



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 02:27 PM JST

PDB ID : 7F1Q
EMDB ID : EMD-31422
Title : Cryo-EM structure of the chemokine receptor CCR5 in complex with MIP-1a and Gi
Authors : Zhang, H.; Chen, K.; Tan, Q.; Han, S.; Zhu, Y.; Zhao, Q.; Wu, B.
Deposited on : 2021-06-09
Resolution : 2.90 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

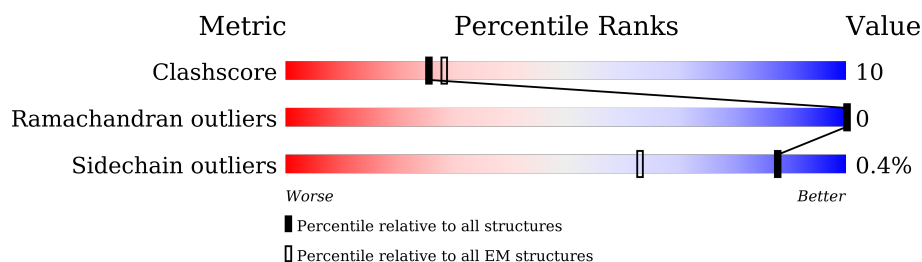
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	R	457	
2	A	354	
3	B	340	
4	C	71	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7123 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 C-C motif chemokine 3,C-C chemokine receptor type 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	367	Total	C	N	O	S	0	0
			2864	1901	455	486	22		

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	15	CYS	THR	engineered mutation	UNP P10147
R	74	GLY	-	linker	UNP P10147
R	75	SER	-	linker	UNP P10147
R	76	GLY	-	linker	UNP P10147
R	77	SER	-	linker	UNP P10147
R	78	GLY	-	linker	UNP P10147
R	79	SER	-	linker	UNP P10147
R	80	GLY	-	linker	UNP P10147
R	81	SER	-	linker	UNP P10147
R	82	GLY	-	linker	UNP P10147
R	83	SER	-	linker	UNP P10147
R	84	GLY	-	linker	UNP P10147
R	85	SER	-	linker	UNP P10147
R	86	GLY	-	linker	UNP P10147
R	87	SER	-	linker	UNP P10147
R	88	GLY	-	linker	UNP P10147
R	89	SER	-	linker	UNP P10147
R	90	GLY	-	linker	UNP P10147
R	91	SER	-	linker	UNP P10147
R	92	GLY	-	linker	UNP P10147
R	93	SER	-	linker	UNP P10147
R	94	GLY	-	linker	UNP P10147
R	95	SER	-	linker	UNP P10147
R	96	GLY	-	linker	UNP P10147
R	97	SER	-	linker	UNP P10147
R	112	CYS	THR	engineered mutation	UNP P51681
R	259	ASN	GLY	engineered mutation	UNP P51681
R	416	LEU	-	expression tag	UNP P51681

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Chain	Residue	Modelled	Actual	Comment	Reference
R	417	GLU	-	expression tag	UNP P51681
R	418	VAL	-	expression tag	UNP P51681
R	419	LEU	-	expression tag	UNP P51681
R	420	PHE	-	expression tag	UNP P51681
R	421	GLN	-	expression tag	UNP P51681
R	422	GLY	-	expression tag	UNP P51681
R	423	PRO	-	expression tag	UNP P51681
R	424	GLY	-	expression tag	UNP P51681
R	425	SER	-	expression tag	UNP P51681
R	426	TRP	-	expression tag	UNP P51681
R	427	SER	-	expression tag	UNP P51681
R	428	HIS	-	expression tag	UNP P51681
R	429	PRO	-	expression tag	UNP P51681
R	430	GLN	-	expression tag	UNP P51681
R	431	PHE	-	expression tag	UNP P51681
R	432	GLU	-	expression tag	UNP P51681
R	433	LYS	-	expression tag	UNP P51681
R	434	GLY	-	expression tag	UNP P51681
R	435	SER	-	expression tag	UNP P51681
R	436	GLY	-	expression tag	UNP P51681
R	437	ALA	-	expression tag	UNP P51681
R	438	GLY	-	expression tag	UNP P51681
R	439	ALA	-	expression tag	UNP P51681
R	440	SER	-	expression tag	UNP P51681
R	441	ALA	-	expression tag	UNP P51681
R	442	GLY	-	expression tag	UNP P51681
R	443	SER	-	expression tag	UNP P51681
R	444	TRP	-	expression tag	UNP P51681
R	445	SER	-	expression tag	UNP P51681
R	446	HIS	-	expression tag	UNP P51681
R	447	PRO	-	expression tag	UNP P51681
R	448	GLN	-	expression tag	UNP P51681
R	449	PHE	-	expression tag	UNP P51681
R	450	GLU	-	expression tag	UNP P51681
R	451	LYS	-	expression tag	UNP P51681
R	452	GLY	-	expression tag	UNP P51681
R	453	SER	-	expression tag	UNP P51681
R	454	ASP	-	expression tag	UNP P51681
R	455	TYR	-	expression tag	UNP P51681
R	456	LYS	-	expression tag	UNP P51681
R	457	ASP	-	expression tag	UNP P51681
R	458	ASP	-	expression tag	UNP P51681

