



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 8K9E / pdb_00008k9e
EMDB ID : EMD-36984
Title : Cryo-EM structure of the photosynthetic alternative complex III from *Chloroflexus aurantiacus* at 3.3 angstrom
Authors : Xu, X.
Deposited on : 2023-08-01
Resolution : 3.33 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:

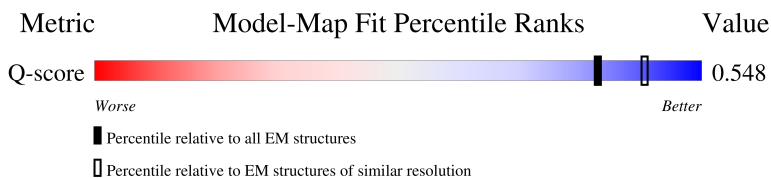
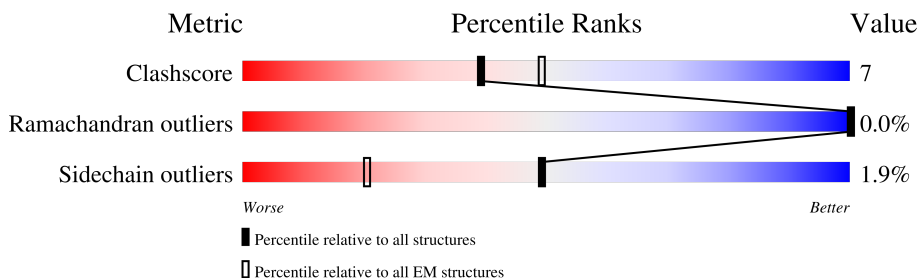
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.33 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	14484 (2.83 - 3.83)

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	219	 80% 16% 5%
2	B	1029	 80% 12% 8% 5%
3	C	486	 76% 16% 8% 5%
4	D	179	 79% 18% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	205	
6	F	411	
7	G	112	
8	I	37	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 19954 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 Cytochrome c7-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1763	1129	306	313	15		

- Molecule 2 is a protein called Fe-S-cluster-containing hydrogenase components 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	951	Total	C	N	O	S	0	0
			7350	4622	1303	1395	30		

- Molecule 3 is a protein called Polysulphide reductase NrfD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3655	2476	576	586	17		

- Molecule 4 is a protein called Quinol:cytochrome c oxidoreductase membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1350	884	215	245	6		

- Molecule 5 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	164	Total	C	N	O	S	0	0
			1292	819	220	246	7		

- Molecule 6 is a protein called Quinol:cytochrome c oxidoreductase quinone-binding subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	397	Total	C	N	O	S	0	0
			3128	2091	506	514	17		

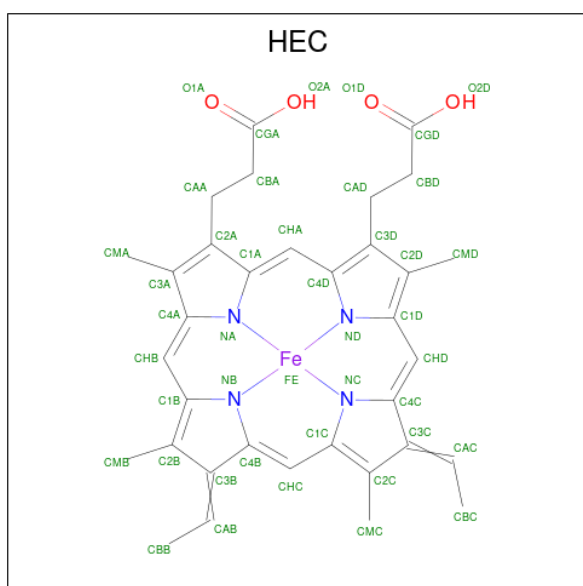
- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	N	O	S	0	0
			623	404	108	107	4		

- Molecule 8 is a protein called unknown.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			305	212	42	48	3		

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



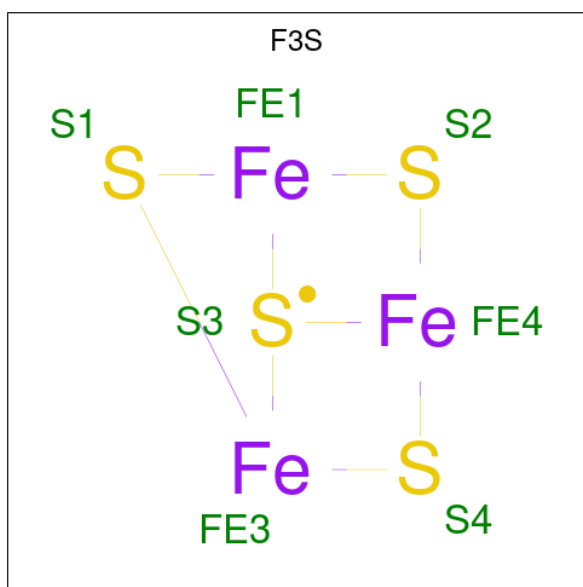
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



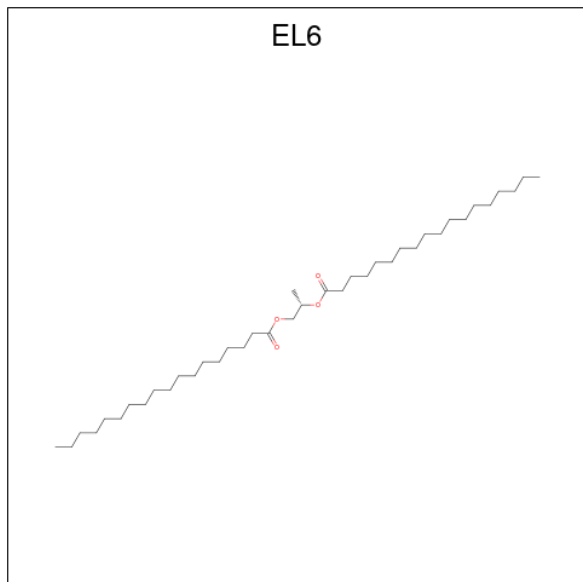
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



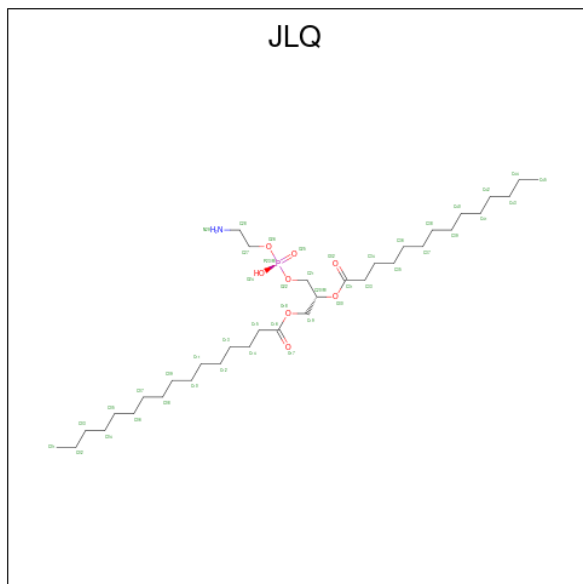
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is [(2S)-2-octadecanoyloxypropyl] octadecanoate (CCD ID: EL6) (formula: $C_{39}H_{76}O_4$).



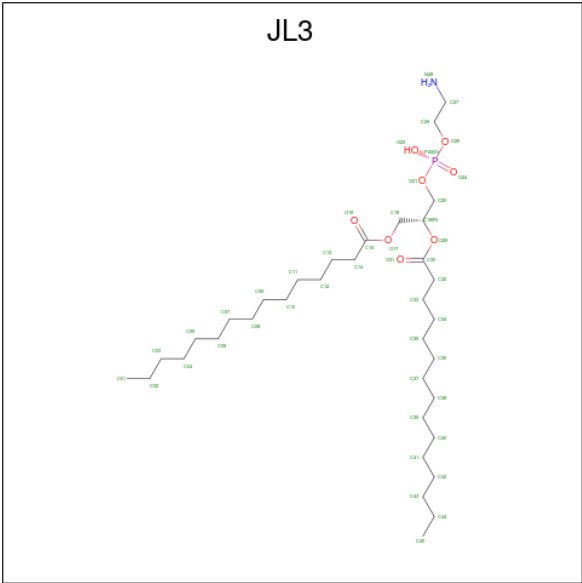
Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			27	23	4	
12	E	1	Total	C	O	0
			28	24	4	

- Molecule 13 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (CCD ID: JLQ) (formula: $C_{35}H_{70}NO_8P$).



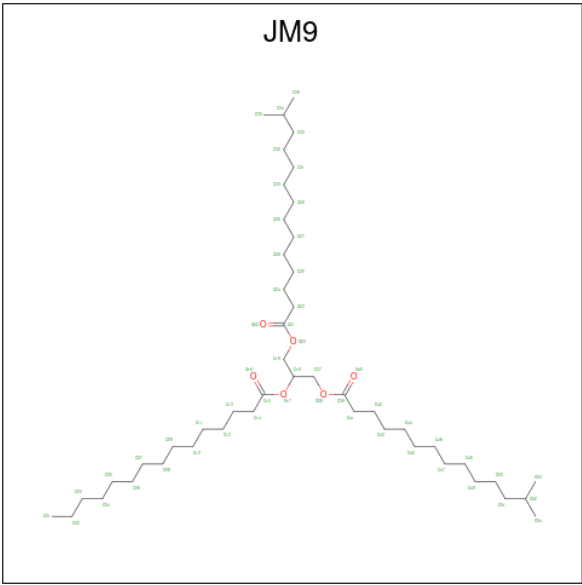
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 14 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-pentadecanoyloxy-propyl] pentadecanoate (CCD ID: JL3) (formula: C₃₅H₇₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 15 is 1,3-bis(13-methyltetradecanoyloxy)propan-2-yl pentadecanoate (CCD ID: JM9) (formula: C₄₈H₉₂O₆).

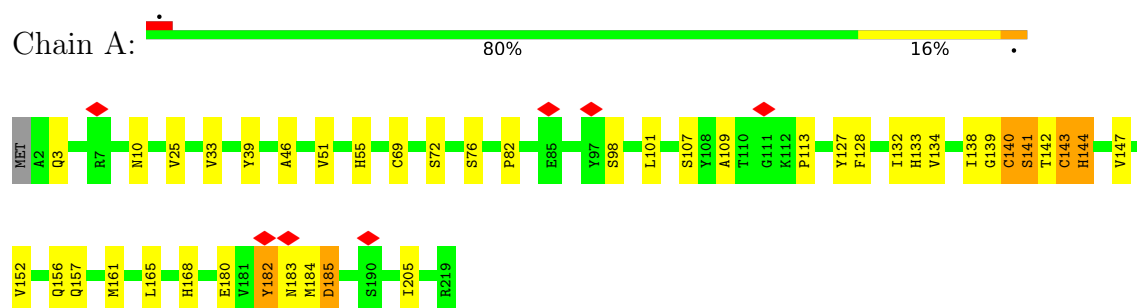


Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	C	O	0
			54	48	6	

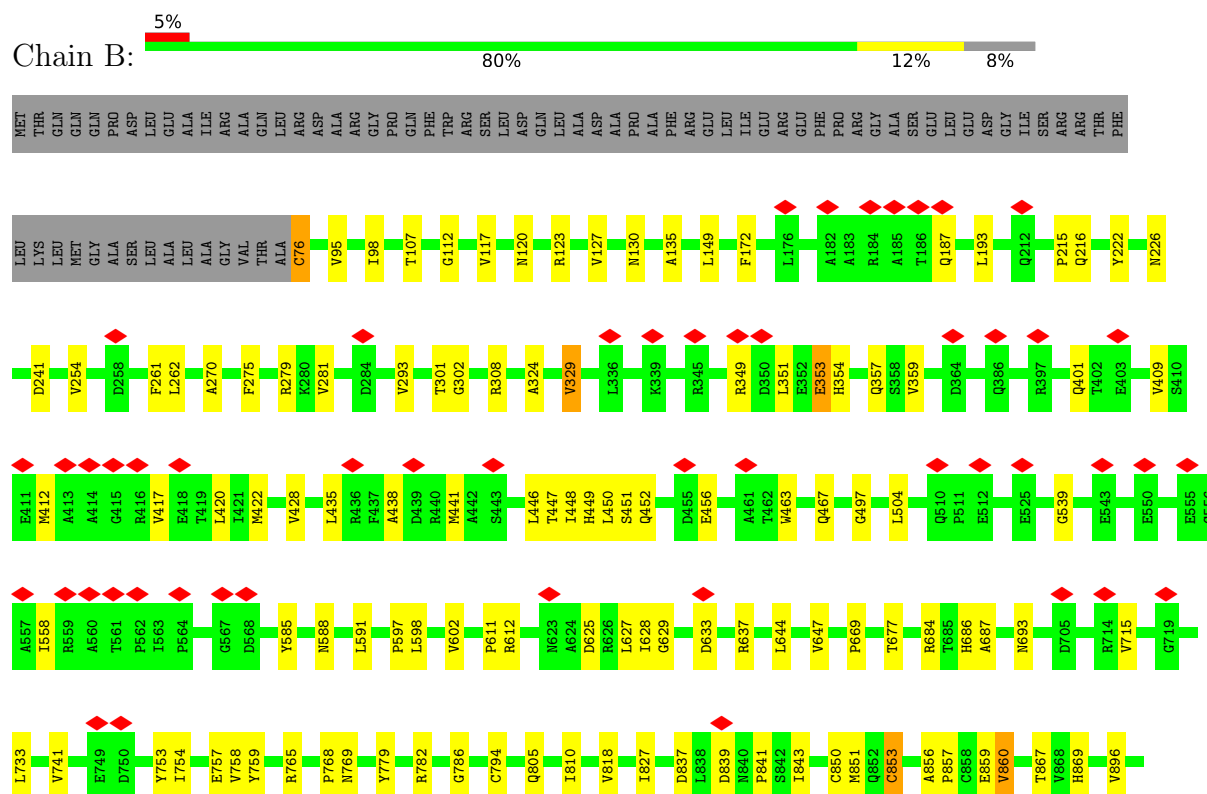
3 Residue-property plots

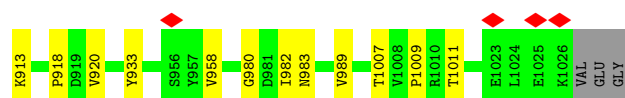
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytochrome c7-like domain-containing protein

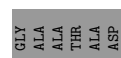
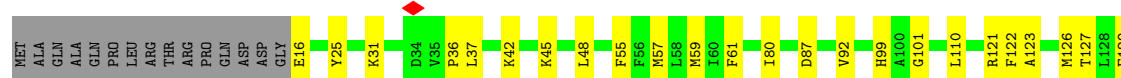
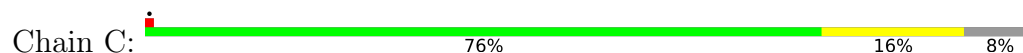


- Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein

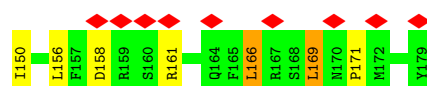
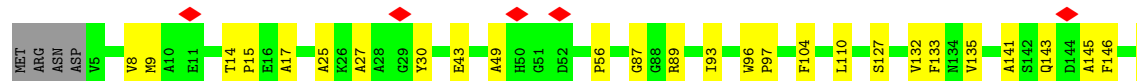
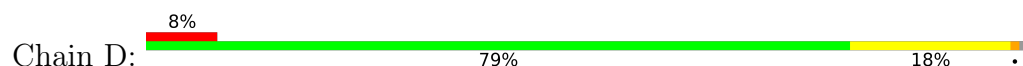




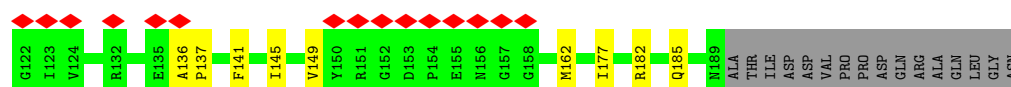
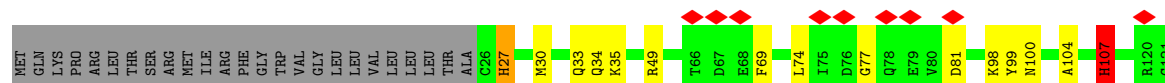
• Molecule 3: Polysulphide reductase NrfD



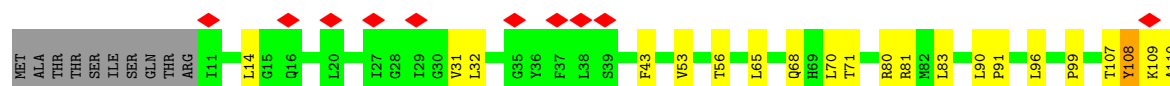
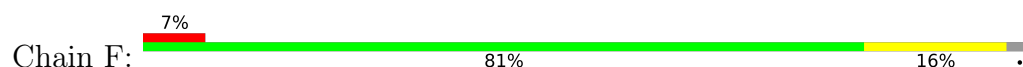
• Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

