



wwPDB EM Validation Summary Report ⓘ

Jun 16, 2025 – 11:13 PM JST

PDB ID : 7CA5 / pdb_00007ca5
EMDB ID : EMD-30324
Title : Cryo-EM structure of human GABA(B) receptor in apo state
Authors : Kim, Y.; Jeong, E.; Jeong, J.; Kim, Y.; Cho, Y.
Deposited on : 2020-06-08
Resolution : 7.60 Å(reported)

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

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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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

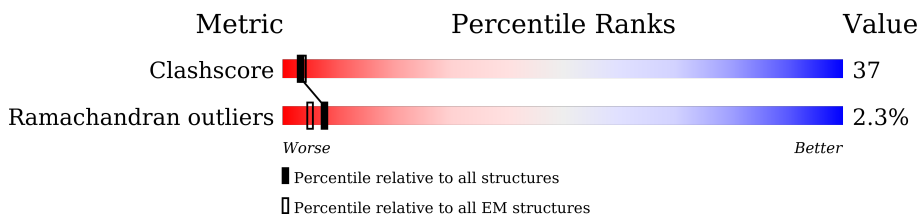
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

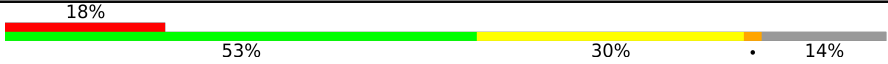

The reported resolution of this entry is 7.60 Å.

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

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	771	
2	B	822	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6484 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	660	Total	C	N	O	0	0
			3257	1937	660	660		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q9UBS5
A	140	ARG	-	expression tag	UNP Q9UBS5
A	141	LEU	-	expression tag	UNP Q9UBS5
A	142	LEU	-	expression tag	UNP Q9UBS5
A	143	THR	-	expression tag	UNP Q9UBS5
A	144	ALA	-	expression tag	UNP Q9UBS5
A	145	LEU	-	expression tag	UNP Q9UBS5
A	146	PHE	-	expression tag	UNP Q9UBS5
A	147	ALA	-	expression tag	UNP Q9UBS5
A	148	TYR	-	expression tag	UNP Q9UBS5
A	149	PHE	-	expression tag	UNP Q9UBS5
A	150	ILE	-	expression tag	UNP Q9UBS5
A	151	VAL	-	expression tag	UNP Q9UBS5
A	152	ALA	-	expression tag	UNP Q9UBS5
A	153	LEU	-	expression tag	UNP Q9UBS5
A	154	ILE	-	expression tag	UNP Q9UBS5
A	155	LEU	-	expression tag	UNP Q9UBS5
A	156	ALA	-	expression tag	UNP Q9UBS5
A	157	PHE	-	expression tag	UNP Q9UBS5
A	158	SER	-	expression tag	UNP Q9UBS5
A	159	VAL	-	expression tag	UNP Q9UBS5
A	160	SER	-	expression tag	UNP Q9UBS5
A	161	ALA	-	expression tag	UNP Q9UBS5
A	162	LYS	-	expression tag	UNP Q9UBS5
A	163	SER	-	expression tag	UNP Q9UBS5
A	164	MET	-	expression tag	UNP Q9UBS5
A	901	SER	-	expression tag	UNP Q9UBS5
A	902	GLY	-	expression tag	UNP Q9UBS5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	903	ARG	-	expression tag	UNP Q9UBS5
A	904	LEU	-	expression tag	UNP Q9UBS5
A	905	GLU	-	expression tag	UNP Q9UBS5
A	906	VAL	-	expression tag	UNP Q9UBS5
A	907	LEU	-	expression tag	UNP Q9UBS5
A	908	PHE	-	expression tag	UNP Q9UBS5
A	909	GLN	-	expression tag	UNP Q9UBS5

- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	655	Total	C	N	O	0	0
			3227	1917	655	655		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	788	SER	-	expression tag	UNP O75899
B	789	GLY	-	expression tag	UNP O75899
B	790	ARG	-	expression tag	UNP O75899
B	791	GLY	-	expression tag	UNP O75899
B	792	GLY	-	expression tag	UNP O75899
B	793	SER	-	expression tag	UNP O75899
B	794	GLU	-	expression tag	UNP O75899
B	795	ASN	-	expression tag	UNP O75899
B	796	LEU	-	expression tag	UNP O75899
B	797	TYR	-	expression tag	UNP O75899
B	798	PHE	-	expression tag	UNP O75899
B	799	GLN	-	expression tag	UNP O75899
B	800	GLY	-	expression tag	UNP O75899
B	801	GLY	-	expression tag	UNP O75899
B	802	SER	-	expression tag	UNP O75899
B	803	GLY	-	expression tag	UNP O75899
B	804	SER	-	expression tag	UNP O75899
B	805	GLY	-	expression tag	UNP O75899
B	806	GLY	-	expression tag	UNP O75899
B	807	ASP	-	expression tag	UNP O75899
B	808	TYR	-	expression tag	UNP O75899
B	809	LYS	-	expression tag	UNP O75899
B	810	ASP	-	expression tag	UNP O75899
B	811	ASP	-	expression tag	UNP O75899
B	812	ASP	-	expression tag	UNP O75899

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Chain	Residue	Modelled	Actual	Comment	Reference
B	813	ASP	-	expression tag	UNP O75899
B	814	LYS	-	expression tag	UNP O75899
B	815	ASP	-	expression tag	UNP O75899
B	816	TYR	-	expression tag	UNP O75899
B	817	LYS	-	expression tag	UNP O75899
B	818	ASP	-	expression tag	UNP O75899
B	819	ASP	-	expression tag	UNP O75899
B	820	ASP	-	expression tag	UNP O75899
B	821	ASP	-	expression tag	UNP O75899
B	822	LYS	-	expression tag	UNP O75899

GLU	ASN	LEU	TYR	PHE	GLN	GLY	GLY	SER	SER	GLY	GLY	ASP	TYR	LYS	ASP	ASP	ASP	LYS	ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187029	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.545, 46.545, 46.545	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.52	1/3252 (0.0%)	0.92	28/4519 (0.6%)
2	B	0.49	0/3219	0.87	24/4465 (0.5%)
All	All	0.50	1/6471 (0.0%)	0.89	52/8984 (0.6%)

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
2	B	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	MET	CA-CB	-5.66	1.44	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	PRO	N-CA-CB	11.77	110.70	102.81
1	A	183	PRO	N-CA-CB	10.61	109.79	102.79
2	B	463	PRO	N-CA-CB	8.37	111.20	103.08
1	A	733	PRO	N-CA-CB	8.22	111.88	103.25
1	A	571	GLY	N-CA-C	-7.85	104.92	115.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	SER	Peptide
2	B	161	PRO	Peptide
2	B	285	TYR	Peptide
2	B	349	VAL	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	3257	0	1469	187	0
2	B	3227	0	1434	158	0
All	All	6484	0	2903	345	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 37.

The worst 5 of 345 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:472:GLU:CB	2:B:642:ARG:CA	1.93	1.45
1:A:657:ASN:O	1:A:661:PHE:CB	1.78	1.29
2:B:60:GLY:O	2:B:103:LEU:HA	1.48	1.12
2:B:472:GLU:CB	2:B:643:PRO:N	2.20	1.05
1:A:310:ALA:HB3	1:A:361:ILE:O	1.60	1.02

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	650/771 (84%)	488 (75%)	144 (22%)	18 (3%)	4	24
2	B	639/822 (78%)	470 (74%)	157 (25%)	12 (2%)	6	32
All	All	1289/1593 (81%)	958 (74%)	301 (23%)	30 (2%)	7	28

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	A	244	PRO
1	A	280	PHE
1	A	288	PRO
1	A	652	TYR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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-30324. These allow visual inspection of the internal detail of the map and identification of artifacts.

