24	J	401	NDP	C5D-O5D-PN-O1N
24	J	401	NDP	C5D-O5D-PN-O2N
27	N	201	PLX	C2-O1-P1-O4
27	N	201	PLX	C2-O1-P1-O3
28	N	202	CDL	CB3-OB5-PB2-OB4
27	N	201	PLX	C35-C36-C37-C38
22	C	302	PEE	C16-C17-C18-C19
23	G	201	8Q1	C7-C8-C9-C10
22	C	302	PEE	C19-C20-C21-C22
24	J	401	NDP	PN-O3-PA-O2A
23	G	201	8Q1	C29-C32-C34-O35
24	J	401	NDP	O4D-C1D-N1N-C6N
28	N	202	CDL	O1-C1-CA2-OA2
22	C	302	PEE	C38-C39-C40-C41
23	G	201	8Q1	C12-C13-C14-C15
27	N	201	PLX	C27-C28-C29-C30
21	A	503	NAI	O4D-C1D-N1N-C2N
21	A	503	NAI	C2D-C1D-N1N-C2N
27	N	201	PLX	C26-C27-C28-C29
22	C	302	PEE	C32-C33-C34-C35
22	C	302	PEE	C36-C37-C38-C39
24	J	401	NDP	O4B-C4B-C5B-O5B
27	N	201	PLX	C15-C16-C17-C18
28	N	202	CDL	C52-C51-CB5-OB6
24	J	401	NDP	PN-O3-PA-O1A
23	G	201	8Q1	C9-C10-C11-C12
28	N	202	CDL	OA5-CA3-CA4-OA6
27	N	201	PLX	C25-C24-O8-C5
28	N	202	CDL	OB6-CB4-CB6-OB8
22	C	302	PEE	C40-C41-C42-C43

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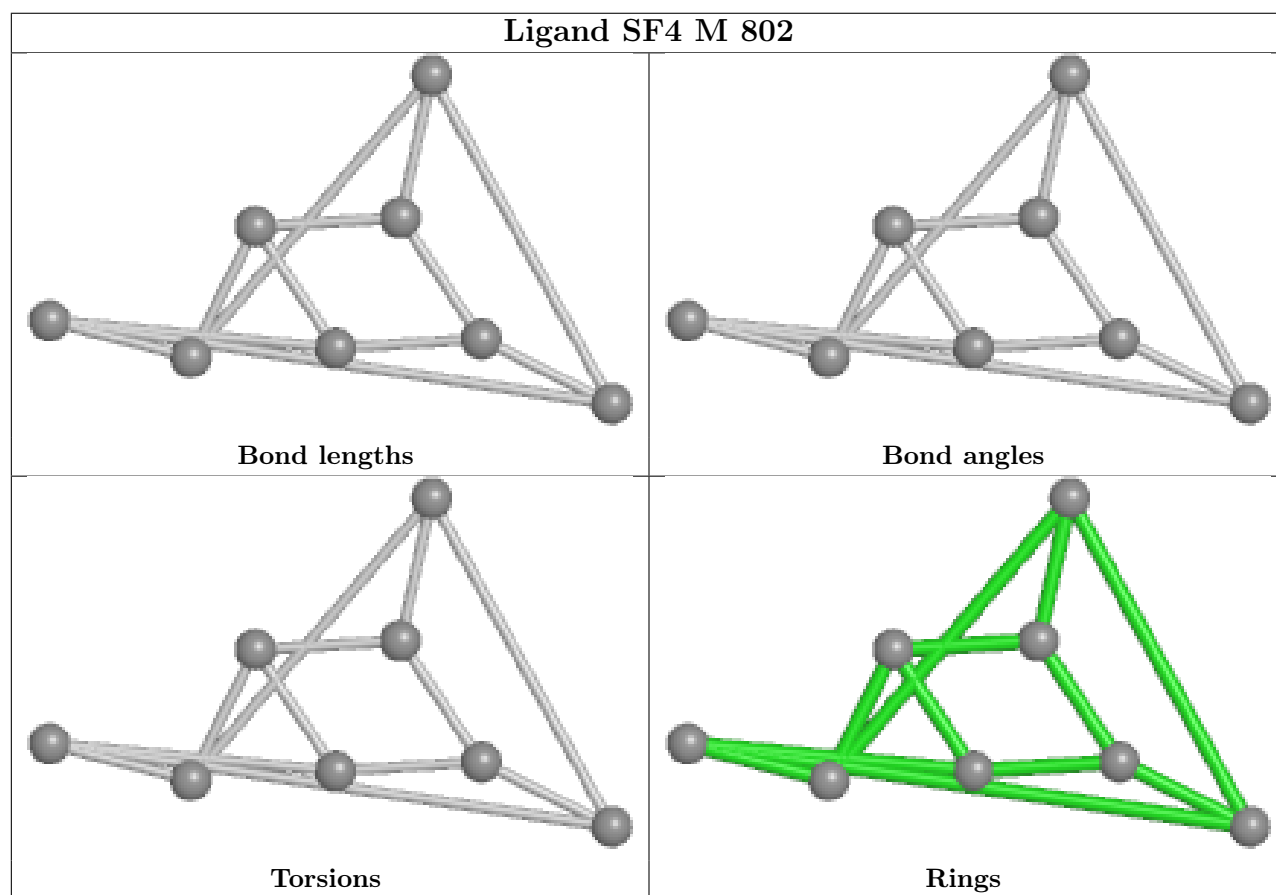
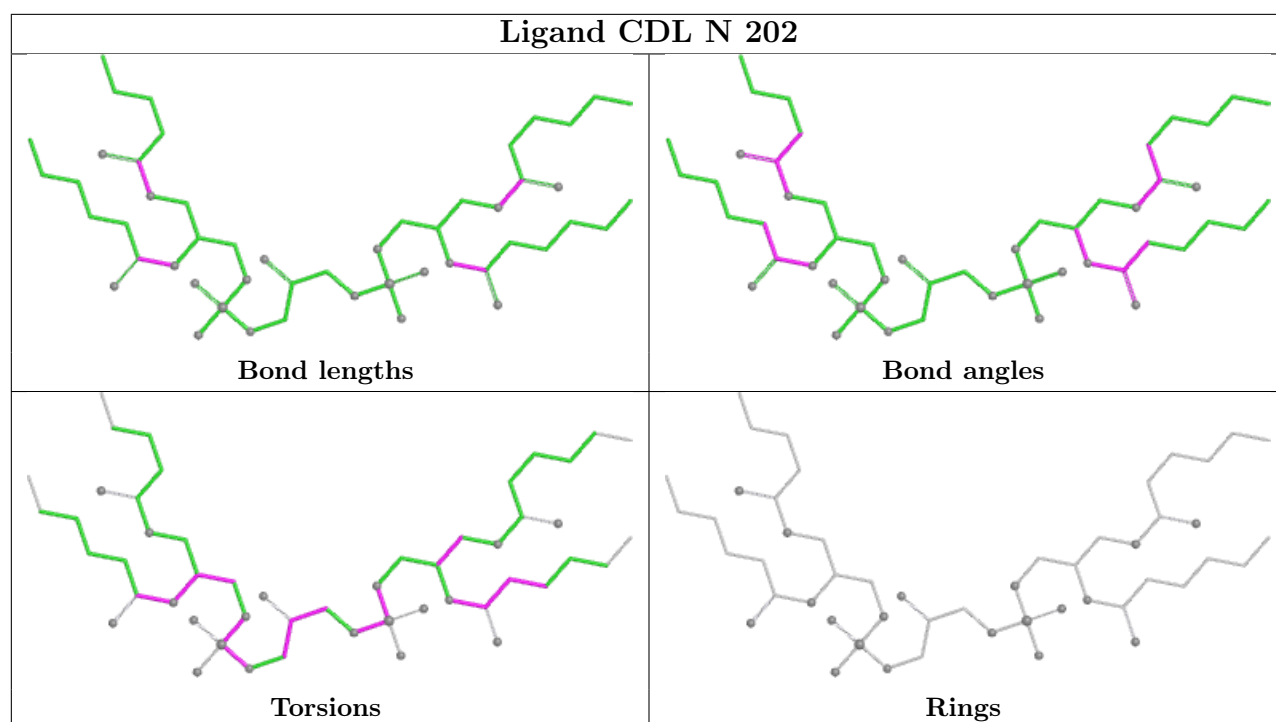
Mol	Chain	Res	Type	Atoms
28	N	202	CDL	C52-C51-CB5-OB7
22	C	302	PEE	O3-C30-C31-C32

