



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:01 AM UTC

PDB ID : 8X2J / pdb_00008x2j
EMDB ID : EMD-38012
Title : Cryo-EM structure of the photosynthetic alternative complex III with a quinone inhibitor HQNO from *Chloroflexus aurantiacus*
Authors : Xu, X.
Deposited on : 2023-11-09
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

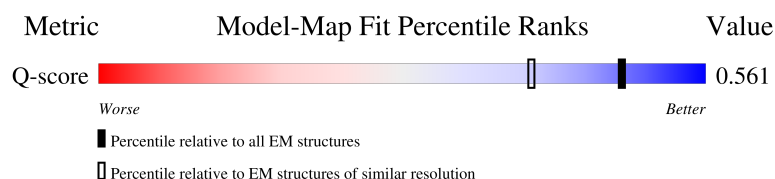
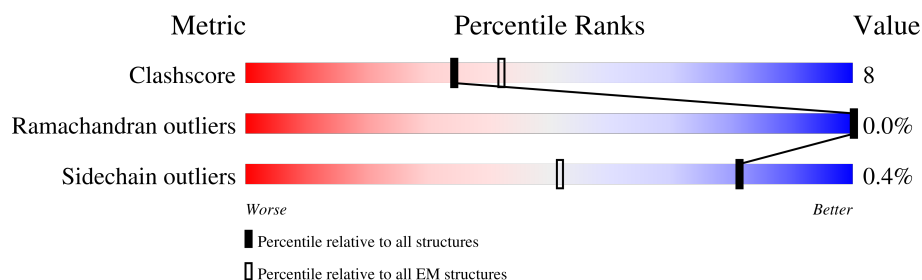
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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% 19%
2	B	1029	72% 21% 8%
3	C	486	75% 17% 8%
4	D	179	77% 21% .

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

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
11	F3S	B	1104	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 19918 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		

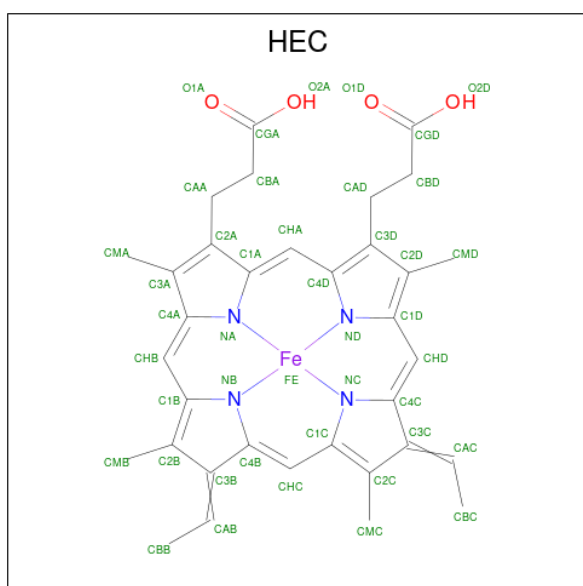
- Molecule 7 is a protein called Uncharacterized protein.

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: $C_{34}H_{34}FeN_4O_4$).



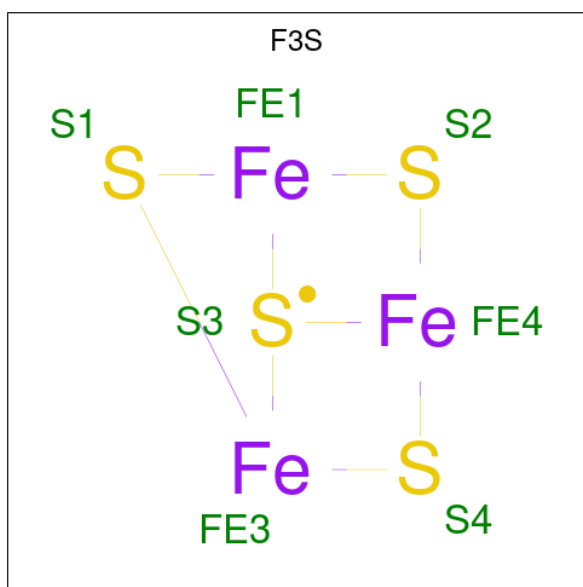
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



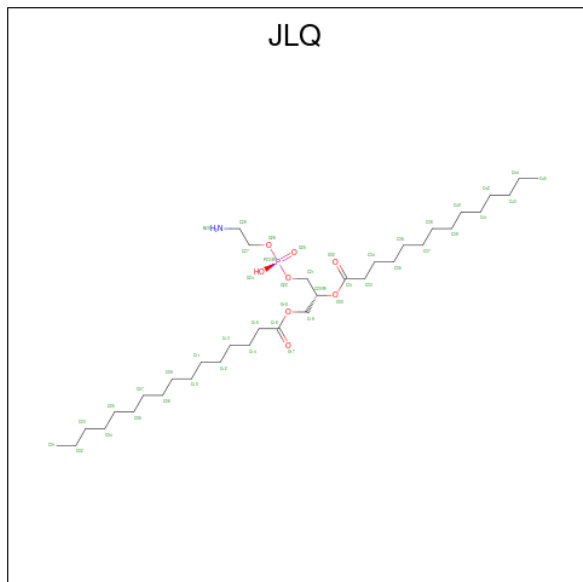
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	
10	B	1	Total	Fe	S	0
			8	4	4	

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



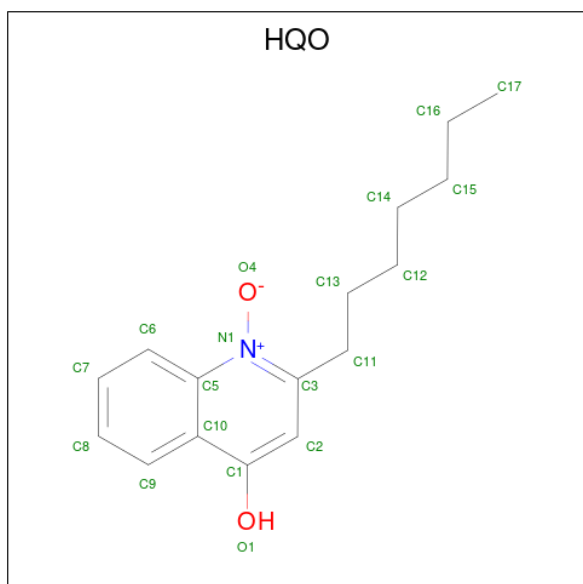
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	Fe	S	0
			7	3	4	

- Molecule 12 is [(2 {R})-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-tetradecanoyloxy-propyl] hexadecanoate (CCD ID: JLQ) (formula: $C_{35}H_{70}NO_8P$).



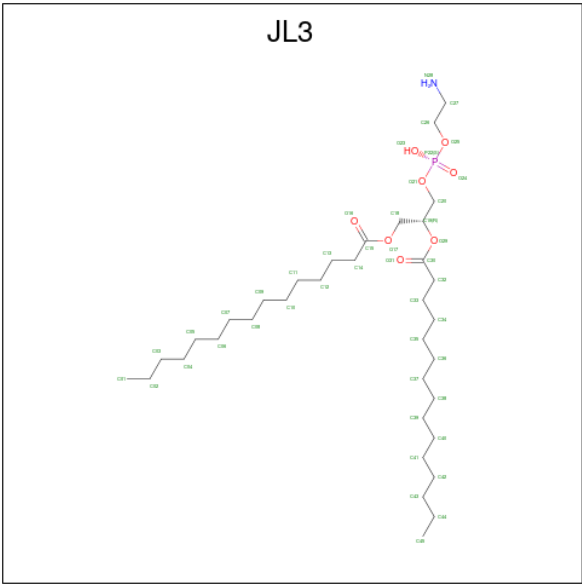
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (CCD ID: HQO) (formula: $C_{16}H_{21}NO_2$).



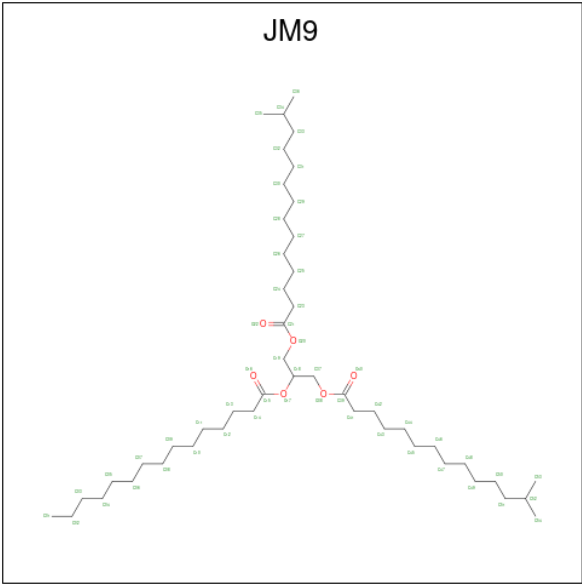
Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total	C	N	O	0
			19	16	1	2	

- 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
			Total	C	N	O	P	
14	C	1	45	35	1	8	1	0

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

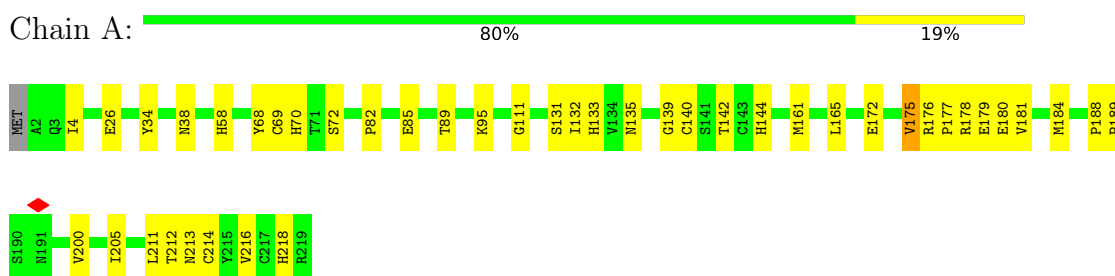


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	C	1	54	48	6	0

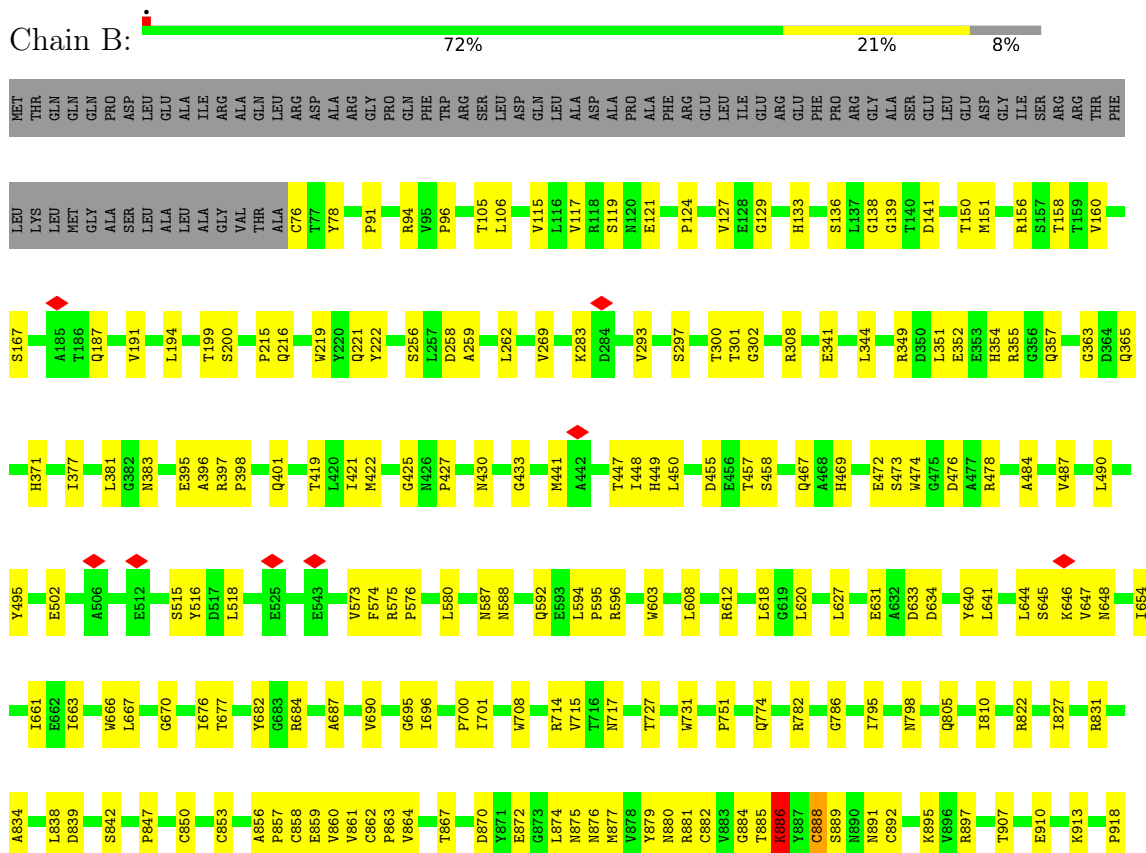
3 Residue-property plots

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

- Molecule 1: Cytochrome c7-like domain-containing protein



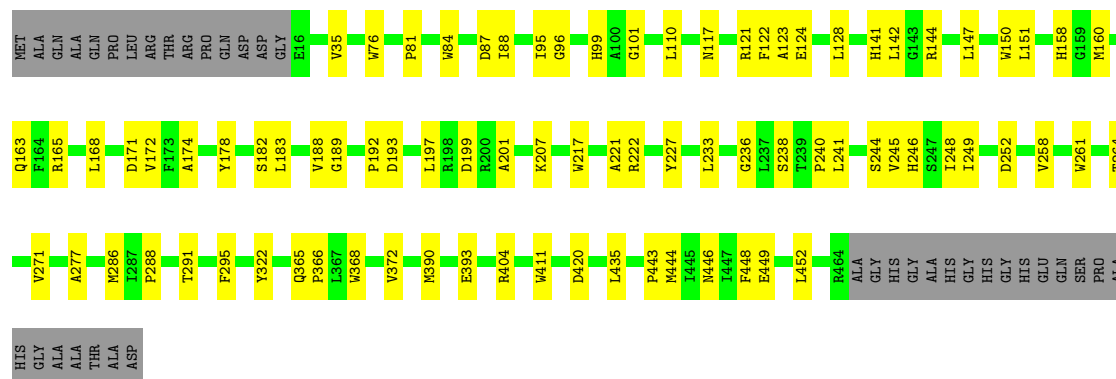
- Molecule 2: Fe-S-cluster-containing hydrogenase components 1-like protein





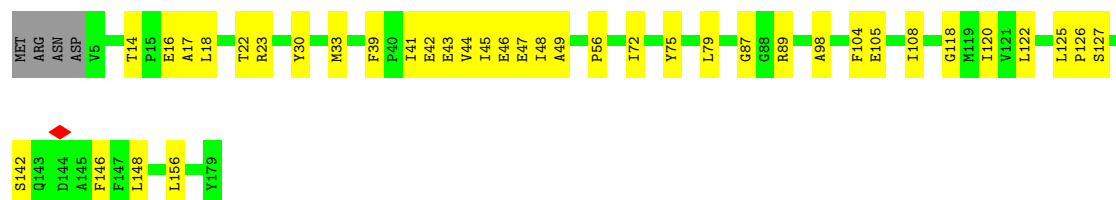
• Molecule 3: Polysulphide reductase NrfD

Chain C: 75% 17% 8%



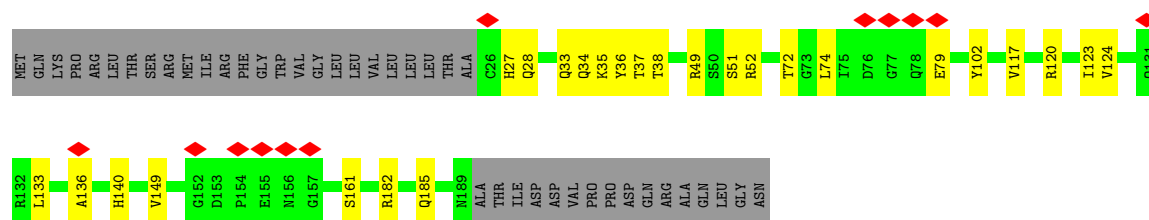
• Molecule 4: Quinol:cytochrome c oxidoreductase membrane protein

Chain D: 77% 21% .



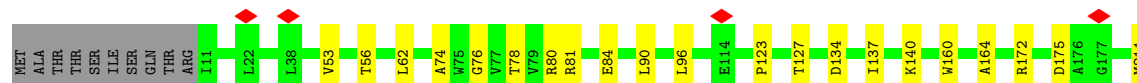
• Molecule 5: Cytochrome c domain-containing protein

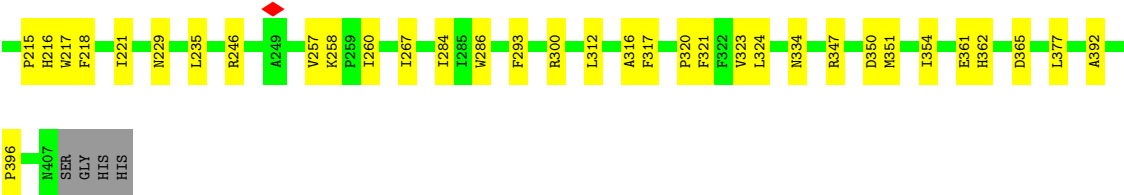
Chain E: 6% 67% 13% 20%



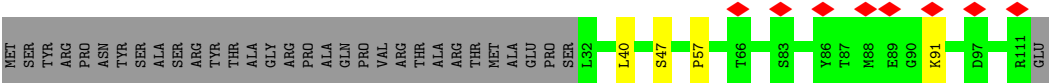
• Molecule 6: Quinol:cytochrome c oxidoreductase quinone-binding subunit 2

Chain F: 83% 13% .





