



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 06:14 pm GMT

PDB ID : 4BOO
EMDB ID : EMD-2381
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes class C
Authors : Zuber, B.; Unwin, N.
Deposited on : 2013-05-21
Resolution : 42.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

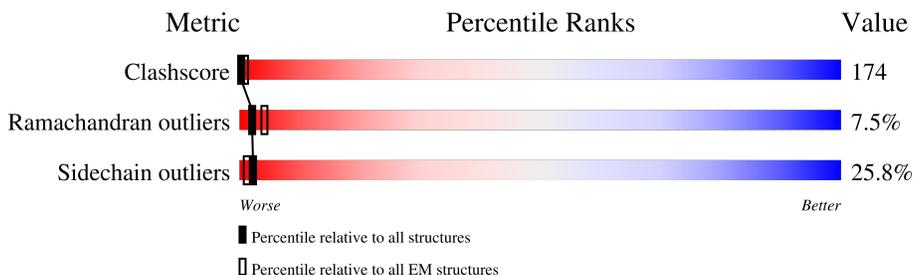
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 42.00 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 $\leq 5\%$. 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	505	

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

F466	G469	H470	L471	N472	Q473	V474	P475	E476	F477	PRO	PHE	PRO	GLY	ASP	PRO	ARG	LYS	TYR	VAL	VAL	PRO																																																								
ASP	LEU	ALA	ASN	PHE	ALA	PRO	GLU	ILE	S414	C415	V416	E417	A418	C419	N420	F421	T422	A423	K424	S425	Q429	N430	D431	S432	G433	S434	E435	N436	E437	N438	V439	V440	L441	T442	G443	K444	V445	I446	D447	K448	A449	C450	F451	N452	L453	A454	L455	L456	L457	F458	S459	L460	G461	T462	L463	A464	I465																				
GLY	LYS	PRO	GLN	ARG	ARG	ARG	SER	SER	PHE	GLY	ILE	MET	ILE	LYS	ALA	GLU	TYR	ILE	ILE	LYS	TYR	PRO	ARG	SER	GLU	ASP	PHE	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																						
K284	Y285	L286	I287	F288	V289	M290	F291	V292	S293	L294	V295	I296	V297	T298	N299	C300	V301	I302	V303	L304	N305	V306	S307	I308	R309	T310	C311	N312	T313	H314	SER	LEU	SER	GLU	LYS	LYS	ASP	ARG	HIS	GLY	LEU	LYS	ARG	VAL	ASN	LYS	PRO	TYR	LEU	LEU	LEU	PHE	LEU	GLU	LEU	F264	F265	F266	L267	I268	A269	Q270	Q271	V272	P273	E274	T275	S276	L277	R216	K217	N278	V279	P280	L281	I282	G283
G164	GLU	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	M180	G181	E182	W183	T184	I185	I186	H187	R188	P189	A190	K191	K192	L193	Y194	N195	V196	V257	L258	L259	A260	Q261	T262	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	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	T252	L253	S254	I255	S256	V257	L258	L259	A260	Q261	T262	D202	I203	D204	F205	Q206	E207	I208	I209	F210	F211	L212	I213	I214	Q215	R216	K217	P218	L219	F220	Y221	I222	I223																		

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	3564	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	80213	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	1.092	Depositor
Minimum voxel value	-0.624	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	0.066	Depositor
Recommended contour level	0.248	Depositor
Tomogram size (\AA)	448.8, 448.8, 448.8	wwPDB
Tomogram dimensions	60, 60, 60	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\AA)	7.48, 7.48, 7.48	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	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
1	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
2	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
3	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
4	E	0.74	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20883 (0.2%)

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	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-8.38	1.14	1.34
1	A	118	TRP	CB-CG	7.89	1.64	1.50
1	D	208	GLN	C-N	7.59	1.51	1.34
4	E	8	GLU	CB-CG	6.55	1.64	1.52
3	C	265	LEU	C-N	6.17	1.48	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	ALA	N-CA-CB	10.40	124.66	110.10
4	E	198	LEU	CA-CB-CG	7.18	131.82	115.30
3	C	315	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	209	ARG	NE-CZ-NH2	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.65	96.77	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	63	TYR	Sidechain
3	C	74	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	72	TYR	Sidechain

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	3005	1078	0
1	D	2991	0	3006	1061	0
2	B	2972	0	2953	1087	0
3	C	2983	0	2987	1149	0
4	E	2987	0	2994	1084	0
All	All	14924	0	14945	5193	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 174.