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Chain	Residue	Modelled	Actual	Comment	Reference
R	459	ASP	-	expression tag	UNP P51681
R	460	ASP	-	expression tag	UNP P51681
R	461	LYS	-	expression tag	UNP P51681

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	216	Total	C	N	O	S	0	0
			1646	1058	285	291	12		

There are 5 discrepancies between the modelled and reference sequences:

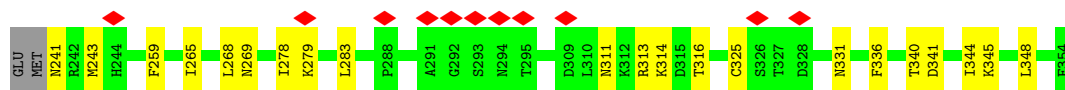
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	SER	engineered mutation	UNP P63096
A	202	THR	GLY	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

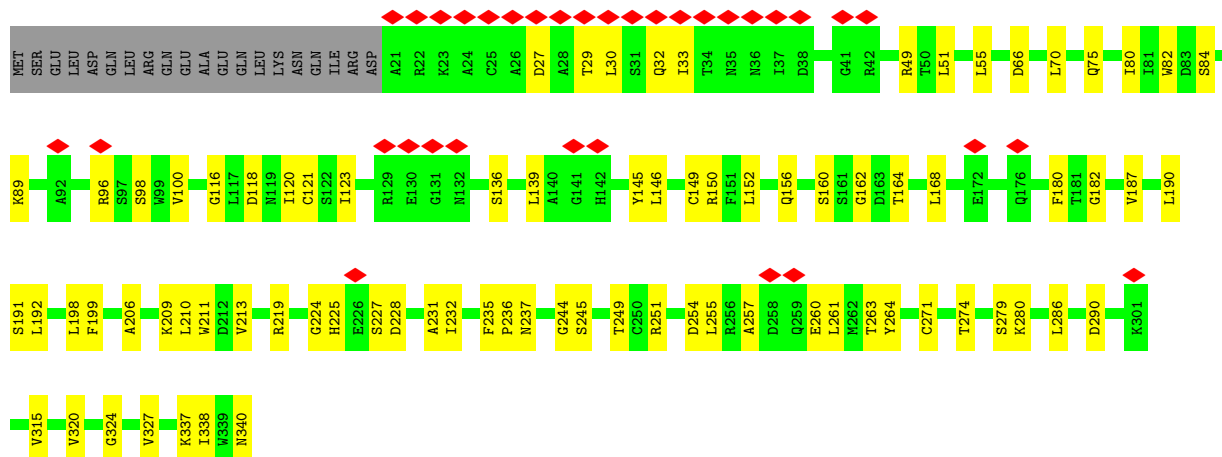
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	320	Total	C	N	O	S	0	0
			2370	1474	420	457	19		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

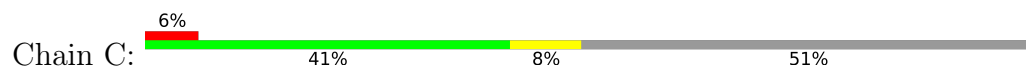
Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	35	Total	C	N	O	S	0	0
			243	155	38	48	2		



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7095732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.1875	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.229	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0293	Depositor
Map size (\AA)	267.52, 267.52, 267.52	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.045, 1.045, 1.045	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	R	0.25	0/2940	0.43	1/4013 (0.0%)
2	A	0.24	0/1674	0.38	0/2257
3	B	0.24	0/2416	0.45	0/3287
4	C	0.24	0/249	0.34	0/344
All	All	0.25	0/7279	0.42	1/9901 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	372	ASP	CB-CG-OD2	5.26	123.03	118.30

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	R	2864	0	2830	72	0
2	A	1646	0	1593	20	0
3	B	2370	0	2237	52	0
4	C	243	0	218	6	0
All	All	7123	0	6878	141	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 10.

