



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 12:16 AM UTC

PDB ID : 9BLL / pdb_00009bll
EMDB ID : EMD-44666
Title : Cryo-EM of RBD(EG5.1)/1301B7 Fab Complex
Authors : Walter, M.R.; Green, T.J.
Deposited on : 2024-04-30
Resolution : 4.10 Å (reported)
Based on initial models : ., 8iou

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:

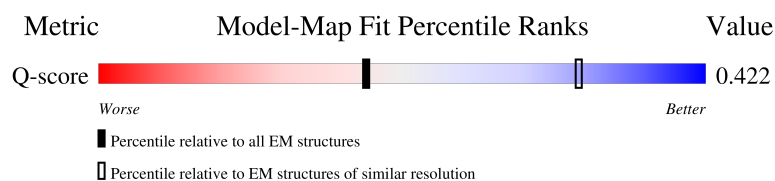
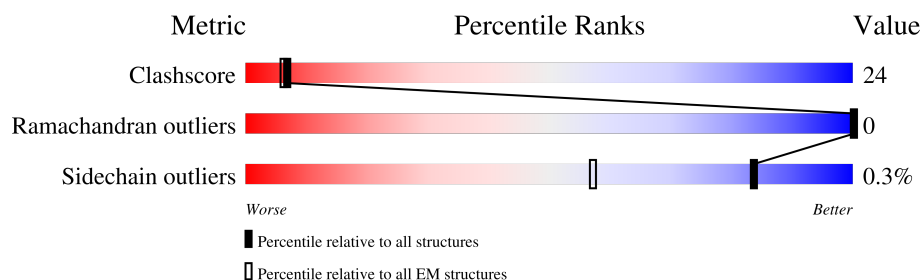
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 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	6458 (3.60 - 4.60)

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	H	128	 45% 55%
2	L	110	 48% 52%
3	T	1244	 10% 6% 84%
4	G	2	 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3428 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 1301B7 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	128	Total	C	N	O	S	0	0
			970	616	159	191	4		

- Molecule 2 is a protein called 1301B7 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	110	Total	C	N	O	S	0	0
			811	504	145	160	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	203	Total	C	N	O	S	0	0
			1605	1031	271	295	8		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	7	MET	-	initiating methionine	UNP P0DTC2
T	8	ARG	-	expression tag	UNP P0DTC2
T	9	PRO	-	expression tag	UNP P0DTC2
T	10	THR	-	expression tag	UNP P0DTC2
T	11	LEU	-	expression tag	UNP P0DTC2
T	12	LEU	-	expression tag	UNP P0DTC2
T	13	TRP	-	expression tag	UNP P0DTC2
T	14	SER	-	expression tag	UNP P0DTC2
T	15	LEU	-	expression tag	UNP P0DTC2
T	16	LEU	-	expression tag	UNP P0DTC2
T	17	LEU	-	expression tag	UNP P0DTC2
T	18	LEU	-	expression tag	UNP P0DTC2
T	19	LEU	-	expression tag	UNP P0DTC2
T	20	GLY	-	expression tag	UNP P0DTC2
T	21	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	22	PHE	-	expression tag	UNP P0DTC2
T	23	ALA	-	expression tag	UNP P0DTC2
T	24	ALA	-	expression tag	UNP P0DTC2
T	25	ALA	-	expression tag	UNP P0DTC2
T	26	ALA	-	expression tag	UNP P0DTC2
T	27	ALA	-	expression tag	UNP P0DTC2
T	53	HIS	GLN	conflict	UNP P0DTC2
T	84	ALA	VAL	conflict	UNP P0DTC2
T	143	ASP	GLY	conflict	UNP P0DTC2
T	?	-	TYR	deletion	UNP P0DTC2
T	146	GLN	HIS	conflict	UNP P0DTC2
T	183	GLU	GLN	conflict	UNP P0DTC2
T	213	GLU	VAL	conflict	UNP P0DTC2
T	252	VAL	GLY	conflict	UNP P0DTC2
T	339	HIS	GLY	conflict	UNP P0DTC2
T	346	THR	ARG	conflict	UNP P0DTC2
T	368	ILE	LEU	conflict	UNP P0DTC2
T	371	PHE	SER	conflict	UNP P0DTC2
T	373	PRO	SER	conflict	UNP P0DTC2
T	375	PHE	SER	conflict	UNP P0DTC2
T	376	ALA	THR	conflict	UNP P0DTC2
T	405	ASN	ASP	conflict	UNP P0DTC2
T	408	SER	ARG	conflict	UNP P0DTC2
T	417	ASN	LYS	conflict	UNP P0DTC2
T	445	PRO	VAL	conflict	UNP P0DTC2
T	446	SER	GLY	conflict	UNP P0DTC2
T	456	LEU	PHE	conflict	UNP P0DTC2
T	460	LYS	ASN	conflict	UNP P0DTC2
T	477	ASN	SER	conflict	UNP P0DTC2
T	478	LYS	THR	conflict	UNP P0DTC2
T	484	ALA	GLU	conflict	UNP P0DTC2
T	486	PRO	PHE	conflict	UNP P0DTC2
T	490	SER	PHE	conflict	UNP P0DTC2
T	498	ARG	GLN	conflict	UNP P0DTC2
T	501	TYR	ASN	conflict	UNP P0DTC2
T	505	HIS	TYR	conflict	UNP P0DTC2
T	614	GLY	ASP	conflict	UNP P0DTC2
T	655	TYR	HIS	conflict	UNP P0DTC2
T	679	LYS	ASN	conflict	UNP P0DTC2
T	681	HIS	PRO	conflict	UNP P0DTC2
T	682	GLY	ARG	conflict	UNP P0DTC2
T	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	685	GLY	ARG	conflict	UNP P0DTC2
T	764	LYS	ASN	conflict	UNP P0DTC2
T	796	TYR	ASP	conflict	UNP P0DTC2
T	817	PRO	PHE	conflict	UNP P0DTC2
T	892	PRO	ALA	conflict	UNP P0DTC2
T	899	PRO	ALA	conflict	UNP P0DTC2
T	942	PRO	ALA	conflict	UNP P0DTC2
T	954	HIS	GLN	conflict	UNP P0DTC2
T	969	LYS	ASN	conflict	UNP P0DTC2
T	986	PRO	LYS	conflict	UNP P0DTC2
T	987	PRO	VAL	conflict	UNP P0DTC2
T	1211	ALA	-	expression tag	UNP P0DTC2
T	1212	SER	-	expression tag	UNP P0DTC2
T	1213	SER	-	expression tag	UNP P0DTC2
T	1214	GLY	-	expression tag	UNP P0DTC2
T	1215	TYR	-	expression tag	UNP P0DTC2
T	1216	ILE	-	expression tag	UNP P0DTC2
T	1217	PRO	-	expression tag	UNP P0DTC2
T	1218	GLU	-	expression tag	UNP P0DTC2
T	1219	ALA	-	expression tag	UNP P0DTC2
T	1220	PRO	-	expression tag	UNP P0DTC2
T	1221	ARG	-	expression tag	UNP P0DTC2
T	1222	ASP	-	expression tag	UNP P0DTC2
T	1223	GLY	-	expression tag	UNP P0DTC2
T	1224	GLN	-	expression tag	UNP P0DTC2
T	1225	ALA	-	expression tag	UNP P0DTC2
T	1226	TYR	-	expression tag	UNP P0DTC2
T	1227	VAL	-	expression tag	UNP P0DTC2
T	1228	ARG	-	expression tag	UNP P0DTC2
T	1229	LYS	-	expression tag	UNP P0DTC2
T	1230	ASP	-	expression tag	UNP P0DTC2
T	1231	GLY	-	expression tag	UNP P0DTC2
T	1232	GLU	-	expression tag	UNP P0DTC2
T	1233	TRP	-	expression tag	UNP P0DTC2
T	1234	VAL	-	expression tag	UNP P0DTC2
T	1235	LEU	-	expression tag	UNP P0DTC2
T	1236	LEU	-	expression tag	UNP P0DTC2
T	1237	SER	-	expression tag	UNP P0DTC2
T	1238	THR	-	expression tag	UNP P0DTC2
T	1239	PHE	-	expression tag	UNP P0DTC2
T	1240	LEU	-	expression tag	UNP P0DTC2
T	1241	GLU	-	expression tag	UNP P0DTC2