The worst 5 of 5193 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)
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.50
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.48
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.47
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.45
3:C:316:THR:CG2	3:C:317:PRO:HD2	1.53	1.39

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%)	289 (79%)	48 (13%)	29 (8%)	1	13
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	12
2	B	364/493 (74%)	273 (75%)	59 (16%)	32 (9%)	1	11
3	C	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	2	20
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	14
All	All	1825/2442 (75%)	1425 (78%)	264 (14%)	136 (8%)	2	13

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	27	HIS
1	A	76	LYS
1	A	83	ASP
1	A	102	ILE

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%)	248 (72%)	95 (28%)	0	3
1	D	343/427 (80%)	258 (75%)	85 (25%)	0	3
2	B	340/449 (76%)	262 (77%)	78 (23%)	1	4
3	C	335/475 (70%)	243 (72%)	92 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	337/463 (73%)	249 (74%)	88 (26%)	0	3
All	All	1698/2241 (76%)	1260 (74%)	438 (26%)	2	3

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	274	THR
1	D	94	ASN
4	E	184	THR
3	C	296	MET
3	C	471	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
4	E	156	ASN
1	D	42	ASN
4	E	153	HIS
4	E	215	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

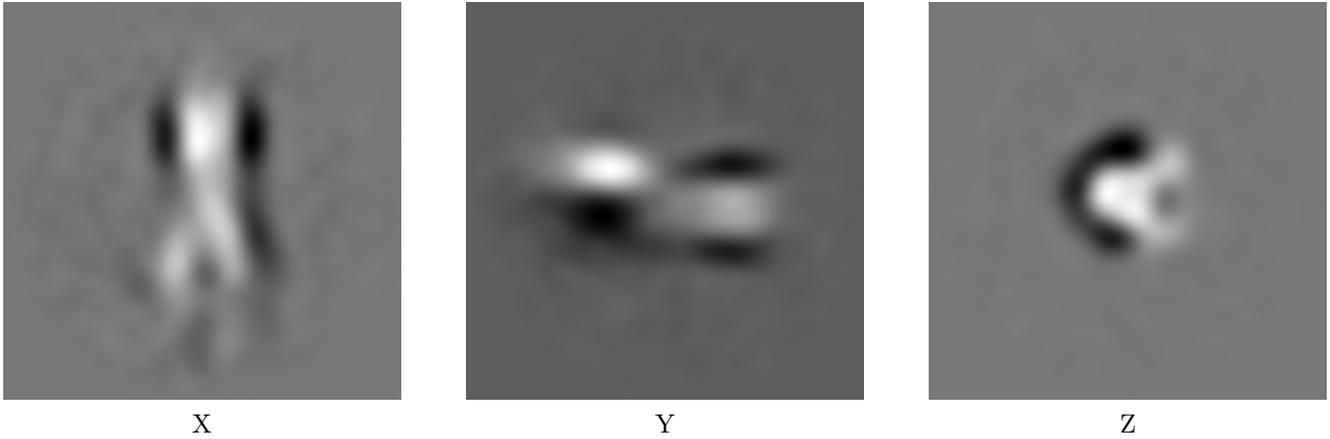
All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	129:THR	C	130:ILE	N	1.14