● 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	160264	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)	1000	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.694	Depositor
Minimum map value	-1.435	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	200.88, 200.88, 200.88	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: HEC, F3S, JM9, JL3, SF4, HQO, 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	0.28	0/1812	0.55	0/2472
2	B	0.29	0/7518	0.52	0/10249
3	C	0.26	0/3787	0.51	0/5179
4	D	0.36	0/1388	0.58	0/1895
5	E	0.19	0/1327	0.43	0/1803
6	F	0.25	0/3226	0.52	0/4408
7	G	0.19	0/635	0.49	0/865
8	I	0.22	0/318	0.48	0/436
All	All	0.27	0/20011	0.52	0/27307

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1713	36	0
2	B	7350	0	7178	159	0
3	C	3655	0	3686	64	0
4	D	1350	0	1341	37	0
5	E	1292	0	1216	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3128	0	3175	31	0
7	G	623	0	660	4	0
8	I	305	0	302	5	0
9	A	215	0	150	10	0
9	E	43	0	30	2	0
10	B	24	0	0	1	0
11	B	7	0	0	5	0
12	C	45	0	0	0	0
13	C	19	0	20	1	0
14	C	45	0	0	0	0
15	C	54	0	0	0	0
All	All	19918	0	19471	319	0

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

All (319) 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)
2:B:888:CYS:SG	11:B:1104:F3S:FE1	1.42	1.09
4:D:156:LEU:HD12	4:D:156:LEU:O	1.65	0.95
3:C:171:ASP:OD1	3:C:248:ILE:HG22	1.80	0.81
5:E:124:VAL:O	5:E:124:VAL:HG13	1.82	0.80
2:B:620:LEU:HD13	2:B:647:VAL:HG21	1.66	0.78
4:D:120:ILE:HD12	4:D:125:LEU:HD23	1.66	0.77
4:D:45:ILE:HG23	4:D:49:ALA:HB3	1.69	0.75
2:B:297:SER:HB3	2:B:677:THR:HG21	1.70	0.74
1:A:216:VAL:HG13	9:A:302:HEC:HBA1	1.74	0.70
5:E:123:ILE:O	5:E:124:VAL:HG12	1.91	0.69
2:B:881:ARG:HH12	3:C:150:TRP:HB3	1.58	0.69
4:D:156:LEU:O	4:D:156:LEU:CD1	2.41	0.69
1:A:142:THR:HG23	1:A:176:ARG:HH21	1.57	0.68
2:B:133:HIS:HB3	2:B:136:SER:HB3	1.77	0.67
4:D:30:TYR:CE1	4:D:156:LEU:CD1	2.78	0.67
2:B:888:CYS:HG	11:B:1104:F3S:FE1	0.38	0.66
4:D:75:TYR:O	4:D:79:LEU:HB2	1.96	0.66
9:A:301:HEC:HHB	2:B:881:ARG:HD3	1.77	0.66
2:B:888:CYS:SG	11:B:1104:F3S:S1	2.95	0.64
2:B:618:LEU:HD22	2:B:717:ASN:HB2	1.79	0.64
2:B:870:ASP:HB2	2:B:874:LEU:H	1.63	0.64
2:B:119:SER:HB3	2:B:490:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:HIS:HD1	2:B:458:SER:HG	1.48	0.61
3:C:277:ALA:HB2	3:C:390:MET:HG2	1.83	0.61
1:A:211:LEU:HD21	9:A:302:HEC:HBD1	1.83	0.61
2:B:676:ILE:HD12	2:B:715:VAL:HG21	1.83	0.61
3:C:171:ASP:OD1	3:C:248:ILE:CG2	2.48	0.61
2:B:425:GLY:O	2:B:430:ASN:ND2	2.35	0.60
6:F:300:ARG:NH2	6:F:354:ILE:O	2.34	0.59
1:A:70:HIS:HE1	9:A:304:HEC:ND	2.01	0.59
2:B:94:ARG:NH1	5:E:52:ARG:O	2.35	0.59
4:D:30:TYR:CE1	4:D:156:LEU:HD12	2.38	0.59
2:B:862:CYS:O	3:C:163:GLN:NE2	2.34	0.59
2:B:78:TYR:O	5:E:28:GLN:NE2	2.35	0.58
6:F:80:ARG:HD2	6:F:396:PRO:HG3	1.85	0.58
2:B:573:VAL:HB	2:B:677:THR:HG22	1.84	0.58
2:B:805:GLN:HG3	2:B:810:ILE:HB	1.86	0.58
2:B:221:GLN:HG2	2:B:397:ARG:HH21	1.69	0.58
2:B:863:PRO:HB3	3:C:168:LEU:HB2	1.85	0.58
2:B:881:ARG:HE	3:C:160:MET:HE2	1.69	0.58
2:B:150:THR:OG1	2:B:588:ASN:ND2	2.37	0.57
5:E:49:ARG:O	5:E:52:ARG:NH2	2.37	0.57
1:A:140:CYS:HB2	1:A:184:MET:HE1	1.87	0.57
2:B:684:ARG:HE	2:B:687:ALA:HB2	1.70	0.57
3:C:221:ALA:HB1	4:D:45:ILE:HG12	1.86	0.57
1:A:135:ASN:O	1:A:178:ARG:NE	2.36	0.57
6:F:81:ARG:NH1	6:F:175:ASP:OD2	2.38	0.57
2:B:907:THR:HA	5:E:34:GLN:HG2	1.87	0.57
1:A:218:HIS:CE1	9:A:301:HEC:ND	2.73	0.56
2:B:885:THR:HG22	3:C:142:LEU:HD11	1.87	0.56
3:C:264:THR:HA	6:F:284:ILE:HD13	1.87	0.56
6:F:134:ASP:OD2	6:F:216:HIS:NE2	2.36	0.56
1:A:200:VAL:HG13	1:A:205:ILE:HB	1.87	0.56
6:F:320:PRO:O	6:F:324:LEU:HB2	2.06	0.56
4:D:120:ILE:O	4:D:126:PRO:HD3	2.06	0.56
4:D:118:GLY:O	4:D:122:LEU:HB2	2.06	0.56
6:F:229:ASN:ND2	6:F:351:MET:SD	2.79	0.56
1:A:69:CYS:HB3	1:A:82:PRO:HG3	1.88	0.56
2:B:352:GLU:HA	2:B:355:ARG:HE	1.71	0.56
4:D:22:THR:HG21	4:D:44:VAL:HG13	1.86	0.56
2:B:864:VAL:HB	2:B:881:ARG:CZ	2.36	0.56
3:C:121:ARG:NH2	3:C:446:ASN:OD1	2.38	0.55
5:E:124:VAL:O	5:E:124:VAL:CG1	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ARG:NH2	2:B:121:GLU:OE1	2.39	0.55
2:B:441:MET:HE3	2:B:447:THR:HG21	1.88	0.55
4:D:46:GLU:HG3	4:D:47:GLU:OE1	2.06	0.55
2:B:427:PRO:HD2	2:B:457:THR:HG21	1.87	0.55
2:B:258:ASP:O	2:B:365:GLN:NE2	2.40	0.55
4:D:30:TYR:CE1	4:D:156:LEU:HD11	2.42	0.55
2:B:888:CYS:HB2	2:B:897:ARG:NE	2.22	0.55
3:C:35:VAL:HG11	3:C:444:MET:HE1	1.88	0.54
6:F:62:LEU:HD12	6:F:164:ALA:HB2	1.89	0.54
2:B:478:ARG:HA	2:B:484:ALA:H	1.72	0.54
3:C:249:ILE:O	3:C:252:ASP:OD1	2.23	0.54
3:C:217:TRP:HA	4:D:125:LEU:HD11	1.90	0.54
4:D:87:GLY:O	4:D:89:ARG:NH1	2.38	0.54
2:B:256:SER:HB2	2:B:293:VAL:HG12	1.89	0.54
1:A:139:GLY:HA3	1:A:176:ARG:CZ	2.38	0.54
3:C:449:GLU:HA	3:C:452:LEU:HB3	1.89	0.54
2:B:858:CYS:SG	2:B:875:ASN:ND2	2.80	0.54
2:B:913:LYS:HG2	5:E:34:GLN:HB3	1.90	0.54
2:B:676:ILE:CD1	2:B:715:VAL:HG21	2.38	0.53
2:B:850:CYS:SG	2:B:930:LYS:NZ	2.81	0.53
2:B:877:MET:SD	2:B:897:ARG:NH2	2.81	0.53
6:F:90:LEU:HD13	6:F:160:TRP:HB3	1.89	0.53
2:B:640:TYR:O	2:B:644:LEU:HG	2.09	0.53
5:E:136:ALA:O	5:E:182:ARG:NH2	2.38	0.53
2:B:654:ILE:HG12	2:B:715:VAL:HG22	1.90	0.53
6:F:96:LEU:HD13	6:F:377:LEU:HD11	1.90	0.53
2:B:381:LEU:HD23	2:B:383:ASN:HD21	1.73	0.53
3:C:221:ALA:HB3	4:D:48:ILE:HD11	1.91	0.53
2:B:575:ARG:HE	2:B:576:PRO:HD2	1.74	0.52
2:B:283:LYS:HG2	2:B:751:PRO:HG2	1.90	0.52
2:B:222:TYR:HA	2:B:401:GLN:HB3	1.92	0.52
2:B:262:LEU:HD12	2:B:301:THR:HA	1.90	0.52
2:B:986:ASN:O	2:B:991:LYS:NZ	2.42	0.52
2:B:117:VAL:HG22	2:B:127:VAL:HG22	1.91	0.52
4:D:156:LEU:HD12	4:D:156:LEU:C	2.34	0.52
2:B:774:GLN:NE2	6:F:286:TRP:O	2.43	0.52
5:E:149:VAL:HG11	9:E:301:HEC:HBD1	1.92	0.52
2:B:884:GLY:HA3	3:C:142:LEU:O	2.10	0.52
3:C:117:ASN:ND2	3:C:449:GLU:O	2.41	0.52
3:C:201:ALA:HB3	3:C:207:LYS:HD3	1.92	0.52
6:F:316:ALA:HB1	6:F:347:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:182:ARG:NH1	5:E:185:GLN:OE1	2.43	0.51
4:D:30:TYR:CD1	4:D:156:LEU:HD11	2.46	0.51
2:B:199:THR:HG22	2:B:395:GLU:HA	1.92	0.51
2:B:219:TRP:HB3	2:B:397:ARG:NH1	2.25	0.51
3:C:96:GLY:HA2	3:C:246:HIS:HE1	1.75	0.51
3:C:121:ARG:NH2	3:C:189:GLY:O	2.42	0.51
4:D:23:ARG:NH1	4:D:47:GLU:OE2	2.44	0.51
2:B:91:PRO:HB2	2:B:94:ARG:HB2	1.93	0.51
3:C:178:TYR:HB2	3:C:245:VAL:HG21	1.91	0.51
5:E:38:THR:O	5:E:51:SER:OG	2.29	0.51
2:B:888:CYS:SG	11:B:1104:F3S:S3	3.10	0.50
4:D:33:MET:HE3	4:D:148:LEU:HD11	1.93	0.50
2:B:645:SER:O	2:B:646:LYS:HB3	2.12	0.50
2:B:822:ARG:NH2	3:C:76:TRP:O	2.44	0.50
3:C:147:LEU:HD11	5:E:27:HIS:HE1	1.76	0.50
2:B:882:CYS:O	3:C:144:ARG:NH2	2.40	0.50
2:B:885:THR:HG22	3:C:142:LEU:CD1	2.42	0.50
2:B:921:THR:OG1	5:E:33:GLN:NE2	2.42	0.50
6:F:76:GLY:O	6:F:80:ARG:HB2	2.12	0.50
1:A:139:GLY:HA2	1:A:181:VAL:HG13	1.94	0.50
3:C:366:PRO:HB2	3:C:372:VAL:HG11	1.92	0.50
1:A:4:ILE:HD13	3:C:207:LYS:HB3	1.94	0.50
2:B:354:HIS:HB3	2:B:357:GLN:HB2	1.94	0.49
5:E:72:THR:HG23	5:E:74:LEU:H	1.77	0.49
1:A:144:HIS:CE1	9:A:303:HEC:ND	2.80	0.49
2:B:308:ARG:NH1	2:B:670:GLY:O	2.45	0.49
3:C:122:PHE:HB3	3:C:286:MET:HE1	1.94	0.49
3:C:258:VAL:HB	3:C:261:TRP:HB2	1.93	0.49
2:B:139:GLY:O	2:B:269:VAL:HG11	2.13	0.49
2:B:641:LEU:HD22	2:B:838:LEU:HD12	1.94	0.49
2:B:892:CYS:O	2:B:895:LYS:NZ	2.42	0.49
3:C:87:ASP:OD1	3:C:87:ASP:N	2.46	0.49
4:D:14:THR:HG23	4:D:17:ALA:H	1.76	0.49
1:A:132:ILE:HB	2:B:943:ILE:HG23	1.95	0.49
1:A:214:CYS:HB2	2:B:876:ASN:HD22	1.78	0.49
4:D:125:LEU:O	4:D:127:SER:N	2.38	0.49
2:B:918:PRO:HA	5:E:35:LYS:HD2	1.93	0.48
5:E:123:ILE:O	5:E:124:VAL:CG1	2.58	0.48
2:B:341:GLU:HA	2:B:344:LEU:HD12	1.96	0.48
2:B:455:ASP:OD1	2:B:684:ARG:NH2	2.47	0.48
2:B:515:SER:HA	2:B:518:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:595:PRO:HG3	2:B:727:THR:HG21	1.96	0.48
3:C:264:THR:HG23	6:F:221:ILE:H	1.78	0.48
6:F:172:ARG:HE	6:F:392:ALA:HB2	1.79	0.48
1:A:111:GLY:O	5:E:49:ARG:NH2	2.47	0.47
6:F:211:MET:HE3	6:F:218:PHE:HA	1.95	0.47
4:D:125:LEU:N	4:D:126:PRO:CD	2.78	0.47
6:F:81:ARG:NE	6:F:84:GLU:OE1	2.46	0.47
2:B:221:GLN:HG2	2:B:397:ARG:NH2	2.29	0.47
3:C:452:LEU:HB2	4:D:39:PHE:HB2	1.96	0.47
2:B:194:LEU:HB3	2:B:422:MET:HG3	1.97	0.47
3:C:192:PRO:HG2	3:C:448:PHE:CE1	2.49	0.47
2:B:618:LEU:HD22	2:B:717:ASN:CA	2.44	0.47
2:B:731:TRP:CD1	2:B:831:ARG:HH12	2.32	0.47
2:B:608:LEU:HD23	2:B:666:TRP:HB3	1.95	0.47
2:B:897:ARG:HA	2:B:930:LYS:HB3	1.95	0.47
3:C:238:SER:HA	3:C:241:LEU:HB3	1.96	0.47
2:B:857:PRO:HB2	2:B:891:ASN:O	2.14	0.47
3:C:174:ALA:HB1	3:C:245:VAL:HG22	1.95	0.47
2:B:592:GLN:HG3	2:B:603:TRP:HA	1.97	0.46
2:B:682:TYR:HB3	2:B:695:GLY:HA3	1.97	0.46
2:B:879:TYR:HE1	2:B:929:GLU:HA	1.80	0.46
6:F:246:ARG:NH2	6:F:334:ASN:OD1	2.47	0.46
2:B:618:LEU:HD22	2:B:717:ASN:N	2.30	0.46
3:C:124:GLU:OE2	3:C:182:SER:OG	2.33	0.46
2:B:618:LEU:HD22	2:B:717:ASN:CB	2.45	0.46
6:F:320:PRO:HA	6:F:323:VAL:HG22	1.97	0.46
2:B:877:MET:CE	2:B:882:CYS:HB2	2.46	0.46
7:G:40:LEU:HD13	8:I:21:THR:HG23	1.96	0.46
2:B:580:LEU:HD21	2:B:592:GLN:HE22	1.80	0.46
2:B:910:GLU:OE1	5:E:36:TYR:OH	2.32	0.46
3:C:171:ASP:HB3	13:C:502:HQQ:O4	2.16	0.46
3:C:233:LEU:HD11	4:D:56:PRO:HG3	1.97	0.46
3:C:165:ARG:HA	4:D:98:ALA:HB1	1.97	0.46
6:F:317:PHE:O	6:F:321:PHE:HB3	2.16	0.46
1:A:218:HIS:CG	2:B:880:ASN:HD21	2.33	0.46
2:B:199:THR:HB	2:B:478:ARG:HB2	1.98	0.46
2:B:648:ASN:HD21	2:B:731:TRP:HH2	1.64	0.46
4:D:18:LEU:HD22	4:D:146:PHE:HB3	1.98	0.46
2:B:396:ALA:O	2:B:398:PRO:HD3	2.16	0.46
2:B:870:ASP:HB3	2:B:872:GLU:H	1.81	0.46
2:B:661:ILE:HB	2:B:701:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:ILE:O	4:D:42:GLU:HB3	2.15	0.45
2:B:156:ARG:NH2	2:B:472:GLU:OE2	2.48	0.45
3:C:197:LEU:HD11	3:C:443:PRO:HD3	1.97	0.45
5:E:37:THR:HG22	5:E:38:THR:H	1.80	0.45
1:A:34:TYR:OH	2:B:76:CYS:O	2.32	0.45
1:A:72:SER:O	1:A:72:SER:OG	2.33	0.45
9:A:301:HEC:HMA1	2:B:881:ARG:HD2	1.98	0.45
2:B:377:ILE:O	2:B:381:LEU:HB2	2.16	0.45
2:B:654:ILE:HG12	2:B:715:VAL:HG13	1.99	0.45
2:B:633:ASP:OD1	2:B:633:ASP:N	2.49	0.45
2:B:867:THR:OG1	2:B:875:ASN:OD1	2.35	0.45
3:C:110:LEU:HD11	3:C:236:GLY:HA2	1.97	0.45
6:F:53:VAL:O	6:F:56:THR:OG1	2.26	0.45
1:A:165:LEU:HD22	1:A:212:THR:HG23	1.99	0.45
2:B:860:VAL:HG13	2:B:861:VAL:HG13	1.99	0.45
5:E:161:SER:HB2	9:E:301:HEC:HBD2	1.99	0.45
2:B:574:PHE:HB2	2:B:708:TRP:HA	1.98	0.45
1:A:72:SER:HB2	2:B:96:PRO:HD2	1.99	0.45
2:B:106:LEU:HD12	2:B:115:VAL:HG11	1.98	0.45
2:B:786:GLY:HA3	2:B:982:ILE:HD11	1.98	0.45
3:C:420:ASP:OD1	3:C:420:ASP:N	2.50	0.45
2:B:105:THR:HB	2:B:487:VAL:HG22	1.98	0.44
2:B:646:LYS:HD2	2:B:646:LYS:C	2.42	0.44
3:C:240:PRO:HB2	4:D:104:PHE:HZ	1.82	0.44
5:E:123:ILE:C	5:E:124:VAL:HG12	2.43	0.44
1:A:26:GLU:OE1	7:G:47:SER:OG	2.34	0.44
2:B:782:ARG:O	2:B:983:ASN:ND2	2.43	0.44
2:B:850:CYS:HB3	2:B:931:CYS:HB3	1.99	0.44
6:F:140:LYS:NZ	6:F:215:PRO:O	2.38	0.44
2:B:363:GLY:O	2:B:371:HIS:NE2	2.51	0.44
2:B:897:ARG:NH1	10:B:1103:SF4:S4	2.86	0.44
3:C:222:ARG:NH1	8:I:4:GLU:OE1	2.50	0.44
6:F:217:TRP:HD1	6:F:293:PHE:HA	1.83	0.44
1:A:38:ASN:HB2	7:G:57:PRO:HD2	2.00	0.44
2:B:587:ASN:HA	2:B:690:VAL:O	2.18	0.44
2:B:648:ASN:HB3	2:B:666:TRP:CE3	2.53	0.44
1:A:213:ASN:HB2	1:A:216:VAL:HG23	2.00	0.43
2:B:351:LEU:HD22	2:B:381:LEU:HD21	2.00	0.43
2:B:422:MET:HG2	2:B:427:PRO:HG2	1.99	0.43
2:B:300:THR:HB	2:B:795:ILE:HB	1.99	0.43
3:C:151:LEU:HB3	3:C:172:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:PRO:HA	3:C:291:THR:HG22	2.00	0.43
4:D:14:THR:OG1	4:D:16:GLU:OE1	2.35	0.43
2:B:450:LEU:HG	2:B:467:GLN:HB2	2.01	0.43
2:B:859:GLU:HA	2:B:867:THR:HG23	2.00	0.43
2:B:1022:GLU:HG3	2:B:1026:LYS:HE2	1.99	0.43
3:C:121:ARG:NH1	3:C:193:ASP:OD2	2.39	0.43
2:B:1022:GLU:HA	2:B:1026:LYS:HB2	1.99	0.43
1:A:132:ILE:HG23	1:A:133:HIS:HD2	1.83	0.43
2:B:631:GLU:HA	2:B:634:ASP:HB2	2.01	0.43
7:G:91:LYS:HA	7:G:91:LYS:HD2	1.85	0.43
1:A:176:ARG:O	1:A:177:PRO:C	2.60	0.43
2:B:937:ARG:NH1	2:B:970:GLN:OE1	2.44	0.43
3:C:99:HIS:CE1	3:C:271:VAL:HG13	2.54	0.43
6:F:123:PRO:O	6:F:127:THR:OG1	2.29	0.43
2:B:502:GLU:HG3	2:B:515:SER:HB2	2.01	0.43
2:B:612:ARG:NH2	2:B:839:ASP:OD2	2.49	0.43
2:B:933:TYR:OH	2:B:1011:THR:OG1	2.30	0.43
1:A:131:SER:O	1:A:135:ASN:ND2	2.45	0.42
2:B:422:MET:HE2	2:B:449:HIS:HD2	1.84	0.42
2:B:663:ILE:HA	2:B:696:ILE:HD12	1.99	0.42
2:B:596:ARG:NH2	2:B:682:TYR:OH	2.44	0.42
2:B:853:CYS:HB3	2:B:1007:THR:HB	2.00	0.42
1:A:95:LYS:HD2	1:A:95:LYS:HA	1.86	0.42
2:B:256:SER:HB3	2:B:259:ALA:HB3	2.00	0.42
1:A:161:MET:HG3	9:A:301:HEC:NC	2.33	0.42
2:B:293:VAL:HG21	2:B:302:GLY:HA2	2.01	0.42
2:B:474:TRP:CD1	2:B:516:TYR:HB2	2.55	0.42
3:C:128:LEU:HD11	3:C:183:LEU:HA	2.02	0.42
3:C:244:SER:OG	4:D:105:GLU:OE2	2.34	0.42
8:I:8:ASP:HB3	8:I:11:VAL:HG23	2.00	0.42
2:B:888:CYS:SG	11:B:1104:F3S:S2	3.17	0.42
3:C:241:LEU:HB2	4:D:108:ILE:HG21	2.00	0.42
6:F:74:ALA:O	6:F:78:THR:OG1	2.37	0.42
6:F:362:HIS:HB2	6:F:365:ASP:HB2	2.01	0.42
2:B:594:LEU:HD11	2:B:798:ASN:HB3	2.02	0.42
6:F:137:ILE:HG12	6:F:215:PRO:HB2	2.01	0.42
5:E:79:GLU:HG2	5:E:140:HIS:HB2	2.01	0.42
2:B:648:ASN:CG	2:B:667:LEU:H	2.27	0.42
2:B:895:LYS:HD2	3:C:81:PRO:HA	2.02	0.42
3:C:101:GLY:HA2	3:C:123:ALA:HB1	2.02	0.42
3:C:365:GLN:HA	3:C:368:TRP:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:PRO:HG2	8:I:6:SER:HB3	2.01	0.42
2:B:124:PRO:HG3	2:B:490:LEU:HB2	2.01	0.41
2:B:187:GLN:HG2	2:B:215:PRO:HD2	2.02	0.41
2:B:151:MET:O	2:B:156:ARG:NH1	2.44	0.41
2:B:349:ARG:HA	2:B:349:ARG:HD3	1.81	0.41
2:B:834:ALA:O	2:B:842:SER:OG	2.34	0.41
2:B:935:VAL:HA	2:B:938:ILE:HB	2.02	0.41
3:C:322:TYR:OH	3:C:393:GLU:OE1	2.33	0.41
3:C:435:LEU:HD23	3:C:435:LEU:HA	1.95	0.41
6:F:257:VAL:HA	6:F:260:ILE:HD12	2.02	0.41
2:B:421:ILE:HG13	2:B:448:ILE:HD13	2.02	0.41
2:B:433:GLY:HA3	2:B:700:PRO:HA	2.02	0.41
2:B:827:ILE:HD11	2:B:847:PRO:HB3	2.03	0.41
9:A:305:HEC:O1D	5:E:120:ARG:NH1	2.54	0.41
2:B:141:ASP:OD1	2:B:141:ASP:N	2.51	0.41
4:D:72:ILE:HD13	4:D:72:ILE:HA	1.96	0.41
1:A:58:HIS:CE1	9:A:305:HEC:NA	2.88	0.41
2:B:618:LEU:HB3	2:B:717:ASN:HB2	2.02	0.41
2:B:856:ALA:HB3	2:B:859:GLU:HB2	2.02	0.41
3:C:188:VAL:O	3:C:227:TYR:OH	2.34	0.41
3:C:404:ARG:HG2	3:C:411:TRP:CD2	2.56	0.41
2:B:160:VAL:O	2:B:167:SER:N	2.52	0.41
2:B:200:SER:OG	2:B:476:ASP:OD1	2.38	0.41
3:C:84:TRP:CG	3:C:88:ILE:HG13	2.56	0.41
3:C:199:ASP:OD2	4:D:142:SER:OG	2.36	0.41
6:F:235:LEU:HB3	6:F:267:ILE:HG12	2.03	0.41
1:A:161:MET:HB3	3:C:158:HIS:HA	2.03	0.41
2:B:158:THR:HA	2:B:495:TYR:HB3	2.03	0.41
1:A:68:TYR:HD2	5:E:102:TYR:HA	1.85	0.41
2:B:469:HIS:O	2:B:473:SER:HB3	2.21	0.41
2:B:627:LEU:HD21	2:B:644:LEU:HD12	2.03	0.41
3:C:95:ILE:HG21	3:C:249:ILE:HD13	2.03	0.41
5:E:133:LEU:O	5:E:185:GLN:NE2	2.48	0.41
8:I:10:GLU:HA	8:I:13:PRO:HG2	2.03	0.41
1:A:172:GLU:HA	1:A:175:VAL:HG22	2.03	0.40
2:B:191:VAL:HA	2:B:419:THR:HB	2.04	0.40
3:C:295:PHE:HE2	3:C:444:MET:HE2	1.86	0.40
6:F:312:LEU:HD11	6:F:350:ASP:HA	2.03	0.40
2:B:129:GLY:HA3	2:B:138:GLY:C	2.46	0.40
2:B:714:ARG:HD3	2:B:714:ARG:N	2.37	0.40
4:D:43:GLU:HA	4:D:46:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:O	1:A:89:THR:OG1	2.37	0.40
2:B:646:LYS:HB3	2:B:646:LYS:HE3	1.88	0.40
4:D:22:THR:HG21	4:D:44:VAL:CG1	2.50	0.40
5:E:117:VAL:HG12	5:E:123:ILE:HG13	2.03	0.40
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.92	0.40
2:B:187:GLN:HB3	2:B:216:GLN:HG3	2.04	0.40
4:D:45:ILE:C	4:D:47:GLU:N	2.79	0.40
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.91	0.40
2:B:885:THR:O	2:B:886:LYS:C	2.65	0.40
6:F:258:LYS:HA	6:F:258:LYS:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
2	B	949/1029 (92%)	892 (94%)	56 (6%)	1 (0%)	48	73
3	C	447/486 (92%)	432 (97%)	15 (3%)	0	100	100
4	D	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
5	E	162/205 (79%)	155 (96%)	7 (4%)	0	100	100
6	F	395/411 (96%)	380 (96%)	15 (4%)	0	100	100
7	G	78/112 (70%)	75 (96%)	3 (4%)	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	2455/2678 (92%)	2334 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	886	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/199 (100%)	195 (98%)	3 (2%)	57	81
2	B	768/830 (92%)	765 (100%)	3 (0%)	84	93
3	C	382/405 (94%)	381 (100%)	1 (0%)	86	94
4	D	143/147 (97%)	143 (100%)	0	100	100
5	E	135/171 (79%)	135 (100%)	0	100	100
6	F	318/330 (96%)	317 (100%)	1 (0%)	86	94
7	G	69/95 (73%)	69 (100%)	0	100	100
8	I	32/32 (100%)	32 (100%)	0	100	100
All	All	2045/2209 (93%)	2037 (100%)	8 (0%)	81	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	A	179	GLU
1	A	180	GLU
2	B	886	LYS
2	B	888	CYS
2	B	889	SER
3	C	141	HIS
6	F	361	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	155	GLN

