



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 07:34 am BST

PDB ID : 9F60 / pdb_00009f60
EMDB ID : EMD-50205
Title : Structure of the Chlamydomonas reinhardtii respiratory complex IV from respiratory supercomplex
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

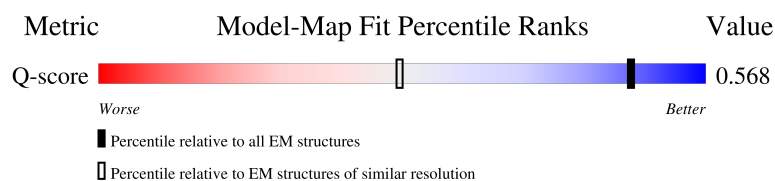
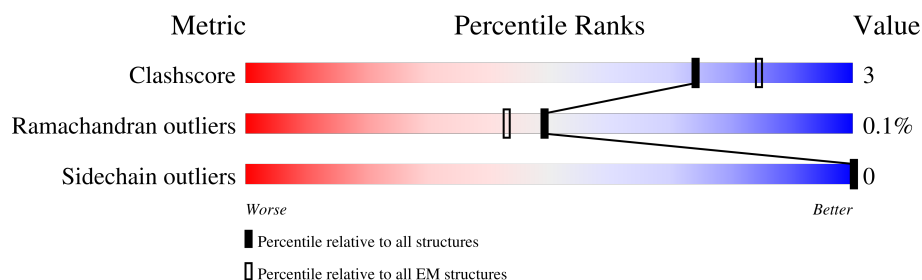
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.39 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.



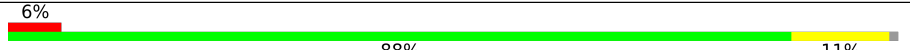
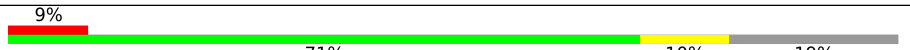
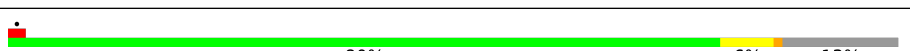
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	2A	505	
2	2B	284	
3	2C	153	
4	2D	382	

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Mol	Chain	Length	Quality of chain
5	2E	175	
6	2F	96	
7	2G	125	
8	2H	148	
9	2I	101	
10	2J	105	
11	2K	58	
12	2L	87	

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
18	CUA	2C	301	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 14202 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		

- Molecule 2 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		

- Molecule 3 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		

- Molecule 5 is a protein called Cox5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		

- Molecule 6 is a protein called Cox5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

- Molecule 7 is a protein called Cox6a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		

- Molecule 8 is a protein called Cox6b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		

- Molecule 9 is a protein called Cox7c.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	2I	72	Total	C	N	O	0	0
			594	393	98	103		

- Molecule 10 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		

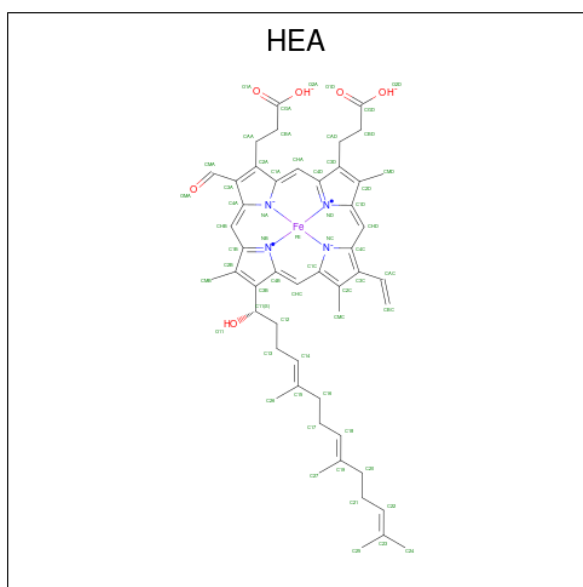
- Molecule 11 is a protein called Cox7a.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	2K	47	Total	C	N	O	0	0
			382	249	63	70		

- Molecule 12 is a protein called CoxIn.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		

- Molecule 13 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
13	2A	1	Total 60	C 49	Fe 1	N 4	O 6	0
13	2A	1	Total 60	C 49	Fe 1	N 4	O 6	0

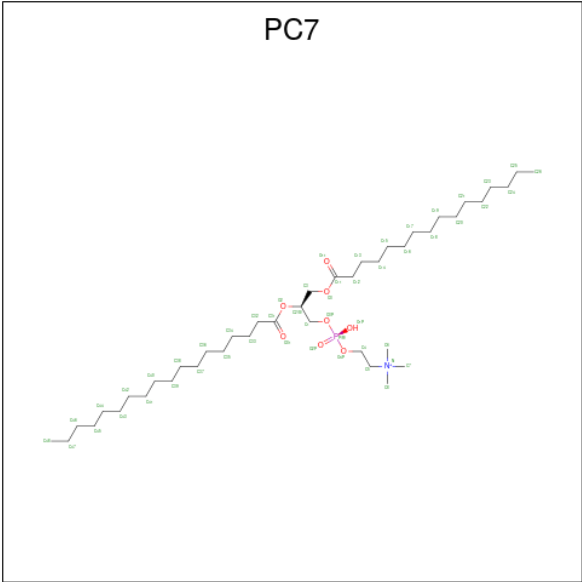
- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
14	2A	1	Total	Cu	0
			1	1	

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

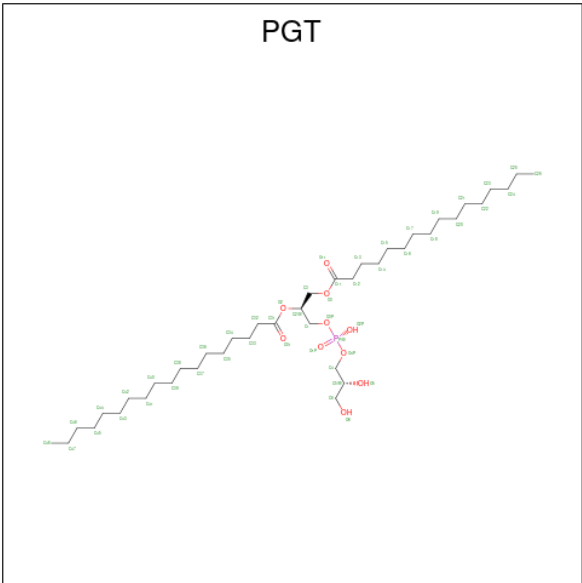
Mol	Chain	Residues	Atoms		AltConf
15	2A	1	Total	Mg	0
			1	1	

- Molecule 16 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



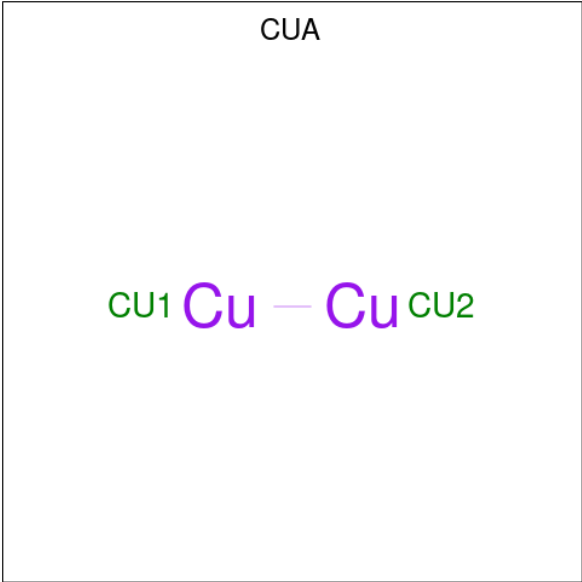
Mol	Chain	Residues	Atoms					AltConf
16	2A	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 17 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



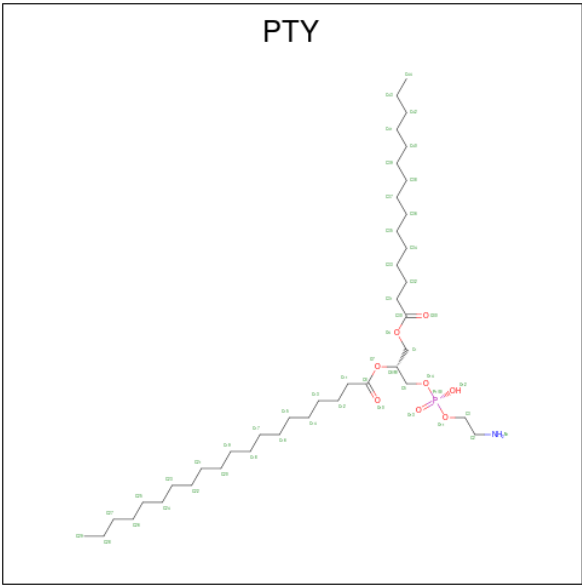
Mol	Chain	Residues	Atoms				AltConf
17	2A	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 18 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
18	2C	1	Total	Cu	0
			2	2	

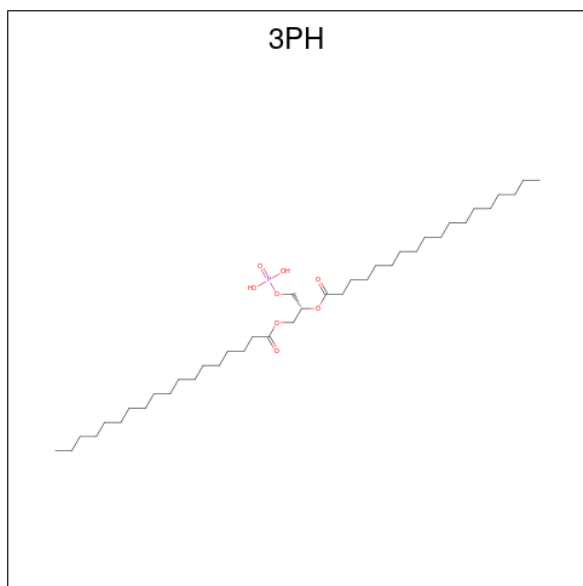
- Molecule 19 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
19	2D	1	Total	C	N	O	P	0
			35	25	1	8	1	
19	2F	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 20 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:

C₃₉H₇₇O₈P).

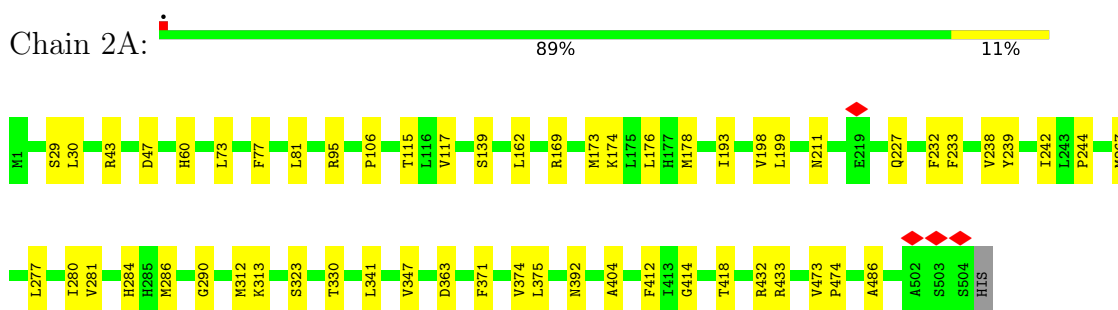


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	2D	1	32	23	8	1	0
20	2I	1	42	33	8	1	0

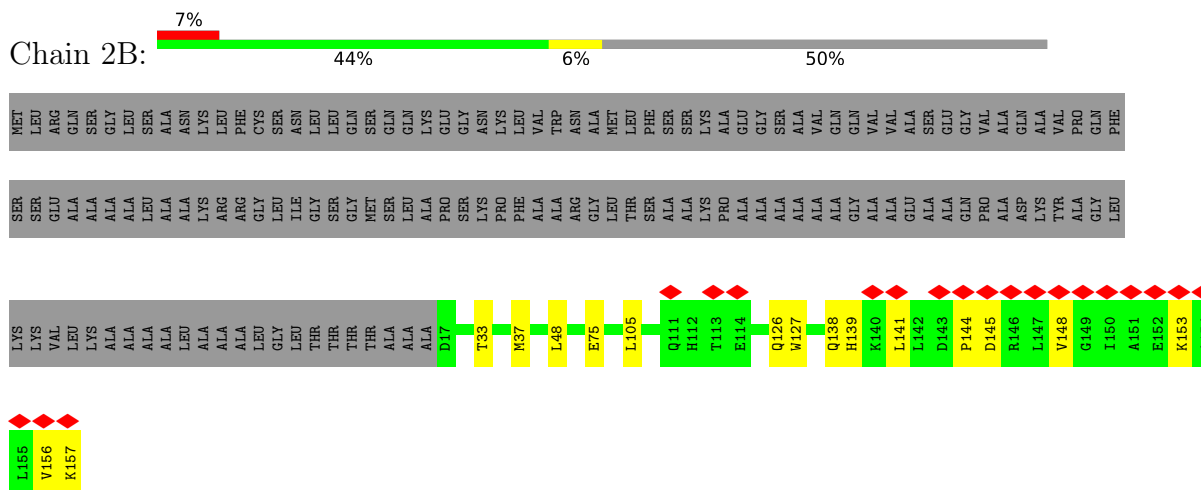
3 Residue-property plots

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

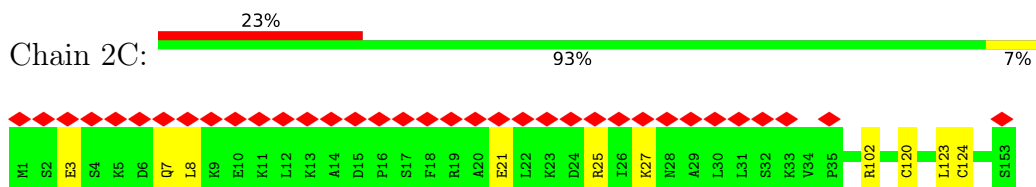
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase polypeptide II