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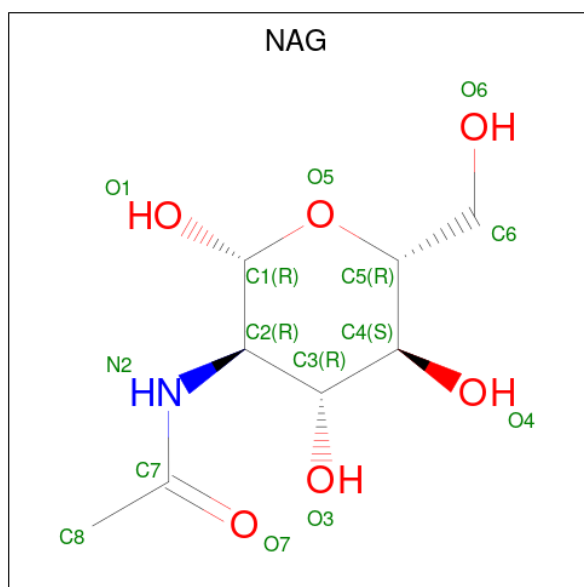
Chain	Residue	Modelled	Actual	Comment	Reference
T	1242	GLY	-	expression tag	UNP P0DTC2
T	1243	THR	-	expression tag	UNP P0DTC2
T	1244	LYS	-	expression tag	UNP P0DTC2
T	1245	HIS	-	expression tag	UNP P0DTC2
T	1246	HIS	-	expression tag	UNP P0DTC2
T	1247	HIS	-	expression tag	UNP P0DTC2
T	1248	HIS	-	expression tag	UNP P0DTC2
T	1249	HIS	-	expression tag	UNP P0DTC2
T	1250	HIS	-	expression tag	UNP P0DTC2

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.443	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.048	Depositor
Map size (Å)	357.69998, 357.69998, 357.69998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89425, 0.89425, 0.89425	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: 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	H	0.27	0/993	0.57	0/1350
2	L	0.31	0/829	0.49	0/1129
3	T	0.36	0/1654	0.48	1/2255 (0.0%)
All	All	0.33	0/3476	0.51	1/4734 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	431	GLY	CA-C-O	-5.01	117.67	122.13

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	H	970	0	935	56	0
2	L	811	0	792	50	0
3	T	1605	0	1536	62	0
4	G	28	0	25	0	0
5	T	14	0	13	0	0
All	All	3428	0	3301	164	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 24.

