



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:26 AM UTC

PDB ID : 4AV2 / pdb_00004av2
EMDB ID : EMD-2105
Title : Single particle electron microscopy of PilQ dodecameric complexes from *Neisseria meningitidis*.
Authors : Berry, J.L.; Phelan, M.M.; Collins, R.F.; Adomavicius, T.; Tonjum, T.; Frye, S.A.; Bird, L.; Owens, R.; Ford, R.C.; Lian, L.Y.; Derrick, J.P.
Deposited on : 2012-05-23
Resolution : 26.00 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 ⓘ 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

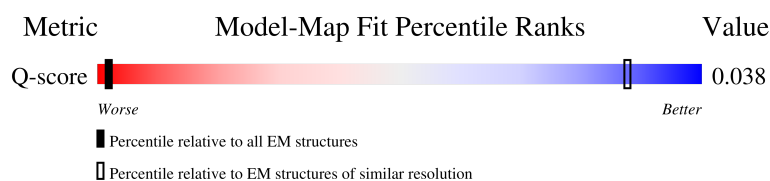
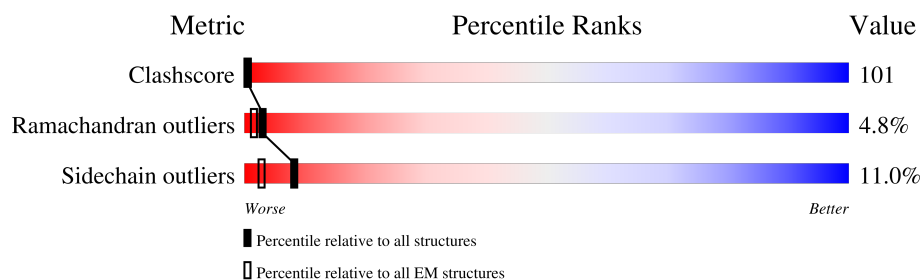
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8 (26.00 - 26.50)

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	745	
1	B	745	
1	C	745	
1	D	745	

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Mol	Chain	Length	Quality of chain
1	E	745	8% 23% 5% 63%
1	F	745	8% 23% 5% 63%
1	G	745	8% 23% 5% 63%
1	H	745	8% 23% 5% 63%
1	I	745	8% 24% 5% 63%
1	J	745	8% 23% 5% 63%
1	K	745	8% 23% 5% 63%
1	L	745	8% 24% 5% 63%
2	M	181	40% 10% 29% 6% 55%
2	N	181	39% 10% 29% 6% 55%
2	O	181	40% 10% 29% 6% 55%
2	P	181	40% 11% 28% 6% 55%
2	Q	181	39% 12% 27% 7% 55%
2	R	181	40% 10% 29% 6% 55%
2	S	181	40% 10% 28% 7% 55%
2	T	181	39% 10% 30% 6% 55%
2	U	181	40% 12% 27% 7% 55%
2	V	181	40% 10% 29% 6% 55%
2	W	181	39% 11% 28% 6% 55%
2	X	181	40% 10% 29% 6% 55%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34704 atoms, of which 1152 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 TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	B	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	C	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	D	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	E	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	F	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	G	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	H	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	I	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	J	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	K	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		
1	L	275	Total	C	N	O	S	0	1
			2152	1354	379	415	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	PHE	LEU	variant	UNP Q70M91
B	428	PHE	LEU	variant	UNP Q70M91
C	428	PHE	LEU	variant	UNP Q70M91
D	428	PHE	LEU	variant	UNP Q70M91
E	428	PHE	LEU	variant	UNP Q70M91

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	PHE	LEU	variant	UNP Q70M91
G	428	PHE	LEU	variant	UNP Q70M91
H	428	PHE	LEU	variant	UNP Q70M91
I	428	PHE	LEU	variant	UNP Q70M91
J	428	PHE	LEU	variant	UNP Q70M91
K	428	PHE	LEU	variant	UNP Q70M91
L	428	PHE	LEU	variant	UNP Q70M91

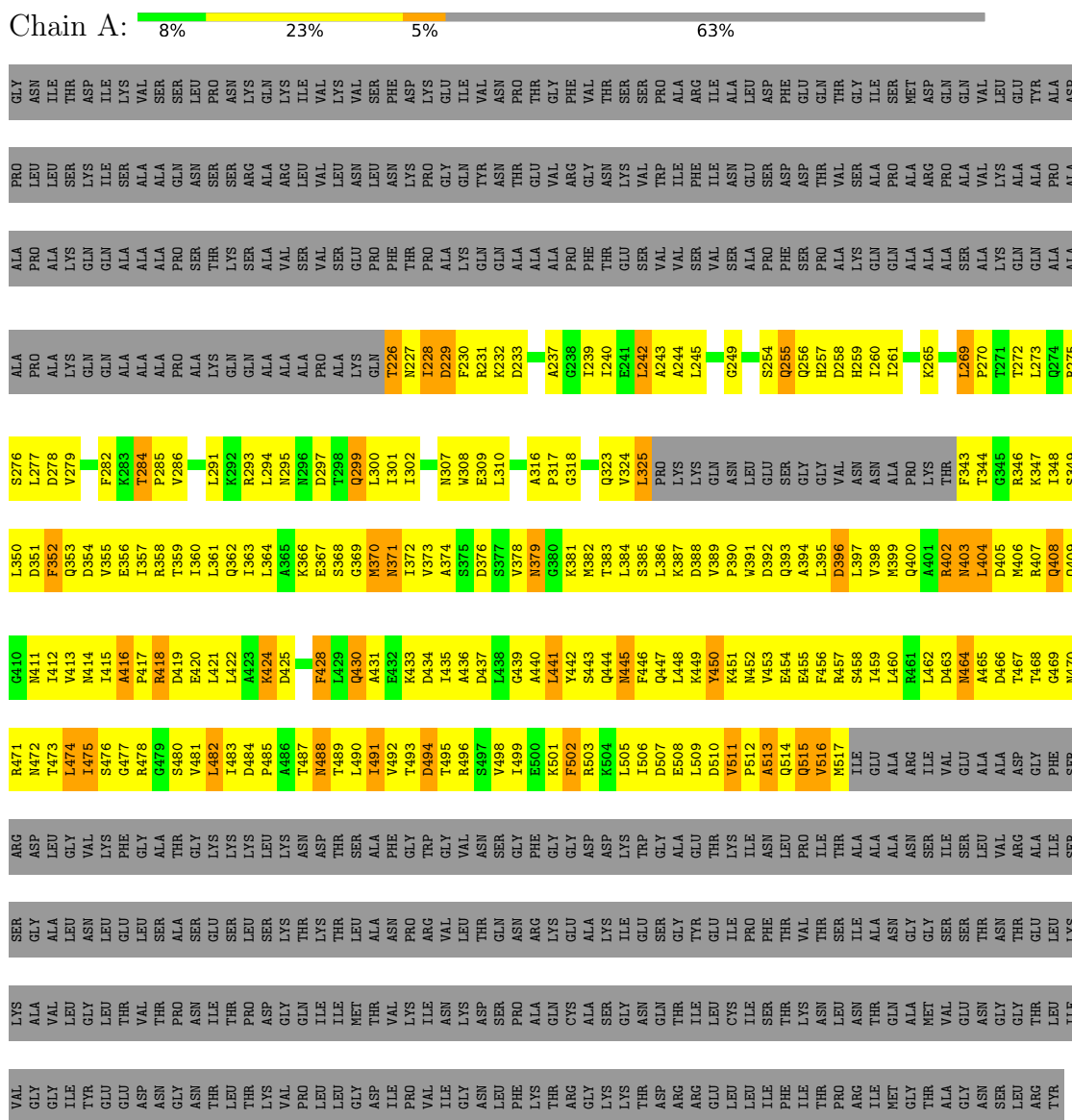
- Molecule 2 is a protein called PILP PROTEIN.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	N	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	O	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	P	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	Q	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	R	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	S	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	T	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	U	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	V	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	W	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		
2	X	82	Total	C	H	N	O	S	0	0
			740	407	96	105	131	1		

