



Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 05:08 PM JST

PDB ID : 22FY / pdb_000022fy
EMDB ID : EMD-68252
Title : Structure of MERS-CoV S protein with 3down-RBDs
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2026-01-09
Resolution : 3.24 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
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

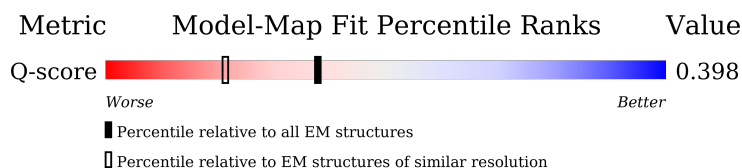
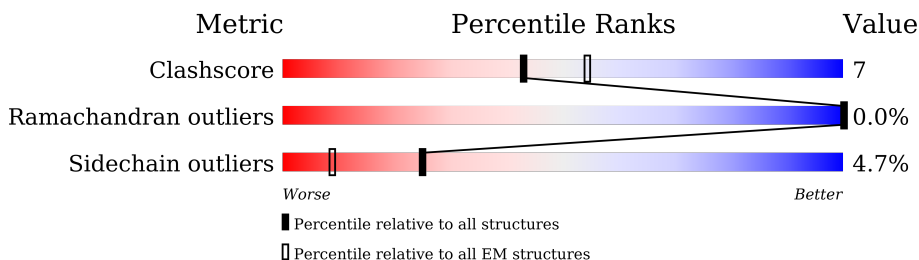
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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	14594 (2.74 - 3.74)

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	1340	
1	B	1340	
1	C	1340	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27996 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1207	Total	C	N	O	S	0	0
			9332	5919	1553	1809	51		
1	C	1207	Total	C	N	O	S	0	0
			9332	5919	1553	1809	51		
1	B	1207	Total	C	N	O	S	0	0
			9332	5919	1553	1809	51		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	GLY	-	expression tag	UNP K9N5Q8
A	1293	SER	-	expression tag	UNP K9N5Q8
A	1294	GLY	-	expression tag	UNP K9N5Q8
A	1295	TYR	-	expression tag	UNP K9N5Q8
A	1296	ILE	-	expression tag	UNP K9N5Q8
A	1297	PRO	-	expression tag	UNP K9N5Q8
A	1298	GLU	-	expression tag	UNP K9N5Q8
A	1299	ALA	-	expression tag	UNP K9N5Q8
A	1300	PRO	-	expression tag	UNP K9N5Q8
A	1301	ARG	-	expression tag	UNP K9N5Q8
A	1302	ASP	-	expression tag	UNP K9N5Q8
A	1303	GLY	-	expression tag	UNP K9N5Q8
A	1304	GLN	-	expression tag	UNP K9N5Q8
A	1305	ALA	-	expression tag	UNP K9N5Q8
A	1306	TYR	-	expression tag	UNP K9N5Q8
A	1307	VAL	-	expression tag	UNP K9N5Q8
A	1308	ARG	-	expression tag	UNP K9N5Q8
A	1309	LYS	-	expression tag	UNP K9N5Q8
A	1310	ASP	-	expression tag	UNP K9N5Q8
A	1311	GLY	-	expression tag	UNP K9N5Q8
A	1312	GLU	-	expression tag	UNP K9N5Q8
A	1313	TRP	-	expression tag	UNP K9N5Q8
A	1314	VAL	-	expression tag	UNP K9N5Q8
A	1315	LEU	-	expression tag	UNP K9N5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1316	LEU	-	expression tag	UNP K9N5Q8
A	1317	SER	-	expression tag	UNP K9N5Q8
A	1318	THR	-	expression tag	UNP K9N5Q8
A	1319	PHE	-	expression tag	UNP K9N5Q8
A	1320	LEU	-	expression tag	UNP K9N5Q8
A	1321	GLY	-	expression tag	UNP K9N5Q8
A	1322	ARG	-	expression tag	UNP K9N5Q8
A	1323	SER	-	expression tag	UNP K9N5Q8
A	1324	LEU	-	expression tag	UNP K9N5Q8
A	1325	GLU	-	expression tag	UNP K9N5Q8
A	1326	VAL	-	expression tag	UNP K9N5Q8
A	1327	LEU	-	expression tag	UNP K9N5Q8
A	1328	PHE	-	expression tag	UNP K9N5Q8
A	1329	GLN	-	expression tag	UNP K9N5Q8
A	1330	GLY	-	expression tag	UNP K9N5Q8
A	1331	PRO	-	expression tag	UNP K9N5Q8
A	1332	GLY	-	expression tag	UNP K9N5Q8
A	1333	HIS	-	expression tag	UNP K9N5Q8
A	1334	HIS	-	expression tag	UNP K9N5Q8
A	1335	HIS	-	expression tag	UNP K9N5Q8
A	1336	HIS	-	expression tag	UNP K9N5Q8
A	1337	HIS	-	expression tag	UNP K9N5Q8
A	1338	HIS	-	expression tag	UNP K9N5Q8
A	1339	HIS	-	expression tag	UNP K9N5Q8
A	1340	HIS	-	expression tag	UNP K9N5Q8
C	1292	GLY	-	expression tag	UNP K9N5Q8
C	1293	SER	-	expression tag	UNP K9N5Q8
C	1294	GLY	-	expression tag	UNP K9N5Q8
C	1295	TYR	-	expression tag	UNP K9N5Q8
C	1296	ILE	-	expression tag	UNP K9N5Q8
C	1297	PRO	-	expression tag	UNP K9N5Q8
C	1298	GLU	-	expression tag	UNP K9N5Q8
C	1299	ALA	-	expression tag	UNP K9N5Q8
C	1300	PRO	-	expression tag	UNP K9N5Q8
C	1301	ARG	-	expression tag	UNP K9N5Q8
C	1302	ASP	-	expression tag	UNP K9N5Q8
C	1303	GLY	-	expression tag	UNP K9N5Q8
C	1304	GLN	-	expression tag	UNP K9N5Q8
C	1305	ALA	-	expression tag	UNP K9N5Q8
C	1306	TYR	-	expression tag	UNP K9N5Q8
C	1307	VAL	-	expression tag	UNP K9N5Q8
C	1308	ARG	-	expression tag	UNP K9N5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1309	LYS	-	expression tag	UNP K9N5Q8
C	1310	ASP	-	expression tag	UNP K9N5Q8
C	1311	GLY	-	expression tag	UNP K9N5Q8
C	1312	GLU	-	expression tag	UNP K9N5Q8
C	1313	TRP	-	expression tag	UNP K9N5Q8
C	1314	VAL	-	expression tag	UNP K9N5Q8
C	1315	LEU	-	expression tag	UNP K9N5Q8
C	1316	LEU	-	expression tag	UNP K9N5Q8
C	1317	SER	-	expression tag	UNP K9N5Q8
C	1318	THR	-	expression tag	UNP K9N5Q8
C	1319	PHE	-	expression tag	UNP K9N5Q8
C	1320	LEU	-	expression tag	UNP K9N5Q8
C	1321	GLY	-	expression tag	UNP K9N5Q8
C	1322	ARG	-	expression tag	UNP K9N5Q8
C	1323	SER	-	expression tag	UNP K9N5Q8
C	1324	LEU	-	expression tag	UNP K9N5Q8
C	1325	GLU	-	expression tag	UNP K9N5Q8
C	1326	VAL	-	expression tag	UNP K9N5Q8
C	1327	LEU	-	expression tag	UNP K9N5Q8
C	1328	PHE	-	expression tag	UNP K9N5Q8
C	1329	GLN	-	expression tag	UNP K9N5Q8
C	1330	GLY	-	expression tag	UNP K9N5Q8
C	1331	PRO	-	expression tag	UNP K9N5Q8
C	1332	GLY	-	expression tag	UNP K9N5Q8
C	1333	HIS	-	expression tag	UNP K9N5Q8
C	1334	HIS	-	expression tag	UNP K9N5Q8
C	1335	HIS	-	expression tag	UNP K9N5Q8
C	1336	HIS	-	expression tag	UNP K9N5Q8
C	1337	HIS	-	expression tag	UNP K9N5Q8
C	1338	HIS	-	expression tag	UNP K9N5Q8
C	1339	HIS	-	expression tag	UNP K9N5Q8
C	1340	HIS	-	expression tag	UNP K9N5Q8
B	1292	GLY	-	expression tag	UNP K9N5Q8
B	1293	SER	-	expression tag	UNP K9N5Q8
B	1294	GLY	-	expression tag	UNP K9N5Q8
B	1295	TYR	-	expression tag	UNP K9N5Q8
B	1296	ILE	-	expression tag	UNP K9N5Q8
B	1297	PRO	-	expression tag	UNP K9N5Q8
B	1298	GLU	-	expression tag	UNP K9N5Q8
B	1299	ALA	-	expression tag	UNP K9N5Q8
B	1300	PRO	-	expression tag	UNP K9N5Q8
B	1301	ARG	-	expression tag	UNP K9N5Q8

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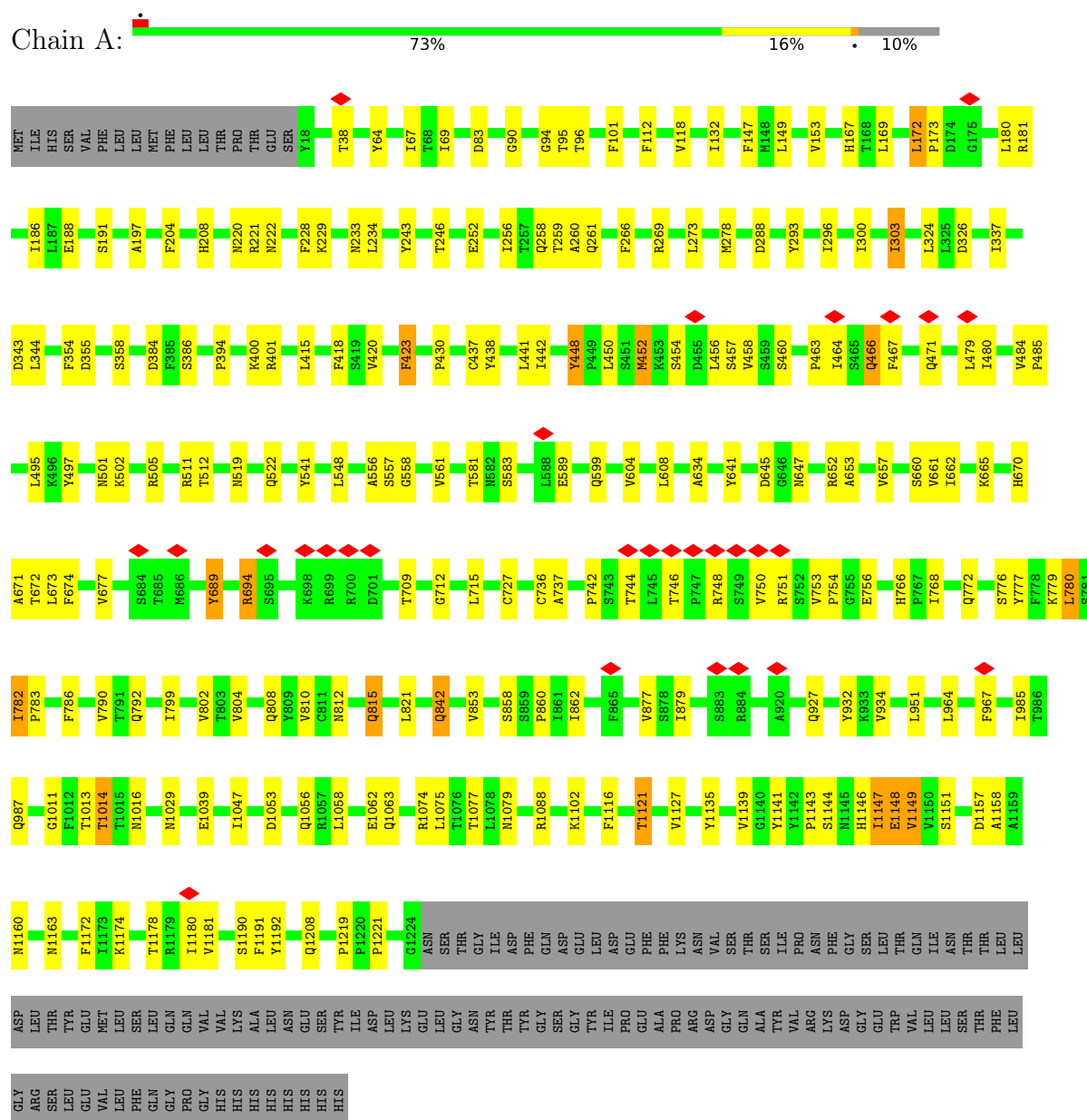
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1302	ASP	-	expression tag	UNP K9N5Q8
B	1303	GLY	-	expression tag	UNP K9N5Q8
B	1304	GLN	-	expression tag	UNP K9N5Q8
B	1305	ALA	-	expression tag	UNP K9N5Q8
B	1306	TYR	-	expression tag	UNP K9N5Q8
B	1307	VAL	-	expression tag	UNP K9N5Q8
B	1308	ARG	-	expression tag	UNP K9N5Q8
B	1309	LYS	-	expression tag	UNP K9N5Q8
B	1310	ASP	-	expression tag	UNP K9N5Q8
B	1311	GLY	-	expression tag	UNP K9N5Q8
B	1312	GLU	-	expression tag	UNP K9N5Q8
B	1313	TRP	-	expression tag	UNP K9N5Q8
B	1314	VAL	-	expression tag	UNP K9N5Q8
B	1315	LEU	-	expression tag	UNP K9N5Q8
B	1316	LEU	-	expression tag	UNP K9N5Q8
B	1317	SER	-	expression tag	UNP K9N5Q8
B	1318	THR	-	expression tag	UNP K9N5Q8
B	1319	PHE	-	expression tag	UNP K9N5Q8
B	1320	LEU	-	expression tag	UNP K9N5Q8
B	1321	GLY	-	expression tag	UNP K9N5Q8
B	1322	ARG	-	expression tag	UNP K9N5Q8
B	1323	SER	-	expression tag	UNP K9N5Q8
B	1324	LEU	-	expression tag	UNP K9N5Q8
B	1325	GLU	-	expression tag	UNP K9N5Q8
B	1326	VAL	-	expression tag	UNP K9N5Q8
B	1327	LEU	-	expression tag	UNP K9N5Q8
B	1328	PHE	-	expression tag	UNP K9N5Q8
B	1329	GLN	-	expression tag	UNP K9N5Q8
B	1330	GLY	-	expression tag	UNP K9N5Q8
B	1331	PRO	-	expression tag	UNP K9N5Q8
B	1332	GLY	-	expression tag	UNP K9N5Q8
B	1333	HIS	-	expression tag	UNP K9N5Q8
B	1334	HIS	-	expression tag	UNP K9N5Q8
B	1335	HIS	-	expression tag	UNP K9N5Q8
B	1336	HIS	-	expression tag	UNP K9N5Q8
B	1337	HIS	-	expression tag	UNP K9N5Q8
B	1338	HIS	-	expression tag	UNP K9N5Q8
B	1339	HIS	-	expression tag	UNP K9N5Q8
B	1340	HIS	-	expression tag	UNP K9N5Q8

