



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 05:43 PM JST

PDB ID : 7WCR
EMDB ID : EMD-32428
Title : RBD-1 of SARS-CoV-2 Beta spike in complex with S5D2 Fab
Authors : Wang, Y.F.; Cong, Y.
Deposited on : 2021-12-20
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

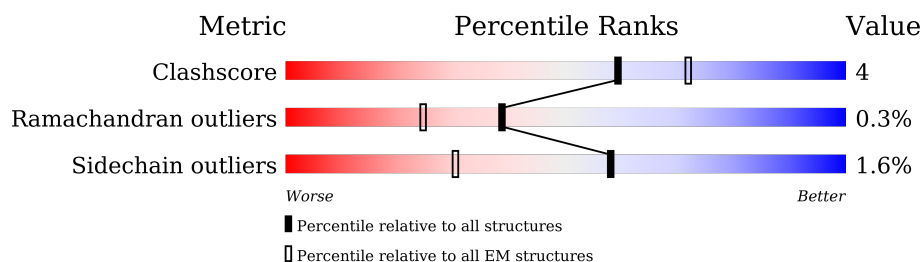
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1258	
2	a	214	
3	b	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4880 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	197	Total	C	N	O	S	0	0
			1563	1005	260	290	8		

There are 71 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	LEU	variant	UNP P0DTC2
A	83	ALA	ASP	variant	UNP P0DTC2
A	218	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	246	ILE	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of S5D2 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	214	Total	C	N	O	S	0	0
			1627	1031	260	329	7		

- Molecule 3 is a protein called Light chain of S5D2 Fab.

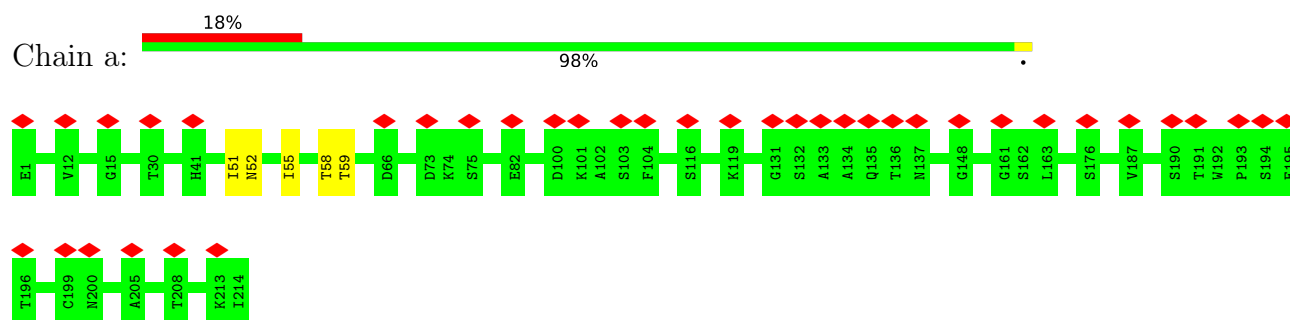
Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	217	Total	C	N	O	S	0	0
			1690	1058	280	346	6		

- Molecule 1: Spike glycoprotein

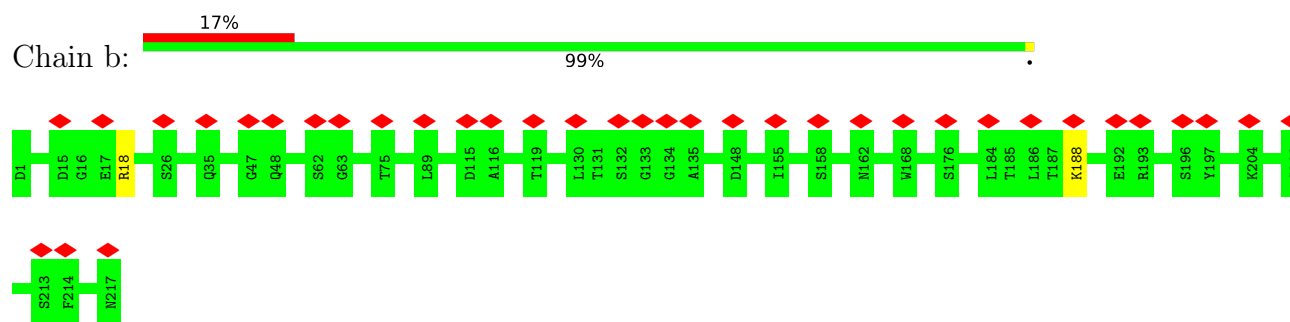


HIS	HIS	LEU	PRO	ALA	ALA	ASN	MET
		GLN	LEU	ILE	SER	THR	GLN
HIS	HIS	GLN	GLN	CYS	ALA	LEU	MET
		LEU	PRO	HIS	ASN	VAL	ALA
HIS	HIS	GLY	GLU	ASP	GLY	LEU	TYR
		LYS	LEU	GLY	ALA	GLN	ARG
HIS	HIS	TYR	ASP	LYS	ALA	LEU	PHE
		GLU	SER	ALA	THR	SER	ASN
HIS	HIS	GLY	PHE	HIS	LYS	SER	ILE
		LYS	GLY	PHE	MET	ASN	GLY
HIS	HIS	SER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

