wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 06:41 pm GMT

PDB ID	:	4CYL
EMDB ID	:	EMD-2530
Title	:	Tomographic subvolume average of EFF-1 fusogen on extracellular vesicles
Authors	:	Zeev-Ben-Mordehai, T.; Vasishtan, D.; Siebert, C.A.; Grunewald, K.
Deposited on	:	2014-04-13
Resolution	:	22.20 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:

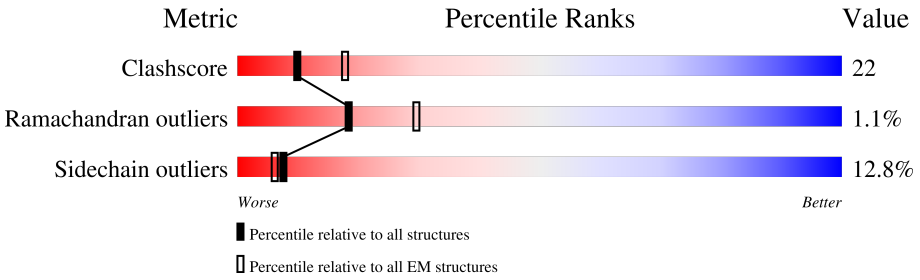
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 22.20 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	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	658	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3644 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 EFF-1A.

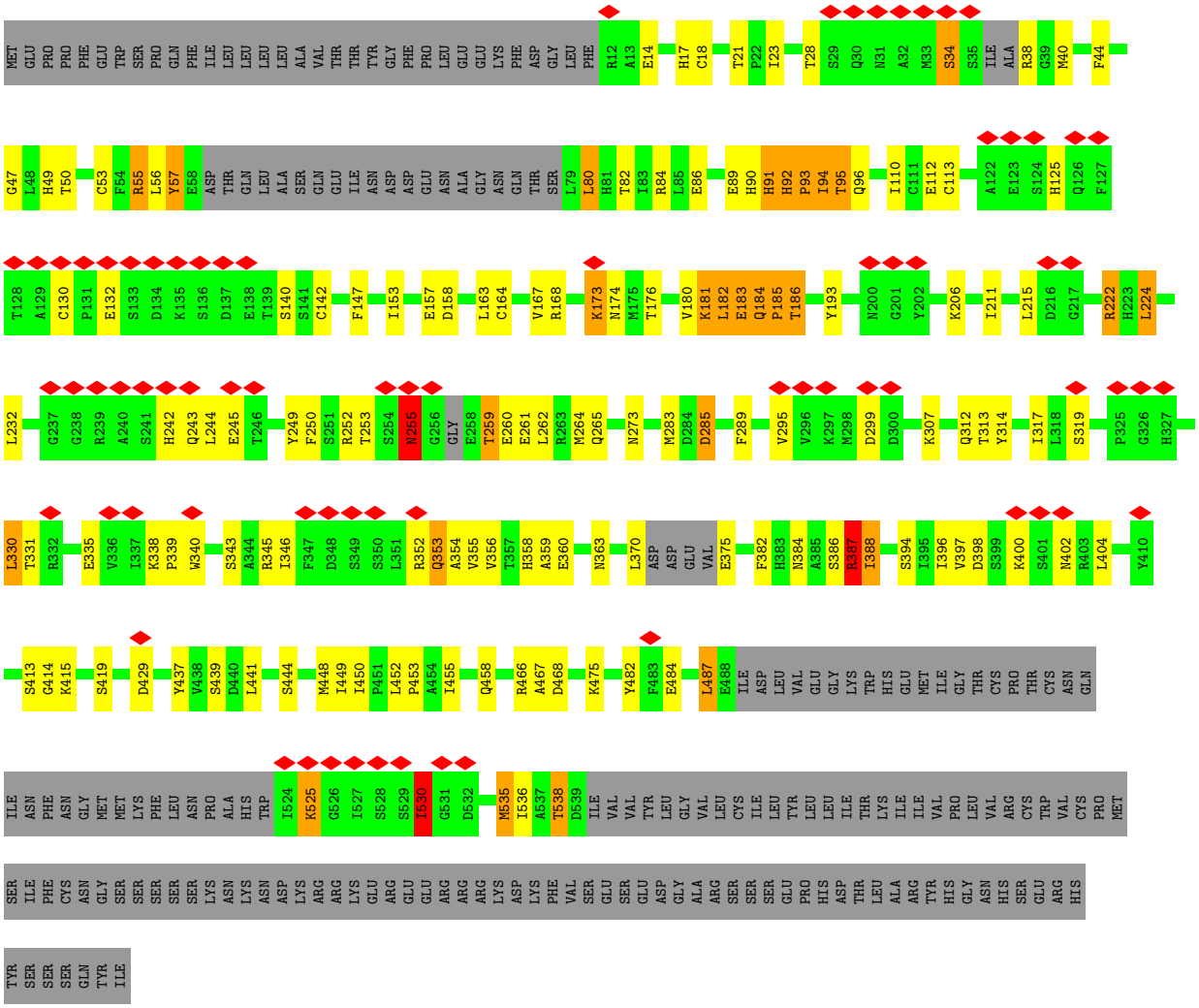
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	466	3644	2277	650	690	27	0	5