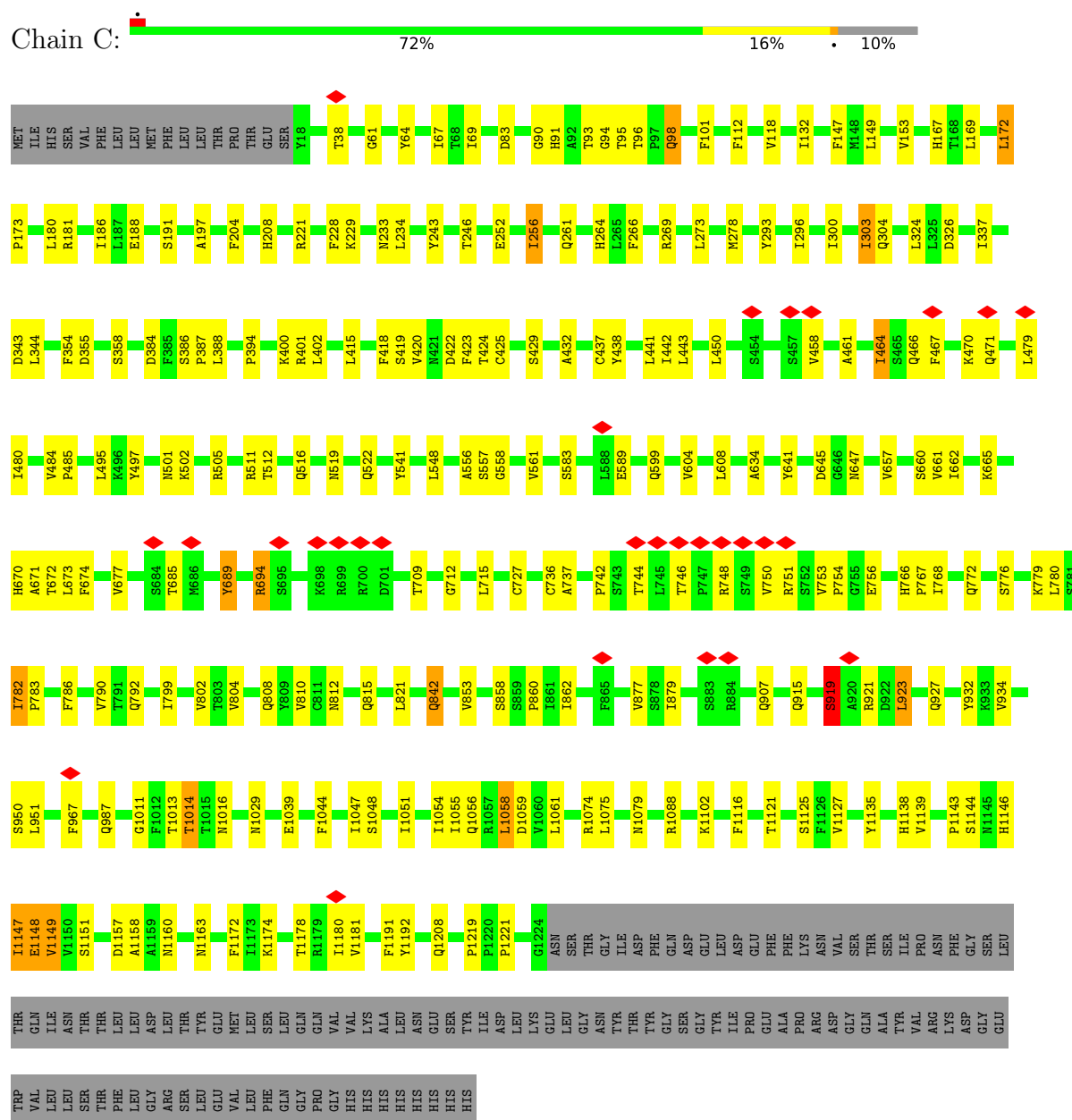
3 Residue-property plots

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.

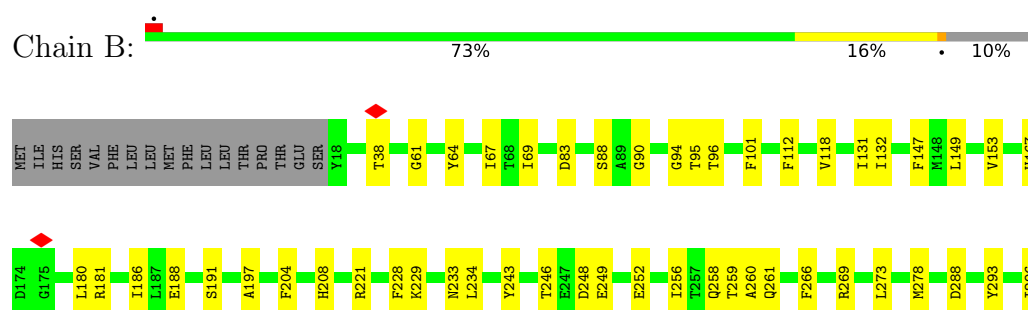
• Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6626	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.385	Depositor
Minimum map value	-0.603	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/9551	0.29	0/12999
1	B	0.12	0/9551	0.29	0/12999
1	C	0.17	0/9551	0.31	0/12999
All	All	0.14	0/28653	0.30	0/38997

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	9332	0	9036	133	0
1	B	9332	0	9036	141	0
1	C	9332	0	9036	138	0
All	All	27996	0	27108	365	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 7.

