



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 04:21 PM JST

PDB ID : 7FAS
EMDB ID : EMD-31505
Title : VAR2CSA 3D7 ectodomain core region
Authors : Wang, L.; Zhaoning, W.
Deposited on : 2021-07-07
Resolution : 3.60 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

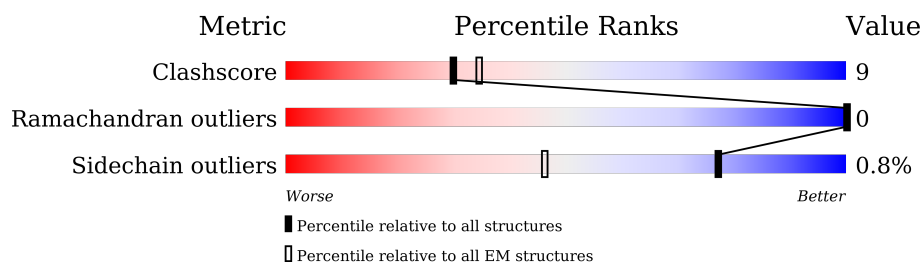
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	1977	

2 Entry composition

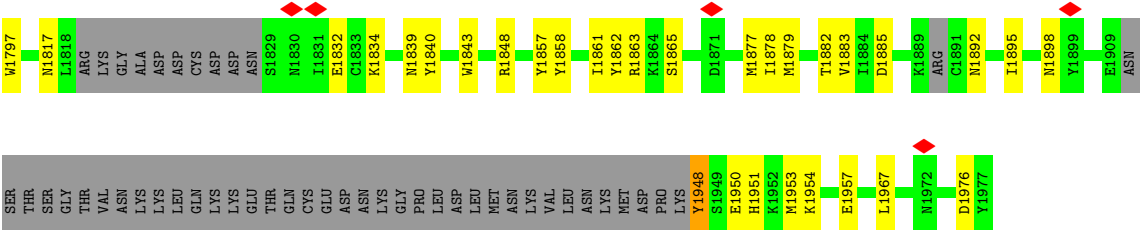
There is only 1 type of molecule in this entry. The entry contains 10173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Erythrocyte membrane protein 1, PfEMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1229	Total	C	N	O	S	0	0
			10173	6414	1753	1931	75		

