wwPDB EM Validation Summary Report (i)

Apr 30, 2024 – 06:53 pm BST

PDB ID	:	5A6U
EMDB ID	:	EMD-3068
Title	:	Native mammalian ribosome-bound Sec61 protein-conducting channel in the 'non-inserting' state
Authors	:	Pfeffer, S.; Burbaum, L.; Unverdorben, P.; Pech, M.; Chen, Y.; Zimmermann, R.; Beckmann, R.; Foerster, F.
Deposited on	:	2015-07-01
Resolution	:	9.00 Å(reported)
Based on initial model	:	3J7Q

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:

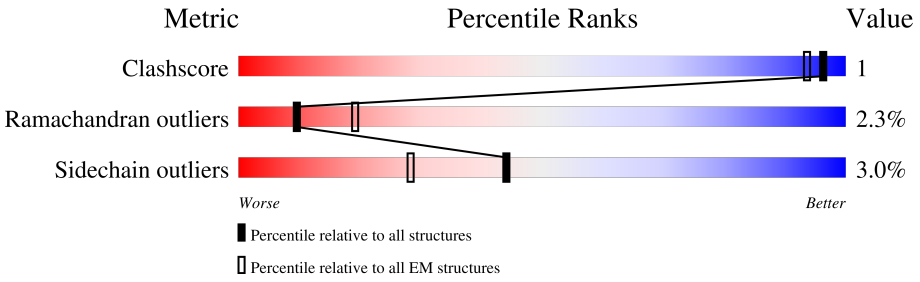
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 9.00 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	451	40%; 70%; 14%; •; 12%
2	B	36	53%; 78%; 17%; •; •
3	G	62	42%; 73%; 26%; •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7770 atoms, of which 3992 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 SEC61A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	396	6180	1967	3165	497	532	19	0	4

- Molecule 2 is a protein called SEC61B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	36	576	186	297	44	47	2	0	0

- Molecule 3 is a protein called SEC61G.

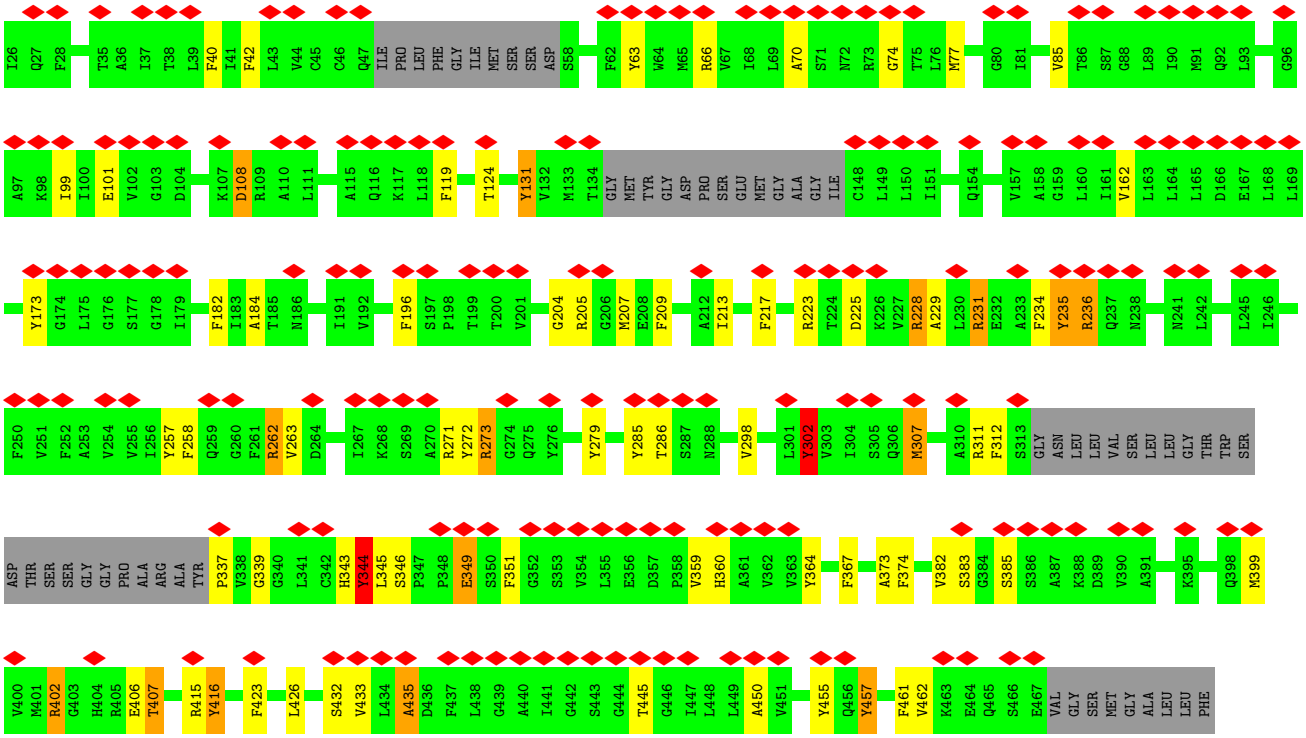
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	G	62	1014	316	530	86	79	3	0	0

