wwPDB EM Validation Summary Report (i)

Apr 30, 2024 – 11:37 pm BST

PDB ID	:	1OED
EMDB ID	:	EMD-1044
Title	:	STRUCTURE OF ACETYLCHOLINE RECEPTOR PORE FROM ELECTRON IMAGES
Authors	:	Miyazawa, A.; Fujiyoshi, Y.; Unwin, N.
Deposited on	:	2003-03-24
Resolution	:	4.00 Å(reported)

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:

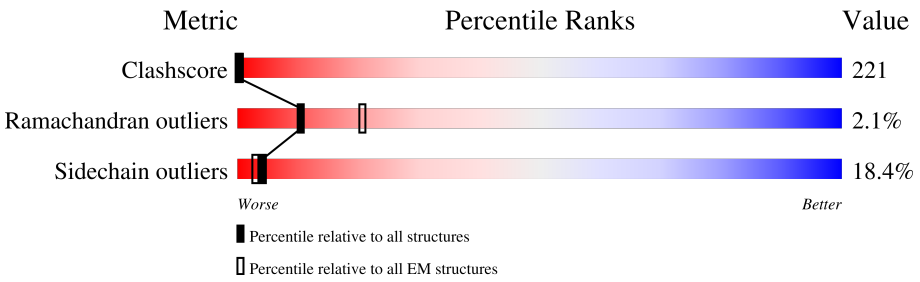
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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 <=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	227	37%; 5%, 40%, 10%, 44%
1	D	227	30%; 5%, 41%, 9%, 44%
2	B	250	32%; •, 34%, 11%, •, 49%
3	C	260	34%; 6%, 33%, 8%, •, 51%
4	E	260	32%; 7%, 30%, 12%, 51%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4926 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
			Total	C	N	O	S		
1	A	127	978	659	144	167	8	0	0
1	D	127	978	659	144	167	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLY	VAL	variant	UNP P02711
A	291	ILE	VAL	variant	UNP P02711
A	318	ASP	ASN	variant	UNP P02711
D	230	GLY	VAL	variant	UNP P02711
D	291	ILE	VAL	variant	UNP P02711
D	318	ASP	ASN	variant	UNP P02711

- Molecule 2 is a protein called Acetylcholine receptor beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	127	995	677	147	165	6	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	ILE	VAL	variant	UNP Q6S3I0
B	259	VAL	LEU	variant	UNP Q6S3I0
B	282	ARG	SER	variant	UNP Q6S3I0
B	442	VAL	ILE	variant	UNP Q6S3I0
B	444	PHE	ILE	variant	UNP Q6S3I0
B	445	VAL	THR	variant	UNP Q6S3I0
B	446	ILE	MET	variant	UNP Q6S3I0

- Molecule 3 is a protein called Acetylcholine receptor delta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	127	982	660	151	163	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	244	SER	ALA	variant	UNP Q6S3H8
C	262	SER	CYS	variant	UNP Q6S3H8
C	303	ILE	VAL	variant	UNP Q6S3H8
C	343	ALA	VAL	variant	UNP Q6S3H8
C	346	SER	ILE	variant	UNP Q6S3H8
C	480	HIS	ARG	variant	UNP Q6S3H8

- Molecule 4 is a protein called Acetylcholine receptor gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	128	993	676	149	161	7	0	0

There are 7 discrepancies between the modelled and reference sequences:

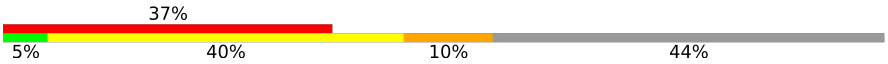
Chain	Residue	Modelled	Actual	Comment	Reference
E	295	MET	LEU	variant	UNP Q6S3H9
E	296	LEU	VAL	variant	UNP Q6S3H9
E	299	MET	THR	variant	UNP Q6S3H9
E	327	GLY	GLU	variant	UNP Q6S3H9
E	336	GLN	HIS	variant	UNP Q6S3H9
E	461	ILE	LEU	variant	UNP Q6S3H9
E	472	PHE	LEU	variant	UNP Q6S3H9

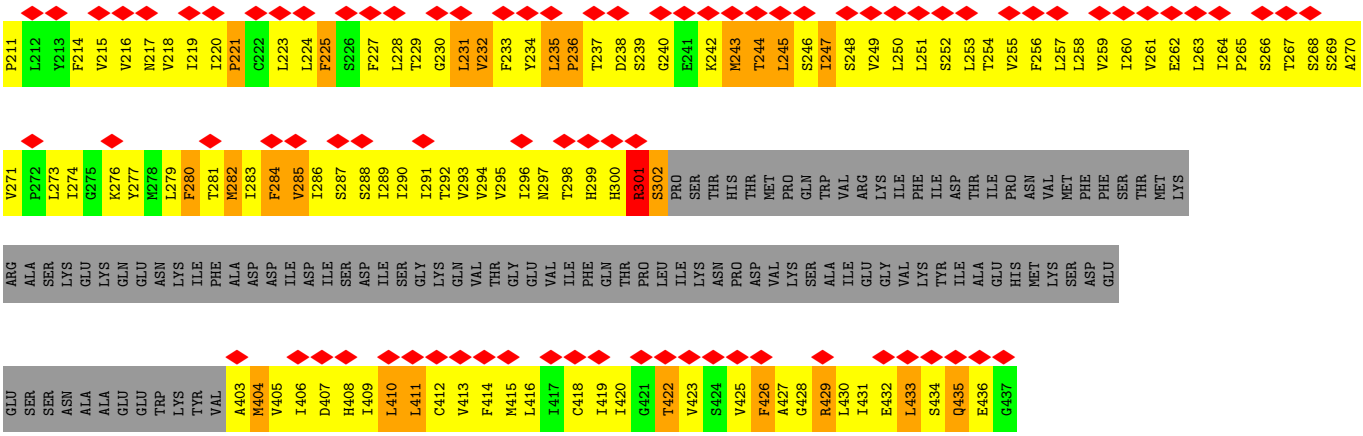
3 Residue-property plots (i)