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Mol	Chain	Res	Type
2	B	82	GLN
2	B	383	ASN
2	B	588	ASN
2	B	693	ASN
2	B	769	ASN
2	B	880	ASN
3	C	141	HIS
3	C	246	HIS
5	E	147	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](#)

14 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	$\# Z > 2$
15	JM9	C	504	-	53,53,53	0.98	5 (9%)	58,58,58	0.90	3 (5%)
9	HEC	A	302	1	46,50,50	1.94	7 (15%)	58,82,82	1.86	9 (15%)
9	HEC	E	301	5	46,50,50	1.89	6 (13%)	58,82,82	2.00	2 (3%)
9	HEC	A	304	1	46,50,50	1.93	7 (15%)	58,82,82	1.63	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SF4	B	1103	2	0,12,12	-	-	-		
9	HEC	A	303	1	46,50,50	1.86	5 (10%)	58,82,82	1.47	3 (5%)
9	HEC	A	301	1	46,50,50	1.92	6 (13%)	58,82,82	1.84	7 (12%)
13	HQO	C	502	-	19,20,20	3.37	3 (15%)	20,26,26	1.30	3 (15%)
12	JLQ	C	501	-	44,44,44	1.00	4 (9%)	47,49,49	1.12	4 (8%)
14	JL3	C	503	-	44,44,44	0.98	3 (6%)	47,49,49	1.15	5 (10%)
9	HEC	A	305	1	46,50,50	1.90	6 (13%)	58,82,82	1.78	2 (3%)
10	SF4	B	1102	2	0,12,12	-	-	-		
11	F3S	B	1104	2	0,9,9	-	-	-		
10	SF4	B	1101	2	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
15	JM9	C	504	-	-	28/56/56/56	-
9	HEC	A	302	1	-	8/14/54/54	-
9	HEC	E	301	5	-	8/14/54/54	-
9	HEC	A	304	1	-	6/14/54/54	-
13	HQO	C	502	-	-	3/7/7/7	0/2/2/2
9	HEC	A	303	1	-	6/14/54/54	-
9	HEC	A	301	1	-	4/14/54/54	-
10	SF4	B	1103	2	-	-	0/6/5/5
12	JLQ	C	501	-	-	30/48/48/48	-
14	JL3	C	503	-	-	25/48/48/48	-
9	HEC	A	305	1	-	4/14/54/54	-
10	SF4	B	1102	2	-	-	0/6/5/5
11	F3S	B	1104	2	-	-	0/3/3/3
10	SF4	B	1101	2	-	-	0/6/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HQO	O4-N1	-13.81	1.23	1.38
9	A	304	HEC	CAC-C3C	6.47	1.56	1.35
9	A	305	HEC	CAC-C3C	6.22	1.55	1.35
9	A	301	HEC	CAC-C3C	6.22	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	302	HEC	CAC-C3C	6.22	1.55	1.35
9	E	301	HEC	CAC-C3C	6.16	1.55	1.35
9	A	303	HEC	CAB-C3B	6.16	1.55	1.35
9	A	304	HEC	CAB-C3B	6.11	1.54	1.35
9	E	301	HEC	CAB-C3B	6.11	1.54	1.35
9	A	305	HEC	CAB-C3B	6.11	1.54	1.35
9	A	301	HEC	CAB-C3B	6.10	1.54	1.35
9	A	303	HEC	CAC-C3C	6.04	1.54	1.35
9	A	302	HEC	CAB-C3B	6.03	1.54	1.35
9	A	305	HEC	C3D-C2D	5.36	1.52	1.38
9	A	303	HEC	C3D-C2D	5.25	1.52	1.38
9	A	302	HEC	C3D-C2D	5.24	1.52	1.38
9	E	301	HEC	C3D-C2D	5.07	1.52	1.38
9	A	304	HEC	C3D-C2D	5.07	1.52	1.38
9	A	301	HEC	C3D-C2D	4.92	1.51	1.38
15	C	504	JM9	O20-C21	2.97	1.42	1.33
14	C	503	JL3	O29-C19	-2.78	1.40	1.46
13	C	502	HQO	C10-C5	2.77	1.46	1.42
15	C	504	JM9	O17-C15	2.68	1.41	1.34
9	A	302	HEC	C3B-C2B	-2.68	1.32	1.41
12	C	501	JLQ	O30-C20	-2.64	1.40	1.46
13	C	502	HQO	C1-C10	2.58	1.47	1.42
9	A	303	HEC	C3C-C2C	-2.51	1.32	1.41
15	C	504	JM9	O38-C39	2.45	1.40	1.33
12	C	501	JLQ	O30-C31	2.43	1.41	1.34
9	A	301	HEC	C2A-C3A	-2.43	1.31	1.36
9	E	301	HEC	C3B-C2B	-2.42	1.33	1.41
9	A	305	HEC	C3B-C2B	-2.40	1.33	1.41
9	A	301	HEC	C3B-C2B	-2.40	1.33	1.41
9	A	304	HEC	C3B-C2B	-2.39	1.33	1.41
9	E	301	HEC	C3C-C2C	-2.39	1.33	1.41
14	C	503	JL3	O17-C15	2.34	1.40	1.33
15	C	504	JM9	O17-C18	-2.33	1.41	1.46
12	C	501	JLQ	O18-C16	2.32	1.40	1.33
9	A	303	HEC	C3B-C2B	-2.32	1.33	1.41
9	A	301	HEC	C3C-C2C	-2.29	1.33	1.41
12	C	501	JLQ	O18-C19	-2.27	1.40	1.45
9	A	305	HEC	C3C-C2C	-2.26	1.33	1.41
9	A	304	HEC	CMB-C2B	2.25	1.55	1.50
9	A	302	HEC	C3C-C2C	-2.22	1.33	1.41
9	A	304	HEC	C3C-C2C	-2.22	1.33	1.41
9	A	304	HEC	C2A-C3A	-2.12	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	302	HEC	CMC-C2C	2.10	1.55	1.50
14	C	503	JL3	O29-C30	2.07	1.40	1.34
9	A	302	HEC	CHA-C1A	-2.07	1.34	1.38
15	C	504	JM9	O38-C37	-2.04	1.40	1.45
9	A	305	HEC	CMC-C2C	2.00	1.54	1.50
9	E	301	HEC	C2A-C3A	-2.00	1.32	1.36