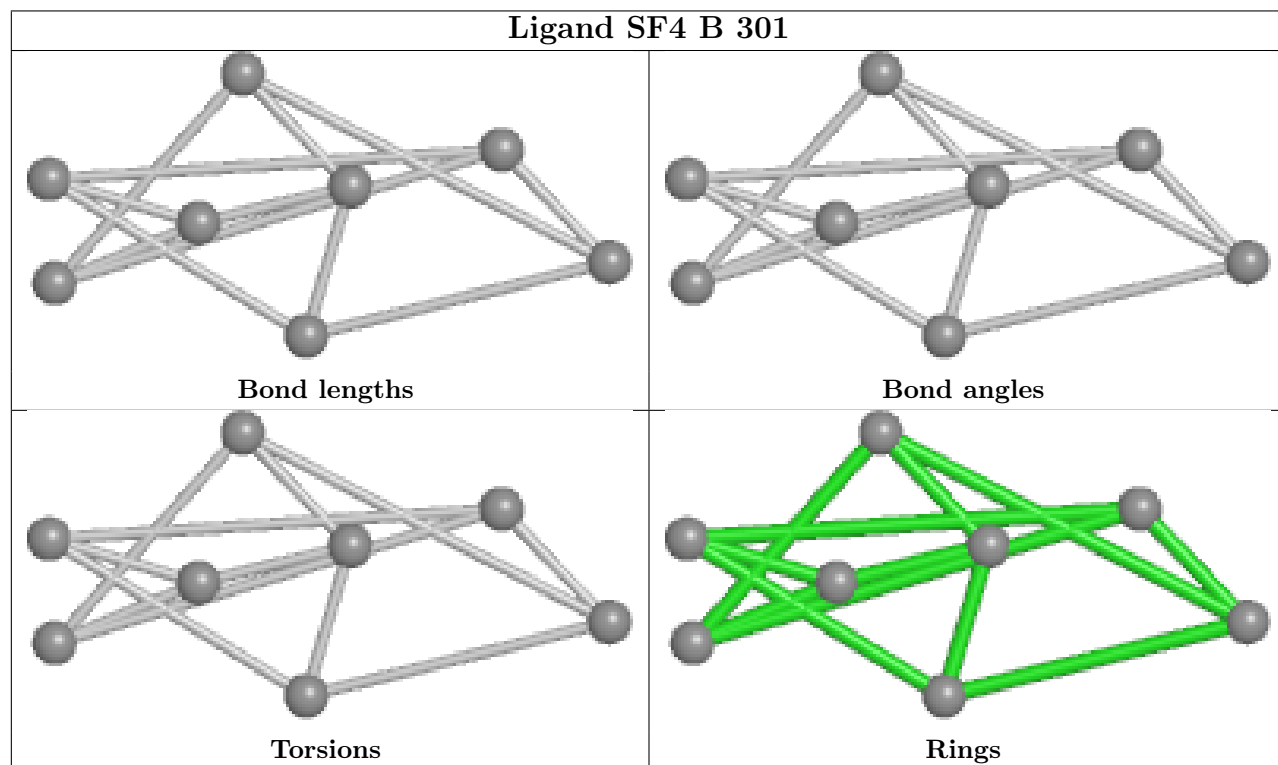
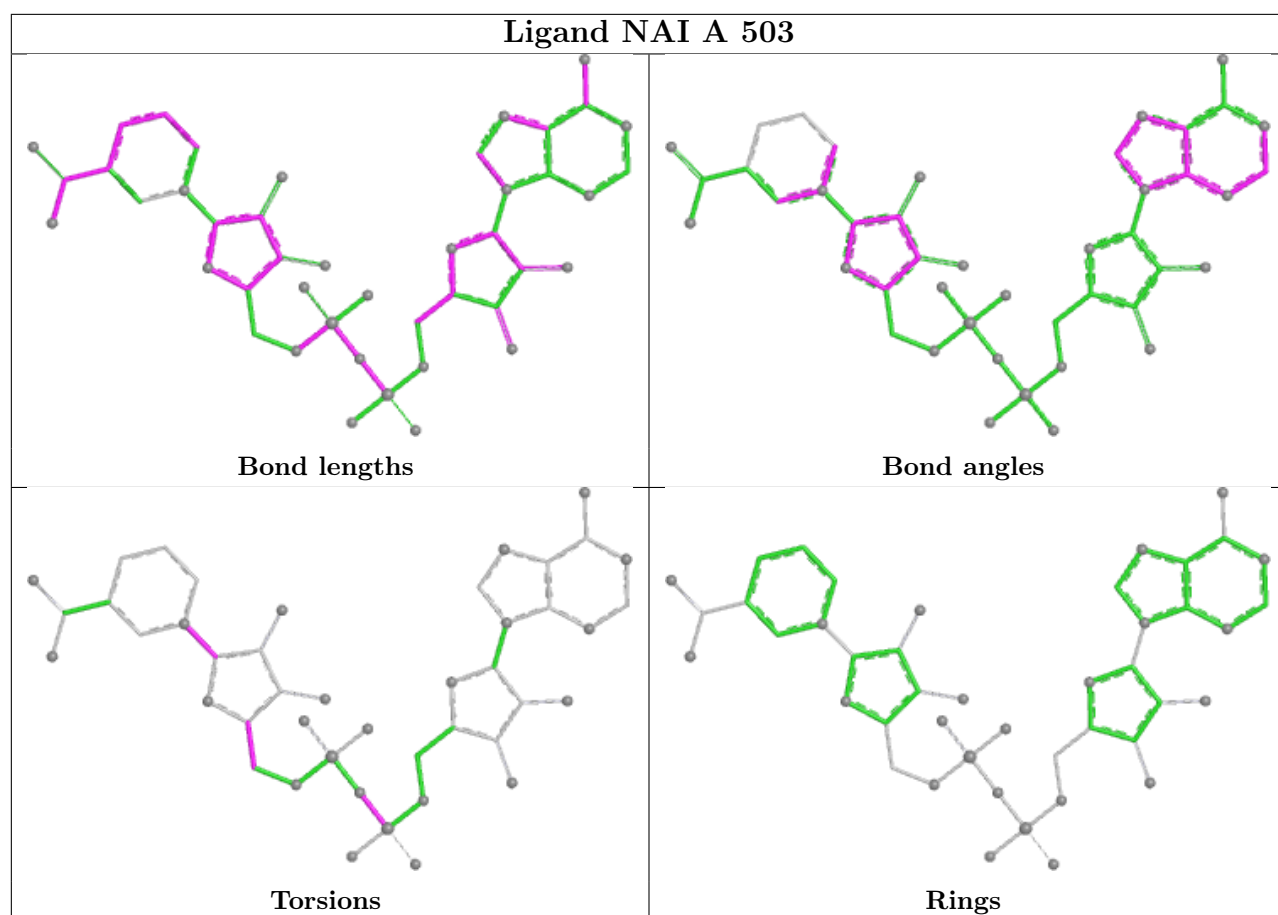
There are no ring outliers.

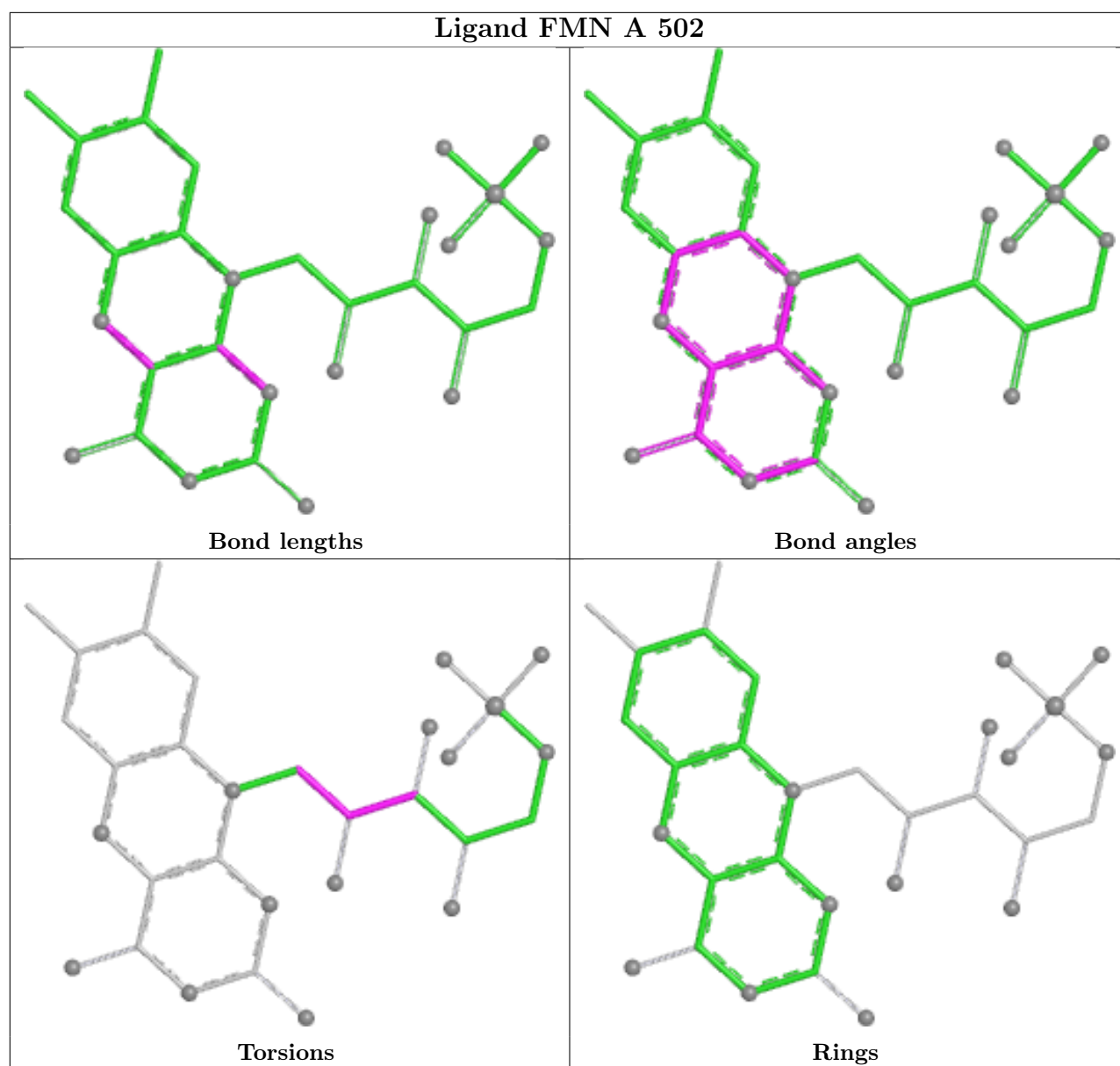
9 monomers are involved in 47 short contacts:

