



Full wwPDB EM Validation Report ⓘ

Mar 10, 2024 – 12:27 AM JST

PDB ID : 8WEJ
EMDB ID : EMD-37477
Title : Structure of human phagocyte NADPH oxidase in the activated state
Authors : Chen, L.; Liu, X.
Deposited on : 2023-09-18
Resolution : 2.79 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:

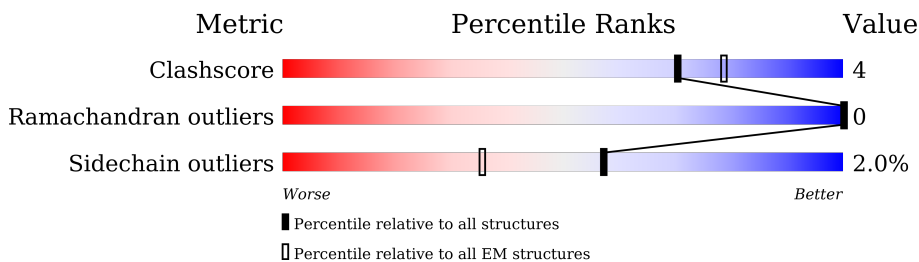
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.79 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	195	
2	B	570	
3	C	286	
4	D	306	
5	E	192	
6	H	251	
7	L	236	
8	F	3	

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 10659 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 b-245 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	134	1030	681	171	173	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	ALA	VAL	conflict	UNP P13498

- Molecule 2 is a protein called Cytochrome b-245 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	569	4549	2974	773	778	24	0	0

- Molecule 3 is a protein called Neutrophil cytosol factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	10	67	45	10	12	0	0

- Molecule 4 is a protein called Neutrophil cytosolic factor 2 (65kDa, chronic granulomatous disease, autosomal 2), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	219	1643	1068	283	282	10	0	0

- Molecule 5 is a protein called Rac family small GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	178	1328	858	220	241	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	LEU	GLN	conflict	UNP A0A8C8XFZ1

- Molecule 6 is a protein called 7D5 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	119	935	595	154	182	4	0	0

- Molecule 7 is a protein called 7D5 Fab light chain.

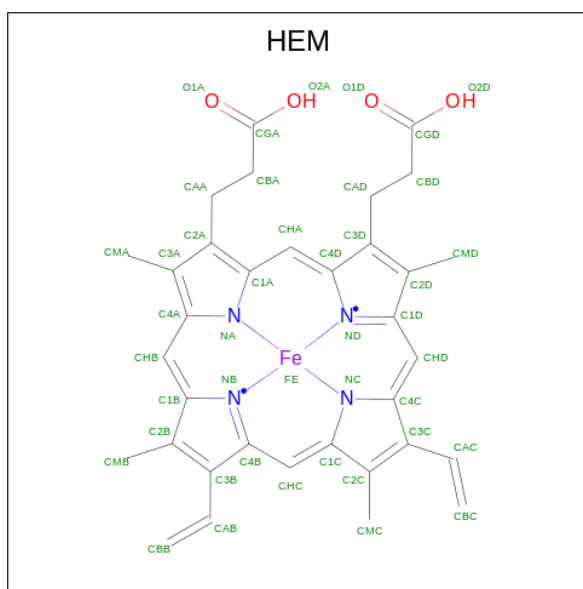
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	107	818	520	138	158	2	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



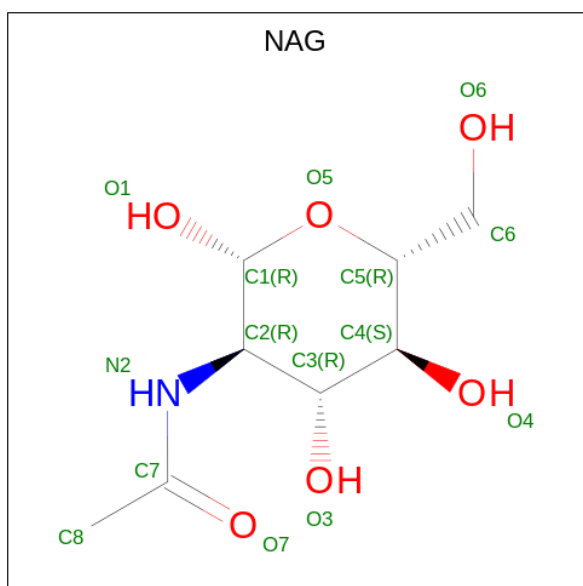
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	F	3	39	22	2	15	0	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
10	B	1	14	8	1	5	0

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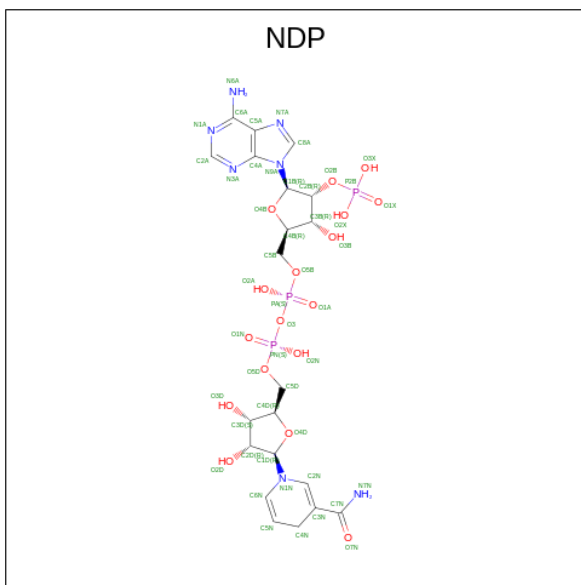
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	B	1	14	8	1	5	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

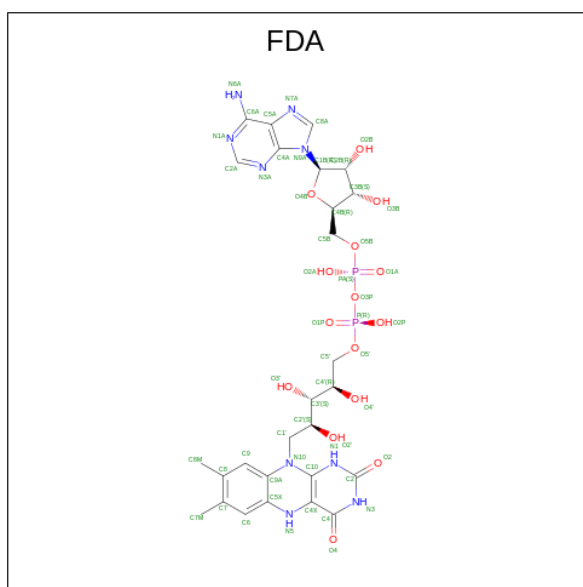
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	B	1	1	1	0
11	E	1	1	1	0

- Molecule 12 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



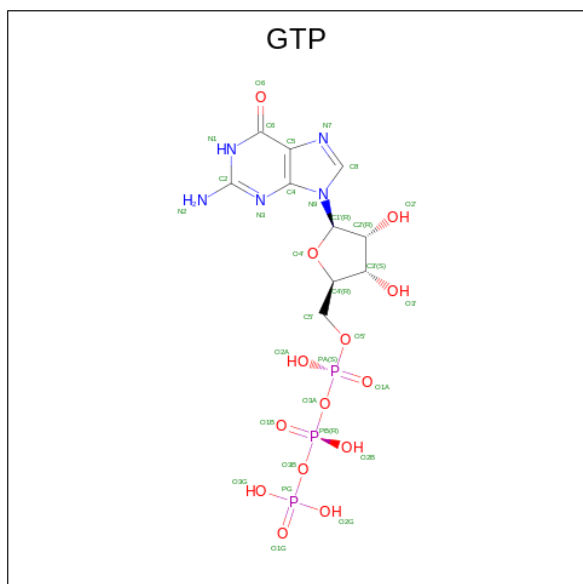
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	B	1	48	21	7	17	3	0

- Molecule 13 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	B	1	53	27	9	15	2	0

- Molecule 14 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	E	1	32	10	5	14	3	0

- Molecule 15 is water.

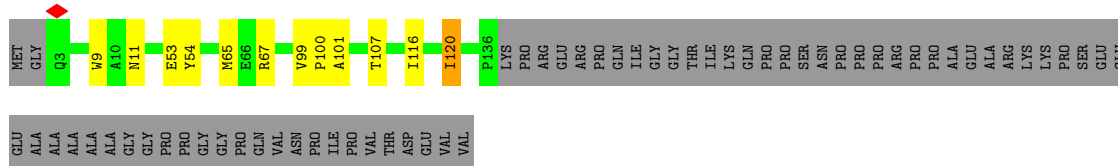
Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

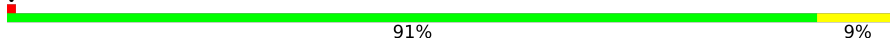
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

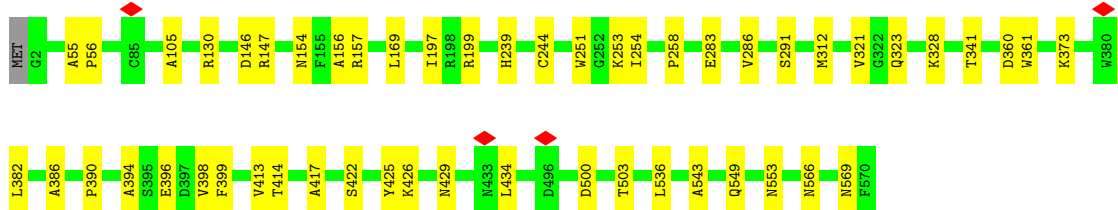
- Molecule 1: Cytochrome b-245 light chain

Chain A: 



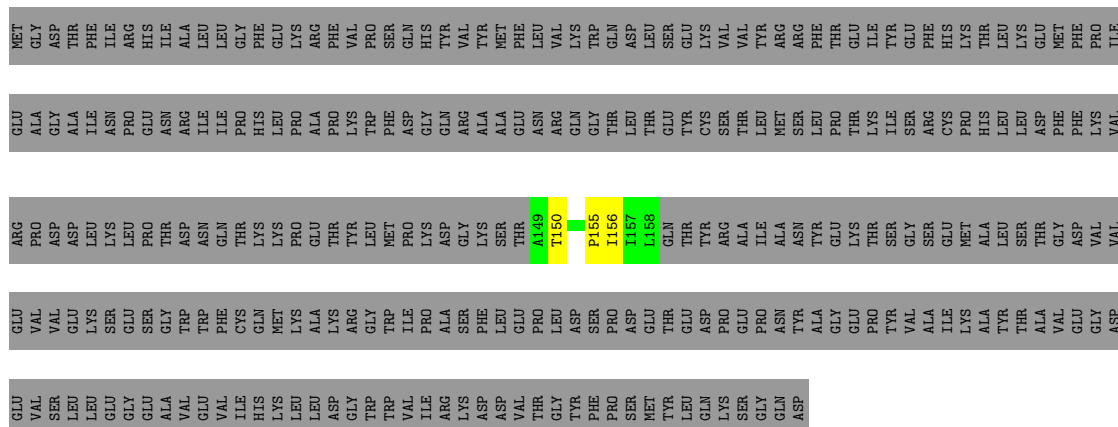
- Molecule 2: Cytochrome b-245 heavy chain

Chain B: 



- Molecule 3: Neutrophil cytosol factor 1

Chain C: 



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
EMM3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.115	Depositor
Minimum map value	-3.348	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	328.96, 328.96, 328.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.028, 1.028, 1.028	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: HEM, NAG, FDA, NDP, GTP, MG, BMA

