wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 03:40 AM JST

PDB ID	:	7E2D
EMDB ID	:	EMD-30955
Title	:	Monomer of TRAPPII (Closed)
Authors	:	Sui, S.F.; Sun, S.; Mi, C.C.
Deposited on	:	2021-02-05
Resolution	:	3.71 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:

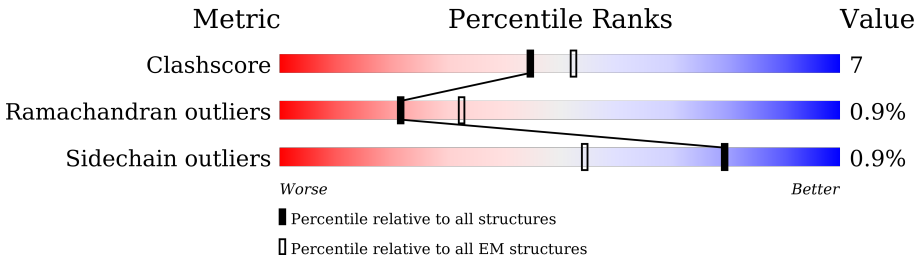
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.71 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	152	85% 10% 5%
2	C	191	85% 10%
2	F	191	81% 14% 5%
3	B	268	60% 15% 25%
4	D	159	72% 22% 5%
5	E	219	57% 16% 24%
6	G	283	62% 10% 28%
7	H	175	74% 10% 16%

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Mol	Chain	Length	Quality of chain
8	I	1102	
9	J	1289	
10	K	560	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23331 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 TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	144	Total	C	N	O	S	0	0
			1160	753	182	221	4		

- Molecule 2 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	184	Total	C	N	O	S	0	0
			1482	947	244	280	11		
2	F	182	Total	C	N	O	S	0	0
			1470	939	242	278	11		

- Molecule 3 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	202	Total	C	N	O	S	0	0
			1630	1051	274	297	8		

- Molecule 4 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total	C	N	O	S	0	0
			1235	793	209	227	6		

- Molecule 5 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	166	Total	C	N	O	S	0	0
			1341	866	214	251	10		

- Molecule 6 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	204	Total	C	N	O	S	0	0
			1648	1052	285	302	9		

- Molecule 7 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	147	Total	C	N	O	S	0	0
			1180	763	195	217	5		

- Molecule 8 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	788	Total	C	N	O	S	0	0
			4204	2558	811	833	2		

- Molecule 9 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	872	Total	C	N	O	S	0	0
			6332	4034	1094	1185	19		

- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 65.

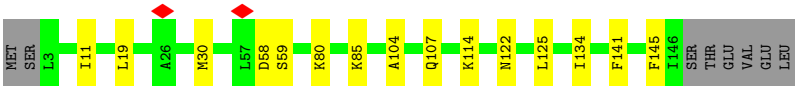
Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	251	Total	C	N	O	S	0	0
			1649	1041	291	315	2		

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.

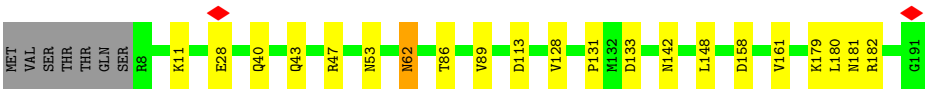
• Molecule 1: TRAPP-associated protein TCA17

Chain A:



• Molecule 2: Trafficking protein particle complex subunit BET3

Chain C:

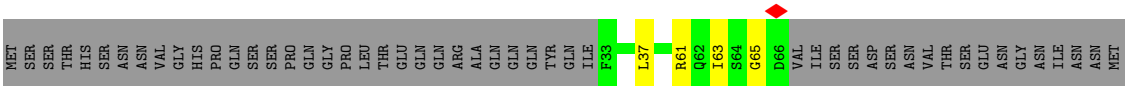


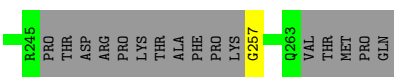
• Molecule 2: Trafficking protein particle complex subunit BET3

Chain F:

• Molecule 3: Trafficking protein particle complex subunit 33

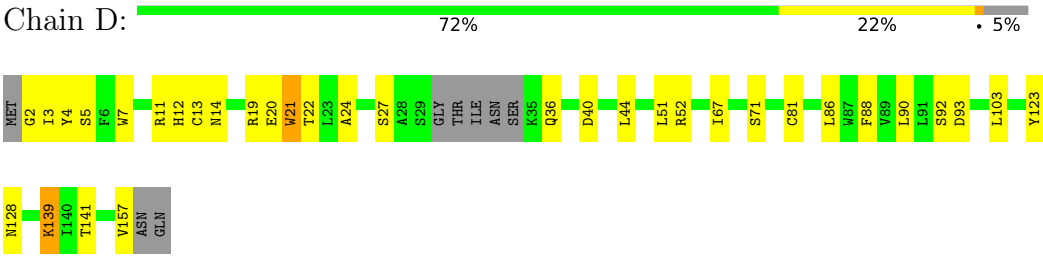
Chain B:





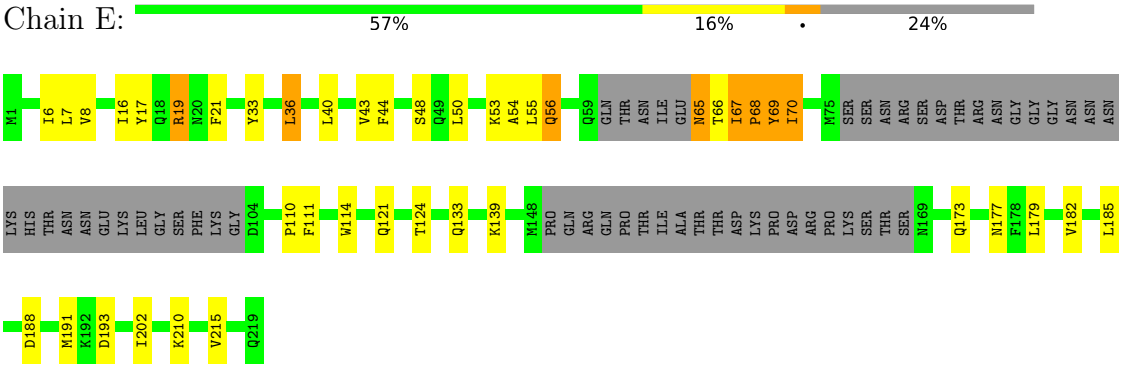
• Molecule 4: Trafficking protein particle complex subunit BET5

Chain D:



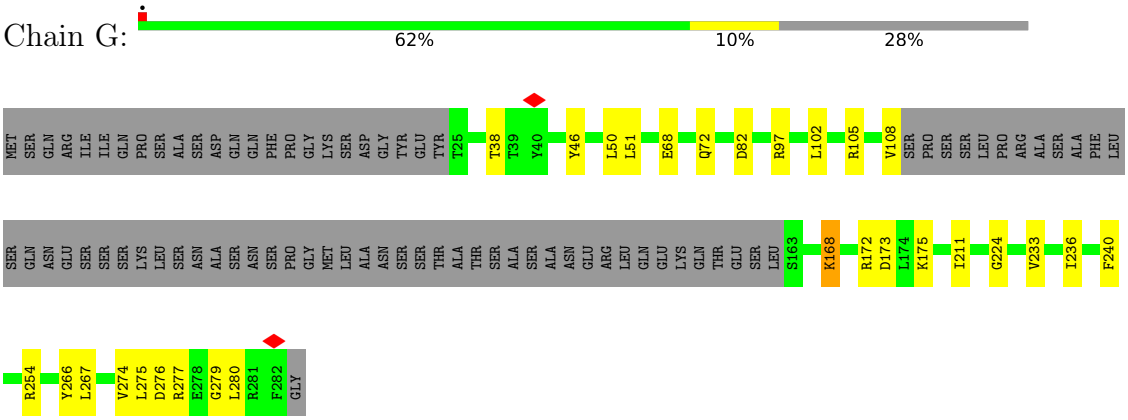
• Molecule 5: Trafficking protein particle complex subunit 23

Chain E:



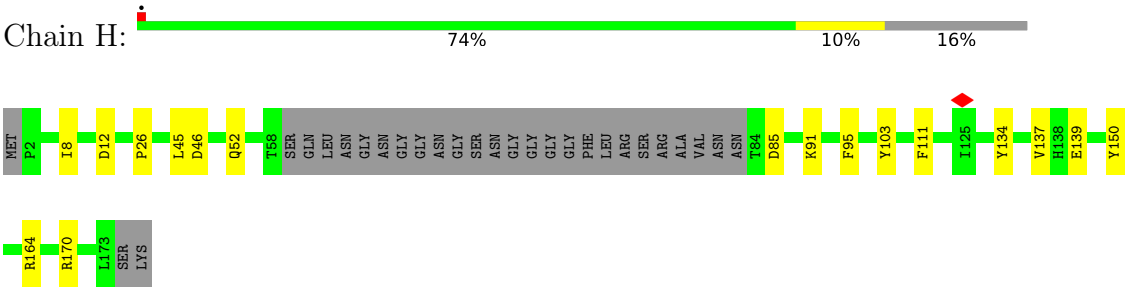
• Molecule 6: Trafficking protein particle complex subunit 31

Chain G:



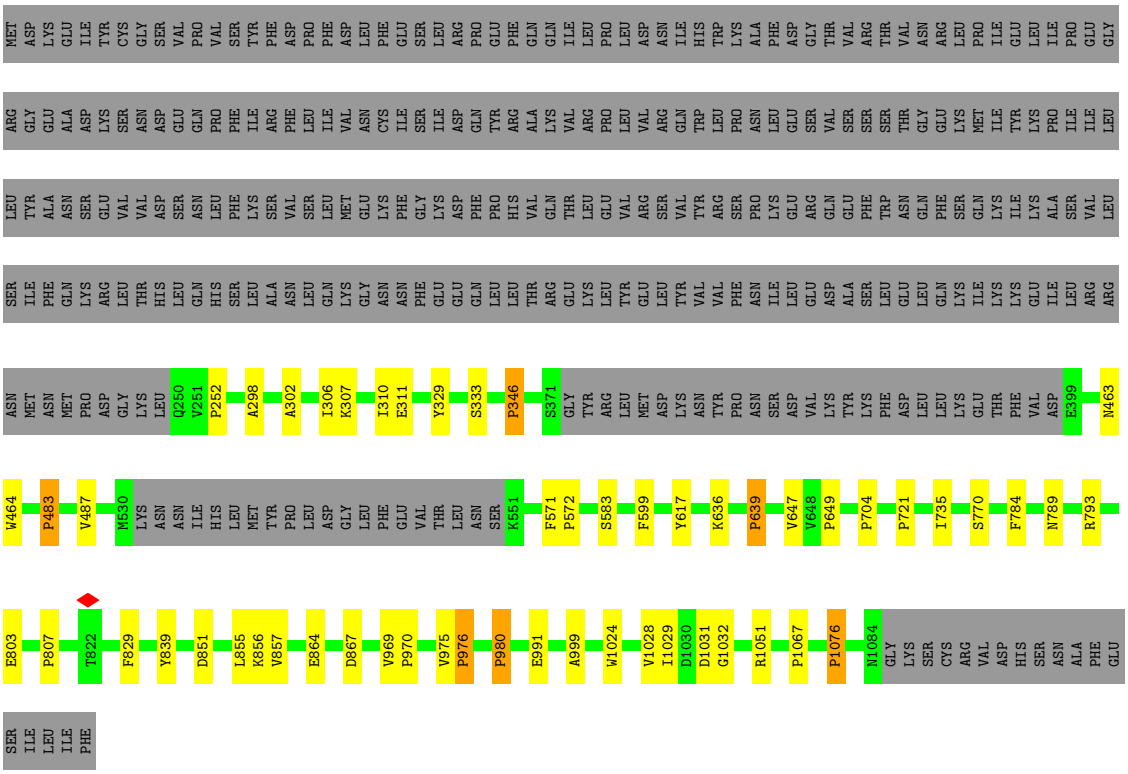
• Molecule 7: Trafficking protein particle complex subunit 20

Chain H:



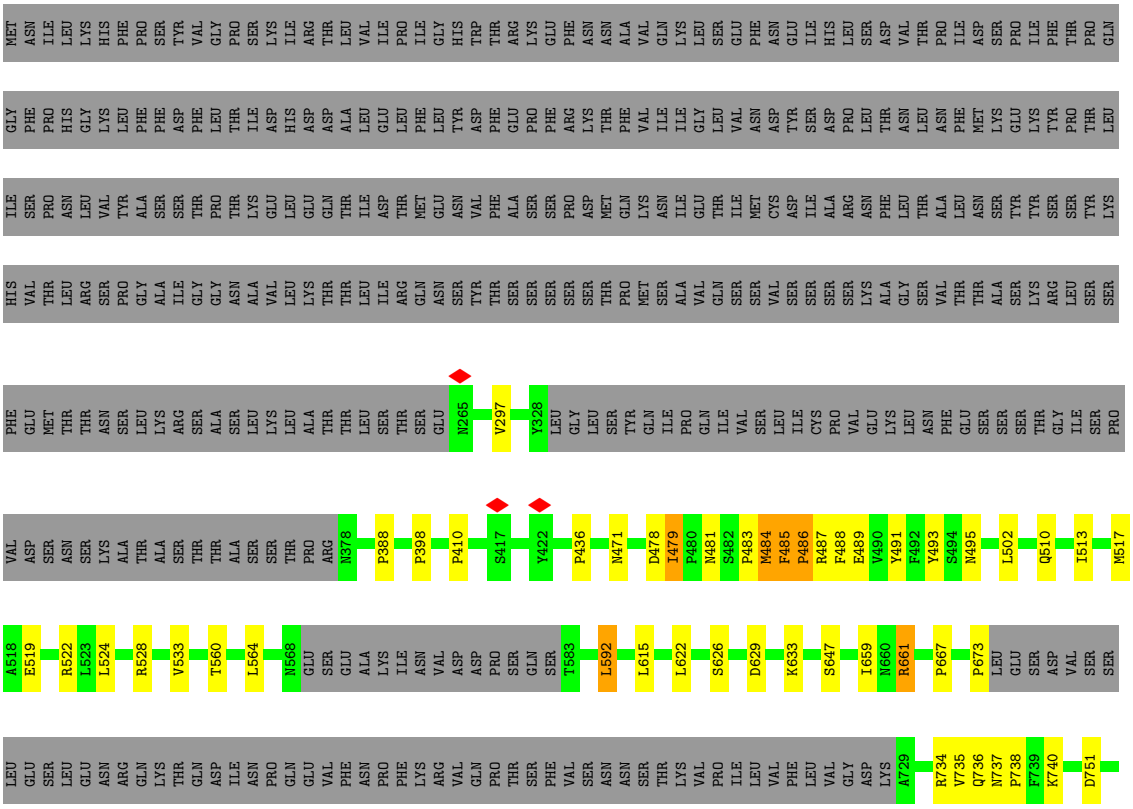
• Molecule 8: Trafficking protein particle complex II-specific subunit 130

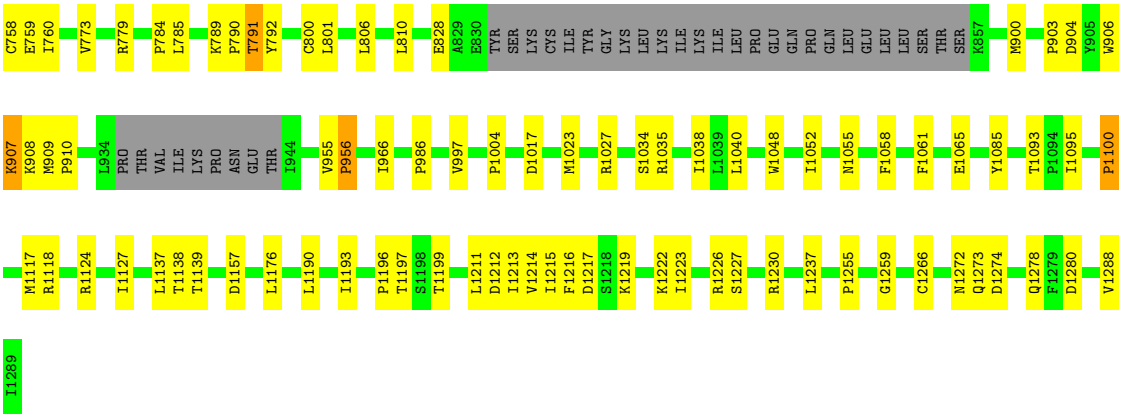
Chain I:



• Molecule 9: Trafficking protein particle complex II-specific subunit 120

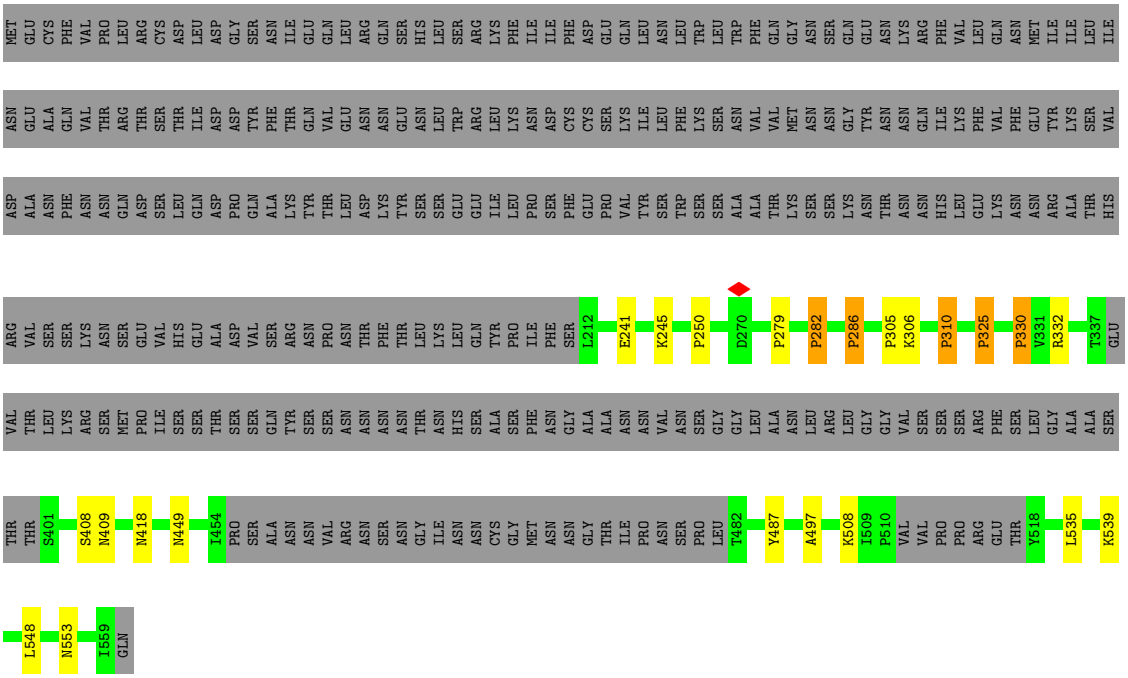
Chain J:





• Molecule 10: Trafficking protein particle complex II-specific subunit 65

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181003	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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	0.35	0/1180	0.73	1/1592 (0.1%)
2	C	0.42	0/1509	0.80	2/2040 (0.1%)
2	F	0.38	0/1497	0.78	2/2024 (0.1%)
3	B	0.40	0/1658	0.83	3/2229 (0.1%)
4	D	0.39	0/1263	0.77	2/1704 (0.1%)
5	E	0.38	0/1365	0.85	7/1840 (0.4%)
6	G	0.39	0/1683	0.70	2/2269 (0.1%)
7	H	0.38	0/1211	0.87	5/1643 (0.3%)
8	I	0.30	0/4226	0.65	13/5864 (0.2%)
9	J	0.37	0/6437	0.83	25/8760 (0.3%)
10	K	0.33	0/1663	0.85	9/2268 (0.4%)
All	All	0.37	0/23692	0.78	71/32233 (0.2%)

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	1052	ILE	CG1-CB-CG2	-11.09	87.00	111.40
9	J	1274	ASP	CB-CG-OD1	9.80	127.12	118.30
7	H	46	ASP	CB-CG-OD1	8.60	126.04	118.30
9	J	659	ILE	CG1-CB-CG2	-8.18	93.42	111.40
9	J	806	LEU	CA-CB-CG	7.80	133.25	115.30

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	1160	0	1184	11	0
2	C	1482	0	1490	13	0
2	F	1470	0	1476	37	0
3	B	1630	0	1640	30	0
4	D	1235	0	1202	32	0
5	E	1341	0	1349	44	0
6	G	1648	0	1630	19	0
7	H	1180	0	1132	9	0
8	I	4204	0	2169	20	0
9	J	6332	0	5658	107	0
10	K	1649	0	1338	16	0
All	All	23331	0	20268	295	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 7.

