



## Full wwPDB EM Validation Report ⓘ

Jun 30, 2026 – 01:24 pm BST

PDB ID : 9S67 / pdb\_00009s67  
EMDB ID : EMD-54623  
Title : CryoEM structure of WIV1 spike monomer in complex with neutralizing antibody VA14\_26  
Authors : Upadhyay, A.; Alguel, Y.; Cherepanov, P.  
Deposited on : 2025-07-31  
Resolution : 4.12 Å(reported)  
Based on initial model : 8TC0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

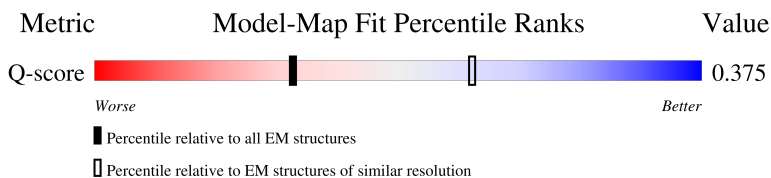
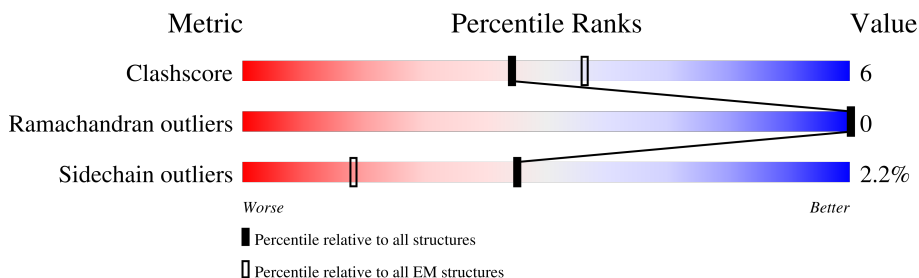
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 4.12 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	5662 ( 3.62 - 4.62 )

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  $\geq 3$ , 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	213	 75% 24%
2	B	238	 80% 13% • 6%
3	C	1239	 39% 6% 55%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7889 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 VA14\_26 Antibody Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	213	1643	1027	279	332	5	0	0

- Molecule 2 is a protein called VA14\_26 antibody Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1677	1064	278	330	5	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	560	4457	2869	738	831	19	0	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	668	SER	ARG	engineered mutation	UNP U5WI05
C	969	PRO	LYS	engineered mutation	UNP U5WI05
C	970	PRO	VAL	engineered mutation	UNP U5WI05
C	1192	SER	-	expression tag	UNP U5WI05
C	1193	GLY	-	expression tag	UNP U5WI05
C	1194	ARG	-	expression tag	UNP U5WI05
C	1195	GLU	-	expression tag	UNP U5WI05
C	1196	ASN	-	expression tag	UNP U5WI05
C	1197	LEU	-	expression tag	UNP U5WI05
C	1198	TYR	-	expression tag	UNP U5WI05
C	1199	PHE	-	expression tag	UNP U5WI05
C	1200	GLN	-	expression tag	UNP U5WI05
C	1201	GLY	-	expression tag	UNP U5WI05
C	1202	GLY	-	expression tag	UNP U5WI05
C	1203	GLY	-	expression tag	UNP U5WI05

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1204	GLY	-	expression tag	UNP U5WI05
C	1205	SER	-	expression tag	UNP U5WI05
C	1206	GLY	-	expression tag	UNP U5WI05
C	1207	TYR	-	expression tag	UNP U5WI05
C	1208	ILE	-	expression tag	UNP U5WI05
C	1209	PRO	-	expression tag	UNP U5WI05
C	1210	GLU	-	expression tag	UNP U5WI05
C	1211	ALA	-	expression tag	UNP U5WI05
C	1212	PRO	-	expression tag	UNP U5WI05
C	1213	ARG	-	expression tag	UNP U5WI05
C	1214	ASP	-	expression tag	UNP U5WI05
C	1215	GLY	-	expression tag	UNP U5WI05
C	1216	GLN	-	expression tag	UNP U5WI05
C	1217	ALA	-	expression tag	UNP U5WI05
C	1218	TYR	-	expression tag	UNP U5WI05
C	1219	VAL	-	expression tag	UNP U5WI05
C	1220	ARG	-	expression tag	UNP U5WI05
C	1221	LYS	-	expression tag	UNP U5WI05
C	1222	ASP	-	expression tag	UNP U5WI05
C	1223	GLY	-	expression tag	UNP U5WI05
C	1224	GLU	-	expression tag	UNP U5WI05
C	1225	TRP	-	expression tag	UNP U5WI05
C	1226	VAL	-	expression tag	UNP U5WI05
C	1227	LEU	-	expression tag	UNP U5WI05
C	1228	LEU	-	expression tag	UNP U5WI05
C	1229	SER	-	expression tag	UNP U5WI05
C	1230	THR	-	expression tag	UNP U5WI05
C	1231	PHE	-	expression tag	UNP U5WI05
C	1232	LEU	-	expression tag	UNP U5WI05
C	1233	GLY	-	expression tag	UNP U5WI05
C	1234	HIS	-	expression tag	UNP U5WI05
C	1235	HIS	-	expression tag	UNP U5WI05
C	1236	HIS	-	expression tag	UNP U5WI05
C	1237	HIS	-	expression tag	UNP U5WI05
C	1238	HIS	-	expression tag	UNP U5WI05
C	1239	HIS	-	expression tag	UNP U5WI05

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

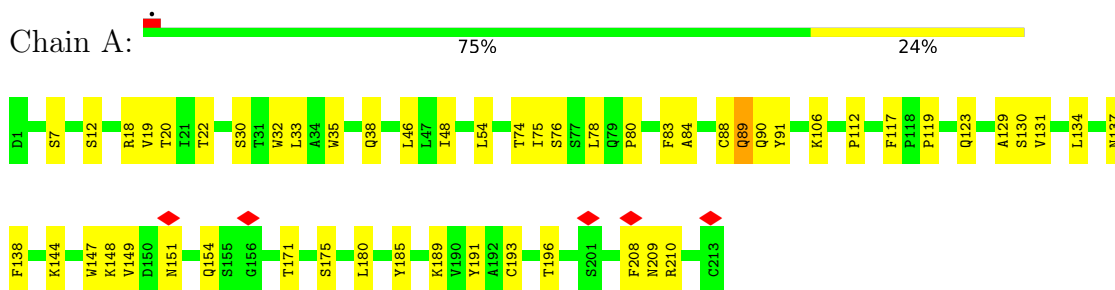


Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

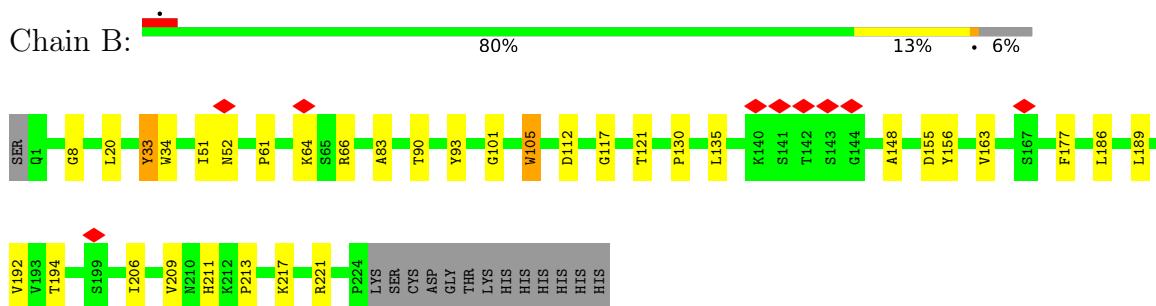
### 3 Residue-property plots [i](#)

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.

