



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 10:38 pm GMT

PDB ID : 4AQ9
EMDB ID : EMD-2072
Title : Gating movement in acetylcholine receptor analysed by time- resolved electron cryo-microscopy (open class)
Authors : Unwin, N.; Fujiyoshi, Y.
Deposited on : 2012-04-13
Resolution : 6.20 Å(reported)
Based on initial model : 2BG9

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

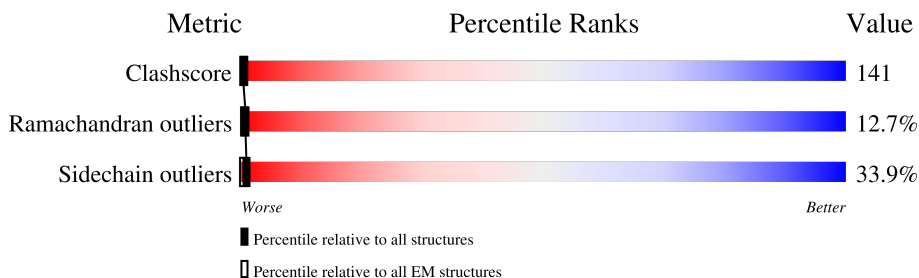
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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 $\leq 5\%$. 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	461	
1	D	461	
2	B	493	
3	C	522	
4	E	488	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14924 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
1	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

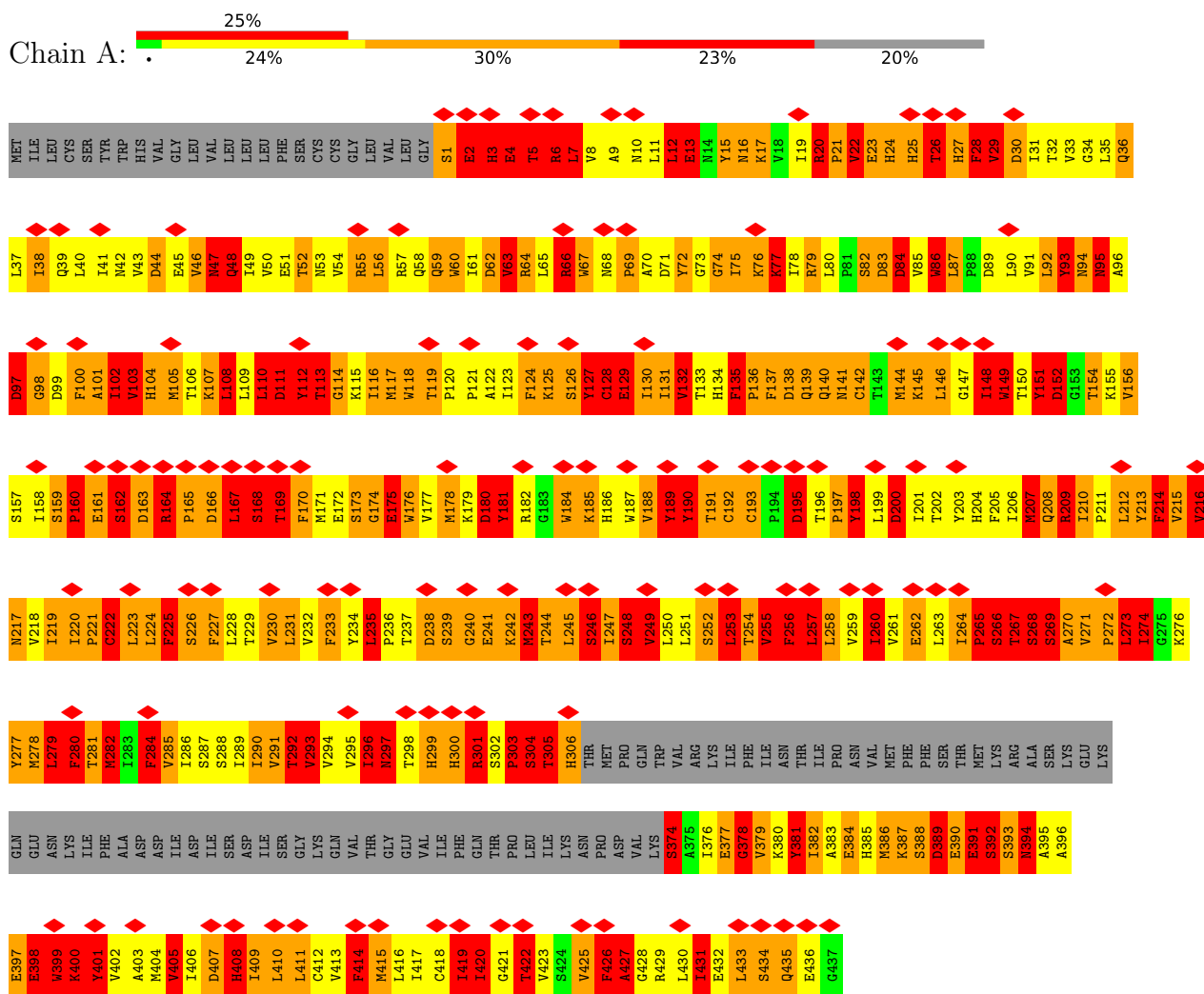
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

