



wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 05:00 PM JST

PDB ID : 7V9L
EMDB ID : EMD-31824
Title : Cryo-EM structure of the SV1-Gs complex.
Authors : Cong, Z.T.; Zhou, F.L.; Zhang, C.; Zou, X.Y.; Zhang, H.B.; Wang, Y.Z.; Zhou, Q.T.; Cai, X.Q.; Liu, Q.F.; Li, J.; Shao, L.J.; Mao, C.Y.; Wang, X.; Wu, J.H.; Xia, T.; Zhao, L.H.; Jiang, H.L.; Zhang, Y.; Xu, H.E.; Cheng, X.; Yang, D.H.; Wang, M.W.
Deposited on : 2021-08-26
Resolution : 2.60 Å(reported)

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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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

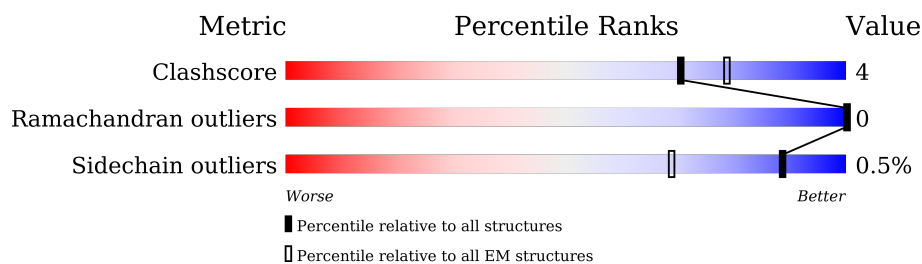
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





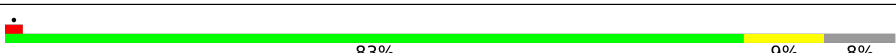
The reported resolution of this entry is 2.60 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	360	 60% 6% 34%
2	R	522	 5% 43% 6% 51%
3	Y	71	 11% 79% 18%
4	N	140	 79% 11% 10%
5	B	371	 83% 9% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8047 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	237	Total	C	N	O	S	0	0
			1964	1243	352	361	8		

- Molecule 2 is a protein called GHRH receptor splice variant 1,GHRH receptor splice variant 1,GHRH receptor splice variant 1,SV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	257	Total	C	N	O	S	0	0
			2064	1377	336	344	7		

- 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	Y	58	Total	C	N	O	S	0	0
			445	278	78	86	3		

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.


Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	341	Total	C	N	O	S	0	0
			2613	1611	470	511	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311


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

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

Chain Y:  11% 79% 18%


MET ALA SER ASN ASN T6 A7 S8 T9 A10 R13 K14 D26 D48 P60 E63 LYS LYS PHE PHE CYS ALA ILE LEU

- Molecule 4: Nanobody 35

Chain N:  79% 11% 10%

MET ALA Q1 V12 A24 F27 T28 F29 G42 V48 V64 R67 F68 R72 M83 L86 K87 P88 E89 D90 T91 Y117 V124 T125 V126 SER SER HIS HIS HIS HIS HIS HIS PRO GLU ALA

- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:  83% 9% 8%

MET GLY SER LEU GLN SER E3 L4 R8 Q9 R22 L30 L51 Y105 V112 I123 Y124 E130 G131 N132 V133 R134 V135 L139 D163 T164 T165 C166 W169 F180 D186 C204 D228 F234 D254 I255 R256 A257 D258 L261 M262

S281 L286 A302 G310 M325 A326 V327 L336 K337 S343 GLY GLY GLY SER SER SER VAL SER GLY TRP ARG LEU PHE LYS ILE SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	377241	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.785	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0644	Depositor
Map size (Å)	234.07999, 234.07999, 234.07999	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	A	0.29	0/2003	0.47	0/2697
2	R	0.29	0/2124	0.45	0/2896
3	Y	0.25	0/451	0.42	0/609
4	N	0.32	0/981	0.51	0/1329
5	B	0.30	0/2660	0.53	0/3606
All	All	0.29	0/8219	0.49	0/11137