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: EFF-1A

Chain A: 11% 48% 18% • 29%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	801	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	78950	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	34.337	Depositor
Minimum voxel value	-38.063	Depositor
Average voxel value	-2.665	Depositor
Voxel value standard deviation	3.182	Depositor
Recommended contour level	18.8	Depositor
Tomogram size (Å)	342.0, 342.0, 342.0	wwPDB
Tomogram dimensions	90, 90, 90	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	3.8, 3.8, 3.8	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	0.55	0/3720	1.72	10/5027 (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	A	0	10

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	SER	O-C-N	-64.72	19.14	122.70
1	A	57	TYR	O-C-N	-61.84	23.75	122.70
1	A	487	LEU	O-C-N	-50.81	41.41	122.70
1	A	538	THR	O-C-N	-21.48	88.33	122.70
1	A	255	ASN	O-C-N	-12.51	101.94	123.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	SER	Mainchain
1	A	57	TYR	Mainchain
1	A	93	PRO	Peptide
1	A	94	ILE	Peptide
1	A	95	THR	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	3644	0	3534	157	0
All	All	3644	0	3534	157	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 22.

The worst 5 of 157 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:182:LEU:HD11	1:A:262:LEU:HD13	1.28	1.12
1:A:94:ILE:HD11	1:A:181:LYS:HD3	1.13	1.09
1:A:387:ARG:HD3	1:A:413:SER:HB3	1.22	1.09
1:A:92:HIS:HA	1:A:183:GLU:HA	1.31	1.07
1:A:250:PHE:HZ	1:A:330:LEU:HD21	1.19	1.05

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	454/658 (69%)	412 (91%)	37 (8%)	5 (1%)	14 52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	ILE
1	A	157	GLU
1	A	255	ASN
1	A	285	ASP
1	A	295	VAL

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	406/584 (70%)	354 (87%)	52 (13%)	4 18

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ARG
1	A	343	SER
1	A	525	LYS
1	A	259	THR
1	A	299	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	402	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 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.

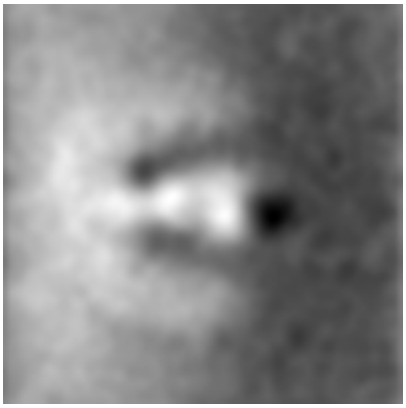
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

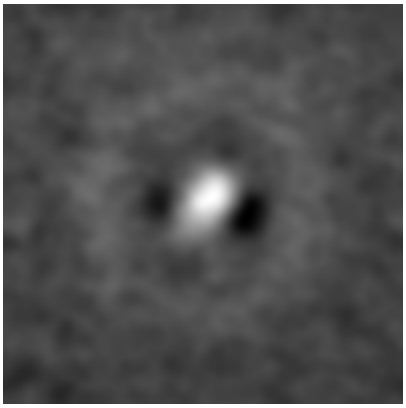
6 Tomogram visualisation (i)

This section contains visualisations of the EMDB entry EMD-2530. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

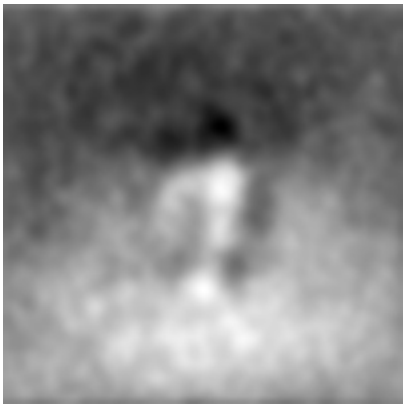
6.1 Orthogonal projections (i)