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.

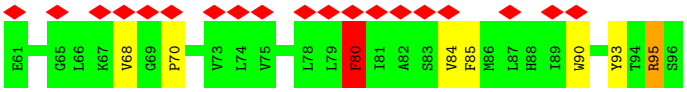
- Molecule 1: SEC61A

Chain A: 40% 70% 14% • 12%



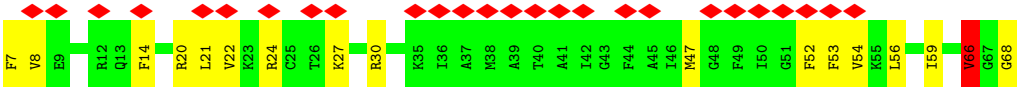
- Molecule 2: SEC61B

Chain B: 53% 78% 17% • •



- Molecule 3: SEC61G

Chain G: 42% 73% 26% •


F7
V8
E9
R12
Q13
F14
R20
L21
V22
K23
R24
C25
T26
K27
R30
K35
I36
A37
M38
A39
T40
A41
I42
G43
F44
A45
I46
M47
G48
F49
I50
G51
F52
F53
V54
K55
L56
I59
V66
G67
G68

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	17653	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH TILT IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum voxel value	20.314	Depositor
Minimum voxel value	-16.746	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Tomogram size (Å)	576.39996, 576.39996, 576.39996	wwPDB
Tomogram dimensions	220, 220, 220	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	2.62, 2.62, 2.62	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	1.73	25/3078 (0.8%)	1.94	72/4186 (1.7%)
2	B	1.61	1/287 (0.3%)	1.90	7/389 (1.8%)
3	G	1.74	2/494 (0.4%)	2.01	15/663 (2.3%)
All	All	1.72	28/3859 (0.7%)	1.95	94/5238 (1.8%)

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	2	11
2	B	0	2
3	G	0	1
All	All	2	14

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ARG	CZ-NH2	8.32	1.43	1.33
1	A	337	PRO	N-CA	6.93	1.59	1.47
1	A	432	SER	CA-CB	6.80	1.63	1.52
1	A	311	ARG	CZ-NH2	6.23	1.41	1.33
1	A	63	TYR	CG-CD2	6.04	1.47	1.39

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	A	235	TYR	CB-CG-CD2	-12.74	113.36	121.00
1	A	257	TYR	CB-CG-CD1	-12.55	113.47	121.00
1	A	131	TYR	CB-CG-CD2	-11.61	114.04	121.00
1	A	344	TYR	CB-CG-CD1	11.57	127.94	121.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	188	CYS	CA
1	A	447	ILE	CB

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	TYR	Sidechain
1	A	228	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	235	TYR	Sidechain
1	A	40	PHE	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	3015	3165	2959	4	0
2	B	279	297	284	1	0
3	G	484	530	477	1	0
All	All	3778	3992	3720	6	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 1.

The worst 5 of 6 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:74:GLY:H	1:A:77:MET:HB3	1.73	0.54
2:B:80:PHE:O	2:B:84:VAL:HG23	2.12	0.49
1:A:302:TYR:CZ	1:A:345:LEU:HD13	2.49	0.48
1:A:339:GLY:O	1:A:343:HIS:CD2	2.69	0.45
1:A:184:ALA:HB2	1:A:450:ALA:CB	2.46	0.45

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	388/451 (86%)	338 (87%)	41 (11%)	9 (2%)	6 34
2	B	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
3	G	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4 26
All	All	482/549 (88%)	428 (89%)	43 (9%)	11 (2%)	9 34

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ILE
1	A	406	GLU
1	A	407	THR
1	A	445	THR
1	A	349	GLU

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	290/374 (78%)	280 (97%)	10 (3%)	37 60
2	B	30/32 (94%)	30 (100%)	0	100 100
3	G	43/53 (81%)	42 (98%)	1 (2%)	50 70
All	All	363/459 (79%)	352 (97%)	11 (3%)	44 63

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	VAL
1	A	402	ARG
3	G	21	LEU
1	A	433	VAL
1	A	307	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	154	GLN
1	A	259	GLN
1	A	343	HIS

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.

