



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 02:44 pm BST

PDB ID : 9TAL / pdb_00009tal
EMDB ID : EMD-55750
Title : Local refinement of E. coli Complex I WT hydrophilic domain in LMNG
Authors : Kovalova, T.; Beghiah, A.; Kaila, V.R.I.
Deposited on : 2025-11-18
Resolution : 2.66 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

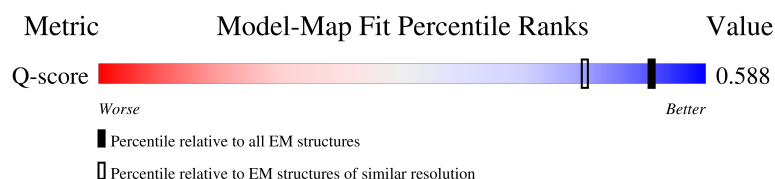
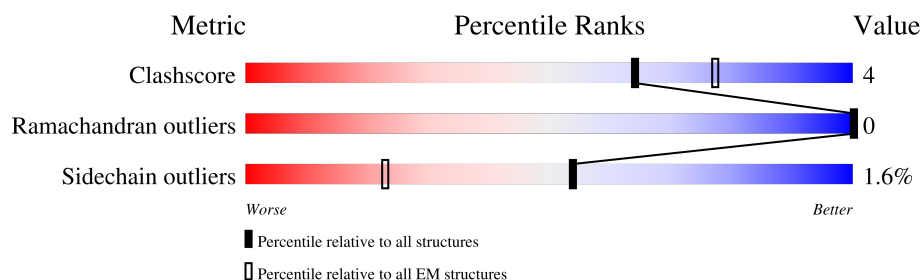
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 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.



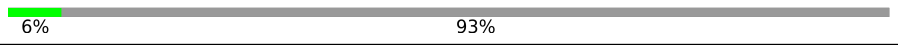
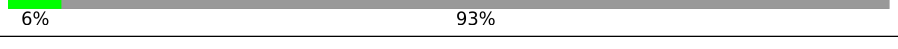
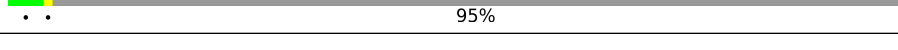
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	E	166	 87% 7% 6%
2	F	461	 88% 7% 5%
3	G	910	 89% 10% .
4	I	180	 73% 8% 19%

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Mol	Chain	Length	Quality of chain
5	B	220	
6	C	600	
7	A	147	
8	H	325	
8	J	325	
8	K	325	
8	L	325	

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
12	SF4	B	301	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20425 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-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	156	Total	C	N	O	S	0	0
			1220	768	215	229	8		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	439	Total	C	N	O	S	0	0
			3407	2162	596	629	20		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	MET	-	initiating methionine	UNP P31979
F	-14	ARG	-	expression tag	UNP P31979
F	-13	GLY	-	expression tag	UNP P31979
F	-12	SER	-	expression tag	UNP P31979
F	-11	HIS	-	expression tag	UNP P31979
F	-10	HIS	-	expression tag	UNP P31979
F	-9	HIS	-	expression tag	UNP P31979
F	-8	HIS	-	expression tag	UNP P31979
F	-7	HIS	-	expression tag	UNP P31979
F	-6	HIS	-	expression tag	UNP P31979
F	-5	THR	-	expression tag	UNP P31979
F	-4	ASP	-	expression tag	UNP P31979
F	-3	PRO	-	expression tag	UNP P31979
F	-2	ALA	-	expression tag	UNP P31979
F	-1	LEU	-	expression tag	UNP P31979
F	0	ARG	-	expression tag	UNP P31979
F	1	ALA	-	expression tag	UNP P31979

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	905	Total	C	N	O	S	0	0
			7027	4392	1269	1329	37		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P33602
G	2	LEU	-	expression tag	UNP P33602

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	145	Total	C	N	O	S	0	0
			1149	728	192	217	12		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	197	Total	C	N	O	S	0	0
			1566	994	271	285	16		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	589	Total	C	N	O	S	0	0
			4760	3049	828	859	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P33599
C	2	VAL	-	expression tag	UNP P33599
C	3	ASN	-	expression tag	UNP P33599
C	4	ASN	-	expression tag	UNP P33599

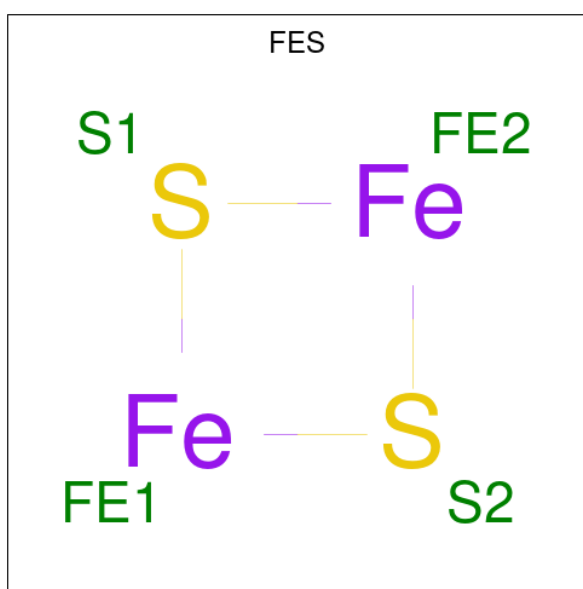
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	19	Total	C	N	O	S	0	0
			133	88	23	19	3		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	22	Total	C	N	O	S	0	0
			177	121	25	30	1		
8	J	42	Total	C	N	O	S	0	0
			342	232	51	56	3		
8	K	22	Total	C	N	O	S	0	0
			166	110	26	29	1		
8	L	16	Total	C	N	O	S	0	0
			120	76	22	20	2		

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

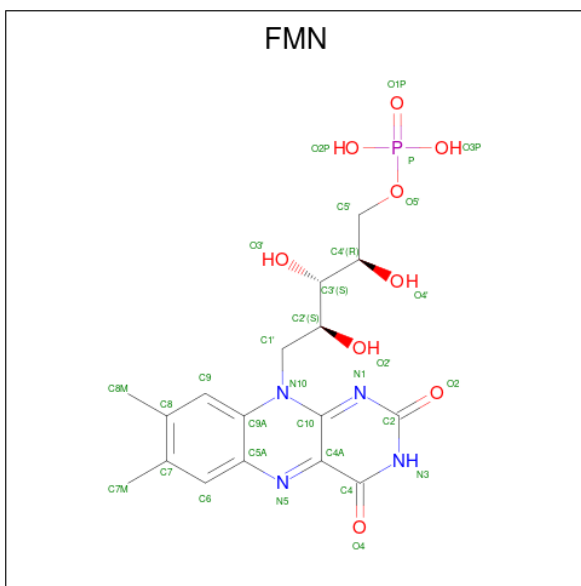


Mol	Chain	Residues	Atoms			AltConf
9	E	1	Total	Fe	S	0
			4	2	2	
9	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

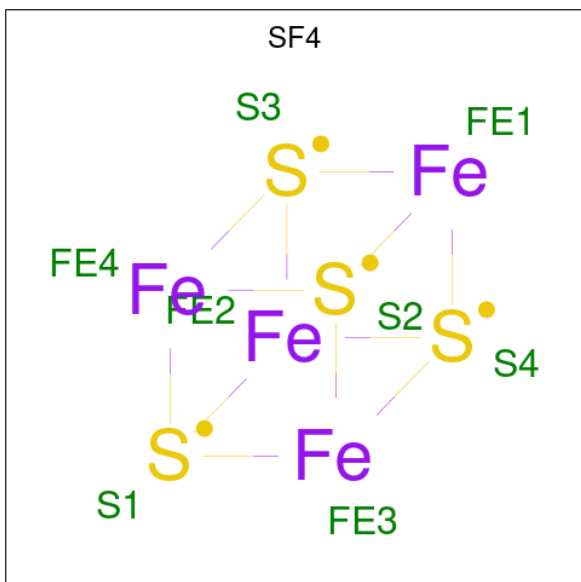
Mol	Chain	Residues	Atoms		AltConf
10	E	1	Total	Ca	0
			1	1	
10	G	3	Total	Ca	0
			3	3	
10	I	1	Total	Ca	0
			1	1	

- Molecule 11 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	F	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
12	G	1	Total 8	Fe 4	S 4	0
12	G	1	Total 8	Fe 4	S 4	0
12	G	1	Total 8	Fe 4	S 4	0
12	I	1	Total 8	Fe 4	S 4	0
12	I	1	Total 8	Fe 4	S 4	0
12	B	1	Total 8	Fe 4	S 4	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	E	4	Total 4	O 4	0
13	F	40	Total 40	O 40	0
13	G	138	Total 138	O 138	0
13	I	18	Total 18	O 18	0
13	B	5	Total 5	O 5	0
13	C	53	Total 53	O 53	0

3 Residue-property plots [i](#)

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

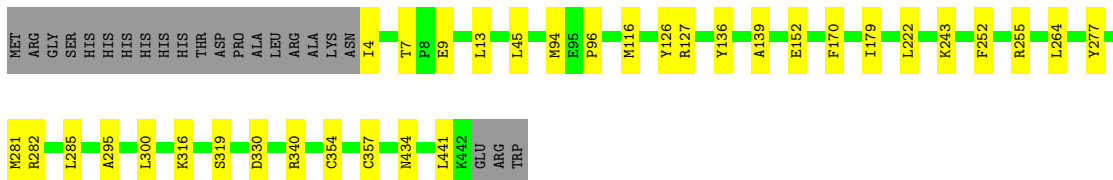
- Molecule 1: NADH-quinone oxidoreductase subunit E

Chain E: 



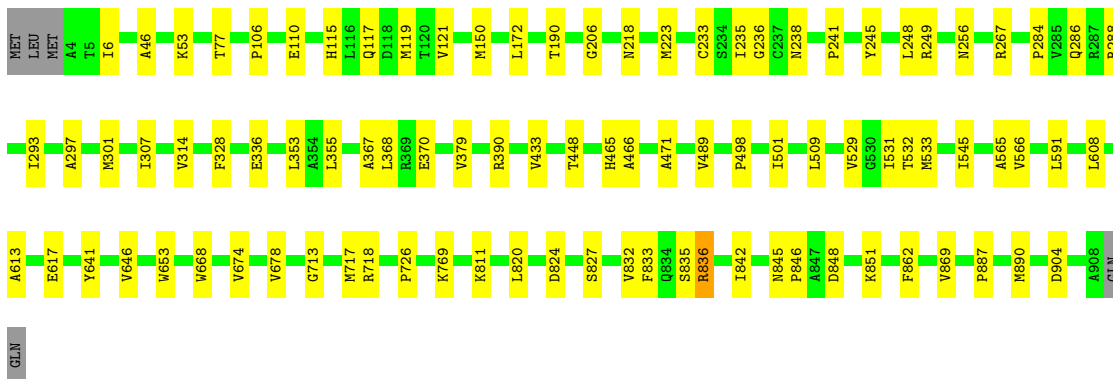
- Molecule 2: NADH-quinone oxidoreductase subunit F

Chain F: 



- Molecule 3: NADH-quinone oxidoreductase subunit G

Chain G: 



- Molecule 4: NADH-quinone oxidoreductase subunit I

Chain I: 

ASN
LEU
LEU
VAL
THR
ALA
ALA
VAL
ILE
LEU
TRP
GLN
ALA
GLN

● Molecule 8: NADH-quinone oxidoreductase subunit H



MET
SER
TRP
ILE
SER
MET
THR
PRO
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LEU
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S33
F34
G35
E36
R37
R38
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L40
G41
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.044	Depositor
Minimum map value	-0.911	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.26	Depositor
Map size ($\text{\AA}$)	585.75, 585.75, 585.75	wwPDB
Map dimensions	710, 710, 710	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FMN, SF4, CA

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	E	0.13	0/1248	0.25	0/1691
2	F	0.13	0/3486	0.24	0/4713
3	G	0.14	0/7178	0.25	0/9733
4	I	0.14	0/1176	0.27	0/1590
5	B	0.15	0/1598	0.31	0/2162
6	C	0.14	0/4891	0.29	0/6637
7	A	0.12	0/135	0.44	0/180
8	H	0.10	0/182	0.30	0/243
8	J	0.15	0/352	0.42	0/475
8	K	0.12	0/170	0.31	0/230
8	L	0.08	0/121	0.23	0/159
All	All	0.14	0/20537	0.27	0/27813

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	E	1220	0	1187	7	0
2	F	3407	0	3374	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	7027	0	6829	51	0
4	I	1149	0	1113	9	0
5	B	1566	0	1561	35	0
6	C	4760	0	4677	46	0
7	A	133	0	139	1	0
8	H	177	0	171	0	0
8	J	342	0	350	9	0
8	K	166	0	162	1	0
8	L	120	0	120	2	0
9	E	4	0	0	0	0
9	G	4	0	0	0	0
10	E	1	0	0	0	0
10	G	3	0	0	0	0
10	I	1	0	0	0	0
11	F	31	0	19	1	0
12	B	8	0	0	2	0
12	F	8	0	0	1	0
12	G	24	0	0	0	0
12	I	16	0	0	0	0
13	B	5	0	0	0	0
13	C	53	0	0	0	0
13	E	4	0	0	0	0
13	F	40	0	0	1	0
13	G	138	0	0	1	0
13	I	18	0	0	0	0
All	All	20425	0	19702	165	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 4.

