wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 01:00 AM EDT

PDB ID	:	7TMW
EMDB ID	:	EMD-26003
Title	:	Cryo-EM structure of the relaxin receptor RXFP1 in complex with heterotrimeric Gs
Authors	:	Erlandson, S.C.; Rawson, S.; Kruse, A.C.
Deposited on	:	2022-01-20
Resolution	:	3.20 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:

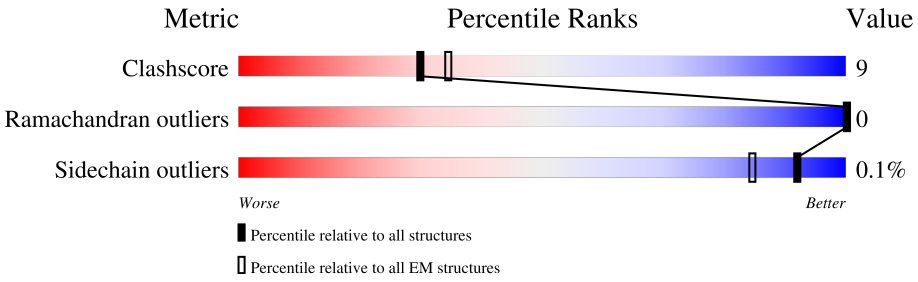
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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 <=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	R	984	5% 41% 10% 49%
2	B	350	8% 65% 20% 15%
3	C	71	6% 10% 90%
4	N	159	8% 57% 22% 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7320 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 Relaxin receptor 1, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	499	Total	C	N	O	S	0	0
			4075	2672	678	702	23		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	2	ASP	-	expression tag	UNP Q9HBX9
R	3	TYR	-	expression tag	UNP Q9HBX9
R	4	LYS	-	expression tag	UNP Q9HBX9
R	5	ASP	-	expression tag	UNP Q9HBX9
R	6	ASP	-	expression tag	UNP Q9HBX9
R	7	ASP	-	expression tag	UNP Q9HBX9
R	8	ASP	-	expression tag	UNP Q9HBX9
R	9	GLY	-	expression tag	UNP Q9HBX9
R	10	GLY	-	expression tag	UNP Q9HBX9
R	11	SER	-	expression tag	UNP Q9HBX9
R	12	LEU	-	expression tag	UNP Q9HBX9
R	13	GLU	-	expression tag	UNP Q9HBX9
R	14	VAL	-	expression tag	UNP Q9HBX9
R	15	LEU	-	expression tag	UNP Q9HBX9
R	16	PHE	-	expression tag	UNP Q9HBX9
R	17	GLN	-	expression tag	UNP Q9HBX9
R	18	GLY	-	expression tag	UNP Q9HBX9
R	19	PRO	-	expression tag	UNP Q9HBX9
R	20	GLY	-	expression tag	UNP Q9HBX9
R	21	GLY	-	expression tag	UNP Q9HBX9
R	22	SER	-	expression tag	UNP Q9HBX9
R	1001	ASN	-	linker	UNP Q9HBX9
R	1002	SER	-	linker	UNP Q9HBX9
R	1003	LYS	-	linker	UNP Q9HBX9
R	1004	THR	-	linker	UNP Q9HBX9
R	1005	GLU	-	linker	UNP Q9HBX9
R	1006	ASP	-	linker	UNP Q9HBX9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1007	GLN	-	linker	UNP Q9HBX9
R	1008	ARG	-	linker	UNP Q9HBX9
R	1009	ASN	-	linker	UNP Q9HBX9
R	1010	GLU	-	linker	UNP Q9HBX9
R	1011	GLU	-	linker	UNP Q9HBX9
R	1012	LYS	-	linker	UNP Q9HBX9
R	1013	ALA	-	linker	UNP Q9HBX9
R	1014	GLN	-	linker	UNP Q9HBX9
R	1015	ARG	-	linker	UNP Q9HBX9
R	1016	GLU	-	linker	UNP Q9HBX9
R	1017	ALA	-	linker	UNP Q9HBX9
R	1018	ASN	-	linker	UNP Q9HBX9
R	1019	LYS	-	linker	UNP Q9HBX9
R	1020	LYS	-	linker	UNP Q9HBX9
R	1021	ILE	-	linker	UNP Q9HBX9
R	1022	GLU	-	linker	UNP Q9HBX9
R	1023	LYS	-	linker	UNP Q9HBX9
R	1024	GLN	-	linker	UNP Q9HBX9
R	1025	LEU	-	linker	UNP Q9HBX9
R	1026	GLN	-	linker	UNP Q9HBX9
R	1027	LYS	-	linker	UNP Q9HBX9
R	1028	ASP	-	linker	UNP Q9HBX9
R	1029	LYS	-	linker	UNP Q9HBX9
R	1030	GLN	-	linker	UNP Q9HBX9
R	1031	VAL	-	linker	UNP Q9HBX9
R	1032	TYR	-	linker	UNP Q9HBX9
R	1033	ARG	-	linker	UNP Q9HBX9
R	1034	ALA	-	linker	UNP Q9HBX9
R	1035	THR	-	linker	UNP Q9HBX9
R	1036	HIS	-	linker	UNP Q9HBX9
R	1037	ARG	-	linker	UNP Q9HBX9
R	1038	LEU	-	linker	UNP Q9HBX9
R	1039	LEU	-	linker	UNP Q9HBX9
R	1040	LEU	-	linker	UNP Q9HBX9
R	1041	LEU	-	linker	UNP Q9HBX9
R	1042	GLY	-	linker	UNP Q9HBX9
R	1043	ALA	-	linker	UNP Q9HBX9
R	1044	ASP	-	linker	UNP Q9HBX9
R	1045	ASN	-	linker	UNP Q9HBX9
R	1046	SER	-	linker	UNP Q9HBX9
R	1047	GLY	-	linker	UNP Q9HBX9
R	1048	LYS	-	linker	UNP Q9HBX9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1049	SER	-	linker	UNP Q9HBX9
R	1050	THR	-	linker	UNP Q9HBX9
R	1051	ILE	-	linker	UNP Q9HBX9
R	1052	VAL	-	linker	UNP Q9HBX9
R	1053	LYS	-	linker	UNP Q9HBX9
R	1054	GLN	-	linker	UNP Q9HBX9
R	1055	MET	-	linker	UNP Q9HBX9
R	1056	ARG	-	linker	UNP Q9HBX9
R	1057	ILE	-	linker	UNP Q9HBX9
R	1058	TYR	-	linker	UNP Q9HBX9
R	1190	HIS	-	linker	UNP Q9HBX9
R	1191	GLY	-	linker	UNP Q9HBX9
R	1192	GLY	-	linker	UNP Q9HBX9
R	1193	SER	-	linker	UNP Q9HBX9
R	1194	GLY	-	linker	UNP Q9HBX9
R	1195	GLY	-	linker	UNP Q9HBX9
R	1196	SER	-	linker	UNP Q9HBX9
R	1197	GLY	-	linker	UNP Q9HBX9
R	1198	GLY	-	linker	UNP Q9HBX9
R	1244	ASP	ALA	conflict	UNP P63092
R	1247	ASP	SER	conflict	UNP P63092
R	?	-	ASN	deletion	UNP P63092
R	?	-	MET	deletion	UNP P63092
R	?	-	VAL	deletion	UNP P63092
R	?	-	ILE	deletion	UNP P63092
R	?	-	ARG	deletion	UNP P63092
R	?	-	GLU	deletion	UNP P63092
R	?	-	ASP	deletion	UNP P63092
R	?	-	ASN	deletion	UNP P63092
R	?	-	GLN	deletion	UNP P63092
R	?	-	THR	deletion	UNP P63092
R	1357	ALA	ILE	conflict	UNP P63092
R	1360	ILE	VAL	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2273	1410	403	440	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P62873
B	2	HIS	-	expression tag	UNP P62873
B	3	HIS	-	expression tag	UNP P62873
B	4	HIS	-	expression tag	UNP P62873
B	5	HIS	-	expression tag	UNP P62873
B	6	HIS	-	expression tag	UNP P62873
B	7	HIS	-	expression tag	UNP P62873
B	8	GLY	-	expression tag	UNP P62873
B	9	SER	-	expression tag	UNP P62873
B	10	SER	-	expression tag	UNP P62873
B	11	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	7	Total	C	N	O	0	0
			54	35	7	12		

