



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:04 AM JST

PDB ID : 7X8Z
EMDB ID : EMD-33061
Title : The SARS-CoV-2 receptor binding domain bound with the Fab fragment of a human neutralizing antibody Ab188
Authors : Kamada, K.; Shirouzu, M.
Deposited on : 2022-03-15
Resolution : 4.10 Å(reported)
Based on initial model : 5CCK

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

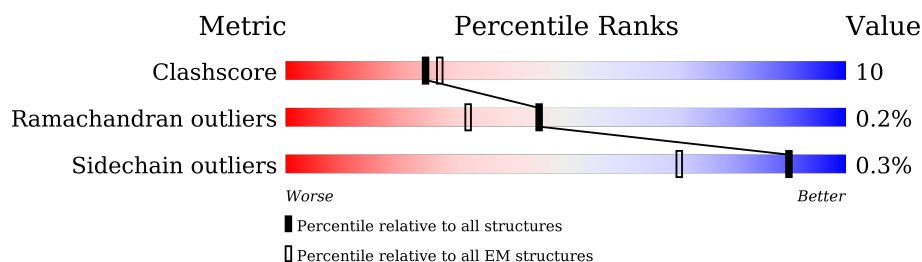
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1278	 13% . 85%
2	H	265	 5% 33% 12% 55%
3	L	248	 8% 34% 11% 55%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6493 atoms, of which 3160 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	194	Total	C	H	N	O	S	0	0
			2988	985	1452	256	287	8		

There are 79 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	ALA	-	expression tag	UNP P0DTC2
A	1210	ALA	-	expression tag	UNP P0DTC2
A	1211	ALA	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	SER	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ARG	-	expression tag	UNP P0DTC2
A	1246	GLU	-	expression tag	UNP P0DTC2
A	1247	ASN	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	TYR	-	expression tag	UNP P0DTC2
A	1250	PHE	-	expression tag	UNP P0DTC2
A	1251	GLN	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	LEU	-	expression tag	UNP P0DTC2
A	1259	ASN	-	expression tag	UNP P0DTC2
A	1260	ASP	-	expression tag	UNP P0DTC2
A	1261	ILE	-	expression tag	UNP P0DTC2
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	ALA	-	expression tag	UNP P0DTC2
A	1265	GLN	-	expression tag	UNP P0DTC2
A	1266	LYS	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2

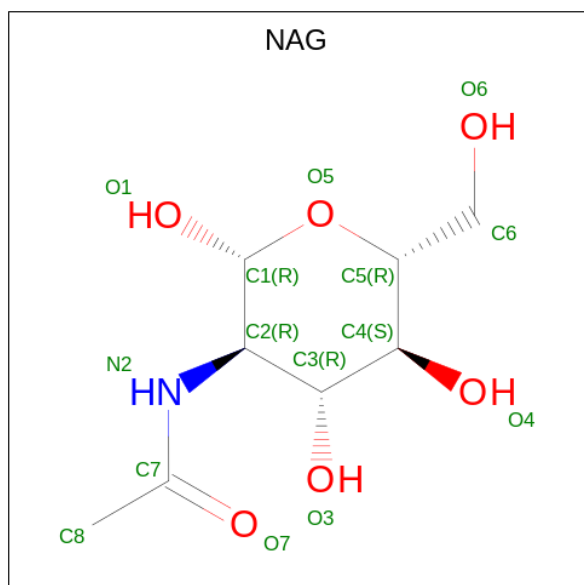
- Molecule 2 is a protein called Ab188 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	120	Total	C	H	N	O	S	0	0
			1789	575	871	156	181	6		

- Molecule 3 is a protein called Ab188 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	112	Total	C	H	N	O	S	0	0
			1689	546	824	142	174	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

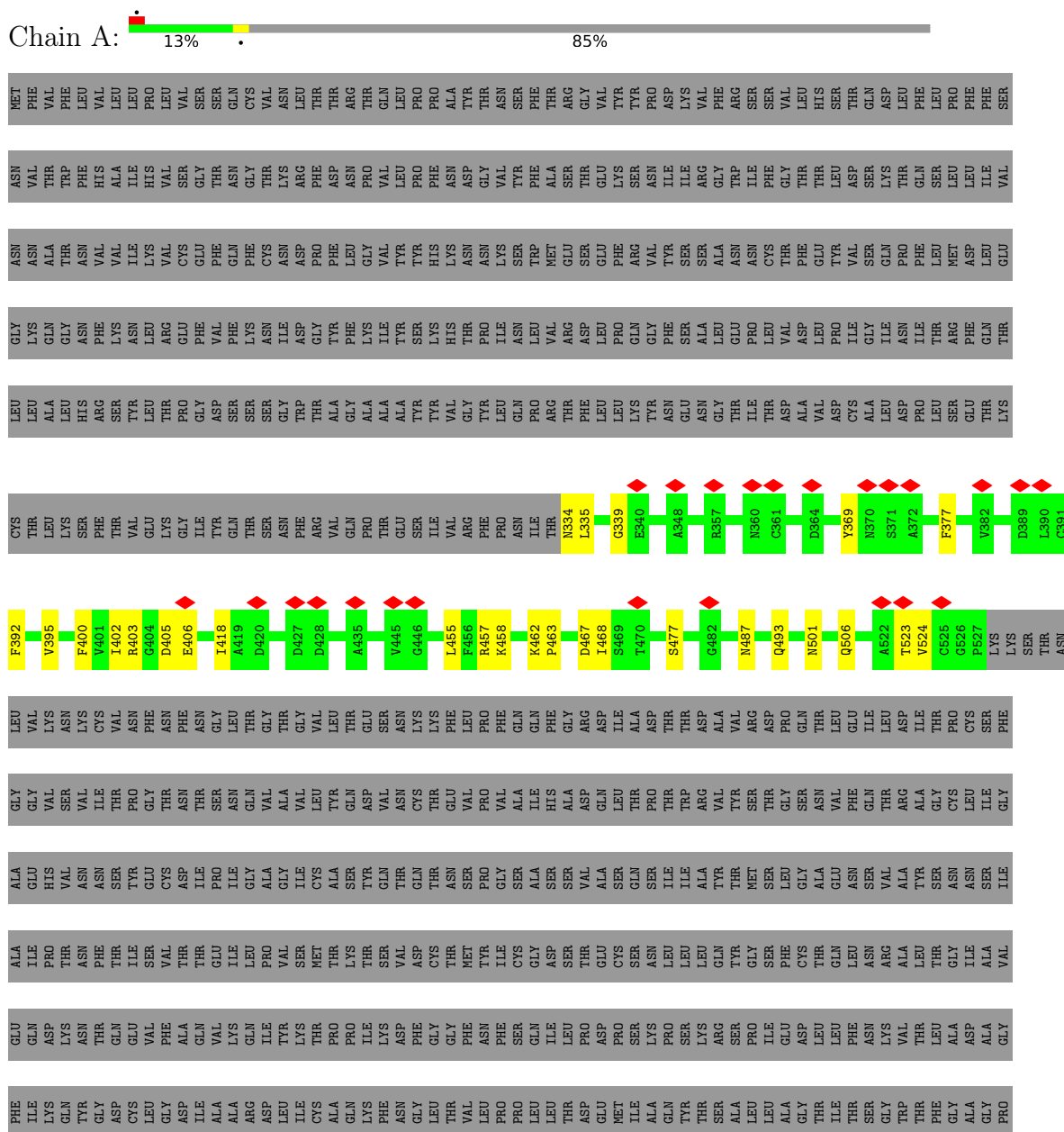


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
4	A	1	27	8	13	1	5	0

3 Residue-property plots

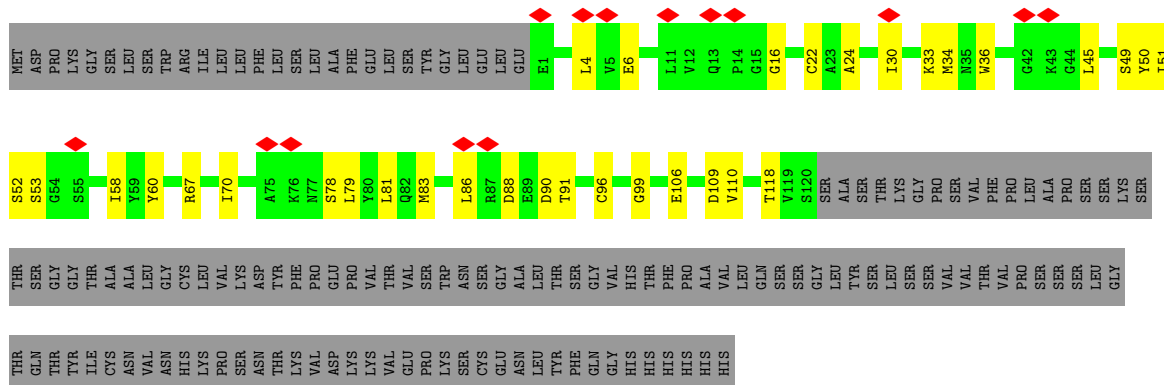
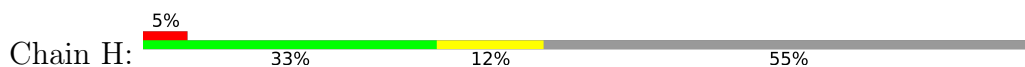
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