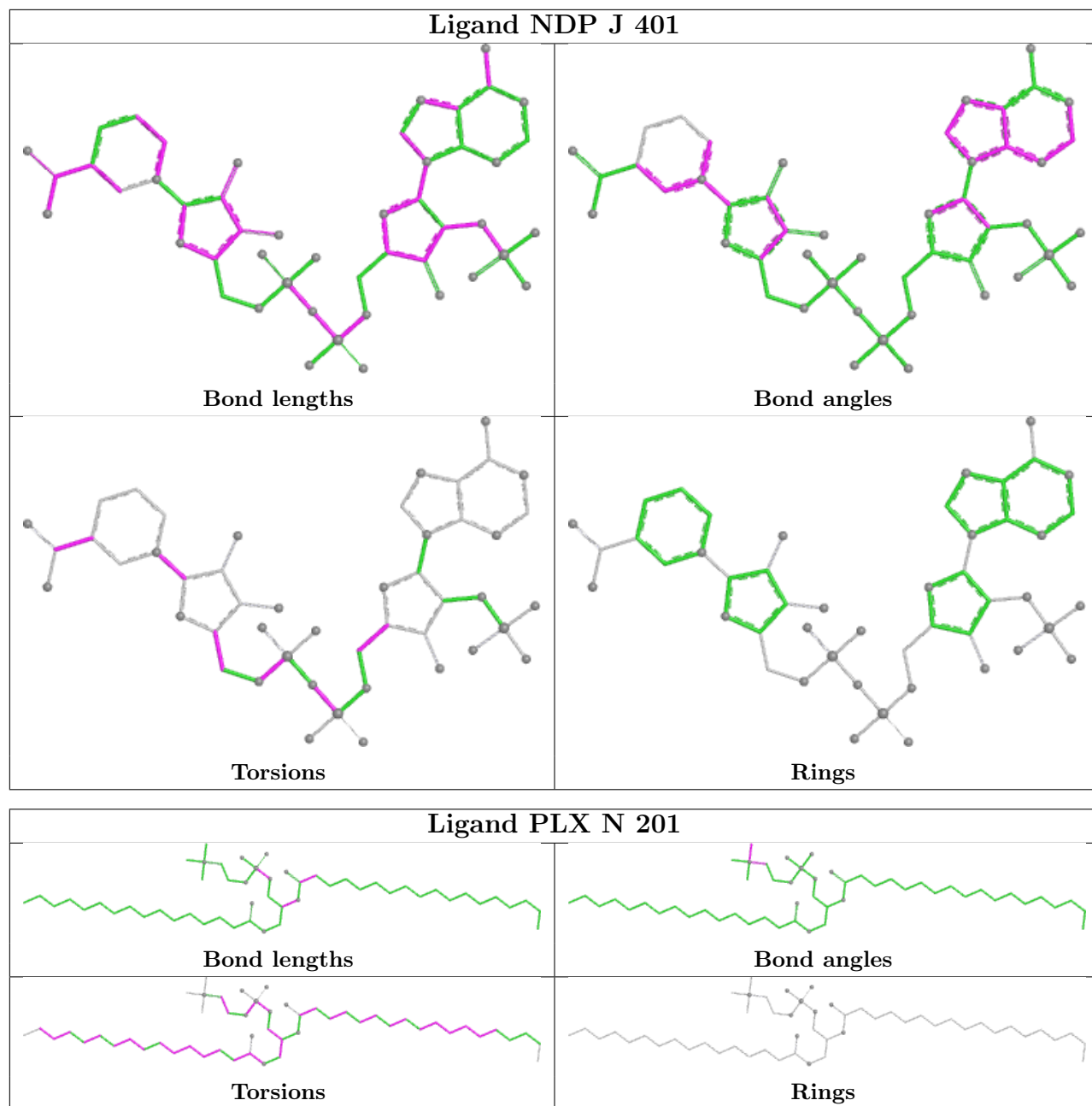
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	N	202	CDL	12	0
19	M	802	SF4	1	0
21	A	503	NAI	5	0
20	A	502	FMN	4	0
24	J	401	NDP	6	0
27	N	201	PLX	2	0
19	A	501	SF4	2	0
23	G	201	8Q1	1	0
22	C	302	PEE	14	0

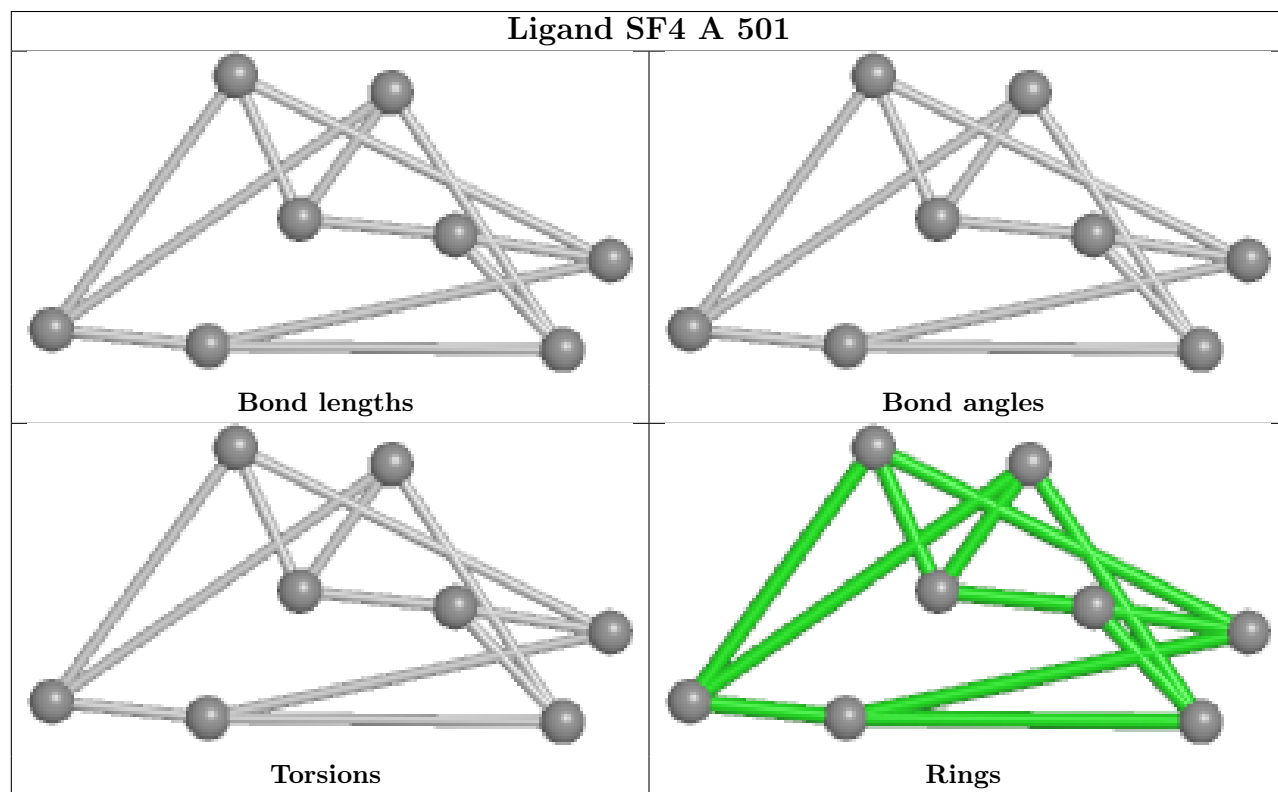
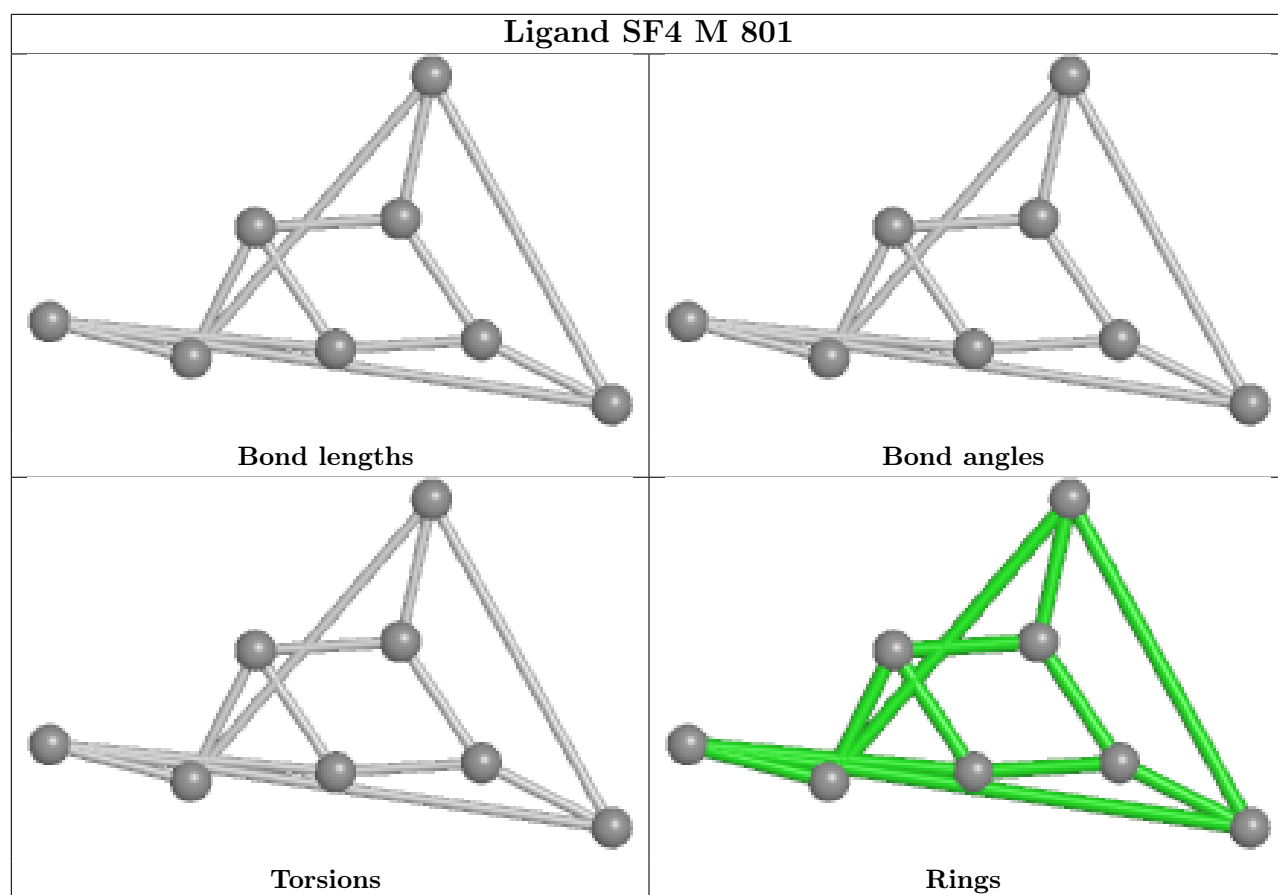
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