- Molecule 4 is a protein called Camelid antibody VHH fragment Nb35.

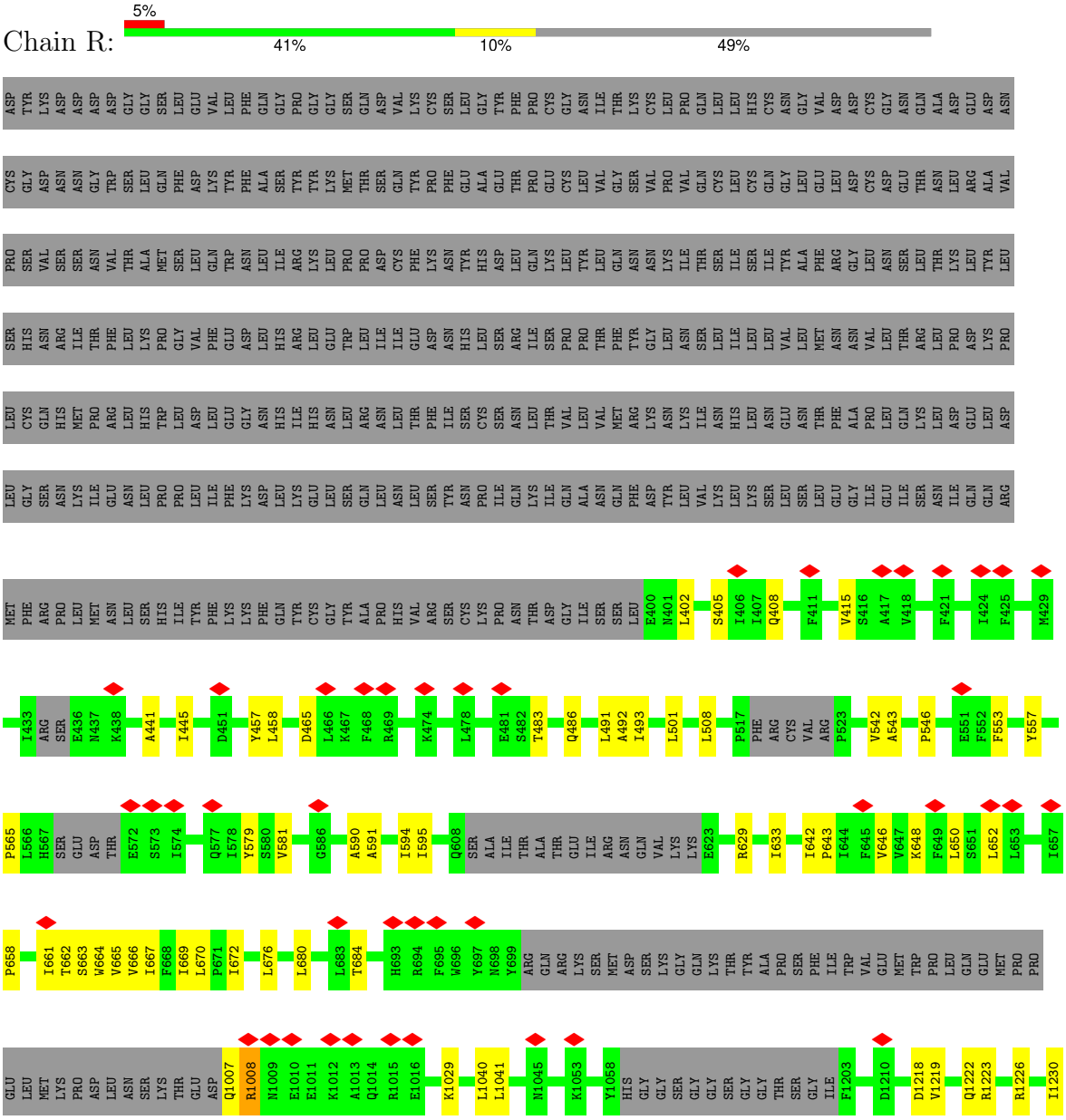
Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total	C	N	O	S	0	0
			918	578	154	180	6		

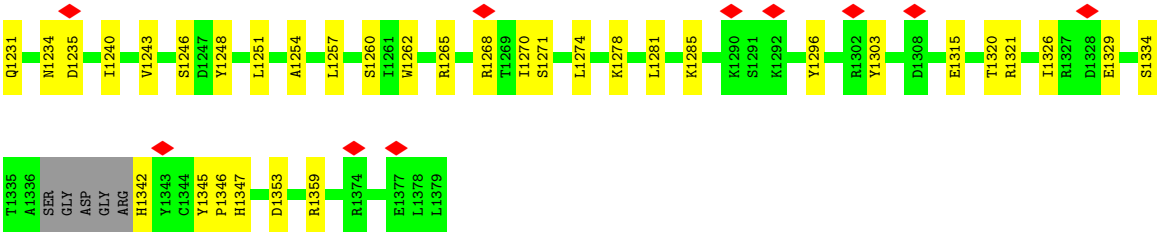
3 Residue-property plots (i)

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.

