



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:12 PM UTC

PDB ID : 8D48 / pdb_00008d48
EMDB ID : EMD-27177
Title : sd1.040 Fab in complex with SARS-CoV-2 Spike 2P glycoprotein
Authors : Abernathy, M.E.; Barnes, C.O.
Deposited on : 2022-06-01
Resolution : 3.70 Å (reported)
Based on initial models : 6VXX, 7D0D, 5AZE

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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

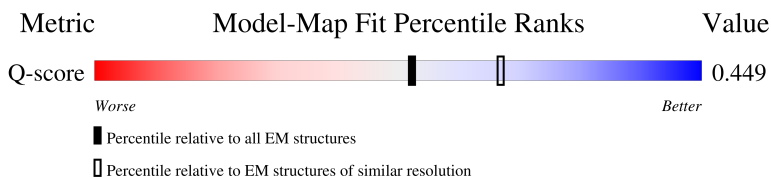
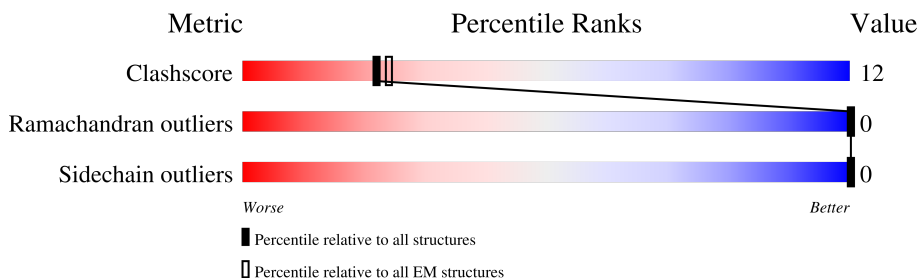
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1259	6% 17% 5% 78%
2	H	233	10% 71% 24%
3	L	220	11% 78% 22%
4	B	2	50% 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5545 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	2	0
			2143	1366	359	408	10		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called sd1.040 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	223	Total	C	N	O	S	0	0
			1663	1044	279	333	7		

- Molecule 3 is a protein called sd1.040 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	220	Total	C	N	O	S	1	0
			1711	1072	286	346	7		

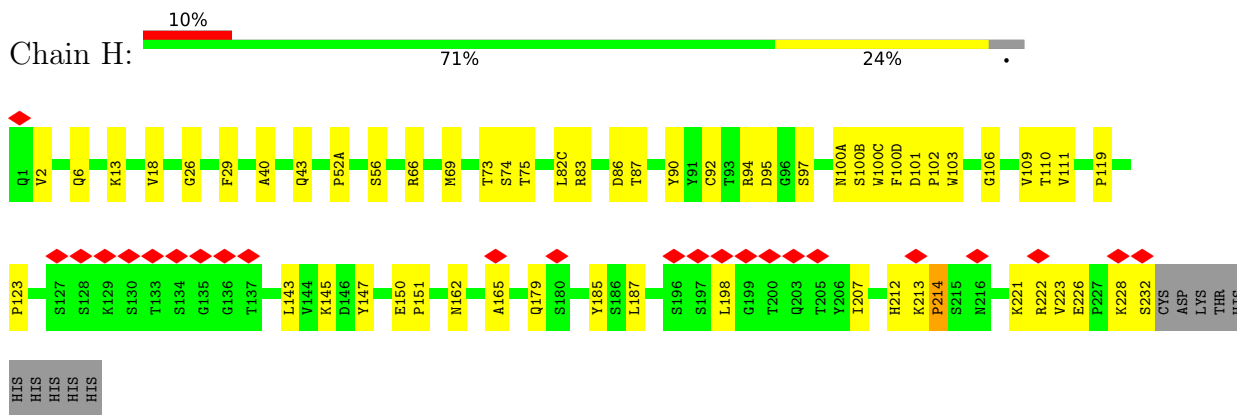
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



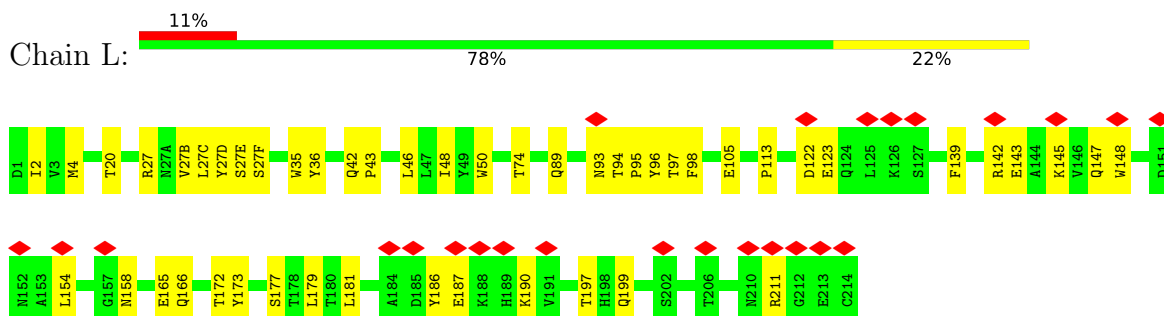
Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

HIS HIS	Tyr	Ala	Ile	Pro	Arg	Ile	Ala	Phe	Gly
	Asp	Pro	Asp	Leu	Arg	Leu	Leu	Asn	Asp
HIS HIS	Leu	Ala	Leu	Ala	Ala	Ala	Leu	Met	Cys
	Gln	Ile	Gln	Ile	Ser	Ser	Thr	Met	Leu
HIS HIS	Leu	His	Leu	Cys	Ala	Ala	Val	Ala	Gly
	Pro	His	Pro	His	Asn	Asn	Lys	Thr	Asp
HIS HIS	Glu	Asp	Glu	Asp	Leu	Leu	Lys	Thr	Ile
	Leu	Gly	Leu	Gly	Ala	Ala	Gln	Arg	Ala
HIS HIS	Asp	Lys	Asp	Lys	Thr	Thr	Ser	Phe	Arg
	Ser	Ala	Ser	Ala	Thr	Thr	Ser	Asn	Ala
HIS HIS	Gln	His	Gln	His	Met	Met	Asn	Gly	Asp
	Tyr	Phe	Tyr	Phe	Ser	Ser	Asn	Ile	Leu
HIS HIS	Glu	Pro	Glu	Pro	Ser	Ser	Phe	Gly	Ile
	Leu	Arg	Leu	Arg	Glu	Glu	Gly	Val	Cys
HIS HIS	Trp	Leu	Trp	Leu	Val	Val	Ala	Thr	Gln
	Pro	Gly	Pro	Gly	Val	Val	Ile	Gln	Lys
HIS HIS	Ser	Val	Ser	Val	Gly	Gly	Ser	Leu	Leu
	Gly	Phe	Gly	Phe	Gly	Gly	Ser	Val	Phe
HIS HIS	Arg	Lys	Arg	Lys	Gln	Gln	Val	Leu	Gly
	Leu	Ser	Leu	Ser	Ser	Ser	Val	Leu	Asn
HIS HIS	Val	Asn	Val	Asn	Lys	Lys	Asn	Glu	Gly
	Pro	His	Pro	His	Arg	Arg	Asp	Glu	Thr
HIS HIS	Thr	Thr	Thr	Thr	Val	Val	Ile	Gln	Val
	Ser	His	Ser	His	Asp	Asp	Leu	Lys	Leu
HIS HIS	Pro	Trp	Pro	Trp	Phe	Phe	Ser	Leu	Pro
	Asp	Phe	Asp	Phe	Cys	Cys	Arg	Leu	Pro
HIS HIS	Val	Val	Val	Val	Gly	Gly	Leu	Ile	Leu
	Gly	Thr	Gly	Thr	Lys	Lys	Asp	Gln	Leu
HIS HIS	Tyr	Gln	Tyr	Gln	Gly	Gly	Pro	Gln	Thr
	Leu	Arg	Leu	Arg	Tyr	Tyr	Pro	Phe	Asp
HIS HIS	Ile	Asn	Ile	Asn	His	His	Glu	Asn	Glu
	Asp	Ala	Asp	Ala	Ile	Ile	Ala	Ser	Met
HIS HIS	Gly	Ser	Gly	Ser	Met	Met	Glu	Ala	Ile
	Ala	Glu	Ala	Glu	Phe	Phe	Val	Ile	Ala
HIS HIS	Pro	Pro	Pro	Pro	Pro	Pro	Gln	Gly	Gln
	Arg	Gln	Arg	Gln	Pro	Pro	Ile	Lys	Tyr
HIS HIS	Asp	Ile	Asp	Ile	Gln	Gln	Asp	Ile	Thr
	Ala	Ala	Ala	Ala	Ala	Ala	Leu	Gln	Ser
HIS HIS	Gln	Val	Gln	Val	Ala	Ala	Ile	Ser	Leu
	Val	Thr	Val	Thr	Pro	Pro	Thr	Leu	Leu
HIS HIS	Tyr	Asn	Tyr	Asn	His	His	Thr	Gly	Ala
	Val	Asn	Val	Asn	Gly	Gly	Gly	Ser	Ala
HIS HIS	Arg	Gln	Arg	Gln	Val	Val	Arg	Ser	Ala
	Gln	Thr	Gln	Thr	Val	Val	Arg	Ser	Ala
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	Glu	Val	Glu	Val	Ala	Ala	Gln	Thr	Ile
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HIS HIS	His	Val	His	Val	Thr	Thr	Gln	Val	Ala
	His	Val	His	Val	Thr	Thr	Gln	Val	Ala
HIS HIS	His	Val	His						