X



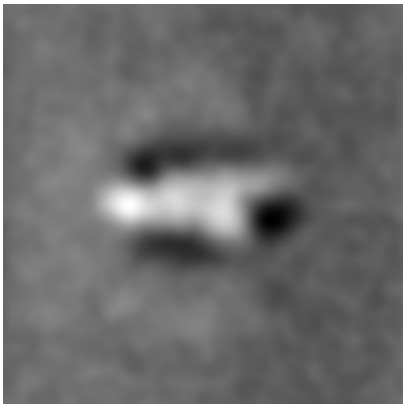
Y



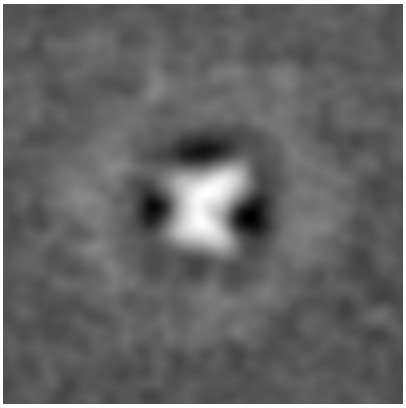
Z

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

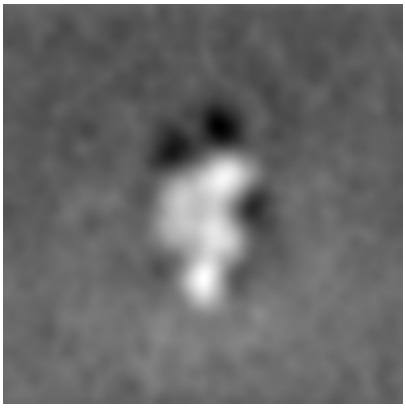
6.2 Central slices (i)



X Index: 45



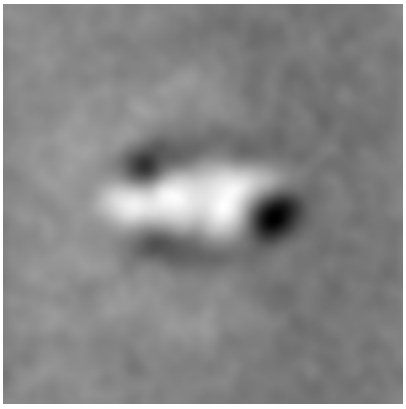
Y Index: 45



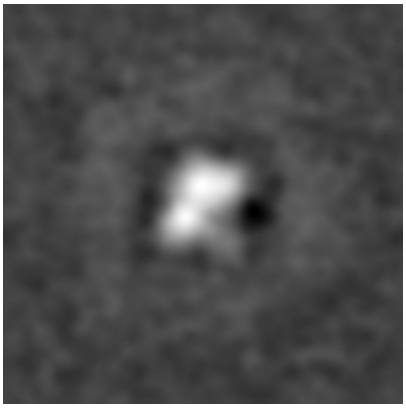
Z Index: 45

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

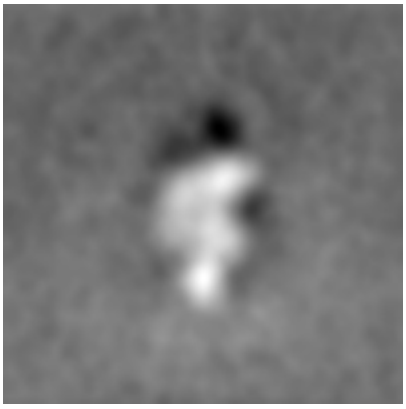
6.3 Largest variance slices (i)