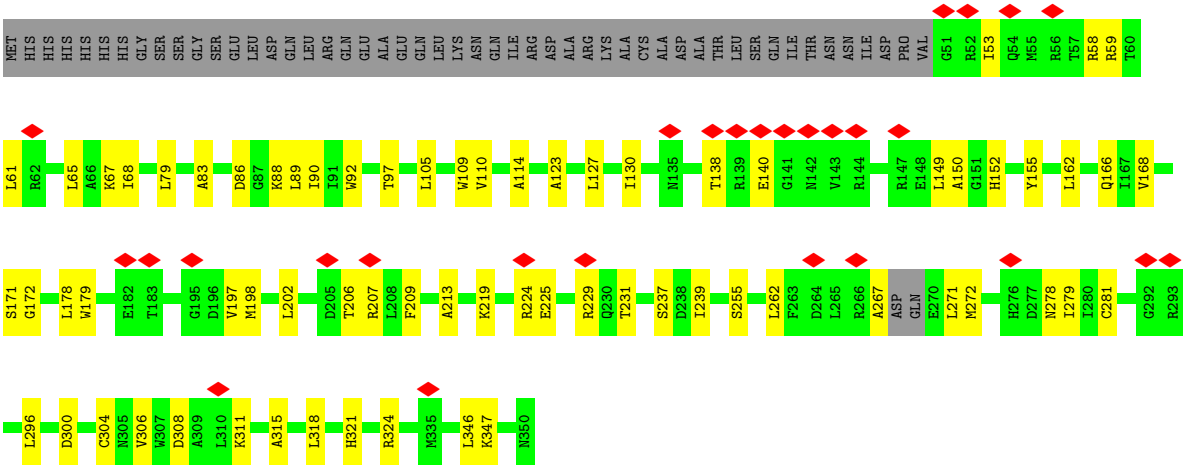
• Molecule 1: Relaxin receptor 1, Guanine nucleotide-binding protein G(s) subunit alpha isoforms short fusion

Chain R:

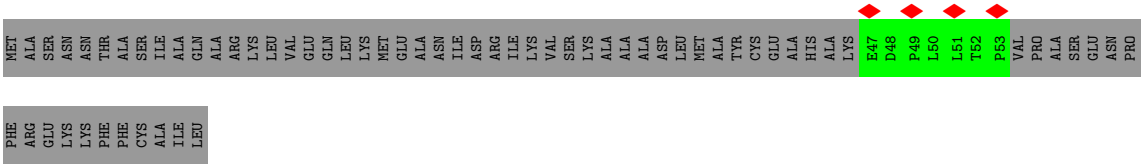




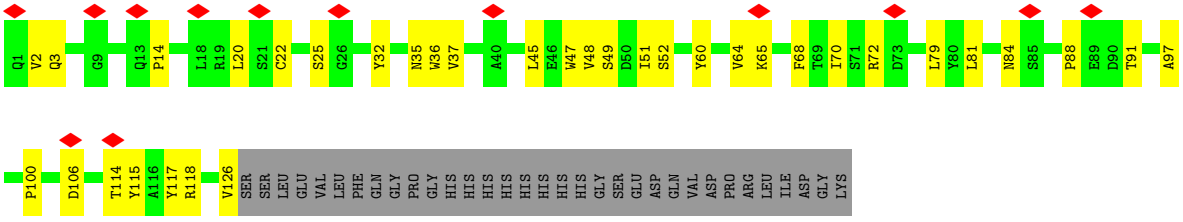
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



• Molecule 4: Camelid antibody VHH fragment Nb35



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	188250	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	116.471	Depositor
Minimum map value	-2.673	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.936	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	R	0.28	0/4170	0.51	0/5640
2	B	0.26	0/2318	0.60	0/3145
3	C	0.22	0/55	0.38	0/76
4	N	0.30	0/938	0.53	0/1276
All	All	0.28	0/7481	0.54	0/10137

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	R	4075	0	4106	64	0
2	B	2273	0	2169	48	0
3	C	54	0	52	0	0
4	N	918	0	852	27	0
All	All	7320	0	7179	129	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 129 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)
2:B:79:LEU:HA	2:B:92:TRP:O	1.67	0.94
2:B:162:LEU:HD11	2:B:168:VAL:HG13	1.64	0.77
4:N:37:VAL:HA	4:N:47:TRP:HA	1.73	0.71
1:R:633:ILE:HG12	1:R:680:LEU:HD21	1.72	0.70
1:R:1222:GLN:HE22	2:B:127:LEU:HD22	1.59	0.68

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	R	483/984 (49%)	474 (98%)	9 (2%)	0	100	100
2	B	294/350 (84%)	282 (96%)	12 (4%)	0	100	100
3	C	5/71 (7%)	5 (100%)	0	0	100	100
4	N	124/159 (78%)	121 (98%)	3 (2%)	0	100	100
All	All	906/1564 (58%)	882 (97%)	24 (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	R	444/893 (50%)	443 (100%)	1 (0%)	92	97
2	B	244/291 (84%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	7/58 (12%)	7 (100%)	0	100 100
4	N	93/133 (70%)	93 (100%)	0	100 100
All	All	788/1375 (57%)	787 (100%)	1 (0%)	92 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	1008	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	1252	GLN
1	R	1256	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.

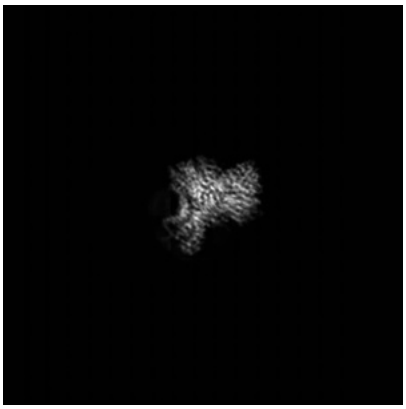
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26003. 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.

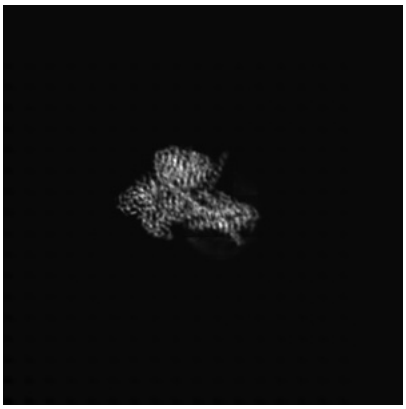
6.1 Orthogonal projections

6.1.1 Primary map



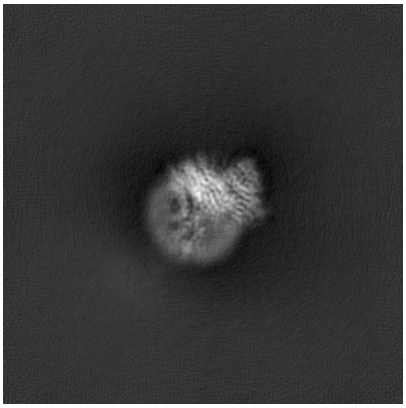
X

Y

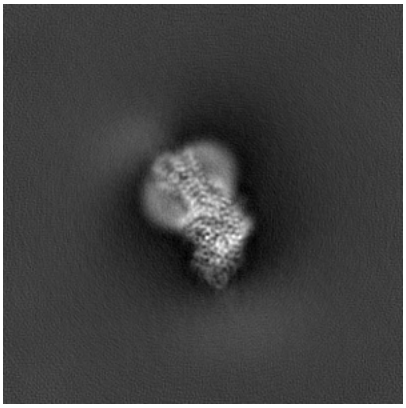


Z

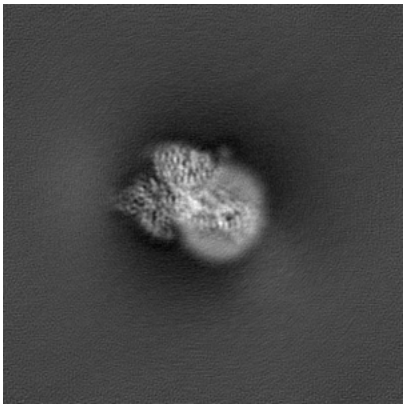
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