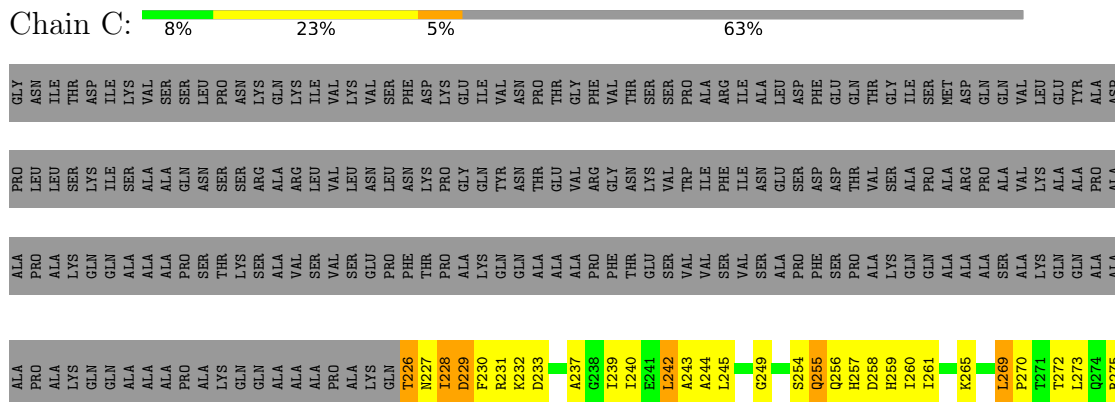
3 Residue-property plots

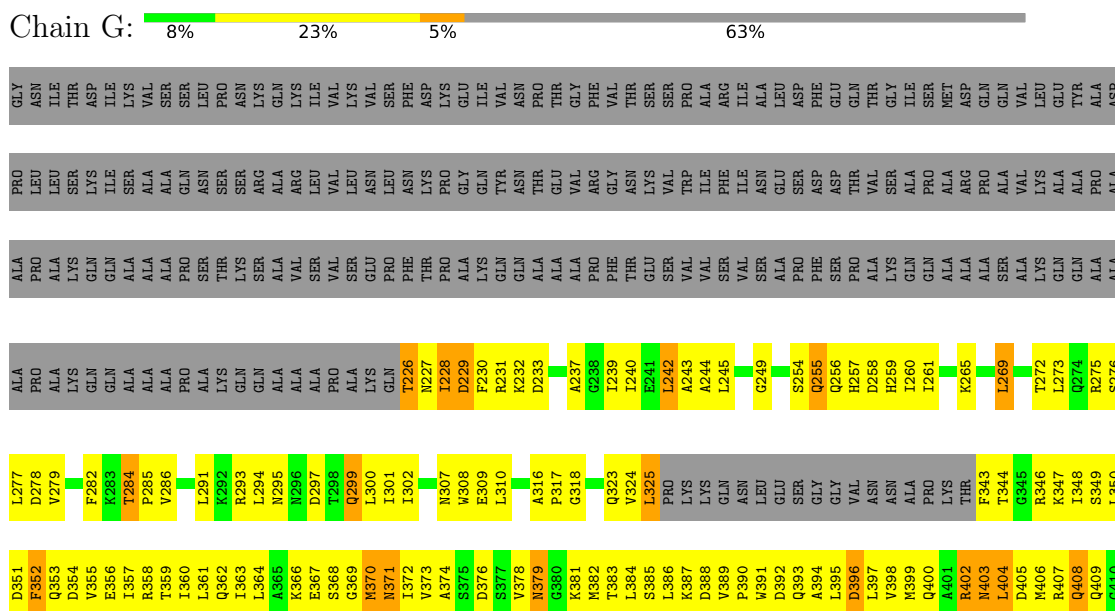
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

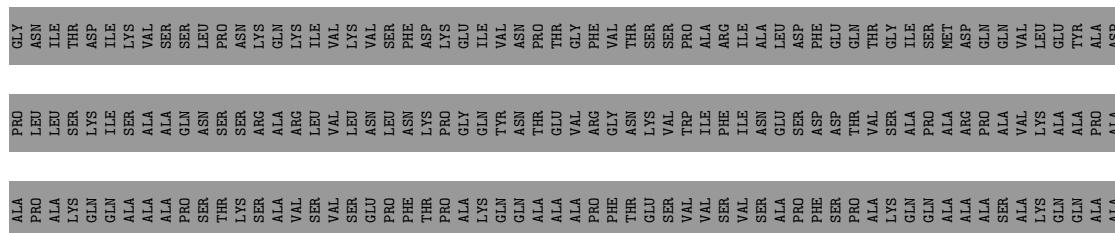
• Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



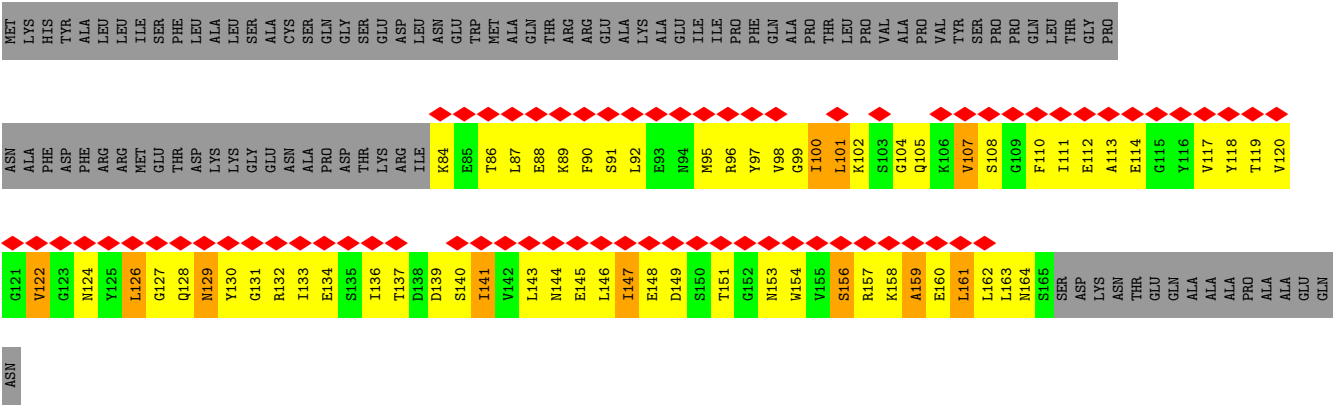
• Molecule 1: TYPE IV PILUS BIOGENESIS AND COMPETENCE PROTEIN PILQ