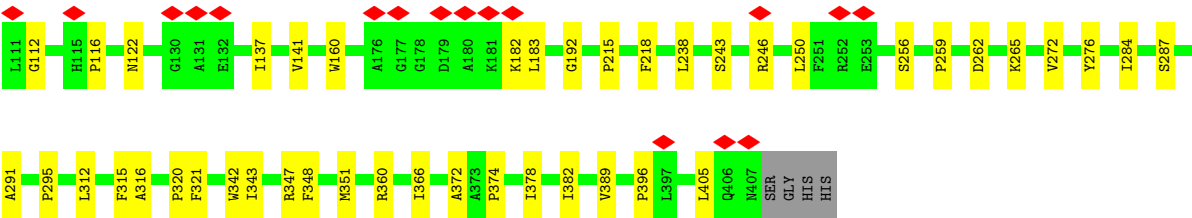


• Molecule 5: Cytochrome c domain-containing protein

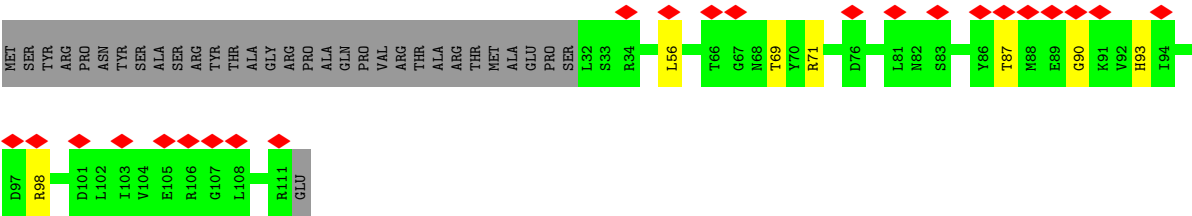


• Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

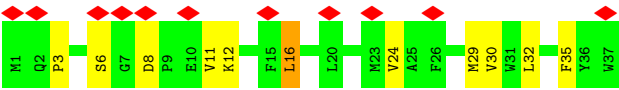




• Molecule 7: Uncharacterized protein



• Molecule 8: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425867	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.411	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	209.99998, 209.99998, 209.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JL3, HEC, SF4, EL6, F3S, JM9, JLQ

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	0.58	1/1812 (0.1%)	0.81	4/2472 (0.2%)
2	B	0.90	0/7518	1.15	7/10249 (0.1%)
3	C	0.69	0/3787	0.92	2/5179 (0.0%)
4	D	0.48	0/1388	0.74	0/1895
5	E	0.54	1/1327 (0.1%)	0.72	3/1803 (0.2%)
6	F	0.89	0/3226	1.15	2/4408 (0.0%)
7	G	0.48	0/635	0.72	1/865 (0.1%)
8	I	1.04	1/318 (0.3%)	1.13	3/436 (0.7%)
All	All	0.78	3/20011 (0.0%)	1.02	22/27307 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	107	HIS	CE1-NE2	7.36	1.40	1.32
8	I	30	VAL	C-O	-5.53	1.17	1.24
1	A	144	HIS	CE1-NE2	5.43	1.38	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	693	ASN	CA-CB-CG	10.61	123.21	112.60
3	C	223	HIS	N-CA-C	-10.05	99.81	113.18
2	B	647	VAL	N-CA-C	-8.82	104.10	112.83
5	E	27	HIS	N-CA-C	7.95	120.03	111.36
1	A	185	ASP	N-CA-C	-7.91	103.20	113.17
5	E	107	HIS	CE1-NE2-CD2	-7.27	101.73	109.00
2	B	839	ASP	N-CA-C	-7.25	104.59	113.50
2	B	353	GLU	N-CA-C	-7.10	104.88	113.97
1	A	142	THR	N-CA-C	-7.07	104.53	113.02
8	I	35	PHE	N-CA-C	6.41	122.17	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	209	LEU	N-CA-C	-6.37	104.20	112.68
1	A	141	SER	N-CA-C	-6.02	105.17	113.18
7	G	98	ARG	N-CA-C	-5.91	105.73	113.12
8	I	12	LYS	CA-C-N	-5.63	112.80	119.05
8	I	12	LYS	C-N-CA	-5.63	112.80	119.05
2	B	625	ASP	N-CA-C	-5.54	106.56	113.38
5	E	107	HIS	CG-CD2-NE2	5.45	112.65	107.20
6	F	141	VAL	N-CA-CB	5.40	113.90	110.50
2	B	497	GLY	CA-C-O	-5.13	118.13	122.29
6	F	108	TYR	CA-C-O	-5.08	115.98	121.87
1	A	144	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
2	B	261	PHE	N-CA-C	-5.02	107.32	113.50

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	1763	0	1713	52	0
2	B	7350	0	7179	73	0
3	C	3655	0	3688	56	0
4	D	1350	0	1341	27	0
5	E	1292	0	1216	20	0
6	F	3128	0	3175	57	0
7	G	623	0	660	3	0
8	I	305	0	302	8	0
9	A	215	0	153	25	0
9	E	43	0	30	4	0
10	B	24	0	0	1	0
11	B	7	0	0	0	0
12	B	27	0	0	1	0
12	E	28	0	0	0	0
13	C	45	0	0	10	0
14	F	45	0	0	2	0
15	F	54	0	0	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19954	0	19457	281	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 7.

All (281) 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)
1:A:140:CYS:SG	9:A:303:HEC:CAB	2.02	1.45
2:B:76:CYS:SG	12:B:1105:EL6:C1	2.16	1.32
1:A:140:CYS:SG	9:A:303:HEC:CBB	1.14	1.23
6:F:272:VAL:HG23	15:F:502:JM9:C31	1.70	1.19
6:F:272:VAL:CG2	15:F:502:JM9:C31	2.23	1.16
1:A:140:CYS:SG	9:A:303:HEC:C3B	2.33	1.14
1:A:140:CYS:SG	9:A:303:HEC:HBB2	0.96	1.14
13:C:501:JLQ:O32	6:F:71:THR:HG21	1.58	1.02
13:C:501:JLQ:O32	6:F:71:THR:CG2	2.11	0.96
1:A:140:CYS:SG	9:A:303:HEC:HBB3	1.15	0.94
1:A:168:HIS:CE1	9:A:301:HEC:HBC1	2.02	0.94
1:A:140:CYS:SG	9:A:303:HEC:HBB1	2.05	0.93
6:F:265:LYS:HE3	14:F:501:JL3:C13	2.01	0.90
6:F:272:VAL:HG21	15:F:502:JM9:C31	2.04	0.87
8:I:16:LEU:C	8:I:16:LEU:HD13	2.00	0.86
3:C:313:THR:HG21	13:C:501:JLQ:C11	2.07	0.85
3:C:233:LEU:HD23	15:F:502:JM9:O16	1.77	0.84
3:C:313:THR:HG21	13:C:501:JLQ:C13	2.07	0.84
1:A:133:HIS:HD1	9:A:303:HEC:HAC	1.44	0.83
9:A:301:HEC:HMC1	9:A:301:HEC:CBC	2.09	0.82
9:A:301:HEC:HMC1	9:A:301:HEC:HBC2	1.64	0.79
5:E:162:MET:HE1	9:E:301:HEC:C4B	2.12	0.79
1:A:168:HIS:ND1	9:A:301:HEC:HBC1	1.98	0.78
4:D:104:PHE:CD1	15:F:502:JM9:C54	2.67	0.78
8:I:16:LEU:HD13	8:I:16:LEU:O	1.82	0.77
6:F:262:ASP:HB3	14:F:501:JL3:O16	1.85	0.77
6:F:56:THR:HG21	6:F:351:MET:HE1	1.67	0.75
4:D:104:PHE:HD1	15:F:502:JM9:C54	2.02	0.72
2:B:602:VAL:HG21	2:B:818:VAL:HG11	1.72	0.71
6:F:272:VAL:HG21	15:F:502:JM9:C30	2.21	0.70
6:F:321:PHE:CE1	15:F:502:JM9:C06	2.74	0.70
6:F:321:PHE:HE1	15:F:502:JM9:C07	2.05	0.70
13:C:501:JLQ:C31	6:F:71:THR:HG22	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:272:VAL:CG2	15:F:502:JM9:C30	2.71	0.68
2:B:786:GLY:HA3	2:B:982:ILE:HD11	1.75	0.67
2:B:324:ALA:HB1	2:B:329:VAL:HG22	1.75	0.67
1:A:140:CYS:HB3	1:A:144:HIS:HD2	1.59	0.67
8:I:16:LEU:C	8:I:16:LEU:CD1	2.67	0.67
5:E:162:MET:HE1	9:E:301:HEC:NB	2.10	0.66
1:A:133:HIS:ND1	9:A:303:HEC:HAC	2.11	0.65
6:F:321:PHE:HE1	15:F:502:JM9:C06	2.08	0.65
13:C:501:JLQ:O30	6:F:71:THR:HG22	1.97	0.64
1:A:132:ILE:HD13	9:A:302:HEC:HAA2	1.79	0.64
2:B:628:ILE:HA	2:B:837:ASP:HA	1.80	0.64
2:B:733:LEU:HD12	2:B:733:LEU:O	1.97	0.63
13:C:501:JLQ:O32	6:F:71:THR:HG22	1.93	0.63
3:C:99:HIS:CD2	3:C:275:VAL:HG22	2.34	0.63
1:A:69:CYS:HB3	1:A:82:PRO:HG3	1.80	0.62
3:C:233:LEU:CD2	15:F:502:JM9:O16	2.47	0.62
1:A:51:VAL:HG12	1:A:51:VAL:O	1.99	0.62
8:I:8:ASP:HB3	8:I:11:VAL:HG23	1.81	0.62
3:C:390:MET:HE3	3:C:394:ARG:HH12	1.63	0.62
13:C:501:JLQ:C31	6:F:71:THR:CG2	2.79	0.61
2:B:120:ASN:HD22	2:B:123:ARG:NH2	1.99	0.61
1:A:168:HIS:HD1	9:A:301:HEC:CBC	2.15	0.60
1:A:140:CYS:H	9:A:303:HEC:HBB3	1.68	0.59
3:C:222:ARG:HG3	4:D:49:ALA:HB2	1.85	0.58
1:A:39:TYR:HH	2:B:76:CYS:N	2.01	0.58
6:F:116:PRO:HG2	6:F:122:ASN:HA	1.86	0.57
2:B:450:LEU:HG	2:B:467:GLN:HB2	1.86	0.57
6:F:90:LEU:HD13	6:F:160:TRP:HB3	1.87	0.57
1:A:46:ALA:HB1	1:A:152:VAL:CG1	2.35	0.57
5:E:149:VAL:H	5:E:162:MET:HB3	1.70	0.56
2:B:293:VAL:HG11	2:B:302:GLY:HA2	1.86	0.56
2:B:611:PRO:HB3	2:B:644:LEU:HD21	1.88	0.56
3:C:255:ILE:HG23	6:F:287:SER:HB3	1.88	0.56
2:B:241:ASP:OD1	2:B:241:ASP:O	2.23	0.56
3:C:57:MET:HB2	3:C:429:GLY:HA3	1.87	0.56
3:C:255:ILE:HD12	6:F:287:SER:HB2	1.88	0.56
2:B:117:VAL:HG22	2:B:127:VAL:HG22	1.86	0.55
2:B:187:GLN:HB2	2:B:216:GLN:HG3	1.87	0.55
1:A:168:HIS:ND1	9:A:301:HEC:CBC	2.69	0.55
2:B:422:MET:HE1	2:B:441:MET:HE3	1.88	0.55
4:D:87:GLY:O	4:D:89:ARG:NH1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG22	8:I:32:LEU:HD13	1.88	0.55
2:B:779:TYR:HD1	2:B:782:ARG:HD2	1.72	0.55
1:A:168:HIS:HD1	9:A:301:HEC:HBC1	1.71	0.55
3:C:101:GLY:HA2	3:C:123:ALA:HB1	1.89	0.55
7:G:69:THR:HG23	7:G:71:ARG:H	1.72	0.55
6:F:53:VAL:HG11	6:F:374:PRO:HB3	1.88	0.54
6:F:378:ILE:O	6:F:382:ILE:HG12	2.08	0.54
2:B:172:PHE:HE1	2:B:448:ILE:HD13	1.73	0.54
3:C:363:ALA:O	3:C:366:PRO:HD2	2.07	0.53
6:F:256:SER:O	6:F:259:PRO:HD2	2.08	0.53
1:A:3:GLN:HB2	4:D:133:PHE:HB3	1.90	0.53
2:B:794:CYS:HG	10:B:1101:SF4:FE4	1.25	0.53
4:D:169:LEU:O	4:D:171:PRO:HD3	2.08	0.53
2:B:222:TYR:HA	2:B:401:GLN:HB3	1.90	0.52
2:B:172:PHE:CE1	2:B:448:ILE:HD13	2.45	0.52
2:B:351:LEU:C	2:B:353:GLU:H	2.17	0.52
1:A:156:GLN:HB3	1:A:157:GLN:OE1	2.09	0.52
6:F:312:LEU:O	6:F:316:ALA:HB3	2.09	0.52
3:C:245:VAL:O	3:C:249:ILE:HG12	2.10	0.52
6:F:272:VAL:HG21	15:F:502:JM9:C29	2.39	0.52
1:A:82:PRO:HG2	9:A:304:HEC:HHD	1.91	0.51
1:A:161:MET:HE2	3:C:158:HIS:HB3	1.93	0.51
2:B:187:GLN:HB3	2:B:215:PRO:HD2	1.92	0.51
2:B:293:VAL:HG13	2:B:308:ARG:HG3	1.91	0.51
5:E:107:HIS:HD2	9:E:301:HEC:NC	2.04	0.51
1:A:128:PHE:HE1	1:A:133:HIS:CE1	2.29	0.51
5:E:107:HIS:CE1	9:E:301:HEC:NA	2.77	0.51
5:E:149:VAL:HG12	5:E:162:MET:H	1.75	0.51
3:C:126:MET:HE3	3:C:285:LEU:HD12	1.92	0.51
3:C:277:ALA:HB2	3:C:390:MET:HG3	1.91	0.51
3:C:25:TYR:HD1	3:C:451:ARG:HB2	1.77	0.50
1:A:72:SER:OG	1:A:76:SER:OG	2.28	0.50
3:C:390:MET:HE3	3:C:394:ARG:NH1	2.27	0.50
1:A:134:VAL:HG13	1:A:180:GLU:HG3	1.93	0.50
2:B:449:HIS:HD1	2:B:451:SER:HB2	1.76	0.50
6:F:276:TYR:CD1	15:F:502:JM9:C36	2.95	0.50
6:F:96:LEU:O	6:F:99:PRO:HD2	2.12	0.49
2:B:135:ALA:HA	2:B:270:ALA:HB2	1.94	0.49
3:C:87:ASP:OD1	3:C:87:ASP:N	2.43	0.49
2:B:612:ARG:HH21	2:B:628:ILE:HD11	1.77	0.49
2:B:446:LEU:HD11	2:B:463:TRP:HD1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:LYS:HG2	5:E:34:GLN:HB3	1.94	0.49
3:C:254:ALA:HB1	6:F:284:ILE:HG12	1.93	0.49
3:C:313:THR:CG2	13:C:501:JLQ:C13	2.86	0.49
5:E:182:ARG:NH1	5:E:185:GLN:OE1	2.46	0.49
1:A:140:CYS:N	9:A:303:HEC:HBB3	2.26	0.49
2:B:412:MET:HG2	2:B:417:VAL:HG21	1.94	0.49
3:C:253:PHE:O	3:C:261:TRP:HB3	2.12	0.49
4:D:141:ALA:HA	4:D:145:ALA:HB3	1.95	0.49
4:D:96:TRP:CG	4:D:97:PRO:HD3	2.48	0.48
2:B:120:ASN:ND2	2:B:123:ARG:NH2	2.61	0.48
1:A:51:VAL:O	1:A:51:VAL:CG1	2.61	0.48
2:B:187:GLN:HB2	2:B:216:GLN:CG	2.44	0.48
1:A:141:SER:HB2	1:A:184:MET:HB3	1.96	0.48
3:C:122:PHE:HB3	3:C:286:MET:HE1	1.94	0.48
5:E:74:LEU:HD22	5:E:77:GLY:C	2.39	0.48
2:B:149:LEU:HB3	2:B:588:ASN:HD21	1.78	0.48
2:B:805:GLN:HG3	2:B:810:ILE:HB	1.95	0.48
1:A:127:TYR:OH	5:E:35:LYS:NZ	2.47	0.48
2:B:409:VAL:HG21	2:B:435:LEU:HD22	1.94	0.48
3:C:258:VAL:HB	3:C:261:TRP:HB2	1.95	0.48
4:D:56:PRO:HB3	15:F:502:JM9:C42	2.44	0.48
2:B:324:ALA:HB1	2:B:329:VAL:CG2	2.43	0.48
6:F:81:ARG:HG2	6:F:396:PRO:HD3	1.96	0.48
3:C:121:ARG:HD3	3:C:186:TRP:HE1	1.78	0.47
2:B:226:ASN:HD22	2:B:401:GLN:HB2	1.79	0.47
4:D:25:ALA:C	4:D:27:ALA:H	2.22	0.47
1:A:98:SER:OG	1:A:101:LEU:HB2	2.14	0.47
1:A:140:CYS:SG	9:A:303:HEC:C4B	3.00	0.47
2:B:422:MET:HB2	2:B:449:HIS:CD2	2.49	0.47
6:F:81:ARG:NH2	6:F:396:PRO:HB3	2.29	0.47
3:C:92:VAL:HG12	3:C:394:ARG:HE	1.80	0.47
1:A:205:ILE:HG23	9:A:302:HEC:HBD1	1.96	0.47
3:C:36:PRO:O	3:C:37:LEU:HB2	2.15	0.47
3:C:250:SER:OG	3:C:266:PHE:HB3	2.15	0.47
4:D:96:TRP:CD1	4:D:97:PRO:HD3	2.50	0.47
3:C:123:ALA:O	3:C:127:THR:HG23	2.14	0.47
5:E:30:MET:HB3	5:E:33:GLN:HE21	1.80	0.47
2:B:853:CYS:HA	2:B:1009:PRO:HA	1.97	0.47
4:D:132:VAL:HG12	4:D:133:PHE:H	1.80	0.47
1:A:128:PHE:CE1	1:A:133:HIS:CE1	3.03	0.46
6:F:243:SER:HB2	6:F:246:ARG:HH21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:276:TYR:HB2	15:F:502:JM9:C36	2.46	0.46
1:A:55:HIS:HE1	9:A:304:HEC:C4D	2.28	0.46
9:A:301:HEC:HMC1	9:A:301:HEC:HBC3	1.95	0.46
4:D:104:PHE:CE1	15:F:502:JM9:C54	2.97	0.46
1:A:182:TYR:O	1:A:183:ASN:C	2.59	0.46
2:B:733:LEU:HD12	2:B:733:LEU:C	2.40	0.46
7:G:87:THR:HG23	7:G:90:GLY:H	1.81	0.46
5:E:98:LYS:HB3	5:E:177:ILE:HD11	1.98	0.46
2:B:354:HIS:HB3	2:B:357:GLN:HB2	1.98	0.46
2:B:684:ARG:HE	2:B:687:ALA:HB2	1.81	0.46
3:C:221:ALA:O	3:C:222:ARG:HB2	2.16	0.46
6:F:315:PHE:O	6:F:320:PRO:HD3	2.16	0.46
1:A:25:VAL:HG13	8:I:29:MET:HE2	1.97	0.46
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.77	0.46
2:B:585:TYR:HB3	2:B:591:LEU:HD12	1.98	0.46
3:C:61:PHE:HB2	3:C:426:GLY:CA	2.45	0.46
2:B:856:ALA:H	4:D:87:GLY:HA2	1.81	0.45
3:C:197:LEU:HD11	3:C:443:PRO:HD3	1.96	0.45
4:D:9:MET:HG3	4:D:135:VAL:HG21	1.99	0.45
3:C:61:PHE:HB2	3:C:426:GLY:HA3	1.98	0.45
1:A:10:ASN:OD1	4:D:127:SER:HA	2.16	0.45
2:B:980:GLY:N	2:B:989:VAL:HG21	2.31	0.45
3:C:421:TRP:O	3:C:425:ILE:HD12	2.17	0.45
2:B:782:ARG:O	2:B:983:ASN:ND2	2.47	0.45
3:C:45:LYS:HA	3:C:48:LEU:HD12	1.99	0.45
3:C:405:ASP:H	3:C:411:TRP:NE1	2.14	0.45
3:C:408:PRO:HA	3:C:411:TRP:CE2	2.52	0.45
3:C:420:ASP:OD1	3:C:420:ASP:N	2.50	0.45
8:I:3:PRO:HG2	8:I:6:SER:HB3	1.99	0.45
5:E:99:TYR:O	5:E:104:ALA:N	2.50	0.44
2:B:107:THR:HG22	2:B:112:GLY:HA2	1.99	0.44
2:B:449:HIS:ND1	2:B:451:SER:HB2	2.32	0.44
2:B:275:PHE:CE2	2:B:279:ARG:HD2	2.52	0.44
2:B:669:PRO:HB2	2:B:841:PRO:HG3	1.99	0.44
1:A:107:SER:C	1:A:109:ALA:H	2.26	0.44
2:B:254:VAL:HG22	2:B:359:VAL:HG12	1.99	0.44
2:B:117:VAL:CG2	2:B:127:VAL:HG22	2.47	0.44
3:C:265:VAL:O	3:C:268:PRO:HD2	2.18	0.44
3:C:332:SER:HB3	6:F:218:PHE:CE1	2.52	0.44
9:A:301:HEC:CBC	9:A:301:HEC:CMC	2.85	0.44
3:C:322:TYR:OH	3:C:356:LEU:HD11	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:PHE:O	5:E:145:ILE:HG13	2.18	0.44
4:D:14:THR:HG23	4:D:17:ALA:H	1.82	0.44
1:A:161:MET:HB3	3:C:158:HIS:HA	2.00	0.43
2:B:629:GLY:HA3	2:B:637:ARG:HD3	1.99	0.43
2:B:850:CYS:HA	2:B:896:VAL:HG21	2.00	0.43
3:C:327:PHE:O	3:C:331:TYR:HB2	2.17	0.43
6:F:315:PHE:HB3	6:F:342:TRP:HZ2	1.82	0.43
1:A:138:ILE:HG21	9:A:302:HEC:HBC2	2.00	0.43
2:B:757:GLU:O	2:B:758:VAL:HB	2.19	0.43
3:C:55:PHE:O	3:C:59:MET:HG2	2.18	0.43
7:G:87:THR:HB	7:G:93:HIS:NE2	2.34	0.43
2:B:853:CYS:HB3	2:B:1007:THR:HB	2.00	0.43
6:F:14:LEU:HD21	6:F:389:VAL:HG13	1.99	0.43
6:F:108:TYR:O	6:F:109:LYS:HB2	2.18	0.43
5:E:136:ALA:O	5:E:182:ARG:NH2	2.52	0.43
1:A:33:VAL:HG22	8:I:32:LEU:CD1	2.48	0.43
4:D:8:VAL:O	4:D:149:CYS:HA	2.18	0.43
6:F:137:ILE:HG12	6:F:215:PRO:HB2	2.01	0.43
2:B:633:ASP:O	2:B:637:ARG:HG3	2.18	0.43
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.83	0.43
5:E:149:VAL:N	5:E:162:MET:HB3	2.32	0.43
1:A:140:CYS:HB3	1:A:144:HIS:CD2	2.47	0.43
2:B:627:LEU:O	2:B:637:ARG:HD2	2.19	0.43
6:F:56:THR:CG2	6:F:351:MET:HE1	2.41	0.43
3:C:313:THR:CG2	13:C:501:JLQ:C11	2.88	0.43
6:F:83:LEU:HD21	6:F:238:LEU:HD11	2.01	0.43
1:A:157:GLN:OE1	1:A:157:GLN:N	2.52	0.42
4:D:132:VAL:HG12	4:D:133:PHE:N	2.34	0.42
2:B:420:LEU:HB3	2:B:447:THR:HG22	2.01	0.42
6:F:65:LEU:HD12	6:F:68:GLN:HE21	1.83	0.42
2:B:262:LEU:HD12	2:B:301:THR:HA	2.01	0.42
3:C:239:THR:HB	3:C:240:PRO:HD3	2.01	0.42
2:B:428:VAL:HG13	2:B:438:ALA:HB2	2.00	0.42
6:F:360:ARG:HD3	6:F:366:ILE:HA	2.00	0.42
2:B:765:ARG:HH21	2:B:769:ASN:H	1.67	0.42
6:F:31:VAL:HG13	6:F:372:ALA:HB1	2.01	0.42
2:B:851:MET:HA	2:B:1011:THR:HB	2.02	0.42
3:C:217:TRP:O	3:C:218:ARG:C	2.62	0.42
6:F:110:ALA:C	6:F:112:GLY:H	2.27	0.42
3:C:154:TYR:CE2	3:C:156:ASN:HB3	2.53	0.42
4:D:30:TYR:CD2	4:D:150:ILE:HD13	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLY:O	1:A:143:CYS:HB2	2.20	0.42
1:A:183:ASN:C	1:A:185:ASP:H	2.28	0.42
4:D:8:VAL:HG12	4:D:166:LEU:HD12	2.02	0.42
6:F:291:ALA:O	6:F:295:PRO:HD3	2.19	0.42
4:D:43:GLU:HA	4:D:43:GLU:OE2	2.20	0.42
6:F:348:PHE:CE2	6:F:374:PRO:HB2	2.55	0.42
2:B:149:LEU:HB3	2:B:588:ASN:ND2	2.35	0.41
2:B:860:VAL:HG11	4:D:89:ARG:NH2	2.34	0.41
3:C:110:LEU:HD11	3:C:236:GLY:HA2	2.01	0.41
1:A:46:ALA:HB1	1:A:152:VAL:HG11	2.02	0.41
6:F:250:LEU:HD23	6:F:250:LEU:HA	1.86	0.41
3:C:129:PHE:CD1	3:C:434:LEU:HD23	2.56	0.41
1:A:134:VAL:HG13	1:A:180:GLU:CG	2.50	0.41
3:C:31:LYS:HD2	3:C:298:TYR:CE2	2.56	0.41
3:C:42:LYS:HE2	3:C:42:LYS:HB2	1.81	0.41
6:F:81:ARG:HH21	6:F:396:PRO:HB3	1.85	0.41
1:A:113:PRO:HB3	5:E:49:ARG:HH11	1.85	0.41
2:B:95:VAL:HB	2:B:98:ILE:HD12	2.03	0.41
2:B:918:PRO:HA	5:E:35:LYS:HD2	2.02	0.41
6:F:32:LEU:HG	6:F:43:PHE:HD1	1.86	0.41
2:B:456:GLU:HG3	2:B:686:HIS:HB2	2.02	0.41
2:B:597:PRO:O	2:B:598:LEU:HB2	2.21	0.41
4:D:15:PRO:HD3	4:D:146:PHE:CZ	2.56	0.41
2:B:130:ASN:ND2	2:B:539:GLY:HA3	2.36	0.41
2:B:859:GLU:HA	2:B:867:THR:HG23	2.03	0.41
3:C:99:HIS:CE1	3:C:271:VAL:HG13	2.56	0.41
6:F:343:ILE:O	6:F:347:ARG:HG2	2.21	0.41
3:C:319:VAL:HA	3:C:322:TYR:CD2	2.56	0.41
6:F:65:LEU:O	6:F:68:GLN:HG3	2.21	0.41
6:F:90:LEU:N	6:F:91:PRO:HD2	2.36	0.41
3:C:80:ILE:HD13	3:C:80:ILE:HA	1.89	0.40
6:F:405:LEU:HD23	6:F:405:LEU:HA	1.89	0.40
2:B:451:SER:O	2:B:452:GLN:HB3	2.22	0.40
2:B:759:TYR:CD2	2:B:768:PRO:HD3	2.56	0.40
3:C:267:PRO:HB2	3:C:268:PRO:HD3	2.02	0.40
4:D:93:ILE:HD12	4:D:93:ILE:HA	1.91	0.40
5:E:100:ASN:HA	5:E:104:ALA:HB2	2.02	0.40
6:F:70:LEU:HD11	6:F:192:GLY:HA2	2.02	0.40
6:F:182:LYS:O	6:F:183:LEU:HB2	2.21	0.40
2:B:856:ALA:HA	2:B:857:PRO:HD2	1.98	0.40
6:F:80:ARG:HE	6:F:80:ARG:HB2	1.77	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ASP:CG	4:D:161:ARG:HB2	2.47	0.40
5:E:81:ASP:N	5:E:137:PRO:HB3	2.36	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	216/219 (99%)	200 (93%)	16 (7%)	0	100	100
2	B	949/1029 (92%)	911 (96%)	38 (4%)	0	100	100
3	C	447/486 (92%)	434 (97%)	13 (3%)	0	100	100
4	D	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
5	E	162/205 (79%)	155 (96%)	6 (4%)	1 (1%)	21	51
6	F	395/411 (96%)	379 (96%)	16 (4%)	0	100	100
7	G	78/112 (70%)	73 (94%)	5 (6%)	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	2455/2678 (92%)	2346 (96%)	108 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	107	HIS