The worst 5 of 141 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:A:184:ILE:HD12	2:A:201:VAL:HG12	1.67	0.77
3:B:249:THR:HA	3:B:264:TYR:O	1.86	0.76
1:R:135:LEU:HD12	1:R:136:VAL:N	2.02	0.75
1:R:353:LEU:HD23	1:R:360:PHE:CE2	2.20	0.74
1:R:175:PHE:HE2	1:R:383:MET:HG2	1.60	0.66

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	363/457 (79%)	352 (97%)	11 (3%)	0	100	100
2	A	210/354 (59%)	207 (99%)	3 (1%)	0	100	100
3	B	318/340 (94%)	309 (97%)	9 (3%)	0	100	100
4	C	33/71 (46%)	32 (97%)	1 (3%)	0	100	100
All	All	924/1222 (76%)	900 (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	306/397 (77%)	304 (99%)	2 (1%)	81	94
2	A	164/306 (54%)	163 (99%)	1 (1%)	84	95
3	B	244/283 (86%)	244 (100%)	0	100	100
4	C	23/58 (40%)	23 (100%)	0	100	100
All	All	737/1044 (71%)	734 (100%)	3 (0%)	88	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	60	LYS
1	R	359	PHE
2	A	279	LYS

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 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

There are no chain breaks in this entry.

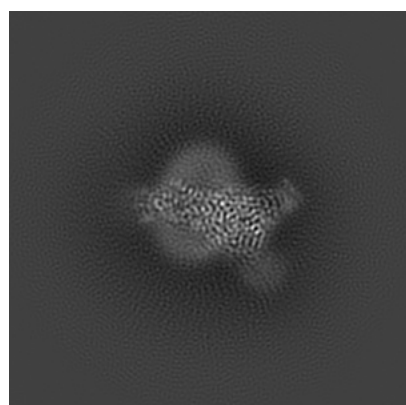
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31422. These allow visual inspection of the internal detail of the map and identification of artifacts.

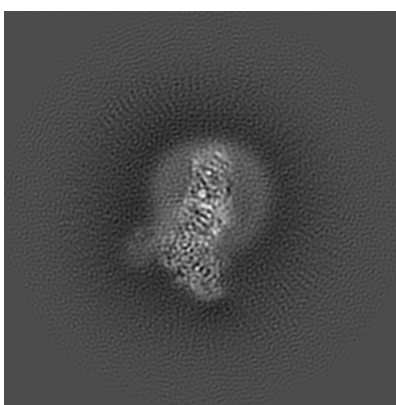
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

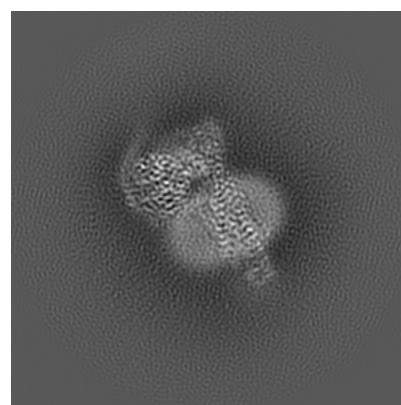
6.1.1 Primary map



X



Y

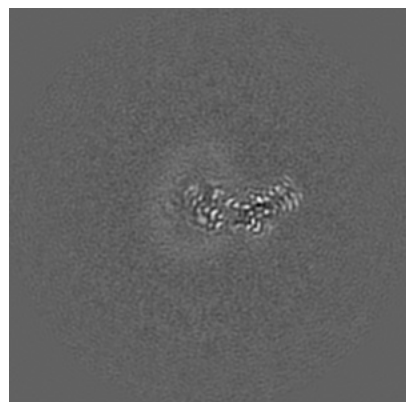


Z

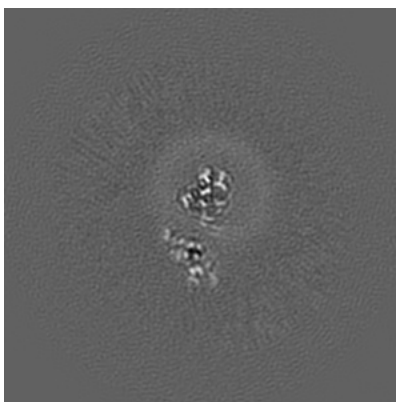
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

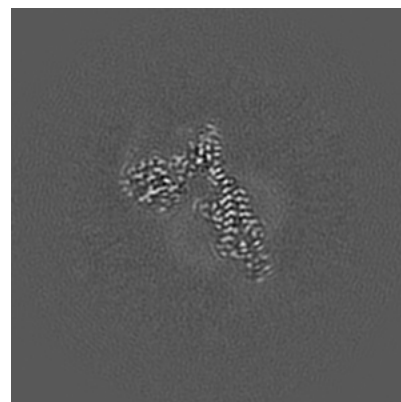
6.2.1 Primary map



X Index: 128



Y Index: 128

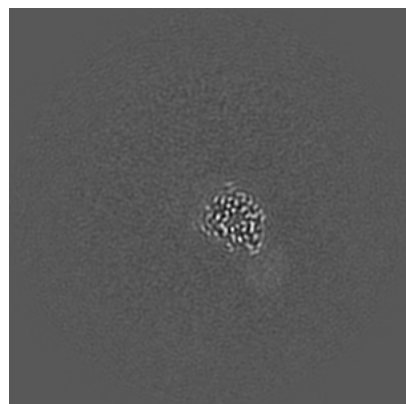


Z Index: 128

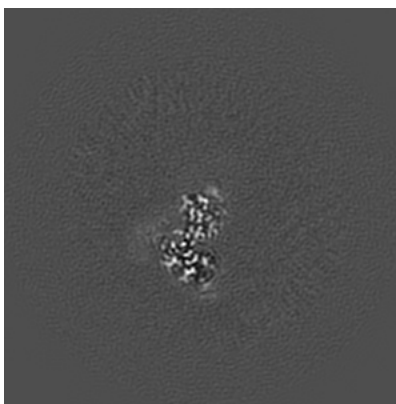
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