- Molecule 2: Heavy chain of S5D2 Fab



- Molecule 3: Light chain of S5D2 Fab



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100064	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.731	Depositor
Minimum map value	-2.670	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	437.2, 437.2, 437.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	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	0.28	0/1608	0.48	0/2189
2	a	0.27	0/1670	0.49	0/2283
3	b	0.25	0/1729	0.47	0/2349
All	All	0.27	0/5007	0.48	0/6821

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	502	GLY	Peptide

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	1563	0	1487	19	0
2	a	1627	0	1572	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	b	1690	0	1621	0	0
All	All	4880	0	4680	19	0

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

The worst 5 of 19 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:455:LEU:CD1	1:A:493:GLN:OE1	1.71	1.37
1:A:455:LEU:CD1	1:A:493:GLN:CD	1.96	1.33
1:A:455:LEU:HD12	1:A:493:GLN:NE2	1.55	1.18
1:A:455:LEU:HD12	1:A:493:GLN:CD	1.60	1.04
1:A:455:LEU:HD11	1:A:493:GLN:CD	1.62	1.01

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	195/1258 (16%)	184 (94%)	10 (5%)	1 (0%)	25	59
2	a	212/214 (99%)	208 (98%)	3 (1%)	1 (0%)	25	59
3	b	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
All	All	622/1689 (37%)	603 (97%)	17 (3%)	2 (0%)	38	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	51	ILE
1	A	491	PRO

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	170/1095 (16%)	167 (98%)	3 (2%)	54	74
2	a	186/186 (100%)	182 (98%)	4 (2%)	47	70
3	b	193/194 (100%)	191 (99%)	2 (1%)	73	84
All	All	549/1475 (37%)	540 (98%)	9 (2%)	58	76

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	18	ARG
3	b	188	LYS
2	a	52	ASN
2	a	55	ILE
2	a	58	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
2	a	6	GLN
2	a	203	HIS
3	b	43	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.

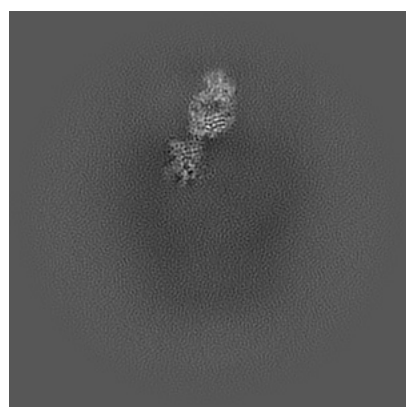
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32428. These allow visual inspection of the internal detail of the map and identification of artifacts.

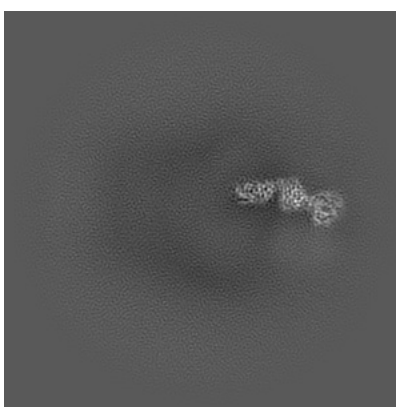
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

