wwPDB EM Validation Summary Report (i)

Nov 9, 2024 – 01:44 pm GMT

PDB ID	:	4AQ5
EMDB ID	:	EMD-2071
Title	:	Gating movement in acetylcholine receptor analysed by time-resolved electron cryo-microscopy (closed class)
Authors	:	Unwin, N.; Fujiyoshi, Y.
Deposited on	:	2012-04-12
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 (i) 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 (i)) were used in the production of this report:

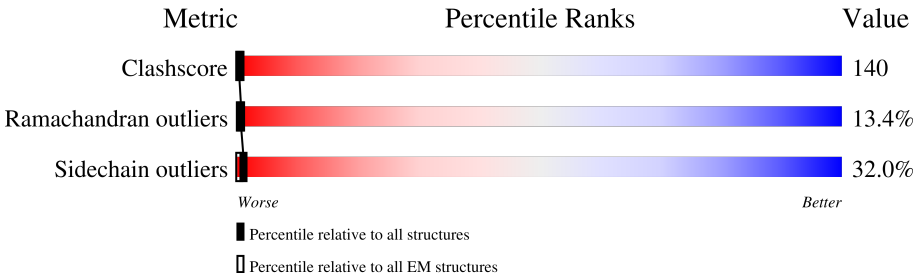
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (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)
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 <=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	31% · 23% 28% 25% 20%
1	D	461	30% · 24% 26% 26% 20%
2	B	493	32% · 22% 27% 21% 25%
3	C	522	31% · 19% 28% 21% 29%
4	E	488	28% · 23% 26% 24% 24%

2 Entry composition (i)

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.

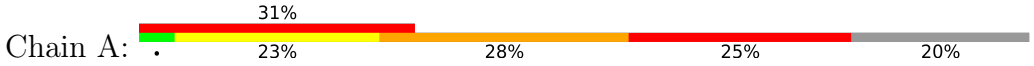
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

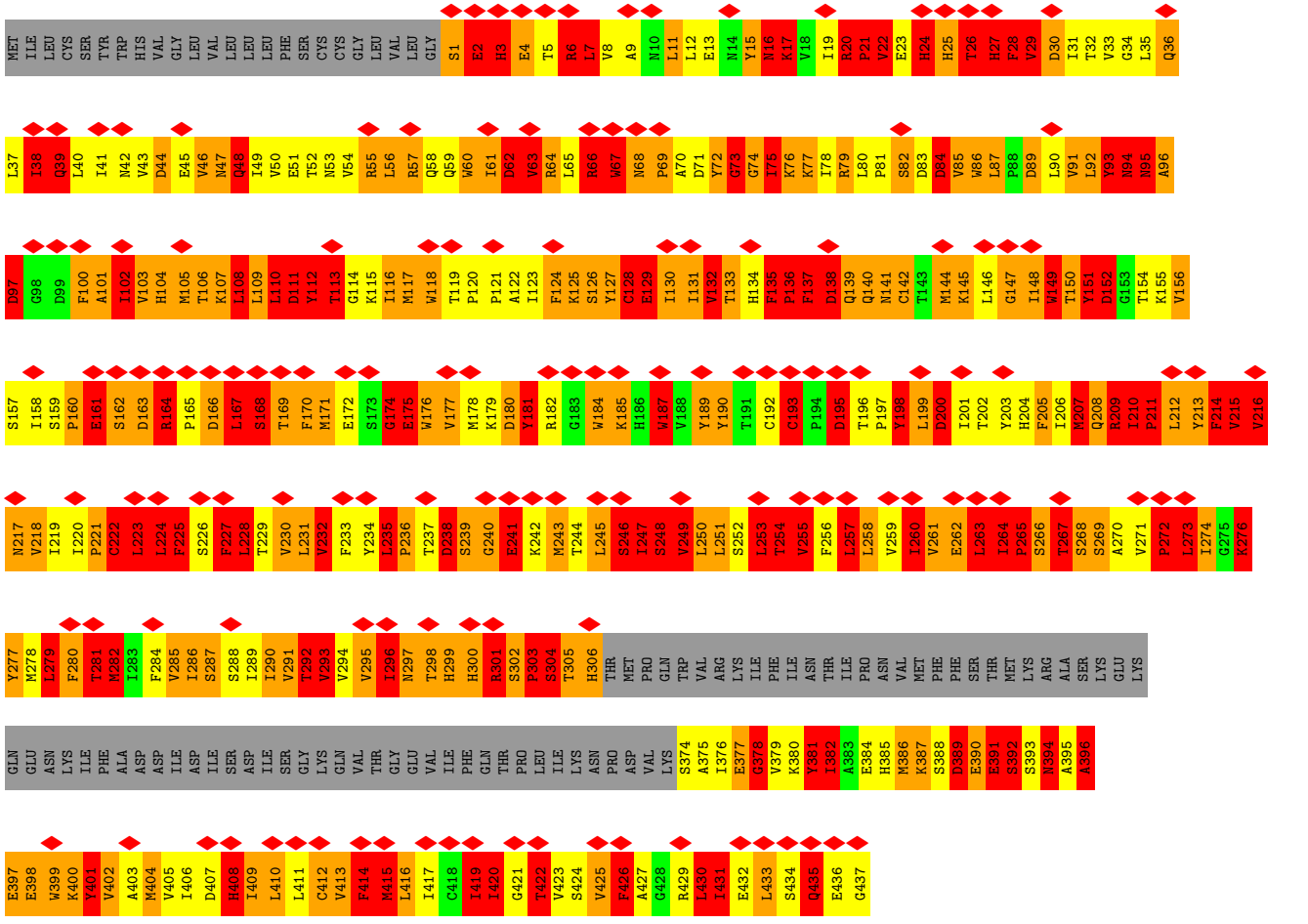
3 Residue-property plots (i)

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

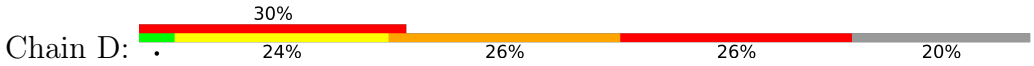
Chain A:

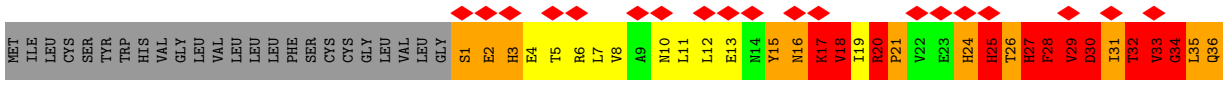


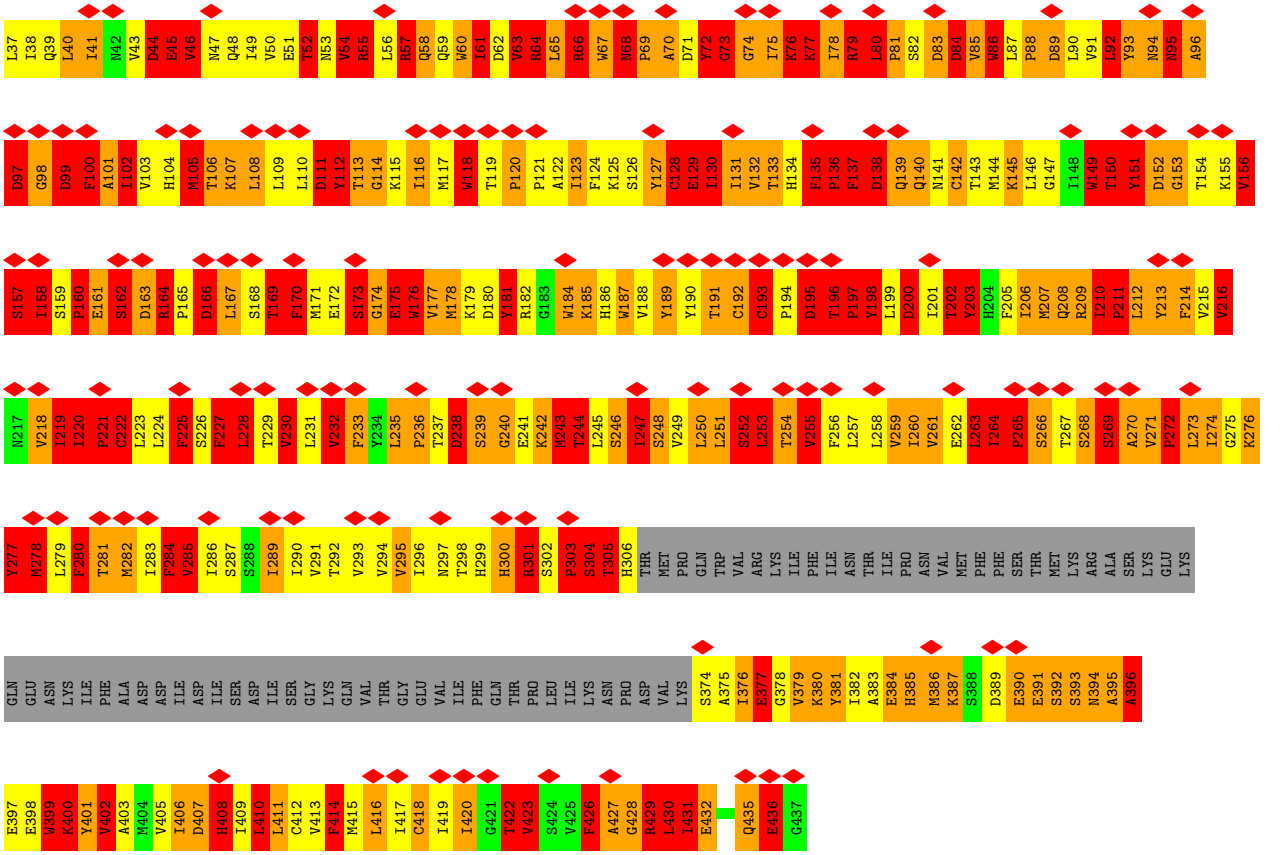


• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

Chain D:

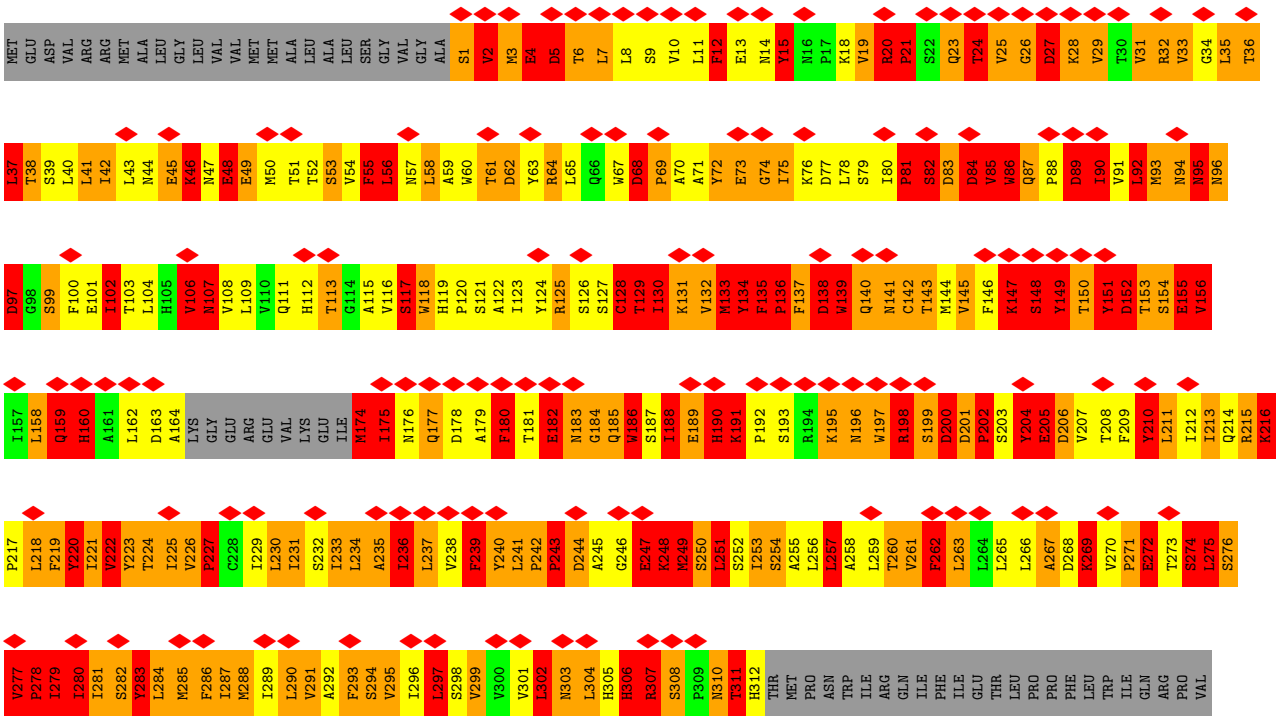


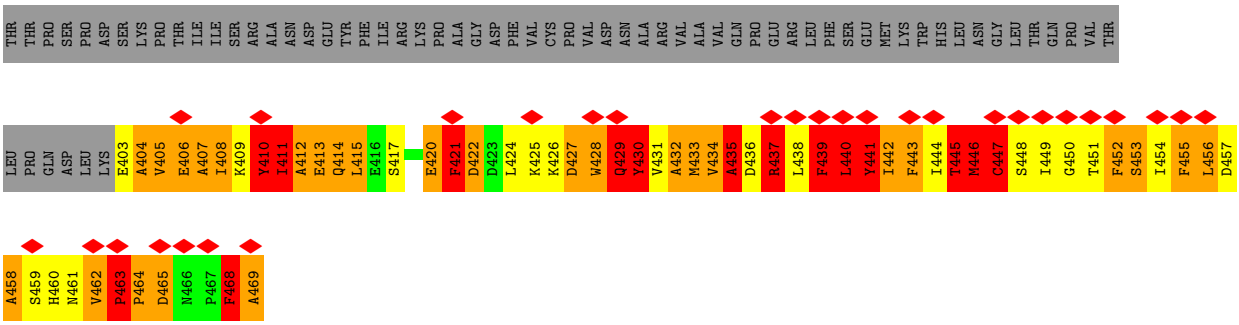




• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

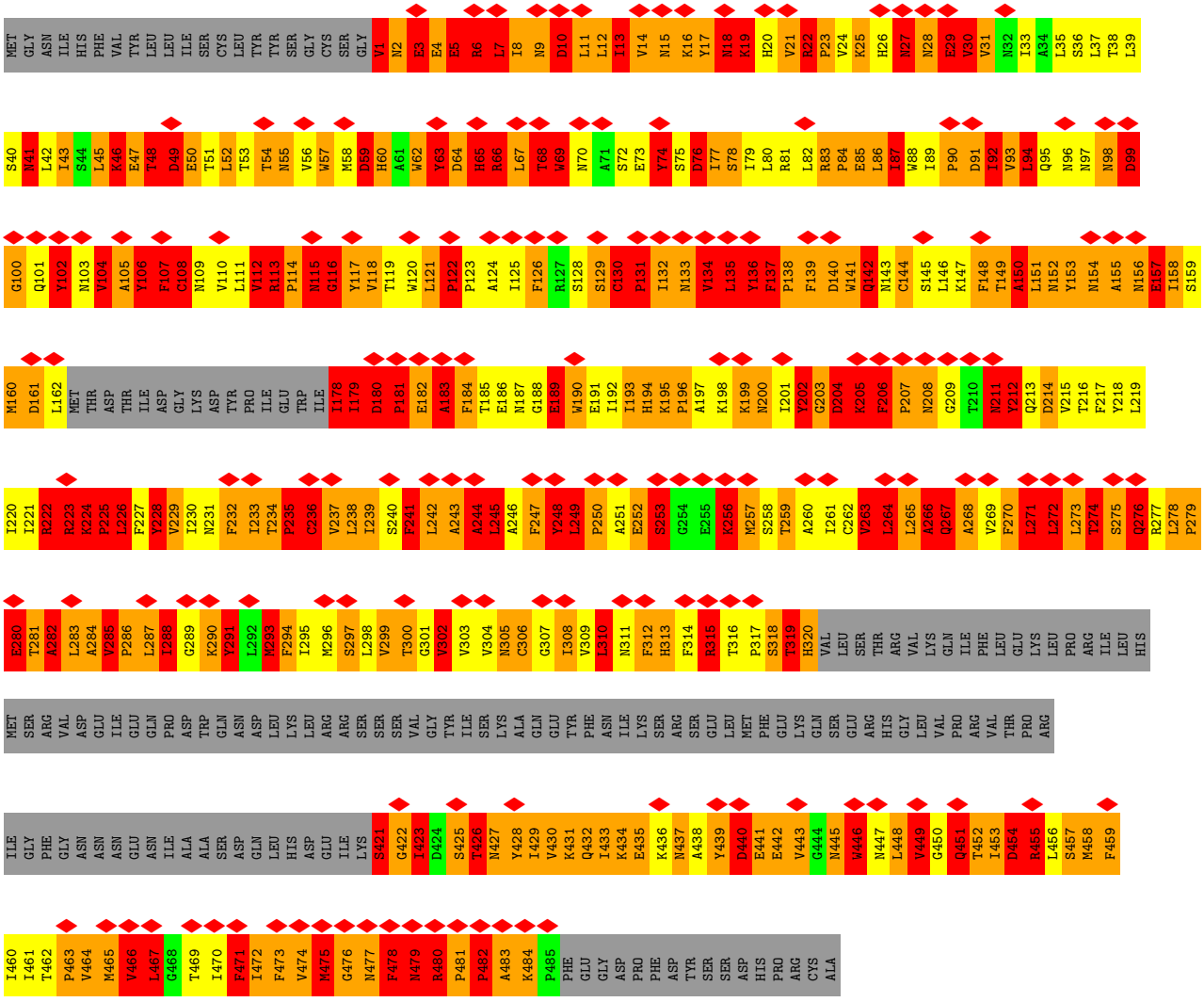
Chain B:





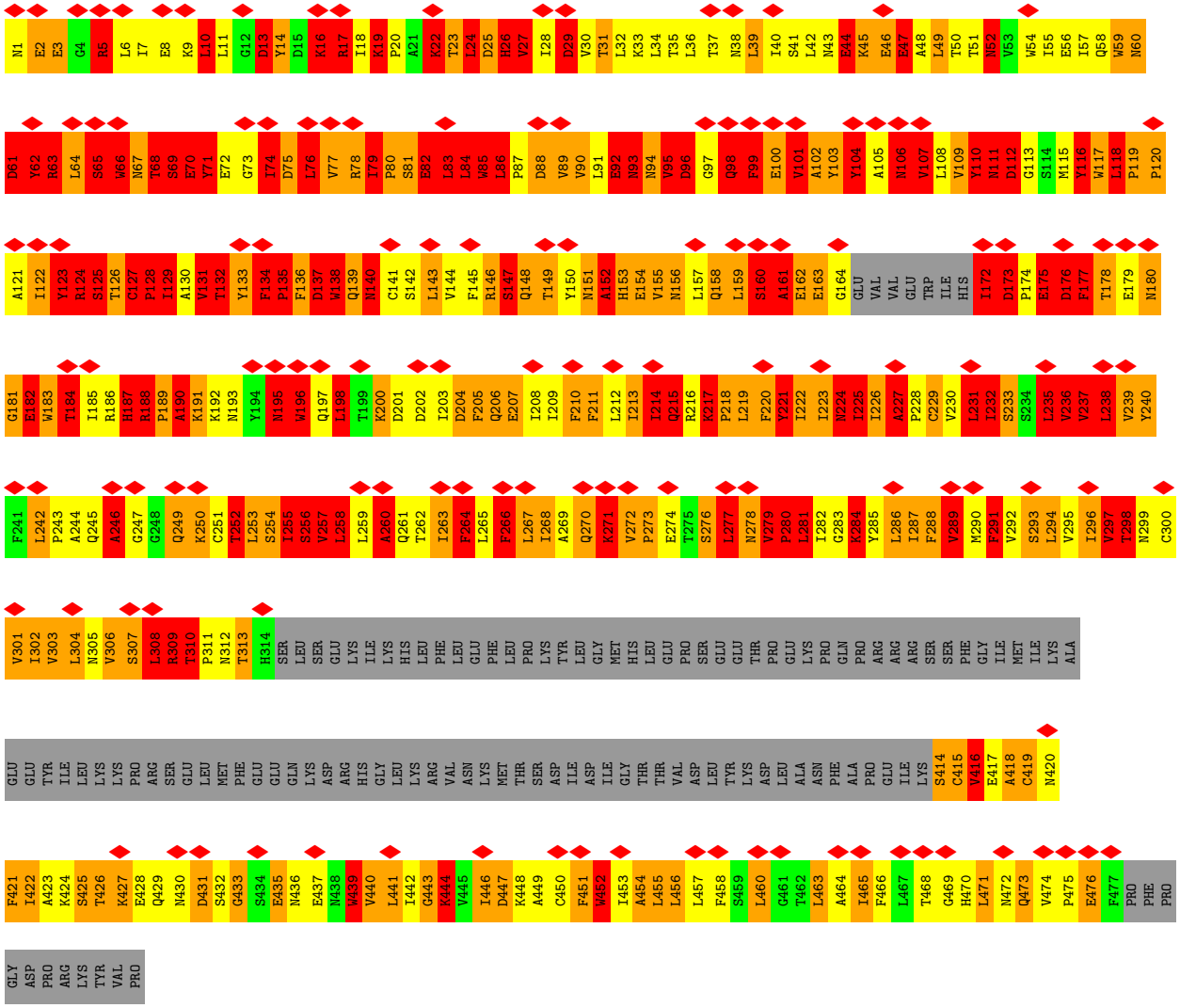
• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain C:



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E:


N1 E2 E3 G4 R5 L6 I7 E8 K9 L10 L11 G12 D13 Y14 D15 K16 R17 I18 K19 P20 A21 K22 T23 L24 D25 H26 V27 I28 D29 V30 T31 L32 K33 L34 T35 L36 T37 N38 L39 I40 S41 L42 N43 E44 K45 E46 E47 A48 L49 T50 T51 N52 V53 W54 I55 E56 I57 Q58 W59 N60
D61 Y62 R63 L64 S65 W66 N67 T68 S69 E70 Y71 E72 G73 I74 D75 L76 V77 R78 I79 P80 S81 E82 L83 L84 V85 L86 P87 D88 V89 V90 L91 E92 N93 N94 V95 D96 G97 Q98 F99 E100 V101 A102 Y103 Y104 A105 N106 V107 L108 V109 Y110 N111 D112 G113 S114 M115 Y116 W117 L118 P119 P120
A121 I122 Y123 R124 S125 T126 C127 P128 I129 A130 W131 T132 Y133 F134 P135 F136 D137 W138 Q139 N140 C141 S142 L143 V144 F145 R146 S147 Q148 T149 Y150 N151 A152 H153 E154 V155 N156 L157 Q158 L159 S160 A161 E162 E163 G164 GLU VAL VAL GLU TRP ILE HIS I172 D173 P174 E175 D176 F177 T178 E179 N180
G181 E182 W183 T184 I185 R186 H187 R188 P189 A190 K191 K192 N193 Y194 N195 W196 Q197 L198 T199 K200 D201 D202 I203 D204 F205 Q206 E207 I208 I209 F210 F211 L212 I213 I214 Q215 R216 K217 P218 L219 F220 Y221 I222 I223 N224 I225 I226 A227 P228 C229 V230 L231 I232 S233 S234 L235 V236 V237 L238 V239 Y240
F241 L242 P243 A244 Q245 A246 G247 G248 Q249 K250 C251 T252 L253 S254 I255 S256 V257 L258 L259 A260 Q261 T262 I263 F264 L265 F266 L267 I268 A269 Q270 K271 V272 P273 E274 T275 S276 L277 N278 V279 P280 L281 I282 G283 K284 Y285 L286 I287 F288 V289 M290 F291 V292 S293 L294 V295 I296 V297 T298 N299 C300
V301 I302 V303 L304 N305 V306 S307 L308 R309 T310 P311 N312 T313 H314 SER LEU SER GLU LYS ILE LYS HIS LEU PHE LEU GLU PHE LEU PRO LYS TYR LEU GLY MET HIS LEU GLU PRO SER GLU GLU THR PRO GLU LYS PRO GLN PRO ARG ARG ARG SER SER PHE GLY ILE MET ILE LYS ALA
GLU GLU TYR ILE LEU LYS LYS PRO ARG SER GLU LEU MET PHE GLU GLU GLN LYS ASP ARG HIS GLY LEU LYS ARG VAL ASN LYS MET THR SER ASP ILE ASP ILE GLY THR THR VAL ASP LEU TYR LYS ASP LEU ALA ASN PHE ALA PRO GLU ILE LYS S414 C415 V416 E417 A418 C419 N420
F421 I422 A423 K424 S425 T426 K427 E428 Q429 N430 D431 S432 G433 S434 E435 N436 E437 N438 W439 V440 L441 I442 G443 K444 V445 I446 D447 K448 A449 C450 F451 W452 I453 A454 L455 L456 L457 F458 S459 L460 G461 T462 L463 A464 I465 F466 L467 T468 G469 H470 L471 N472 Q473 V474 P475 E476 F477 PRO PHE PRO
GLY ASP PRO ARG LYS TYR VAL PRO

4 Experimental information (i)

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 ($e^-/Å^2$)	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	4.906	Depositor
Minimum map value	-3.900	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.2	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%)	2.70	244/4186 (5.8%)
1	D	1.70	13/3069 (0.4%)	2.80	272/4186 (6.5%)
2	B	1.70	14/3048 (0.5%)	2.78	261/4162 (6.3%)
3	C	1.63	11/3059 (0.4%)	2.83	284/4175 (6.8%)
4	E	1.67	17/3057 (0.6%)	2.80	266/4174 (6.4%)
All	All	1.68	70/15302 (0.5%)	2.78	1327/20883 (6.4%)

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	7	116
1	D	6	125
2	B	6	112
3	C	6	125
4	E	12	107
All	All	37	585