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	301	HEC	CBB-CAB-C3B	-9.18	109.09	127.43
9	E	301	HEC	CBC-CAC-C3C	-8.85	109.75	127.43
9	A	305	HEC	CBB-CAB-C3B	-8.70	110.05	127.43
9	A	302	HEC	CBB-CAB-C3B	-7.81	111.83	127.43
9	A	305	HEC	CBC-CAC-C3C	-7.46	112.52	127.43
9	A	301	HEC	CBB-CAB-C3B	-7.18	113.09	127.43
9	A	303	HEC	CBB-CAB-C3B	-6.98	113.48	127.43
9	A	304	HEC	CBB-CAB-C3B	-6.30	114.85	127.43
9	A	301	HEC	CBC-CAC-C3C	-6.29	114.86	127.43
9	A	302	HEC	CBC-CAC-C3C	-5.66	116.12	127.43
12	C	501	JLQ	O30-C31-C33	5.27	122.88	111.48
9	A	304	HEC	CBC-CAC-C3C	-5.11	117.21	127.43
9	A	303	HEC	CBC-CAC-C3C	-4.92	117.60	127.43
14	C	503	JL3	O29-C30-C32	4.28	120.74	111.48
9	A	302	HEC	CAD-C3D-C4D	3.88	132.51	124.94
15	C	504	JM9	O17-C15-C14	3.73	119.56	111.48
13	C	502	HQO	C1-C2-C3	3.34	120.97	118.45
15	C	504	JM9	O38-C39-C41	2.79	120.36	111.83
14	C	503	JL3	C19-O29-C30	-2.70	111.35	117.80
12	C	501	JLQ	O18-C16-C15	2.69	120.04	111.83
14	C	503	JL3	O17-C18-C19	-2.65	100.76	108.40
13	C	502	HQO	C2-C3-N1	2.63	121.83	118.94
14	C	503	JL3	O17-C15-C14	2.62	119.83	111.83
9	A	301	HEC	CMD-C2D-C1D	2.62	129.40	125.42
15	C	504	JM9	O20-C21-C23	2.59	119.74	111.83
9	A	302	HEC	C2A-C1A-NA	2.48	112.72	110.32
9	A	301	HEC	C4B-NB-C1B	-2.47	101.80	105.82
14	C	503	JL3	O23-P22-O24	-2.42	101.21	112.44
9	A	302	HEC	C4A-NA-C1A	-2.40	101.90	105.82
12	C	501	JLQ	O24-P23-O25	-2.37	101.40	112.44
9	A	304	HEC	C3D-C4D-ND	2.35	112.76	110.15
9	A	301	HEC	C3D-C4D-ND	2.30	112.71	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	HQO	O1-C1-C10	2.27	120.31	116.42
9	A	304	HEC	C4B-NB-C1B	-2.26	102.13	105.82
9	A	301	HEC	CMC-C2C-C1C	-2.22	122.05	125.42
9	A	302	HEC	CBD-CAD-C3D	2.16	118.52	112.53
9	A	302	HEC	O1D-CGD-CBD	-2.12	116.36	123.09
9	A	302	HEC	C4B-NB-C1B	-2.11	102.38	105.82
9	A	302	HEC	C4D-C3D-C2D	-2.08	103.65	106.87
9	A	303	HEC	C1C-CHC-C4B	-2.07	118.27	124.66
9	A	301	HEC	CHC-C1C-C2C	-2.05	121.48	127.43
12	C	501	JLQ	O30-C31-O32	-2.04	118.94	123.70
9	A	304	HEC	C4C-NC-C1C	-2.00	102.56	105.82

There are no chirality outliers.

All (122) 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	301	HEC	C4C-C3C-CAC-CBC
9	A	302	HEC	C2C-C3C-CAC-CBC
9	A	302	HEC	C4C-C3C-CAC-CBC
9	A	302	HEC	C4D-C3D-CAD-CBD
9	A	303	HEC	C2B-C3B-CAB-CBB
9	A	303	HEC	C2C-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	C2C-C3C-CAC-CBC
12	C	501	JLQ	C21-O22-P23-O24
12	C	501	JLQ	C21-O22-P23-O25
12	C	501	JLQ	C21-O22-P23-O26
12	C	501	JLQ	C27-O26-P23-O25
12	C	501	JLQ	O32-C31-O30-C20
12	C	501	JLQ	C33-C31-O30-C20
13	C	502	HQO	C3-C11-C13-C12
14	C	503	JL3	C20-O21-P22-O24
14	C	503	JL3	C20-O21-P22-O25
14	C	503	JL3	C26-O25-P22-O21
14	C	503	JL3	C26-O25-P22-O23
14	C	503	JL3	C32-C30-O29-C19

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Mol	Chain	Res	Type	Atoms
15	C	504	JM9	O17-C18-C19-O20
15	C	504	JM9	O40-C39-O38-C37
14	C	503	JL3	O31-C30-O29-C19
14	C	503	JL3	C14-C15-O17-C18
15	C	504	JM9	C41-C39-O38-C37
14	C	503	JL3	O16-C15-O17-C18
9	A	302	HEC	C2A-CAA-CBA-CGA
12	C	501	JLQ	C15-C16-O18-C19
9	A	302	HEC	C2D-C3D-CAD-CBD
12	C	501	JLQ	C31-C33-C34-C35
14	C	503	JL3	C30-C32-C33-C34
12	C	501	JLQ	O17-C16-O18-C19
12	C	501	JLQ	C13-C14-C15-C16
15	C	504	JM9	C49-C50-C51-C52
14	C	503	JL3	C08-C09-C10-C11
12	C	501	JLQ	C08-C09-C10-C11
15	C	504	JM9	C39-C41-C42-C43
15	C	504	JM9	C47-C48-C49-C50
15	C	504	JM9	C29-C30-C31-C32
13	C	502	HQO	C12-C14-C15-C16
9	A	302	HEC	C3D-CAD-CBD-CGD
12	C	501	JLQ	C06-C07-C08-C09
12	C	501	JLQ	C07-C08-C09-C10
14	C	503	JL3	C32-C33-C34-C35
12	C	501	JLQ	C38-C39-C40-C41
14	C	503	JL3	C40-C41-C42-C43
14	C	503	JL3	C05-C06-C07-C08
12	C	501	JLQ	C34-C35-C36-C37
15	C	504	JM9	C48-C49-C50-C51
15	C	504	JM9	C45-C46-C47-C48
12	C	501	JLQ	C36-C37-C38-C39
15	C	504	JM9	C09-C10-C11-C12
15	C	504	JM9	C43-C44-C45-C46
12	C	501	JLQ	C10-C11-C12-C13
15	C	504	JM9	C11-C12-C13-C14
15	C	504	JM9	C41-C42-C43-C44
15	C	504	JM9	C05-C06-C07-C08
14	C	503	JL3	C03-C04-C05-C06
15	C	504	JM9	C25-C26-C27-C28
12	C	501	JLQ	C01-C02-C03-C04
12	C	501	JLQ	C39-C40-C41-C42
15	C	504	JM9	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
14	C	503	JL3	C07-C08-C09-C10
15	C	504	JM9	C37-C18-C19-O20
13	C	502	HQO	C14-C15-C16-C17
14	C	503	JL3	O17-C18-C19-O29
15	C	504	JM9	C27-C28-C29-C30
12	C	501	JLQ	C35-C36-C37-C38
14	C	503	JL3	C37-C38-C39-C40
14	C	503	JL3	C04-C05-C06-C07
15	C	504	JM9	C46-C47-C48-C49
12	C	501	JLQ	O18-C19-C20-C21
14	C	503	JL3	C35-C36-C37-C38
12	C	501	JLQ	C19-C20-C21-O22
15	C	504	JM9	C10-C11-C12-C13
9	A	302	HEC	C4B-C3B-CAB-CBB
9	A	303	HEC	C4B-C3B-CAB-CBB
9	A	303	HEC	C4C-C3C-CAC-CBC
9	A	305	HEC	C4B-C3B-CAB-CBB
9	A	305	HEC	C4C-C3C-CAC-CBC
9	E	301	HEC	C4B-C3B-CAB-CBB
9	E	301	HEC	C4C-C3C-CAC-CBC
12	C	501	JLQ	O30-C20-C21-O22
12	C	501	JLQ	O18-C19-C20-O30
12	C	501	JLQ	C11-C12-C13-C14
15	C	504	JM9	C06-C07-C08-C09
14	C	503	JL3	O17-C18-C19-C20
12	C	501	JLQ	C42-C43-C44-C45
9	A	302	HEC	C2B-C3B-CAB-CBB
9	A	305	HEC	C2B-C3B-CAB-CBB
9	E	301	HEC	C2B-C3B-CAB-CBB
9	E	301	HEC	C2C-C3C-CAC-CBC
14	C	503	JL3	O25-C26-C27-N28
12	C	501	JLQ	C09-C10-C11-C12
15	C	504	JM9	C07-C08-C09-C10
14	C	503	JL3	C11-C12-C13-C14
12	C	501	JLQ	C41-C42-C43-C44
9	A	304	HEC	CAA-CBA-CGA-O2A
12	C	501	JLQ	C40-C41-C42-C43
14	C	503	JL3	C34-C35-C36-C37
9	A	304	HEC	CAA-CBA-CGA-O1A
9	A	303	HEC	CAA-CBA-CGA-O2A
14	C	503	JL3	C33-C34-C35-C36
9	A	303	HEC	CAA-CBA-CGA-O1A

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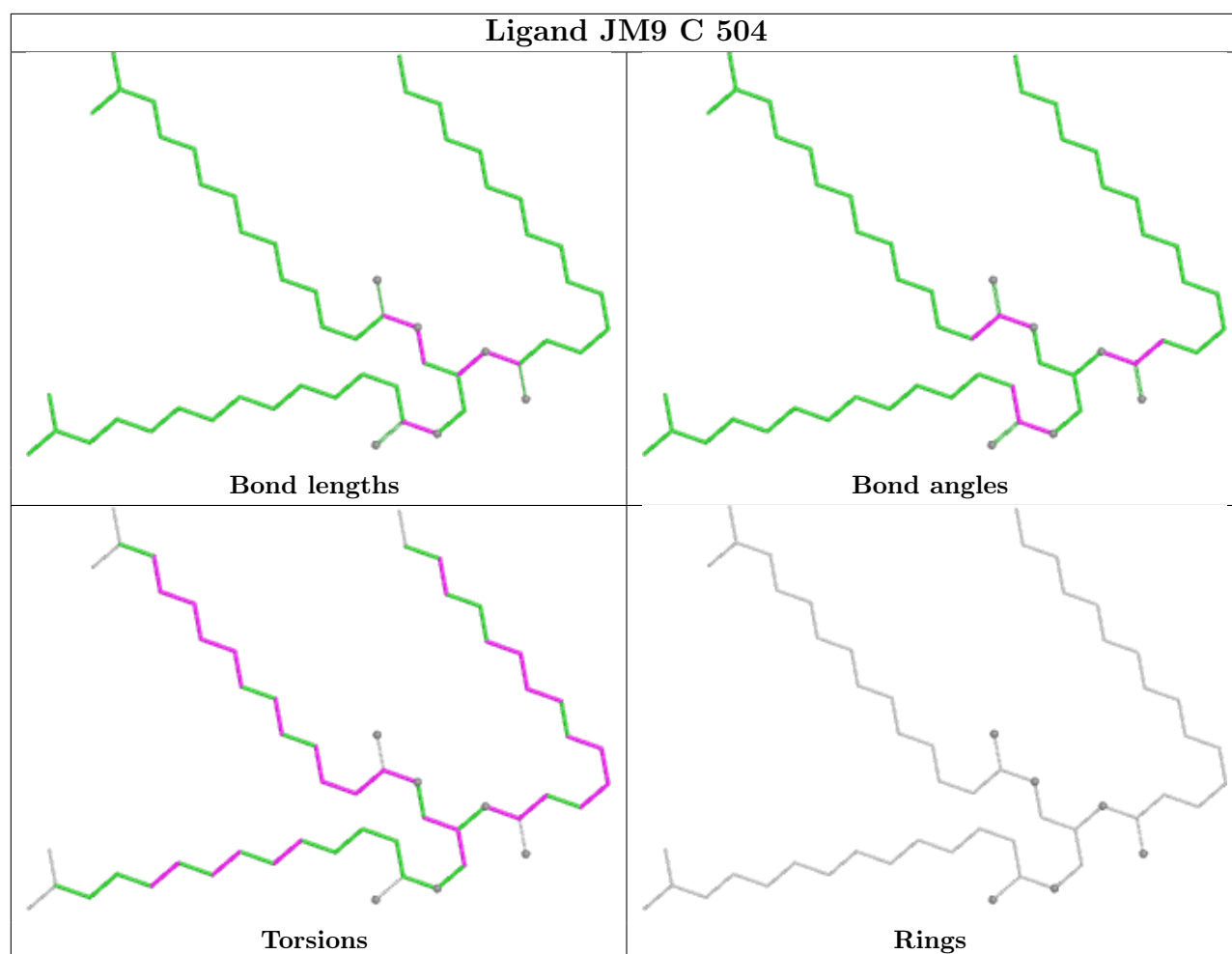
Mol	Chain	Res	Type	Atoms
15	C	504	JM9	C19-C18-C37-O38
9	E	301	HEC	CAA-CBA-CGA-O2A
15	C	504	JM9	O16-C15-O17-C18
14	C	503	JL3	C10-C11-C12-C13
9	E	301	HEC	CAA-CBA-CGA-O1A
9	E	301	HEC	CAD-CBD-CGD-O2D
15	C	504	JM9	O38-C39-C41-C42
15	C	504	JM9	C14-C15-O17-C18
12	C	501	JLQ	C37-C38-C39-C40
9	E	301	HEC	CAD-CBD-CGD-O1D
15	C	504	JM9	C13-C14-C15-O17
15	C	504	JM9	O40-C39-C41-C42

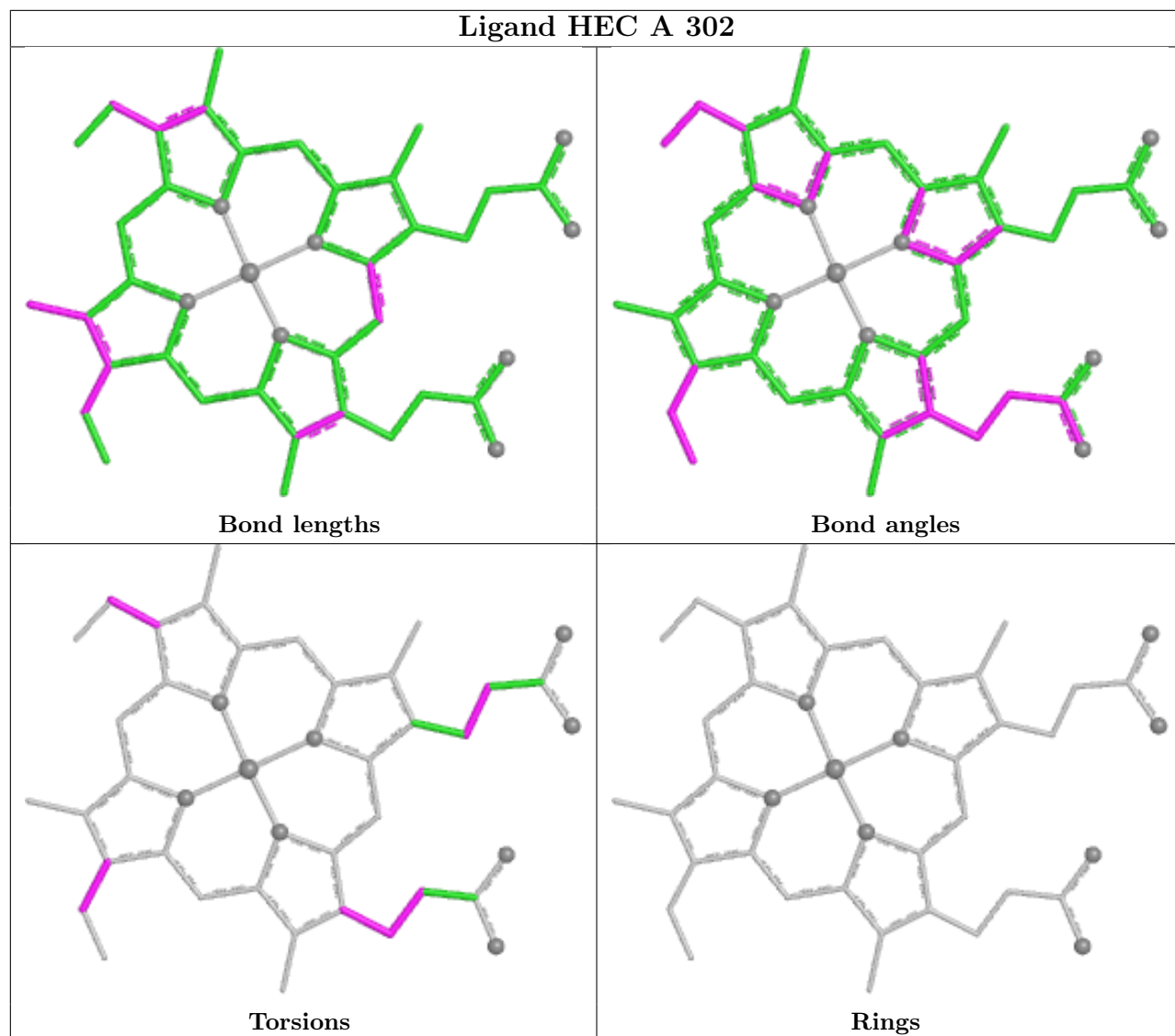
There are no ring outliers.