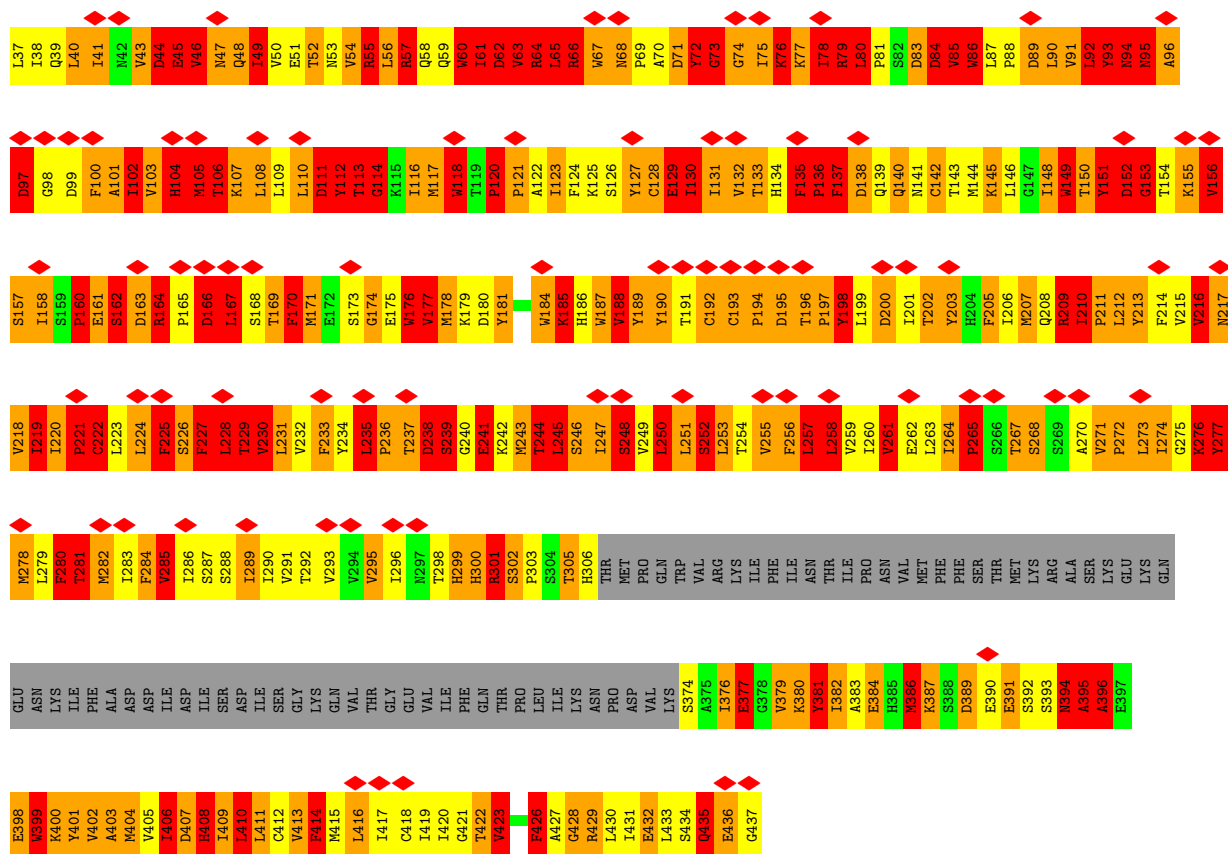
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

3 Residue-property plots

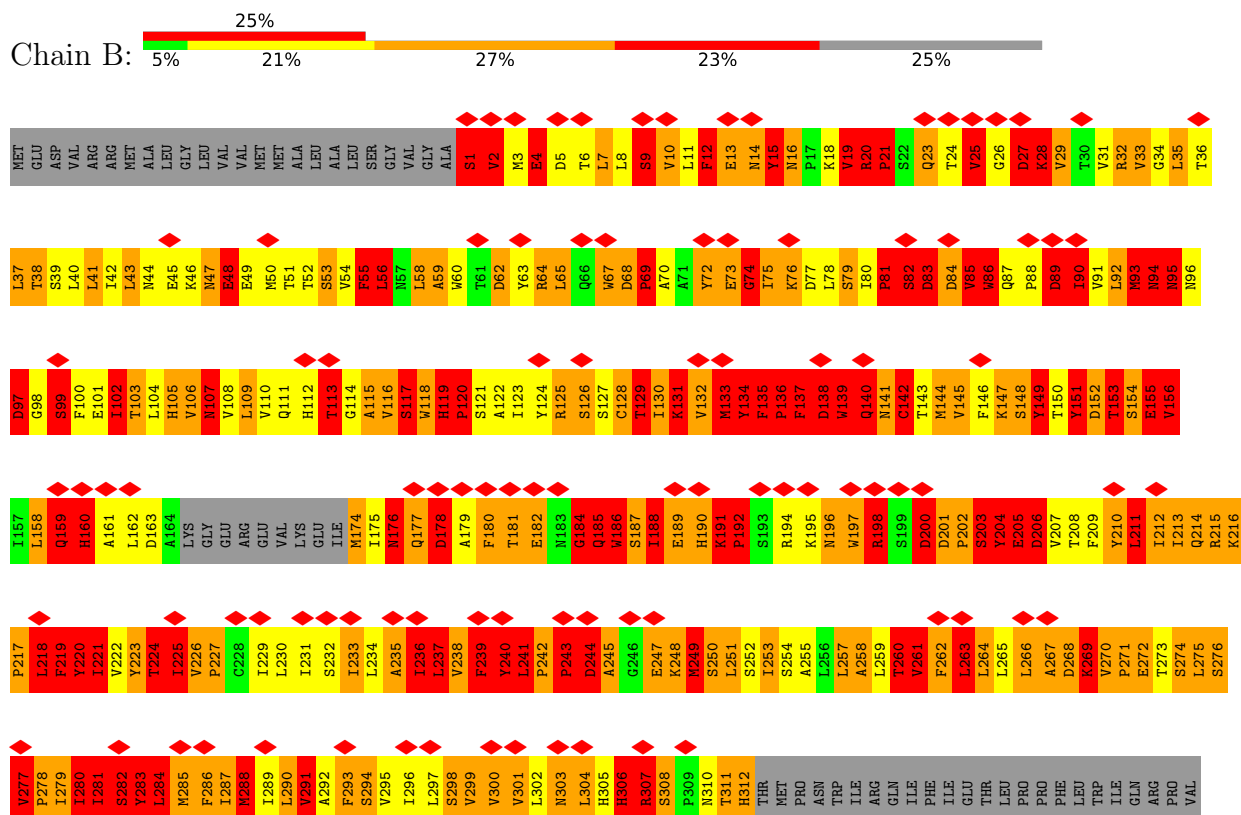
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

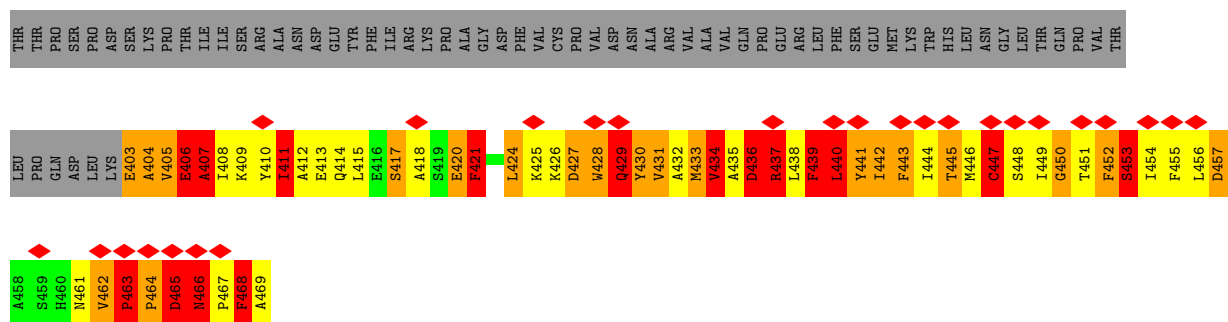
• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA



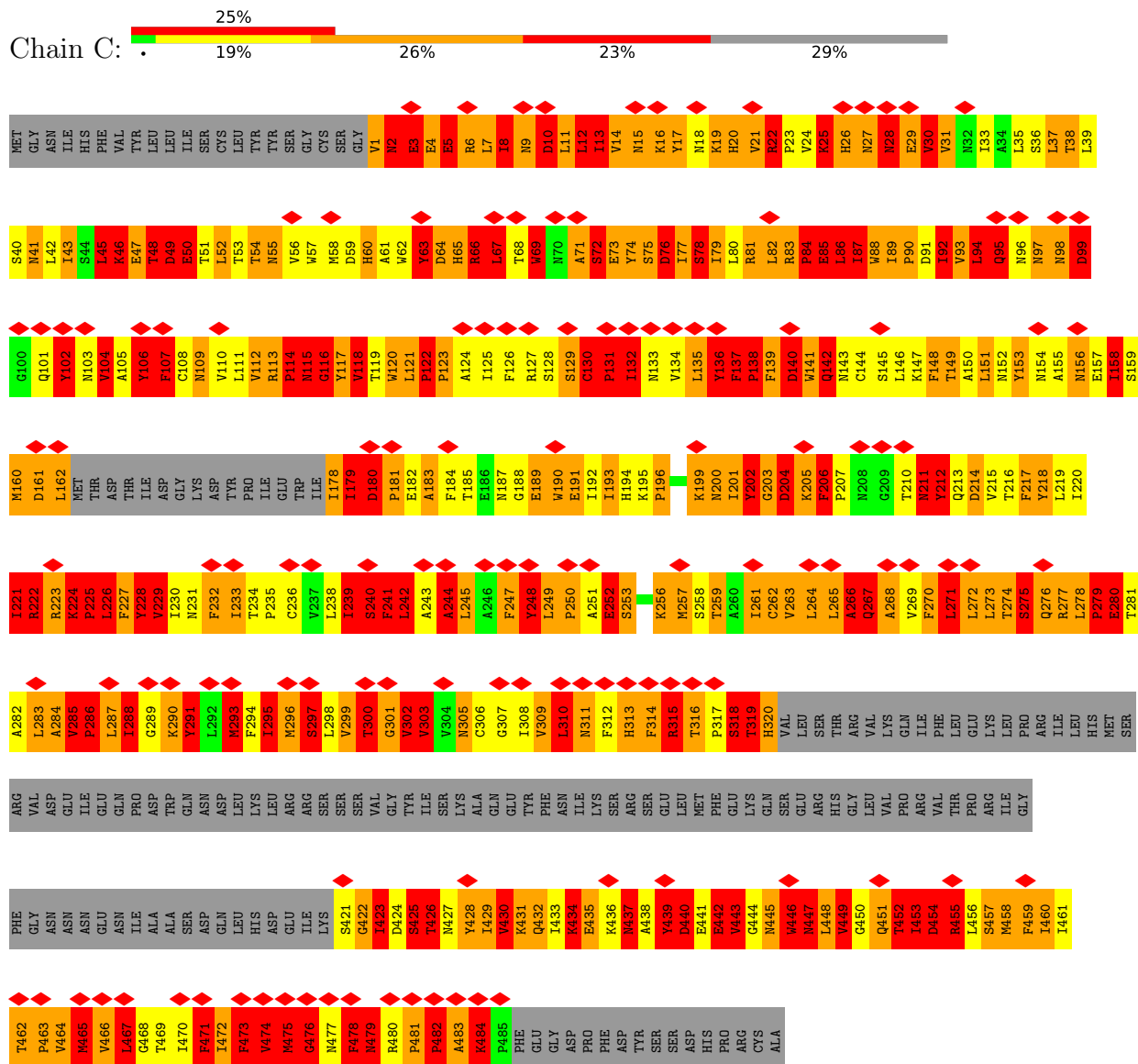


• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

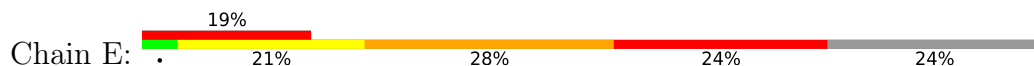


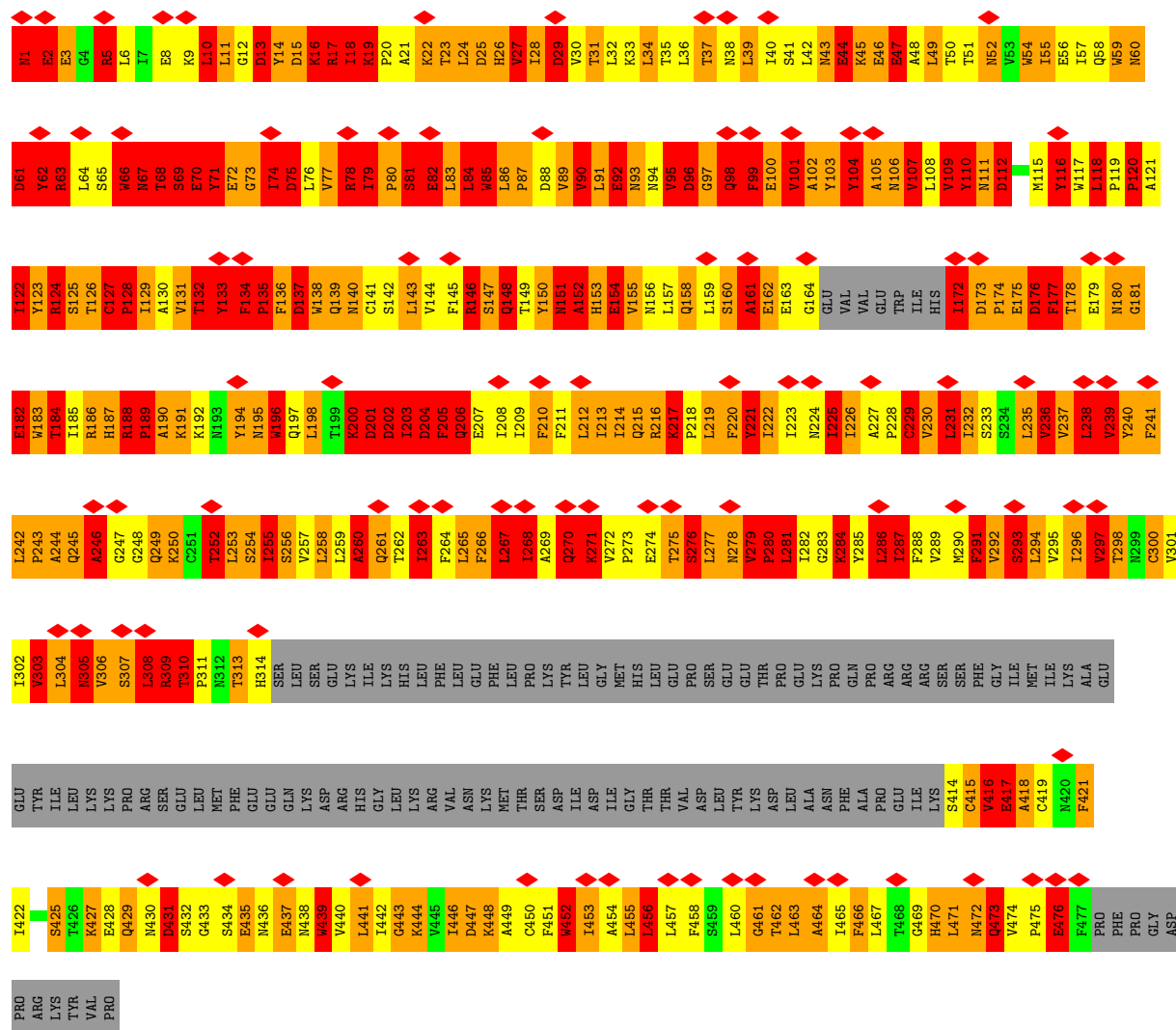


● Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT



● Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	EACH TUBE IMAGE	Depositor
Microscope	JEOL 3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	38500	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	5.148	Depositor
Minimum map value	-3.483	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	128.0, 128.0, 168.0	wwPDB
Map dimensions	128, 128, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	A	1.68	15/3069 (0.5%)	2.74	258/4186 (6.2%)
1	D	1.68	10/3069 (0.3%)	2.84	300/4186 (7.2%)
2	B	1.68	13/3048 (0.4%)	2.82	301/4162 (7.2%)
3	C	1.69	10/3059 (0.3%)	2.80	285/4175 (6.8%)
4	E	1.69	12/3057 (0.4%)	2.85	295/4174 (7.1%)
All	All	1.68	60/15302 (0.4%)	2.81	1439/20883 (6.9%)

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	6	122
1	D	5	120
2	B	11	128
3	C	5	120
4	E	9	118
All	All	36	608

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	GLN	C-N	9.62	1.56	1.34
2	B	129	THR	C-N	-9.40	1.12	1.34
4	E	311	PRO	N-CD	8.91	1.60	1.47
1	A	118	TRP	CB-CG	8.41	1.65	1.50
1	A	222	CYS	CB-SG	-8.07	1.68	1.82

The worst 5 of 1439 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	63	ARG	NE-CZ-NH1	22.18	131.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	17	ARG	NE-CZ-NH2	-21.30	109.65	120.30
1	A	190	TYR	CB-CG-CD2	-18.56	109.87	121.00
1	D	164	ARG	NE-CZ-NH1	18.36	129.48	120.30
1	A	209	ARG	NE-CZ-NH2	17.98	129.29	120.30

5 of 36 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	SER	CA
1	A	149	TRP	CA
1	A	162	SER	CA
1	A	267	THR	CB
1	A	304	SER	CA

5 of 608 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASN	Mainchain
1	A	20	ARG	Mainchain
1	A	22	VAL	Mainchain
1	A	5	THR	Mainchain
1	A	6	ARG	Peptide