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-9.22	1.12	1.34
4	E	8	GLU	CB-CG	8.90	1.69	1.52
1	A	118	TRP	CB-CG	8.84	1.66	1.50
1	D	175	GLU	CD-OE1	8.46	1.34	1.25
1	A	222	CYS	CB-SG	-7.49	1.69	1.82

The worst 5 of 1327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	309	ARG	NE-CZ-NH1	25.87	133.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	307	ARG	NE-CZ-NH2	24.36	132.48	120.30
3	C	277	ARG	NE-CZ-NH2	21.78	131.19	120.30
3	C	17	TYR	CB-CG-CD1	-19.82	109.11	121.00
4	E	17	ARG	NE-CZ-NH2	-18.78	110.91	120.30

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	SER	CA
1	A	209	ARG	CA
1	A	267	THR	CB
1	A	292	THR	CB
1	A	304	SER	CA

5 of 585 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASN	Mainchain
1	A	24	HIS	Mainchain
1	A	25	HIS	Mainchain
1	A	28	PHE	Mainchain
1	A	3	HIS	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	3004	897	0
1	D	2991	0	3005	854	0
2	B	2972	0	2951	830	0
3	C	2983	0	2985	848	0
4	E	2987	0	2988	947	0
All	All	14924	0	14933	4181	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 140.

The worst 5 of 4181 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:A:282:MET:CE	1:A:282:MET:SD	2.01	1.46
1:D:86:TRP:CD2	1:D:86:TRP:O	1.71	1.40
2:B:306:HIS:O	2:B:306:HIS:ND1	1.62	1.29
1:A:113:THR:CG2	1:A:113:THR:O	1.76	1.28
1:A:236:PRO:HB3	1:A:299:HIS:CE1	1.69	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%)	260 (71%)	58 (16%)	48 (13%)	0	4
1	D	366/461 (79%)	264 (72%)	56 (15%)	46 (13%)	0	4
2	B	364/493 (74%)	243 (67%)	65 (18%)	56 (15%)	0	3
3	C	364/522 (70%)	252 (69%)	68 (19%)	44 (12%)	0	4
4	E	365/488 (75%)	234 (64%)	80 (22%)	51 (14%)	0	3
All	All	1825/2425 (75%)	1253 (69%)	327 (18%)	245 (13%)	0	4

5 of 245 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PRO
1	A	24	HIS
1	A	27	HIS
1	A	48	GLN
1	A	76	LYS

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%)	231 (67%)	112 (33%)	0	2
1	D	343/427 (80%)	230 (67%)	113 (33%)	0	2
2	B	340/449 (76%)	235 (69%)	105 (31%)	0	2
3	C	335/475 (70%)	235 (70%)	100 (30%)	0	2
4	E	337/447 (75%)	224 (66%)	113 (34%)	0	1
All	All	1698/2225 (76%)	1155 (68%)	543 (32%)	1	2

5 of 543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	101	VAL
4	E	140	ASN
4	E	96	ASP
4	E	284	LYS
2	B	283	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	479	ASN
4	E	472	ASN
1	D	408	HIS
4	E	299	ASN
4	E	156	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 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	3
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	306:VAL	C	307:SER	N	1.19
1	E	309:ARG	C	310:THR	N	1.19
1	B	129:THR	C	130:ILE	N	1.12

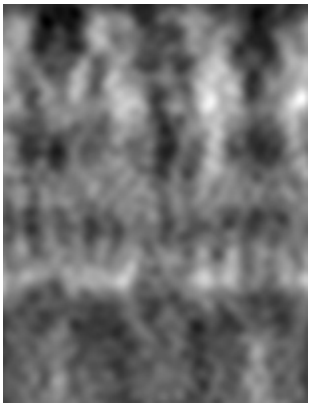
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2071. These allow visual inspection of the internal detail of the map and identification of artifacts.

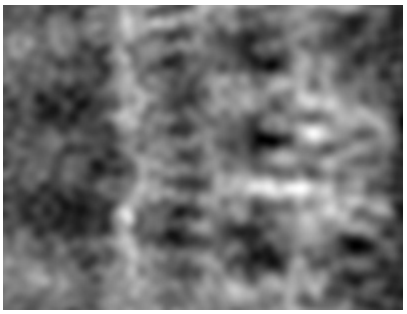
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

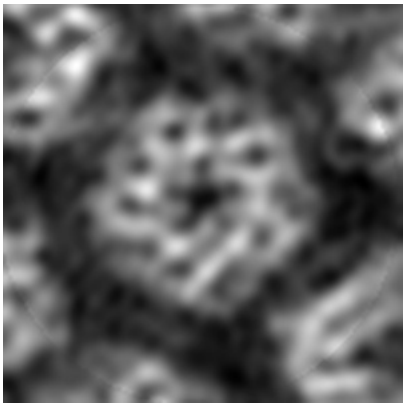
6.1.1 Primary map



X



Y



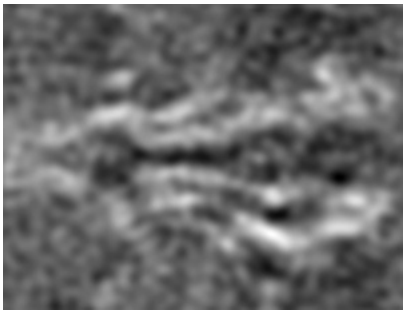
Z

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

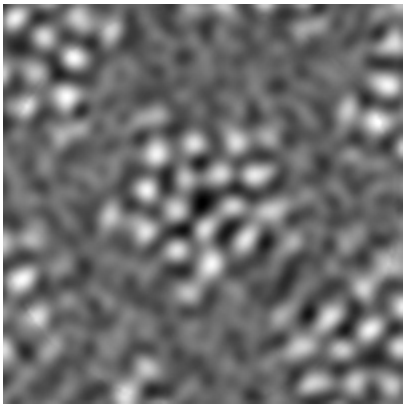
6.2 Central slices

6.2.1 Primary map

X Index: 64



Y Index: 64



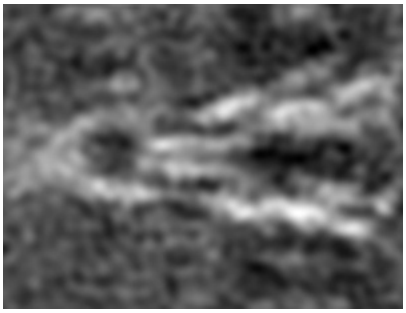
Z Index: 84

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

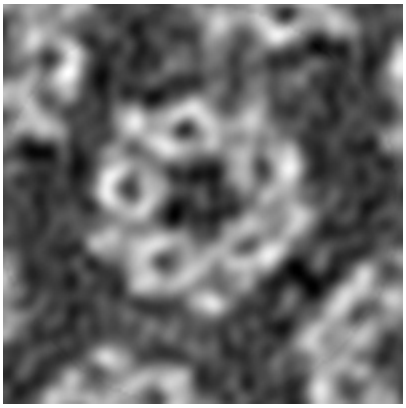
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 7