All (164) 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:L:86:TYR:O	2:L:101:GLY:HA2	1.67	0.93
2:L:54:ARG:NH2	2:L:59:PRO:O	2.11	0.81
1:H:33:PRO:HG2	1:H:106:TYR:CE1	2.14	0.81
1:H:90:PHE:O	1:H:117:GLY:HA2	1.81	0.81
2:L:6:GLN:HE22	2:L:101:GLY:H	1.28	0.80
2:L:54:ARG:NH1	2:L:58:ILE:O	2.16	0.79
2:L:38:HIS:HB3	2:L:85:ASP:HB2	1.65	0.78
1:H:33:PRO:HB3	1:H:52:ILE:HA	1.65	0.76
1:H:6:GLU:OE2	1:H:117:GLY:N	2.18	0.74
1:H:72:ASP:HB3	1:H:76:GLY:HA2	1.73	0.70
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.74	0.69
3:T:355:ARG:HD2	3:T:396:TYR:HD2	1.57	0.68
3:T:474:GLN:NE2	3:T:480:CYS:SG	2.66	0.68
2:L:49:TYR:OH	2:L:53:ASN:ND2	2.27	0.68
1:H:84:SER:HA	1:H:122:VAL:HG11	1.76	0.67
2:L:34:HIS:HB3	2:L:89:GLN:HG3	1.77	0.65
3:T:448:ASN:OD1	3:T:449:TYR:N	2.29	0.65
3:T:422:ASN:HD21	3:T:454:ARG:H	1.45	0.65
1:H:51:ILE:HG13	1:H:57:VAL:HG22	1.79	0.64
3:T:420:ASP:OD2	3:T:460:LYS:NZ	2.31	0.64
3:T:386:LYS:HG3	3:T:390:LEU:HD23	1.80	0.64
3:T:379:CYS:HB2	3:T:384:PRO:HG3	1.81	0.63
1:H:15:GLY:N	1:H:82(C):LEU:O	2.23	0.63
2:L:30:VAL:HG12	2:L:93:ARG:HH22	1.63	0.63
3:T:333:THR:HG23	3:T:334:ASN:OD1	1.99	0.62
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.83	0.61
2:L:53:ASN:OD1	2:L:54:ARG:N	2.34	0.60
1:H:12:LYS:HD2	1:H:82(C):LEU:HD12	1.84	0.60
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.35	0.60
1:H:99:TYR:O	1:H:103:LEU:HD23	2.02	0.59
1:H:28:THR:OG1	3:T:505:HIS:ND1	2.35	0.59
3:T:446:SER:O	3:T:498:ARG:NE	2.29	0.59
3:T:448:ASN:OD1	3:T:450:ASN:N	2.32	0.59
3:T:474:GLN:NE2	3:T:478:LYS:O	2.36	0.59
3:T:437:ASN:OD1	3:T:438:SER:N	2.36	0.58
1:H:38:ARG:HH21	1:H:63:PHE:HZ	1.49	0.58
3:T:474:GLN:NE2	3:T:488:CYS:SG	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:338:PHE:HD2	3:T:368:ILE:HD11	1.69	0.58
3:T:387:LEU:HD23	3:T:390:LEU:HD11	1.86	0.58
1:H:38:ARG:HG3	1:H:48:VAL:HG21	1.86	0.57
3:T:497:PHE:CE2	3:T:507:PRO:HB3	2.39	0.57
3:T:332:ILE:HD12	3:T:335:LEU:HD21	1.85	0.57
1:H:30:GLY:O	1:H:31:SER:OG	2.22	0.56
3:T:353:TRP:HZ3	3:T:355:ARG:HE	1.54	0.56
2:L:65:SER:OG	2:L:66:LYS:N	2.38	0.56
2:L:85:ASP:OD1	2:L:103:ARG:HG2	2.05	0.56
3:T:342:PHE:CE2	3:T:368:ILE:HD12	2.41	0.55
2:L:6:GLN:NE2	2:L:101:GLY:H	2.03	0.55
3:T:342:PHE:HE2	3:T:368:ILE:HG23	1.71	0.55
3:T:350:VAL:HG21	3:T:418:ILE:HD11	1.89	0.54
3:T:428:ASP:OD1	3:T:428:ASP:N	2.41	0.53
1:H:36:TRP:CZ3	1:H:92:CYS:HB3	2.43	0.53
2:L:9:SER:HA	2:L:102:THR:HG23	1.91	0.53
3:T:422:ASN:OD1	3:T:454:ARG:HB2	2.09	0.53
1:H:21:SER:HB2	1:H:79:HIS:CE1	2.43	0.53
2:L:17:GLN:H	2:L:78:LEU:H	1.56	0.53
3:T:407:VAL:HG21	3:T:508:TYR:HD2	1.74	0.53
2:L:54:ARG:HH21	2:L:62:PHE:N	2.06	0.53
1:H:12:LYS:O	1:H:123:SER:N	2.42	0.52
1:H:53:ILE:HG13	1:H:73:THR:HG21	1.91	0.52
3:T:434:ILE:HB	3:T:511:VAL:CG2	2.39	0.52
1:H:31:SER:OG	1:H:98:ASP:HB2	2.08	0.52
1:H:68:THR:OG1	1:H:81:GLU:OE2	2.28	0.52
3:T:359:SER:OG	3:T:394:ASN:OD1	2.11	0.52
1:H:39:GLN:HB3	1:H:89:VAL:HB	1.91	0.52
1:H:48:VAL:HG13	1:H:63:PHE:HD2	1.74	0.52
1:H:71:GLY:HA2	1:H:78:ALA:HA	1.92	0.51
1:H:97:TYR:CG	1:H:102:ARG:HD2	2.45	0.51
3:T:457:ARG:NH1	3:T:467:ASP:OD2	2.37	0.51
3:T:378:LYS:HB3	3:T:380:TYR:CE1	2.46	0.51
3:T:342:PHE:CE1	3:T:511:VAL:HG21	2.45	0.51
3:T:427:ASP:N	3:T:427:ASP:OD1	2.41	0.51
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.46	0.51
3:T:347:PHE:CE1	3:T:509:ARG:HD3	2.46	0.51
3:T:399:SER:HB3	3:T:511:VAL:HG12	1.92	0.51
1:H:97:TYR:CD1	1:H:102:ARG:HD2	2.46	0.50
2:L:86:TYR:O	2:L:101:GLY:CA	2.52	0.50
3:T:358:ILE:HB	3:T:395:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:GLY:HA3	3:T:456:LEU:HG	1.93	0.50
3:T:438:SER:O	3:T:438:SER:OG	2.25	0.50
1:H:2:VAL:HG21	1:H:94:ARG:NH1	2.26	0.49
1:H:18:VAL:O	1:H:81:GLU:HA	2.12	0.49
1:H:33:PRO:HG2	1:H:106:TYR:CD1	2.47	0.49
2:L:33:VAL:HG22	2:L:51:ASN:OD1	2.11	0.49
2:L:27:ARG:NH1	2:L:27:ARG:HB3	2.27	0.49
2:L:31:TYR:CZ	2:L:91:TYR:HD2	2.31	0.49
3:T:474:GLN:OE1	3:T:475:ALA:N	2.46	0.48
3:T:452:LEU:HG	3:T:494:SER:HA	1.95	0.48
1:H:23:LYS:HD2	1:H:77:SER:HB3	1.95	0.48
2:L:18:ARG:HA	2:L:75:ILE:O	2.11	0.48
3:T:447:GLY:HA2	3:T:498:ARG:HG2	1.95	0.48
1:H:111:MET:HB2	2:L:36:TYR:OH	2.14	0.48
3:T:457:ARG:HG2	3:T:458:LYS:H	1.79	0.47
2:L:32:ALA:HA	2:L:51:ASN:HD21	1.79	0.47
1:H:47:TRP:HZ3	2:L:95(A):GLY:HA3	1.80	0.47
3:T:358:ILE:HB	3:T:395:VAL:CG2	2.43	0.47
3:T:434:ILE:HB	3:T:511:VAL:HG23	1.97	0.47
1:H:12:LYS:HZ3	1:H:18:VAL:HB	1.79	0.47
1:H:94:ARG:NH2	1:H:96:SER:OG	2.48	0.47
2:L:83:GLU:HA	2:L:104:LEU:O	2.15	0.47
2:L:85:ASP:O	2:L:86:TYR:HD1	1.98	0.47
3:T:344:ALA:O	3:T:345:THR:OG1	2.29	0.47
1:H:82(B):GLY:O	1:H:83:ARG:NE	2.45	0.47
1:H:83:ARG:NH2	1:H:86:ASP:OD2	2.48	0.46
3:T:418:ILE:HD12	3:T:422:ASN:HB2	1.97	0.46
2:L:13:GLY:N	2:L:105:THR:O	2.49	0.46
3:T:347:PHE:CD2	3:T:399:SER:HB2	2.51	0.46
3:T:362:VAL:HG13	3:T:525:CYS:O	2.16	0.46
2:L:45:LYS:HG2	2:L:46:LEU:N	2.31	0.45
1:H:5:VAL:N	1:H:23:LYS:O	2.48	0.45
3:T:377:PHE:HD1	3:T:434:ILE:HD13	1.81	0.45
2:L:3:GLY:HA2	2:L:97:VAL:CG2	2.46	0.45
2:L:34:HIS:O	2:L:88:CYS:HA	2.16	0.45
2:L:49:TYR:CD1	2:L:55:PRO:HG3	2.52	0.45
1:H:31:SER:O	1:H:33:PRO:HD3	2.17	0.45
1:H:53:ILE:CG1	1:H:73:THR:HG21	2.47	0.45
2:L:78:LEU:HD12	2:L:79:GLN:H	1.81	0.44
3:T:357:ARG:HH22	3:T:394:ASN:HD21	1.65	0.44
1:H:67:VAL:HB	1:H:82:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:ARG:HH21	2:L:62:PHE:H	1.63	0.44
1:H:80:MET:HE1	1:H:90:PHE:CE2	2.53	0.44
1:H:59:TYR:CD2	1:H:67:VAL:HG13	2.54	0.43
2:L:17:GLN:O	2:L:77:GLY:N	2.51	0.43
2:L:49:TYR:HD1	2:L:55:PRO:HG3	1.83	0.43
2:L:54:ARG:NH2	2:L:62:PHE:H	2.17	0.43
3:T:353:TRP:CD1	3:T:353:TRP:H	2.35	0.43
1:H:103:LEU:O	1:H:106:TYR:HB2	2.19	0.43
3:T:438:SER:OG	3:T:441:LEU:HB2	2.19	0.43
2:L:92:ASP:O	2:L:93:ARG:C	2.62	0.43
1:H:31:SER:HB3	1:H:53:ILE:HD12	2.01	0.43
3:T:338:PHE:O	3:T:341:VAL:HG12	2.19	0.43
1:H:7:SER:O	1:H:118:THR:OG1	2.32	0.42
2:L:38:HIS:CD2	2:L:44:PRO:HG3	2.54	0.42
2:L:13:GLY:HA3	2:L:106:VAL:HG22	2.00	0.42
1:H:70:THR:O	1:H:79:HIS:N	2.50	0.42
1:H:98:ASP:N	1:H:103:LEU:HD21	2.34	0.42
3:T:350:VAL:HG13	3:T:422:ASN:HD22	1.85	0.42
3:T:365:TYR:HD2	3:T:387:LEU:HD13	1.84	0.42
1:H:25:SER:C	1:H:27:GLY:H	2.28	0.42
1:H:21:SER:OG	1:H:22:CYS:N	2.53	0.42
2:L:61:ARG:HA	2:L:76:THR:HG22	2.01	0.42
1:H:112:ASP:OD2	1:H:113:VAL:HG23	2.19	0.41
3:T:365:TYR:CD2	3:T:387:LEU:HD13	2.55	0.41
2:L:66:LYS:HA	2:L:71:ALA:HA	2.01	0.41
1:H:99:TYR:H	1:H:103:LEU:HD23	1.85	0.41
2:L:27:ARG:HB3	2:L:27:ARG:HH11	1.84	0.41
3:T:530:SER:OG	3:T:531:THR:N	2.52	0.41
3:T:352:ALA:HB1	3:T:466:ARG:HH21	1.85	0.41
1:H:27:GLY:HA3	1:H:75:ALA:HA	2.03	0.41
3:T:338:PHE:HA	3:T:341:VAL:HG12	2.03	0.41
2:L:17:GLN:N	2:L:17:GLN:OE1	2.54	0.41
2:L:39:VAL:HB	2:L:42:ALA:HB3	2.03	0.41
2:L:54:ARG:CZ	2:L:60:ASP:HA	2.51	0.41
3:T:353:TRP:O	3:T:466:ARG:NH1	2.53	0.41
3:T:422:ASN:ND2	3:T:454:ARG:H	2.17	0.41
1:H:3:GLN:HA	1:H:3:GLN:OE1	2.19	0.41
1:H:29:PHE:CE1	1:H:34:ILE:HD11	2.56	0.41
2:L:59:PRO:O	2:L:61:ARG:N	2.54	0.40
2:L:61:ARG:HH22	2:L:79:GLN:HB2	1.85	0.40
3:T:342:PHE:HB3	3:T:371:PHE:HE2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:516:GLU:C	3:T:517:LEU:HD22	2.46	0.40
2:L:54:ARG:HH12	2:L:58:ILE:C	2.23	0.40
1:H:39:GLN:O	1:H:88:ALA:HB1	2.21	0.40
3:T:393:THR:HG21	3:T:518:LEU:H	1.86	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	H	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
2	L	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
3	T	201/1244 (16%)	175 (87%)	26 (13%)	0	100	100
All	All	435/1482 (29%)	379 (87%)	56 (13%)	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	H	102/102 (100%)	102 (100%)	0	100	100
2	L	88/88 (100%)	87 (99%)	1 (1%)	65	74
3	T	176/1078 (16%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	366/1268 (29%)	365 (100%)	1 (0%)	84	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	94	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	G	1	4,1	14,14,15	0.63	1 (7%)	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.49	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
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	-2.15	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