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	A	2991	0	3001	903	0
1	D	2991	0	3004	903	0
2	B	2972	0	2952	783	0
3	C	2983	0	2983	892	0
4	E	2987	0	2989	900	0
All	All	14924	0	14929	4213	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 141.

The worst 5 of 4213 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:D:86:TRP:CD2	1:D:86:TRP:O	1.68	1.44
4:E:217:LYS:O	4:E:217:LYS:CE	1.74	1.36
4:E:284:LYS:N	4:E:284:LYS:HE3	1.42	1.29
2:B:130:ILE:HB	2:B:134:TYR:CD2	1.67	1.27
1:D:86:TRP:O	1:D:86:TRP:CG	1.83	1.26

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	366/461 (79%)	251 (69%)	68 (19%)	47 (13%)	0	4
1	D	366/461 (79%)	265 (72%)	54 (15%)	47 (13%)	0	4
2	B	364/493 (74%)	238 (65%)	85 (23%)	41 (11%)	0	5
3	C	364/522 (70%)	244 (67%)	74 (20%)	46 (13%)	0	4
4	E	365/488 (75%)	239 (66%)	76 (21%)	50 (14%)	0	4
All	All	1825/2425 (75%)	1237 (68%)	357 (20%)	231 (13%)	1	4

5 of 231 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	7	LEU
1	A	48	GLN
1	A	83	ASP
1	A	93	TYR

5.3.2 Protein sidechains ⓘ

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	343/427 (80%)	224 (65%)	119 (35%)	0	1
1	D	343/427 (80%)	222 (65%)	121 (35%)	0	1
2	B	340/449 (76%)	240 (71%)	100 (29%)	0	2
3	C	335/475 (70%)	217 (65%)	118 (35%)	0	1
4	E	337/447 (75%)	219 (65%)	118 (35%)	0	1
All	All	1698/2225 (76%)	1122 (66%)	576 (34%)	1	1

5 of 576 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	19	LYS
4	E	471	LEU
4	E	66	TRP
4	E	18	ILE
4	E	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	140	ASN
4	E	156	ASN
4	E	472	ASN
3	C	15	ASN
3	C	9	ASN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	126:THR	C	127:CYS	N	1.19
1	E	309:ARG	C	310:THR	N	1.19
1	B	129:THR	C	130:ILE	N	1.12

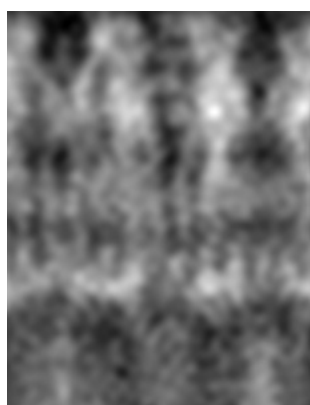
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2072. These allow visual inspection of the internal detail of the map and identification of artifacts.