Y Index: 71

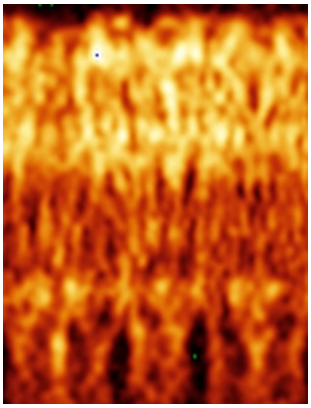


Z Index: 145

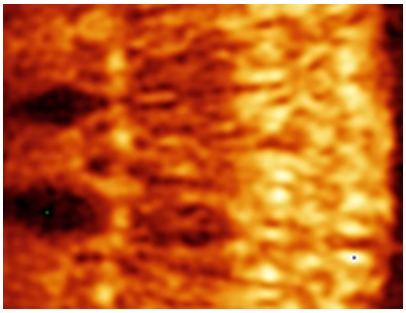
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

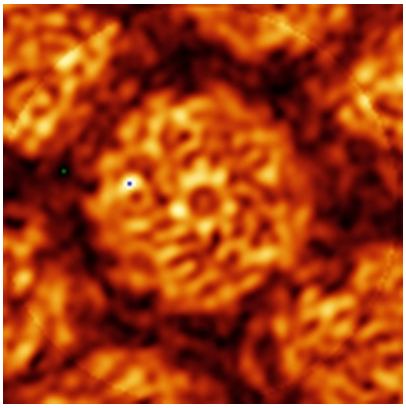
6.4.1 Primary map



X



Y

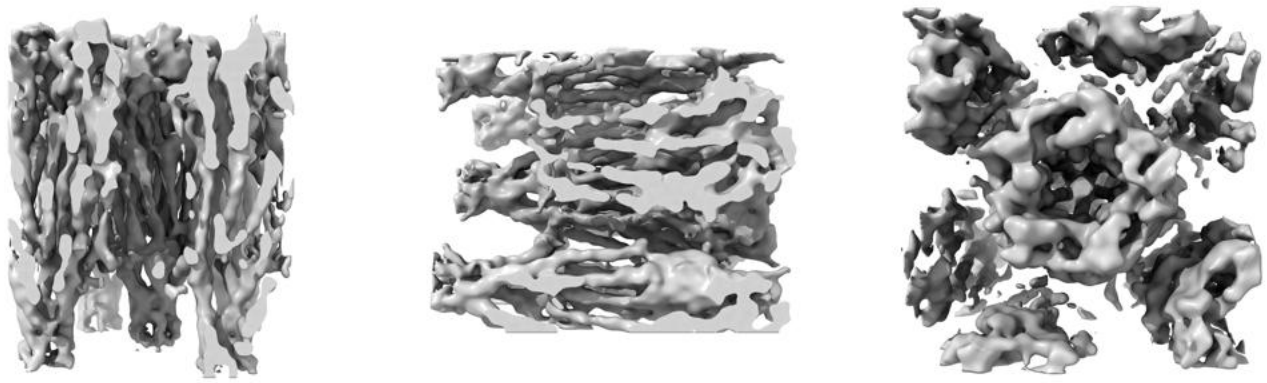


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

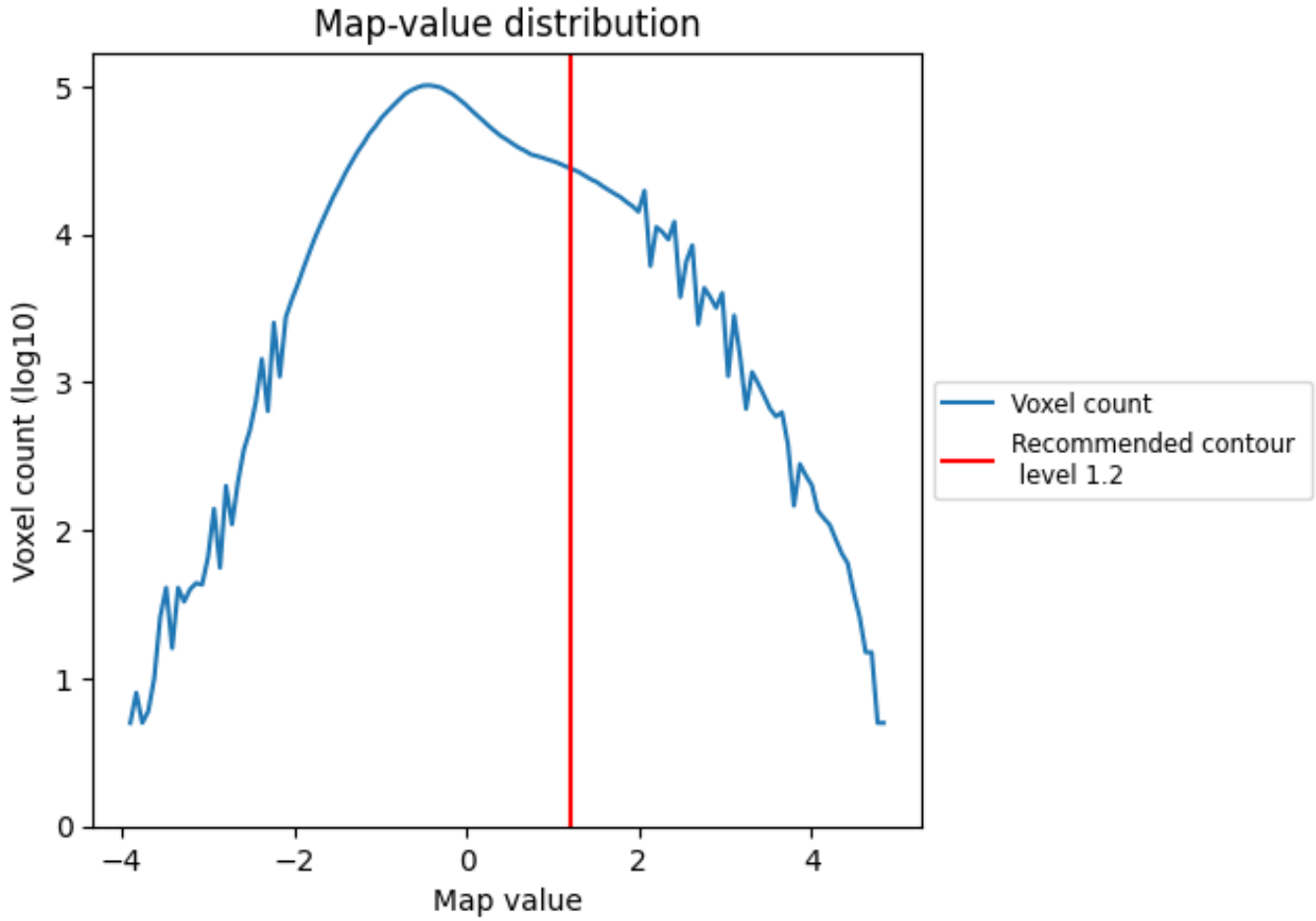
6.6 Mask visualisation (i)

