



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 10:35 AM UTC

PDB ID : 4AQ9 / pdb_00004aq9
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

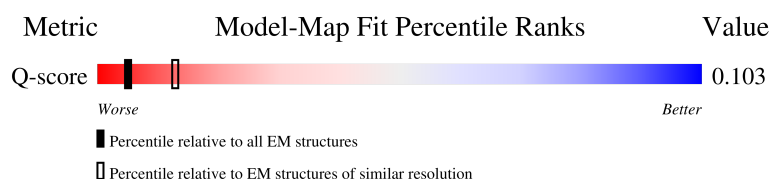
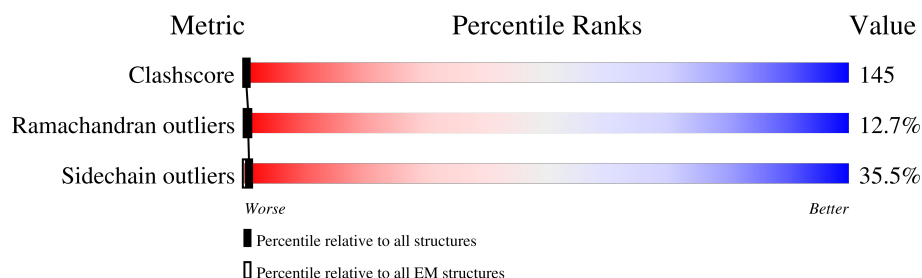
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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	25% 12% 33% 34% 20%
1	D	461	21% 15% 31% 33% 20%
2	B	493	25% 13% 29% 31% 25%
3	C	522	25% 13% 26% 30% 29%

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Mol	Chain	Length	Quality of chain
4	E	488	19% 15% 27% 33% 24%

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		

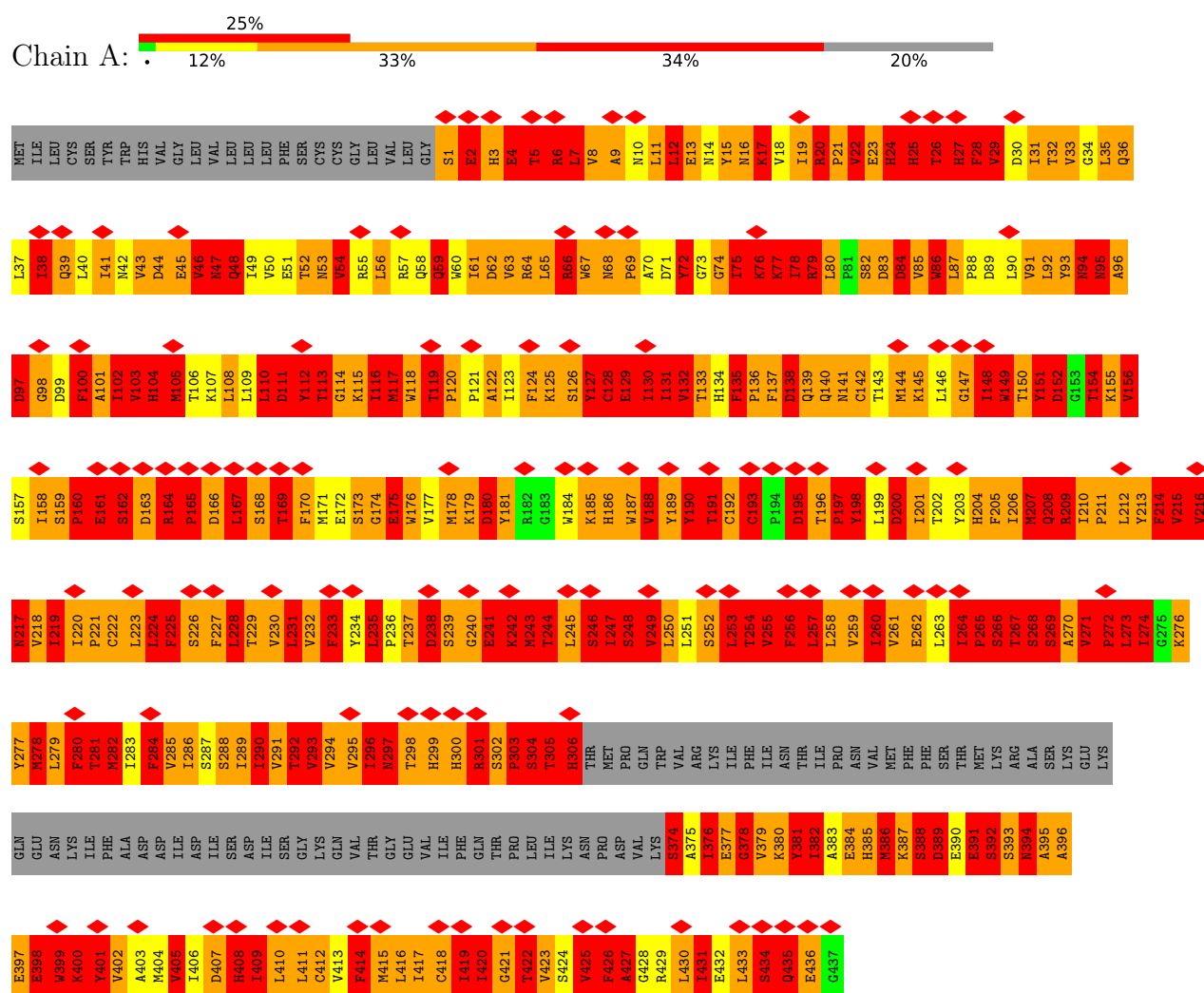
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