K1701	S1708	S1709	M1710	K1711	M1712	D1713	K1717	R1720	M1726	I1729	ALA	VAL	PRO	ASN	ASN	ILE	THR	GLY	ALA	ASN	LYS	D1741	P1742	L1748	Q1754	D1762	E1763	E1764	LYS	GLU	LYS	K1769	P1770	M1771	E1772	M1773	C1777	M1778	H1782	Q1789	F1790	I1791	N1792	M1793	L1794	E1795	E1796					
LYS	G1582	N1583	W1587	S1588	K1589	K1590	K1594	LEU	GLU	ASN	GLY	T1600	L1601	Y1605	W1606	P1607	P1608	R1609	R1610	L1613	E1617	L1618	P1619	P1620	I1621	I1622	I1623	K1624	N1625	M1627	L1637	E1638	T1639	I1642	R1646	N1659	K1667	R1674	D1679	L1680	Y1694	I1698										
ASP	LEU	LEU	GLU	LYS	ASN	PRO	GLY	CYS	THR	ILE	PHE	THR	ASN	ASN	ASN	ASP	PHE	ASN	ASN	ASN	GLU	TYR	THR	GLY	LYS	TYR	SER	ILE	SER	GLY	GLN	VAL	LYS	TYR	TYR	GLU	ASN	ALA	LYS	ASN	N1574	L1577	E1580									
M1417	K1418	K1419	GLN	LYS	ASN	GLY	THR	PHE	THR	ASN	PRO	PHE	THR	PRO	THR	GLY	D1440	E1441	D1442	S1446	W1447	R1467	D1468	A1469	C1470	T1471	ASN	ASN	GLY	GLY	ALA	D1477	K1478	G1481	K1484	C1487	T1506	E1509	N1510	V1513	G1514	LYS	SER	ALA	SER							
N1351	M1352	I1353	L1354	G1355	THR	SER	VAL	ASN	ILE	TYR	GLN	K1290	I1291	K1292	N1293	A1294	I1295	Q1296	L1301	Y1305	H1306	ASP	LYS	ILE	GLU	LYS	THR	GLY	THR	LYS	GLN	ASN	GLY	PRO	MET	LYS	GLY	GLN	VAL	N1395	A1396	W1397	W1398	K1399	G1403	E1404	D1407	C1411	T1414	K1415	I1416	
LYS	ASN	ASP	THR	LYS	GLU	SER	LEU	LYS	GLN	ILE	PHE	K1290	I1291	K1292	N1293	A1294	I1295	Q1296	L1301	Y1305	H1306	ASP	LYS	ILE	GLU	LYS	THR	GLY	THR	LYS	GLN	ASN	GLY	PRO	MET	LYS	GLY	GLN	VAL	N1395	A1396	W1397	W1398	K1399	G1403	E1404	D1407	C1411	T1414	K1415	I1416	
GLY	CYS	PRO	PRO	ILE	TYR	ASP	GLY	LYS	ILE	PHE	PRO	PRO	GLN	TRP	ILE	CYS	LYS	ASP	TRP	ILE	HIS	GLY	ASP	THR	ILE	ILE	ILE	GLY	THR	ASN	GLY	ASN	GLY	ALA	CYS	ILE	PRO	PRO	GLY	VAL	GLY	GLU	LEU	TRP	ASP	ARG	TYR	GLY	ARG	SER	ASN	ILE
SER	LYS	ILE	THR	HIS	THR	GLU	ASP	LYS	LYS	E1086	C1087	C1088	C1089	Y1091	I1095	Q1101	K1104	M1108	K1111	F1112	Q1113	R1114	K1115	Q1116	I1117	TYR	ASP	ALA	ASN	GLY	LYS	GLY	GLN	ASN	LYS	K1128	S1131	L1136	F1137	F1138	E1143	Y1144	I1145	Q1146	LYS	Y1148	G1151	ASP	TRP			
K1004	PRO	THR	THR	VAL	ARG	SER	ASN	SER	LYS	N1083	C1084	K1085	E1086	C1087	C1088	C1089	Y1091	I1095	Q1101	K1104	M1108	K1111	F1112	Q1113	R1114	K1115	Q1116	I1117	TYR	ASP	ALA	ASN	GLY	LYS	GLY	GLN	ASN	LYS	K1128	S1131	L1136	F1137	F1138	E1143	Y1144	I1145	Q1146	LYS	Y1148	G1151	ASP	TRP
ASN	LYS	GLU	THR	VAL	ARG	SER	ASN	GLN	CYS	N933	T934	A935	P941	S942	P943	L944	K952	I959	P960	T961	N962	E963	S964	D967	D968	R969	K970	N974	Q975	W976	S977	C978	G979	S980	ALA	ARG	THR	MET	LYS	ARG	GLY	TYR	LYS	ASN	D991	E994	Y998	H999	G1000			
D896	T897	S898	Y899	SER	SER	L702	L705	M721	N728	S729	C732	CYS	GLY	ASP	GLY	VAL	THR	GLY	SER	GLY	S743	D746	P749	I750	I751	I754	R759	F760	L761	Q762	R772	Q773	V776	K777	P778	V779	I780	E781	C783	K787	GLU	SER	GLY	GLY	THR	CYS						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	304160	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	338.256, 338.256, 338.256	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.044, 1.044, 1.044	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	0.24	0/10355	0.44	0/13872

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	10173	0	9830	177	0
All	All	10173	0	9830	177	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 9.

The worst 5 of 177 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:1817:ASN:HB2	1:A:1951:HIS:CE1	2.13	0.83
1:A:1817:ASN:ND2	1:A:1951:HIS:HE1	1.84	0.76
1:A:1609:ARG:NH1	1:A:1679:ASP:OD2	2.19	0.75
1:A:169:ASP:O	1:A:274:GLN:NE2	2.21	0.74
1:A:772:ARG:NH1	1:A:901:CYS:O	2.22	0.72

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	1135/1977 (57%)	1089 (96%)	46 (4%)	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	1122/1796 (62%)	1113 (99%)	9 (1%)	79	88

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

Mol	Chain	Res	Type
1	A	1877	MET
1	A	1948	TYR
1	A	1336	LYS
1	A	1419	LYS
1	A	1610	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1340	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1343	GLN
1	A	1951	HIS
1	A	1817	ASN
1	A	832	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.

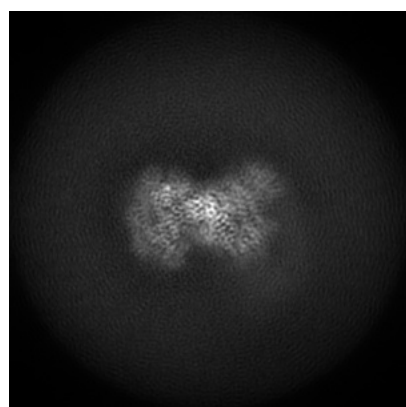
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31505. These allow visual inspection of the internal detail of the map and identification of artifacts.