All (365) 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:C:919:SER:HB2	1:B:652:ARG:HE	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:ARG:H	1:C:694:ARG:HH11	1.32	0.76
1:B:694:ARG:HH11	1:B:694:ARG:H	1.33	0.75
1:A:694:ARG:HH11	1:A:694:ARG:H	1.33	0.74
1:A:1208:GLN:HE22	1:B:987:GLN:HG3	1.56	0.71
1:C:919:SER:HB2	1:B:652:ARG:HH21	1.56	0.70
1:C:919:SER:HB2	1:B:652:ARG:NE	2.06	0.69
1:C:919:SER:C	1:B:652:ARG:NH2	2.50	0.69
1:C:987:GLN:HG3	1:B:1208:GLN:HE22	1.58	0.68
1:C:497:TYR:HB2	1:C:561:VAL:HB	1.78	0.66
1:A:497:TYR:HB2	1:A:561:VAL:HB	1.78	0.65
1:B:497:TYR:HB2	1:B:561:VAL:HB	1.78	0.65
1:B:672:THR:HB	1:B:715:LEU:HB2	1.78	0.65
1:A:672:THR:HB	1:A:715:LEU:HB2	1.78	0.64
1:C:919:SER:HB2	1:B:652:ARG:NH2	2.13	0.64
1:B:736:CYS:SG	1:B:737:ALA:N	2.71	0.64
1:A:736:CYS:SG	1:A:737:ALA:N	2.71	0.64
1:A:1208:GLN:OE1	1:B:987:GLN:NE2	2.30	0.64
1:C:657:VAL:HG13	1:C:677:VAL:HG21	1.80	0.64
1:C:736:CYS:SG	1:C:737:ALA:N	2.71	0.64
1:B:1075:LEU:O	1:B:1079:ASN:ND2	2.30	0.64
1:C:672:THR:HB	1:C:715:LEU:HB2	1.79	0.63
1:A:657:VAL:HG13	1:A:677:VAL:HG21	1.80	0.63
1:A:94:GLY:HA2	1:A:303:ILE:HB	1.81	0.63
1:B:94:GLY:HA2	1:B:303:ILE:HB	1.81	0.62
1:C:662:ILE:HB	1:C:671:ALA:HB3	1.80	0.62
1:C:1029:ASN:OD1	1:C:1088:ARG:NH2	2.31	0.62
1:A:987:GLN:HG3	1:C:1208:GLN:HE22	1.63	0.62
1:B:657:VAL:HG13	1:B:677:VAL:HG21	1.80	0.62
1:A:1157:ASP:HB3	1:A:1160:ASN:HB2	1.82	0.62
1:C:1075:LEU:O	1:C:1079:ASN:ND2	2.31	0.62
1:B:662:ILE:HB	1:B:671:ALA:HB3	1.81	0.62
1:B:1029:ASN:OD1	1:B:1088:ARG:NH2	2.32	0.62
1:C:246:THR:O	1:C:269:ARG:NH2	2.33	0.61
1:C:790:VAL:HG22	1:C:1139:VAL:HG22	1.82	0.61
1:C:987:GLN:NE2	1:B:1208:GLN:OE1	2.33	0.61
1:A:246:THR:O	1:A:269:ARG:NH2	2.34	0.61
1:A:662:ILE:HB	1:A:671:ALA:HB3	1.81	0.61
1:C:167:HIS:H	1:C:186:ILE:HG12	1.65	0.61
1:B:1157:ASP:HB3	1:B:1160:ASN:HB2	1.82	0.61
1:C:69:ILE:HD11	1:B:634:ALA:HA	1.82	0.61
1:C:853:VAL:HB	1:C:951:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:O	1:B:269:ARG:NH2	2.34	0.61
1:B:709:THR:OG1	1:B:712:GLY:O	2.20	0.60
1:A:709:THR:OG1	1:A:712:GLY:O	2.20	0.60
1:A:1075:LEU:O	1:A:1079:ASN:ND2	2.30	0.60
1:C:810:VAL:O	1:C:1074:ARG:NH1	2.35	0.60
1:A:1029:ASN:OD1	1:A:1088:ARG:NH2	2.32	0.60
1:B:167:HIS:H	1:B:186:ILE:HG12	1.67	0.60
1:B:853:VAL:HB	1:B:951:LEU:HD21	1.84	0.60
1:A:634:ALA:HA	1:B:69:ILE:HD11	1.84	0.59
1:B:790:VAL:HG22	1:B:1139:VAL:HG22	1.83	0.59
1:A:853:VAL:HB	1:A:951:LEU:HD21	1.84	0.59
1:A:266:PHE:HB3	1:A:278:MET:HB3	1.85	0.58
1:C:1157:ASP:HB3	1:C:1160:ASN:HB2	1.83	0.58
1:B:266:PHE:HB3	1:B:278:MET:HB3	1.85	0.58
1:B:810:VAL:O	1:B:1074:ARG:NH1	2.37	0.58
1:A:167:HIS:H	1:A:186:ILE:HG12	1.67	0.58
1:A:790:VAL:HG22	1:A:1139:VAL:HG22	1.83	0.58
1:A:358:SER:HB2	1:A:665:LYS:H	1.69	0.58
1:A:810:VAL:O	1:A:1074:ARG:NH1	2.37	0.58
1:A:252:GLU:OE2	1:A:269:ARG:NH1	2.37	0.58
1:B:252:GLU:OE2	1:B:269:ARG:NH1	2.37	0.57
1:C:252:GLU:OE2	1:C:269:ARG:NH1	2.37	0.57
1:C:94:GLY:HA2	1:C:303:ILE:HB	1.86	0.57
1:C:153:VAL:HG21	1:B:548:LEU:HD22	1.86	0.57
1:B:112:PHE:HD1	1:B:293:TYR:HB3	1.69	0.57
1:C:783:PRO:HG2	1:C:1192:TYR:HB2	1.85	0.57
1:C:772:GLN:HB2	1:C:776:SER:HB3	1.87	0.57
1:B:358:SER:HB2	1:B:665:LYS:H	1.69	0.57
1:A:343:ASP:HB2	1:A:661:VAL:HG22	1.87	0.57
1:C:266:PHE:HB3	1:C:278:MET:HB3	1.85	0.56
1:B:501:ASN:H	1:B:558:GLY:HA2	1.70	0.56
1:A:783:PRO:HG2	1:A:1192:TYR:HB2	1.86	0.56
1:C:112:PHE:HD1	1:C:293:TYR:HB3	1.69	0.56
1:B:783:PRO:HG2	1:B:1192:TYR:HB2	1.86	0.56
1:A:501:ASN:H	1:A:558:GLY:HA2	1.70	0.56
1:B:181:ARG:NH2	1:B:221:ARG:O	2.39	0.56
1:C:358:SER:HB2	1:C:665:LYS:H	1.70	0.56
1:A:112:PHE:HD1	1:A:293:TYR:HB3	1.69	0.56
1:C:188:GLU:HB3	1:C:233:ASN:HB2	1.88	0.56
1:A:548:LEU:HD22	1:B:153:VAL:HG21	1.87	0.56
1:B:792:GLN:NE2	1:B:1135:TYR:OH	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLN:HB2	1:A:776:SER:HB3	1.88	0.56
1:C:181:ARG:NH2	1:C:221:ARG:O	2.38	0.56
1:B:786:PHE:HA	1:B:1144:SER:HB3	1.88	0.56
1:B:343:ASP:HB2	1:B:661:VAL:HG22	1.87	0.55
1:C:423:PHE:HA	1:C:480:ILE:HD12	1.87	0.55
1:B:753:VAL:HG23	1:B:756:GLU:H	1.72	0.55
1:A:792:GLN:NE2	1:A:1135:TYR:OH	2.39	0.55
1:A:181:ARG:NH2	1:A:221:ARG:O	2.39	0.55
1:A:188:GLU:HB3	1:A:233:ASN:HB2	1.89	0.55
1:A:753:VAL:HG23	1:A:756:GLU:H	1.72	0.55
1:A:1219:PRO:HB2	1:A:1221:PRO:HD2	1.89	0.55
1:C:792:GLN:NE2	1:C:1135:TYR:OH	2.39	0.55
1:A:987:GLN:NE2	1:C:1208:GLN:OE1	2.40	0.55
1:C:877:VAL:HG12	1:C:879:ILE:H	1.72	0.55
1:C:1219:PRO:HB2	1:C:1221:PRO:HD2	1.88	0.55
1:A:415:LEU:HD22	1:A:420:VAL:HG21	1.89	0.55
1:A:786:PHE:HA	1:A:1144:SER:HB3	1.88	0.55
1:C:753:VAL:HG23	1:C:756:GLU:H	1.72	0.54
1:B:188:GLU:HB3	1:B:233:ASN:HB2	1.89	0.54
1:C:786:PHE:HA	1:C:1144:SER:HB3	1.89	0.54
1:C:343:ASP:HB2	1:C:661:VAL:HG22	1.89	0.54
1:B:415:LEU:HD22	1:B:420:VAL:HG21	1.89	0.54
1:A:69:ILE:HD11	1:C:634:ALA:HA	1.89	0.54
1:A:877:VAL:HG12	1:A:879:ILE:H	1.71	0.54
1:B:772:GLN:HB2	1:B:776:SER:HB3	1.88	0.54
1:B:877:VAL:HG12	1:B:879:ILE:H	1.71	0.54
1:C:709:THR:OG1	1:C:712:GLY:O	2.20	0.54
1:B:208:HIS:HB3	1:B:300:ILE:HG13	1.89	0.54
1:B:1219:PRO:HB2	1:B:1221:PRO:HD2	1.89	0.54
1:B:258:GLN:NE2	1:B:288:ASP:O	2.41	0.54
1:A:645:ASP:OD2	1:A:647:ASN:ND2	2.41	0.54
1:B:384:ASP:OD1	1:B:386:SER:OG	2.26	0.53
1:A:780:LEU:HG	1:B:965:SER:HB2	1.89	0.53
1:A:768:ILE:HG22	1:B:860:PRO:HG3	1.90	0.53
1:A:208:HIS:HB3	1:A:300:ILE:HG13	1.89	0.53
1:B:344:LEU:HD13	1:B:670:HIS:HB3	1.91	0.53
1:C:645:ASP:OD2	1:C:647:ASN:ND2	2.41	0.53
1:C:919:SER:HB2	1:B:652:ARG:CZ	2.38	0.53
1:C:402:LEU:HB2	1:C:443:LEU:HB3	1.90	0.53
1:B:645:ASP:OD2	1:B:647:ASN:ND2	2.41	0.52
1:B:259:THR:HG23	1:B:261:GLN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:NE2	1:A:288:ASP:O	2.41	0.52
1:C:344:LEU:HD13	1:C:670:HIS:HB3	1.91	0.52
1:A:90:GLY:HA2	1:A:101:PHE:HB3	1.91	0.52
1:A:768:ILE:HA	1:B:860:PRO:HD3	1.90	0.52
1:A:344:LEU:HD13	1:A:670:HIS:HB3	1.91	0.52
1:B:90:GLY:HA2	1:B:101:PHE:HB3	1.91	0.52
1:A:1151:SER:OG	1:A:1172:PHE:O	2.23	0.52
1:A:259:THR:HG23	1:A:261:GLN:H	1.74	0.52
1:C:208:HIS:HB3	1:C:300:ILE:HG13	1.90	0.52
1:C:779:LYS:HB3	1:C:1149:VAL:HG13	1.92	0.52
1:A:808:GLN:O	1:A:812:ASN:ND2	2.43	0.51
1:A:261:GLN:HG3	1:C:442:ILE:HD11	1.93	0.51
1:C:808:GLN:O	1:C:812:ASN:ND2	2.43	0.51
1:B:191:SER:HA	1:B:197:ALA:HB3	1.92	0.51
1:C:112:PHE:HA	1:C:293:TYR:HD1	1.76	0.51
1:C:501:ASN:H	1:C:558:GLY:HA2	1.74	0.51
1:B:808:GLN:O	1:B:812:ASN:ND2	2.43	0.51
1:C:90:GLY:HA2	1:C:101:PHE:HB3	1.93	0.51
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.93	0.51
1:C:402:LEU:HD12	1:C:443:LEU:HD23	1.93	0.51
1:C:660:SER:HB2	1:C:673:LEU:HB3	1.92	0.50
1:C:858:SER:HB2	1:B:766:HIS:HB2	1.94	0.50
1:C:802:VAL:HG22	1:C:934:VAL:HG22	1.94	0.50
1:A:260:ALA:O	1:C:401:ARG:NH1	2.44	0.50
1:B:742:PRO:HG2	1:B:754:PRO:HD3	1.93	0.50
1:A:401:ARG:HG3	1:A:442:ILE:HG23	1.94	0.50
1:A:858:SER:H	1:C:767:PRO:HD2	1.77	0.50
1:A:780:LEU:CG	1:B:965:SER:HB2	2.41	0.50
1:B:1151:SER:OG	1:B:1172:PHE:O	2.23	0.50
1:A:112:PHE:HA	1:A:293:TYR:HD1	1.76	0.50
1:A:191:SER:HA	1:A:197:ALA:HB3	1.92	0.50
1:A:660:SER:HB2	1:A:673:LEU:HB3	1.94	0.50
1:A:858:SER:HB2	1:C:766:HIS:HB2	1.94	0.49
1:A:742:PRO:HG2	1:A:754:PRO:HD3	1.93	0.49
1:C:860:PRO:HD3	1:B:768:ILE:HA	1.93	0.49
1:B:112:PHE:HA	1:B:293:TYR:HD1	1.76	0.49
1:C:401:ARG:HG3	1:C:442:ILE:HG23	1.94	0.49
1:B:541:TYR:HD2	1:B:556:ALA:HB3	1.78	0.49
1:A:355:ASP:OD1	1:A:355:ASP:N	2.46	0.49
1:C:191:SER:HA	1:C:197:ALA:HB3	1.94	0.49
1:C:1151:SER:OG	1:C:1172:PHE:O	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1174:LYS:HD3	1:C:1178:THR:HG21	1.93	0.49
1:B:1174:LYS:HD3	1:B:1178:THR:HG21	1.95	0.49
1:A:802:VAL:HG22	1:A:934:VAL:HG22	1.95	0.49
1:C:464:ILE:HG12	1:C:470:LYS:HG3	1.94	0.49
1:C:742:PRO:HG2	1:C:754:PRO:HD3	1.94	0.49
1:C:355:ASP:OD1	1:C:355:ASP:N	2.46	0.49
1:A:229:LYS:HG2	1:A:234:LEU:HD13	1.95	0.49
1:B:401:ARG:HG3	1:B:442:ILE:HG23	1.94	0.49
1:A:442:ILE:HD11	1:B:261:GLN:HG3	1.95	0.49
1:A:541:TYR:HD2	1:A:556:ALA:HB3	1.78	0.49
1:B:355:ASP:N	1:B:355:ASP:OD1	2.46	0.48
1:B:1058:LEU:O	1:B:1063:GLN:NE2	2.47	0.48
1:A:810:VAL:HG11	1:A:821:LEU:HD13	1.95	0.48
1:B:802:VAL:HG22	1:B:934:VAL:HG22	1.95	0.48
1:C:502:LYS:O	1:C:557:SER:N	2.47	0.48
1:C:589:GLU:HB3	1:B:512:THR:HA	1.95	0.48
1:B:660:SER:HB2	1:B:673:LEU:HB3	1.94	0.48
1:B:810:VAL:HG11	1:B:821:LEU:HD13	1.96	0.48
1:A:502:LYS:O	1:A:557:SER:N	2.46	0.48
1:C:919:SER:CB	1:B:652:ARG:HH21	2.26	0.48
1:C:471:GLN:HB2	1:C:479:LEU:HD22	1.96	0.48
1:C:541:TYR:HD2	1:C:556:ALA:HB3	1.78	0.48
1:C:674:PHE:HB3	1:C:677:VAL:HB	1.96	0.48