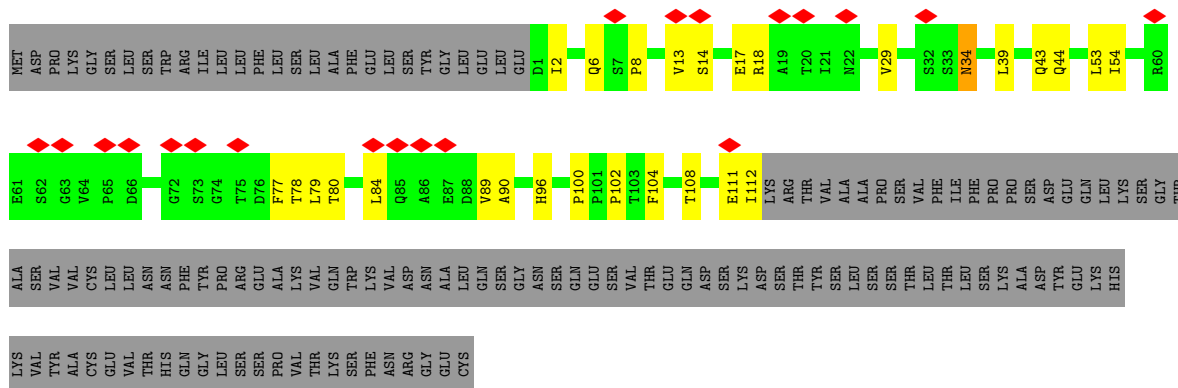
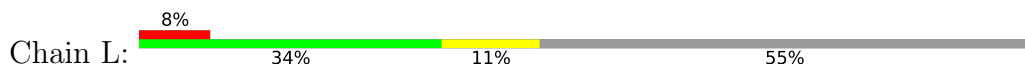


GLY	LEU	VAL	LYS	ILE	ASN	ALA
GLY	ASN	ASN	ASN	ARG	GLN	ALA
GLY	GLU	ASN	PHE	LEU	ASN	LEU
SER	SER	THR	THR	GLU	ALA	ILE
LEU	ILE	TYR	ALA	ILE	ALA	PHE
ASN	ASP	ASP	PRO	ARG	LEU	PRO
ASP	LEU	PRO	GLY	ARG	ASN	MET
ILE	GLN	GLN	ILE	SER	THR	GLN
PHE	GLU	GLN	CYS	ALA	LEU	MET
GLU	LEU	PRO	HIS	ASN	VAL	ALA
ALA	GLY	GLU	ASP	LEU	LYS	TYR
GLN	LYS	LEU	GLY	ALA	GLN	ARG
LYS	TYR	ASP	LYS	ALA	LEU	PHE
ILE	GLU	SER	ALA	THR	SER	ASN
GLU	GLN	PHE	GLN	LYS	GLY	GLY
TRP	ALA	LYS	PHE	MET	ASN	ILE
HIS	ALA	GLU	PRO	SER	PHE	GLY
GLU	ALA	GLU	ARG	GLU	GLY	VAL
GLY	GLY	GLU	LEU	CYS	ALA	THR
HIS	SER	ASP	GLY	VAL	ILE	GLN
HIS	GLY	ASP	VAL	LEU	SER	ASN
HIS	TYR	TYR	PHE	GLY	SER	VAL
ILE	TYR	PHE	VAL	GLN	VAL	LEU
PRO	LYS	SER	SER	SER	LEU	TYR
GLU	ASN	GLU	ASN	LYS	ASN	ASN
ALA	HIS	HIS	GLY	ARG	ASP	GLN
PRO	PRO	THR	VAL	VAL	ILE	GLN
ARG	SER	SER	HIS	ASP	LEU	LYS
ASP	PRO	PRO	TRP	PHE	SER	LEU
GLY	ASP	ASP	PHE	CYS	ARG	ILE
ALA	VAL	VAL	VAL	GLY	LEU	ALA
TYR	ALA	ASP	THR	LYS	ASP	ASN
TYR	VAL	LEU	GLN	GLY	PRO	GLN
VAL	GLY	GLY	ARG	TYR	PRO	PHE
ARG	ASP	ASP	ASN	HIS	GLU	ASN
LYS	ILE	ILE	PHE	LEU	ALA	SER
ASP	SER	SER	TYR	MET	GLU	ALA
GLY	GLY	GLY	GLU	SER	VAL	ILE
GLU	ILE	ILE	PRO	PHE	GLN	GLY
TRP	VAL	ASN	GLN	PRO	ILE	LYS
VAL	ALA	ALA	ILE	GLN	ASP	ILE
LEU	SER	LEU	ILE	SER	ARG	GLN
LEU	VAL	VAL	THR	ALA	LEU	ASP
THR	VAL	VAL	THR	PRO	ILE	SER
THR	ASN	ASN	ASN	HIS	THR	LEU
PHE	ILE	ILE	ASN	GLY	GLY	SER
LEU	LYS	GLN	THR	VAL	ARG	SER
GLY	GLY	LYS	PHE	VAL	LEU	THR
SER	SER	VAL	VAL	PHE	GLN	PRO
SER	ILE	ILE	SER	SER	LEU	ALA
GLY	GLY	ASP	GLY	HIS	LEU	LEU
ARG	ARG	ARG	ASN	VAL	GLN	LEU
GLU	LEU	LEU	CYS	THR	THR	GLY
ASN	ASN	VAL	VAL	TYR	TYR	LYS
LEU	GLU	GLU	VAL	VAL	VAL	LYS
TYR	TYR	VAL	THR	PRO	THR	GLN
PHE	PHE	ALA	ILE	ALA	ASP	ASN
GLN	GLY	LYS	THR	GLN	GLN	VAL
HIS	HIS	ASN	TYR	GLU	LEU	VAL

- Molecule 2: Ab188 heavy chain



- Molecule 3: Ab188 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0107	Depositor
Map size (Å)	130.982, 130.982, 130.982	wwPDB
Map dimensions	158, 158, 158	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82899994, 0.82899994, 0.82899994	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	A	0.27	0/1580	0.50	0/2151
2	H	0.26	0/937	0.54	0/1267
3	L	0.27	0/888	0.50	0/1210
All	All	0.27	0/3405	0.51	0/4628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1536	1452	1452	20	0
2	H	918	871	873	25	0
3	L	865	824	827	25	0
4	A	14	13	13	1	0
All	All	3333	3160	3165	67	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 10.