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

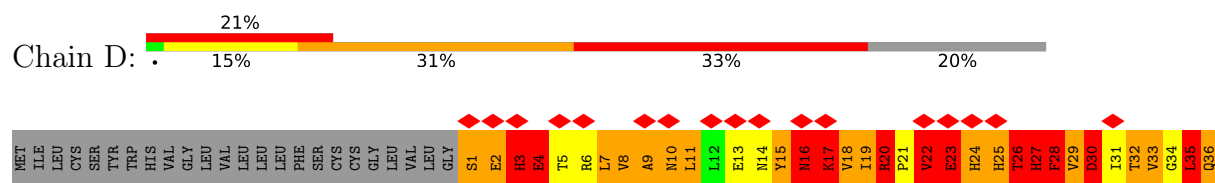
3 Residue-property plots

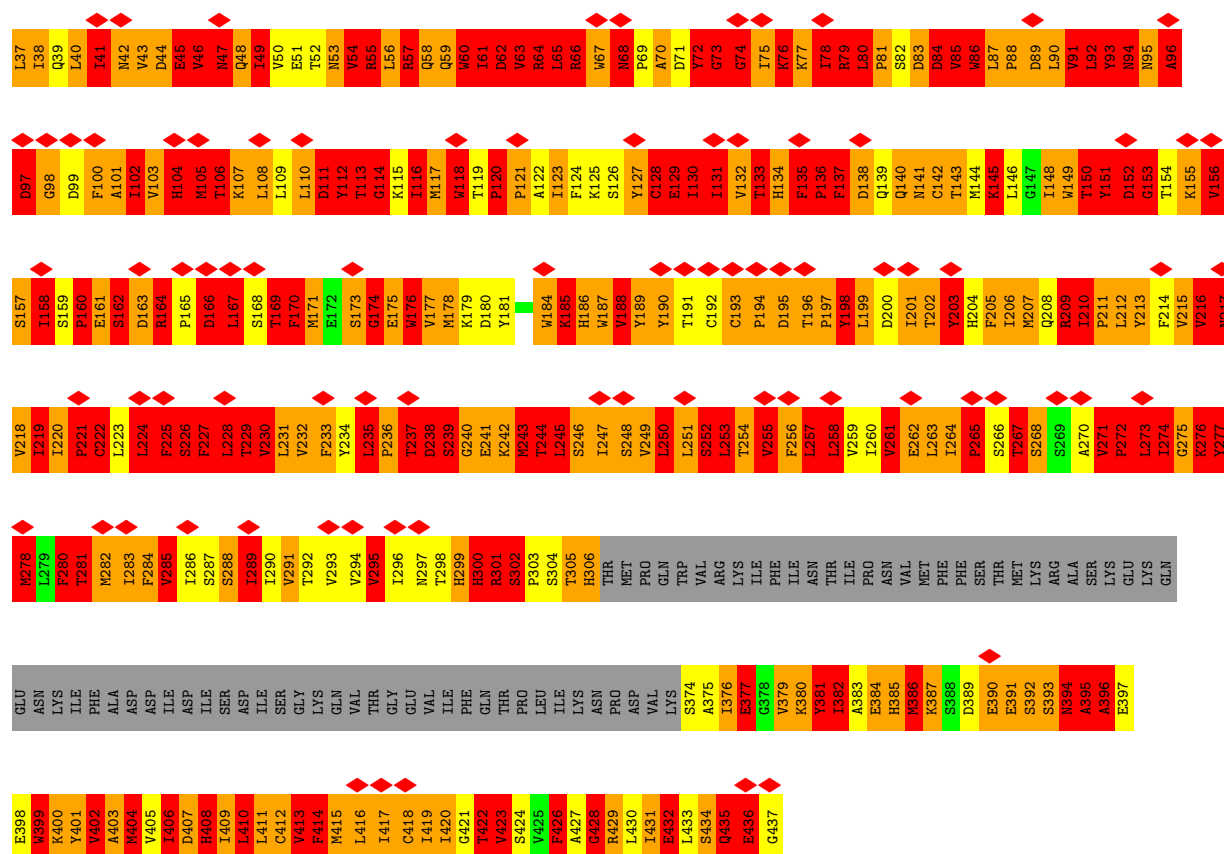
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