All (165) 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)
5:B:101:THR:HG21	6:C:254:ARG:HD3	1.60	0.83
6:C:74:LEU:HB3	6:C:133:ASN:HD22	1.47	0.79
8:J:60:LEU:HD21	8:L:34:PHE:HB2	1.76	0.68
6:C:236:GLN:HG2	6:C:243:VAL:HB	1.77	0.67
8:J:88:MET:HA	8:J:88:MET:HE3	1.76	0.67
6:C:408:SER:HB2	6:C:463:CYS:HB2	1.79	0.64
3:G:218:ASN:HD22	3:G:249:ARG:HD2	1.63	0.64
3:G:106:PRO:HD3	6:C:515:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:72:PHE:HD1	5:B:73:THR:H	1.47	0.63
3:G:848:ASP:HA	3:G:851:LYS:HE3	1.81	0.61
6:C:378:ARG:O	6:C:382:GLU:HG3	2.01	0.61
3:G:355:LEU:HD21	3:G:545:ILE:HG13	1.83	0.60
6:C:76:ASP:HB3	6:C:562:ARG:HG3	1.87	0.57
6:C:468:MET:HE3	6:C:468:MET:HA	1.87	0.57
6:C:391:LEU:HD22	6:C:478:LEU:HD12	1.87	0.56
3:G:301:MET:HE3	3:G:653:TRP:CE3	2.40	0.56
3:G:718:ARG:HD3	3:G:726:PRO:HG3	1.86	0.56
5:B:21:LYS:HE2	5:B:23:GLU:HG2	1.86	0.56
5:B:96:MET:HE1	5:B:114:TYR:HB2	1.88	0.55
4:I:47:ARG:CZ	5:B:208:ARG:HD2	2.36	0.55
5:B:138:ILE:HG23	5:B:140:SER:H	1.71	0.55
2:F:357:CYS:HB3	12:F:502:SF4:S4	2.47	0.55
3:G:368:LEU:HD21	3:G:390:ARG:HB3	1.89	0.54
5:B:98:VAL:HG11	5:B:145:VAL:HG21	1.89	0.54
2:F:434:ASN:HB3	4:I:146:PRO:HD2	1.90	0.54
3:G:307:ILE:HG21	3:G:591:LEU:HD13	1.91	0.53
5:B:60:GLY:HA3	5:B:65:TYR:HB2	1.91	0.53
6:C:144:LEU:HB3	6:C:169:LEU:HB2	1.89	0.53
8:J:79:ASP:HB3	8:J:82:ILE:HG22	1.91	0.53
5:B:62:SER:HB3	12:B:301:SF4:S1	2.49	0.53
5:B:63:CYS:HB2	12:B:301:SF4:S2	2.49	0.53
8:J:82:ILE:HD11	8:K:132:PHE:HB3	1.90	0.52
2:F:441:LEU:HD21	6:C:496:ASP:HB2	1.91	0.52
6:C:175:ALA:HB2	6:C:258:LYS:HE3	1.91	0.52
3:G:466:ALA:HB3	3:G:489:VAL:HG21	1.90	0.52
8:J:61:VAL:O	8:J:65:ILE:HG13	2.11	0.51
1:E:98:HIS:HA	1:E:102:TYR:HD1	1.77	0.50
2:F:300:LEU:HD21	2:F:319:SER:HB2	1.93	0.50
6:C:501:THR:HG23	6:C:521:GLN:HB3	1.92	0.50
5:B:73:THR:HA	5:B:76:HIS:NE2	2.27	0.50
5:B:103:PHE:HE1	6:C:254:ARG:HG3	1.77	0.49
3:G:115:HIS:CE1	3:G:119:MET:HE3	2.46	0.49
6:C:200:LYS:HB2	6:C:203:GLU:HG2	1.94	0.49
3:G:117:GLN:HG2	6:C:516:ILE:HG23	1.94	0.49
3:G:218:ASN:ND2	3:G:249:ARG:HD2	2.26	0.49
7:A:37:LEU:HB3	8:J:69:PHE:CD2	2.48	0.49
6:C:397:ALA:O	6:C:401:ASN:HB2	2.12	0.49
6:C:576:ILE:HD11	6:C:583:ASP:HB3	1.95	0.49
6:C:403:ILE:HB	6:C:407:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:21:LEU:HD22	6:C:30:ARG:HH22	1.77	0.49
5:B:64:CYS:HB3	5:B:99:ALA:HB1	1.95	0.48
3:G:367:ALA:HB3	3:G:370:GLU:HG3	1.94	0.48
6:C:24:PRO:O	6:C:28:GLU:HG3	2.14	0.48
6:C:387:MET:N	6:C:388:PRO:HD2	2.29	0.48
6:C:201:PRO:HG2	6:C:208:ARG:HD3	1.96	0.47
4:I:48:ILE:HG12	4:I:116:LEU:HG	1.97	0.47
5:B:21:LYS:CE	5:B:23:GLU:HG2	2.44	0.47
3:G:284:PRO:HD3	3:G:646:VAL:HB	1.97	0.47
2:F:282:ARG:HB2	2:F:285:LEU:HD12	1.95	0.47
3:G:613:ALA:HB1	3:G:617:GLU:HB2	1.95	0.47
3:G:115:HIS:HE1	3:G:119:MET:HE3	1.78	0.47
3:G:288:ARG:HD2	3:G:293:ILE:HD13	1.97	0.47
5:B:60:GLY:HA3	5:B:65:TYR:CD1	2.50	0.47
3:G:531:ILE:HD11	3:G:533:MET:HE2	1.97	0.46
6:C:77:LEU:HB3	6:C:137:TYR:HB3	1.97	0.46
2:F:45:LEU:HD12	2:F:45:LEU:HA	1.83	0.46
6:C:73:MET:HE2	6:C:423:GLY:HA2	1.97	0.46
3:G:353:LEU:HD22	3:G:509:LEU:HG	1.98	0.46
1:E:116:LYS:HE3	1:E:116:LYS:HA	1.98	0.46
3:G:236:GLY:HA2	13:G:1101:HOH:O	2.16	0.46
6:C:211:GLU:HG3	6:C:214:ASP:HB2	1.97	0.46
5:B:101:THR:HA	5:B:129:CYS:HB3	1.98	0.45
6:C:328:GLN:HA	6:C:333:MET:HA	1.98	0.45
6:C:565:SER:HB3	6:C:593:PHE:HB2	1.98	0.45
5:B:25:VAL:HG11	5:B:193:TYR:CE1	2.51	0.45
2:F:136:TYR:HB3	2:F:139:ALA:HB3	1.99	0.45
3:G:328:PHE:CG	3:G:678:VAL:HG22	2.52	0.45
3:G:190:THR:HG21	3:G:836:ARG:HD3	1.98	0.45
6:C:405:LYS:HB2	6:C:405:LYS:HE3	1.79	0.45
3:G:887:PRO:HB2	3:G:890:MET:HG3	1.99	0.45
5:B:72:PHE:CZ	5:B:166:MET:HB2	2.51	0.45
6:C:212:ASN:HA	6:C:215:PHE:CE2	2.52	0.45
5:B:85:VAL:HG22	5:B:86:LEU:H	1.82	0.44
2:F:94:MET:HE3	2:F:94:MET:HB2	1.87	0.44
3:G:713:GLY:O	3:G:717:MET:HG3	2.18	0.44
6:C:74:LEU:HD23	6:C:133:ASN:HB2	1.99	0.44
6:C:65:LYS:HE2	6:C:65:LYS:HB3	1.71	0.44
3:G:301:MET:HE3	3:G:653:TRP:HE3	1.81	0.44
3:G:379:VAL:HB	3:G:433:VAL:HG12	1.99	0.44
4:I:42:PRO:HB3	5:B:215:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ARG:HG2	2:F:170:PHE:HE2	1.83	0.44
3:G:314:VAL:HG22	3:G:565:ALA:HB3	1.98	0.43
5:B:148:PHE:HD2	5:B:149:ILE:HG23	1.83	0.43
6:C:65:LYS:HD3	6:C:130:LEU:HD22	1.99	0.43
2:F:116:MET:HG2	2:F:222:LEU:HD13	2.00	0.43
2:F:7:THR:HG23	2:F:9:GLU:H	1.82	0.43
5:B:45:MET:HG2	8:J:65:ILE:HD13	1.99	0.43
6:C:165:LYS:HD3	6:C:165:LYS:HA	1.67	0.43
6:C:168:PRO:HA	6:C:173:TYR:CD1	2.53	0.43
5:B:38:PHE:O	5:B:42:LEU:HD22	2.18	0.43
2:F:96:PRO:HB2	2:F:295:ALA:HB2	2.00	0.43
3:G:6:ILE:HG22	3:G:77:THR:HB	2.01	0.43
3:G:845:ASN:OD1	3:G:846:PRO:HD2	2.18	0.43
6:C:405:LYS:O	6:C:409:GLN:HB2	2.17	0.43
3:G:238:ASN:ND2	3:G:256:ASN:HD22	2.17	0.43
1:E:161:LEU:HD12	1:E:161:LEU:HA	1.86	0.43
2:F:354:CYS:HA	3:G:46:ALA:O	2.19	0.43
11:F:501:FMN:HM81	11:F:501:FMN:HM73	1.84	0.43
3:G:110:GLU:HG3	3:G:206:GLY:HA2	2.01	0.43
3:G:233:CYS:SG	3:G:235:ILE:HG12	2.59	0.43
3:G:827:SER:HB3	3:G:833:PHE:CE2	2.54	0.43
4:I:100:ILE:HG21	5:B:135:MET:HB3	2.01	0.43
2:F:340:ARG:HD3	13:F:612:HOH:O	2.19	0.43
3:G:150:MET:O	3:G:150:MET:HE3	2.19	0.42
3:G:501:ILE:HG12	3:G:532:THR:HB	2.01	0.42
3:G:848:ASP:O	3:G:851:LYS:HG2	2.19	0.42
6:C:233:ILE:HD13	6:C:247:PRO:HA	1.99	0.42
5:B:148:PHE:CD2	5:B:149:ILE:HG23	2.55	0.42
8:L:29:GLY:HA2	8:L:32:MET:HE3	2.02	0.42
3:G:824:ASP:HB3	3:G:827:SER:HB2	2.02	0.42
1:E:25:GLU:CD	1:E:38:GLU:HG2	2.44	0.42
6:C:144:LEU:HA	6:C:168:PRO:HD2	2.02	0.42
6:C:169:LEU:HD23	6:C:169:LEU:HA	1.84	0.42
1:E:90:ARG:HA	1:E:129:LEU:O	2.20	0.42
3:G:465:HIS:HA	3:G:471:ALA:HB3	2.02	0.42
2:F:126:TYR:CZ	2:F:127:ARG:HD2	2.54	0.42
3:G:53:LYS:HE3	3:G:53:LYS:HB2	1.88	0.42
6:C:402:THR:HA	6:C:405:LYS:HB3	2.02	0.42
1:E:158:ILE:HD13	1:E:158:ILE:HA	1.88	0.42
2:F:255:ARG:HD3	2:F:330:ASP:OD2	2.20	0.42
3:G:121:VAL:HG21	6:C:520:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:498:PRO:HG2	3:G:529:VAL:HG23	2.01	0.42
3:G:433:VAL:HG23	3:G:448:THR:HG23	2.01	0.41
5:B:73:THR:HA	5:B:76:HIS:CD2	2.54	0.41
5:B:204:LYS:O	5:B:208:ARG:HG3	2.20	0.41
3:G:267:ARG:HB2	3:G:820:LEU:HG	2.02	0.41
2:F:179:ILE:HD12	2:F:179:ILE:HA	1.86	0.41
3:G:245:TYR:HA	3:G:641:TYR:CZ	2.55	0.41
4:I:36:GLU:HA	4:I:37:PRO:HD3	1.91	0.41
5:B:48:TRP:HA	5:B:51:LYS:HG2	2.01	0.41
5:B:140:SER:HB3	6:C:160:MET:HE1	2.03	0.41
6:C:569:LEU:HD13	6:C:572:ILE:HD12	2.01	0.41
1:E:117:PRO:HA	1:E:128:LEU:HB3	2.03	0.41
3:G:297:ALA:HB1	3:G:668:TRP:CH2	2.56	0.41
5:B:180:ARG:HB2	5:B:193:TYR:HB2	2.02	0.41
2:F:152:GLU:HA	2:F:152:GLU:OE1	2.21	0.41
2:F:281:MET:HE3	2:F:281:MET:HB3	1.87	0.41
3:G:674:VAL:O	3:G:678:VAL:HG23	2.21	0.41
5:B:117:MET:HE2	5:B:117:MET:HB3	1.90	0.41
6:C:597:ASP:OD1	6:C:597:ASP:C	2.63	0.41
8:J:58:LEU:HD23	8:J:58:LEU:HA	1.88	0.41
2:F:264:LEU:HD21	2:F:277:TYR:CZ	2.55	0.41
4:I:106:GLU:HG3	4:I:115:GLN:HA	2.03	0.41
5:B:68:MET:HE3	5:B:126:MET:SD	2.61	0.41
6:C:587:TYR:O	6:C:591:ILE:HG23	2.20	0.41
3:G:241:PRO:HB3	3:G:248:LEU:HD11	2.03	0.40
3:G:862:PHE:HA	3:G:904:ASP:O	2.21	0.40
4:I:141:GLY:HA3	5:B:212:THR:HA	2.02	0.40
3:G:811:LYS:HB3	3:G:811:LYS:HE2	1.84	0.40
6:C:217:PHE:HE1	6:C:236:GLN:HB2	1.85	0.40
3:G:286:GLN:HB2	3:G:608:LEU:HD13	2.03	0.40
4:I:127:ARG:NH1	5:B:132:SER:HB3	2.35	0.40
5:B:182:PRO:HG3	5:B:191:GLY:H	1.86	0.40
8:J:74:ILE:HD13	8:J:74:ILE:HA	1.87	0.40
2:F:243:LYS:HE3	2:F:243:LYS:HB3	1.85	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	E	154/166 (93%)	149 (97%)	5 (3%)	0	100	100
2	F	437/461 (95%)	427 (98%)	10 (2%)	0	100	100
3	G	903/910 (99%)	874 (97%)	29 (3%)	0	100	100
4	I	143/180 (79%)	140 (98%)	3 (2%)	0	100	100
5	B	189/220 (86%)	177 (94%)	12 (6%)	0	100	100
6	C	587/600 (98%)	557 (95%)	30 (5%)	0	100	100
7	A	17/147 (12%)	17 (100%)	0	0	100	100
8	H	20/325 (6%)	18 (90%)	2 (10%)	0	100	100
8	J	40/325 (12%)	39 (98%)	1 (2%)	0	100	100
8	K	20/325 (6%)	17 (85%)	3 (15%)	0	100	100
8	L	14/325 (4%)	14 (100%)	0	0	100	100
All	All	2524/3984 (63%)	2429 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	129/139 (93%)	128 (99%)	1 (1%)	73	85
2	F	353/372 (95%)	349 (99%)	4 (1%)	65	80
3	G	733/738 (99%)	723 (99%)	10 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	124/154 (80%)	122 (98%)	2 (2%)	55	74
5	B	173/192 (90%)	166 (96%)	7 (4%)	28	47
6	C	509/519 (98%)	501 (98%)	8 (2%)	55	74
7	A	12/119 (10%)	12 (100%)	0	100	100
8	H	18/269 (7%)	17 (94%)	1 (6%)	19	32
8	J	37/269 (14%)	36 (97%)	1 (3%)	39	61
8	K	16/269 (6%)	16 (100%)	0	100	100
8	L	12/269 (4%)	12 (100%)	0	100	100
All	All	2116/3309 (64%)	2082 (98%)	34 (2%)	54	74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	149	THR
2	F	4	ILE
2	F	13	LEU
2	F	252	PHE
2	F	316	LYS
3	G	172	LEU
3	G	223	MET
3	G	336	GLU
3	G	566	VAL
3	G	769	LYS
3	G	832	VAL
3	G	835	SER
3	G	836	ARG
3	G	842	ILE
3	G	869	VAL
4	I	77	LEU
4	I	147	GLU
5	B	8	ILE
5	B	63	CYS
5	B	69	VAL
5	B	101	THR
5	B	183	LEU
5	B	207	GLU
5	B	219	GLU
6	C	36	ASP
6	C	124	VAL