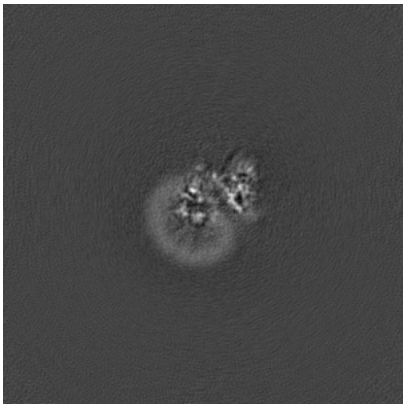
6.2.1 Primary map

X Index: 144

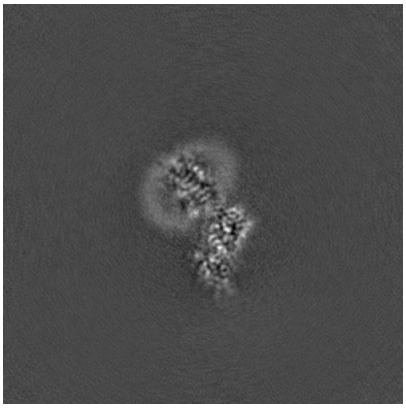
Y Index: 144

Z Index: 144

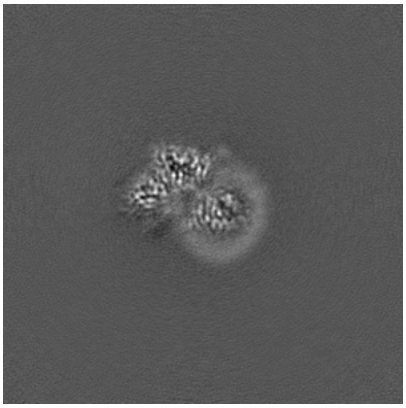
6.2.2 Raw map



X Index: 144



Y Index: 144



Z Index: 144

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

6.3 Largest variance slices (i)

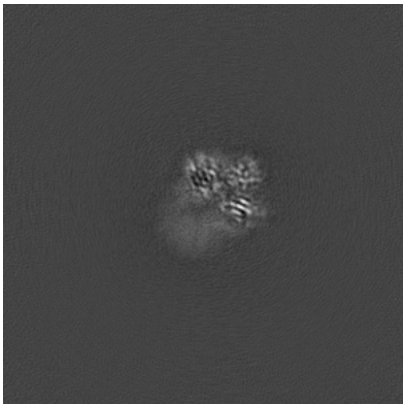
6.3.1 Primary map

X Index: 120

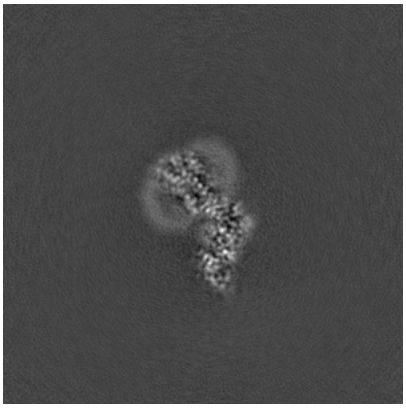
Y Index: 138

Z Index: 155

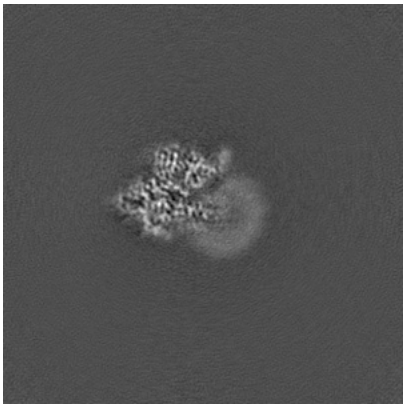
6.3.2 Raw map



X Index: 128



Y Index: 141

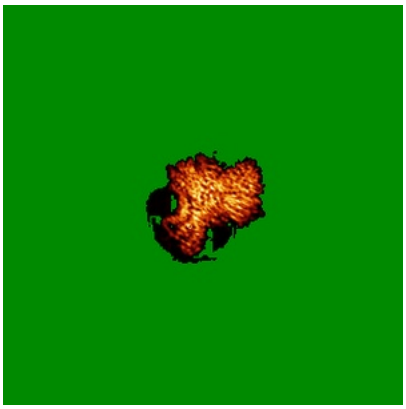


Z Index: 155

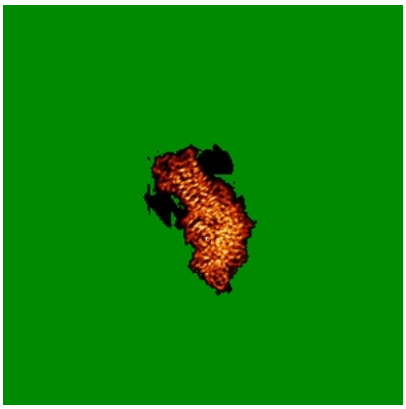
The images above show the largest variance slices of the map in three orthogonal directions.