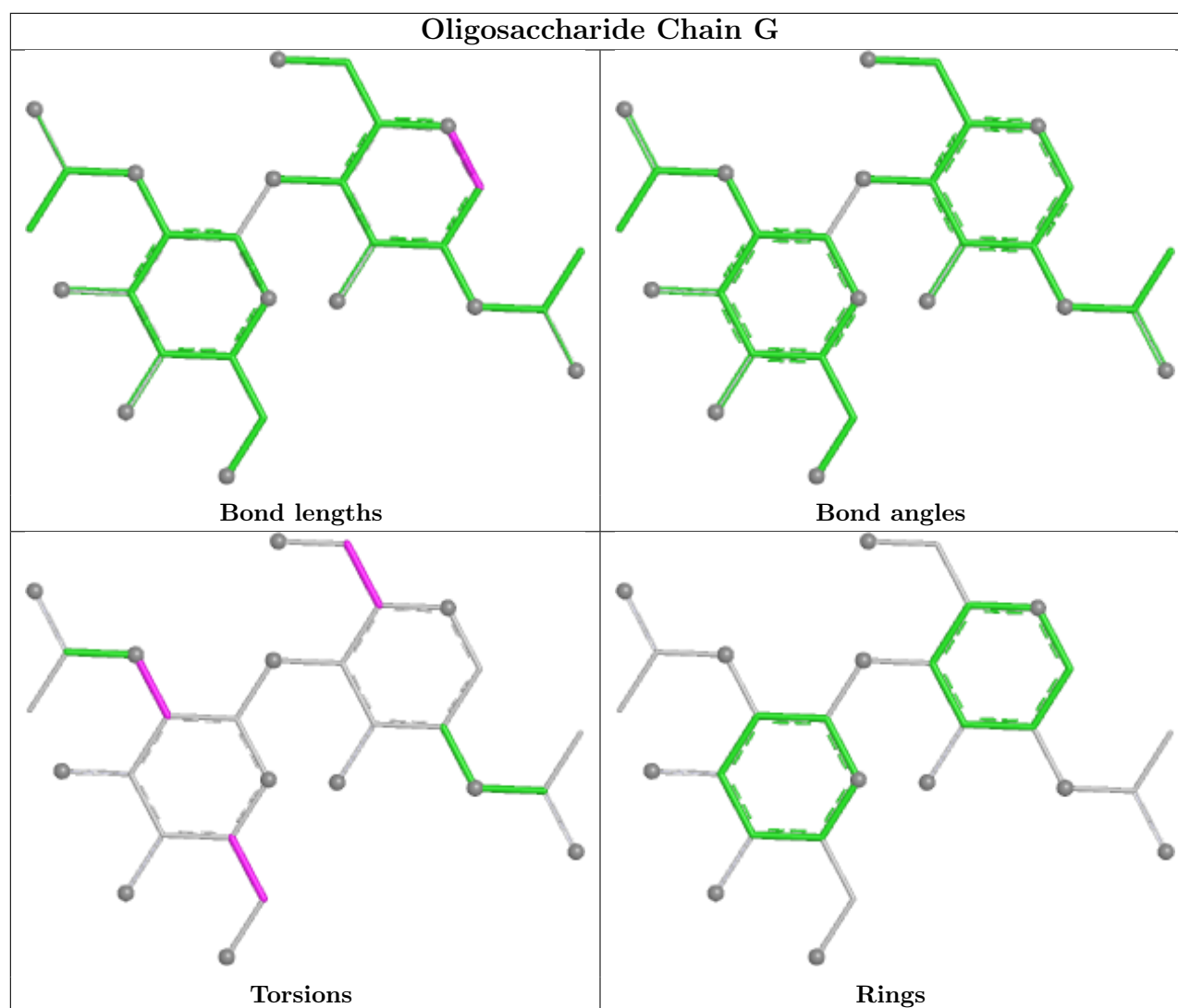
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7

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](#)

1 ligand is 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	$\# Z > 2$
5	NAG	T	1301	3	14,14,15	0.20	0	17,19,21	0.44	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
5	NAG	T	1301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

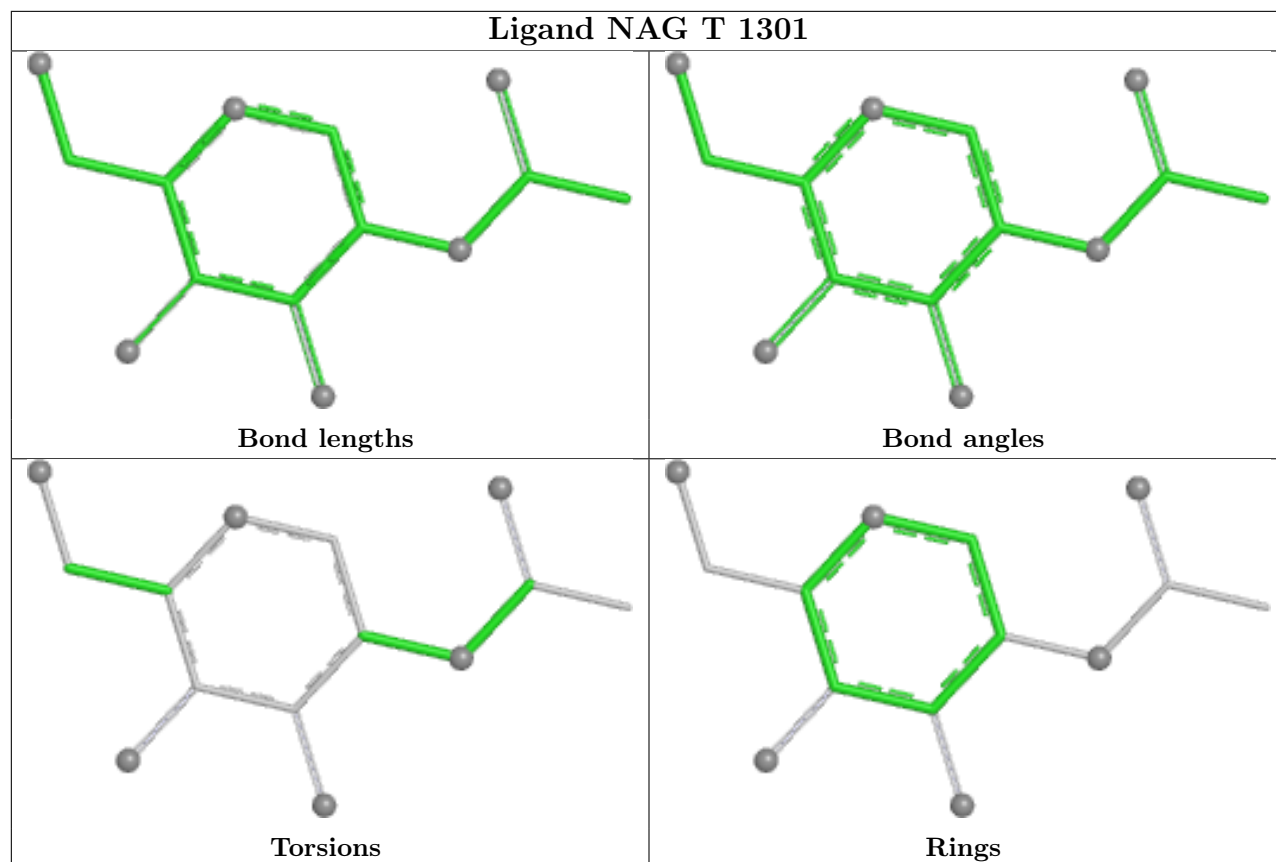
There are no chirality outliers.

There are no torsion outliers.

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 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.

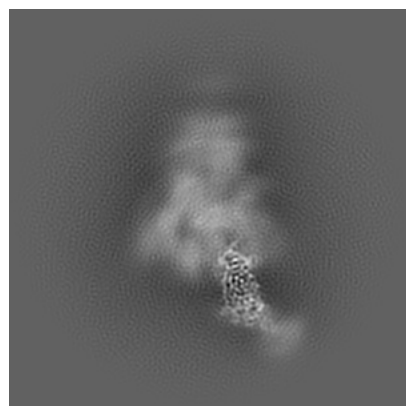
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44666. These allow visual inspection of the internal detail of the map and identification of artifacts.

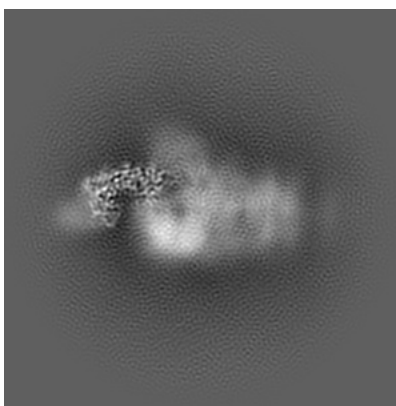
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