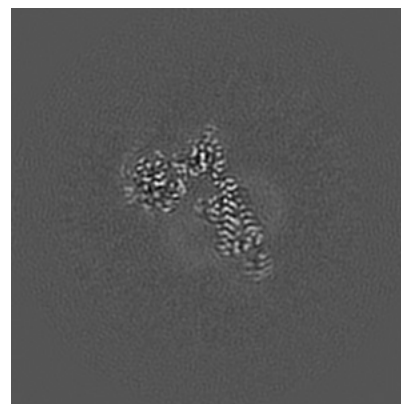
6.3.1 Primary map



X Index: 96



Y Index: 152

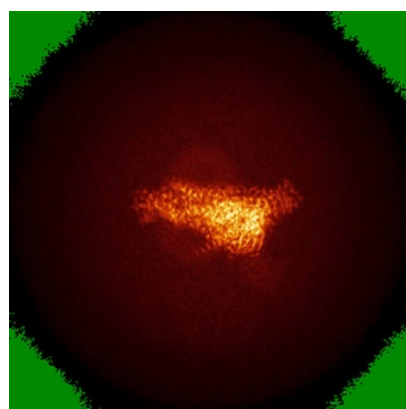


Z Index: 126

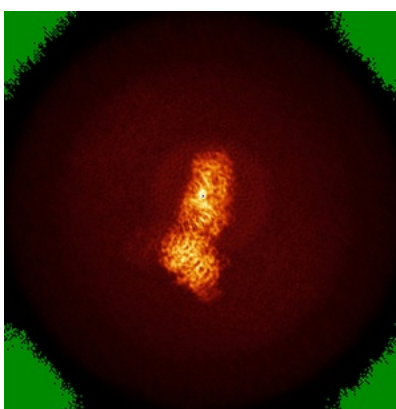
The images above show the largest variance slices of the map in three orthogonal directions.

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

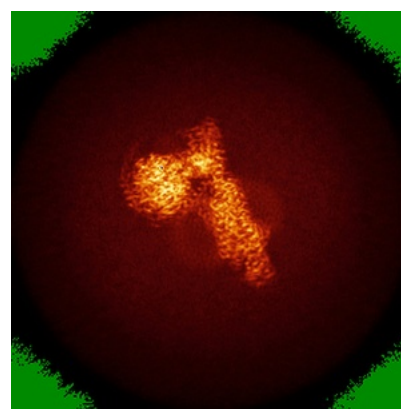
6.4.1 Primary map



X



Y

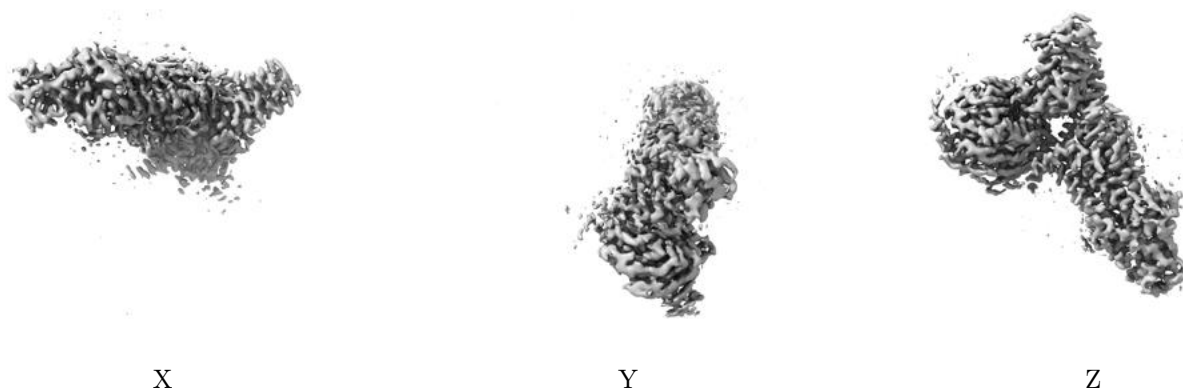


Z

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 0.0293. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