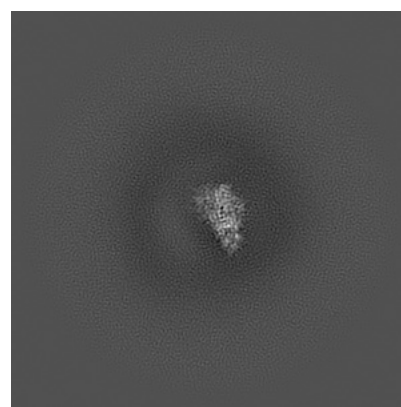
6.1.1 Primary map



X



Y

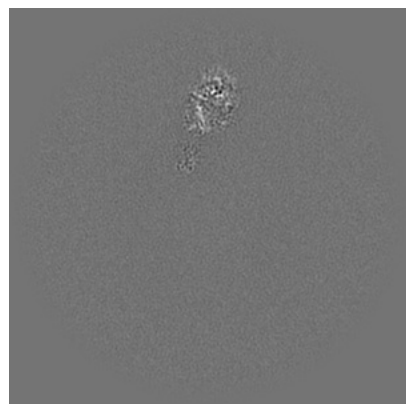


Z

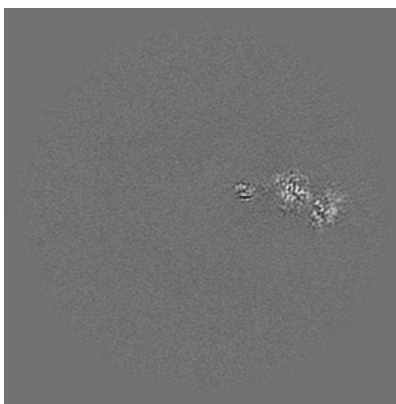
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

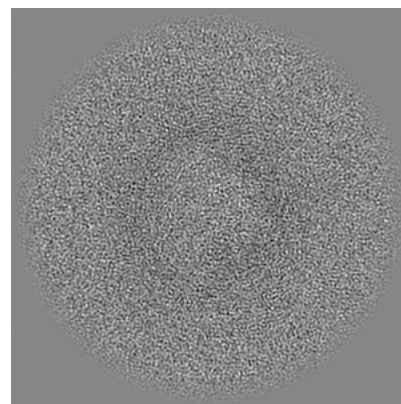
6.2.1 Primary map



X Index: 200



Y Index: 200

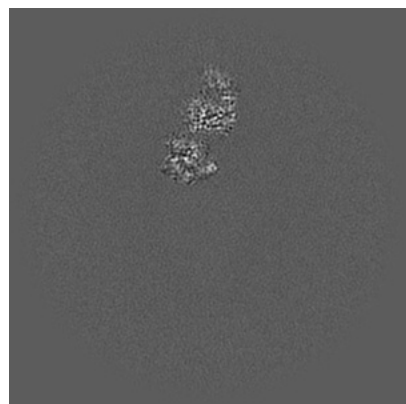


Z Index: 200

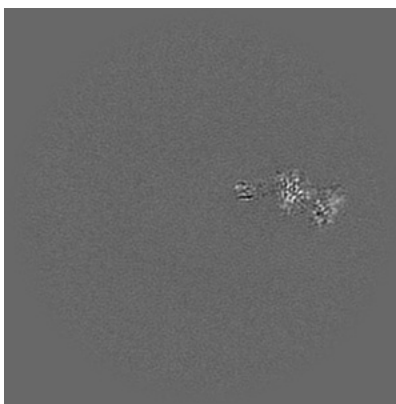
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

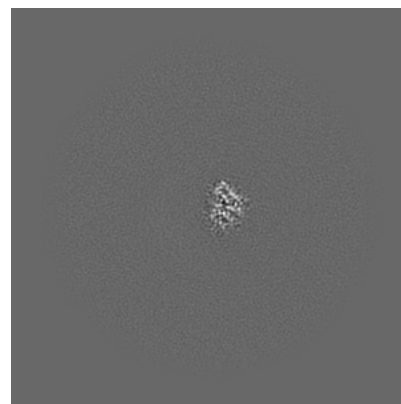
6.3.1 Primary map



X Index: 213



Y Index: 199

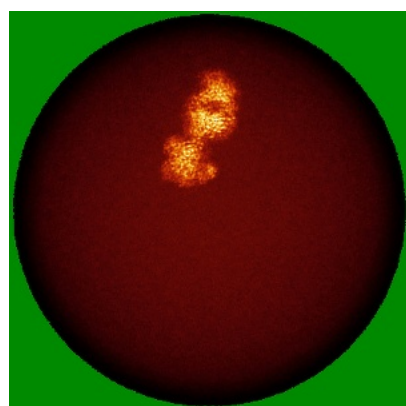


Z Index: 292

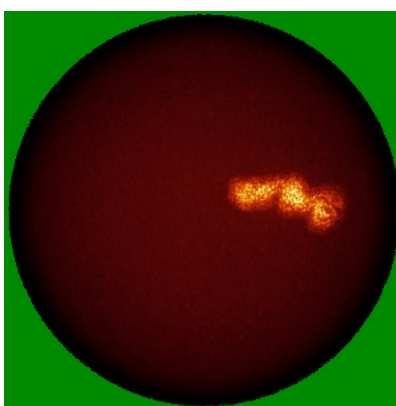
The images above show the largest variance slices of the map in three orthogonal directions.