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Mol	Chain	Res	Type
6	C	210	THR
6	C	243	VAL
6	C	275	ILE
6	C	327	ILE
6	C	342	ASP
6	C	356	PHE
8	H	228	GLU
8	J	68	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	24	HIS
1	E	27	HIS
1	E	56	HIS
2	F	159	ASN
2	F	341	ASN
2	F	386	GLN
2	F	425	GLN
3	G	113	ASN
3	G	310	GLN
3	G	397	GLN
3	G	425	GLN
3	G	598	GLN
3	G	607	HIS
3	G	630	GLN
3	G	655	HIS
3	G	743	ASN
3	G	745	GLN
3	G	806	GLN
3	G	839	GLN
4	I	64	ASN
5	B	111	GLN
6	C	20	HIS
6	C	133	ASN
6	C	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
12	SF4	F	502	2	0,12,12	-	-	-		
9	FES	G	1003	3	0,4,4	-	-	-		
9	FES	E	201	1	0,4,4	-	-	-		
12	SF4	I	203	4	0,12,12	-	-	-		
12	SF4	G	1001	3	0,12,12	-	-	-		
11	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.19	6 (12%)
12	SF4	I	202	4	0,12,12	-	-	-		
12	SF4	G	1002	3	0,12,12	-	-	-		
12	SF4	G	1007	3	0,12,12	-	-	-		
12	SF4	B	301	5	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SF4	F	502	2	-	-	0/6/5/5
9	FES	G	1003	3	-	-	0/1/1/1
9	FES	E	201	1	-	-	0/1/1/1
12	SF4	I	203	4	-	-	0/6/5/5
12	SF4	G	1001	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FMN	F	501	-	-	5/18/18/18	0/3/3/3
12	SF4	I	202	4	-	-	0/6/5/5
12	SF4	G	1002	3	-	-	0/6/5/5
12	SF4	G	1007	3	-	-	0/6/5/5
12	SF4	B	301	5	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	501	FMN	C4A-N5	3.71	1.38	1.30
11	F	501	FMN	C10-N1	2.41	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	501	FMN	C4-N3-C2	-3.07	119.97	125.64
11	F	501	FMN	C4A-C4-N3	2.65	119.92	113.19
11	F	501	FMN	C4A-C10-N10	2.63	120.33	116.48
11	F	501	FMN	O4-C4-C4A	-2.55	119.84	126.60
11	F	501	FMN	C10-C4A-N5	-2.26	120.05	124.86
11	F	501	FMN	C4A-C10-N1	-2.06	119.94	124.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	501	FMN	C1'-C2'-C3'-O3'
11	F	501	FMN	C1'-C2'-C3'-C4'
11	F	501	FMN	O2'-C2'-C3'-O3'
11	F	501	FMN	O2'-C2'-C3'-C4'
11	F	501	FMN	N10-C1'-C2'-O2'

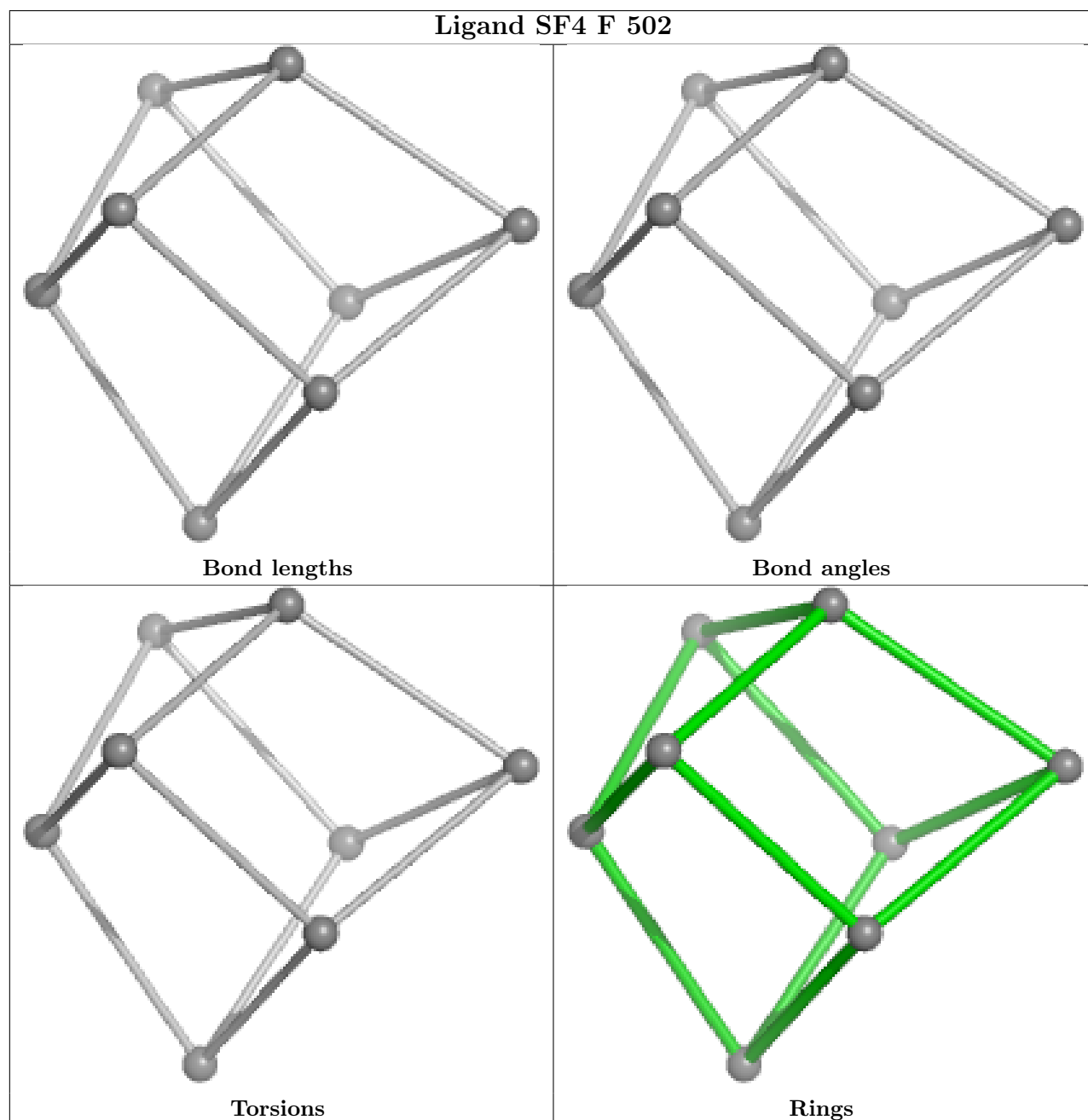
There are no ring outliers.

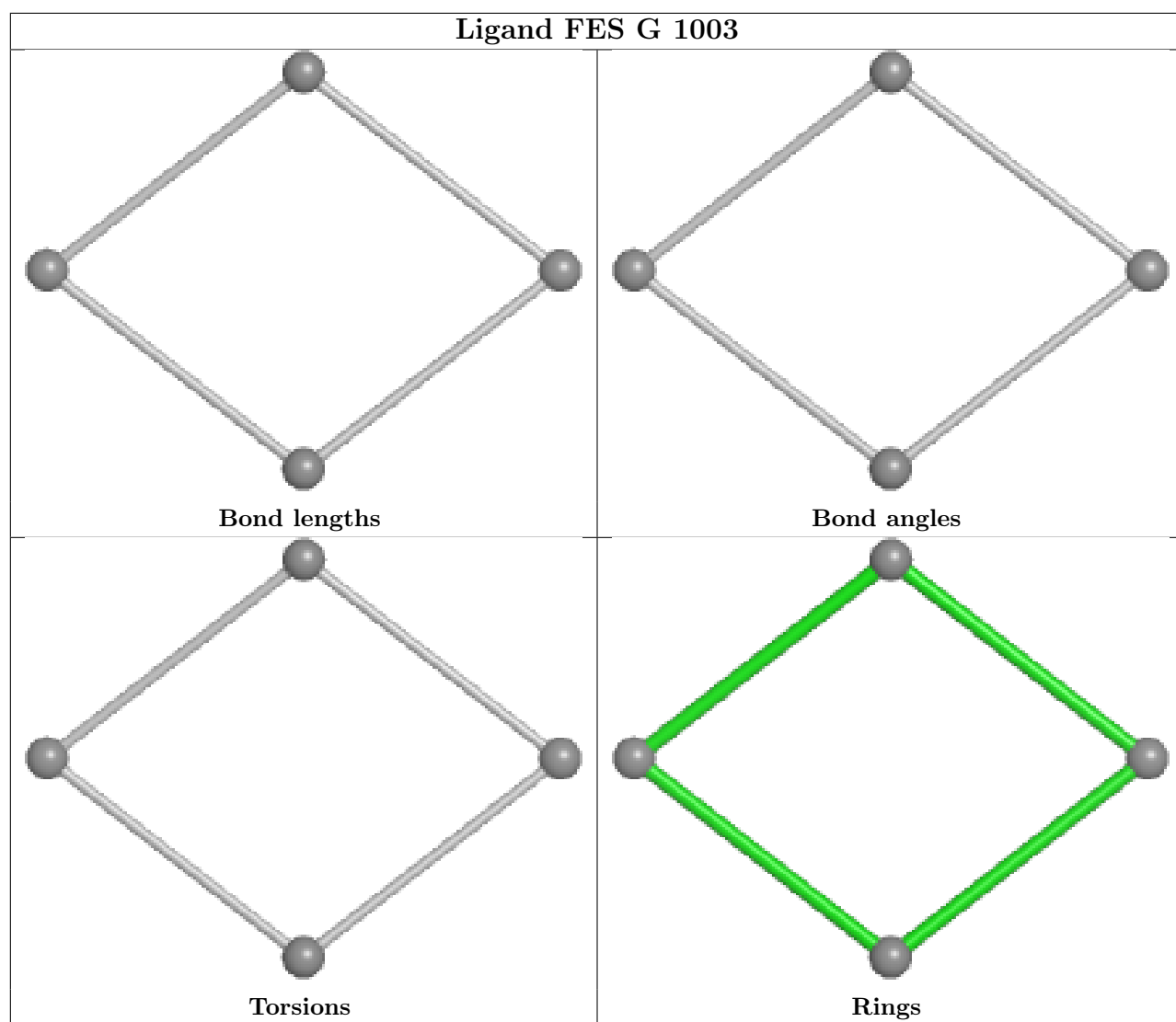
3 monomers are involved in 4 short contacts:

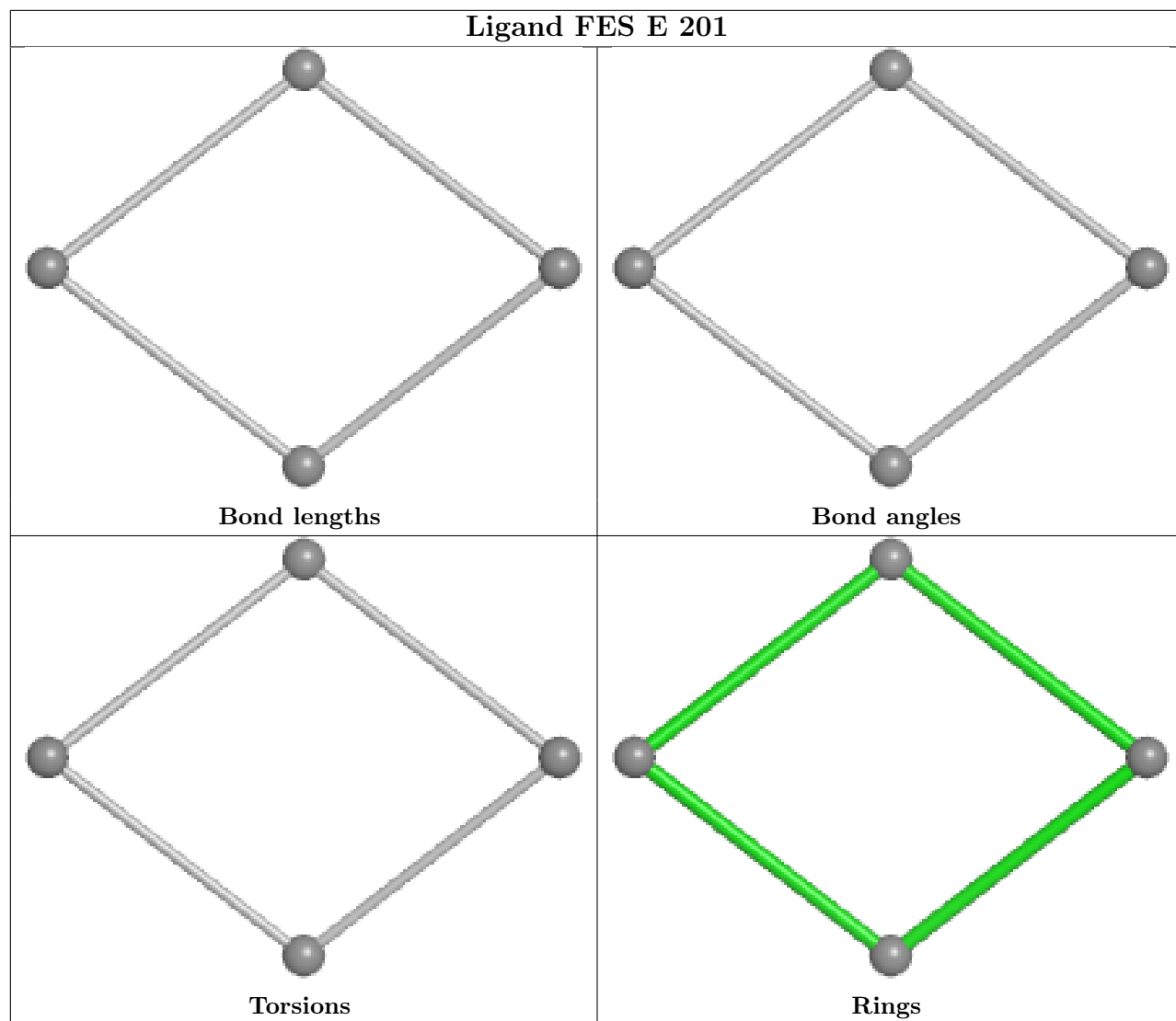
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	502	SF4	1	0
11	F	501	FMN	1	0
12	B	301	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

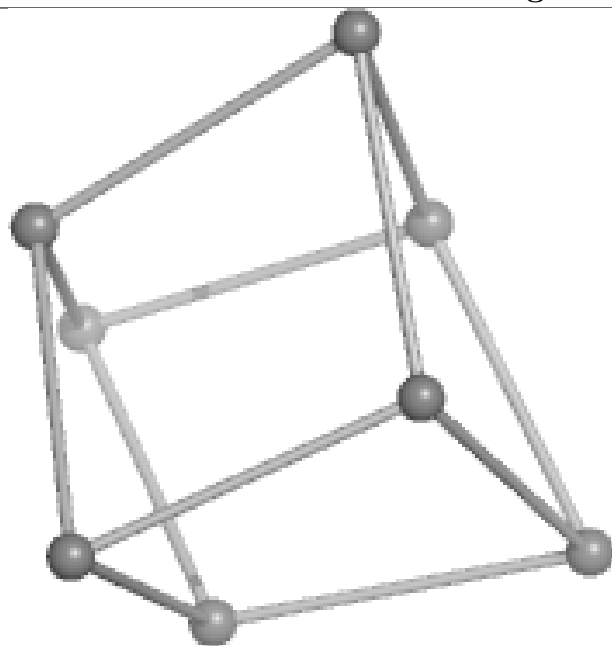
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