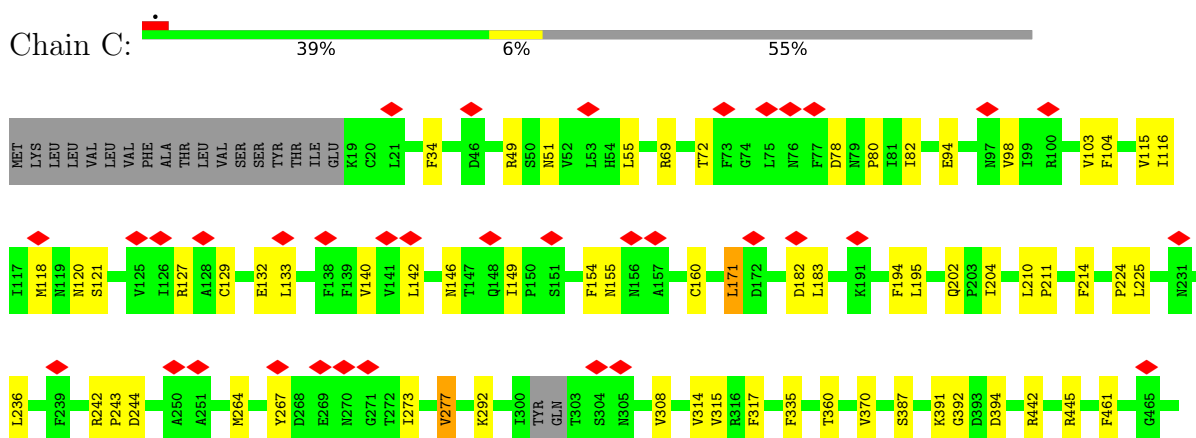
- Molecule 1: VA14\_26 Antibody Light Chain



- Molecule 2: VA14\_26 antibody Heavy Chain



- Molecule 3: Spike glycoprotein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1460644	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 ( $e^-/\text{\AA}^2$ )	32.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.801	Depositor
Minimum map value	-2.924	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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	0.13	0/1678	0.31	0/2279
2	B	0.15	0/1723	0.33	0/2355
3	C	0.12	0/4585	0.28	0/6242
All	All	0.13	0/7986	0.30	0/10876

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	1643	0	1603	29	0
2	B	1677	0	1638	24	0
3	C	4457	0	4278	51	0
4	C	112	0	104	0	0
All	All	7889	0	7623	99	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 6.