9 monomers are involved in 19 short contacts:

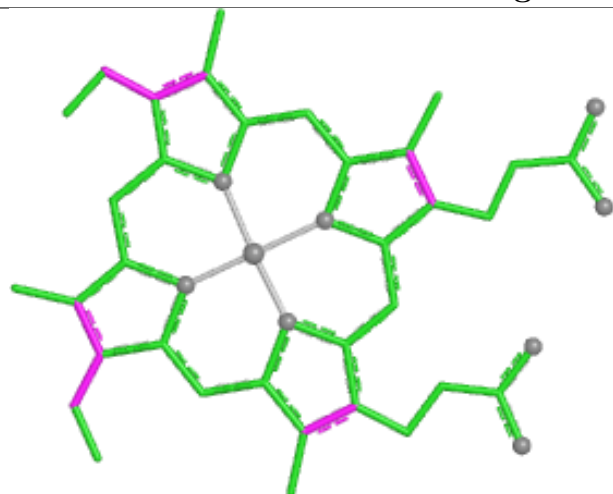
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	302	HEC	2	0
9	E	301	HEC	2	0
9	A	304	HEC	1	0
10	B	1103	SF4	1	0
9	A	303	HEC	1	0
9	A	301	HEC	4	0
13	C	502	HQO	1	0
9	A	305	HEC	2	0
11	B	1104	F3S	5	0

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.