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

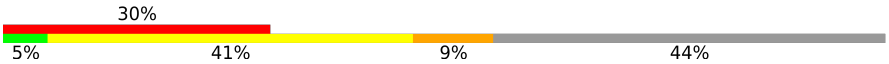
Chain A:

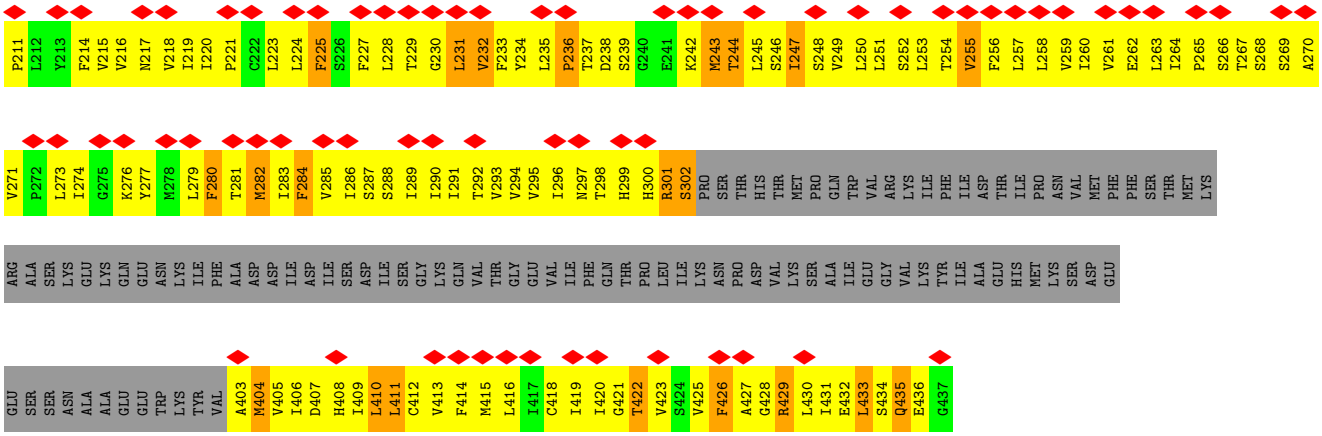




• Molecule 1: Acetylcholine receptor subunit alpha

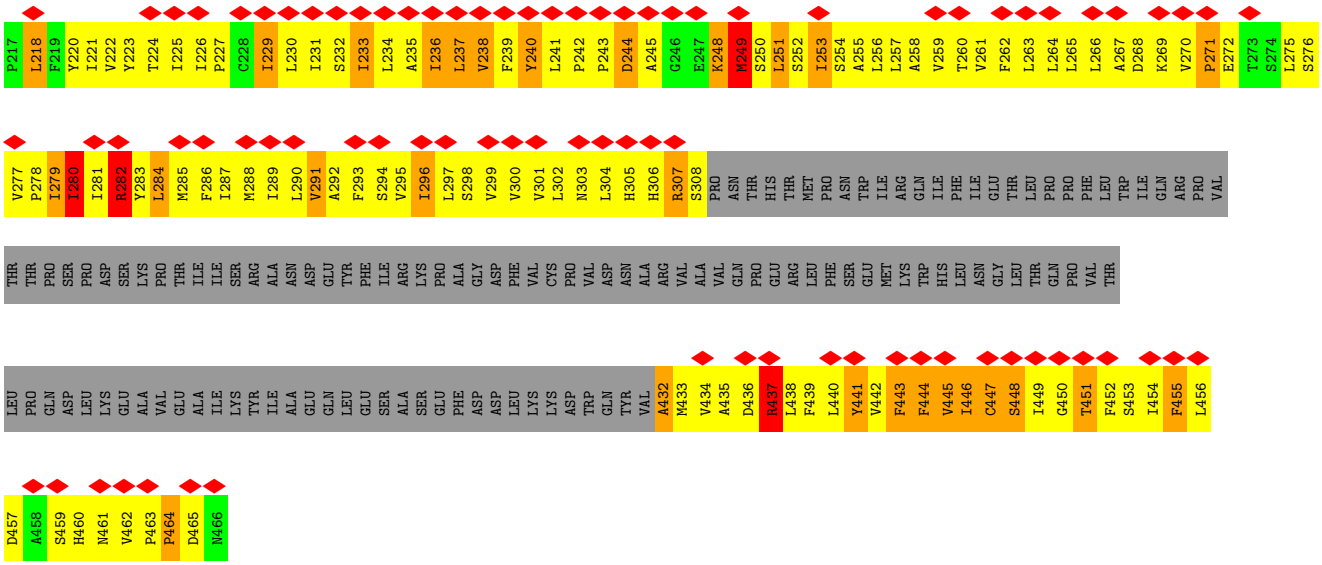
Chain D:





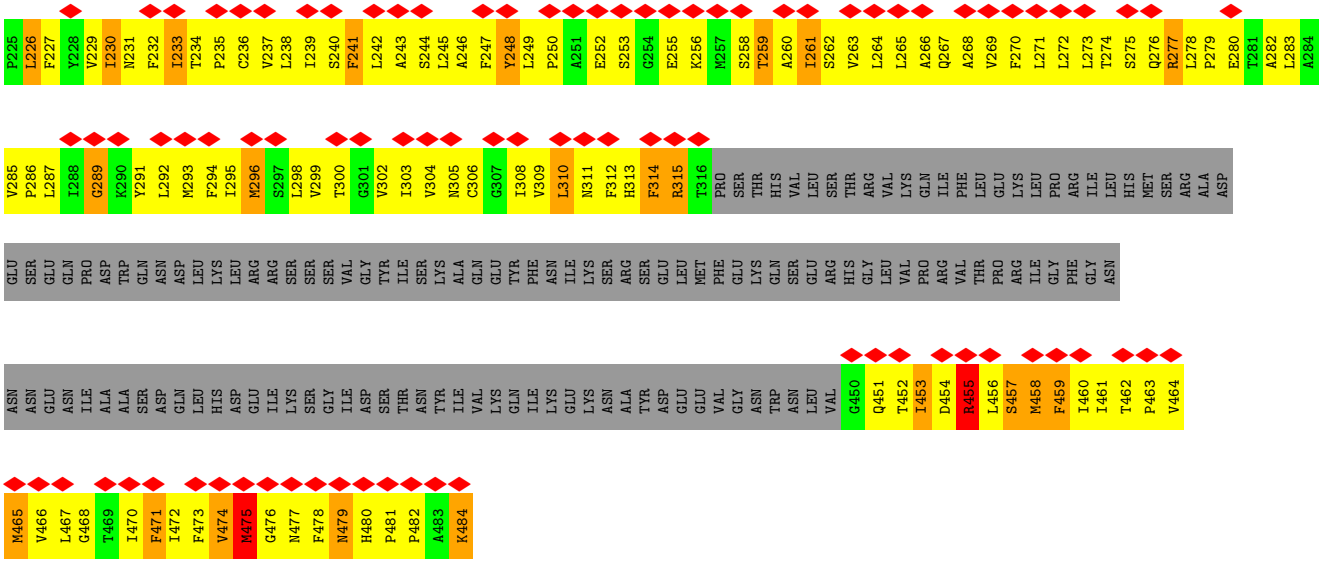
• Molecule 2: Acetylcholine receptor beta subunit

Chain B:



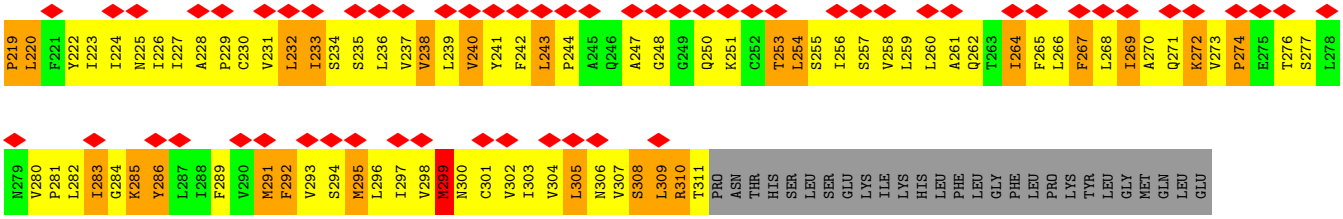
- Molecule 3: Acetylcholine receptor delta subunit

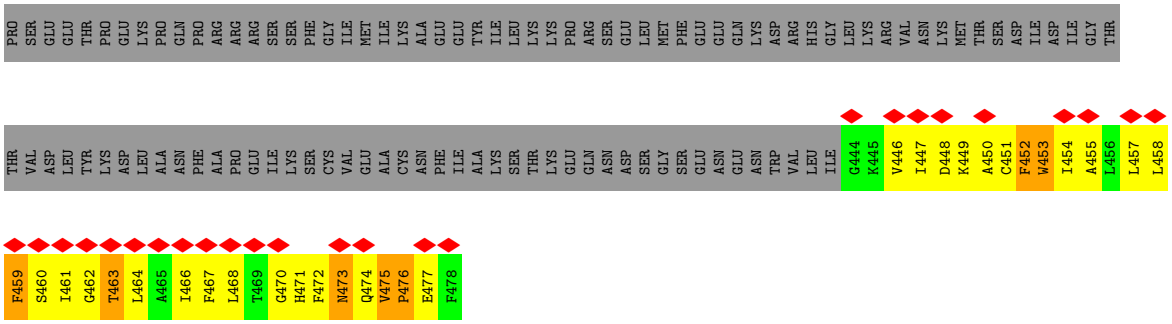
Chain C:



- Molecule 4: Acetylcholine receptor gamma subunit

Chain E:




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 SER CYS VAL GLU ALA CYS ASN PHE ILE ALA LYS SER THR LYS GLU GLN ASN ASP SER GLY SER GLU ASN GLU ASN TRP VAL LEU ILE G444 K445 V446 I447 D448 K449 A450 C451 F452 W453 I454 A455 L456 L457 L458
F459 S460 I461 G462 T463 L464 A465 I466 F467 L468 T469 G470 H471 F472 N473 Q474 V475 P476 E477 F478

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	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	36800	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.320	Depositor
Minimum map value	-2.439	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.18	Depositor
Map size (Å)	128, 128, 168	wwPDB
Map dimensions	128, 128, 55	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1, 1, 1	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	0.70	1/996 (0.1%)	1.11	8/1357 (0.6%)
1	D	0.71	1/996 (0.1%)	1.11	7/1357 (0.5%)
2	B	0.99	4/1019 (0.4%)	1.16	7/1393 (0.5%)
3	C	0.75	0/1005	1.16	6/1367 (0.4%)
4	E	0.72	0/1014	1.17	5/1381 (0.4%)
All	All	0.78	6/5030 (0.1%)	1.14	33/6855 (0.5%)

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
4	E	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	271	PRO	N-CD	-18.04	1.22	1.47
2	B	445	VAL	CB-CG1	9.40	1.72	1.52
1	A	403	ALA	C-O	8.17	1.38	1.23
1	D	403	ALA	C-O	8.16	1.38	1.23
2	B	448	SER	CB-OG	-6.73	1.33	1.42

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	445	VAL	CG1-CB-CG2	-8.62	97.11	110.90
3	C	315	ARG	NE-CZ-NH2	7.83	124.21	120.30
3	C	455	ARG	NE-CZ-NH2	7.74	124.17	120.30
2	B	307	ARG	NE-CZ-NH2	7.61	124.10	120.30
4	E	310	ARG	NE-CZ-NH2	7.35	123.98	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	476	PRO	Mainchain

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	978	0	1059	510	0
1	D	978	0	1059	528	0
2	B	995	0	1064	503	0
3	C	982	0	1040	441	0
4	E	993	0	1077	513	0
All	All	4926	0	5299	2261	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 221.

