



Full wwPDB EM Validation Report ⓘ

Jul 20, 2026 – 02:15 PM EDT

PDB ID : 9YSG / pdb_00009ysg
EMDB ID : EMD-73392
Title : Cryo-EM structure of SARS-CoV-2 Omicron neutralizing antibody AB2-122
with BA.5 RBD and SP1-77 Fab complex
Authors : Jonaid, G.; Batra, H.; Kibria, G.; Chen, B.; Alt, F.W.
Deposited on : 2025-10-18
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

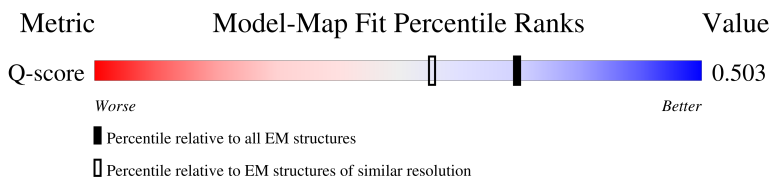
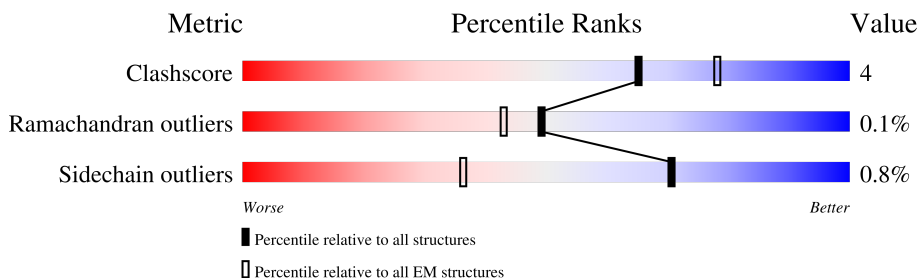
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.00 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.



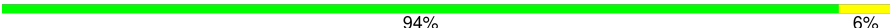
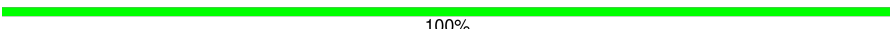
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	676	
2	D	451	
3	E	213	
4	F	449	

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Mol	Chain	Length	Quality of chain
5	G	214	 94%6%
6	T	3	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17426 atoms, of which 8569 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
			Total	C	H	N	O	S		
1	A	270	4210	1373	2067	364	397	9	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P0DTC2
A	-1	PHE	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	THR	-	expression tag	UNP P0DTC2
A	3	THR	-	expression tag	UNP P0DTC2
A	4	LYS	-	expression tag	UNP P0DTC2
A	5	ARG	-	expression tag	UNP P0DTC2
A	6	THR	-	expression tag	UNP P0DTC2
A	25	ILE	THR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	30	SER	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	143	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	213	GLY	VAL	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	452	ARG	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2
A	486	VAL	PHE	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2

- Molecule 2 is a protein called SP1-77 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	225	Total	C	H	N	O	S	0	0
			3371	1076	1666	291	331	7		

- Molecule 3 is a protein called SP1-77 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3193	1016	1563	269	340	5		

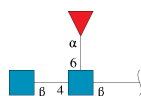
- Molecule 4 is a protein called AB2-122 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	220	Total	C	H	N	O	S	0	0
			3308	1057	1635	281	326	9		

- Molecule 5 is a protein called AB2-122 Fab light chain.

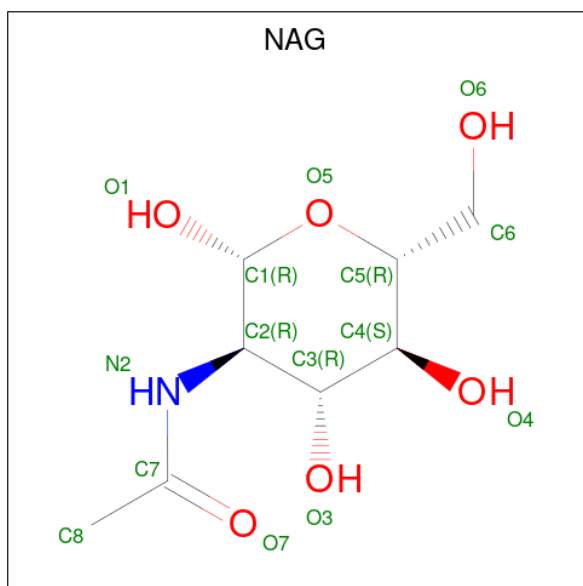
Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	214	Total	C	H	N	O	S	0	0
			3241	1035	1587	273	340	6		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	3	Total	C	H	N	O	0	0
			75	22	37	2	14		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