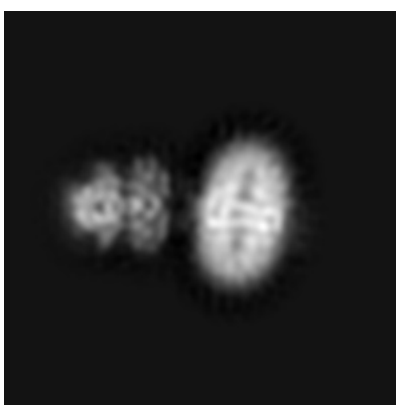
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

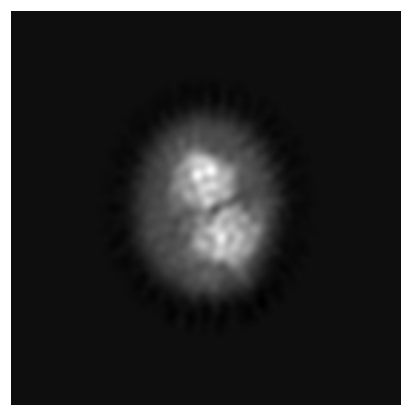
6.1.1 Primary map



X



Y



Z

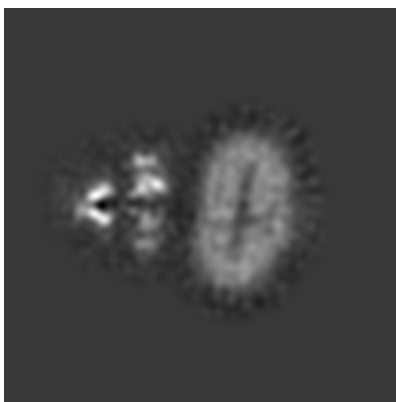
The images above show the map projected in three orthogonal directions.

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](#)

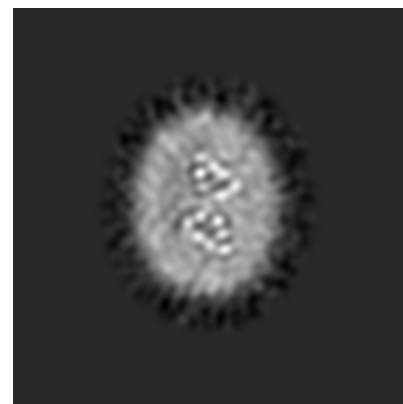
6.3.1 Primary map



X Index: 128



Y Index: 114



Z Index: 142

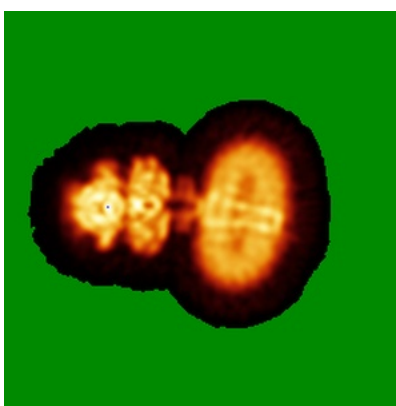
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