1:A:384:ASP:OD1	1:A:386:SER:OG	2.26	0.48
1:A:1174:LYS:HD3	1:A:1178:THR:HG21	1.95	0.48
1:C:689:TYR:HE1	1:C:694:ARG:HH12	1.62	0.48
1:B:456:LEU:HD21	1:B:463:PRO:HB2	1.96	0.48
1:C:229:LYS:HG2	1:C:234:LEU:HD13	1.95	0.47
1:A:779:LYS:HB3	1:A:1149:VAL:HG13	1.97	0.47
1:B:229:LYS:HG2	1:B:234:LEU:HD13	1.95	0.47
1:A:1058:LEU:O	1:A:1063:GLN:NE2	2.47	0.47
1:B:1121:THR:HG23	1:B:1141:TYR:HB3	1.97	0.47
1:A:782:ILE:HD13	1:A:1143:PRO:HA	1.97	0.47
1:A:1121:THR:HG23	1:A:1141:TYR:HB3	1.96	0.47
1:B:502:LYS:O	1:B:557:SER:N	2.46	0.47
1:B:779:LYS:HB3	1:B:1149:VAL:HG13	1.97	0.47
1:A:780:LEU:HD12	1:B:965:SER:HB2	1.97	0.47
1:C:810:VAL:HG11	1:C:821:LEU:HD13	1.95	0.47
1:A:674:PHE:HB3	1:A:677:VAL:HB	1.97	0.47
1:B:418:PHE:HA	1:B:485:PRO:HG3	1.97	0.47
1:B:466:GLN:HB3	1:B:467:PHE:H	1.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:VAL:HA	1:C:932:TYR:HA	1.97	0.47
1:C:782:ILE:HD13	1:C:1143:PRO:HA	1.96	0.47
1:C:1011:GLY:O	1:C:1016:ASN:ND2	2.48	0.47
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.97	0.46
1:C:388:LEU:HD22	1:C:443:LEU:HD21	1.96	0.46
1:A:860:PRO:HD3	1:C:768:ILE:HA	1.98	0.46
1:C:923:LEU:H	1:C:923:LEU:HG	1.54	0.46
1:A:153:VAL:HG21	1:C:548:LEU:HD22	1.97	0.46
1:B:782:ILE:HD13	1:B:1143:PRO:HA	1.97	0.46
1:A:766:HIS:HB2	1:B:858:SER:HB2	1.98	0.46
1:A:1011:GLY:O	1:A:1016:ASN:ND2	2.49	0.46
1:B:1011:GLY:O	1:B:1016:ASN:ND2	2.49	0.46
1:A:804:VAL:HA	1:A:932:TYR:HA	1.98	0.46
1:C:1058:LEU:C	1:B:429:SER:HB2	2.41	0.46
1:C:418:PHE:HA	1:C:485:PRO:HG3	1.97	0.46
1:A:418:PHE:HA	1:A:485:PRO:HG3	1.97	0.46
1:A:799:ILE:HG12	1:A:842:GLN:HG3	1.97	0.45
1:C:919:SER:C	1:B:652:ARG:HH21	2.22	0.45
1:B:674:PHE:HB3	1:B:677:VAL:HB	1.97	0.45
1:A:64:TYR:HB3	1:A:67:ILE:HD11	1.98	0.45
1:C:64:TYR:HB3	1:C:67:ILE:HD11	1.99	0.45
1:B:799:ILE:HG12	1:B:842:GLN:HG3	1.97	0.45
1:B:804:VAL:HA	1:B:932:TYR:HA	1.98	0.45
1:A:689:TYR:HE1	1:A:694:ARG:HH12	1.65	0.45
1:B:64:TYR:HB3	1:B:67:ILE:HD11	1.98	0.45
1:B:862:ILE:H	1:B:862:ILE:HG12	1.60	0.45
1:B:1102:LYS:NZ	1:B:1116:PHE:O	2.47	0.45
1:C:1102:LYS:NZ	1:C:1116:PHE:O	2.47	0.45
1:B:228:PHE:HD2	1:B:234:LEU:HD11	1.81	0.45
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.97	0.45
1:B:452:MET:HE2	1:B:452:MET:HB2	1.69	0.45
1:A:1053:ASP:HA	1:A:1056:GLN:HG2	1.99	0.45
1:C:467:PHE:HE1	1:C:516:GLN:H	1.63	0.45
1:C:860:PRO:HG3	1:B:768:ILE:HG22	1.98	0.45
1:B:689:TYR:HE1	1:B:694:ARG:HH12	1.65	0.45
1:C:384:ASP:OD1	1:C:386:SER:OG	2.27	0.44
1:C:423:PHE:HA	1:C:480:ILE:HG23	1.99	0.44
1:C:858:SER:OG	1:C:950:SER:OG	2.25	0.44
1:A:438:TYR:CE1	1:A:441:LEU:HB2	2.52	0.44
1:B:438:TYR:CE1	1:B:441:LEU:HB2	2.52	0.44
1:A:172:LEU:HD23	1:A:173:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:HD2	1:A:234:LEU:HD11	1.81	0.44
1:A:782:ILE:HG12	1:A:1143:PRO:HB3	1.99	0.44
1:C:415:LEU:HD22	1:C:420:VAL:HG21	1.99	0.44
1:B:172:LEU:HD23	1:B:173:PRO:HD2	1.99	0.44
1:A:1102:LYS:NZ	1:A:1116:PHE:O	2.47	0.44
1:C:438:TYR:CE1	1:C:441:LEU:HB2	2.52	0.44
1:C:1180:ILE:HG22	1:C:1181:VAL:HG13	1.99	0.44
1:B:149:LEU:HD22	1:B:169:LEU:HD23	2.00	0.44
1:A:423:PHE:HB3	1:C:461:ALA:HB3	2.00	0.43
1:A:1058:LEU:HB3	1:A:1062:GLU:HB2	2.00	0.43
1:B:1058:LEU:HB3	1:B:1062:GLU:HB2	2.00	0.43
1:A:149:LEU:HD22	1:A:169:LEU:HD23	2.00	0.43
1:C:783:PRO:HB3	1:C:1191:PHE:HA	1.99	0.43
1:B:1053:ASP:HA	1:B:1056:GLN:HG2	1.99	0.43
1:C:149:LEU:HD22	1:C:169:LEU:HD23	1.99	0.43
1:C:782:ILE:HG12	1:C:1143:PRO:HB3	1.99	0.43
1:C:61:GLY:HA2	1:B:581:THR:HG22	2.00	0.43
1:C:172:LEU:HD23	1:C:173:PRO:HD2	1.99	0.43
1:B:782:ILE:HG12	1:B:1143:PRO:HB3	1.99	0.43
1:A:581:THR:HG22	1:B:61:GLY:HA2	2.01	0.43
1:A:1157:ASP:OD1	1:A:1158:ALA:N	2.52	0.43
1:C:1157:ASP:OD1	1:C:1158:ALA:N	2.52	0.43
1:A:204:PHE:HE2	1:A:296:ILE:HG12	1.83	0.43
1:A:1013:THR:O	1:A:1014:THR:HG22	2.19	0.43
1:C:204:PHE:HE2	1:C:296:ILE:HG12	1.83	0.43
1:B:204:PHE:HE2	1:B:296:ILE:HG12	1.83	0.43
1:B:423:PHE:HA	1:B:480:ILE:HD12	2.01	0.42
1:A:423:PHE:HA	1:A:480:ILE:HD12	2.01	0.42
1:B:1157:ASP:OD1	1:B:1158:ALA:N	2.52	0.42
1:A:456:LEU:HD21	1:A:463:PRO:HB2	2.01	0.42
1:A:783:PRO:HB3	1:A:1191:PHE:HA	2.01	0.42
1:C:1013:THR:O	1:C:1014:THR:HG22	2.19	0.42
1:B:1013:THR:O	1:B:1014:THR:HG22	2.19	0.42
1:A:512:THR:HA	1:B:589:GLU:HB3	2.00	0.42
1:A:1147:ILE:HG12	1:A:1148:GLU:N	2.35	0.42
1:A:452:MET:HB2	1:A:452:MET:HE2	1.69	0.42
1:B:248:ASP:OD1	1:B:249:GLU:N	2.45	0.42
1:B:782:ILE:HG21	1:B:1143:PRO:HB3	2.01	0.42
1:C:303:ILE:HD13	1:C:303:ILE:H	1.85	0.42
1:C:324:LEU:HB3	1:C:337:ILE:HB	2.02	0.42
1:B:783:PRO:HB3	1:B:1191:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ILE:HG21	1:A:1143:PRO:HB3	2.01	0.42
1:A:1039:GLU:HG2	1:A:1077:THR:HG21	2.02	0.42
1:C:93:THR:HA	1:C:304:GLN:HB2	2.00	0.42
1:C:429:SER:HB3	1:C:432:ALA:HB3	2.01	0.42
1:C:1039:GLU:HG3	1:C:1044:PHE:HZ	1.84	0.42
1:B:324:LEU:HB3	1:B:337:ILE:HB	2.01	0.42
1:A:519:ASN:HB2	1:A:522:GLN:HB2	2.02	0.42
1:C:118:VAL:HG21	1:C:147:PHE:CZ	2.55	0.42
1:C:799:ILE:HG13	1:C:842:GLN:HG3	2.00	0.42
1:A:1160:ASN:HB3	1:A:1163:ASN:OD1	2.20	0.42
1:B:118:VAL:HG21	1:B:147:PHE:CZ	2.54	0.42
1:B:303:ILE:HD13	1:B:303:ILE:H	1.85	0.42
1:A:324:LEU:HB3	1:A:337:ILE:HB	2.01	0.41
1:C:91:HIS:H	1:C:101:PHE:HB2	1.84	0.41
1:A:589:GLU:HB3	1:C:512:THR:HA	2.02	0.41
1:A:652:ARG:HG3	1:A:653:ALA:H	1.85	0.41
1:C:228:PHE:HD2	1:C:234:LEU:HD11	1.84	0.41
1:B:180:LEU:N	1:B:243:TYR:O	2.54	0.41
1:B:1147:ILE:HG12	1:B:1148:GLU:N	2.35	0.41
1:A:118:VAL:HG21	1:A:147:PHE:CZ	2.54	0.41
1:A:448:TYR:HD1	1:A:448:TYR:HA	1.77	0.41
1:A:463:PRO:HA	1:A:466:GLN:HB2	2.03	0.41
1:B:608:LEU:HD13	1:B:641:TYR:CG	2.55	0.41
1:A:471:GLN:HB2	1:A:479:LEU:HD22	2.02	0.41
1:C:180:LEU:N	1:C:243:TYR:O	2.54	0.41
1:A:777:TYR:HA	1:B:969:ALA:HB1	2.01	0.41
1:A:985:ILE:HG12	1:A:1190:SER:HB2	2.03	0.41
1:B:386:SER:OG	1:B:387:PRO:HD3	2.21	0.41
1:B:652:ARG:HG3	1:B:653:ALA:H	1.85	0.41
1:A:303:ILE:H	1:A:303:ILE:HD13	1.85	0.41
1:A:780:LEU:CD1	1:B:965:SER:HB2	2.51	0.41
1:C:927:GLN:HG2	1:C:932:TYR:CE2	2.56	0.41
1:B:448:TYR:HD1	1:B:448:TYR:HA	1.77	0.41
1:B:1160:ASN:HB3	1:B:1163:ASN:OD1	2.20	0.41
1:A:927:GLN:HG2	1:A:932:TYR:CE2	2.56	0.41
1:B:471:GLN:HB2	1:B:479:LEU:HD22	2.02	0.41
1:B:827:PHE:HD2	1:B:1075:LEU:HD13	1.85	0.41
1:B:898:VAL:HG23	1:B:900:ILE:HG22	2.03	0.41
1:C:256:ILE:HA	1:C:264:HIS:O	2.21	0.41
1:C:919:SER:CB	1:B:652:ARG:HE	2.24	0.41
1:C:1125:SER:OG	1:C:1138:HIS:ND1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:CYS:HB3	1:A:583:SER:HB3	2.03	0.41
1:A:608:LEU:HD13	1:A:641:TYR:CG	2.55	0.41
1:C:437:CYS:HB3	1:C:583:SER:HB3	2.03	0.41
1:C:599:GLN:NE2	1:C:604:VAL:HG11	2.36	0.41
1:C:685:THR:HG21	1:C:694:ARG:HB3	2.03	0.41
1:C:1061:LEU:HD12	1:C:1061:LEU:H	1.85	0.41
1:B:842:GLN:HE21	1:B:842:GLN:HB3	1.64	0.41
1:B:985:ILE:HG12	1:B:1190:SER:HB2	2.03	0.41
1:B:1039:GLU:HG2	1:B:1077:THR:HG21	2.02	0.41
1:A:149:LEU:HB2	1:A:169:LEU:HB3	2.03	0.41
1:A:326:ASP:HB2	1:A:354:PHE:CZ	2.56	0.41
1:A:401:ARG:NH1	1:B:260:ALA:O	2.51	0.41
1:A:466:GLN:HB3	1:A:467:PHE:H	1.42	0.41
1:A:599:GLN:NE2	1:A:604:VAL:HG11	2.36	0.41
1:C:386:SER:OG	1:C:387:PRO:HD3	2.21	0.41
1:B:599:GLN:NE2	1:B:604:VAL:HG11	2.36	0.41
1:A:220:ASN:ND2	1:A:222:ASN:H	2.19	0.40
1:A:964:LEU:HD23	1:A:964:LEU:H	1.86	0.40
1:A:1180:ILE:HG22	1:A:1181:VAL:HG13	2.03	0.40
1:A:815:GLN:HE21	1:A:815:GLN:HB3	1.70	0.40
1:C:1160:ASN:HB3	1:C:1163:ASN:OD1	2.20	0.40
1:B:326:ASP:HB2	1:B:354:PHE:CZ	2.56	0.40
1:A:180:LEU:N	1:A:243:TYR:O	2.54	0.40
1:A:430:PRO:HB3	1:C:461:ALA:HB2	2.03	0.40
1:C:326:ASP:HB2	1:C:354:PHE:CZ	2.57	0.40
1:C:1147:ILE:HG12	1:C:1148:GLU:N	2.36	0.40
1:B:519:ASN:HB2	1:B:522:GLN:HB2	2.02	0.40
1:C:98:GLN:H	1:C:98:GLN:HG2	1.77	0.40
1:C:149:LEU:HB2	1:C:169:LEU:HB3	2.02	0.40
1:C:466:GLN:HG3	1:C:467:PHE:H	1.84	0.40
1:C:519:ASN:HB2	1:C:522:GLN:HB2	2.03	0.40
1:C:608:LEU:HD13	1:C:641:TYR:CG	2.56	0.40
1:B:88:SER:HB2	1:B:131:ILE:HD12	2.03	0.40
1:B:505:ARG:HG2	1:B:554:LEU:HD13	2.03	0.40
1:C:782:ILE:HG21	1:C:1143:PRO:HB3	2.03	0.40
1:B:437:CYS:HB3	1:B:583:SER:HB3	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	1205/1340 (90%)	1131 (94%)	74 (6%)	0	100	100
1	B	1205/1340 (90%)	1129 (94%)	76 (6%)	0	100	100
1	C	1205/1340 (90%)	1129 (94%)	75 (6%)	1 (0%)	48	77
All	All	3615/4020 (90%)	3389 (94%)	225 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	919	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	1039/1159 (90%)	994 (96%)	45 (4%)	26	56
1	B	1039/1159 (90%)	994 (96%)	45 (4%)	26	56
1	C	1039/1159 (90%)	983 (95%)	56 (5%)	20	50
All	All	3117/3477 (90%)	2971 (95%)	146 (5%)	25	54