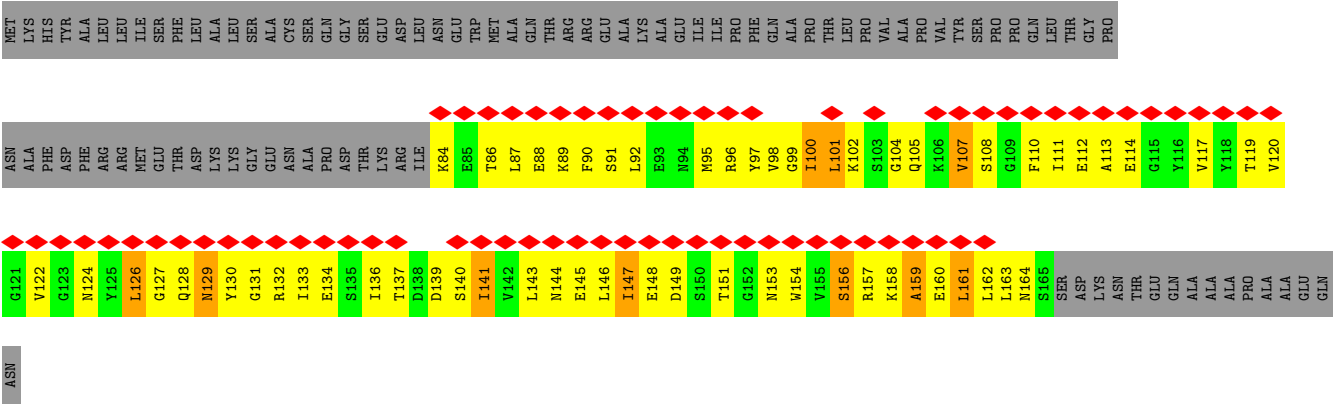
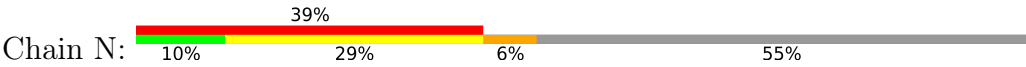




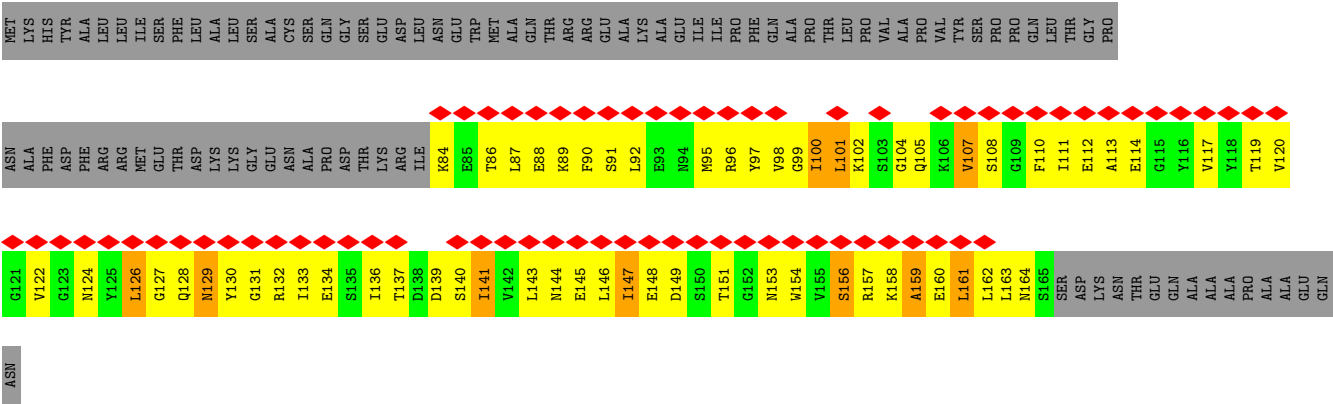
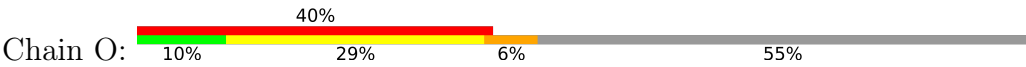




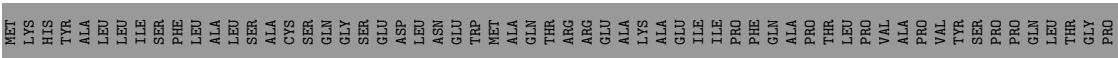
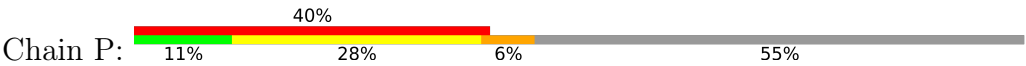
• Molecule 2: PILP PROTEIN



• Molecule 2: PILP PROTEIN

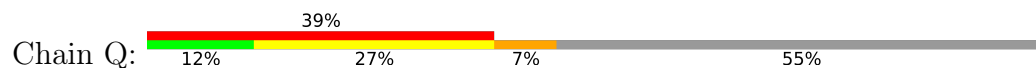


• Molecule 2: PILP PROTEIN

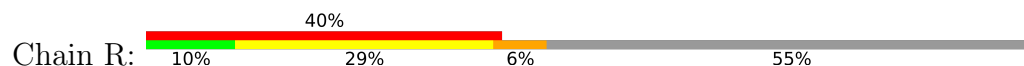




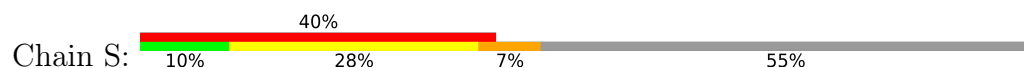
• Molecule 2: PILP PROTEIN

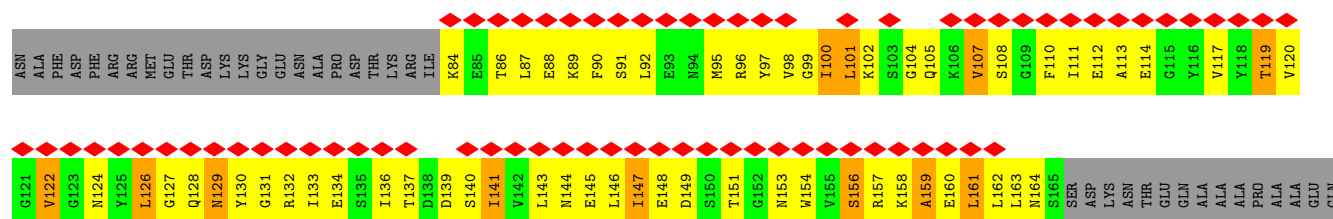


• Molecule 2: PILP PROTEIN

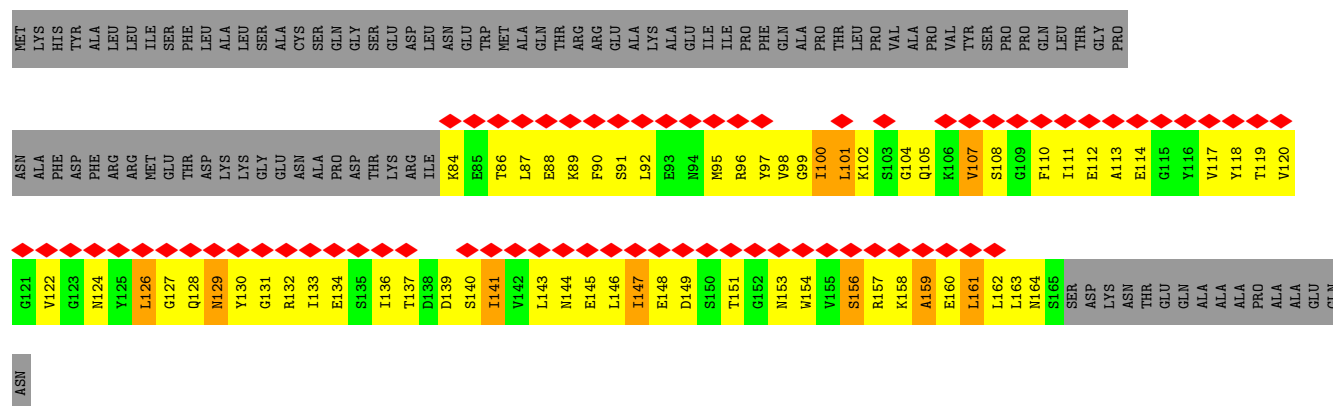
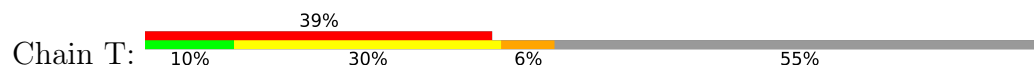