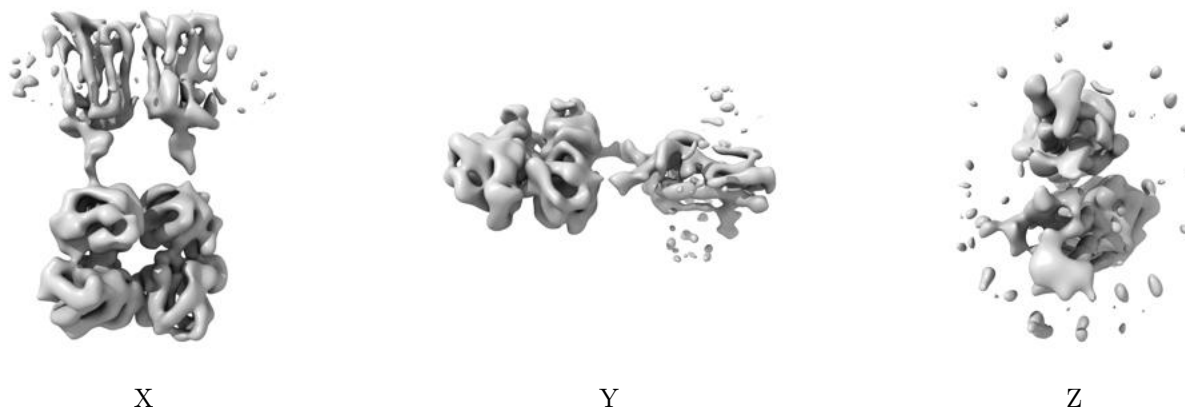


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

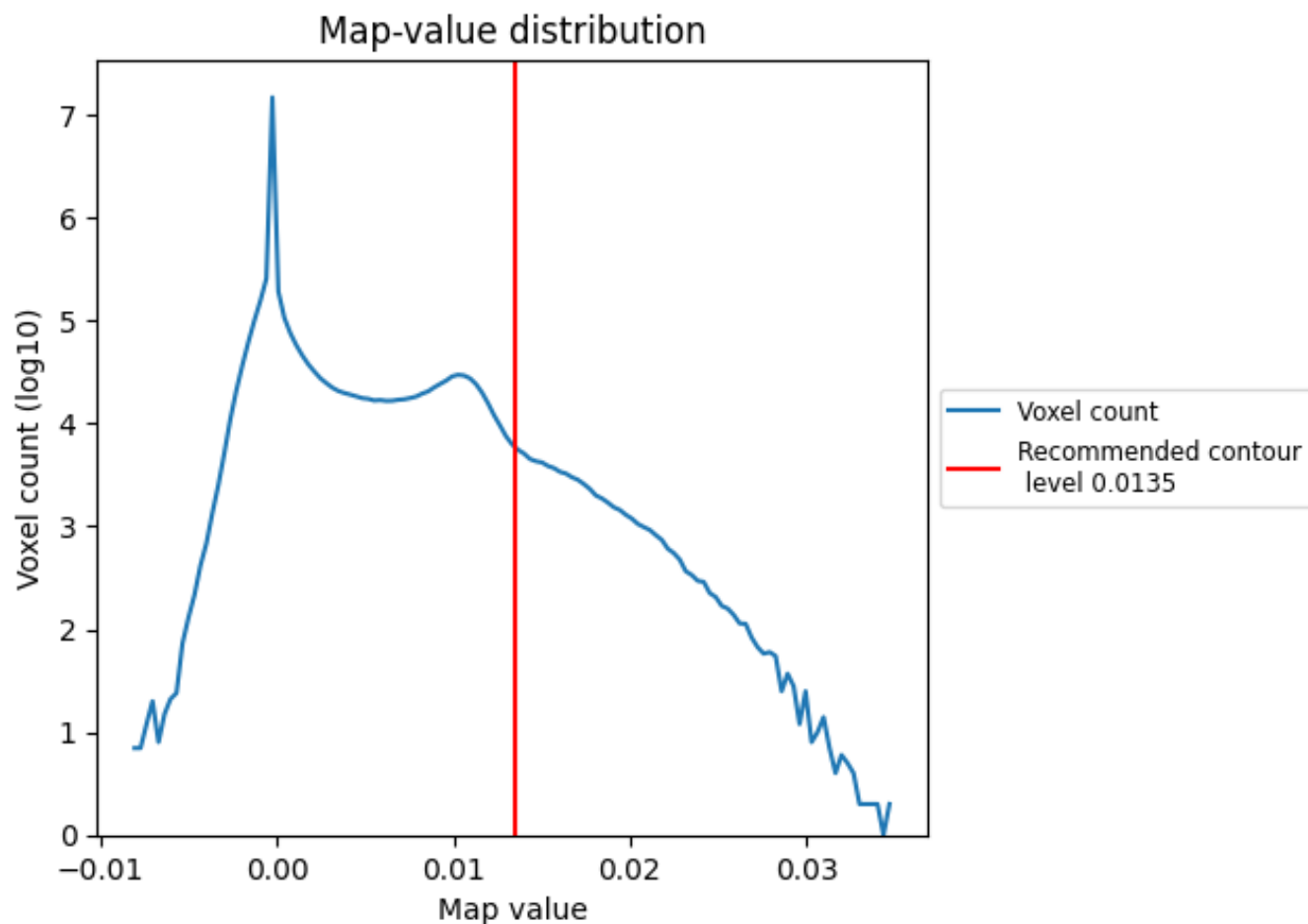
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