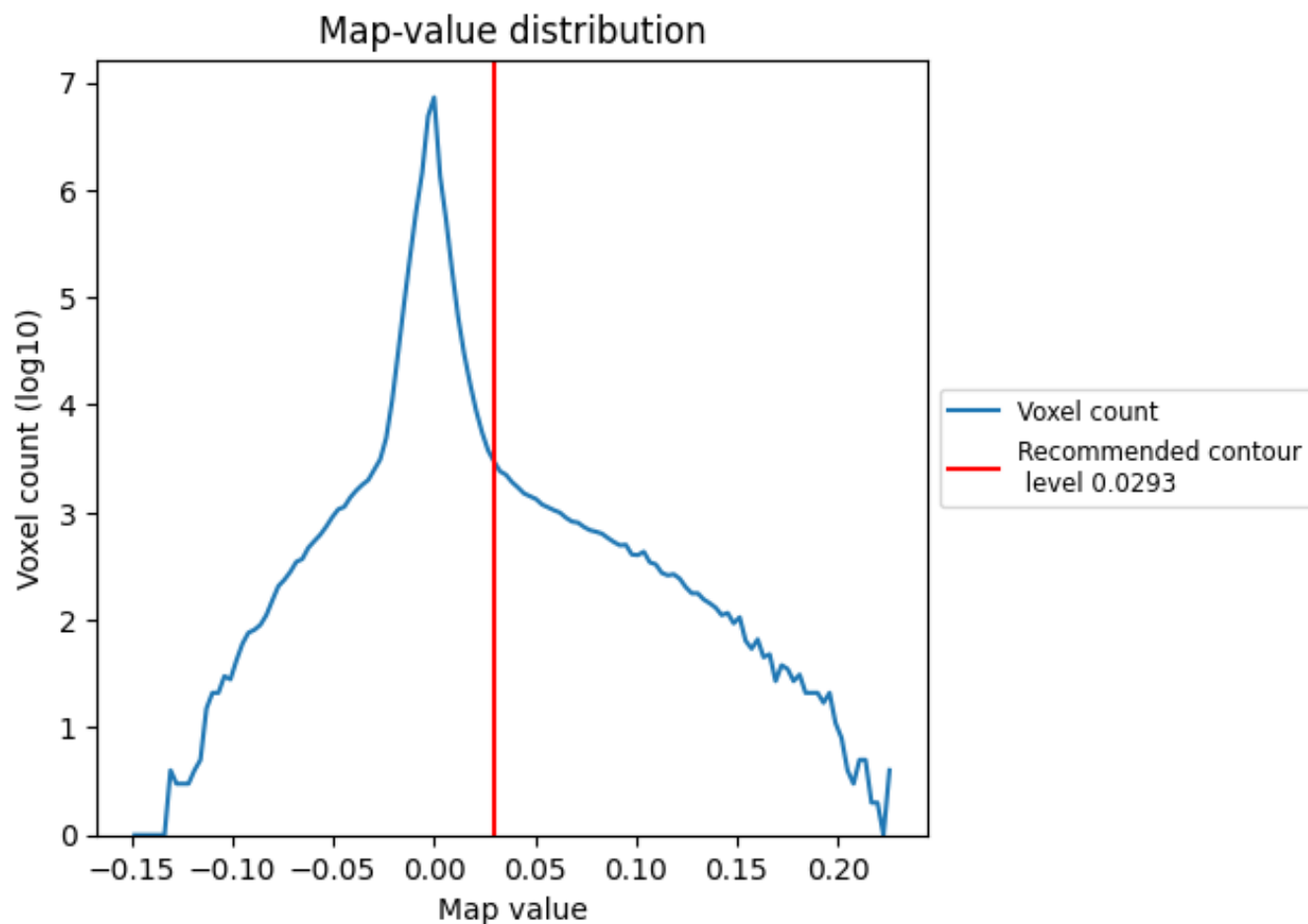
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