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

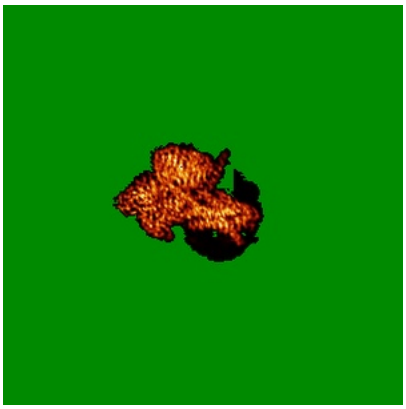
6.4.1 Primary map



X

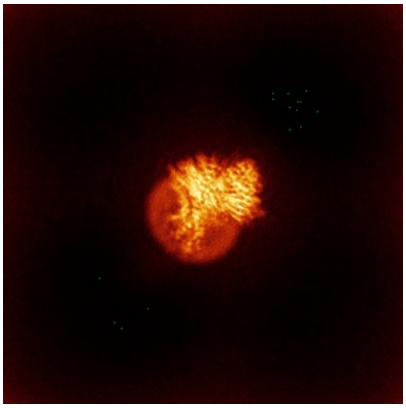


Y

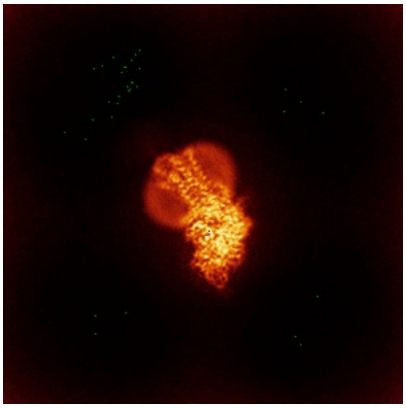


Z

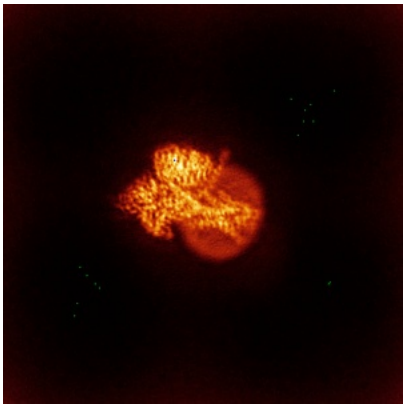
6.4.2 Raw map



X



Y

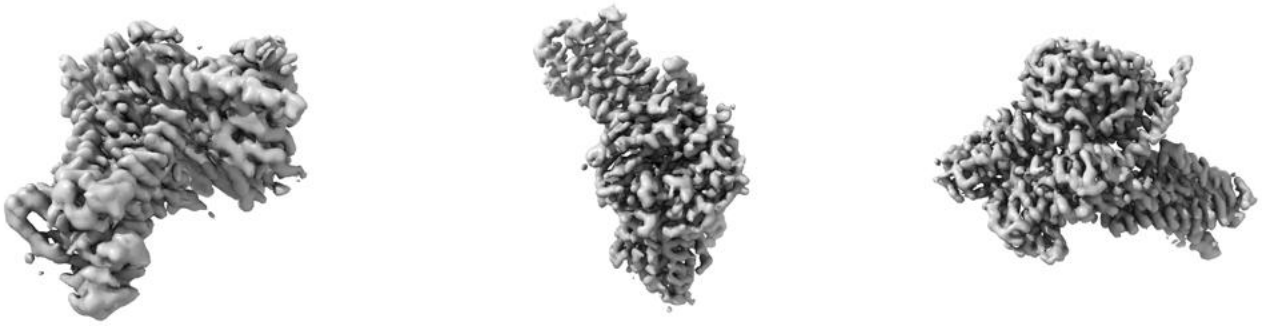


Z

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 5.5. 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.

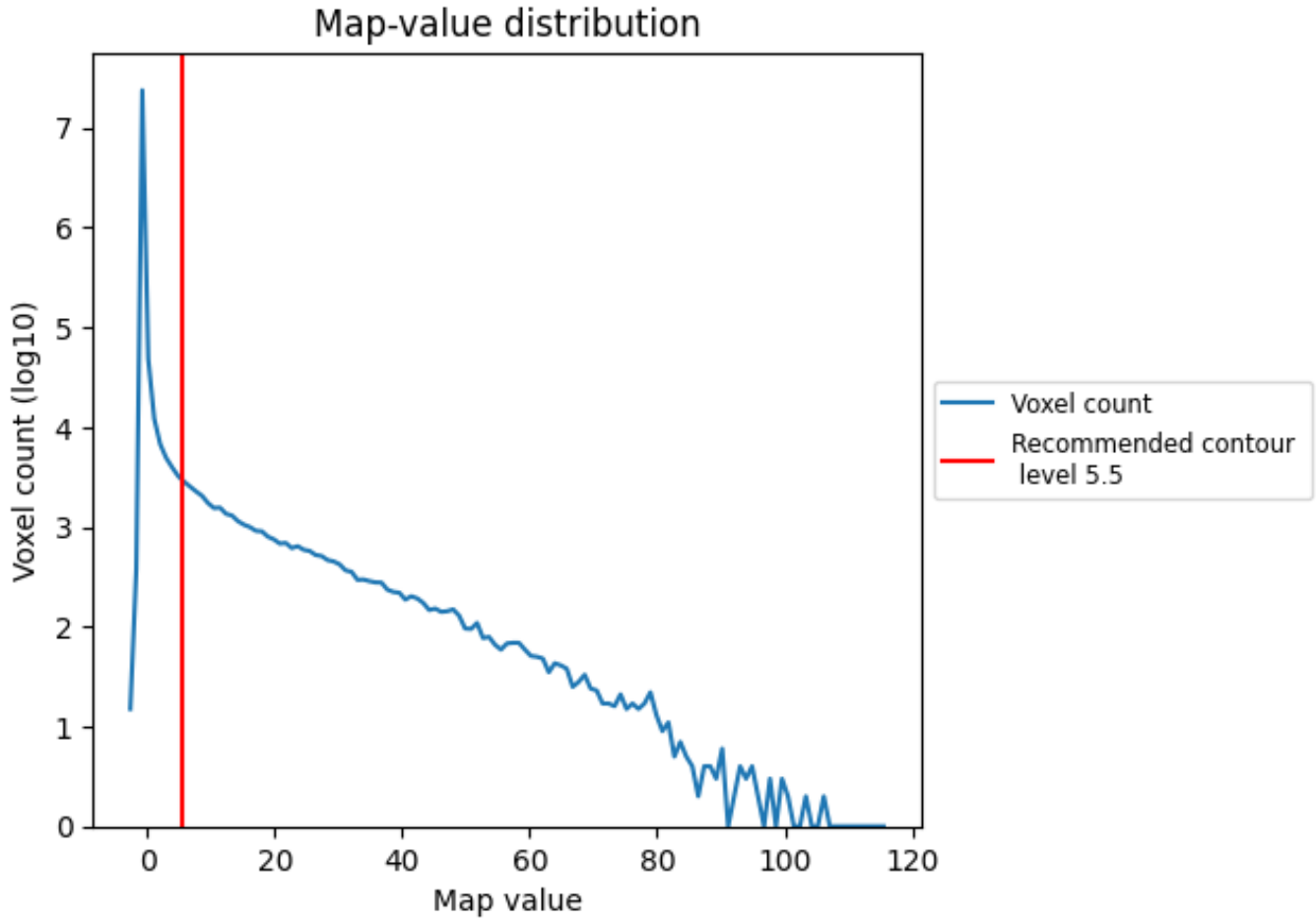
6.6 Mask visualisation (i)