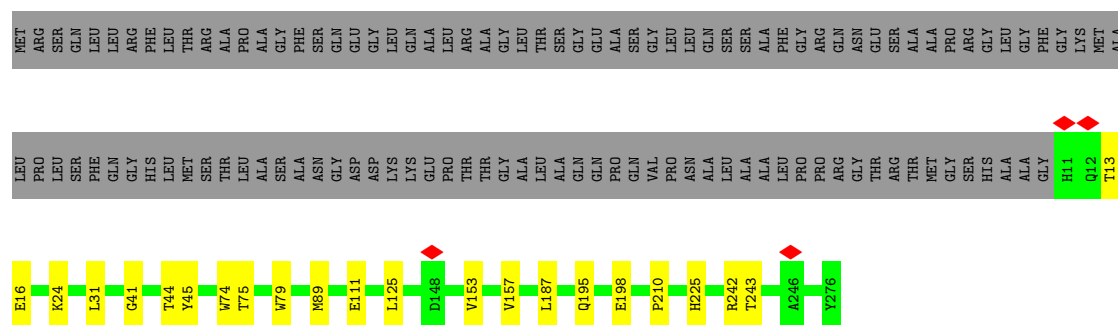


- Molecule 3: cytochrome-c oxidase



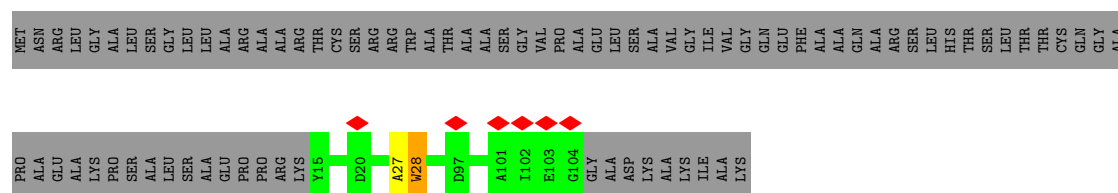
- Molecule 4: Cytochrome c oxidase subunit 3

Chain 2D: 



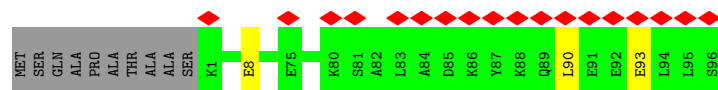
• Molecule 5: Cox5b

Chain 2E: 



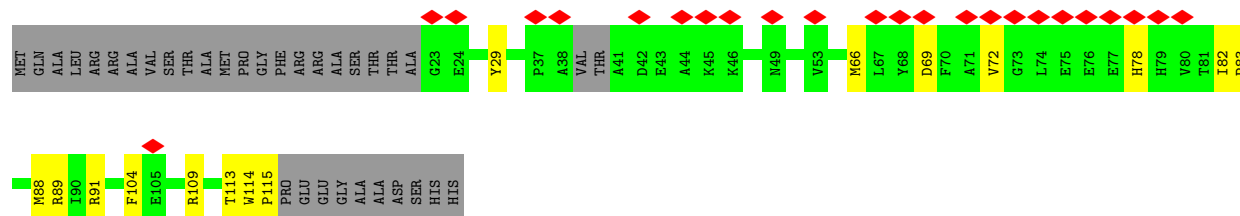
• Molecule 6: Cox5c

Chain 2F: 



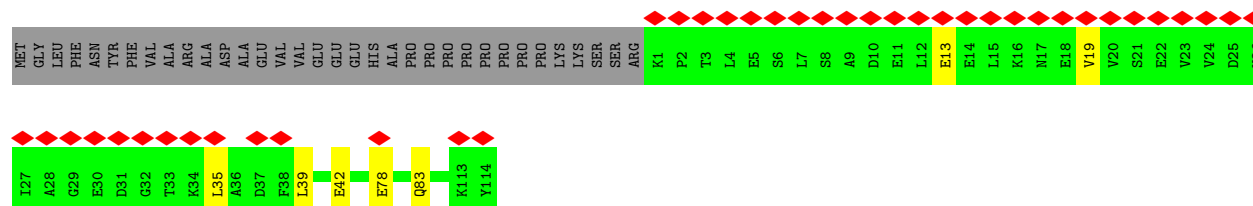
• Molecule 7: Cox6a

Chain 2G: 



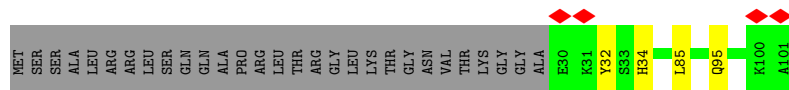
• Molecule 8: Cox6b

Chain 2H: 

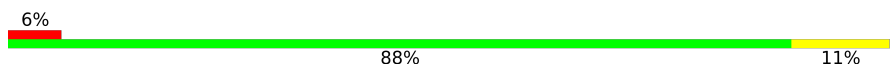


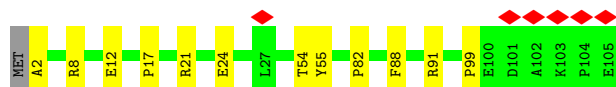
• Molecule 9: Cox7c

Chain 2I:  67% 29%



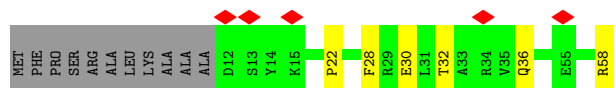
• Molecule 10: Cytochrome c oxidase subunit

Chain 2J:  6% 88% 11%



• Molecule 11: Cox7a

Chain 2K:  9% 71% 10% 19%



• Molecule 12: CoxIn

Chain 2L:  80% 6% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	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 ($e^-/\text{\AA}^2$)	36.27	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.850	Depositor
Minimum map value	-0.453	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	589.6, 589.6, 589.6	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0027211, 1.0027211, 1.0027211	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: HEA, PTY, PGT, PC7, CU, MG, 3PH, CUA

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	2A	0.26	0/4011	0.51	3/5484 (0.1%)
2	2B	0.23	0/1204	0.45	0/1641
3	2C	0.21	0/1237	0.41	0/1676
4	2D	0.23	0/2152	0.47	0/2937
5	2E	0.24	0/757	0.62	3/1029 (0.3%)
6	2F	0.19	0/726	0.35	0/974
7	2G	0.27	0/762	0.57	0/1038
8	2H	0.19	0/980	0.42	0/1325
9	2I	0.23	0/619	0.46	0/839
10	2J	0.21	0/839	0.39	0/1143
11	2K	0.20	0/392	0.39	0/531
12	2L	0.25	0/621	0.59	1/841 (0.1%)
All	All	0.24	0/14300	0.48	7/19458 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	2L	75	VAL	N-CA-C	-6.79	106.19	112.43
5	2E	27	ALA	CA-C-N	6.58	134.12	121.54
5	2E	27	ALA	C-N-CA	6.58	134.12	121.54
1	2A	176	LEU	N-CA-C	-6.50	107.22	114.62
1	2A	486	ALA	CA-C-N	5.27	131.18	121.70
1	2A	486	ALA	C-N-CA	5.27	131.18	121.70
5	2E	28	TRP	N-CA-C	-5.15	99.83	110.80

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	2A	3888	0	3936	36	0
2	2B	1169	0	1191	14	0
3	2C	1212	0	1243	11	0
4	2D	2079	0	2039	15	0
5	2E	737	0	706	0	0
6	2F	706	0	685	2	0
7	2G	733	0	708	12	0
8	2H	954	0	900	6	0
9	2I	594	0	553	4	0
10	2J	816	0	807	9	0
11	2K	382	0	367	6	0
12	2L	605	0	588	4	0
13	2A	120	0	108	2	0
14	2A	1	0	0	0	0
15	2A	1	0	0	0	0
16	2A	27	0	28	1	0
17	2A	33	0	36	1	0
18	2C	2	0	0	3	0
19	2D	35	0	43	1	0
19	2F	34	0	41	0	0
20	2D	32	0	37	0	0
20	2I	42	0	60	0	0
All	All	14202	0	14076	91	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 3.

All (91) 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)
3:2C:120:CYS:SG	18:2C:301:CUA:CU2	1.01	1.51
7:2G:78:HIS:O	7:2G:109:ARG:NH1	1.85	1.09
3:2C:124:CYS:SG	18:2C:301:CUA:CU1	1.75	0.74
1:2A:375:LEU:HD13	13:2A:602:HEA:HAC	1.74	0.69
3:2C:120:CYS:HG	18:2C:301:CUA:CU2	1.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2D:301:PTY:HC52	7:2G:104:PHE:HD2	1.64	0.62
1:2A:47:ASP:HA	10:2J:54:THR:HG21	1.83	0.59
1:2A:211:ASN:O	11:2K:58:ARG:NH2	2.33	0.58
10:2J:88:PHE:O	10:2J:91:ARG:NH1	2.34	0.58
2:2B:156:VAL:HG13	2:2B:157:LYS:HG2	1.87	0.57
2:2B:139:HIS:HB3	8:2H:39:LEU:HD22	1.86	0.57
7:2G:78:HIS:O	7:2G:109:ARG:CZ	2.55	0.55
4:2D:75:THR:OG1	11:2K:36:GLN:OE1	2.25	0.55
4:2D:111:GLU:OE1	4:2D:225:HIS:NE2	2.33	0.55
1:2A:238:VAL:HB	13:2A:601:HEA:HAC	1.89	0.54
7:2G:82:ILE:HG21	7:2G:88:MET:HE2	1.90	0.54
1:2A:474:PRO:HG3	10:2J:8:ARG:HE	1.72	0.54
2:2B:126:GLN:NE2	3:2C:124:CYS:O	2.35	0.54
3:2C:3:GLU:O	3:2C:7:GLN:N	2.38	0.54
12:2L:69:ARG:HB2	12:2L:74:LYS:HB2	1.90	0.54
4:2D:195:GLN:NE2	4:2D:198:GLU:OE1	2.42	0.53
1:2A:392:ASN:ND2	10:2J:12:GLU:OE1	2.40	0.53
1:2A:77:PHE:O	1:2A:81:LEU:HB2	2.09	0.52
1:2A:281:VAL:O	1:2A:284:HIS:ND1	2.24	0.52
1:2A:106:PRO:HB3	4:2D:45:TYR:HB2	1.92	0.52
3:2C:25:ARG:NH1	8:2H:13:GLU:OE2	2.43	0.52
1:2A:323:SER:OG	2:2B:75:GLU:OE1	2.27	0.52
1:2A:117:VAL:O	1:2A:139:SER:OG	2.28	0.51
1:2A:414:GLY:O	1:2A:418:THR:OG1	2.26	0.51
1:2A:173:MET:HE3	1:2A:178:MET:HG2	1.92	0.50
10:2J:17:PRO:HG2	10:2J:24:GLU:HB3	1.92	0.50
12:2L:31:ARG:NH2	12:2L:61:SER:OG	2.34	0.50
2:2B:153:LYS:HA	2:2B:156:VAL:HG12	1.93	0.50
3:2C:21:GLU:OE2	3:2C:25:ARG:NH2	2.44	0.50
1:2A:371:PHE:HA	1:2A:374:VAL:HG22	1.93	0.50
4:2D:41:GLY:O	4:2D:44:THR:OG1	2.26	0.50
1:2A:43:ARG:HB2	10:2J:55:TYR:HB3	1.94	0.50
1:2A:267:MET:SD	1:2A:313:LYS:NZ	2.81	0.50
7:2G:69:ASP:HA	7:2G:72:VAL:HG12	1.93	0.50
4:2D:125:LEU:HD13	4:2D:210:PRO:HB3	1.93	0.49
1:2A:290:GLY:O	3:2C:102:ARG:NH2	2.47	0.48
4:2D:13:THR:OG1	4:2D:16:GLU:OE1	2.32	0.48
1:2A:199:LEU:HB2	1:2A:233:PHE:CG	2.49	0.48
1:2A:239:TYR:HA	1:2A:242:ILE:HG22	1.96	0.48
3:2C:8:LEU:HD22	8:2H:19:VAL:HG21	1.96	0.47
1:2A:115:THR:O	9:2I:95:GLN:NE2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:330:THR:HG21	1:2A:404:ALA:HB1	1.96	0.47
1:2A:277:LEU:HD23	1:2A:280:ILE:HD11	1.97	0.47
4:2D:153:VAL:HG12	7:2G:66:MET:HE3	1.97	0.47
9:2I:32:TYR:HE1	11:2K:30:GLU:HG3	1.80	0.46
2:2B:144:PRO:HB2	3:2C:27:LYS:HE3	1.96	0.46
2:2B:145:ASP:N	2:2B:145:ASP:OD1	2.48	0.46
9:2I:34:HIS:CD2	11:2K:22:PRO:HG3	2.51	0.46
2:2B:33:THR:HG22	2:2B:37:MET:HE3	1.97	0.45
7:2G:83:PRO:HB3	7:2G:114:TRP:CZ2	2.51	0.45
11:2K:28:PHE:O	11:2K:32:THR:OG1	2.34	0.45
4:2D:24:LYS:HG3	7:2G:29:TYR:CZ	2.52	0.45
6:2F:90:LEU:HA	6:2F:93:GLU:HB2	1.99	0.45
1:2A:95:ARG:HG3	4:2D:31:LEU:HD13	1.98	0.44
4:2D:74:TRP:HE1	11:2K:32:THR:HG21	1.82	0.44
4:2D:157:VAL:HG13	4:2D:187:LEU:HD22	1.99	0.44
7:2G:78:HIS:HB2	7:2G:109:ARG:NH2	2.32	0.44
1:2A:227:GLN:HB2	1:2A:286:MET:HE3	2.00	0.44
1:2A:162:LEU:HD12	1:2A:193:ILE:HD12	1.98	0.44
1:2A:363:ASP:HA	1:2A:432:ARG:HD3	2.00	0.44
7:2G:89:ARG:O	7:2G:89:ARG:HG2	2.18	0.44
2:2B:126:GLN:HA	2:2B:127:TRP:HA	1.74	0.43
8:2H:78:GLU:HA	8:2H:83:GLN:HE22	1.83	0.43
1:2A:198:VAL:HG11	1:2A:232:PHE:HD2	1.83	0.43
1:2A:341:LEU:HD11	1:2A:412:PHE:HE1	1.84	0.43
1:2A:433:ARG:HD3	3:2C:123:LEU:HD22	2.01	0.42
2:2B:141:LEU:HD21	8:2H:35:LEU:HD13	2.00	0.42
1:2A:312:MET:SD	12:2L:14:LEU:HD11	2.60	0.42
2:2B:138:GLN:HE21	8:2H:42:GLU:HB3	1.84	0.42
4:2D:242:ARG:HG2	4:2D:243:THR:HG23	2.02	0.42
2:2B:145:ASP:HA	2:2B:148:VAL:HB	2.01	0.42
1:2A:30:LEU:HB3	1:2A:60:HIS:HB2	2.02	0.41
16:2A:605:PC7:H132	16:2A:605:PC7:H331	2.01	0.41
7:2G:91:ARG:HD3	7:2G:91:ARG:HA	1.95	0.41
1:2A:73:LEU:HB3	1:2A:244:PRO:HB2	2.03	0.41
1:2A:473:VAL:HA	1:2A:474:PRO:HD3	1.88	0.41
17:2A:606:PGT:O1P	4:2D:79:TRP:NE1	2.47	0.41
6:2F:8:GLU:OE2	10:2J:2:ALA:N	2.54	0.41
1:2A:169:ARG:HH21	1:2A:174:LYS:HA	1.86	0.40
4:2D:89:MET:HE3	4:2D:89:MET:HB3	1.99	0.40
1:2A:347:VAL:HB	2:2B:48:LEU:HD13	2.03	0.40
10:2J:82:PRO:HG2	10:2J:99:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:29:SER:HB2	9:2I:85:LEU:HA	2.03	0.40
10:2J:21:ARG:NH2	10:2J:24:GLU:O	2.52	0.40
2:2B:105:LEU:HB2	12:2L:75:VAL:HG13	2.04	0.40
7:2G:113:THR:O	7:2G:115:PRO:HD3	2.20	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	2A	502/505 (99%)	489 (97%)	13 (3%)	0	100	100
2	2B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100
3	2C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
4	2D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
5	2E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	18
6	2F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
7	2G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
8	2H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
9	2I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
10	2J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
11	2K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
12	2L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
All	All	1718/2219 (77%)	1657 (96%)	60 (4%)	1 (0%)	49	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	2E	28	TRP