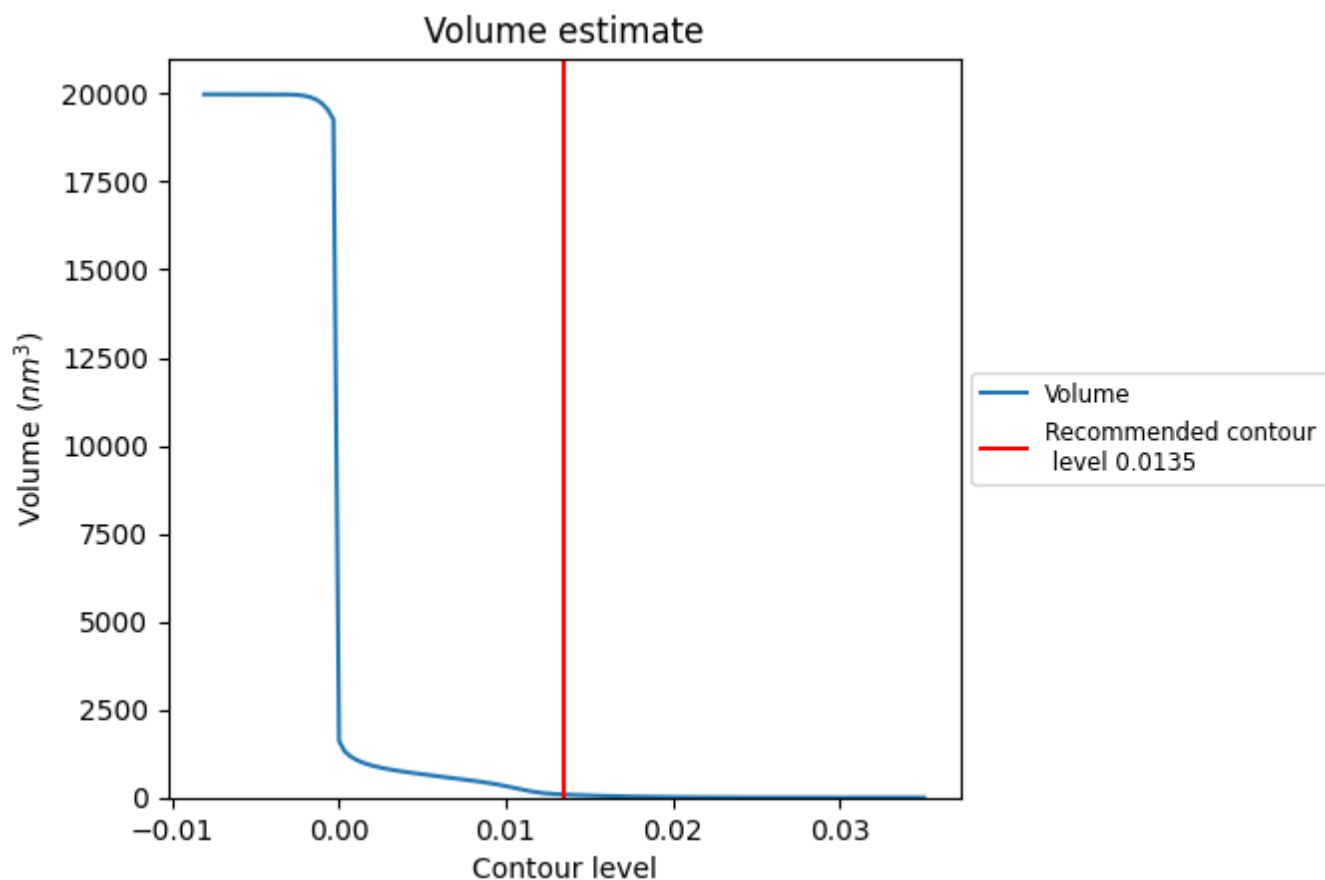
This section contains the results of statistical analysis of the map.

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.