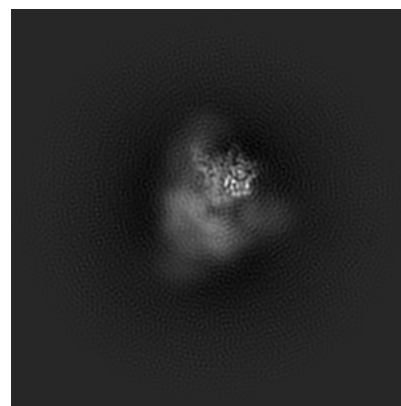
6.1.1 Primary map



X

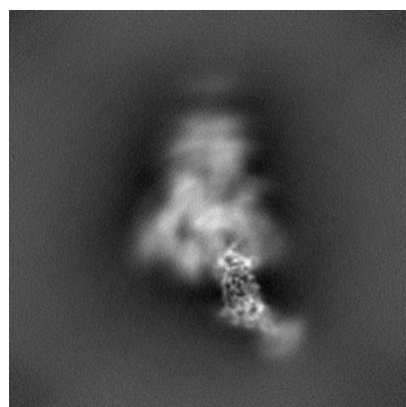


Y

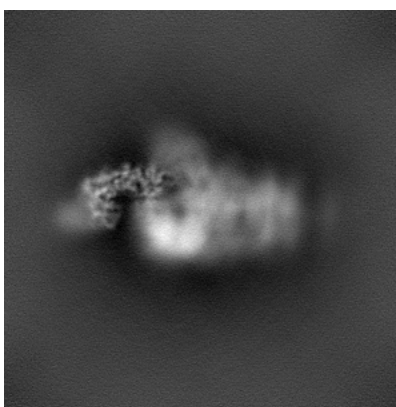


Z

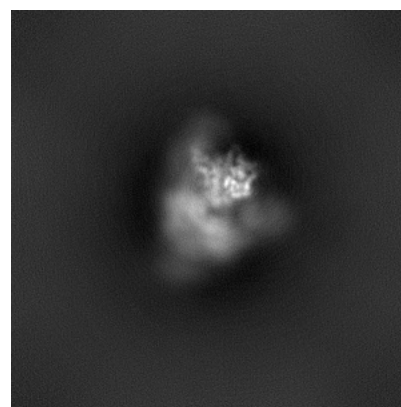
6.1.2 Raw map



X



Y

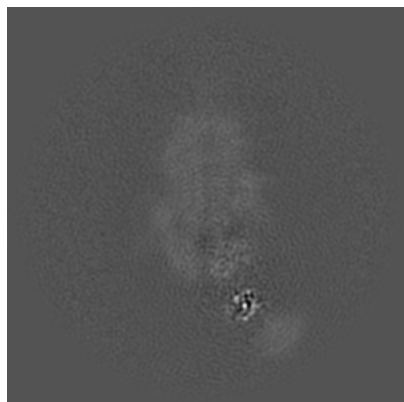


Z

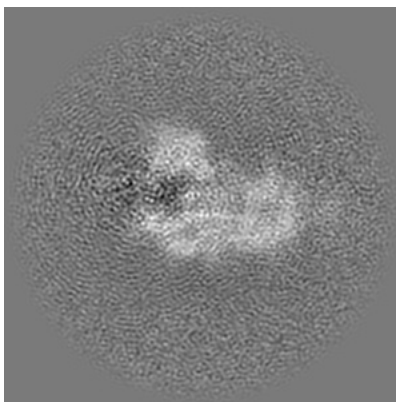
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

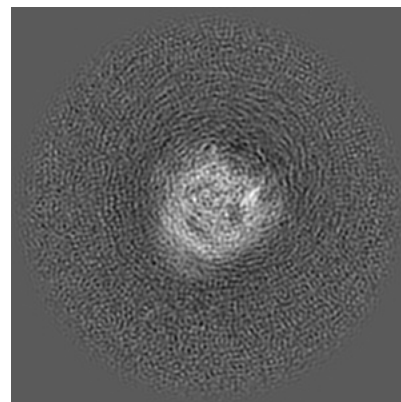
6.2.1 Primary map



X Index: 200



Y Index: 200

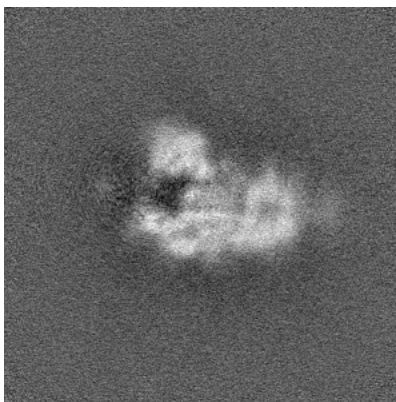


Z Index: 200

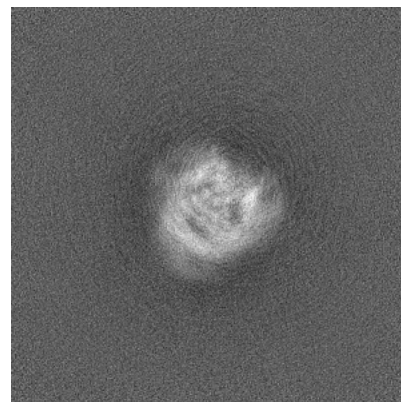
6.2.2 Raw map



X Index: 200



Y Index: 200

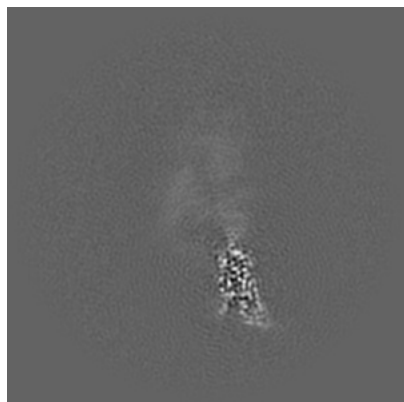


Z Index: 200

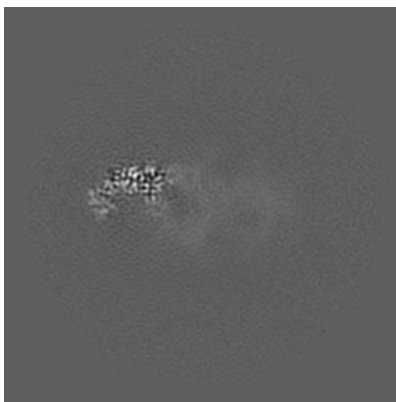
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

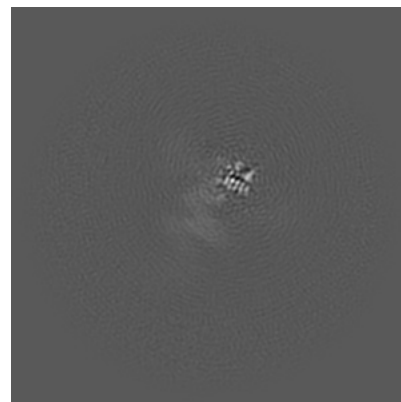
6.3.1 Primary map



X Index: 228

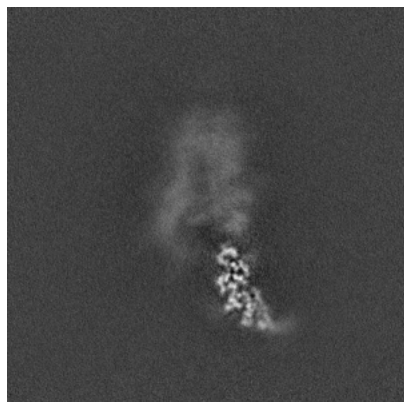


Y Index: 227

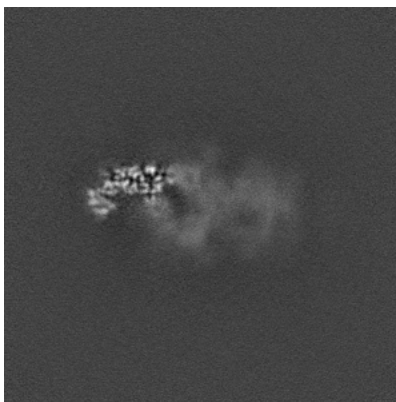


Z Index: 142

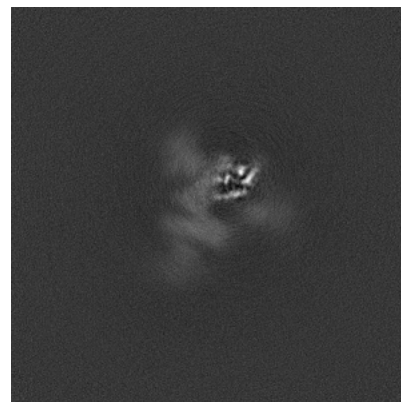
6.3.2 Raw map



X Index: 221



Y Index: 227

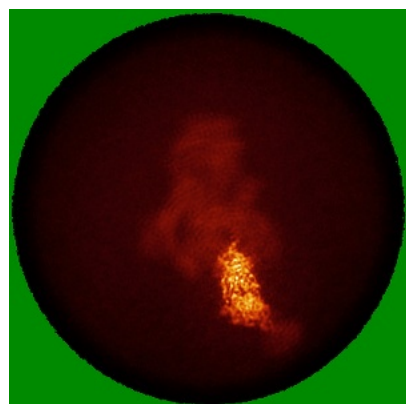


Z Index: 149

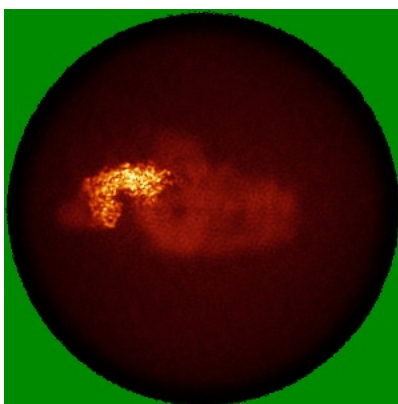
The images above show the largest variance slices of the map in three orthogonal directions.