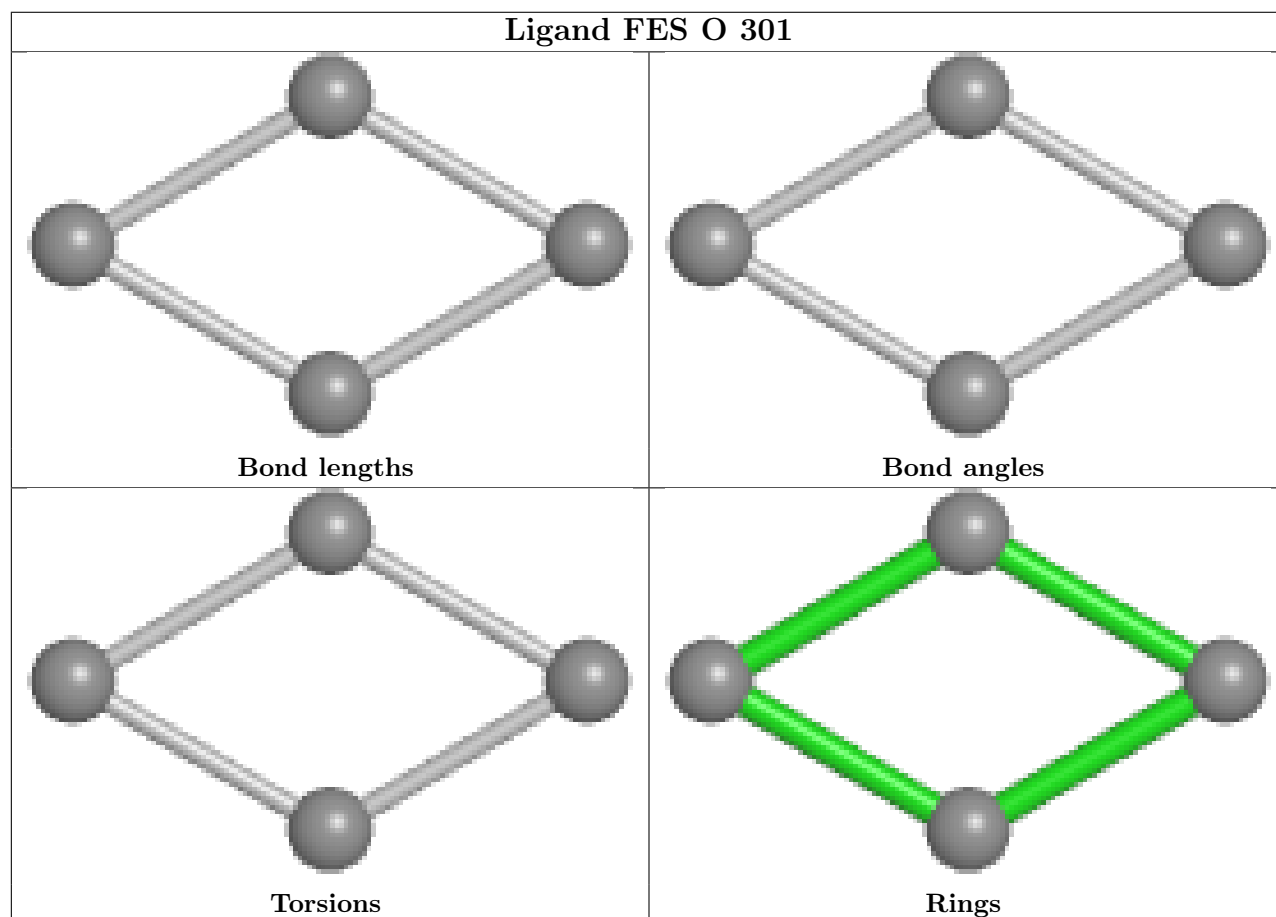
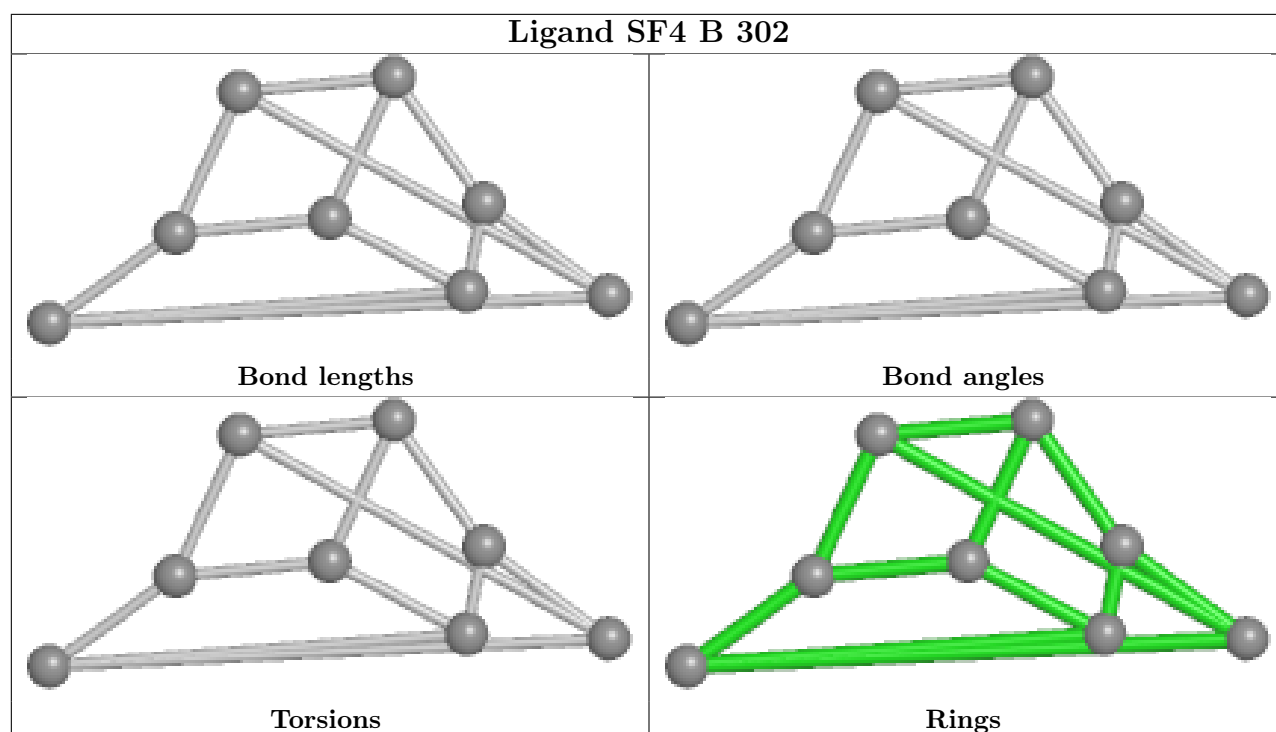