X Index: 47



Y Index: 49



Z Index: 44

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

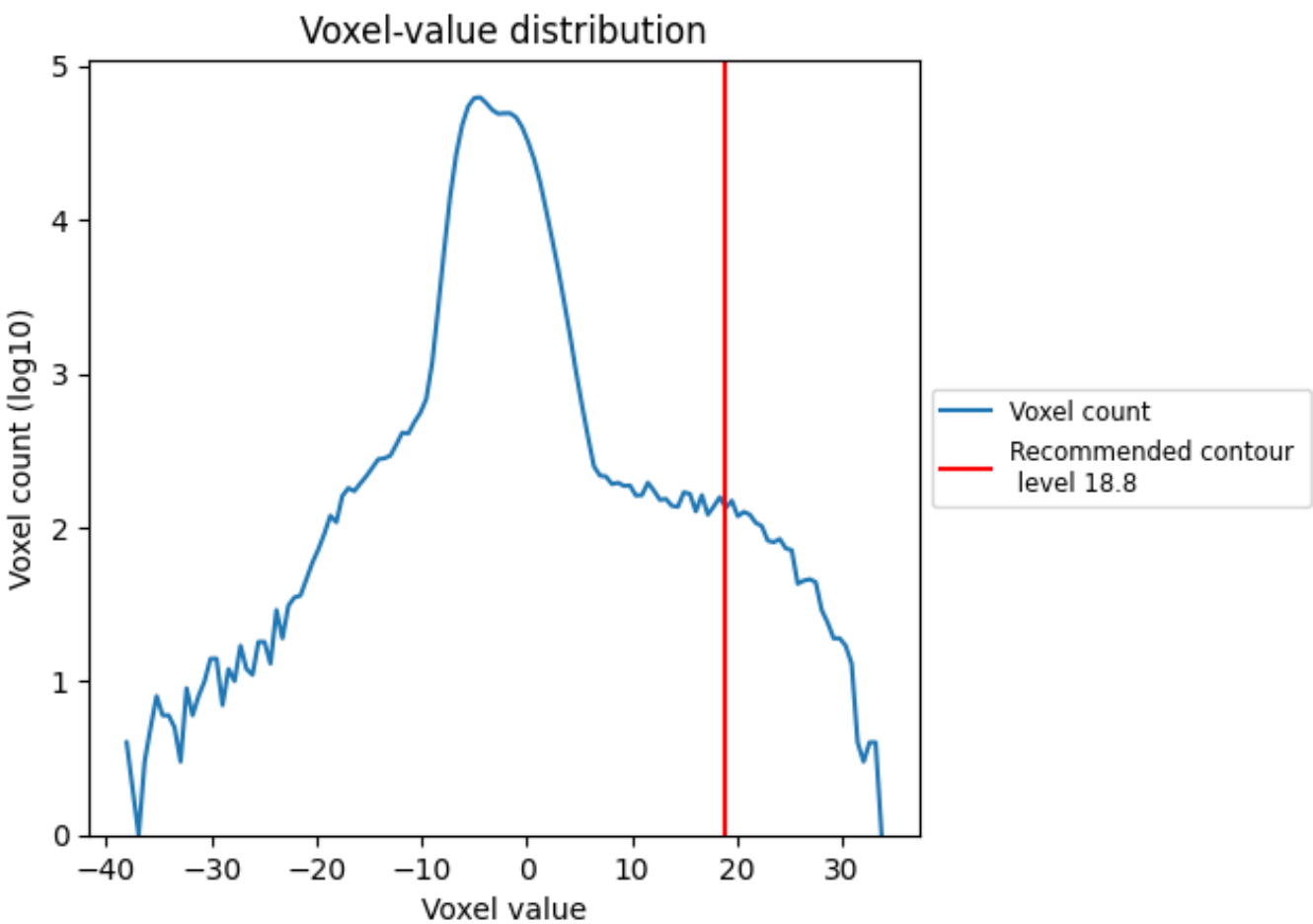
6.4 Mask visualisation (i)

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.

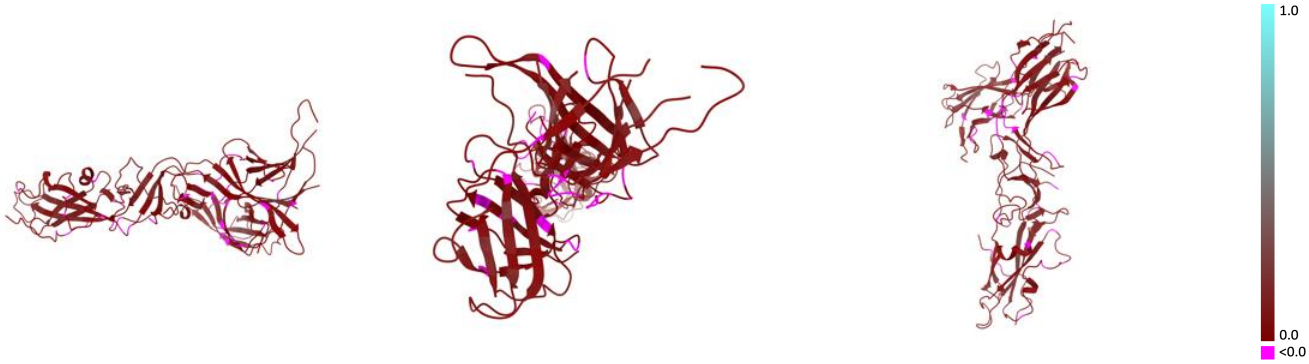
8 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2530 and PDB model 4CYL. 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)



