Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 08:56 am BST

PDB ID	:	8R8K
EMDB ID	:	EMD-19002
Title	:	XBB-4 Fab in complex with SARS-CoV-2 BA.2.12.1 Spike Glycoprotein
Authors	:	Duyvesteyn, H.M.E.; Ren, J.; Stuart, D.I.
Deposited on	:	2023-11-29
Resolution	:	3.41 Å(reported)
Based on initial model	:	8CIM

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:

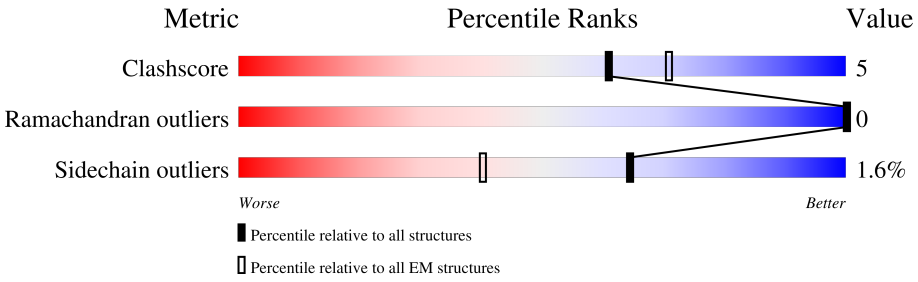
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1285	19% · 78%
2	H	233	47% 7% 45%
3	L	214	46% · 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4005 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
			Total	C	N	O	S		
1	A	280	2222	1425	378	409	10	0	0

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	conflict	UNP A0A7L9WCR1
A	?	-	LEU	deletion	UNP A0A7L9WCR1
A	?	-	PRO	deletion	UNP A0A7L9WCR1
A	?	-	PRO	deletion	UNP A0A7L9WCR1
A	24	SER	ALA	conflict	UNP A0A7L9WCR1
A	139	ASP	GLY	conflict	UNP A0A7L9WCR1
A	210	GLY	VAL	conflict	UNP A0A7L9WCR1
A	336	ASP	GLY	conflict	UNP A0A7L9WCR1
A	368	PHE	SER	conflict	UNP A0A7L9WCR1
A	370	PRO	SER	conflict	UNP A0A7L9WCR1
A	372	PHE	SER	conflict	UNP A0A7L9WCR1
A	373	ALA	THR	conflict	UNP A0A7L9WCR1
A	402	ASN	ASP	conflict	UNP A0A7L9WCR1
A	405	SER	ARG	conflict	UNP A0A7L9WCR1
A	414	ASN	LYS	conflict	UNP A0A7L9WCR1
A	437	LYS	ASN	conflict	UNP A0A7L9WCR1
A	449	GLN	LEU	conflict	UNP A0A7L9WCR1
A	474	ASN	SER	conflict	UNP A0A7L9WCR1
A	475	LYS	THR	conflict	UNP A0A7L9WCR1
A	481	ALA	GLU	conflict	UNP A0A7L9WCR1
A	490	ARG	GLN	conflict	UNP A0A7L9WCR1
A	495	ARG	GLN	conflict	UNP A0A7L9WCR1
A	498	TYR	ASN	conflict	UNP A0A7L9WCR1
A	502	HIS	TYR	conflict	UNP A0A7L9WCR1
A	652	TYR	HIS	conflict	UNP A0A7L9WCR1
A	676	LYS	ASN	conflict	UNP A0A7L9WCR1
A	701	LEU	SER	conflict	UNP A0A7L9WCR1
A	761	LYS	ASN	conflict	UNP A0A7L9WCR1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	793	TYR	ASP	conflict	UNP A0A7L9WCR1
A	951	HIS	GLN	conflict	UNP A0A7L9WCR1
A	966	LYS	ASN	conflict	UNP A0A7L9WCR1
A	1206	GLY	-	expression tag	UNP A0A7L9WCR1
A	1207	SER	-	expression tag	UNP A0A7L9WCR1
A	1208	GLY	-	expression tag	UNP A0A7L9WCR1
A	1209	TYR	-	expression tag	UNP A0A7L9WCR1
A	1210	ILE	-	expression tag	UNP A0A7L9WCR1
A	1211	PRO	-	expression tag	UNP A0A7L9WCR1
A	1212	GLU	-	expression tag	UNP A0A7L9WCR1
A	1213	ALA	-	expression tag	UNP A0A7L9WCR1
A	1214	PRO	-	expression tag	UNP A0A7L9WCR1
A	1215	ARG	-	expression tag	UNP A0A7L9WCR1
A	1216	ASP	-	expression tag	UNP A0A7L9WCR1
A	1217	GLY	-	expression tag	UNP A0A7L9WCR1
A	1218	GLN	-	expression tag	UNP A0A7L9WCR1
A	1219	ALA	-	expression tag	UNP A0A7L9WCR1
A	1220	TYR	-	expression tag	UNP A0A7L9WCR1
A	1221	VAL	-	expression tag	UNP A0A7L9WCR1
A	1222	ARG	-	expression tag	UNP A0A7L9WCR1
A	1223	LYS	-	expression tag	UNP A0A7L9WCR1
A	1224	ASP	-	expression tag	UNP A0A7L9WCR1
A	1225	GLY	-	expression tag	UNP A0A7L9WCR1
A	1226	GLU	-	expression tag	UNP A0A7L9WCR1
A	1227	TRP	-	expression tag	UNP A0A7L9WCR1
A	1228	VAL	-	expression tag	UNP A0A7L9WCR1
A	1229	LEU	-	expression tag	UNP A0A7L9WCR1
A	1230	LEU	-	expression tag	UNP A0A7L9WCR1
A	1231	SER	-	expression tag	UNP A0A7L9WCR1
A	1232	THR	-	expression tag	UNP A0A7L9WCR1
A	1233	PHE	-	expression tag	UNP A0A7L9WCR1
A	1234	LEU	-	expression tag	UNP A0A7L9WCR1
A	1235	GLY	-	expression tag	UNP A0A7L9WCR1
A	1236	ARG	-	expression tag	UNP A0A7L9WCR1
A	1237	SER	-	expression tag	UNP A0A7L9WCR1
A	1238	LEU	-	expression tag	UNP A0A7L9WCR1
A	1239	GLU	-	expression tag	UNP A0A7L9WCR1
A	1240	VAL	-	expression tag	UNP A0A7L9WCR1
A	1241	LEU	-	expression tag	UNP A0A7L9WCR1
A	1242	PHE	-	expression tag	UNP A0A7L9WCR1
A	1243	GLN	-	expression tag	UNP A0A7L9WCR1
A	1244	GLY	-	expression tag	UNP A0A7L9WCR1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1245	PRO	-	expression tag	UNP A0A7L9WCR1
A	1246	GLY	-	expression tag	UNP A0A7L9WCR1
A	1247	HIS	-	expression tag	UNP A0A7L9WCR1
A	1248	HIS	-	expression tag	UNP A0A7L9WCR1
A	1249	HIS	-	expression tag	UNP A0A7L9WCR1
A	1250	HIS	-	expression tag	UNP A0A7L9WCR1
A	1251	HIS	-	expression tag	UNP A0A7L9WCR1
A	1252	HIS	-	expression tag	UNP A0A7L9WCR1
A	1253	HIS	-	expression tag	UNP A0A7L9WCR1
A	1254	HIS	-	expression tag	UNP A0A7L9WCR1
A	1255	GLY	-	expression tag	UNP A0A7L9WCR1
A	1256	SER	-	expression tag	UNP A0A7L9WCR1
A	1257	ALA	-	expression tag	UNP A0A7L9WCR1
A	1258	TRP	-	expression tag	UNP A0A7L9WCR1
A	1259	SER	-	expression tag	UNP A0A7L9WCR1
A	1260	HIS	-	expression tag	UNP A0A7L9WCR1
A	1261	PRO	-	expression tag	UNP A0A7L9WCR1
A	1262	GLN	-	expression tag	UNP A0A7L9WCR1
A	1263	PHE	-	expression tag	UNP A0A7L9WCR1
A	1264	GLU	-	expression tag	UNP A0A7L9WCR1
A	1265	LYS	-	expression tag	UNP A0A7L9WCR1
A	1266	GLY	-	expression tag	UNP A0A7L9WCR1
A	1267	GLY	-	expression tag	UNP A0A7L9WCR1
A	1268	GLY	-	expression tag	UNP A0A7L9WCR1
A	1269	SER	-	expression tag	UNP A0A7L9WCR1
A	1270	GLY	-	expression tag	UNP A0A7L9WCR1
A	1271	GLY	-	expression tag	UNP A0A7L9WCR1
A	1272	GLY	-	expression tag	UNP A0A7L9WCR1
A	1273	SER	-	expression tag	UNP A0A7L9WCR1
A	1274	GLY	-	expression tag	UNP A0A7L9WCR1
A	1275	GLY	-	expression tag	UNP A0A7L9WCR1
A	1276	SER	-	expression tag	UNP A0A7L9WCR1
A	1277	ALA	-	expression tag	UNP A0A7L9WCR1
A	1278	TRP	-	expression tag	UNP A0A7L9WCR1
A	1279	SER	-	expression tag	UNP A0A7L9WCR1
A	1280	HIS	-	expression tag	UNP A0A7L9WCR1
A	1281	PRO	-	expression tag	UNP A0A7L9WCR1
A	1282	GLN	-	expression tag	UNP A0A7L9WCR1
A	1283	PHE	-	expression tag	UNP A0A7L9WCR1
A	1284	GLU	-	expression tag	UNP A0A7L9WCR1
A	1285	LYS	-	expression tag	UNP A0A7L9WCR1