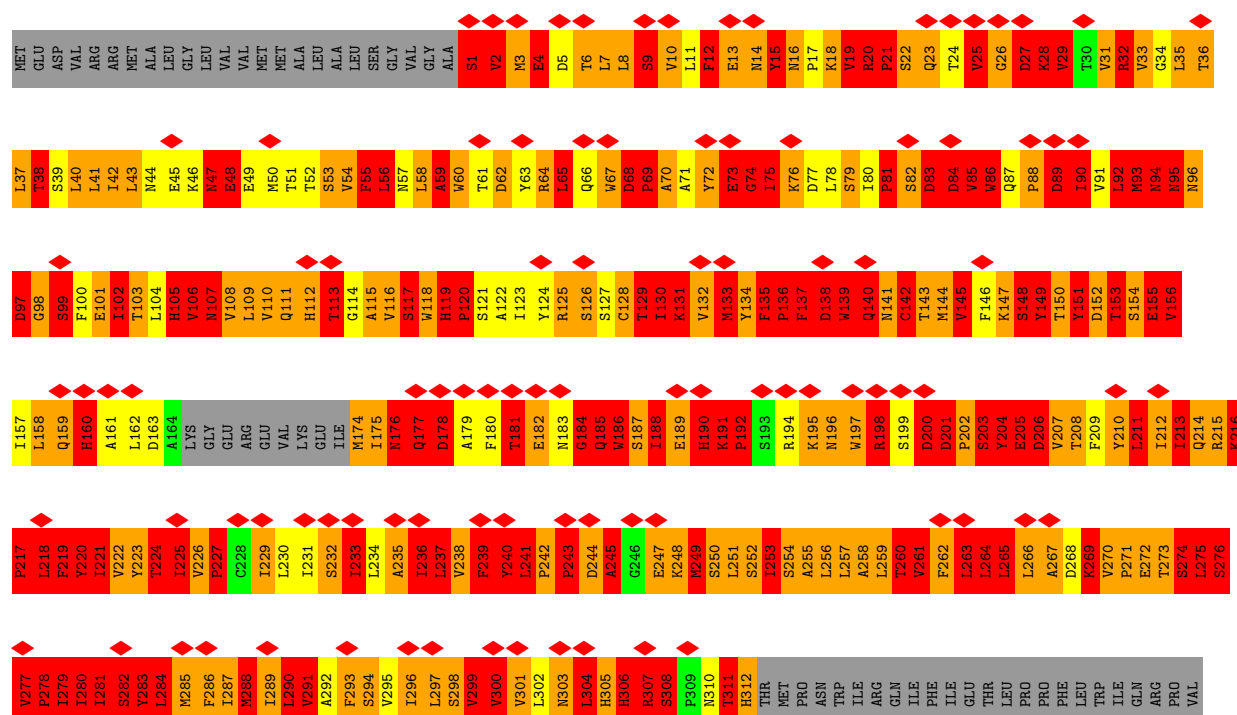


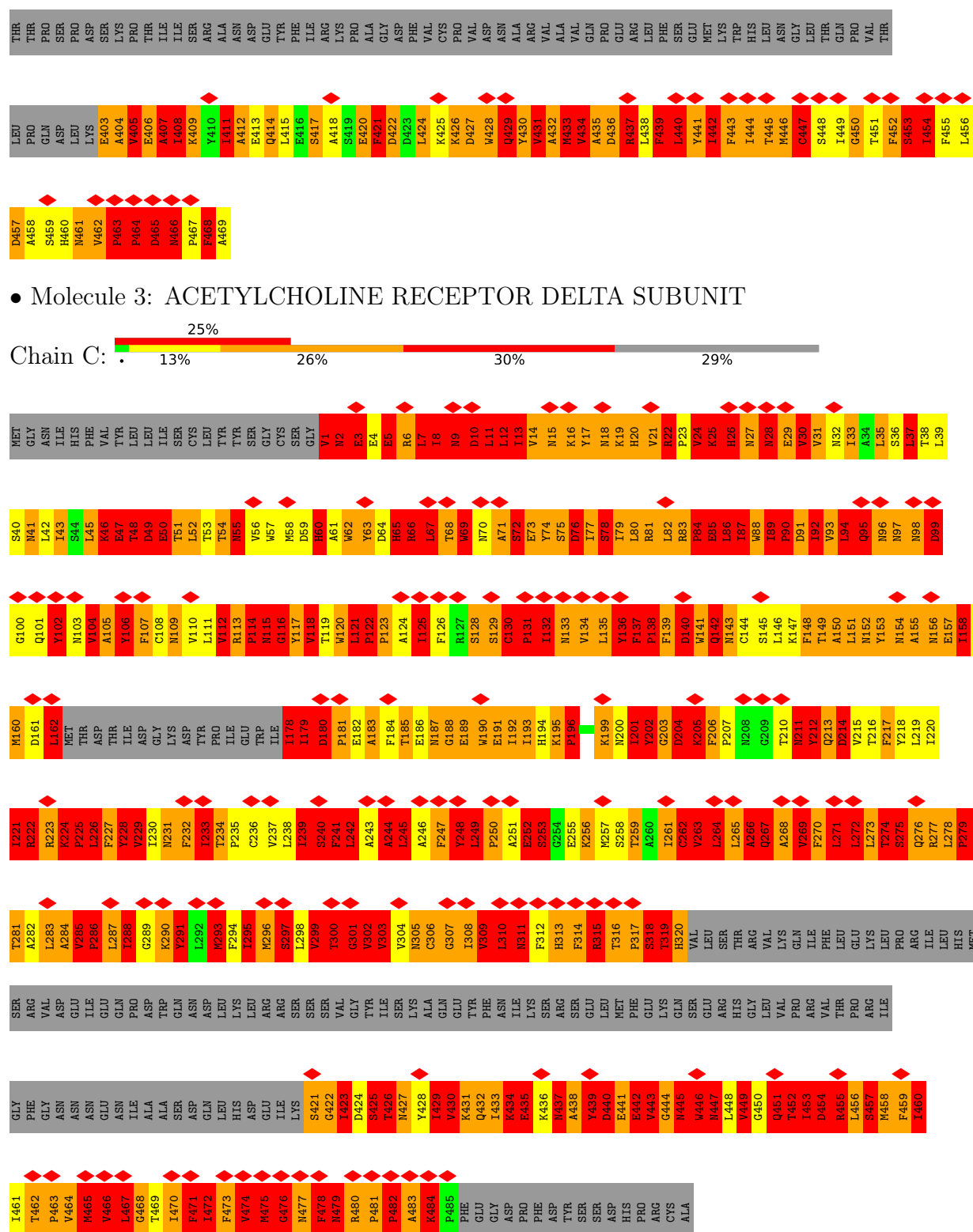
• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA





• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT





• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT



GLY	F421	GLU	GLU	V301	F241	G181	A121	D61
	ASP	GLU	TYR	T302	L242	E182	I122	Y62
PRO	A422	TYR	TYR	V303	P243	W183	Y123	R63
	ARG	ILE	ILE	L304	A244	T184	R124	E3
LYS	S425	LEU	LEU	N305	Q245	I185	S125	G4
	T426	LYS	LYS	V306	A246	R186	T126	R5
VAL	K427	LYS	LYS	S307	G247	H187	C127	W66
	E428	PRO	ARG	L308	G248	R188	P128	N67
PRO	Q429	SER	SER	R309	Q249	P189	I129	T68
	N430	GLU	GLU	T310	K250	A190	A130	E8
ASP	D431	LEU	LEU	F311	C251	K191	V131	K9
	S432	MET	MET	N312	T252	K192	T132	L10
ARG	G433	PHE	PHE	T313	L253	N193	Y133	L11
	S434	GLU	GLU	H314	S254	Y194	F134	G12
LYS	E435	GLU	GLU	SER	T255	M195	P135	D13
	N436	GLN	SER		S256	Q197	F136	D75
TYR	E437	LYS	ASP	LEU	V257	L198	D137	D15
	N438	ASP	GLU	GLU	L258	T199	W138	R17
VAL	W439	ARG	LYS	LYS	L259	K200	Q139	I18
	V440	HIS	ILE	ILE	A260	D201	G141	K19
PRO	L441	GLY	LYS	LYS	Q261	D202	S142	P20
	T442	LEU	HIS	HIS	T262	I203	L143	I19
ARG	G443	LYS	LEU	LEU	T263	D204	V144	S81
	K444	ARG	PHE	PHE	F264	F205	F145	T23
LYS	V445	VAL	LEU	LEU	F266	O206	R146	L24
	I446	ASN	GLU	GLU	L265	E207	S147	D25
VAL	D447	LYS	PHE	PHE	F266	I208	O148	H26
	K448	MET	LEU	LEU	L267	I209	T149	V27
PRO	A449	THR	THR	PRO	L268	F210	Y150	I28
	C450	SER	SER	LYS	A269	F211	M151	D29
GLY	F451	ASP	ASP	TYR	Q270	T211	A152	V30
	W452	ILE	ASP	LEU	K271	L212	H153	T31
ARG	I453	ILE	GLY	GLY	V272	I213	E154	L32
	A454	GLY	THR	MET	P273	I214	Y155	K33
LYS	L455	THR	THR	HIS	E274	Q215	N156	L34
	L456	THR	THR	LEU	E274	R216	L157	T35
VAL	L457	VAL	VAL	PRO	T275	K217	Q158	L36
	F458	ASP	ASP	SER	S276	L219	L159	T37
PRO	S459	LEU	TYR	GLU	L277	F220	S160	N38
	L460	LYS	LYS	THR	N278	Y221	A161	L39
GLY	G461	ASP	ASP	PRO	V279	I222	E162	I40
	T462	LEU	ALA	GLU	P280	I223	Y103	S41
ARG	L463	ALA	ASN	LYS	L281	N224	G164	L42
	A464	PHE	PHE	PRO	G283	I225	VAL	N43
LYS	I465	ALA	ALA	PRO	Y285	I226	VAL	E44
	F466	PRO	PRO	PRO	L286	A227	GLU	K45
VAL	L467	GLU	ILE	ARG	T287	C228	TRP	E46
	G469	LYS	LYS	ARG	F288	V230	HIS	F47
PRO	H470	S414	S415	SER	N289	L231	I172	L48
	L471	C415	V416	PHE	M290	D173	D173	N52
GLY	N472	V416	E417	GLY	V291	S233	P174	V53
	Q473	A418	MET	ILE	V292	S234	E175	G13
VAL	V474	C419	ILE	ILE	S293	L235	D176	W54
	P475	P475	LYS	LYS	V295	V236	F177	E56
PRO	E476	N420	ALA	ALA	I296	V237	T178	T57
	F477	PRO	PHE	PRO	T297	L238	E179	Q58
GLY	P478	PRO	PRO	PRO	T298	V239	N180	W59
	N479	PRO	PRO	PRO	T299	Y240		N60

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	2.16	53/3069 (1.7%)	3.32	520/4186 (12.4%)
1	D	2.20	62/3069 (2.0%)	3.37	551/4186 (13.2%)
2	B	2.20	68/3048 (2.2%)	3.34	559/4162 (13.4%)
3	C	2.17	60/3059 (2.0%)	3.36	542/4175 (13.0%)
4	E	2.17	74/3057 (2.4%)	3.39	548/4174 (13.1%)
All	All	2.18	317/15302 (2.1%)	3.35	2720/20883 (13.0%)

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 317 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-17.79	1.12	1.34
1	D	208	GLN	C-N	16.06	1.56	1.33
2	B	159	GLN	C-N	9.56	1.49	1.33
2	B	144	MET	C-N	9.55	1.46	1.33
2	B	225	ILE	CA-CB	9.52	1.66	1.54

The worst 5 of 2720 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	GLN	OE1-CD-NE2	-20.07	102.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	98	GLN	OE1-CD-NE2	-18.71	103.89	122.60
1	A	20	ARG	CA-C-O	-17.45	106.41	119.32
1	D	251	LEU	O-C-N	15.13	138.16	122.12
4	E	238	LEU	N-CA-C	-14.67	90.92	112.04

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 [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	2991	0	3006	925	0
1	D	2991	0	3006	920	0
2	B	2972	0	2953	815	0
3	C	2983	0	2987	908	0
4	E	2987	0	2994	915	0
All	All	14924	0	14946	4319	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 145.

The worst 5 of 4319 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
3:C:278:LEU:C	3:C:278:LEU:HD12	1.58	1.28
2:B:130:ILE:HB	2:B:134:TYR:CD2	1.67	1.27

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%)	0	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 [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	343/427 (80%)	214 (62%)	129 (38%)	0	1
1	D	343/427 (80%)	219 (64%)	124 (36%)	0	1
2	B	340/449 (76%)	239 (70%)	101 (30%)	0	2
3	C	335/475 (70%)	213 (64%)	122 (36%)	0	1
4	E	337/447 (75%)	211 (63%)	126 (37%)	0	1
All	All	1698/2225 (76%)	1096 (64%)	602 (36%)	1	1

5 of 602 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	387	LYS
4	E	268	ILE
4	E	5	ARG
1	D	385	HIS
4	E	110	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	52	ASN
4	E	261	GLN
4	E	67	ASN
4	E	156	ASN
4	E	429	GLN

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](#)

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

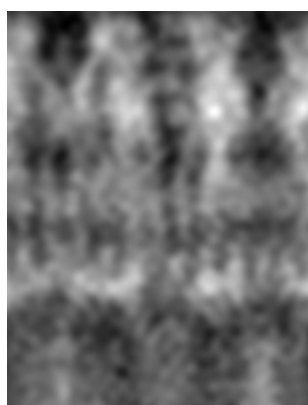
6 Map visualisation [i](#)

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.