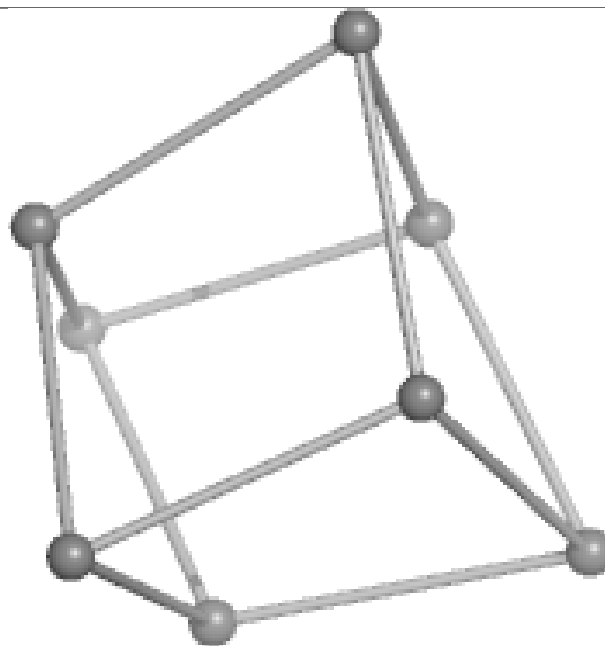




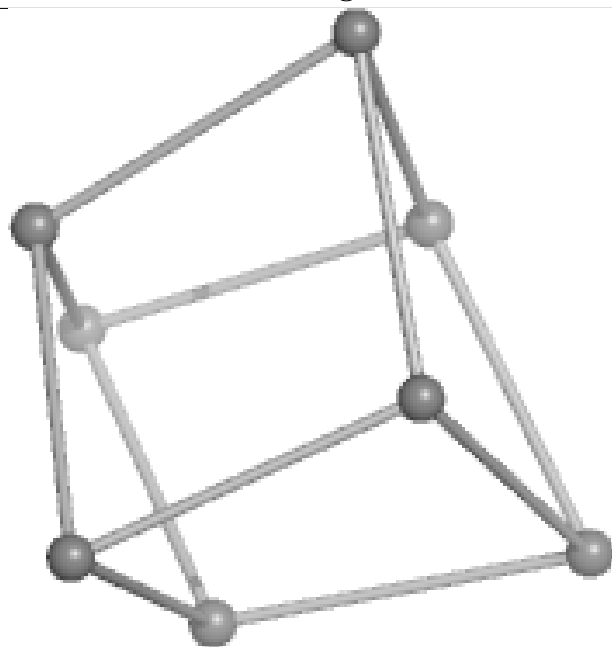
Ligand SF4 I 203



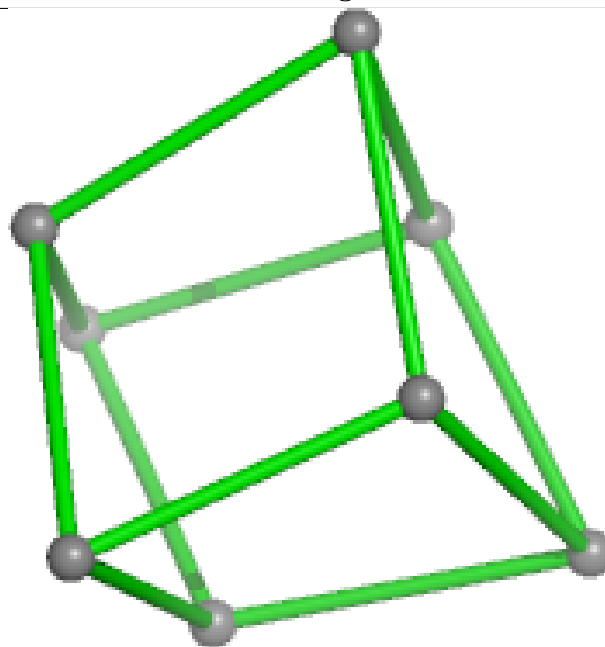
Bond lengths



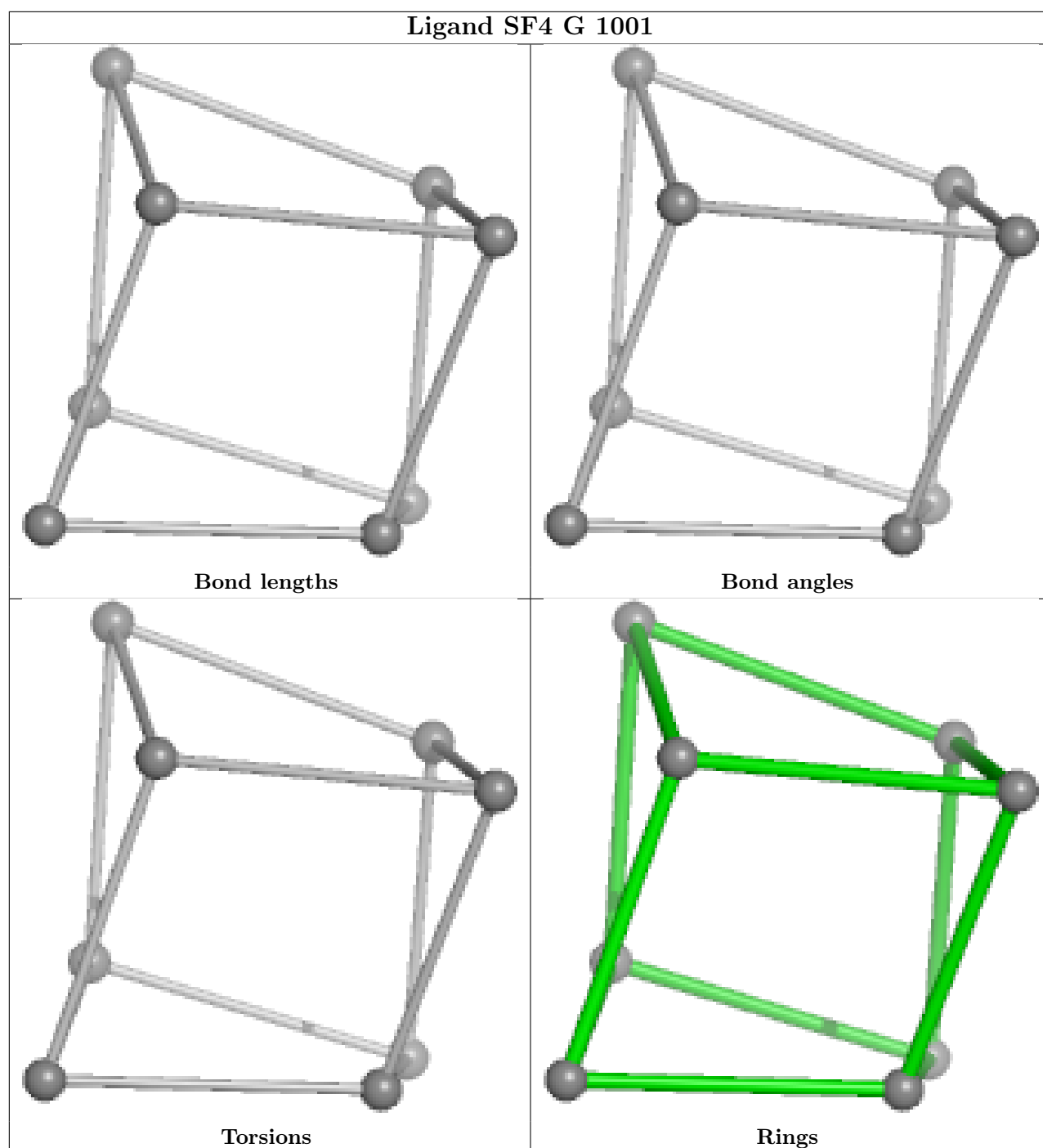
Bond angles

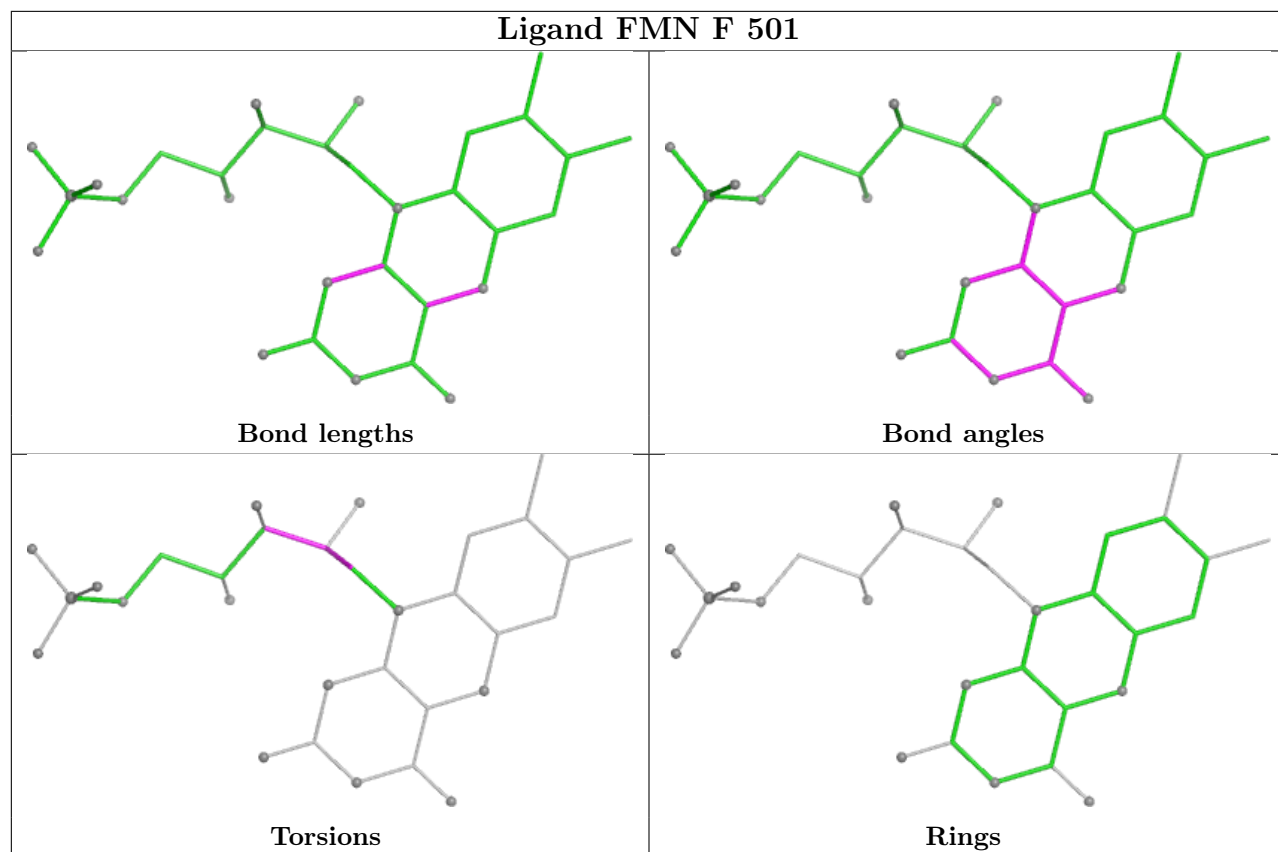


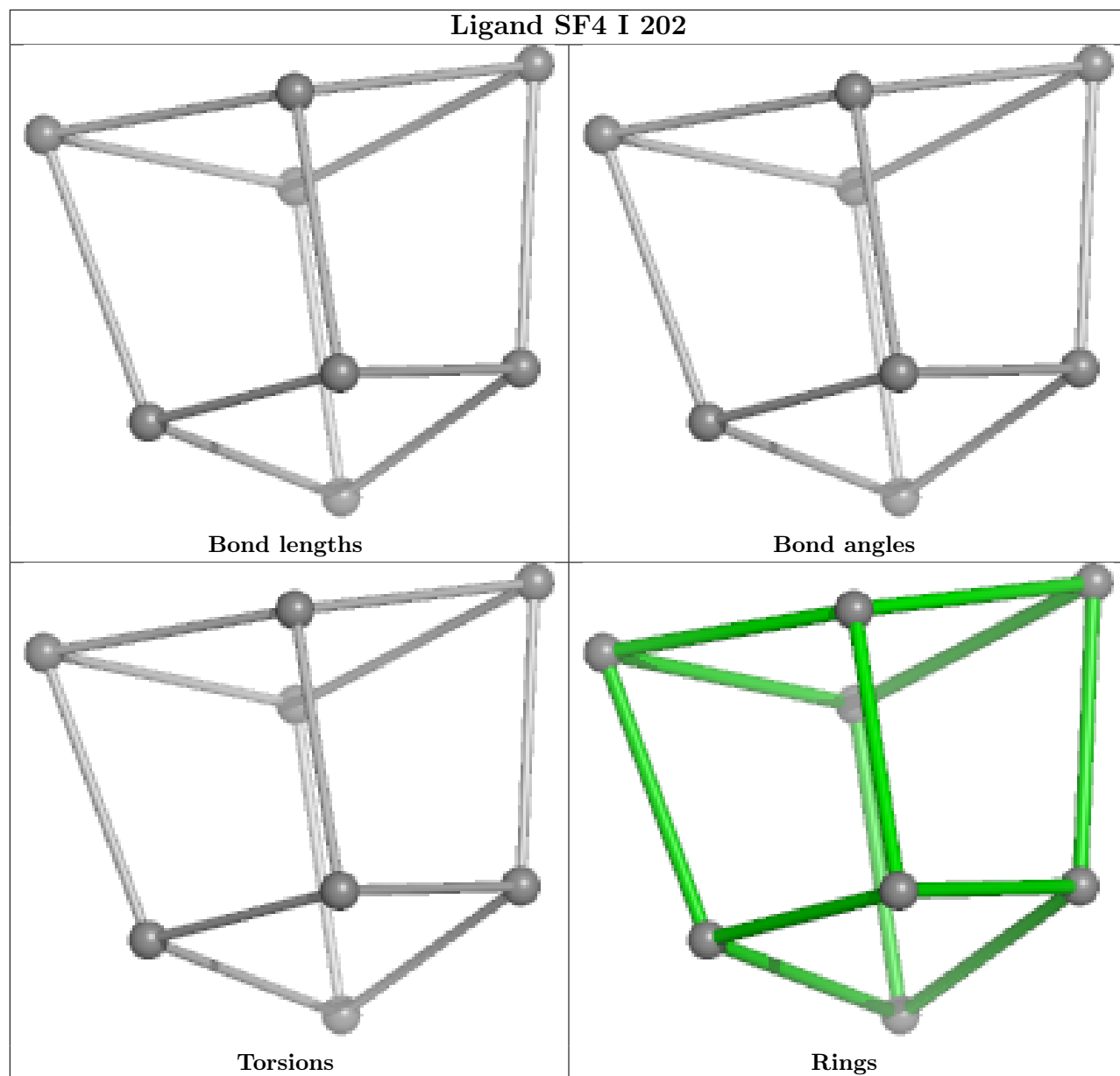
Torsions

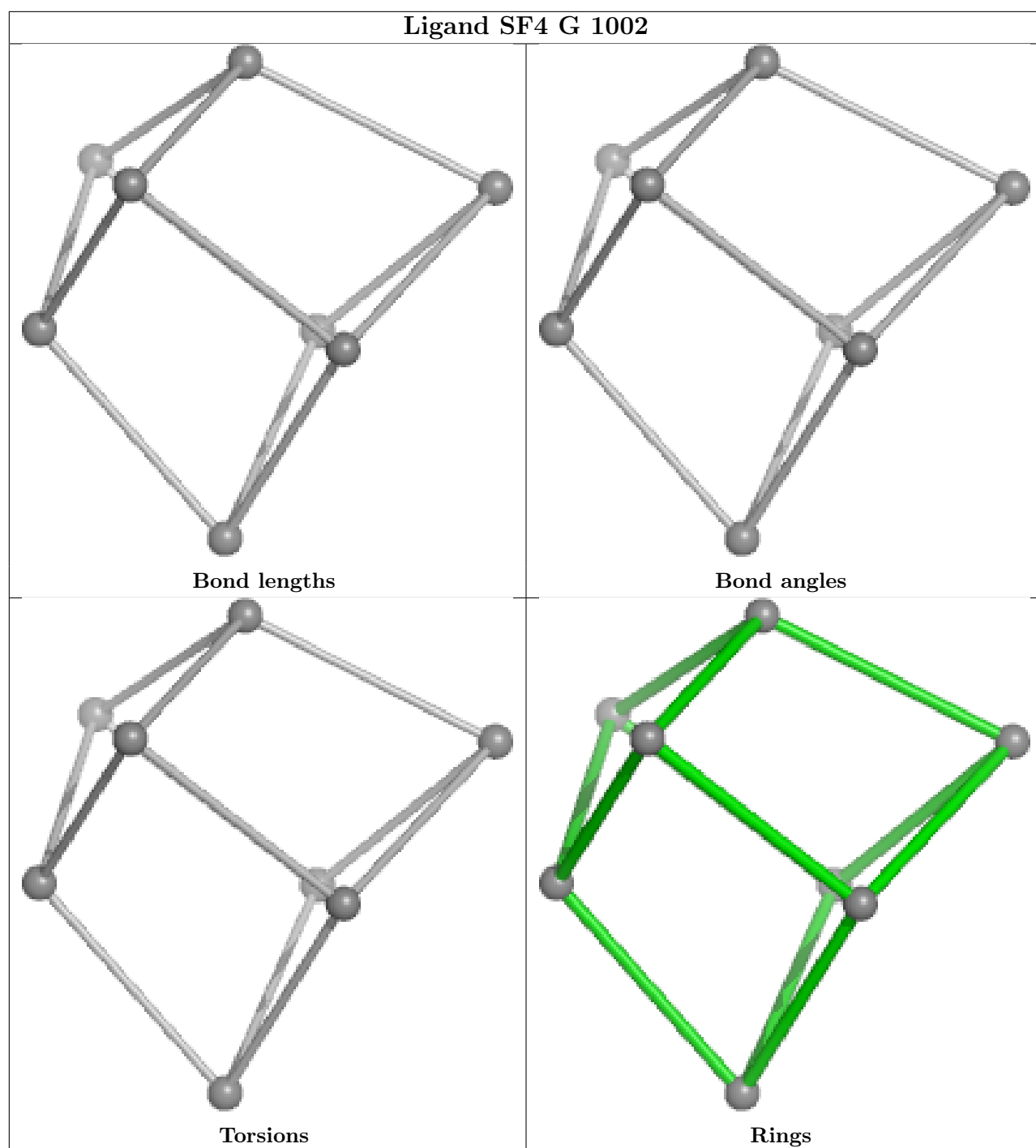


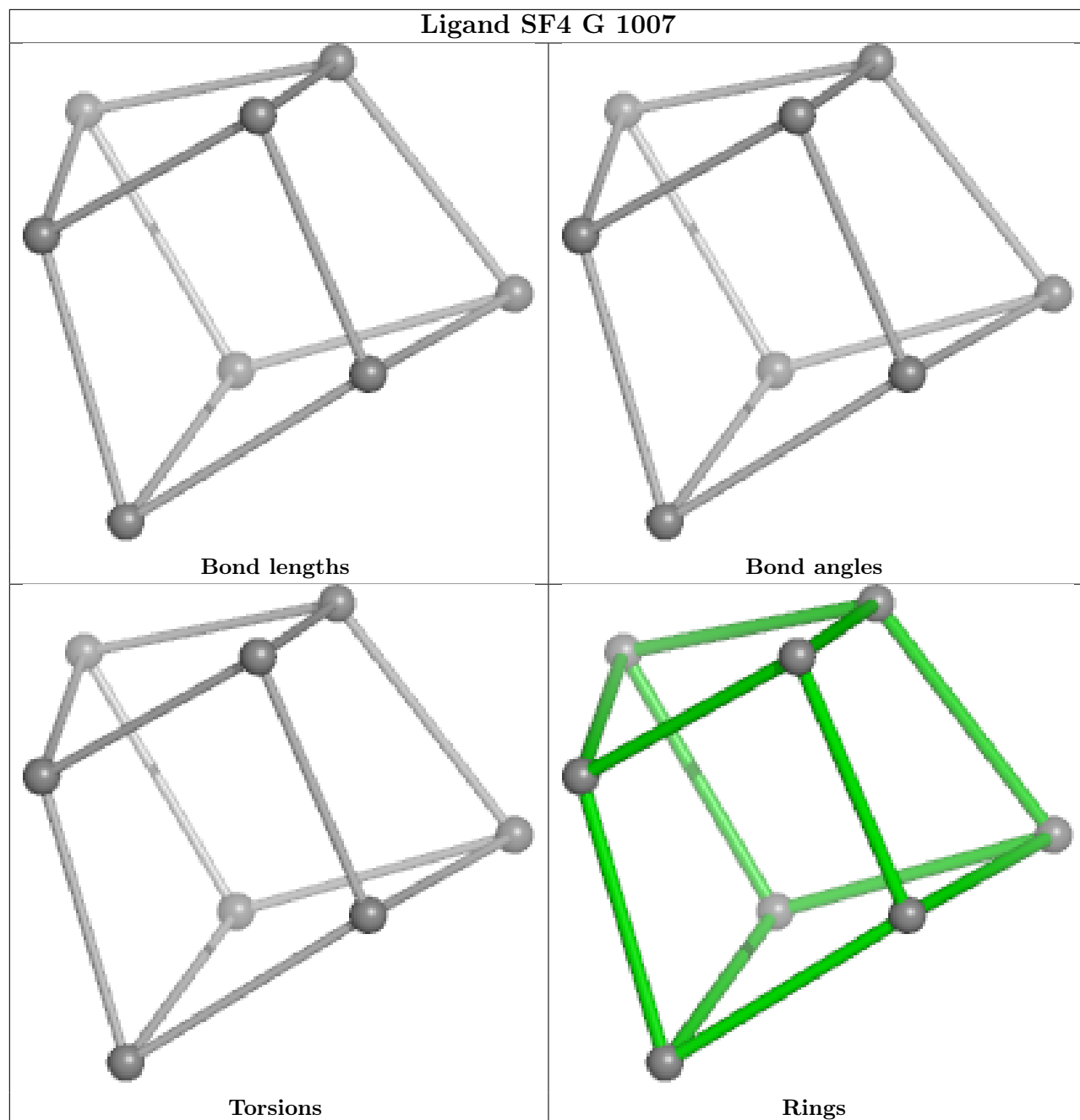
Rings

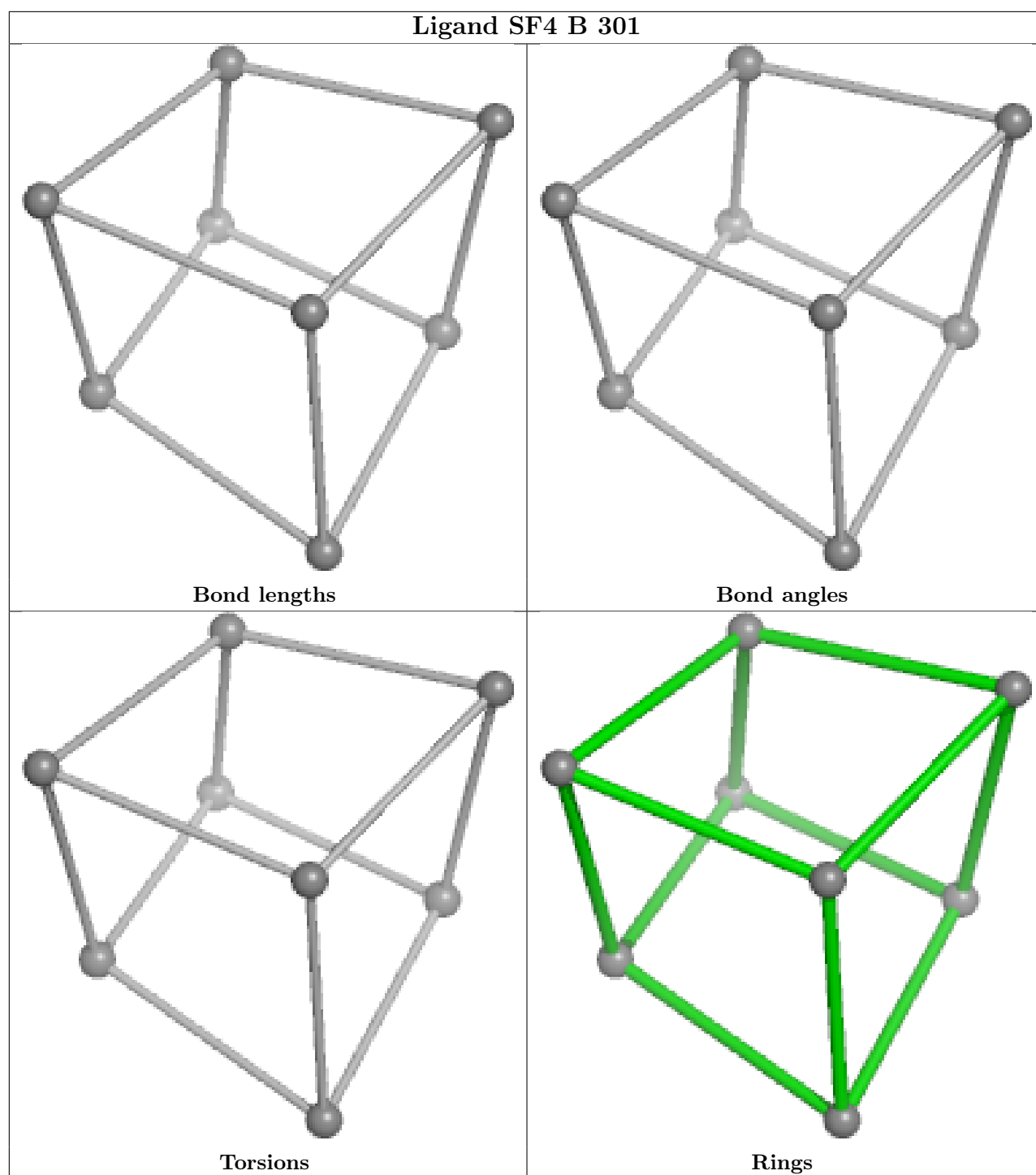












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55750. These allow visual inspection of the internal detail of the map and identification of artifacts.