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

7 Map analysis

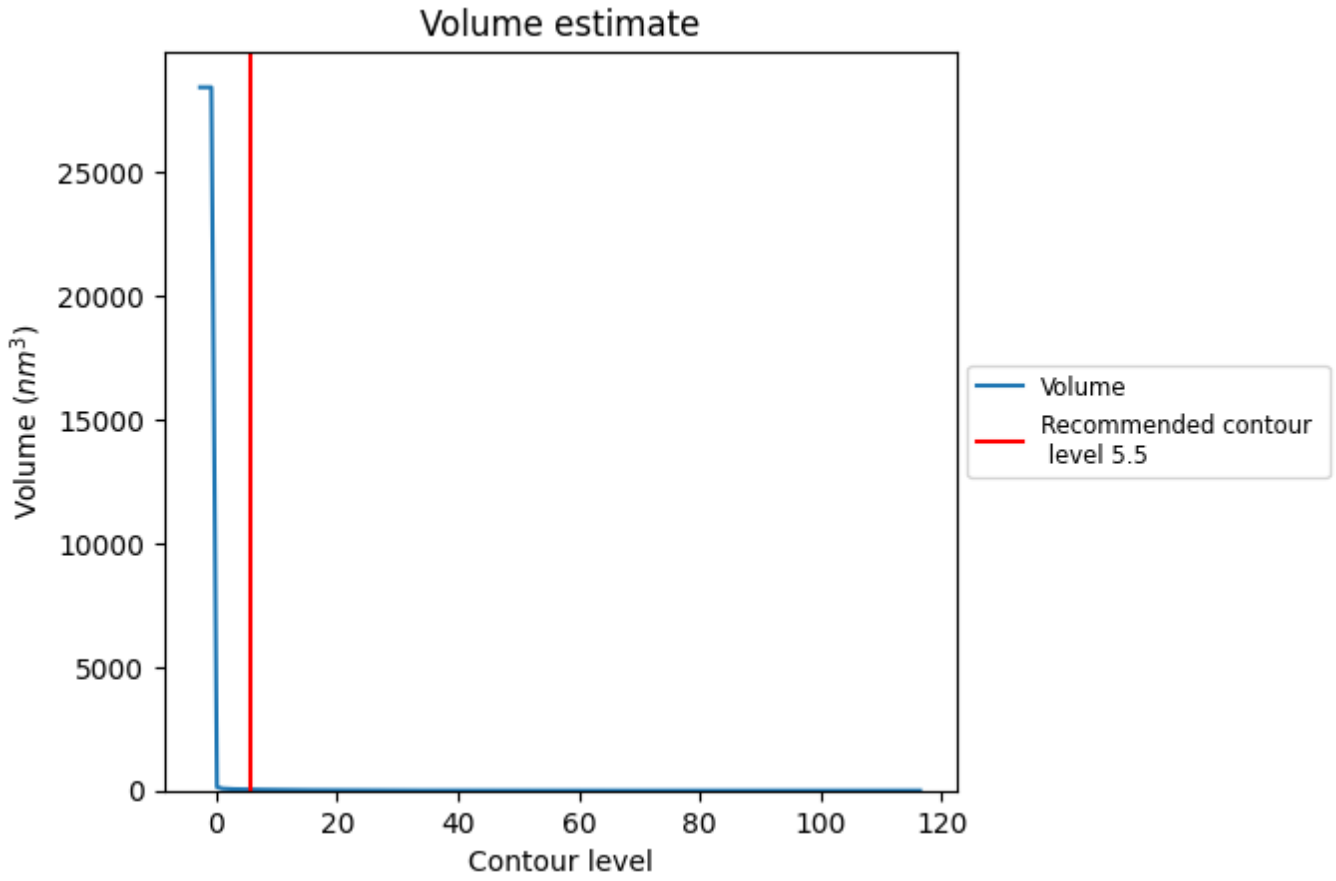
This section contains the results of statistical analysis of the map.

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.

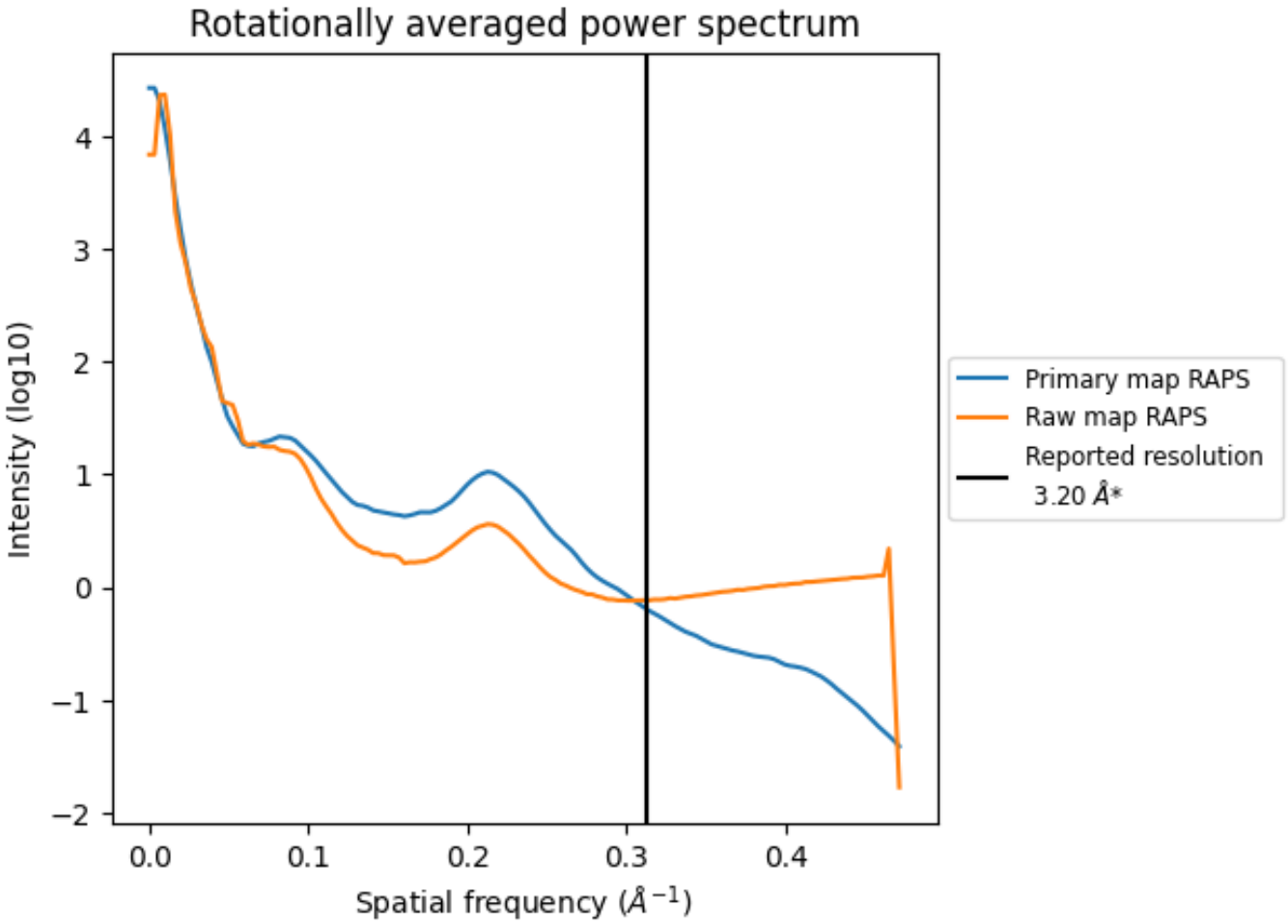
7.2 Volume estimate



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 40 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)