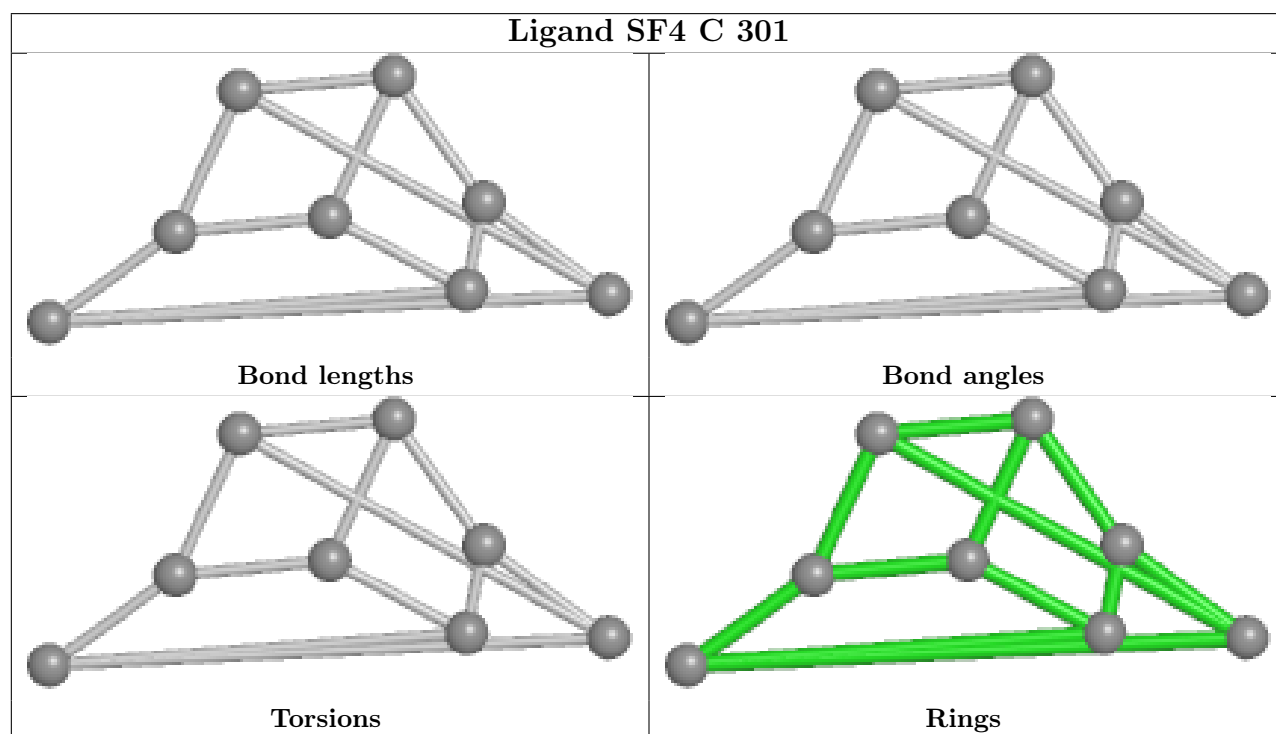
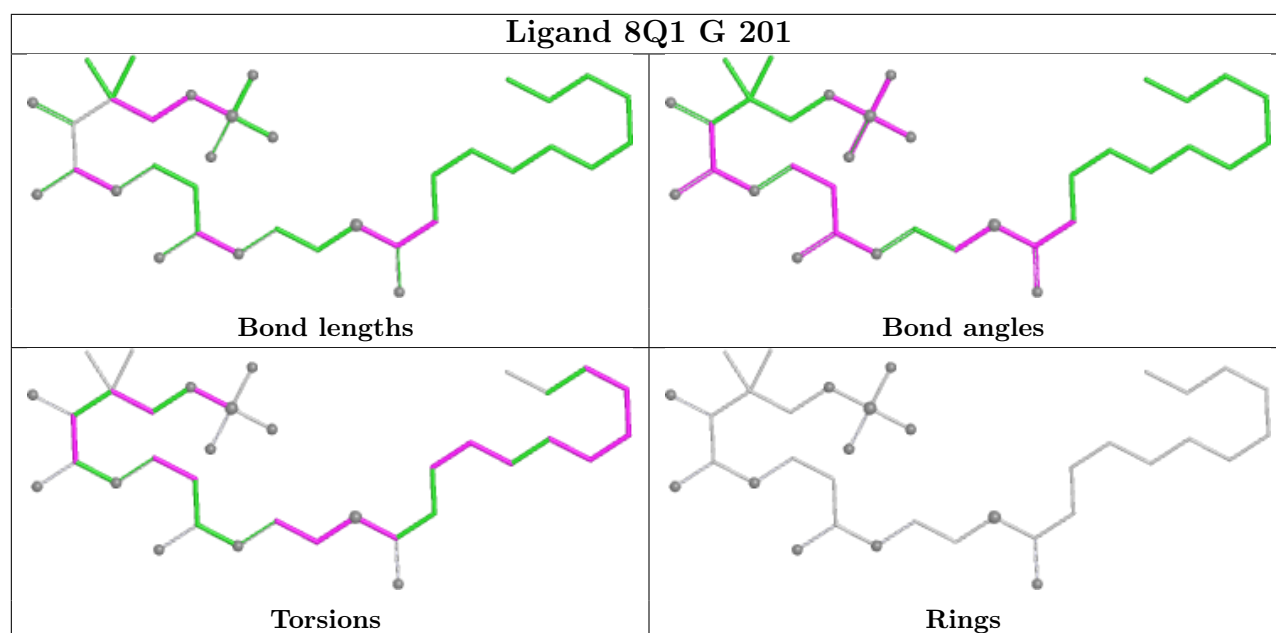


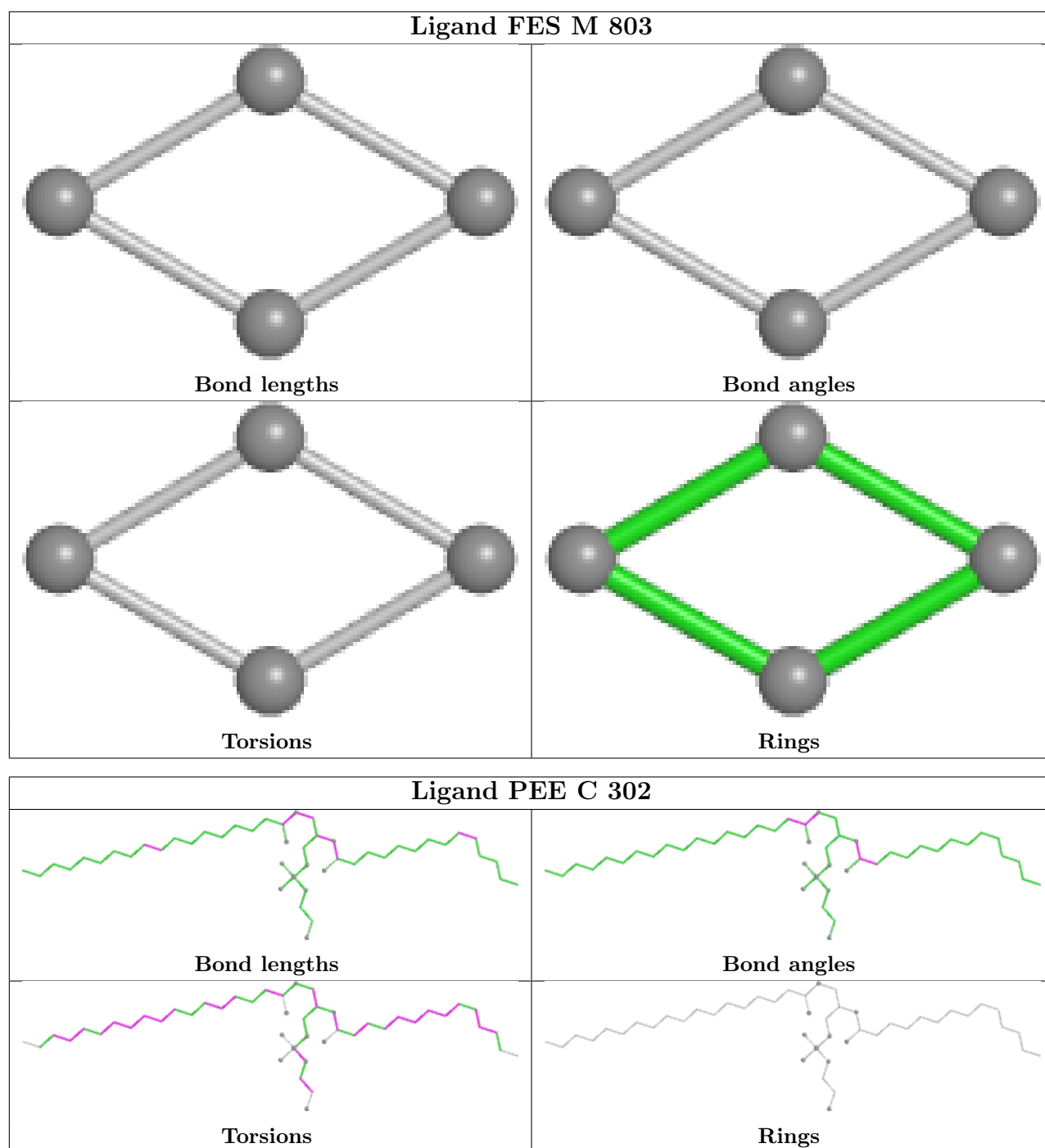












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

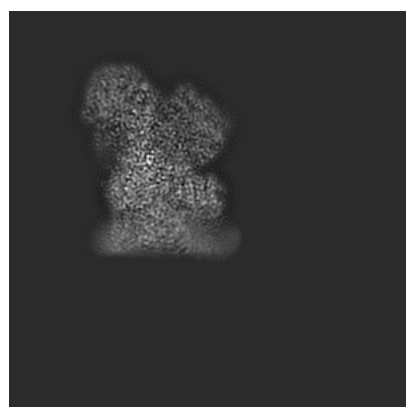
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32198. These allow visual inspection of the internal detail of the map and identification of artifacts.