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

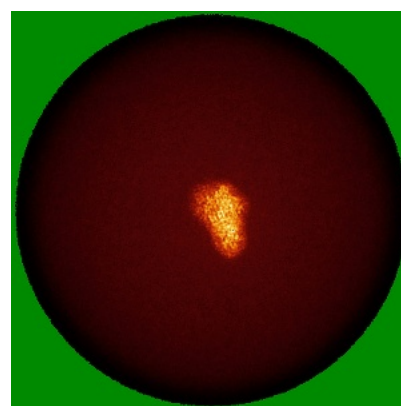
6.4.1 Primary map



X



Y

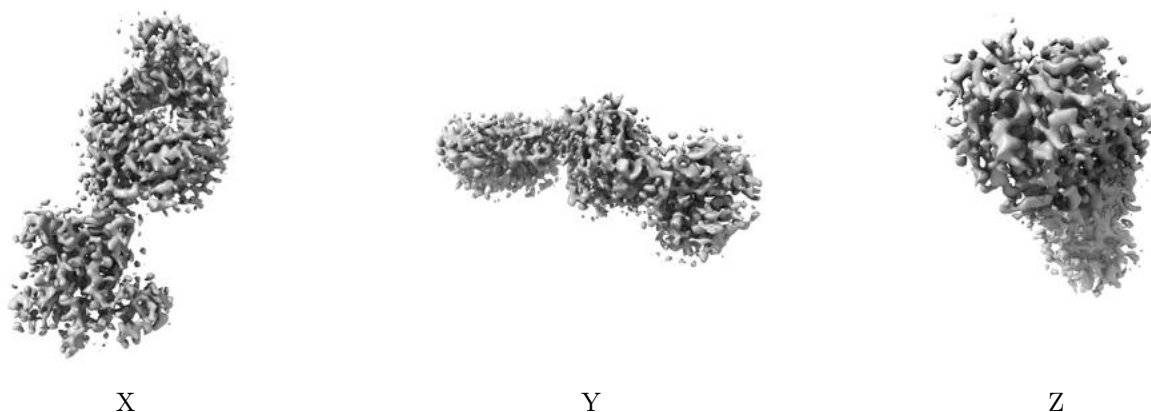


Z

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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

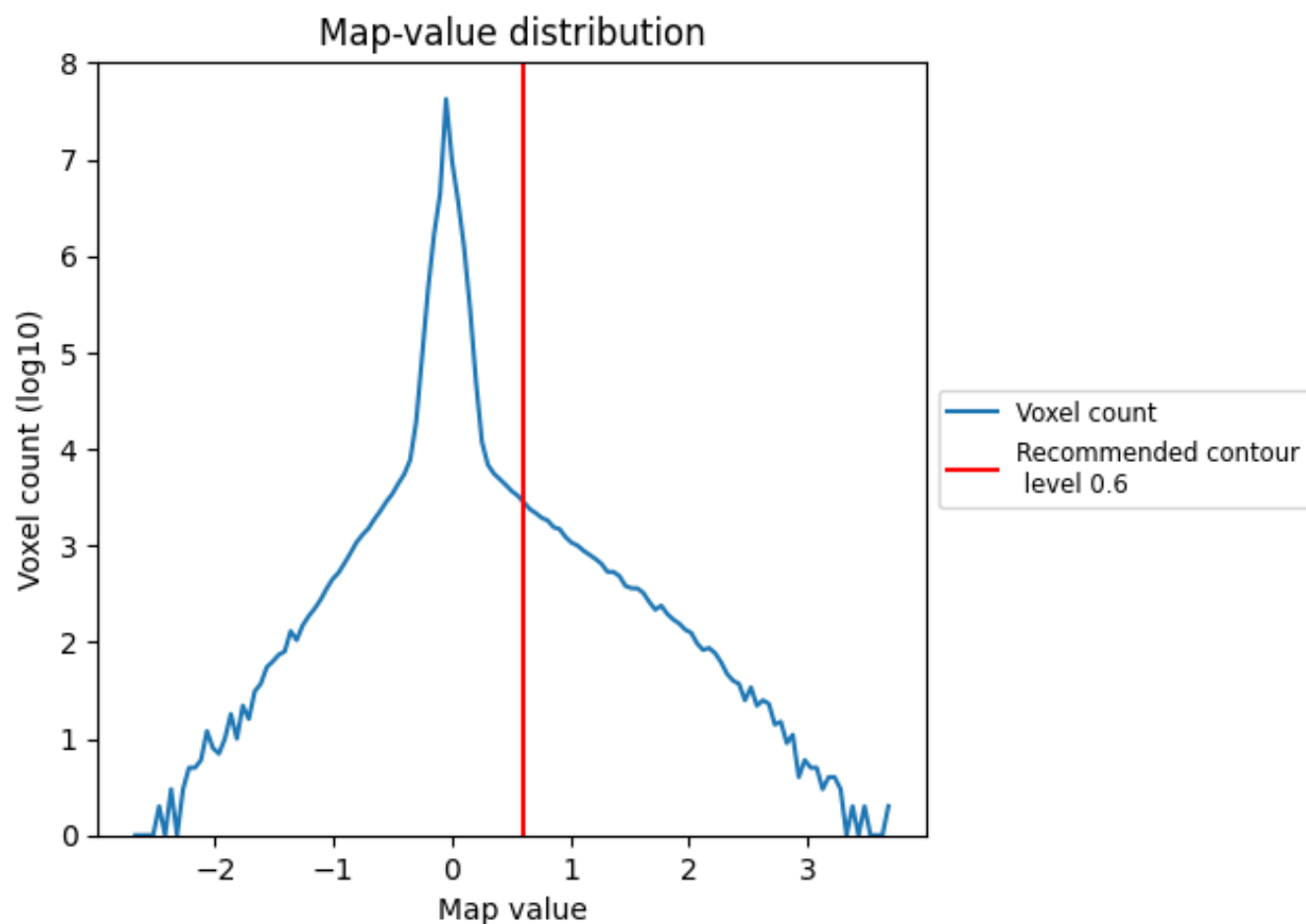
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