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	2A	408/409 (100%)	408 (100%)	0	100	100
2	2B	132/224 (59%)	132 (100%)	0	100	100
3	2C	137/137 (100%)	137 (100%)	0	100	100
4	2D	211/294 (72%)	211 (100%)	0	100	100
5	2E	79/137 (58%)	79 (100%)	0	100	100
6	2F	66/72 (92%)	66 (100%)	0	100	100
7	2G	75/100 (75%)	75 (100%)	0	100	100
8	2H	103/132 (78%)	103 (100%)	0	100	100
9	2I	58/80 (72%)	58 (100%)	0	100	100
10	2J	83/84 (99%)	83 (100%)	0	100	100
11	2K	39/46 (85%)	39 (100%)	0	100	100
12	2L	63/74 (85%)	63 (100%)	0	100	100
All	All	1454/1789 (81%)	1454 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	2A	490	HIS
2	2B	111	GLN
2	2B	112	HIS
4	2D	21	HIS
4	2D	222	HIS
4	2D	275	GLN
6	2F	63	GLN
8	2H	83	GLN

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Mol	Chain	Res	Type
12	2L	56	GLN
12	2L	72	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	PGT	2A	606	-	32,32,50	0.61	0	35,38,56	0.60	0
20	3PH	2I	201	-	41,41,47	0.67	1 (2%)	45,46,52	0.67	1 (2%)
16	PC7	2A	605	-	26,26,51	0.66	0	32,34,59	0.70	0
19	PTY	2D	301	-	34,34,49	0.57	0	37,39,54	0.57	0
20	3PH	2D	302	-	31,31,47	0.77	1 (3%)	35,36,52	0.72	1 (2%)
19	PTY	2F	101	-	33,33,49	0.55	0	36,38,54	0.45	0
13	HEA	2A	601	1	66,67,67	2.44	26 (39%)	78,103,103	2.54	32 (41%)
18	CUA	2C	301	-	0,1,1	-	-	-	-	-
13	HEA	2A	602	1	66,67,67	2.46	23 (34%)	78,103,103	2.58	33 (42%)

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
17	PGT	2A	606	-	-	10/37/37/55	-
20	3PH	2I	201	-	-	14/43/43/49	-
16	PC7	2A	605	-	-	10/30/30/55	-
19	PTY	2D	301	-	-	13/38/38/53	-
20	3PH	2D	302	-	-	19/33/33/49	-
19	PTY	2F	101	-	-	15/37/37/53	-
13	HEA	2A	601	1	-	10/36/76/76	-
13	HEA	2A	602	1	-	7/36/76/76	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2A	602	HEA	C3B-C2B	5.67	1.47	1.34
13	2A	602	HEA	FE-ND	5.60	2.12	1.94
13	2A	601	HEA	FE-NB	5.59	2.12	1.94
13	2A	601	HEA	FE-ND	5.48	2.11	1.94
13	2A	602	HEA	FE-NB	5.38	2.11	1.94
13	2A	601	HEA	C3A-C2A	5.15	1.47	1.36
13	2A	601	HEA	C3B-C2B	5.12	1.46	1.34
13	2A	602	HEA	C3D-C2D	4.97	1.47	1.36
13	2A	601	HEA	C3D-C2D	4.87	1.47	1.36
13	2A	602	HEA	C3A-C2A	4.80	1.47	1.36
13	2A	602	HEA	FE-NC	4.75	2.11	1.95
13	2A	601	HEA	FE-NC	4.70	2.11	1.95
13	2A	602	HEA	CHC-C4B	4.54	1.47	1.38
13	2A	601	HEA	CHD-C1D	4.36	1.47	1.38
13	2A	602	HEA	CHB-C4A	4.29	1.46	1.38
13	2A	602	HEA	CHA-C1A	4.29	1.46	1.38
13	2A	602	HEA	CHD-C1D	4.19	1.47	1.38
13	2A	601	HEA	CHC-C4B	4.18	1.47	1.38
13	2A	601	HEA	CHB-C4A	4.17	1.46	1.38
13	2A	601	HEA	C1A-NA	4.15	1.47	1.39
13	2A	601	HEA	CHA-C1A	4.08	1.46	1.38
13	2A	602	HEA	C1A-NA	4.03	1.47	1.39
13	2A	601	HEA	C4A-NA	3.98	1.47	1.39
13	2A	602	HEA	C4A-NA	3.73	1.47	1.39
13	2A	602	HEA	CHC-C1C	3.66	1.47	1.39
13	2A	601	HEA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2A	602	HEA	CHD-C4C	3.38	1.47	1.39
20	2D	302	3PH	P-O11	3.33	1.70	1.60
13	2A	601	HEA	CHB-C1B	3.33	1.46	1.39
20	2I	201	3PH	P-O11	3.27	1.70	1.60
13	2A	601	HEA	CHC-C1C	3.26	1.46	1.39
13	2A	602	HEA	CHB-C1B	3.23	1.46	1.39
13	2A	602	HEA	CHA-C4D	3.17	1.46	1.39
13	2A	601	HEA	CHA-C4D	3.17	1.46	1.39
13	2A	602	HEA	C1D-ND	-3.08	1.35	1.40
13	2A	602	HEA	C4B-C3B	3.07	1.49	1.44
13	2A	601	HEA	C4B-NB	-2.79	1.35	1.40
13	2A	602	HEA	C1C-C2C	2.74	1.49	1.43
13	2A	601	HEA	C1D-ND	-2.70	1.35	1.40
13	2A	602	HEA	C4C-NC	-2.45	1.35	1.39
13	2A	602	HEA	C4B-NB	-2.42	1.36	1.40
13	2A	601	HEA	C3C-C4C	2.40	1.48	1.42
13	2A	601	HEA	C4B-C3B	2.39	1.48	1.44
13	2A	602	HEA	C4D-C3D	2.36	1.49	1.45
13	2A	601	HEA	C1C-NC	-2.32	1.35	1.39
13	2A	601	HEA	C4C-NC	-2.18	1.35	1.39
13	2A	601	HEA	C1D-C2D	2.16	1.48	1.44
13	2A	601	HEA	C1C-C2C	2.09	1.48	1.43
13	2A	601	HEA	C1B-C2B	2.08	1.48	1.44
13	2A	601	HEA	C1A-C2A	2.08	1.48	1.45
13	2A	602	HEA	C3C-C4C	2.00	1.47	1.42

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2A	602	HEA	C3C-C4C-NC	7.18	114.66	110.25
13	2A	601	HEA	C3D-C4D-ND	6.78	116.92	110.36
13	2A	602	HEA	C3D-C4D-ND	6.73	116.87	110.36
13	2A	601	HEA	C3C-C4C-NC	6.33	114.14	110.25
13	2A	602	HEA	C3C-C2C-C1C	-5.74	100.23	107.16
13	2A	602	HEA	C2B-C1B-NB	5.66	116.66	109.88
13	2A	602	HEA	C2D-C1D-ND	5.64	116.53	109.84
13	2A	601	HEA	C3B-C4B-NB	5.60	116.48	109.84
13	2A	601	HEA	C3C-C2C-C1C	-5.44	100.60	107.16
13	2A	601	HEA	C2D-C1D-ND	5.28	116.10	109.84
13	2A	601	HEA	C2B-C1B-NB	4.95	115.81	109.88
13	2A	602	HEA	C3B-C4B-NB	4.92	115.67	109.84
13	2A	601	HEA	C2C-C1C-NC	4.73	117.28	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2A	602	HEA	C2A-C1A-NA	4.45	114.66	110.32
13	2A	601	HEA	C13-C12-C11	-4.45	107.66	114.35
13	2A	601	HEA	C2A-C1A-NA	4.41	114.61	110.32
13	2A	602	HEA	C4A-NA-C1A	-4.33	101.11	105.35
13	2A	602	HEA	C2C-C1C-NC	4.22	116.51	110.08
13	2A	601	HEA	C1D-C2D-C3D	-4.14	102.61	106.96
13	2A	601	HEA	C4A-NA-C1A	-4.12	101.32	105.35
13	2A	602	HEA	C1D-C2D-C3D	-3.82	102.94	106.96
13	2A	602	HEA	C4D-C3D-C2D	-3.65	101.57	106.90
13	2A	601	HEA	C3A-C2A-C1A	-3.59	103.65	107.08
13	2A	602	HEA	CHA-C4D-ND	-3.50	120.61	124.42
13	2A	602	HEA	C1B-C2B-C3B	-3.33	102.81	106.80
13	2A	601	HEA	C4D-C3D-C2D	-3.29	102.11	106.90
13	2A	601	HEA	CMB-C2B-C1B	3.26	130.00	125.04
13	2A	602	HEA	C3A-C2A-C1A	-3.13	104.09	107.08
13	2A	602	HEA	C4B-C3B-C2B	-3.10	102.11	107.41
13	2A	601	HEA	C4B-C3B-C2B	-3.10	102.12	107.41
13	2A	601	HEA	C1B-C2B-C3B	-3.07	103.13	106.80
13	2A	602	HEA	C27-C19-C20	2.98	120.28	115.27
13	2A	601	HEA	CAD-CBD-CGD	-2.97	107.21	113.60
13	2A	602	HEA	CAD-C3D-C4D	2.97	129.84	124.66
13	2A	602	HEA	C1D-ND-C4D	-2.89	102.09	105.07
13	2A	602	HEA	CMC-C2C-C1C	2.84	129.70	125.37
13	2A	601	HEA	C13-C14-C15	-2.82	120.88	127.66
13	2A	601	HEA	CHC-C1C-C2C	-2.81	119.29	127.24
13	2A	602	HEA	CAD-CBD-CGD	-2.79	107.59	113.60
13	2A	602	HEA	CHB-C4A-NA	-2.77	121.44	124.44
13	2A	601	HEA	C1D-ND-C4D	-2.72	102.27	105.07
13	2A	602	HEA	C13-C14-C15	-2.68	121.21	127.66
13	2A	602	HEA	C26-C15-C16	2.65	119.73	115.27
13	2A	601	HEA	C27-C19-C20	2.61	119.66	115.27
13	2A	601	HEA	C4B-NB-C1B	-2.53	102.46	105.07
13	2A	602	HEA	CHB-C1B-C2B	-2.48	121.11	124.98
13	2A	601	HEA	CHA-C4D-ND	-2.44	121.77	124.42
13	2A	601	HEA	CHA-C4D-C3D	-2.40	121.31	124.84
13	2A	602	HEA	C25-C23-C24	2.35	119.80	114.60
13	2A	601	HEA	CHB-C1B-NB	-2.34	121.88	124.42
13	2A	602	HEA	CHD-C1D-C2D	-2.25	120.47	126.73
13	2A	602	HEA	C4B-NB-C1B	-2.25	102.75	105.07
13	2A	601	HEA	C4C-NC-C1C	-2.24	103.16	105.35
13	2A	601	HEA	CMC-C2C-C3C	2.22	131.96	126.59
13	2A	602	HEA	C4C-NC-C1C	-2.20	103.19	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2I	201	3PH	O13-P-O11	-2.18	100.94	106.73
13	2A	601	HEA	CHD-C1D-C2D	-2.17	120.71	126.73
13	2A	602	HEA	CHA-C1A-NA	-2.14	122.13	124.44
13	2A	602	HEA	CHC-C1C-C2C	-2.13	121.22	127.24
13	2A	602	HEA	CBA-CAA-C2A	-2.12	106.73	112.63
13	2A	602	HEA	CAA-CBA-CGA	-2.08	109.12	113.60
13	2A	601	HEA	C26-C15-C16	2.08	118.77	115.27
13	2A	601	HEA	C25-C23-C24	2.06	119.16	114.60
20	2D	302	3PH	O13-P-O11	-2.05	101.29	106.73
13	2A	601	HEA	CHA-C1A-NA	-2.04	122.23	124.44
13	2A	601	HEA	CMD-C2D-C1D	2.01	128.10	125.04
13	2A	602	HEA	CHB-C1B-NB	-2.01	122.24	124.42

