



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:35 PM UTC

PDB ID : 8WEJ / pdb_00008wej
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:

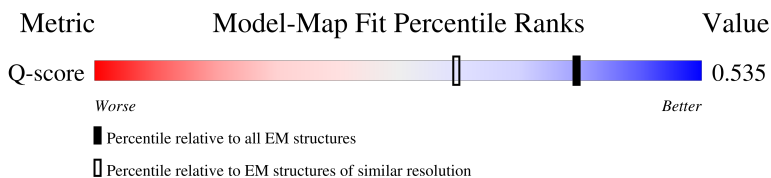
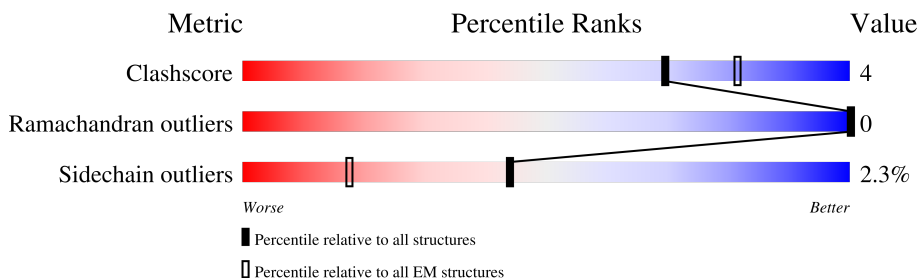
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.79 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	

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Mol	Chain	Length	Quality of chain
5	E	192	 82% 10% 7%
6	H	251	 42% 6% 53%
7	L	236	 40% 5% 55%
8	F	3	 100%

2 Entry composition

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
1	A	134	Total	C	N	O	S	0	0
			1030	681	171	173	5		

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
2	B	569	Total	C	N	O	S	0	0
			4549	2974	773	778	24		

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

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

- 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
4	D	219	Total	C	N	O	S	0	0
			1643	1068	283	282	10		

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

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

There is a discrepancy between the modelled and reference sequences:

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

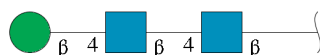
- Molecule 6 is a protein called 7D5 Fab heavy chain.

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

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

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

- 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.



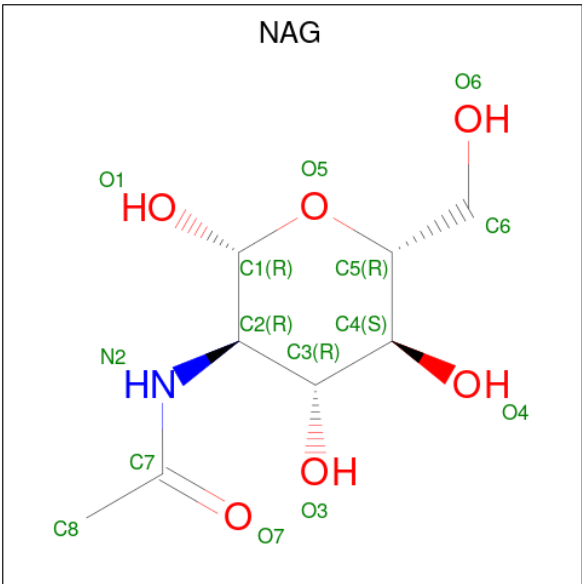
Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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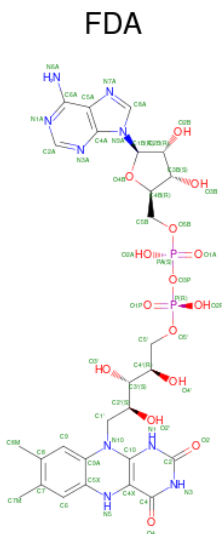
Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	0
			14	8	1	5	

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

- # NDP

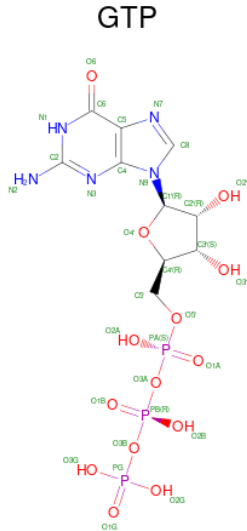
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 48	C 21	N 7	O 17	P 3	0

- WORLDWIDE
PDB
PROTEIN DATA BANK



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

- Molecule 14 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 15 is water.

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

- Chain D:
-
- 10% 63% 8% 28%
- ME D18 D27 D34 W65 K68 H69 L70 A71 A73 A76 Q76 M79 K86 A90 L101 R102 Y109 L114 C121 E122 N126 F129 M130 Y131 A132 E135 E136 W137 T148 S149 M150 K151 S152 E153 P154 R155 H156 S157 K158 I159 D160 V161 V162 V163 V164 V165 V166 V167 V168 V169 V170 V171 V172 V173 V174 V175 V176 V177 V178 V179 V180 V181 V182 V183 V184 V185 V186 V187 V188 V189 V190 V191 V192 V193 V194 V195 V196 V197 V198 V199 V200 V201 V202 V203 V204 V205 V206 V207 V208 V209 V210 V211 V212 V213 V214 V215 V216
- E164 C165 V166 W167 K168 Q169 K170 L171 Y172 E173 I177 V190 L193 D210 Q211 F214 P219 LEU GLN PRO GLN ALA ALA GLU PRO PRO PRO ARG PRO PRO LYS THR PRO GLU ILE PHE ARG ALA LEU LEU GLU GLY GLY GLN HIS ARG VAL LEU PHE GLY PHE VAL PRO GLU THR

- Chain E: 

- [illegible]

- [illegible]

- 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%

HA01
HA02
EM03

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 ($\text{\AA}$)	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 ($\text{\AA}$)	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, NDP, BMA, MG, FDA, NAG, GTP

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	0.21	0/1058	0.40	0/1443
2	B	0.21	0/4680	0.38	0/6360
3	C	0.26	0/67	0.57	0/92
4	D	0.28	1/1677 (0.1%)	0.42	0/2275
5	E	0.24	0/1358	0.41	0/1860
6	H	0.20	0/962	0.40	0/1310
7	L	0.23	0/835	0.41	0/1135
All	All	0.23	1/10637 (0.0%)	0.40	0/14475

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	34	ASP	C-O	-6.01	1.21	1.23

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	30	0
3	C	67	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1643	0	1606	15	0
5	E	1328	0	1304	12	0
6	H	935	0	870	8	0
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:122:GLU:O	4:D:126:ASN:ND2	2.44	0.51
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
2:B:569:ASN:O	13:B:607:FDA:HM82	2.14	0.47
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
7:L:50:TYR:C	7:L:51:THR:HG23	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:19:VAL:HG22	7:L:78:LEU:HD11	2.01	0.42
2:B:299:LYS:NZ	4:D:214:PHE:O	2.47	0.42
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
4:D:90:ALA:CB	4:D:130:MET:HE2	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	48	80
2	B	481/498 (97%)	468 (97%)	13 (3%)	39	74
3	C	7/252 (3%)	5 (71%)	2 (29%)	0	1
4	D	155/262 (59%)	153 (99%)	2 (1%)	61	86
5	E	138/168 (82%)	135 (98%)	3 (2%)	45	78
6	H	103/223 (46%)	101 (98%)	2 (2%)	50	81
7	L	88/209 (42%)	87 (99%)	1 (1%)	65	87
All	All	1072/1762 (61%)	1047 (98%)	25 (2%)	44	78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	120	ILE
2	B	12	ILE
2	B	151	SER
2	B	204	VAL
2	B	254	ILE
2	B	301	VAL
2	B	312	MET
2	B	373	LYS
2	B	381	LYS
2	B	382	LEU
2	B	396	GLU
2	B	398	VAL
2	B	414	THR
2	B	502	ILE
3	C	150	THR
3	C	156	ILE
4	D	79	MET

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Mol	Chain	Res	Type
4	D	101	LEU
5	E	145	MET
5	E	148	GLU
5	E	176	VAL
6	H	49	MET
6	H	81	LEU
7	L	51	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	ASN
4	D	33	GLN

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 ⓘ

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	0.27	0	17,19,21	0.49	0
8	NAG	F	2	8	14,14,15	0.20	0	17,19,21	0.34	0
8	BMA	F	3	8	11,11,12	0.62	0	15,15,17	0.63	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.

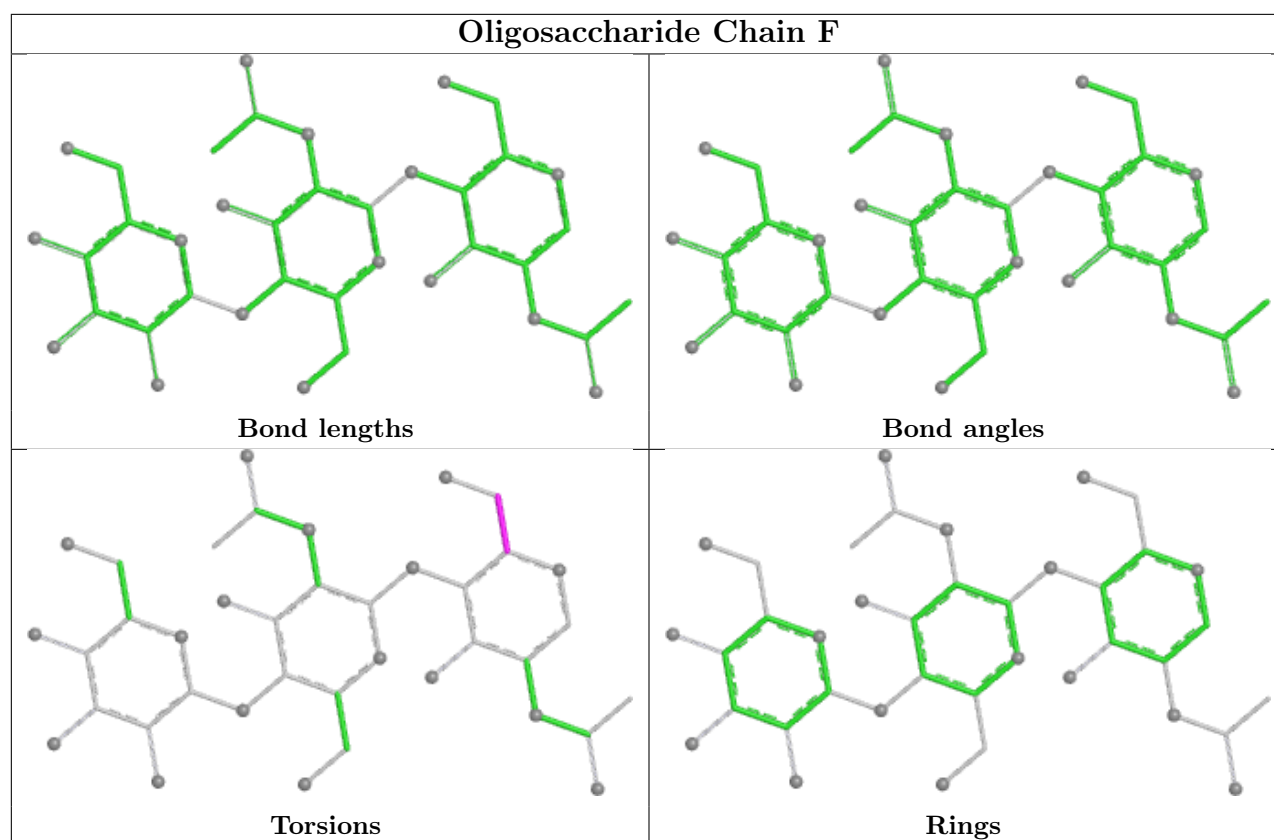
All (2) torsion outliers are listed below:

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	$\# Z > 2$
9	HEM	B	602	2	50,50,50	1.51	8 (16%)	67,82,82	1.28	9 (13%)
13	FDA	B	607	11	57,58,58	1.68	11 (19%)	78,89,89	1.77	21 (26%)
10	NAG	B	604	2	14,14,15	0.26	0	17,19,21	0.43	0
10	NAG	B	603	2	14,14,15	0.21	0	17,19,21	0.44	0
12	NDP	B	606	-	51,52,52	1.26	7 (13%)	71,80,80	1.62	15 (21%)
14	GTP	E	200	11	33,34,34	1.16	3 (9%)	50,54,54	1.60	7 (14%)
9	HEM	B	601	2	50,50,50	1.46	8 (16%)	67,82,82	1.36	12 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	B	602	2	-	7/14/54/54	-
13	FDA	B	607	11	-	6/34/50/50	0/6/6/6
10	NAG	B	604	2	-	2/6/23/26	0/1/1/1
10	NAG	B	603	2	-	1/6/23/26	0/1/1/1
12	NDP	B	606	-	-	7/34/77/77	0/5/5/5
14	GTP	E	200	11	-	3/22/38/38	0/3/3/3
9	HEM	B	601	2	-	2/14/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	607	FDA	C5X-C9A	7.84	1.49	1.40
12	B	606	NDP	C5A-C4A	4.29	1.46	1.39
13	B	607	FDA	C5A-C4A	4.29	1.46	1.39
9	B	601	HEM	FE-NB	3.89	2.06	1.94
9	B	601	HEM	FE-ND	3.72	2.06	1.94
13	B	607	FDA	C8-C7	3.71	1.49	1.40
9	B	602	HEM	FE-NA	3.66	2.07	1.95
9	B	602	HEM	FE-ND	3.62	2.06	1.94
9	B	602	HEM	CAC-C3C	3.40	1.56	1.47
9	B	602	HEM	FE-NB	3.36	2.05	1.94
14	E	200	GTP	C5-C4	3.36	1.48	1.38
9	B	601	HEM	CAC-C3C	3.19	1.55	1.47
9	B	601	HEM	CAB-C3B	3.12	1.55	1.47
9	B	602	HEM	FE-NC	3.10	2.05	1.95
9	B	602	HEM	CAB-C3B	3.00	1.55	1.47
9	B	601	HEM	FE-NC	2.77	2.04	1.95
13	B	607	FDA	C5A-C6A	2.69	1.48	1.41
9	B	601	HEM	FE-NA	2.68	2.04	1.95
13	B	607	FDA	C4-N3	-2.66	1.33	1.38
12	B	606	NDP	C5A-N7A	-2.61	1.34	1.39
13	B	607	FDA	C4X-C4	2.43	1.49	1.41
9	B	602	HEM	CMB-C2B	2.40	1.55	1.50
12	B	606	NDP	C5A-C6A	2.39	1.47	1.41
13	B	607	FDA	C5A-N7A	-2.37	1.34	1.39
13	B	607	FDA	C2-N3	-2.35	1.33	1.37
9	B	601	HEM	CMB-C2B	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	200	GTP	C5-N7	-2.33	1.34	1.39
12	B	606	NDP	C8A-N9A	-2.29	1.33	1.37
12	B	606	NDP	C4A-N9A	-2.26	1.33	1.37
13	B	607	FDA	C8A-N7A	2.20	1.35	1.31
12	B	606	NDP	C8A-N7A	2.20	1.35	1.31
9	B	601	HEM	CMC-C2C	2.19	1.55	1.50
14	E	200	GTP	C6-N1	-2.19	1.34	1.38
13	B	607	FDA	C4A-N9A	-2.16	1.33	1.37
13	B	607	FDA	C5X-N5	-2.10	1.36	1.39
12	B	606	NDP	C6N-C5N	2.06	1.39	1.33
9	B	602	HEM	CMA-C3A	2.03	1.54	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	607	FDA	C5A-C4A-N3A	-5.97	118.50	126.72
12	B	606	NDP	C5A-C4A-N3A	-5.30	119.42	126.72
14	E	200	GTP	C5-C4-N3	-5.16	120.18	128.39
13	B	607	FDA	N3A-C4A-N9A	4.78	135.29	127.17
12	B	606	NDP	N3A-C4A-N9A	4.30	134.48	127.17
14	E	200	GTP	C2-N3-C4	4.27	119.66	112.30
13	B	607	FDA	N3-C2-N1	4.26	122.44	115.74
14	E	200	GTP	N9-C4-N3	4.26	134.47	125.95
13	B	607	FDA	C2A-N3A-C4A	3.76	121.01	111.83
13	B	607	FDA	N3A-C2A-N1A	-3.50	123.28	128.58
13	B	607	FDA	C4A-C5A-N7A	-3.46	106.62	110.58
12	B	606	NDP	C4D-O4D-C1D	-3.42	101.91	109.47
14	E	200	GTP	C6-C5-N7	3.23	136.17	130.29
13	B	607	FDA	C4A-N9A-C8A	3.18	109.08	105.74
12	B	606	NDP	C4A-C5A-N7A	-3.11	107.03	110.58
12	B	606	NDP	C2A-N3A-C4A	3.07	119.34	111.83
9	B	601	HEM	CHC-C1C-NC	2.81	127.51	124.45
13	B	607	FDA	C5A-N7A-C8A	2.80	107.84	103.45
9	B	602	HEM	C3B-C2B-C1B	2.79	108.50	106.41
9	B	601	HEM	CHD-C1D-ND	2.70	127.33	124.42
13	B	607	FDA	C4-N3-C2	-2.70	122.65	126.37
12	B	606	NDP	C4A-N9A-C8A	2.70	108.57	105.74
12	B	606	NDP	N3A-C2A-N1A	-2.67	124.54	128.58
9	B	601	HEM	C3B-C2B-C1B	2.62	108.38	106.41
13	B	607	FDA	N9A-C8A-N7A	-2.60	110.25	113.94
9	B	602	HEM	C3B-C4B-NB	-2.59	107.61	109.47
13	B	607	FDA	C4-C4X-N5	2.56	122.91	116.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	607	FDA	O4-C4-C4X	-2.53	121.16	127.26
13	B	607	FDA	C8M-C8-C9	-2.53	115.12	119.57
12	B	606	NDP	O3B-C3B-C4B	-2.52	103.84	111.08
13	B	607	FDA	C1'-C2'-C3'	2.51	116.46	109.66
12	B	606	NDP	C3N-C7N-N7N	2.47	122.06	117.67
9	B	602	HEM	C4D-ND-C1D	2.46	108.12	105.21
12	B	606	NDP	O4D-C1D-N1N	2.46	112.77	108.08
13	B	607	FDA	C4X-C4-N3	2.43	118.81	112.13
13	B	607	FDA	C8M-C8-C7	2.39	125.64	120.76
9	B	601	HEM	C4D-ND-C1D	2.38	108.02	105.21
9	B	602	HEM	C1B-NB-C4B	2.35	107.99	105.21
14	E	200	GTP	C3'-C2'-C1'	2.28	105.77	101.46
9	B	601	HEM	C1B-NB-C4B	2.24	107.86	105.21
13	B	607	FDA	C5X-C9A-N10	2.23	120.53	118.01
9	B	602	HEM	CHD-C1D-ND	2.23	126.82	124.42
9	B	602	HEM	C3C-C2C-C1C	2.22	109.15	107.05
9	B	601	HEM	C2D-C1D-ND	-2.19	107.37	109.90
13	B	607	FDA	C5'-C4'-C3'	-2.18	108.10	112.22
13	B	607	FDA	O2-C2-N3	-2.17	118.00	121.86
13	B	607	FDA	C2A-N1A-C6A	2.16	122.28	118.73
12	B	606	NDP	C3D-C2D-C1D	2.14	105.52	101.46
9	B	602	HEM	CAB-C3B-C2B	-2.14	121.48	128.43
9	B	602	HEM	C3D-C4D-ND	-2.14	107.83	110.17
9	B	601	HEM	CAC-C3C-C4C	2.13	129.91	124.82
9	B	601	HEM	CBA-CAA-C2A	-2.13	106.64	112.53
14	E	200	GTP	O6-C6-C5	-2.11	120.96	126.53
13	B	607	FDA	C9A-C9-C8	2.09	123.43	119.22
9	B	601	HEM	C3B-C4B-NB	-2.07	107.98	109.47
12	B	606	NDP	O4B-C1B-N9A	2.07	112.07	108.09
12	B	606	NDP	N6A-C6A-N1A	2.07	122.98	118.38
9	B	601	HEM	CHC-C4B-C3B	2.05	129.17	125.07
12	B	606	NDP	C5A-N7A-C8A	2.04	106.66	103.45
14	E	200	GTP	C4-C5-N7	-2.04	107.44	110.67
9	B	602	HEM	C2D-C1D-ND	-2.04	107.55	109.90
9	B	601	HEM	CAB-C3B-C2B	-2.03	121.82	128.43
12	B	606	NDP	C2B-C3B-C4B	2.03	106.35	101.99
9	B	601	HEM	CHB-C4A-NA	2.01	127.50	123.86