- Molecule 2 is a protein called XBB-4 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	128	Total	C	N	O	S	0	0
			981	618	165	194	4		

- Molecule 3 is a protein called XBB-4 Fab Light chain.

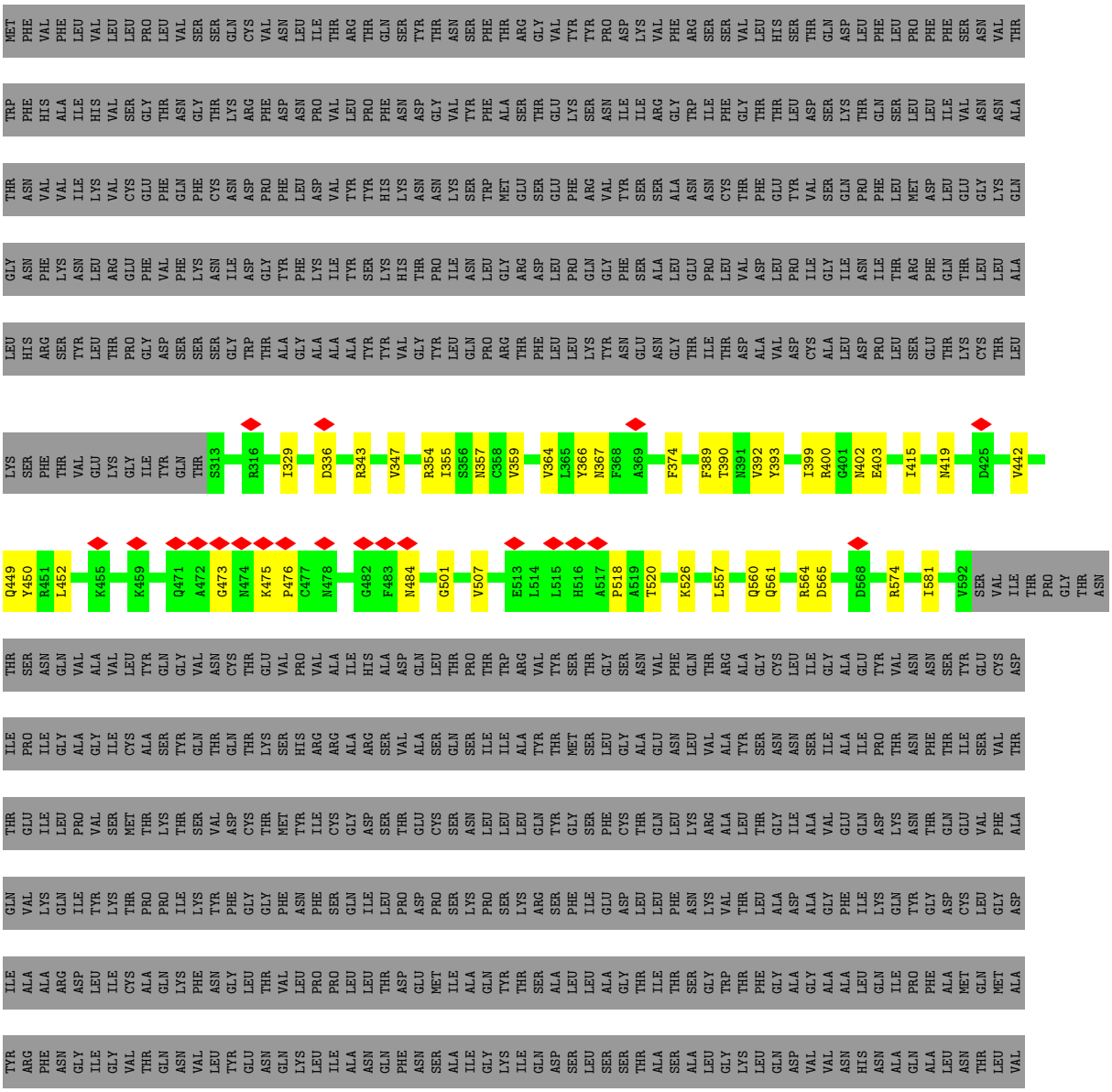
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			802	505	131	163	3		

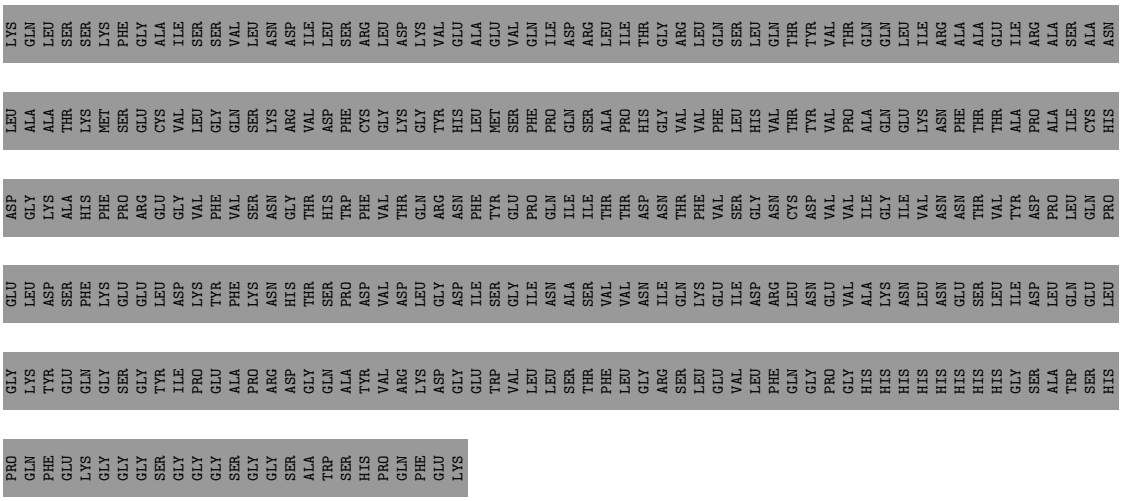
3 Residue-property plots (i)