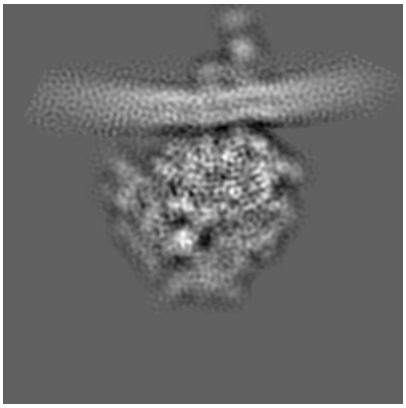
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

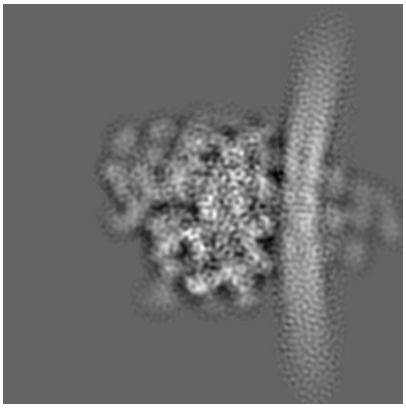
6 Tomogram visualisation (i)

This section contains visualisations of the EMDB entry EMD-3068. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

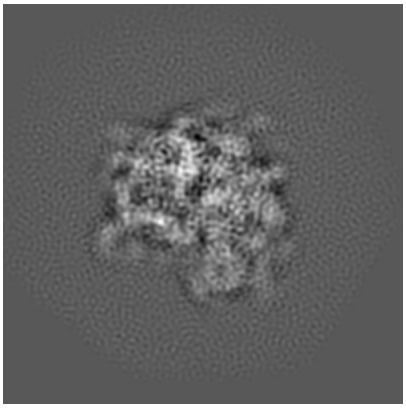
6.1 Orthogonal projections (i)



X



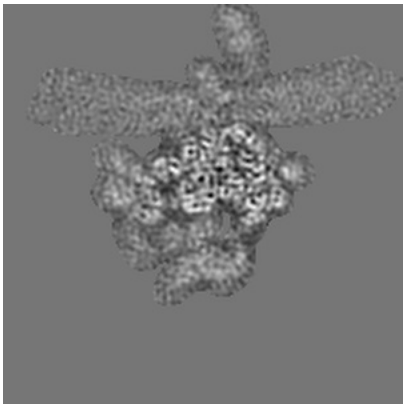
Y



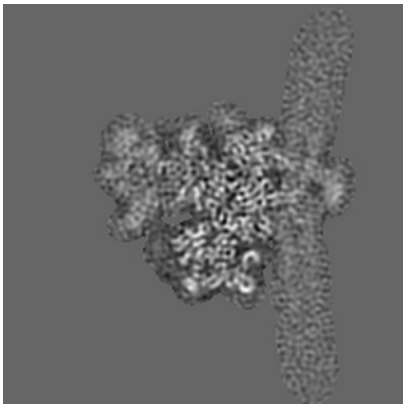
Z

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

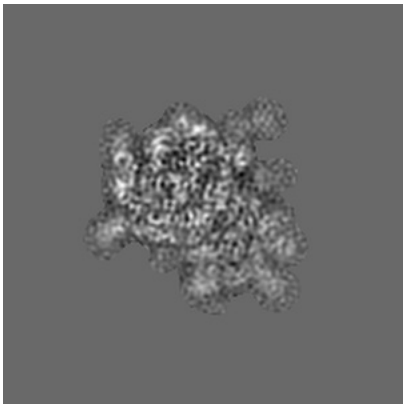
6.2 Central slices (i)