6 Tomogram visualisation [i](#)

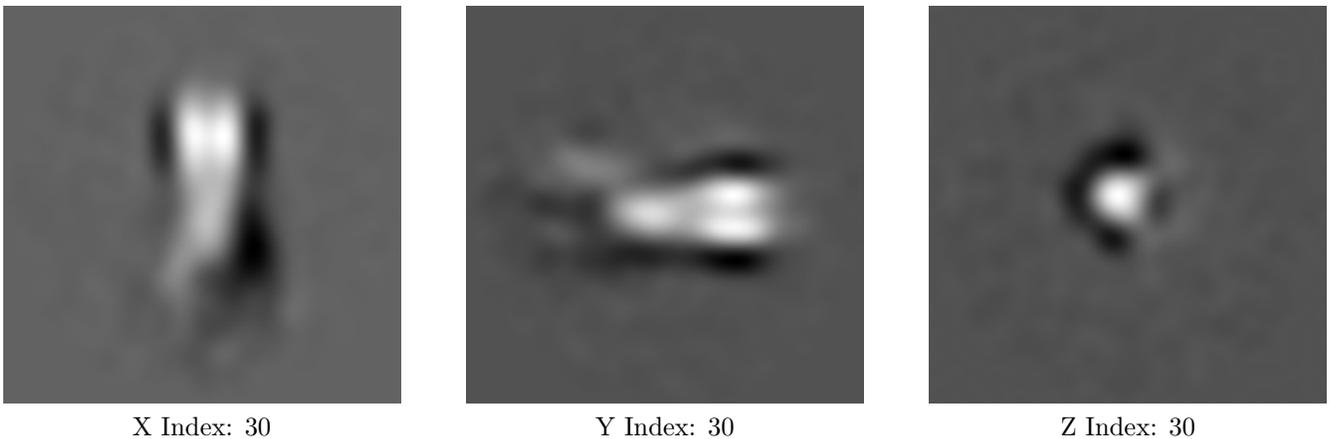
This section contains visualisations of the EMDB entry EMD-2381. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



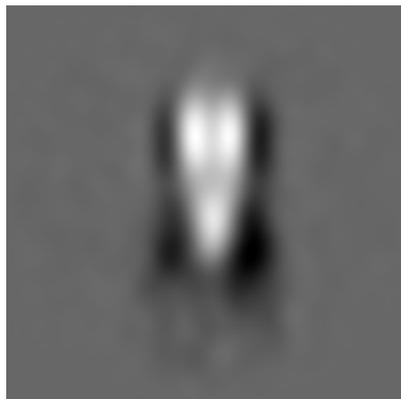
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)

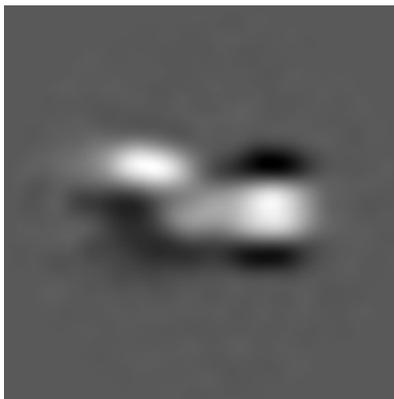


The images above show central slices of the tomogram in three orthogonal directions.

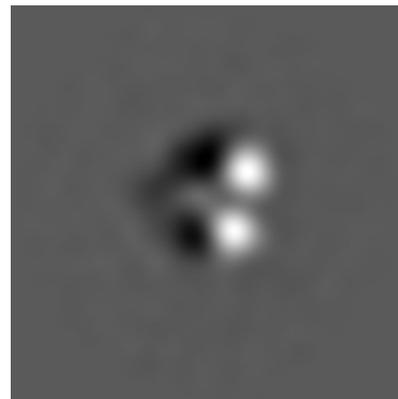
6.3 Largest variance slices [i](#)