All (99) 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)
3:C:51:ASN:HA	3:C:267:TYR:O	1.78	0.82
3:C:94:GLU:O	3:C:182:ASP:HB2	1.84	0.78
3:C:142:LEU:O	3:C:146:ASN:HA	1.87	0.75
1:A:112:PRO:HB3	1:A:138:PHE:HB3	1.73	0.70
3:C:562:SER:HB2	3:C:571:ILE:HD11	1.73	0.69
3:C:315:VAL:HG12	3:C:529:ASN:HB3	1.74	0.68
1:A:148:LYS:HD2	1:A:151:ASN:HA	1.79	0.62
3:C:127:ARG:HH12	3:C:160:CYS:HA	1.65	0.62
1:A:137:ASN:HA	1:A:171:THR:HB	1.81	0.62
1:A:20:THR:HG22	1:A:74:THR:HG22	1.81	0.61
3:C:461:PHE:HB2	3:C:478:PRO:HG3	1.83	0.61
1:A:134:LEU:HD22	2:B:192:VAL:HG21	1.83	0.61
3:C:242:ARG:HD2	3:C:243:PRO:HD2	1.83	0.60
1:A:18:ARG:HD3	1:A:76:SER:HA	1.84	0.59
2:B:163:VAL:HG22	2:B:209:VAL:HG12	1.83	0.58
1:A:48:ILE:HD11	1:A:54:LEU:HD23	1.85	0.58
2:B:211:HIS:CE1	2:B:213:PRO:HG2	2.38	0.57
3:C:264:MET:HB3	3:C:277:VAL:HG23	1.87	0.57
3:C:55:LEU:HD21	3:C:292:LYS:HE3	1.85	0.56
3:C:195:LEU:HD12	3:C:225:LEU:HD12	1.88	0.56
3:C:132:GLU:HB2	3:C:155:ASN:HB3	1.86	0.55
3:C:479:LEU:H	3:C:479:LEU:HD23	1.72	0.54
3:C:133:LEU:HD23	3:C:154:PHE:HB3	1.89	0.54
3:C:547:GLN:HB3	3:C:550:GLN:HG3	1.88	0.54
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.88	0.54
2:B:51:ILE:HG22	2:B:52:ASN:HB2	1.90	0.54
3:C:51:ASN:CA	3:C:267:TYR:O	2.55	0.54
2:B:90:THR:HG23	2:B:121:THR:HA	1.90	0.54
3:C:442:ARG:HH12	3:C:445:ARG:HD2	1.72	0.54
3:C:34:PHE:HE2	3:C:69:ARG:HG2	1.74	0.53
2:B:156:TYR:HB2	2:B:211:HIS:CD2	2.44	0.53
3:C:72:THR:HG22	3:C:78:ASP:H	1.73	0.52
1:A:119:PRO:HD3	1:A:131:VAL:HG22	1.91	0.51
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.46	0.51
3:C:140:VAL:HB	3:C:149:ILE:HB	1.92	0.50
3:C:335:PHE:HD2	3:C:387:SER:HB2	1.76	0.50
1:A:123:GLN:HE22	1:A:130:SER:HB2	1.76	0.50
2:B:33:TYR:HD2	2:B:101:GLY:HA3	1.76	0.50
3:C:80:PRO:HG2	3:C:82:ILE:HD11	1.94	0.50
3:C:335:PHE:CD2	3:C:387:SER:HB2	2.47	0.49
1:A:80:PRO:HA	1:A:83:PHE:HE2	1.77	0.49
2:B:93:TYR:O	2:B:117:GLY:HA2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HG3	1:A:129:ALA:HB1	1.96	0.48
3:C:183:LEU:HB2	3:C:204:ILE:HD13	1.94	0.48
3:C:210:LEU:HD12	3:C:211:PRO:HD2	1.94	0.48
2:B:34:TRP:HB2	2:B:51:ILE:HD12	1.95	0.48
2:B:61:PRO:HA	2:B:64:LYS:HB2	1.95	0.48
3:C:121:SER:HA	3:C:171:LEU:HD21	1.96	0.47
3:C:121:SER:HB2	3:C:171:LEU:HD11	1.96	0.47
1:A:119:PRO:HB3	1:A:130:SER:H	1.80	0.46
2:B:206:ILE:HG12	2:B:221:ARG:HB2	1.96	0.46
3:C:103:VAL:HG22	3:C:116:ILE:HG22	1.97	0.46
3:C:142:LEU:O	3:C:146:ASN:CA	2.60	0.46
1:A:38:GLN:O	1:A:84:ALA:HB1	2.15	0.46
3:C:547:GLN:HG2	3:C:548:PRO:HD2	1.97	0.45
2:B:155:ASP:HA	2:B:186:LEU:HB3	1.97	0.45
3:C:104:PHE:HB2	3:C:115:VAL:HG12	1.99	0.45
1:A:19:VAL:HG21	1:A:78:LEU:HD11	1.98	0.45
2:B:130:PRO:HB3	2:B:156:TYR:HB3	1.97	0.45
3:C:183:LEU:HB3	3:C:202:GLN:O	2.17	0.45
3:C:525:CYS:HA	3:C:537:GLY:O	2.16	0.45
1:A:189:LYS:HE3	1:A:209:ASN:HD21	1.82	0.45
2:B:156:TYR:HB2	2:B:211:HIS:HD2	1.82	0.45
3:C:98:VAL:HG12	3:C:236:LEU:HD12	1.97	0.44
3:C:391:LYS:HG3	3:C:482:TYR:CZ	2.52	0.44
1:A:191:TYR:HB2	1:A:208:PHE:CE1	2.53	0.44
3:C:49:ARG:HB2	3:C:267:TYR:CG	2.53	0.44
1:A:144:LYS:HB2	1:A:196:THR:HB	1.99	0.44
2:B:211:HIS:HE1	2:B:213:PRO:HG2	1.81	0.44
3:C:542:SER:HB3	3:C:571:ILE:HG23	1.99	0.44
3:C:242:ARG:HG3	3:C:244:ASP:H	1.82	0.44
1:A:46:LEU:HB2	2:B:112:ASP:OD2	2.18	0.43
1:A:149:VAL:HG22	1:A:191:TYR:HD2	1.84	0.43
3:C:482:TYR:HD1	3:C:482:TYR:HA	1.71	0.43
1:A:117:PHE:HB3	2:B:135:LEU:HD22	2.01	0.43
1:A:117:PHE:CD2	2:B:135:LEU:HB3	2.54	0.43
3:C:242:ARG:HH11	3:C:243:PRO:HG2	1.84	0.43
3:C:392:GLY:HA2	3:C:495:TYR:CD1	2.53	0.43
2:B:217:LYS:HE2	2:B:217:LYS:HB2	1.83	0.43
2:B:105:TRP:CD1	2:B:105:TRP:N	2.87	0.43
3:C:118:MET:HE1	3:C:120:ASN:HB3	2.00	0.42
3:C:547:GLN:HE22	3:C:549:PHE:HB2	1.84	0.42
1:A:147:TRP:HB2	1:A:154:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:317:PHE:CE2	3:C:515:LYS:HB3	2.54	0.42
3:C:194:PHE:CZ	3:C:224:PRO:HB3	2.55	0.42
2:B:148:ALA:HA	2:B:194:THR:HA	2.01	0.42
3:C:530:PHE:CD2	3:C:563:VAL:HG11	2.54	0.42
1:A:12:SER:HB3	1:A:106:LYS:HG2	2.02	0.41
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.64	0.41
1:A:30:SER:HB3	1:A:32:TRP:CD1	2.56	0.41
1:A:189:LYS:HD2	1:A:210:ARG:HE	1.85	0.41
3:C:214:PHE:HZ	3:C:273:ILE:HG22	1.85	0.41
2:B:66:ARG:HD2	2:B:83:ALA:O	2.20	0.41
3:C:49:ARG:HB2	3:C:267:TYR:CD2	2.56	0.41
3:C:103:VAL:HG13	3:C:116:ILE:HG22	2.02	0.41
3:C:127:ARG:NH1	3:C:129:CYS:HB3	2.36	0.40
3:C:391:LYS:HB2	3:C:394:ASP:CG	2.46	0.40
1:A:175:SER:HB3	2:B:177:PHE:CE2	2.55	0.40
1:A:7:SER:HB3	1:A:22:THR:HG23	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	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
2	B	222/238 (93%)	216 (97%)	6 (3%)	0	100	100
3	C	556/1239 (45%)	526 (95%)	30 (5%)	0	100	100
All	All	989/1690 (58%)	943 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/188 (100%)	180 (96%)	8 (4%)	26	48
2	B	188/201 (94%)	185 (98%)	3 (2%)	55	69
3	C	499/1077 (46%)	491 (98%)	8 (2%)	55	69
All	All	875/1466 (60%)	856 (98%)	19 (2%)	45	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	75	ILE
1	A	89	GLN
1	A	90	GLN
1	A	91	TYR
1	A	180	LEU
1	A	185	TYR
1	A	193	CYS
2	B	33	TYR
2	B	105	TRP
2	B	189	LEU
3	C	171	LEU
3	C	277	VAL
3	C	308	VAL
3	C	314	VAL
3	C	360	THR
3	C	370	VAL
3	C	468	CYS
3	C	482	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	55	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	GLN
1	A	188	HIS
2	B	208	ASN
3	C	97	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands 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	C	1307	3	14,14,15	0.76	0	17,19,21	0.88	0
4	NAG	C	1302	3	14,14,15	0.70	0	17,19,21	1.14	1 (5%)
4	NAG	C	1304	3	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	C	1308	3	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	C	1301	3	14,14,15	0.72	0	17,19,21	0.81	0
4	NAG	C	1306	3	14,14,15	0.77	0	17,19,21	0.85	0
4	NAG	C	1305	3	14,14,15	0.73	0	17,19,21	0.93	0
4	NAG	C	1303	3	14,14,15	0.73	0	17,19,21	0.80	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	C	1307	3	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	3	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	3	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	3	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	3	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	3	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	3	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1302	NAG	C2-N2-C7	3.04	127.24	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	C	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	C	1302	NAG	C3-C2-N2-C7
4	C	1302	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

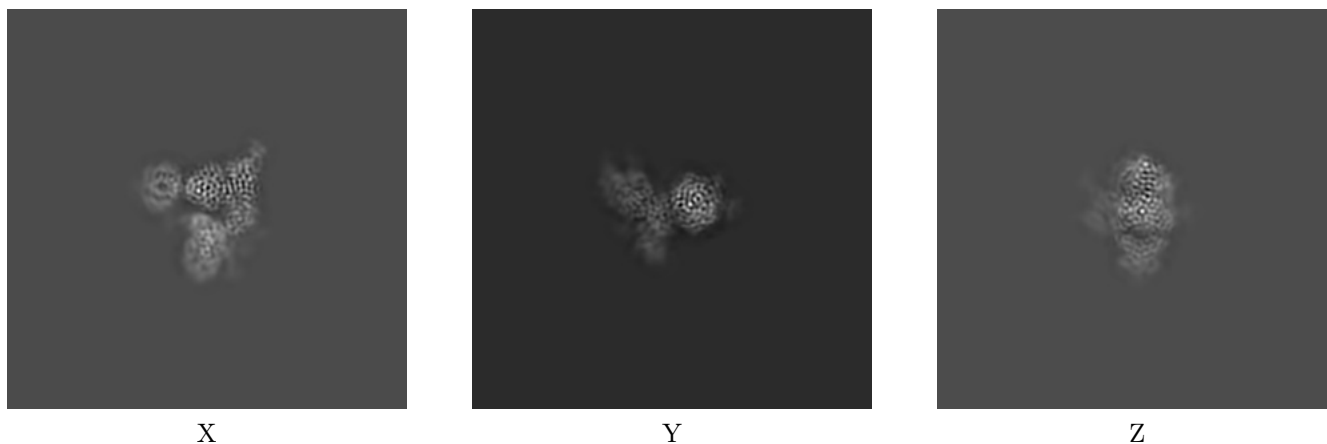
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54623. These allow visual inspection of the internal detail of the map and identification of artifacts.