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: Spike glycoprotein

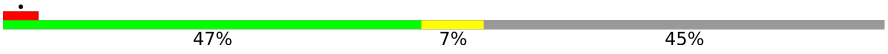
Chain A:

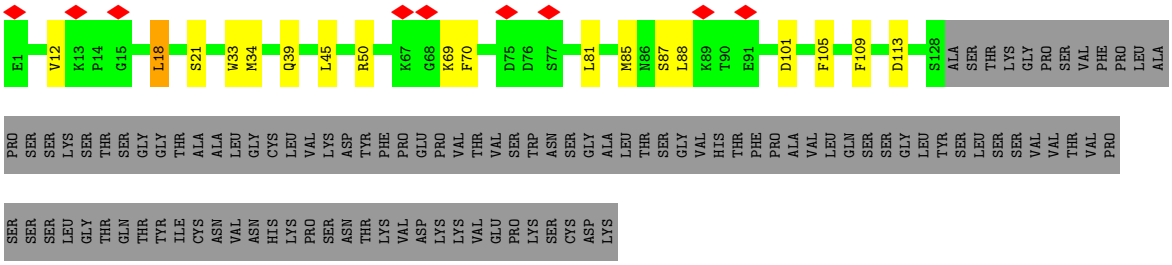




• Molecule 2: XBB-4 Fab Heavy chain

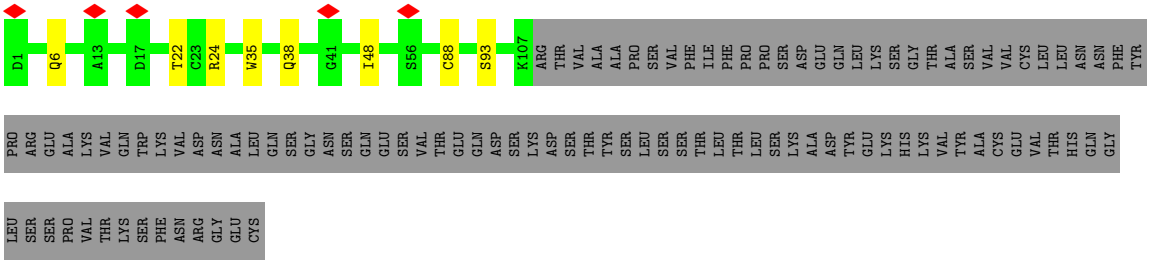
Chain H:





• Molecule 3: XBB-4 Fab Light chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF and Motion correction, on-the-fly.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.571	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.139	Depositor
Map size (Å)	328.635, 328.635, 328.635	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7303, 0.7303, 0.7303	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/2283	0.48	0/3104
2	H	0.26	0/1003	0.49	0/1357
3	L	0.26	0/818	0.49	0/1108
All	All	0.26	0/4104	0.49	0/5569

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

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	2222	0	2140	24	0
2	H	981	0	939	12	0
3	L	802	0	791	5	0
All	All	4005	0	3870	36	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 5.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ARG:HG3	1:A:403:GLU:HB2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LYS:HD3	1:A:476:PRO:HD2	1.78	0.65
1:A:390:THR:O	1:A:520:THR:OG1	2.15	0.64
1:A:355:ILE:HB	1:A:392:VAL:HB	1.82	0.62
2:H:33:TRP:HB2	2:H:101:ASP:HB2	1.82	0.61
1:A:557:LEU:HB2	1:A:560:GLN:HG3	1.82	0.61
1:A:564:ARG:HH11	1:A:564:ARG:HG2	1.67	0.58
3:L:6:GLN:NE2	3:L:88:CYS:SG	2.77	0.57
1:A:473:GLY:HA3	1:A:484:ASN:HD21	1.68	0.56
2:H:69:LYS:HG3	2:H:70:PHE:CD1	2.42	0.55
1:A:402:ASN:ND2	1:A:501:GLY:O	2.36	0.53
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.91	0.52
1:A:343:ARG:NH2	2:H:109:PHE:HB3	2.26	0.51
1:A:343:ARG:HH21	2:H:109:PHE:HB3	1.76	0.51
1:A:357:ASN:H	1:A:520:THR:HB	1.76	0.51
2:H:85:MET:HG3	2:H:88:LEU:HD11	1.93	0.51
2:H:50:ARG:NH1	2:H:113:ASP:OD2	2.45	0.50
1:A:364:VAL:O	1:A:367:ASN:HB2	2.12	0.48
1:A:354:ARG:NH1	1:A:393:TYR:OH	2.47	0.48
1:A:329:ILE:HG22	1:A:359:VAL:HG23	1.96	0.48
1:A:574:ARG:HH21	1:A:581:ILE:HD11	1.79	0.48
3:L:22:THR:OG1	3:L:24:ARG:NH1	2.46	0.48
1:A:449:GLN:HE22	2:H:105:PHE:HE1	1.64	0.46
2:H:34:MET:HB3	2:H:81:LEU:HD22	1.96	0.46
1:A:399:ILE:HD11	1:A:507:VAL:HG21	1.98	0.46
1:A:450:TYR:HE2	1:A:452:LEU:HD13	1.81	0.45
1:A:564:ARG:HG2	1:A:564:ARG:NH1	2.29	0.45
1:A:442:VAL:HG22	3:L:93:SER:HA	1.99	0.45
1:A:518:PRO:HG3	1:A:561:GLN:CD	2.36	0.45
2:H:87:SER:O	2:H:87:SER:OG	2.27	0.43
1:A:347:VAL:HG21	1:A:415:ILE:HD12	2.00	0.43
2:H:39:GLN:NE2	3:L:38:GLN:OE1	2.43	0.42
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.01	0.42
1:A:526:LYS:HA	1:A:526:LYS:HD3	1.84	0.42
2:H:12:VAL:HG11	2:H:18:LEU:HD11	2.01	0.42
1:A:347:VAL:HG22	1:A:419:ASN:HB3	2.02	0.41

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	278/1285 (22%)	269 (97%)	9 (3%)	0	100	100
2	H	126/233 (54%)	125 (99%)	1 (1%)	0	100	100
3	L	105/214 (49%)	102 (97%)	3 (3%)	0	100	100
All	All	509/1732 (29%)	496 (97%)	13 (3%)	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	244/1110 (22%)	239 (98%)	5 (2%)	55	79
2	H	104/195 (53%)	102 (98%)	2 (2%)	57	80
3	L	92/188 (49%)	92 (100%)	0	100	100
All	All	440/1493 (30%)	433 (98%)	7 (2%)	64	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	ASP
1	A	366	TYR
1	A	374	PHE
1	A	389	PHE
1	A	565	ASP

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Mol	Chain	Res	Type
2	H	18	LEU
2	H	21	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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.

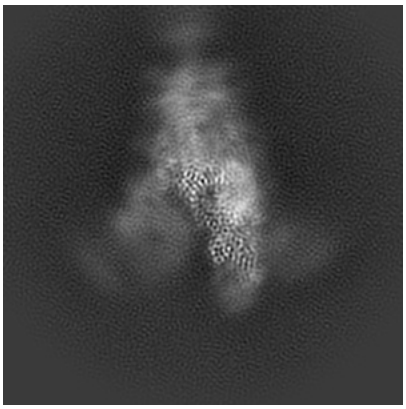
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19002. These allow visual inspection of the internal detail of the map and identification of artifacts.