X Index: 28



Y Index: 33



Z Index: 21

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

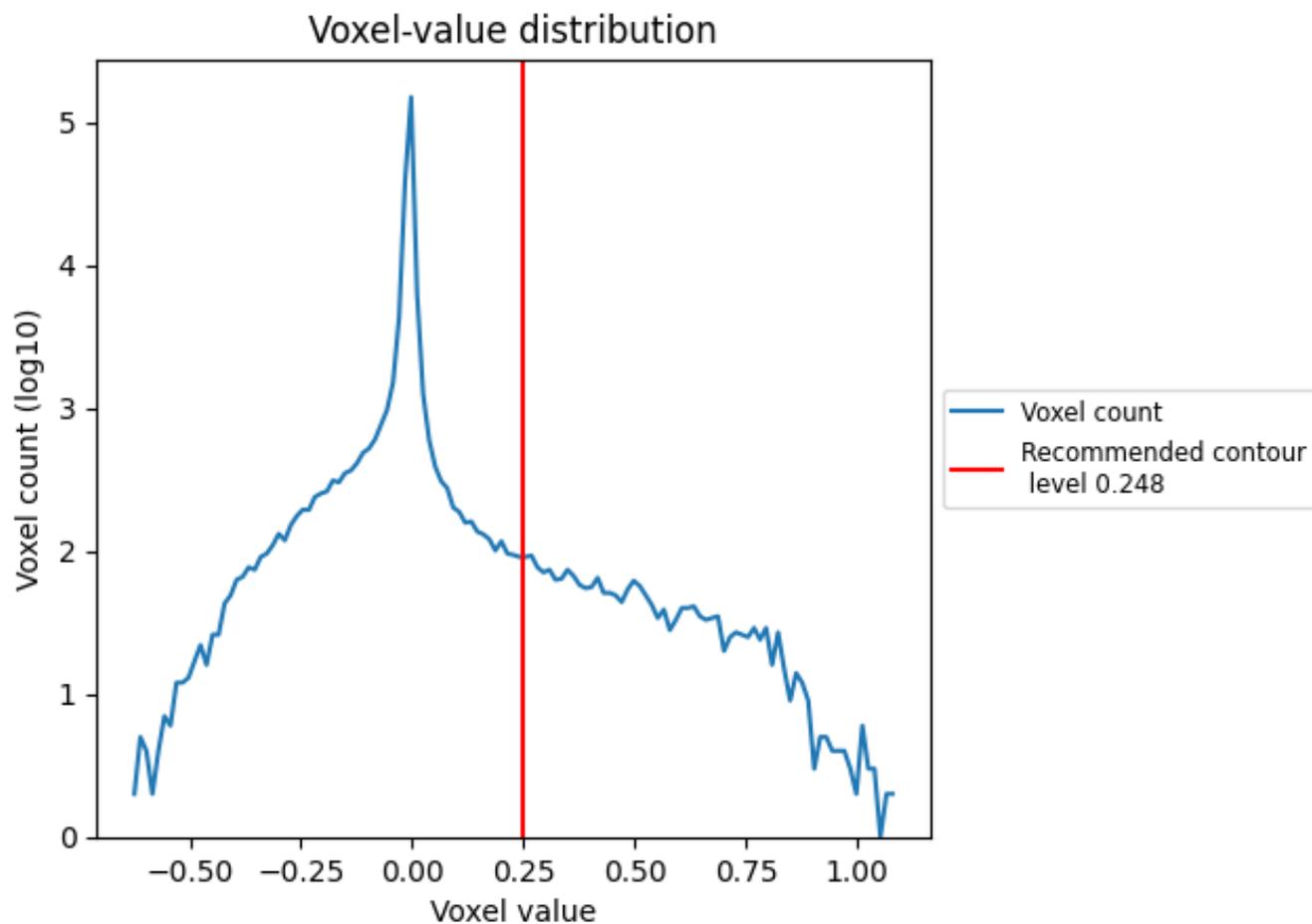
6.4 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

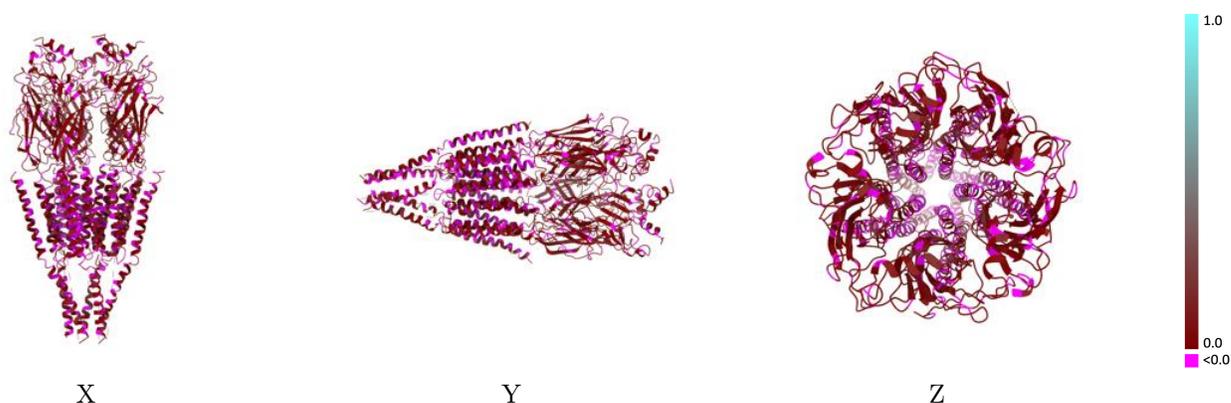
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2381 and PDB model 4BOO. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay [i](#)

This section was not generated.