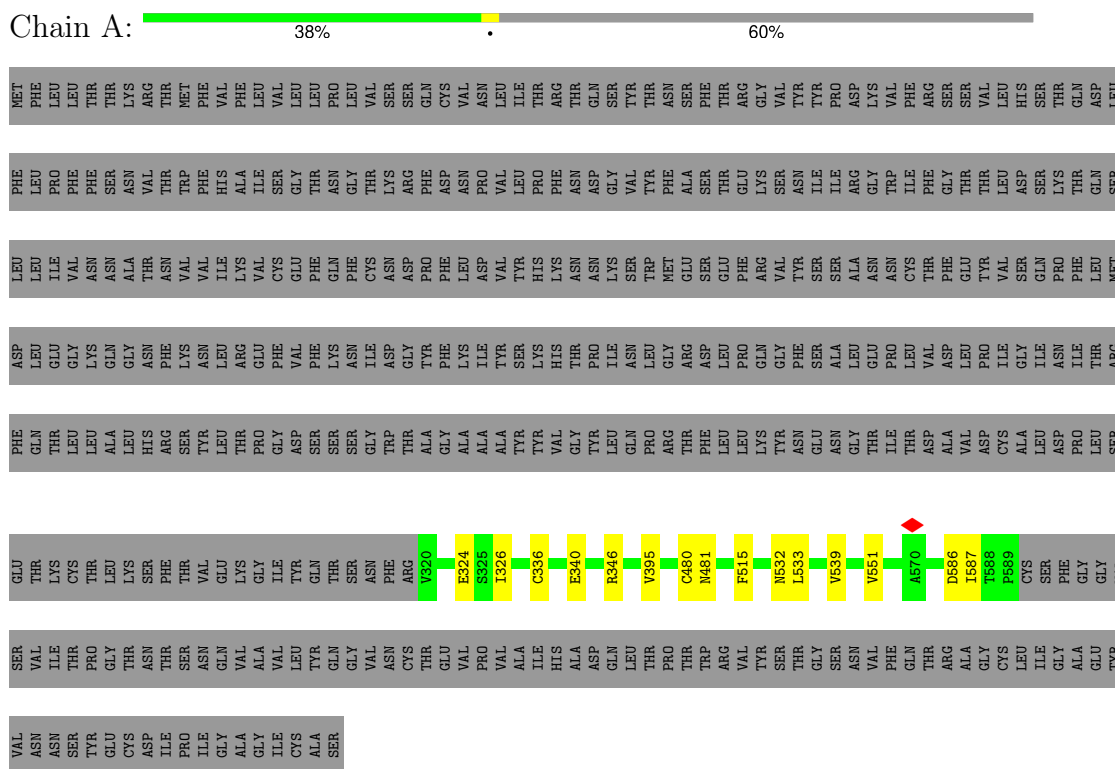


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			28	8	14	1	5	

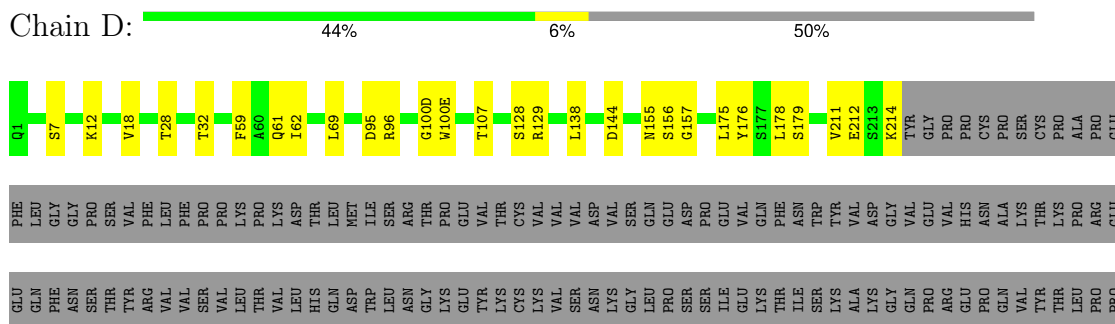
3 Residue-property plots

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



• Molecule 2: SP1-77 Fab heavy chain



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

- Molecule 3: SP1-77 Fab light chain

Chain E: 87% 12%

D1	S7 P8	W35	L47 I48	L78	E81	Y91	L94 P95	E104	V114	E122	G127 T128	N137	E142	D184	K187 H188 K189 V190	V195	N209	G210 R211	E212	CVS
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- Molecule 4: AB2-122 Fab heavy chain

Chain F: 45% . 51%

[illegible]

- Molecule 5: AB2-122 Fab light chain

Chain G: 94% 6%

D1
E55 T56
E123
E143
N152
E161
E165
L175
H189
Q199
R211
G212
E213
G214

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 100%

NAG1
NAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79684	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 ($e^-/\text{\AA}^2$)	52.28	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	294.4, 294.4, 294.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.736, 0.736, 0.736	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, TYS, FUC

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	0.20	0/2201	0.42	0/2997
2	D	0.13	0/1748	0.33	0/2383
3	E	0.13	0/1664	0.34	0/2261
4	F	0.16	0/1699	0.34	0/2312
5	G	0.12	0/1690	0.31	0/2294
All	All	0.15	0/9002	0.35	0/12247

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	2143	2067	2066	9	0
2	D	1705	1666	1666	19	0
3	E	1630	1563	1563	15	0
4	F	1673	1635	1635	14	0
5	G	1654	1587	1587	9	0
6	T	38	37	34	0	0
7	A	14	14	13	0	0
All	All	8857	8569	8564	64	0

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

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:143:GLU:N	5:G:143:GLU:OE2	2.16	0.79
3:E:122:GLU:N	3:E:122:GLU:OE2	2.17	0.76
4:F:140:GLY:O	4:F:141:THR:OG1	2.06	0.73
5:G:123:GLU:N	5:G:123:GLU:OE1	2.23	0.71
1:A:326:ILE:O	1:A:326:ILE:HD12	1.92	0.69
2:D:95:ASP:OD1	2:D:96:ARG:N	2.27	0.68
5:G:55:GLU:OE1	5:G:56:THR:N	2.29	0.65
1:A:324:GLU:OE1	1:A:539:VAL:HG22	1.98	0.62
3:E:212:GLU:N	3:E:212:GLU:OE1	2.37	0.58
5:G:199:GLN:OE1	5:G:199:GLN:N	2.39	0.56
5:G:189:HIS:O	5:G:211:ARG:NH1	2.40	0.55
4:F:89:ASP:OD1	4:F:89:ASP:C	2.49	0.55
4:F:1:GLN:OE1	4:F:1:GLN:N	2.38	0.54
5:G:165:GLU:OE2	5:G:165:GLU:HA	2.08	0.53
4:F:150:ASP:OD1	4:F:150:ASP:N	2.40	0.53
3:E:81:GLU:OE1	3:E:81:GLU:N	2.27	0.52
4:F:33:TYS:O2	4:F:52:ASN:ND2	2.43	0.51
4:F:161:ASN:O	4:F:164:ALA:HB3	2.10	0.51
4:F:184:LEU:C	4:F:184:LEU:HD12	2.36	0.50
3:E:188:HIS:O	3:E:210:ARG:NH1	2.42	0.49
1:A:532:ASN:OD1	1:A:533:LEU:N	2.46	0.49
1:A:346:ARG:NH2	2:D:95:ASP:OD2	2.46	0.49
2:D:156:SER:OG	2:D:157:GLY:N	2.46	0.48
5:G:152:ASN:OD1	5:G:152:ASN:C	2.56	0.48
2:D:61:GLN:HA	2:D:61:GLN:OE1	2.13	0.48
2:D:7:SER:O	2:D:107:THR:HG22	2.12	0.48
3:E:127:GLY:O	3:E:128:THR:HG22	2.14	0.48
1:A:324:GLU:C	1:A:324:GLU:OE2	2.58	0.47
1:A:551:VAL:O	1:A:587:ILE:HD12	2.14	0.47
4:F:127:VAL:HG22	4:F:204:VAL:HG21	1.97	0.47
4:F:134:SER:O	4:F:135:LYS:HB2	2.14	0.47
2:D:212:GLU:OE2	2:D:214:LYS:N	2.49	0.46
2:D:62:ILE:N	2:D:62:ILE:HD12	2.30	0.46
5:G:161:GLU:OE1	5:G:175:LEU:HD11	2.15	0.46
5:G:213:GLU:HA	5:G:213:GLU:OE2	2.15	0.46
2:D:155:ASN:O	2:D:156:SER:OG	2.29	0.46
2:D:32:THR:HG21	2:D:96:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:OD1	1:A:532:ASN:C	2.58	0.46
4:F:133:SER:O	4:F:135:LYS:N	2.49	0.45
2:D:144:ASP:HB2	2:D:175:LEU:HB2	1.98	0.44
2:D:28:THR:O	2:D:28:THR:HG23	2.17	0.44
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.83	0.44
1:A:340:GLU:OE2	1:A:340:GLU:O	2.35	0.44
3:E:184:ASP:OD1	3:E:187:LYS:NZ	2.44	0.44
4:F:133:SER:C	4:F:135:LYS:H	2.25	0.44
4:F:140:GLY:C	4:F:141:THR:HG1	2.19	0.44
2:D:178:LEU:HD12	2:D:179:SER:N	2.33	0.43
3:E:94:LEU:O	3:E:95:PRO:C	2.61	0.43
2:D:212:GLU:HA	2:D:212:GLU:OE1	2.18	0.43
3:E:189:LYS:HG3	3:E:190:VAL:HG23	2.01	0.43
3:E:7:SER:OG	3:E:8:PRO:HD3	2.19	0.42
3:E:142:GLU:OE1	3:E:142:GLU:C	2.62	0.42
2:D:100(D):GLY:HA2	3:E:91:TYR:CD1	2.55	0.42
2:D:138:LEU:HD13	2:D:211:VAL:HG21	2.01	0.42
3:E:114:VAL:HG21	3:E:195:VAL:HG11	2.02	0.42
3:E:209:ASN:OD1	3:E:210:ARG:N	2.53	0.41
3:E:35:TRP:HB2	3:E:48:ILE:HB	2.02	0.41
4:F:32:TYR:CD1	4:F:32:TYR:N	2.89	0.41
2:D:128:SER:O	2:D:129:ARG:C	2.64	0.41
2:D:176:TYR:CD1	2:D:176:TYR:N	2.89	0.41
2:D:59:PHE:CE1	2:D:69:LEU:HD13	2.56	0.41
3:E:137:ASN:OD1	3:E:137:ASN:N	2.53	0.41
4:F:35:TYR:HB2	4:F:106:MET:SD	2.62	0.40
2:D:12:LYS:HG3	2:D:18:VAL:HG13	2.02	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	268/676 (40%)	259 (97%)	9 (3%)	0	100	100
2	D	223/451 (49%)	206 (92%)	16 (7%)	1 (0%)	30	65
3	E	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
4	F	217/449 (48%)	201 (93%)	16 (7%)	0	100	100
5	G	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
All	All	1130/2003 (56%)	1070 (95%)	59 (5%)	1 (0%)	49	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	100(E)	TRP