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	0.29	0/1058	0.57	0/1443
2	B	0.31	0/4680	0.53	0/6360
3	C	0.31	0/67	0.52	0/92
4	D	0.33	0/1677	0.55	0/2275
5	E	0.33	0/1358	0.57	0/1860
6	H	0.31	0/962	0.57	0/1310
7	L	0.33	0/835	0.57	0/1135
All	All	0.32	0/10637	0.55	0/14475

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	1030	0	1041	7	0
2	B	4549	0	4505	29	0
3	C	67	0	74	1	0
4	D	1643	0	1606	14	0
5	E	1328	0	1304	13	0
6	H	935	0	870	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	818	0	793	7	0
8	F	39	0	34	0	0
9	B	86	0	60	6	0
10	B	28	0	26	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	B	48	0	26	0	0
13	B	53	0	33	2	0
14	E	32	0	12	0	0
15	B	1	0	0	0	0
All	All	10659	0	10384	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:ARG:NH2	5:E:145:MET:SD	2.63	0.72
5:E:84:LEU:HD23	5:E:120:ARG:HE	1.55	0.71
7:L:39:LYS:NZ	7:L:81:GLU:O	2.23	0.70
6:H:67:ARG:NH2	6:H:90:ASP:OD2	2.25	0.69
2:B:147:ARG:NH1	6:H:104:ASP:OD2	2.27	0.67
2:B:425:TYR:O	2:B:429:ASN:ND2	2.30	0.62
7:L:88:CYS:O	7:L:99:GLY:N	2.33	0.61
2:B:105:ALA:HB1	9:B:602:HEM:HBB2	1.84	0.60
2:B:244:CYS:O	2:B:251:TRP:NE1	2.33	0.59
2:B:154:ASN:ND2	2:B:156:ALA:O	2.37	0.58
2:B:569:ASN:O	13:B:607:FDA:HM83	2.06	0.56
6:H:47:GLU:OE2	6:H:61:ASN:ND2	2.37	0.56
4:D:129:PHE:N	4:D:172:TYR:OH	2.39	0.55
1:A:65:MET:SD	2:B:199:ARG:NH1	2.79	0.55
6:H:39:ARG:NH1	6:H:90:ASP:OD1	2.37	0.54
2:B:253:LYS:NZ	6:H:101:TYR:O	2.36	0.54
9:B:601:HEM:HBC2	9:B:601:HEM:HHD	1.90	0.54
9:B:601:HEM:HHC	9:B:601:HEM:HBB2	1.91	0.53
9:B:602:HEM:HBB2	9:B:602:HEM:HHC	1.91	0.52
1:A:11:ASN:OD1	1:A:67:ARG:NH2	2.40	0.52
1:A:116:ILE:O	1:A:120:ILE:HG13	2.09	0.52
2:B:239:HIS:ND1	2:B:258:PRO:O	2.42	0.52
2:B:360:ASP:OD1	2:B:361:TRP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:GLU:O	4:D:126:ASN:ND2	2.44	0.51
4:D:91:ILE:HD11	4:D:134:LYS:HZ2	1.75	0.50
2:B:283:GLU:HA	2:B:286:VAL:HG12	1.93	0.49
4:D:102:ARG:NH2	5:E:159:ALA:O	2.46	0.49
2:B:426:LYS:HD3	2:B:434:LEU:HD21	1.95	0.49
4:D:126:ASN:O	4:D:130:MET:HG2	2.13	0.48
3:C:155:PRO:HB3	5:E:42:ALA:HB1	1.95	0.48
5:E:26:ASN:OD1	5:E:162:GLN:NE2	2.43	0.48
4:D:72:VAL:HB	4:D:109:TYR:CE2	2.49	0.48
5:E:2:GLN:HB2	5:E:51:VAL:HG12	1.96	0.47
7:L:29:ILE:O	7:L:71:TYR:OH	2.33	0.47
1:A:101:ALA:O	1:A:107:THR:OG1	2.28	0.47
2:B:321:VAL:HG12	2:B:422:SER:OG	2.14	0.47
2:B:549:GLN:O	2:B:553:ASN:ND2	2.46	0.47
9:B:602:HEM:HMC1	9:B:602:HEM:HBC2	1.96	0.47
4:D:121:CYS:HB3	4:D:150:MET:HG3	1.97	0.46
2:B:105:ALA:CB	9:B:602:HEM:HBB2	2.44	0.46
4:D:76:GLN:HG2	4:D:177:ILE:HD12	1.96	0.46
5:E:148:GLU:HG3	5:E:149:ILE:HG23	1.97	0.46
6:H:54:TYR:O	6:H:72:ARG:NH1	2.49	0.46
4:D:190:VAL:HA	4:D:193:LEU:HD13	1.98	0.45
2:B:341:THR:H	13:B:607:FDA:HN5	1.63	0.45
2:B:500:ASP:OD2	2:B:503:THR:OG1	2.34	0.45
1:A:99:VAL:HB	1:A:100:PRO:HD3	1.98	0.45
2:B:413:VAL:O	2:B:417:ALA:N	2.42	0.45
2:B:321:VAL:HG11	2:B:399:PHE:HE2	1.82	0.44
7:L:33:LEU:HB3	7:L:51:THR:HG22	2.00	0.44
2:B:55:ALA:HB3	2:B:56:PRO:HD3	2.00	0.44
4:D:156:HIS:O	4:D:156:HIS:ND1	2.50	0.44
5:E:155:LEU:HD13	5:E:168:VAL:HA	1.98	0.44
2:B:323:GLN:HB3	2:B:390:PRO:HB2	1.99	0.44
5:E:90:PHE:HB2	5:E:137:ILE:HD11	1.99	0.44
2:B:536:LEU:CD2	2:B:543:ALA:HA	2.48	0.44
2:B:291:SER:HA	2:B:386:ALA:HB1	2.00	0.43
1:A:9:TRP:HA	2:B:197:ILE:HD11	2.00	0.43
5:E:93:VAL:HB	5:E:145:MET:HE2	1.99	0.43
5:E:80:ILE:HG21	5:E:93:VAL:HG13	1.99	0.43
4:D:102:ARG:NH1	5:E:26:ASN:O	2.51	0.43
6:H:32:GLY:HA2	6:H:54:TYR:HB3	2.00	0.43
7:L:19:VAL:HG22	7:L:78:LEU:HD11	2.01	0.42
7:L:50:TYR:C	7:L:51:THR:HG23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ARG:NE	2:B:157:ARG:O	2.48	0.42
2:B:536:LEU:HD23	2:B:543:ALA:HA	2.00	0.41
2:B:156:ALA:HB2	2:B:169:LEU:HD11	2.02	0.41
4:D:72:VAL:HG21	4:D:114:LEU:CD2	2.50	0.41
5:E:8:VAL:HG22	5:E:79:LEU:HD12	2.03	0.41
4:D:65:ASN:OD1	4:D:68:LYS:NZ	2.54	0.41
2:B:130:ARG:NH2	2:B:146:ASP:OD1	2.54	0.41
7:L:18:ARG:HA	7:L:75:ILE:O	2.21	0.41
1:A:54:TYR:O	1:A:67:ARG:NH1	2.54	0.41
2:B:394:ALA:HB1	2:B:566:ASN:HB3	2.03	0.41
4:D:70:LEU:HD23	4:D:73:ALA:HB2	2.04	0.40
6:H:73:ASP:OD1	6:H:75:SER:OG	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/195 (68%)	131 (99%)	1 (1%)	0	100	100
2	B	567/570 (100%)	556 (98%)	11 (2%)	0	100	100
3	C	8/286 (3%)	6 (75%)	2 (25%)	0	100	100
4	D	217/306 (71%)	207 (95%)	10 (5%)	0	100	100
5	E	176/192 (92%)	168 (96%)	8 (4%)	0	100	100
6	H	117/251 (47%)	111 (95%)	6 (5%)	0	100	100
7	L	105/236 (44%)	95 (90%)	10 (10%)	0	100	100
All	All	1322/2036 (65%)	1274 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	100/150 (67%)	98 (98%)	2 (2%)	55 84
2	B	481/498 (97%)	472 (98%)	9 (2%)	57 85
3	C	7/252 (3%)	5 (71%)	2 (29%)	0 1
4	D	155/262 (59%)	153 (99%)	2 (1%)	69 91
5	E	138/168 (82%)	136 (99%)	2 (1%)	67 90
6	H	103/223 (46%)	101 (98%)	2 (2%)	57 85
7	L	88/209 (42%)	86 (98%)	2 (2%)	50 82
All	All	1072/1762 (61%)	1051 (98%)	21 (2%)	57 84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	120	ILE
2	B	254	ILE
2	B	312	MET
2	B	328	LYS
2	B	373	LYS
2	B	381	LYS
2	B	382	LEU
2	B	396	GLU
2	B	398	VAL
2	B	414	THR
3	C	150	THR
3	C	156	ILE
4	D	79	MET
4	D	101	LEU
5	E	145	MET
5	E	148	GLU
6	H	49	MET
6	H	81	LEU
7	L	51	THR

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Mol	Chain	Res	Type
7	L	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 monosaccharides 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
8	NAG	F	1	8,2	14,14,15	0.28	0	17,19,21	0.47	0
8	NAG	F	2	8	14,14,15	0.20	0	17,19,21	0.32	0
8	BMA	F	3	8	11,11,12	0.64	0	15,15,17	0.66	0

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
8	NAG	F	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

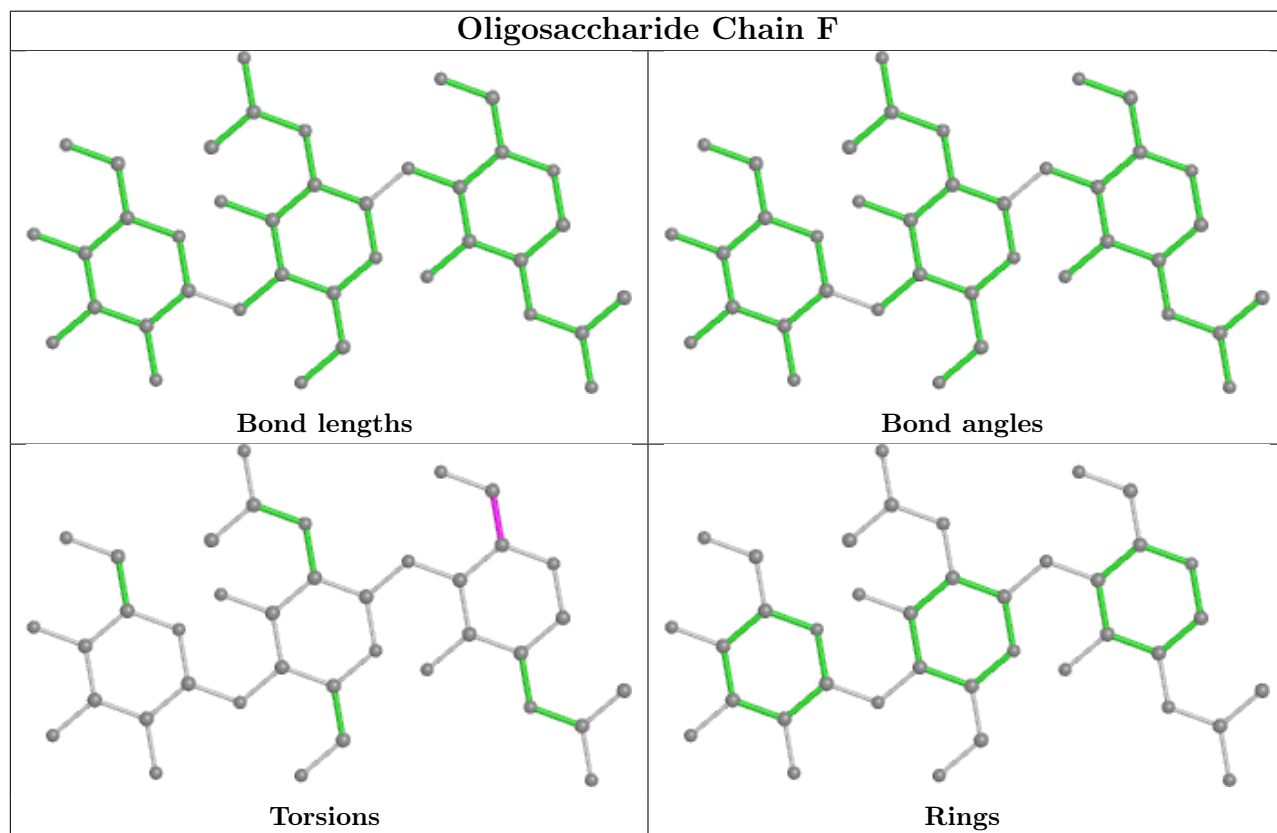
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	1	NAG	O5-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
10	NAG	B	604	2	14,14,15	0.25	0	17,19,21	0.41	0
12	NDP	B	606	-	45,52,52	1.06	3 (6%)	53,80,80	1.42	10 (18%)
13	FDA	B	607	11	52,58,58	1.56	7 (13%)	60,89,89	1.48	15 (25%)
14	GTP	E	200	11	26,34,34	0.93	1 (3%)	32,54,54	1.52	5 (15%)
9	HEM	B	601	2	41,50,50	1.52	5 (12%)	45,82,82	1.75	13 (28%)
9	HEM	B	602	2	41,50,50	1.53	5 (12%)	45,82,82	1.64	11 (24%)
10	NAG	B	603	2	14,14,15	0.22	0	17,19,21	0.42	0