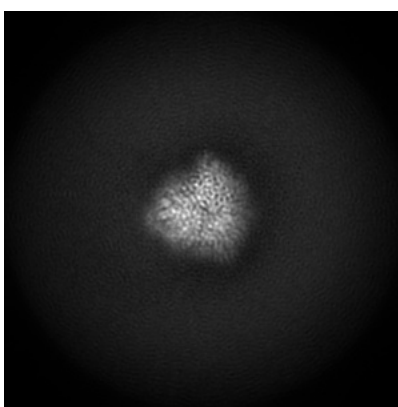
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

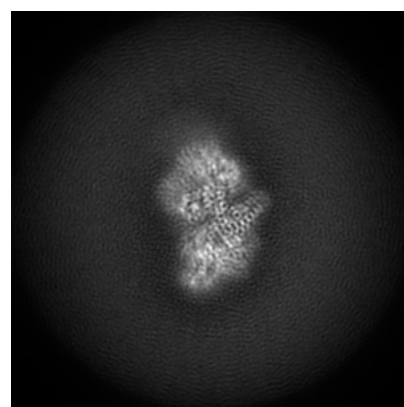
6.1.1 Primary map



X



Y

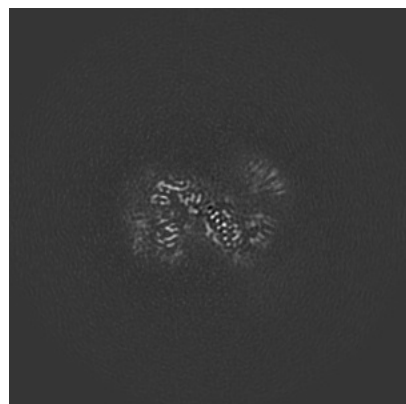


Z

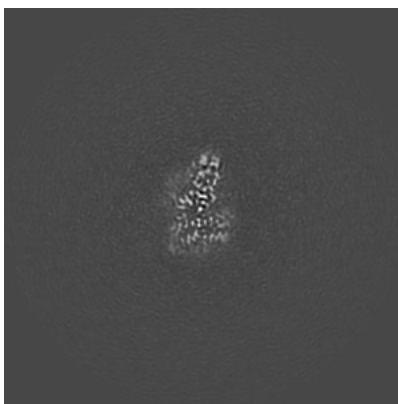
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

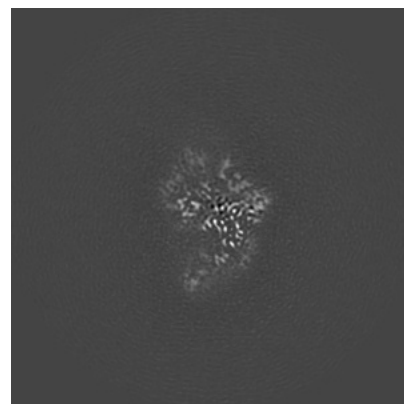
6.2.1 Primary map



X Index: 162



Y Index: 162

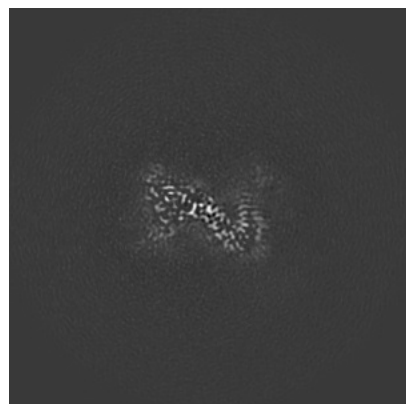


Z Index: 162

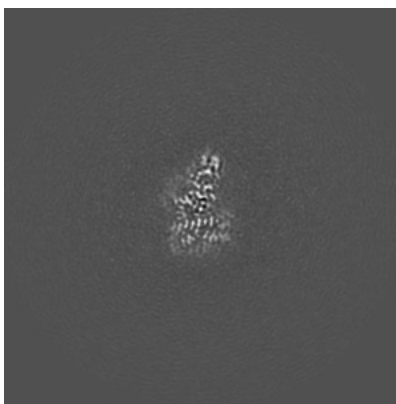
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

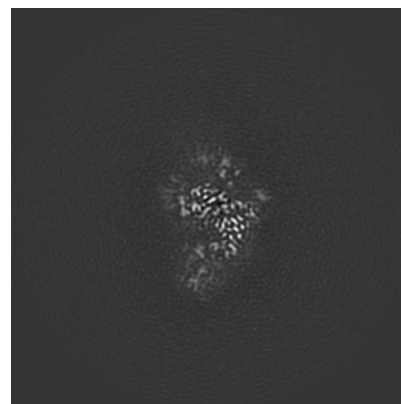
6.3.1 Primary map



X Index: 171



Y Index: 163

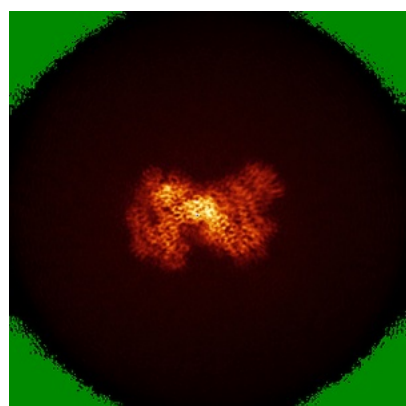


Z Index: 157

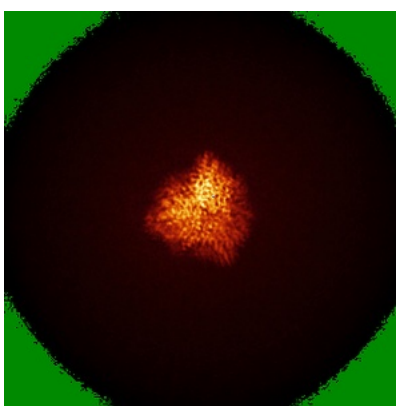
The images above show the largest variance slices of the map in three orthogonal directions.