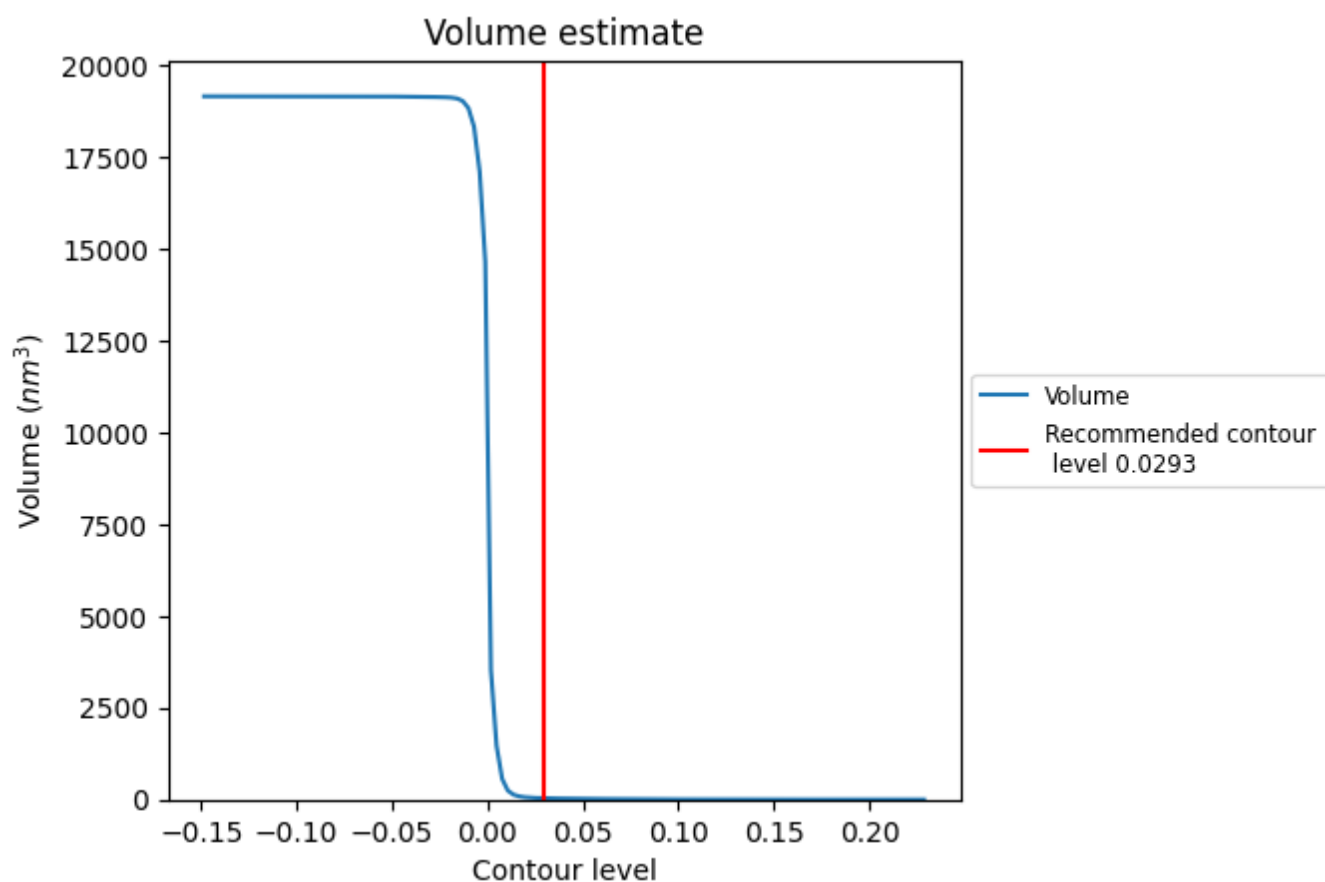
This section contains the results of statistical analysis of the map.

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.

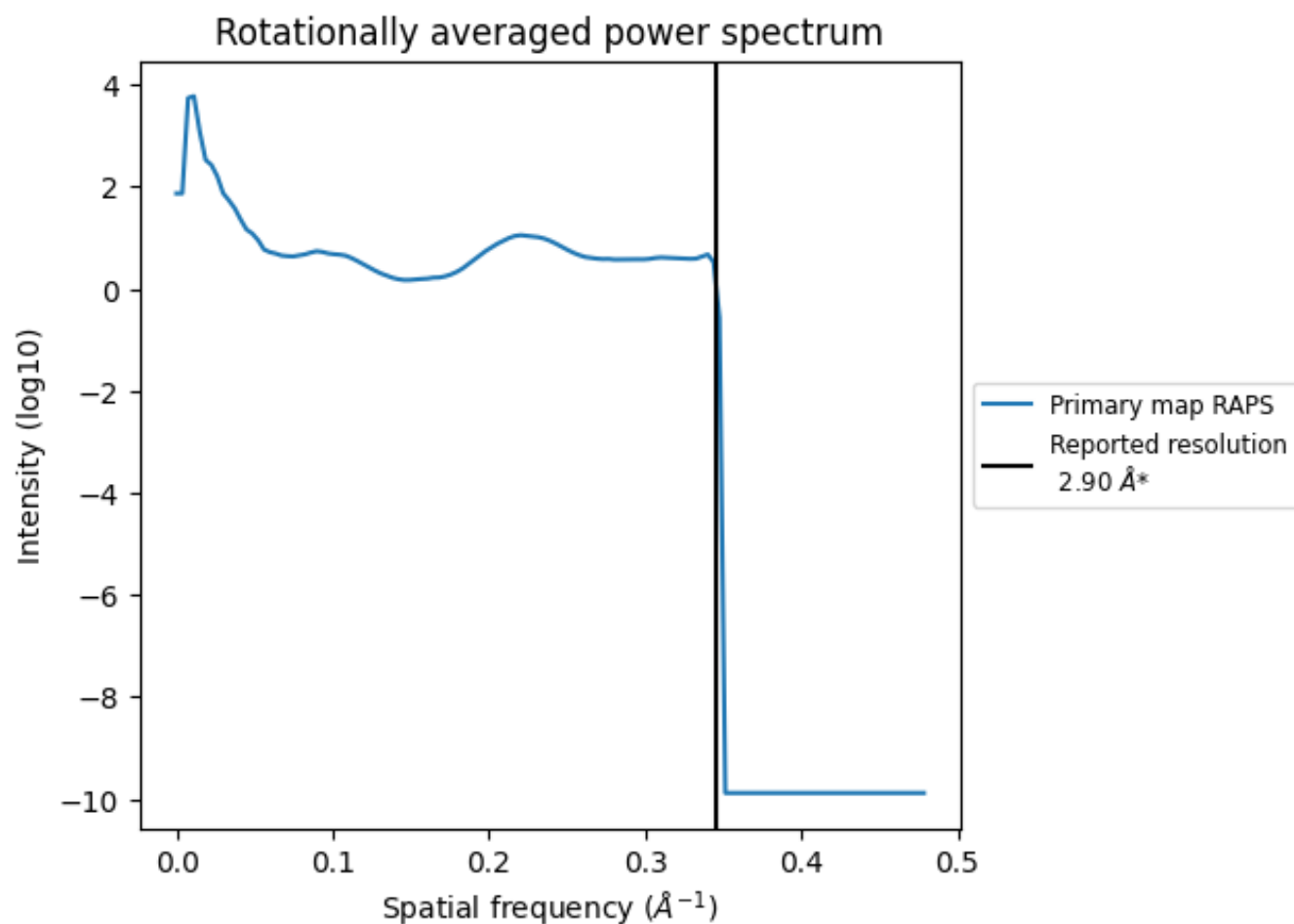
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 37 nm³; this corresponds to an approximate mass of 34 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 0.345 Å⁻¹