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	236/596 (40%)	232 (98%)	4 (2%)	53	78
2	D	190/399 (48%)	190 (100%)	0	100	100
3	E	187/188 (100%)	183 (98%)	4 (2%)	47	75
4	F	185/397 (47%)	185 (100%)	0	100	100
5	G	188/188 (100%)	188 (100%)	0	100	100
All	All	986/1768 (56%)	978 (99%)	8 (1%)	70	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	CYS
1	A	480	CYS
1	A	481	ASN
1	A	586	ASP
3	E	47	LEU
3	E	78	LEU
3	E	104	GLU

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Mol	Chain	Res	Type
3	E	128	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	474	GLN
1	A	493	GLN
2	D	155	ASN
4	F	59	ASN
4	F	62	GLN
4	F	170	HIS
5	G	6	GLN
5	G	137	ASN
5	G	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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	TYS	F	33	4	15,16,17	1.57	2 (13%)	15,22,24	0.87	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	TYS	F	33	4	-	3/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	33	TYS	OH-S	5.01	1.68	1.58
4	F	33	TYS	OH-CZ	-3.08	1.37	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	33	TYS	CZ-OH-S-O2
4	F	33	TYS	CZ-OH-S-O3
4	F	33	TYS	CZ-OH-S-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	33	TYS	1	0

5.5 Carbohydrates [i](#)

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	T	1	6,1	14,14,15	0.74	0	17,19,21	0.93	0
6	NAG	T	2	6	14,14,15	0.71	0	17,19,21	0.82	0
6	FUC	T	3	6	10,10,11	0.76	0	14,14,16	0.96	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
6	NAG	T	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	FUC	T	3	6	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

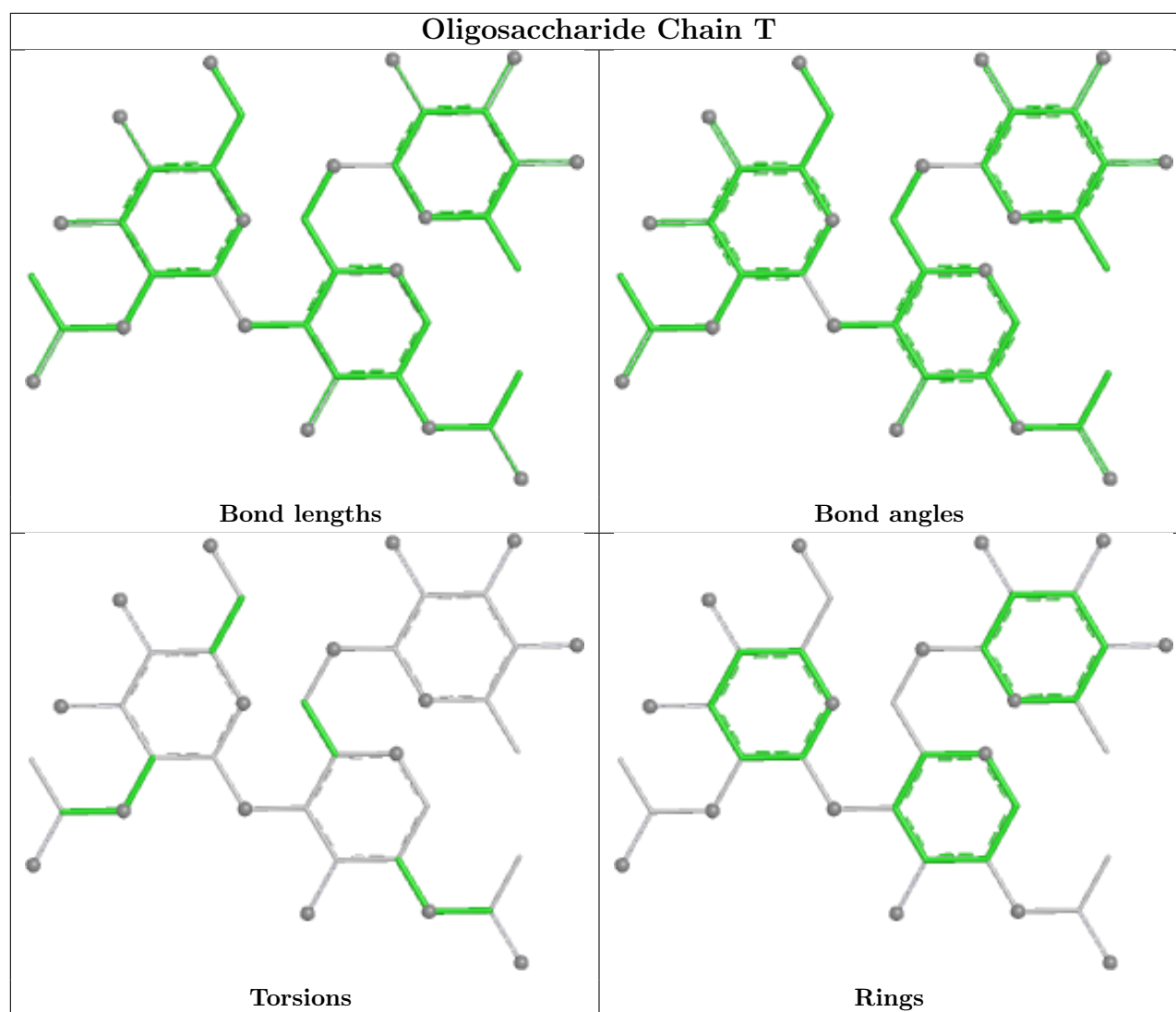
There are no chirality outliers.

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 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	$\# Z > 2$
7	NAG	A	701	1	14,14,15	0.72	0	17,19,21	0.87	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
7	NAG	A	701	1	-	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.

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.

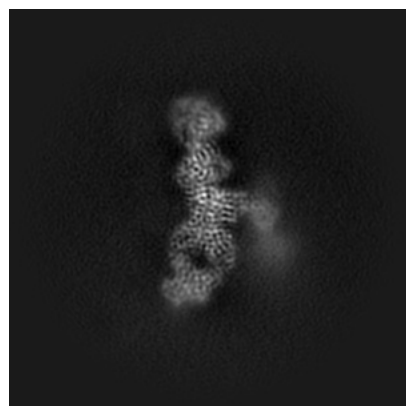
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73392. These allow visual inspection of the internal detail of the map and identification of artifacts.