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

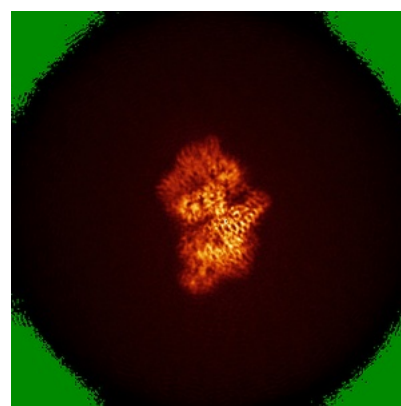
6.4.1 Primary map



X



Y

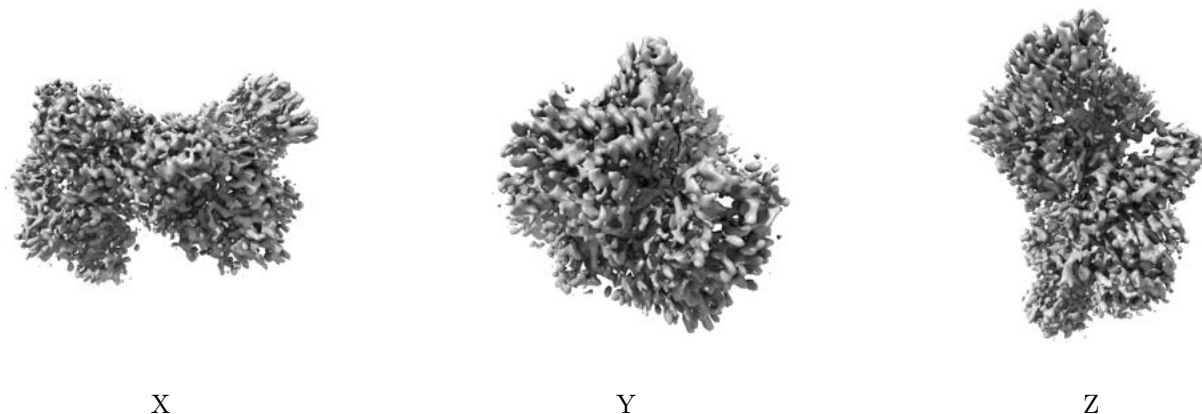


Z

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