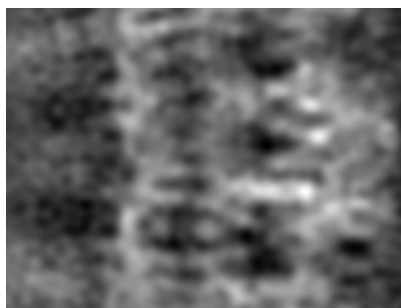
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

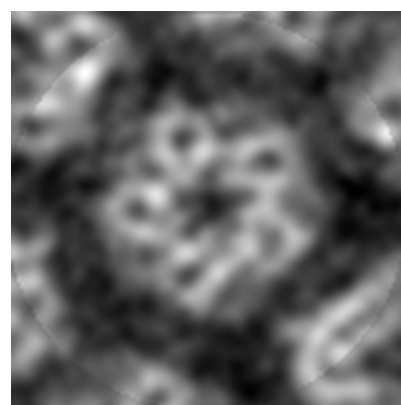
6.1.1 Primary map



X



Y

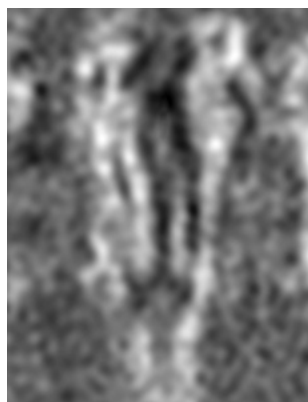


Z

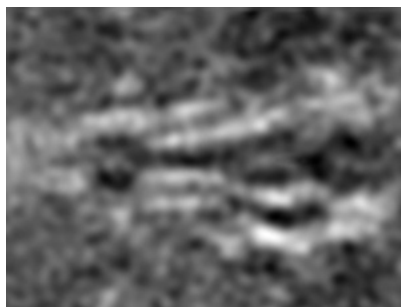
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

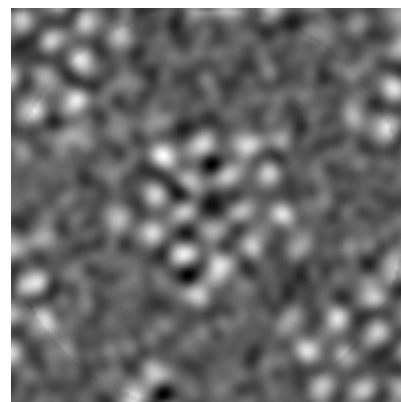
6.2.1 Primary map



X Index: 64



Y Index: 64

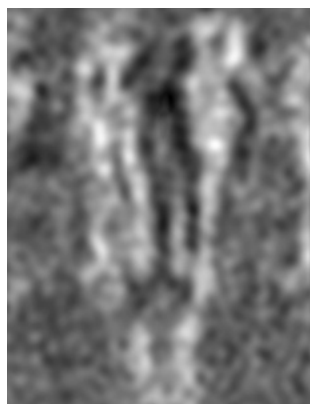


Z Index: 84

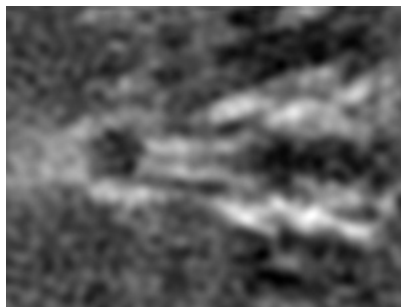
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

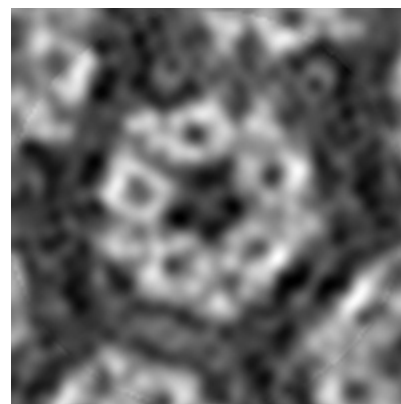
6.3.1 Primary map



X Index: 63



Y Index: 71

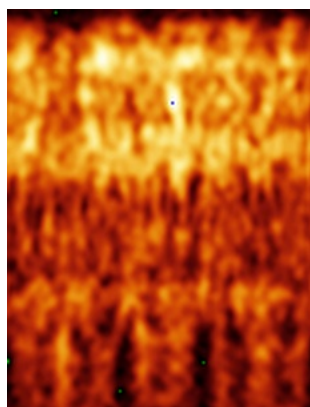


Z Index: 145

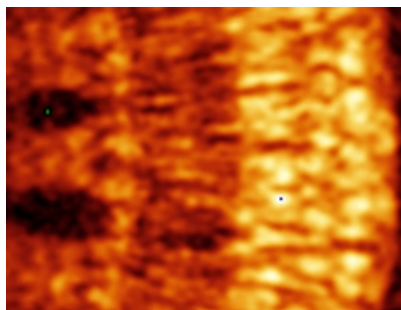
The images above show the largest variance slices of the map in three orthogonal directions.