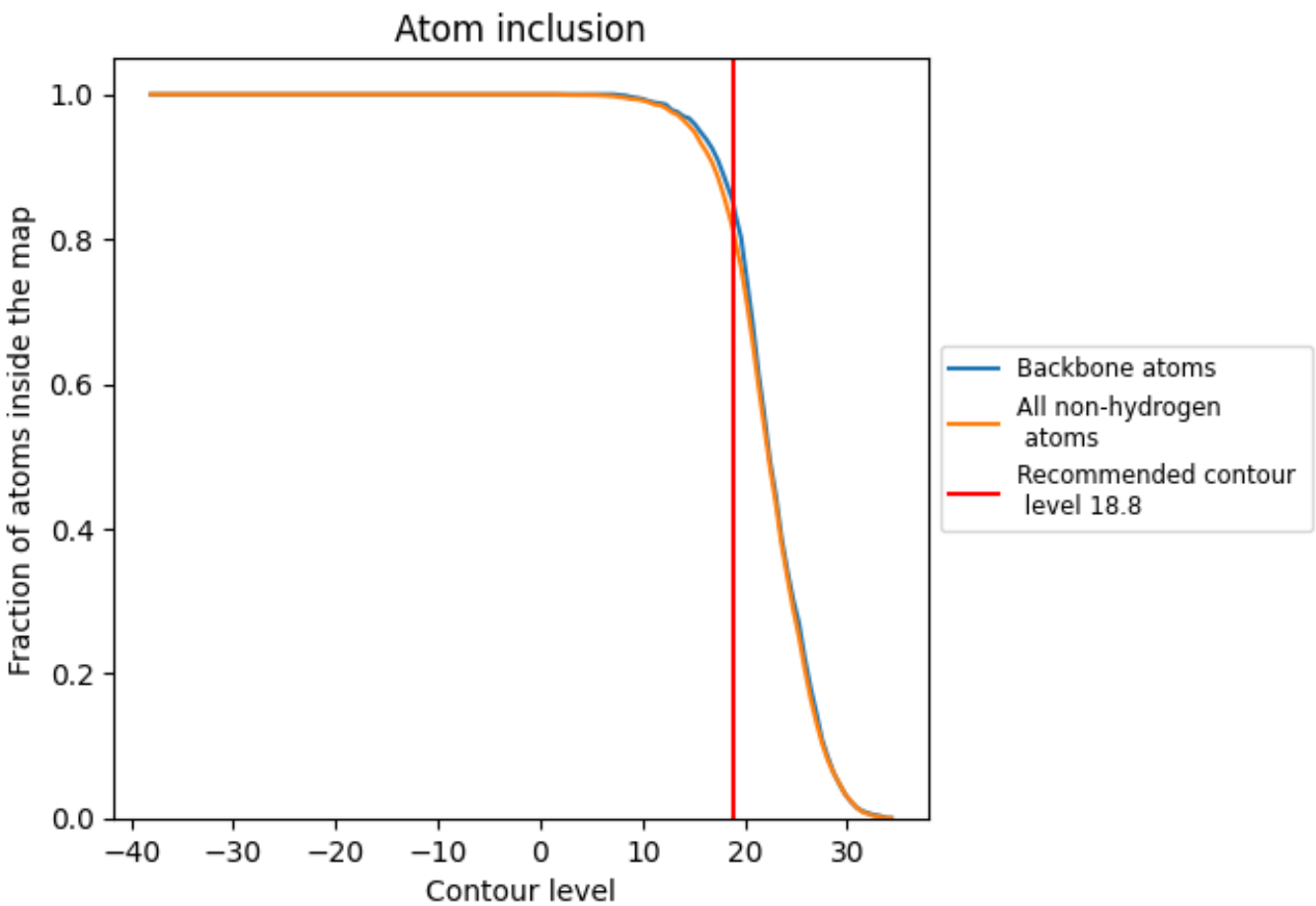
X Y Z

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, 85% of all backbone atoms, 82% 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 (18.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8159	0.0720
A	0.8159	0.0720