5.3.2 Protein sidechains [i](#)

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	198/199 (100%)	194 (98%)	4 (2%)	48	67
2	B	768/830 (92%)	748 (97%)	20 (3%)	40	63
3	C	382/405 (94%)	378 (99%)	4 (1%)	68	75
4	D	143/147 (97%)	139 (97%)	4 (3%)	38	62
5	E	135/171 (79%)	132 (98%)	3 (2%)	45	65
6	F	318/330 (96%)	317 (100%)	1 (0%)	86	85
7	G	69/95 (73%)	68 (99%)	1 (1%)	59	72
8	I	32/32 (100%)	30 (94%)	2 (6%)	16	45
All	All	2045/2209 (93%)	2006 (98%)	39 (2%)	49	68

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	CYS
1	A	143	CYS
1	A	147	VAL
1	A	182	TYR
2	B	76	CYS
2	B	193	LEU
2	B	281	VAL
2	B	329	VAL
2	B	349	ARG
2	B	504	LEU
2	B	558	ILE
2	B	677	THR
2	B	715	VAL
2	B	741	VAL
2	B	753	TYR
2	B	754	ILE
2	B	827	ILE
2	B	843	ILE
2	B	853	CYS
2	B	860	VAL
2	B	869	HIS
2	B	920	VAL
2	B	933	TYR
2	B	958	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	16	GLU
3	C	151	LEU
3	C	255	ILE
3	C	265	VAL
4	D	143	GLN
4	D	156	LEU
4	D	166	LEU
4	D	169	LEU
5	E	27	HIS
5	E	69	PHE
5	E	107	HIS
6	F	107	THR
7	G	56	LEU
8	I	16	LEU
8	I	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	146	GLN
1	A	170	ASN
2	B	82	GLN
2	B	120	ASN
2	B	145	GLN
2	B	187	GLN
2	B	206	GLN
2	B	216	GLN
2	B	357	GLN
2	B	375	HIS
2	B	391	HIS
2	B	449	HIS
2	B	790	ASN
2	B	808	ASN
2	B	817	GLN
2	B	869	HIS
2	B	880	ASN
2	B	900	ASN
3	C	225	HIS
3	C	302	HIS
4	D	143	GLN
5	E	33	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	147	ASN
6	F	139	HIS
6	F	216	HIS
6	F	261	HIS
6	F	407	ASN

5.3.3 RNA [i](#)

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](#)

15 ligands are 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	$\# Z > 2$
9	HEC	A	303	1	46,50,50	1.91	6 (13%)	58,82,82	1.68	3 (5%)
9	HEC	A	301	1	46,50,50	1.89	6 (13%)	58,82,82	1.63	5 (8%)
10	SF4	B	1101	2	0,12,12	-	-	-	-	-
12	EL6	E	302	-	27,27,42	1.17	4 (14%)	29,29,44	1.45	3 (10%)
11	F3S	B	1104	2	0,9,9	-	-	-	-	-
12	EL6	B	1105	-	26,26,42	1.20	4 (15%)	28,28,44	1.49	3 (10%)
9	HEC	E	301	5	46,50,50	1.90	6 (13%)	58,82,82	2.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	JM9	F	502	-	53,53,53	0.99	5 (9%)	58,58,58	0.77	3 (5%)
14	JL3	F	501	-	44,44,44	0.99	4 (9%)	47,49,49	1.10	4 (8%)
13	JLQ	C	501	-	44,44,44	0.97	4 (9%)	47,49,49	1.25	6 (12%)
10	SF4	B	1103	2	0,12,12	-	-	-	-	-
10	SF4	B	1102	2	0,12,12	-	-	-	-	-
9	HEC	A	305	1	46,50,50	1.92	6 (13%)	58,82,82	1.86	3 (5%)
9	HEC	A	302	1	46,50,50	1.90	6 (13%)	58,82,82	1.91	4 (6%)
9	HEC	A	304	1	46,50,50	1.90	6 (13%)	58,82,82	1.85	2 (3%)