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
10	NAG	B	604	2	-	2/6/23/26	0/1/1/1
12	NDP	B	606	-	-	8/30/77/77	0/5/5/5
13	FDA	B	607	11	-	6/30/50/50	0/6/6/6
14	GTP	E	200	11	-	4/18/38/38	0/3/3/3
9	HEM	B	601	2	-	1/12/54/54	-
9	HEM	B	602	2	-	7/12/54/54	-
10	NAG	B	603	2	-	1/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	607	FDA	C5X-C9A	7.58	1.49	1.40
9	B	602	HEM	C3C-CAC	4.21	1.56	1.47
9	B	601	HEM	C3C-C2C	-4.21	1.34	1.40
9	B	601	HEM	C3C-CAC	3.95	1.55	1.47
13	B	607	FDA	C8-C7	3.60	1.49	1.40
9	B	602	HEM	C3C-C2C	-3.39	1.35	1.40
12	B	606	NDP	C6N-C5N	3.38	1.39	1.33
9	B	601	HEM	CAB-C3B	3.04	1.55	1.47
9	B	602	HEM	CAB-C3B	2.93	1.55	1.47
13	B	607	FDA	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	607	FDA	C4X-C4	2.65	1.49	1.42
9	B	602	HEM	CAA-C2A	2.58	1.55	1.52
9	B	602	HEM	CMB-C2B	2.32	1.55	1.50
13	B	607	FDA	C2-N3	-2.28	1.33	1.37
9	B	601	HEM	CMB-C2B	2.24	1.55	1.50
12	B	606	NDP	C5A-C4A	2.20	1.46	1.40
13	B	607	FDA	C5A-C4A	2.19	1.46	1.40
14	E	200	GTP	C6-N1	-2.09	1.34	1.37
13	B	607	FDA	C5X-N5	-2.09	1.36	1.39
12	B	606	NDP	O4B-C1B	2.08	1.44	1.41
9	B	601	HEM	FE-NB	2.02	2.06	1.96

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	607	FDA	N3-C2-N1	4.13	122.44	115.80
9	B	602	HEM	C4B-CHC-C1C	3.87	127.66	122.56
14	E	200	GTP	PA-O3A-PB	-3.83	119.68	132.83
14	E	200	GTP	PB-O3B-PG	-3.67	120.23	132.83
9	B	601	HEM	CBA-CAA-C2A	-3.50	106.64	112.62
9	B	601	HEM	CMA-C3A-C4A	-3.50	123.09	128.46
13	B	607	FDA	N3A-C2A-N1A	-3.45	123.28	128.68
12	B	606	NDP	C4D-O4D-C1D	-3.43	101.91	109.47
9	B	601	HEM	C4C-CHD-C1D	3.41	127.06	122.56
14	E	200	GTP	C3'-C2'-C1'	3.18	105.77	100.98
9	B	601	HEM	C4B-CHC-C1C	3.12	126.68	122.56
12	B	606	NDP	PN-O3-PA	-3.08	122.27	132.83
9	B	601	HEM	CHC-C4B-C3B	3.01	129.17	124.57
9	B	602	HEM	C4D-ND-C1D	2.95	108.12	105.07
9	B	601	HEM	C4D-ND-C1D	2.86	108.02	105.07
9	B	602	HEM	CMA-C3A-C4A	-2.83	124.11	128.46
9	B	602	HEM	C1B-NB-C4B	2.83	107.99	105.07
9	B	602	HEM	CHC-C4B-C3B	2.77	128.81	124.57
9	B	602	HEM	C3B-C2B-C1B	2.72	108.50	106.49
9	B	601	HEM	C1B-NB-C4B	2.70	107.86	105.07
9	B	602	HEM	C4C-CHD-C1D	2.69	126.11	122.56
9	B	601	HEM	CHD-C1D-ND	2.67	127.33	124.43
13	B	607	FDA	C4A-C5A-N7A	-2.66	106.62	109.40
13	B	607	FDA	O4-C4-C4X	-2.65	121.16	127.24
12	B	606	NDP	N3A-C2A-N1A	-2.65	124.54	128.68
13	B	607	FDA	C4-N3-C2	-2.56	122.65	126.34
9	B	601	HEM	C4A-C3A-C2A	2.56	108.77	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	601	HEM	C3B-C2B-C1B	2.55	108.38	106.49
12	B	606	NDP	O3B-C3B-C4B	-2.49	103.84	111.05
12	B	606	NDP	C3N-C7N-N7N	2.47	122.06	117.67
12	B	606	NDP	O4D-C1D-N1N	2.41	112.77	108.06
14	E	200	GTP	C5-C6-N1	2.40	118.19	113.95
13	B	607	FDA	P-O3P-PA	-2.40	124.60	132.83
13	B	607	FDA	C8M-C8-C7	2.39	125.64	120.74
13	B	607	FDA	C1'-C2'-C3'	2.39	116.46	109.79
13	B	607	FDA	C8M-C8-C9	-2.36	115.12	119.49
13	B	607	FDA	C4-C4X-N5	2.30	122.91	116.63
12	B	606	NDP	C4A-C5A-N7A	-2.27	107.03	109.40
9	B	602	HEM	CHD-C1D-ND	2.20	126.82	124.43
13	B	607	FDA	C4X-C4-N3	2.18	118.81	112.31
9	B	602	HEM	CAB-C3B-C2B	-2.16	121.48	128.60
12	B	606	NDP	C3D-C2D-C1D	2.15	105.52	101.43
9	B	601	HEM	CAD-CBD-CGD	-2.14	108.99	113.60
13	B	607	FDA	C5'-C4'-C3'	-2.12	108.10	112.20
9	B	602	HEM	C4A-C3A-C2A	2.12	108.47	107.00
12	B	606	NDP	N6A-C6A-N1A	2.12	122.98	118.57
9	B	602	HEM	C3D-C4D-ND	-2.10	107.83	110.17
9	B	601	HEM	C2D-C1D-ND	-2.10	107.37	109.88
14	E	200	GTP	C8-N7-C5	2.07	106.93	102.99
13	B	607	FDA	C2A-N1A-C6A	2.06	122.28	118.75
9	B	601	HEM	CAB-C3B-C2B	-2.06	121.82	128.60
13	B	607	FDA	C9A-C9-C8	2.05	123.43	119.30
13	B	607	FDA	O2-C2-N3	-2.02	118.00	121.82
12	B	606	NDP	C2B-C3B-C4B	2.01	106.35	101.99

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	602	HEM	C1A-C2A-CAA-CBA
9	B	602	HEM	C3A-C2A-CAA-CBA
12	B	606	NDP	C5D-O5D-PN-O1N
12	B	606	NDP	O4D-C4D-C5D-O5D
12	B	606	NDP	C3D-C4D-C5D-O5D
12	B	606	NDP	O4D-C1D-N1N-C2N
13	B	607	FDA	N10-C1'-C2'-O2'
13	B	607	FDA	N10-C1'-C2'-C3'
13	B	607	FDA	O4'-C4'-C5'-O5'
14	E	200	GTP	C5'-O5'-PA-O1A

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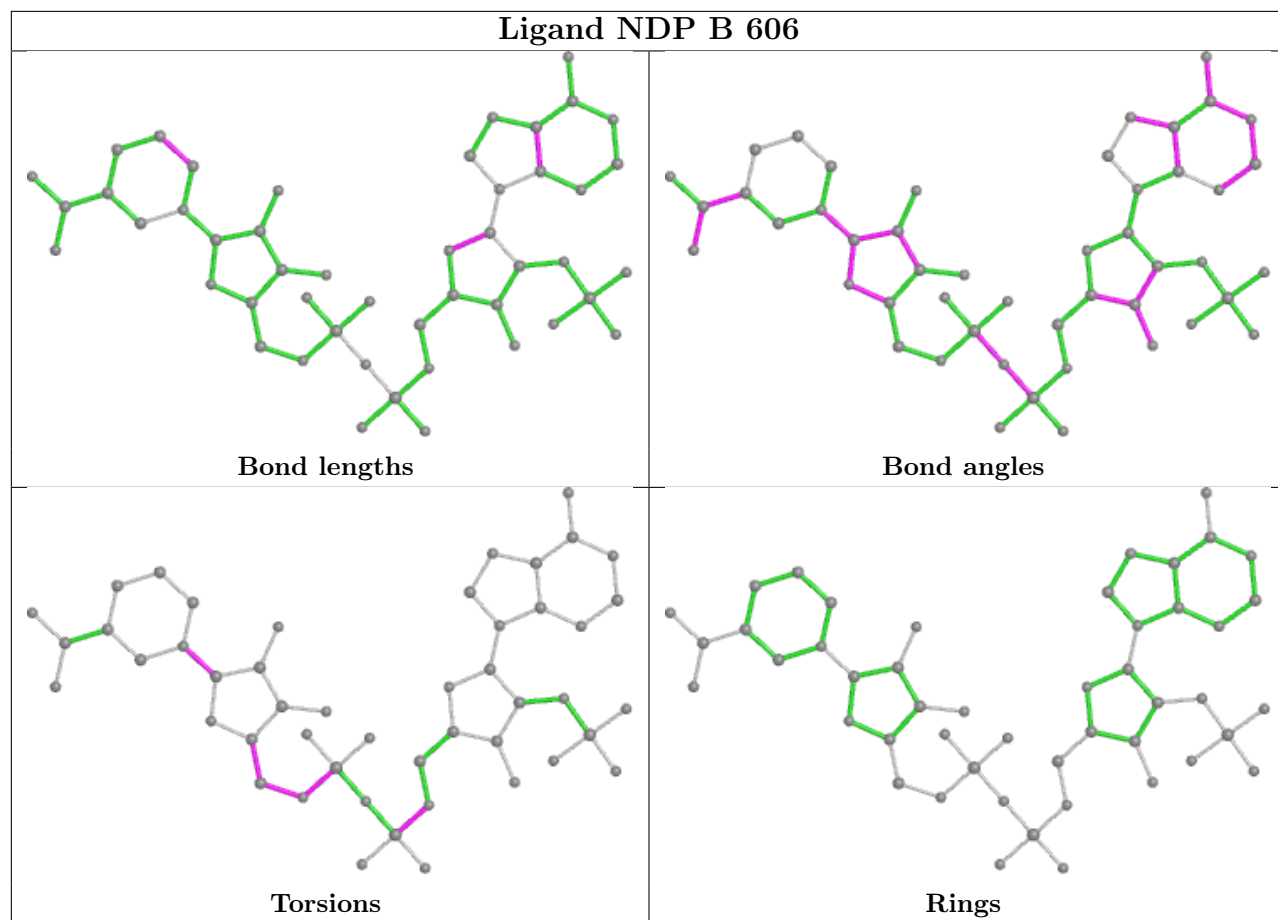
Mol	Chain	Res	Type	Atoms
10	B	603	NAG	O5-C5-C6-O6
9	B	602	HEM	C4D-C3D-CAD-CBD
9	B	602	HEM	C2D-C3D-CAD-CBD
10	B	604	NAG	C4-C5-C6-O6
12	B	606	NDP	C2D-C1D-N1N-C6N
9	B	601	HEM	C4B-C3B-CAB-CBB
9	B	602	HEM	C4B-C3B-CAB-CBB
12	B	606	NDP	C5B-O5B-PA-O3
10	B	604	NAG	O5-C5-C6-O6
9	B	602	HEM	C2A-CAA-CBA-CGA
12	B	606	NDP	C4D-C5D-O5D-PN
13	B	607	FDA	O3'-C3'-C4'-C5'
9	B	602	HEM	C3D-CAD-CBD-CGD
12	B	606	NDP	C2D-C1D-N1N-C2N
13	B	607	FDA	C3B-C4B-C5B-O5B
13	B	607	FDA	C2'-C3'-C4'-C5'
14	E	200	GTP	C5'-O5'-PA-O3A
14	E	200	GTP	PA-O3A-PB-O1B
14	E	200	GTP	PA-O3A-PB-O2B