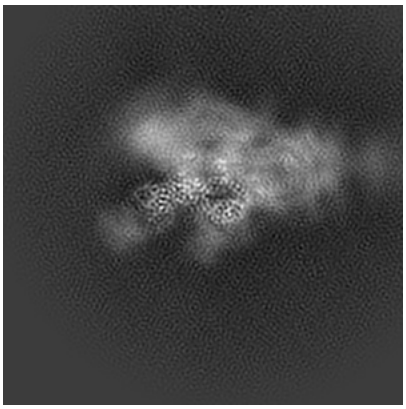
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

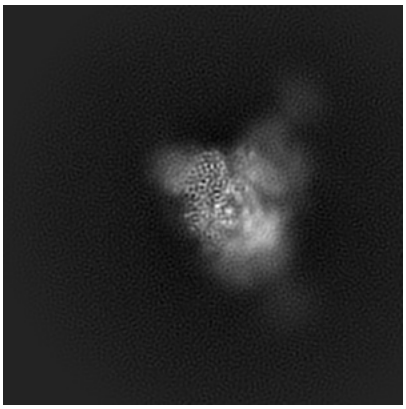
6.1.1 Primary map



X

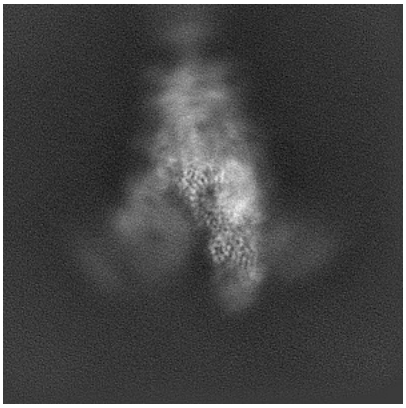


Y

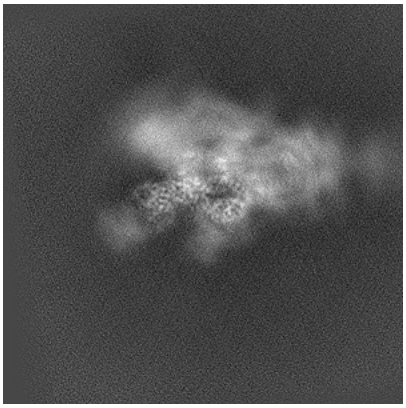


Z

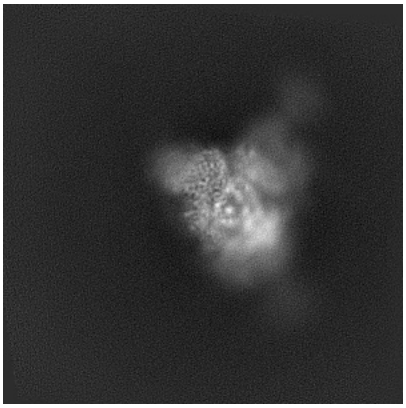
6.1.2 Raw map



X



Y

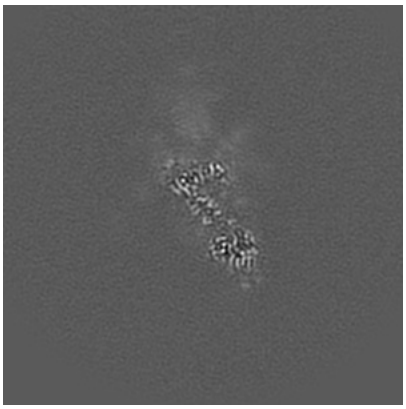


Z

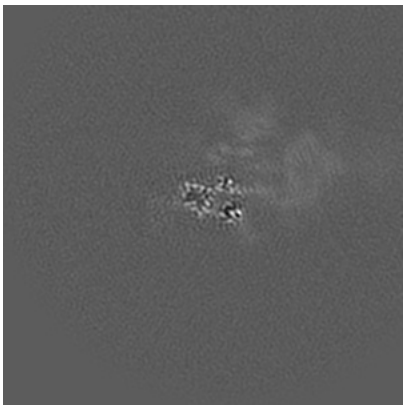
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

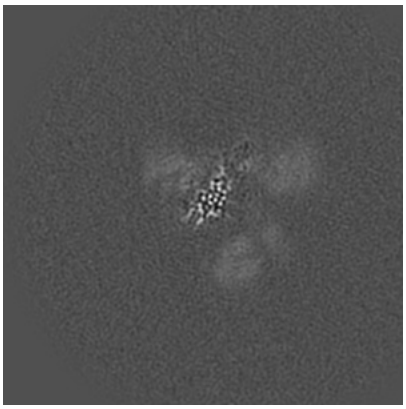
6.2.1 Primary map



X Index: 225

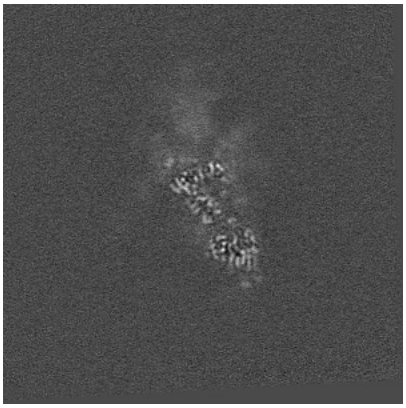


Y Index: 225

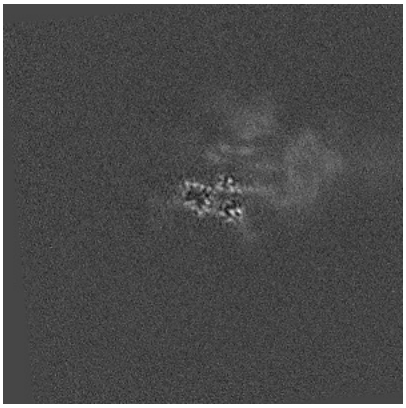


Z Index: 225

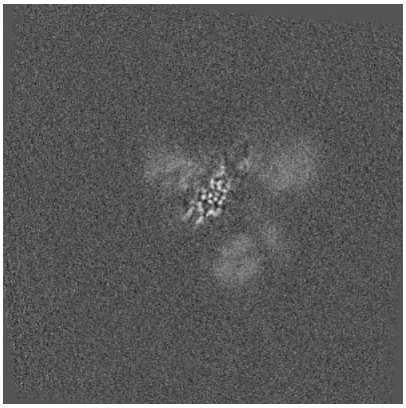
6.2.2 Raw map



X Index: 225



Y Index: 225

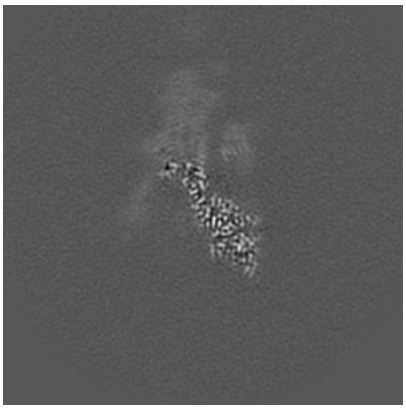


Z Index: 225

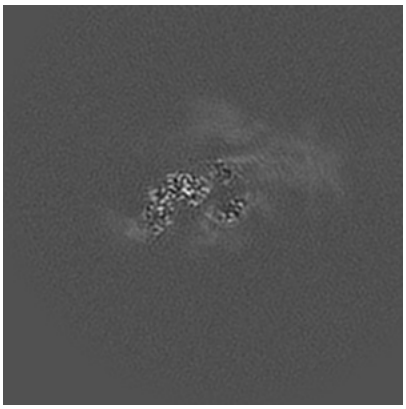
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