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	1964	0	1948	11	0
2	R	2064	0	2096	19	0
3	Y	445	0	454	2	0
4	N	961	0	932	11	0
5	B	2613	0	2516	20	0
All	All	8047	0	7946	58	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 58 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:R:130:HIS:HB3	2:R:133:PHE:N	1.77	0.97
1:A:228:ARG:NH2	5:B:186:ASP:OD1	2.12	0.82
2:R:130:HIS:CB	2:R:133:PHE:N	2.47	0.77
5:B:22:ARG:NH1	5:B:258:ASP:O	2.28	0.65
4:N:117:TYR:OH	5:B:228:ASP:OD1	2.19	0.60

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	233/360 (65%)	224 (96%)	9 (4%)	0	100	100
2	R	251/522 (48%)	242 (96%)	9 (4%)	0	100	100
3	Y	56/71 (79%)	56 (100%)	0	0	100	100
4	N	124/140 (89%)	117 (94%)	7 (6%)	0	100	100
5	B	339/371 (91%)	326 (96%)	13 (4%)	0	100	100
All	All	1003/1464 (68%)	965 (96%)	38 (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	214/314 (68%)	212 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	224/444 (50%)	224 (100%)	0	100	100
3	Y	47/58 (81%)	47 (100%)	0	100	100
4	N	104/116 (90%)	104 (100%)	0	100	100
5	B	282/302 (93%)	280 (99%)	2 (1%)	84	94
All	All	871/1234 (71%)	867 (100%)	4 (0%)	89	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	HIS
1	A	280	ARG
5	B	105	TYR
5	B	234	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	239	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

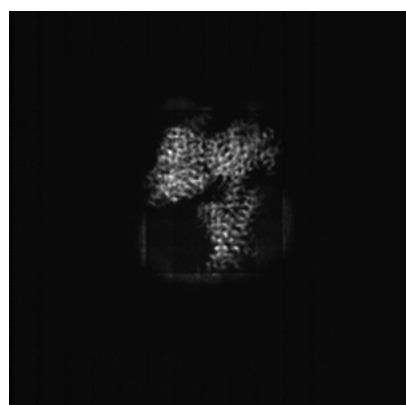
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31824. These allow visual inspection of the internal detail of the map and identification of artifacts.

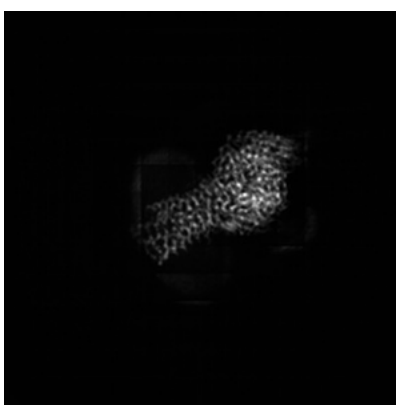
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

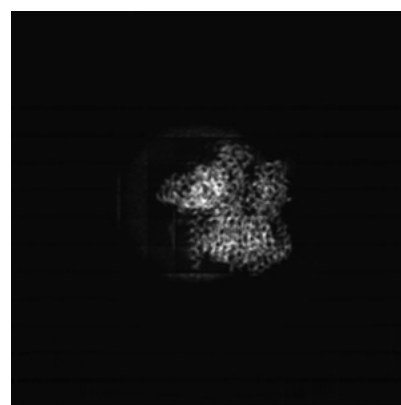
6.1.1 Primary map



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: 112



Y Index: 112

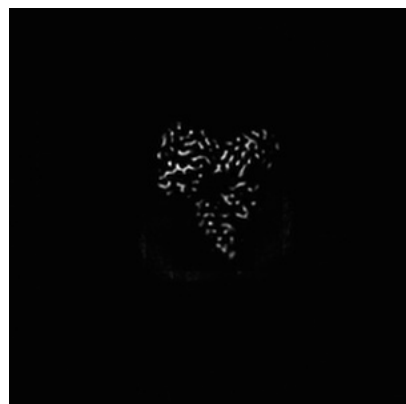


Z Index: 112

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: 116



Y Index: 117



Z Index: 140

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

6.4 Orthogonal surface views [i](#)

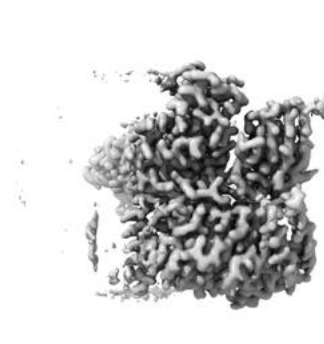
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0644. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