The worst 5 of 2261 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:286:PHE:CE1	2:B:456:LEU:HB3	1.31	1.64
2:B:463:PRO:CG	2:B:464:PRO:HD3	1.26	1.59
3:C:285:VAL:CG1	3:C:286:PRO:HD2	1.33	1.52
1:A:296:ILE:HD11	4:E:239:LEU:CD1	1.38	1.51
2:B:463:PRO:HG2	2:B:464:PRO:CD	1.43	1.48

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	123/227 (54%)	118 (96%)	4 (3%)	1 (1%)	19	58
1	D	123/227 (54%)	117 (95%)	5 (4%)	1 (1%)	19	58
2	B	123/250 (49%)	108 (88%)	10 (8%)	5 (4%)	3	25
3	C	123/260 (47%)	114 (93%)	6 (5%)	3 (2%)	6	36
4	E	124/260 (48%)	114 (92%)	7 (6%)	3 (2%)	6	36
All	All	616/1224 (50%)	571 (93%)	32 (5%)	13 (2%)	10	39

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	218	LEU
2	B	282	ARG
2	B	249	MET
3	C	289	GLY
3	C	451	GLN

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	118/209 (56%)	98 (83%)	20 (17%)	2	14
1	D	118/209 (56%)	101 (86%)	17 (14%)	3	18
2	B	116/229 (51%)	89 (77%)	27 (23%)	1	5
3	C	111/233 (48%)	93 (84%)	18 (16%)	2	15
4	E	114/235 (48%)	90 (79%)	24 (21%)	1	6
All	All	577/1115 (52%)	471 (82%)	106 (18%)	4	10

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	457	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	269	SER
4	E	309	LEU
3	C	465	MET
1	D	225	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	300	HIS
1	D	408	HIS
4	E	473	ASN
1	D	435	GLN
3	C	267	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 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.

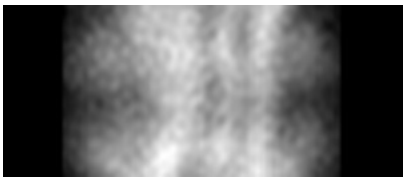
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1044. These allow visual inspection of the internal detail of the map and identification of artifacts.

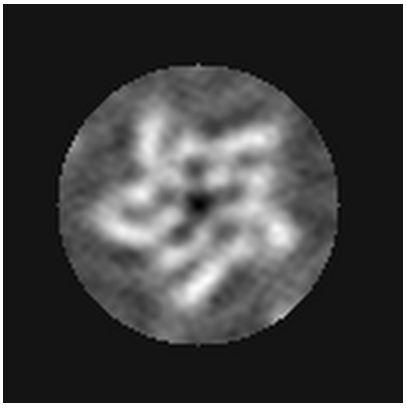
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

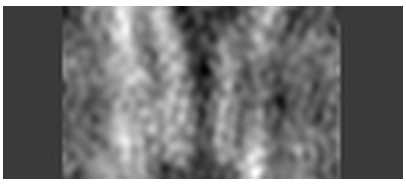
Y

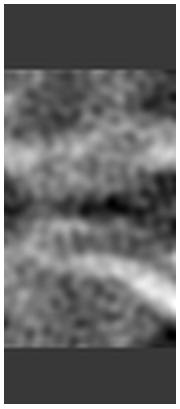

Z

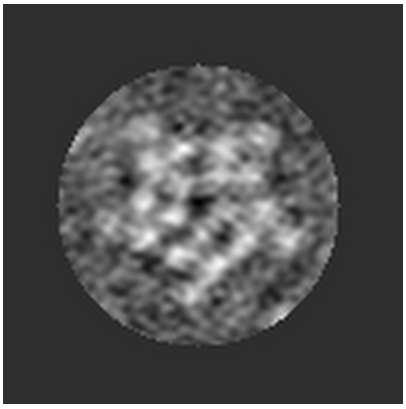
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 64

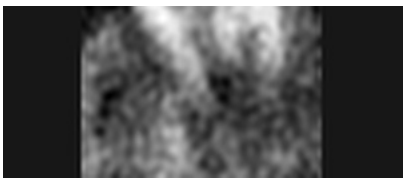

Y Index: 64


Z Index: 27

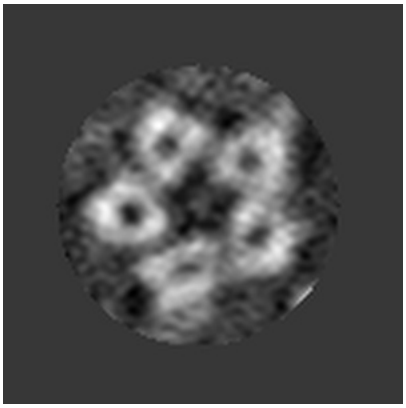
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 86