All (67) 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)
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.65	0.76
2:H:91:THR:OG1	2:H:118:THR:OG1	2.08	0.70
2:H:109:ASP:OD1	2:H:110:VAL:N	2.23	0.69
2:H:83:MET:HG2	2:H:86:LEU:HD21	1.73	0.68
2:H:45:LEU:HD23	3:L:104:PHE:CD1	2.32	0.64
3:L:2:ILE:HG21	3:L:96:HIS:CD2	2.34	0.63
2:H:88:ASP:O	2:H:91:THR:HG22	1.99	0.62
2:H:50:TYR:OH	2:H:106:GLU:OE1	2.15	0.61
2:H:34:MET:SD	2:H:79:LEU:HD23	2.42	0.59
2:H:45:LEU:HD23	3:L:104:PHE:HD1	1.65	0.59
3:L:29:VAL:HG22	3:L:96:HIS:HE1	1.68	0.58
3:L:17:GLU:O	3:L:84:LEU:N	2.36	0.58
2:H:58:ILE:HG22	2:H:60:TYR:CE1	2.39	0.57
3:L:111:GLU:OE2	3:L:112:ILE:HG23	2.04	0.57
3:L:29:VAL:HG22	3:L:96:HIS:CE1	2.40	0.57
3:L:43:GLN:HE21	3:L:90:ALA:HB3	1.69	0.57
2:H:33:LYS:O	2:H:99:GLY:N	2.38	0.56
1:A:400:PHE:HB3	1:A:402:ILE:HD11	1.87	0.55
1:A:487:ASN:N	2:H:106:GLU:OE2	2.39	0.55
3:L:111:GLU:CD	3:L:112:ILE:HG23	2.28	0.54
3:L:43:GLN:NE2	3:L:90:ALA:HB3	2.22	0.53
2:H:52:SER:OG	2:H:53:SER:N	2.42	0.53
1:A:392:PHE:O	1:A:523:THR:N	2.38	0.52
1:A:405:ASP:OD1	1:A:406:GLU:N	2.42	0.52
1:A:457:ARG:NH1	1:A:467:ASP:OD1	2.43	0.52
2:H:51:ILE:HD12	2:H:70:ILE:HG22	1.92	0.52
3:L:39:LEU:HD13	3:L:77:PHE:CE2	2.45	0.52
1:A:468:ILE:HG23	1:A:468:ILE:O	2.09	0.52
3:L:13:VAL:HG11	3:L:18:ARG:O	2.10	0.51
2:H:36:TRP:CD1	2:H:81:LEU:HD12	2.45	0.51
3:L:53:LEU:O	3:L:54:ILE:HD13	2.11	0.51
2:H:22:CYS:O	2:H:78:SER:OG	2.14	0.51
1:A:501:ASN:O	1:A:506:GLN:NE2	2.46	0.48
3:L:6:GLN:NE2	3:L:108:THR:HG23	2.28	0.48
2:H:16:GLY:O	2:H:86:LEU:HD23	2.14	0.48
3:L:79:LEU:HD23	3:L:80:THR:N	2.29	0.48
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.47	0.47
1:A:524:VAL:HG13	1:A:524:VAL:O	2.14	0.47
1:A:462:LYS:HB2	1:A:463:PRO:HD2	1.97	0.47
2:H:58:ILE:HG22	2:H:58:ILE:O	2.14	0.47
3:L:43:GLN:OE1	3:L:53:LEU:HD11	2.15	0.46
3:L:44:GLN:O	3:L:90:ALA:HB1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:13:VAL:O	3:L:13:VAL:HG13	2.17	0.45
2:H:83:MET:HG2	2:H:86:LEU:HD11	1.99	0.45
3:L:89:VAL:O	3:L:89:VAL:HG23	2.17	0.45
2:H:6:GLU:OE2	2:H:96:CYS:N	2.50	0.44
3:L:34:ASN:O	3:L:34:ASN:ND2	2.46	0.44
1:A:402:ILE:HG23	1:A:418:ILE:CD1	2.46	0.44
1:A:339:GLY:HA2	4:A:1301:NAG:H83	2.00	0.44
2:H:4:LEU:HA	2:H:24:ALA:HB2	1.99	0.43
2:H:83:MET:CG	2:H:86:LEU:HD11	2.49	0.43
1:A:334:ASN:O	1:A:335:LEU:HD22	2.19	0.43
1:A:455:LEU:HD22	1:A:493:GLN:OE1	2.18	0.42
1:A:400:PHE:CB	1:A:402:ILE:HD11	2.48	0.42
3:L:39:LEU:HD13	3:L:77:PHE:CD2	2.54	0.42
1:A:369:TYR:HB3	1:A:377:PHE:CE1	2.54	0.42
1:A:457:ARG:O	1:A:458:LYS:HG2	2.20	0.42
1:A:402:ILE:HG22	1:A:403:ARG:O	2.20	0.41
2:H:30:ILE:O	2:H:53:SER:OG	2.34	0.41
2:H:36:TRP:N	2:H:49:SER:OG	2.47	0.41
1:A:402:ILE:HG22	1:A:403:ARG:N	2.34	0.41
2:H:83:MET:SD	2:H:86:LEU:HD11	2.60	0.41
3:L:8:PRO:O	3:L:108:THR:HG22	2.21	0.41
3:L:14:SER:O	3:L:14:SER:OG	2.34	0.41
3:L:78:THR:HG22	3:L:79:LEU:N	2.36	0.40
3:L:100:PRO:O	3:L:102:PRO:HD3	2.21	0.40
1:A:402:ILE:HG23	1:A:418:ILE:HD13	2.03	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	192/1278 (15%)	170 (88%)	21 (11%)	1 (0%)	25 62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	118/265 (44%)	103 (87%)	15 (13%)	0	100	100
3	L	110/248 (44%)	93 (84%)	17 (16%)	0	100	100
All	All	420/1791 (24%)	366 (87%)	53 (13%)	1 (0%)	45	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	SER

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	167/1108 (15%)	167 (100%)	0	100	100
2	H	96/223 (43%)	96 (100%)	0	100	100
3	L	97/219 (44%)	96 (99%)	1 (1%)	73	81
All	All	360/1550 (23%)	359 (100%)	1 (0%)	90	92

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

Mol	Chain	Res	Type
3	L	34	ASN

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

Mol	Chain	Res	Type
3	L	6	GLN
3	L	96	HIS

5.3.3 RNA ⓘ

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](#)

There are no oligosaccharides in this entry.

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	$\# Z > 2$
4	NAG	A	1301	1	14,14,15	0.24	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
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

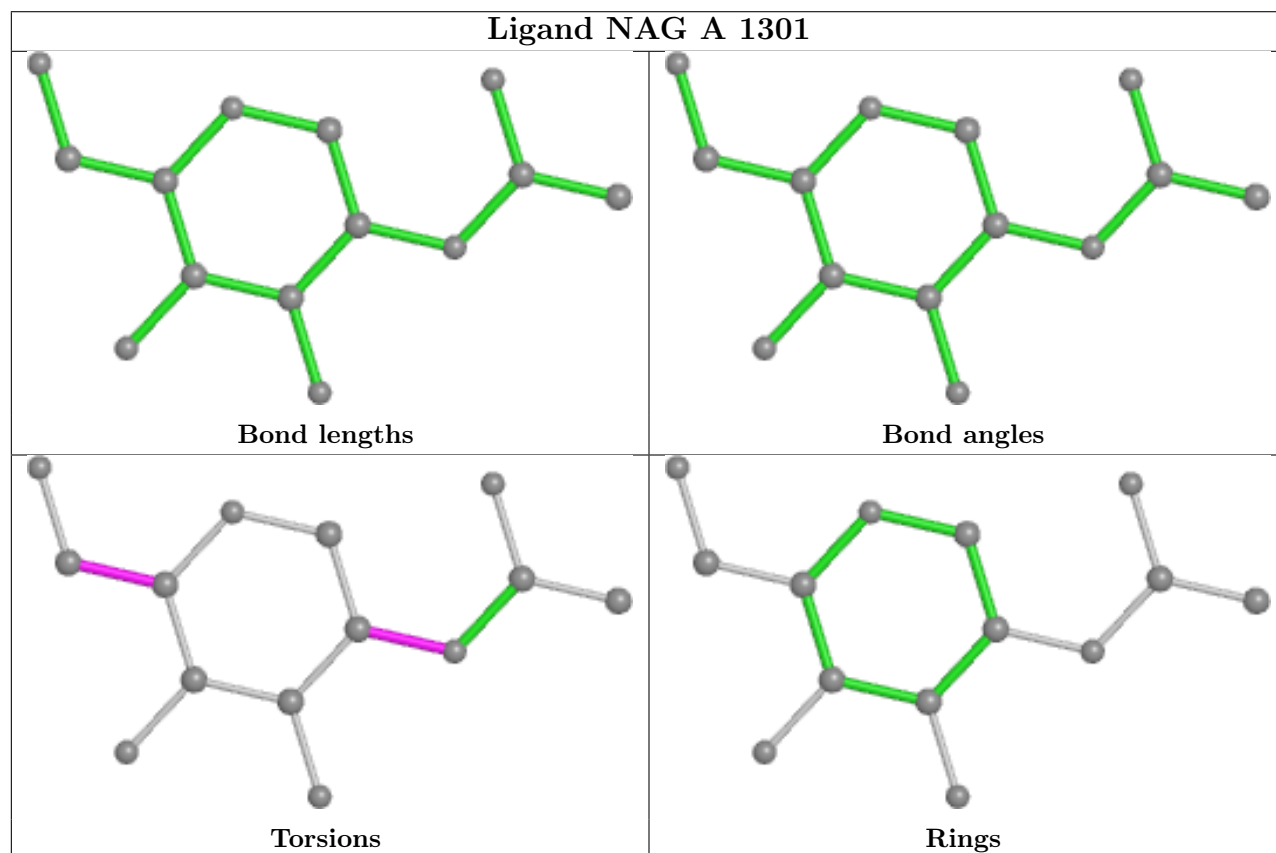
Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	O5-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C1-C2-N2-C7
4	A	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	NAG	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

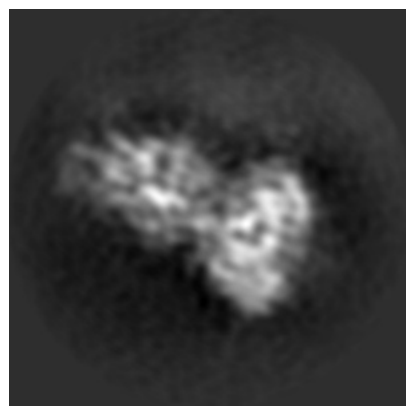
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33061. These allow visual inspection of the internal detail of the map and identification of artifacts.