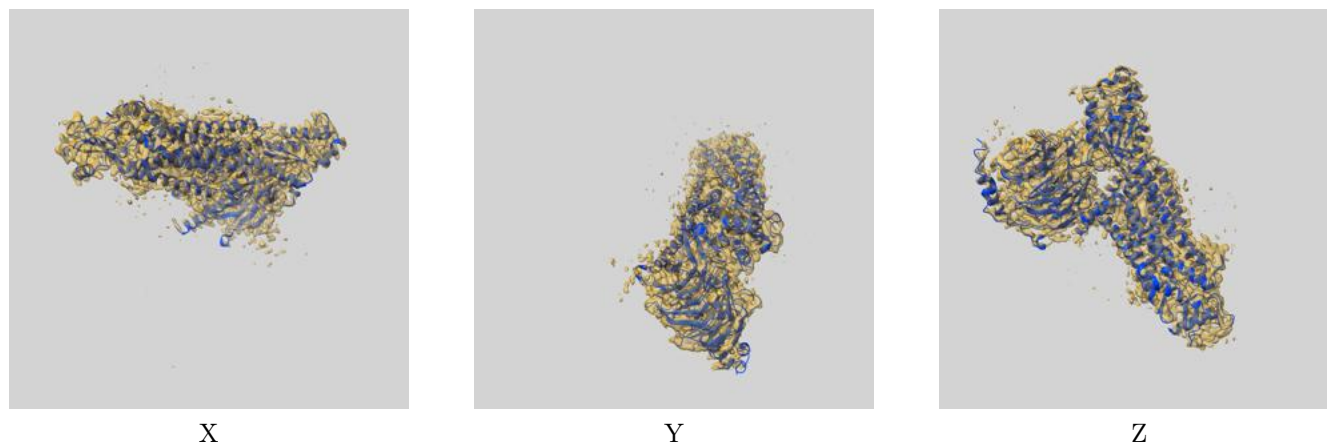
8 Fourier-Shell correlation

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-31422 and PDB model 7F1Q. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



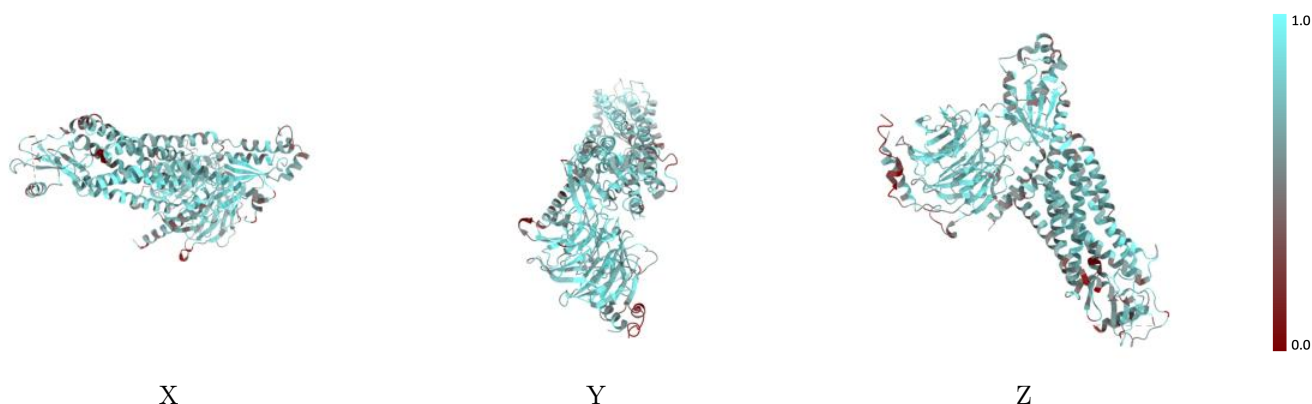
The images above show the 3D surface view of the map at the recommended contour level 0.0293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