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	2A	601	HEA	C2A-C3A-CMA-OMA
13	2A	602	HEA	C3B-C11-C12-C13
13	2A	602	HEA	O11-C11-C12-C13
13	2A	602	HEA	C15-C16-C17-C18
19	2D	301	PTY	C11-C8-O7-C6
19	2F	101	PTY	C3-O11-P1-O12
19	2F	101	PTY	C5-O14-P1-O11
19	2F	101	PTY	C5-O14-P1-O13
20	2D	302	3PH	C1-O11-P-O13
20	2D	302	3PH	C1-O11-P-O14
20	2D	302	3PH	C1-O11-P-O12
20	2D	302	3PH	C22-C21-O21-C2
20	2I	201	3PH	C1-O11-P-O13
20	2I	201	3PH	C1-O11-P-O14
16	2A	605	PC7	O11-C11-O3-C3
19	2D	301	PTY	O10-C8-O7-C6
16	2A	605	PC7	C12-C11-O3-C3
17	2A	606	PGT	C12-C11-O3-C3
20	2D	302	3PH	O22-C21-O21-C2
17	2A	606	PGT	O11-C11-O3-C3
20	2I	201	3PH	C22-C21-O21-C2
13	2A	602	HEA	C19-C20-C21-C22
20	2I	201	3PH	O22-C21-O21-C2
16	2A	605	PC7	C4-O4P-P-O3P
19	2F	101	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
20	2I	201	3PH	C24-C25-C26-C27
17	2A	606	PGT	C11-C12-C13-C14
20	2I	201	3PH	C29-C2A-C2B-C2C
19	2F	101	PTY	N1-C2-C3-O11
19	2F	101	PTY	C11-C8-O7-C6
19	2F	101	PTY	O10-C8-O7-C6
19	2F	101	PTY	C34-C35-C36-C37
20	2D	302	3PH	C32-C31-O31-C3
20	2D	302	3PH	O21-C2-C3-O31
20	2D	302	3PH	C23-C24-C25-C26
20	2D	302	3PH	C22-C23-C24-C25
17	2A	606	PGT	C1-C2-C3-O3
20	2D	302	3PH	C1-C2-C3-O31
19	2D	301	PTY	C17-C18-C19-C20
16	2A	605	PC7	C31-C32-C33-C34
20	2D	302	3PH	O32-C31-O31-C3
20	2I	201	3PH	C1-O11-P-O12
19	2D	301	PTY	C19-C20-C21-C22
16	2A	605	PC7	C2-C1-O3P-P
20	2I	201	3PH	C2-C1-O11-P
19	2D	301	PTY	C16-C17-C18-C19
20	2I	201	3PH	C26-C27-C28-C29
13	2A	602	HEA	C2A-C3A-CMA-OMA
19	2F	101	PTY	C35-C36-C37-C38
16	2A	605	PC7	C32-C33-C34-C35
20	2D	302	3PH	O11-C1-C2-C3
20	2D	302	3PH	C28-C29-C2A-C2B
19	2F	101	PTY	O4-C1-C6-O7
19	2D	301	PTY	C6-C5-O14-P1
16	2A	605	PC7	C4-O4P-P-O2P
19	2F	101	PTY	C2-C3-O11-P1
20	2D	302	3PH	O11-C1-C2-O21
16	2A	605	PC7	C4-C5-N-C6
13	2A	601	HEA	C4A-C3A-CMA-OMA
13	2A	602	HEA	C4A-C3A-CMA-OMA
20	2I	201	3PH	C33-C34-C35-C36
16	2A	605	PC7	C4-C5-N-C8
13	2A	602	HEA	C11-C12-C13-C14
16	2A	605	PC7	C4-C5-N-C7
20	2I	201	3PH	C31-C32-C33-C34
17	2A	606	PGT	O2-C2-C3-O3
19	2D	301	PTY	C3-O11-P1-O14

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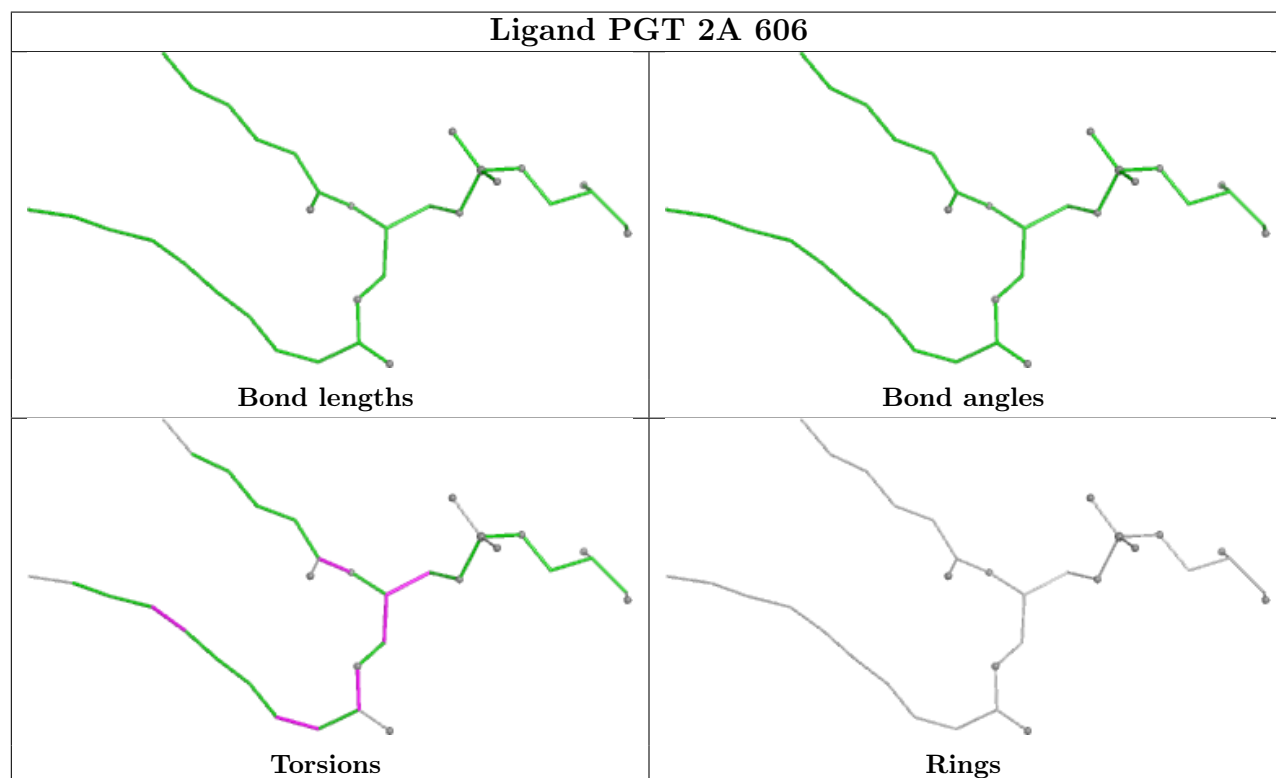
Mol	Chain	Res	Type	Atoms
19	2D	301	PTY	C13-C14-C15-C16
20	2I	201	3PH	C32-C33-C34-C35
17	2A	606	PGT	O31-C31-O2-C2
20	2D	302	3PH	C35-C36-C37-C38
17	2A	606	PGT	O3P-C1-C2-O2
20	2I	201	3PH	C34-C35-C36-C37
17	2A	606	PGT	C32-C31-O2-C2
13	2A	601	HEA	CAA-CBA-CGA-O2A
13	2A	601	HEA	C4C-C3C-CAC-CBC
19	2F	101	PTY	O14-C5-C6-C1
13	2A	601	HEA	C26-C15-C16-C17
17	2A	606	PGT	C15-C16-C17-C18
19	2D	301	PTY	C12-C11-C8-O7
20	2D	302	3PH	C24-C25-C26-C27
13	2A	601	HEA	CAD-CBD-CGD-O2D
19	2F	101	PTY	C11-C12-C13-C14
19	2F	101	PTY	O4-C1-C6-C5
13	2A	601	HEA	CAA-CBA-CGA-O1A
13	2A	601	HEA	CAD-CBD-CGD-O1D
20	2D	302	3PH	O21-C21-C22-C23
19	2D	301	PTY	C15-C16-C17-C18
17	2A	606	PGT	O3P-C1-C2-C3
19	2D	301	PTY	C12-C11-C8-O10
20	2D	302	3PH	C25-C26-C27-C28
20	2I	201	3PH	C36-C37-C38-C39
19	2D	301	PTY	C3-O11-P1-O13
20	2D	302	3PH	O22-C21-C22-C23
13	2A	601	HEA	C2A-CAA-CBA-CGA
19	2D	301	PTY	O14-C5-C6-O7
19	2F	101	PTY	O14-C5-C6-O7
13	2A	601	HEA	C19-C20-C21-C22

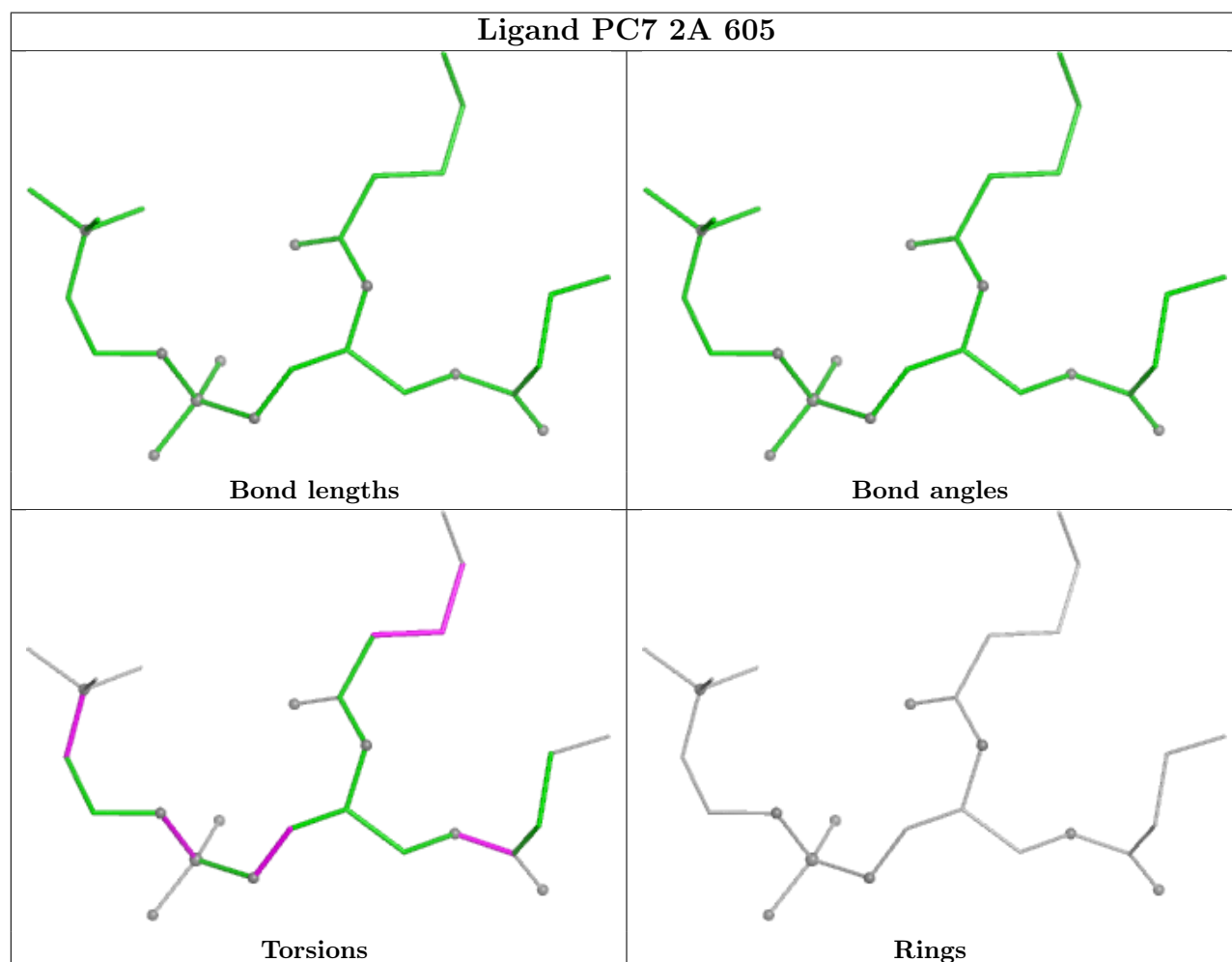
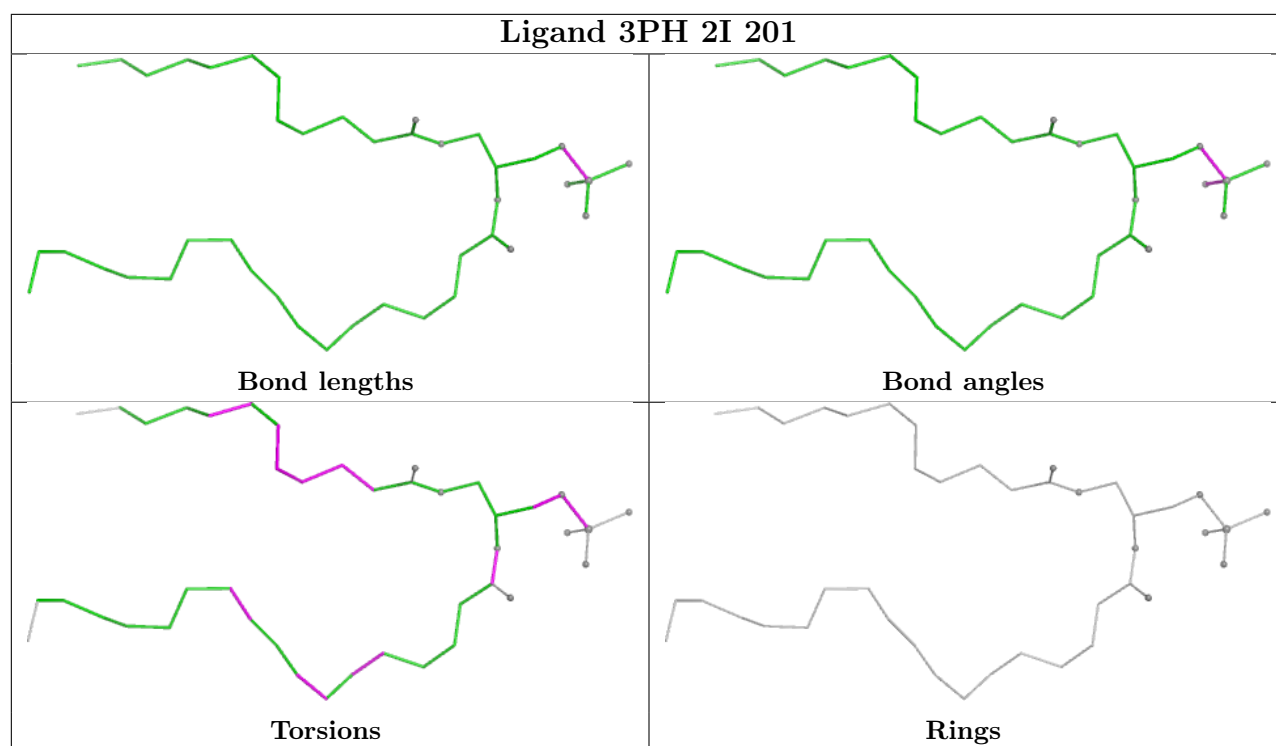
There are no ring outliers.