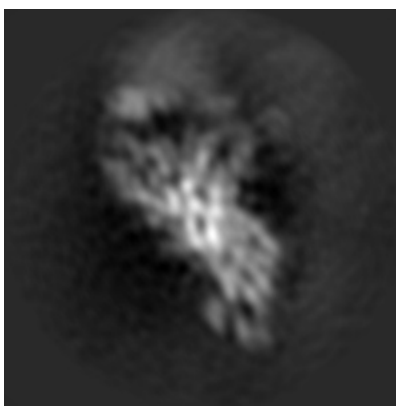
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

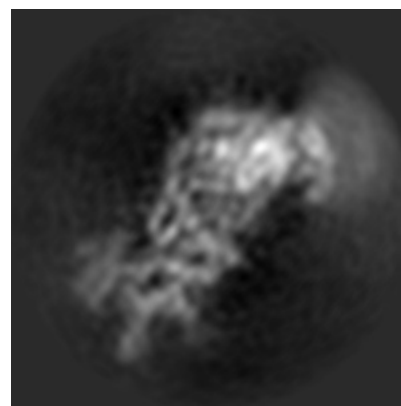
6.1.1 Primary map



X

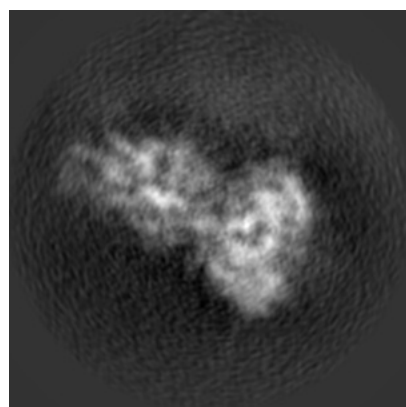


Y

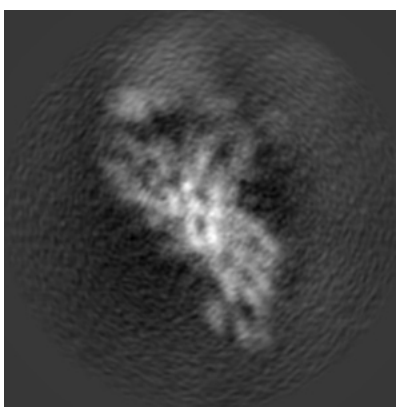


Z

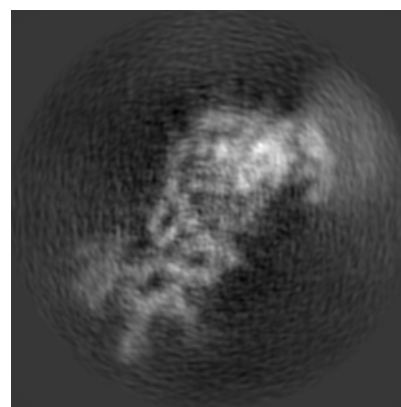
6.1.2 Raw map



X



Y

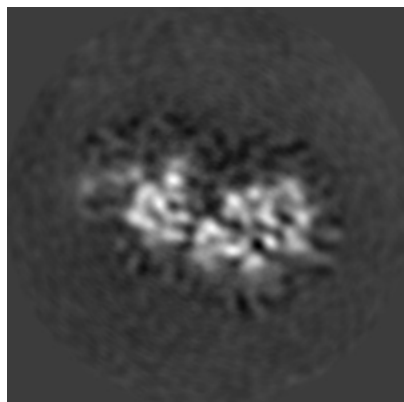


Z

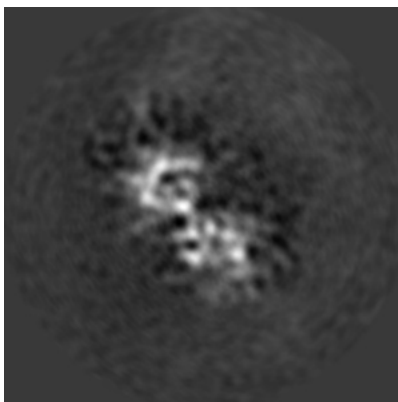
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

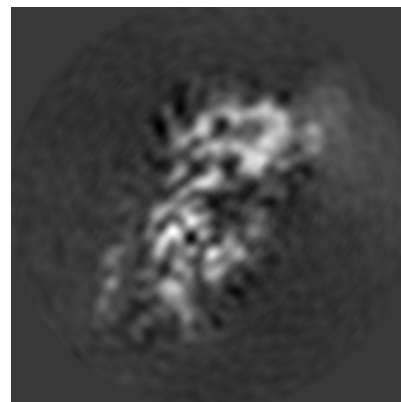
6.2.1 Primary map



X Index: 79

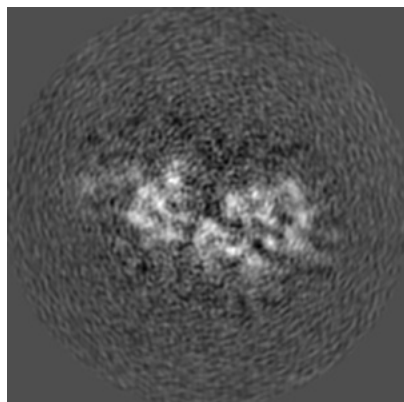


Y Index: 79

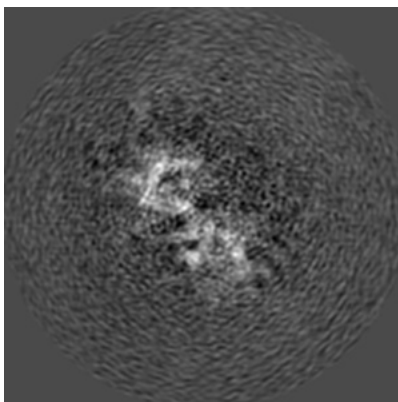


Z Index: 79

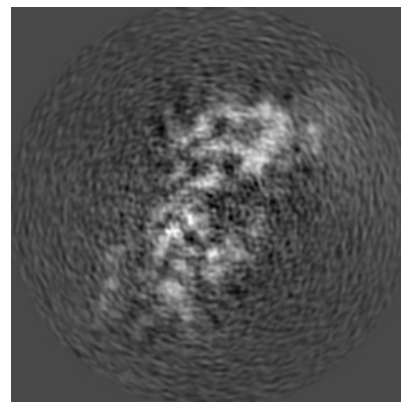
6.2.2 Raw map



X Index: 79



Y Index: 79

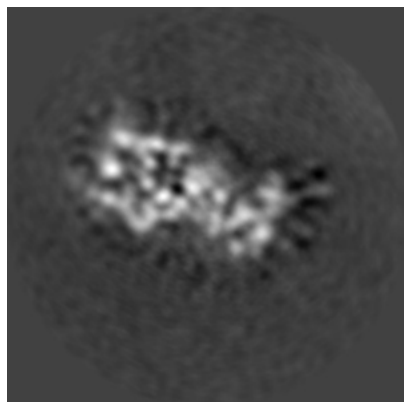


Z Index: 79

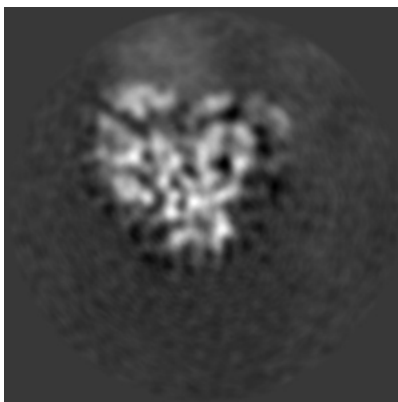
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