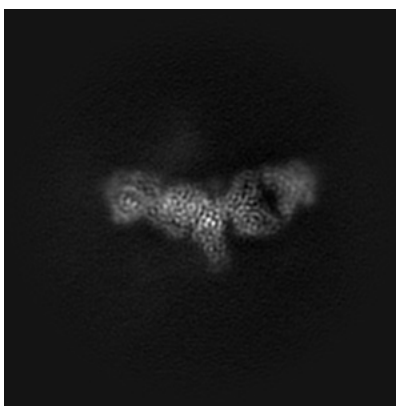
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

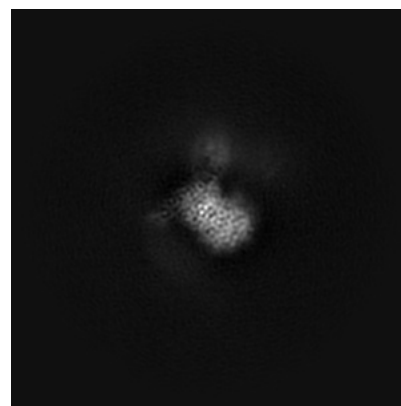
6.1.1 Primary map



X

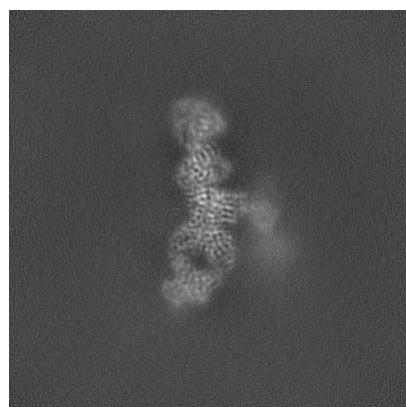


Y

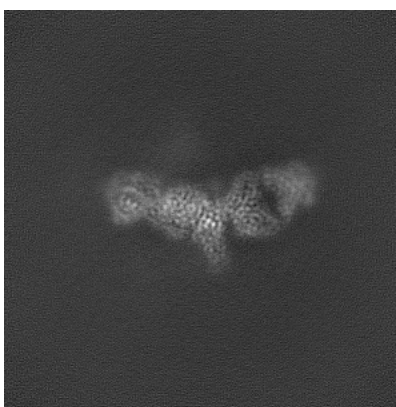


Z

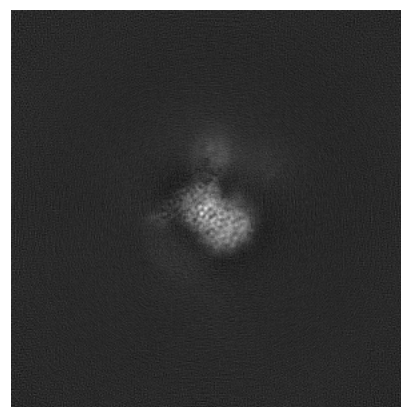
6.1.2 Raw map



X



Y

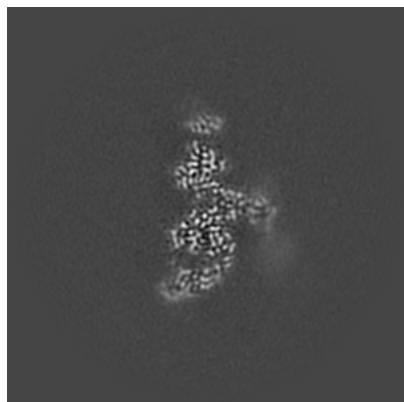


Z

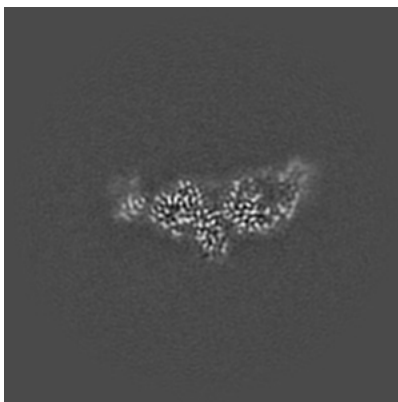
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

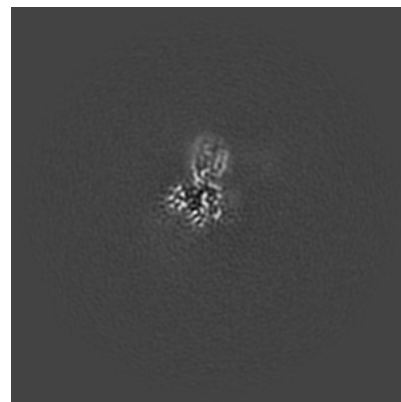
6.2.1 Primary map



X Index: 200

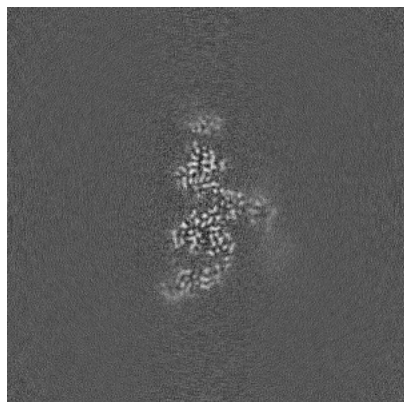


Y Index: 200

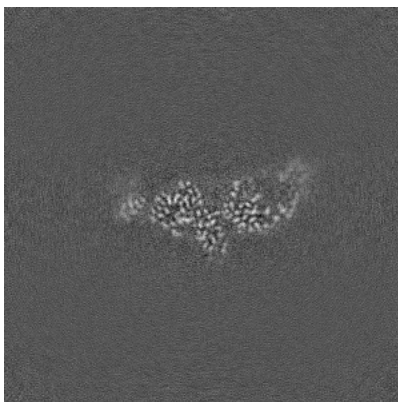


Z Index: 200

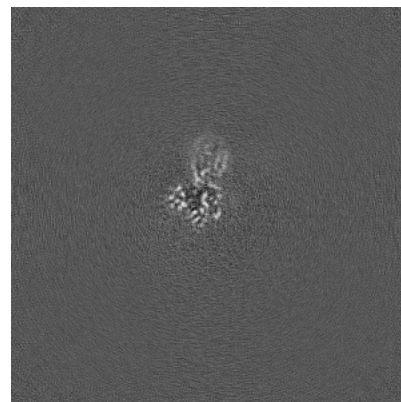
6.2.2 Raw map



X Index: 200



Y Index: 200

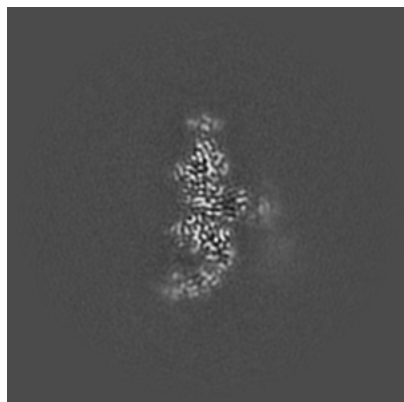


Z Index: 200

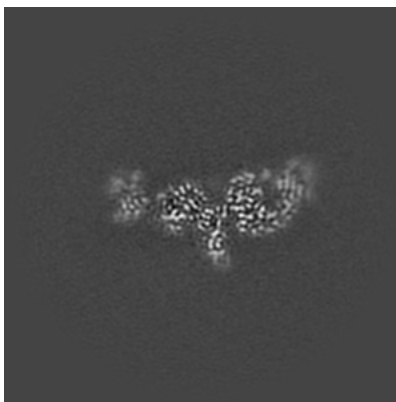
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