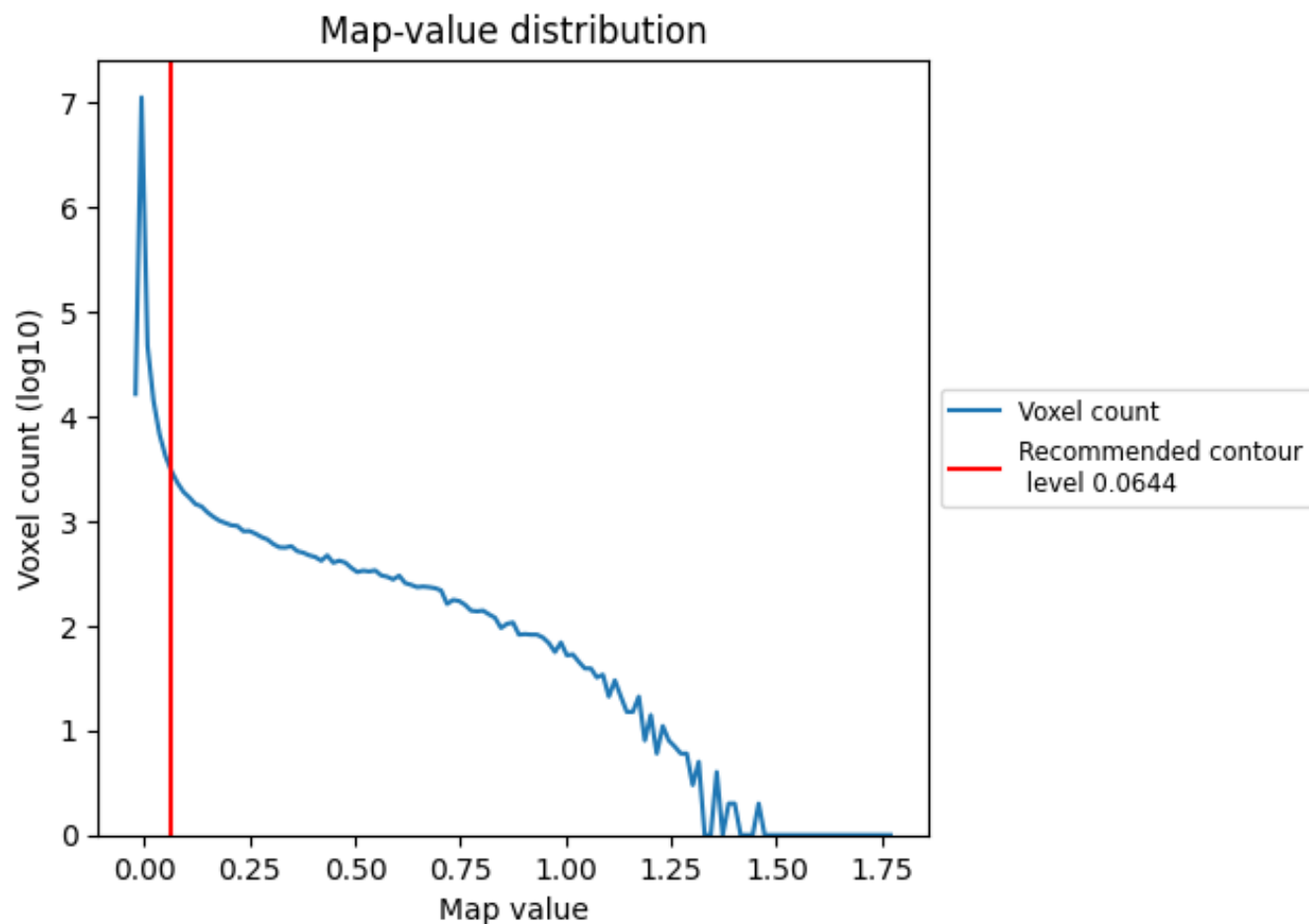
6.5 Mask visualisation

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