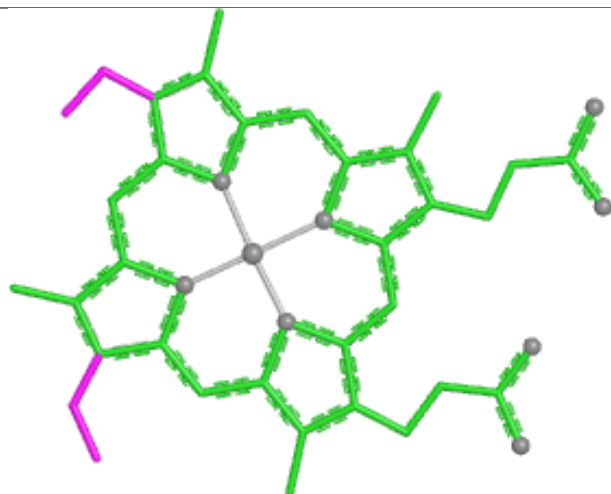




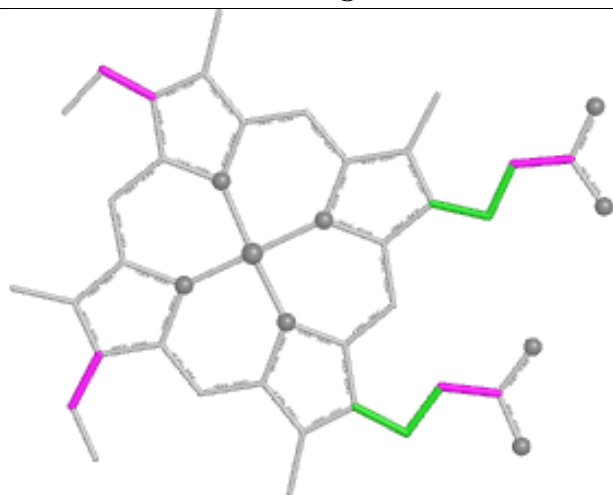
Ligand HEC E 301



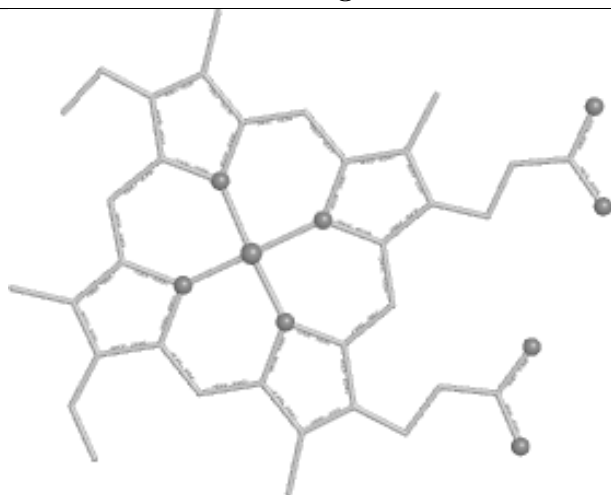
Bond lengths



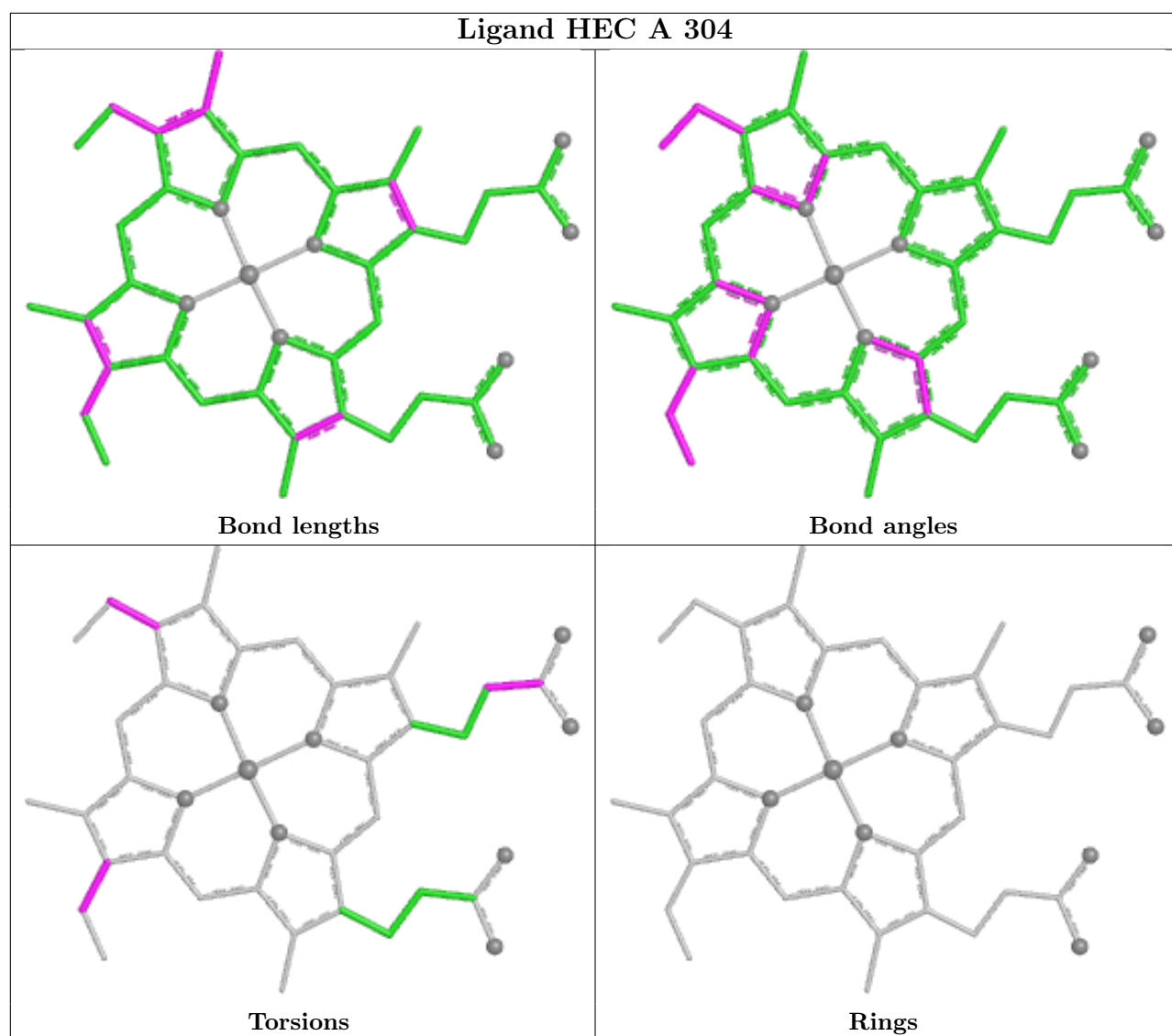
Bond angles

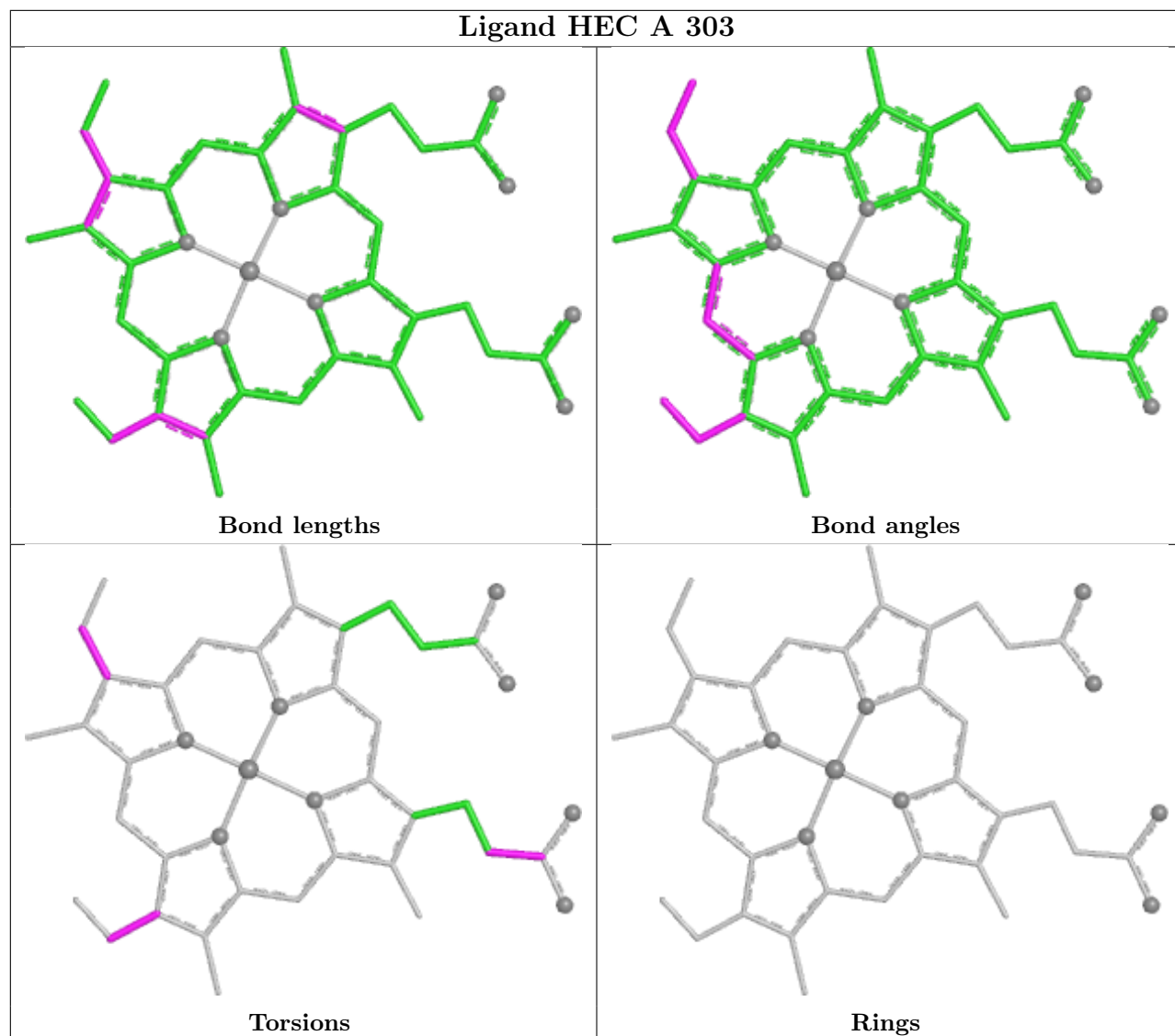


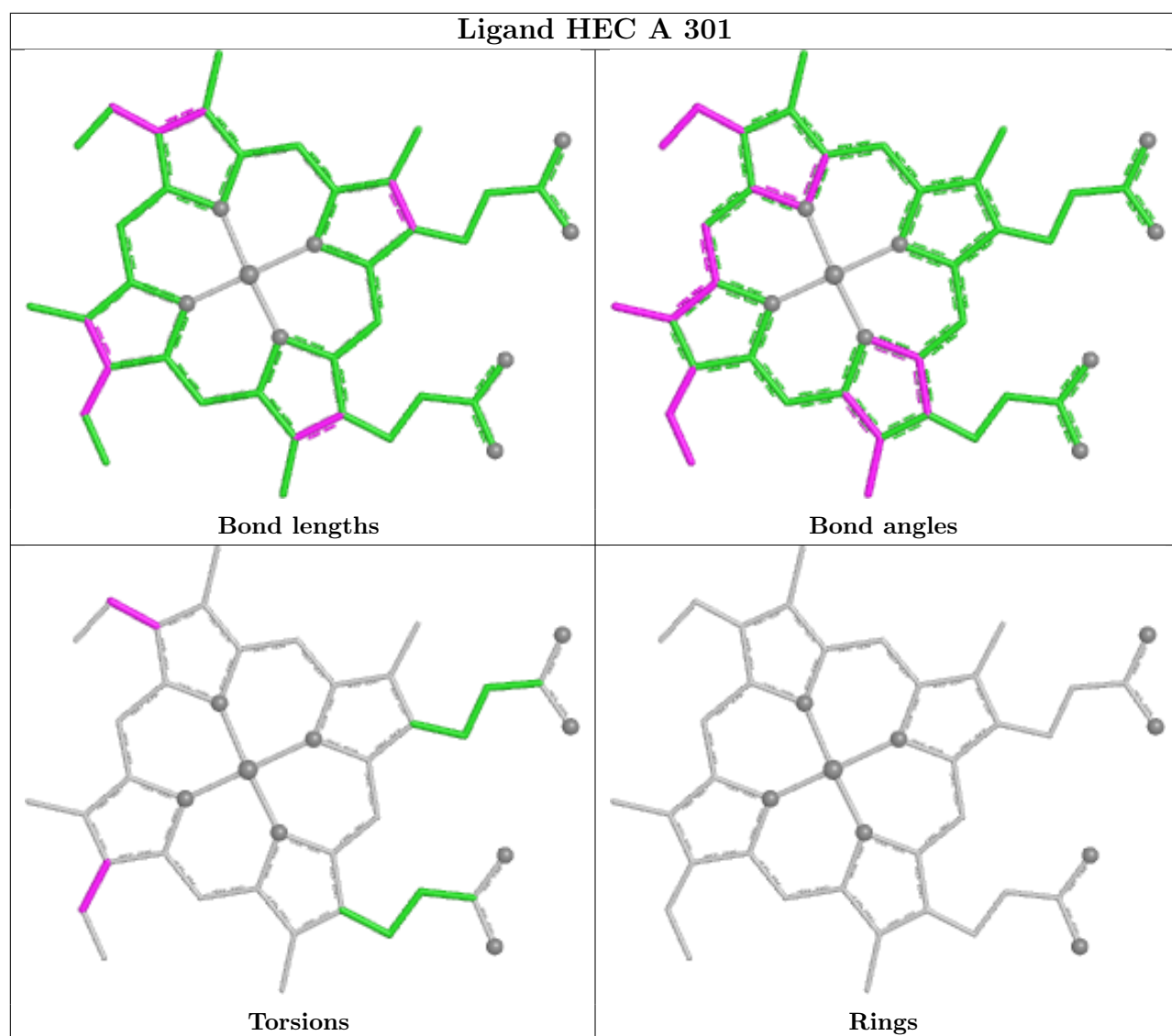
Torsions

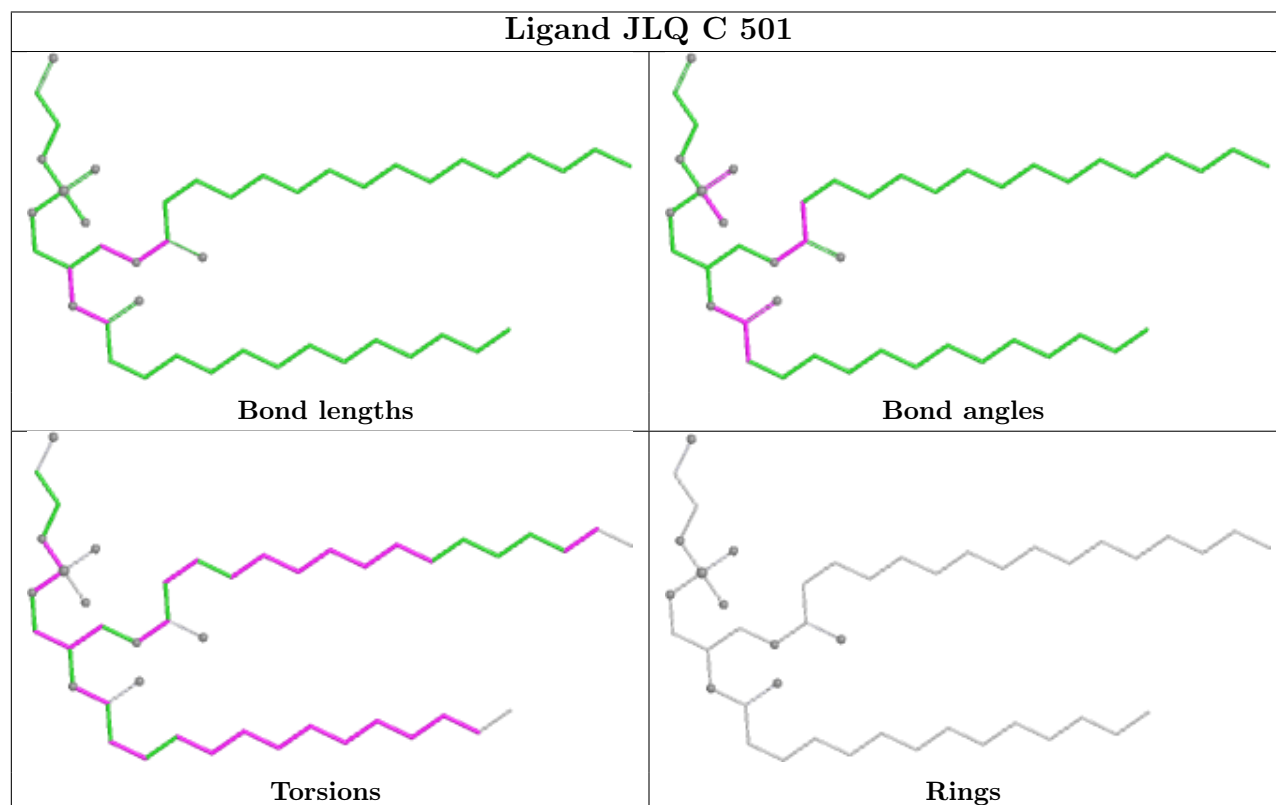
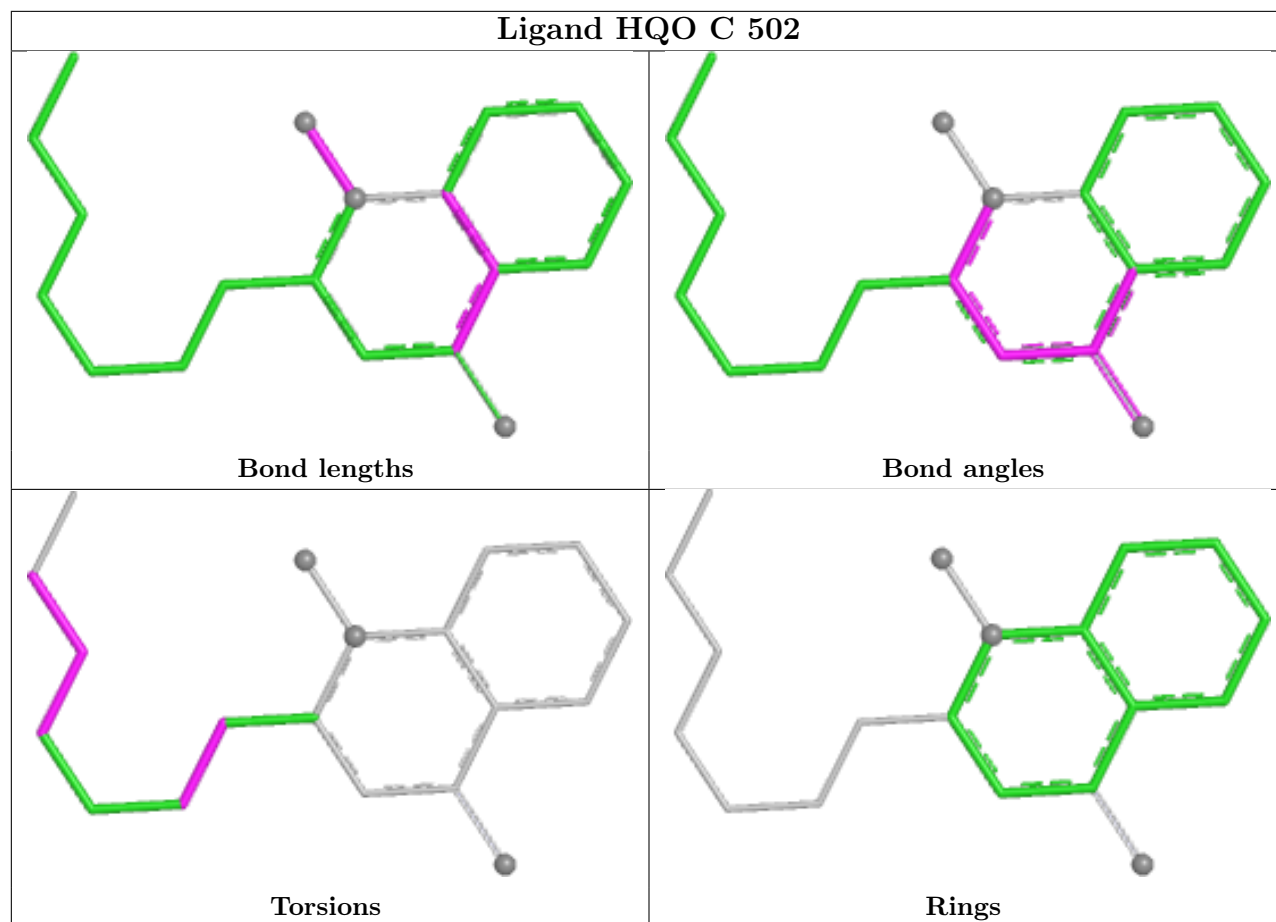


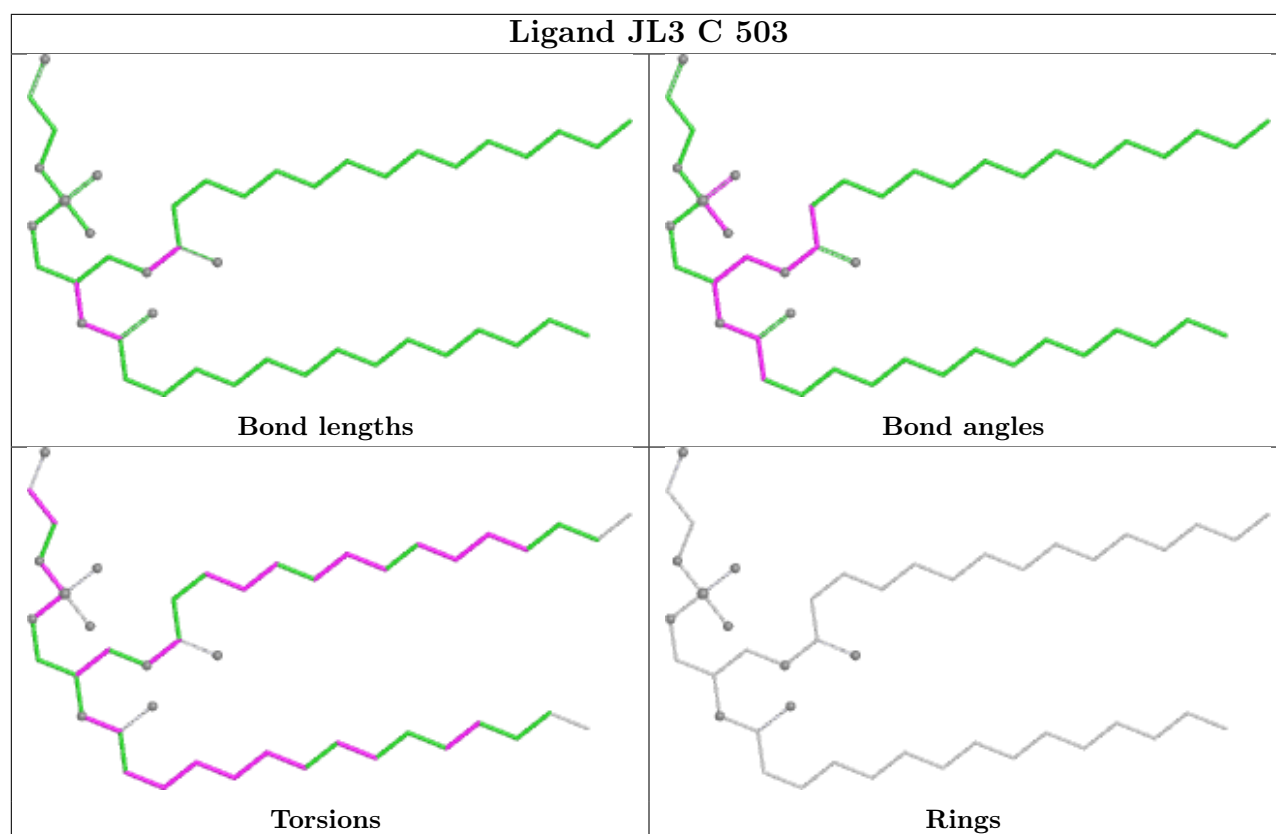
Rings

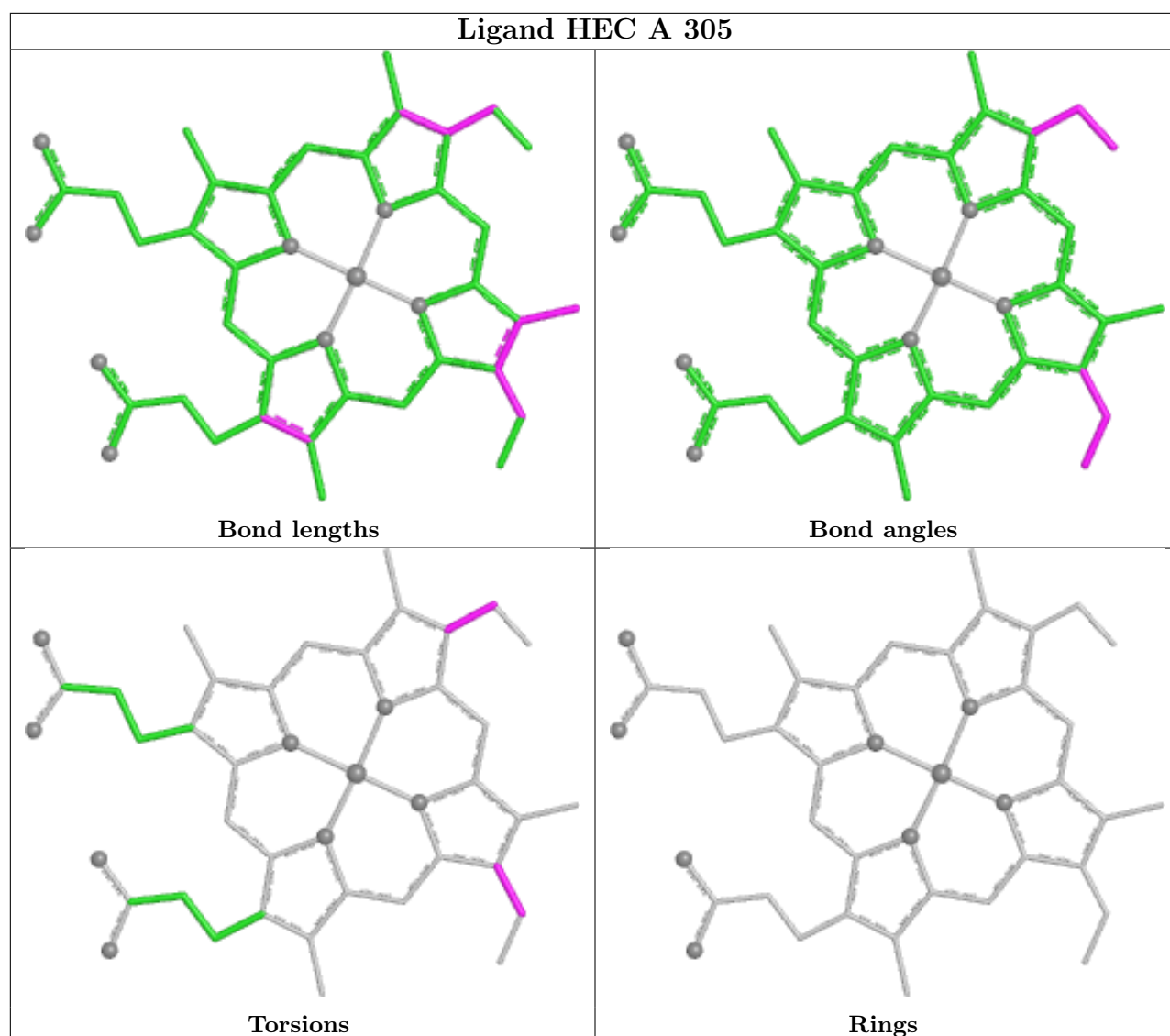












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

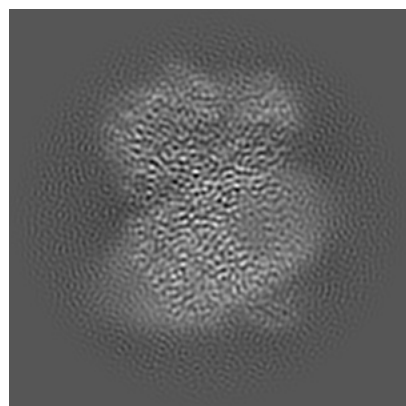
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38012. These allow visual inspection of the internal detail of the map and identification of artifacts.

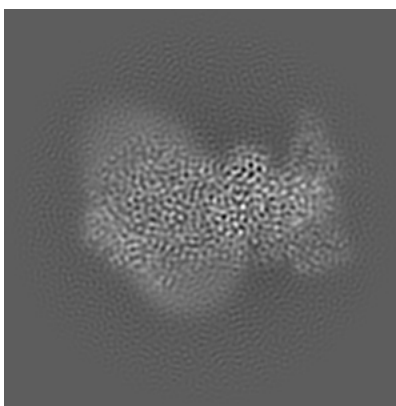
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

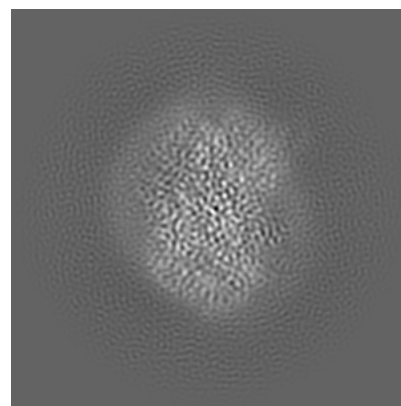
6.1.1 Primary map



X

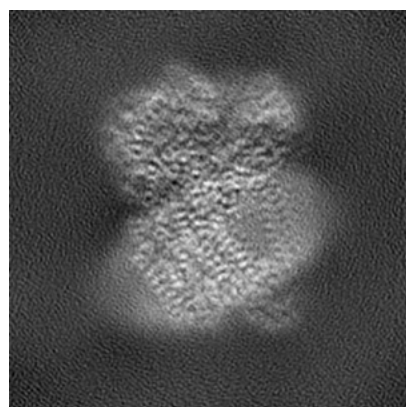


Y

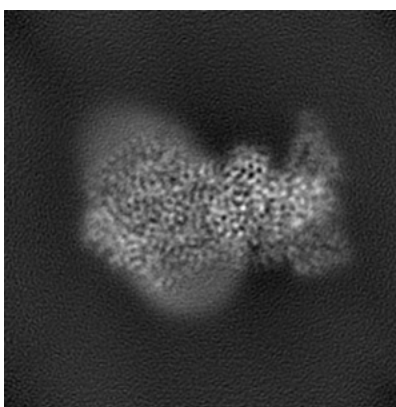


Z

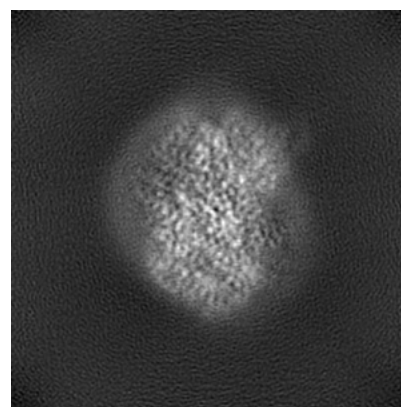
6.1.2 Raw map



X



Y

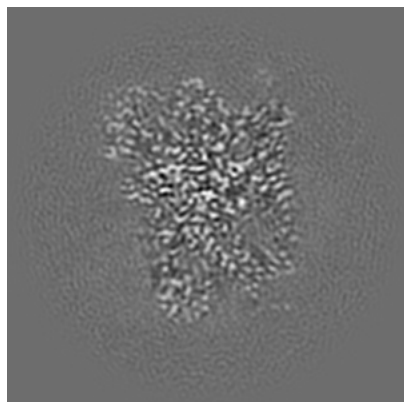


Z

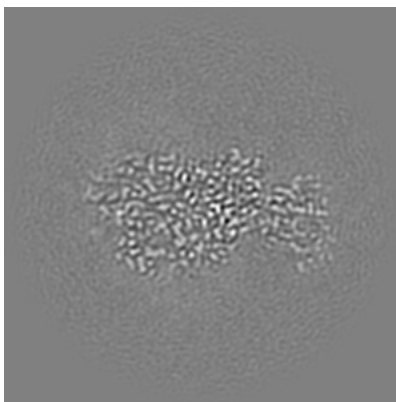
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