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	602	HEM	C1A-C2A-CAA-CBA
12	B	606	NDP	C5D-O5D-PN-O1N
12	B	606	NDP	O4D-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
12	B	606	NDP	C3D-C4D-C5D-O5D
10	B	603	NAG	O5-C5-C6-O6
9	B	602	HEM	C3A-C2A-CAA-CBA
9	B	602	HEM	C4D-C3D-CAD-CBD
9	B	602	HEM	C2D-C3D-CAD-CBD
10	B	604	NAG	C4-C5-C6-O6
9	B	601	HEM	C4B-C3B-CAB-CBB
9	B	601	HEM	C4C-C3C-CAC-CBC
9	B	602	HEM	C4B-C3B-CAB-CBB
10	B	604	NAG	O5-C5-C6-O6
12	B	606	NDP	C2D-C1D-N1N-C6N
13	B	607	FDA	O3'-C3'-C4'-C5'
12	B	606	NDP	C4D-C5D-O5D-PN
9	B	602	HEM	C3D-CAD-CBD-CGD
13	B	607	FDA	C2'-C3'-C4'-C5'
13	B	607	FDA	C3B-C4B-C5B-O5B
9	B	602	HEM	C2A-CAA-CBA-CGA
12	B	606	NDP	C2D-C1D-N1N-C2N
14	E	200	GTP	PA-O3A-PB-O1B
14	E	200	GTP	PA-O3A-PB-O2B

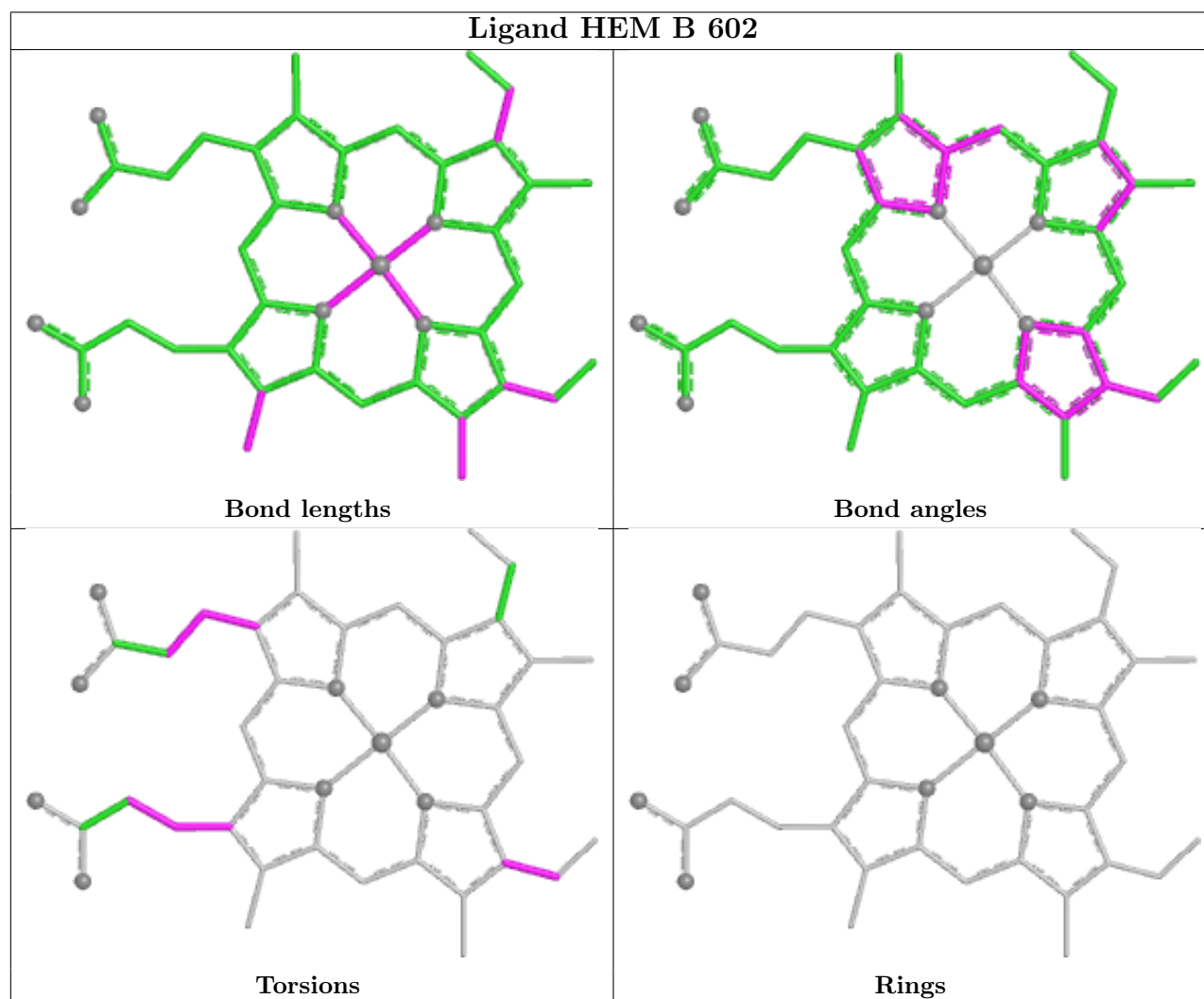
There are no ring outliers.

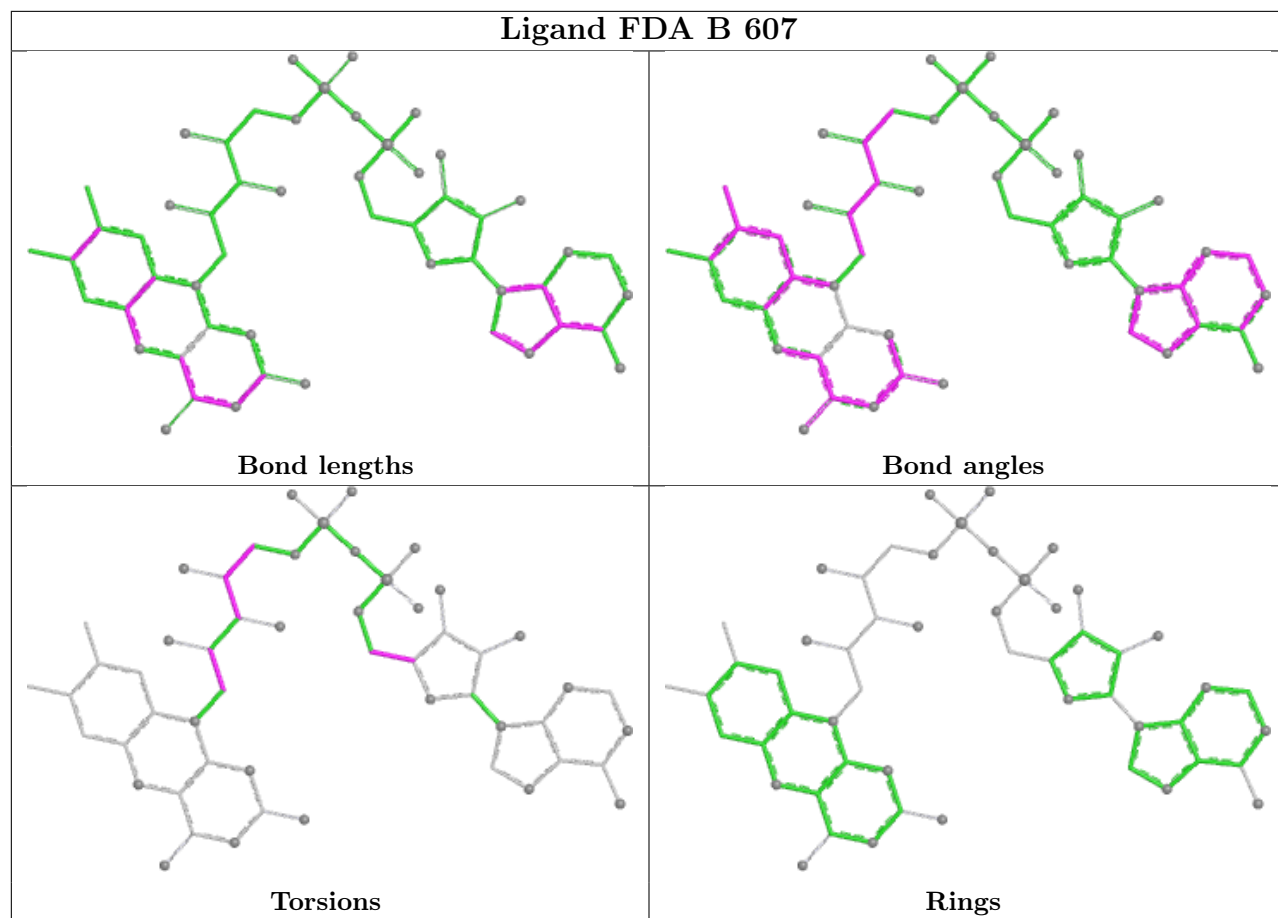
3 monomers are involved in 8 short contacts:

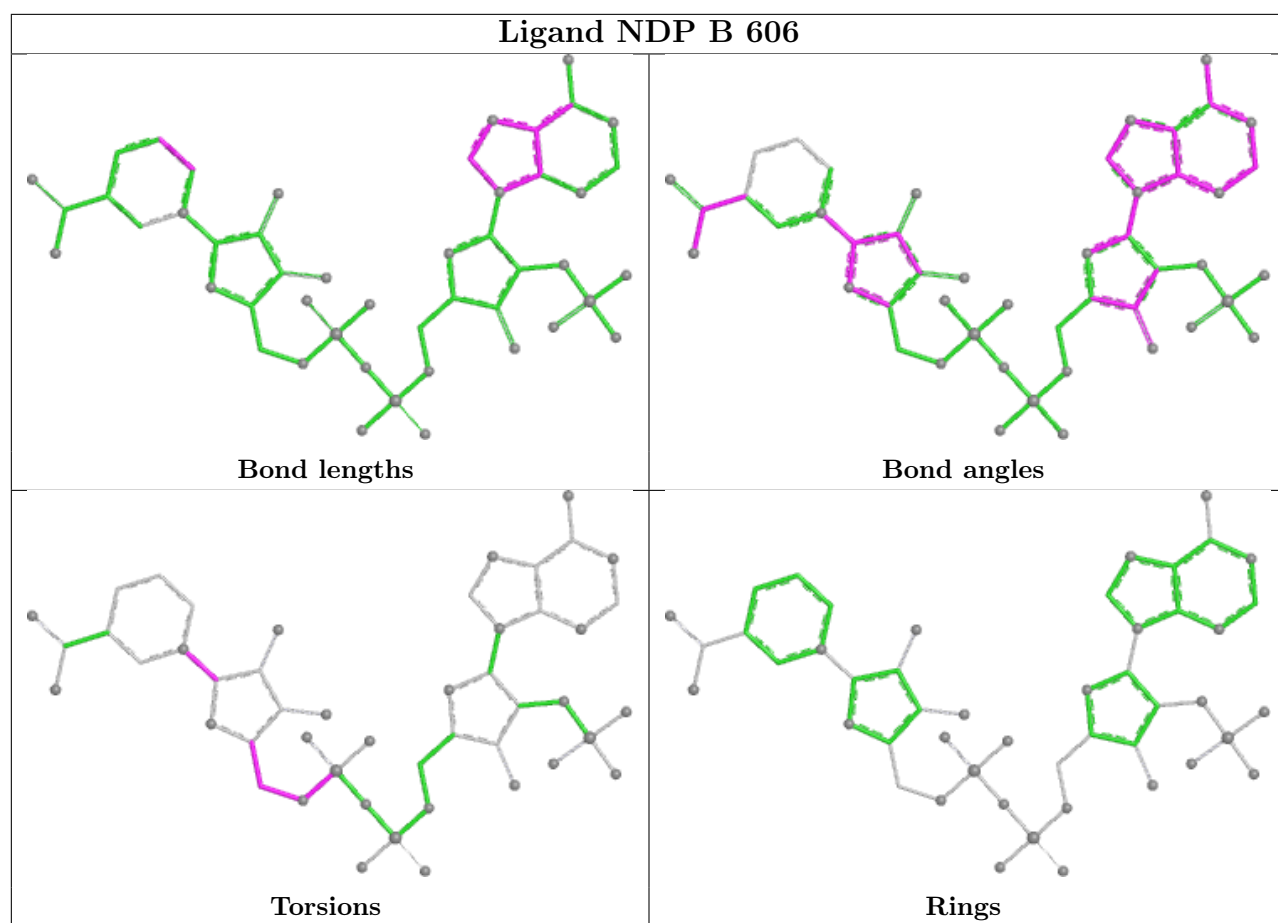
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	602	HEM	4	0
13	B	607	FDA	2	0
9	B	601	HEM	2	0

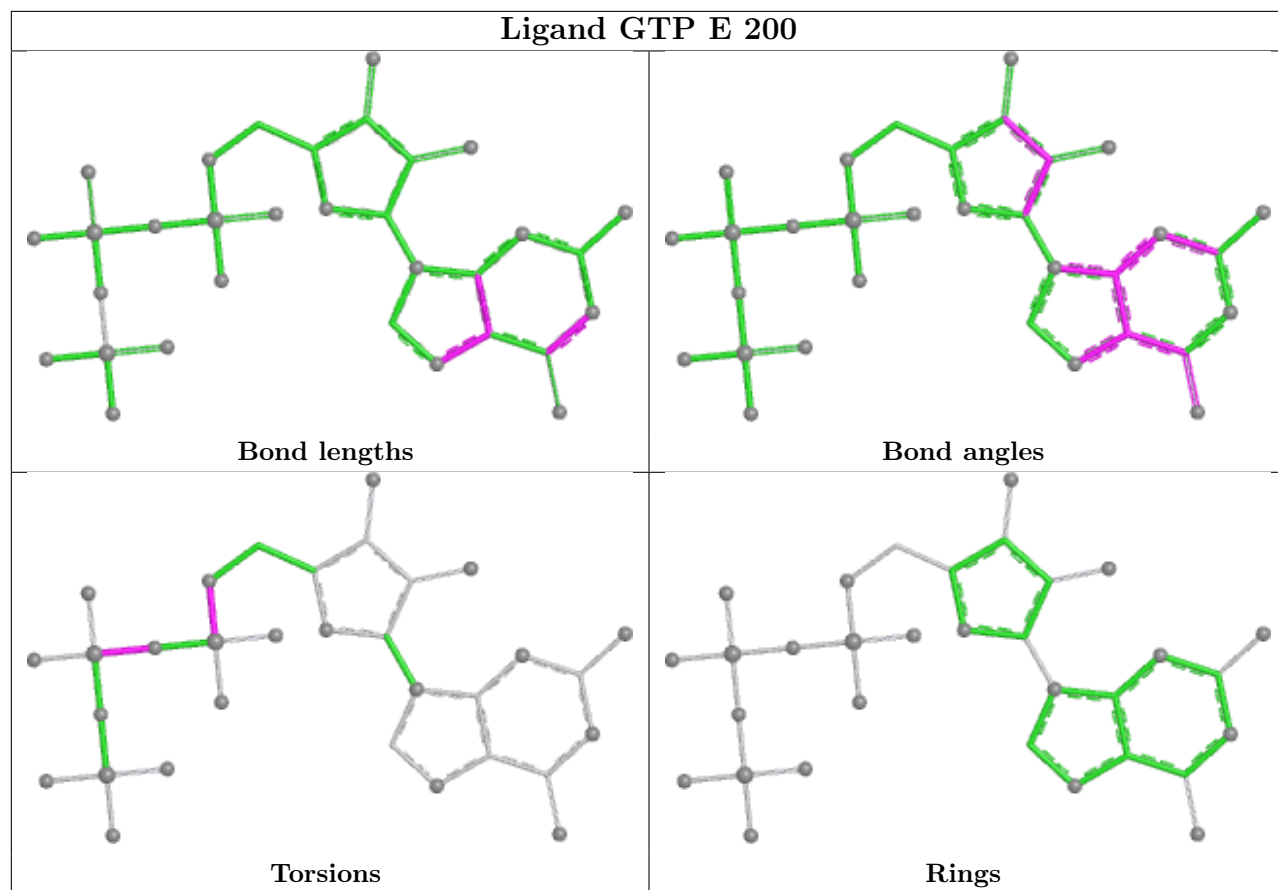
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

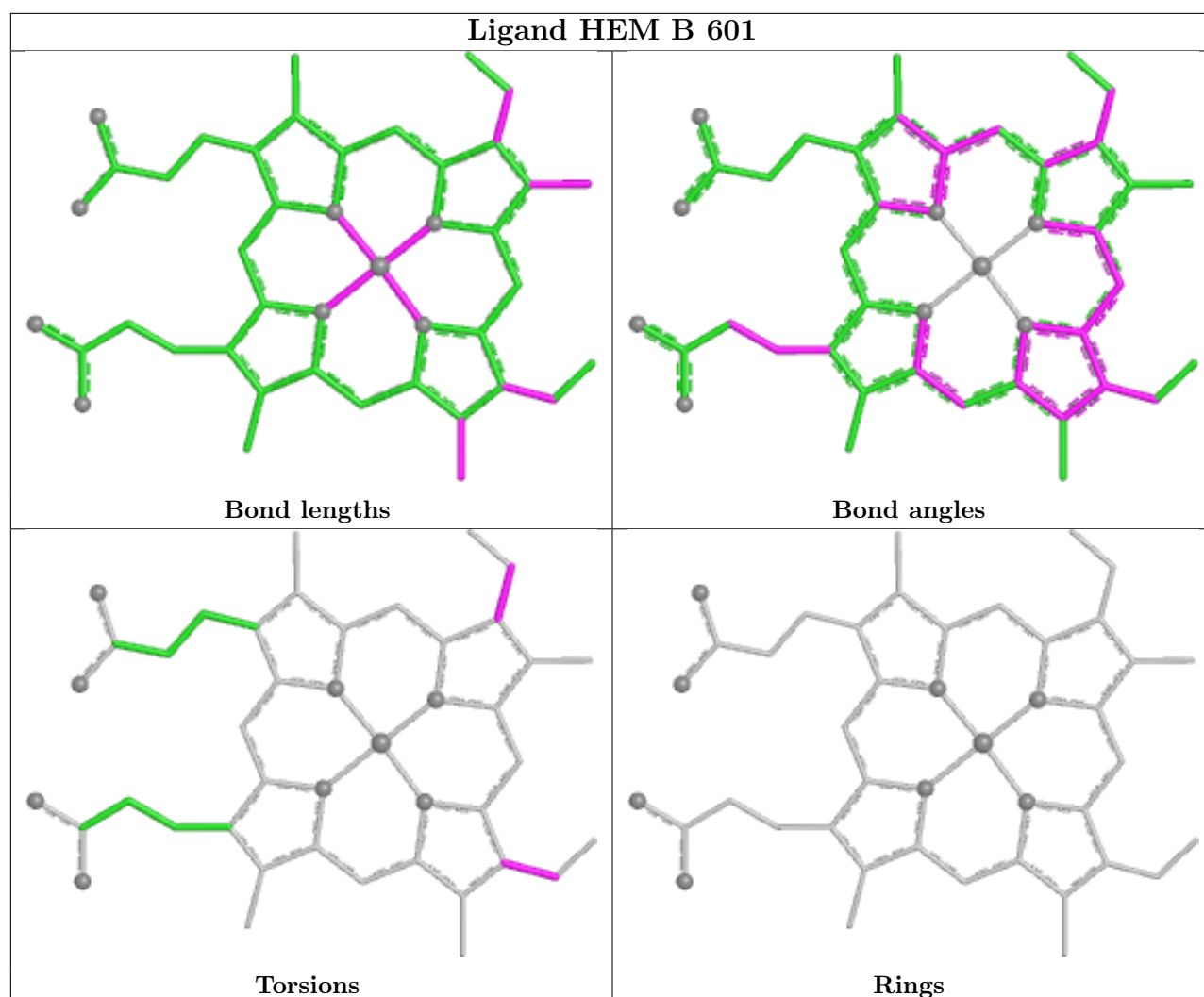
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

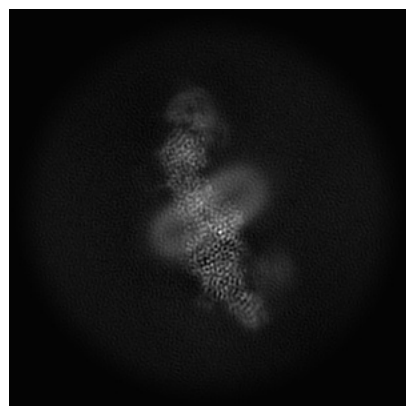
6 Map visualisation [i](#)

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.