7 Map analysis [i](#)

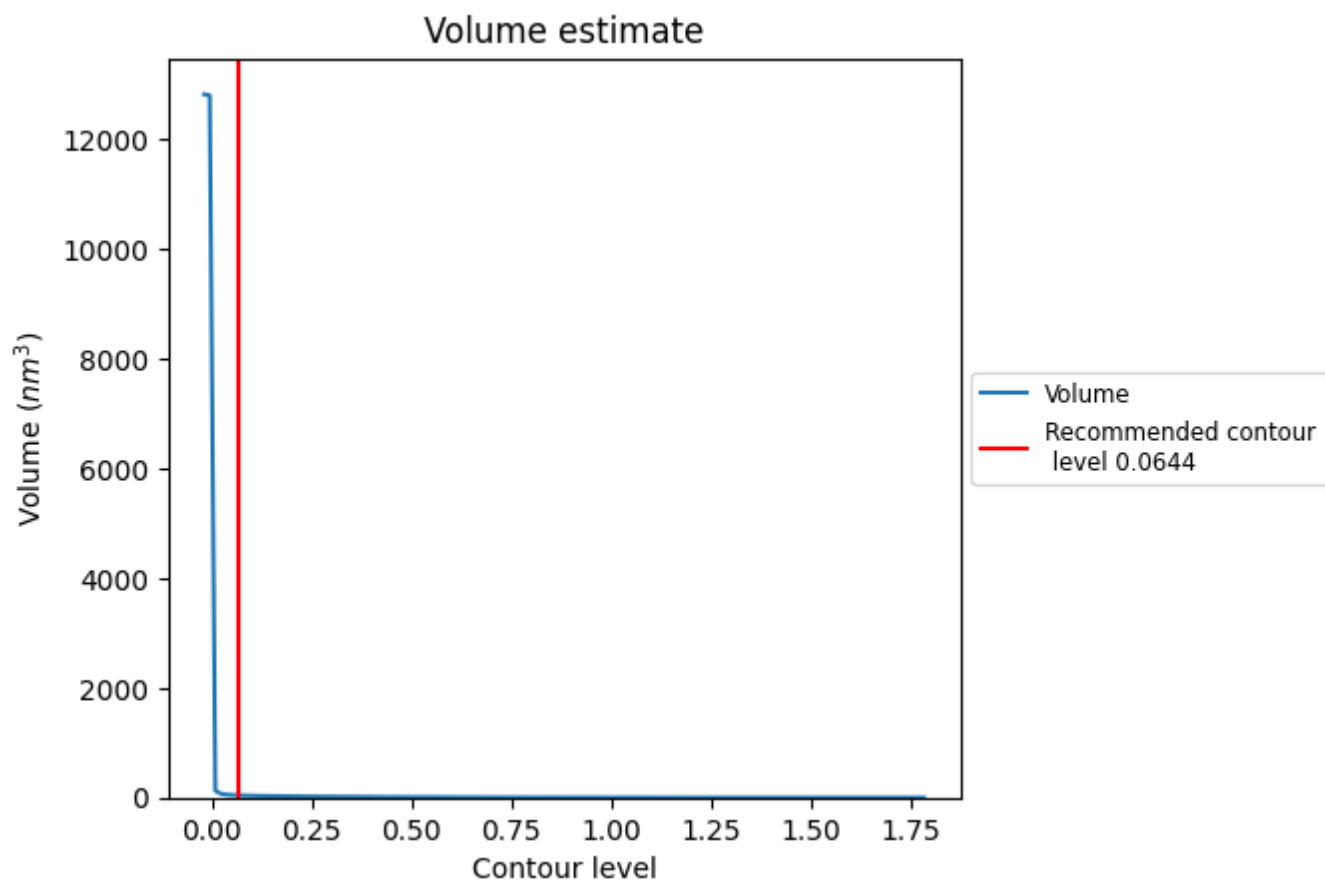
This section contains the results of statistical analysis of the map.