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

7 Map analysis

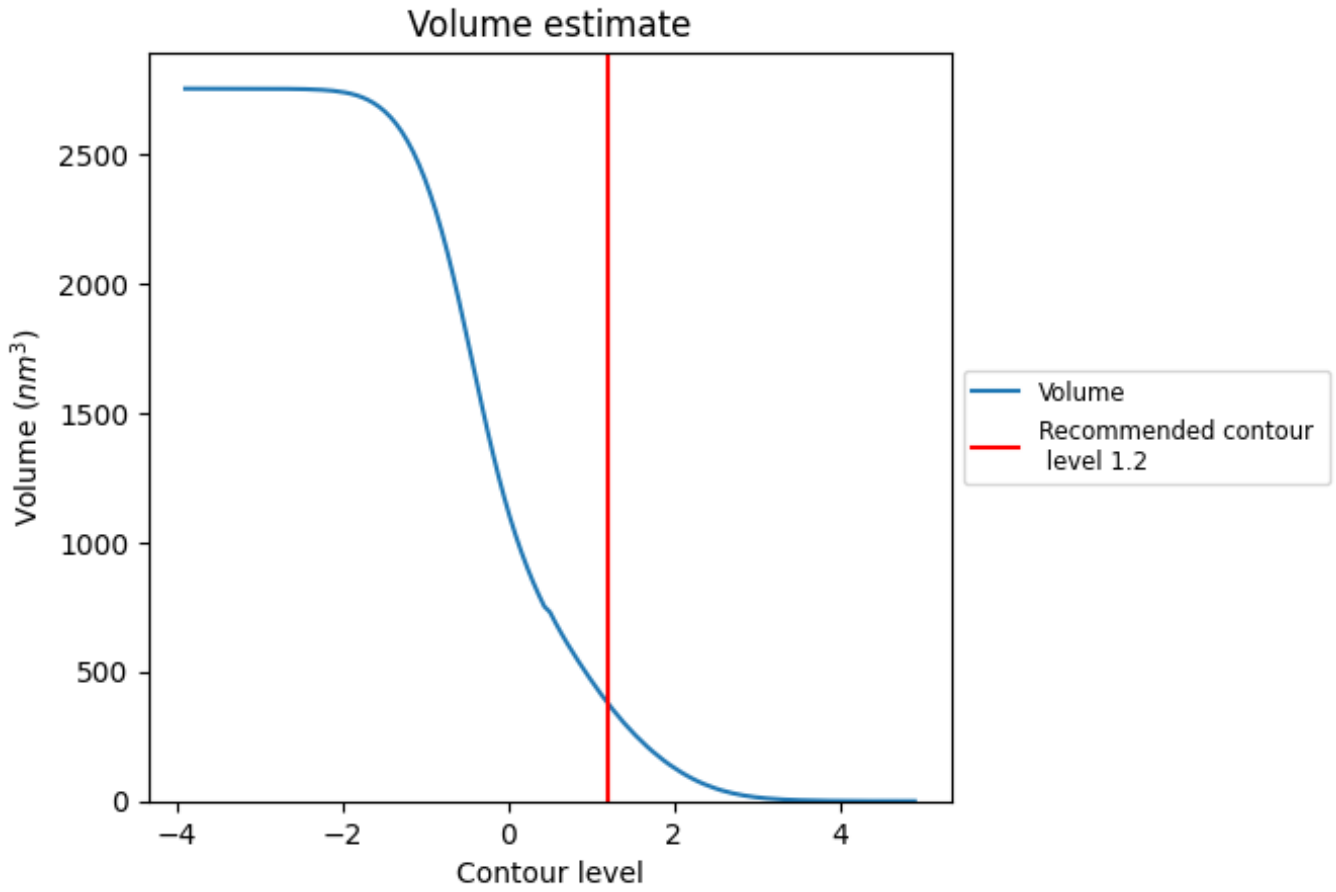
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 379 nm^3; this corresponds to an approximate mass of 342 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.

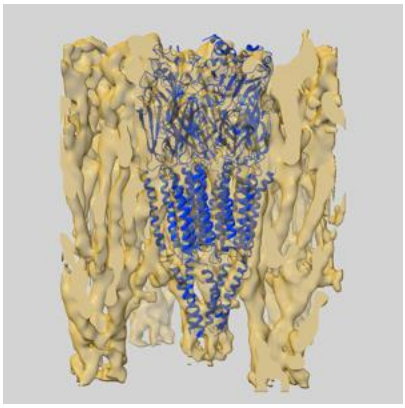
8 Fourier-Shell correlation

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

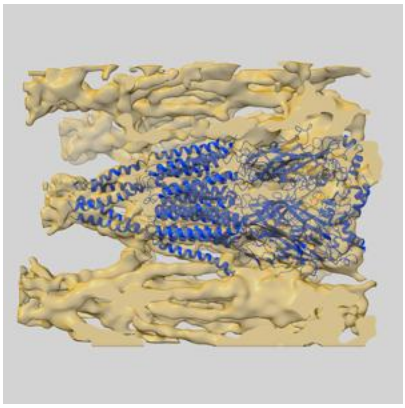
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2071 and PDB model 4AQ5. Per-residue inclusion information can be found in section 3 on page 4.