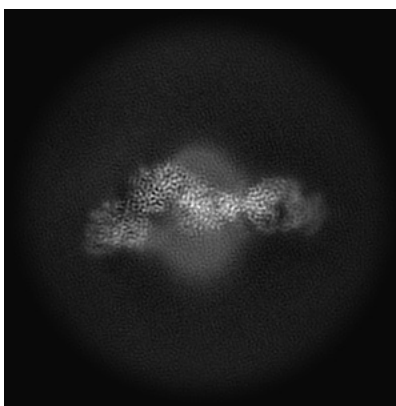
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

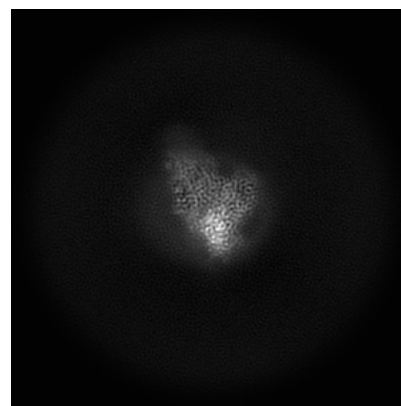
6.1.1 Primary map



X

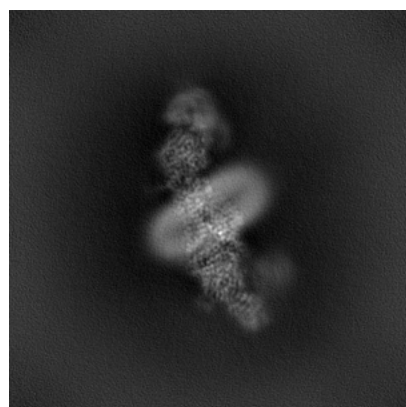


Y

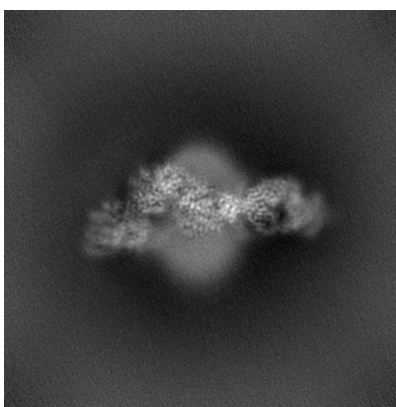


Z

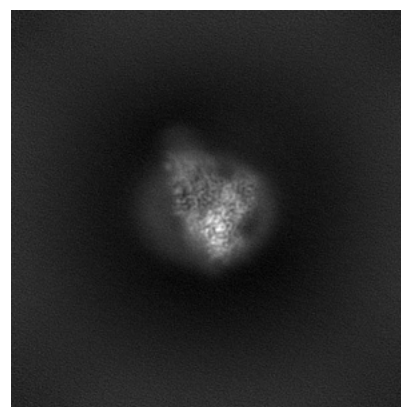
6.1.2 Raw map



X



Y

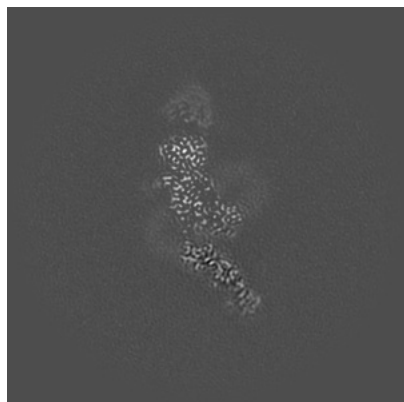


Z

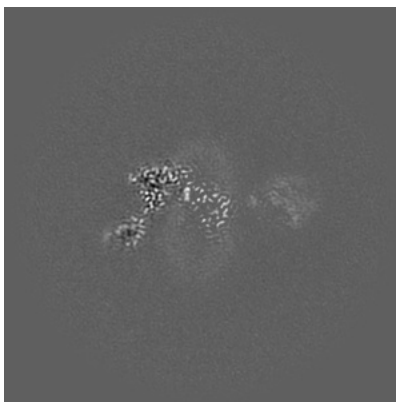
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

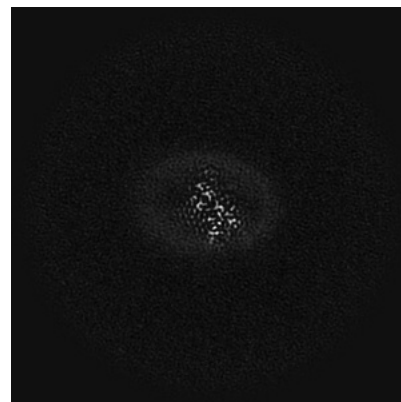
6.2.1 Primary map



X Index: 160

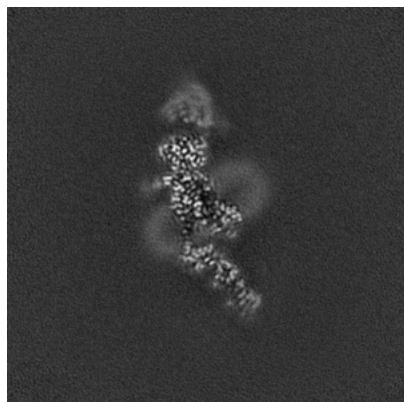


Y Index: 160

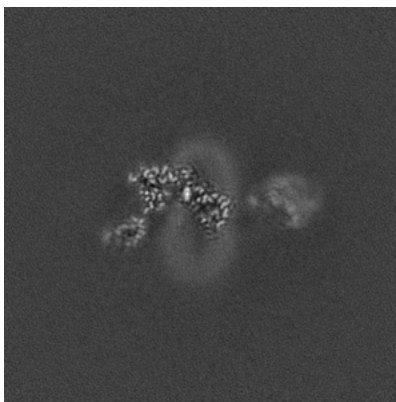


Z Index: 160

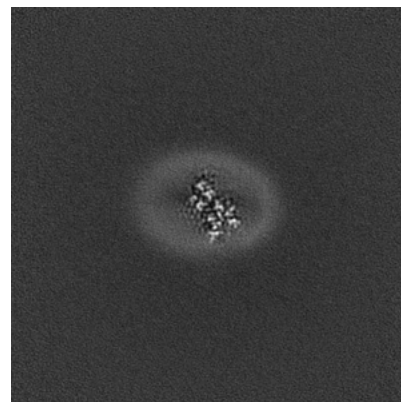
6.2.2 Raw map



X Index: 160



Y Index: 160

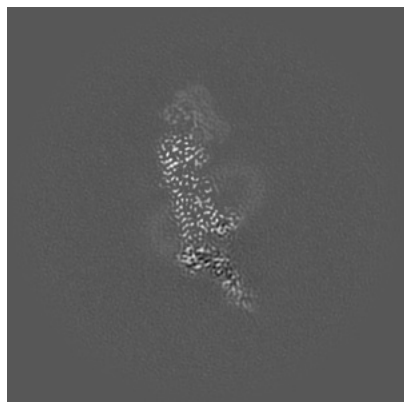


Z Index: 160

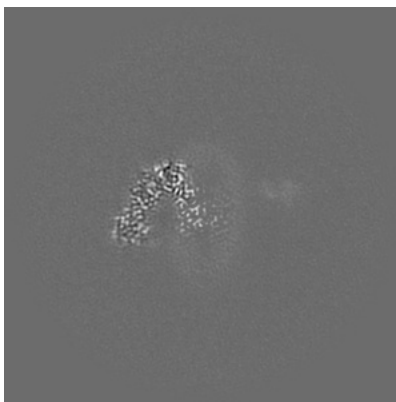
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