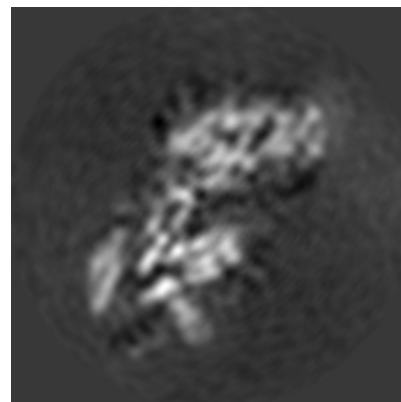
6.3.1 Primary map



X Index: 66

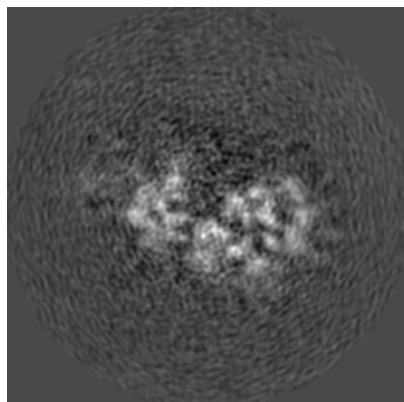


Y Index: 102

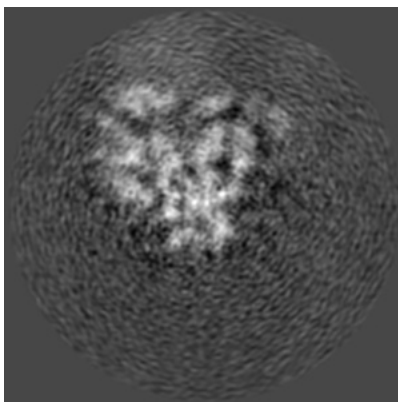


Z Index: 83

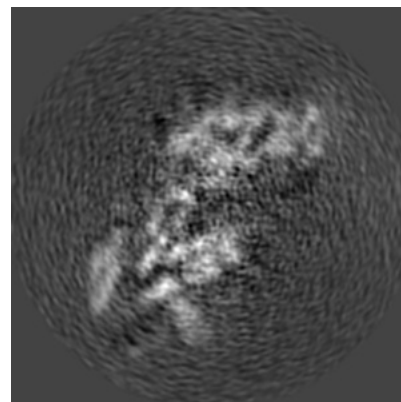
6.3.2 Raw map



X Index: 80



Y Index: 102

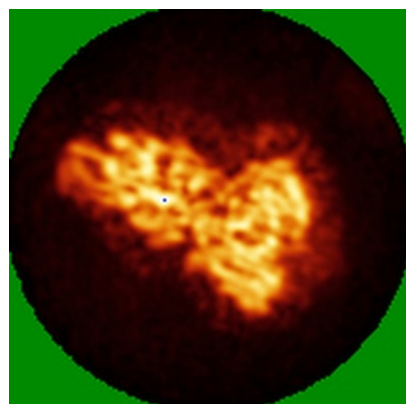


Z Index: 83

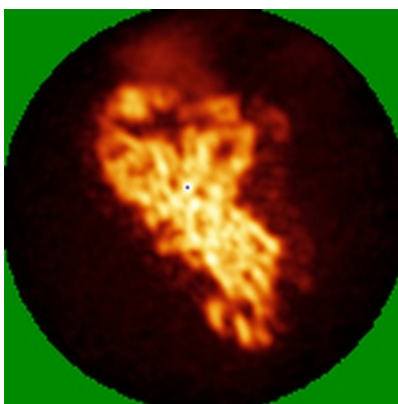
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

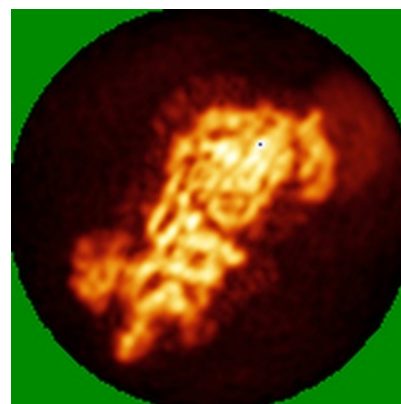
6.4.1 Primary map



X

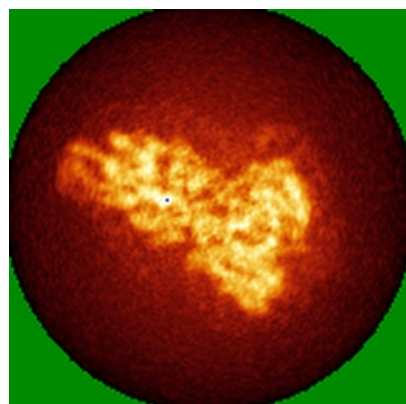


Y

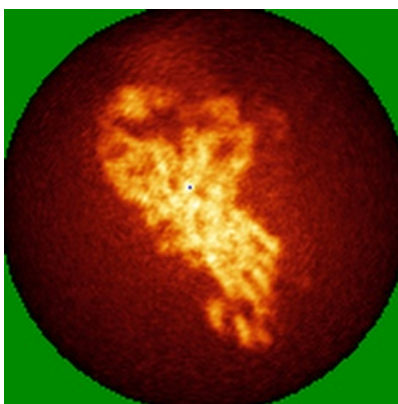


Z

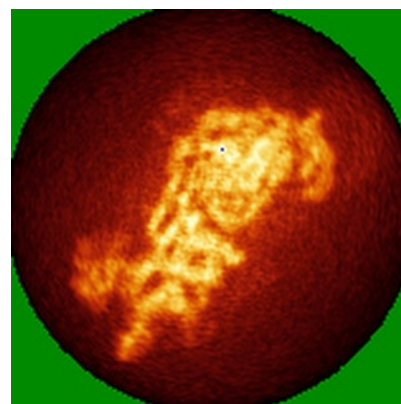
6.4.2 Raw map



X



Y

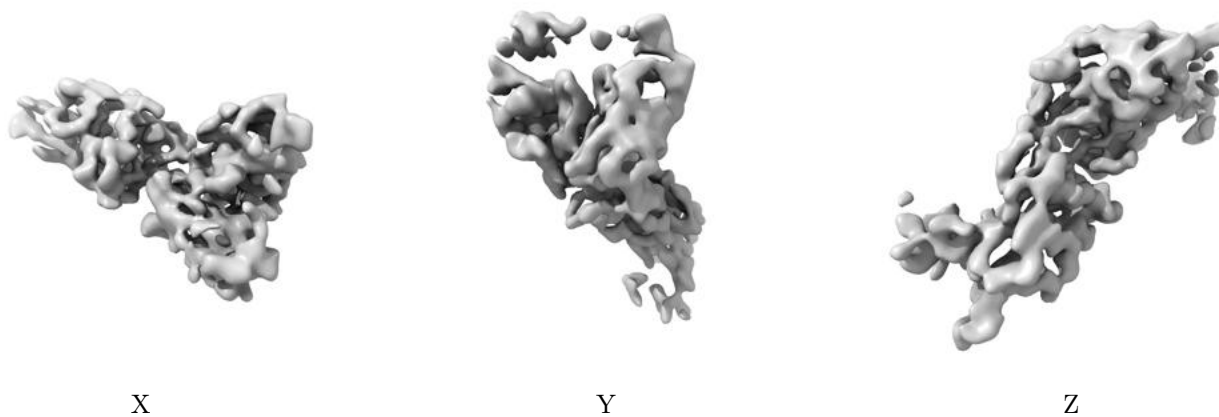


Z

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.

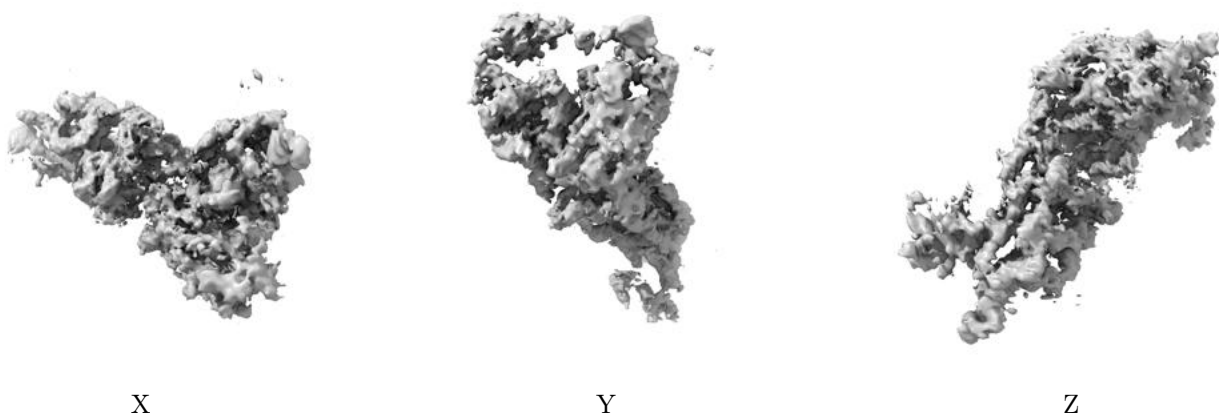
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0107. 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.