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

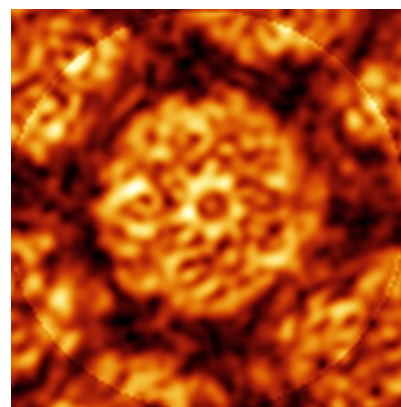
6.4.1 Primary map



X



Y

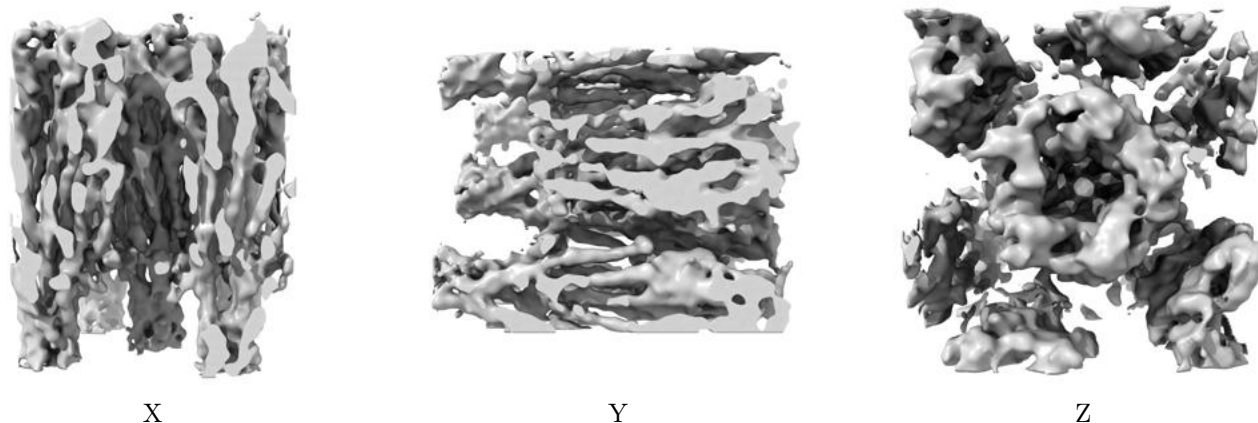


Z

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.

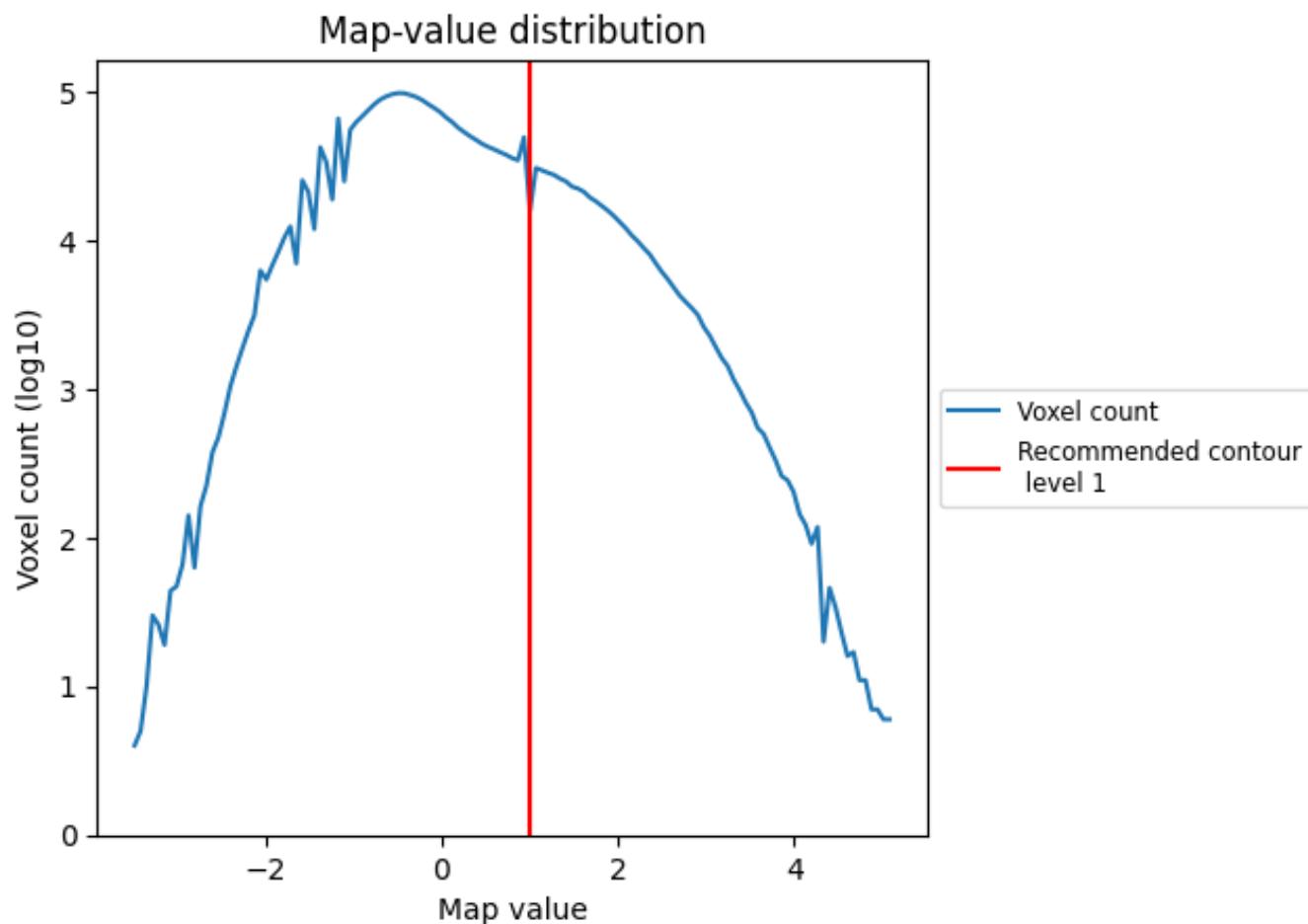
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