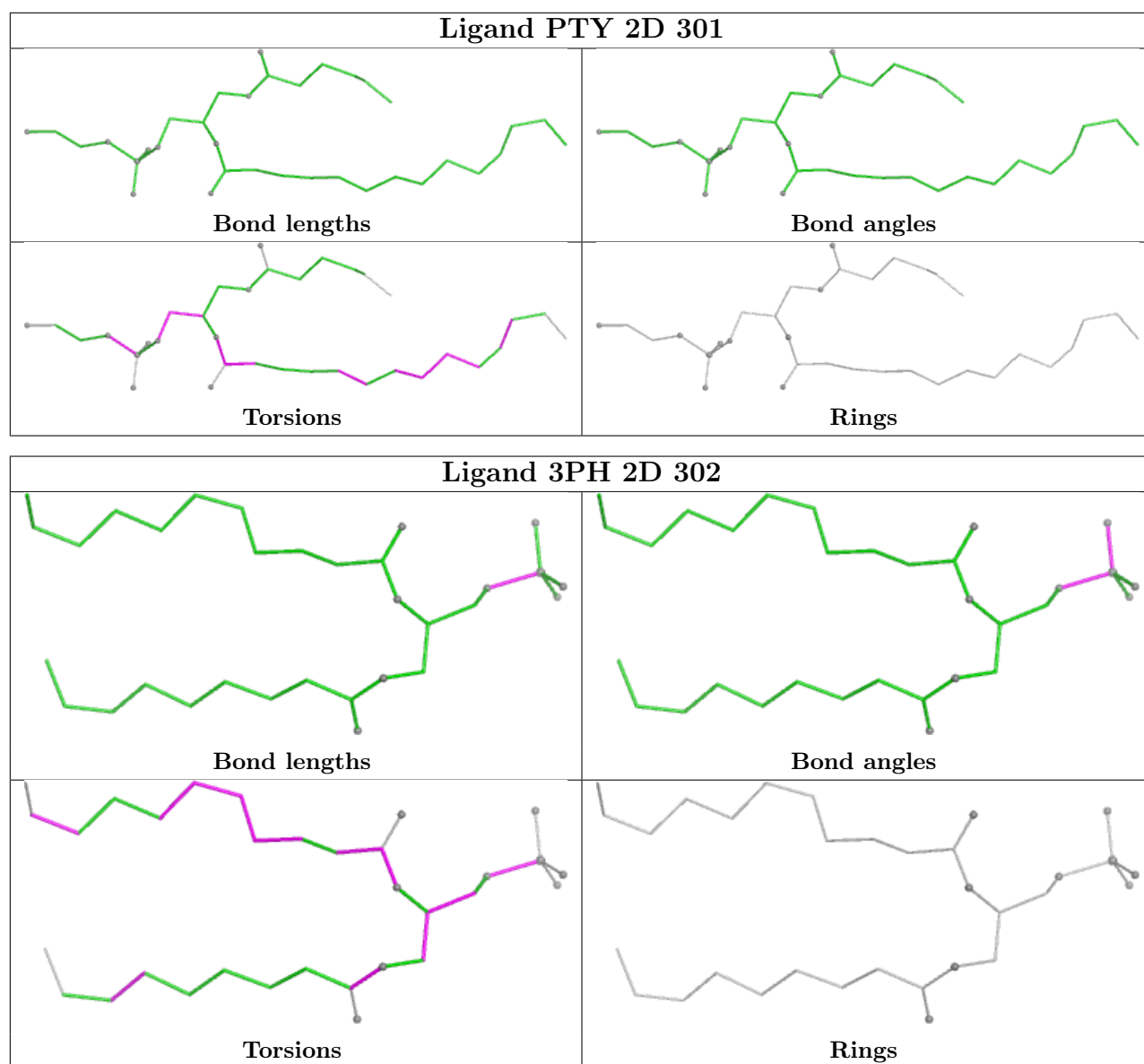
6 monomers are involved in 8 short contacts:

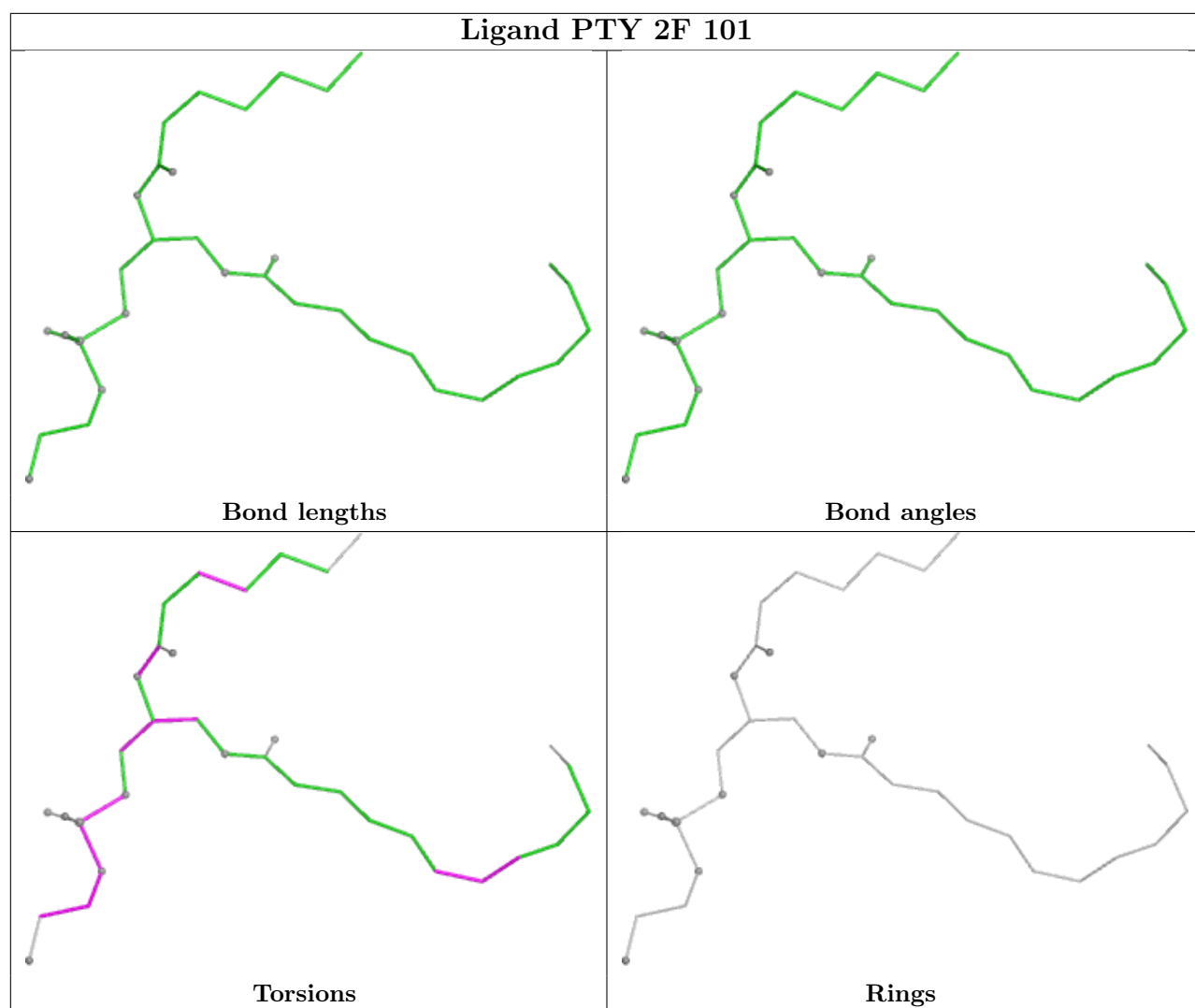
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2A	606	PGT	1	0
16	2A	605	PC7	1	0
19	2D	301	PTY	1	0
13	2A	601	HEA	1	0
18	2C	301	CUA	3	0
13	2A	602	HEA	1	0

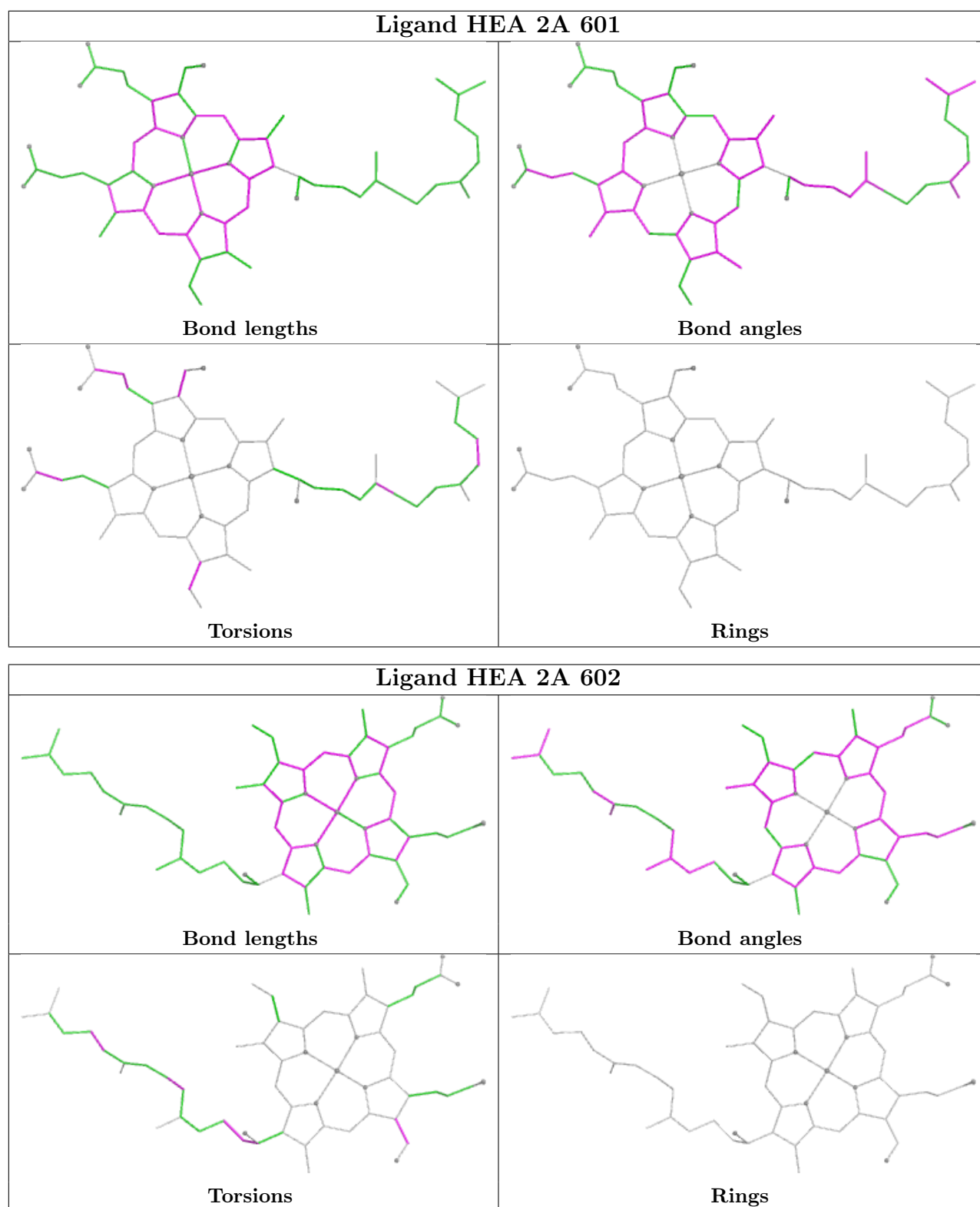
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

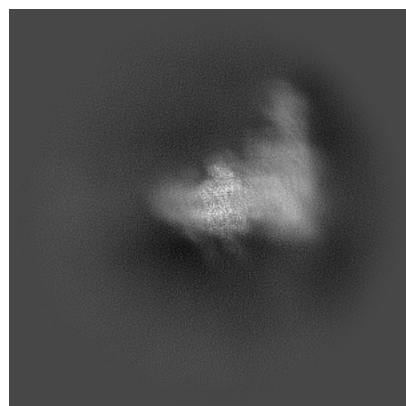
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50205. These allow visual inspection of the internal detail of the map and identification of artifacts.