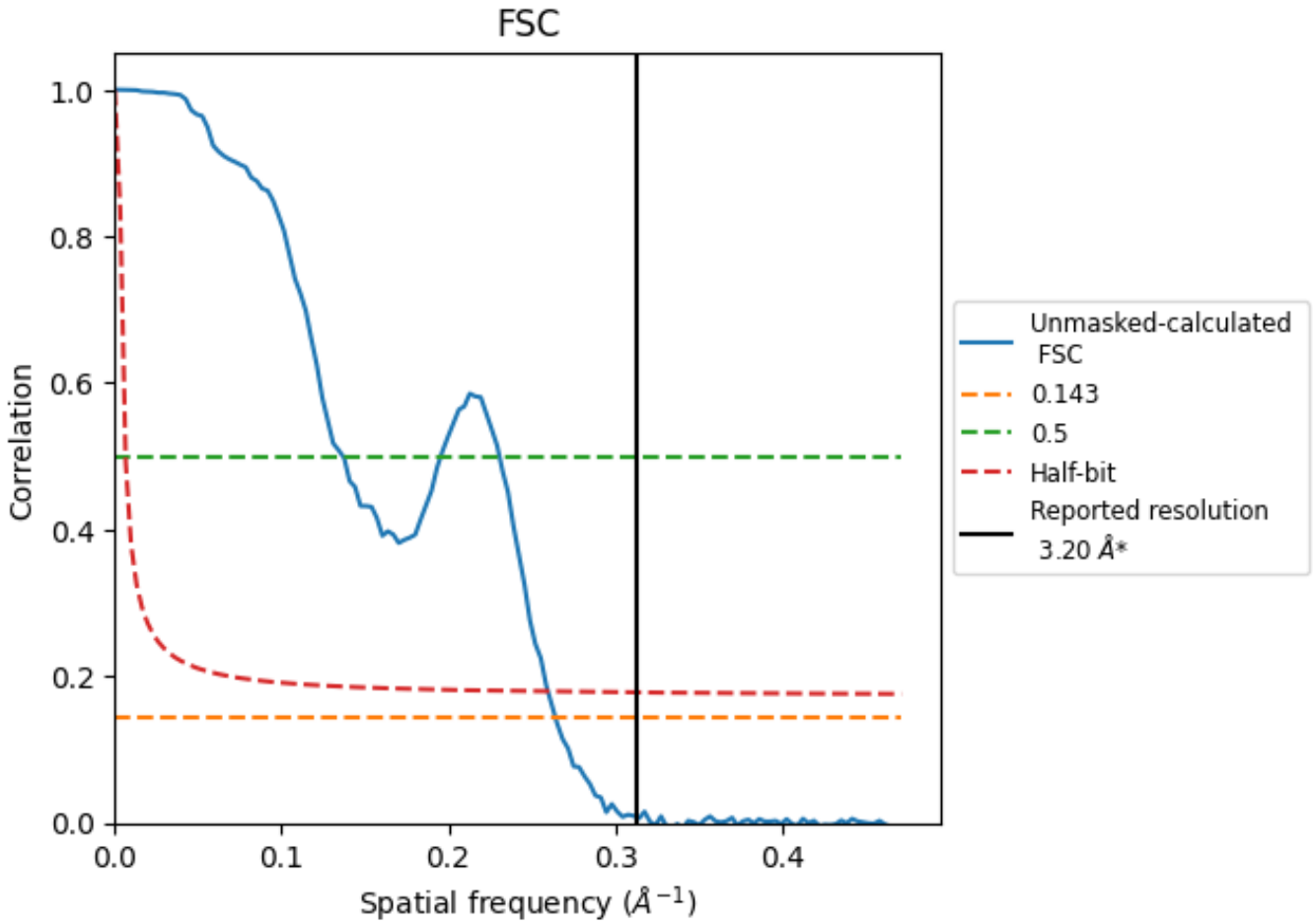


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

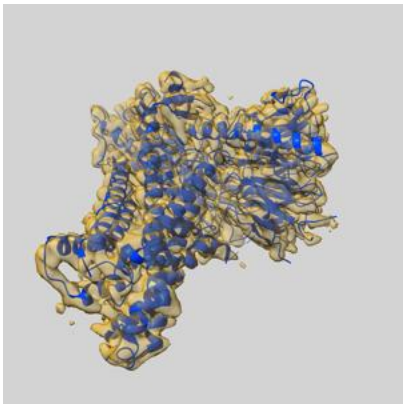
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.31	3.85

*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 3.78 differs from the reported value 3.2 by more than 10 %

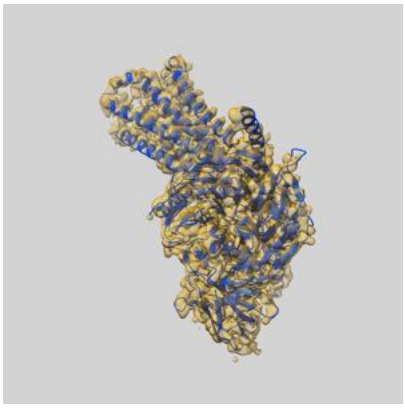
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26003 and PDB model 7TMW. Per-residue inclusion information can be found in section 3 on page 7.