- Molecule 2: sd1.040 Fab heavy chain



- Molecule 3: sd1.040 Fab light chain



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	277530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.501	Depositor
Minimum map value	-1.088	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.187	Depositor
Map size (Å)	368.1072, 368.1072, 368.1072	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8521, 0.8521, 0.8521	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.14	0/2201	0.44	3/2996 (0.1%)
2	H	0.24	0/1705	0.54	1/2325 (0.0%)
3	L	0.29	0/1752	0.47	0/2382
All	All	0.23	0/5658	0.48	4/7703 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	214	PRO	CA-N-CD	-11.13	96.41	112.00
1	A	350	VAL	N-CA-C	7.89	117.99	110.42
1	A	379	CYS	CA-CB-SG	6.20	128.65	114.40
1	A	352	ALA	N-CA-CB	6.17	120.29	111.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2054	54	0
2	H	1663	0	1618	38	0
3	L	1711	0	1648	34	0
4	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5545	0	5345	125	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 12.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:222:ARG:NH2	2:H:226:GLU:OE2	1.57	1.35
1:A:351:TYR:HE2	1:A:452:LEU:CD1	1.49	1.24
1:A:351:TYR:CE2	1:A:452:LEU:HD11	1.84	1.13
1:A:351:TYR:CE2	1:A:452:LEU:CD1	2.38	1.05
1:A:351:TYR:HE2	1:A:452:LEU:HD12	1.33	0.91
1:A:490:PHE:HE1	1:A:493:GLN:HB3	1.34	0.90
1:A:379:CYS:HB2	1:A:432:CYS:HA	1.62	0.81
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.61	0.81
1:A:490:PHE:HD1	1:A:492:LEU:O	1.64	0.80
1:A:490:PHE:CD1	1:A:492:LEU:O	2.36	0.78
1:A:351:TYR:CZ	1:A:452:LEU:HD11	2.20	0.76
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.66	0.76
3:L:94:THR:N	3:L:95:PRO:HD2	2.04	0.73
1:A:379:CYS:CB	1:A:432:CYS:HA	2.18	0.73
1:A:568:ASP:OD1	1:A:569:ILE:N	2.22	0.72
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.72	0.71
2:H:90:TYR:O	2:H:106:GLY:HA2	1.91	0.71
2:H:123:PRO:HB3	2:H:223:VAL:HG12	1.74	0.70
2:H:100(D):PHE:O	2:H:103:TRP:NE1	2.27	0.67
2:H:87:THR:HG22	2:H:111:VAL:H	1.61	0.66
1:A:351:TYR:CE2	1:A:452:LEU:HD12	2.24	0.64
3:L:143:GLU:N	3:L:143:GLU:OE2	2.31	0.64
3:L:199:GLN:OE1	3:L:199:GLN:N	2.30	0.62
2:H:86:ASP:OD1	2:H:90:TYR:OH	2.18	0.61
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.83	0.60
1:A:351:TYR:OH	1:A:452:LEU:HD11	2.01	0.60
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.81	0.60
3:L:181:LEU:HD11	3:L:186:TYR:HD1	1.67	0.59
2:H:207:ILE:HG12	2:H:222:ARG:HB3	1.85	0.58
3:L:93:ASN:HB3	3:L:95:PRO:HD2	1.85	0.58
2:H:207:ILE:HG23	2:H:221:LYS:O	2.03	0.58
3:L:145:LYS:HB3	3:L:197:THR:HB	1.86	0.57
1:A:437:ASN:HD21	1:A:439:ASN:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HG3	1:A:419:ALA:HB2	1.87	0.57
3:L:148:TRP:NE1	3:L:177:SER:OG	2.35	0.57
1:A:472:ILE:HG21	1:A:482:GLY:HA2	1.87	0.56
1:A:490:PHE:CE1	1:A:493:GLN:HB3	2.26	0.56
3:L:94:THR:O	3:L:96:TYR:HD1	1.88	0.56
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.89	0.55
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.72	0.55
1:A:379:CYS:HB2	1:A:431:GLY:O	2.07	0.55
1:A:345:THR:OG1	1:A:346:ARG:NH1	2.39	0.55
3:L:147:GLN:HE21	3:L:154:LEU:HD13	1.72	0.55
1:A:383:SER:OG	1:A:385:THR:O	2.25	0.54
3:L:89:GLN:HB2	3:L:98:PHE:CD1	2.43	0.54
1:A:393:THR:O	1:A:523:THR:OG1	2.27	0.53
2:H:6:GLN:NE2	2:H:92:CYS:SG	2.82	0.53
1:A:458:LYS:HB3	1:A:473:TYR:CE2	2.43	0.52
2:H:73:THR:HG22	2:H:74:SER:H	1.76	0.51
1:A:452:LEU:HD12	1:A:452:LEU:C	2.35	0.51
3:L:27(E):SER:O	3:L:27(F):SER:HB3	2.11	0.51
1:A:444:LYS:HB2	1:A:448:ASN:HB2	1.93	0.51
1:A:498:GLN:OE1	1:A:499:PRO:HD2	2.11	0.51
2:H:97:SER:O	2:H:97:SER:OG	2.26	0.50
2:H:101:ASP:HB2	2:H:102:PRO:HD3	1.92	0.50
1:A:435:ALA:HA	1:A:509:ARG:O	2.12	0.50
1:A:436:TRP:CH2	1:A:509:ARG:HG2	2.47	0.50
3:L:93:ASN:C	3:L:95:PRO:HD2	2.36	0.50
1:A:458:LYS:HB3	1:A:473:TYR:HE2	1.76	0.49
3:L:27(C):LEU:HG	3:L:27(D):TYR:N	2.25	0.49
2:H:213:LYS:HB3	2:H:214:PRO:HD2	1.94	0.49
3:L:94:THR:N	3:L:95:PRO:CD	2.75	0.49
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.94	0.49
1:A:462:LYS:N	1:A:465:GLU:OE1	2.45	0.49
1:A:386:LYS:HG2	1:A:386:LYS:O	2.13	0.49
2:H:100(C):TRP:O	2:H:101:ASP:N	2.45	0.49
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.45	0.49
2:H:66:ARG:NH1	2:H:83:ARG:HH21	2.10	0.48
2:H:73:THR:O	2:H:75:THR:N	2.45	0.48
2:H:2:VAL:H	2:H:26:GLY:HA3	1.78	0.48
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.95	0.48
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.49	0.48
2:H:143:LEU:HD12	2:H:187:LEU:O	2.14	0.48
1:A:409:GLN:HE21	1:A:419:ALA:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:ASN:HB3	2:H:165:ALA:HB3	1.96	0.48
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.79	0.47
3:L:172:THR:OG1	3:L:173:TYR:N	2.48	0.47
1:A:490:PHE:CD1	1:A:490:PHE:O	2.68	0.47
2:H:87:THR:HG22	2:H:110:THR:HA	1.97	0.47
1:A:439:ASN:OD1	1:A:443:SER:OG	2.33	0.47
3:L:165:GLU:HG3	3:L:166:GLN:N	2.29	0.47
1:A:498:GLN:HB3	1:A:501:ASN:OD1	2.14	0.46
3:L:122:ASP:OD2	3:L:123:GLU:N	2.48	0.46
1:A:428:ASP:OD1	1:A:428:ASP:N	2.45	0.46
1:A:329:PHE:O	1:A:580:GLN:NE2	2.49	0.45
2:H:13:LYS:HB2	2:H:13:LYS:HE2	1.78	0.45
3:L:187:GLU:HA	3:L:211:ARG:HH12	1.81	0.45
3:L:190:LYS:NZ	3:L:190:LYS:O	2.49	0.45
2:H:221:LYS:HG3	2:H:222:ARG:H	1.82	0.45
3:L:42:GLN:HG3	3:L:43:PRO:HD2	1.98	0.45
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.99	0.45
2:H:145:LYS:NZ	2:H:179:GLN:OE1	2.43	0.45
2:H:228:LYS:O	2:H:232:SER:C	2.60	0.45
3:L:4:MET:HE3	3:L:4:MET:HB3	1.86	0.45
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.51	0.44
2:H:87:THR:HA	2:H:109:VAL:O	2.16	0.44
1:A:328:ARG:HA	1:A:530:SER:HB3	2.00	0.44
2:H:100(A):ASN:OD1	2:H:100(B):SER:N	2.52	0.43
2:H:151:PRO:O	2:H:212:HIS:HD2	2.02	0.43
1:A:521:PRO:HG3	2:H:56:SER:HB2	2.00	0.43
3:L:20:THR:HG22	3:L:74:THR:HG22	2.00	0.43
1:A:345:THR:OG1	1:A:346:ARG:HG3	2.19	0.43
3:L:158:ASN:OD1	3:L:158:ASN:N	2.51	0.43
3:L:93:ASN:CB	3:L:95:PRO:HD2	2.48	0.43
3:L:105:GLU:OE2	3:L:142:ARG:NH1	2.41	0.42
2:H:69:MET:HE3	2:H:69:MET:HB2	1.82	0.42
1:A:346:ARG:C	1:A:347:PHE:HD1	2.28	0.41
2:H:29:PHE:O	2:H:52(A):PRO:HG2	2.20	0.41
1:A:401:VAL:HG23	1:A:509:ARG:NH2	2.35	0.41
2:H:66:ARG:CZ	2:H:83:ARG:HH21	2.33	0.41
3:L:50:TRP:HA	3:L:50:TRP:CE3	2.55	0.41
2:H:94:ARG:HG2	2:H:102:PRO:HG2	2.02	0.41
3:L:27(B):VAL:O	3:L:27(B):VAL:HG12	2.19	0.41
3:L:179:LEU:HD21	3:L:181:LEU:HD23	2.03	0.41
3:L:2:ILE:O	3:L:97:THR:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:O	1:A:421:TYR:HB2	2.20	0.41
2:H:198:LEU:HD12	2:H:198:LEU:HA	1.94	0.41
2:H:95:ASP:OD1	2:H:95:ASP:C	2.64	0.41
2:H:150:GLU:HB3	2:H:185:TYR:CD2	2.56	0.41
3:L:36:TYR:CD1	3:L:46:LEU:HA	2.55	0.41
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.55	0.40
1:A:405:ASP:OD1	1:A:405:ASP:N	2.55	0.40
3:L:27:ARG:O	3:L:27(B):VAL:HG23	2.20	0.40
2:H:18:VAL:HG23	2:H:82(C):LEU:HD11	2.03	0.40
3:L:145:LYS:HD2	3:L:145:LYS:HA	1.84	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	271/1259 (22%)	261 (96%)	10 (4%)	0	100	100
2	H	221/233 (95%)	196 (89%)	25 (11%)	0	100	100
3	L	219/220 (100%)	203 (93%)	16 (7%)	0	100	100
All	All	711/1712 (42%)	660 (93%)	51 (7%)	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	239/1096 (22%)	239 (100%)	0	100	100
2	H	190/200 (95%)	190 (100%)	0	100	100
3	L	194/194 (100%)	194 (100%)	0	100	100
All	All	623/1490 (42%)	623 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	409	GLN
1	A	437	ASN
1	A	519	HIS
2	H	39	GLN
2	H	212	HIS
3	L	38	GLN
3	L	147	GLN