X Index: 110



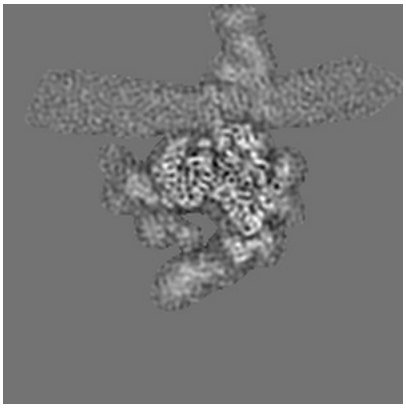
Y Index: 110



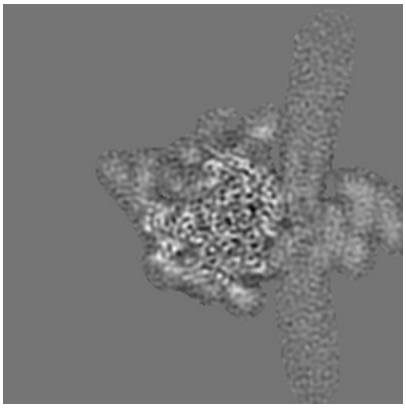
Z Index: 110

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

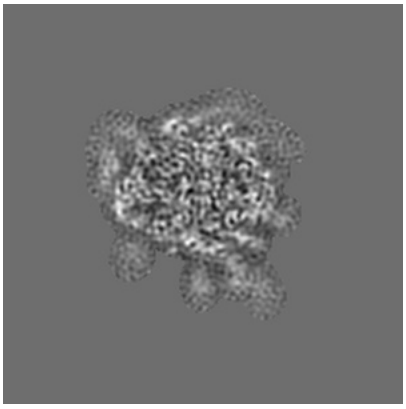
6.3 Largest variance slices (i)



X Index: 102



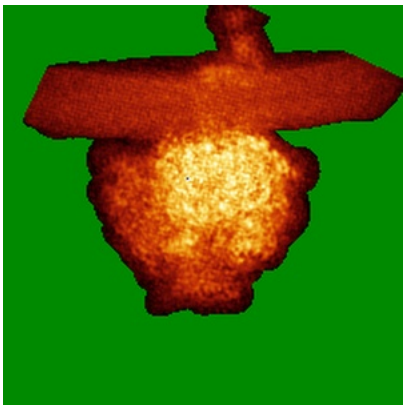
Y Index: 130



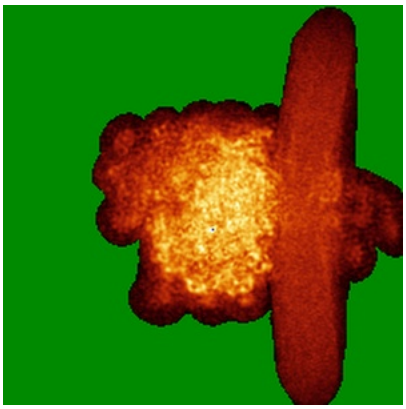
Z Index: 131

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

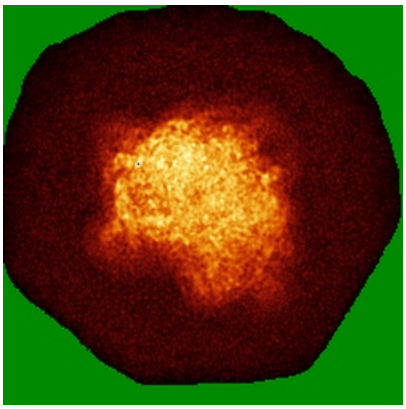
6.4 Orthogonal standard-deviation projections (False-color) (i)