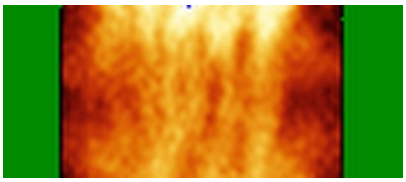
Y Index: 82

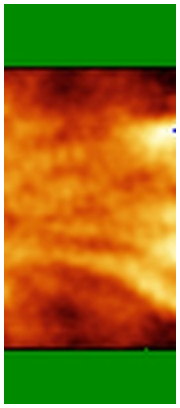

Z Index: 54

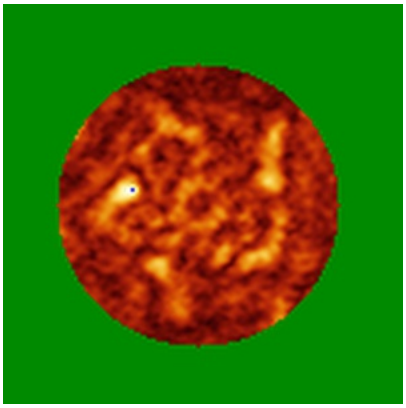
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

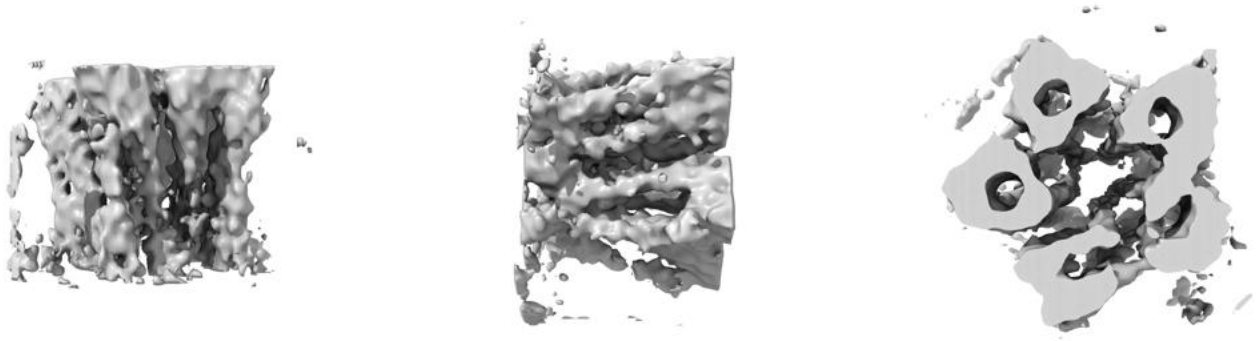

Y


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

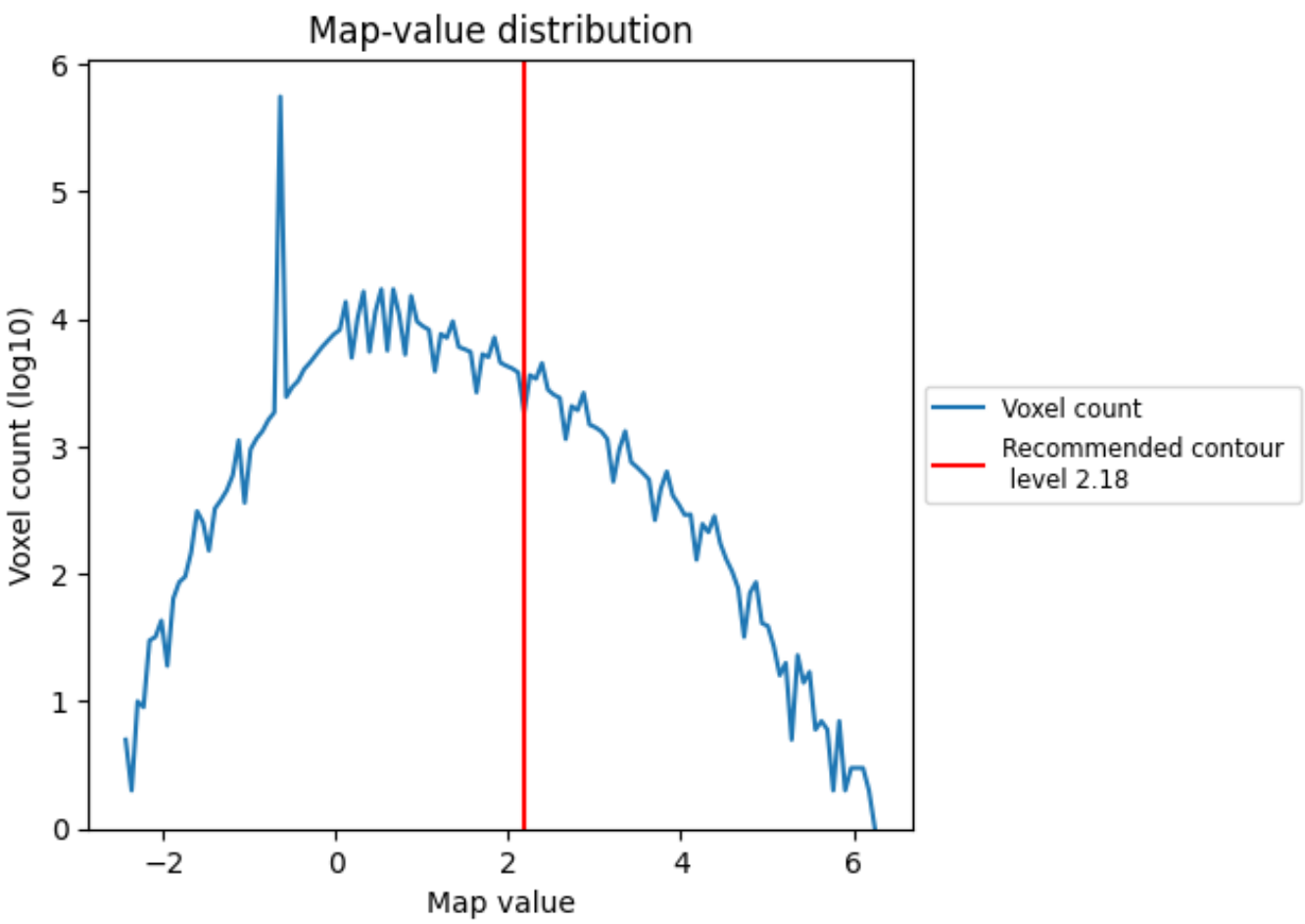
6.6 Mask visualisation (i)