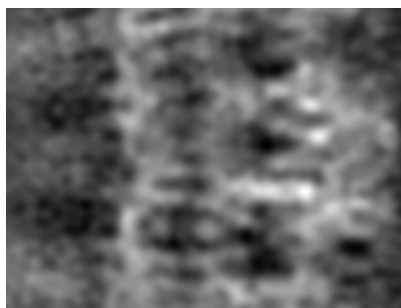
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

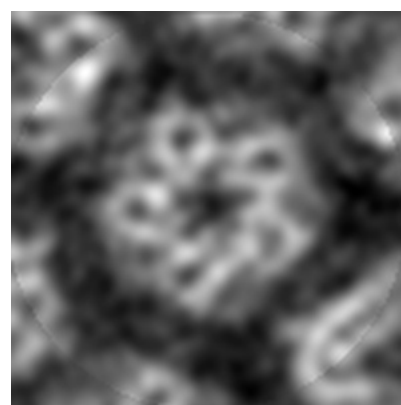
6.1.1 Primary map



X



Y

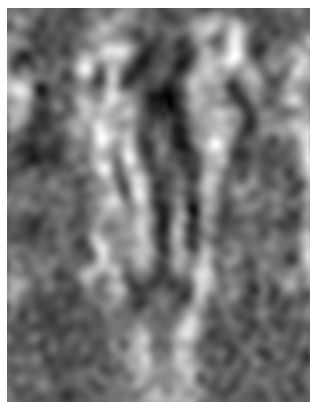


Z

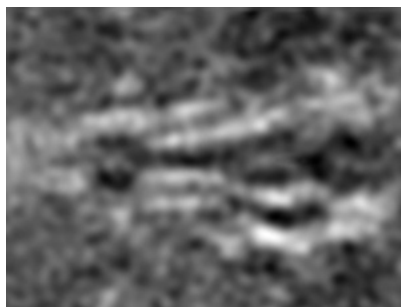
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

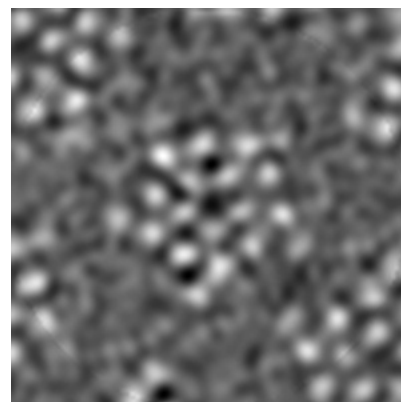
6.2.1 Primary map



X Index: 64



Y Index: 64

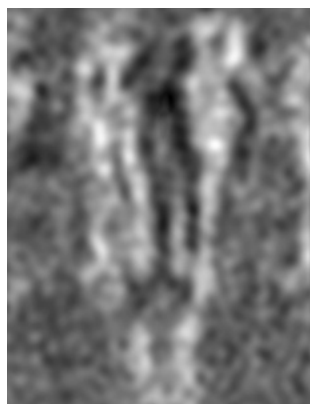


Z Index: 84

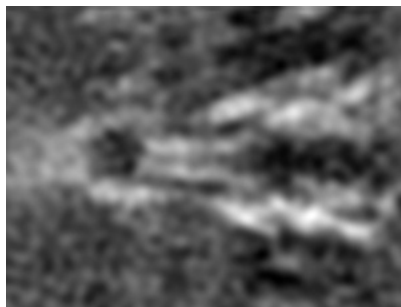
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

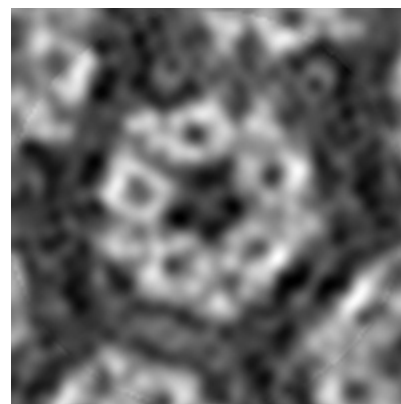
6.3.1 Primary map



X Index: 63



Y Index: 71

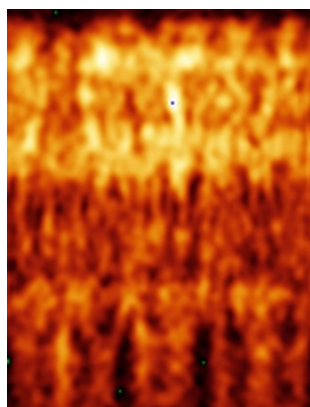


Z Index: 145

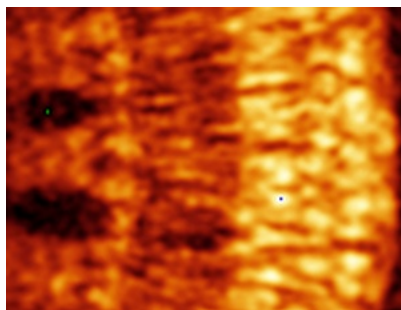
The images above show the largest variance slices of the map in three orthogonal directions.