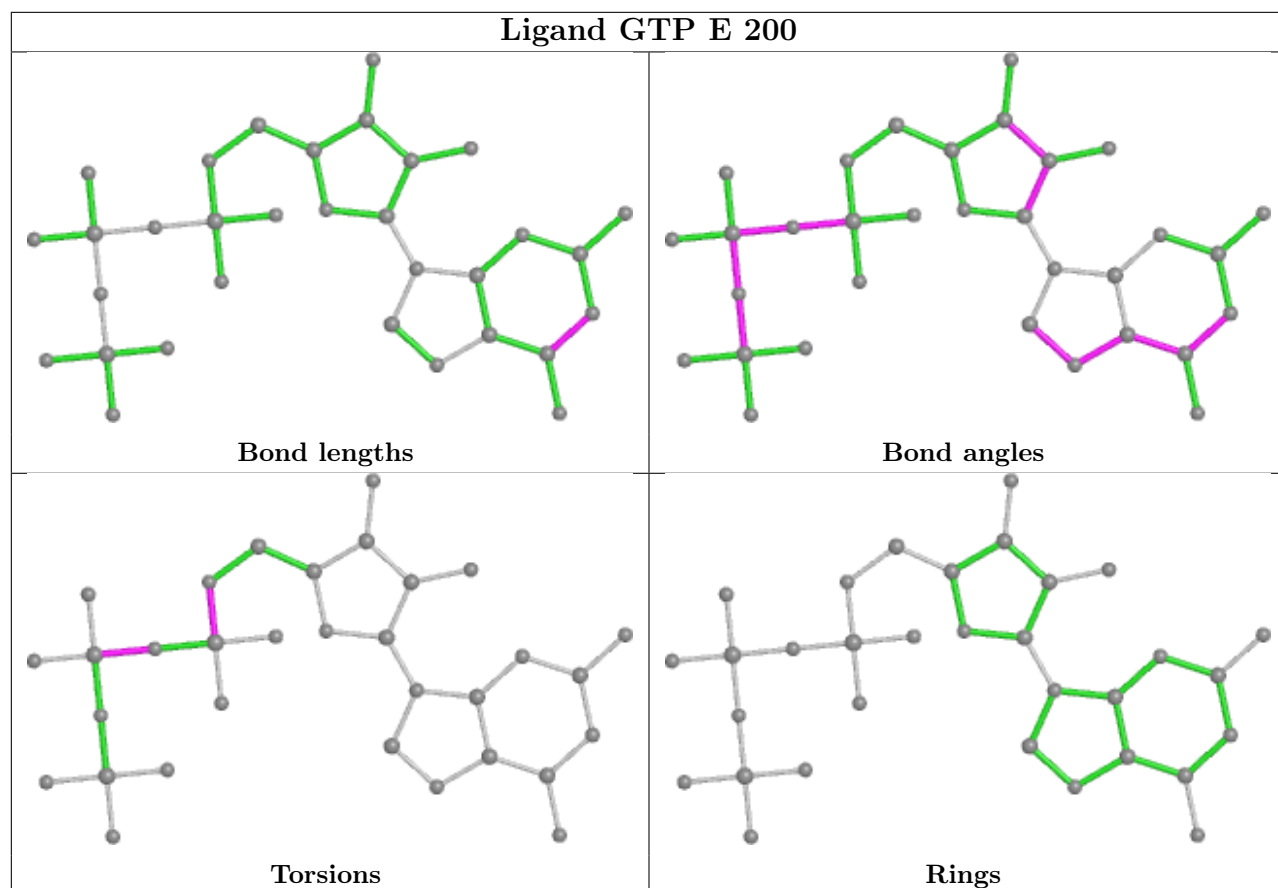
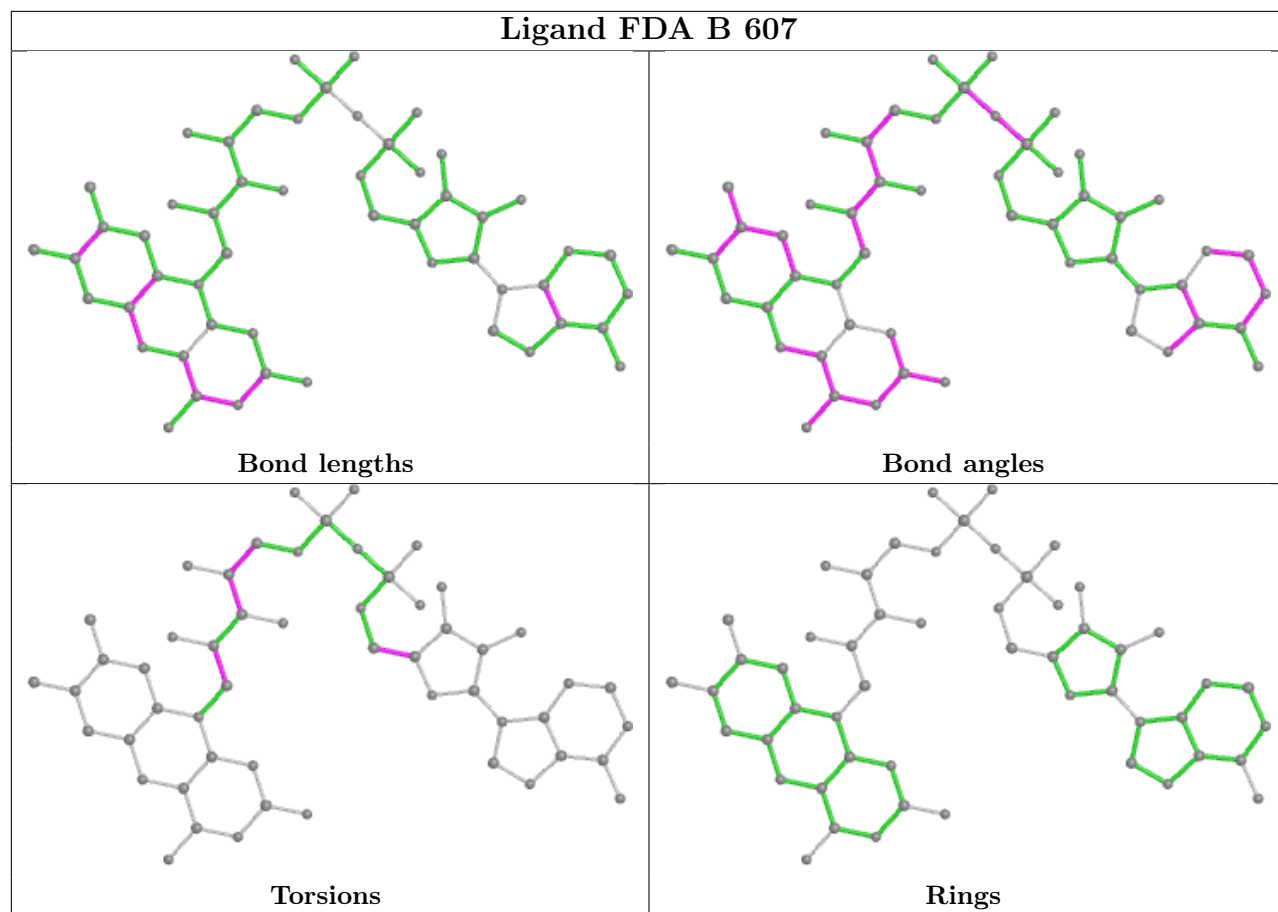
There are no ring outliers.

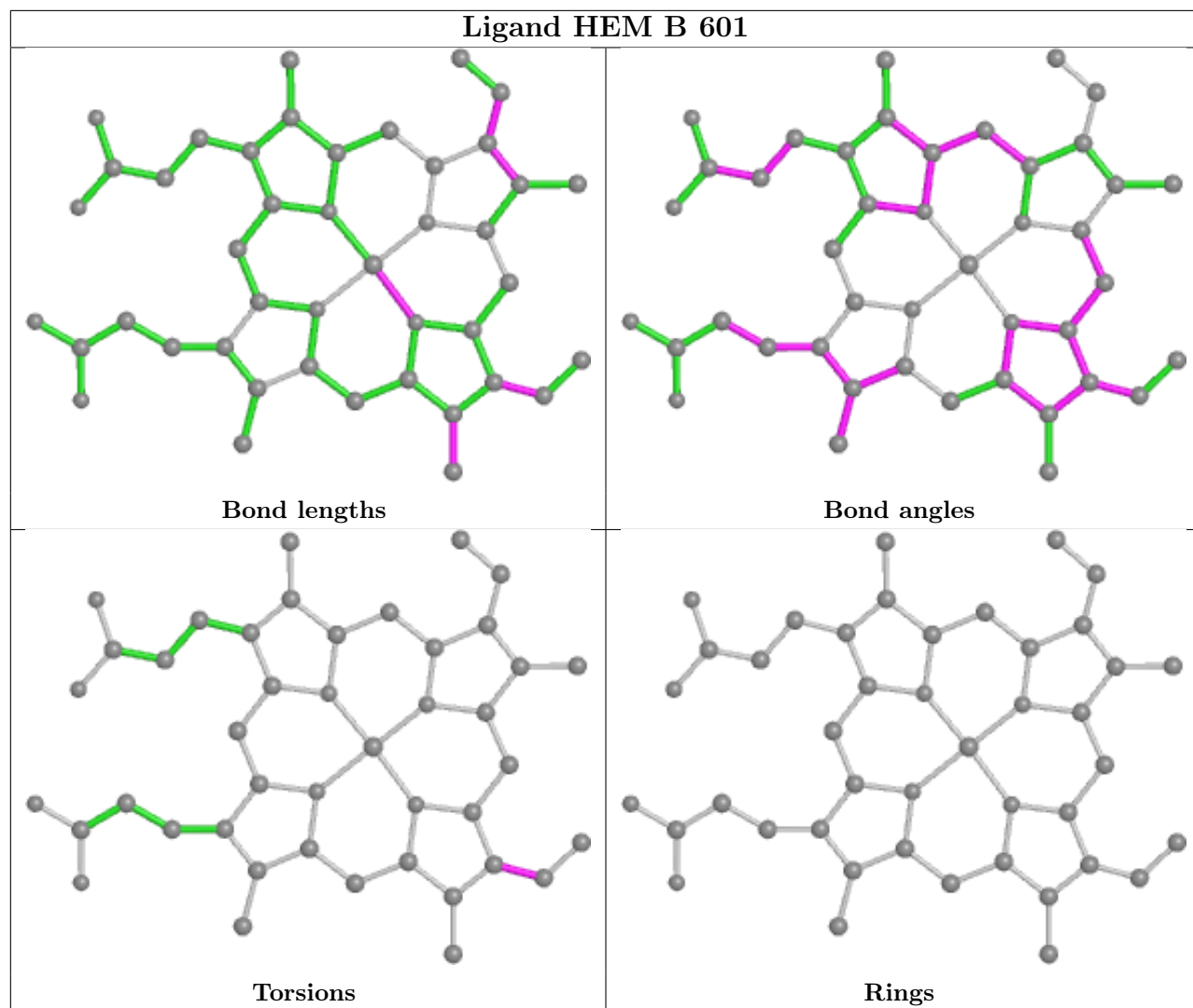
3 monomers are involved in 8 short contacts:

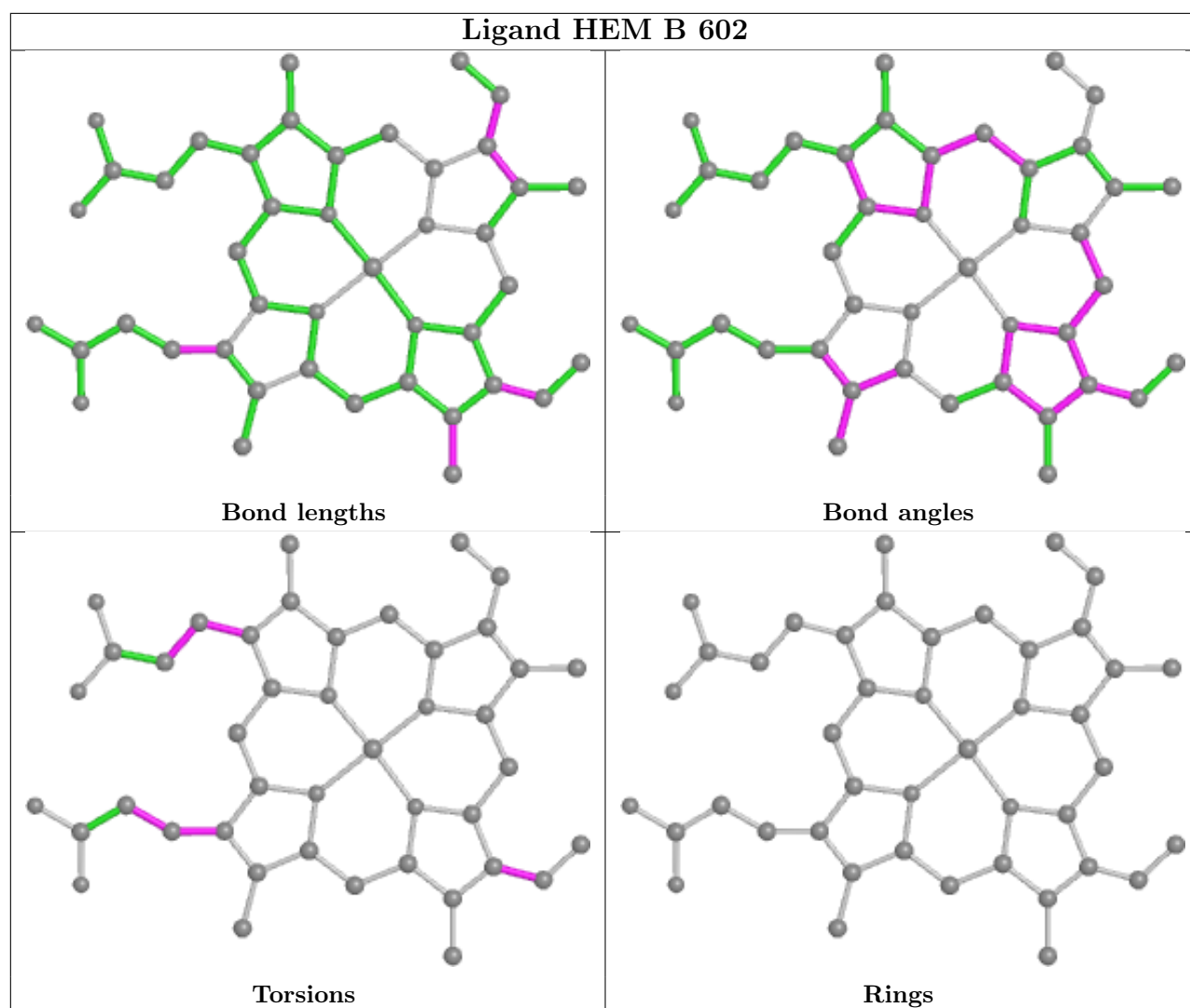
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	607	FDA	2	0
9	B	601	HEM	2	0
9	B	602	HEM	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

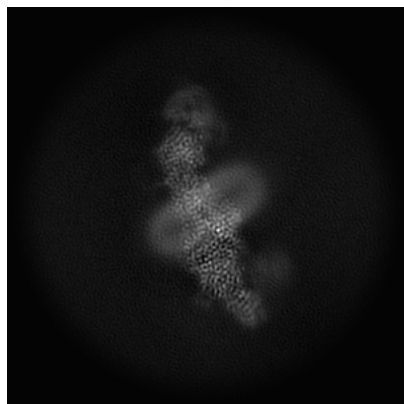
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37477. These allow visual inspection of the internal detail of the map and identification of artifacts.

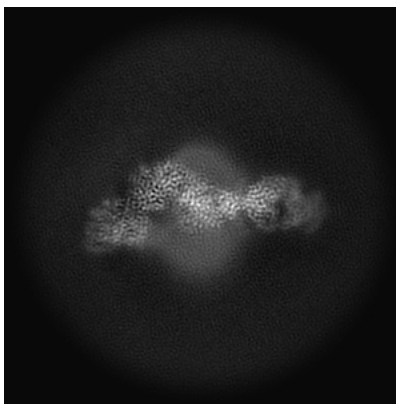
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

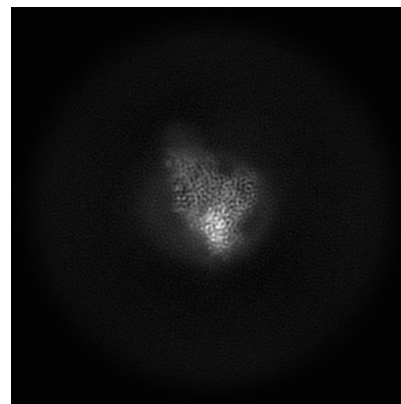
6.1.1 Primary map



X

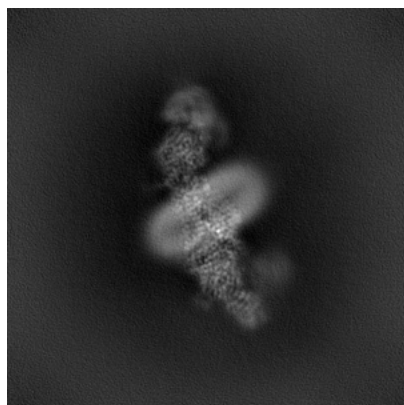


Y

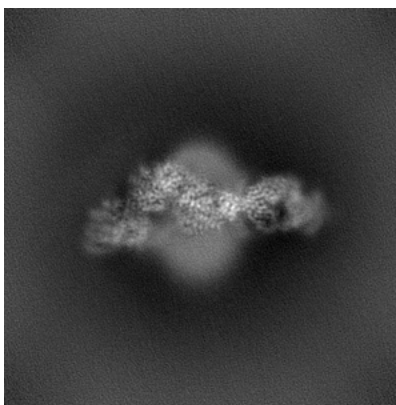


Z

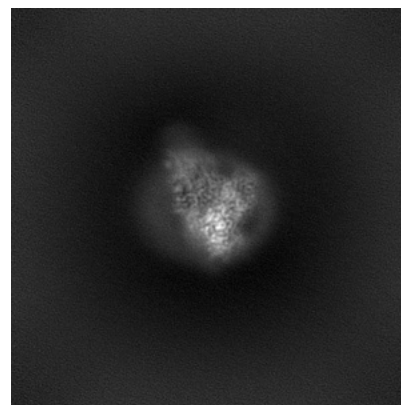
6.1.2 Raw map



X



Y

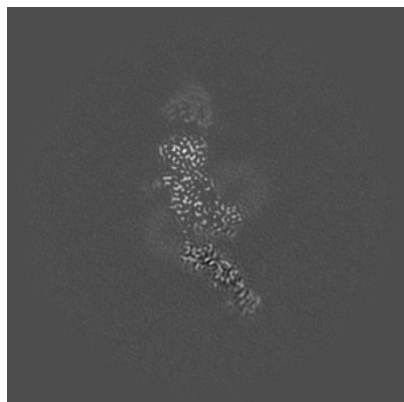


Z

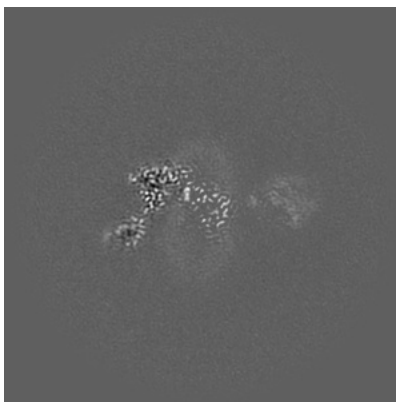
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