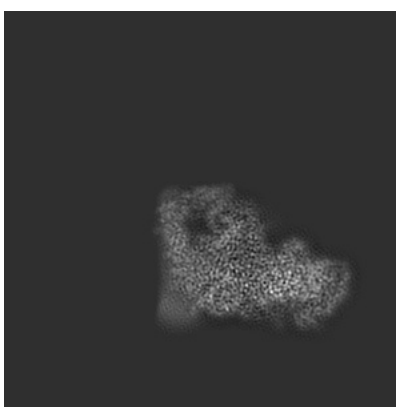
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

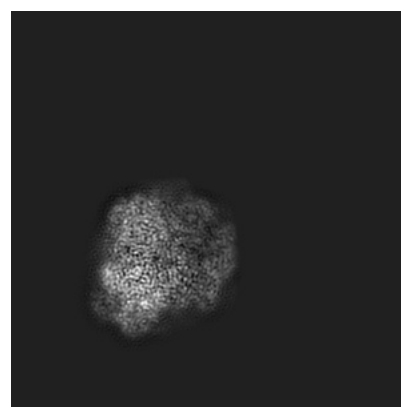
6.1.1 Primary map



X



Y

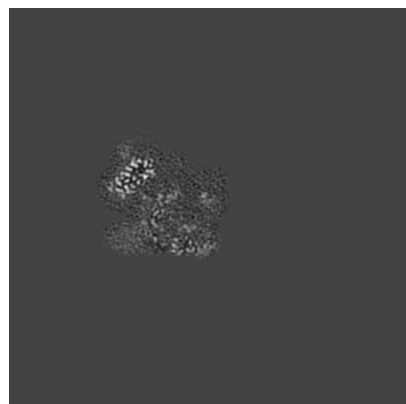


Z

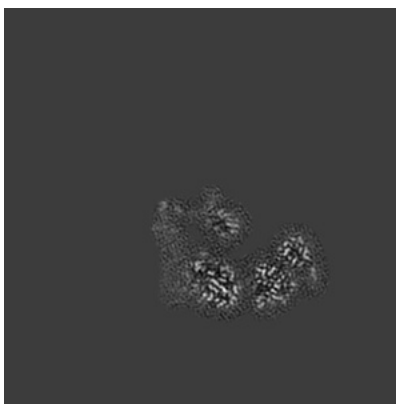
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

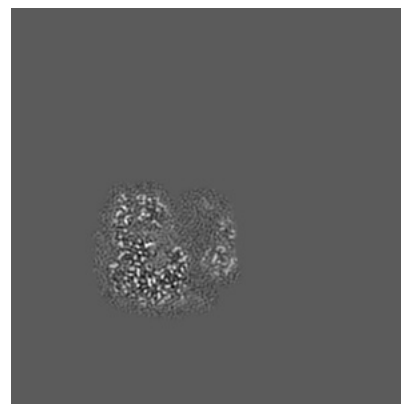
6.2.1 Primary map



X Index: 155



Y Index: 155

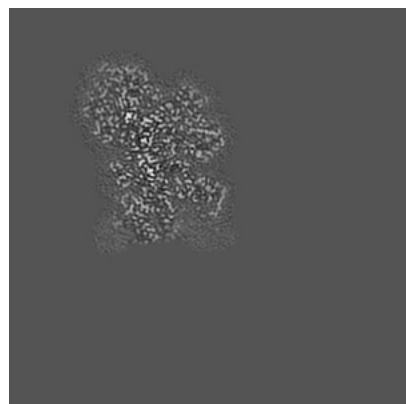


Z Index: 155

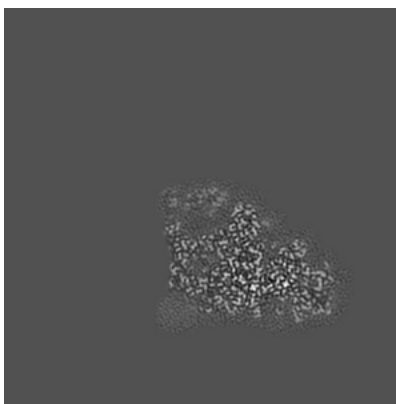
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

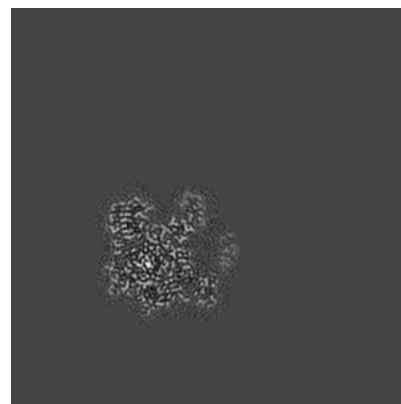
6.3.1 Primary map



X Index: 98



Y Index: 107

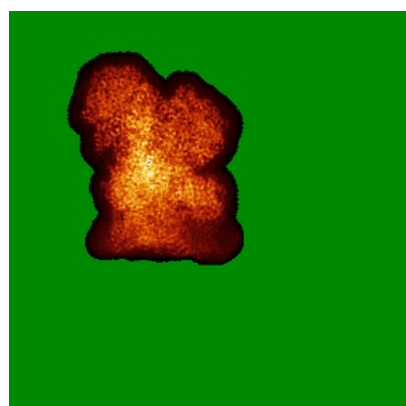


Z Index: 173

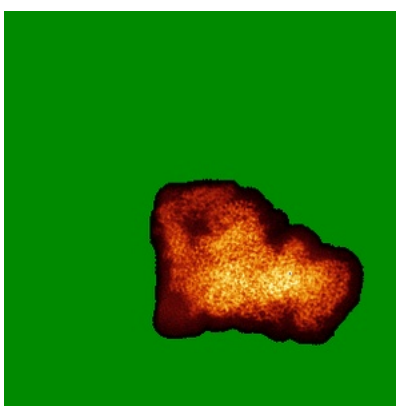
The images above show the largest variance slices of the map in three orthogonal directions.

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

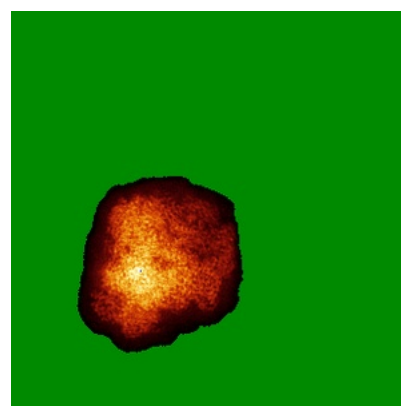
6.4.1 Primary map



X



Y

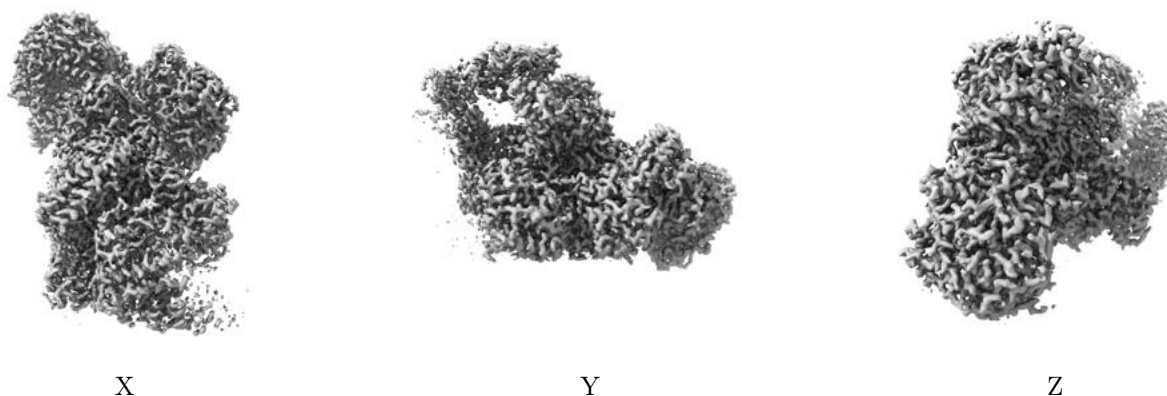


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0301. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