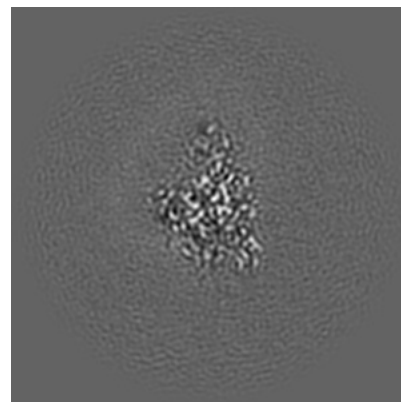
6.2.1 Primary map



X Index: 108

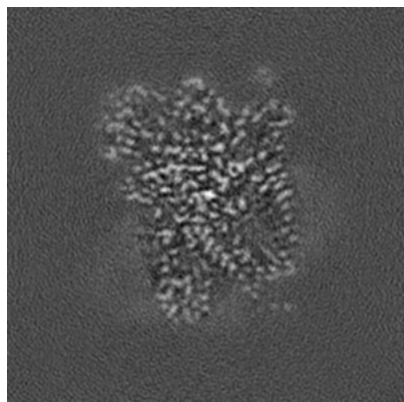


Y Index: 108

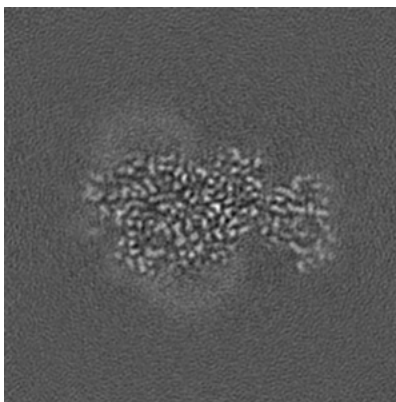


Z Index: 108

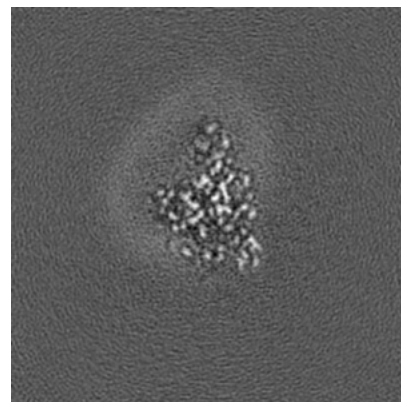
6.2.2 Raw map



X Index: 108



Y Index: 108

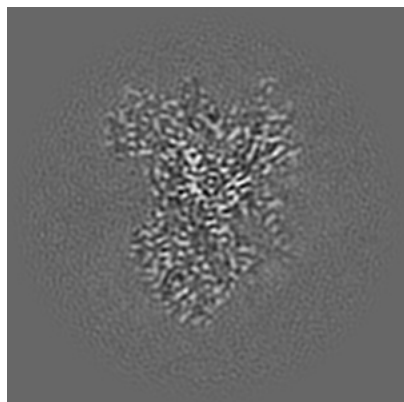


Z Index: 108

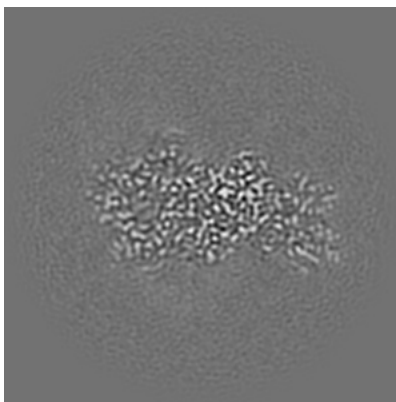
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

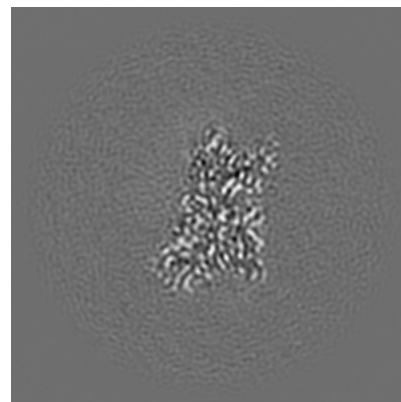
6.3.1 Primary map



X Index: 115

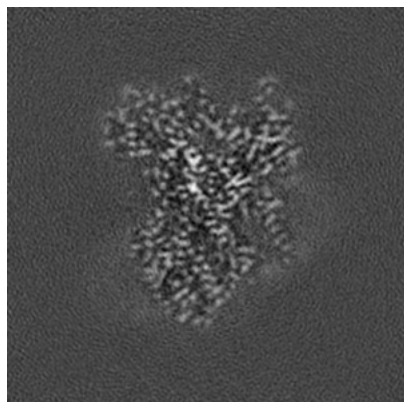


Y Index: 101

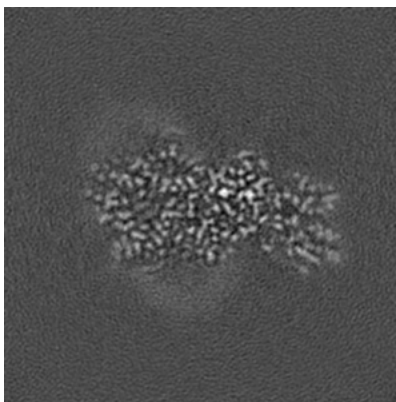


Z Index: 127

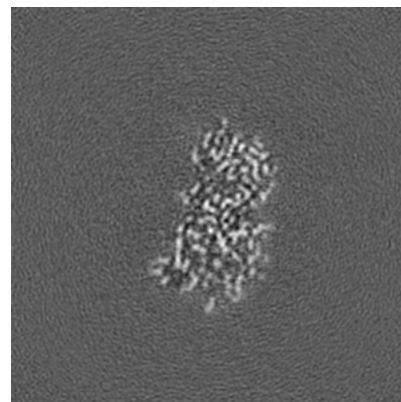
6.3.2 Raw map



X Index: 115



Y Index: 101

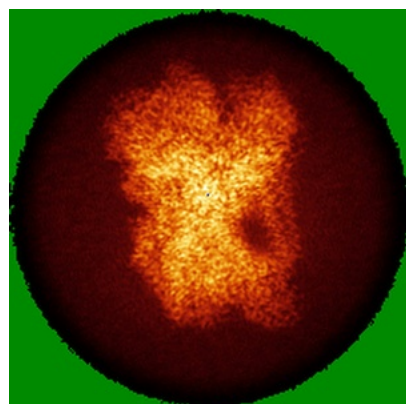


Z Index: 135

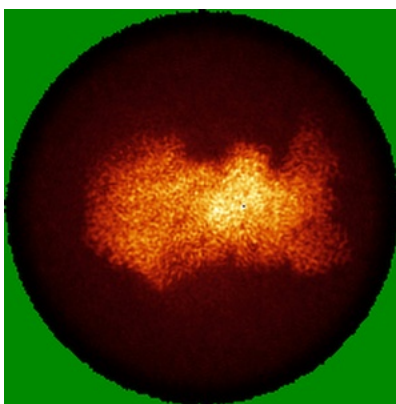
The images above show the largest variance slices of the map in three orthogonal directions.

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

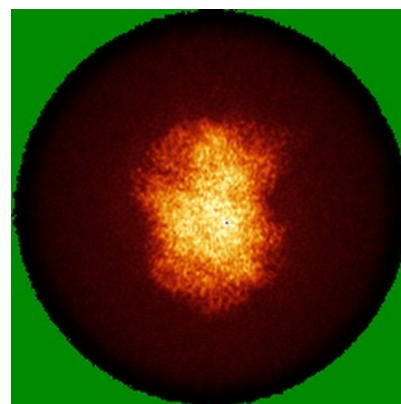
6.4.1 Primary map



X

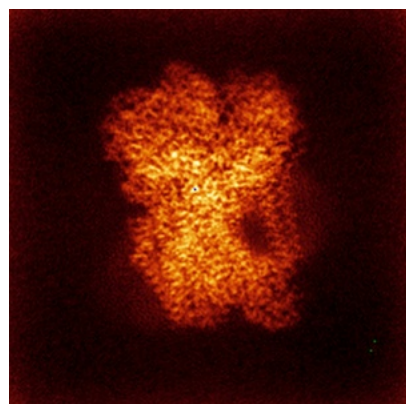


Y

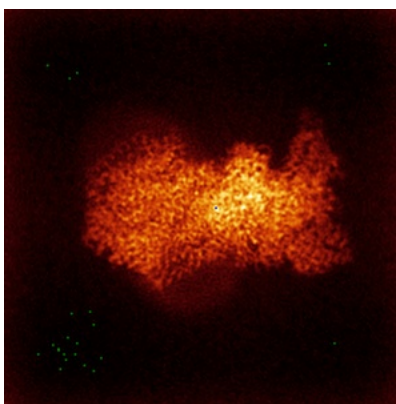


Z

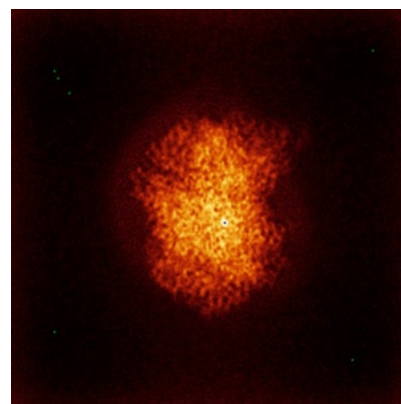
6.4.2 Raw map



X



Y

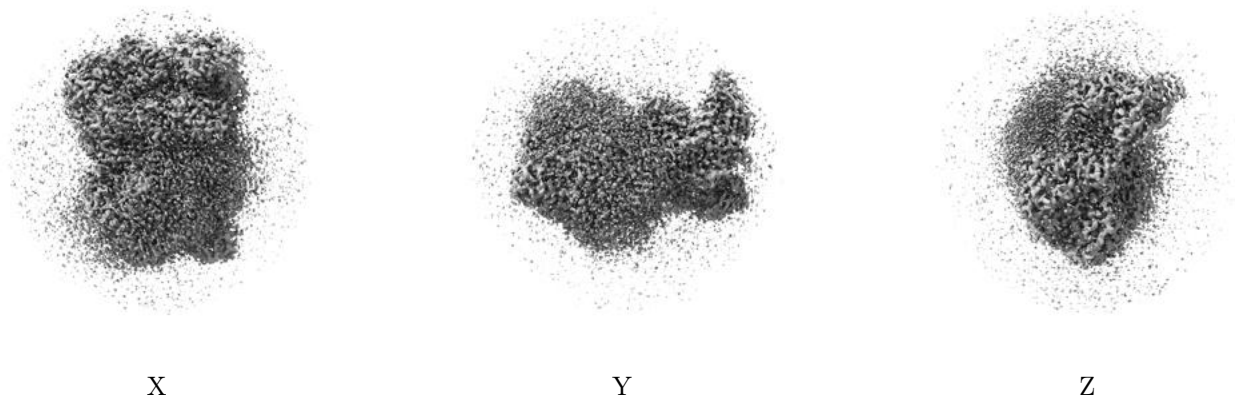


Z

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.

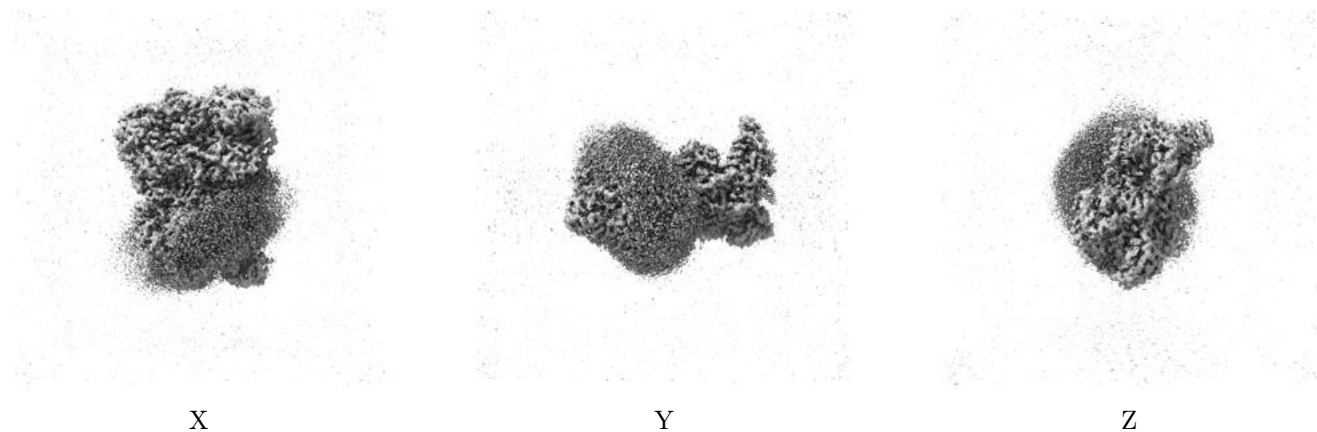
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

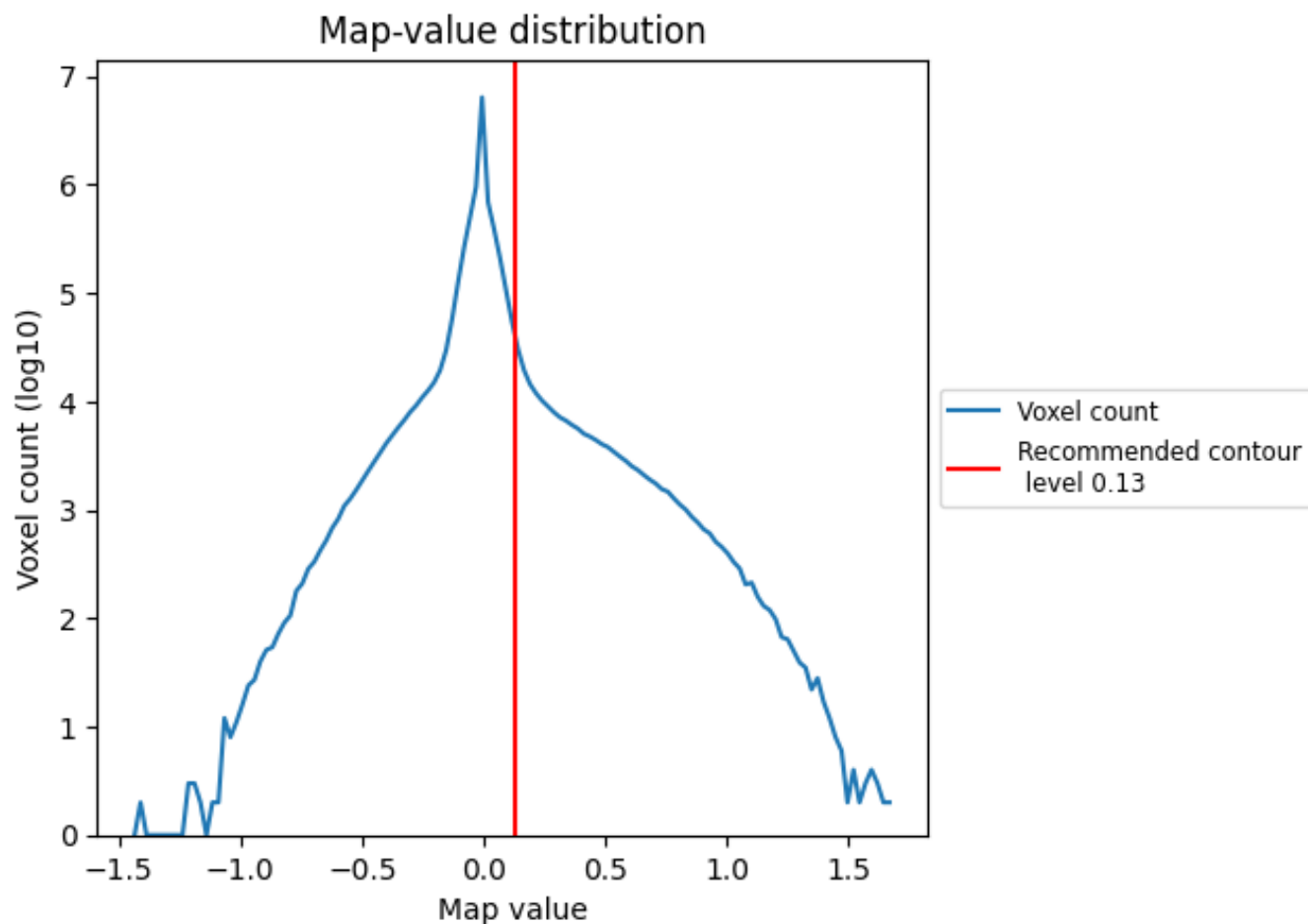
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