X



Y



Z

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

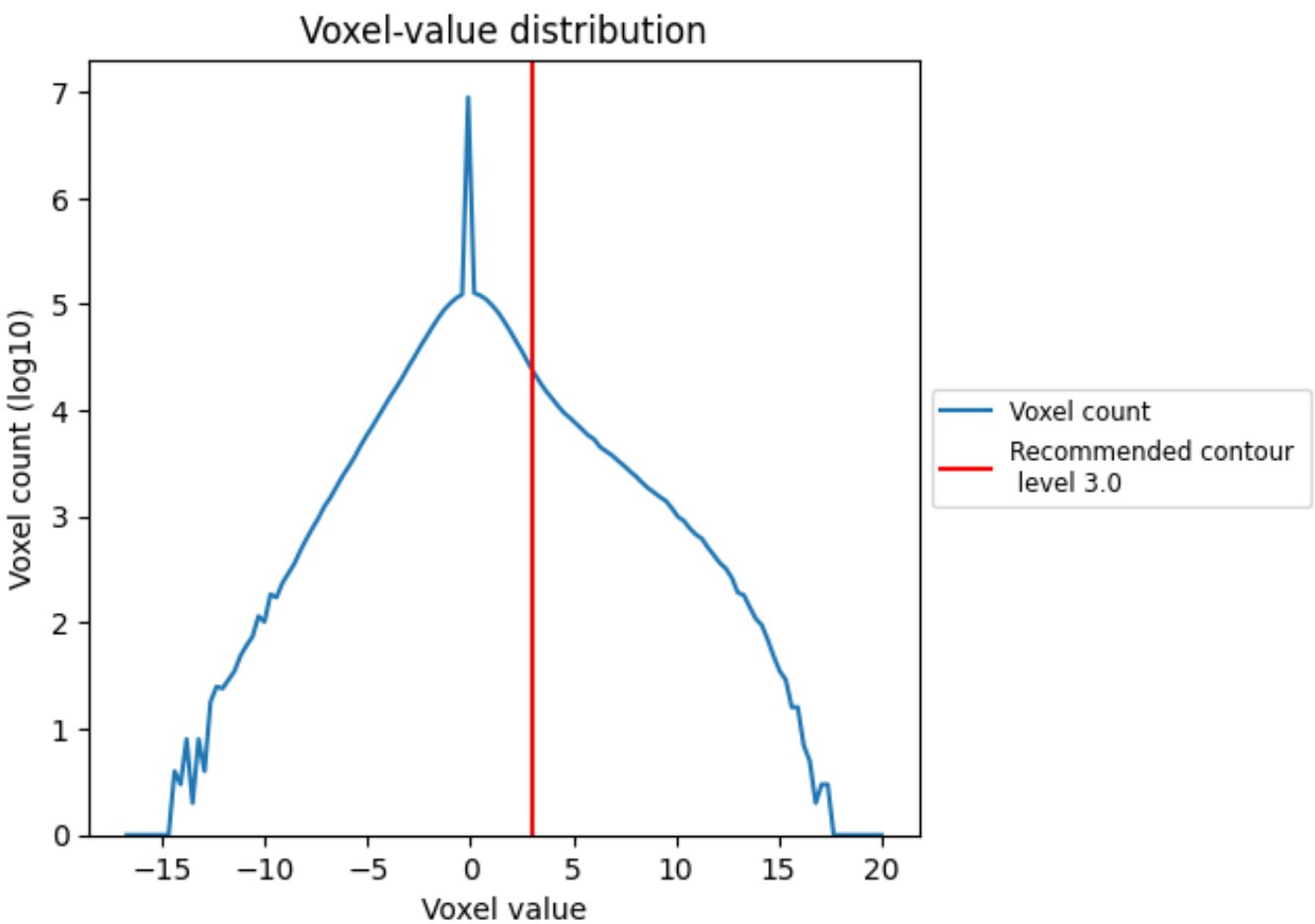
6.5 Mask visualisation (i)

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.

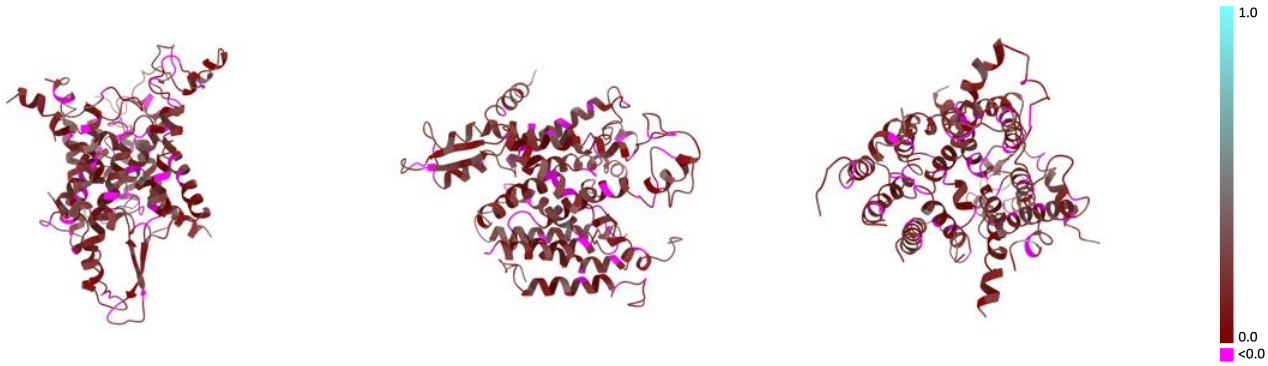
8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3068 and PDB model 5A6U. 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)