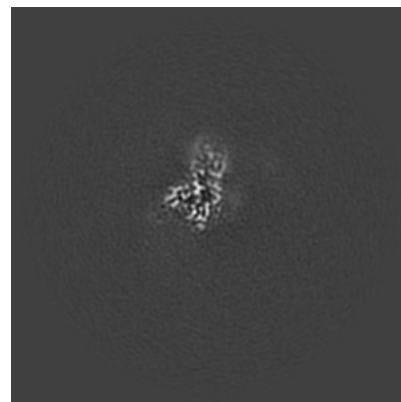
6.3.1 Primary map



X Index: 195

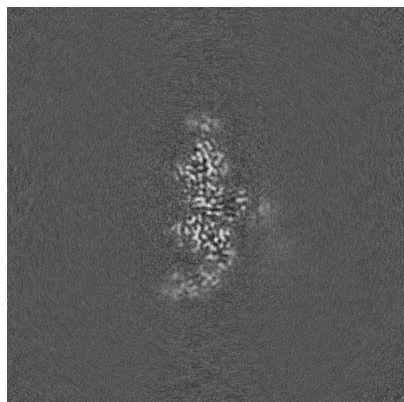


Y Index: 196

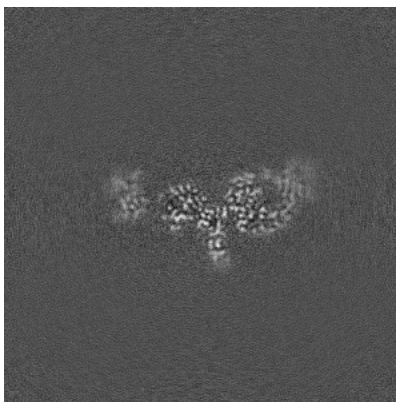


Z Index: 202

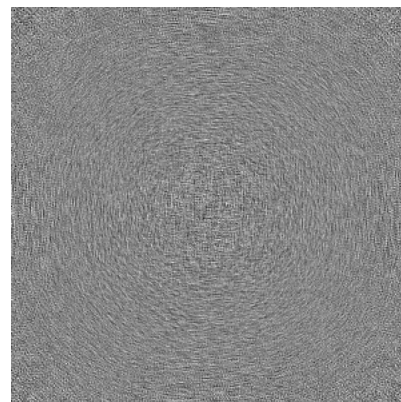
6.3.2 Raw map



X Index: 195



Y Index: 195



Z Index: 0

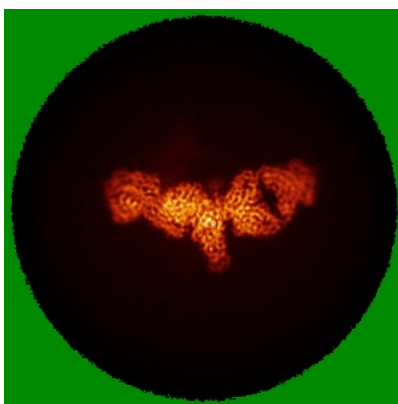
The images above show the largest variance slices of the map in three orthogonal directions.

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

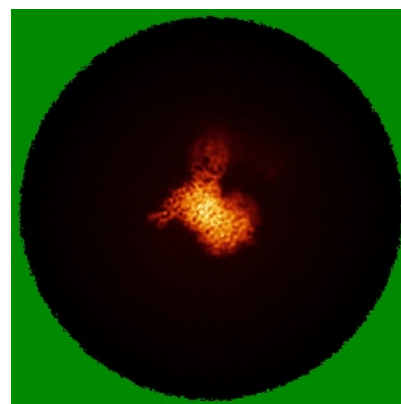
6.4.1 Primary map



X

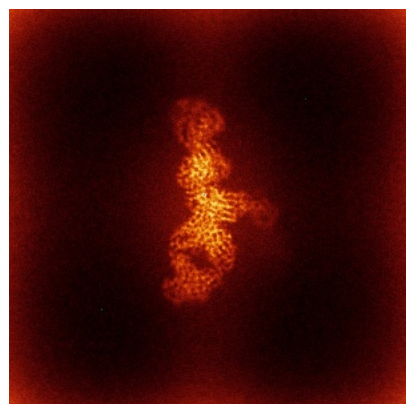


Y

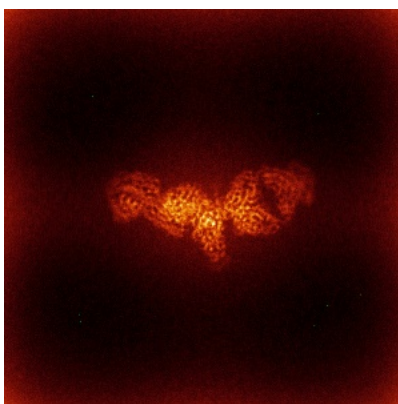


Z

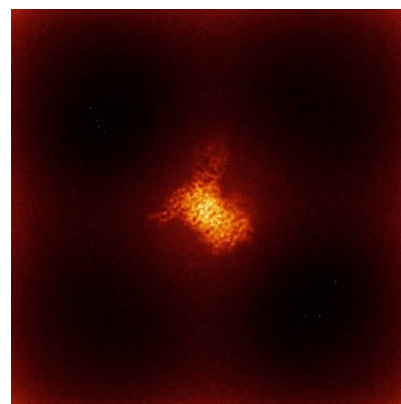
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



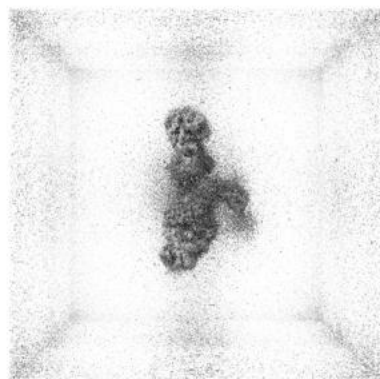
Y



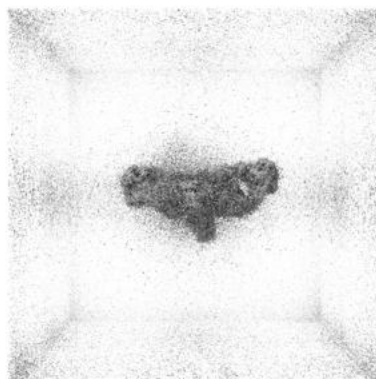
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

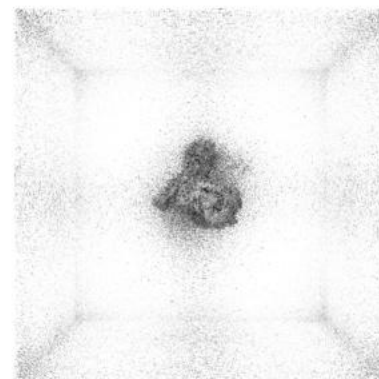
6.5.2 Raw map



X



Y



Z

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

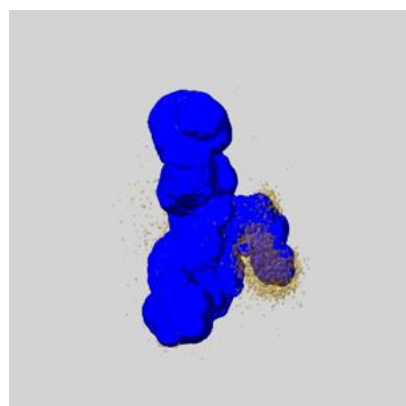
6.6 Mask visualisation [i](#)

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

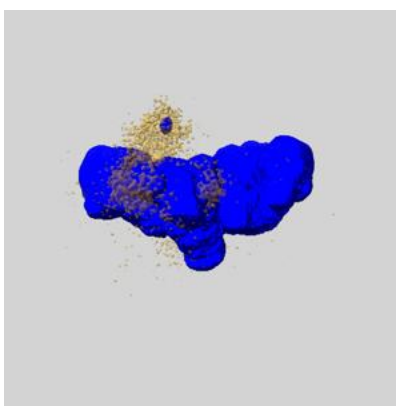
A mask typically either:

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

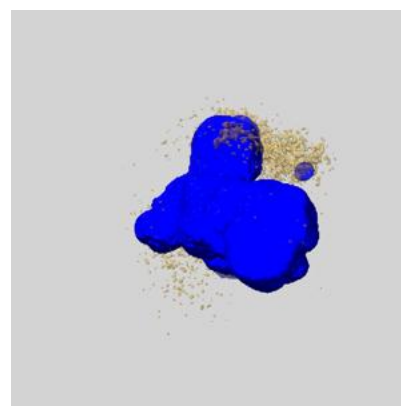
6.6.1 emd_73392_msk_1.map [i](#)