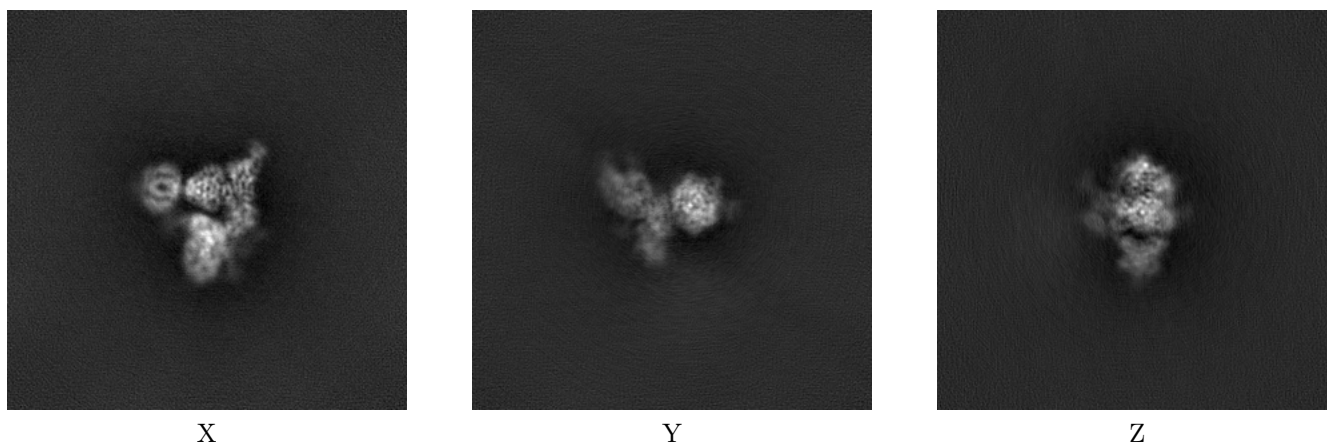
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



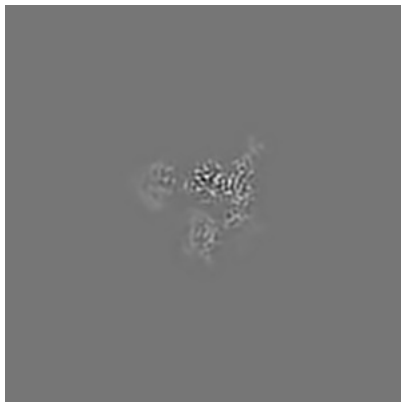
#### 6.1.2 Raw map



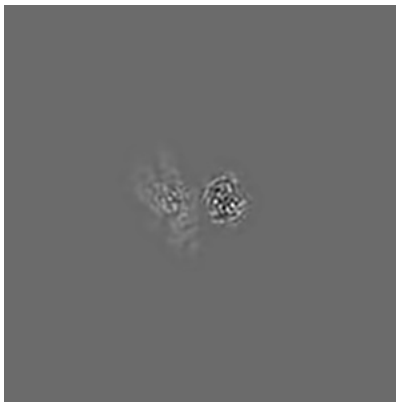
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 160

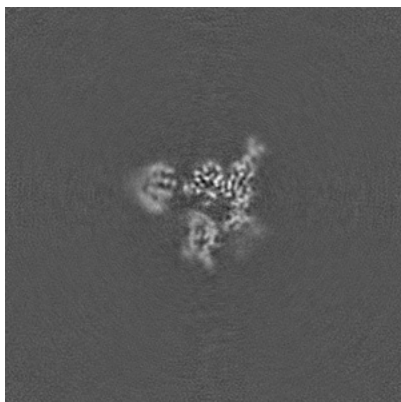


Y Index: 160

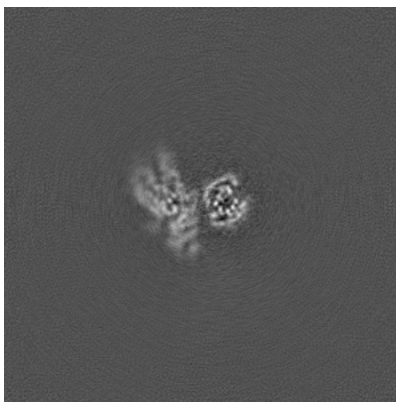


Z Index: 160

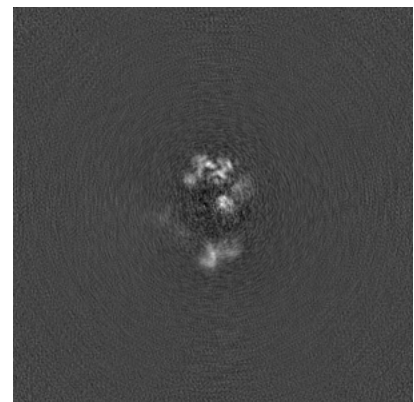
### 6.2.2 Raw map



X Index: 160



Y Index: 160

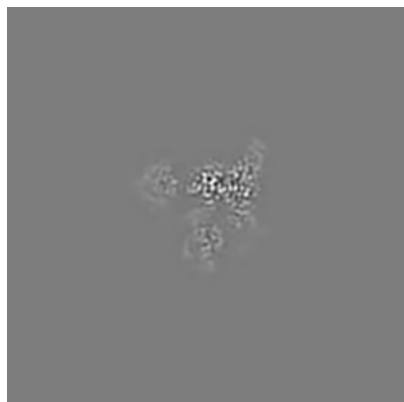


Z Index: 160

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

## 6.3 Largest variance slices [i](#)

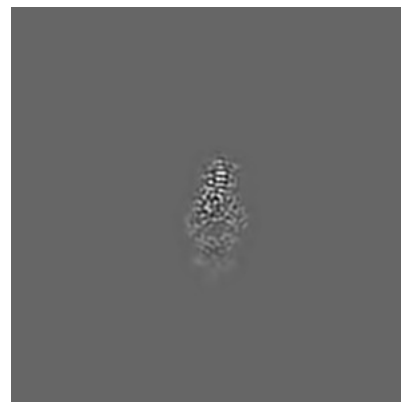
### 6.3.1 Primary map



X Index: 163

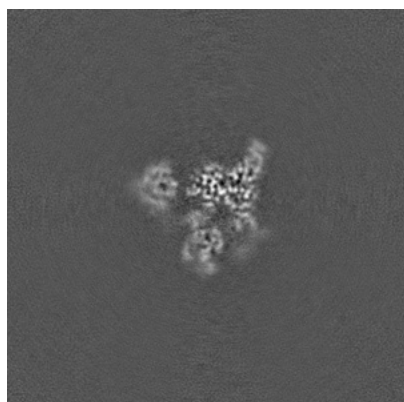


Y Index: 158

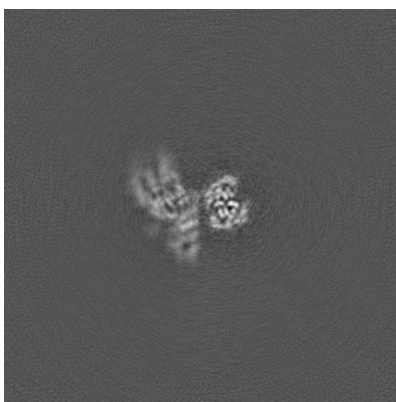


Z Index: 178

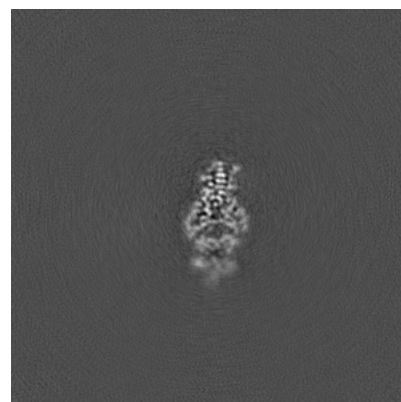
### 6.3.2 Raw map



X Index: 163



Y Index: 158

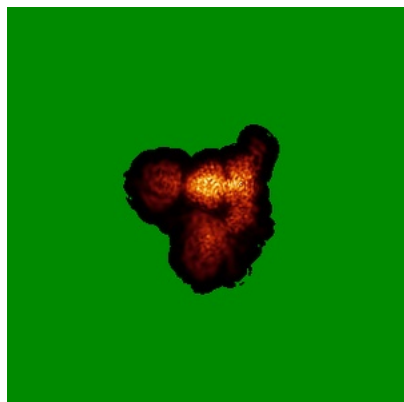


Z Index: 178

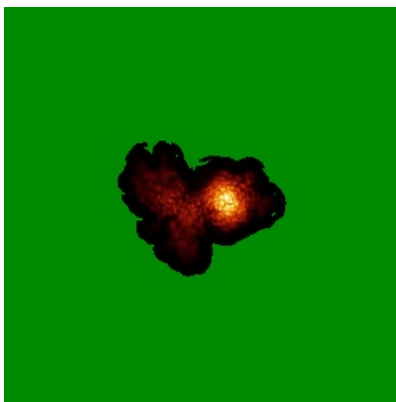
The images above show the largest variance slices of the map in three orthogonal directions.