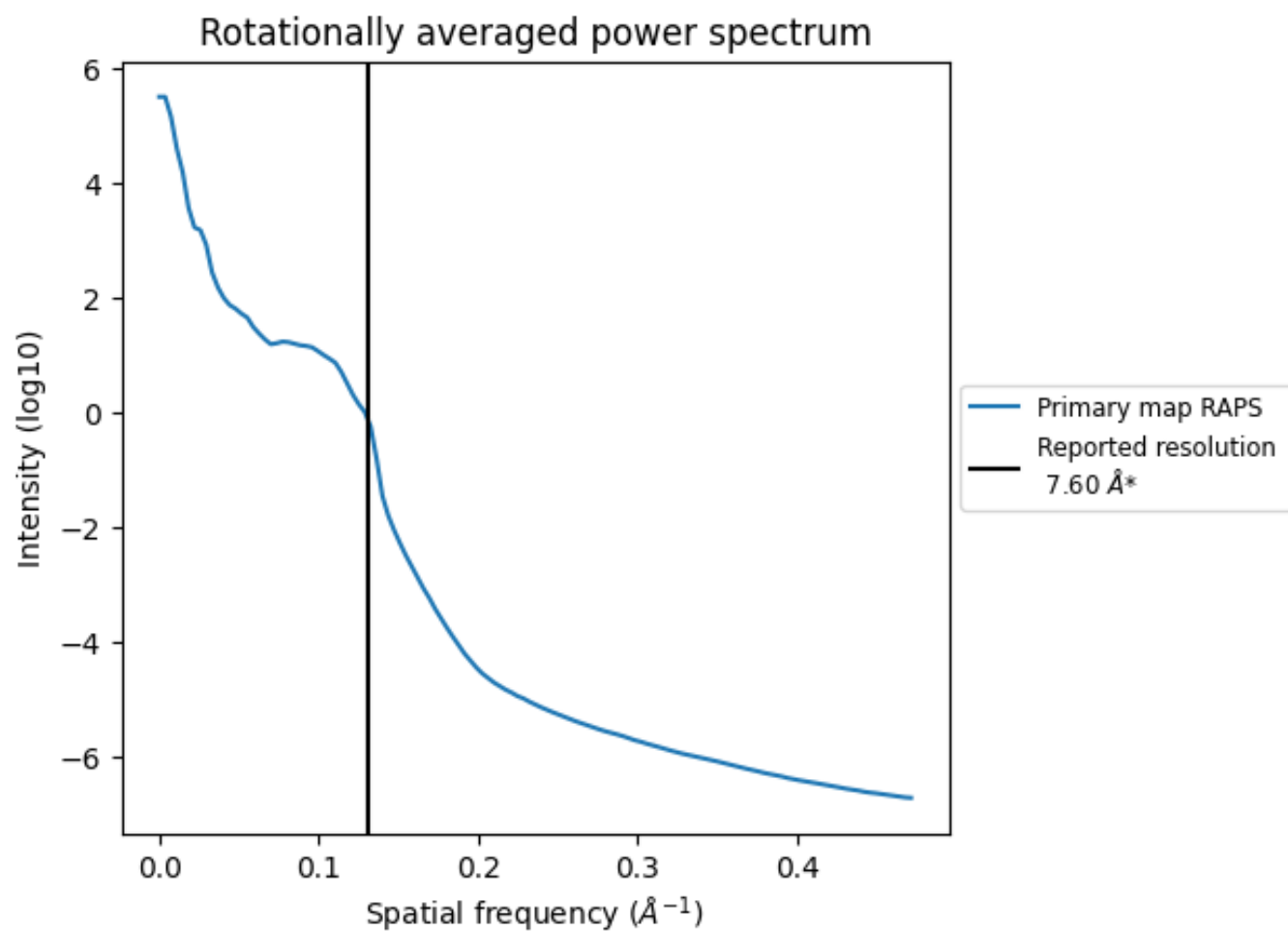
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; 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 0.132 Å⁻¹

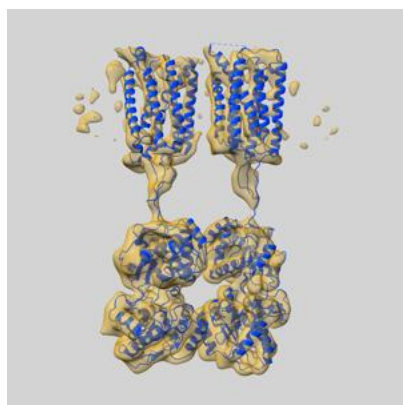
8 Fourier-Shell correlation ⓘ

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

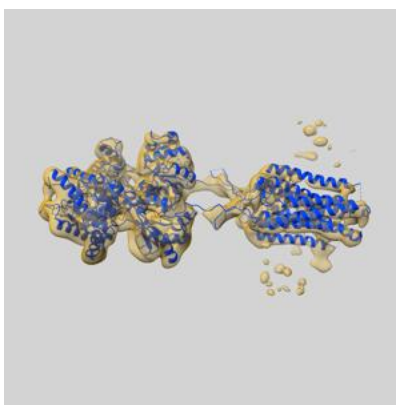
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30324 and PDB model 7CA5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