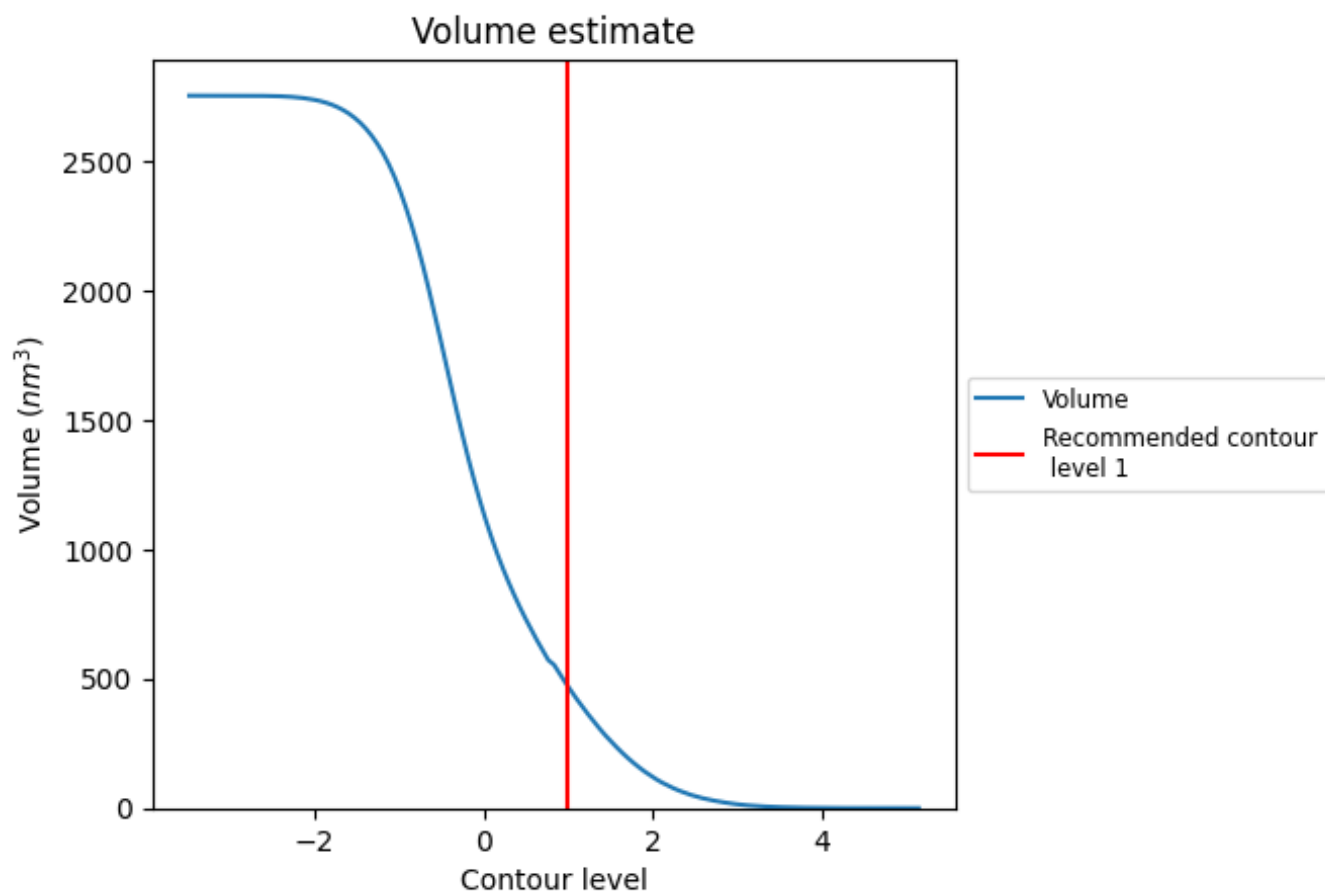
This section contains the results of statistical analysis of the map.

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.

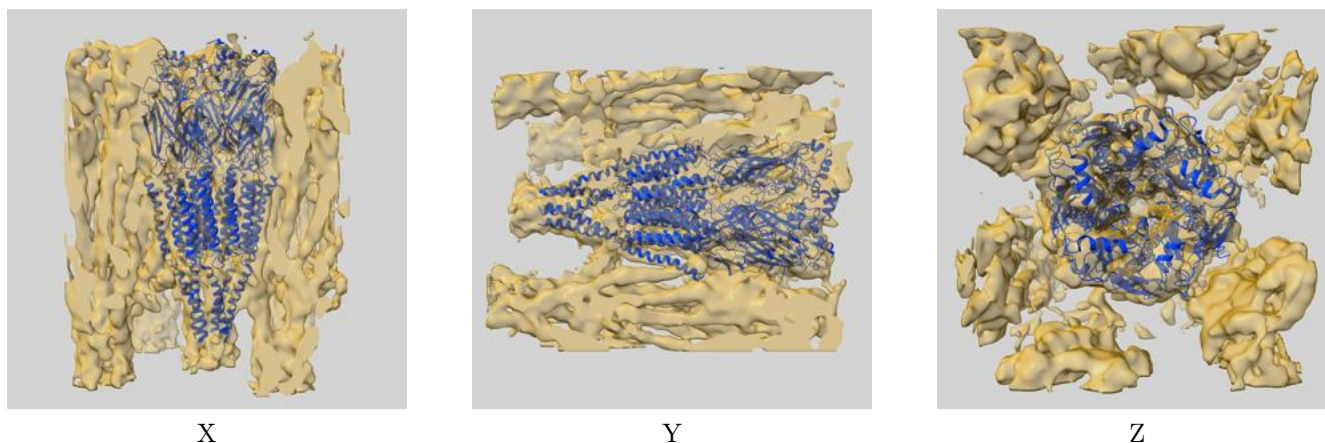
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

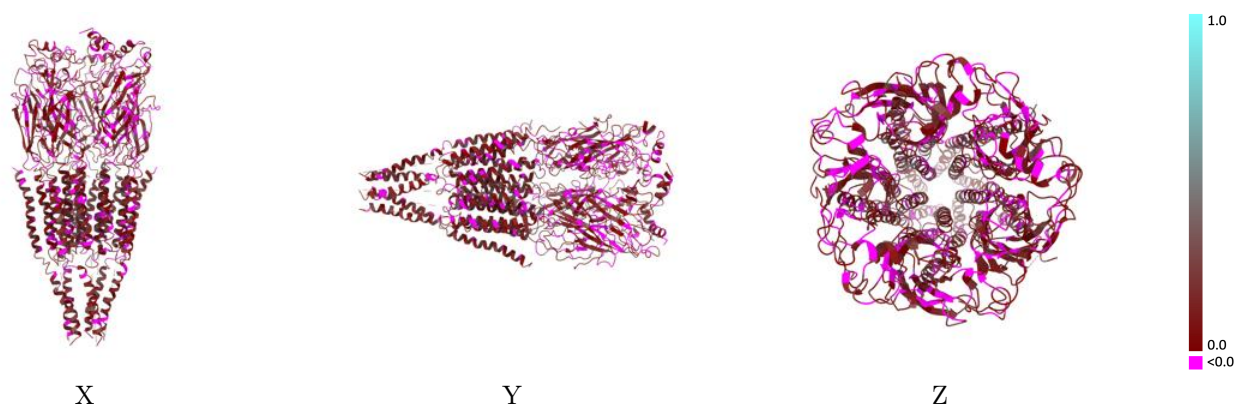
This section contains information regarding the fit between EMDB map EMD-2072 and PDB model 4AQ9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