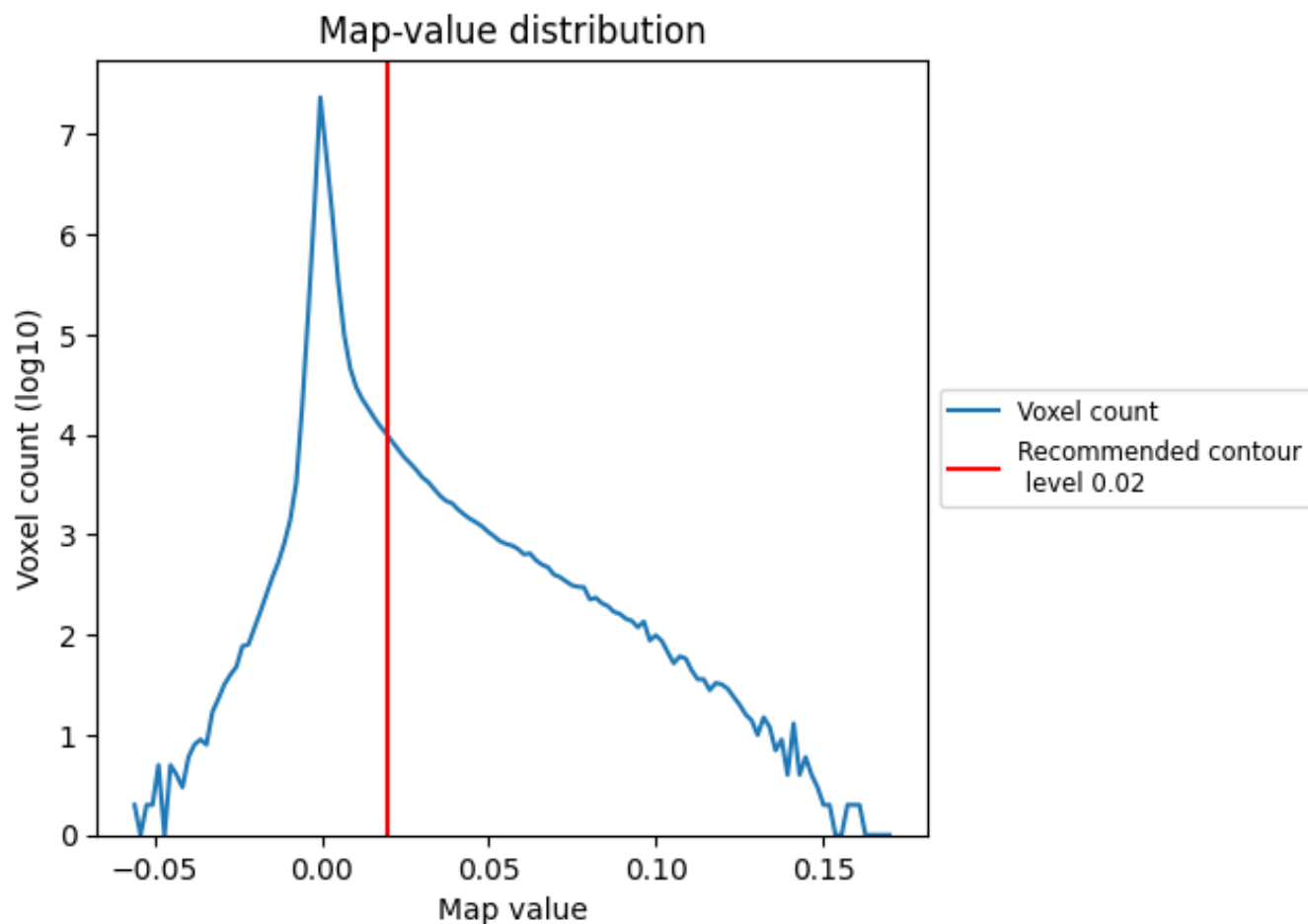
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

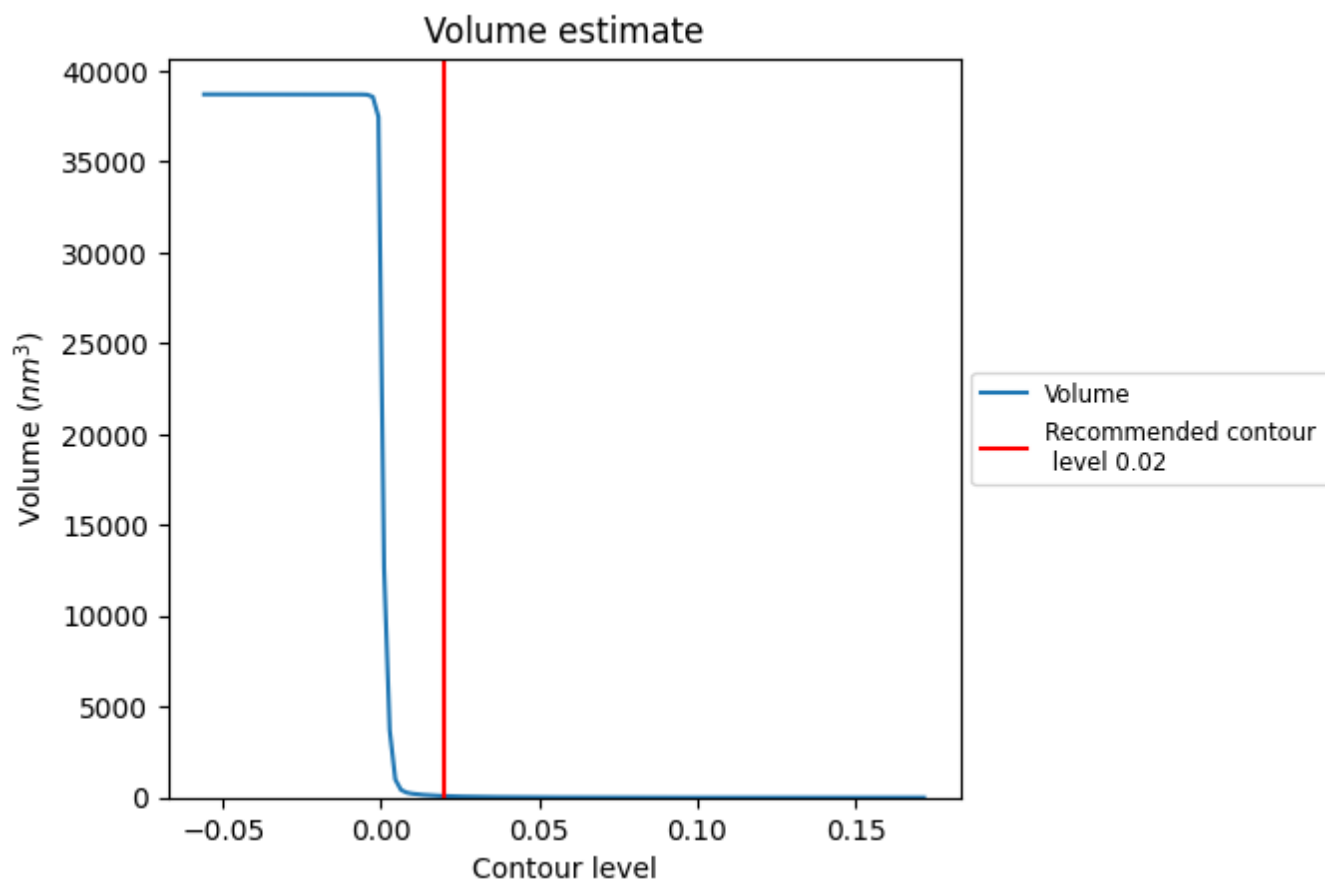
This section contains the results of statistical analysis of the map.