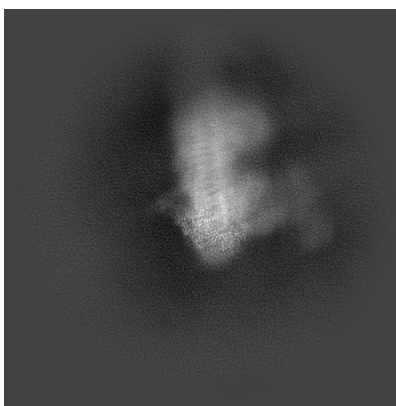
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

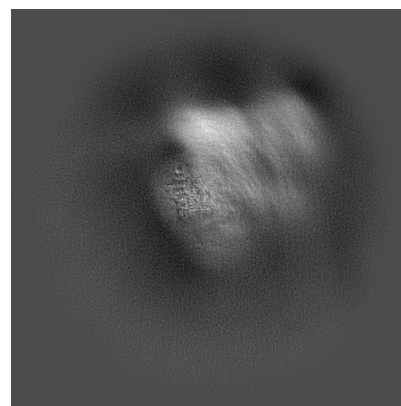
6.1.1 Primary map



X

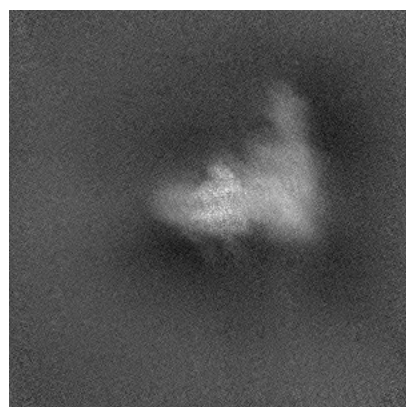


Y

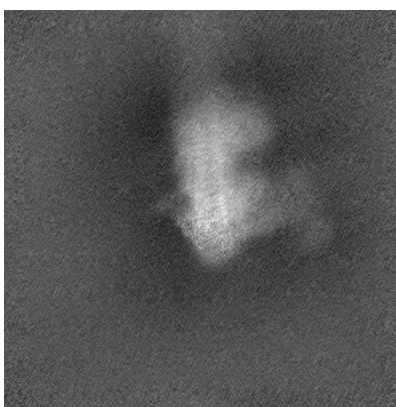


Z

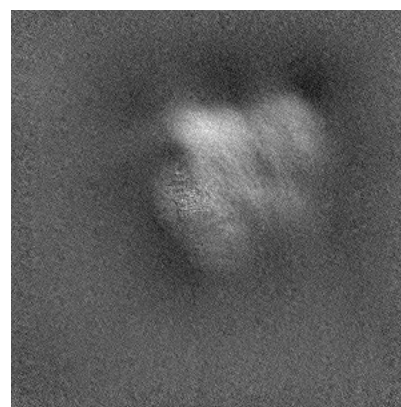
6.1.2 Raw map



X



Y

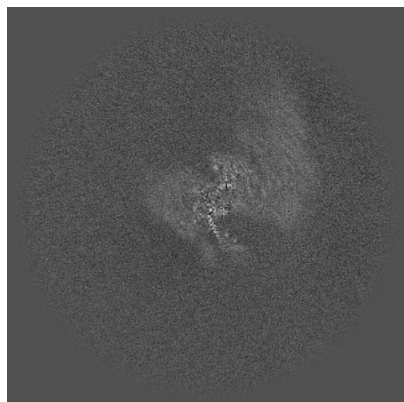


Z

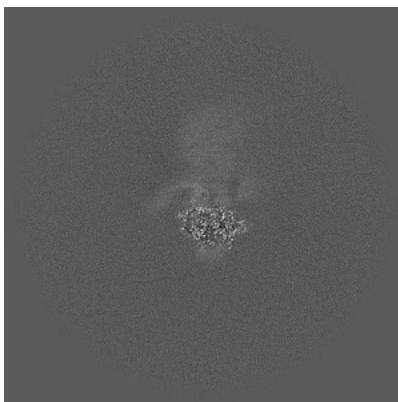
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

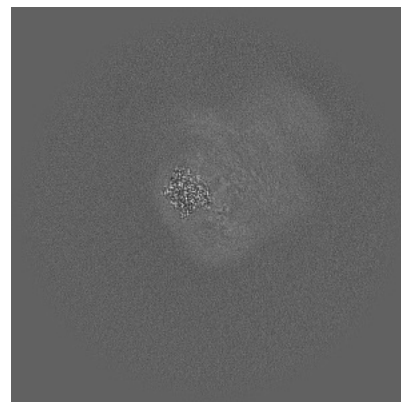
6.2.1 Primary map



X Index: 294

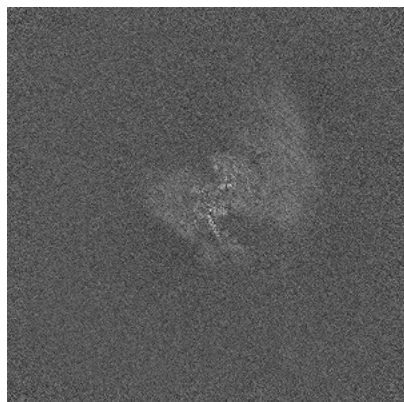


Y Index: 294

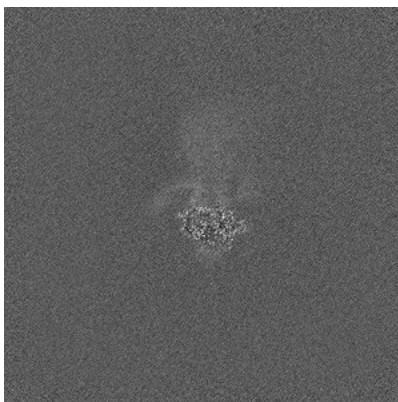


Z Index: 294

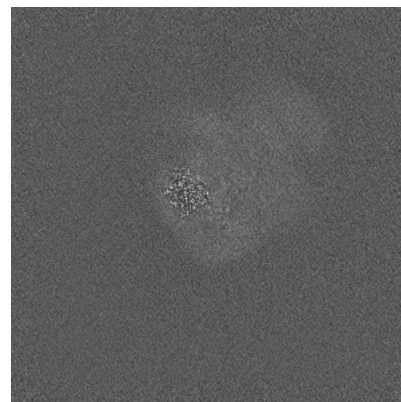
6.2.2 Raw map



X Index: 294



Y Index: 294

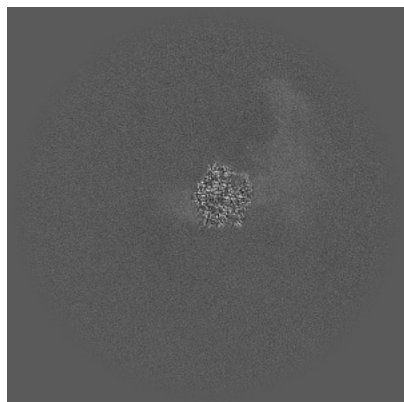


Z Index: 294

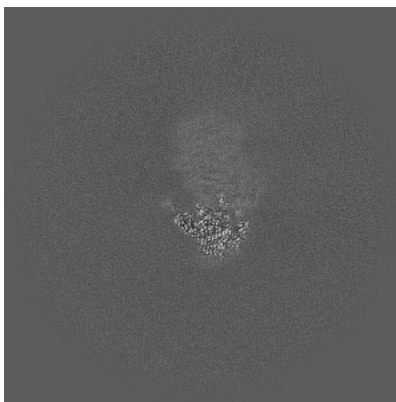
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

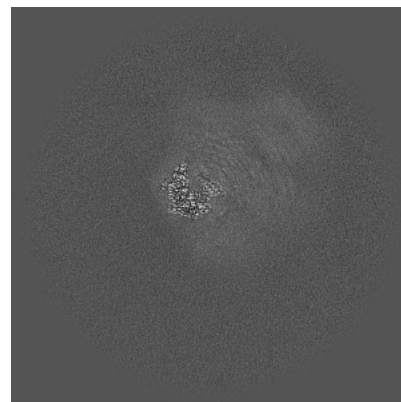
6.3.1 Primary map



X Index: 256

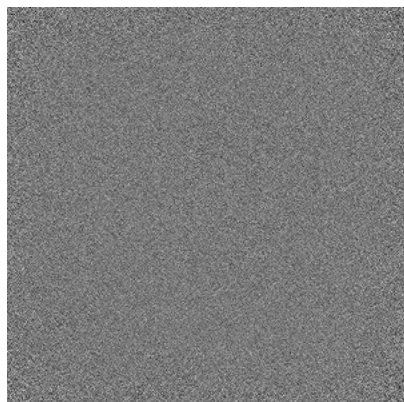


Y Index: 317

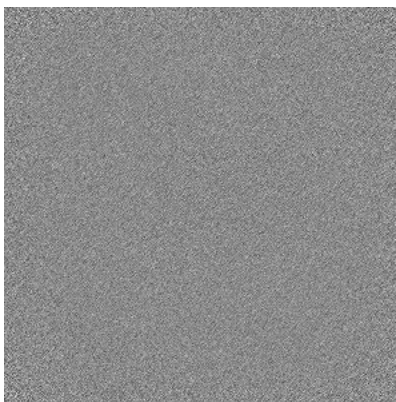


Z Index: 322

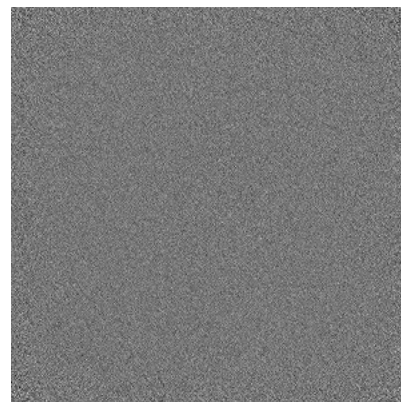
6.3.2 Raw map



X Index: 0



Y Index: 0

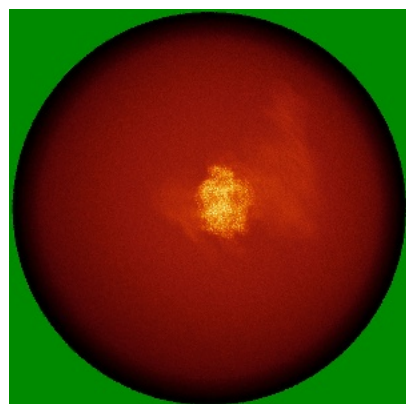


Z Index: 0

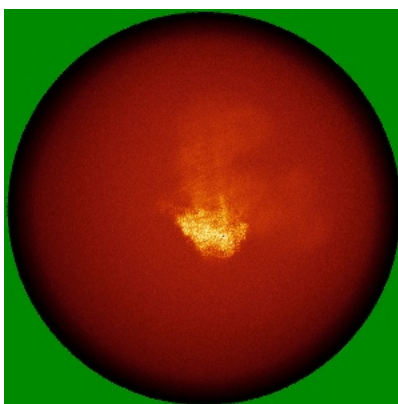
The images above show the largest variance slices of the map in three orthogonal directions.

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

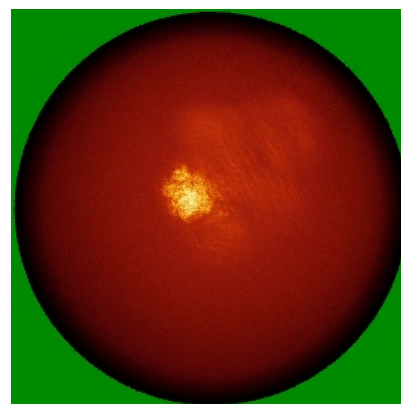
6.4.1 Primary map



X

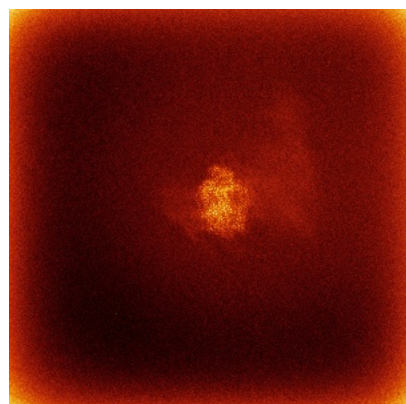


Y

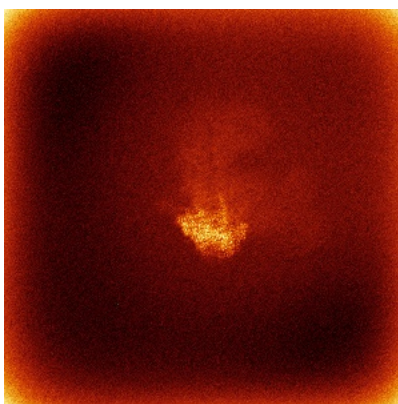


Z

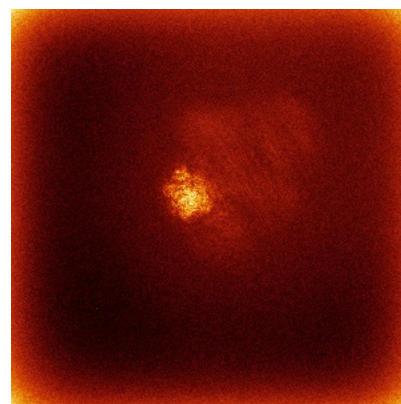
6.4.2 Raw map



X



Y



Z

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

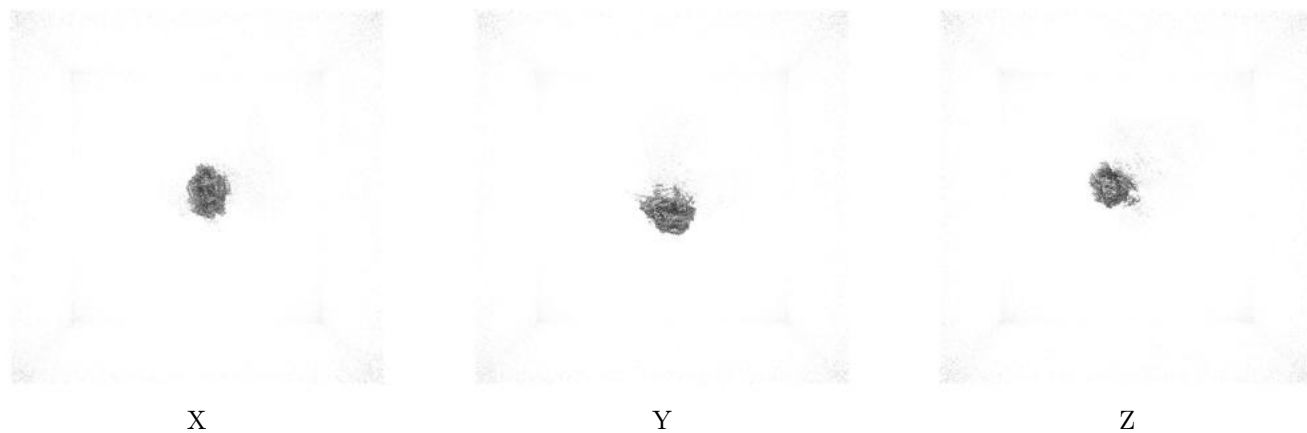
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.135. 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.