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

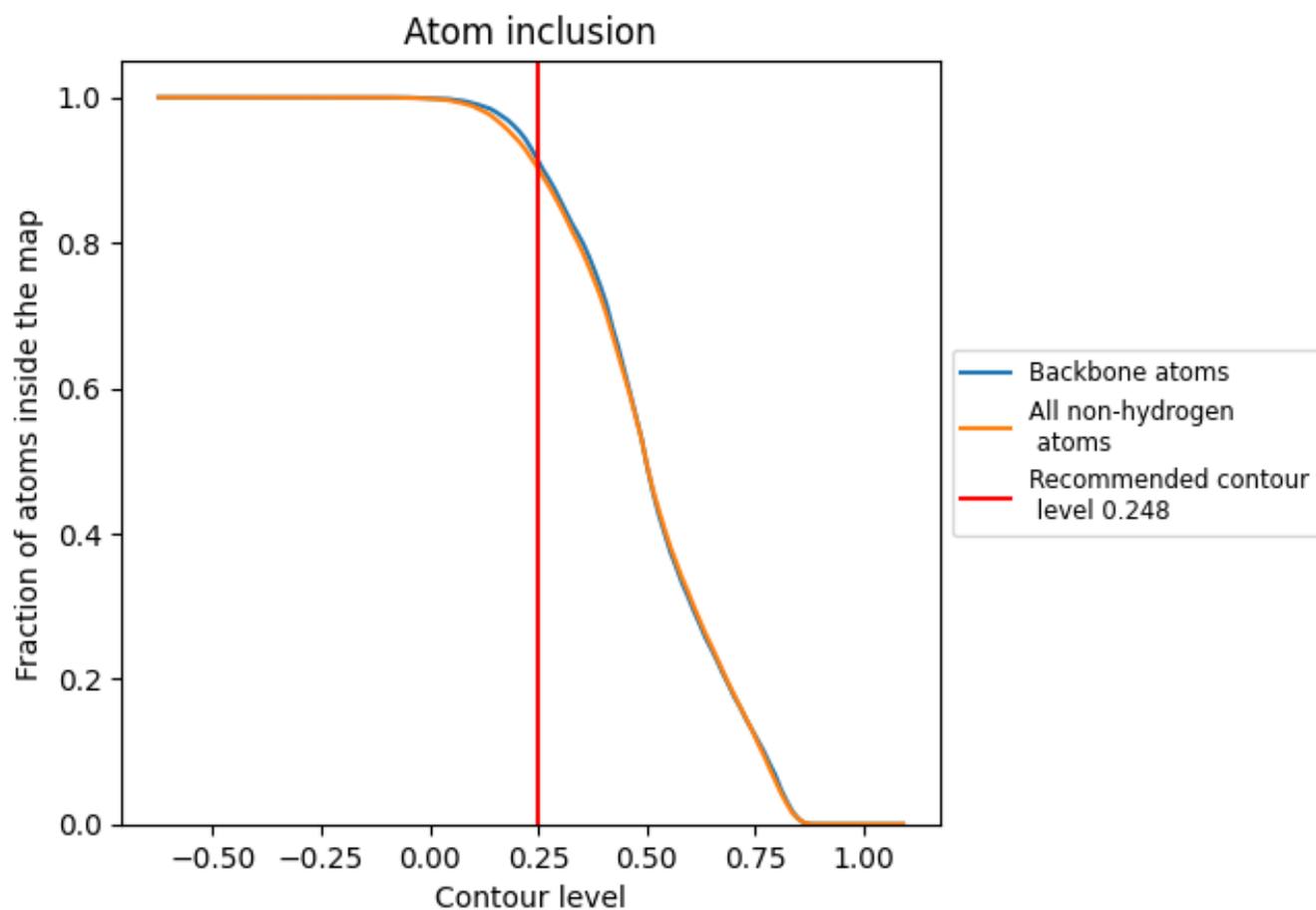


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9046	 0.0420
A	 0.8895	 0.0470
B	 0.9089	 0.0470
C	 0.9141	 0.0410
D	 0.8770	 0.0310
E	 0.9334	 0.0470