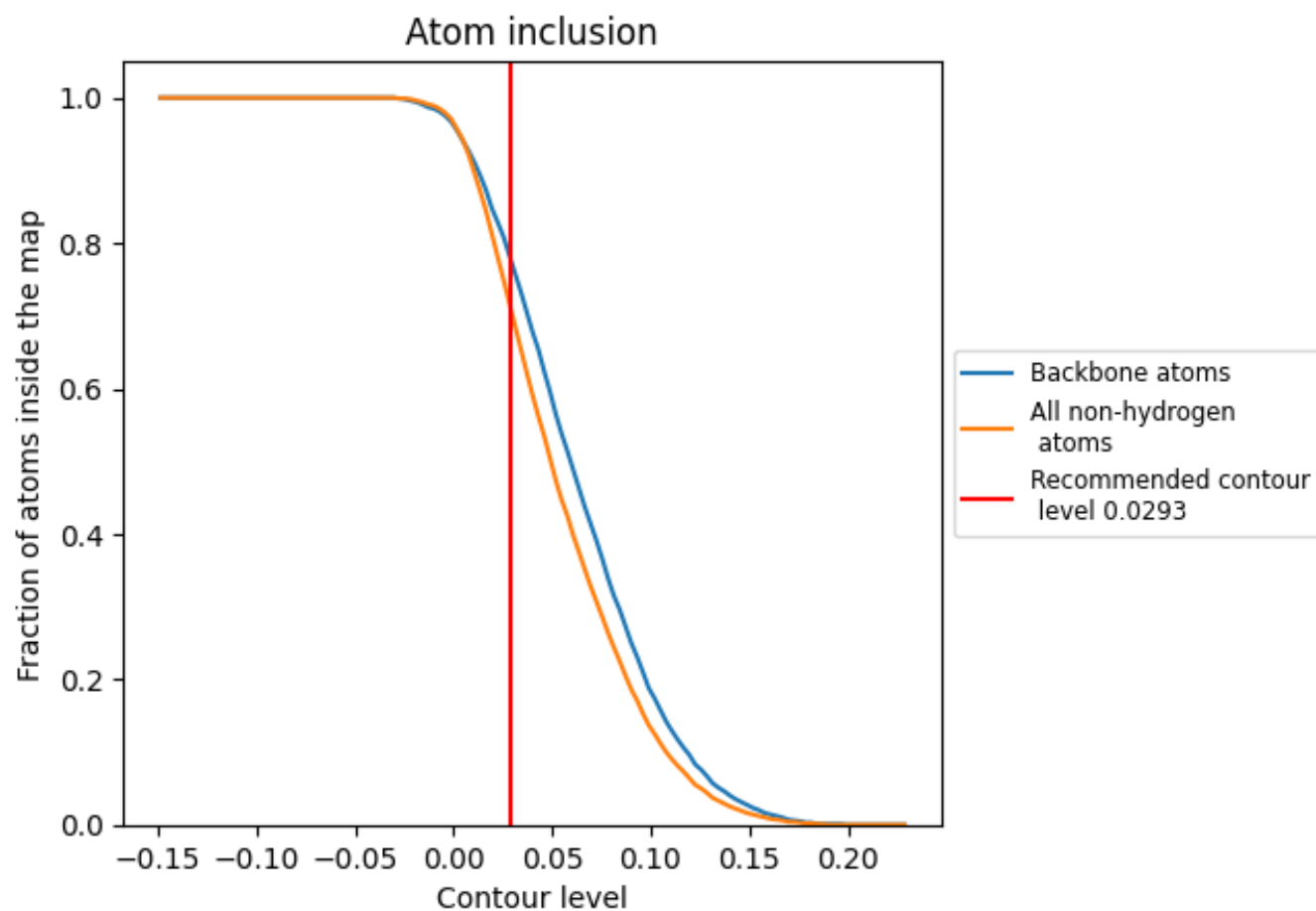
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0293).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.0293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7070	<div></div> 0.4800
A	<div></div> 0.7240	<div></div> 0.5070
B	<div></div> 0.7290	<div></div> 0.4800
C	<div></div> 0.6200	<div></div> 0.4410
R	<div></div> 0.6880	<div></div> 0.4680