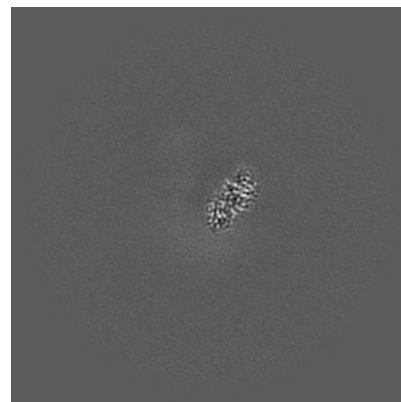
6.3.1 Primary map



X Index: 165

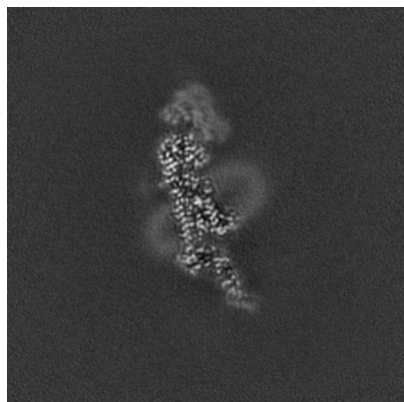


Y Index: 169

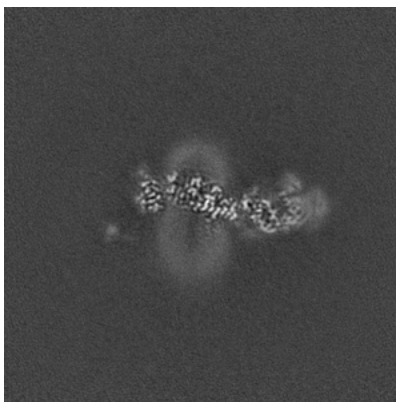


Z Index: 125

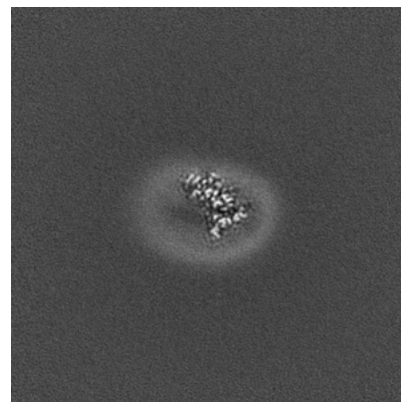
6.3.2 Raw map



X Index: 165



Y Index: 150

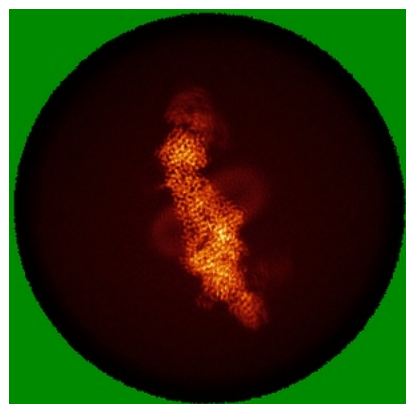


Z Index: 151

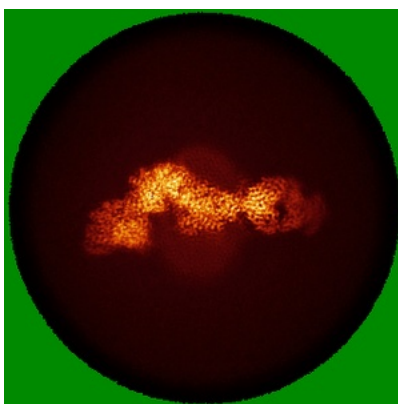
The images above show the largest variance slices of the map in three orthogonal directions.

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

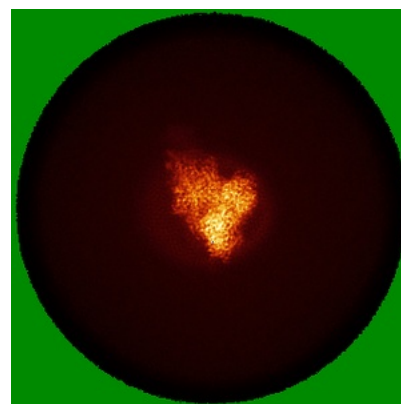
6.4.1 Primary map



X

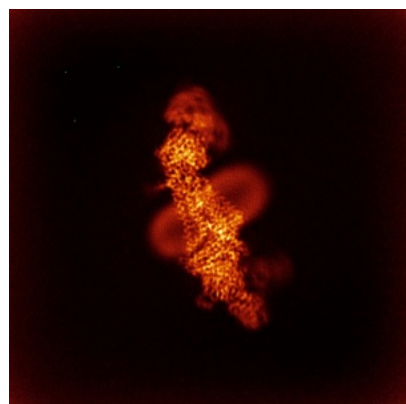


Y

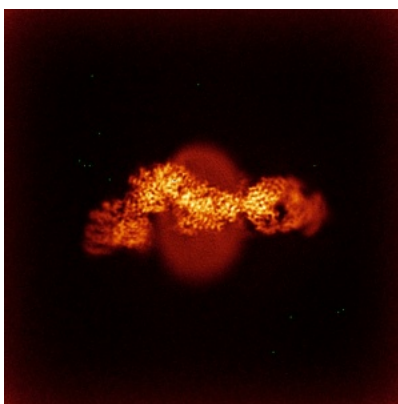


Z

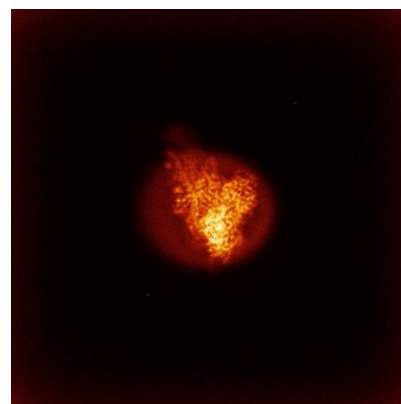
6.4.2 Raw map



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.

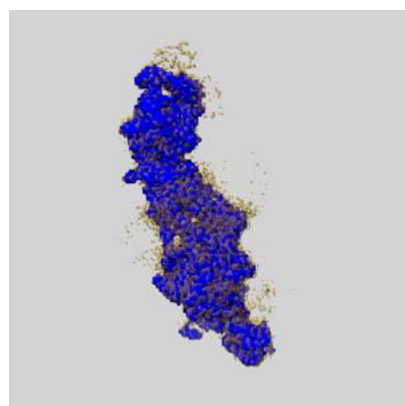
6.6 Mask visualisation [i](#)

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

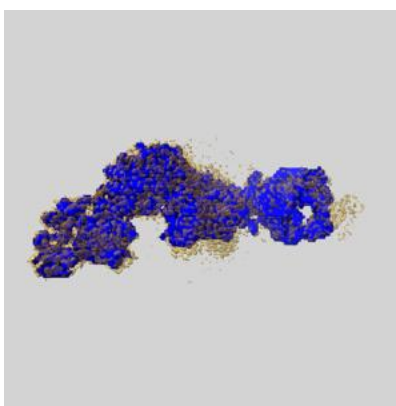
A mask typically either:

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

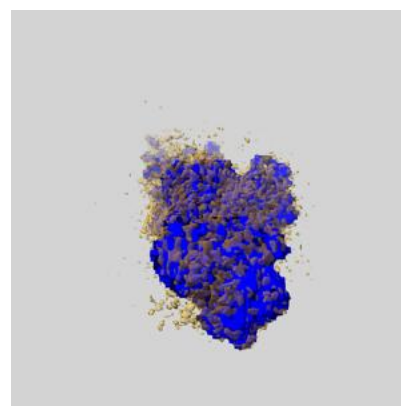
6.6.1 emd_37477_msk_1.map [i](#)