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
9	HEC	A	303	1	-	6/14/54/54	-
9	HEC	A	301	1	-	3/14/54/54	-
10	SF4	B	1101	2	-	-	0/6/5/5
12	EL6	E	302	-	-	10/28/28/43	-
12	EL6	B	1105	-	-	9/27/27/43	-
15	JM9	F	502	-	-	21/56/56/56	-
9	HEC	E	301	5	-	5/14/54/54	-
11	F3S	B	1104	2	-	-	0/3/3/3
14	JL3	F	501	-	-	17/48/48/48	-
13	JLQ	C	501	-	-	18/48/48/48	-
10	SF4	B	1103	2	-	-	0/6/5/5
10	SF4	B	1102	2	-	-	0/6/5/5
9	HEC	A	305	1	-	4/14/54/54	-
9	HEC	A	302	1	-	4/14/54/54	-
9	HEC	A	304	1	-	6/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	303	HEC	CAC-C3C	6.31	1.55	1.35
9	A	303	HEC	CAB-C3B	6.27	1.55	1.35
9	A	304	HEC	CAC-C3C	6.25	1.55	1.35
9	A	305	HEC	CAC-C3C	6.22	1.55	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	305	HEC	CAB-C3B	6.13	1.54	1.35
9	A	302	HEC	CAB-C3B	6.13	1.54	1.35
9	A	301	HEC	CAC-C3C	6.11	1.54	1.35
9	E	301	HEC	CAC-C3C	6.09	1.54	1.35
9	A	301	HEC	CAB-C3B	6.09	1.54	1.35
9	A	304	HEC	CAB-C3B	6.07	1.54	1.35
9	A	302	HEC	CAC-C3C	6.07	1.54	1.35
9	E	301	HEC	CAB-C3B	5.98	1.54	1.35
9	A	305	HEC	C3D-C2D	5.20	1.52	1.38
9	E	301	HEC	C3D-C2D	5.12	1.52	1.38
9	A	303	HEC	C3D-C2D	5.10	1.52	1.38
9	A	302	HEC	C3D-C2D	5.08	1.52	1.38
9	A	304	HEC	C3D-C2D	5.02	1.52	1.38
9	A	301	HEC	C3D-C2D	4.99	1.51	1.38
12	E	302	EL6	O21-C2	-3.80	1.40	1.47
12	B	1105	EL6	O21-C2	-3.60	1.40	1.47
15	F	502	JM9	O20-C21	3.14	1.42	1.33
15	F	502	JM9	O17-C15	2.82	1.42	1.34
14	F	501	JL3	O29-C19	-2.75	1.40	1.46
9	A	303	HEC	C3B-C2B	-2.64	1.32	1.41
9	A	301	HEC	C3C-C2C	-2.63	1.32	1.41
9	A	303	HEC	C3C-C2C	-2.58	1.32	1.41
9	A	304	HEC	C3C-C2C	-2.58	1.32	1.41
9	A	305	HEC	C3C-C2C	-2.56	1.32	1.41
9	A	302	HEC	C3C-C2C	-2.56	1.32	1.41
9	E	301	HEC	C3C-C2C	-2.53	1.32	1.41
15	F	502	JM9	O38-C39	2.52	1.40	1.33
9	E	301	HEC	C3B-C2B	-2.51	1.32	1.41
9	A	302	HEC	C3B-C2B	-2.51	1.32	1.41
9	A	301	HEC	C3B-C2B	-2.51	1.32	1.41
9	A	304	HEC	C3B-C2B	-2.50	1.32	1.41
9	A	305	HEC	C3B-C2B	-2.50	1.32	1.41
12	B	1105	EL6	O31-C31	2.37	1.40	1.33
12	E	302	EL6	O31-C31	2.33	1.40	1.33
14	F	501	JL3	O17-C18	-2.30	1.40	1.45
12	B	1105	EL6	O21-C21	2.29	1.40	1.34
13	C	501	JLQ	O18-C16	2.28	1.40	1.33
12	B	1105	EL6	O31-C3	-2.28	1.40	1.45
12	E	302	EL6	O31-C3	-2.27	1.40	1.45
13	C	501	JLQ	O30-C31	2.26	1.40	1.34
13	C	501	JLQ	O18-C19	-2.26	1.40	1.45
14	F	501	JL3	O17-C15	2.24	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	502	JM9	O17-C18	-2.24	1.41	1.46
12	E	302	EL6	O21-C21	2.23	1.40	1.34
9	A	305	HEC	C2A-C3A	-2.15	1.32	1.36
9	A	304	HEC	C2A-C3A	-2.12	1.32	1.36
13	C	501	JLQ	O30-C20	-2.10	1.41	1.46
9	A	301	HEC	C2A-C3A	-2.10	1.32	1.36
9	A	302	HEC	C2A-C3A	-2.08	1.32	1.36
14	F	501	JL3	O29-C30	2.06	1.40	1.34
15	F	502	JM9	O38-C37	-2.04	1.40	1.45
9	E	301	HEC	C2A-C3A	-2.02	1.32	1.36
9	A	303	HEC	CMA-C3A	2.01	1.54	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	301	HEC	CBC-CAC-C3C	-8.83	109.78	127.43
9	A	304	HEC	CBB-CAB-C3B	-8.63	110.19	127.43
9	E	301	HEC	CBB-CAB-C3B	-8.45	110.55	127.43
9	A	302	HEC	CBC-CAC-C3C	-8.36	110.73	127.43
9	A	305	HEC	CBB-CAB-C3B	-8.17	111.11	127.43
9	A	302	HEC	CBB-CAB-C3B	-8.02	111.41	127.43
9	A	301	HEC	CBB-CAB-C3B	-7.73	111.98	127.43
9	A	304	HEC	CBC-CAC-C3C	-7.40	112.65	127.43
9	A	303	HEC	CBC-CAC-C3C	-7.34	112.76	127.43
9	A	305	HEC	CBC-CAC-C3C	-7.17	113.10	127.43
9	A	303	HEC	CBB-CAB-C3B	-6.69	114.06	127.43
12	B	1105	EL6	O21-C21-C22	4.49	121.19	111.48
13	C	501	JLQ	O30-C31-C33	4.41	121.01	111.48
12	E	302	EL6	O21-C21-C22	4.29	120.76	111.48
14	F	501	JL3	O29-C30-C32	3.89	119.89	111.48
14	F	501	JL3	C01-C02-C03	3.41	136.40	113.36
9	A	301	HEC	CBC-CAC-C3C	-3.32	120.80	127.43
13	C	501	JLQ	O30-C20-C19	3.21	119.85	108.34
13	C	501	JLQ	O30-C20-C21	2.91	118.80	108.34
15	F	502	JM9	O38-C39-C41	2.91	120.70	111.83
13	C	501	JLQ	C21-C20-C19	2.73	118.16	111.78
12	B	1105	EL6	O31-C31-C32	2.72	120.14	111.83
15	F	502	JM9	O17-C15-C14	2.68	117.29	111.48
13	C	501	JLQ	O18-C16-C15	2.50	119.47	111.83
14	F	501	JL3	O17-C15-C14	2.47	119.37	111.83
12	E	302	EL6	C2-O21-C21	-2.45	114.24	117.78
13	C	501	JLQ	O24-P23-O25	-2.42	101.18	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	501	JL3	O23-P22-O24	-2.41	101.21	112.44
12	E	302	EL6	O31-C31-C32	2.40	119.16	111.83
9	E	301	HEC	C4C-NC-C1C	-2.35	101.98	105.82
12	B	1105	EL6	O21-C2-C3	2.26	111.40	106.21
9	A	301	HEC	C4B-NB-C1B	-2.19	102.25	105.82
15	F	502	JM9	O20-C21-C23	2.15	118.38	111.83
9	A	305	HEC	C4B-NB-C1B	-2.13	102.34	105.82
9	A	301	HEC	C4C-NC-C1C	-2.06	102.46	105.82
9	A	301	HEC	C4A-NA-C1A	-2.05	102.47	105.82
9	A	302	HEC	C4C-NC-C1C	-2.02	102.52	105.82
9	A	302	HEC	C4B-NB-C1B	-2.01	102.54	105.82
9	A	303	HEC	C4B-NB-C1B	-2.00	102.56	105.82

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	HEC	C2B-C3B-CAB-CBB
9	A	301	HEC	C4B-C3B-CAB-CBB
9	A	301	HEC	C2C-C3C-CAC-CBC
9	A	302	HEC	C2B-C3B-CAB-CBB
9	A	302	HEC	C4B-C3B-CAB-CBB
9	A	302	HEC	C2C-C3C-CAC-CBC
9	A	303	HEC	C2C-C3C-CAC-CBC
9	A	303	HEC	C4C-C3C-CAC-CBC
9	A	304	HEC	C2B-C3B-CAB-CBB
9	A	304	HEC	C4B-C3B-CAB-CBB
9	A	304	HEC	C2C-C3C-CAC-CBC
9	A	304	HEC	C4C-C3C-CAC-CBC
9	A	305	HEC	C2B-C3B-CAB-CBB
9	A	305	HEC	C4B-C3B-CAB-CBB
9	A	305	HEC	C2C-C3C-CAC-CBC
9	A	305	HEC	C4C-C3C-CAC-CBC
9	E	301	HEC	C2B-C3B-CAB-CBB
9	E	301	HEC	C4B-C3B-CAB-CBB
9	E	301	HEC	C2C-C3C-CAC-CBC
12	B	1105	EL6	O21-C2-C3-O31
13	C	501	JLQ	O18-C19-C20-O30
13	C	501	JLQ	O32-C31-O30-C20
13	C	501	JLQ	C33-C31-O30-C20
14	F	501	JL3	C20-O21-P22-O24
14	F	501	JL3	C20-O21-P22-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	F	501	JL3	C32-C30-O29-C19
15	F	502	JM9	O17-C18-C19-O20
14	F	501	JL3	O16-C15-O17-C18
14	F	501	JL3	O31-C30-O29-C19
14	F	501	JL3	C14-C15-O17-C18
15	F	502	JM9	C41-C39-O38-C37
12	B	1105	EL6	C22-C21-O21-C2
15	F	502	JM9	O40-C39-O38-C37
12	B	1105	EL6	O22-C21-O21-C2
12	B	1105	EL6	C32-C31-O31-C3
13	C	501	JLQ	C15-C16-O18-C19
12	B	1105	EL6	O32-C31-O31-C3
13	C	501	JLQ	O17-C16-O18-C19
12	E	302	EL6	C21-C22-C23-C24
13	C	501	JLQ	C31-C33-C34-C35
14	F	501	JL3	C30-C32-C33-C34
14	F	501	JL3	C05-C06-C07-C08
15	F	502	JM9	C06-C07-C08-C09
15	F	502	JM9	C23-C21-O20-C19
15	F	502	JM9	C45-C46-C47-C48
13	C	501	JLQ	C34-C35-C36-C37
15	F	502	JM9	C47-C48-C49-C50
14	F	501	JL3	C08-C09-C10-C11
15	F	502	JM9	C41-C42-C43-C44
15	F	502	JM9	O22-C21-O20-C19
15	F	502	JM9	C08-C09-C10-C11
12	E	302	EL6	C22-C21-O21-C2
14	F	501	JL3	C35-C36-C37-C38
15	F	502	JM9	C27-C28-C29-C30
12	E	302	EL6	O22-C21-O21-C2
14	F	501	JL3	C01-C02-C03-C04
15	F	502	JM9	C24-C25-C26-C27
13	C	501	JLQ	C36-C37-C38-C39
12	B	1105	EL6	C1-C2-C3-O31
14	F	501	JL3	C33-C34-C35-C36
14	F	501	JL3	O17-C18-C19-C20
14	F	501	JL3	C37-C38-C39-C40
14	F	501	JL3	O17-C18-C19-O29
14	F	501	JL3	C10-C11-C12-C13
12	E	302	EL6	C32-C33-C34-C35
15	F	502	JM9	C37-C18-C19-O20
13	C	501	JLQ	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	501	JLQ	C12-C13-C14-C15
9	A	304	HEC	C3D-CAD-CBD-CGD
12	B	1105	EL6	C31-C32-C33-C34
15	F	502	JM9	C03-C04-C05-C06
9	A	302	HEC	C4C-C3C-CAC-CBC
9	A	303	HEC	C4B-C3B-CAB-CBB
9	E	301	HEC	C4C-C3C-CAC-CBC
15	F	502	JM9	C05-C06-C07-C08
9	A	303	HEC	C2B-C3B-CAB-CBB
13	C	501	JLQ	C27-O26-P23-O22
13	C	501	JLQ	C27-O26-P23-O24
13	C	501	JLQ	C27-O26-P23-O25
12	E	302	EL6	C31-C32-C33-C34
15	F	502	JM9	C46-C47-C48-C49
12	E	302	EL6	C27-C28-C29-C2A
13	C	501	JLQ	C01-C02-C03-C04
13	C	501	JLQ	O18-C19-C20-C21
15	F	502	JM9	C43-C44-C45-C46
15	F	502	JM9	O38-C39-C41-C42
13	C	501	JLQ	C42-C43-C44-C45
15	F	502	JM9	C30-C31-C32-C33
9	A	303	HEC	CAD-CBD-CGD-O2D
12	E	302	EL6	C24-C25-C26-C27
9	A	303	HEC	CAD-CBD-CGD-O1D
12	E	302	EL6	O21-C21-C22-C23
13	C	501	JLQ	O30-C31-C33-C34
12	B	1105	EL6	C33-C34-C35-C36
12	E	302	EL6	C23-C24-C25-C26
15	F	502	JM9	C13-C14-C15-O17
9	A	304	HEC	C1A-C2A-CAA-CBA
14	F	501	JL3	O29-C30-C32-C33
9	E	301	HEC	CAA-CBA-CGA-O2A
12	E	302	EL6	O22-C21-C22-C23
12	B	1105	EL6	C35-C36-C37-C38
13	C	501	JLQ	O32-C31-C33-C34
15	F	502	JM9	C13-C14-C15-O16

There are no ring outliers.

10 monomers are involved in 60 short contacts:

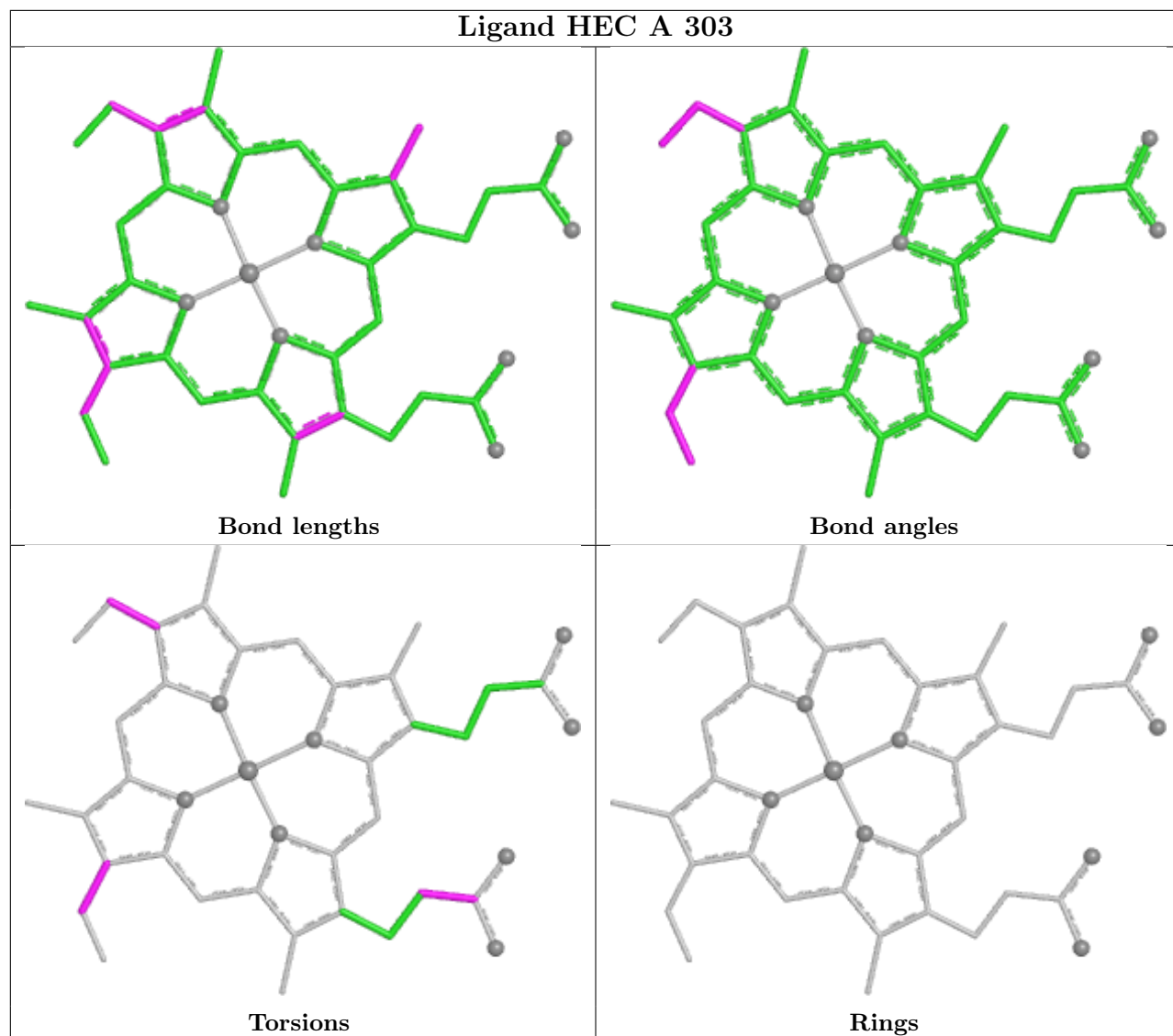
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	303	HEC	11	0

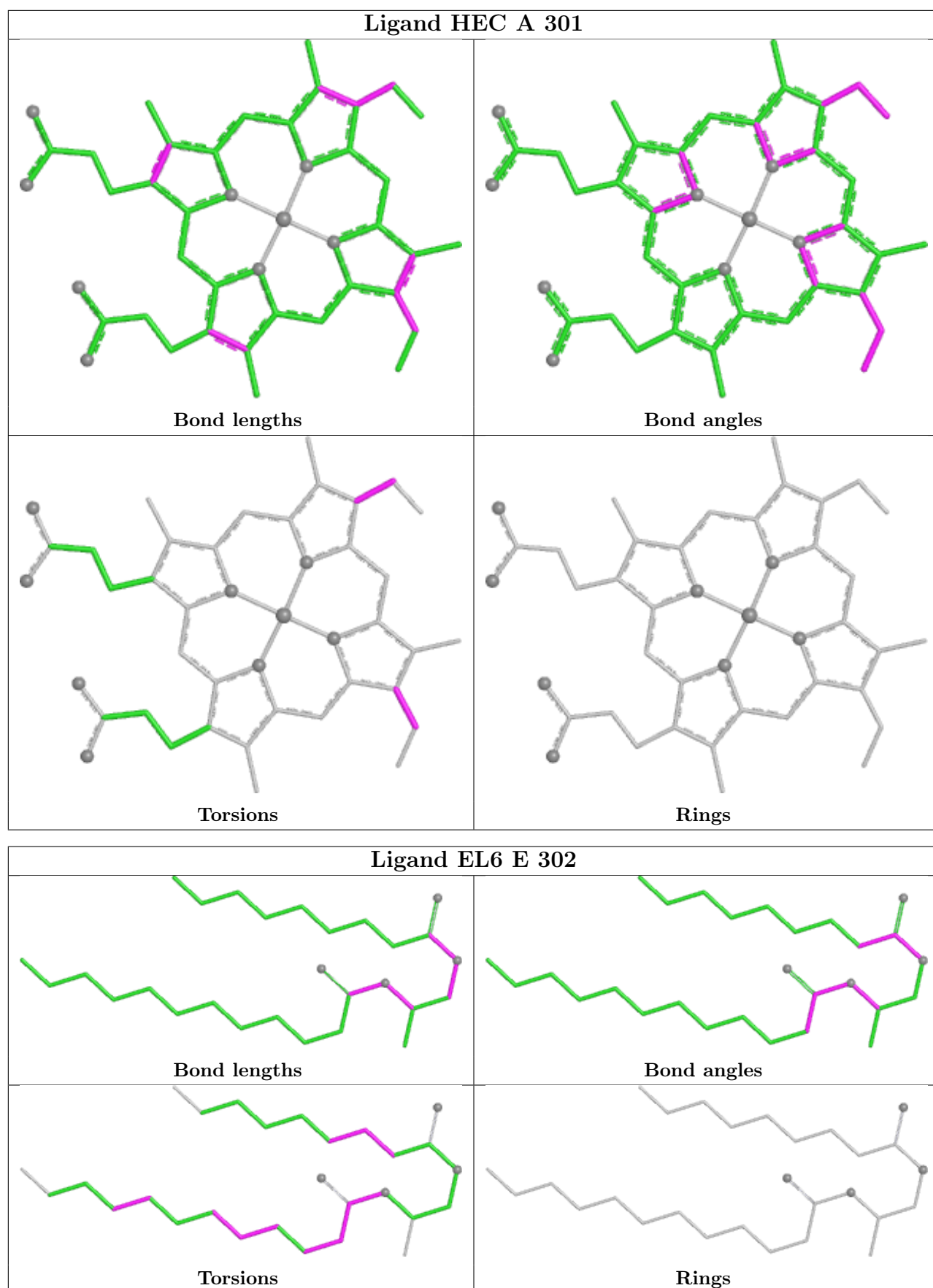
Continued on next page...