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	83	ASP

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Mol	Chain	Res	Type
1	A	95	THR
1	A	96	THR
1	A	132	ILE
1	A	172	LEU
1	A	256	ILE
1	A	273	LEU
1	A	303	ILE
1	A	423	PHE
1	A	448	TYR
1	A	450	LEU
1	A	452	MET
1	A	454	SER
1	A	457	SER
1	A	458	VAL
1	A	460	SER
1	A	464	ILE
1	A	466	GLN
1	A	484	VAL
1	A	495	LEU
1	A	505	ARG
1	A	511	ARG
1	A	689	TYR
1	A	694	ARG
1	A	727	CYS
1	A	744	THR
1	A	746	THR
1	A	748	ARG
1	A	750	VAL
1	A	751	ARG
1	A	780	LEU
1	A	782	ILE
1	A	815	GLN
1	A	842	GLN
1	A	862	ILE
1	A	967	PHE
1	A	1014	THR
1	A	1047	ILE
1	A	1121	THR
1	A	1127	VAL
1	A	1146	HIS
1	A	1147	ILE
1	A	1148	GLU

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Mol	Chain	Res	Type
1	A	1149	VAL
1	C	38	THR
1	C	83	ASP
1	C	95	THR
1	C	96	THR
1	C	98	GLN
1	C	132	ILE
1	C	172	LEU
1	C	256	ILE
1	C	261	GLN
1	C	273	LEU
1	C	303	ILE
1	C	419	SER
1	C	422	ASP
1	C	424	THR
1	C	425	CYS
1	C	450	LEU
1	C	458	VAL
1	C	464	ILE
1	C	484	VAL
1	C	495	LEU
1	C	505	ARG
1	C	511	ARG
1	C	689	TYR
1	C	694	ARG
1	C	727	CYS
1	C	744	THR
1	C	746	THR
1	C	748	ARG
1	C	750	VAL
1	C	751	ARG
1	C	780	LEU
1	C	782	ILE
1	C	815	GLN
1	C	842	GLN
1	C	862	ILE
1	C	907	GLN
1	C	915	GLN
1	C	919	SER
1	C	921	ARG
1	C	923	LEU
1	C	967	PHE

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Mol	Chain	Res	Type
1	C	1014	THR
1	C	1047	ILE
1	C	1048	SER
1	C	1051	ILE
1	C	1054	ILE
1	C	1055	ILE
1	C	1056	GLN
1	C	1058	LEU
1	C	1059	ASP
1	C	1121	THR
1	C	1127	VAL
1	C	1146	HIS
1	C	1147	ILE
1	C	1148	GLU
1	C	1149	VAL
1	B	38	THR
1	B	83	ASP
1	B	95	THR
1	B	96	THR
1	B	132	ILE
1	B	172	LEU
1	B	256	ILE
1	B	273	LEU
1	B	303	ILE
1	B	423	PHE
1	B	448	TYR
1	B	450	LEU
1	B	452	MET
1	B	454	SER
1	B	457	SER
1	B	458	VAL
1	B	460	SER
1	B	464	ILE
1	B	466	GLN
1	B	484	VAL
1	B	495	LEU
1	B	505	ARG
1	B	511	ARG
1	B	689	TYR
1	B	694	ARG
1	B	727	CYS
1	B	744	THR

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Mol	Chain	Res	Type
1	B	746	THR
1	B	748	ARG
1	B	750	VAL
1	B	751	ARG
1	B	780	LEU
1	B	782	ILE
1	B	815	GLN
1	B	842	GLN
1	B	862	ILE
1	B	967	PHE
1	B	1014	THR
1	B	1047	ILE
1	B	1121	THR
1	B	1127	VAL
1	B	1146	HIS
1	B	1147	ILE
1	B	1148	GLU
1	B	1149	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	220	ASN
1	A	222	ASN
1	A	264	HIS
1	A	427	GLN
1	A	516	GLN
1	A	521	ASN
1	A	599	GLN
1	A	628	GLN
1	A	769	GLN
1	A	785	ASN
1	A	792	GLN
1	A	808	GLN
1	A	812	ASN
1	A	815	GLN
1	A	832	ASN
1	A	842	GLN
1	A	907	GLN
1	A	915	GLN
1	A	987	GLN

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Mol	Chain	Res	Type
1	A	1009	GLN
1	A	1020	HIS
1	A	1031	GLN
1	A	1085	GLN
1	A	1097	GLN
1	C	114	ASN
1	C	220	ASN
1	C	222	ASN
1	C	280	GLN
1	C	466	GLN
1	C	516	GLN
1	C	544	GLN
1	C	599	GLN
1	C	719	ASN
1	C	769	GLN
1	C	785	ASN
1	C	792	GLN
1	C	808	GLN
1	C	812	ASN
1	C	815	GLN
1	C	832	ASN
1	C	842	GLN
1	C	915	GLN
1	C	988	GLN
1	C	1009	GLN
1	C	1020	HIS
1	C	1031	GLN
1	C	1056	GLN
1	C	1085	GLN
1	C	1097	GLN
1	C	1208	GLN
1	B	114	ASN
1	B	220	ASN
1	B	222	ASN
1	B	264	HIS
1	B	427	GLN
1	B	516	GLN
1	B	544	GLN
1	B	599	GLN
1	B	628	GLN
1	B	769	GLN
1	B	785	ASN

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Mol	Chain	Res	Type
1	B	792	GLN
1	B	800	GLN
1	B	808	GLN
1	B	812	ASN
1	B	815	GLN
1	B	832	ASN
1	B	842	GLN
1	B	907	GLN
1	B	915	GLN
1	B	1009	GLN
1	B	1020	HIS
1	B	1031	GLN
1	B	1085	GLN
1	B	1097	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

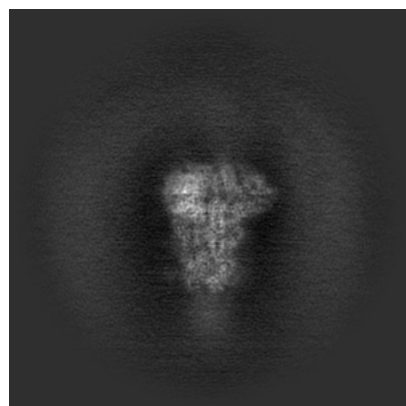
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68252. These allow visual inspection of the internal detail of the map and identification of artifacts.

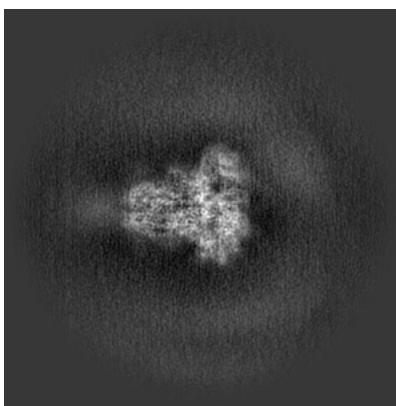
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

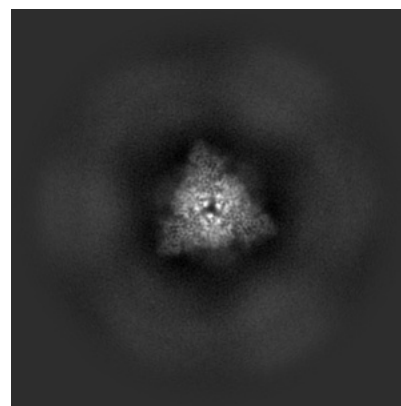
6.1.1 Primary map



X

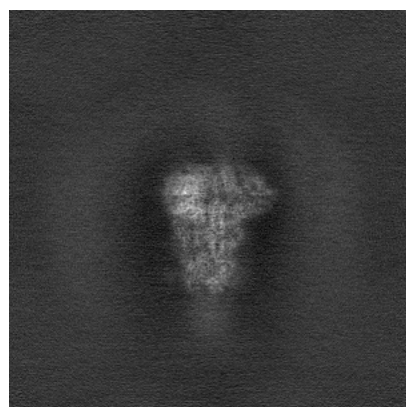


Y

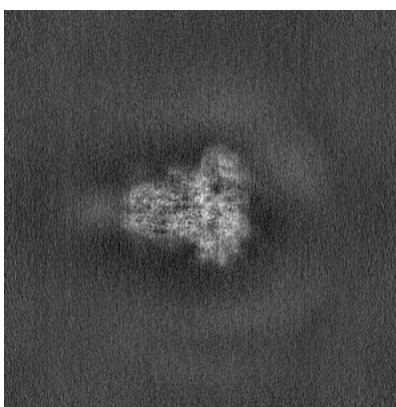


Z

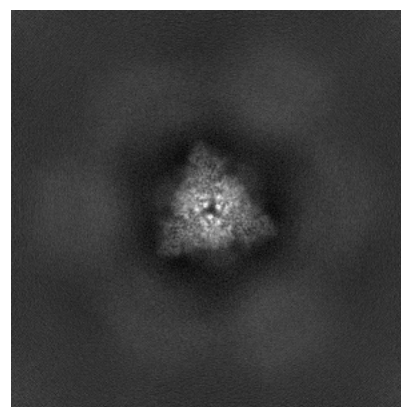
6.1.2 Raw map



X



Y

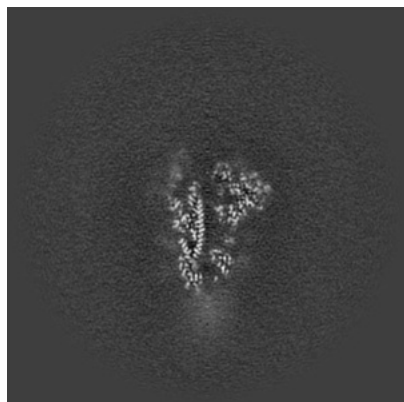


Z

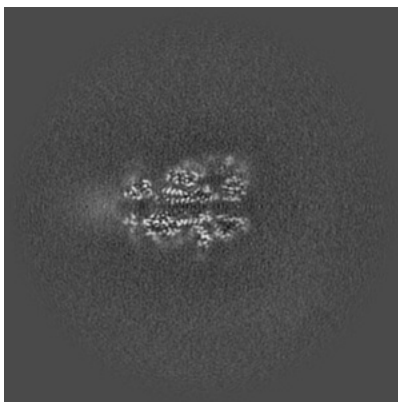
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