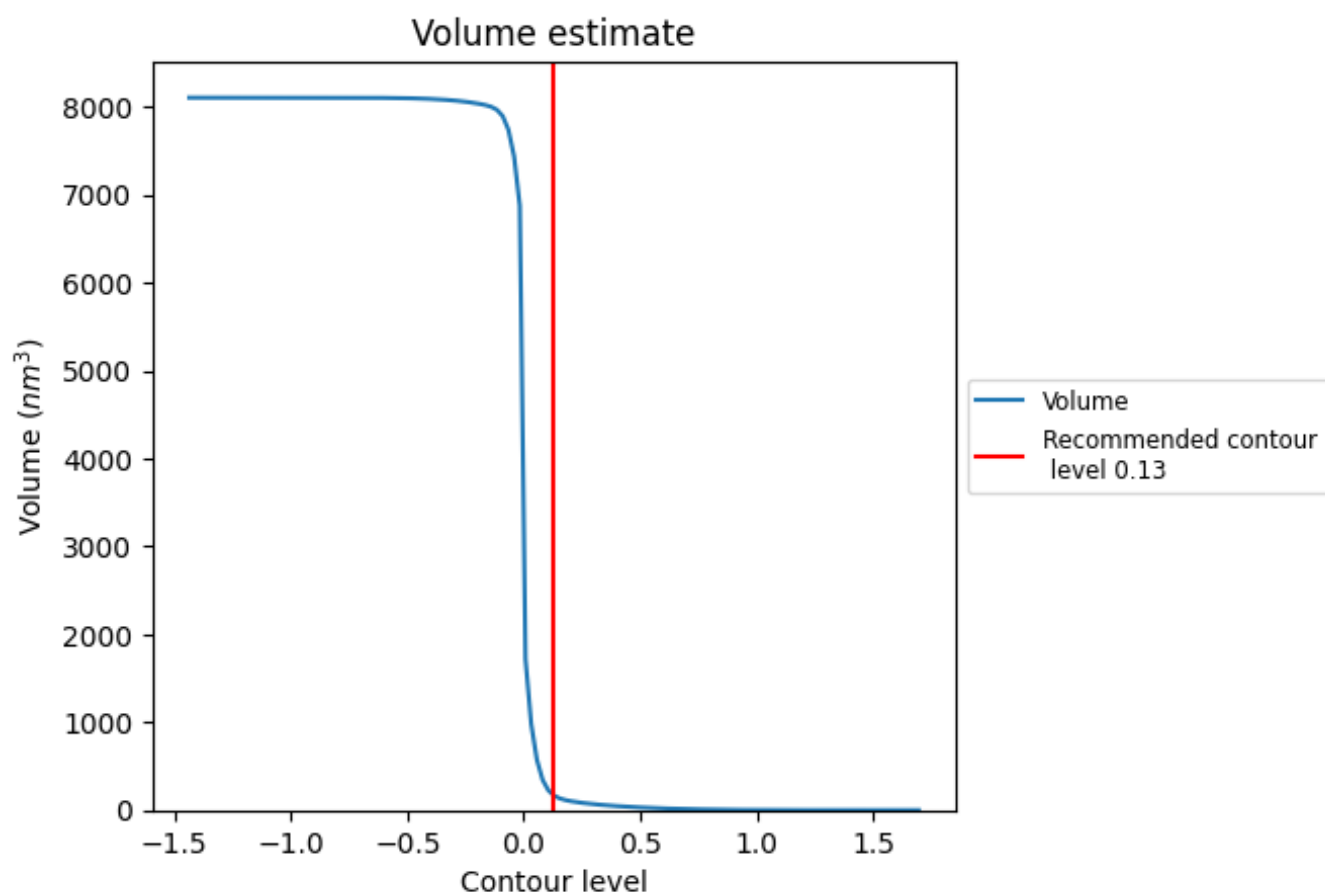
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

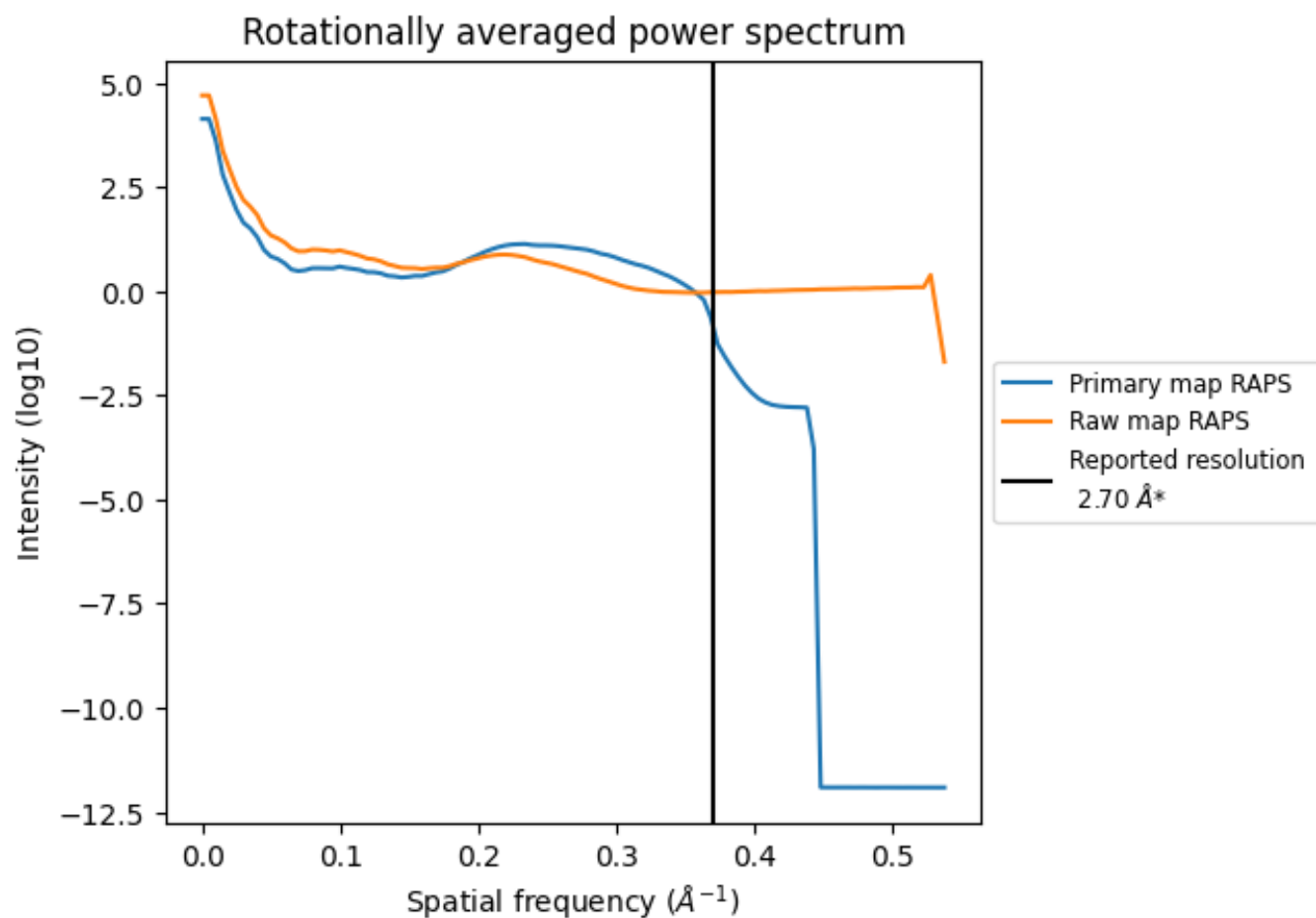
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm^3 ; this corresponds to an approximate mass of 149 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 ⓘ

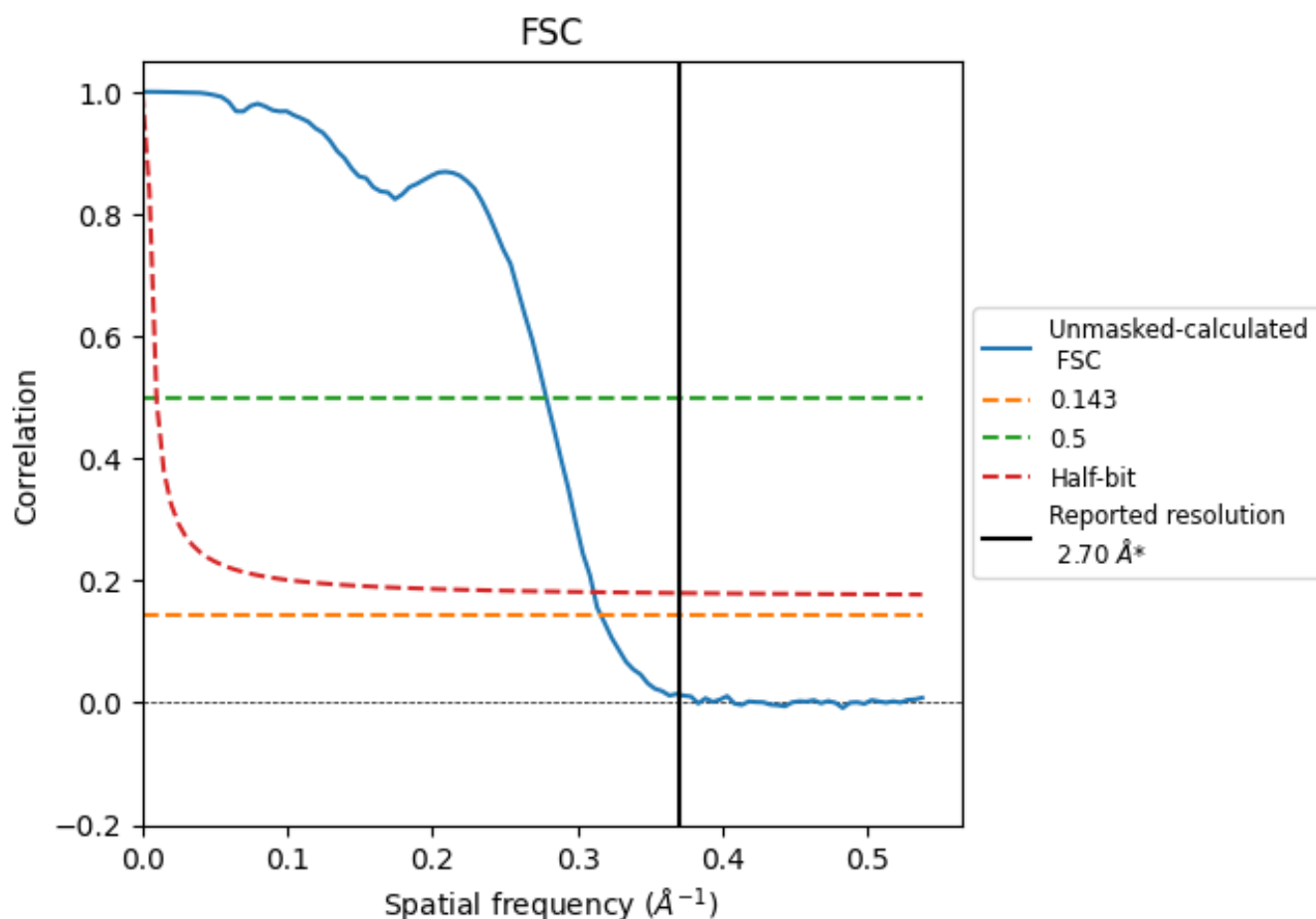


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

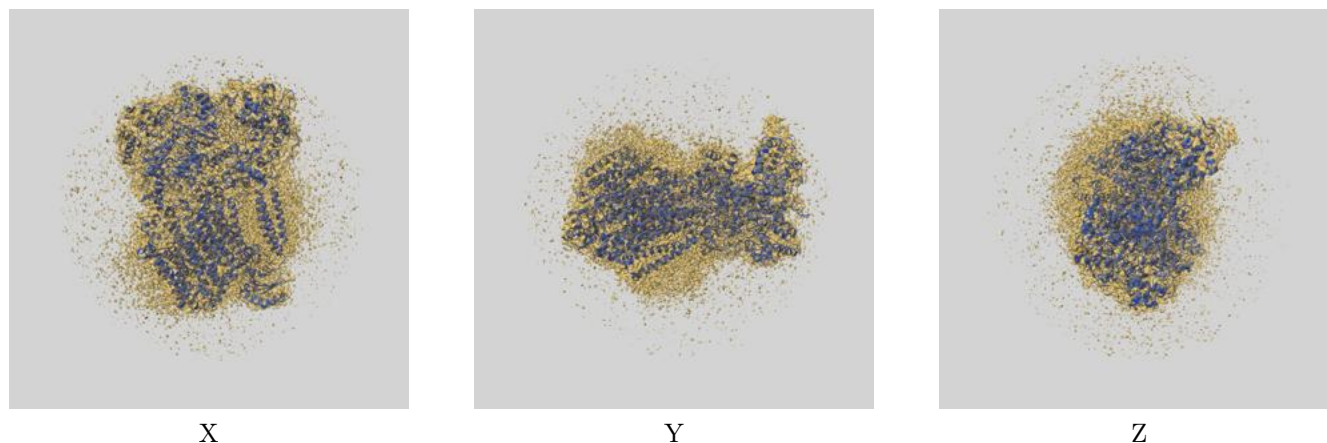
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.59	3.21

*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 3.16 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38012 and PDB model 8X2J. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



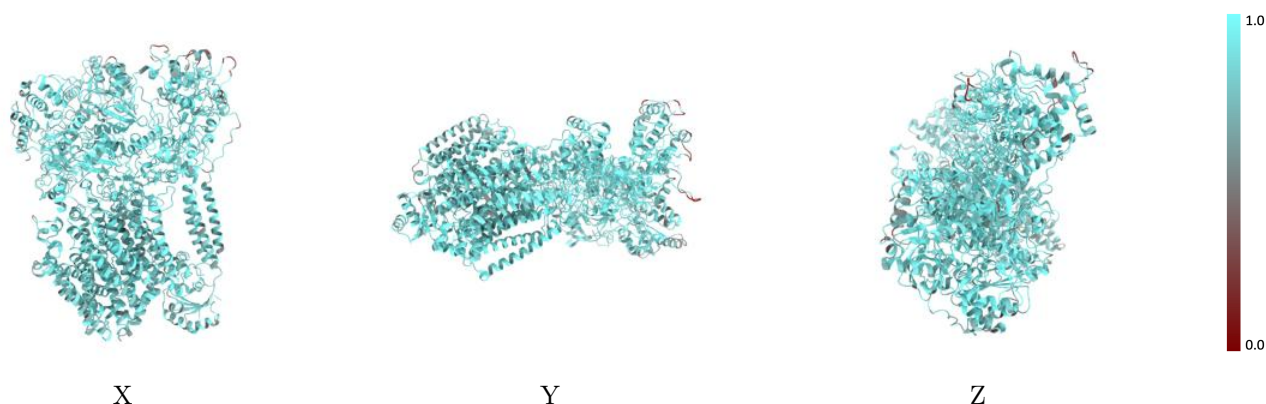
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



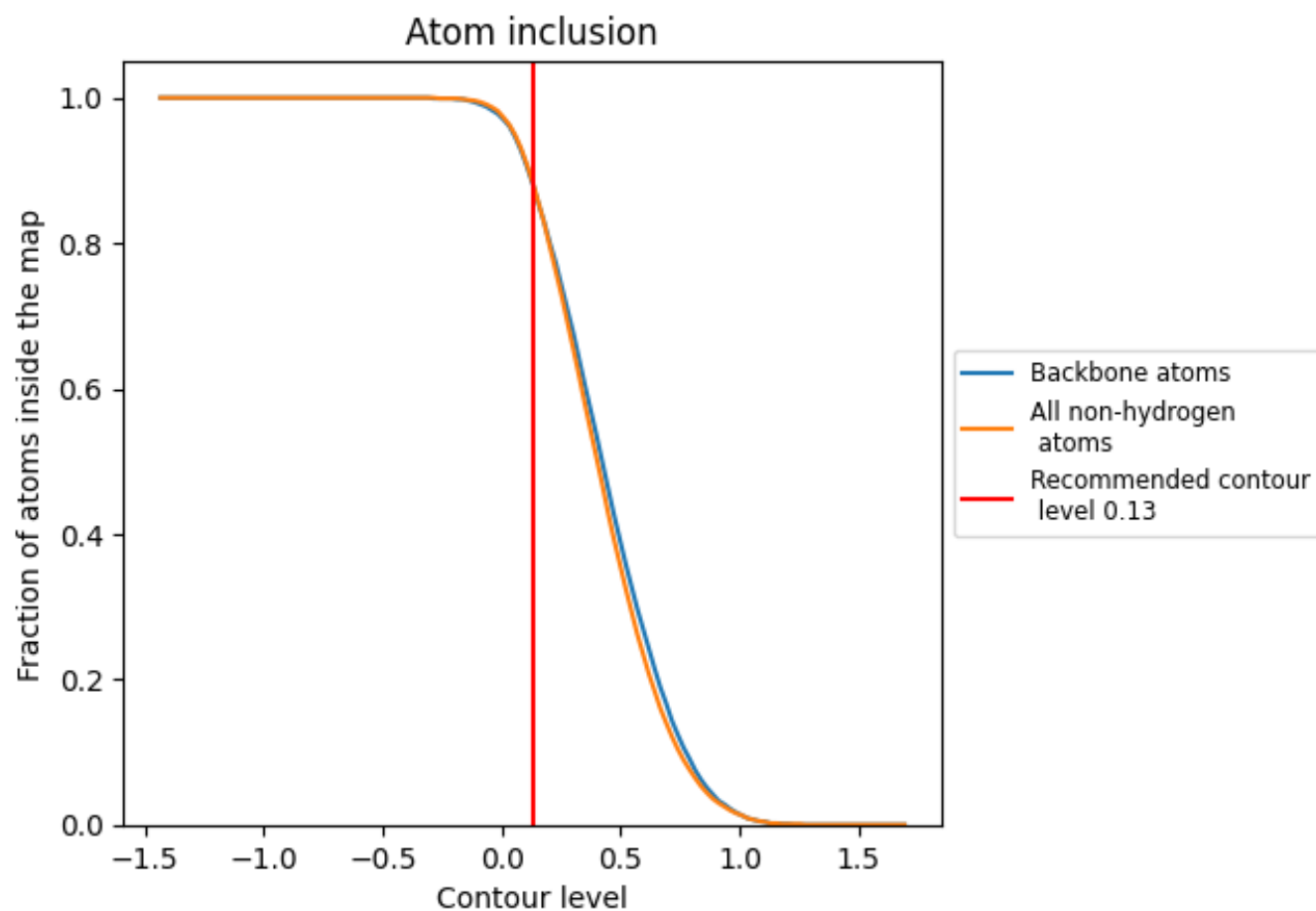
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5610
A	0.9120	0.5750
B	0.8920	0.5670
C	0.9220	0.5890
D	0.8690	0.5500
E	0.8340	0.5190
F	0.8630	0.5440
G	0.7420	0.4800
I	0.8510	0.5290

1.0

0.0

<0.0