The worst 5 of 295 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)
5:E:44:PHE:CE1	2:F:189:PRO:HG3	1.49	1.43
9:J:478:ASP:OD2	9:J:488:PHE:HE1	1.15	1.25
9:J:1216:PHE:CD1	9:J:1222:LYS:HB3	1.71	1.24
5:E:44:PHE:HE1	2:F:189:PRO:CG	1.61	1.14
2:C:181:ASN:O	2:C:182:ARG:HG2	1.48	1.13

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	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
2	C	182/191 (95%)	167 (92%)	15 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	180/191 (94%)	172 (96%)	8 (4%)	0	100	100
3	B	196/268 (73%)	186 (95%)	10 (5%)	0	100	100
4	D	147/159 (92%)	137 (93%)	10 (7%)	0	100	100
5	E	158/219 (72%)	144 (91%)	12 (8%)	2 (1%)	12	47
6	G	200/283 (71%)	190 (95%)	10 (5%)	0	100	100
7	H	143/175 (82%)	133 (93%)	10 (7%)	0	100	100
8	I	782/1102 (71%)	678 (87%)	90 (12%)	14 (2%)	8	41
9	J	860/1289 (67%)	726 (84%)	127 (15%)	7 (1%)	19	56
10	K	243/560 (43%)	212 (87%)	26 (11%)	5 (2%)	7	39
All	All	3233/4589 (70%)	2882 (89%)	323 (10%)	28 (1%)	21	53

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	346	PRO
8	I	483	PRO
8	I	639	PRO
8	I	969	VAL
8	I	976	PRO

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	134/142 (94%)	134 (100%)	0	100	100
2	C	169/176 (96%)	168 (99%)	1 (1%)	86	92
2	F	168/176 (96%)	168 (100%)	0	100	100
3	B	180/248 (73%)	178 (99%)	2 (1%)	73	85
4	D	135/145 (93%)	134 (99%)	1 (1%)	84	91
5	E	152/199 (76%)	148 (97%)	4 (3%)	46	69
6	G	182/249 (73%)	180 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	H	127/152 (84%)	126 (99%)	1 (1%)	81 89
8	I	78/1023 (8%)	78 (100%)	0	100 100
9	J	575/1213 (47%)	567 (99%)	8 (1%)	67 82
10	K	121/518 (23%)	121 (100%)	0	100 100
All	All	2021/4241 (48%)	2002 (99%)	19 (1%)	79 88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	485	PHE
9	J	907	LYS
9	J	1226	ARG
9	J	661	ARG
6	G	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	65	ASN
5	E	133	GLN
9	J	737	ASN
8	I	854	ASN
3	B	143	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.

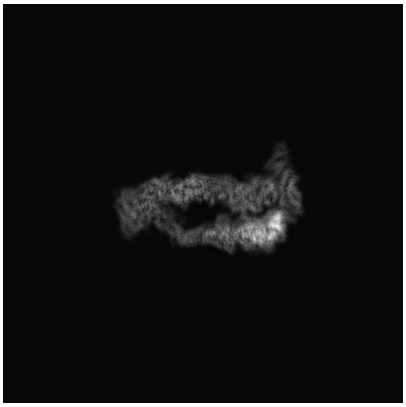
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30955. These allow visual inspection of the internal detail of the map and identification of artifacts.

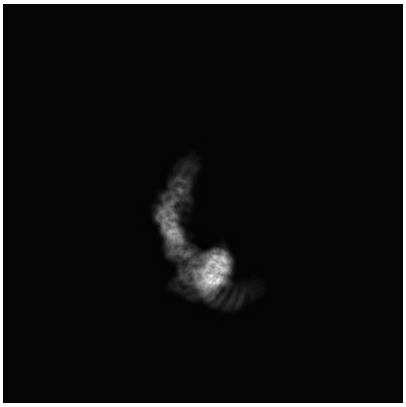
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

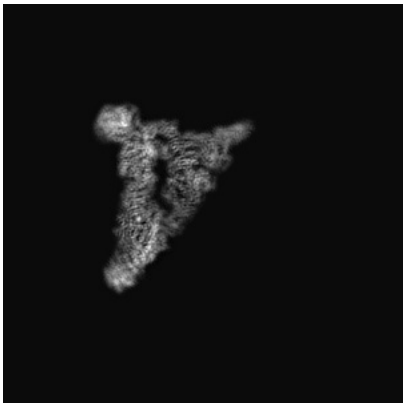
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 240