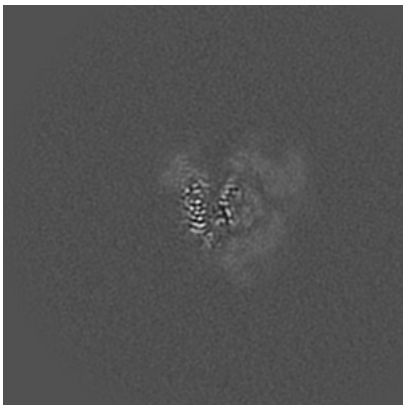
6.3.1 Primary map



X Index: 241

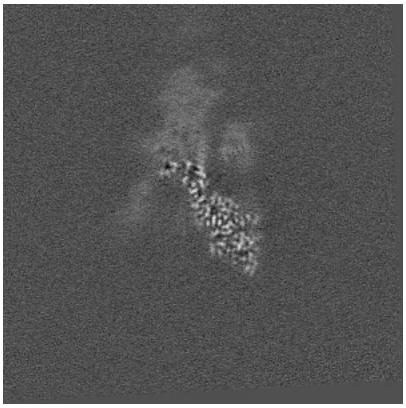


Y Index: 243

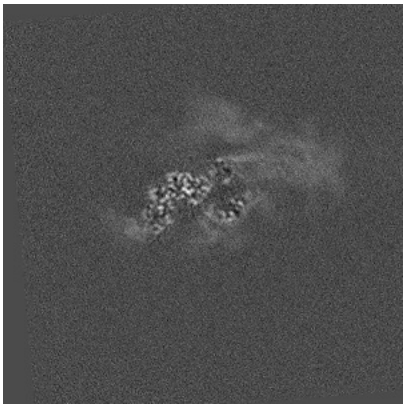


Z Index: 253

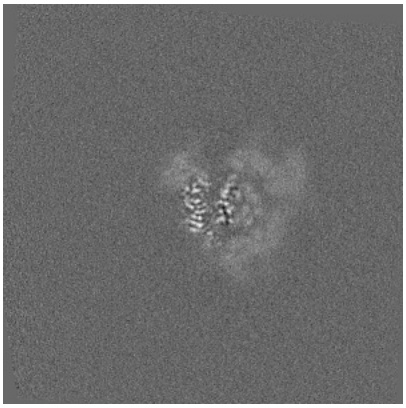
6.3.2 Raw map



X Index: 241



Y Index: 243

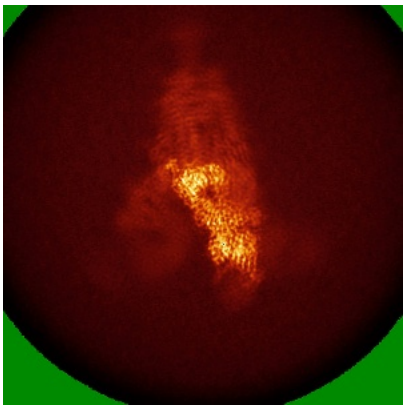


Z Index: 254

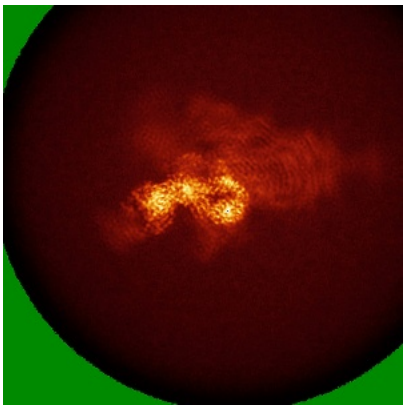
The images above show the largest variance slices of the map in three orthogonal directions.

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

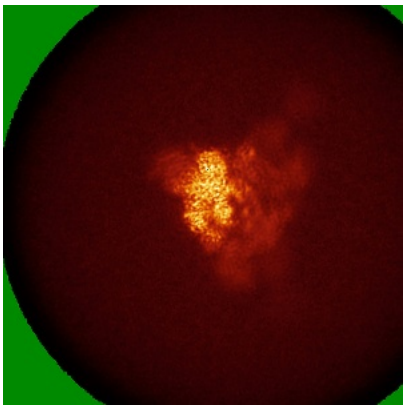
6.4.1 Primary map



X

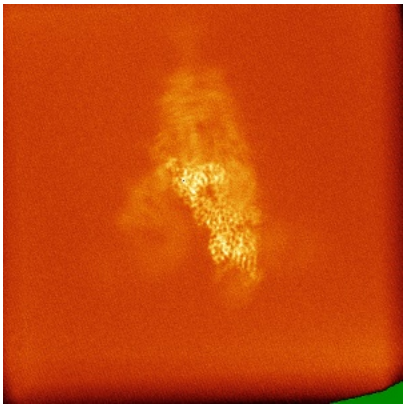


Y

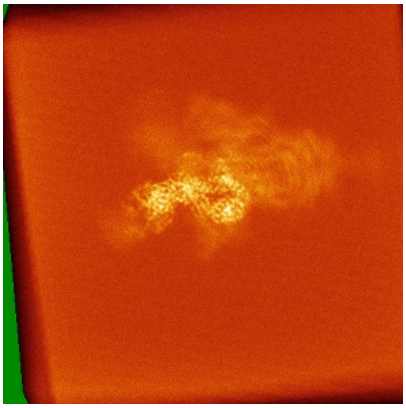


Z

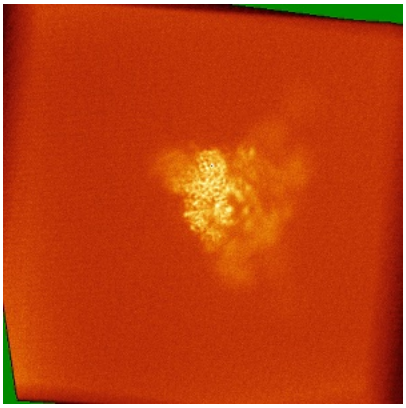
6.4.2 Raw map



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 0.139. 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.