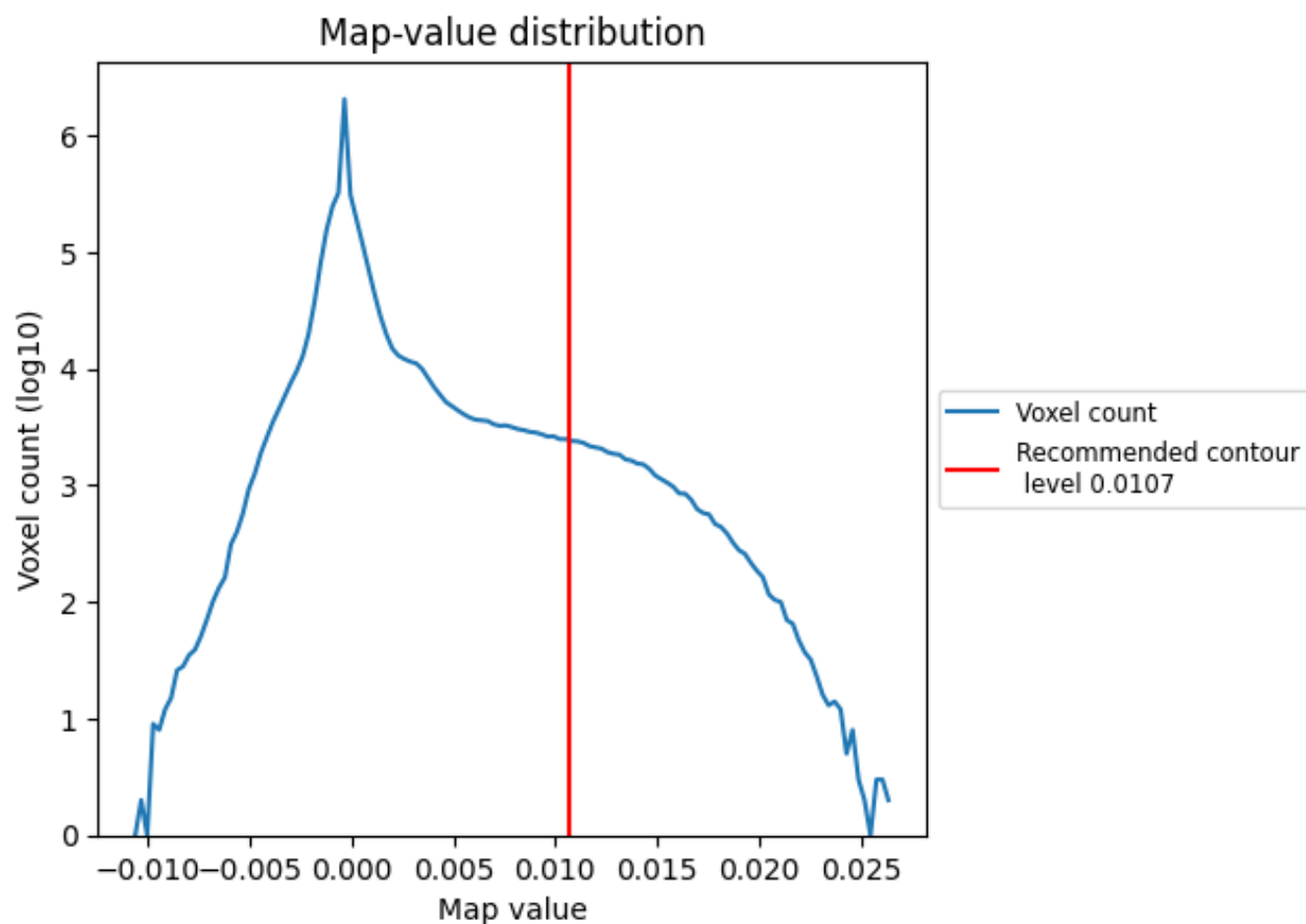
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

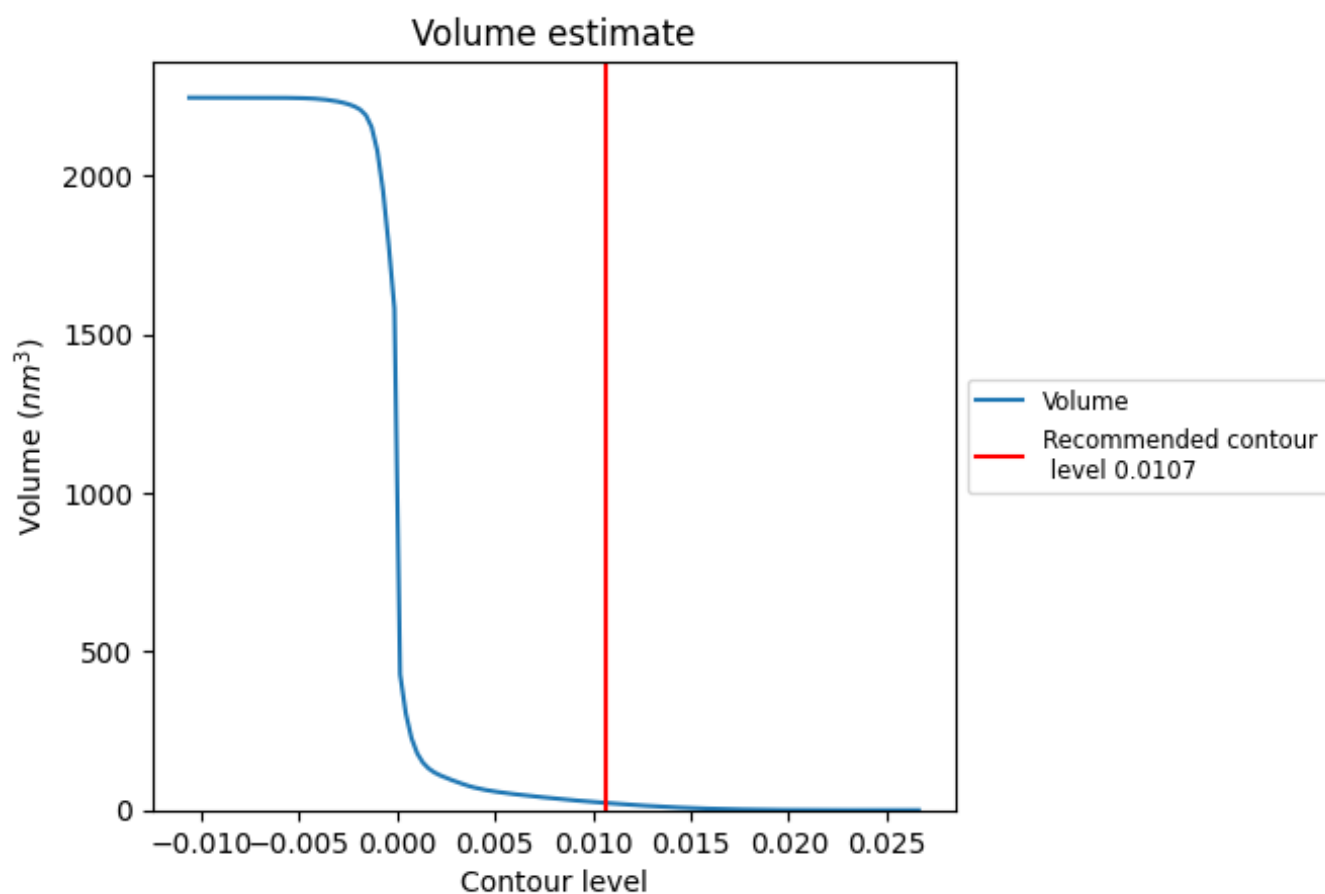
This section contains the results of statistical analysis of the map.

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.