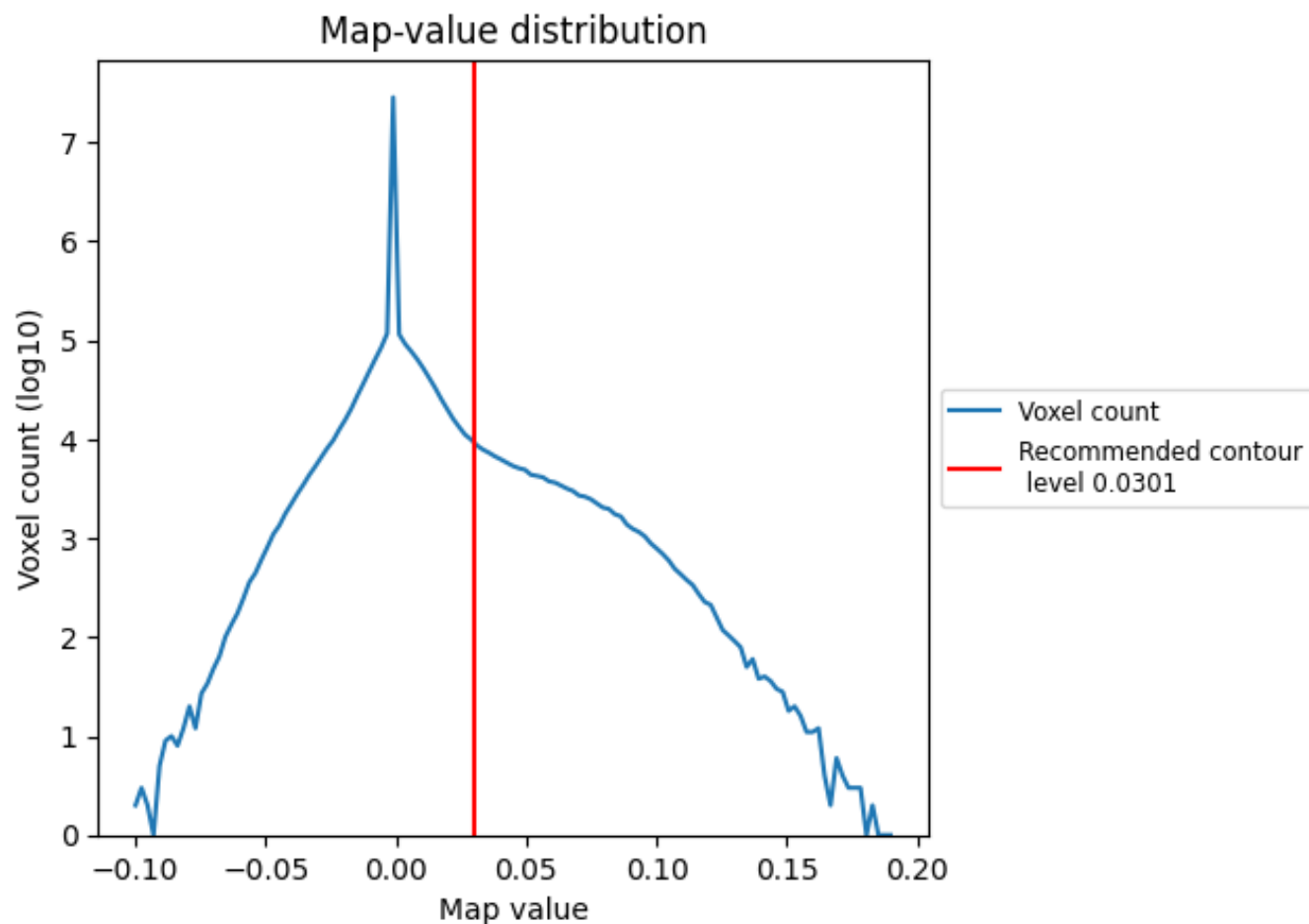
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

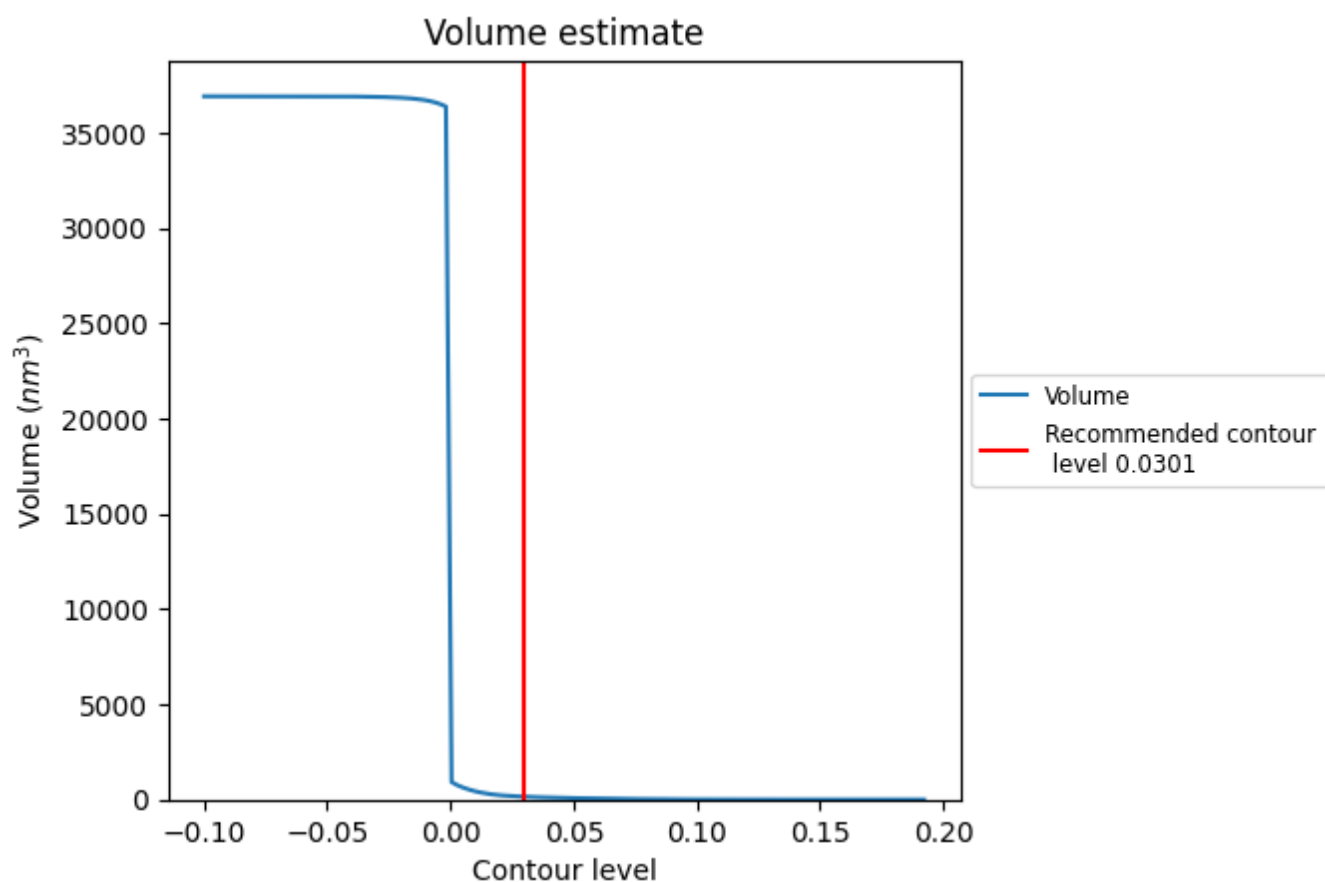
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

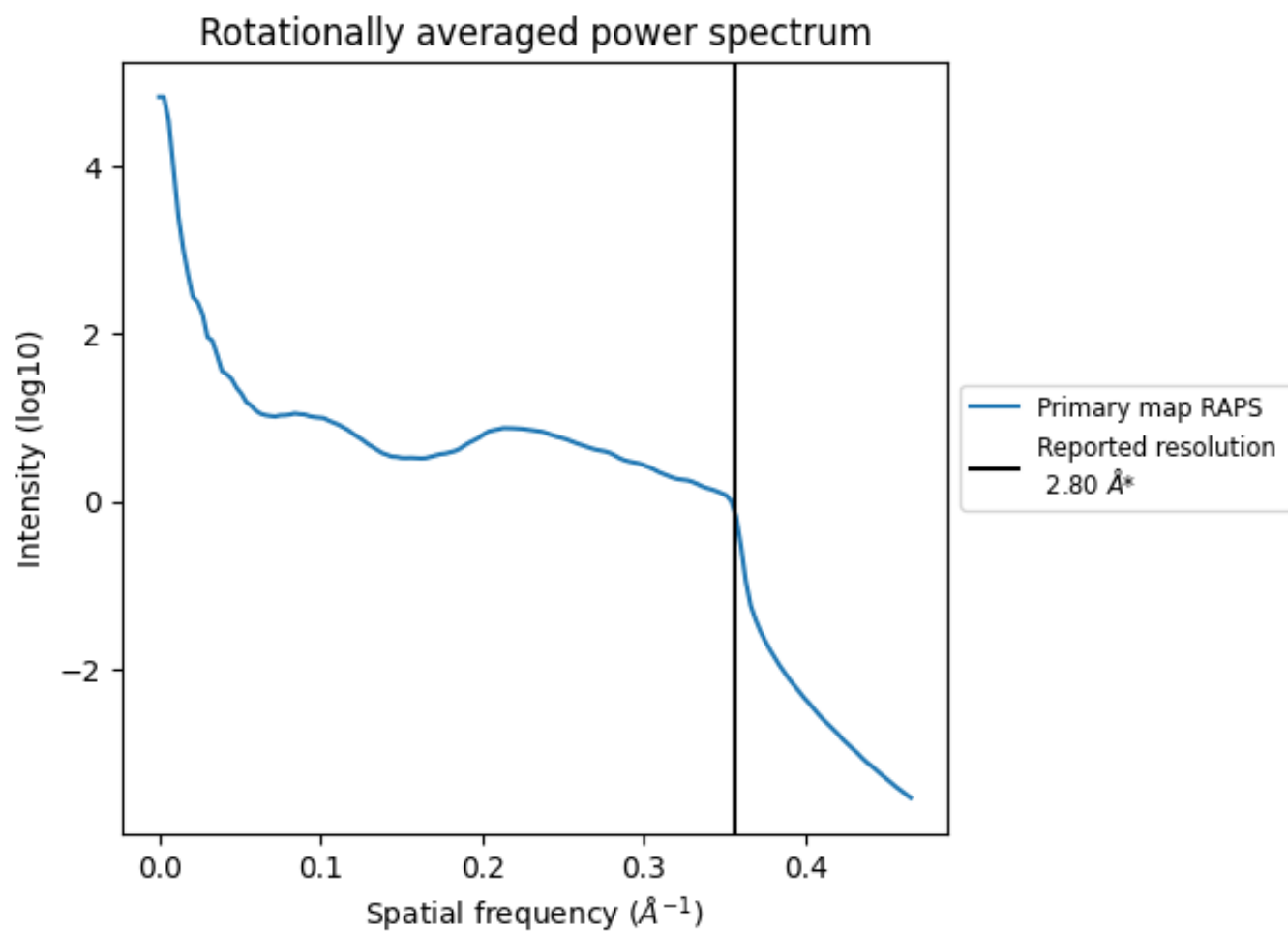
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 135 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