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

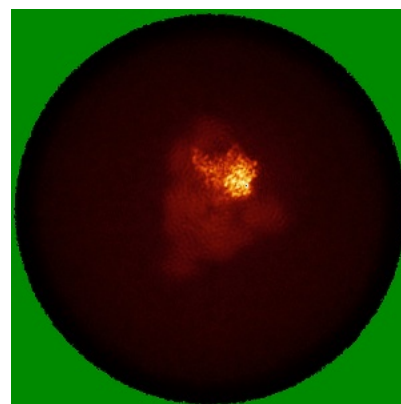
6.4.1 Primary map



X



Y

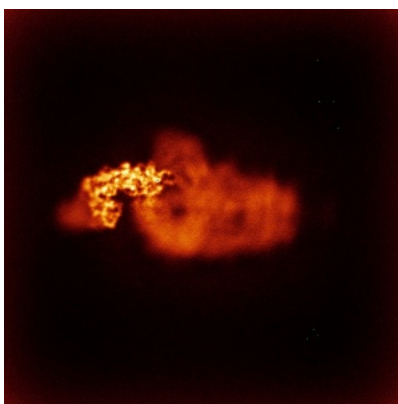


Z

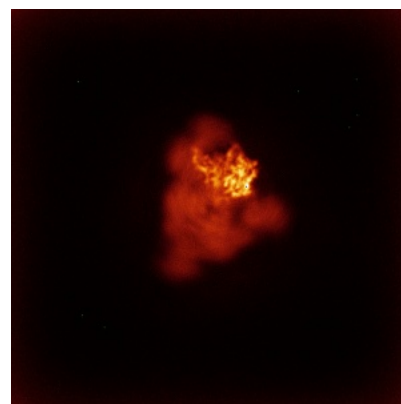
6.4.2 Raw map



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.

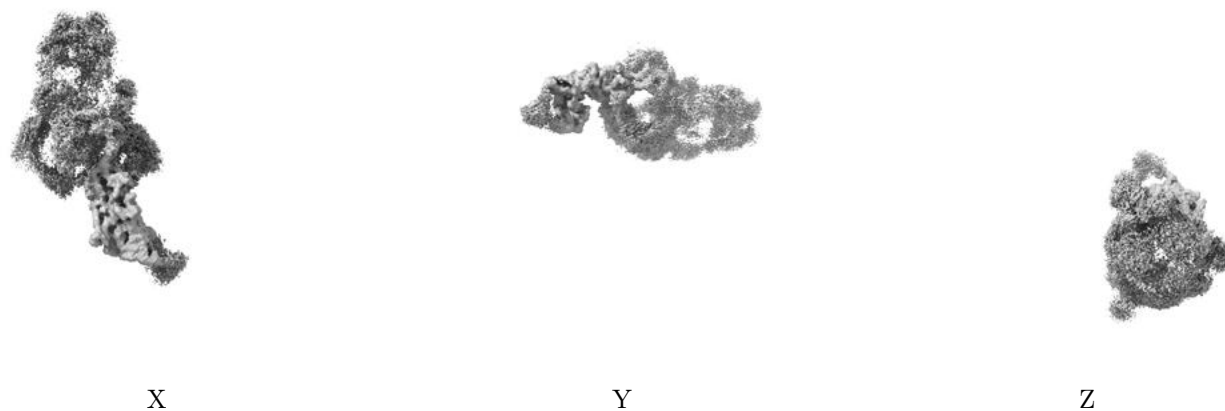
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. 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.

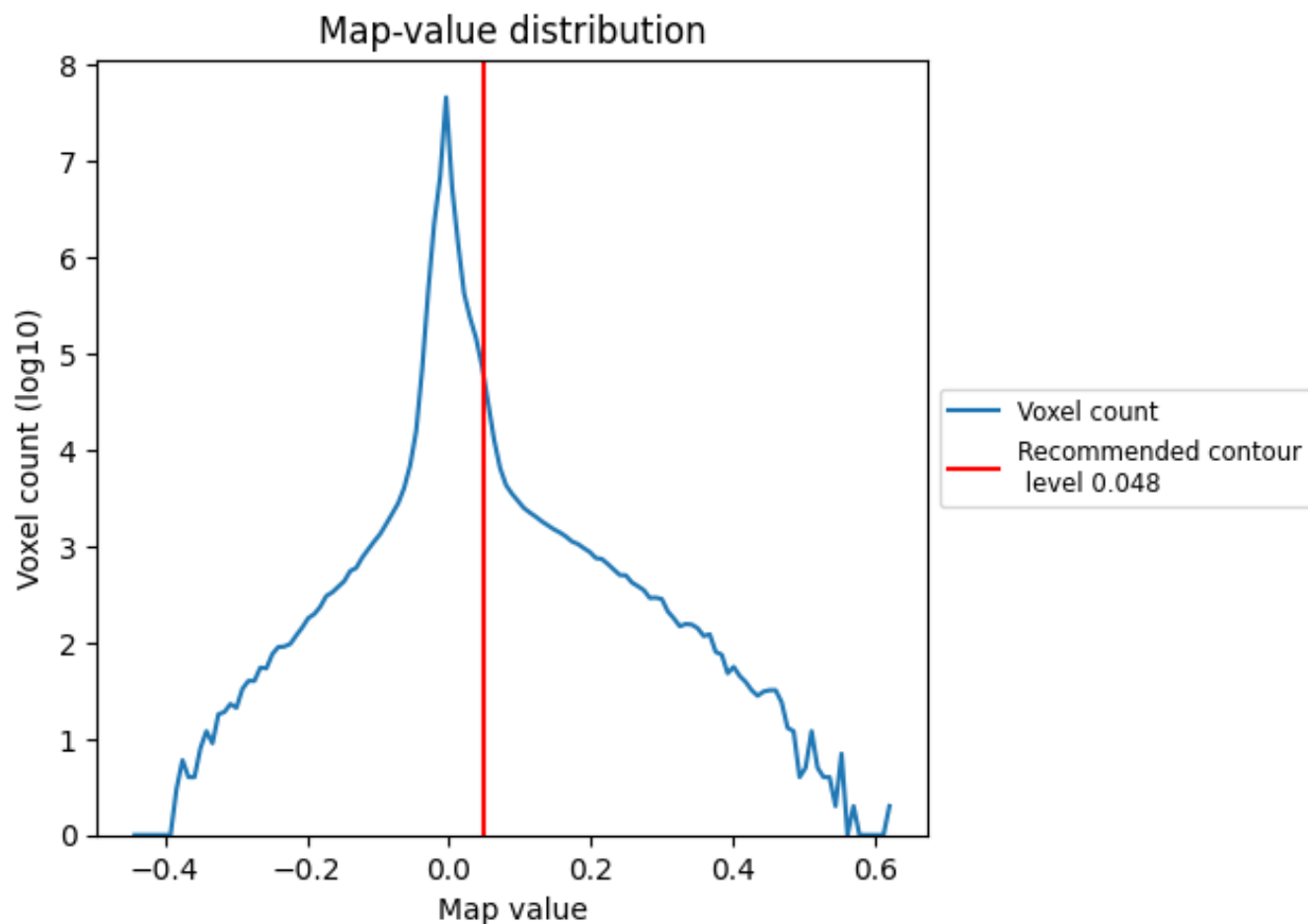
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