X



Y

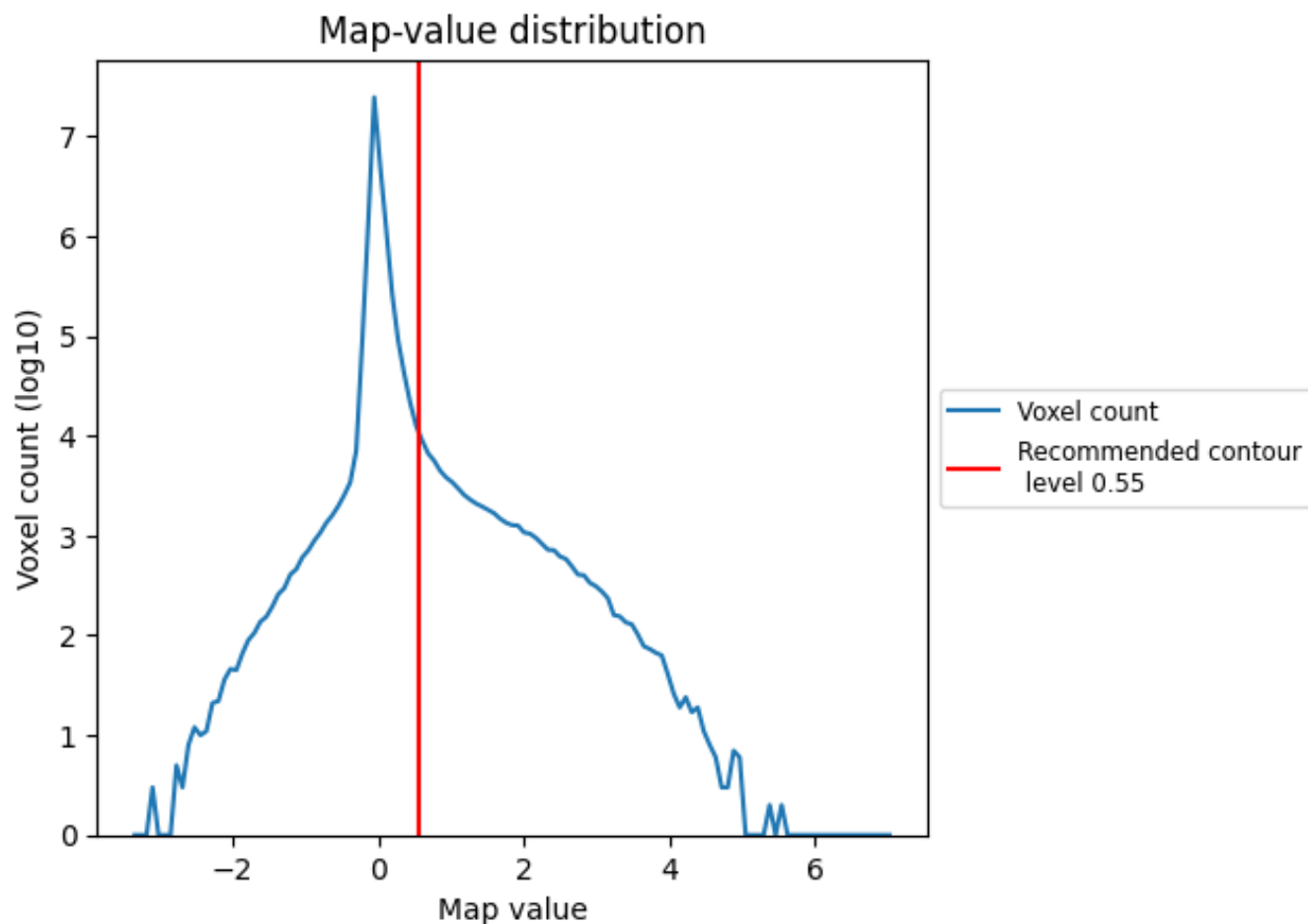


Z

7 Map analysis [i](#)

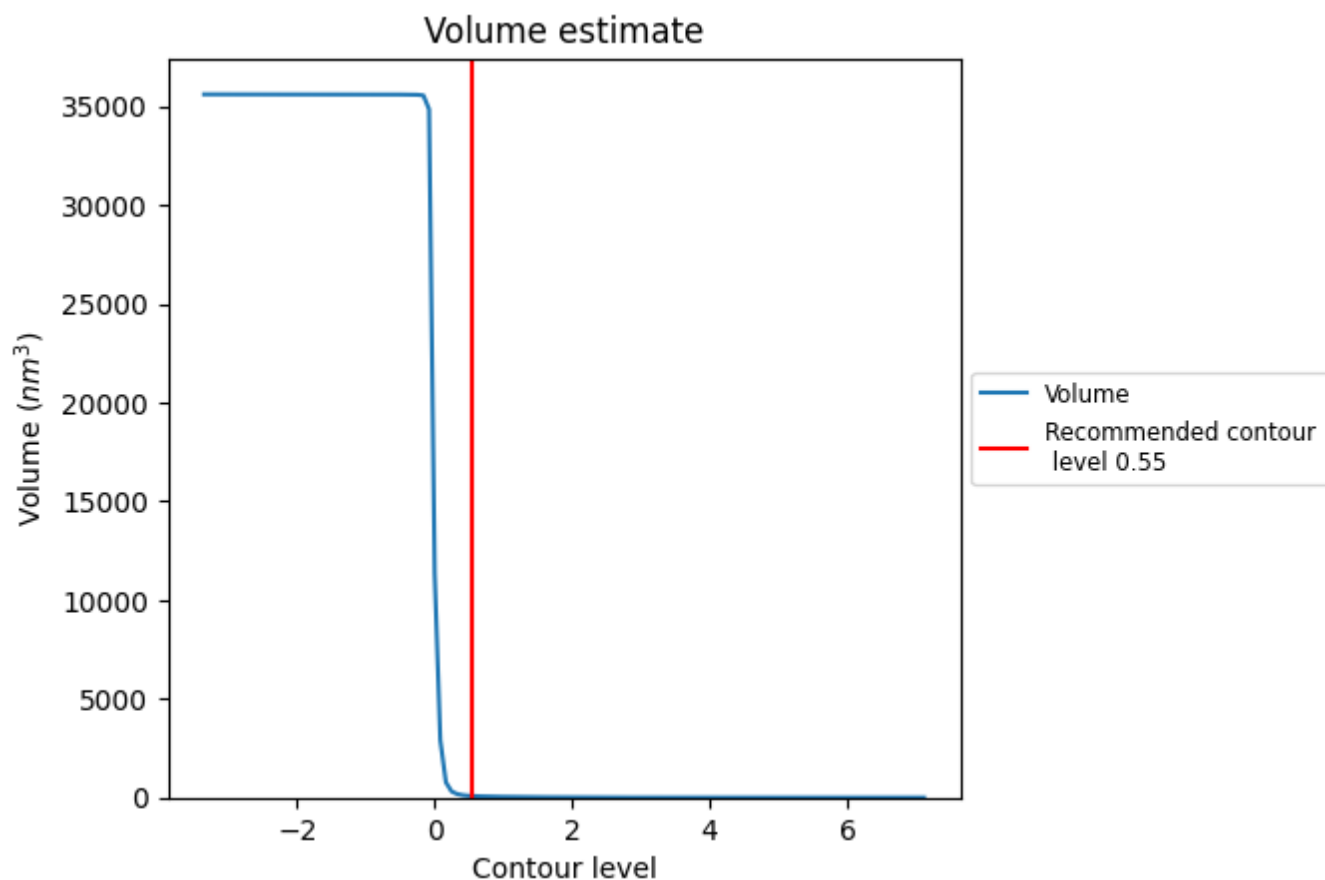
This section contains the results of statistical analysis of the map.

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.

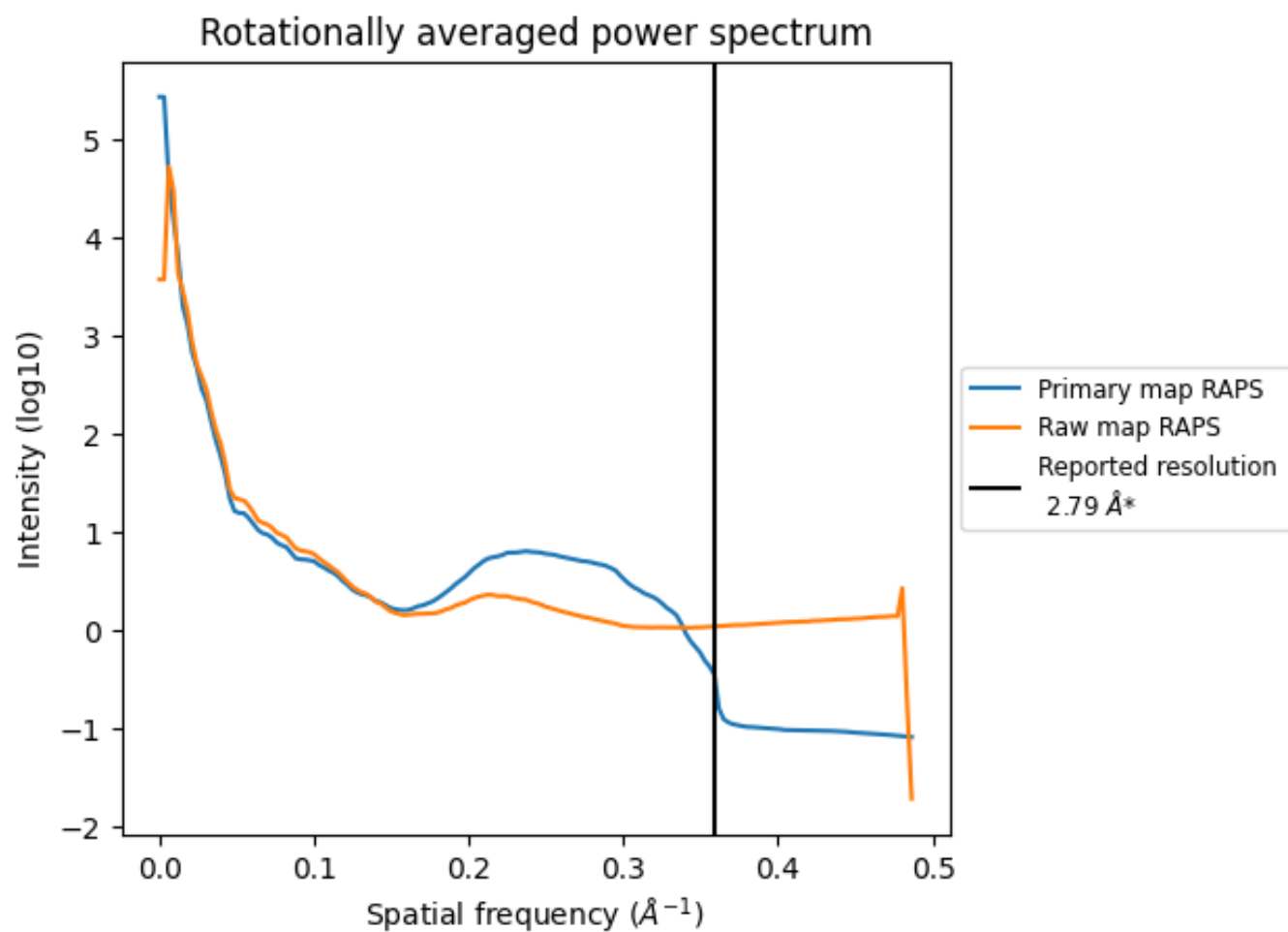
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; 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 ⓘ

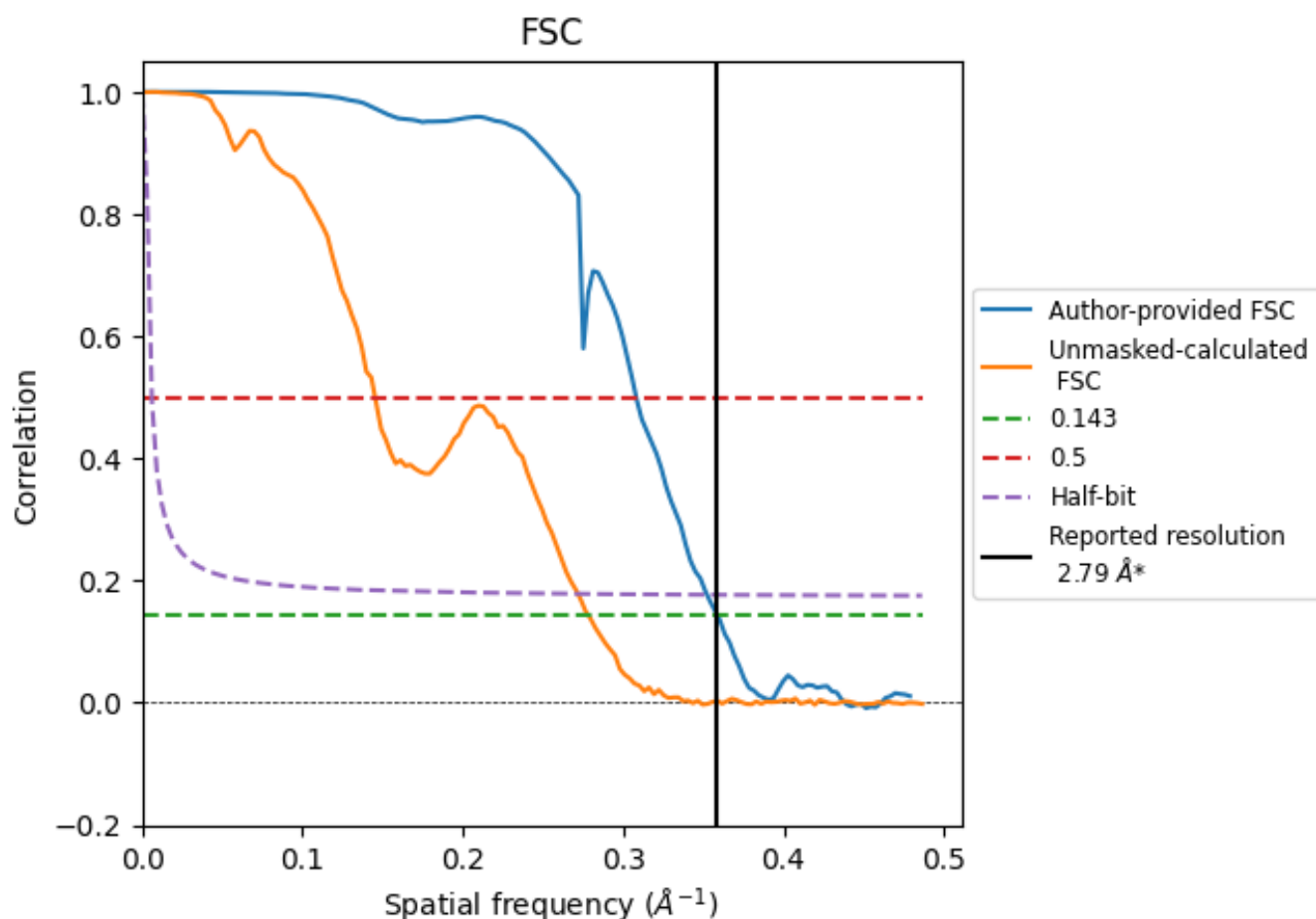


*Reported resolution corresponds to spatial frequency of $0.358 \text{ \AA}^{-1}$