X



Y

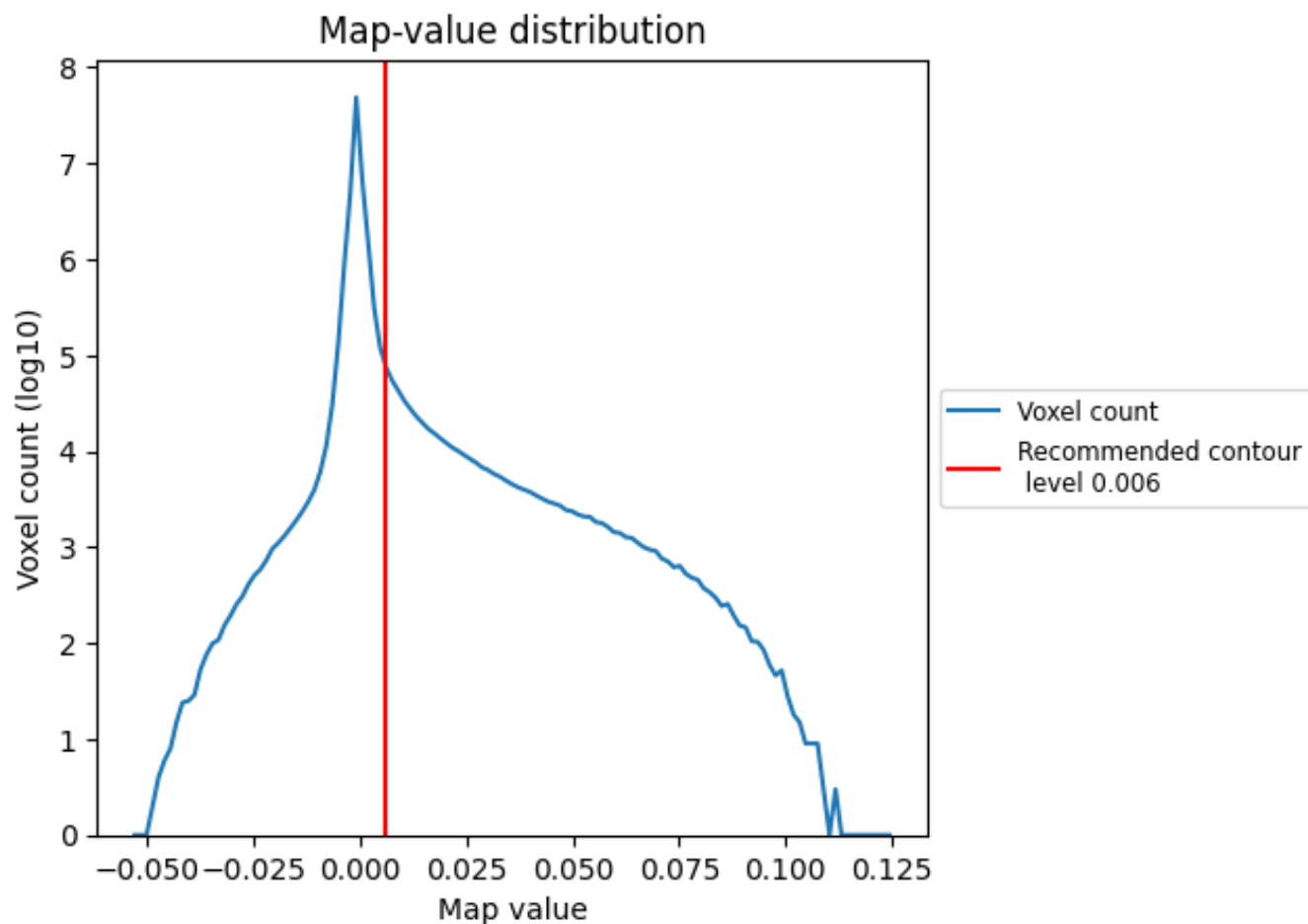


Z

7 Map analysis [i](#)

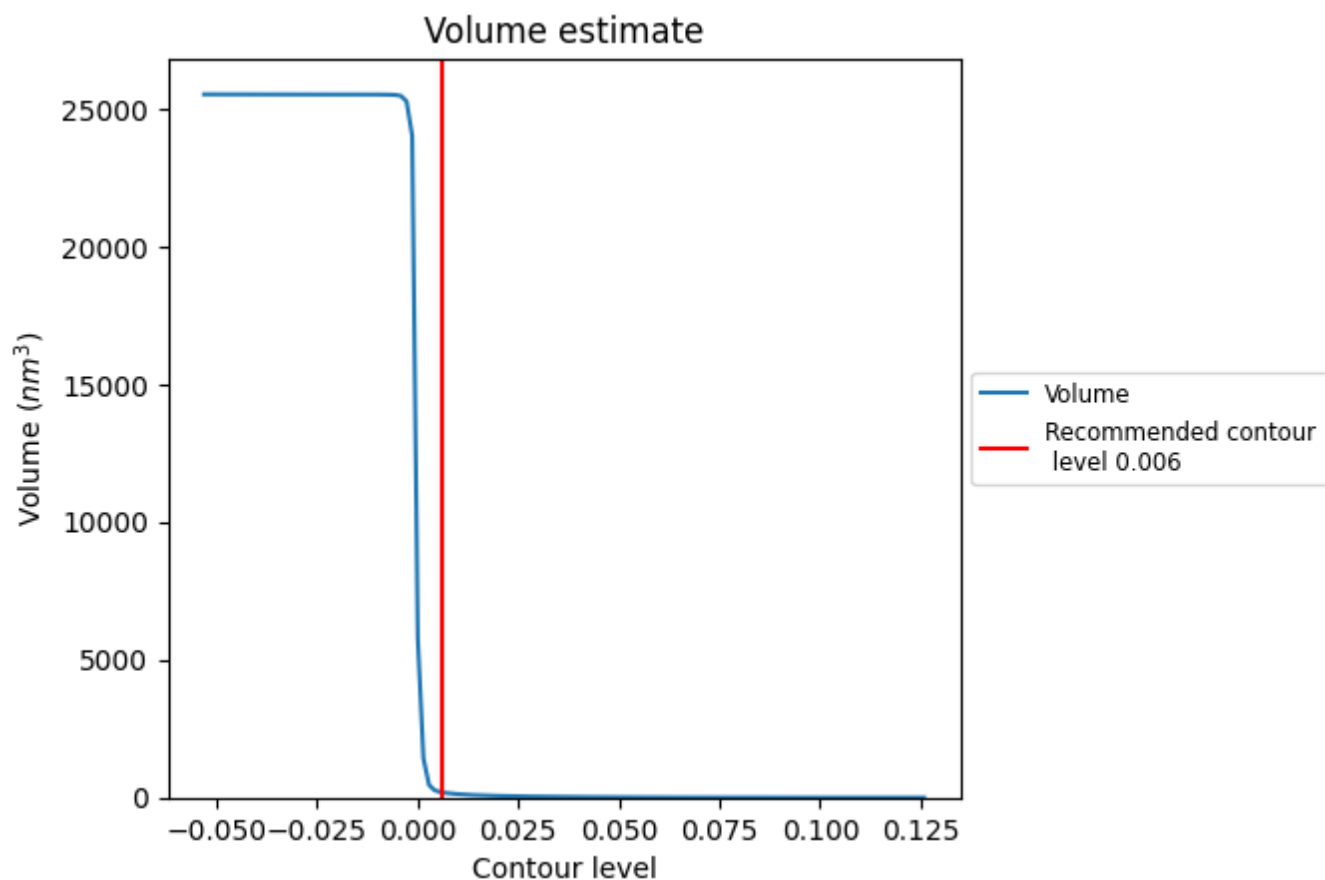
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