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

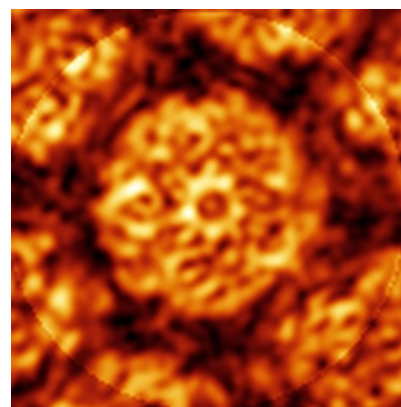
6.4.1 Primary map



X



Y

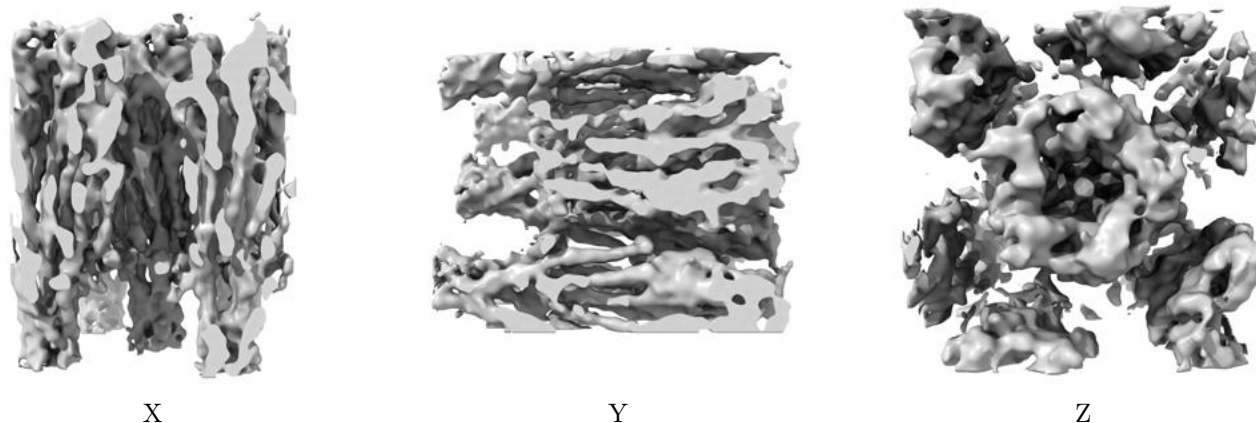


Z

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

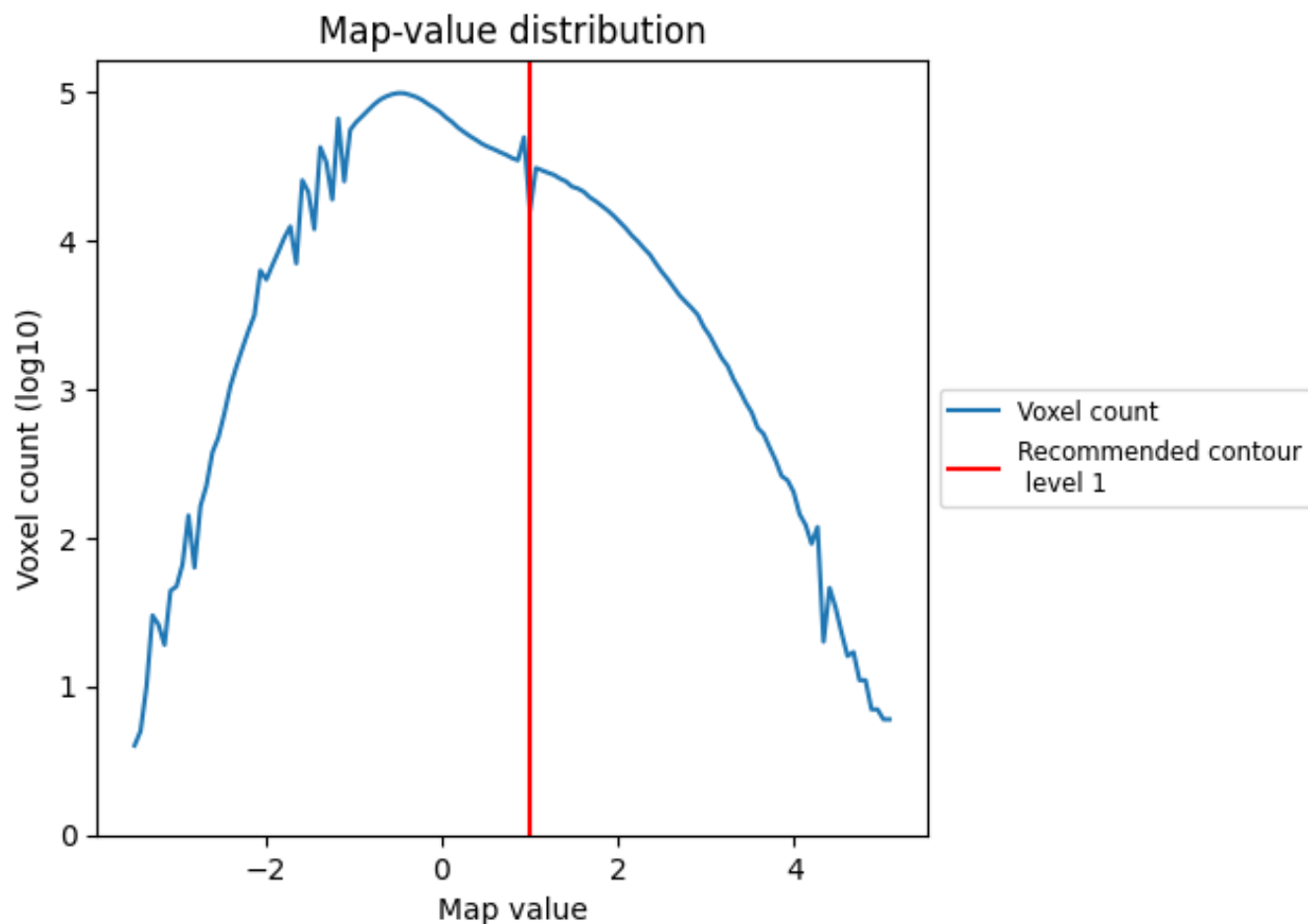
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