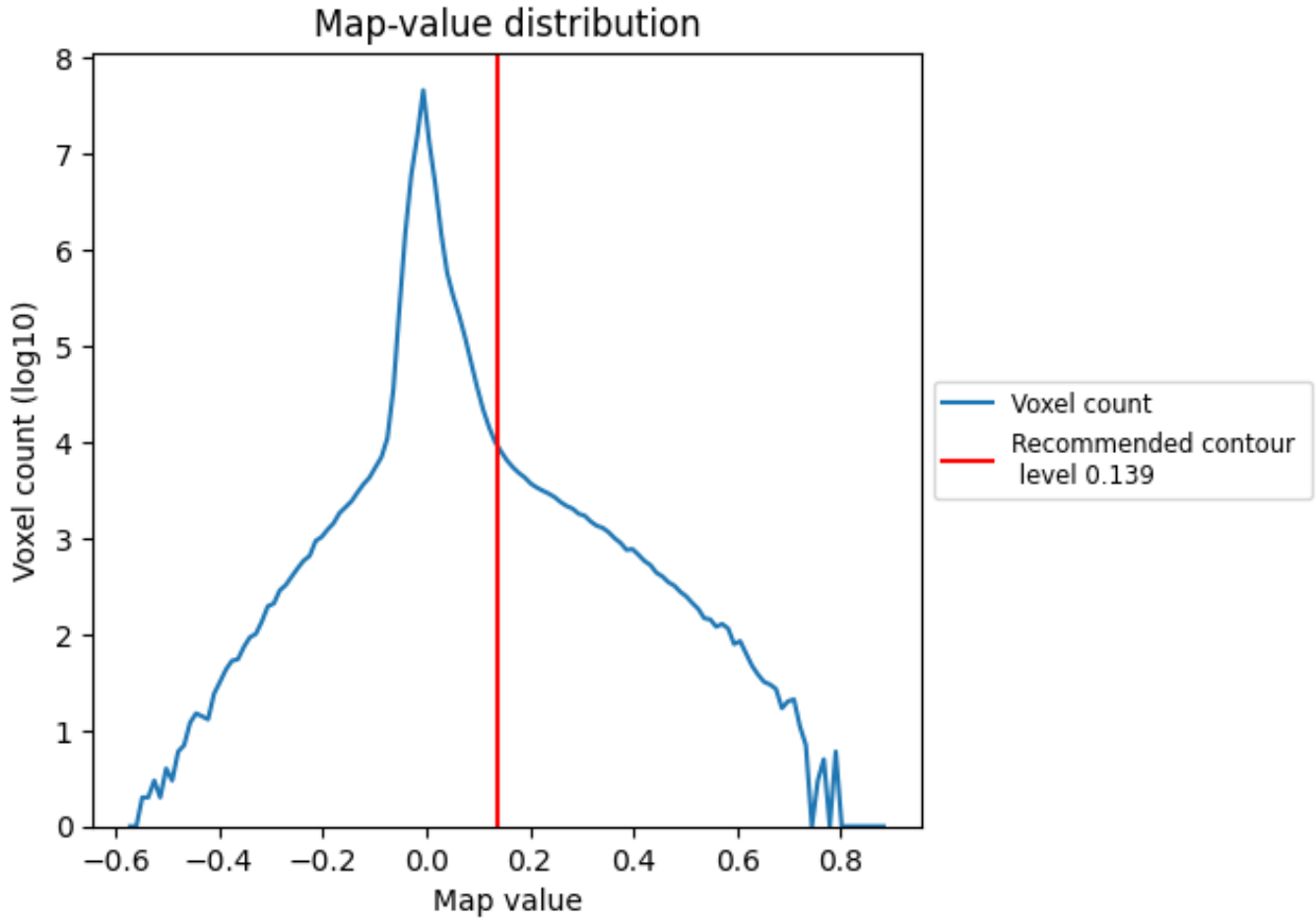
6.6 Mask visualisation (i)

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

7 Map analysis

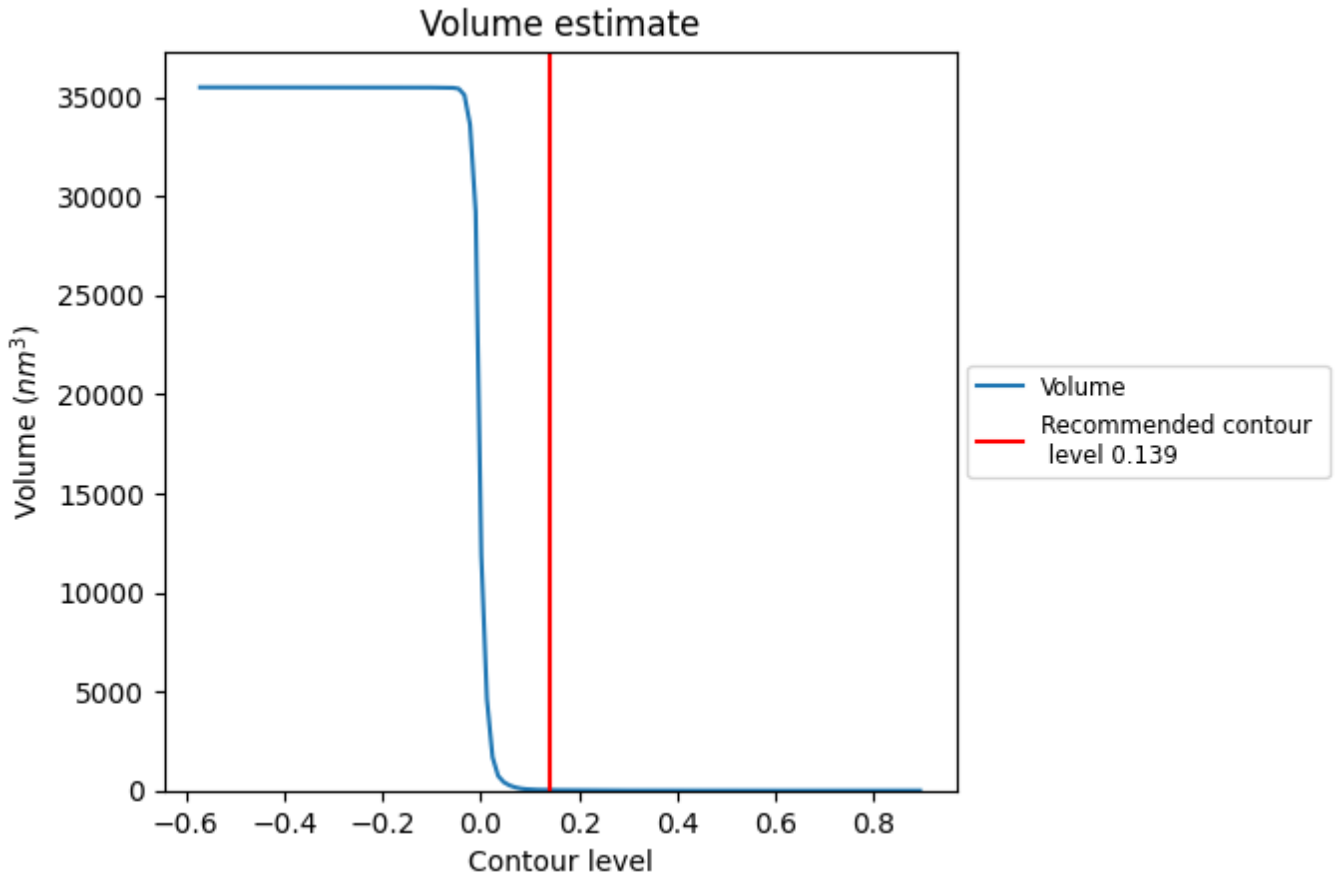
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