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

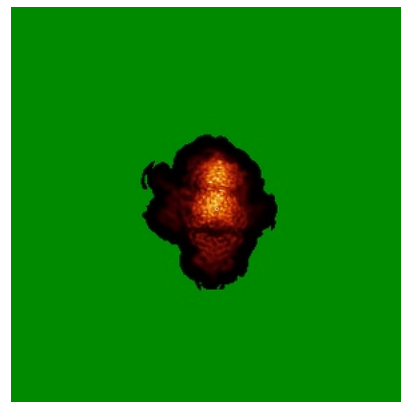
### 6.4.1 Primary map



X

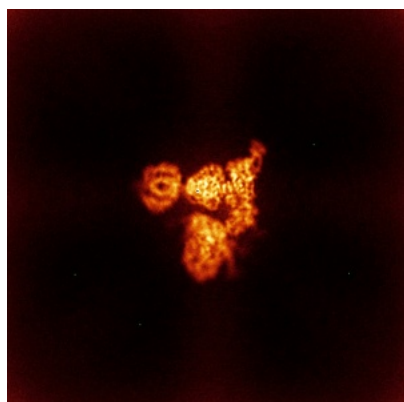


Y

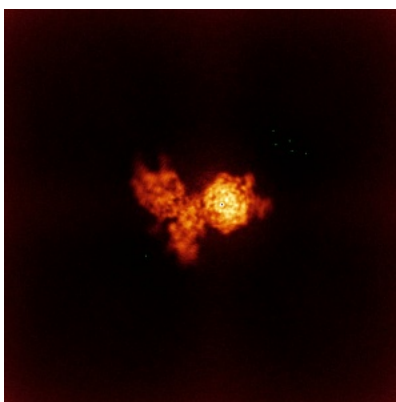


Z

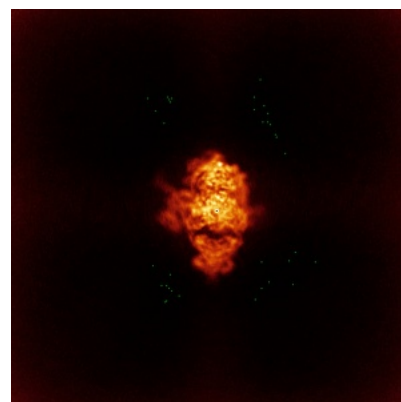
### 6.4.2 Raw map



X



Y

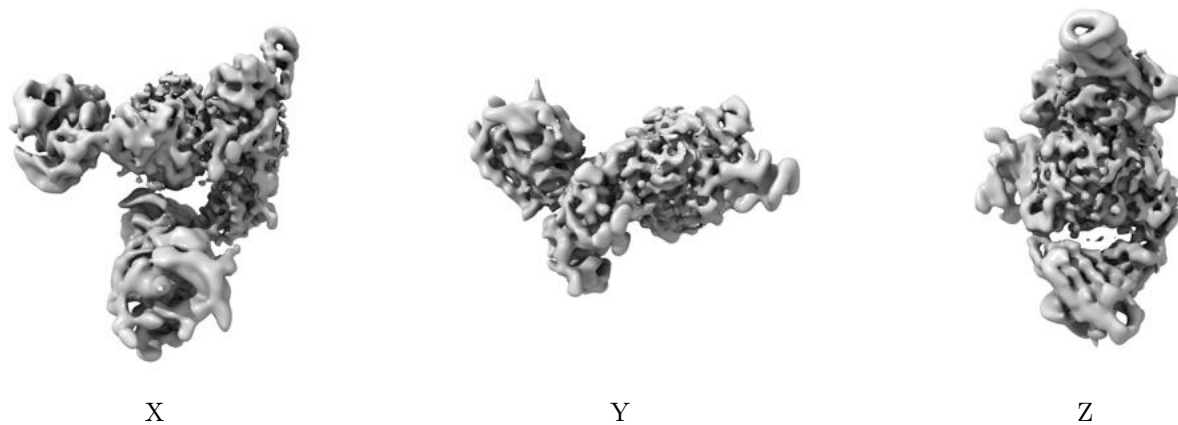


Z

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.

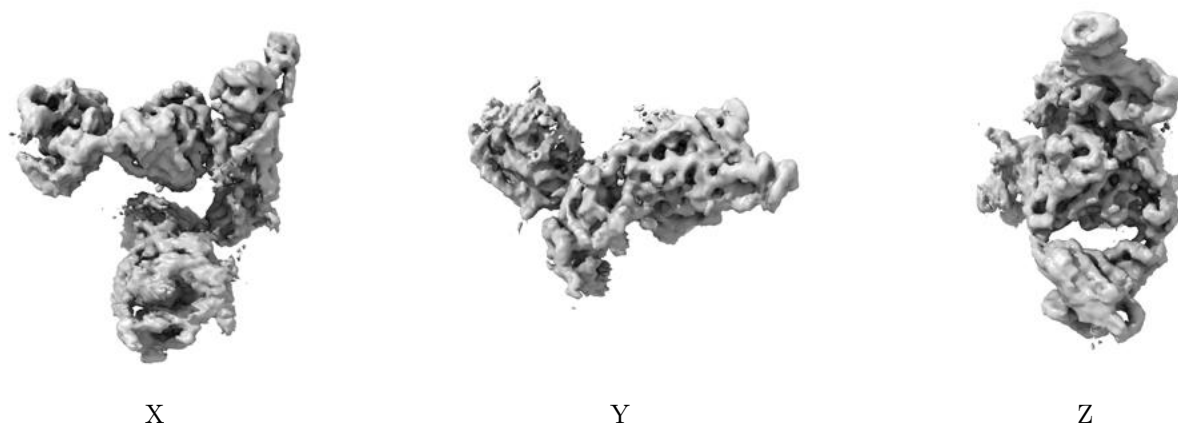
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