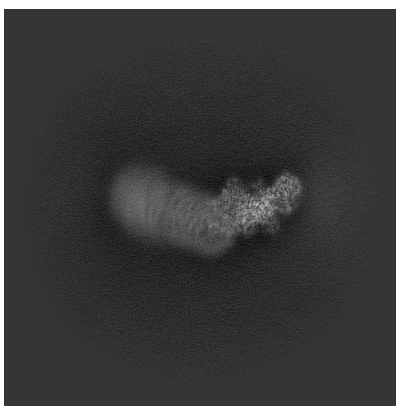
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

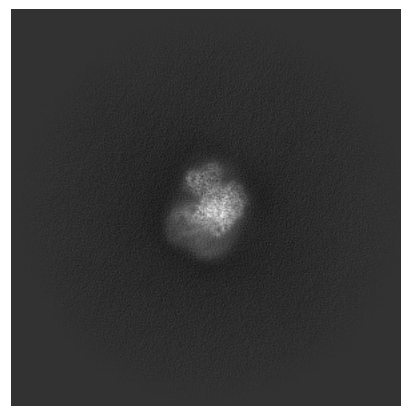
6.1.1 Primary map



X

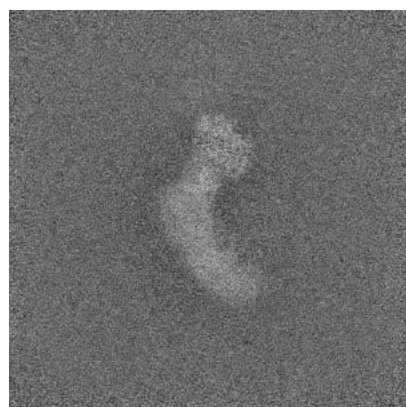


Y

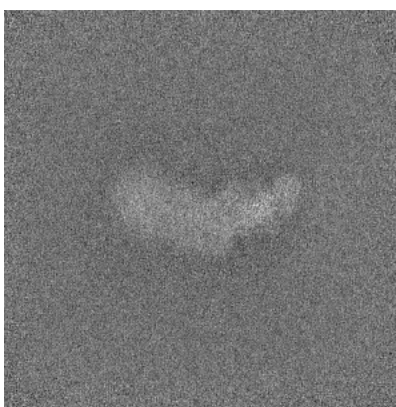


Z

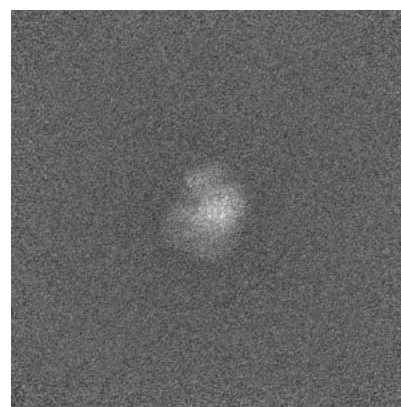
6.1.2 Raw map



X



Y

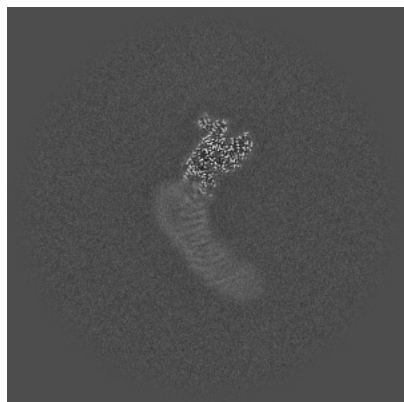


Z

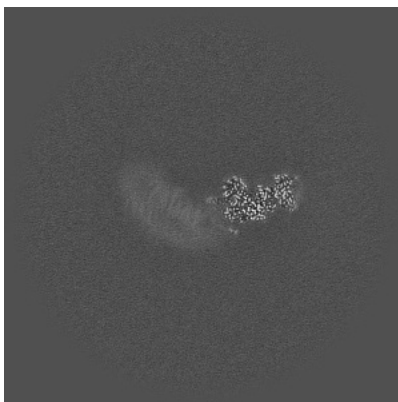
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

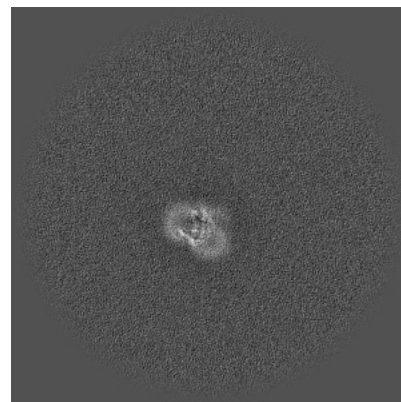
6.2.1 Primary map



X Index: 355

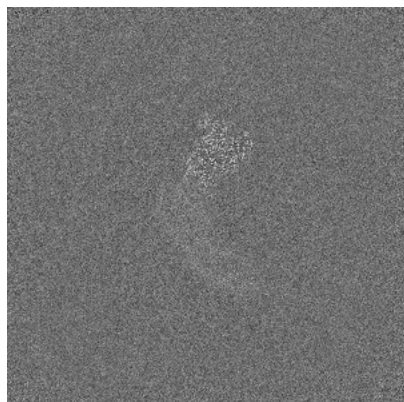


Y Index: 355

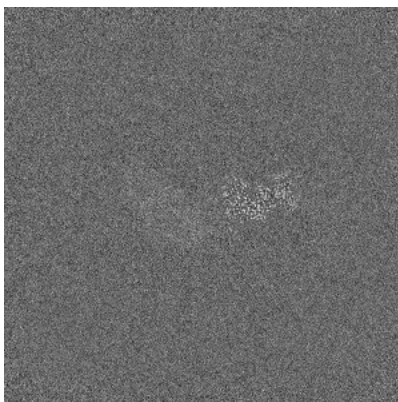


Z Index: 355

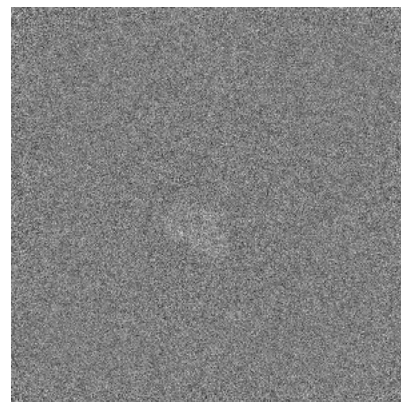
6.2.2 Raw map



X Index: 355



Y Index: 355



Z Index: 355

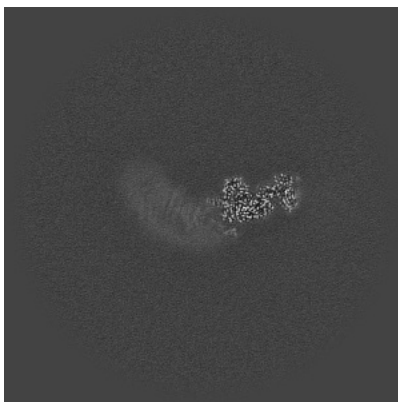
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

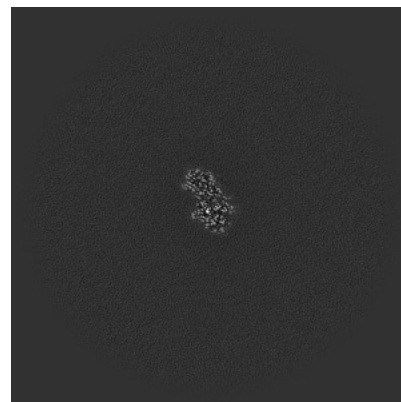
6.3.1 Primary map



X Index: 362

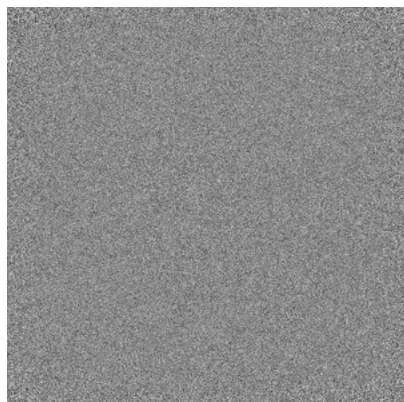


Y Index: 352

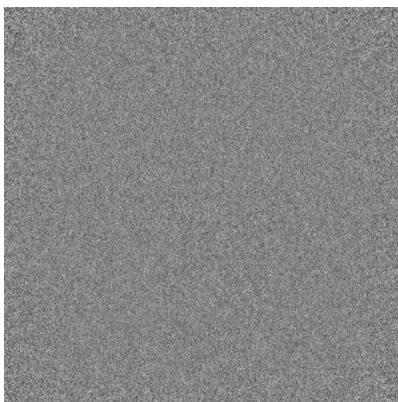


Z Index: 428

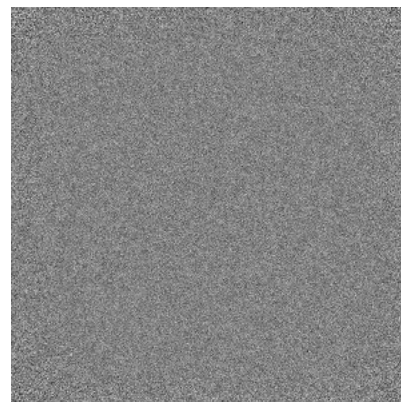
6.3.2 Raw map



X Index: 0



Y Index: 0

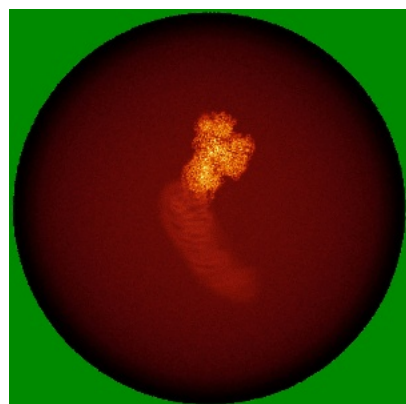


Z Index: 0

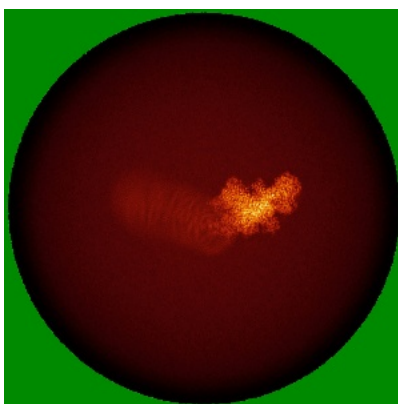
The images above show the largest variance slices of the map in three orthogonal directions.