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](#)

2 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
4	NAG	B	1	4,1	14,14,15	0.50	0	17,19,21	0.68	0
4	NAG	B	2	4	14,14,15	0.83	1 (7%)	17,19,21	1.43	1 (5%)

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
4	NAG	B	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	NAG	O5-C1	2.97	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C1-O5-C5	5.57	119.65	112.19

There are no chirality outliers.

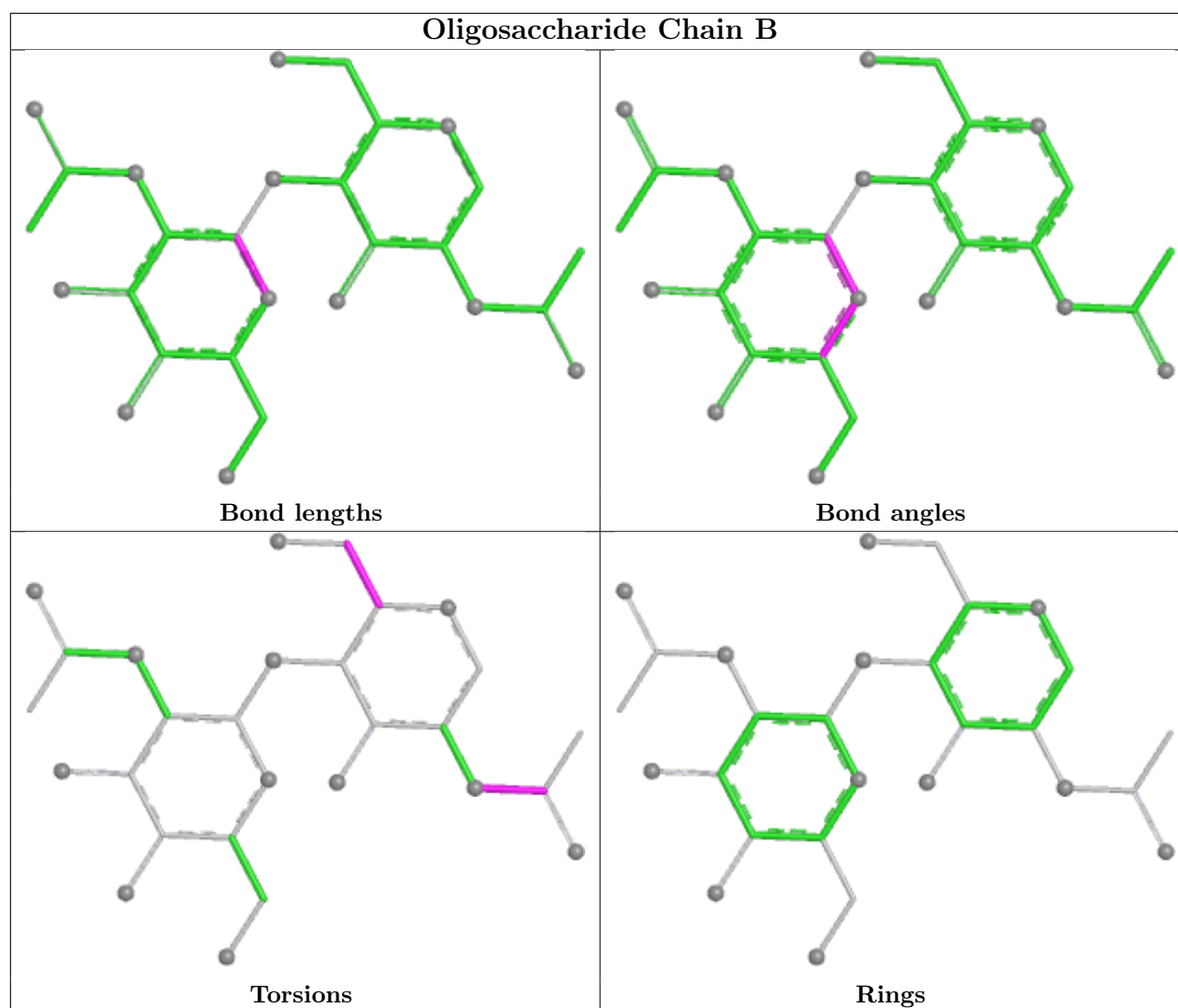
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-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](#)

There are no ligands in this entry.

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.