• Molecule 2: PILP PROTEIN

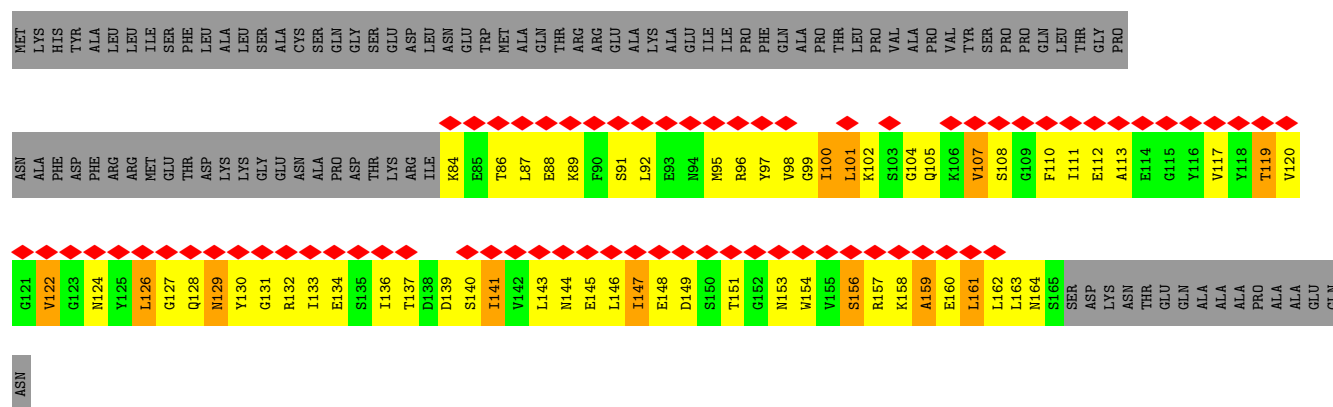
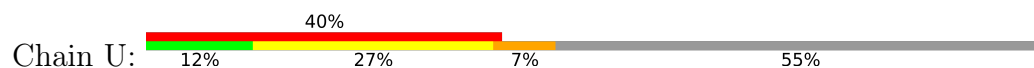




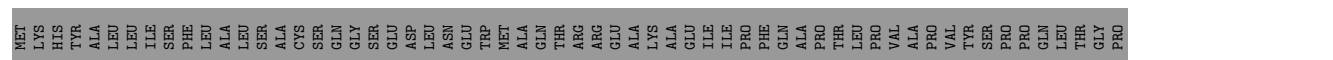
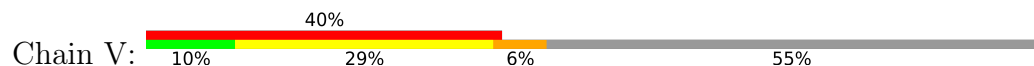
• Molecule 2: PILP PROTEIN

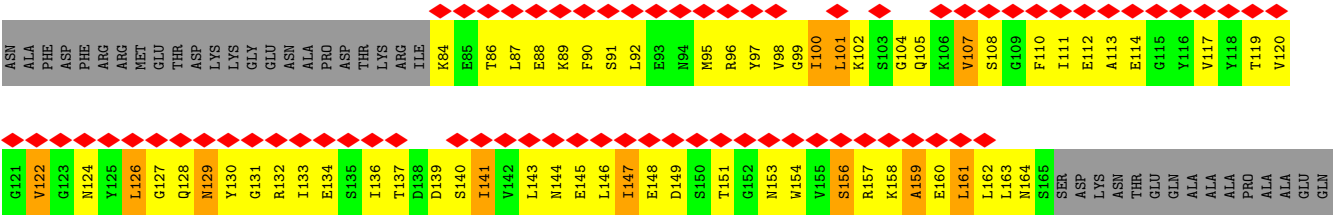


• Molecule 2: PILP PROTEIN

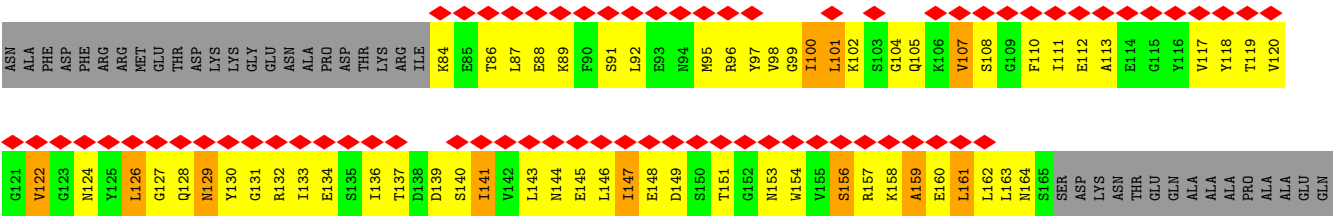
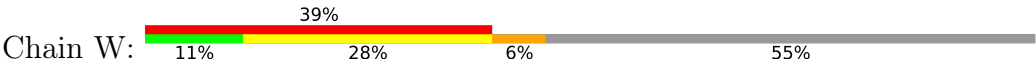


• Molecule 2: PILP PROTEIN

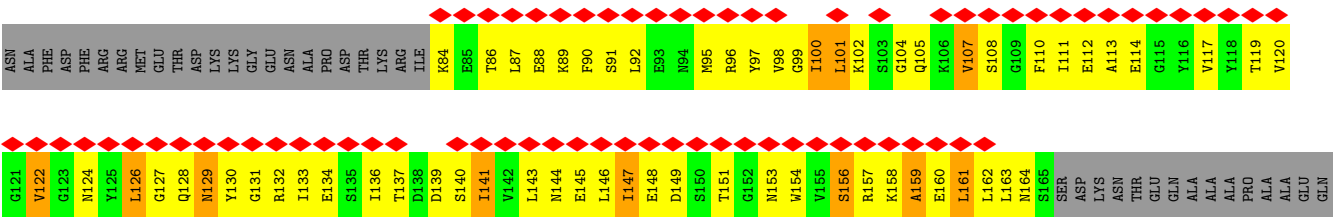
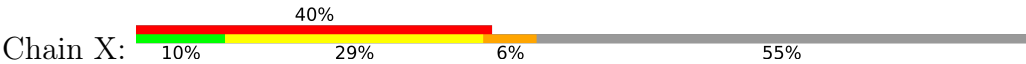