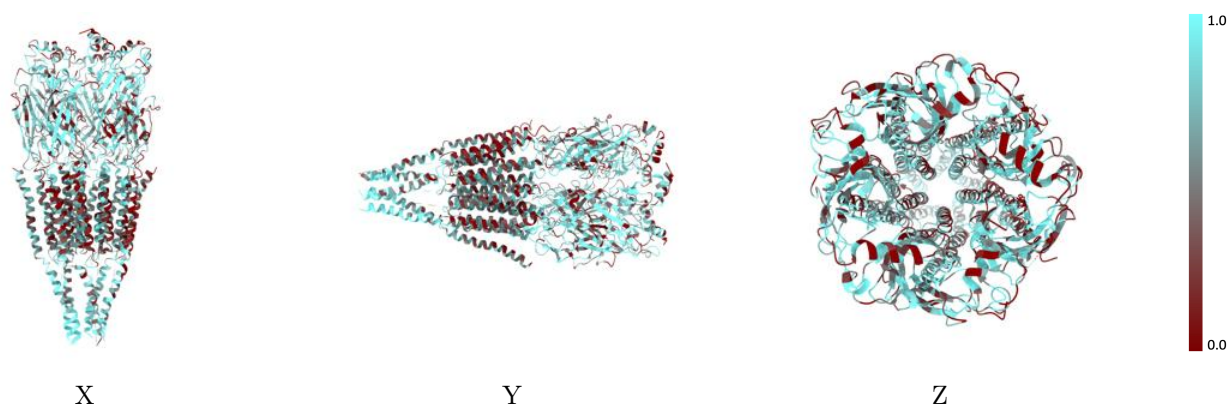
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



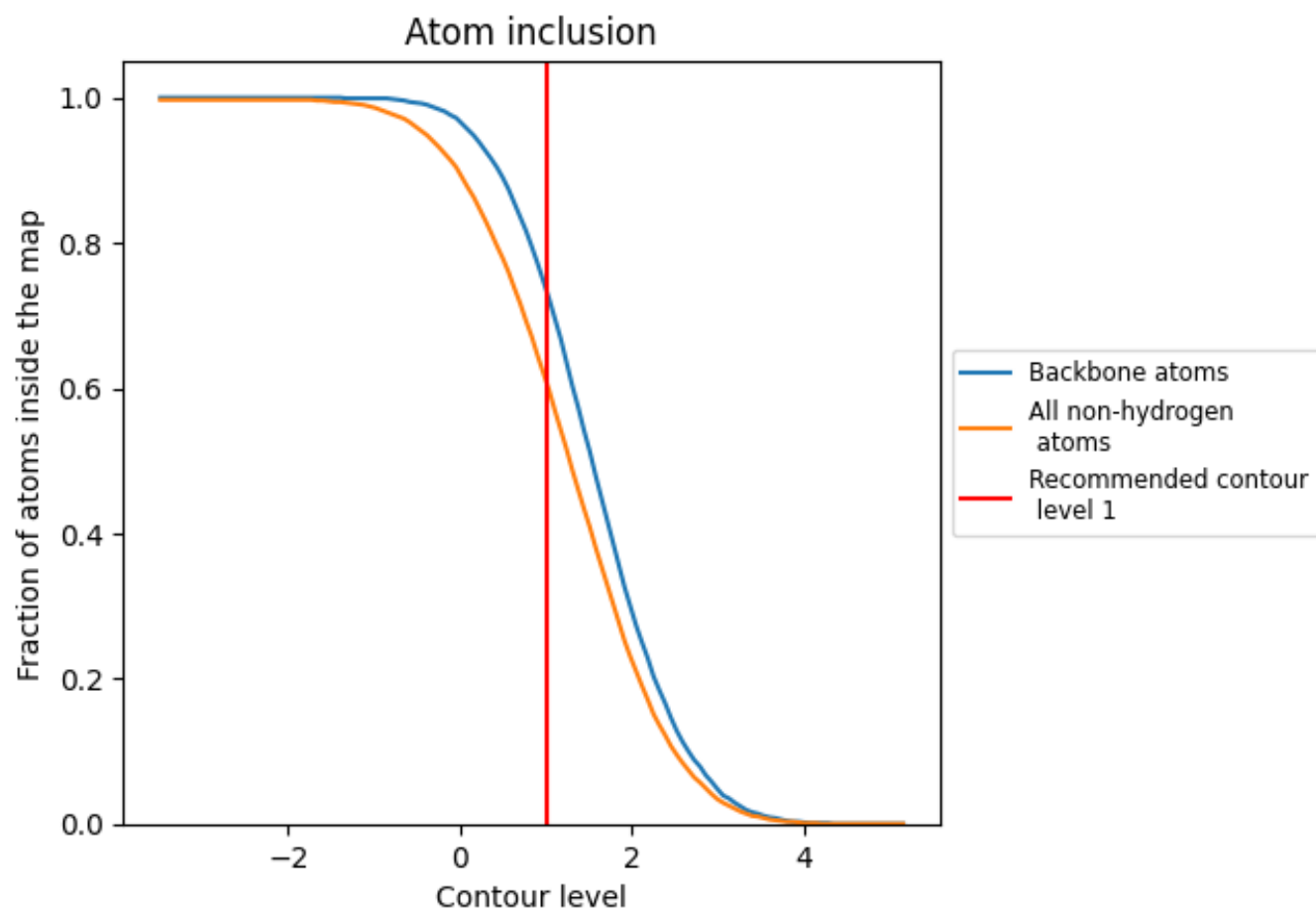
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6100	0.1030
A	0.6080	0.1060
B	0.5780	0.0910
C	0.5740	0.0980
D	0.6270	0.1090
E	0.6610	0.1100