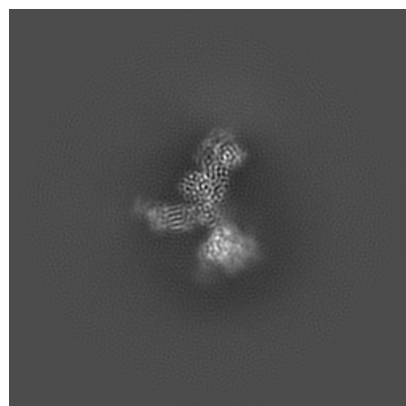
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27177. These allow visual inspection of the internal detail of the map and identification of artifacts.

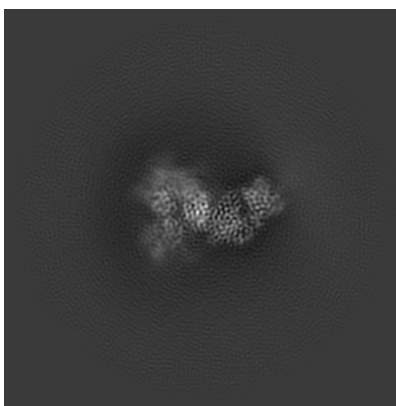
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

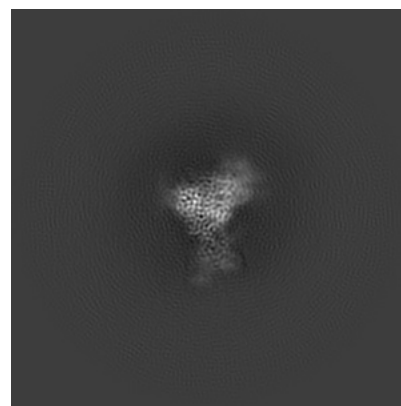
6.1.1 Primary map



X

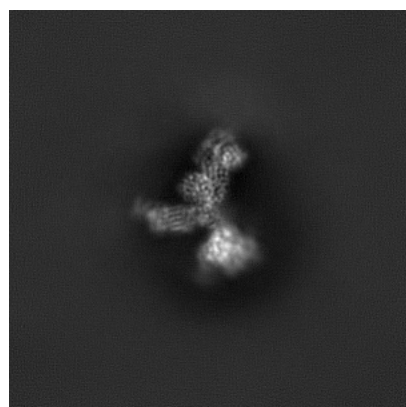


Y

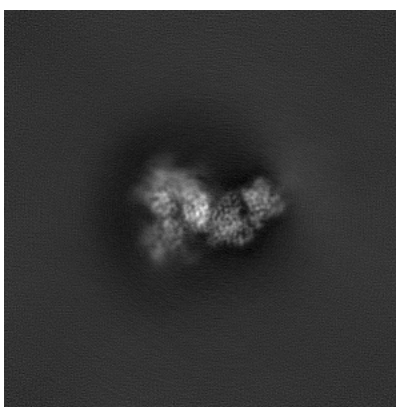


Z

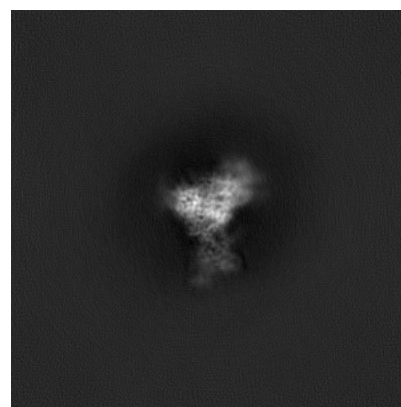
6.1.2 Raw map



X



Y

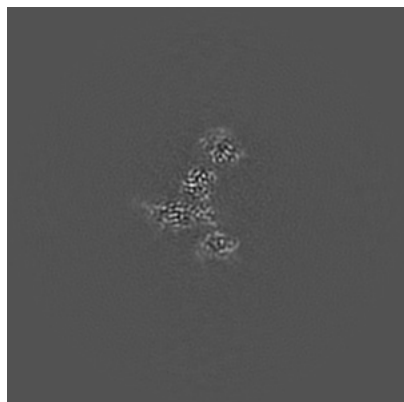


Z

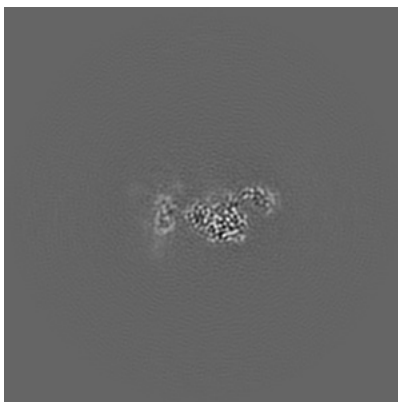
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

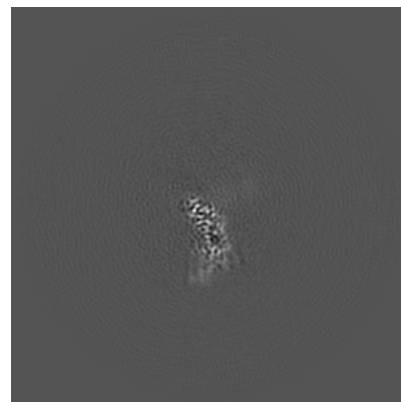
6.2.1 Primary map



X Index: 216

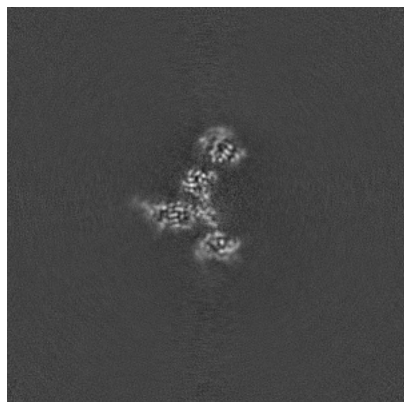


Y Index: 216

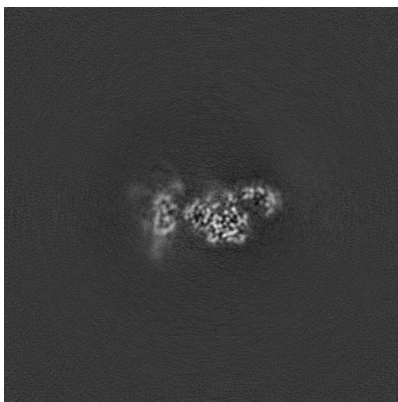


Z Index: 216

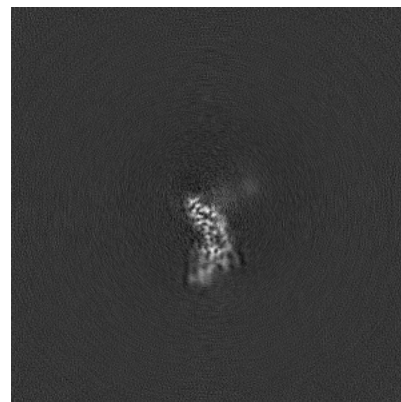
6.2.2 Raw map



X Index: 216



Y Index: 216

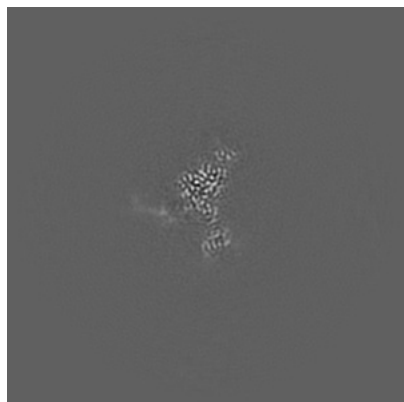


Z Index: 216

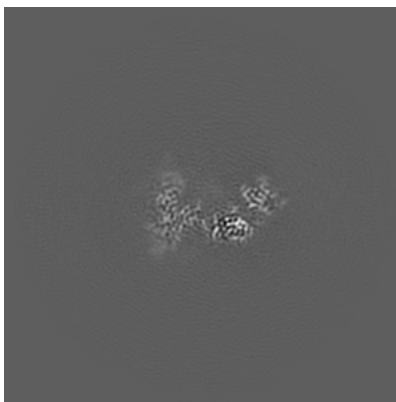
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