• Molecule 2: PILP PROTEIN



• Molecule 2: PILP PROTEIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	25303	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIT EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5100	Depositor
Magnification	33112	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.28	Depositor
Map size ($\text{\AA}$)	289.92, 289.92, 289.92	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.53, 4.53, 4.53	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	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	B	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	C	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	D	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	E	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	F	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	G	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	H	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	I	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	J	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	K	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
1	L	1.14	1/2179 (0.0%)	1.60	24/2950 (0.8%)
2	M	0.28	0/652	0.64	0/878
2	N	0.28	0/652	0.64	0/878
2	O	0.28	0/652	0.64	0/878
2	P	0.28	0/652	0.64	0/878
2	Q	0.28	0/652	0.64	0/878
2	R	0.28	0/652	0.64	0/878
2	S	0.28	0/652	0.64	0/878
2	T	0.28	0/652	0.64	0/878
2	U	0.28	0/652	0.64	0/878
2	V	0.28	0/652	0.64	0/878
2	W	0.28	0/652	0.64	0/878
2	X	0.28	0/652	0.64	0/878
All	All	1.01	12/33972 (0.0%)	1.44	288/45936 (0.6%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	511	VAL	CA-CB	-6.48	1.50	1.54
1	F	511	VAL	CA-CB	-6.48	1.50	1.54
1	I	511	VAL	CA-CB	-6.48	1.50	1.54
1	L	511	VAL	CA-CB	-6.48	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	VAL	CA-CB	-6.39	1.50	1.54

The worst 5 of 288 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	CG-CD-OE1	-38.08	44.65	120.80
1	D	408	GLN	CG-CD-OE1	-38.08	44.65	120.80
1	G	408	GLN	CG-CD-OE1	-38.08	44.65	120.80
1	J	408	GLN	CG-CD-OE1	-38.08	44.65	120.80
1	C	408	GLN	CG-CD-OE1	-38.07	44.66	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2152	0	2190	617	0
1	B	2152	0	2190	625	0
1	C	2152	0	2190	628	0
1	D	2152	0	2190	622	0
1	E	2152	0	2190	619	0
1	F	2152	0	2190	614	0
1	G	2152	0	2190	613	0
1	H	2152	0	2190	621	0
1	I	2152	0	2190	610	0
1	J	2152	0	2190	618	0
1	K	2152	0	2190	621	0
1	L	2152	0	2190	613	0
2	M	644	96	636	122	0
2	N	644	96	636	119	0
2	O	644	96	636	119	0
2	P	644	96	636	121	0
2	Q	644	96	636	124	0
2	R	644	96	636	123	0
2	S	644	96	636	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	644	96	636	122	0
2	U	644	96	636	117	0
2	V	644	96	636	121	0
2	W	644	96	636	119	0
2	X	644	96	636	122	0
All	All	33552	1152	33912	6831	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 101.

The worst 5 of 6831 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:E:347:LYS:NZ	2:Q:104:GLY:HA2	1.29	1.47
1:C:347:LYS:NZ	2:O:104:GLY:HA2	1.30	1.46
1:G:347:LYS:NZ	2:S:104:GLY:HA2	1.30	1.46
1:A:347:LYS:NZ	2:M:104:GLY:HA2	1.30	1.41
1:I:347:LYS:NZ	2:U:104:GLY:HA2	1.30	1.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	B	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	C	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	D	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	E	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	G	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	H	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	I	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	J	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	K	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
1	L	271/745 (36%)	235 (87%)	29 (11%)	7 (3%)	4	25
2	M	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	N	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	O	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	P	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	Q	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	R	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	S	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	T	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	U	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	V	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	W	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
2	X	80/181 (44%)	51 (64%)	19 (24%)	10 (12%)	0	4
All	All	4212/11112 (38%)	3432 (82%)	576 (14%)	204 (5%)	3	16

5 of 204 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	402	ARG
1	B	379	ASN
1	B	402	ARG
1	C	379	ASN

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	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	B	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	C	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	D	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	E	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	F	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	G	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	H	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	I	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	J	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	K	239/615 (39%)	213 (89%)	26 (11%)	6	21
1	L	239/615 (39%)	213 (89%)	26 (11%)	6	21
2	M	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	N	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	O	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	P	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	Q	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	R	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	S	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	T	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	U	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	V	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	W	71/152 (47%)	63 (89%)	8 (11%)	5	19
2	X	71/152 (47%)	63 (89%)	8 (11%)	5	19
All	All	3720/9204 (40%)	3312 (89%)	408 (11%)	8	20

5 of 408 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	475	ILE
1	L	226	THR
2	W	164	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	242	LEU
1	K	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 161 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	307	ASN
2	P	94	ASN
1	K	408	GLN
1	L	403	ASN
2	S	129	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](#)

There are no chain breaks in this entry.

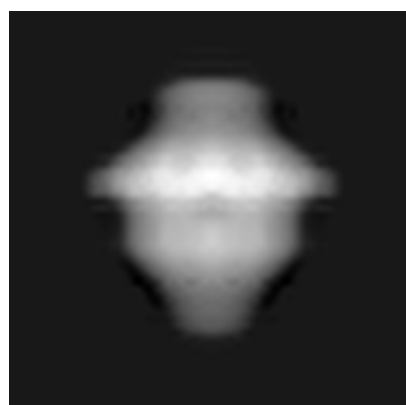
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2105. These allow visual inspection of the internal detail of the map and identification of artifacts.

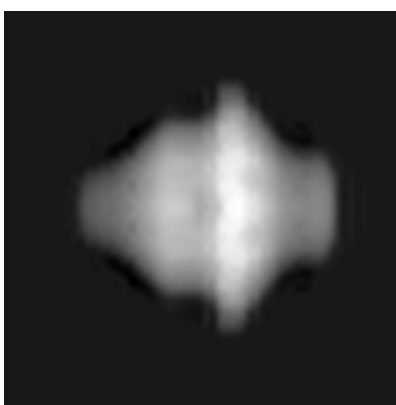
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

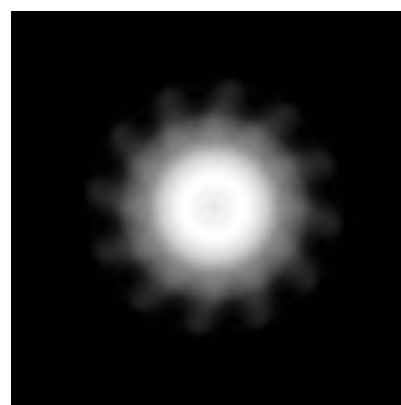
6.1.1 Primary map



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: 32



Y Index: 32



Z Index: 32

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: 32



Y Index: 32



Z Index: 36

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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