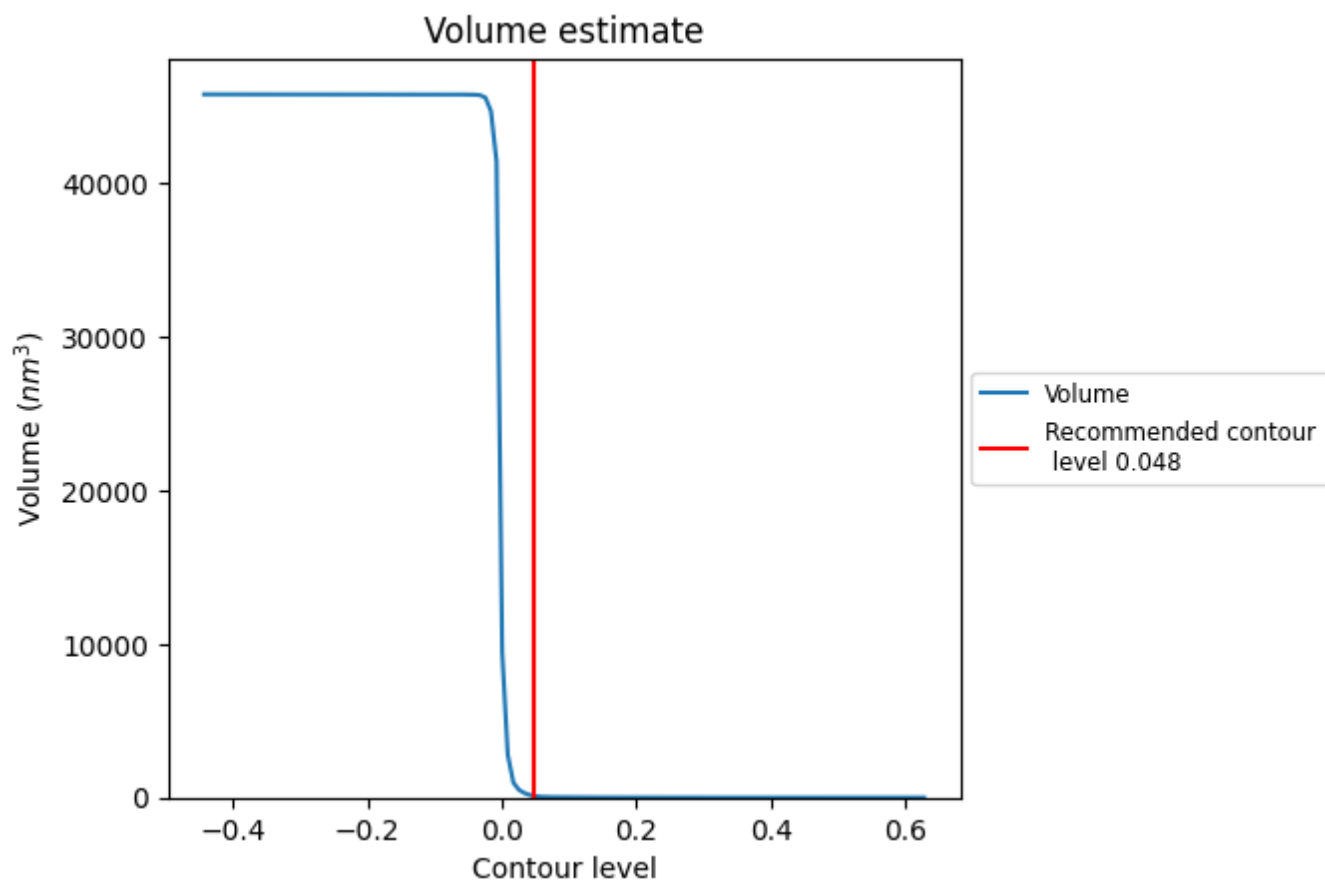
This section contains the results of statistical analysis of the map.

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.

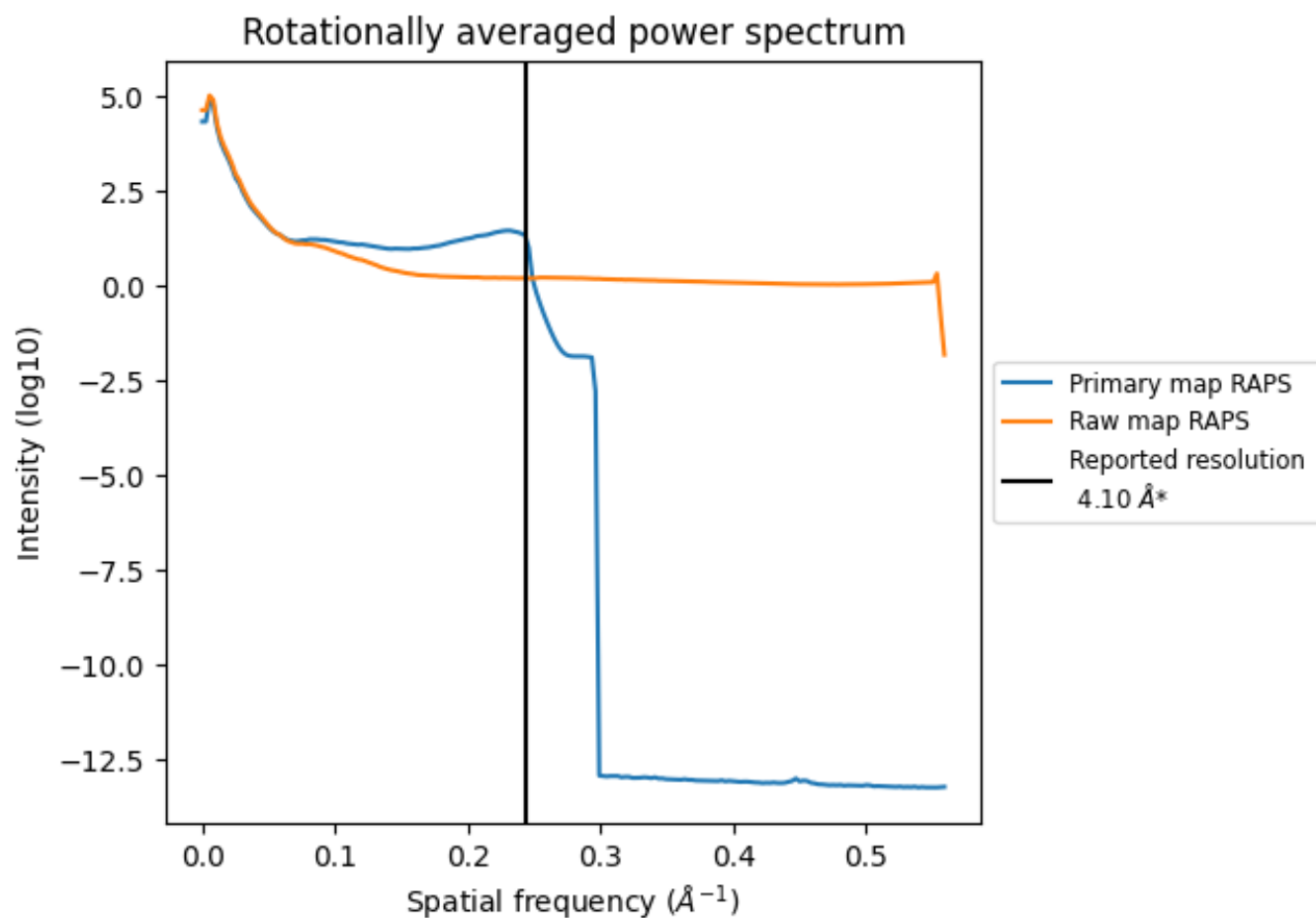
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 97 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 ⓘ