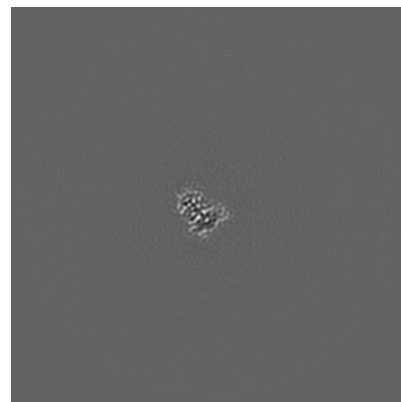
6.3.1 Primary map



X Index: 202

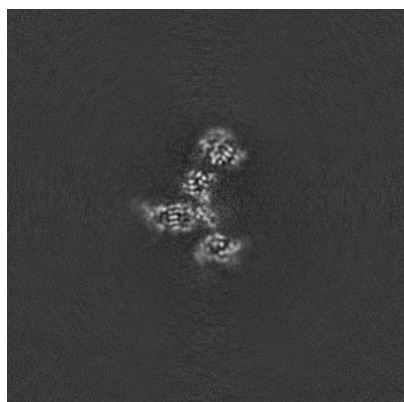


Y Index: 223

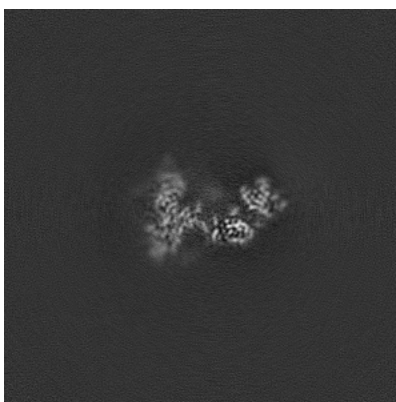


Z Index: 242

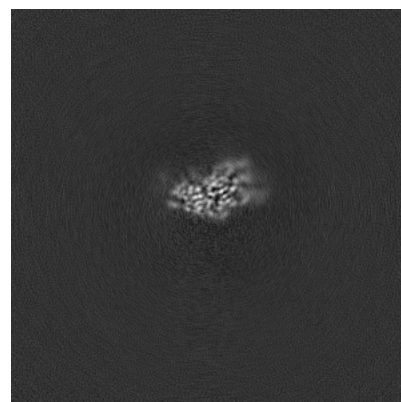
6.3.2 Raw map



X Index: 217



Y Index: 223

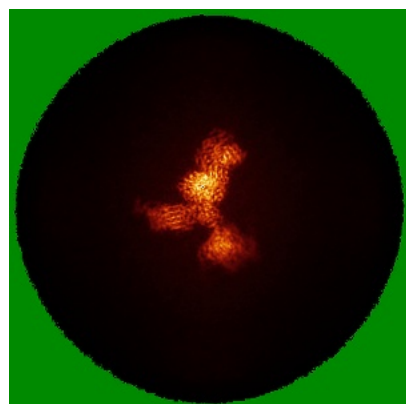


Z Index: 176

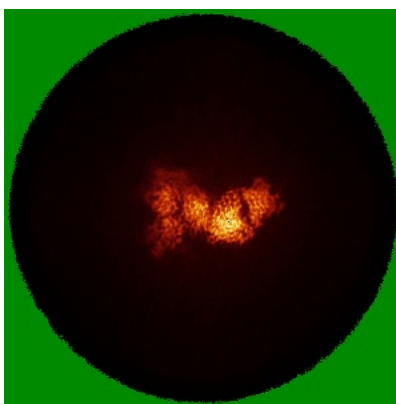
The images above show the largest variance slices of the map in three orthogonal directions.

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

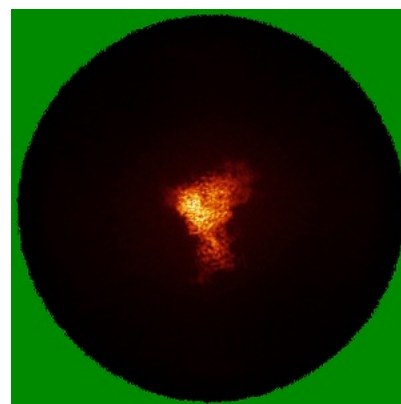
6.4.1 Primary map



X

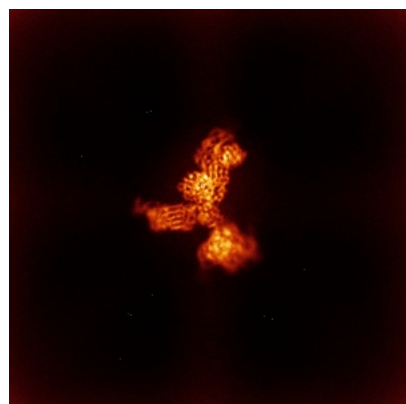


Y

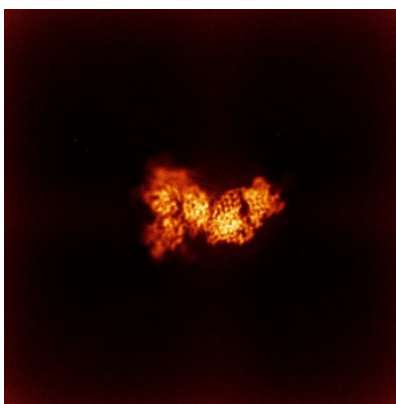


Z

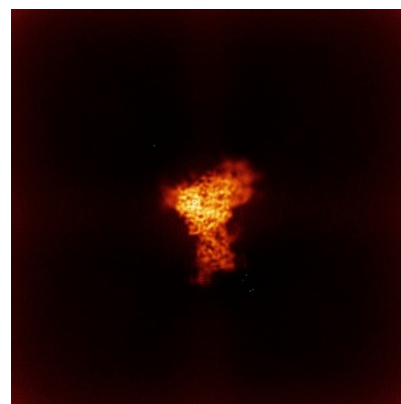
6.4.2 Raw map



X



Y

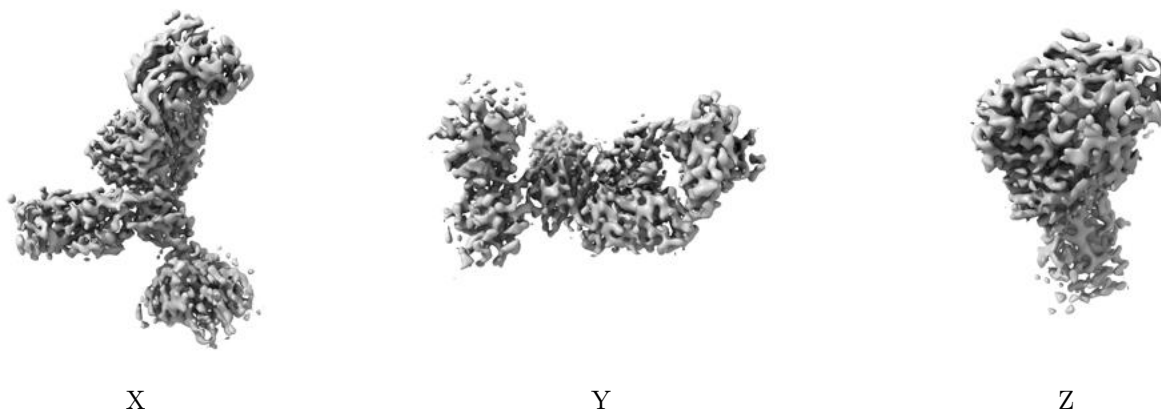


Z

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.