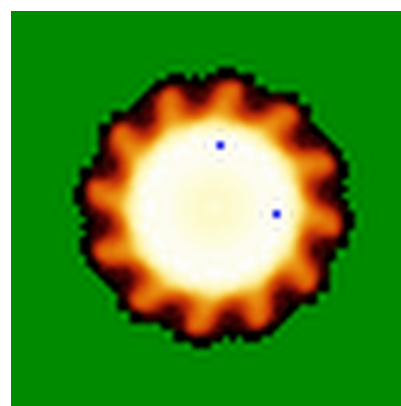
6.4.1 Primary map



X



Y

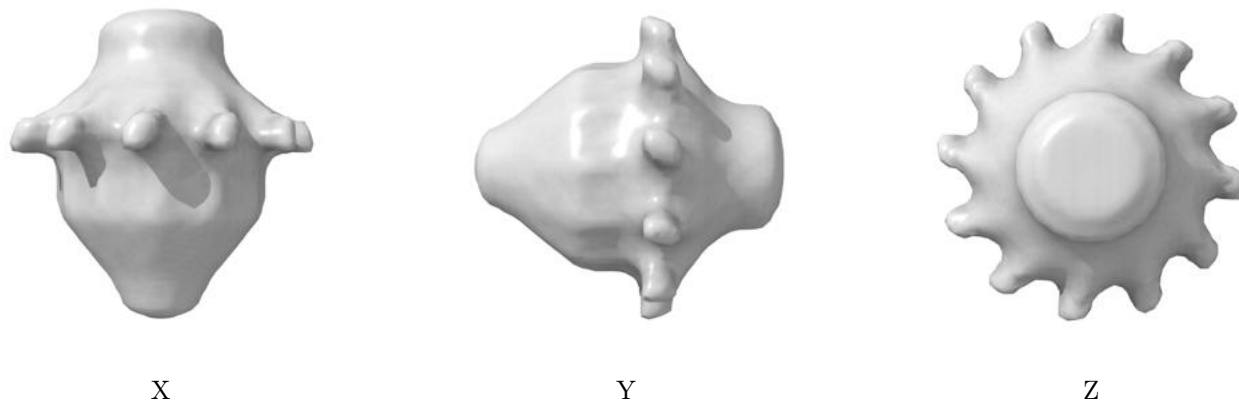


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

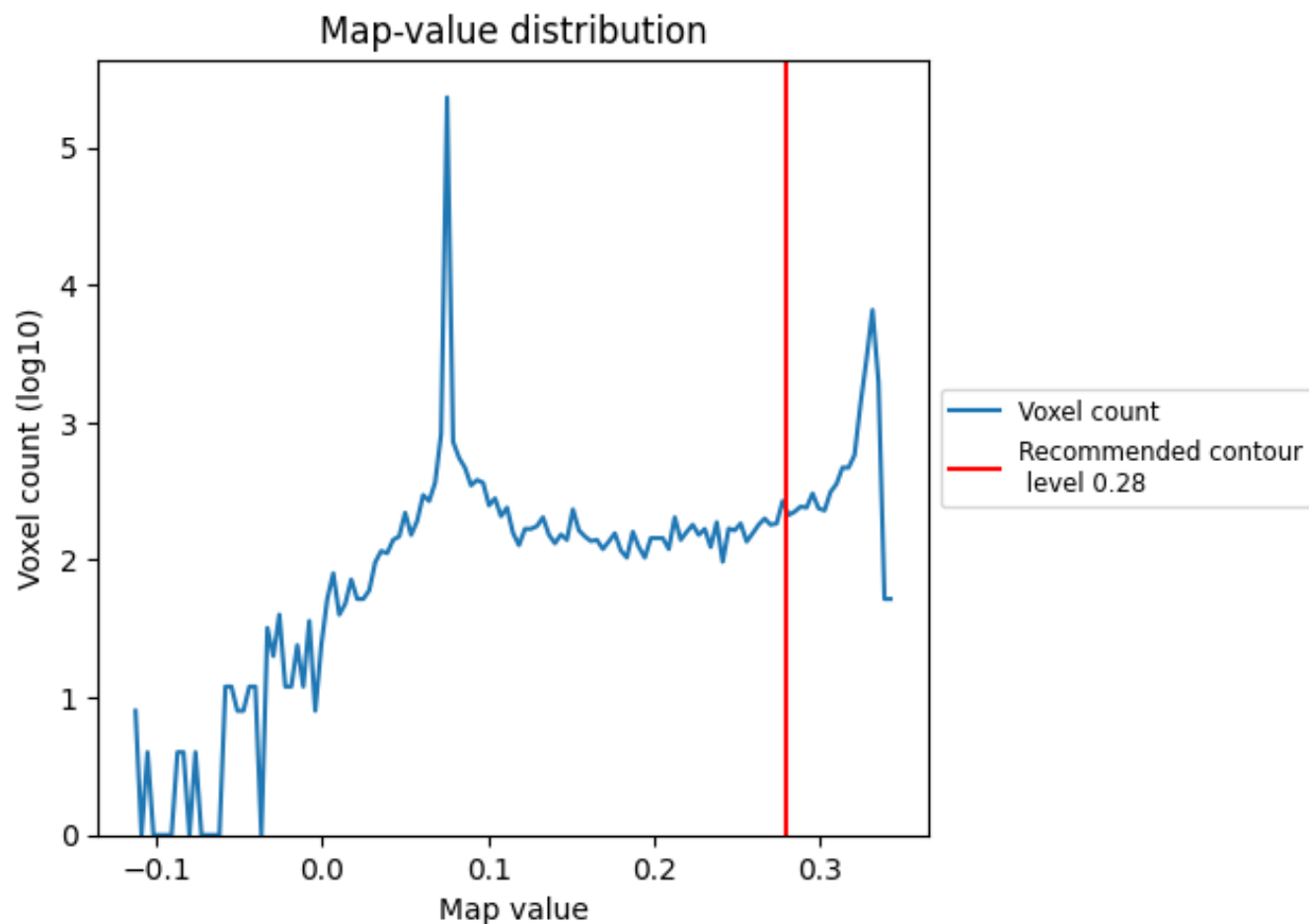
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

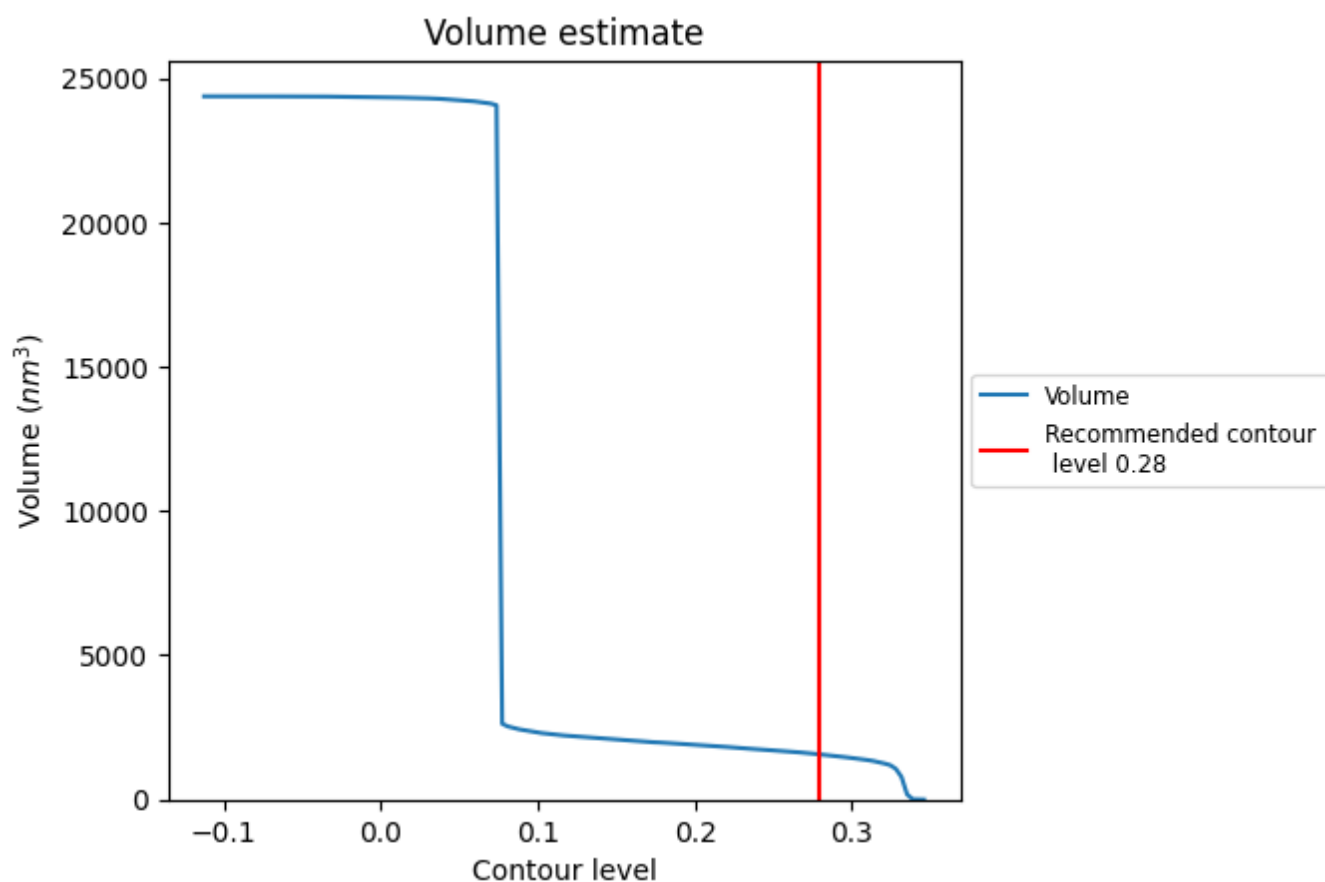
This section contains the results of statistical analysis of the map.