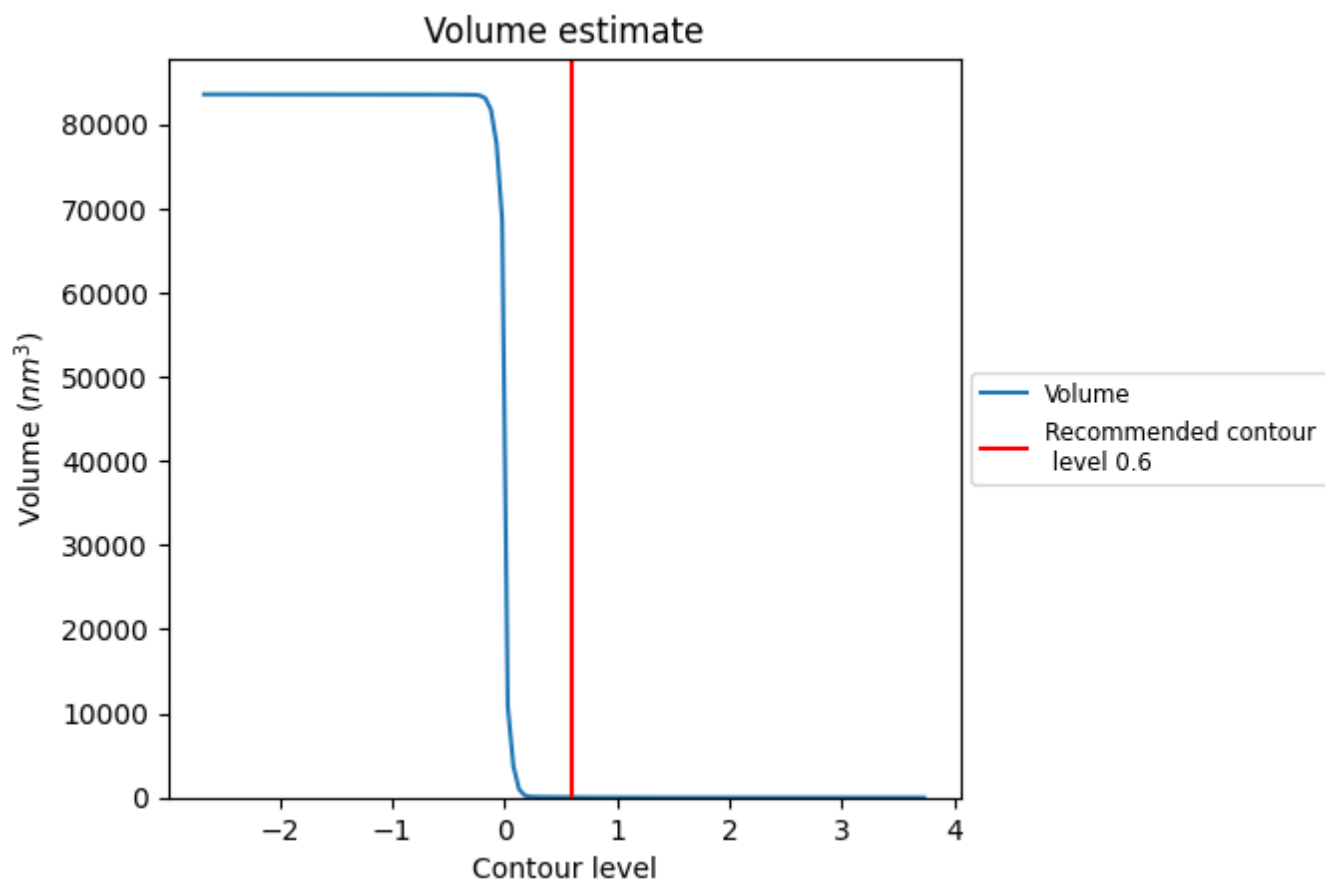
This section contains the results of statistical analysis of the map.