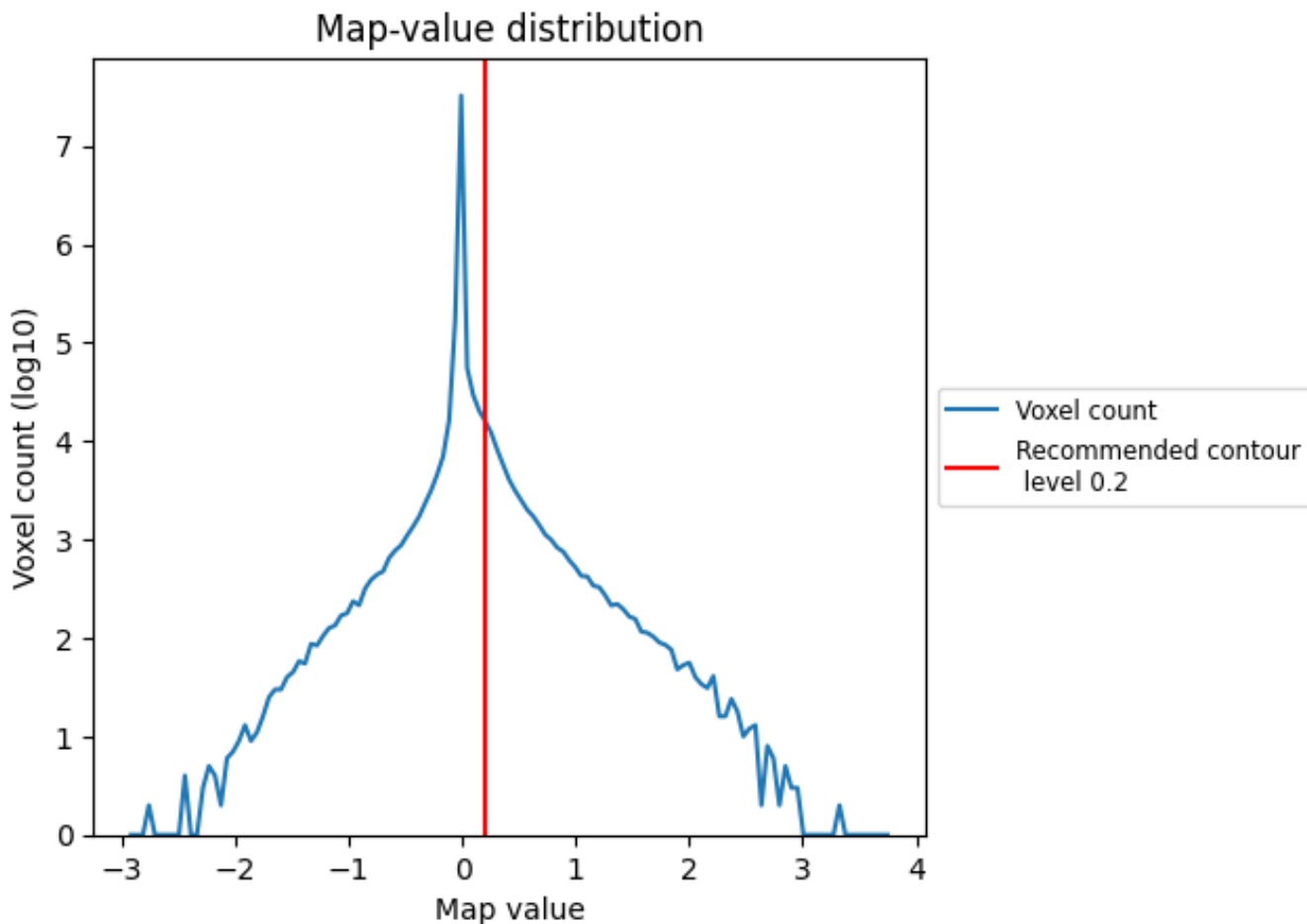
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

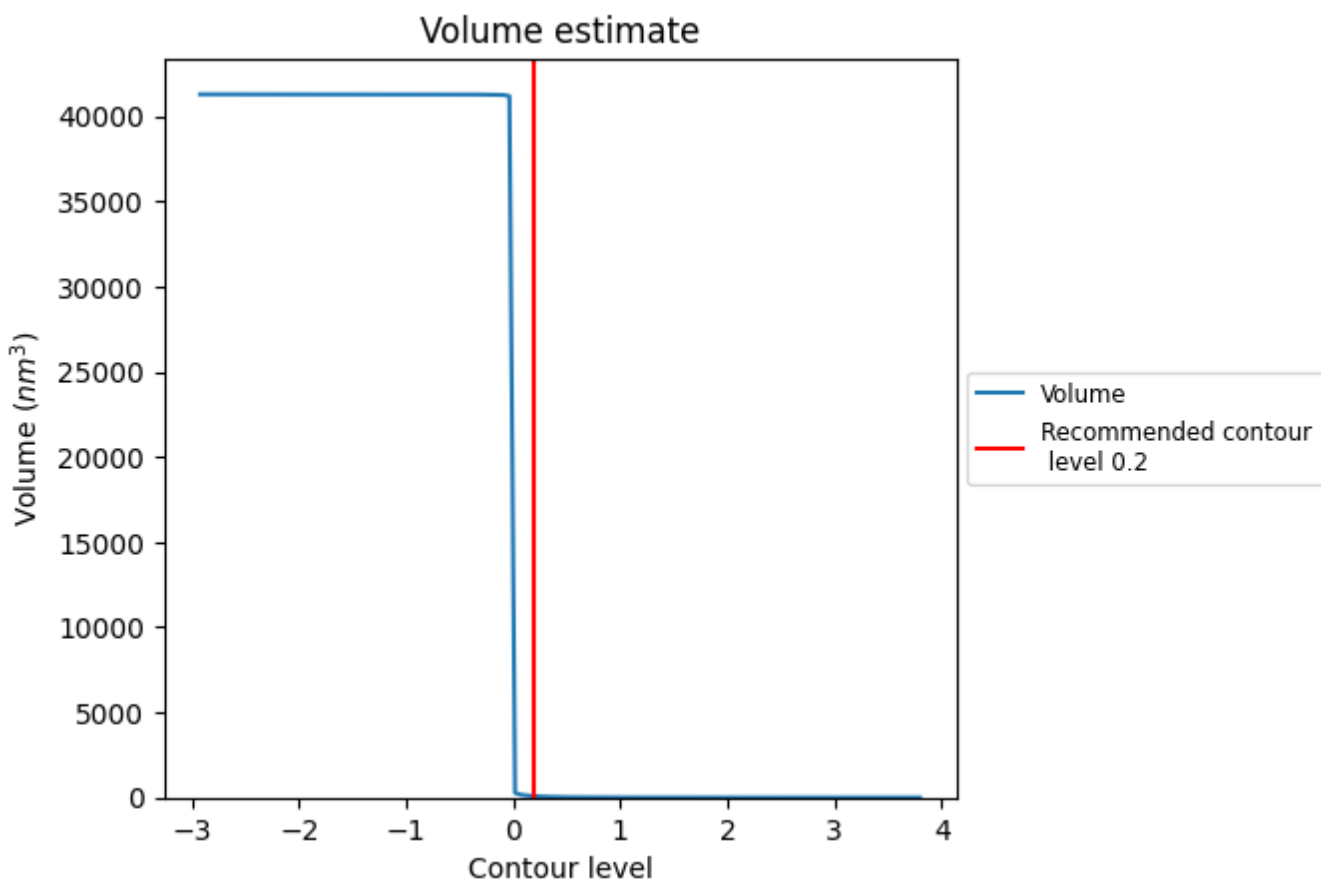
This section contains the results of statistical analysis of the map.