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.

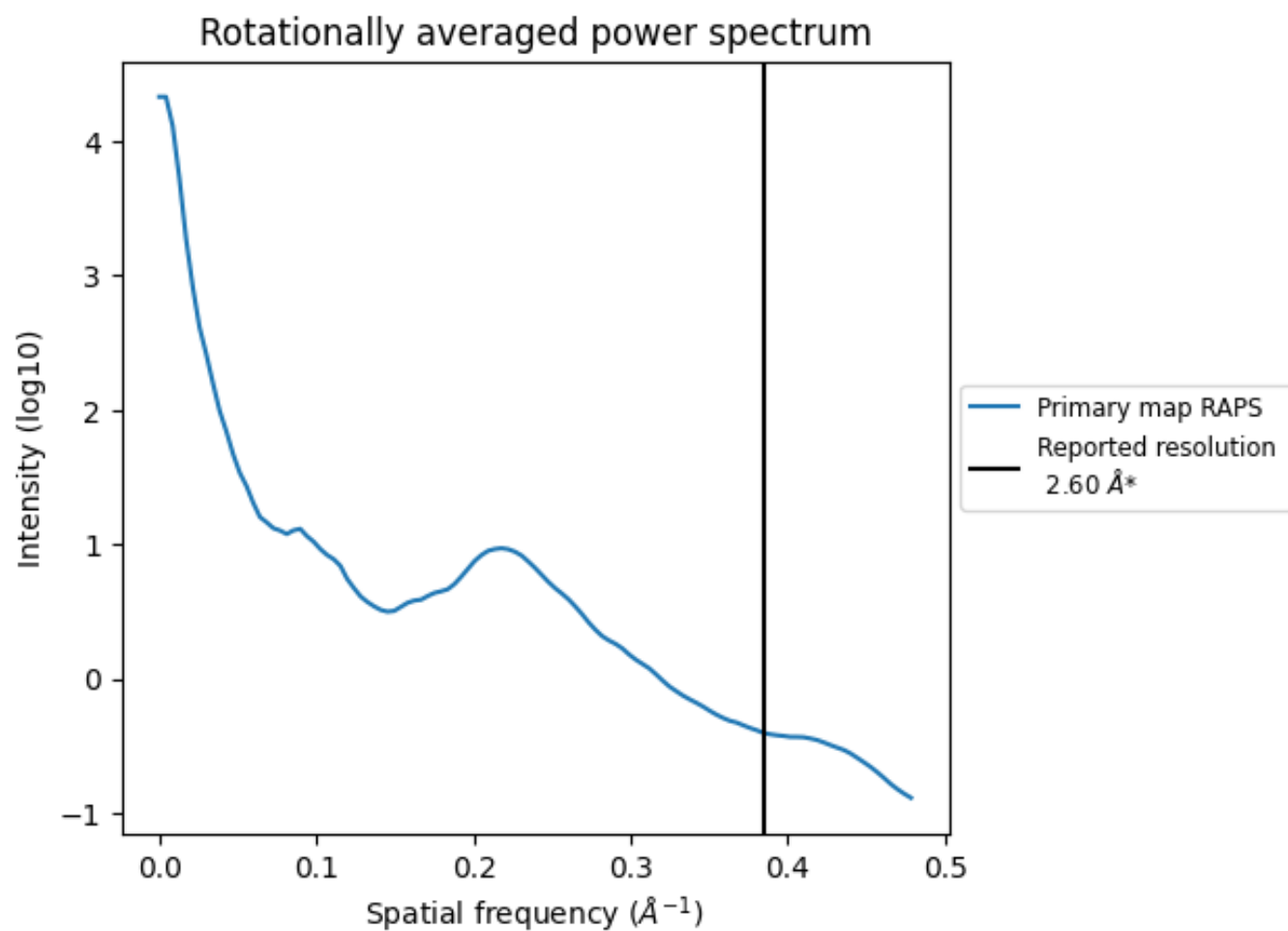
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 0.385 Å⁻¹