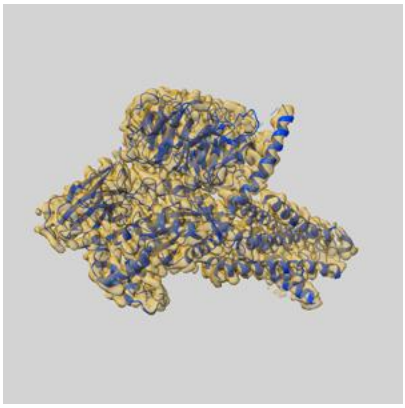
9.1 Map-model overlay



X



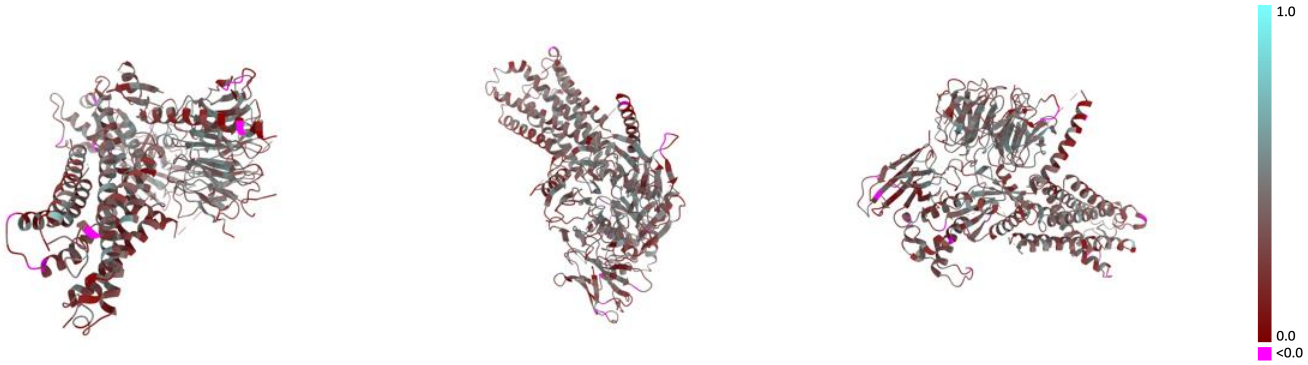
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5 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.

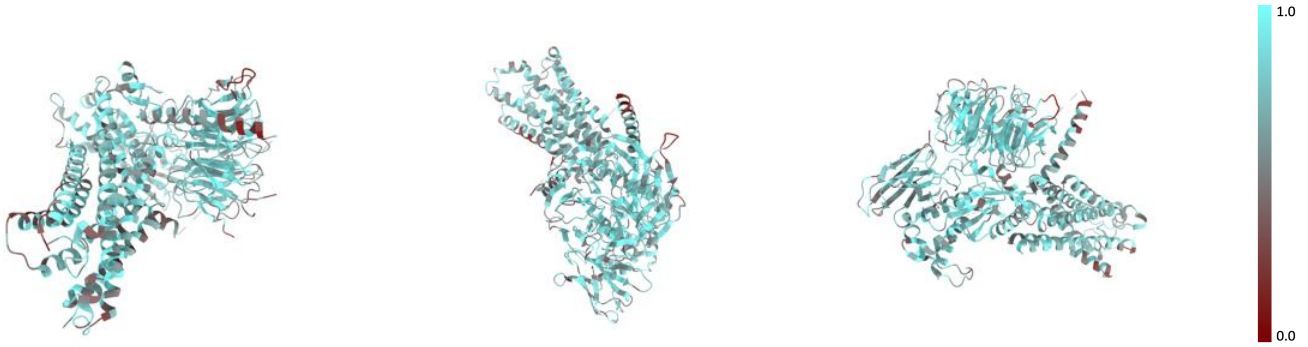
9.2 Q-score mapped to coordinate model (i)



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.

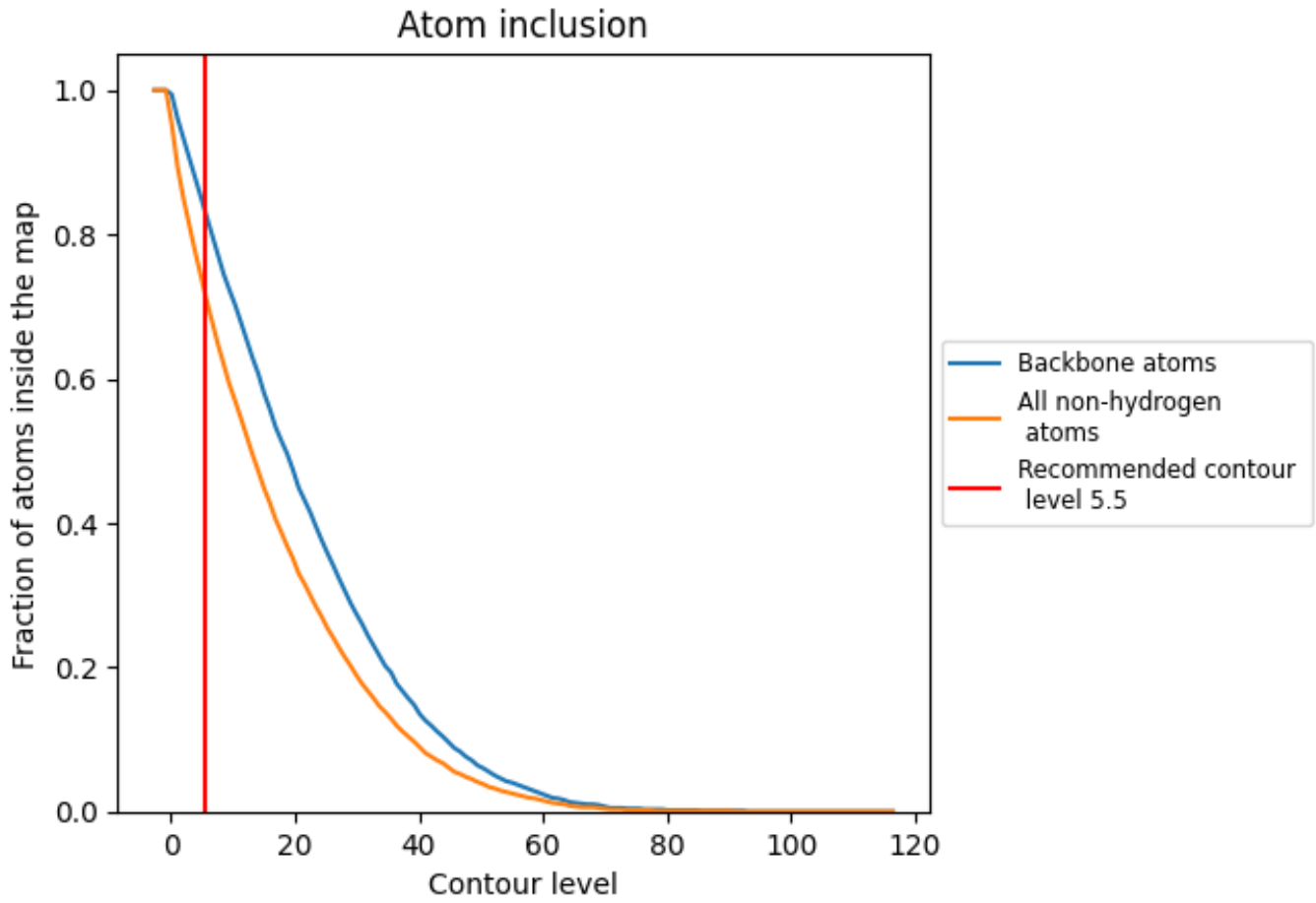
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.5).

9.4 Atom inclusion (i)



At the recommended contour level, 83% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7180	0.3360
B	0.7390	0.3660
C	0.4440	0.2210
N	0.7230	0.3140
R	0.7090	0.3250