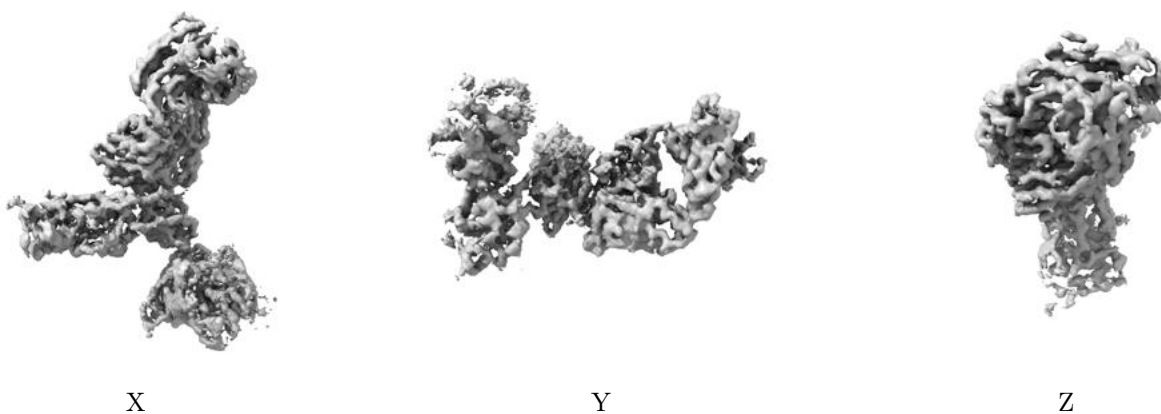
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

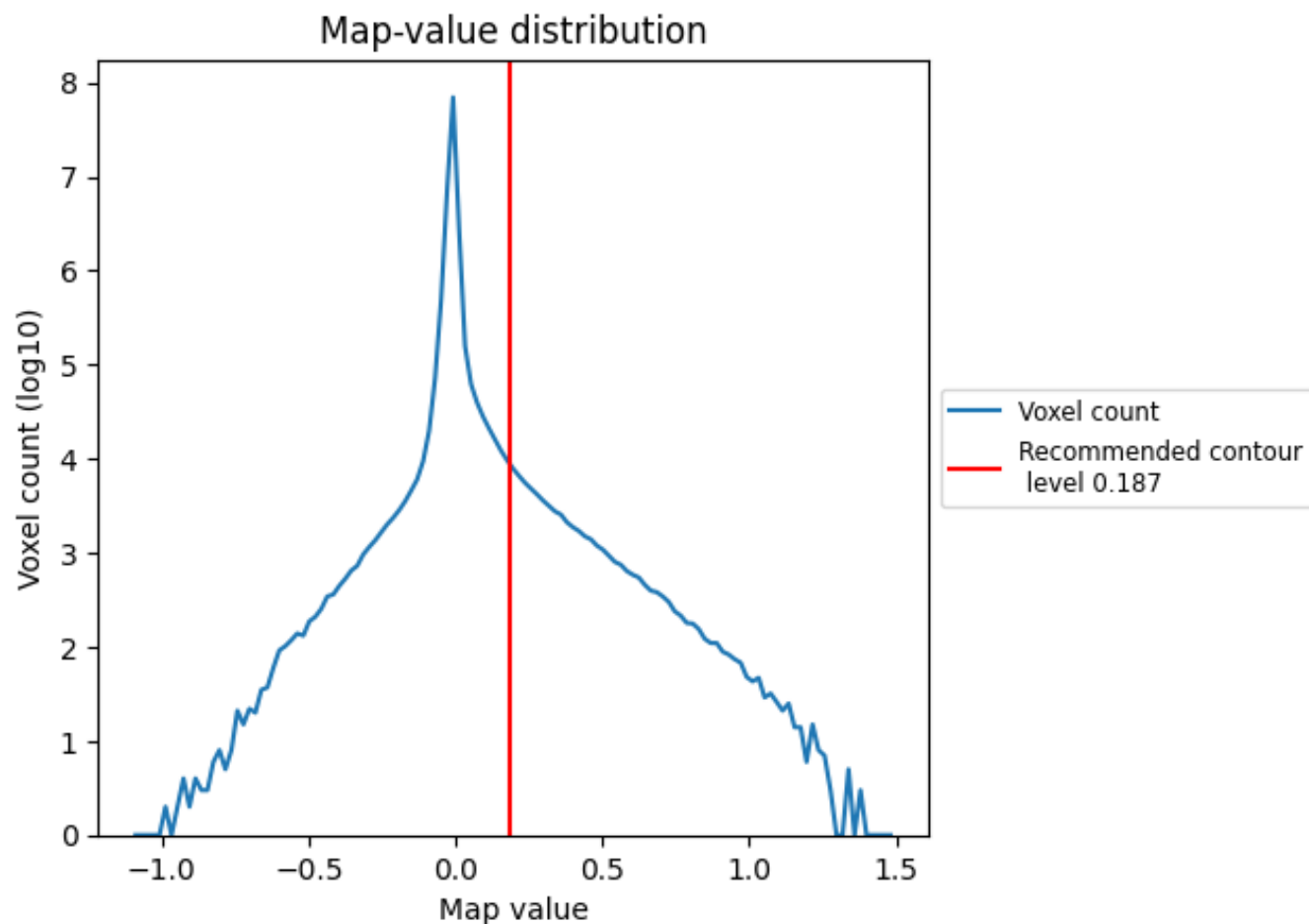
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

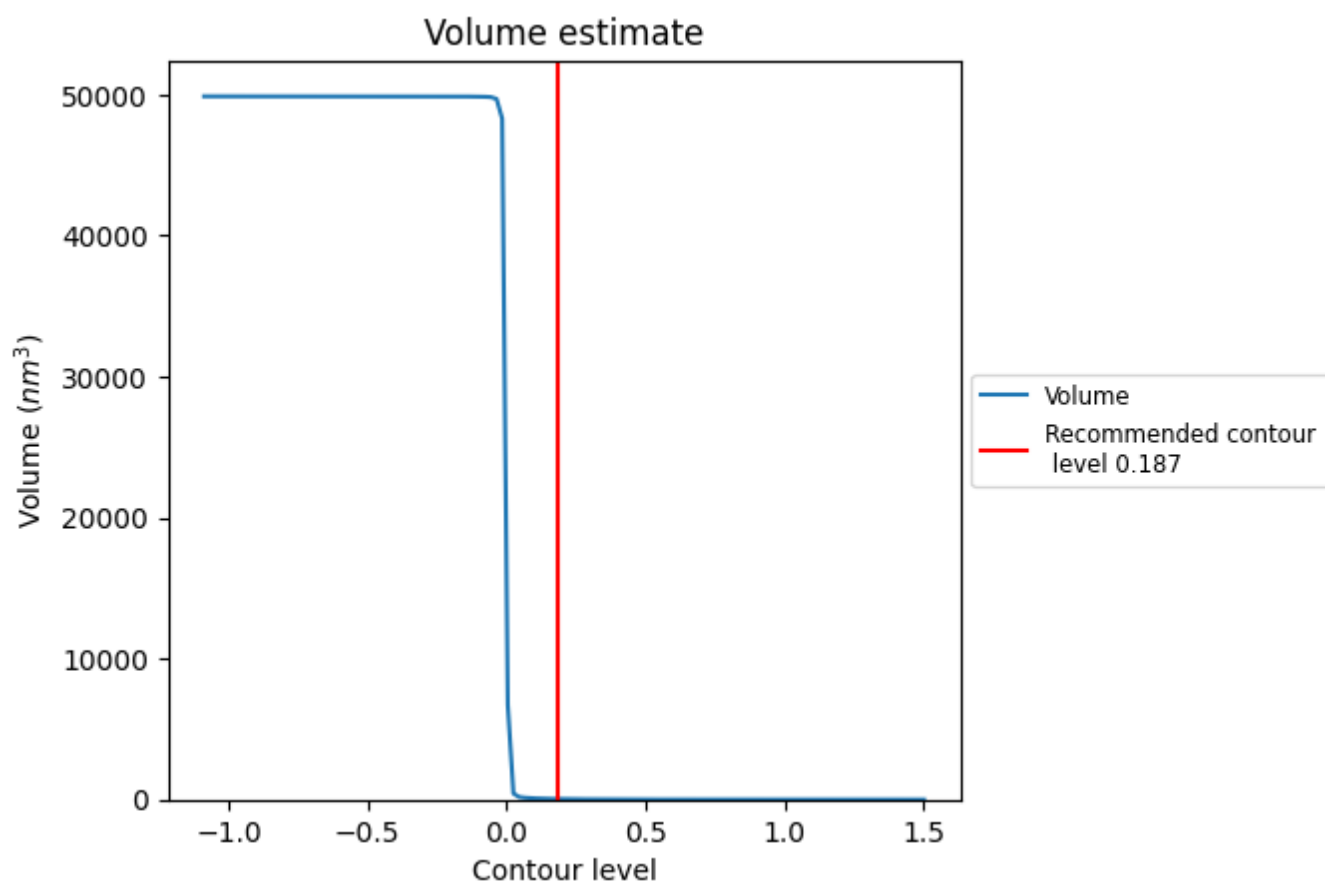
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