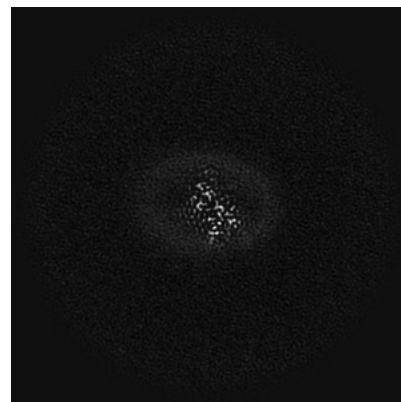
6.2.1 Primary map



X Index: 160

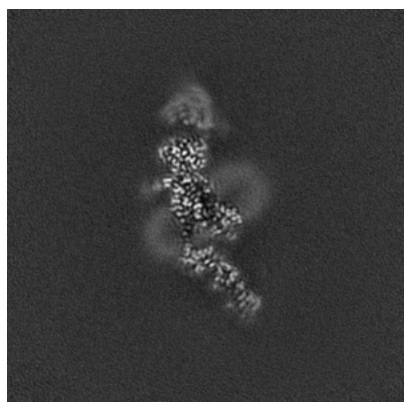


Y Index: 160

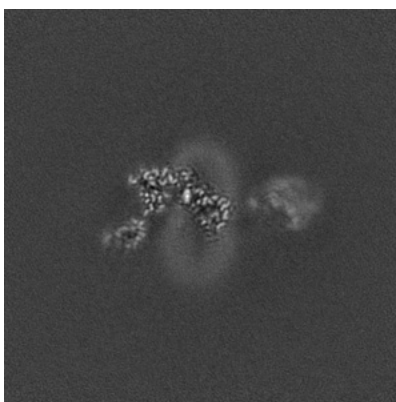


Z Index: 160

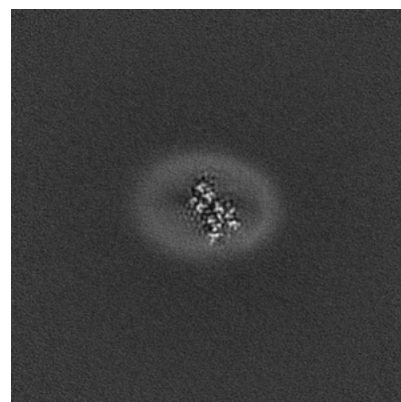
6.2.2 Raw map



X Index: 160



Y Index: 160

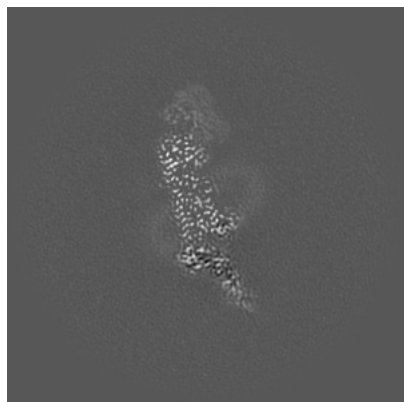


Z Index: 160

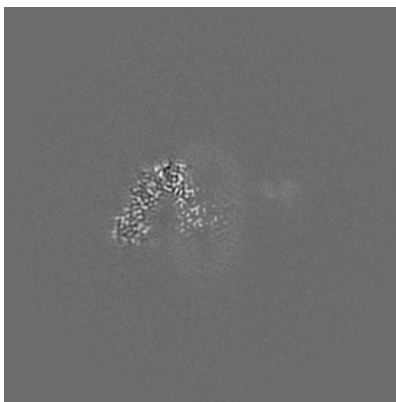
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

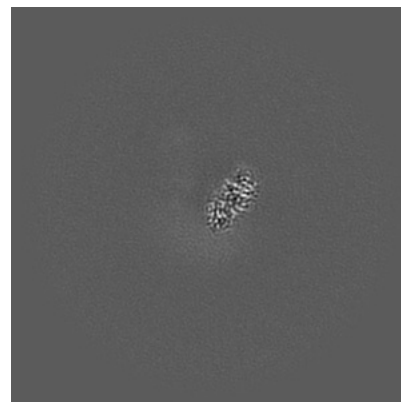
6.3.1 Primary map



X Index: 165

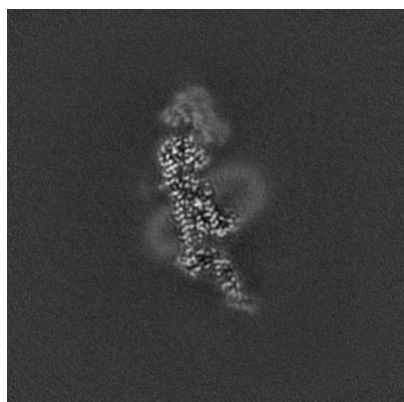


Y Index: 169

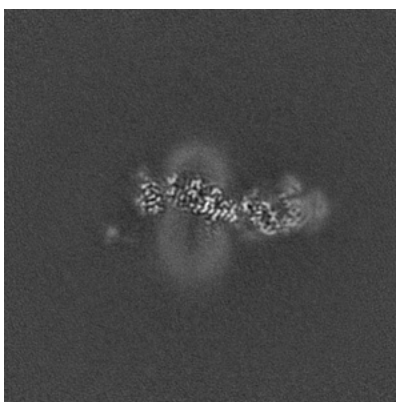


Z Index: 125

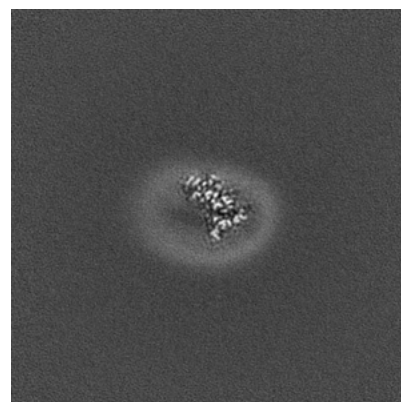
6.3.2 Raw map



X Index: 165



Y Index: 150

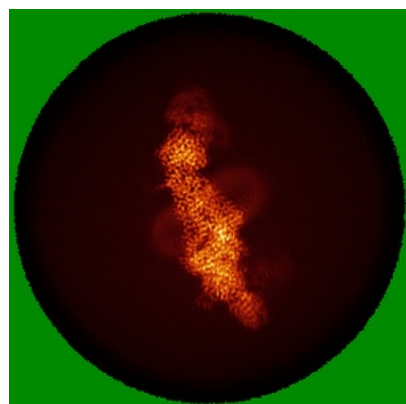


Z Index: 151

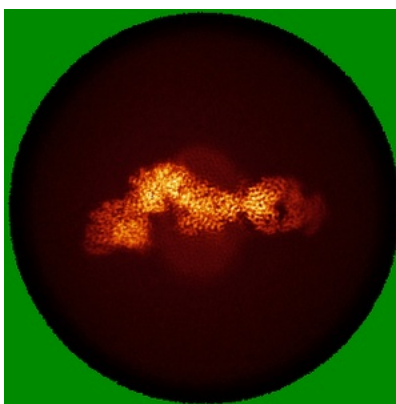
The images above show the largest variance slices of the map in three orthogonal directions.

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

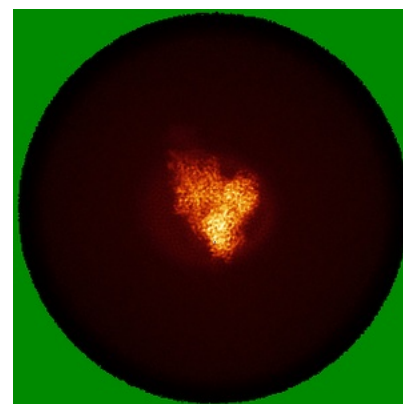
6.4.1 Primary map



X

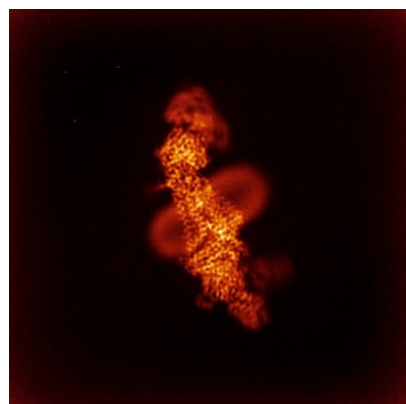


Y

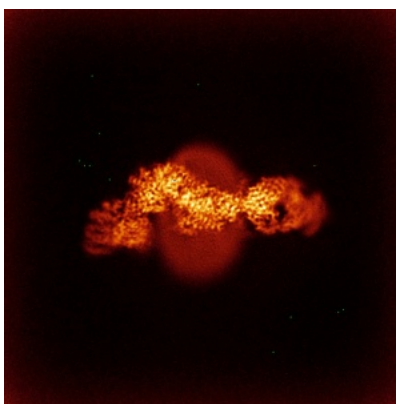


Z

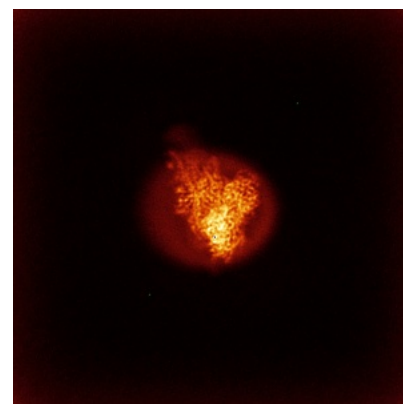
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. 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



X



Y



Z

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.

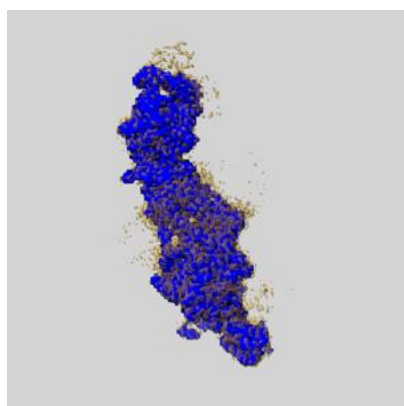
6.6 Mask visualisation [i](#)

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

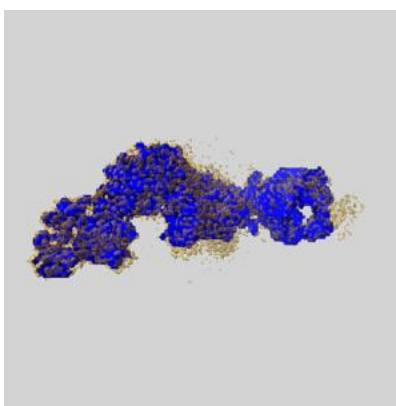
A mask typically either:

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

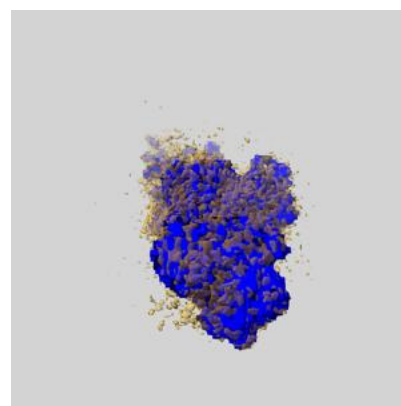
6.6.1 emd_37477_msk_1.map [i](#)