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.

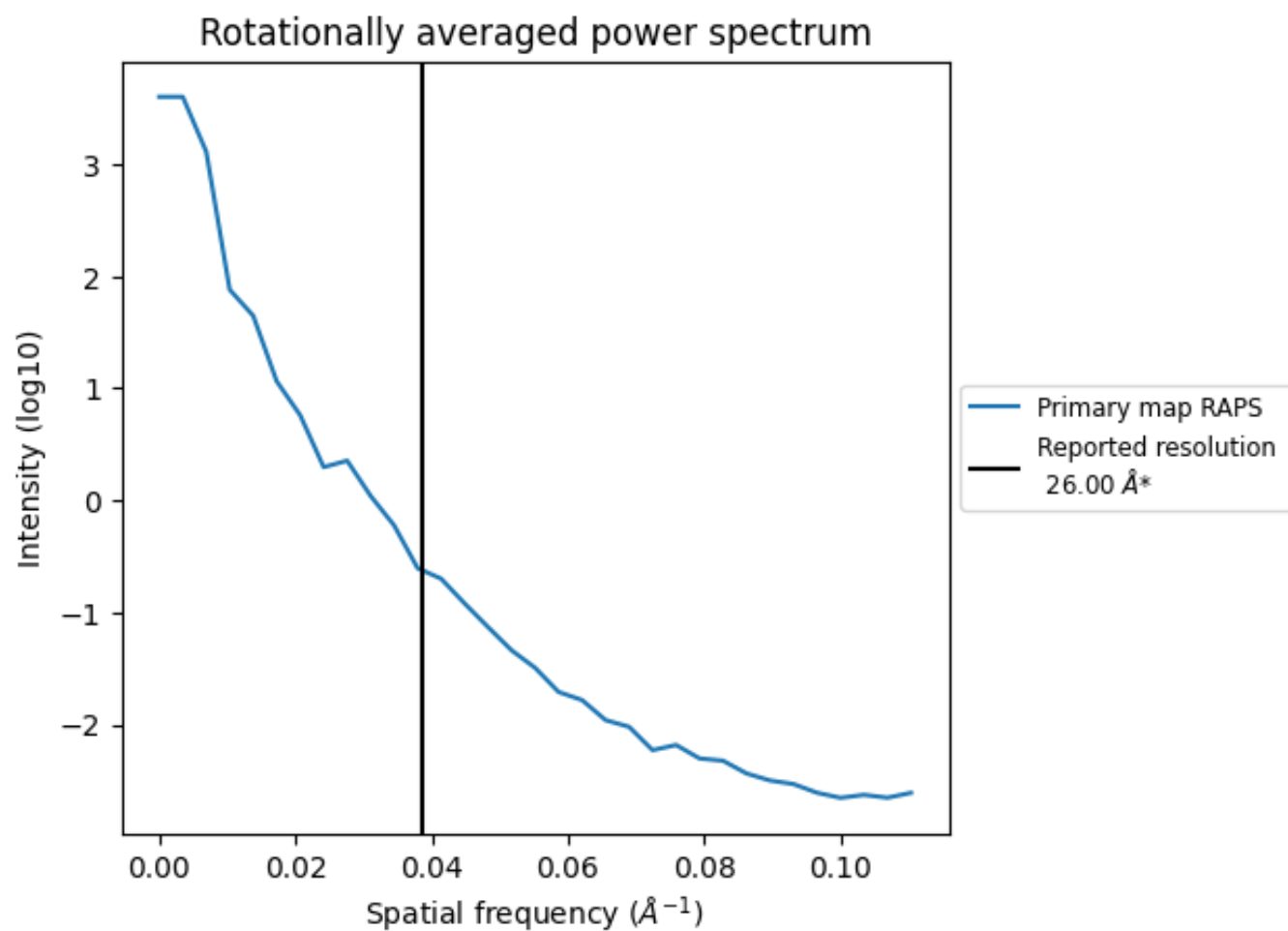
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1565 nm³; this corresponds to an approximate mass of 1414 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.038 Å⁻¹

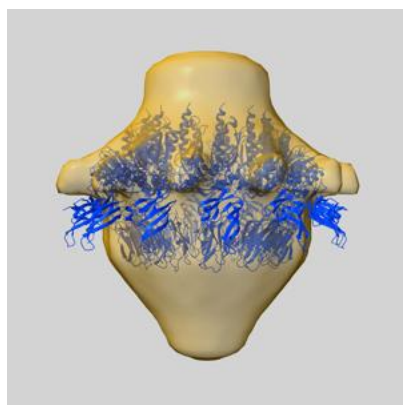
8 Fourier-Shell correlation

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

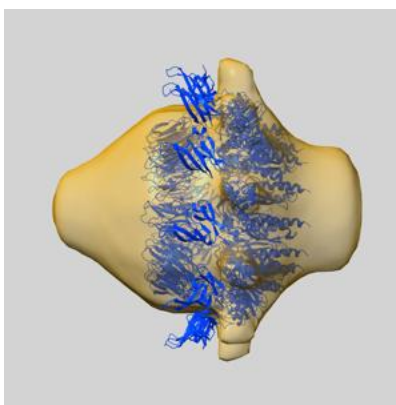
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2105 and PDB model 4AV2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

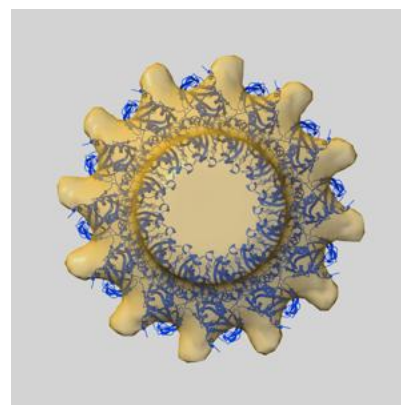
9.1 Map-model overlay [i](#)