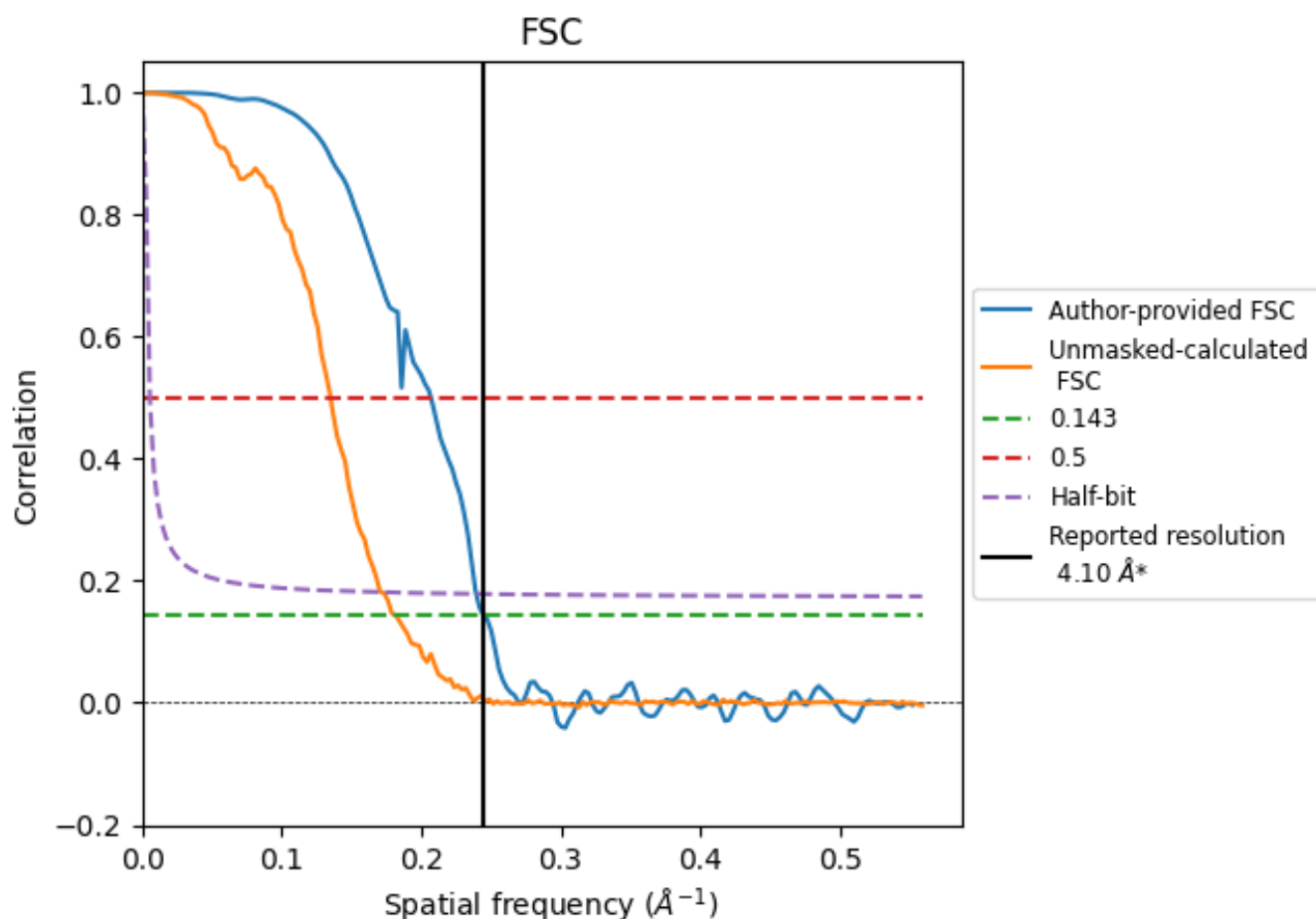


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.83	4.18
Unmasked-calculated*	5.50	7.41	5.82

*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 5.50 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

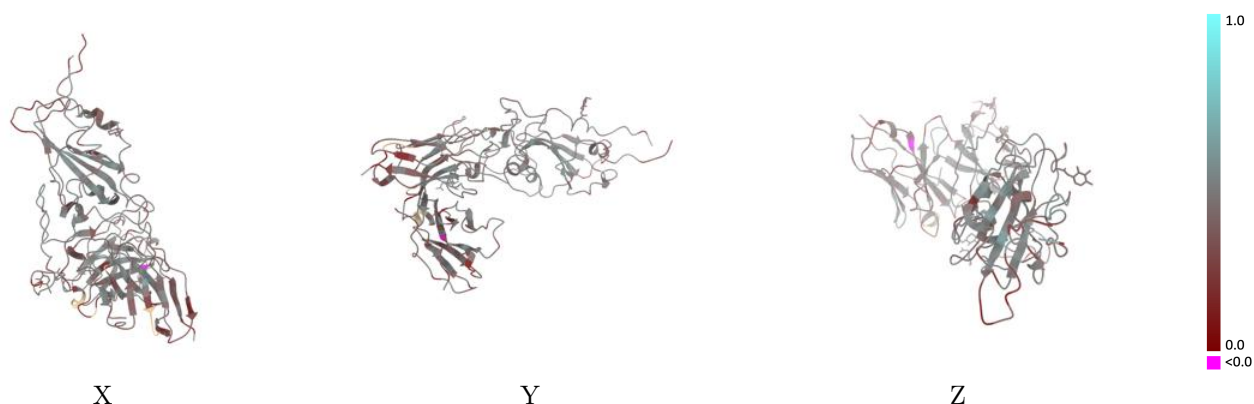
This section contains information regarding the fit between EMDB map EMD-44666 and PDB model 9BLL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



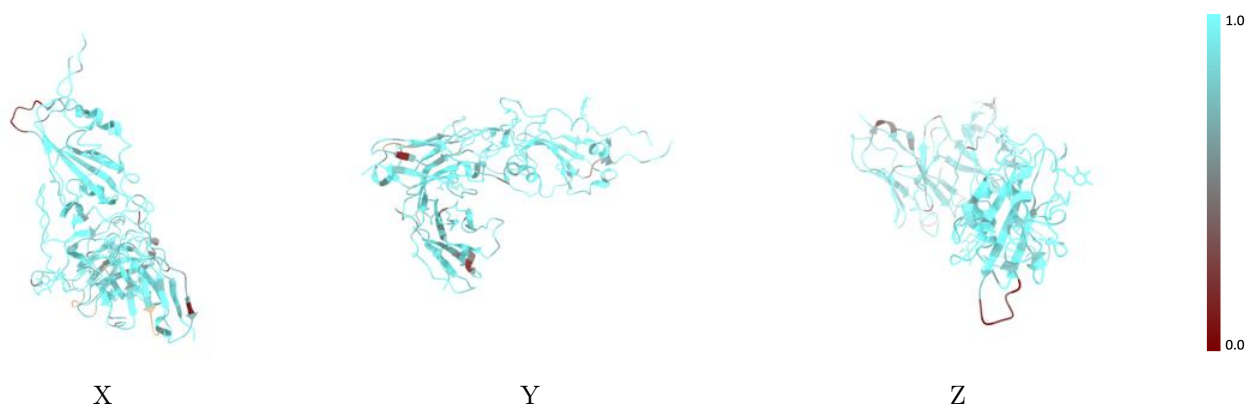
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



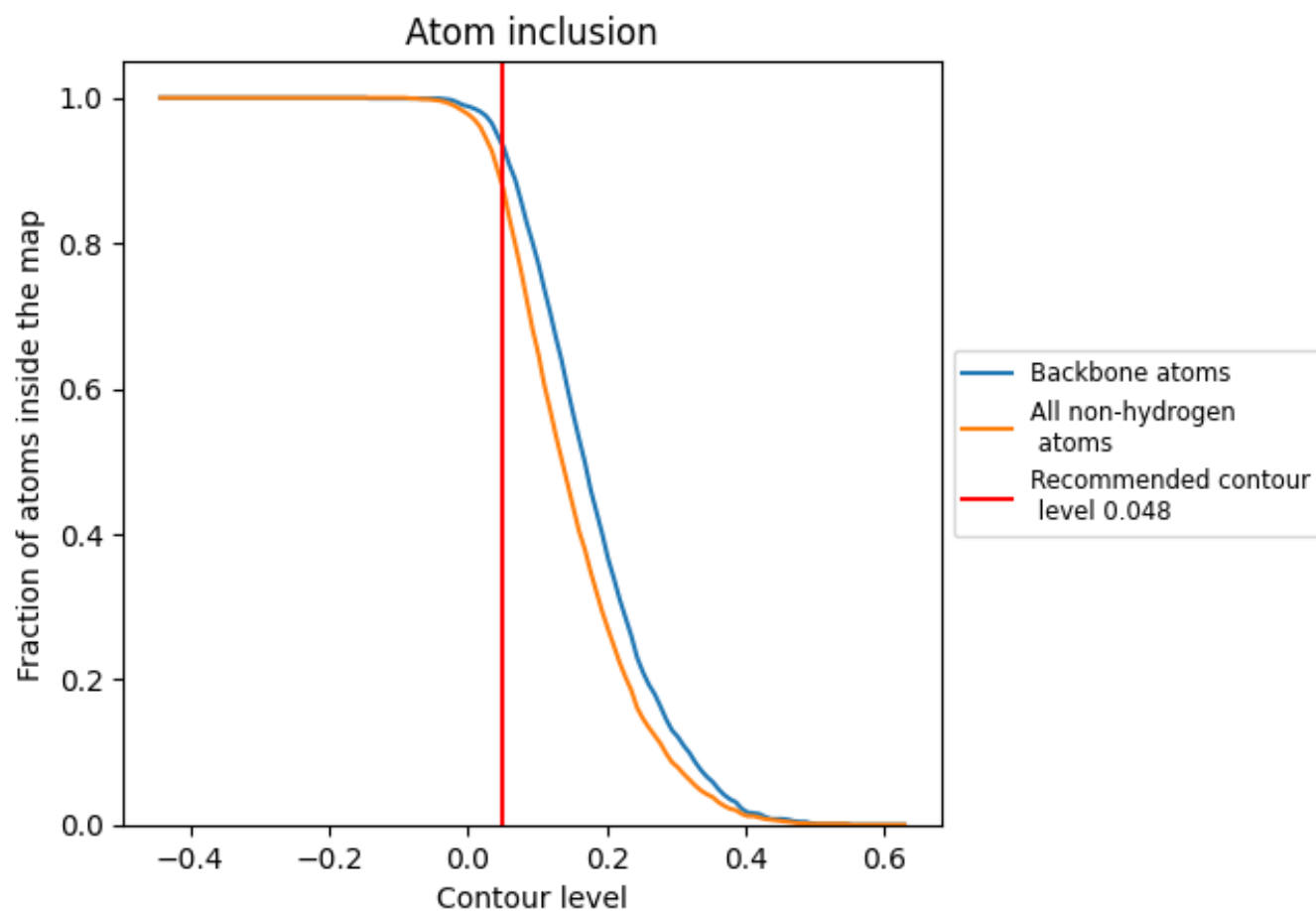
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.048).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.4220
G	0.9640	0.4560
H	0.8770	0.4190
L	0.8540	0.3910
T	0.8990	0.4380