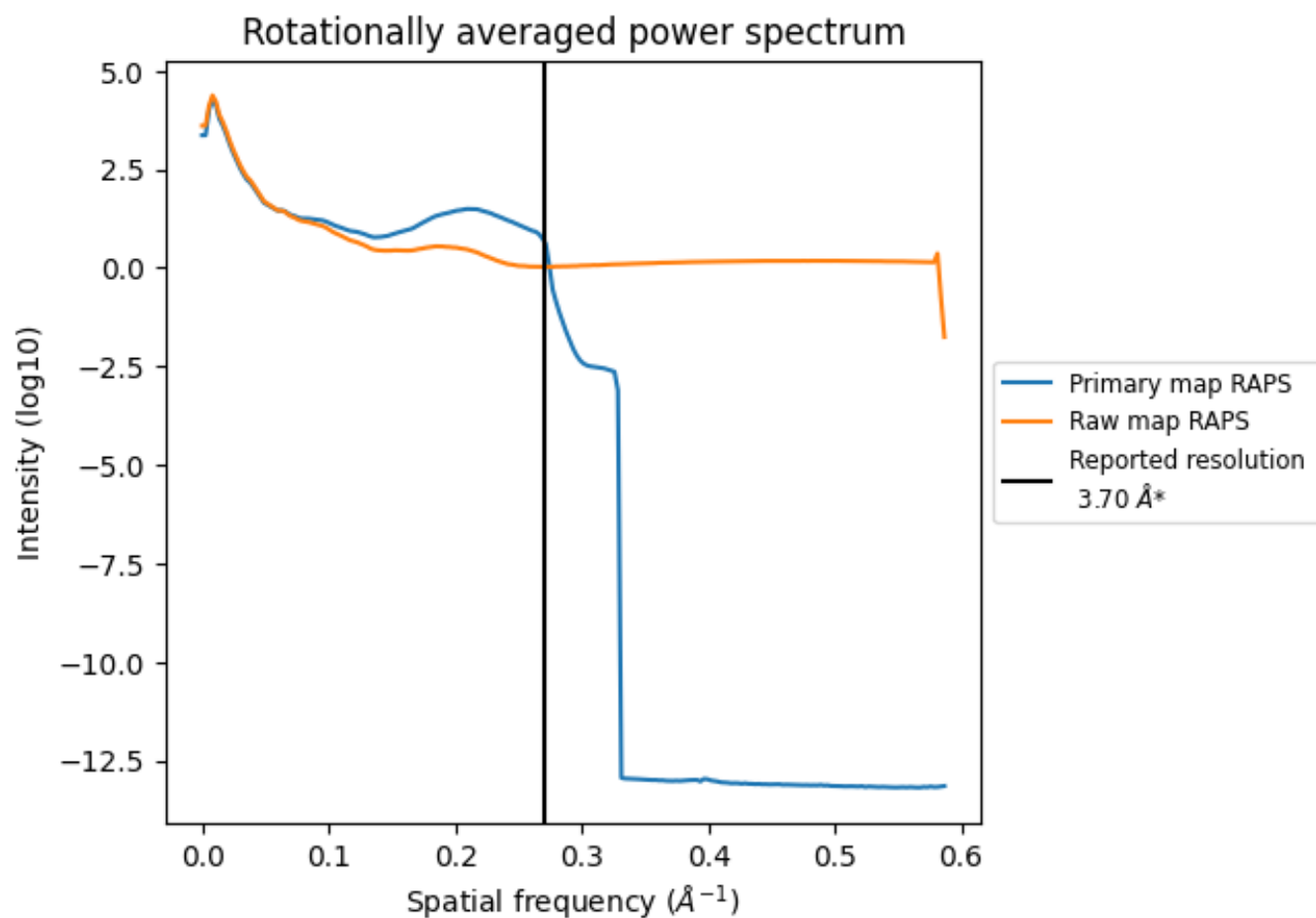
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 ⓘ

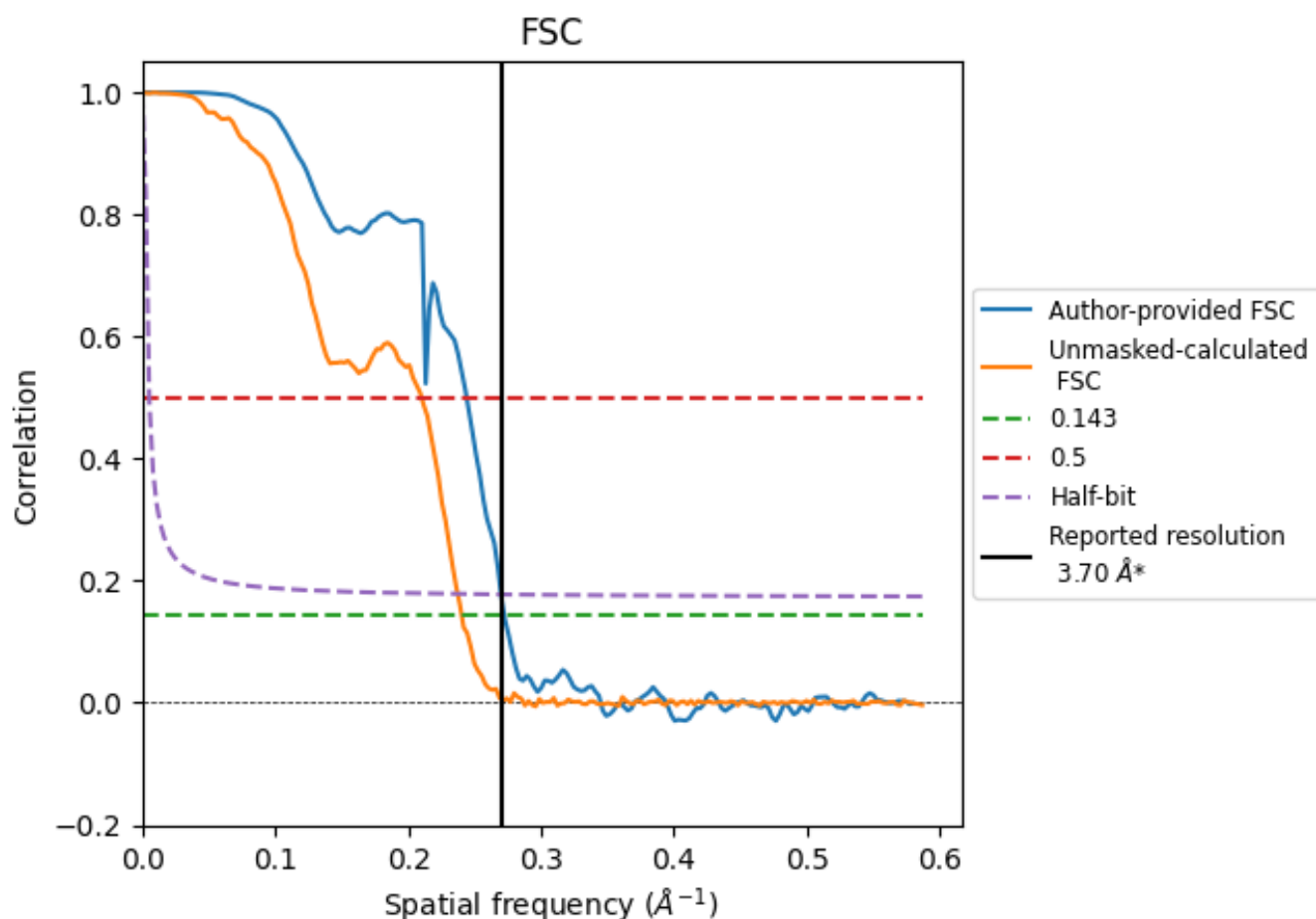


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

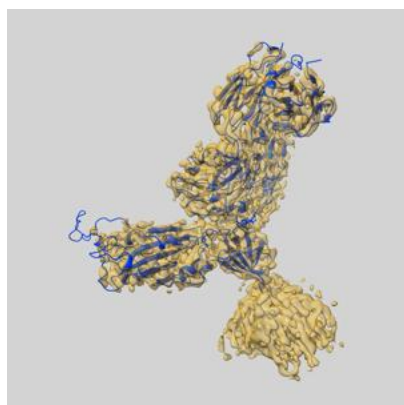
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.10	3.70
Unmasked-calculated*	4.16	4.76	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.7 by more than 10 %

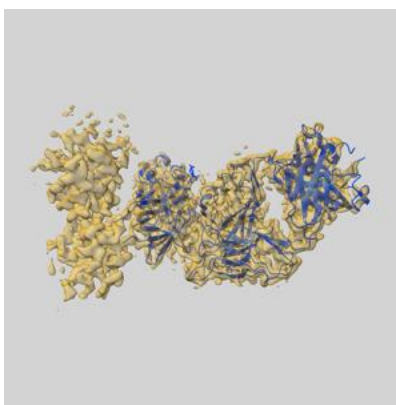
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27177 and PDB model 8D48. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