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 0.358 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

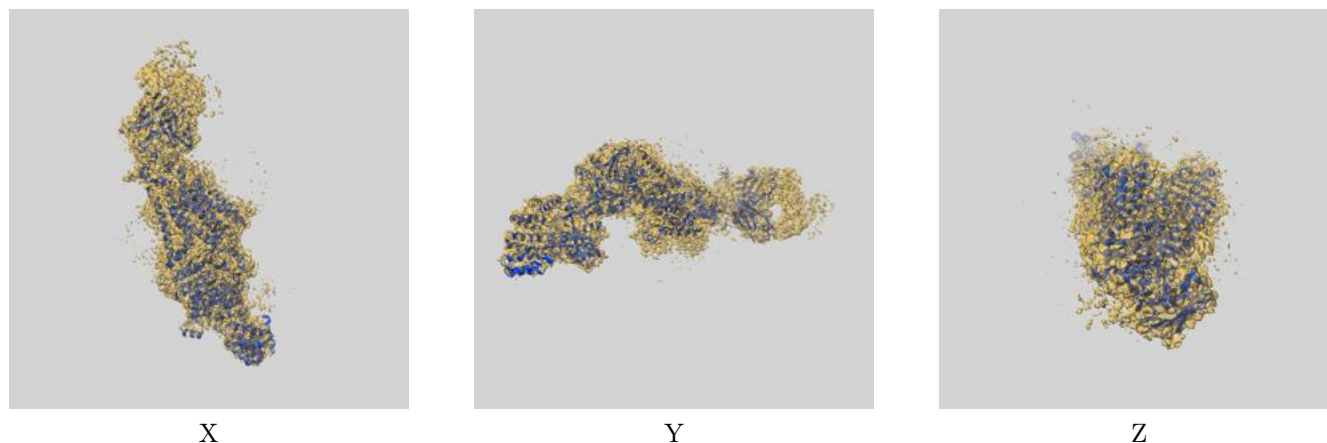
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.25	2.84
Unmasked-calculated*	3.59	6.89	3.68

*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](#)

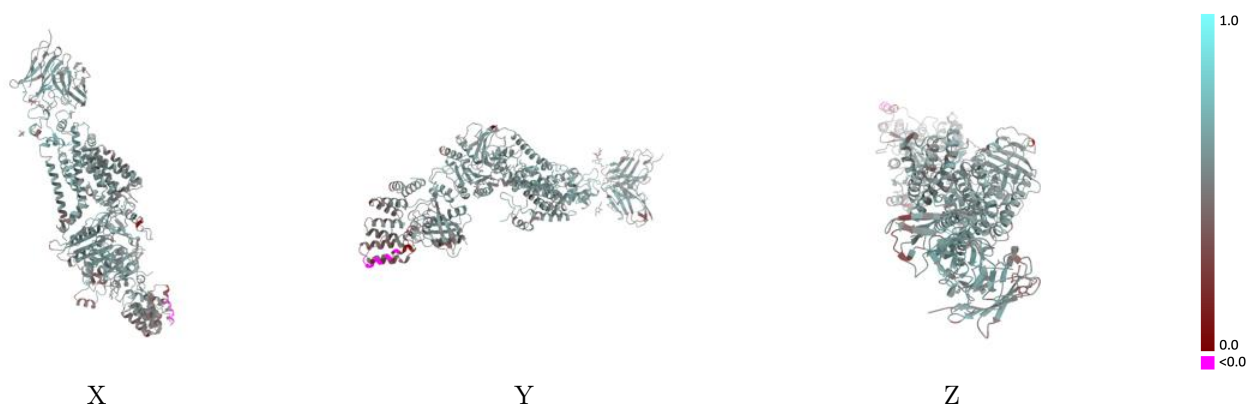
This section contains information regarding the fit between EMDB map EMD-37477 and PDB model 8WEJ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



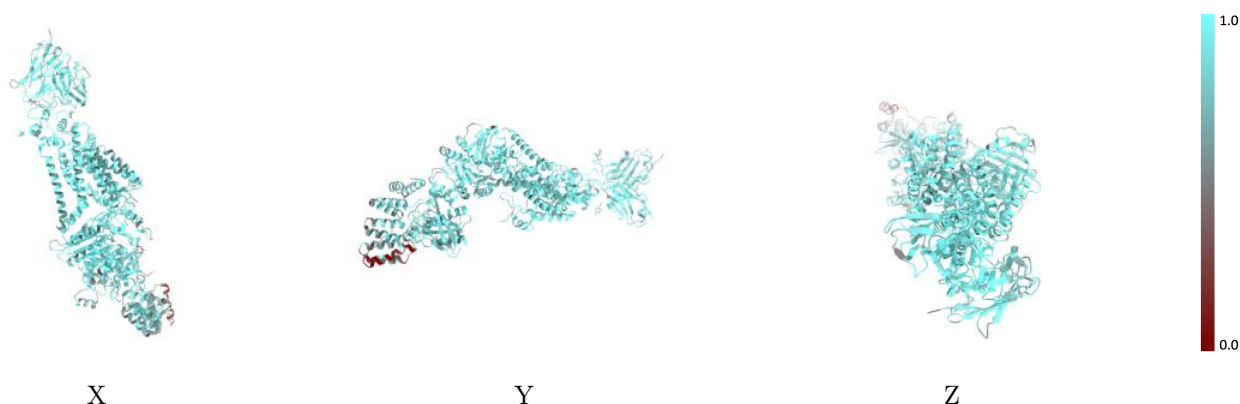
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



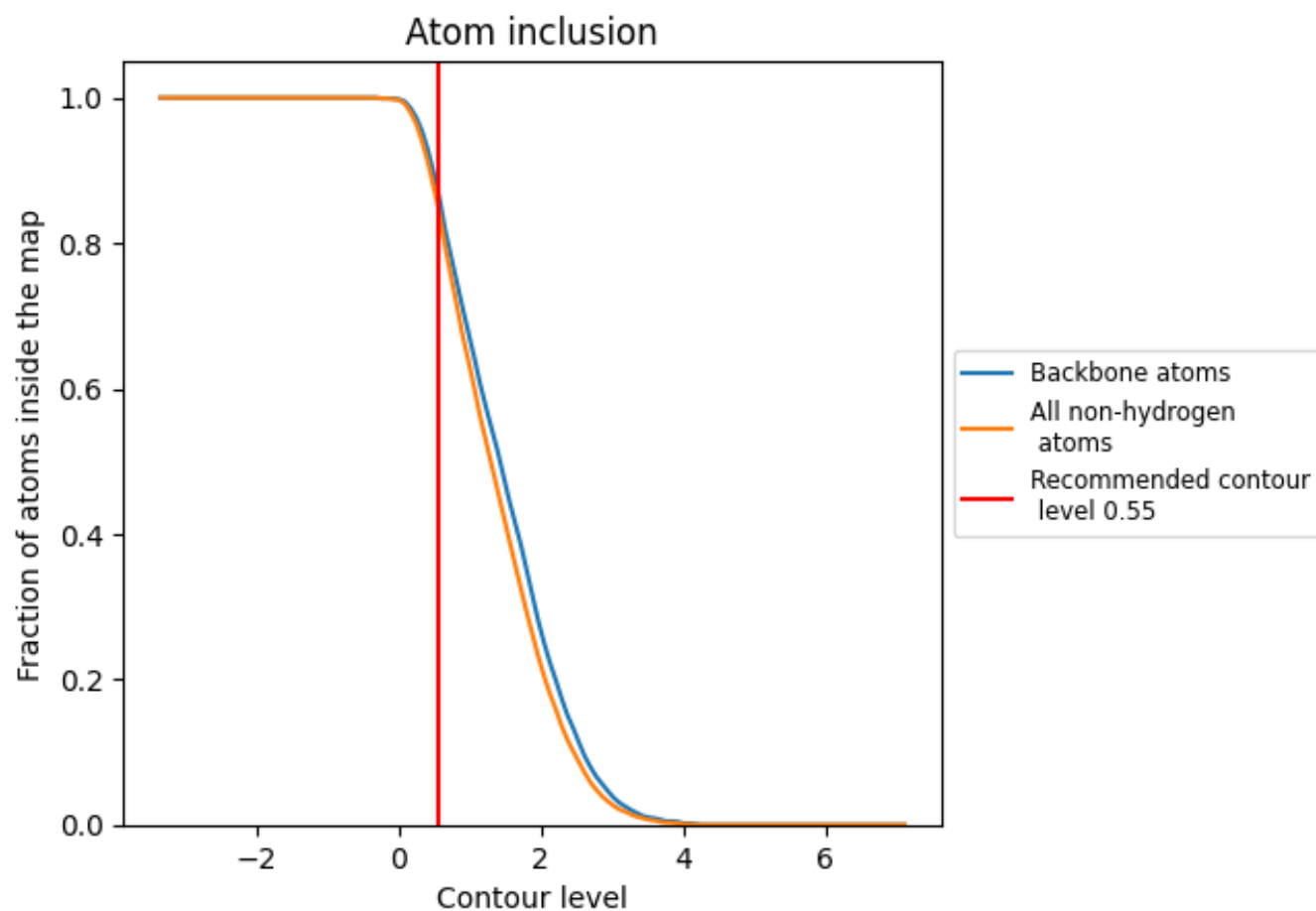
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

1.0

0.0

<0.0