X



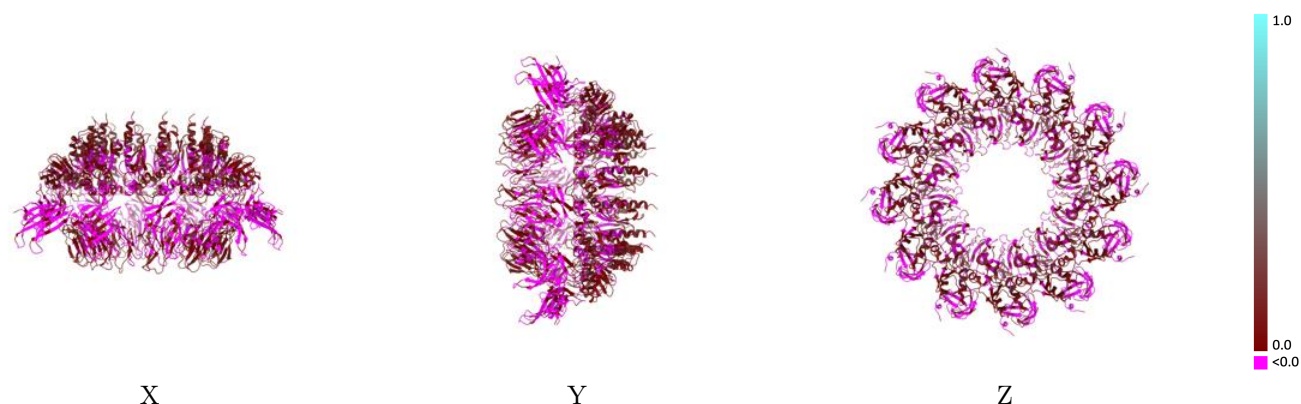
Y



Z

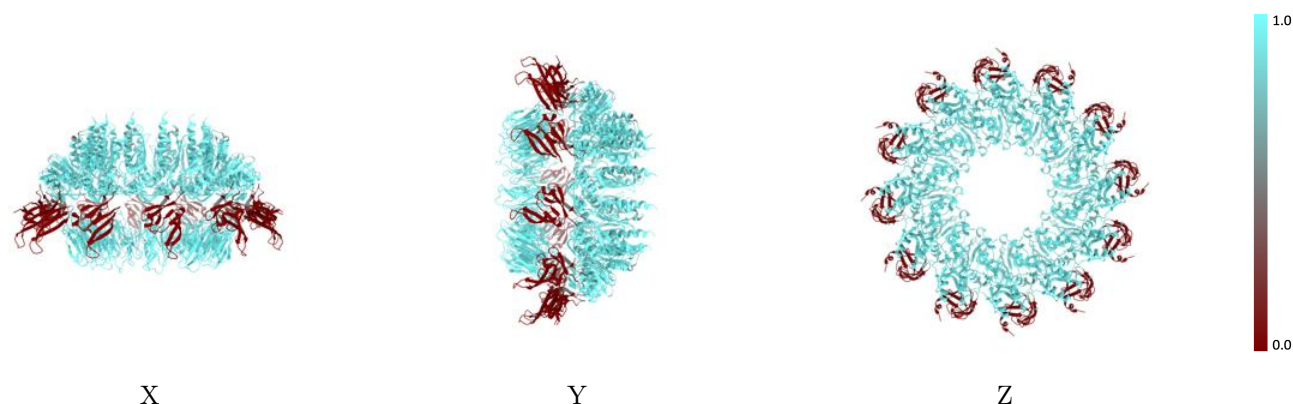
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



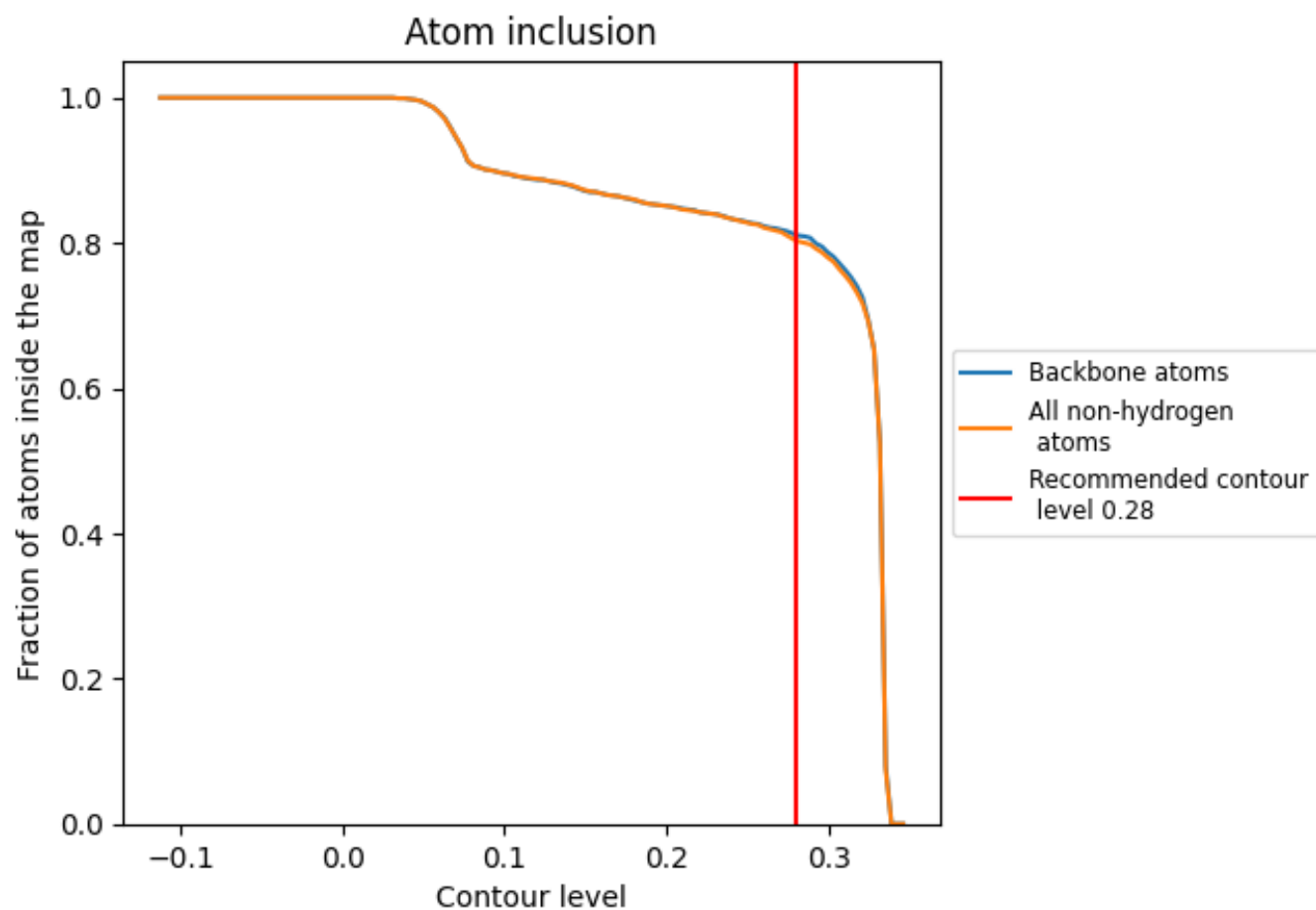
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.28).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.0380
A	 0.9890	 0.0630
B	 0.9890	 0.0590
C	 0.9890	 0.0650
D	 0.9890	 0.0620
E	 0.9890	 0.0600
F	 0.9890	 0.0650
G	 0.9890	 0.0620
H	 0.9890	 0.0600
I	 0.9890	 0.0660
J	 0.9890	 0.0640
K	 0.9890	 0.0610
L	 0.9890	 0.0640
M	 0.0900	 -0.0540
N	 0.0900	 -0.0460
O	 0.0900	 -0.0540
P	 0.0900	 -0.0550
Q	 0.0900	 -0.0380
R	 0.0900	 -0.0470
S	 0.0900	 -0.0440
T	 0.0900	 -0.0320
U	 0.0900	 -0.0440
V	 0.0900	 -0.0460
W	 0.0900	 -0.0370
X	 0.0900	 -0.0520