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.

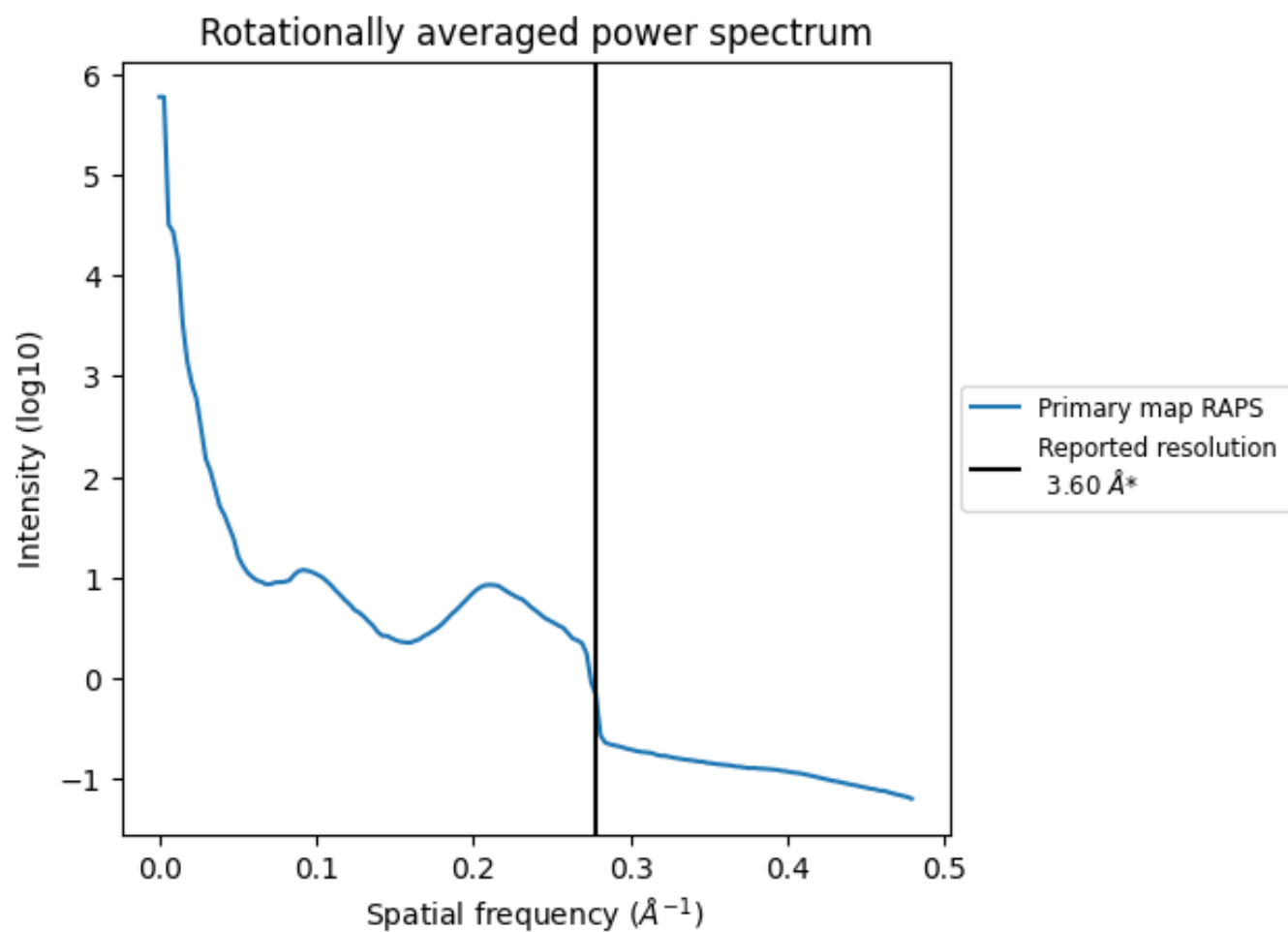
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm^3 ; this corresponds to an approximate mass of 77 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 0.278 Å⁻¹