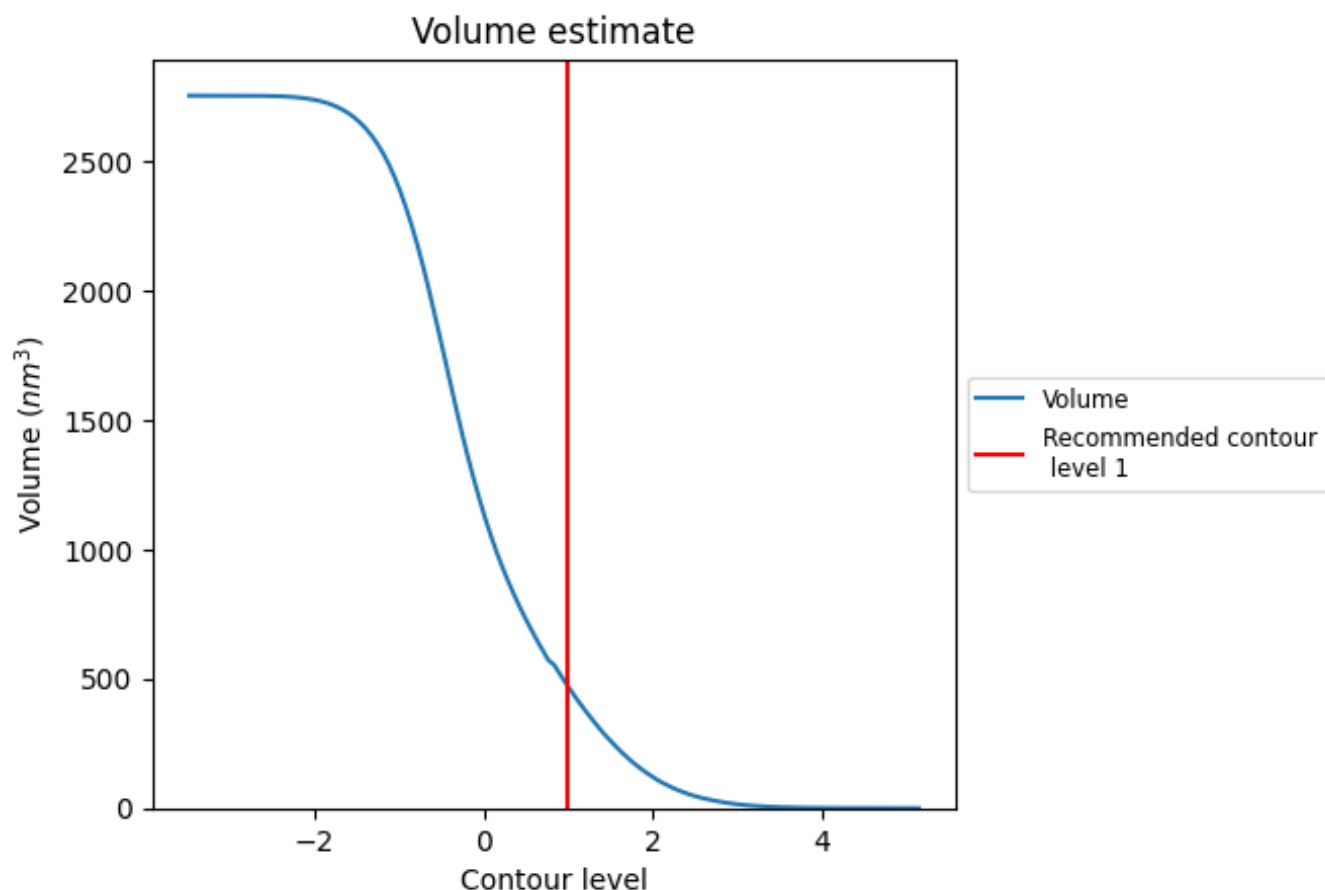
This section contains the results of statistical analysis of the map.

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 469 nm³; this corresponds to an approximate mass of 424 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

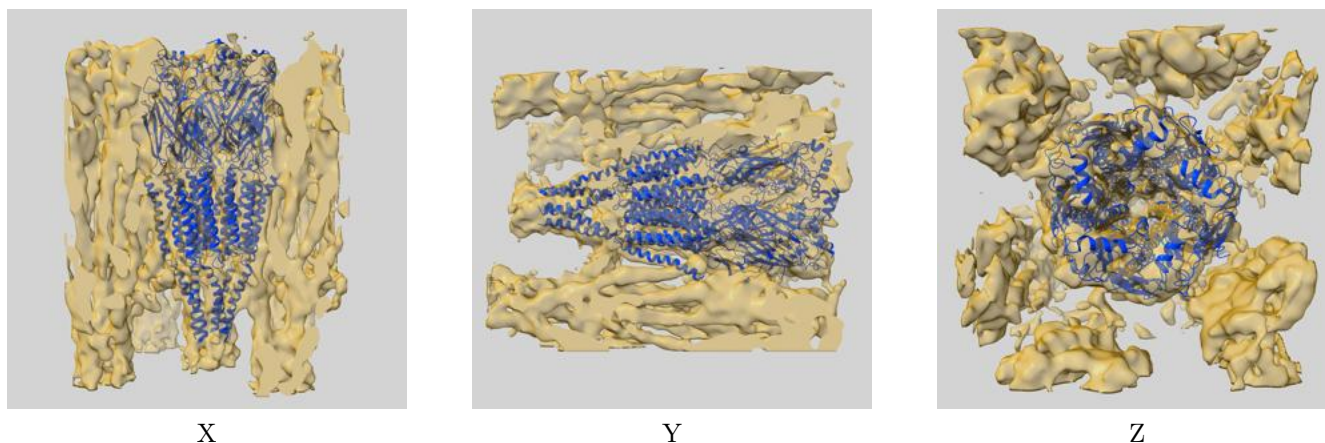
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

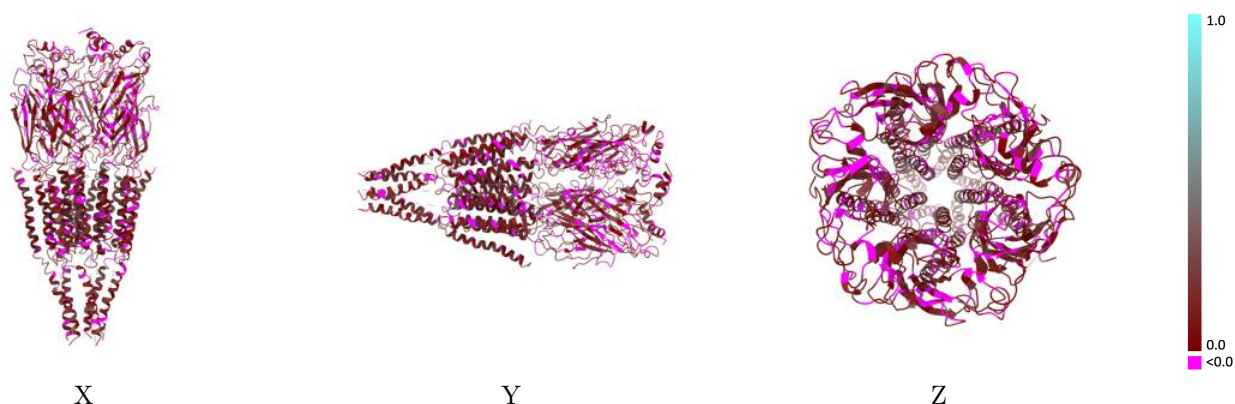
This section contains information regarding the fit between EMDB map EMD-2072 and PDB model 4AQ9. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