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

7 Map analysis (i)

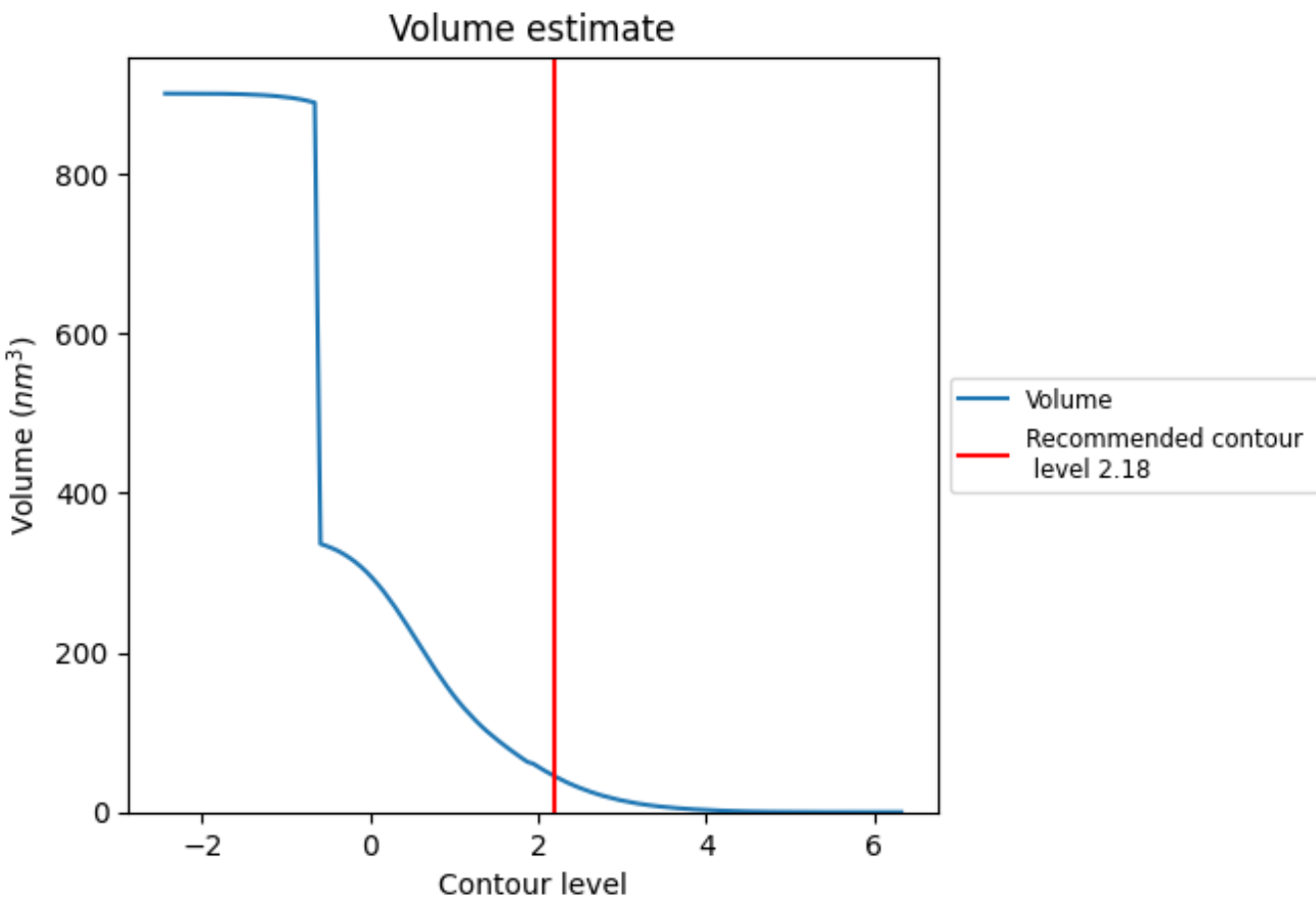
This section contains the results of statistical analysis of the map.

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 46 nm^3; this corresponds to an approximate mass of 41 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.