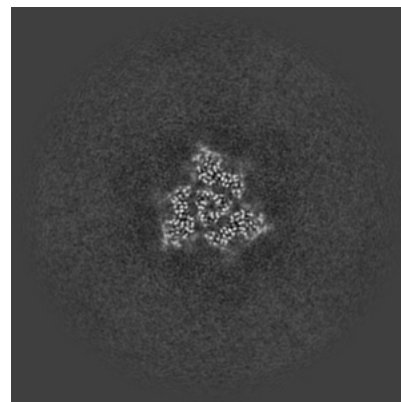
6.2.1 Primary map



X Index: 240

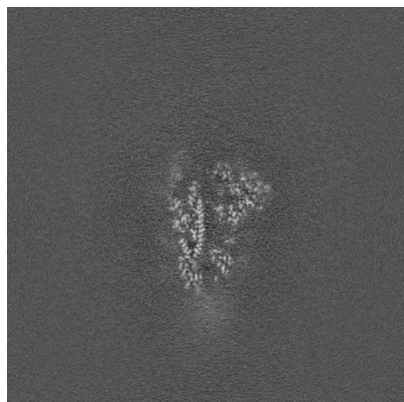


Y Index: 240

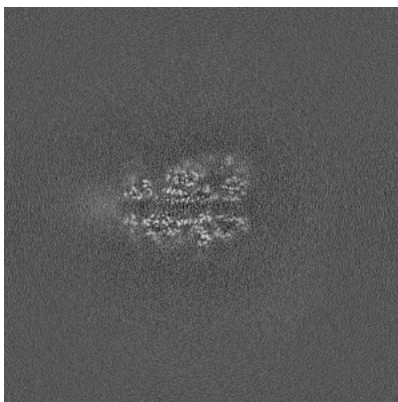


Z Index: 240

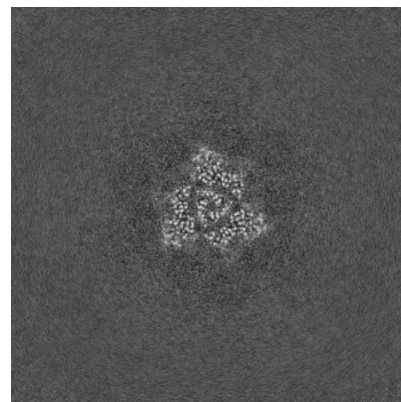
6.2.2 Raw map



X Index: 240



Y Index: 240

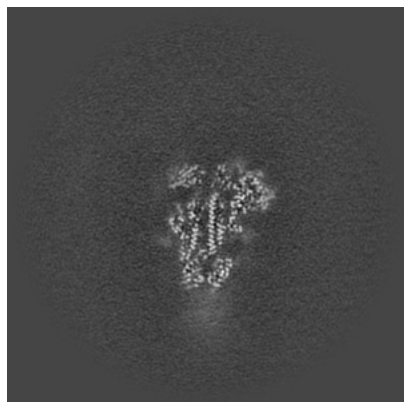


Z Index: 240

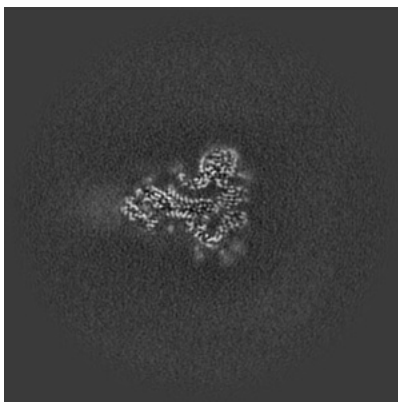
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

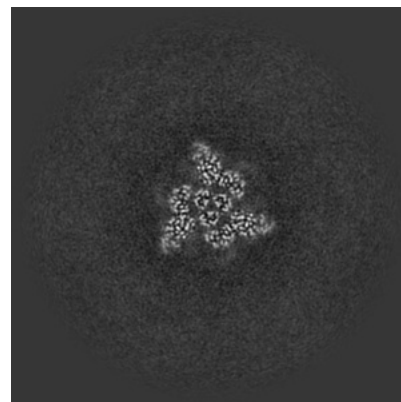
6.3.1 Primary map



X Index: 232

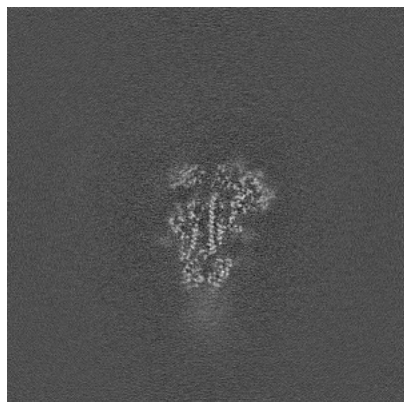


Y Index: 226

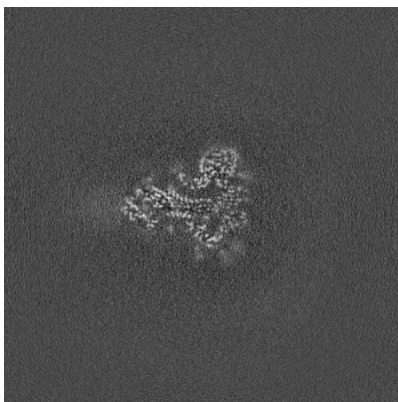


Z Index: 242

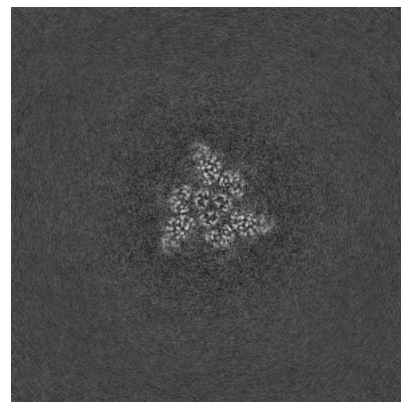
6.3.2 Raw map



X Index: 232



Y Index: 226

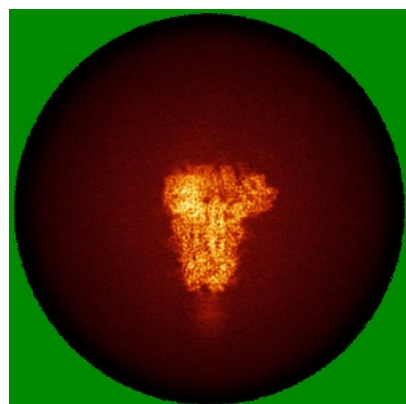


Z Index: 242

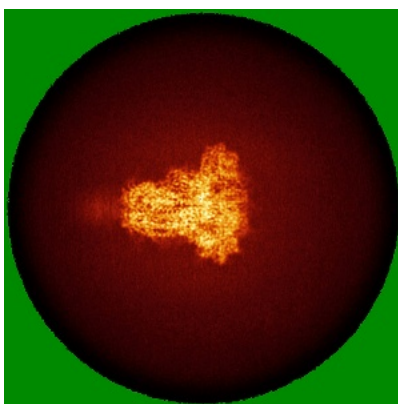
The images above show the largest variance slices of the map in three orthogonal directions.

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

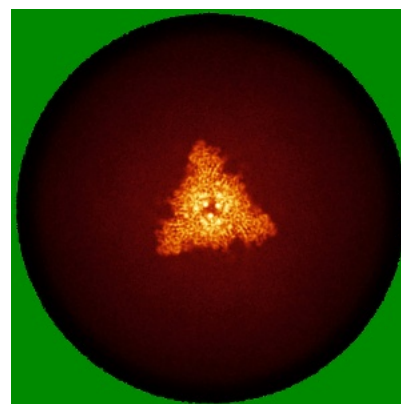
6.4.1 Primary map



X

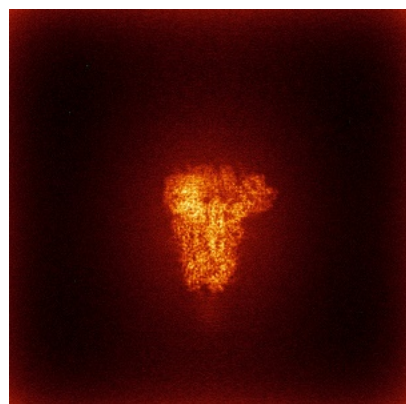


Y

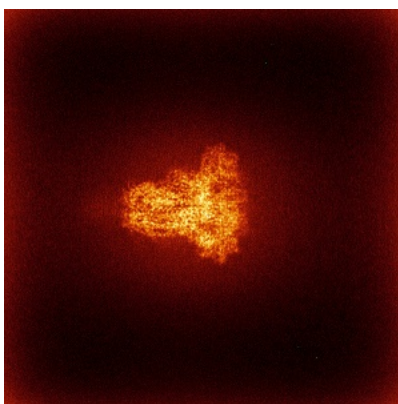


Z

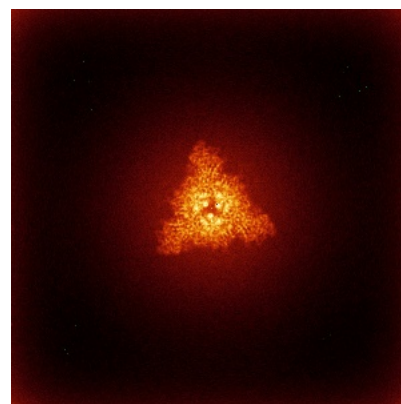
6.4.2 Raw map



X



Y

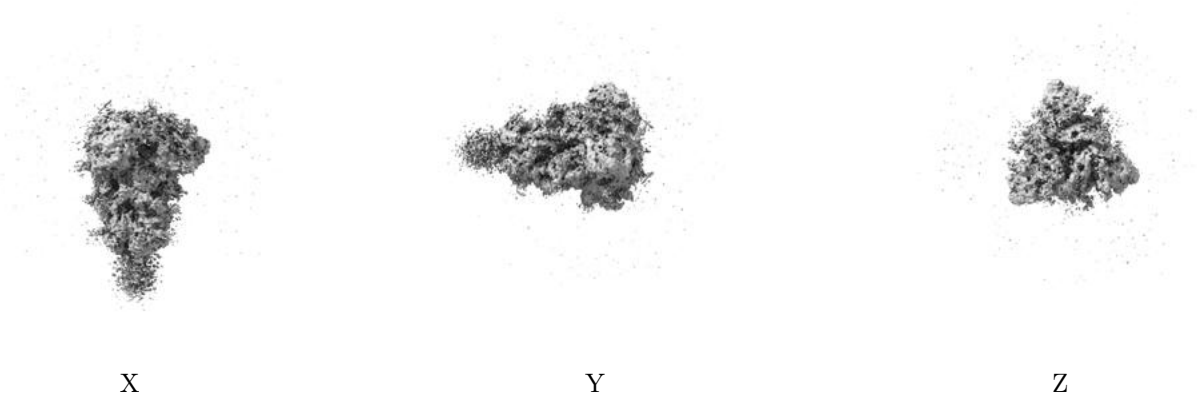


Z

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.