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.

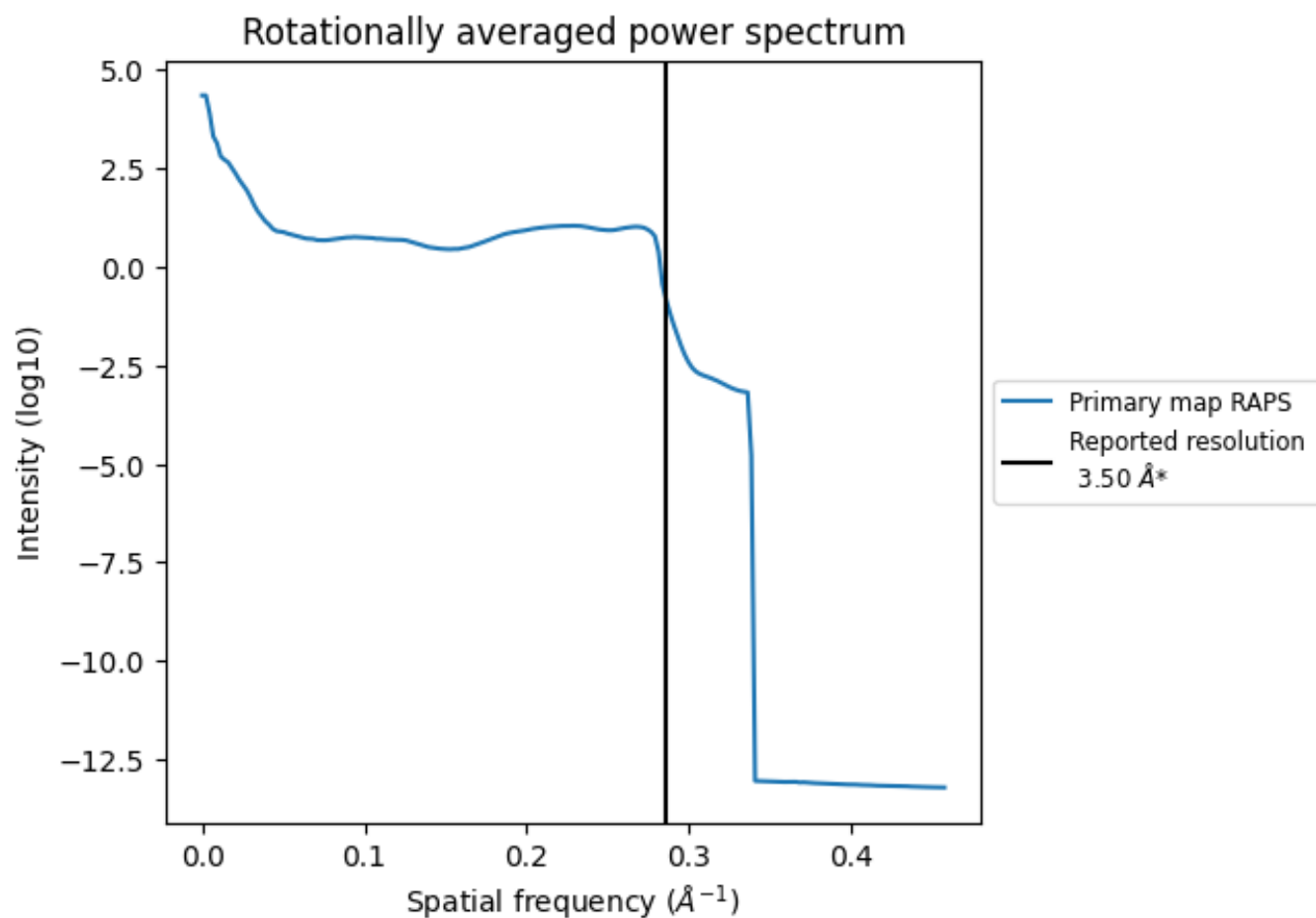
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm^3 ; this corresponds to an approximate mass of 31 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 0.286 Å⁻¹