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

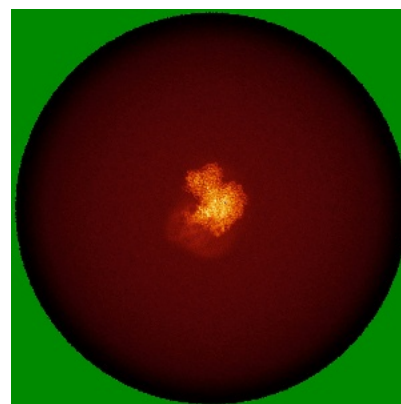
6.4.1 Primary map



X

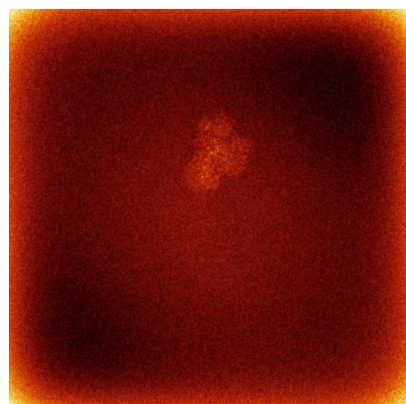


Y

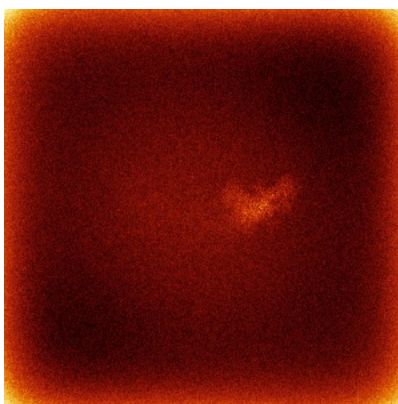


Z

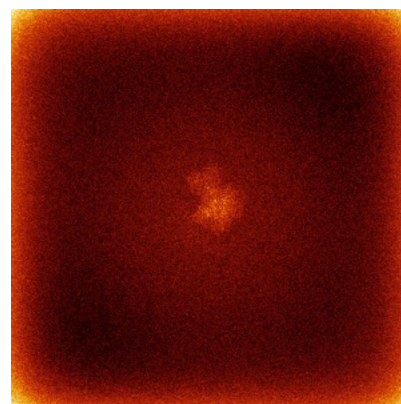
6.4.2 Raw map



X



Y

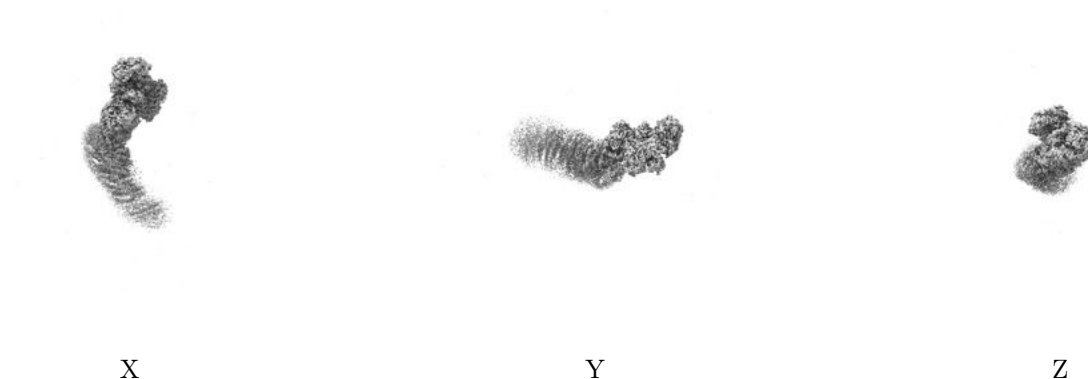


Z

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.

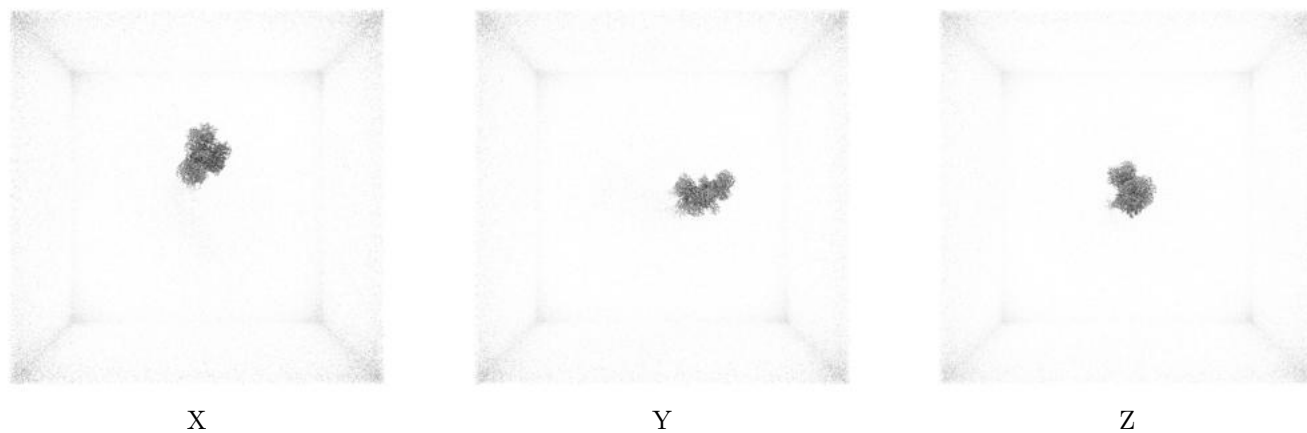
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

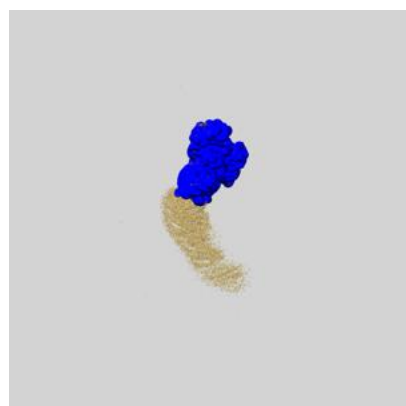
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

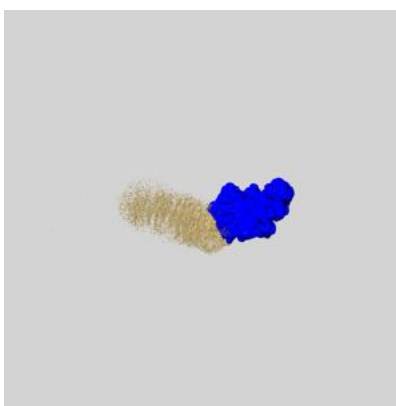
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_55750_msk_1.map [i](#)



X



Y

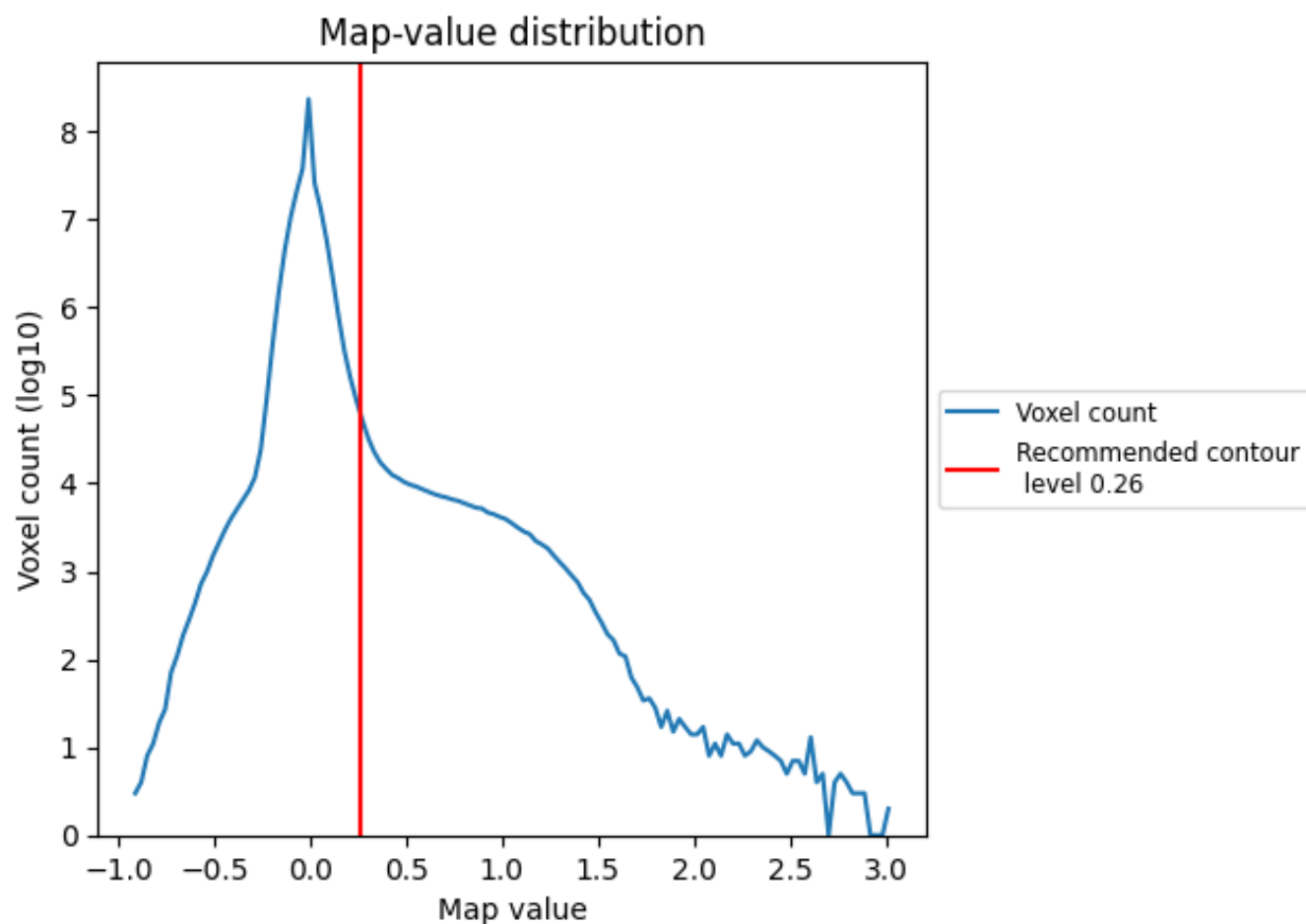


Z

7 Map analysis [i](#)

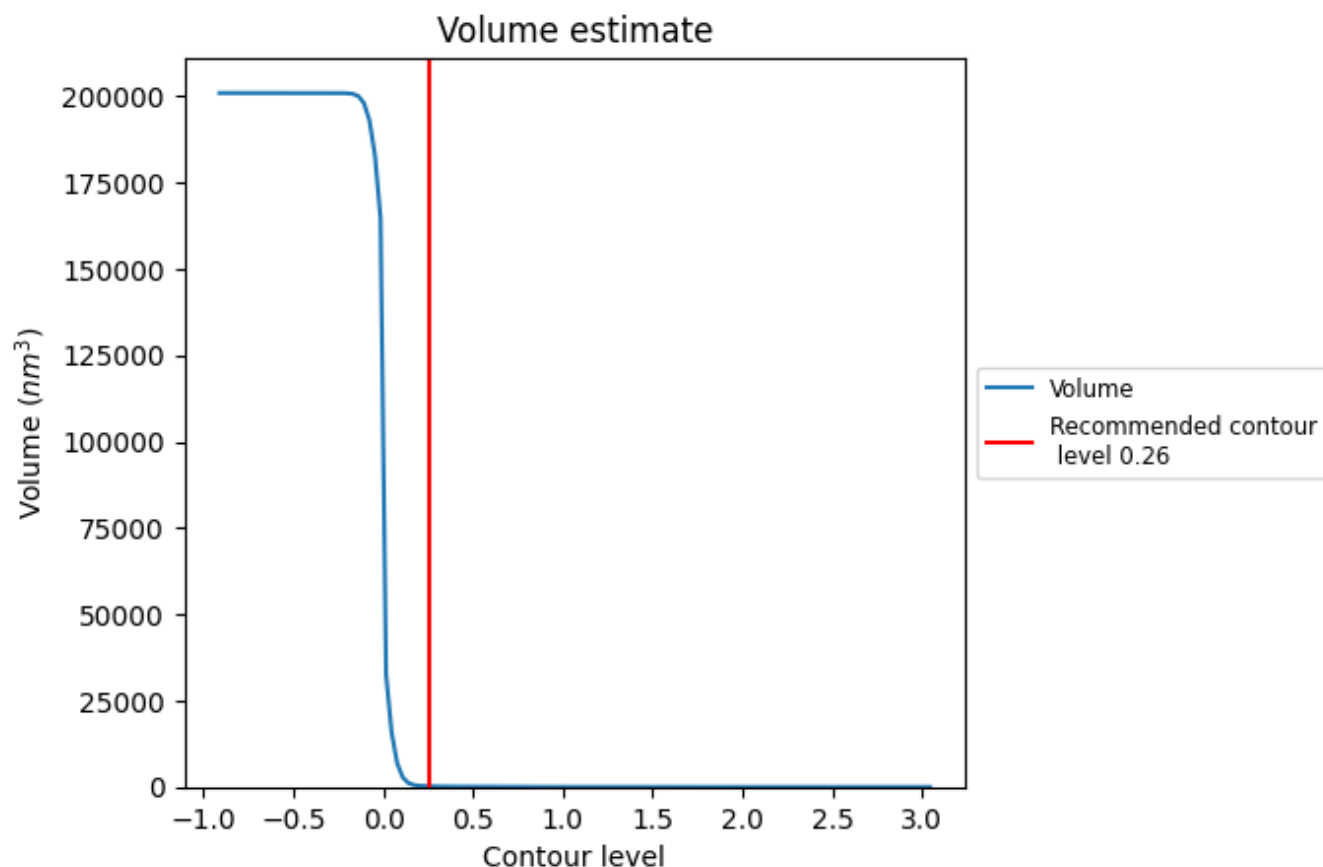
This section contains the results of statistical analysis of the map.

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.