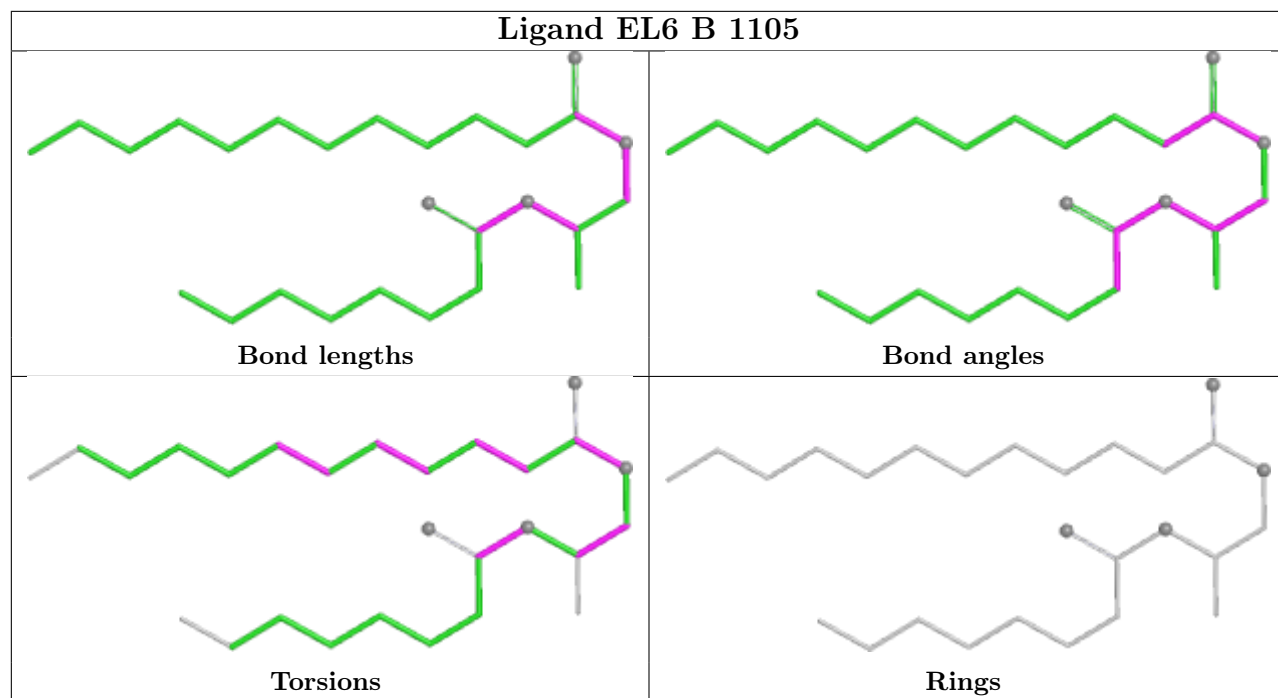
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEC	9	0
10	B	1101	SF4	1	0
12	B	1105	EL6	1	0
9	E	301	HEC	4	0
15	F	502	JM9	17	0
14	F	501	JL3	2	0
13	C	501	JLQ	10	0
9	A	302	HEC	3	0
9	A	304	HEC	2	0

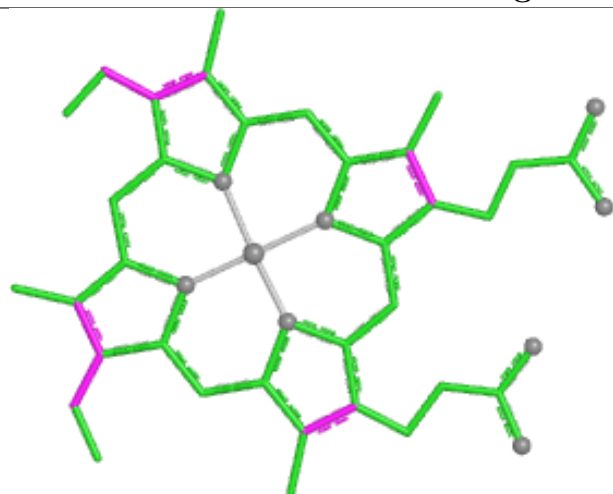
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



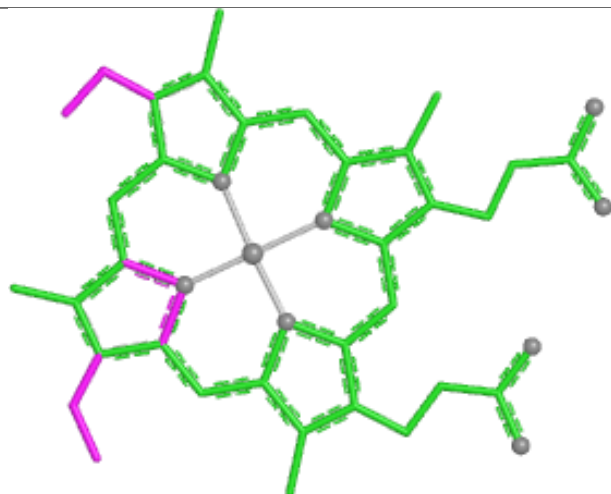




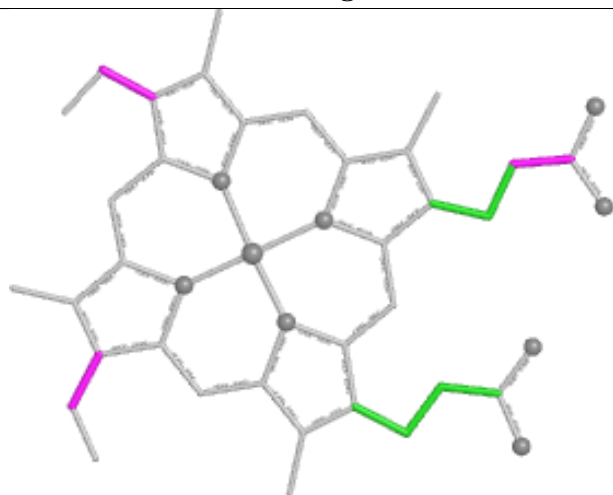
Ligand HEC E 301



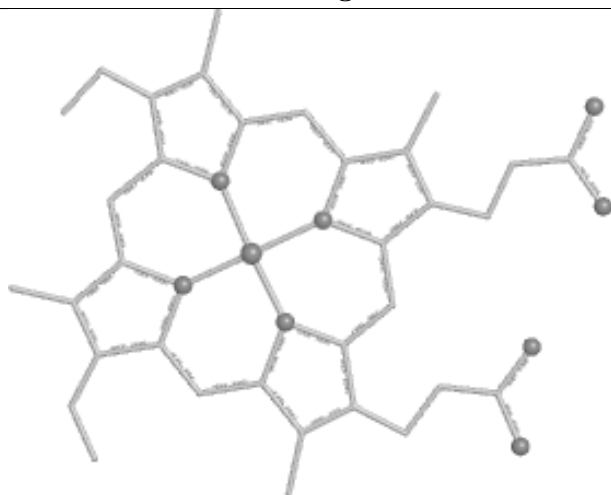
Bond lengths



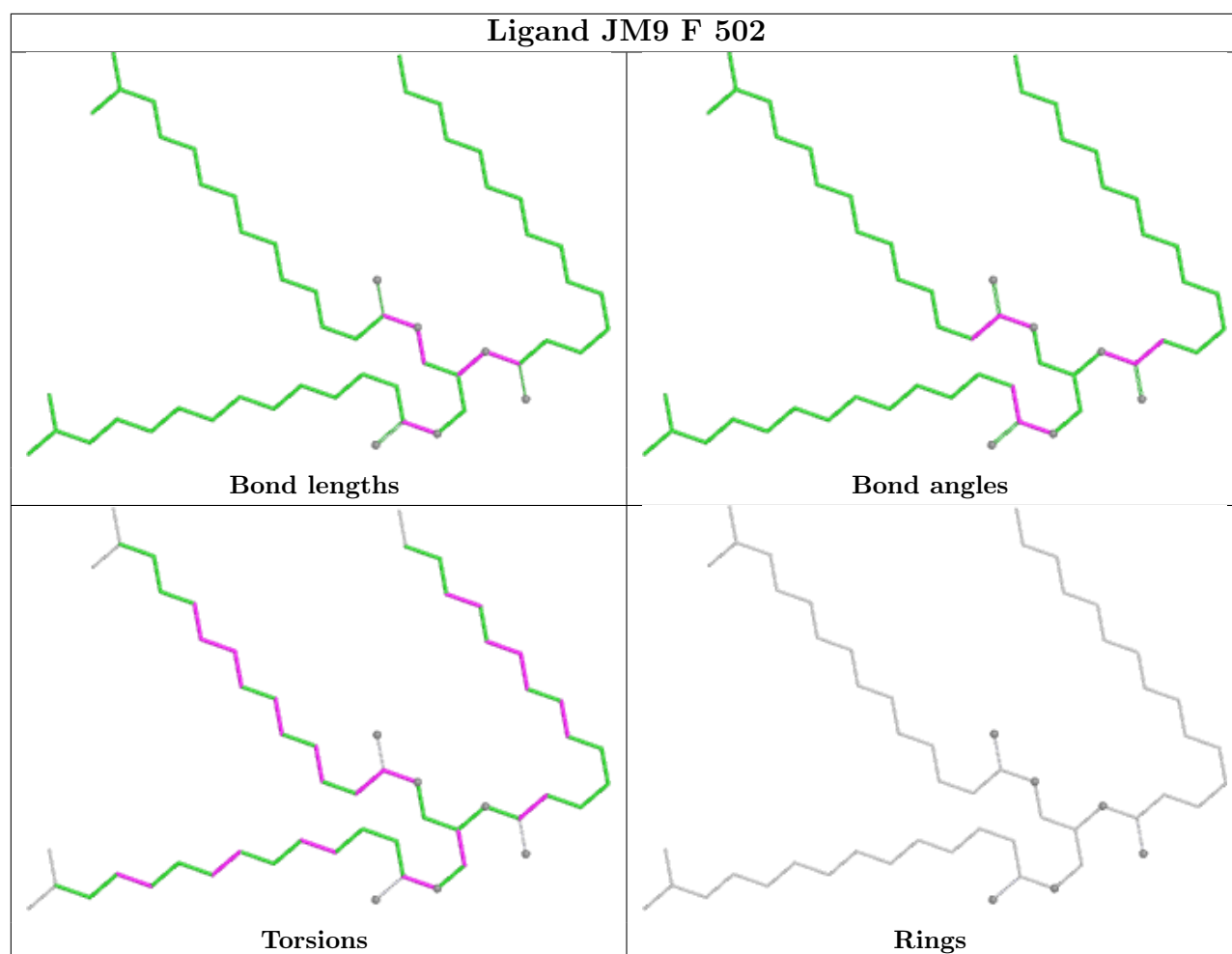
Bond angles

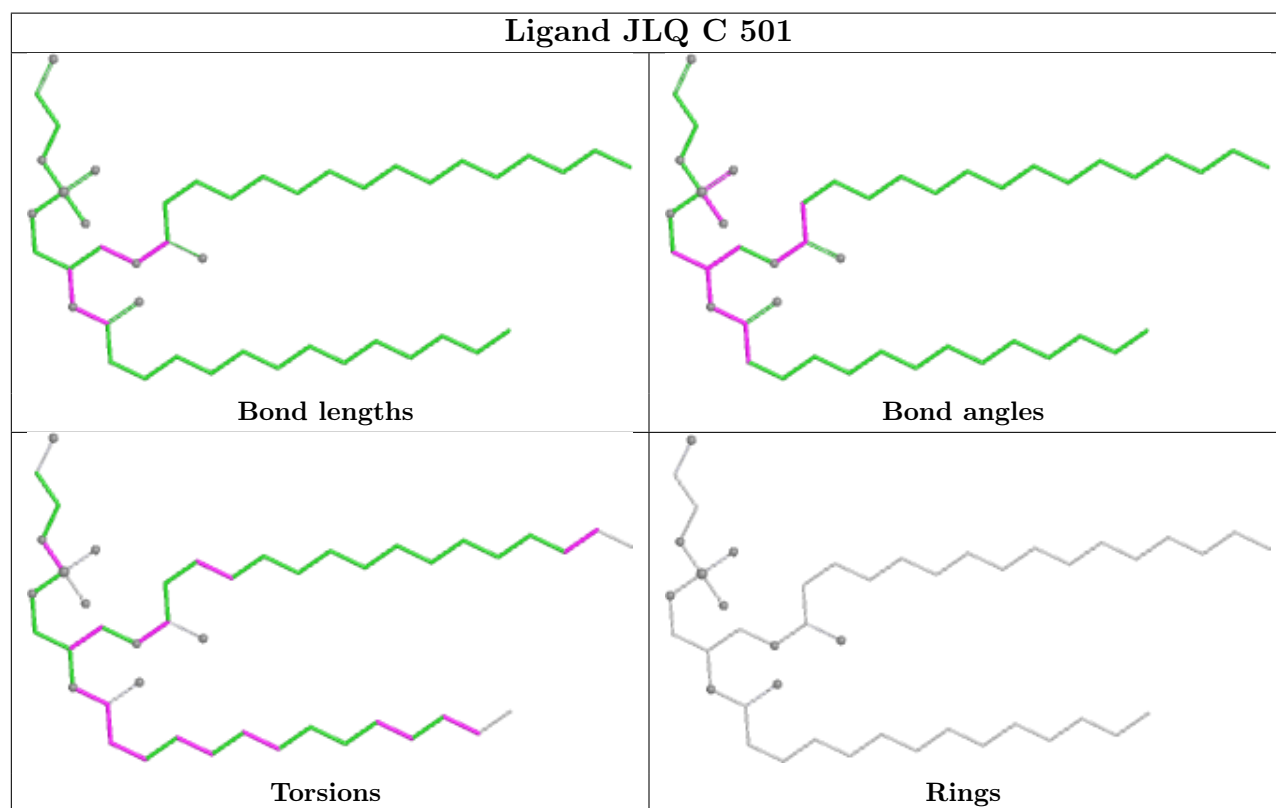
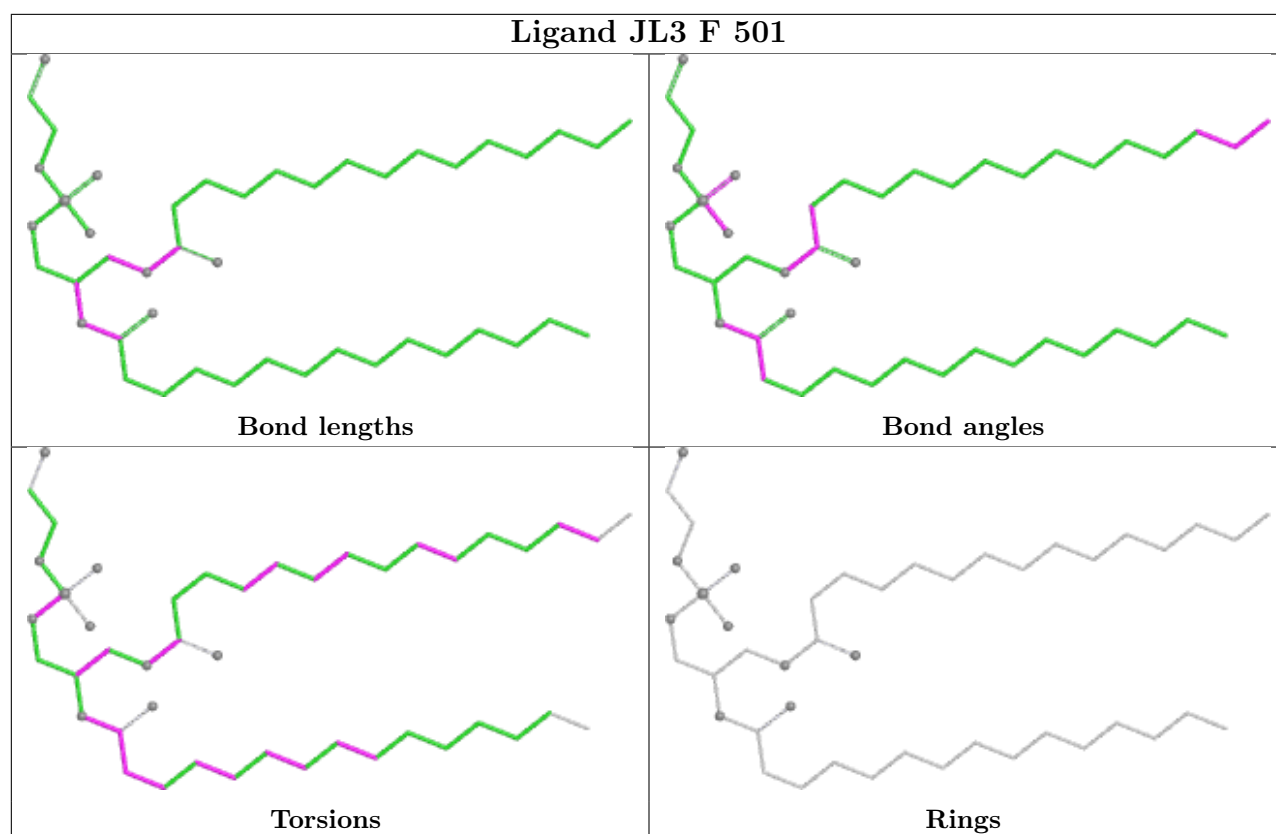