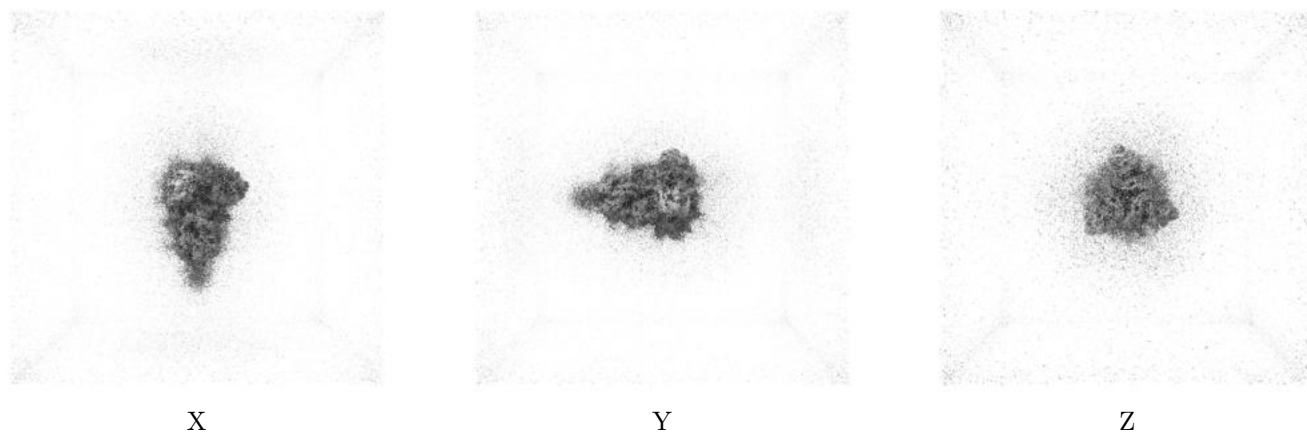
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

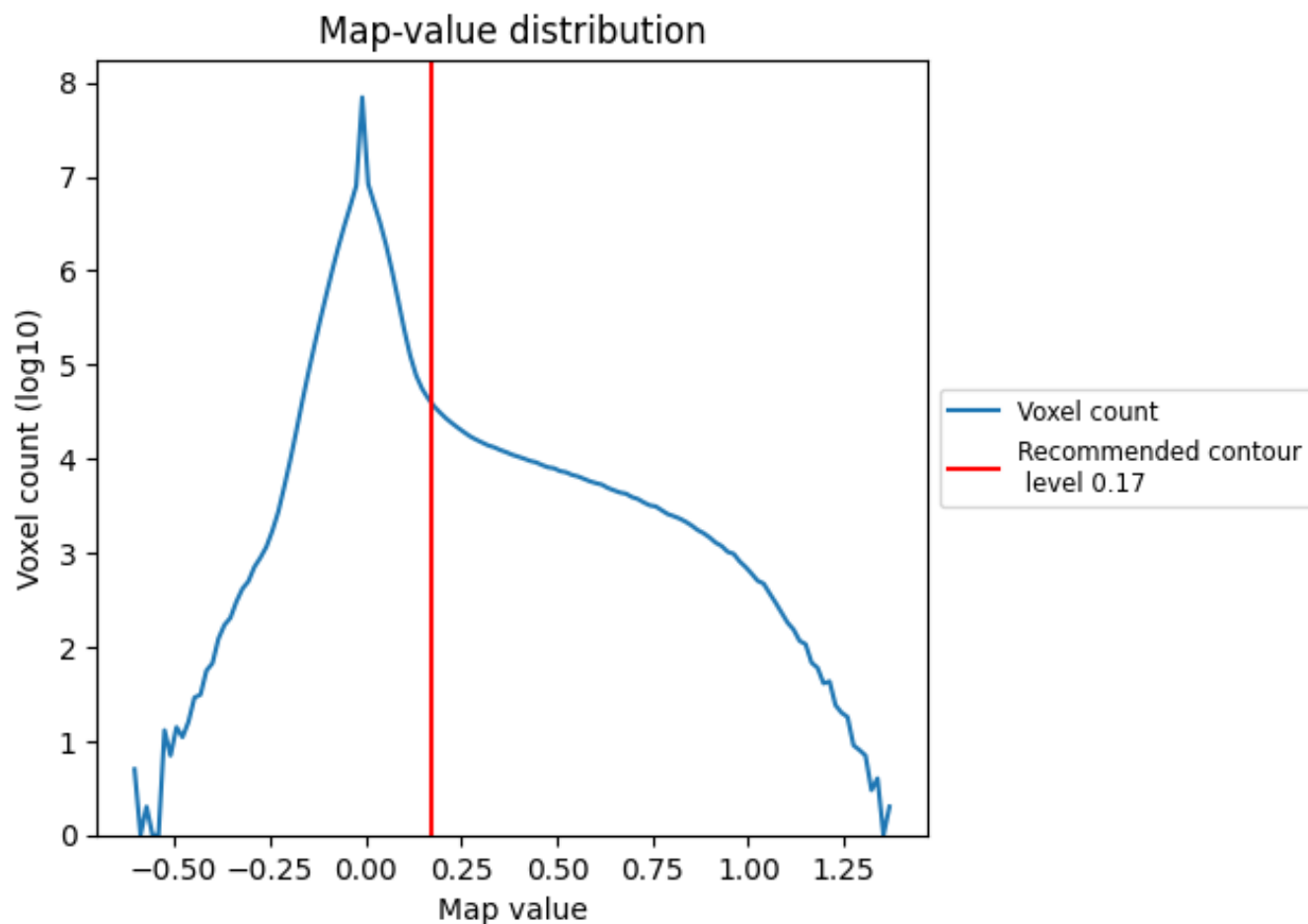
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

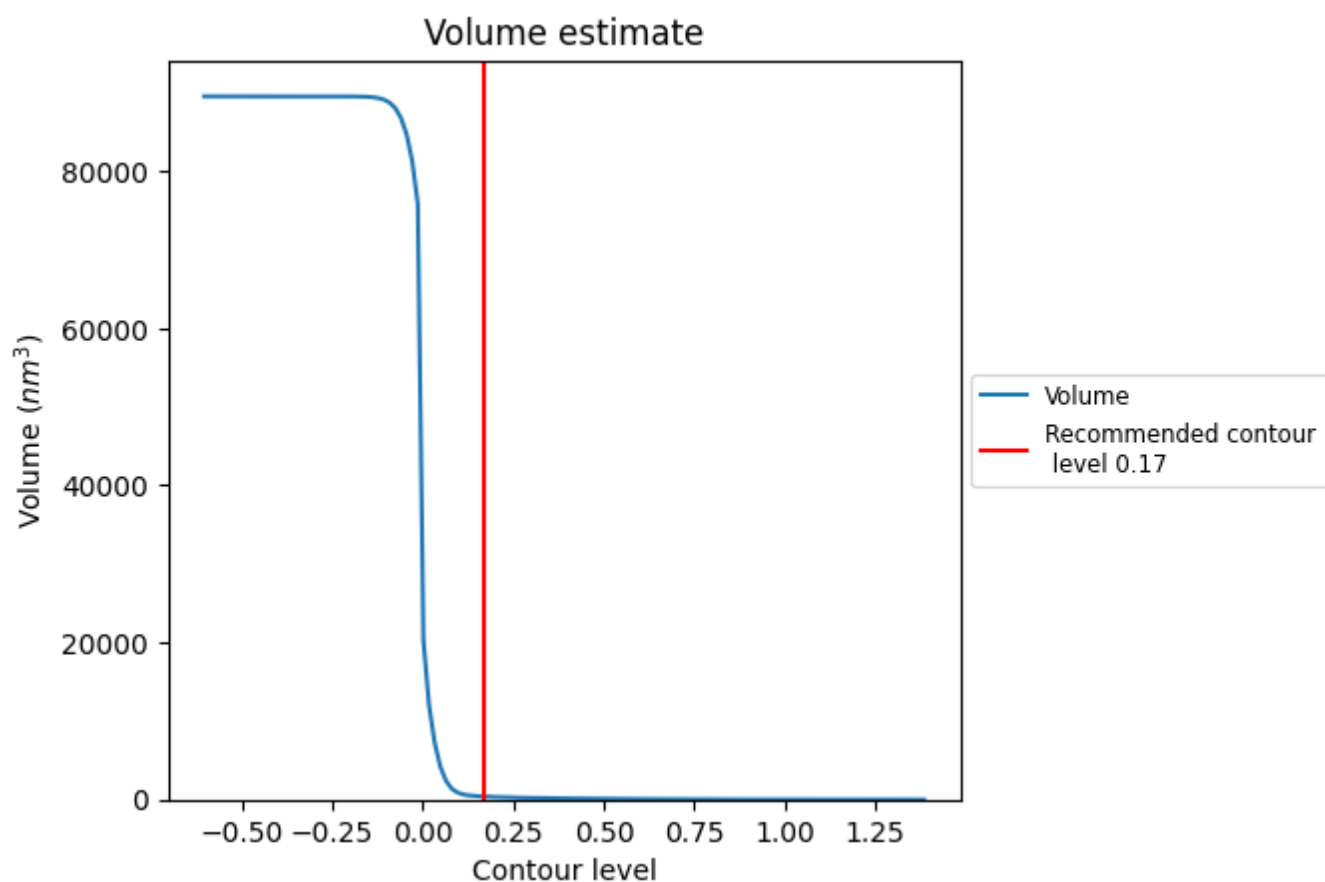
This section contains the results of statistical analysis of the map.

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.

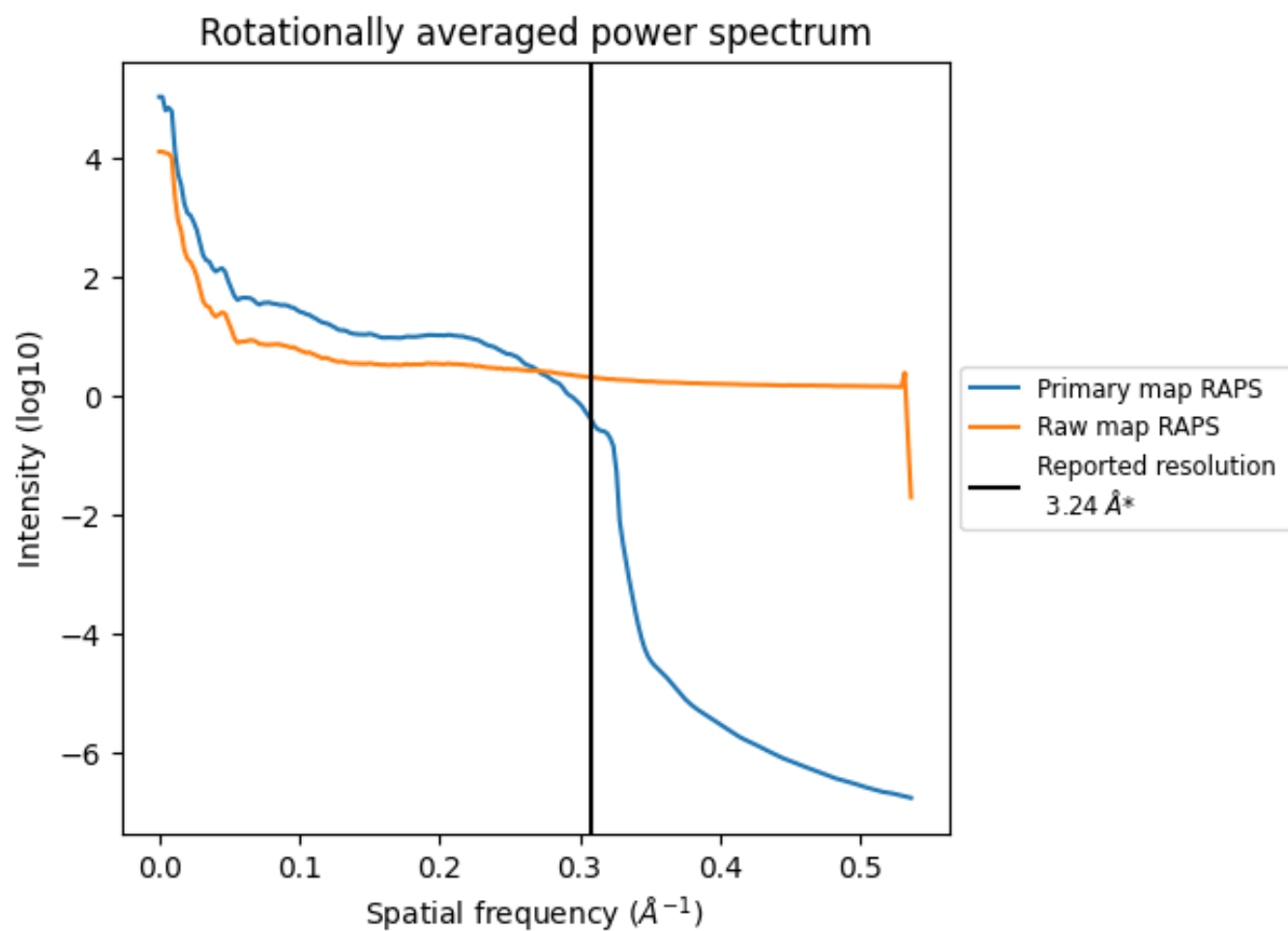
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 346 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 ⓘ