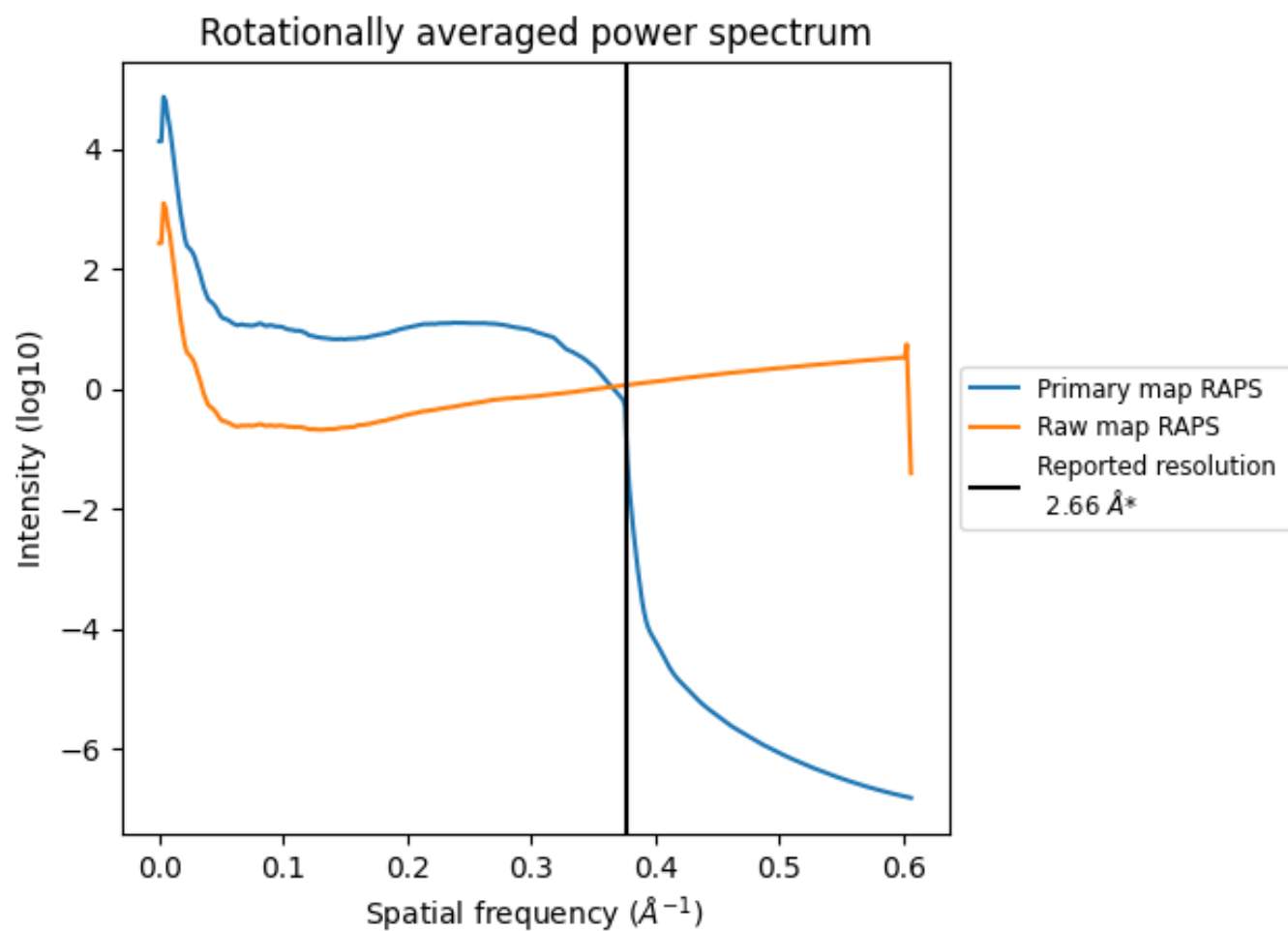
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm^3 ; this corresponds to an approximate mass of 172 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 ⓘ

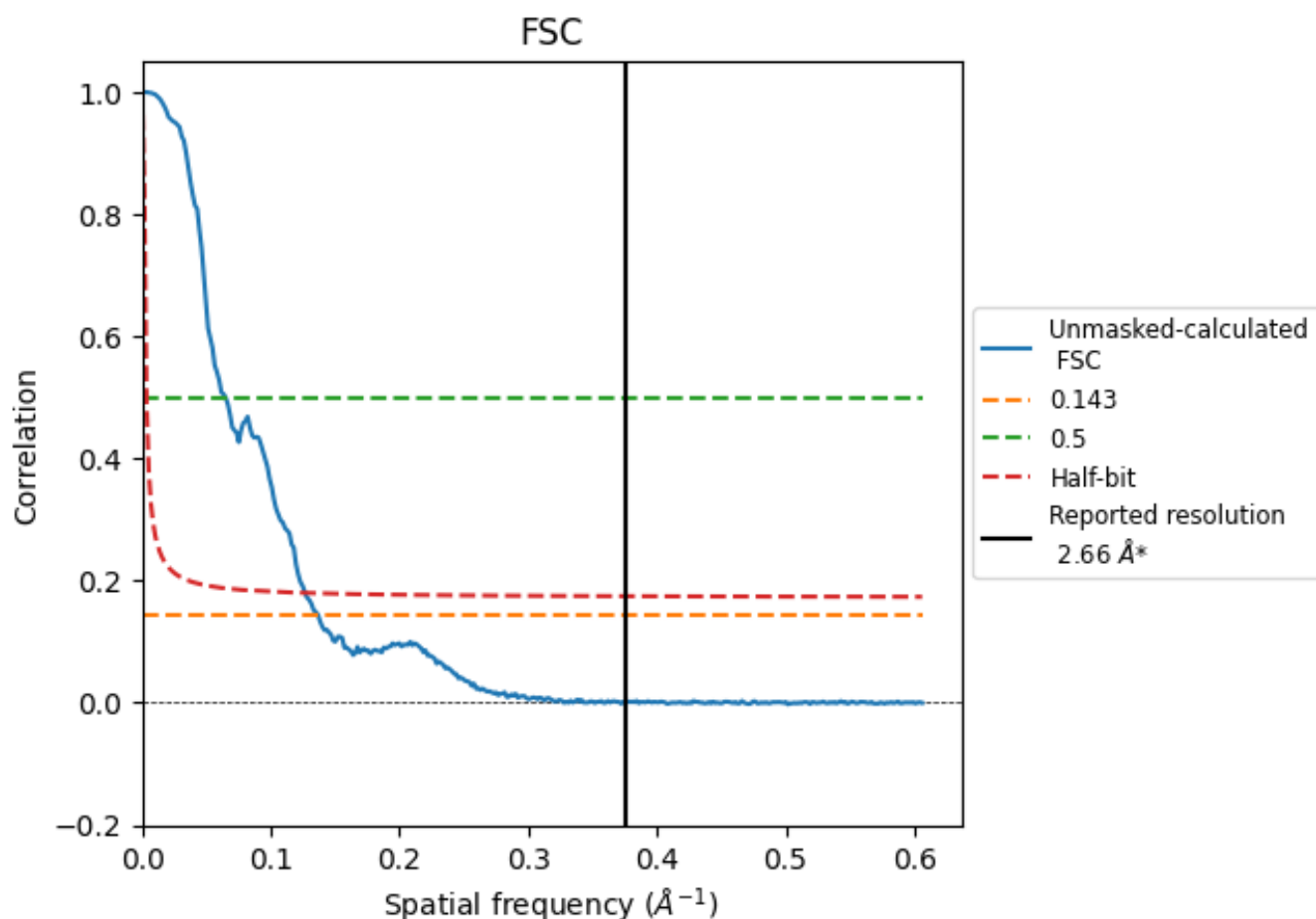


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.376 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

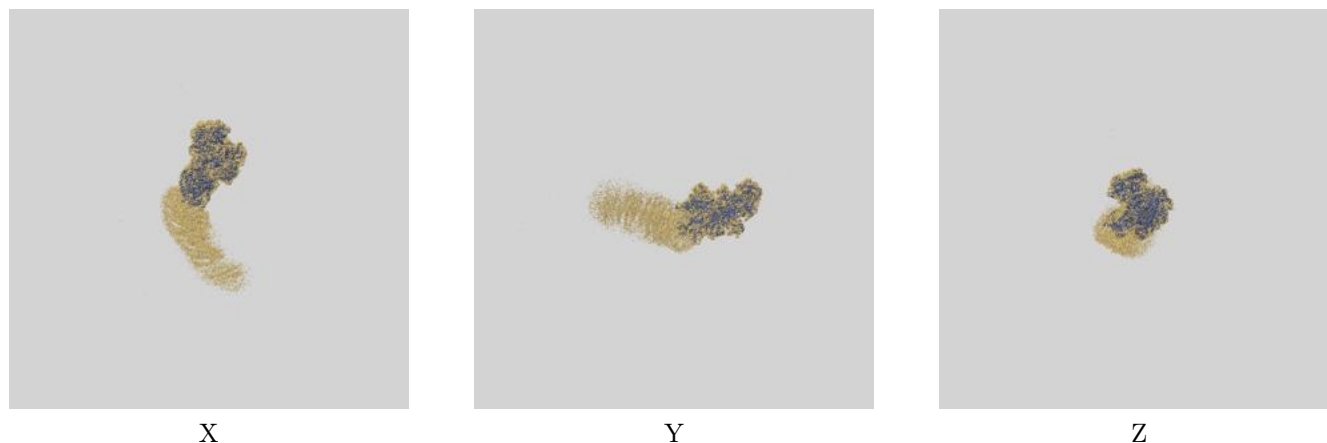
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.32	15.48	7.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.32 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55750 and PDB model 9TAL. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



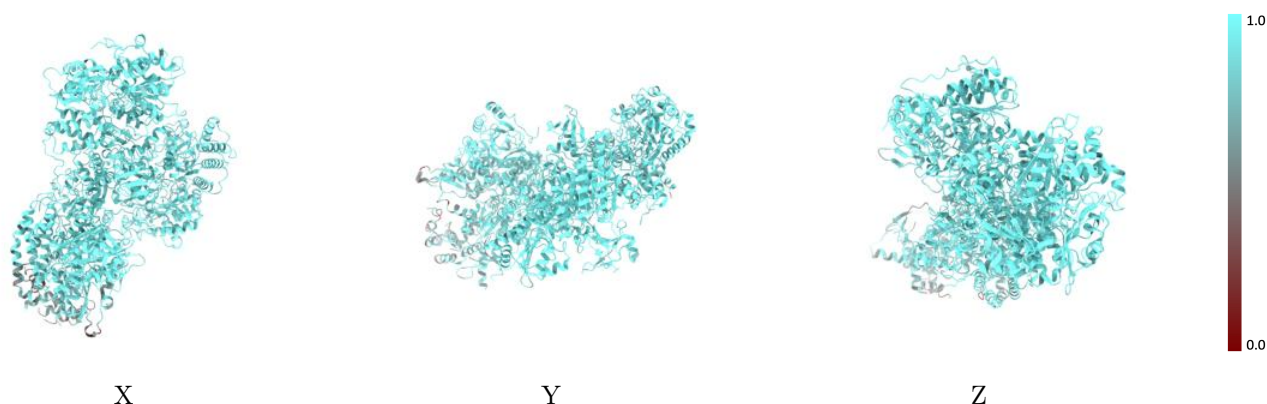
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



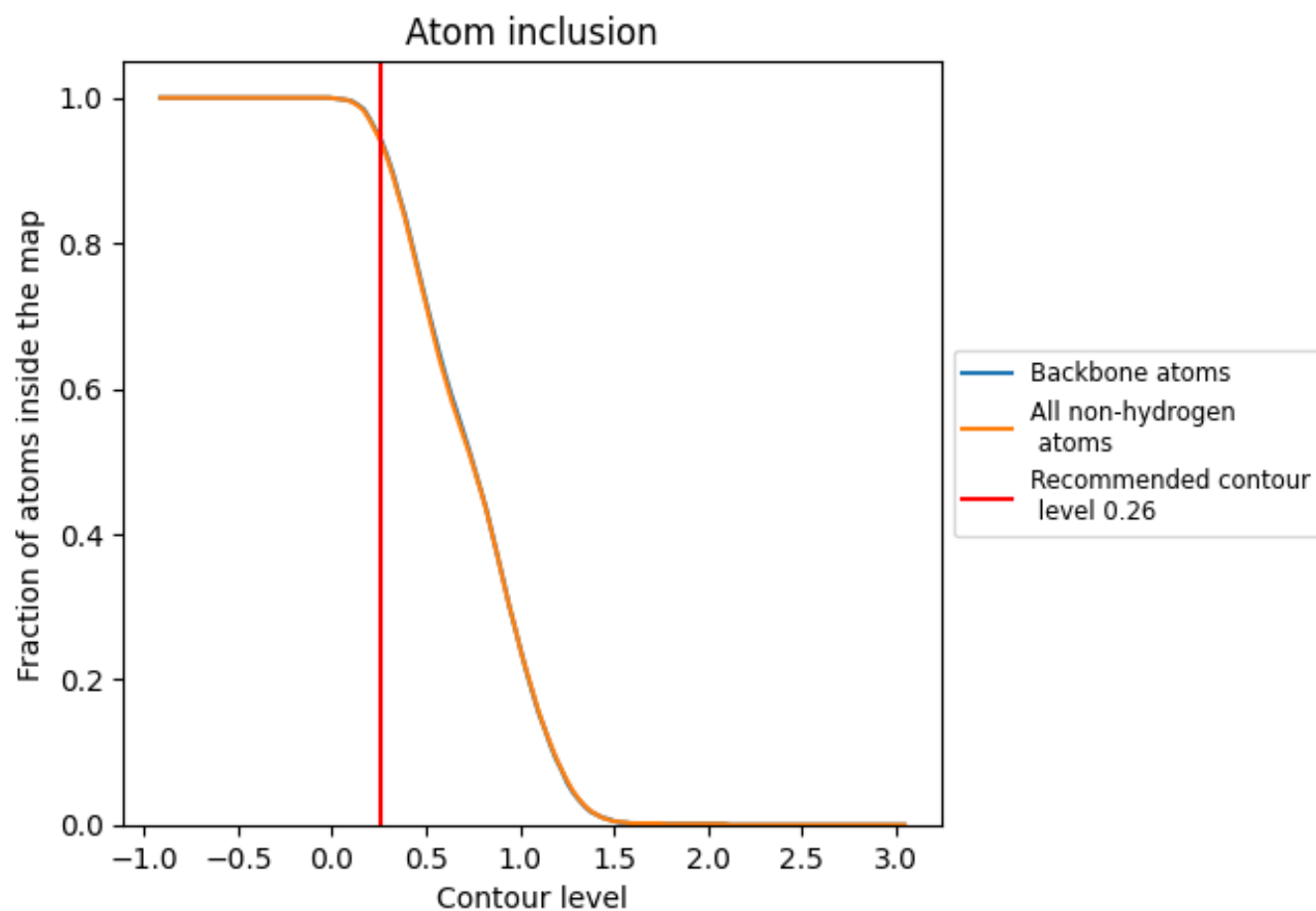
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.5880
A	 0.6770	 0.3920
B	 0.9010	 0.5590
C	 0.9290	 0.5790
E	 0.9590	 0.5960
F	 0.9680	 0.6050
G	 0.9710	 0.6110
H	 0.7770	 0.4630
I	 0.9750	 0.6180
J	 0.7430	 0.4330
K	 0.5580	 0.3570
L	 0.5090	 0.3100