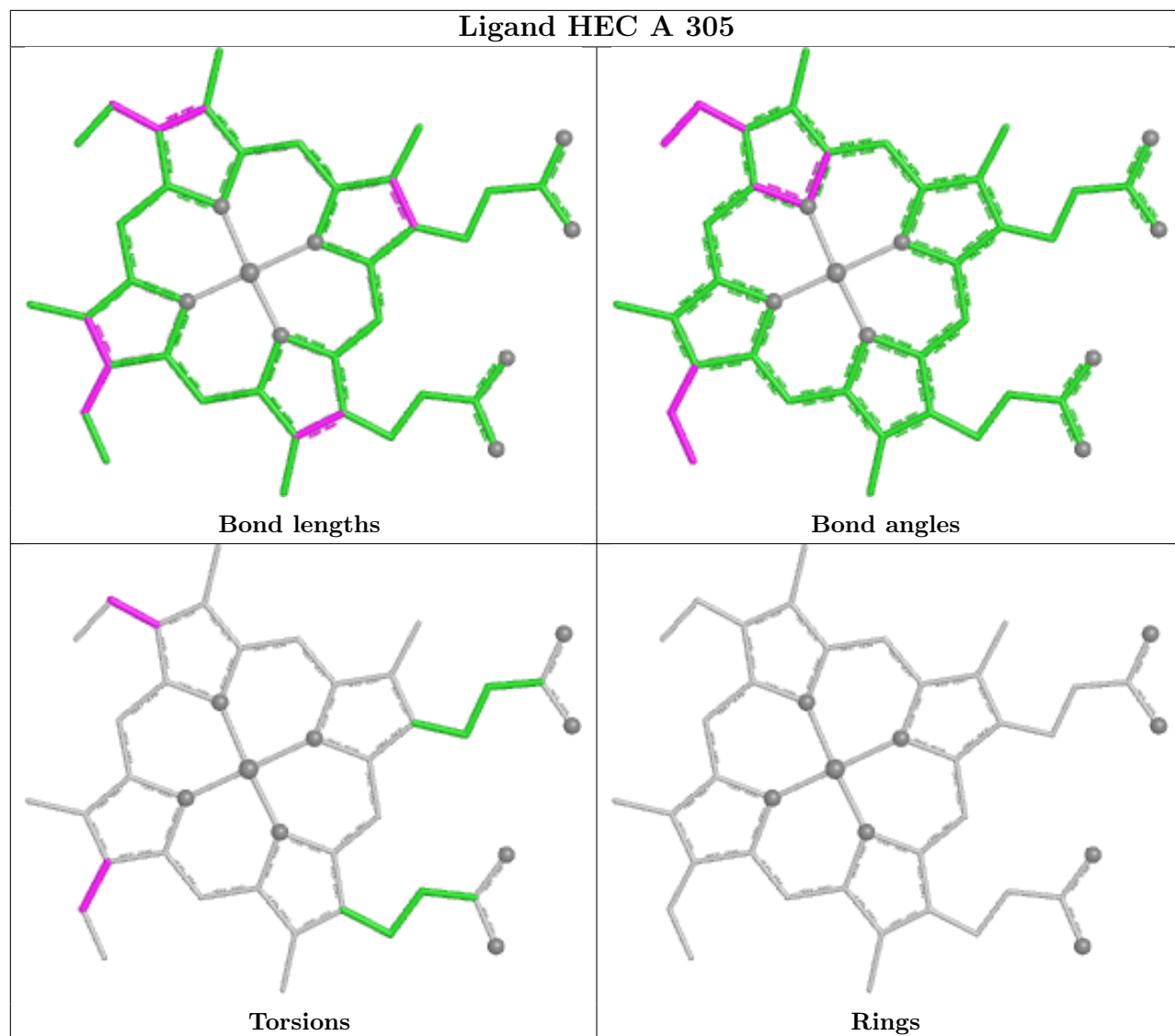
Torsions

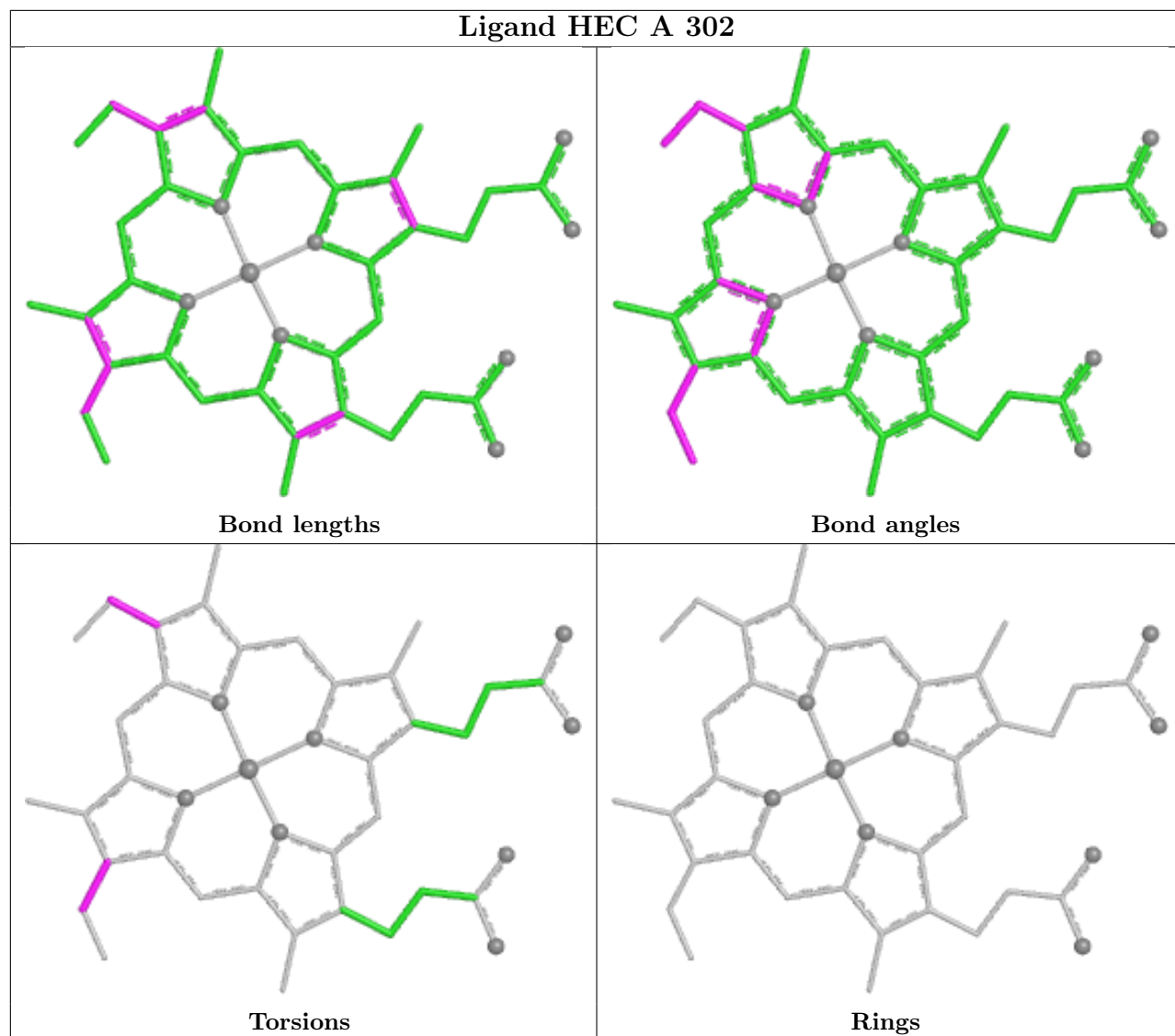


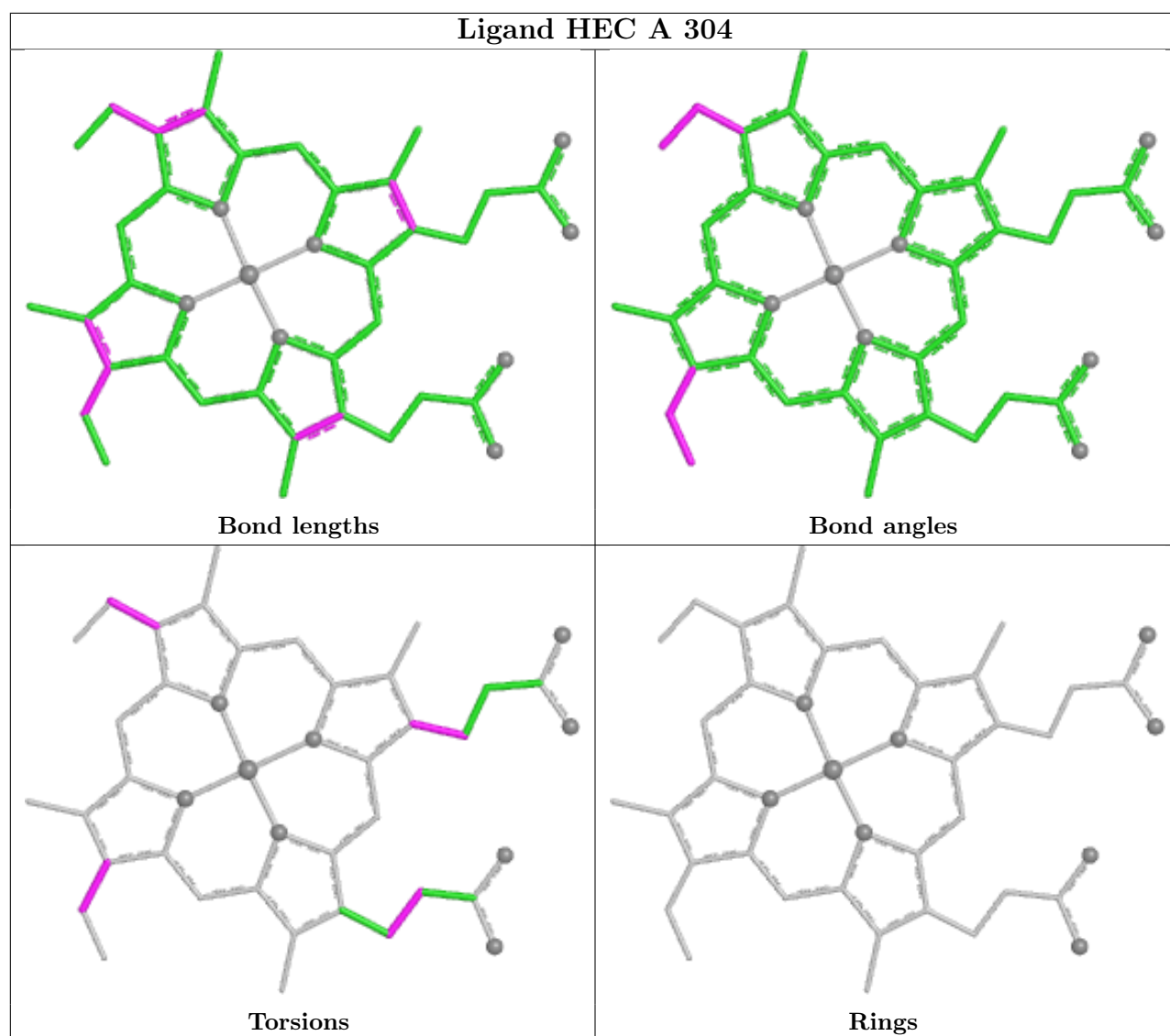
Rings











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.

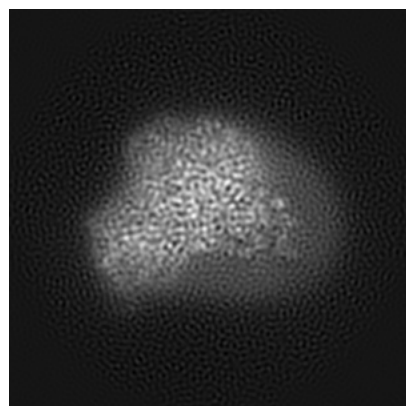
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36984. These allow visual inspection of the internal detail of the map and identification of artifacts.

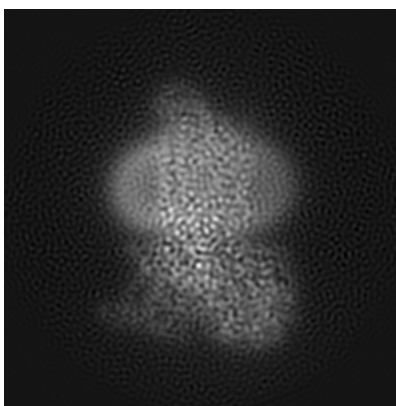
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

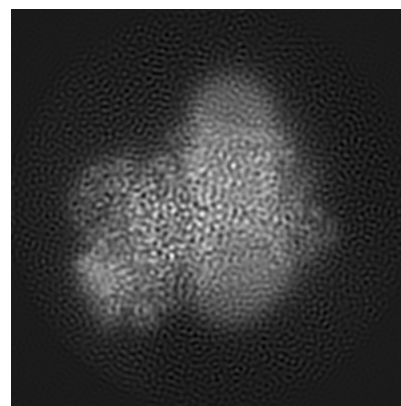
6.1.1 Primary map



X

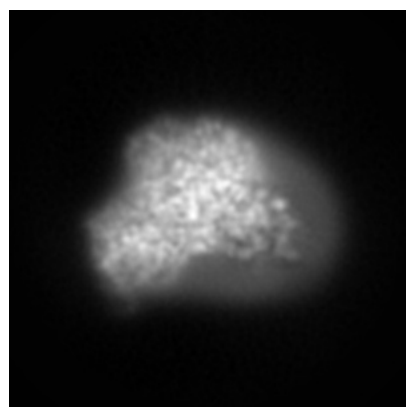


Y

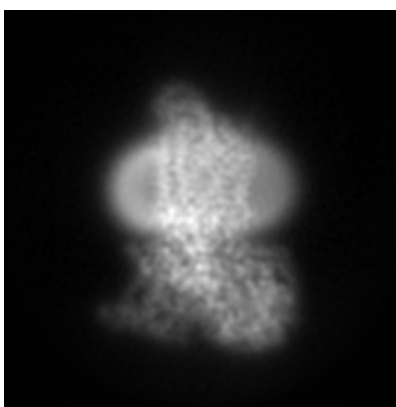


Z

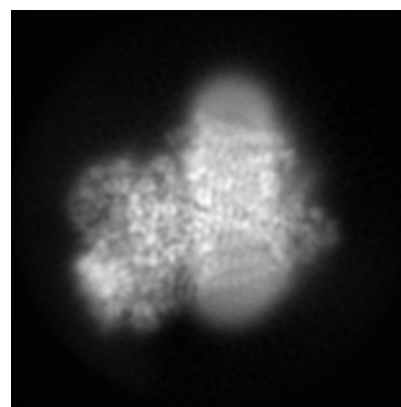
6.1.2 Raw map



X



Y

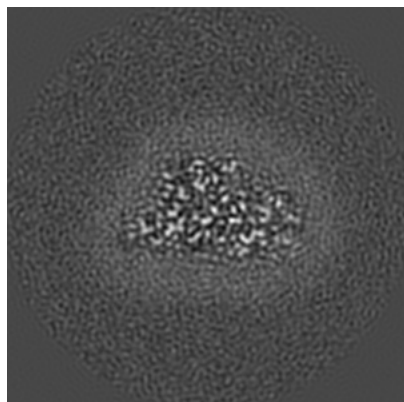


Z

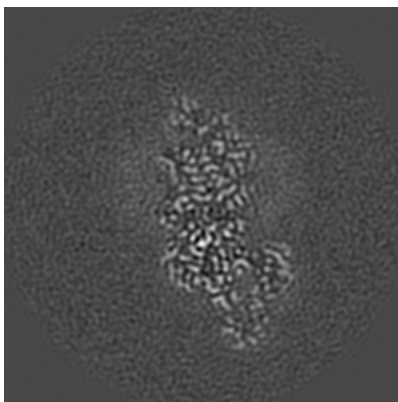
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