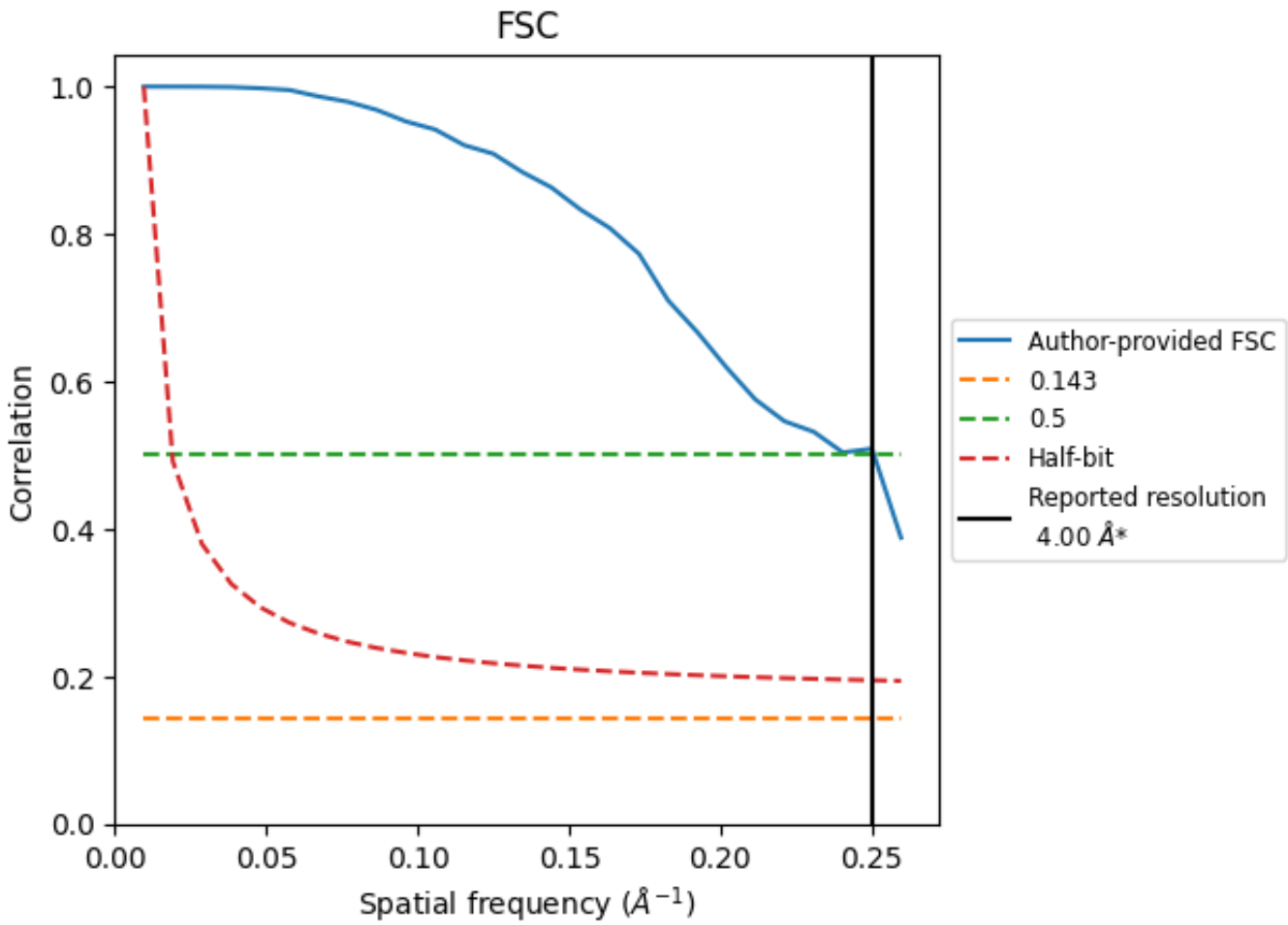
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

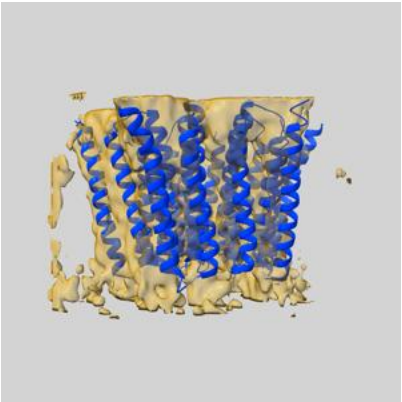
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	4.00	-
Author-provided FSC curve	-	3.99	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

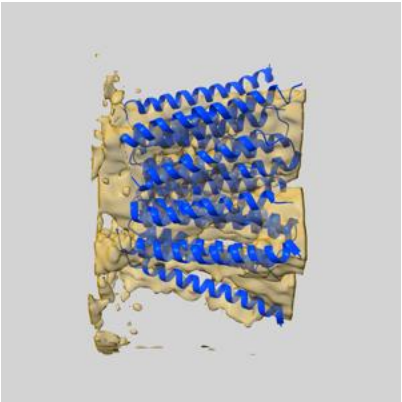
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1044 and PDB model 1OED. Per-residue inclusion information can be found in section 3 on page 5.

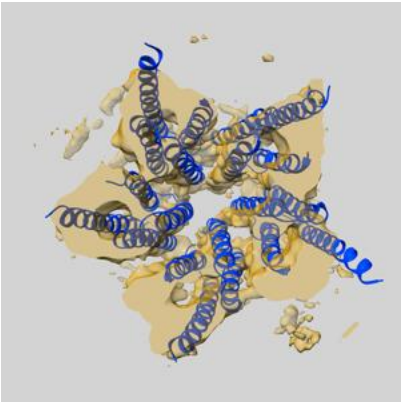
9.1 Map-model overlay (i)



X



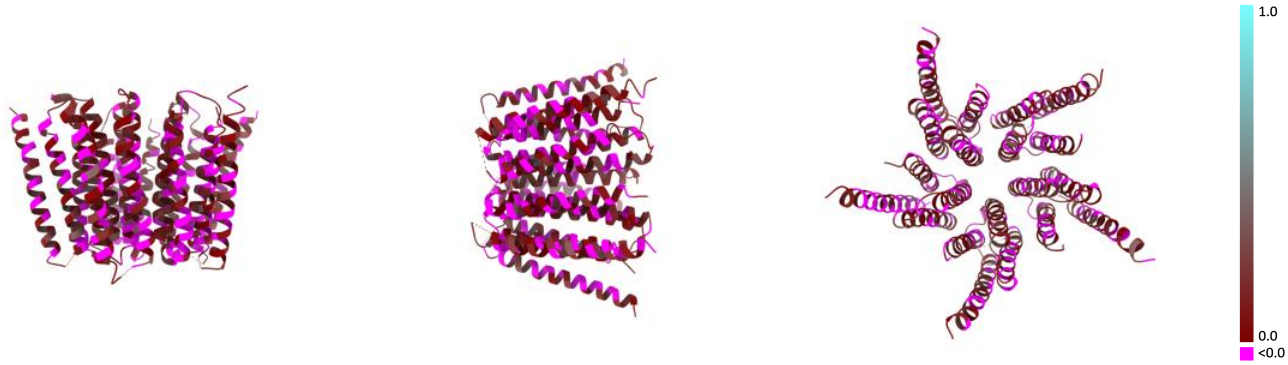
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.18 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.