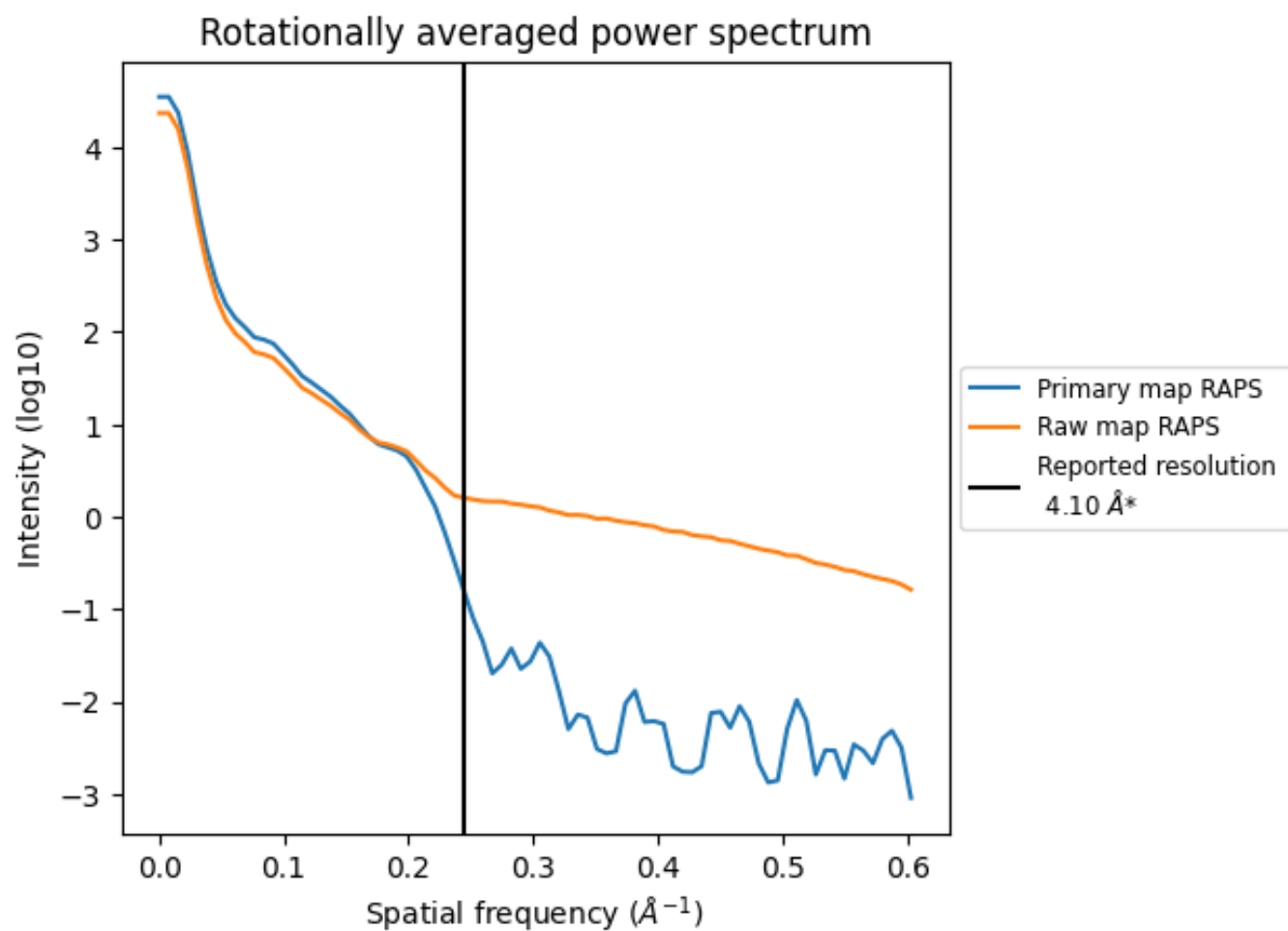
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm³; this corresponds to an approximate mass of 20 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 ⓘ

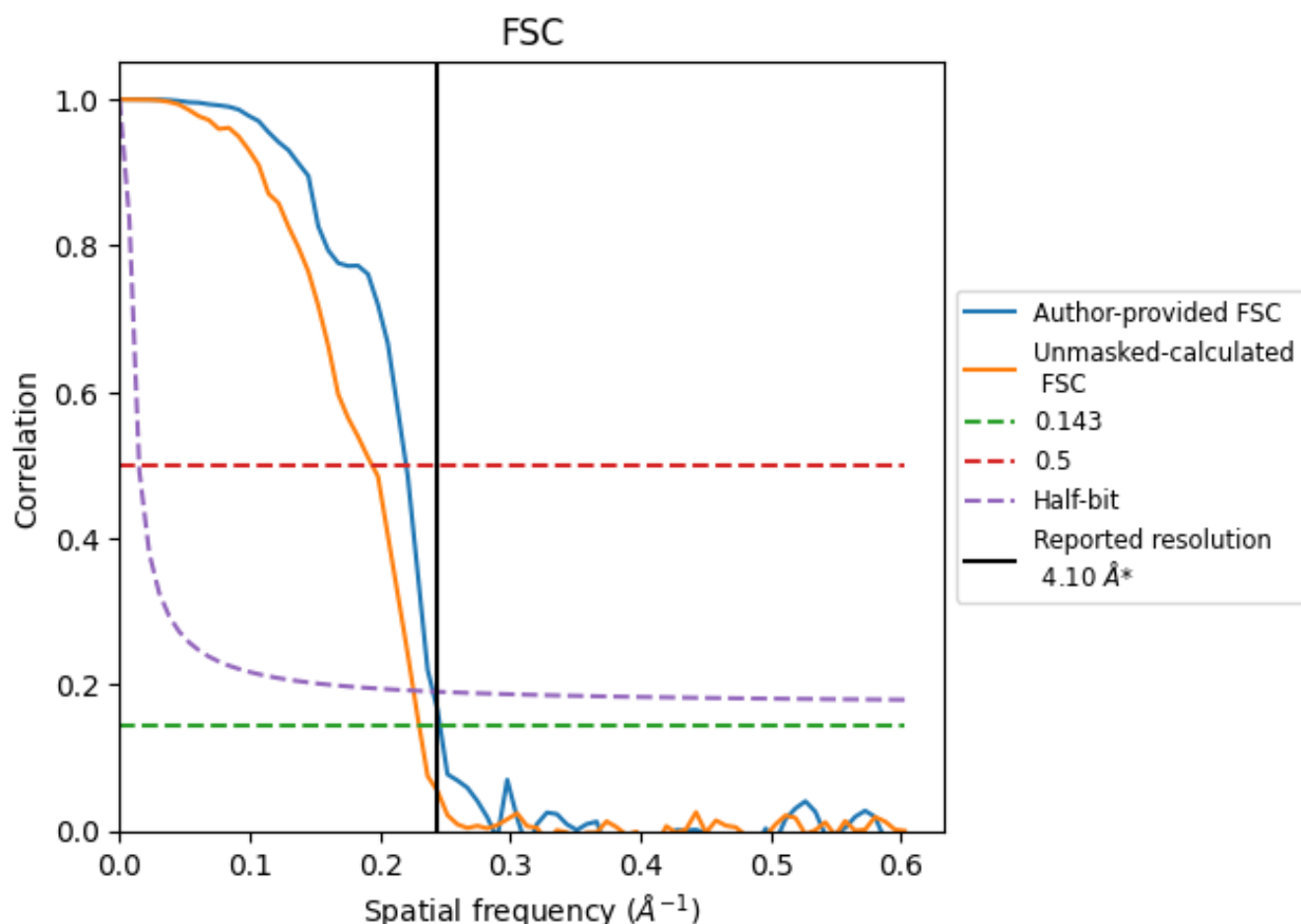


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

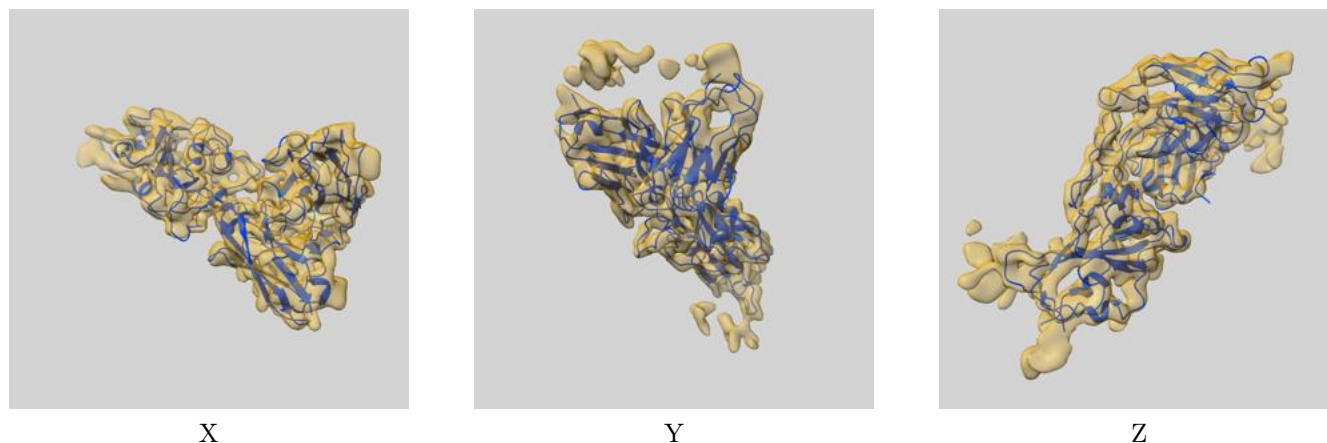
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.06	4.54	4.15
Unmasked-calculated*	4.34	5.16	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