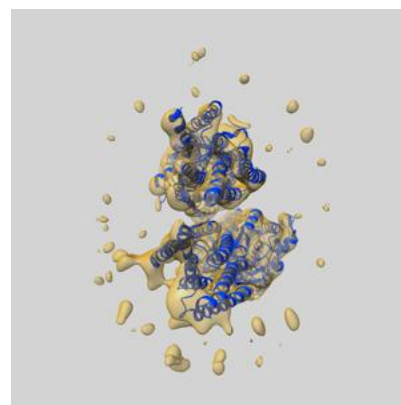
9.1 Map-model overlay [i](#)



X



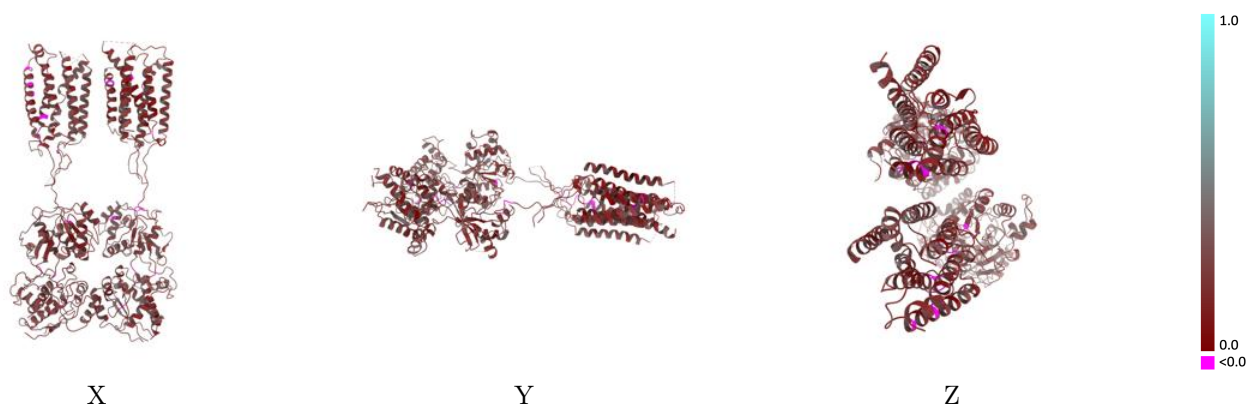
Y



Z

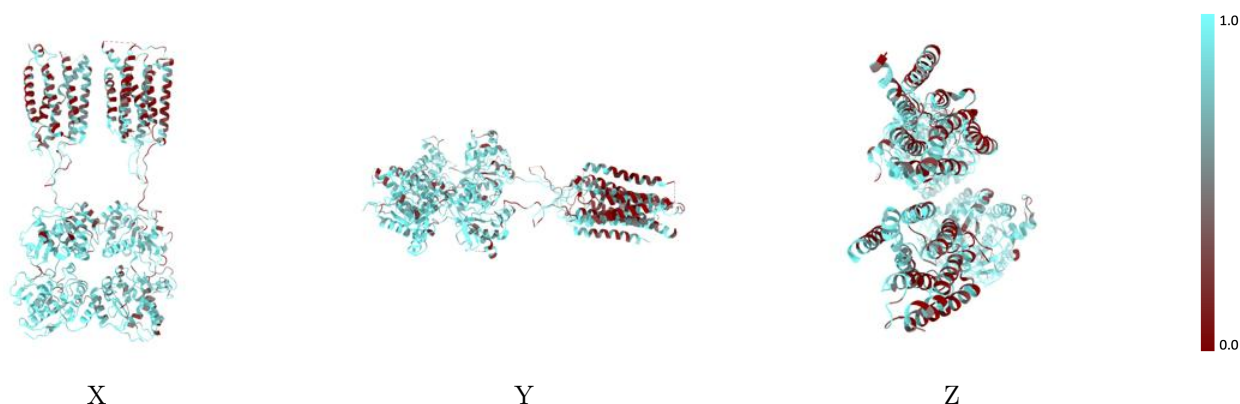
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