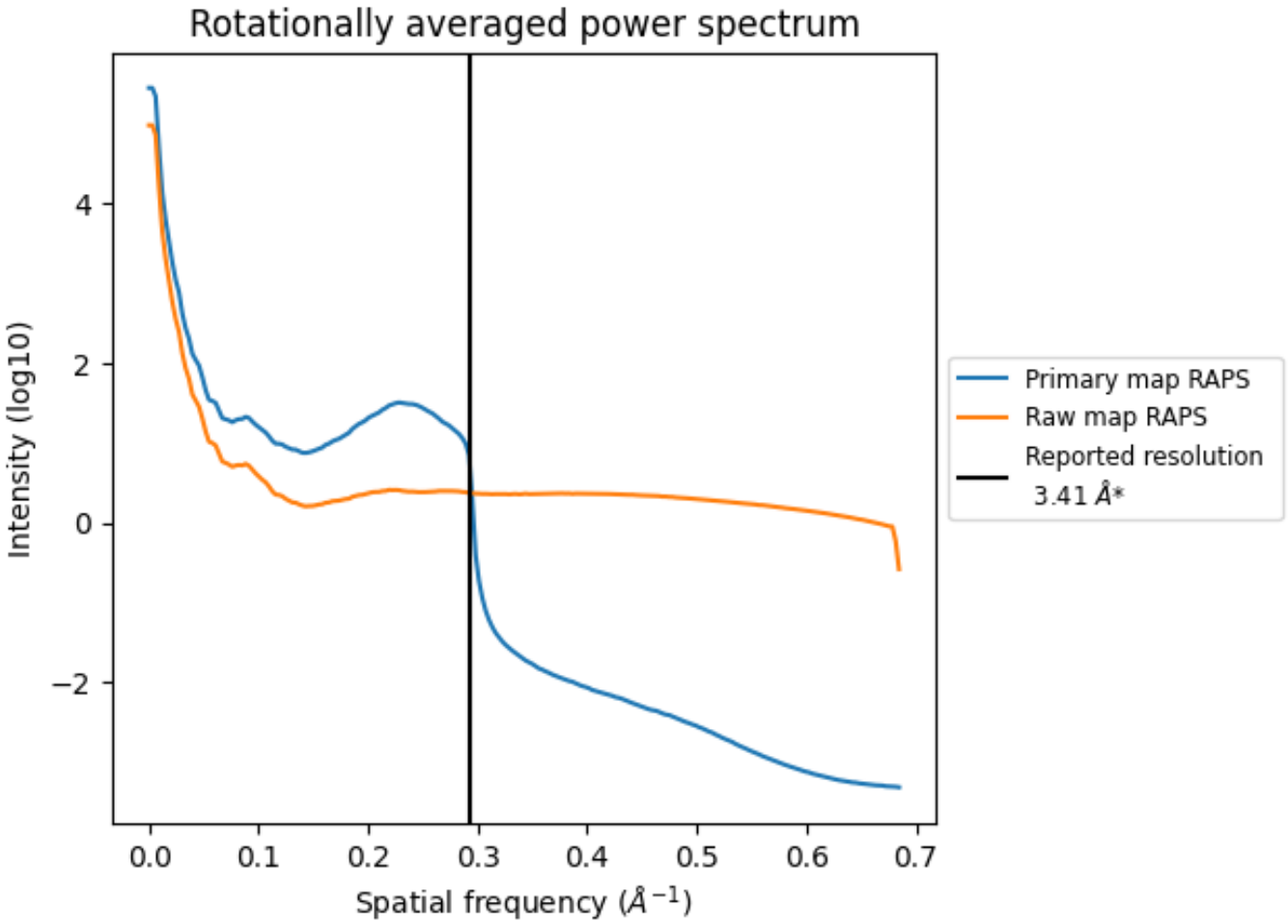
7.2 Volume estimate



The volume at the recommended contour level is 29 nm^3; this corresponds to an approximate mass of 26 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)

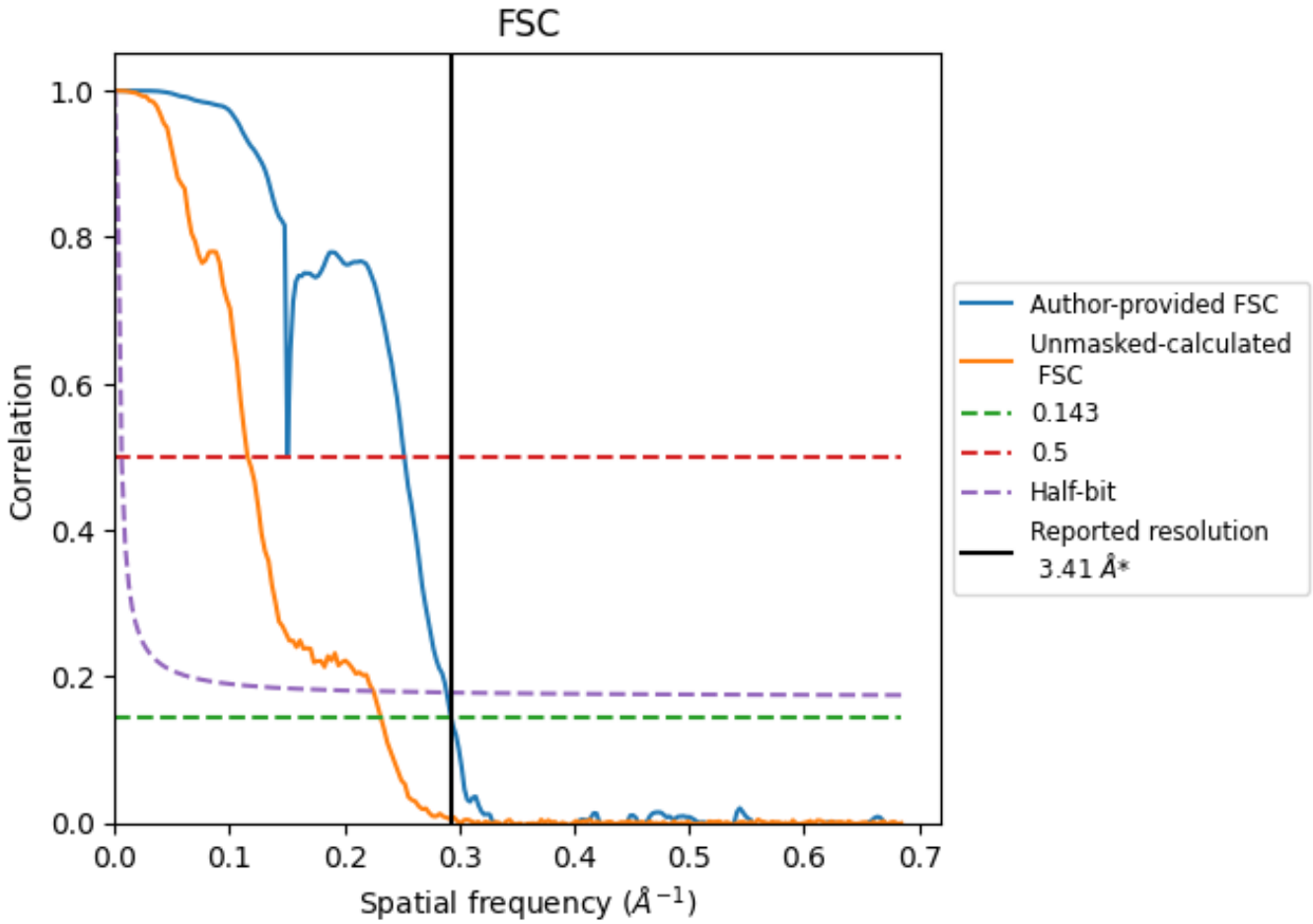


*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.293 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	3.97	3.46
Unmasked-calculated*	4.32	8.65	4.44

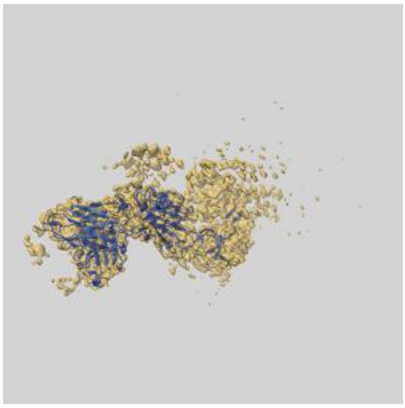
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.41 by more than 10 %