X



Y

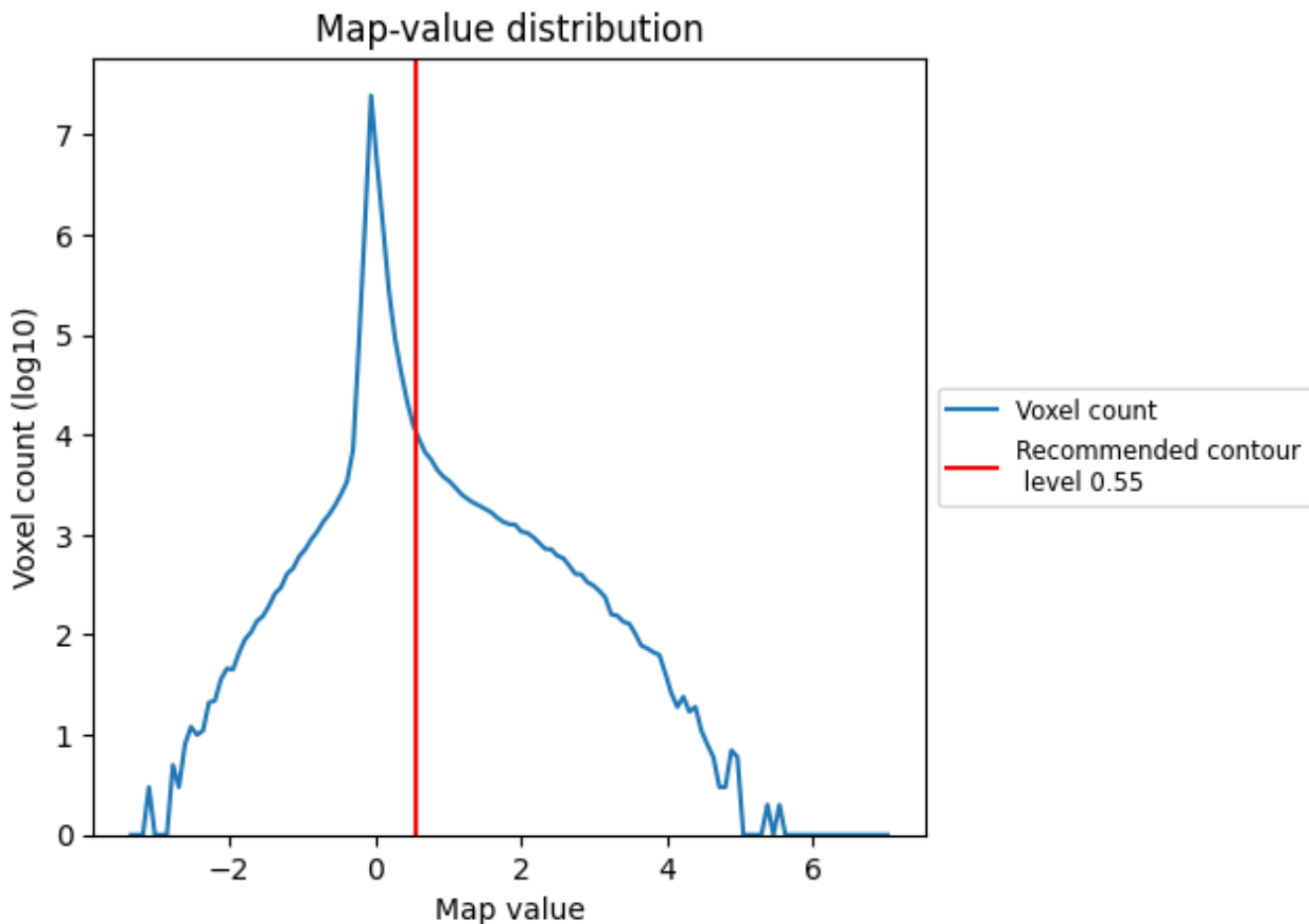


Z

7 Map analysis [i](#)

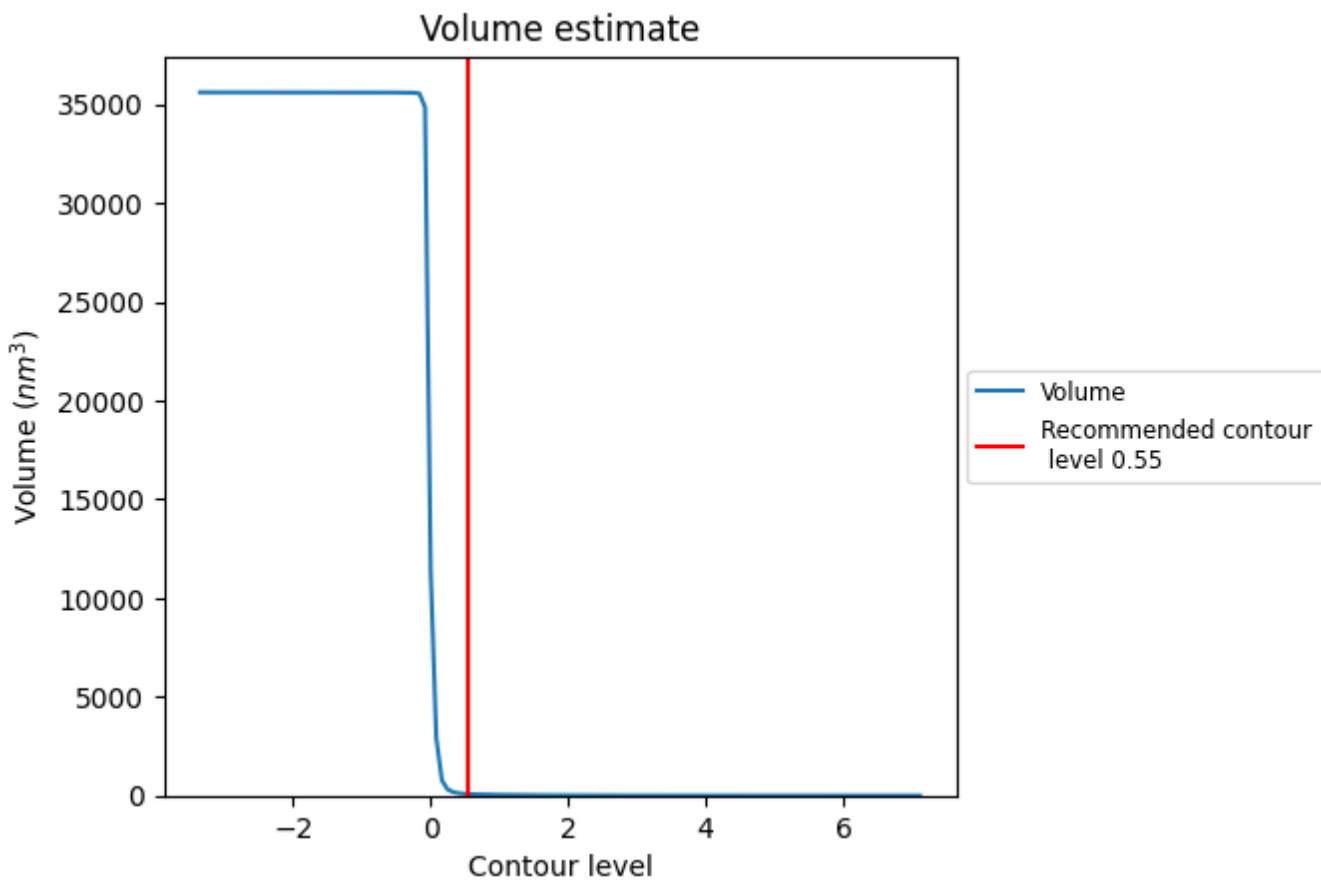
This section contains the results of statistical analysis of the map.

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.

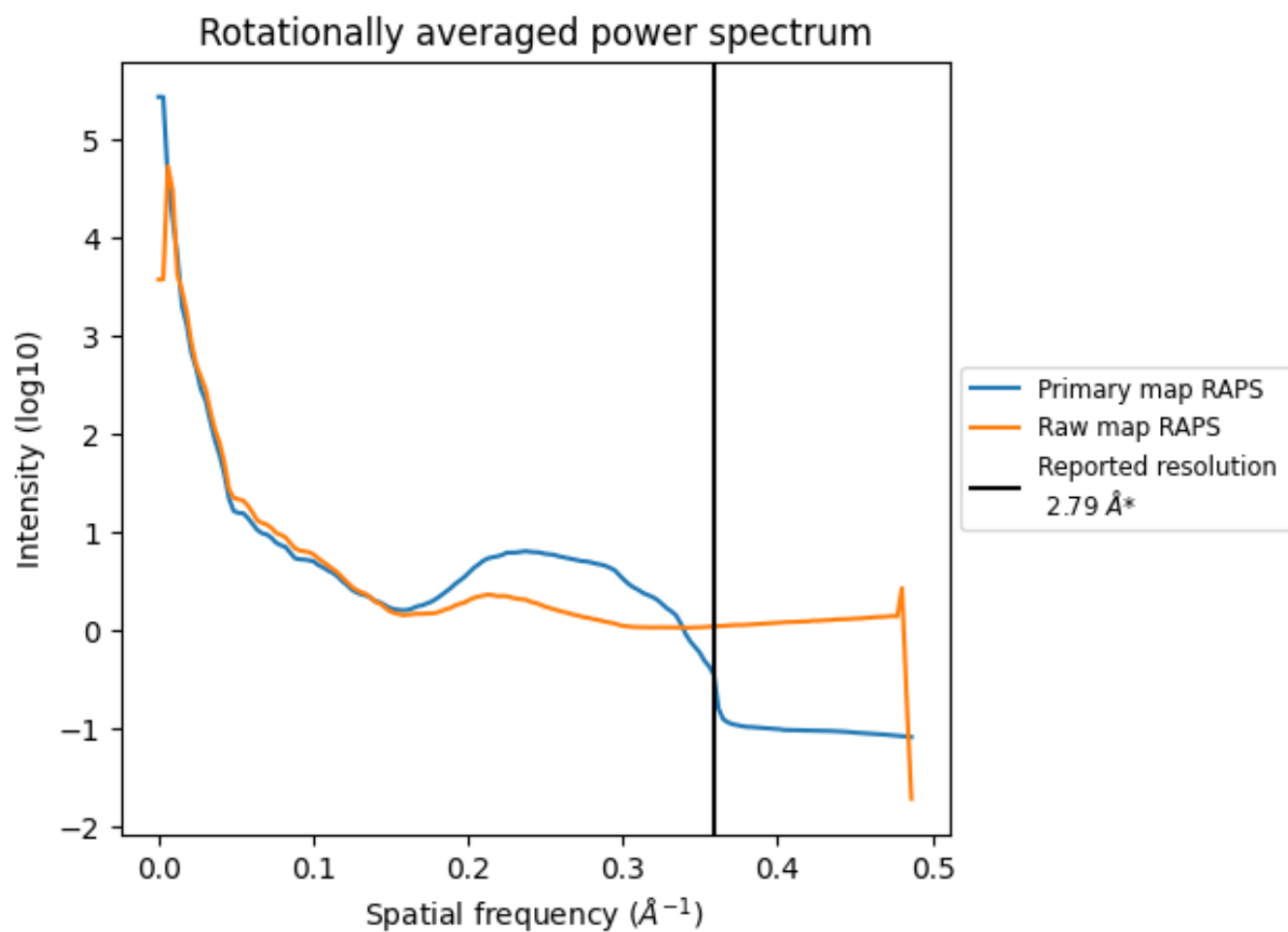
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 71 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 i