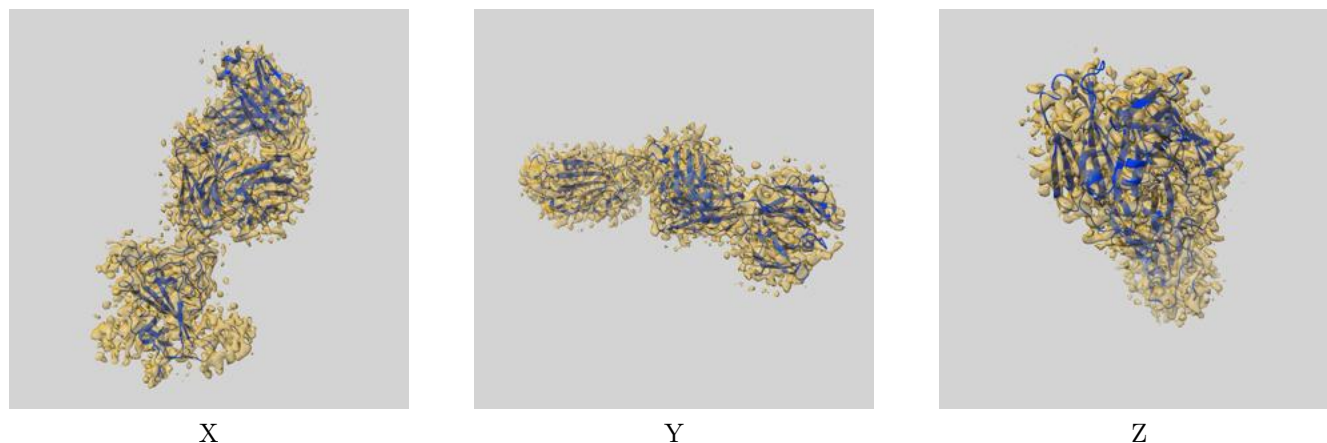
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

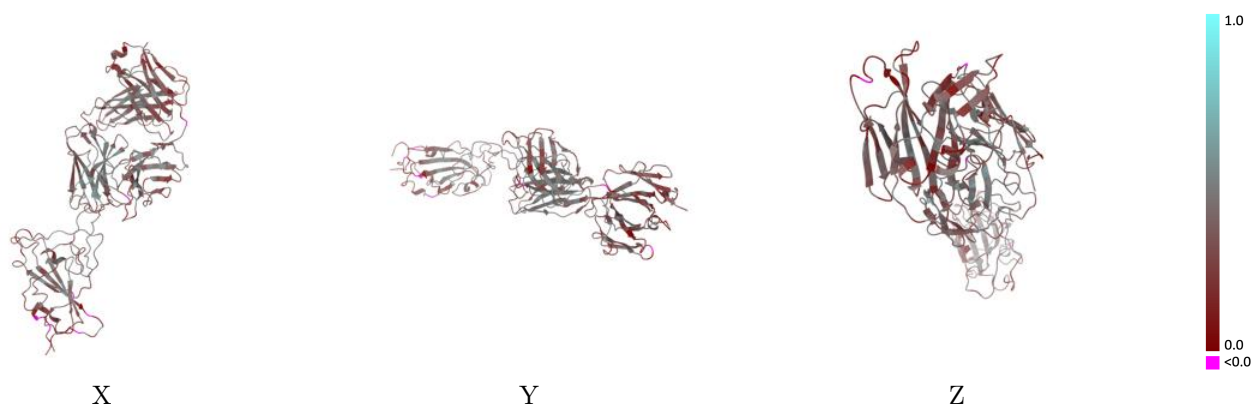
This section contains information regarding the fit between EMDB map EMD-32428 and PDB model 7WCR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



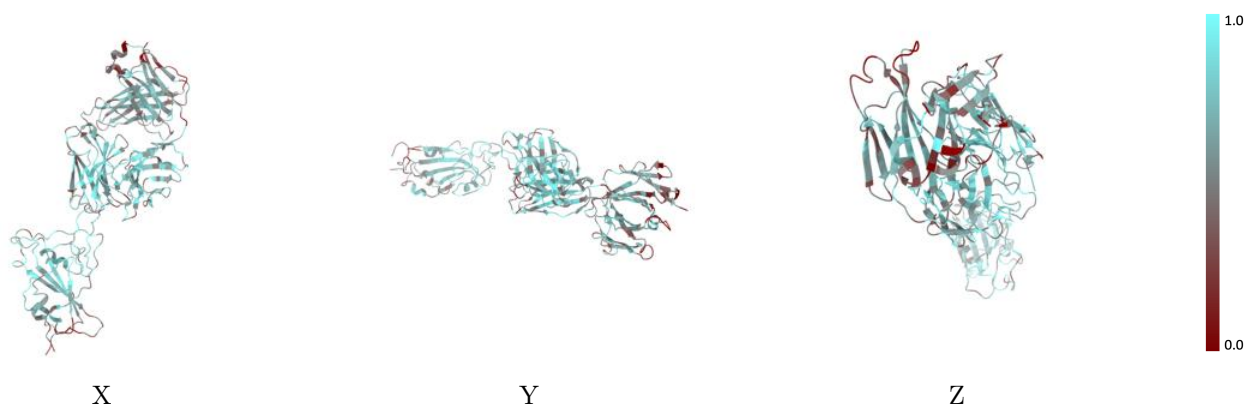
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