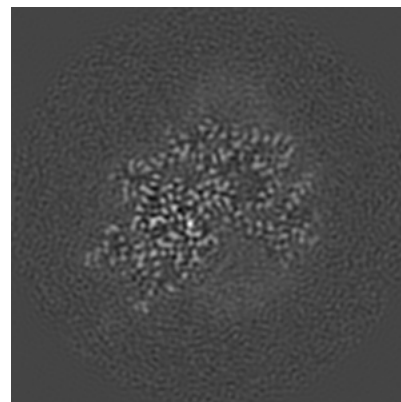
6.2.1 Primary map



X Index: 100

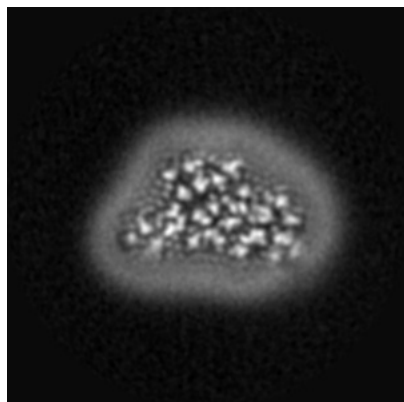


Y Index: 100

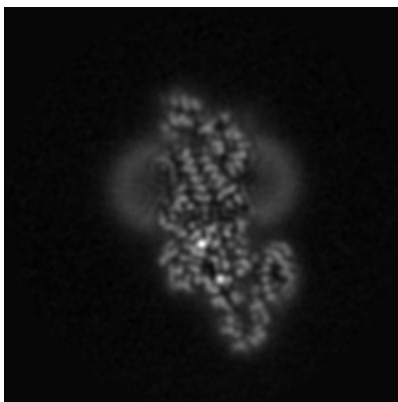


Z Index: 100

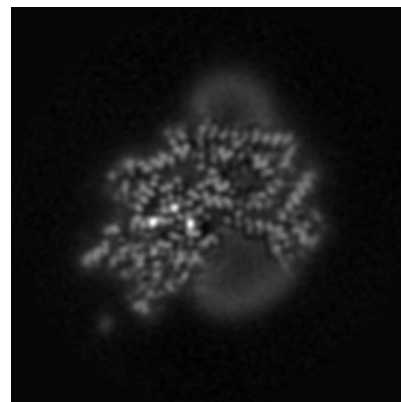
6.2.2 Raw map



X Index: 100



Y Index: 100

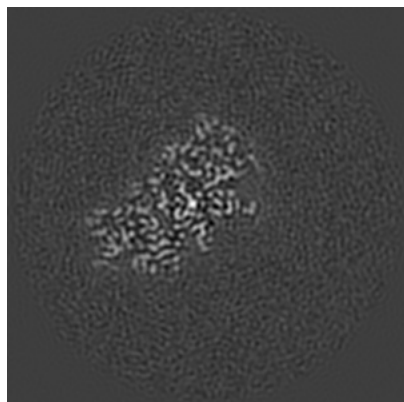


Z Index: 100

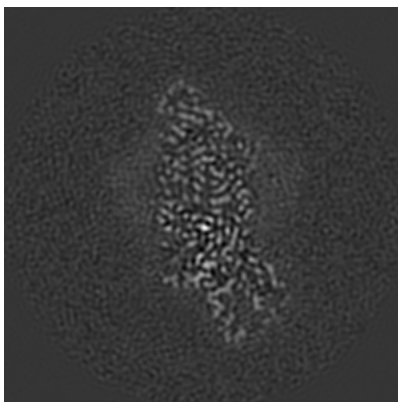
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

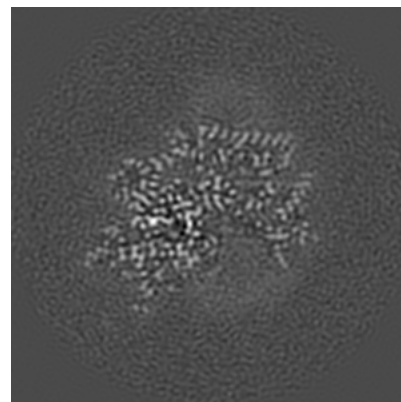
6.3.1 Primary map



X Index: 71

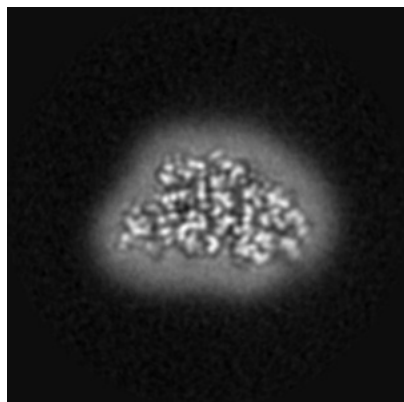


Y Index: 91

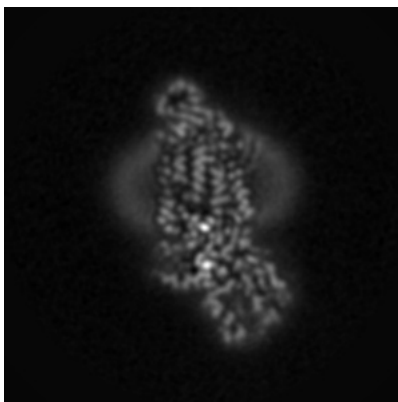


Z Index: 101

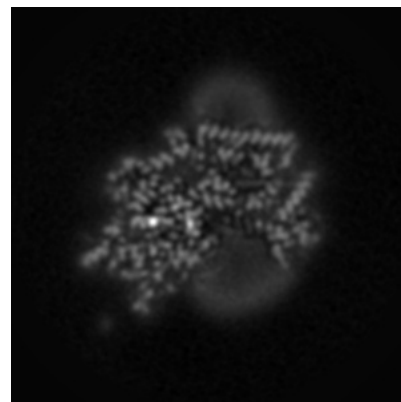
6.3.2 Raw map



X Index: 95



Y Index: 91

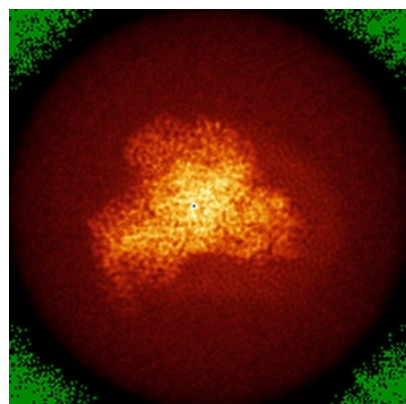


Z Index: 101

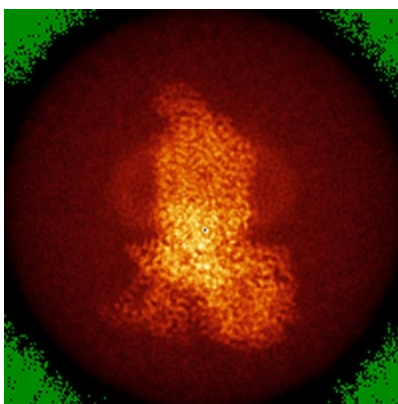
The images above show the largest variance slices of the map in three orthogonal directions.

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

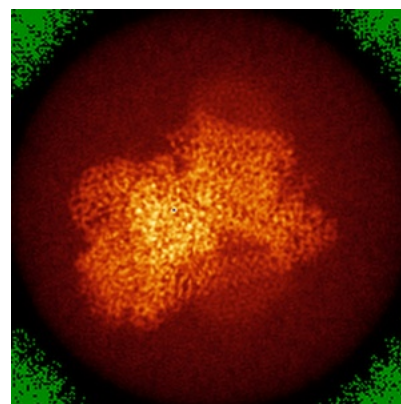
6.4.1 Primary map



X

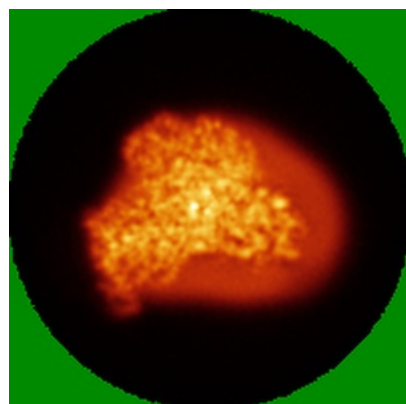


Y

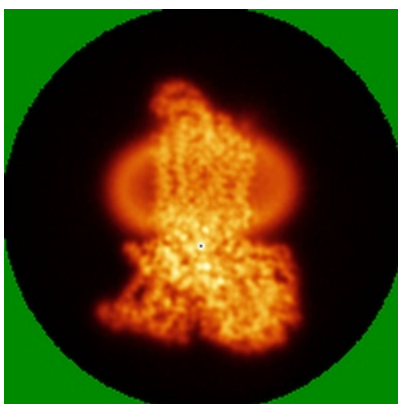


Z

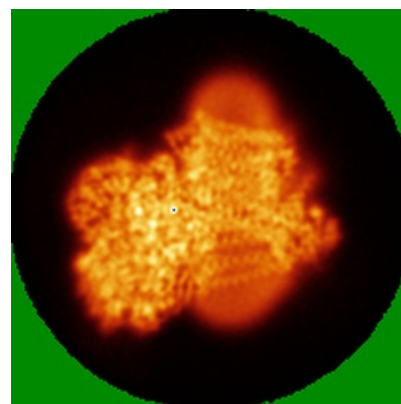
6.4.2 Raw map



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 0.06. 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.

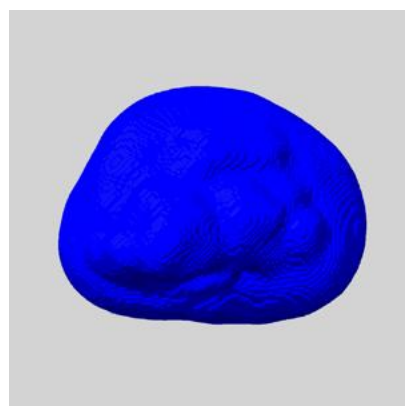
6.6 Mask visualisation [i](#)

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

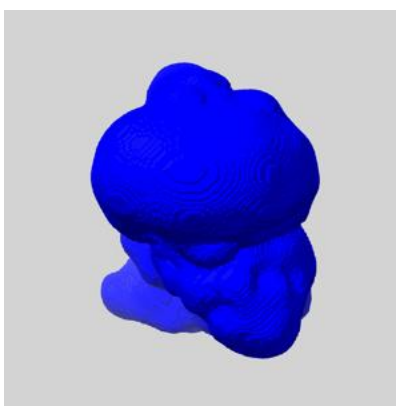
A mask typically either:

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

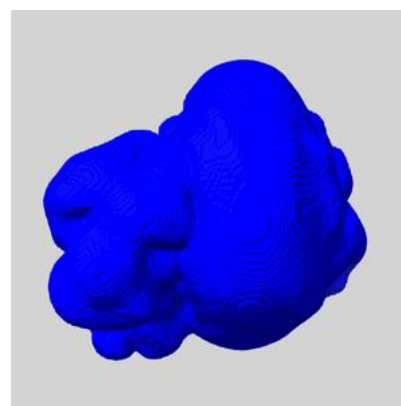
6.6.1 emd_36984_msk_1.map [i](#)



X



Y

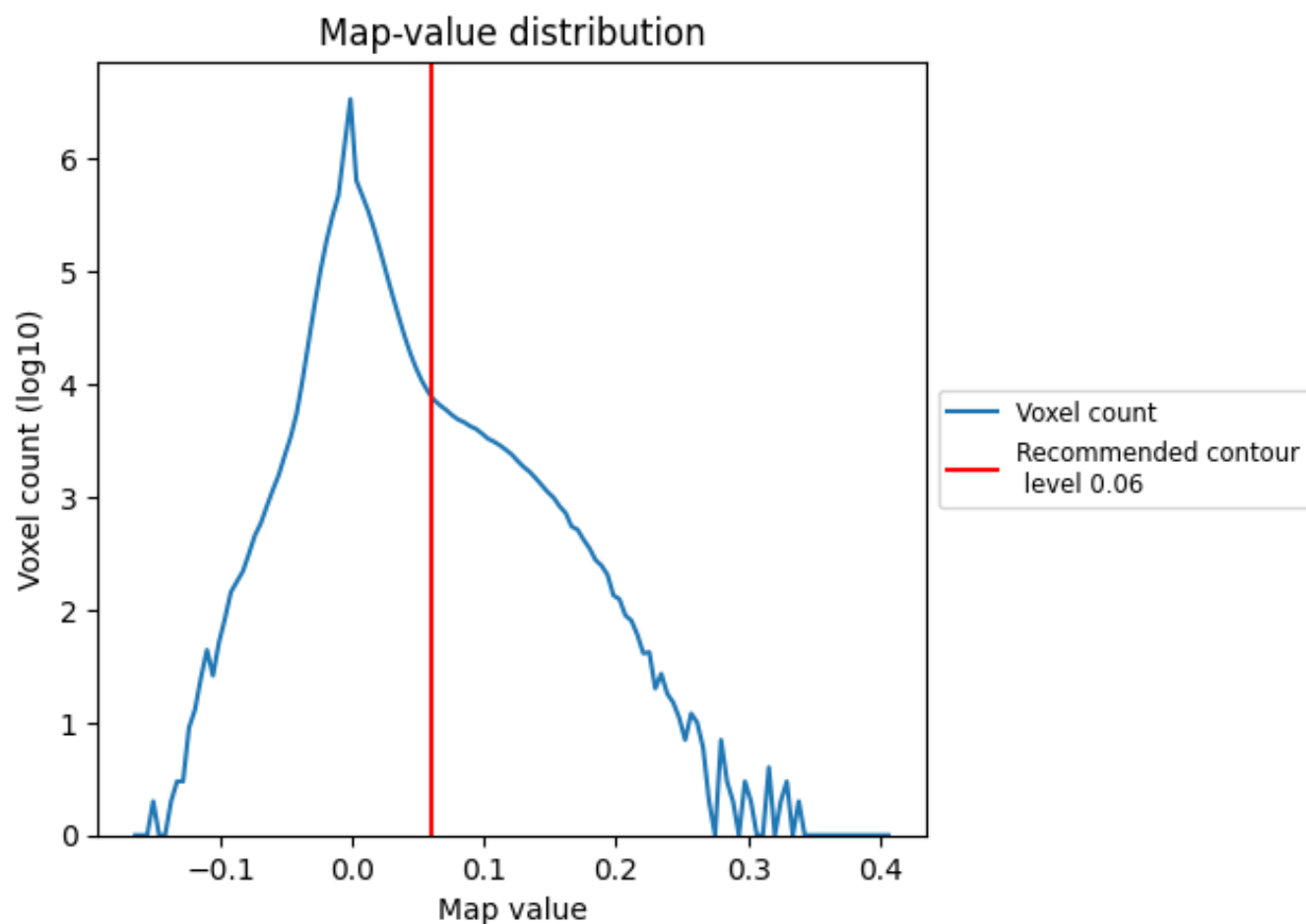


Z

7 Map analysis [i](#)

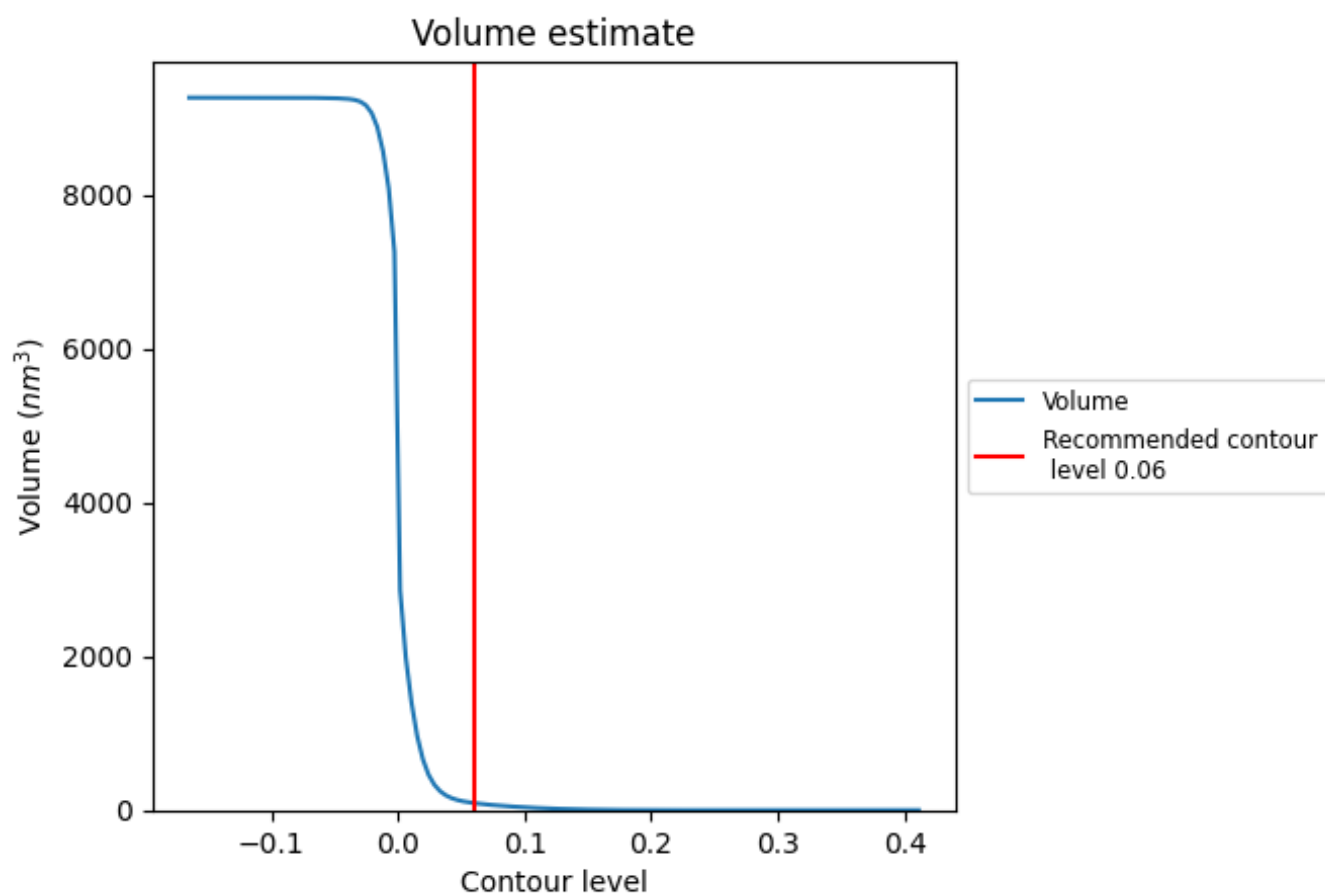
This section contains the results of statistical analysis of the map.