### 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.

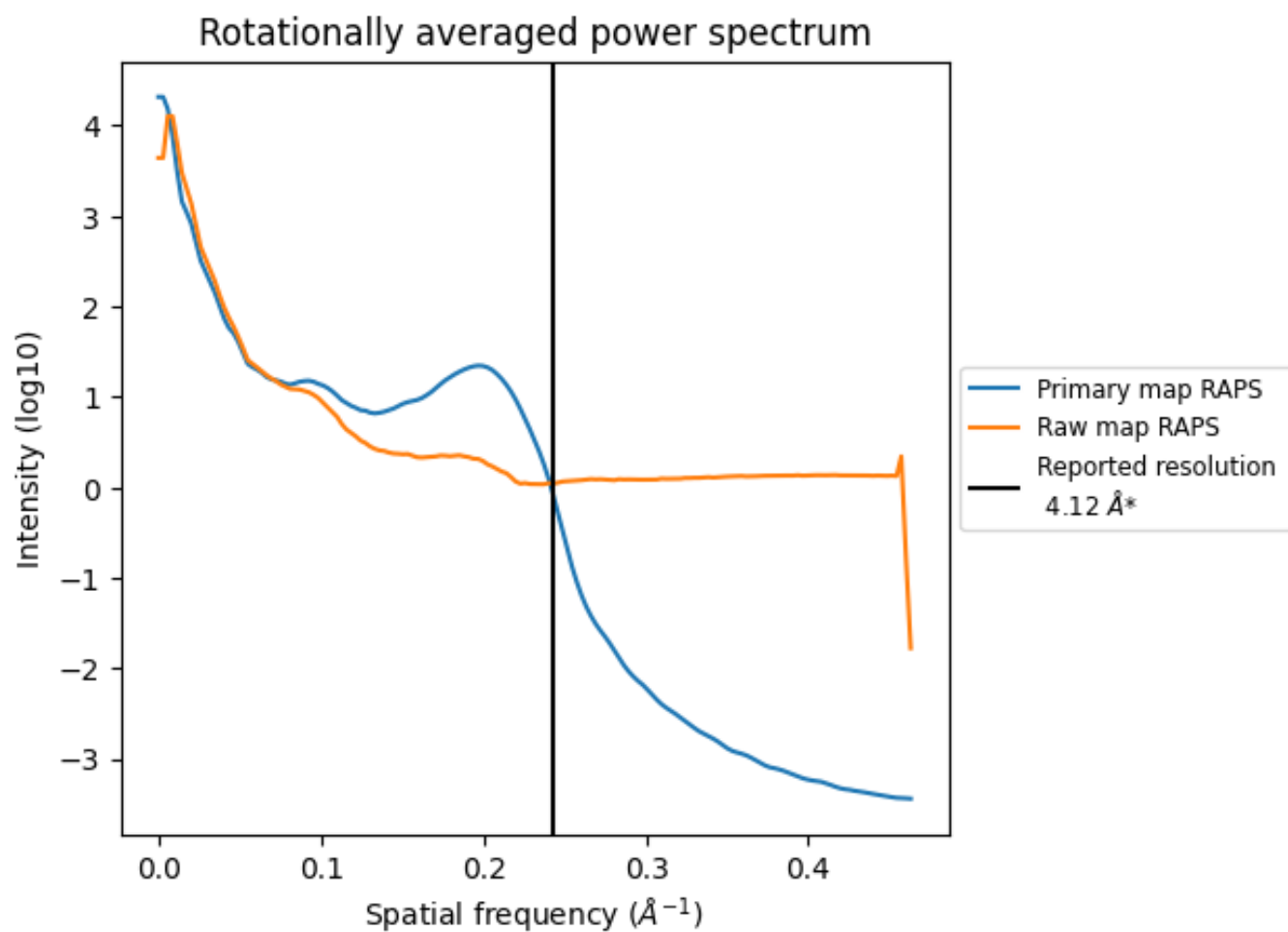
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm<sup>3</sup>; this corresponds to an approximate mass of 75 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](#)