Y Index: 240

Z Index: 240

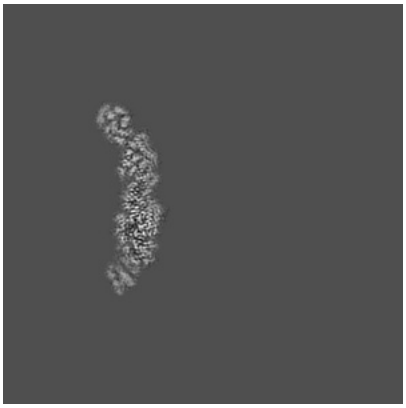
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 159

Y Index: 325

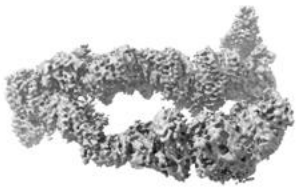


Z Index: 253

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

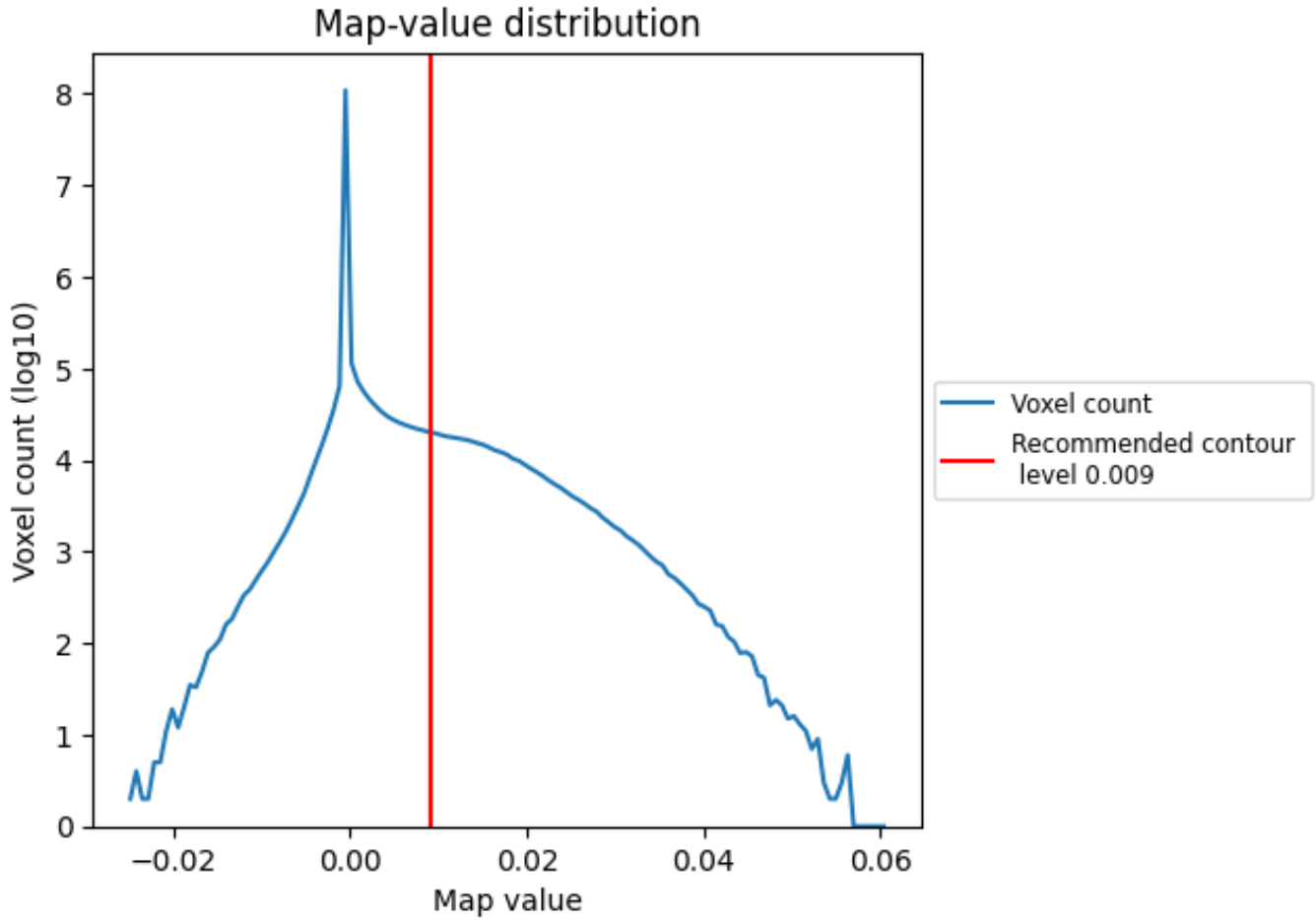
6.5 Mask visualisation (i)