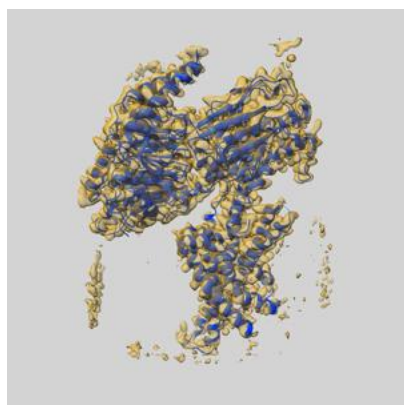
8 Fourier-Shell correlation ⓘ

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

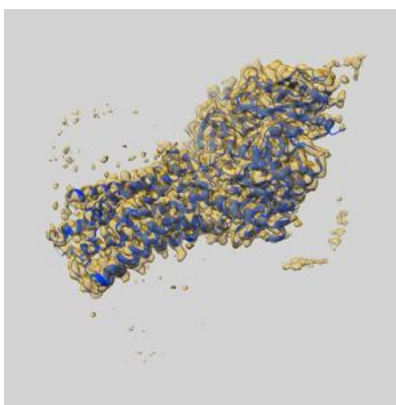
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31824 and PDB model 7V9L. Per-residue inclusion information can be found in section [3](#) on page [5](#).

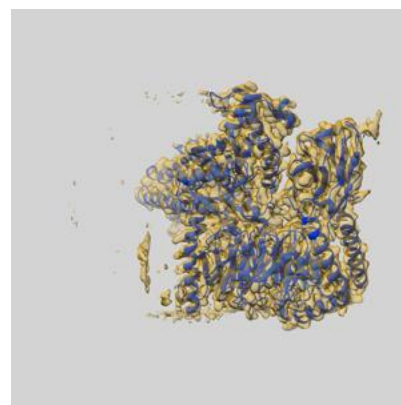
9.1 Map-model overlay [i](#)



X



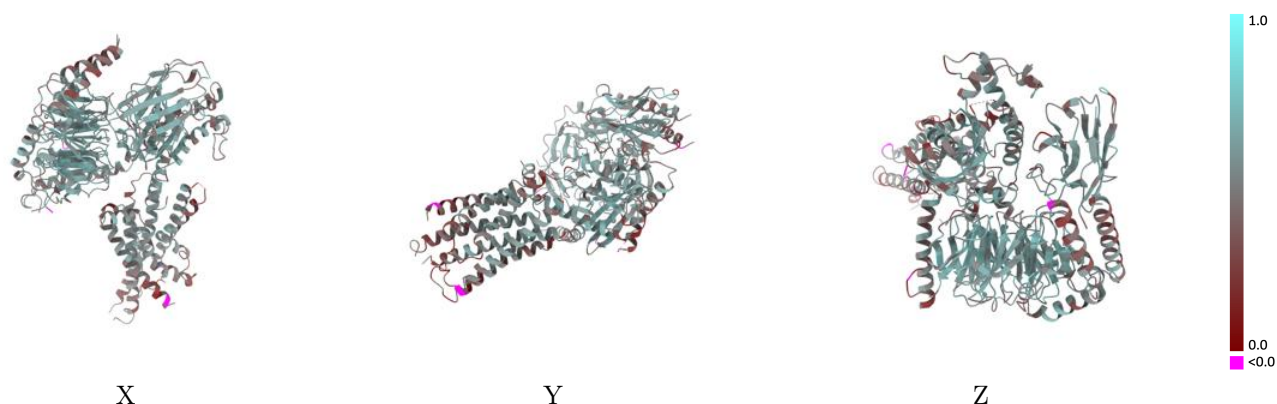
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0644 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](#)