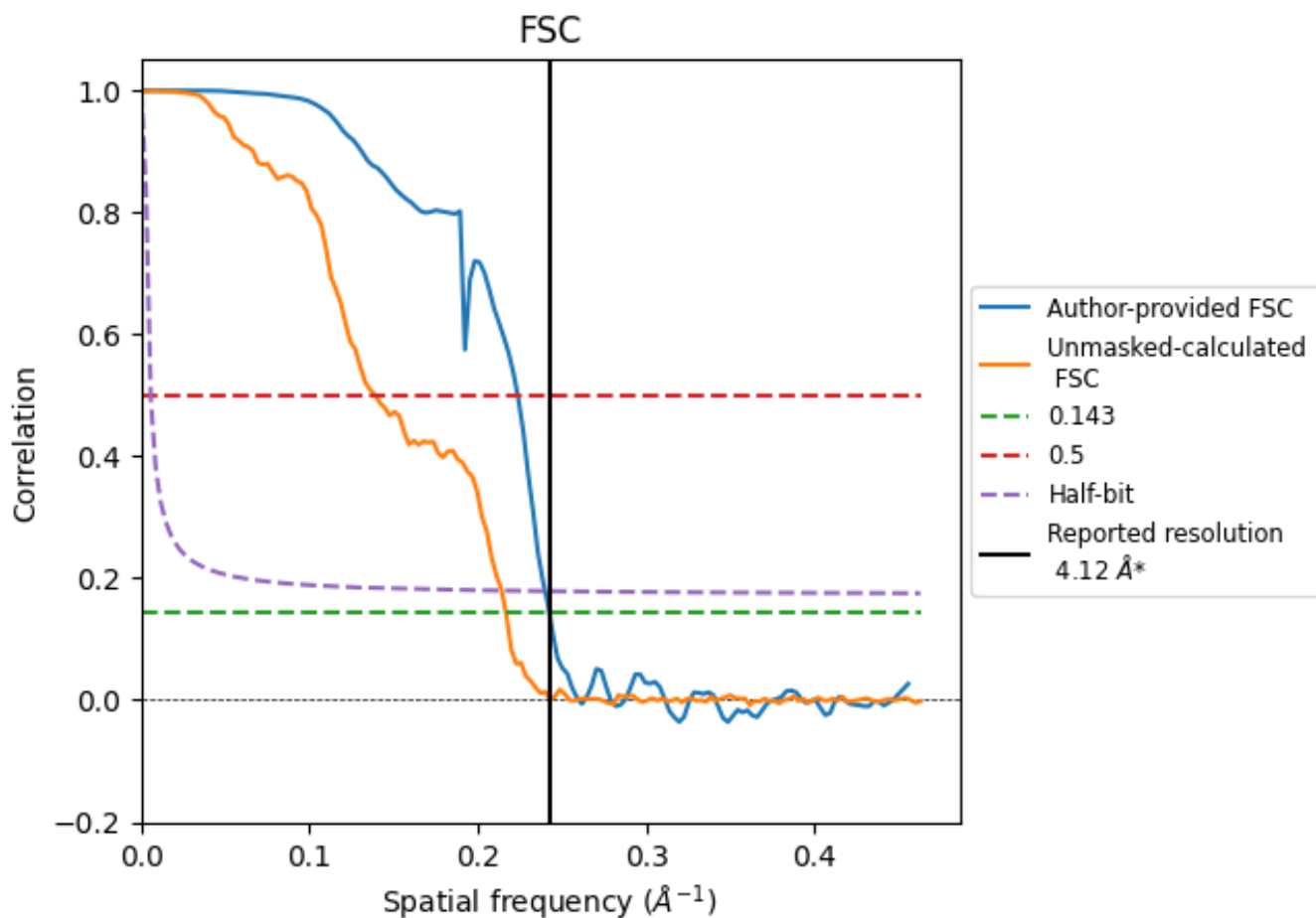


\*Reported resolution corresponds to spatial frequency of 0.243 Å<sup>-1</sup>

## 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 0.243 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

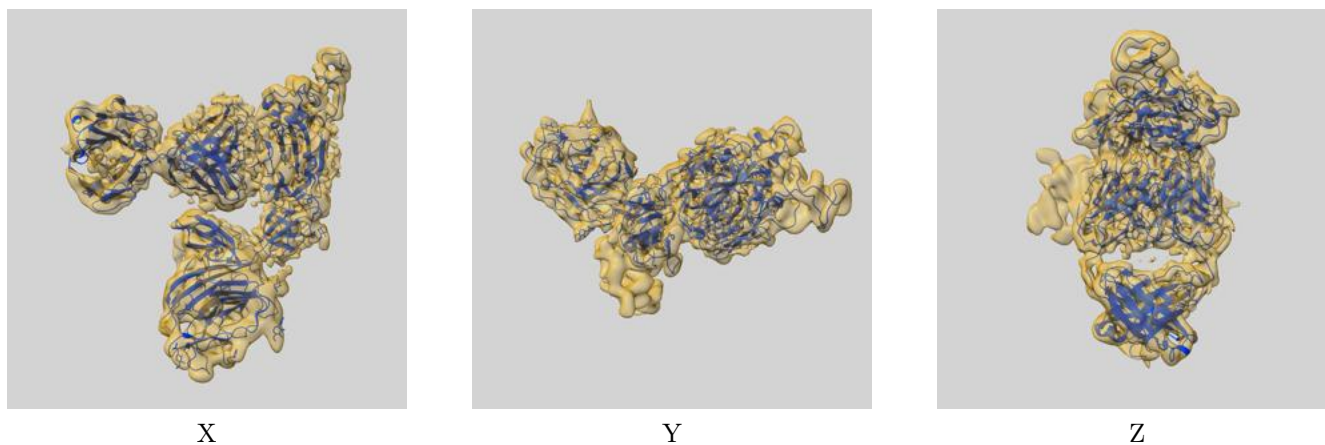
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.12	-	-
Author-provided FSC curve	4.12	4.47	4.17
Unmasked-calculated*	4.61	7.19	4.67

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.61 differs from the reported value 4.12 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54623 and PDB model 9S67. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



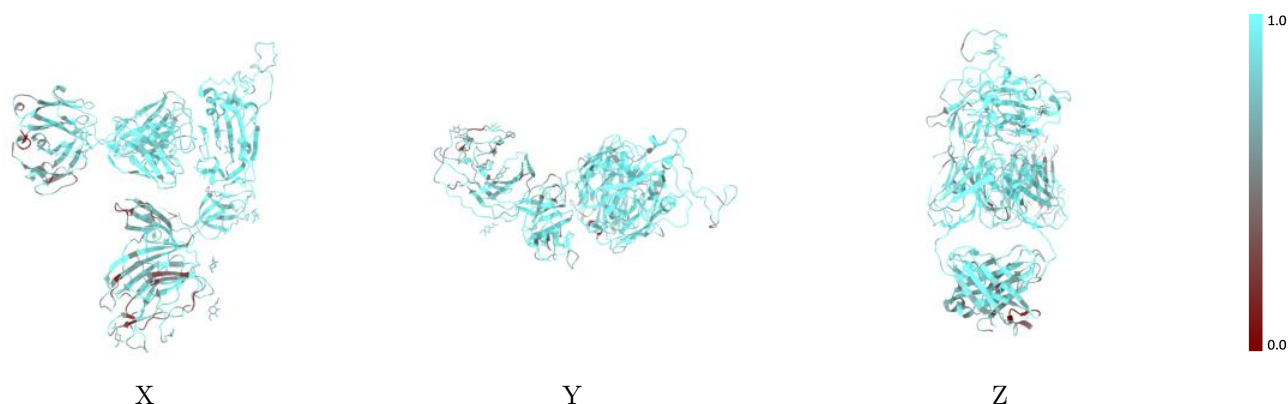
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



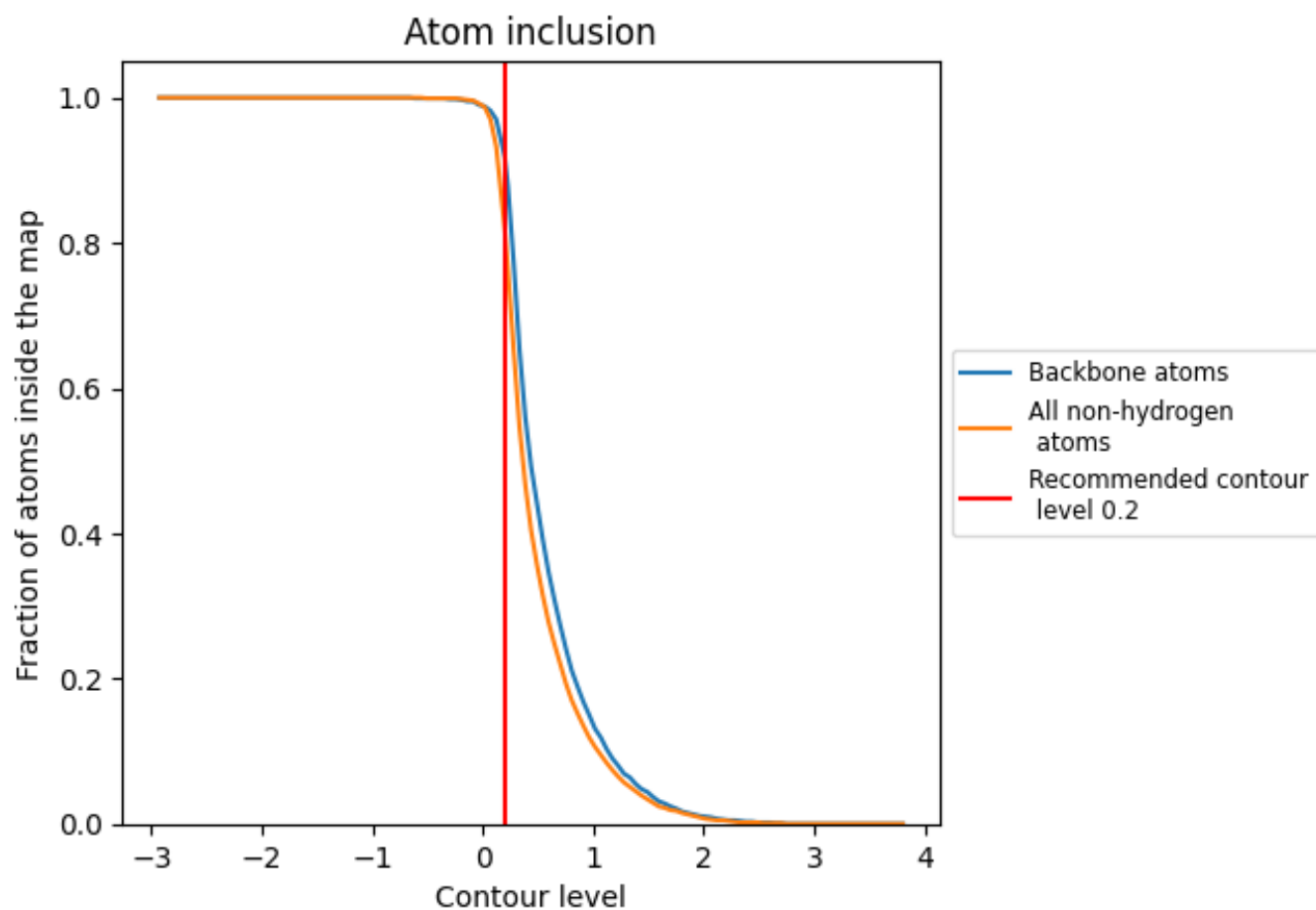
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.3750
A	 0.8290	 0.3750
B	 0.8470	 0.4050
C	 0.8030	 0.3630