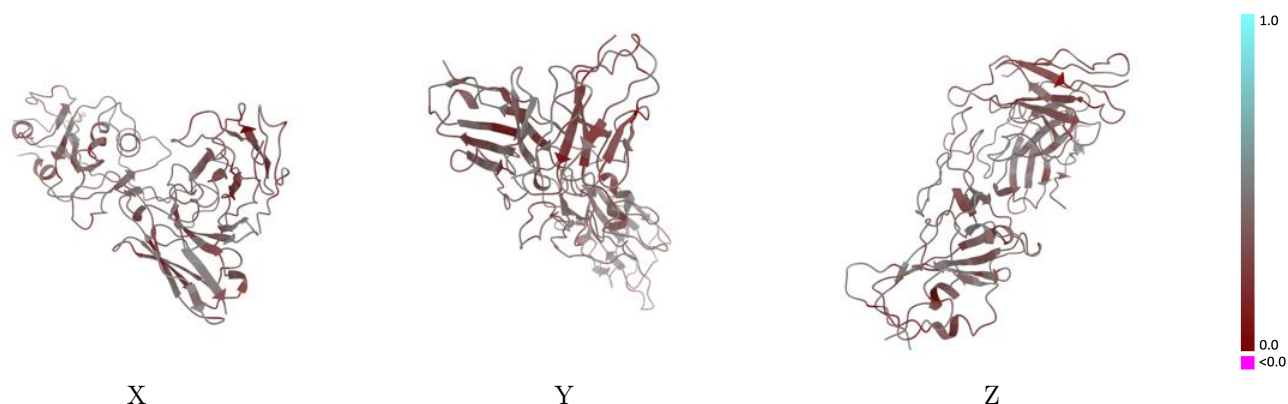
This section contains information regarding the fit between EMDB map EMD-33061 and PDB model 7X8Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



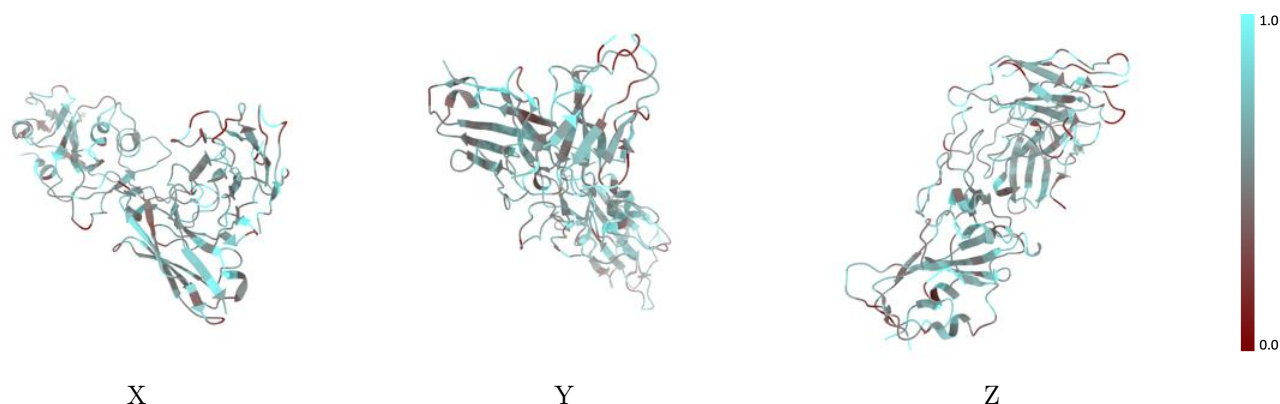
The images above show the 3D surface view of the map at the recommended contour level 0.0107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



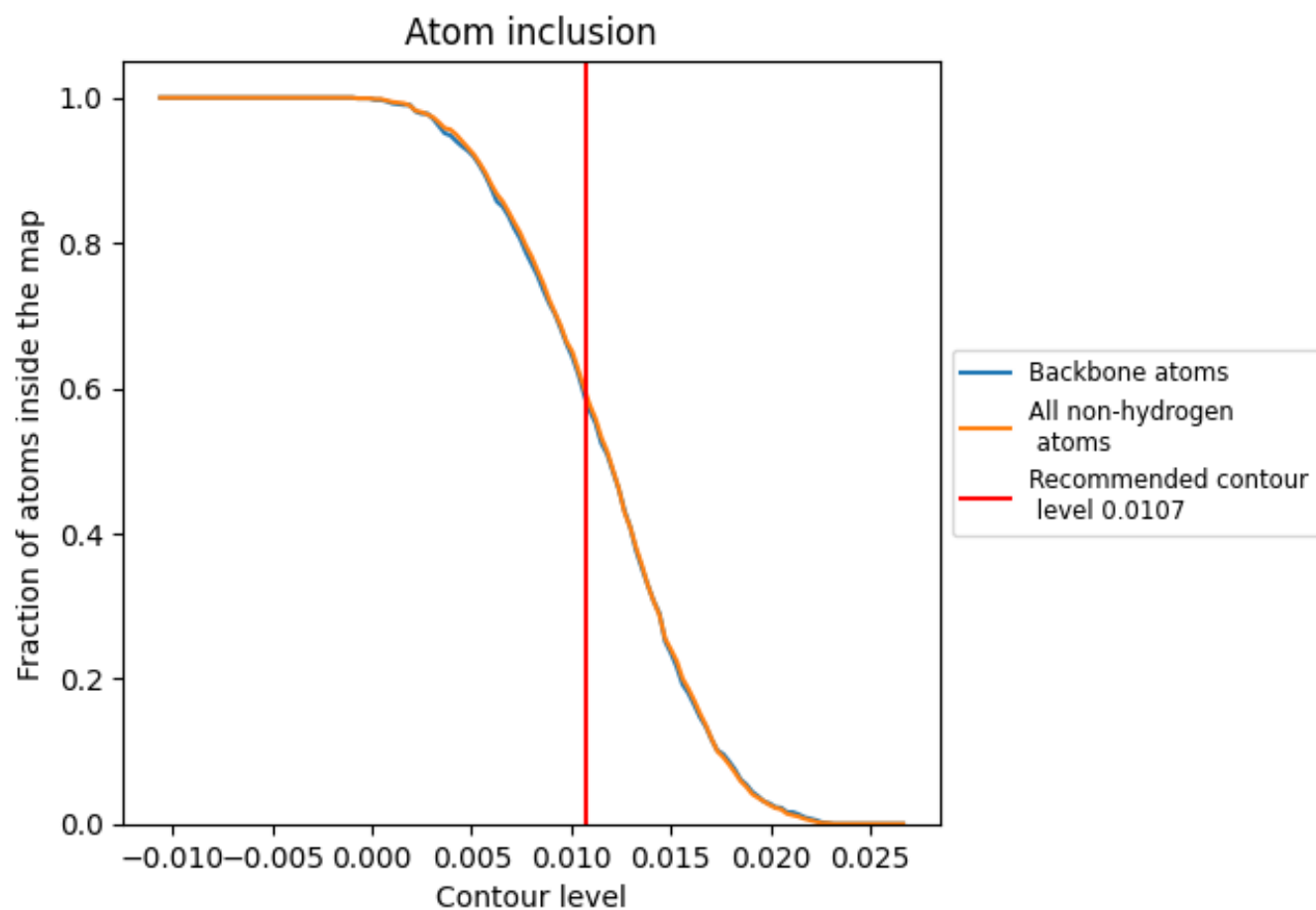
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0107).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 60% 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 (0.0107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5960	<div></div> 0.3680
A	<div></div> 0.6070	<div></div> 0.3770
H	<div></div> 0.5940	<div></div> 0.3790
L	<div></div> 0.5840	<div></div> 0.3390