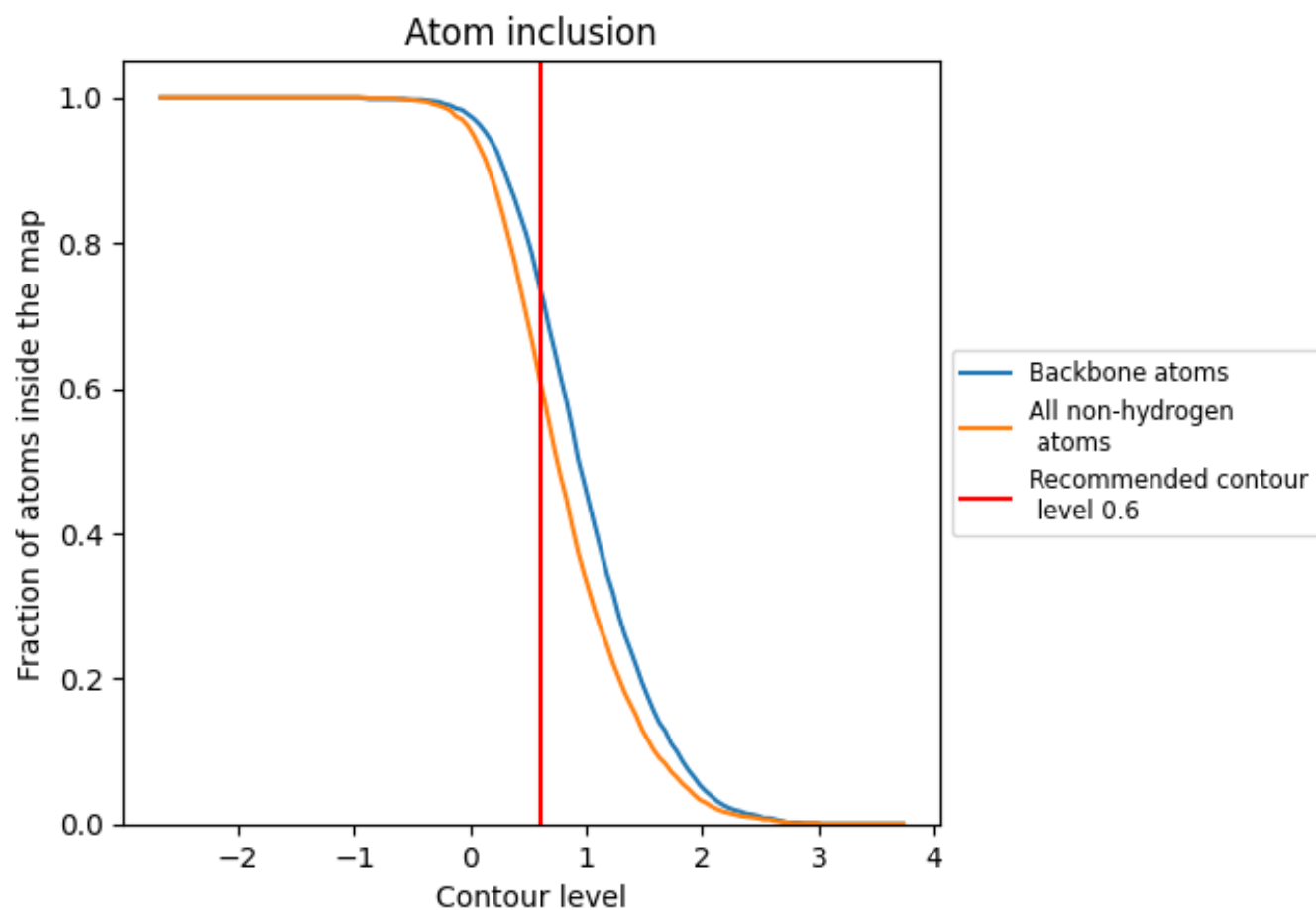
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 61% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6120	<div><div></div></div> 0.3540
A	<div><div></div></div> 0.6240	<div><div></div></div> 0.3410
a	<div><div></div></div> 0.6080	<div><div></div></div> 0.3720
b	<div><div></div></div> 0.6060	<div><div></div></div> 0.3490