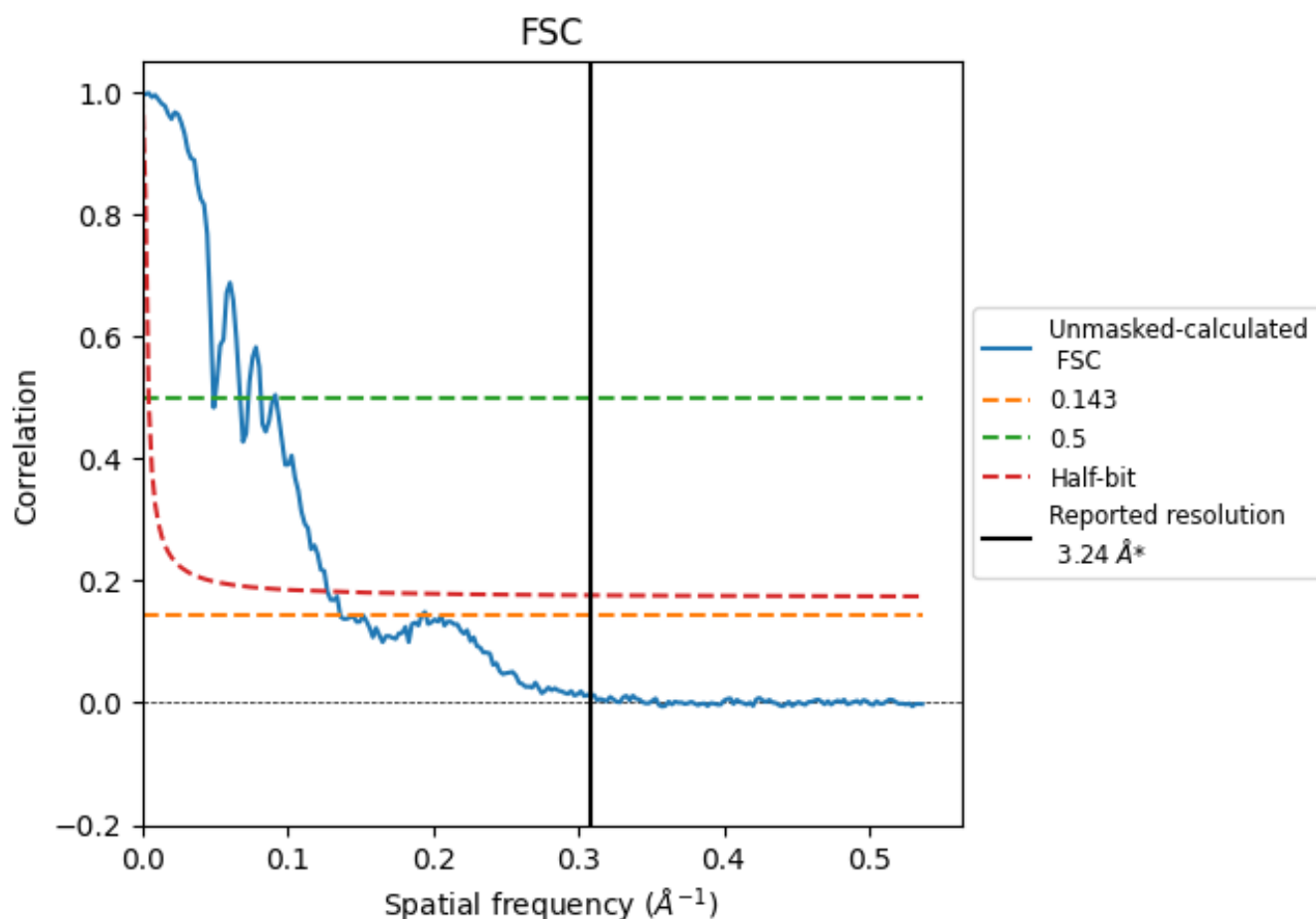


*Reported resolution corresponds to spatial frequency of 0.309 $\text{\AA}^{-1}$

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 0.309 Å⁻¹

8.2 Resolution estimates [i](#)

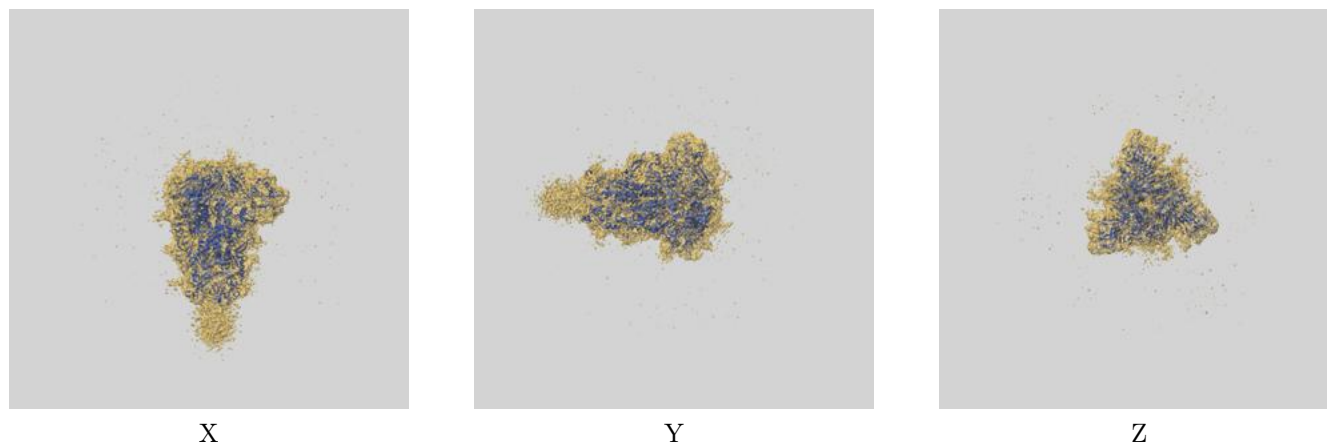
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.34	20.45	7.85

*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 7.34 differs from the reported value 3.24 by more than 10 %

9 Map-model fit [i](#)

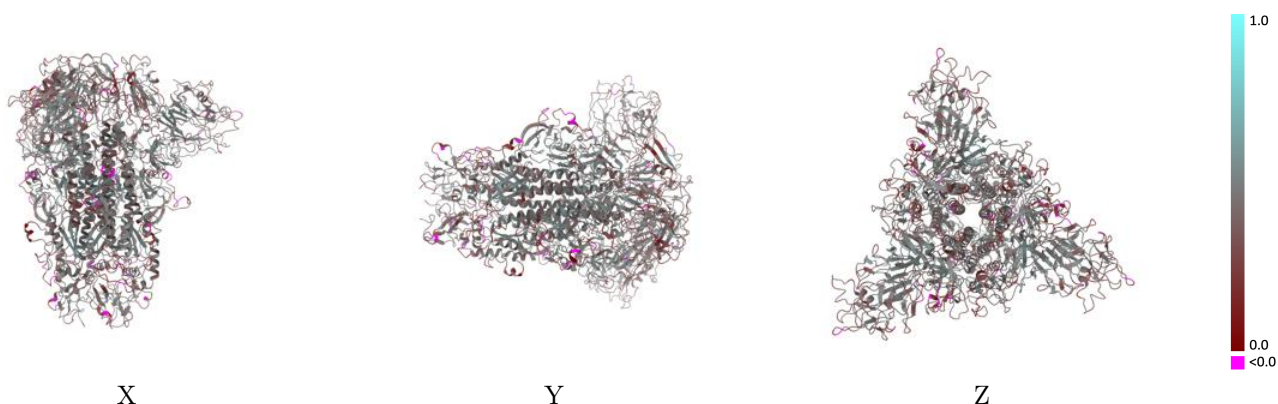
This section contains information regarding the fit between EMDB map EMD-68252 and PDB model 22FY. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



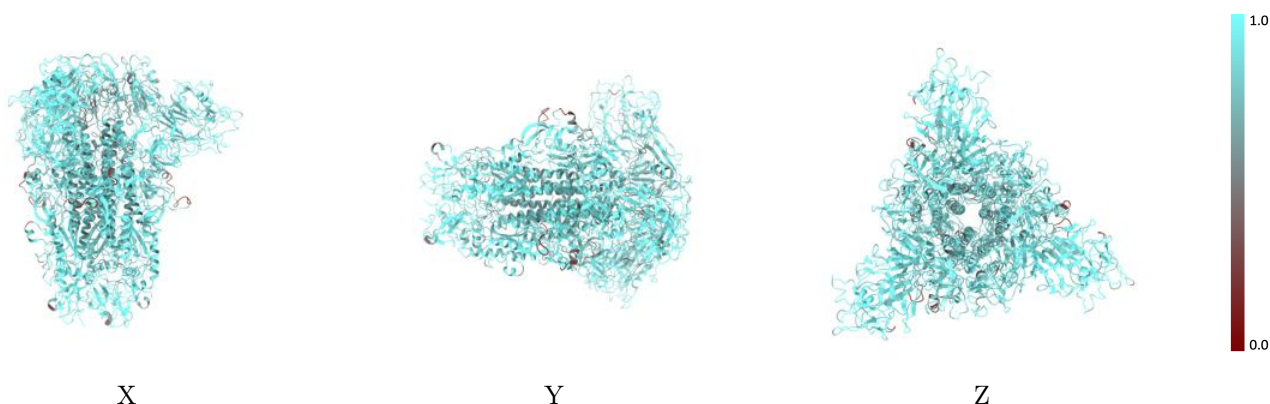
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



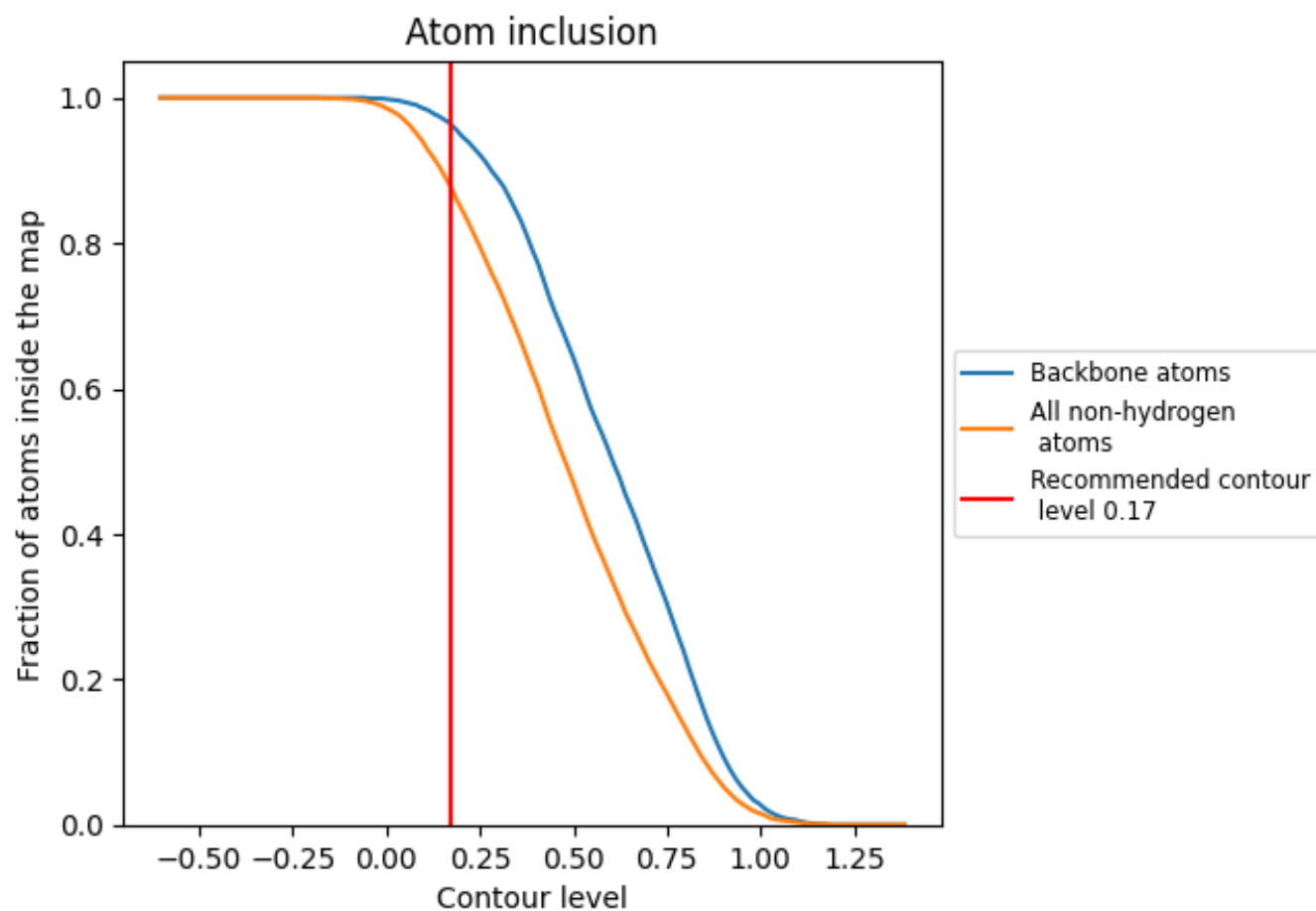
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.3980
A	0.8780	0.3970
B	0.8790	0.3970
C	0.8800	0.3990