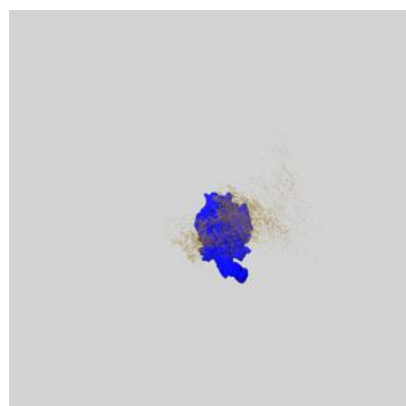
6.6 Mask visualisation [i](#)

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

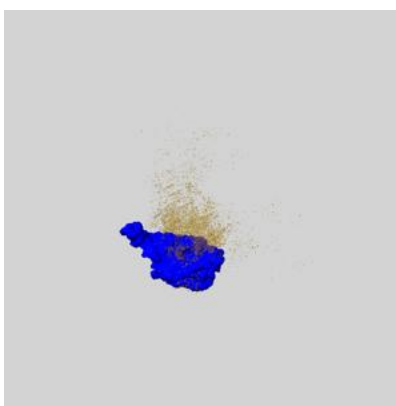
A mask typically either:

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

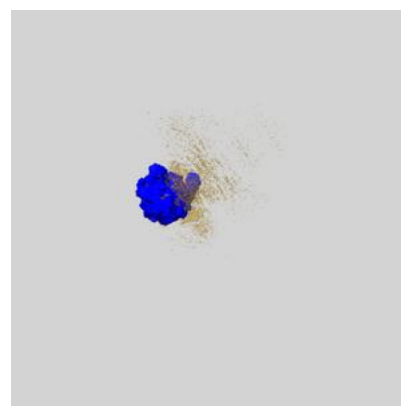
6.6.1 emd_50205_msk_1.map [i](#)



X



Y

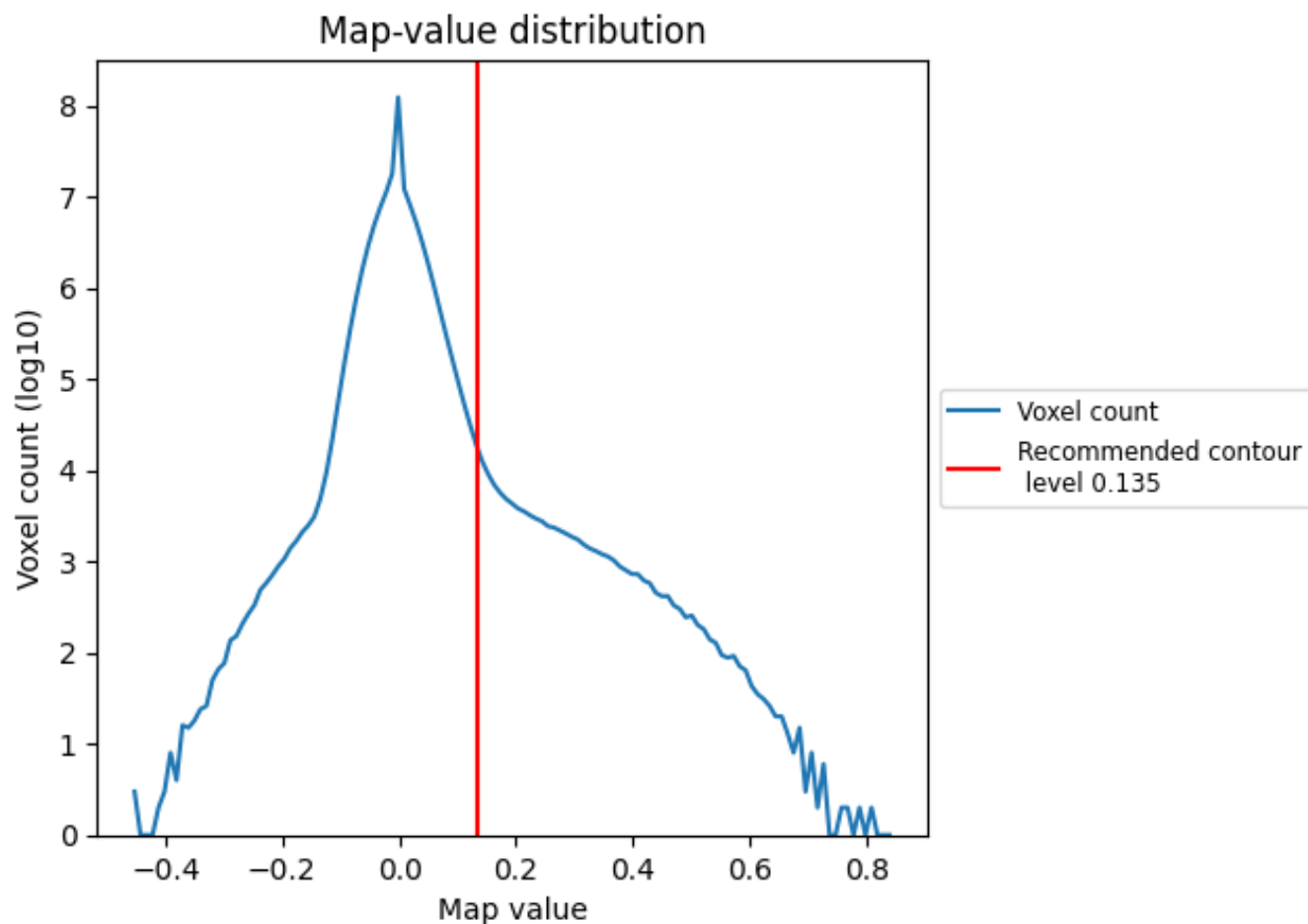


Z

7 Map analysis [i](#)

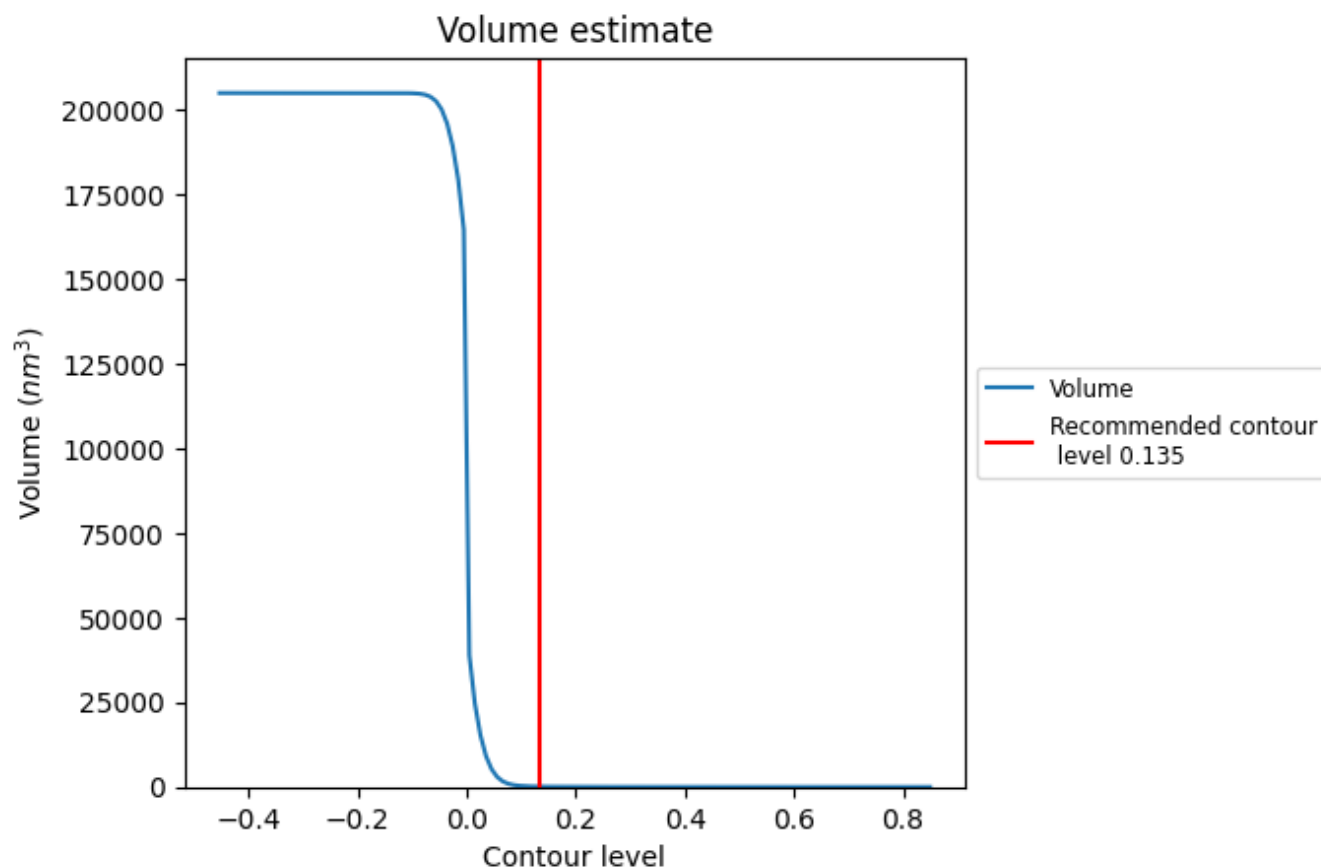
This section contains the results of statistical analysis of the map.

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.

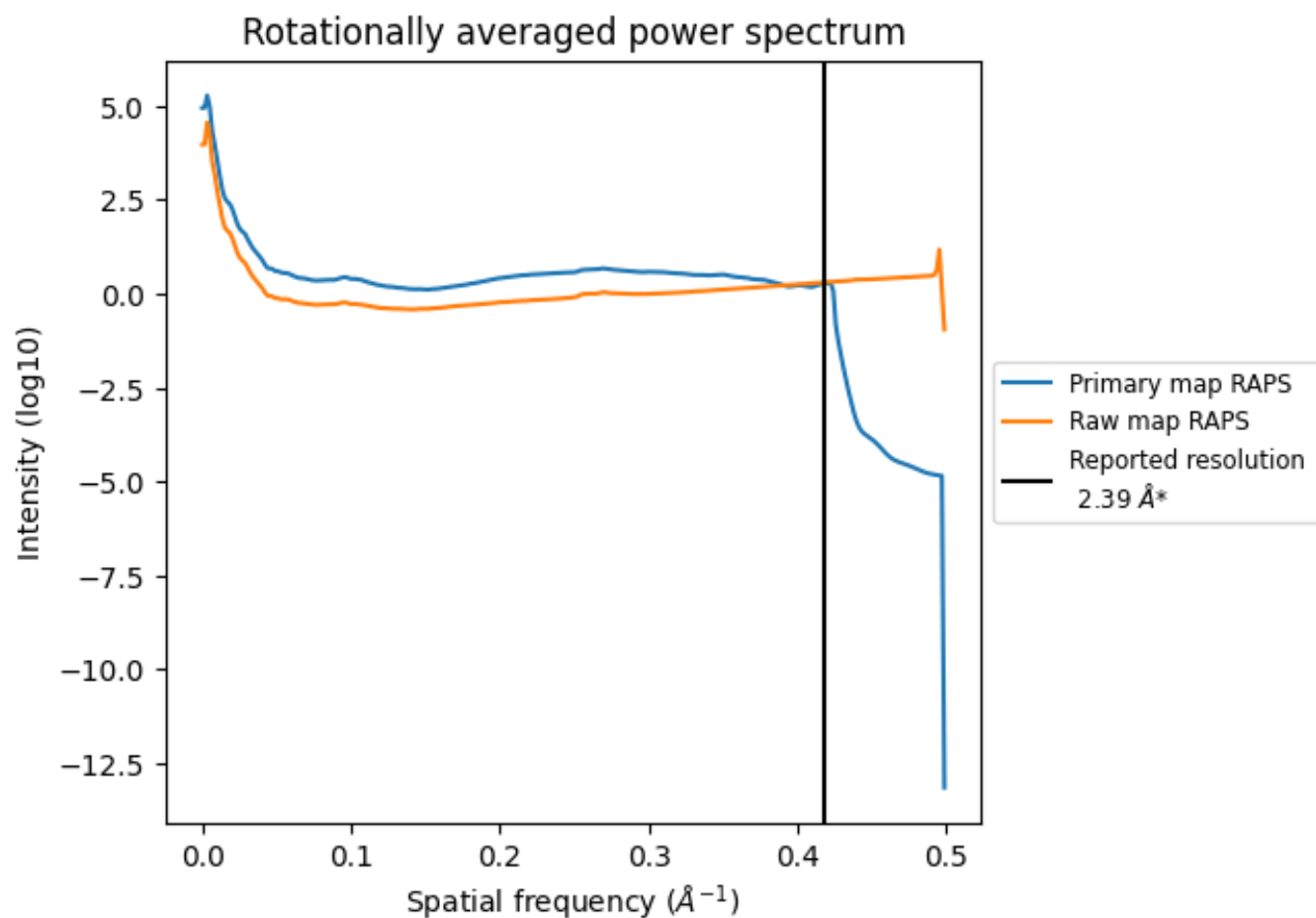
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 92 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 ⓘ