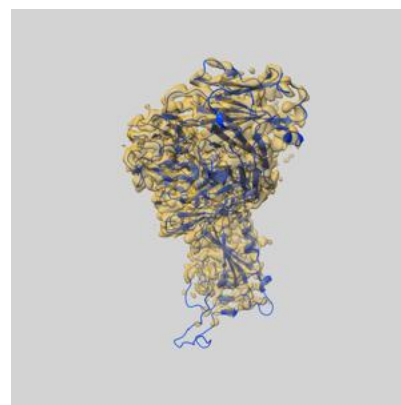
9.1 Map-model overlay [i](#)



X



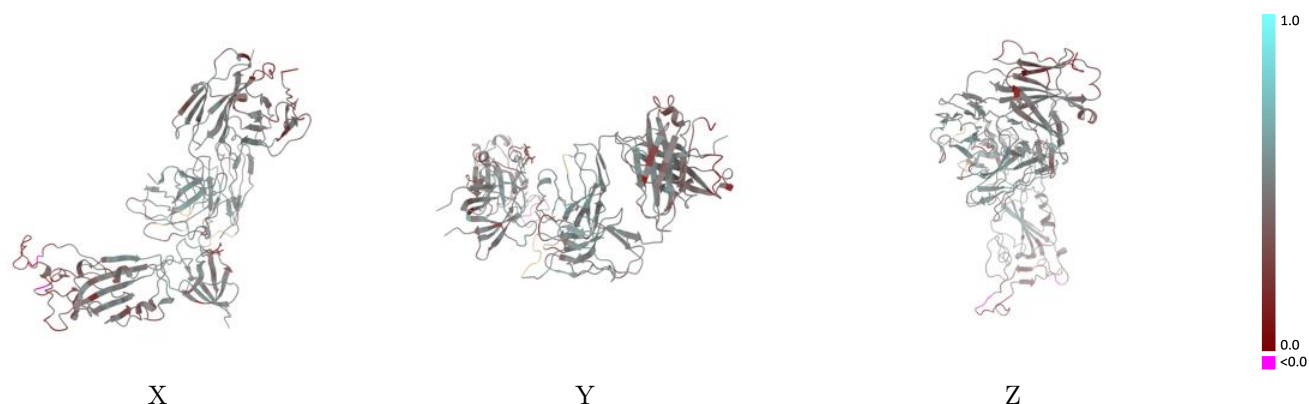
Y



Z

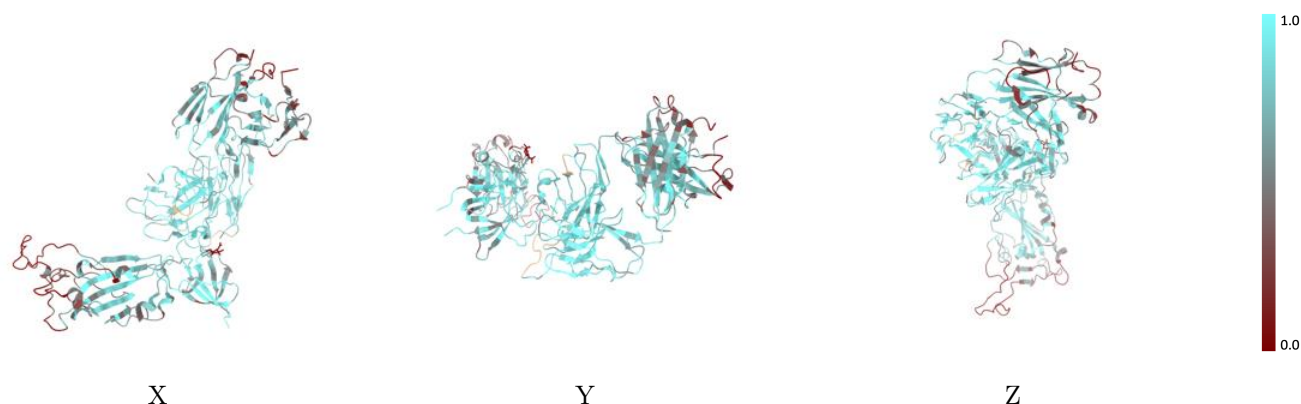
The images above show the 3D surface view of the map at the recommended contour level 0.187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



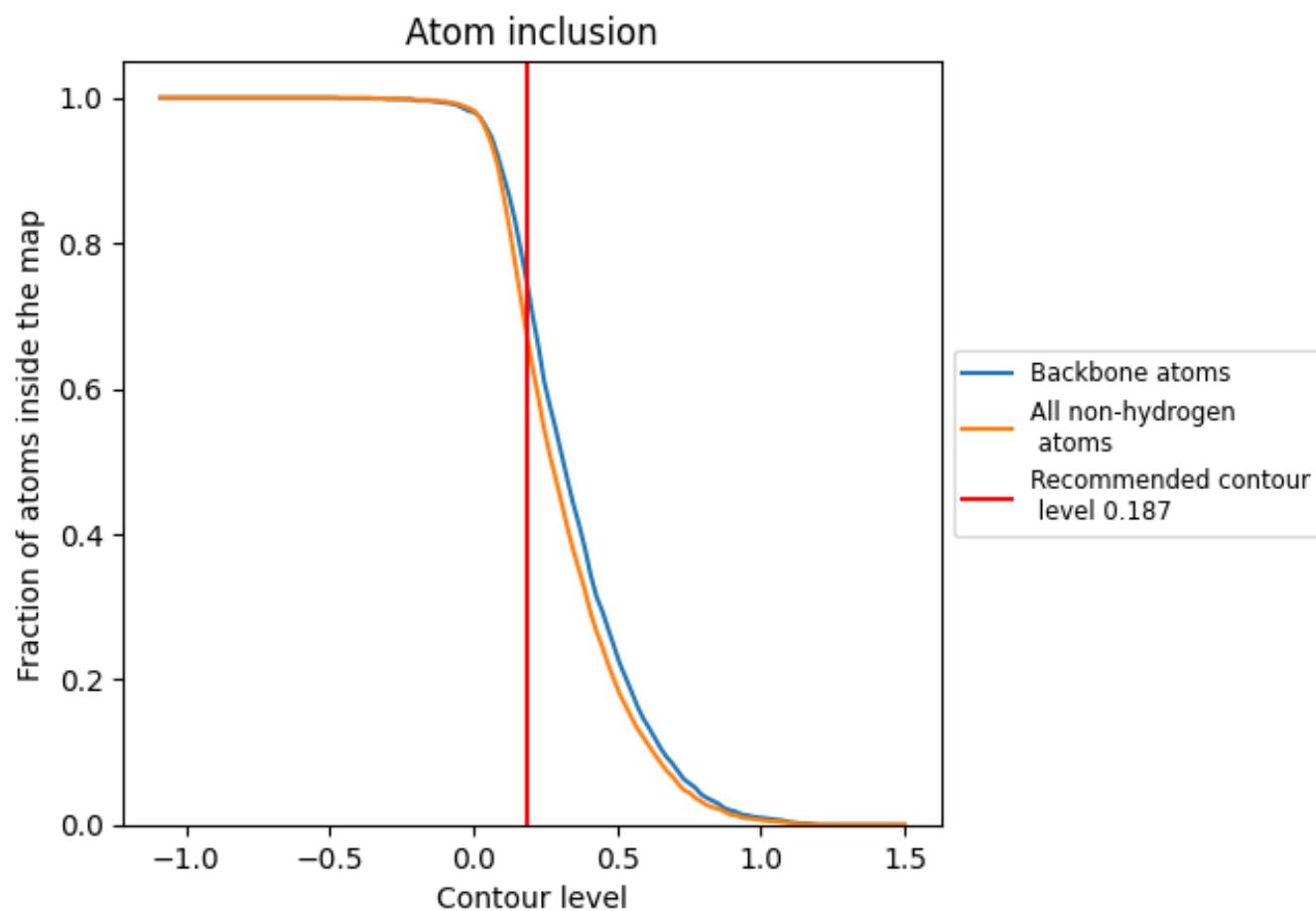
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.187).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.4490
A	0.5930	0.4240
B	0.2860	0.3370
H	0.7430	0.4790
L	0.7100	0.4530