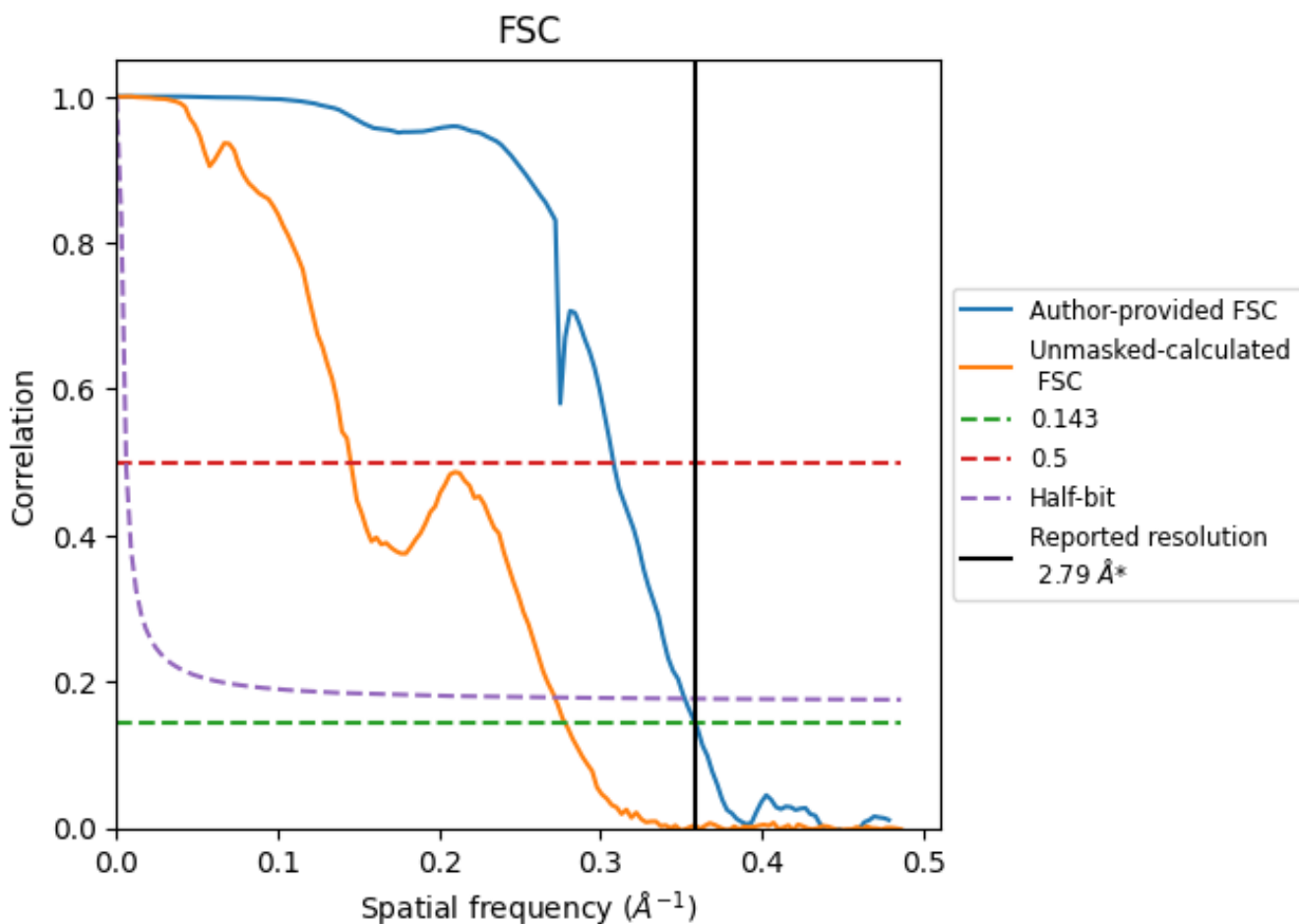


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

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 0.358 \AA^{-1}

8.2 Resolution estimates [i](#)

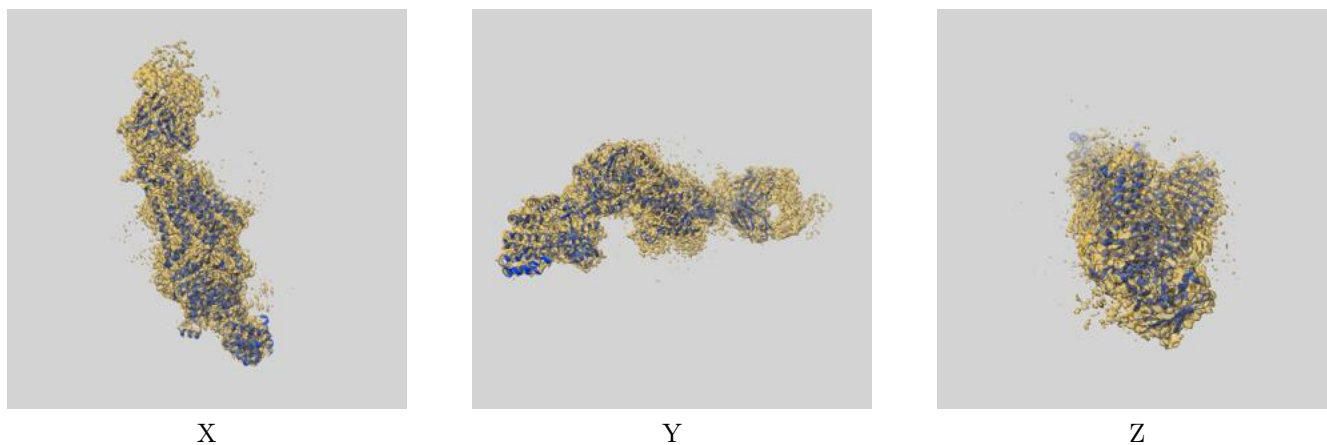
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.25	2.84
Unmasked-calculated*	3.59	6.89	3.68

*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 3.59 differs from the reported value 2.79 by more than 10 %

9 Map-model fit [i](#)

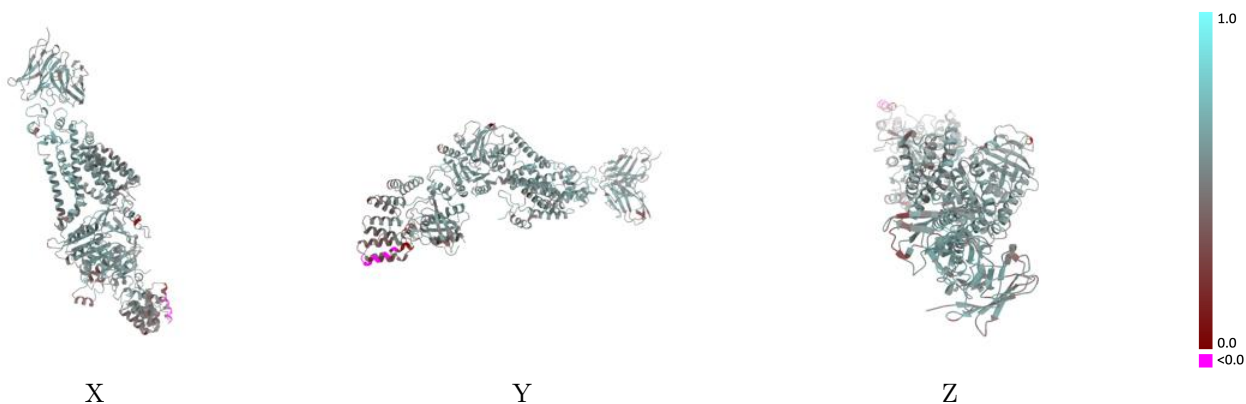
This section contains information regarding the fit between EMDB map EMD-37477 and PDB model 8WEJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



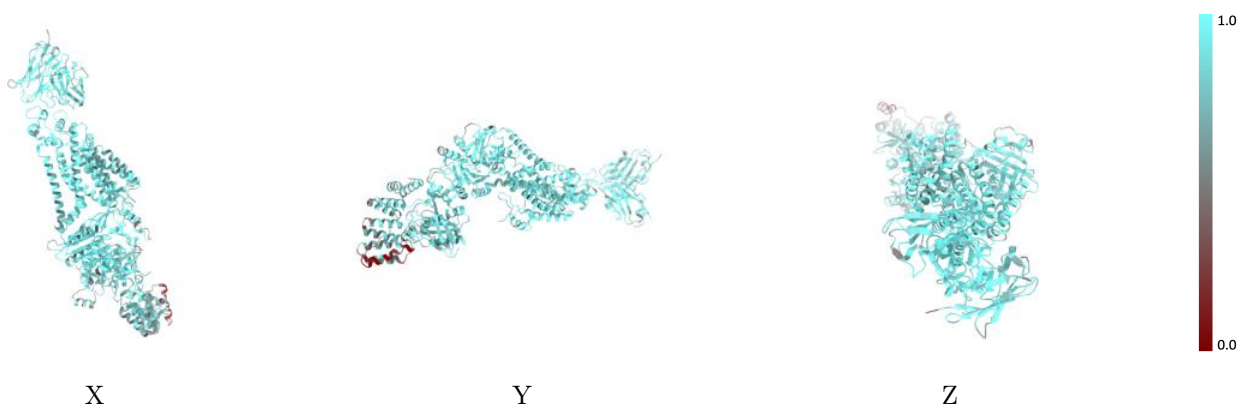
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



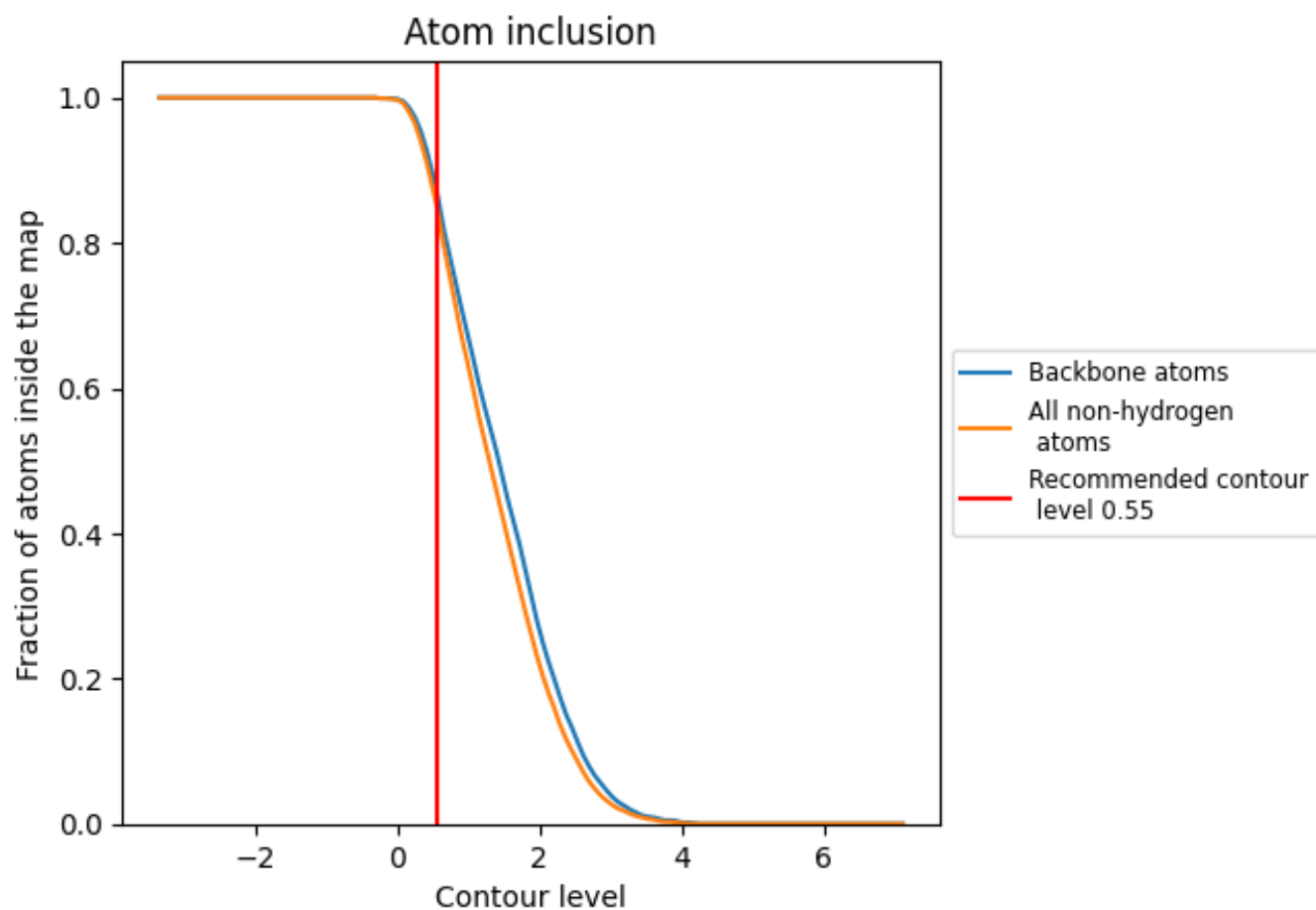
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.5350
A	 0.8650	 0.5370
B	 0.9130	 0.5680
C	 0.7020	 0.5050
D	 0.6930	 0.4540
E	 0.8350	 0.5150
F	 0.6410	 0.4160
H	 0.8740	 0.5400
L	 0.8650	 0.5390