9 Map-model fit

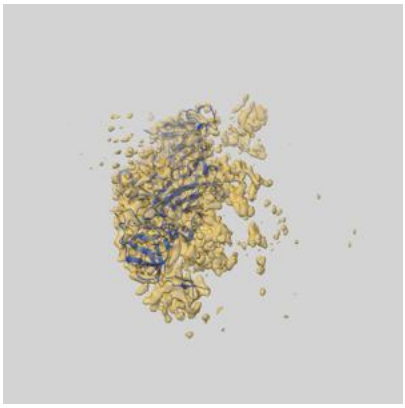
This section contains information regarding the fit between EMDB map EMD-19002 and PDB model 8R8K. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

X



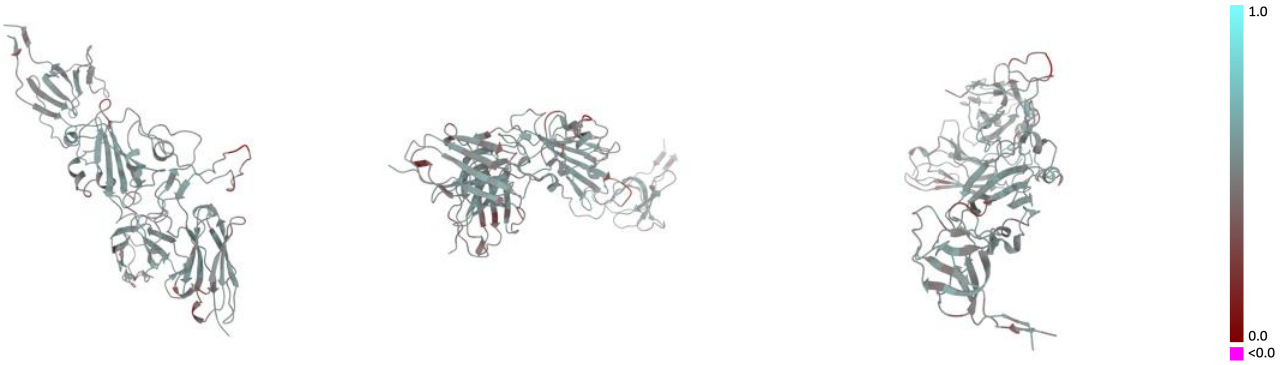
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.139 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.

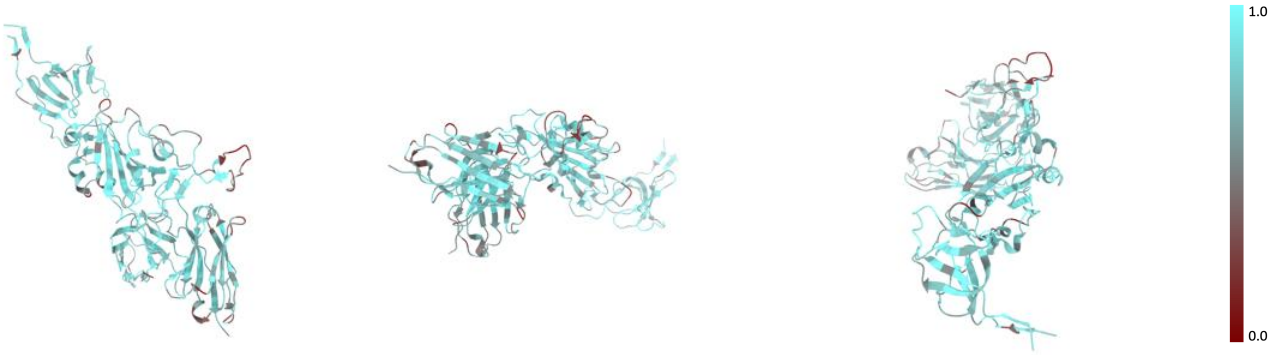
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

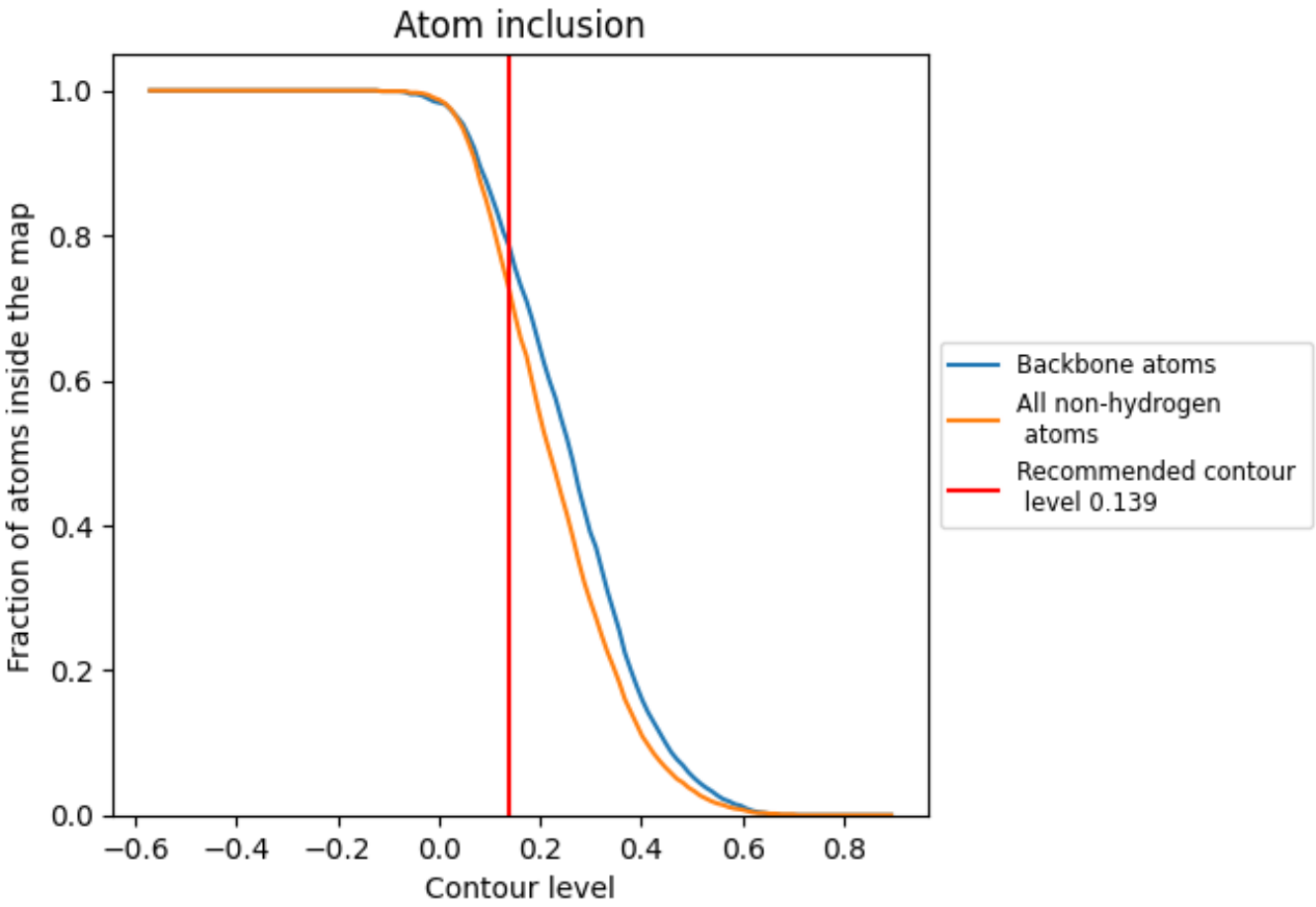
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.139).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.139) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.5040
A	0.7350	0.5060
H	0.7070	0.5070
L	0.7200	0.4940