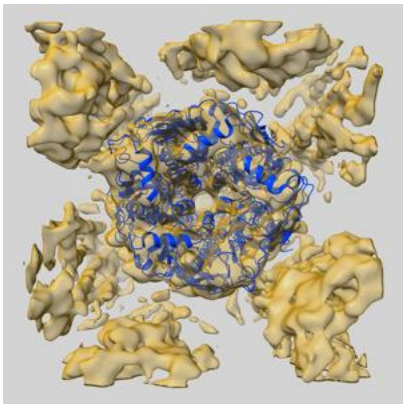
9.1 Map-model overlay



X



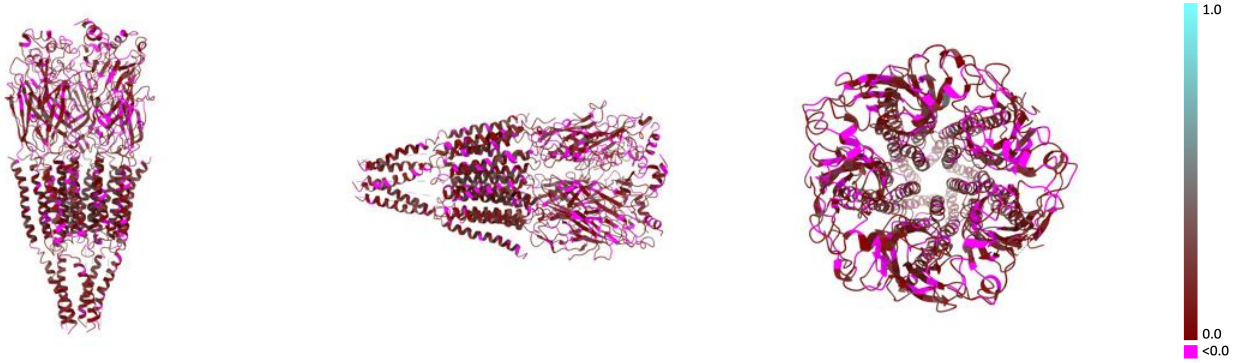
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2 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.

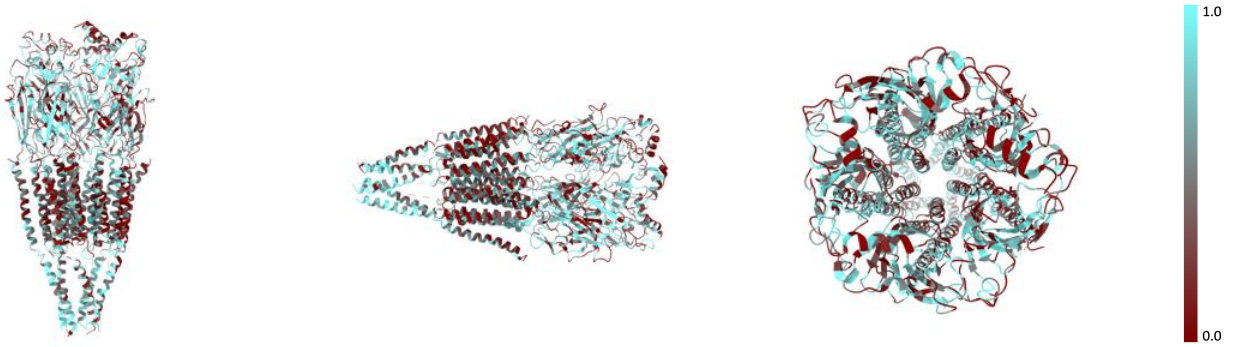
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

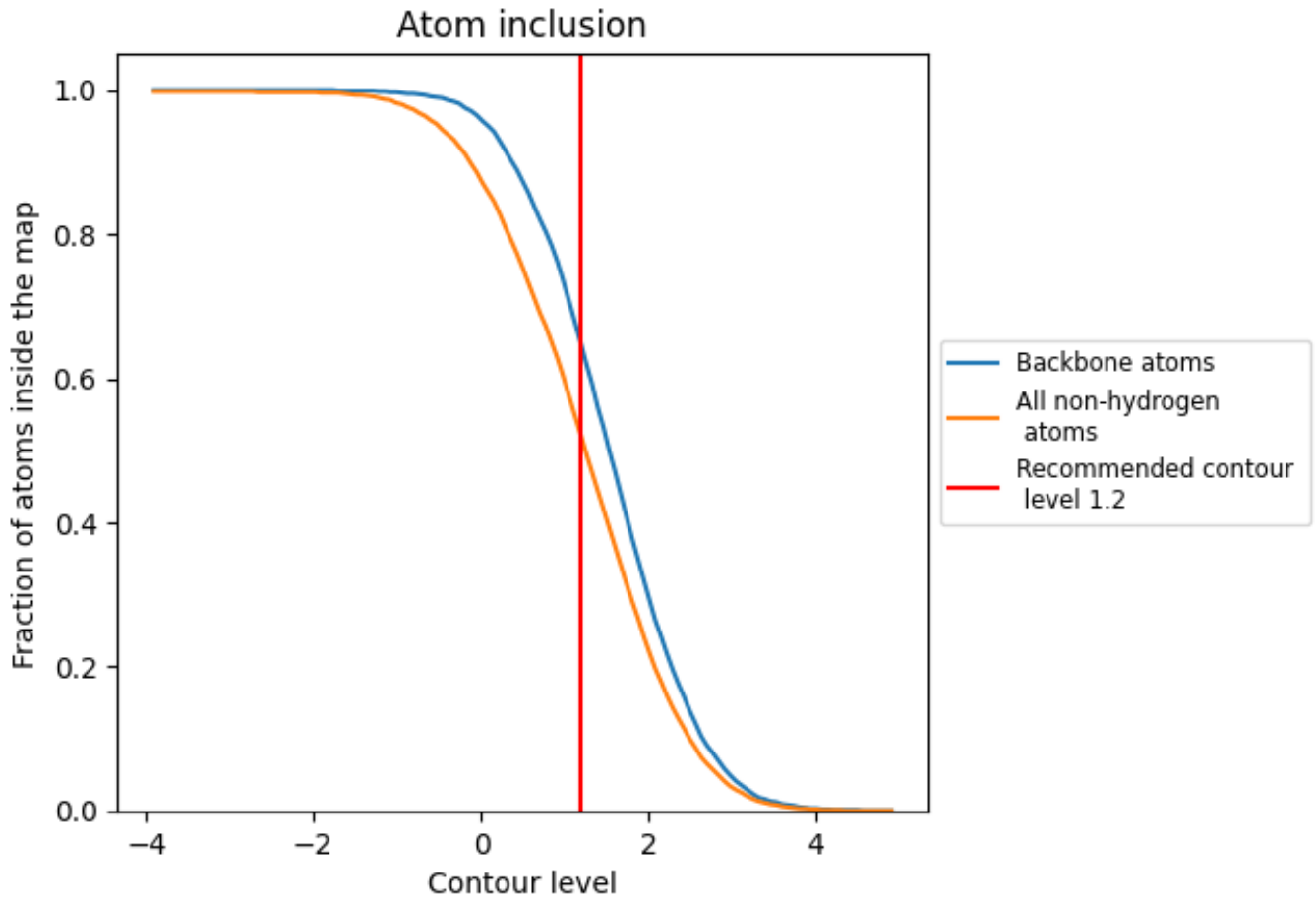
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.2).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 52% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5200	0.1050
A	0.5320	0.1070
B	0.4930	0.0950
C	0.4880	0.0980
D	0.5340	0.1100
E	0.5530	0.1160