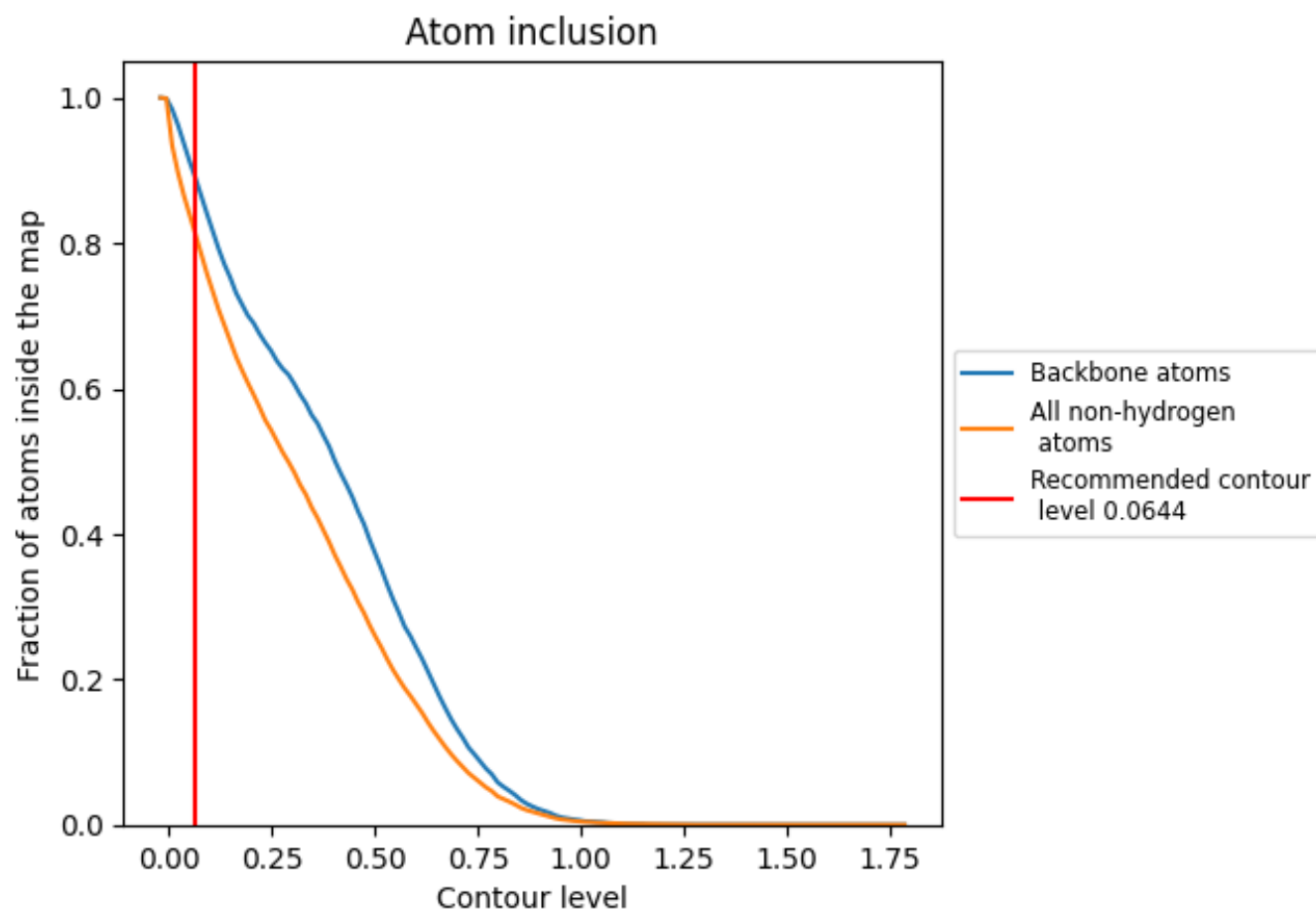
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0644).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.0644) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8112	<div></div> 0.5050
A	<div></div> 0.8110	<div></div> 0.5130
B	<div></div> 0.8719	<div></div> 0.5560
N	<div></div> 0.8412	<div></div> 0.5320
R	<div></div> 0.7427	<div></div> 0.4310
Y	<div></div> 0.7100	<div></div> 0.4610