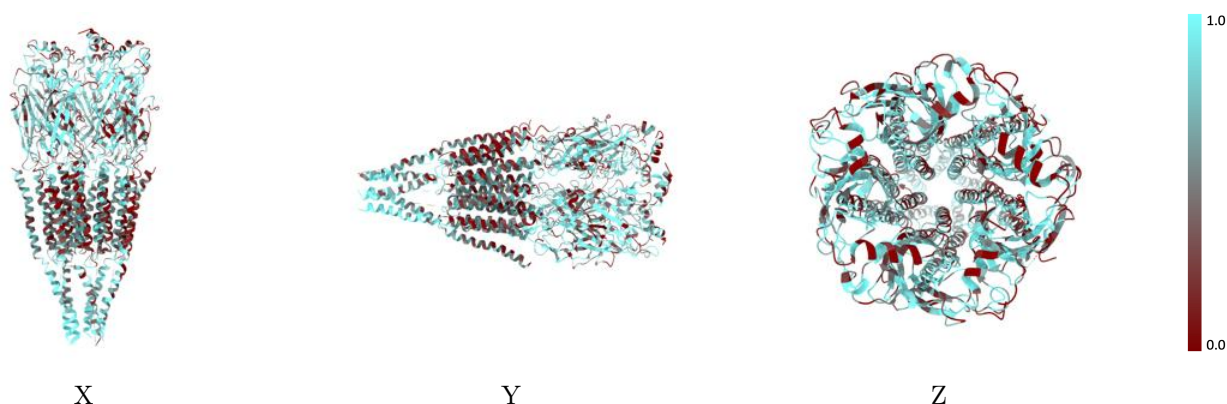
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



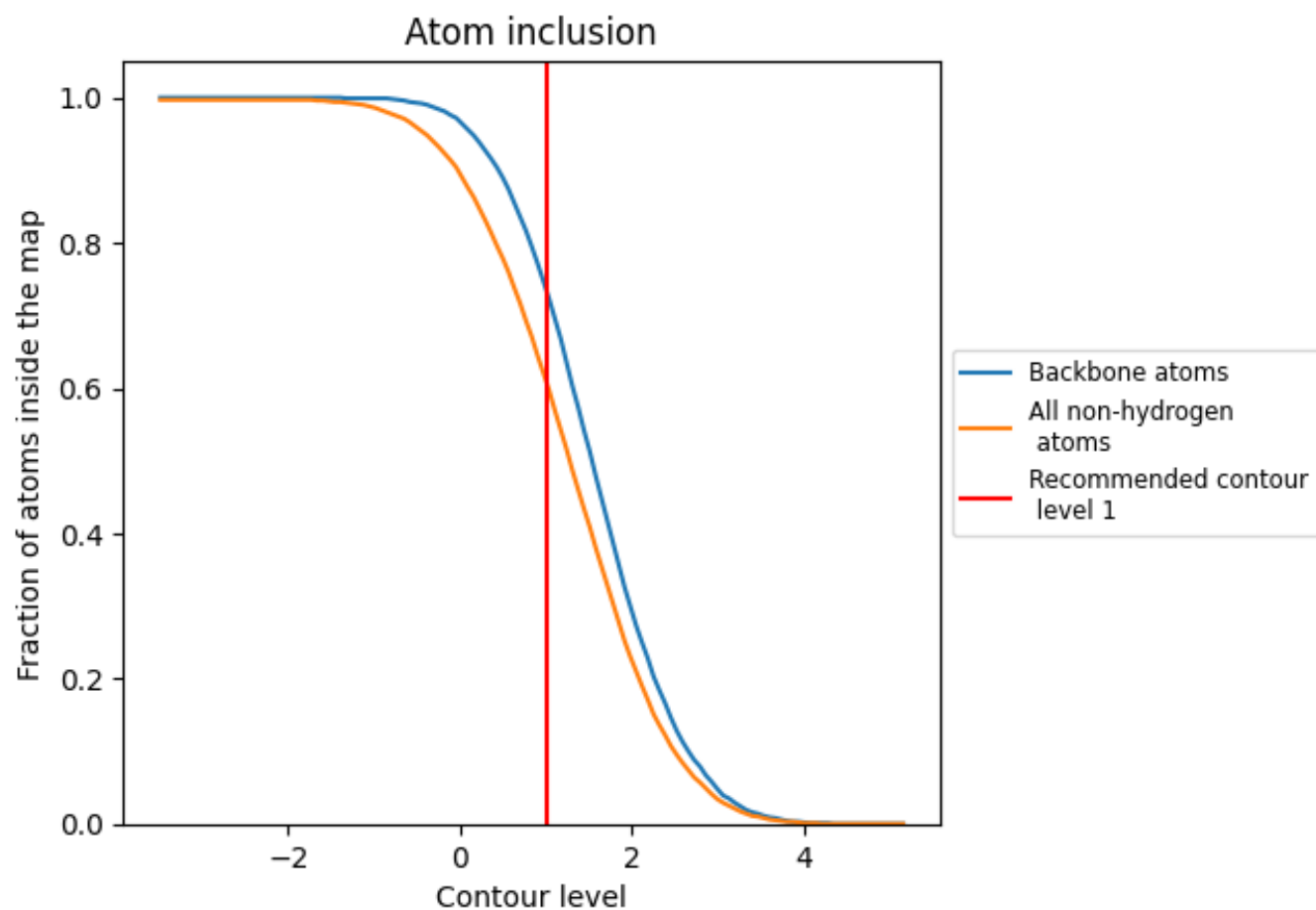
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 61% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6100	<div></div> 0.1030
A	<div></div> 0.6080	<div></div> 0.1060
B	<div></div> 0.5780	<div></div> 0.0910
C	<div></div> 0.5740	<div></div> 0.0980
D	<div></div> 0.6270	<div></div> 0.1090
E	<div></div> 0.6610	<div></div> 0.1100