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.

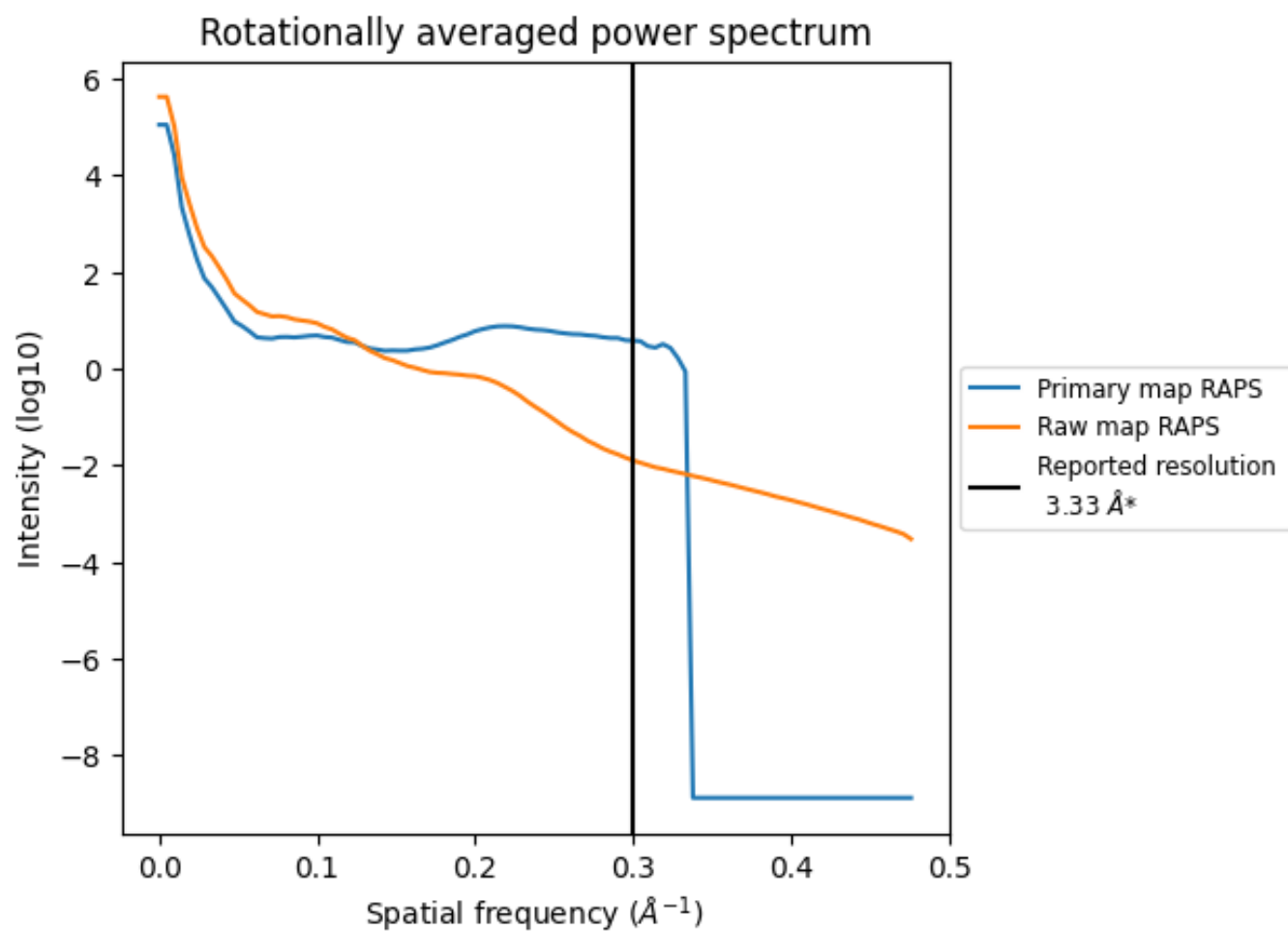
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm^3 ; this corresponds to an approximate mass of 83 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 ⓘ

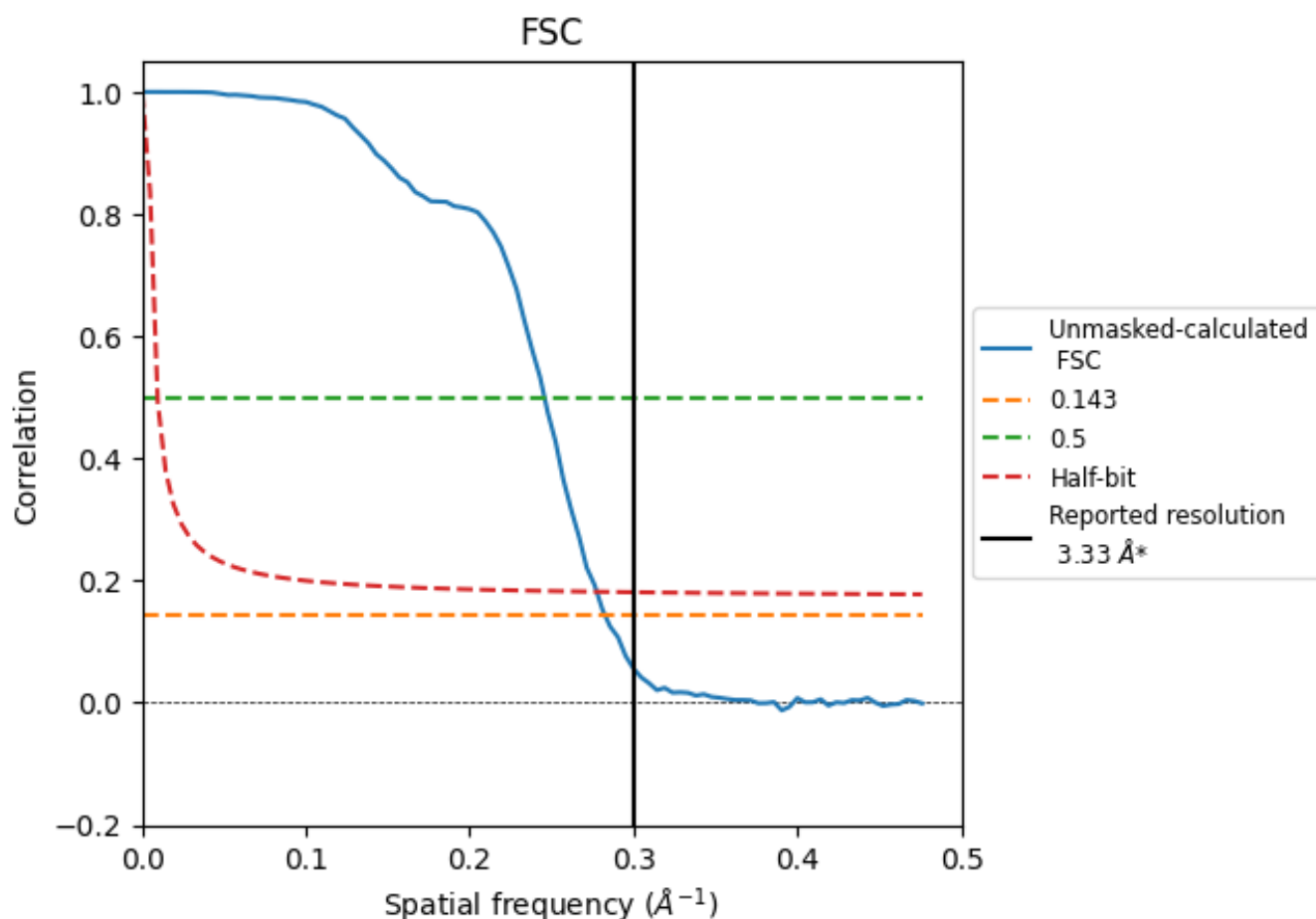


*Reported resolution corresponds to spatial frequency of $0.300 \text{ \AA}^{-1}$

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 $0.300 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

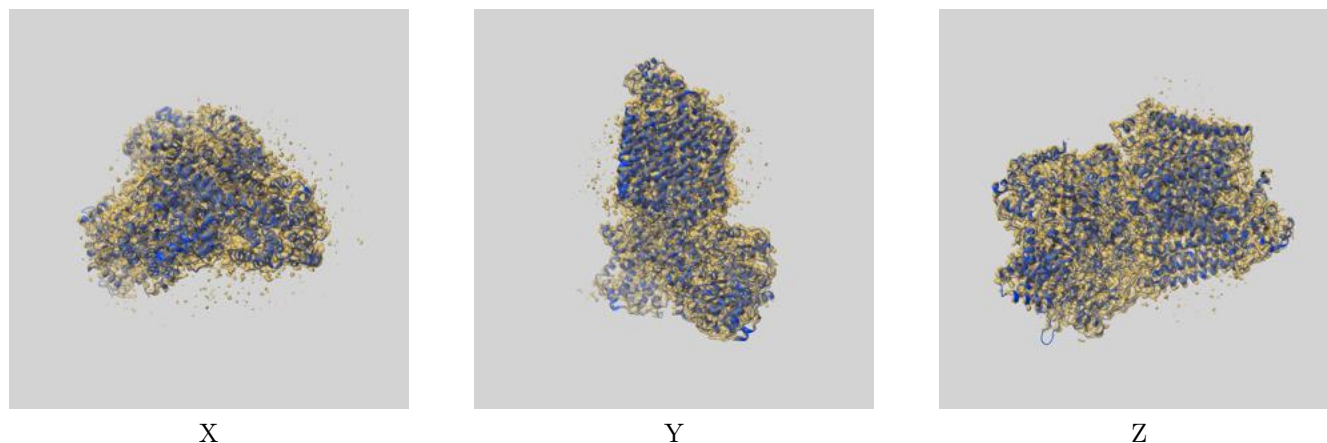
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.07	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

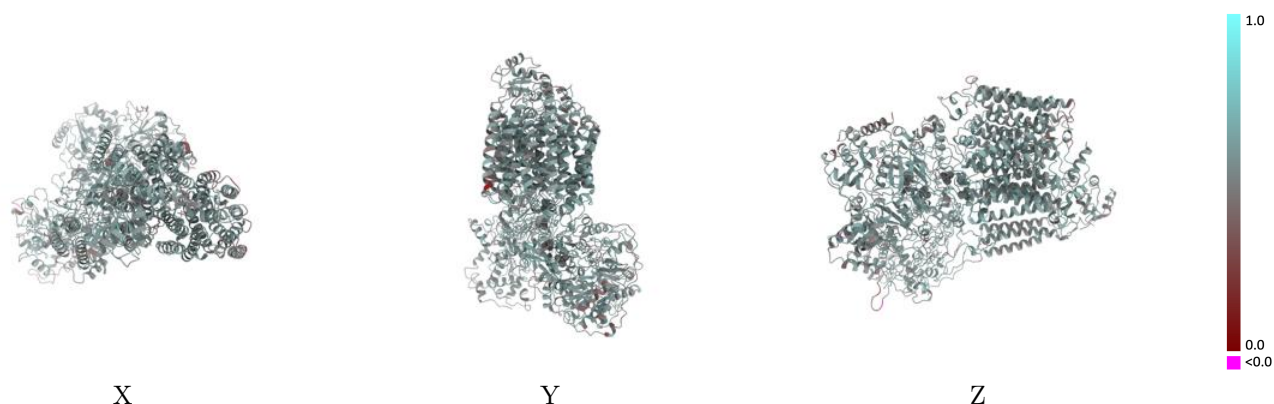
This section contains information regarding the fit between EMDB map EMD-36984 and PDB model 8K9E. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



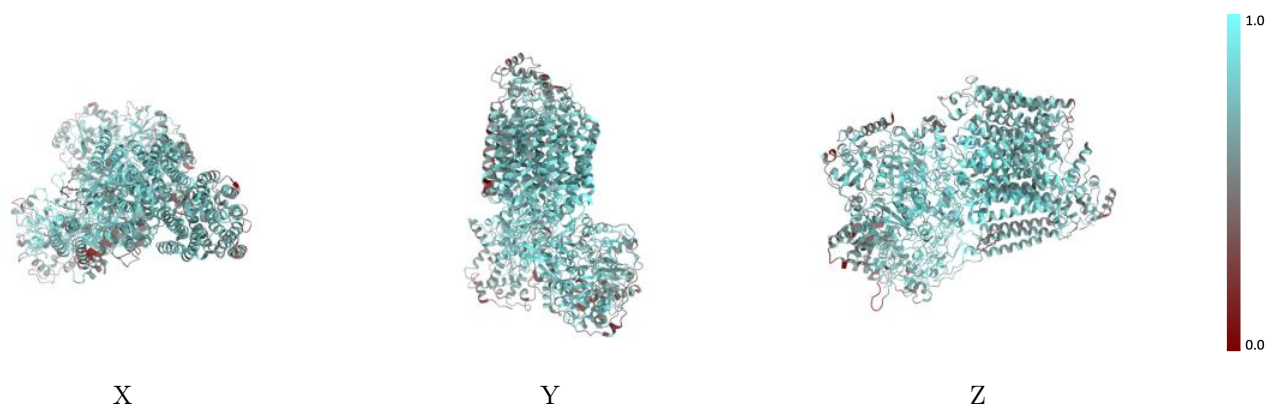
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



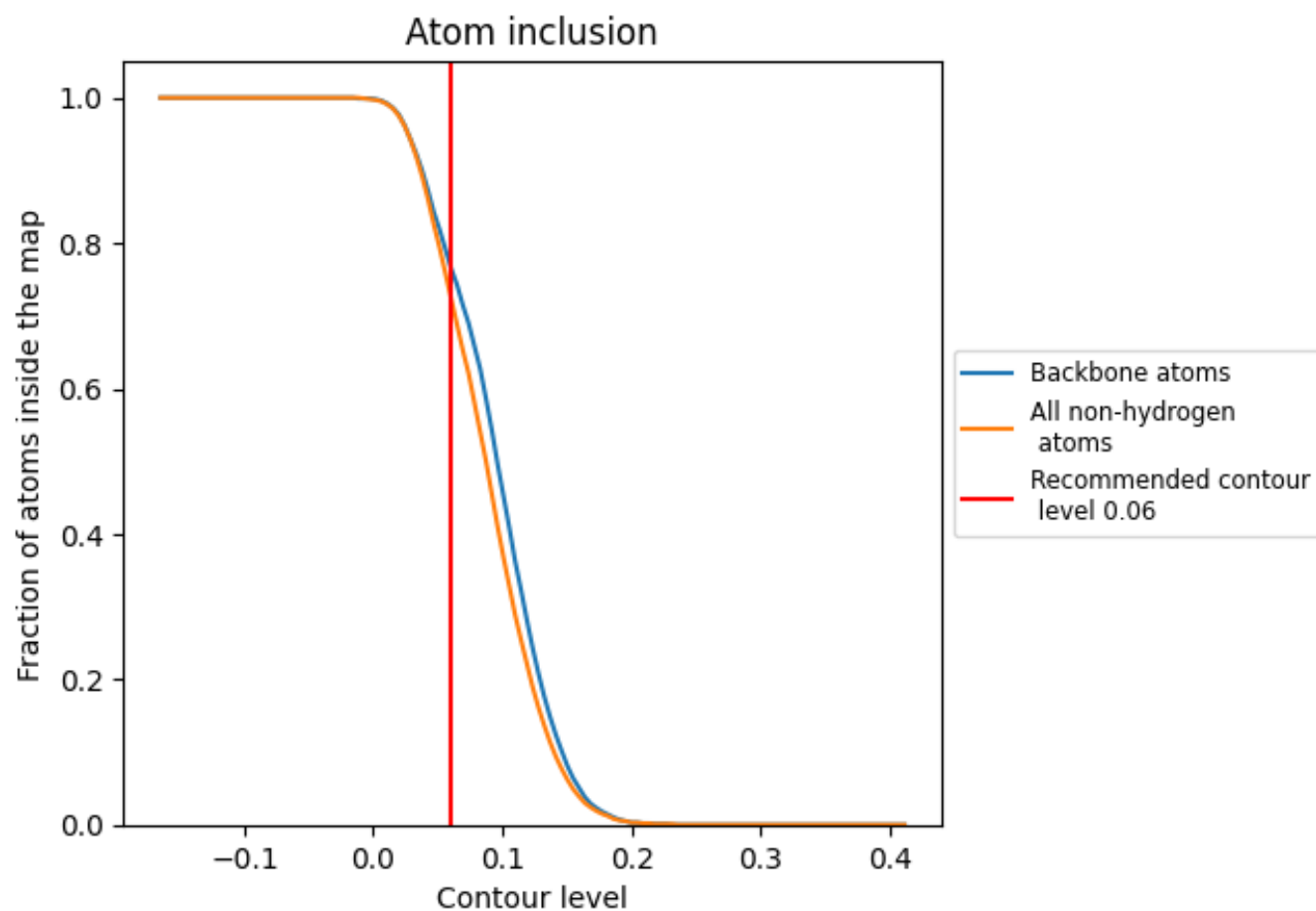
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.5480
A	0.7880	0.5580
B	0.7320	0.5510
C	0.7990	0.5670
D	0.6730	0.5400
E	0.6480	0.5350
F	0.7080	0.5340
G	0.5120	0.5020
I	0.5480	0.5320

1.0

0.0

<0.0