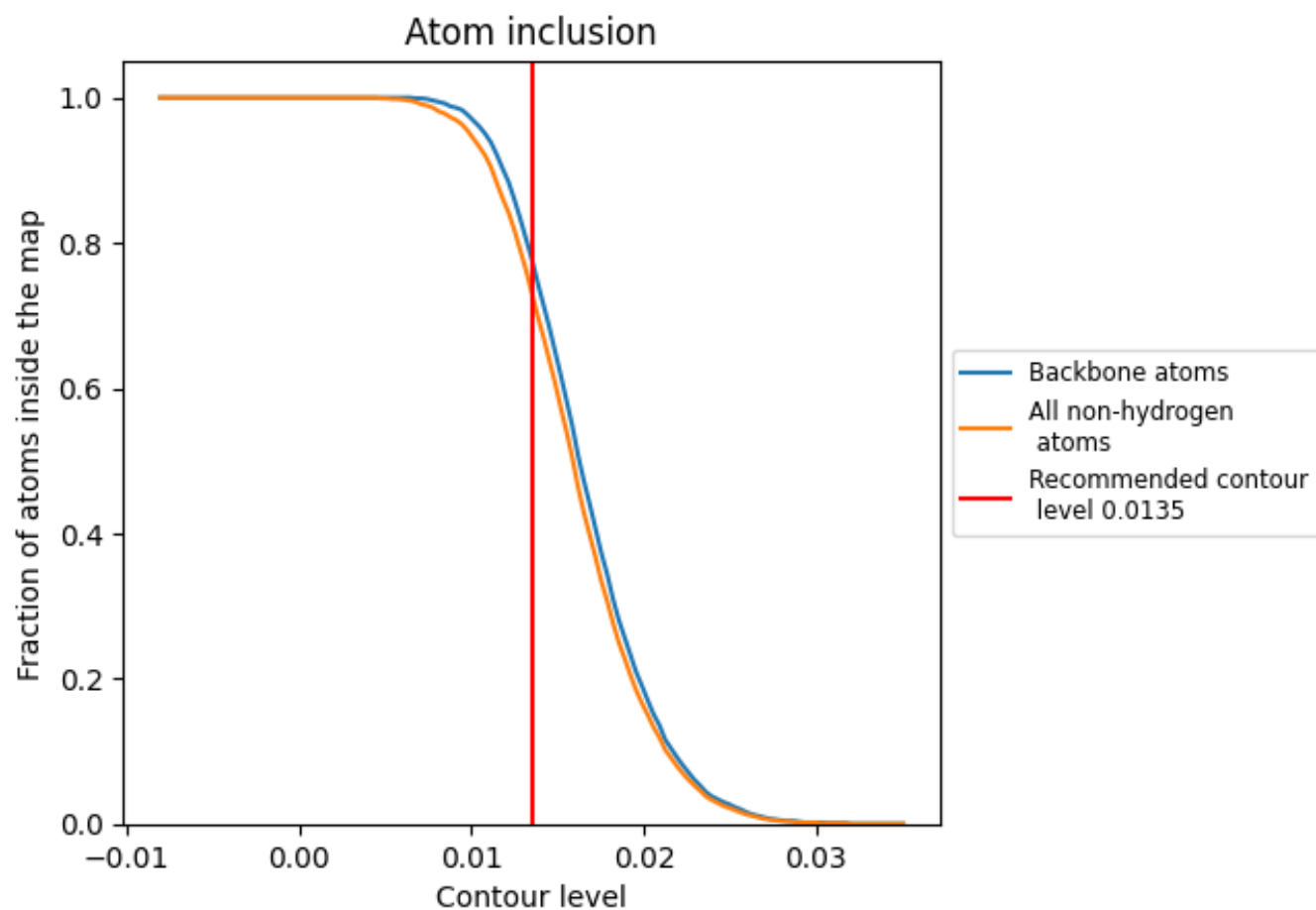
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7310	<div></div> 0.2480
A	<div></div> 0.7540	<div></div> 0.2560
B	<div></div> 0.7080	<div></div> 0.2410