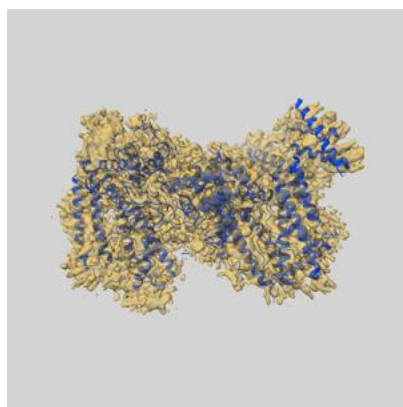
8 Fourier-Shell correlation ⓘ

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

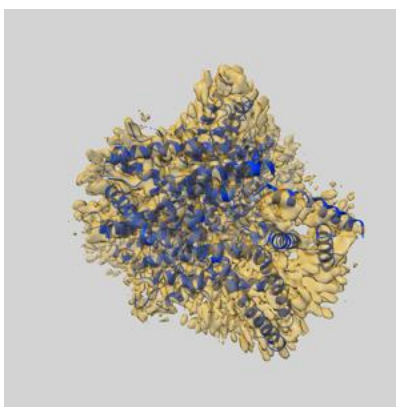
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31505 and PDB model 7FAS. Per-residue inclusion information can be found in section [3](#) on page [4](#).

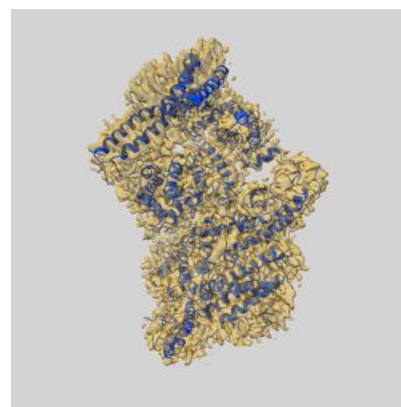
9.1 Map-model overlay [i](#)



X



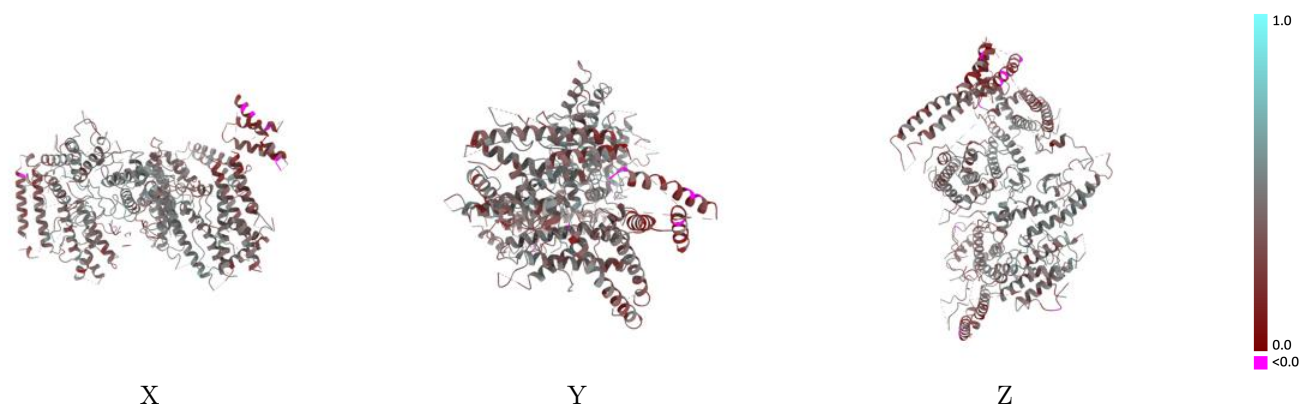
Y



Z

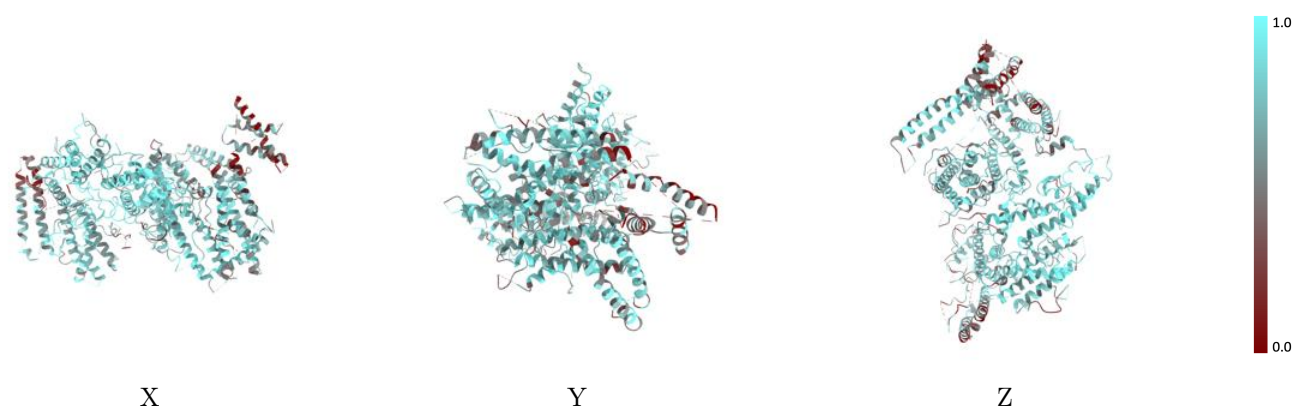
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