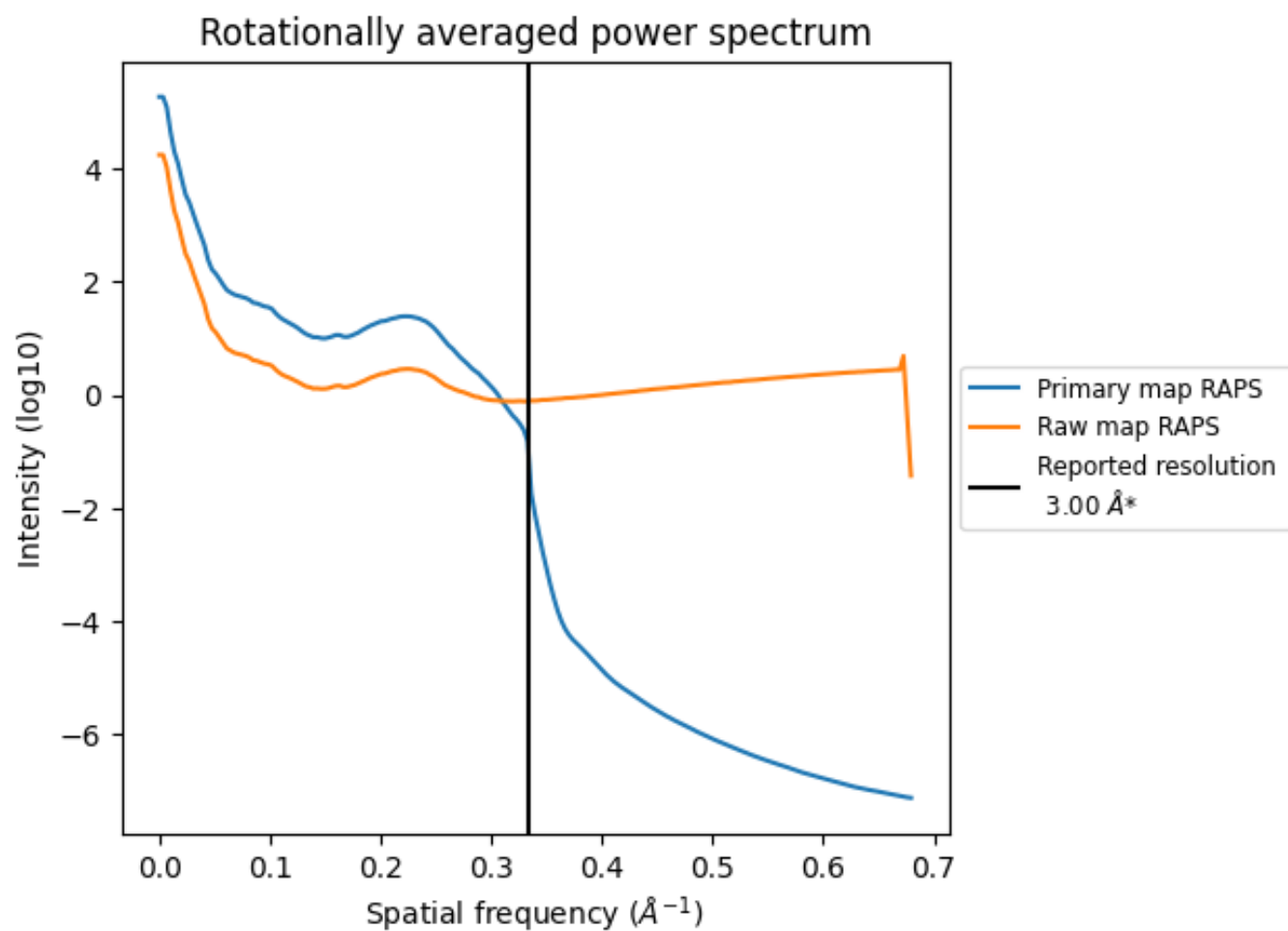
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm^3 ; this corresponds to an approximate mass of 175 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