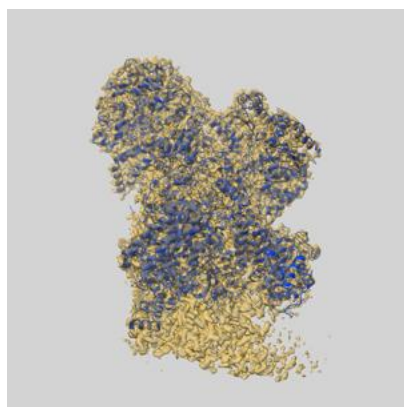
8 Fourier-Shell correlation

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

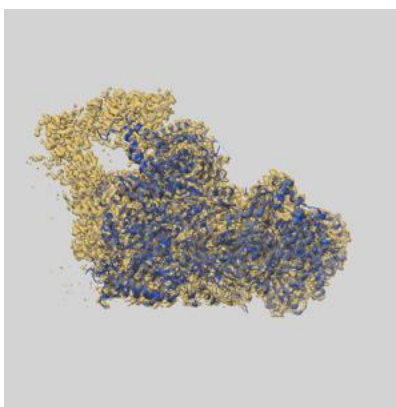
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32198 and PDB model 7VYA. Per-residue inclusion information can be found in section 3 on page 13.

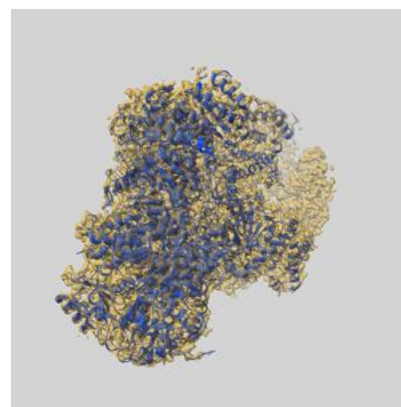
9.1 Map-model overlay [i](#)



X



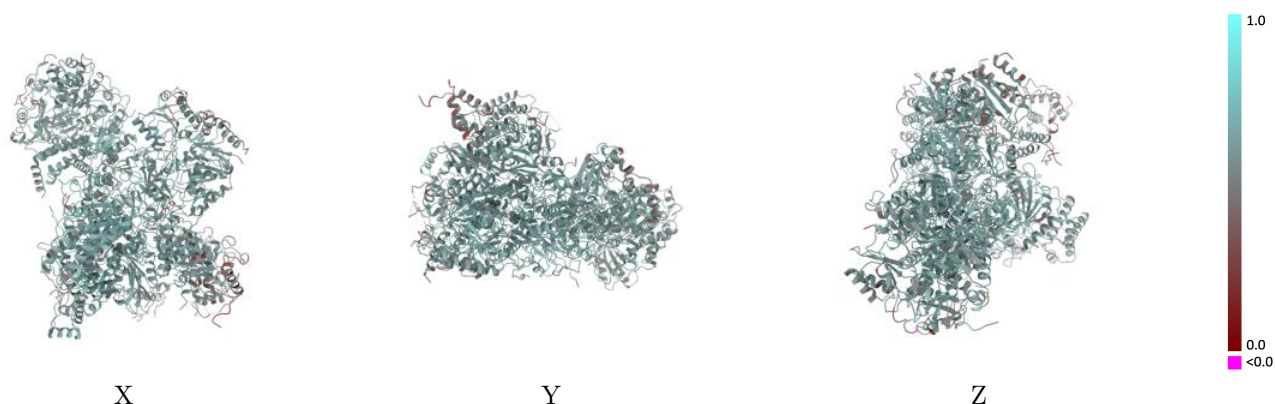
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0301 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](#)

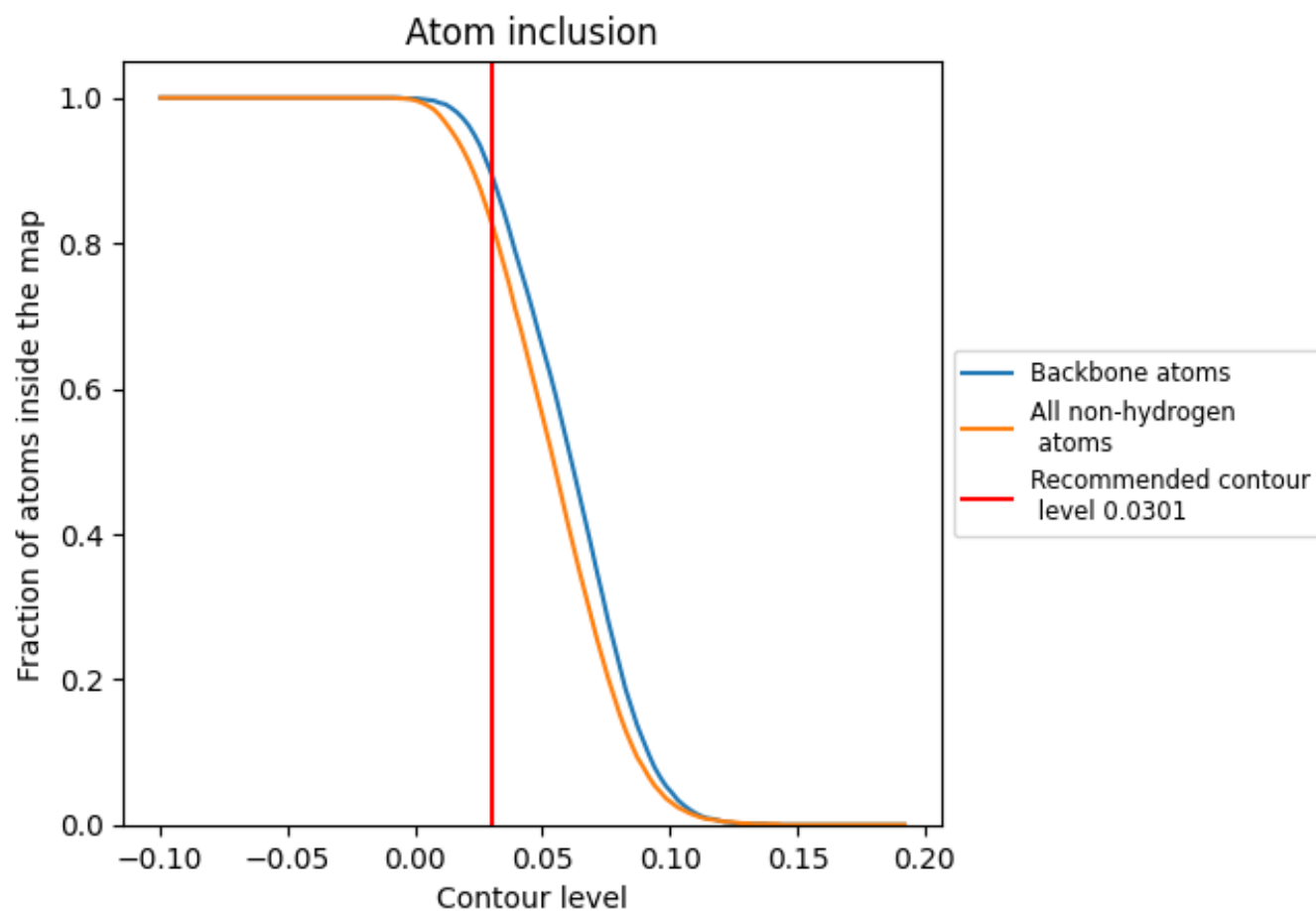


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.0301) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5970
A	 0.8230	 0.5880
B	 0.9190	 0.6380
C	 0.8650	 0.6230
E	 0.7980	 0.5840
F	 0.7230	 0.5330
G	 0.4830	 0.4350
H	 0.7840	 0.5730
I	 0.7680	 0.5830
J	 0.7900	 0.5820
K	 0.7760	 0.5540
L	 0.8410	 0.6050
M	 0.8660	 0.6100
N	 0.7630	 0.5900
O	 0.7530	 0.5590
P	 0.9160	 0.6340
Q	 0.9020	 0.6370
T	 0.8420	 0.6090
W	 0.7690	 0.5810