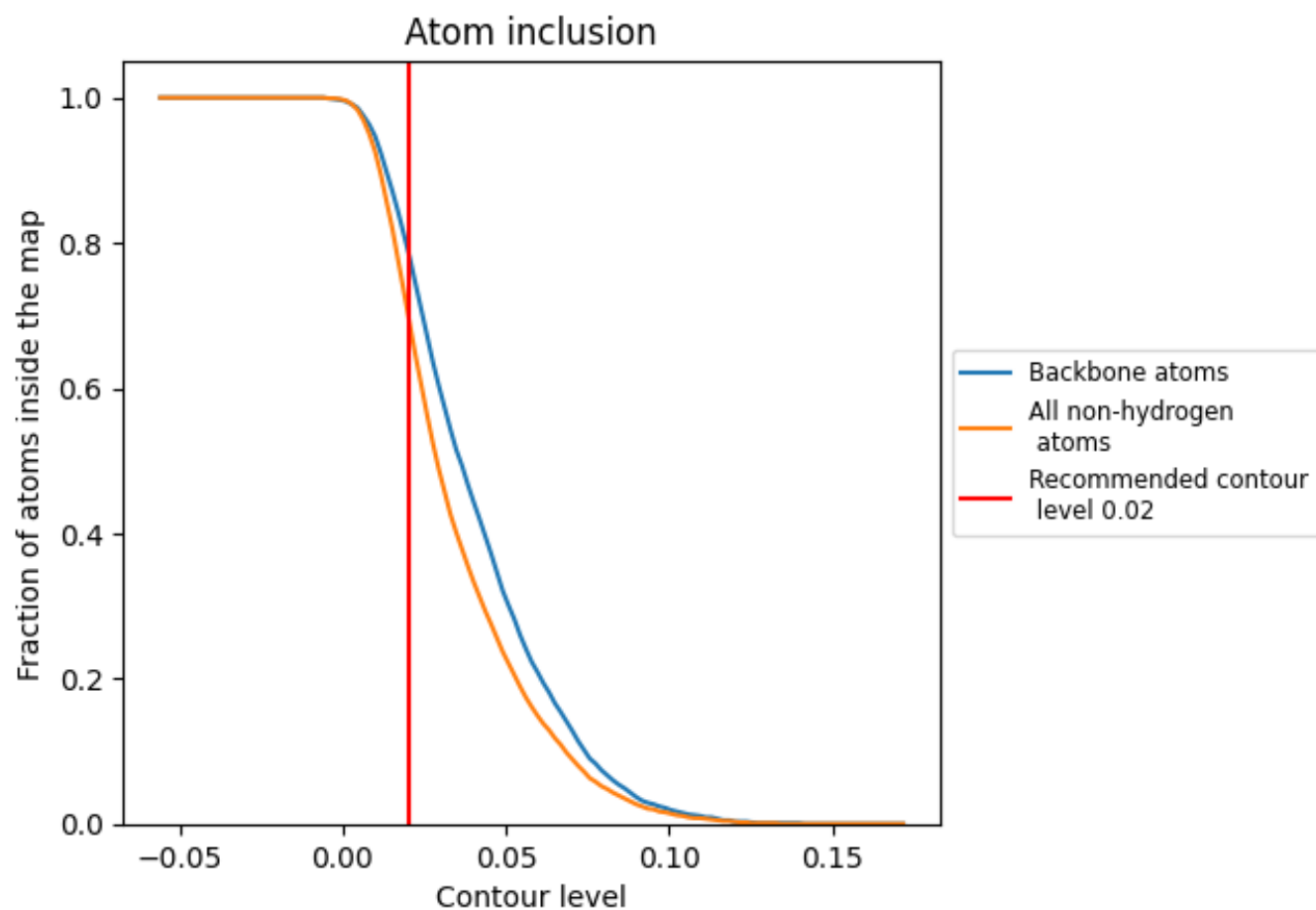
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7000	<div></div> 0.4020
A	<div></div> 0.7000	<div></div> 0.4020