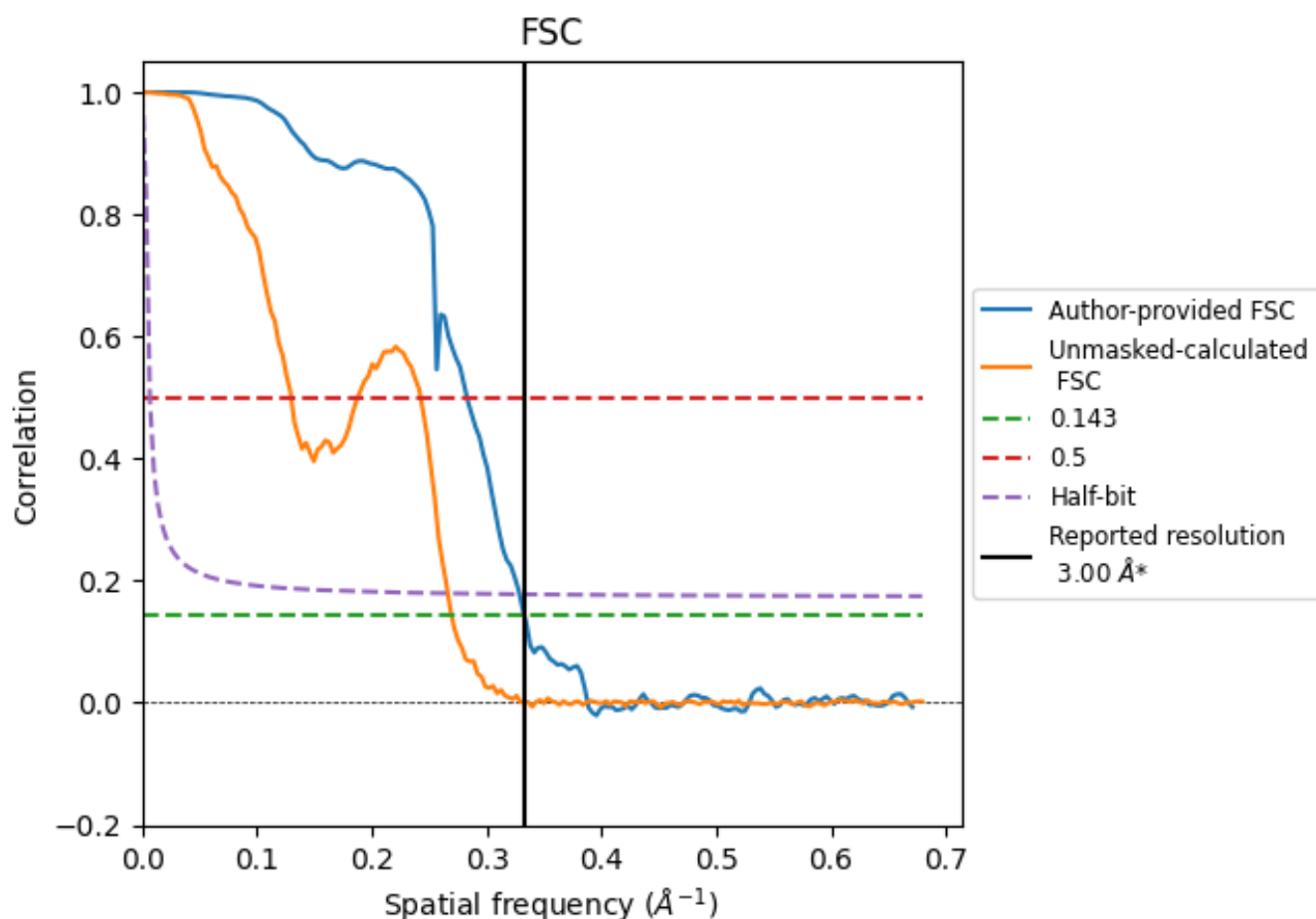


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

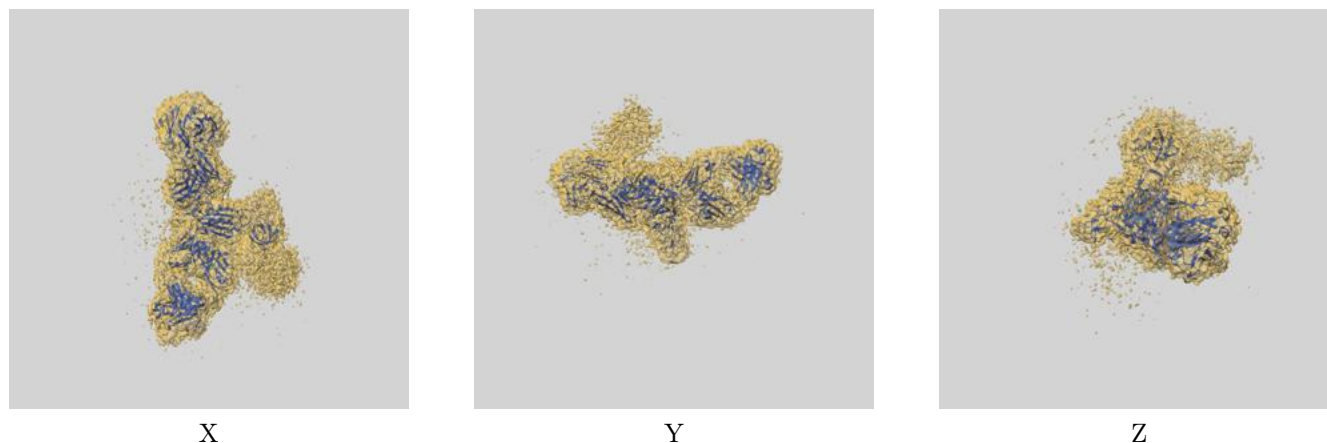
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.53	3.04
Unmasked-calculated*	3.71	7.71	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

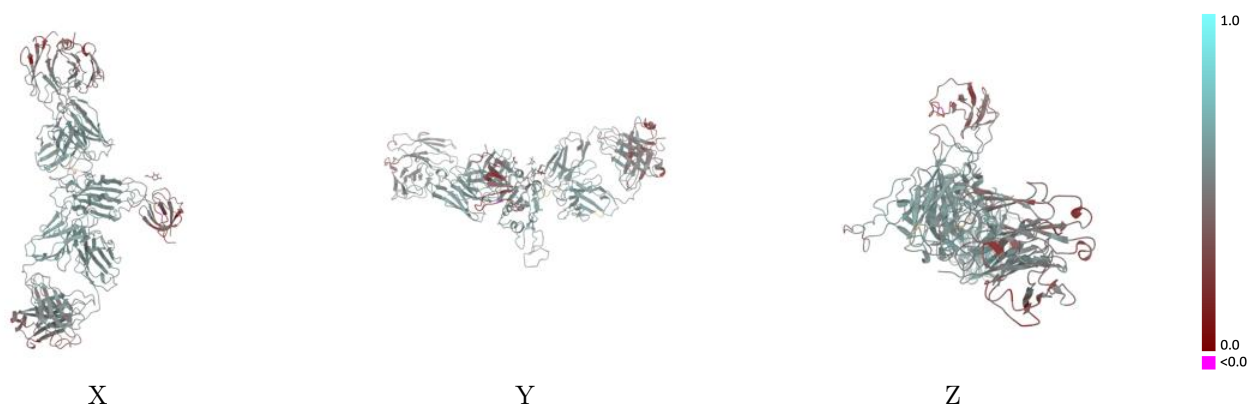
This section contains information regarding the fit between EMDB map EMD-73392 and PDB model 9YSG. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.006 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](#)



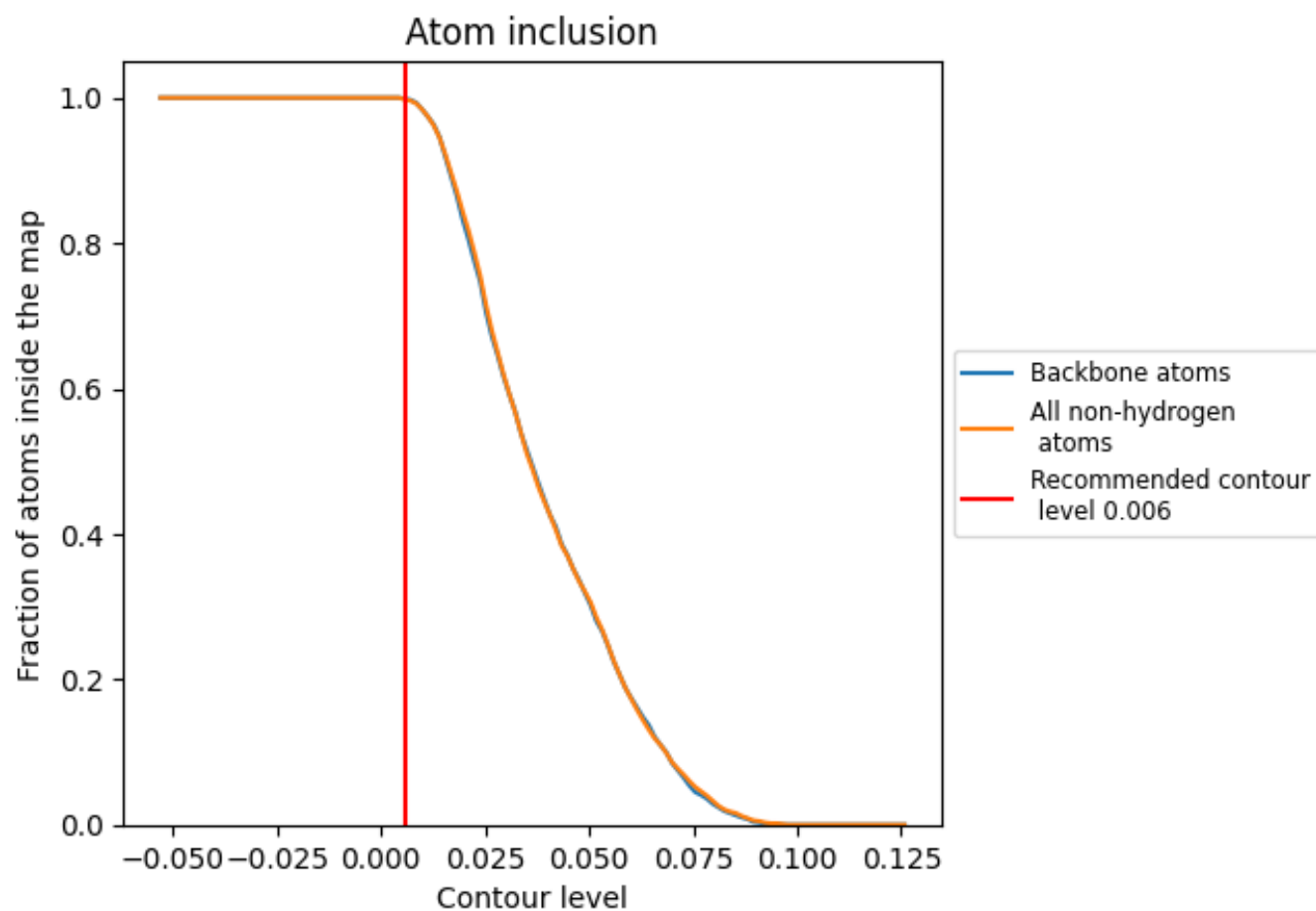
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9970	0.5030
A	0.9900	0.4930
D	0.9990	0.5010
E	1.0000	0.4820
F	0.9980	0.5280
G	0.9980	0.5150
T	1.0000	0.5150

1.0

0.0

<0.0