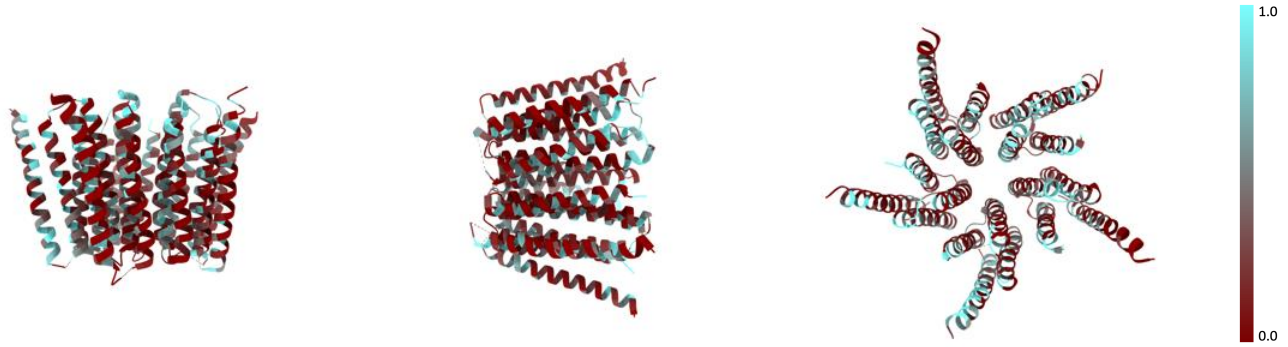
9.2 Q-score mapped to coordinate model (i)



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.

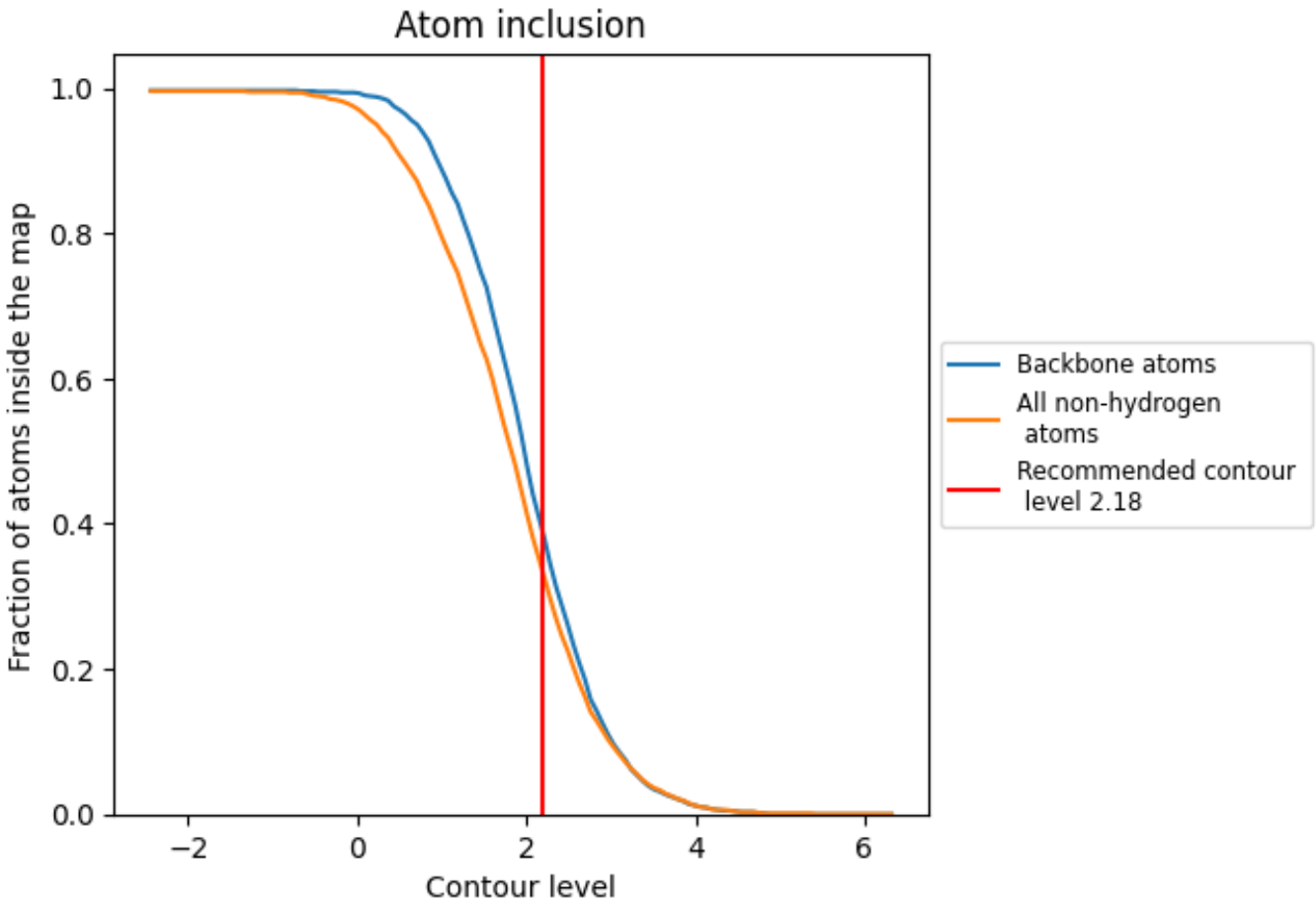
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.18).

9.4 Atom inclusion (i)



At the recommended contour level, 40% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3400	0.0660
A	0.3150	0.0560
B	0.3440	0.0520
C	0.2750	0.0660
D	0.4210	0.0960
E	0.3410	0.0570