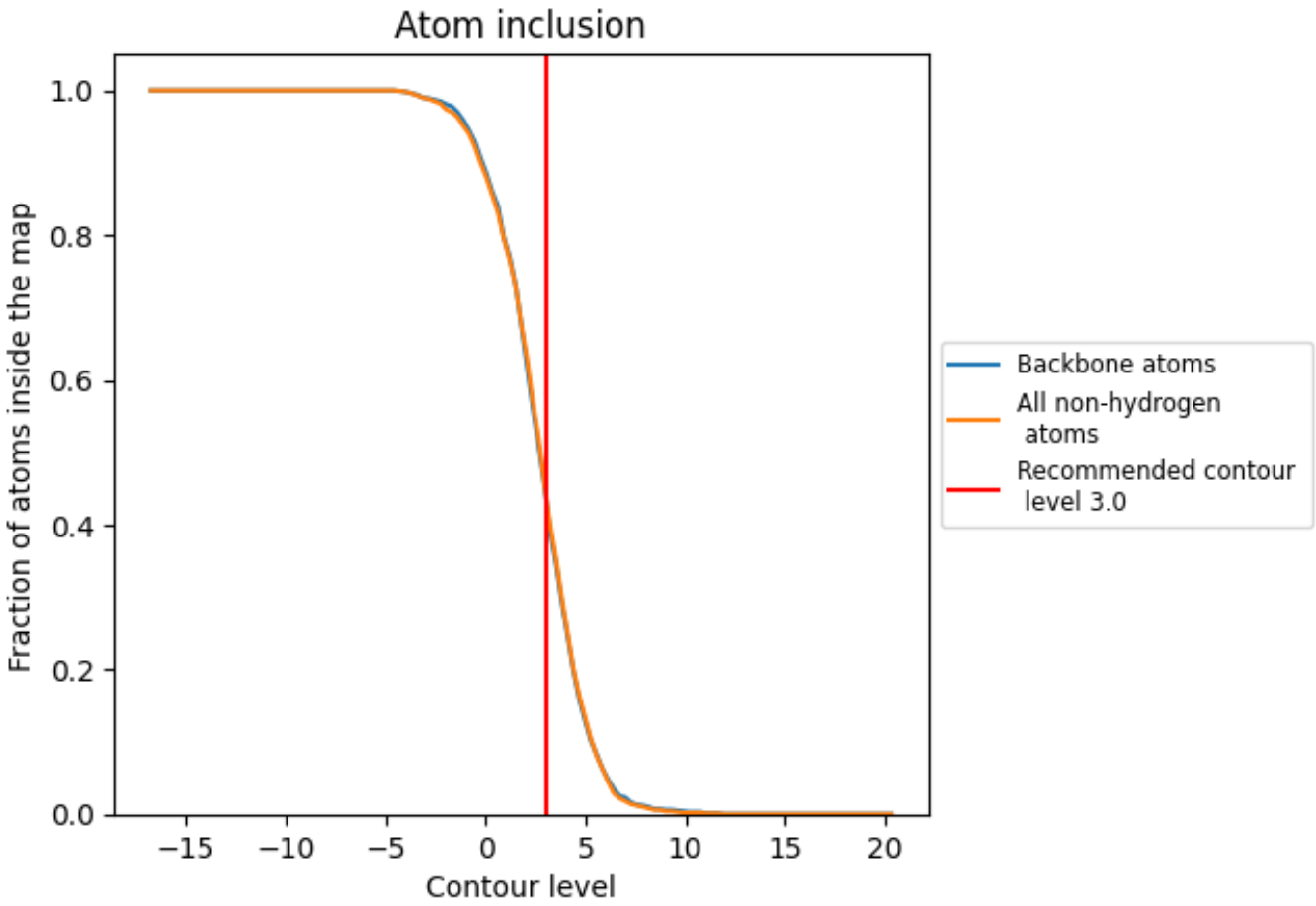
X Y Z

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.

8.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4470	0.1430
A	0.4480	0.1380
B	0.3890	0.1580
G	0.4450	0.1690