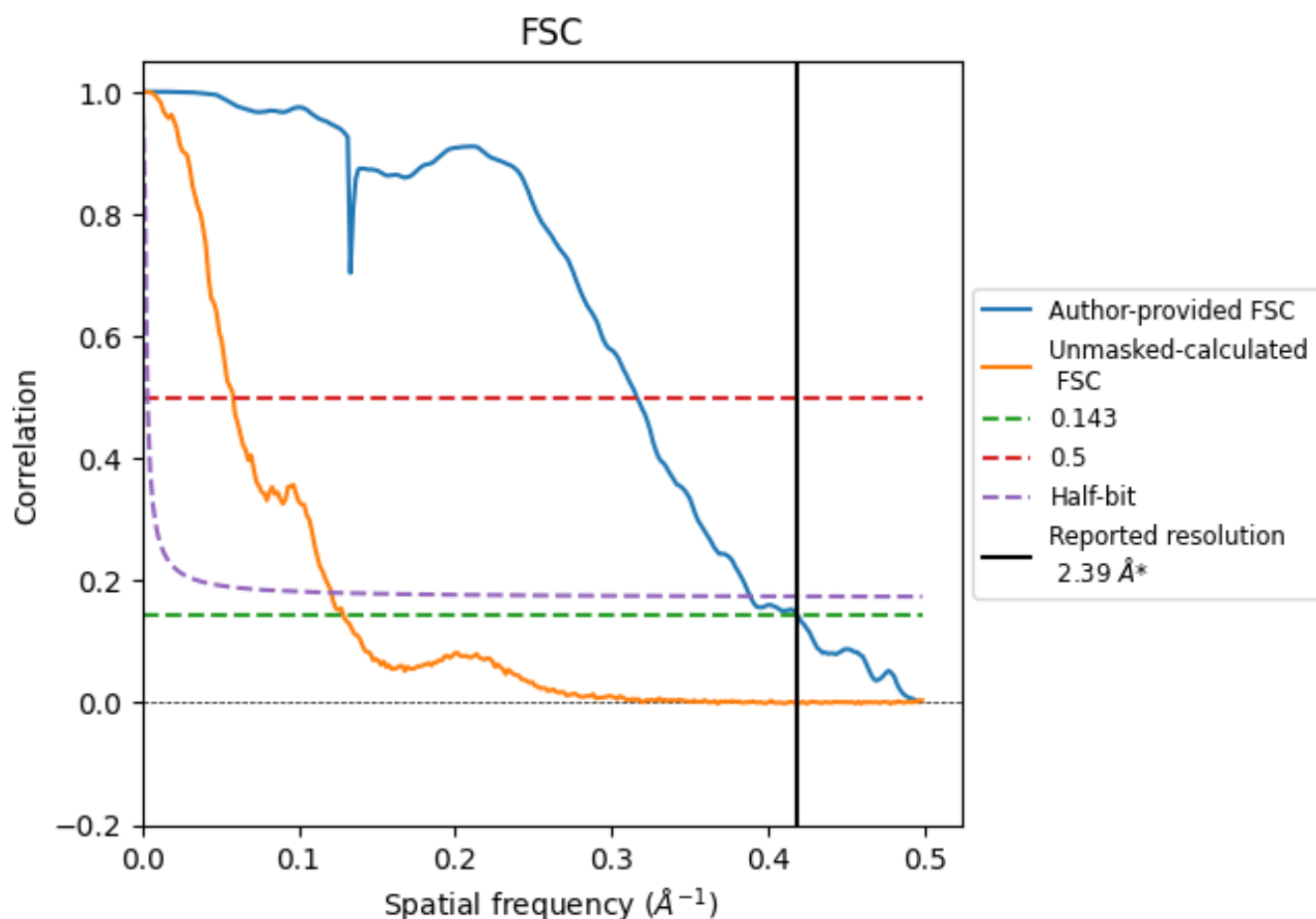


*Reported resolution corresponds to spatial frequency of $0.418 \text{ \AA}^{-1}$

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 0.418 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

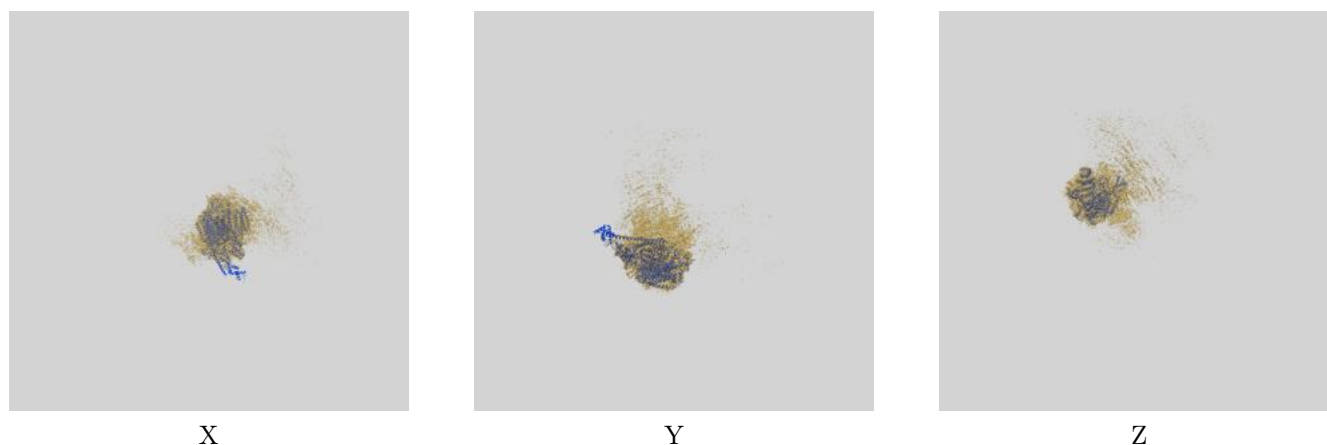
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	3.16	2.57
Unmasked-calculated*	7.78	17.24	8.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.78 differs from the reported value 2.39 by more than 10 %

9 Map-model fit [i](#)

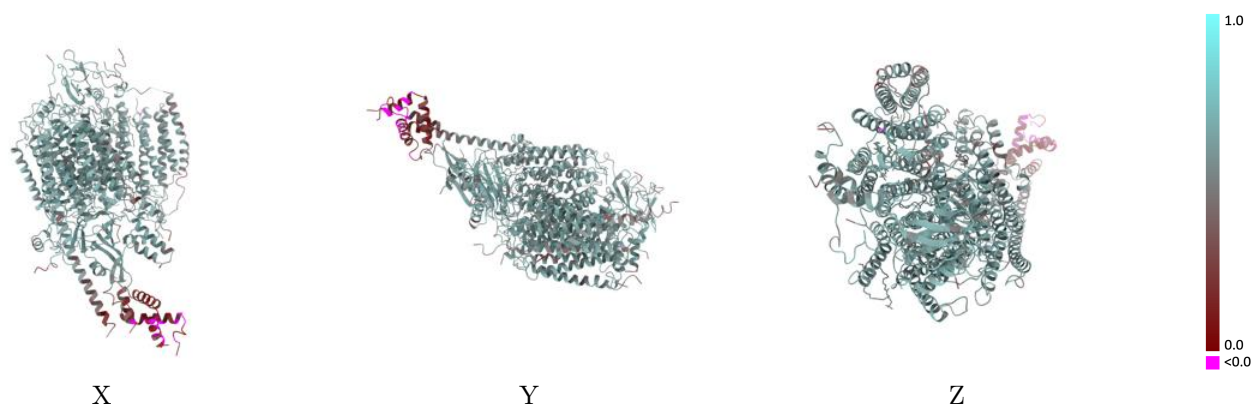
This section contains information regarding the fit between EMDB map EMD-50205 and PDB model 9F60. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



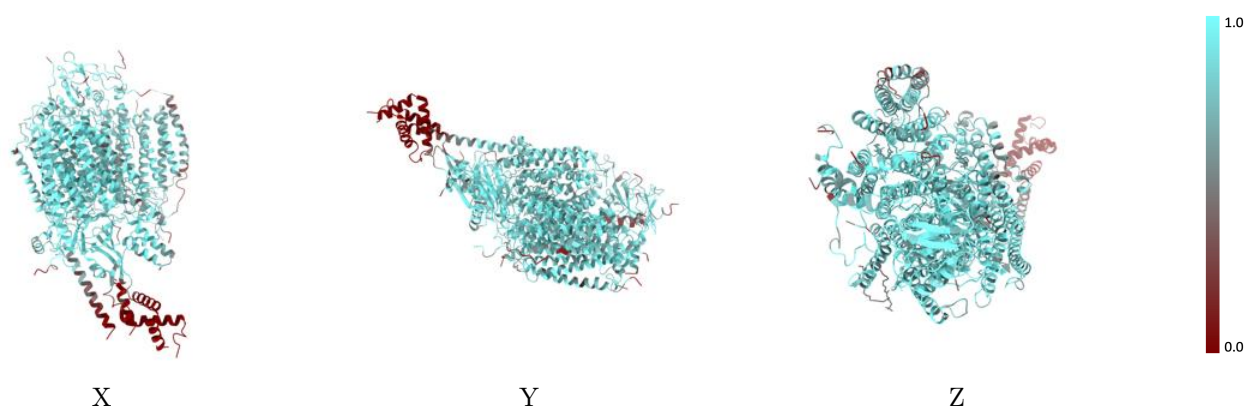
The images above show the 3D surface view of the map at the recommended contour level 0.135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



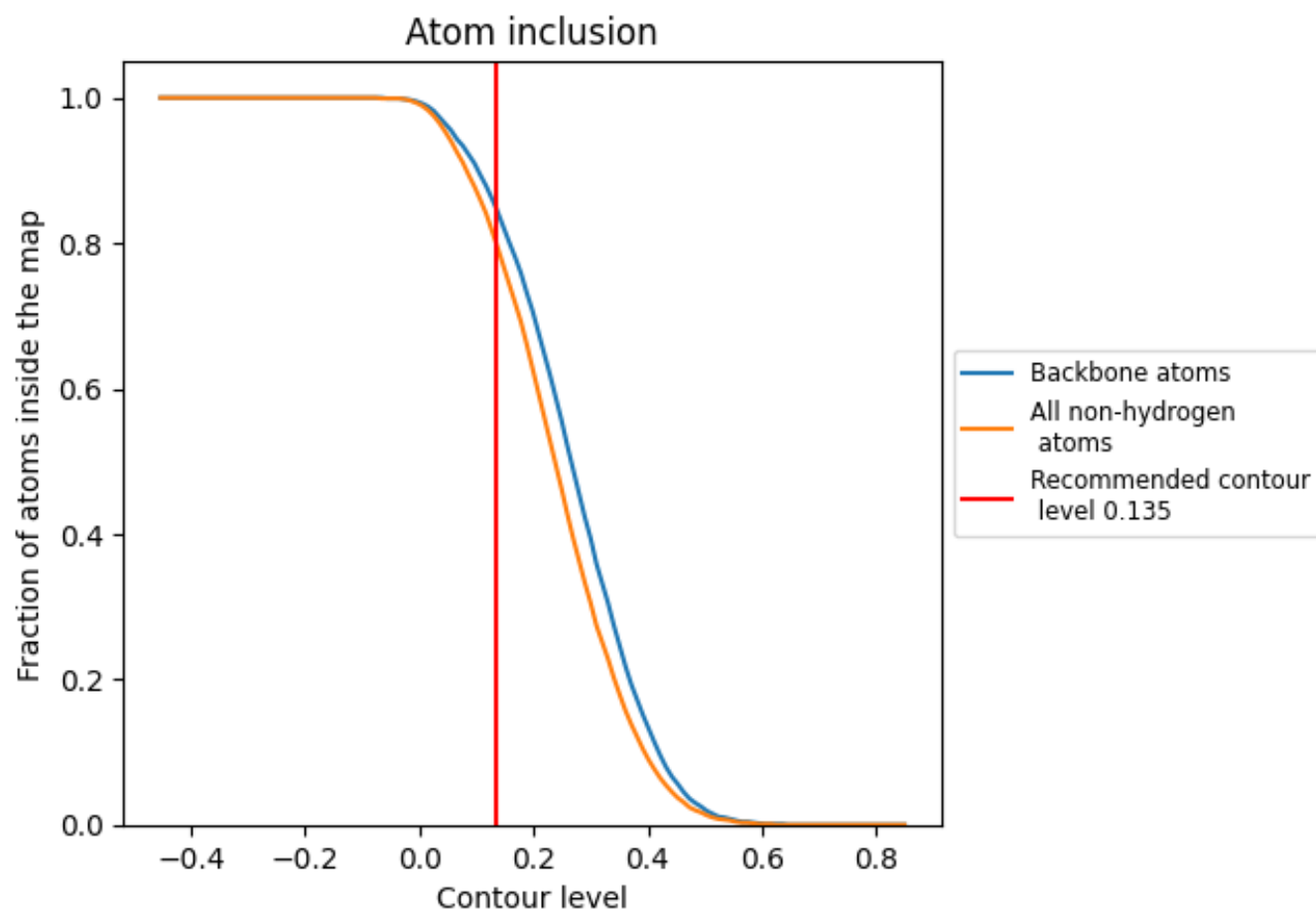
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.5680
2A	0.9200	0.6170
2B	0.7950	0.5700
2C	0.7100	0.5200
2D	0.8600	0.5950
2E	0.7870	0.5620
2F	0.6940	0.5210
2G	0.6300	0.5180
2H	0.5700	0.4410
2I	0.7820	0.5800
2J	0.7970	0.5760
2K	0.7390	0.5640
2L	0.7310	0.5400