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

7 Map analysis

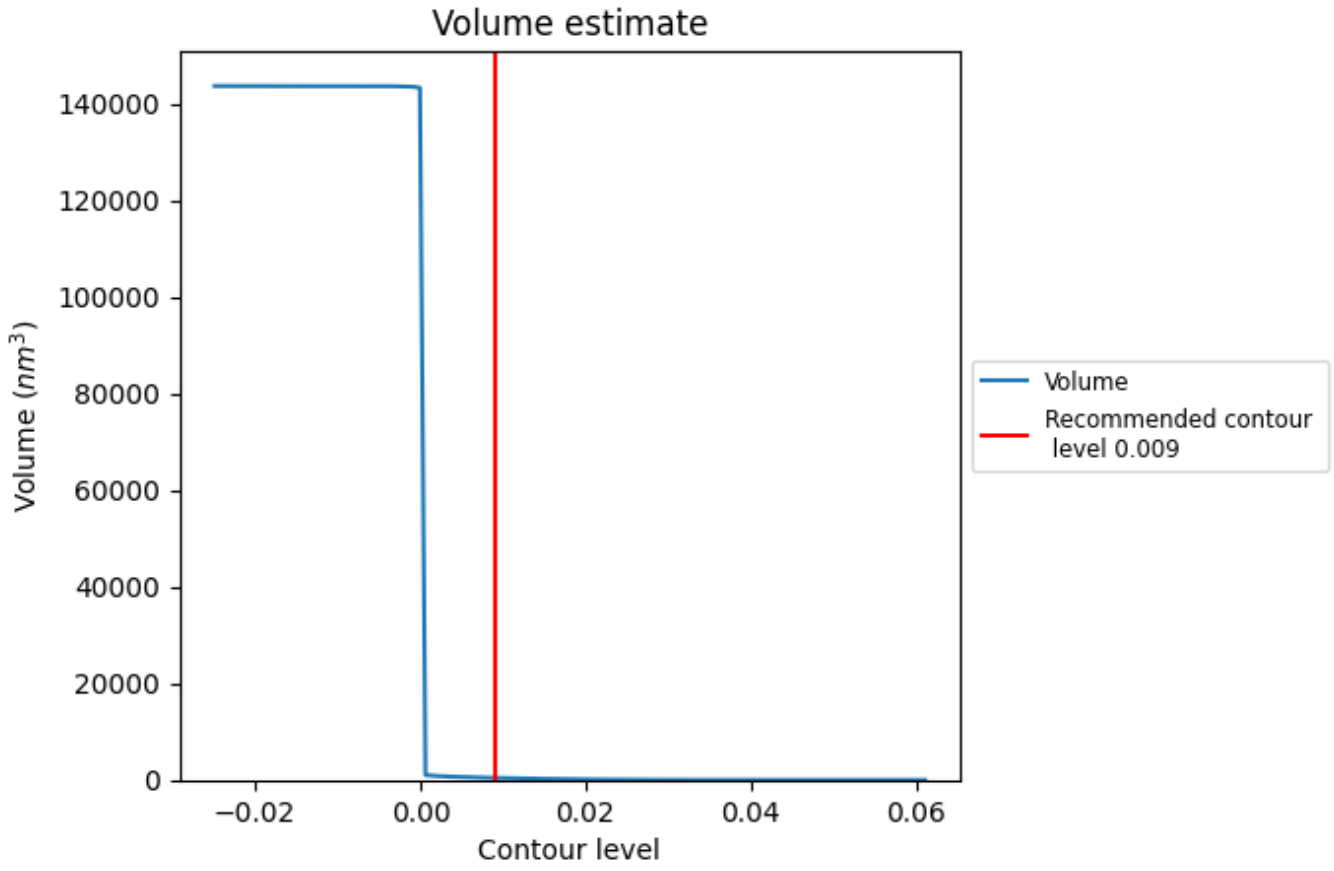
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

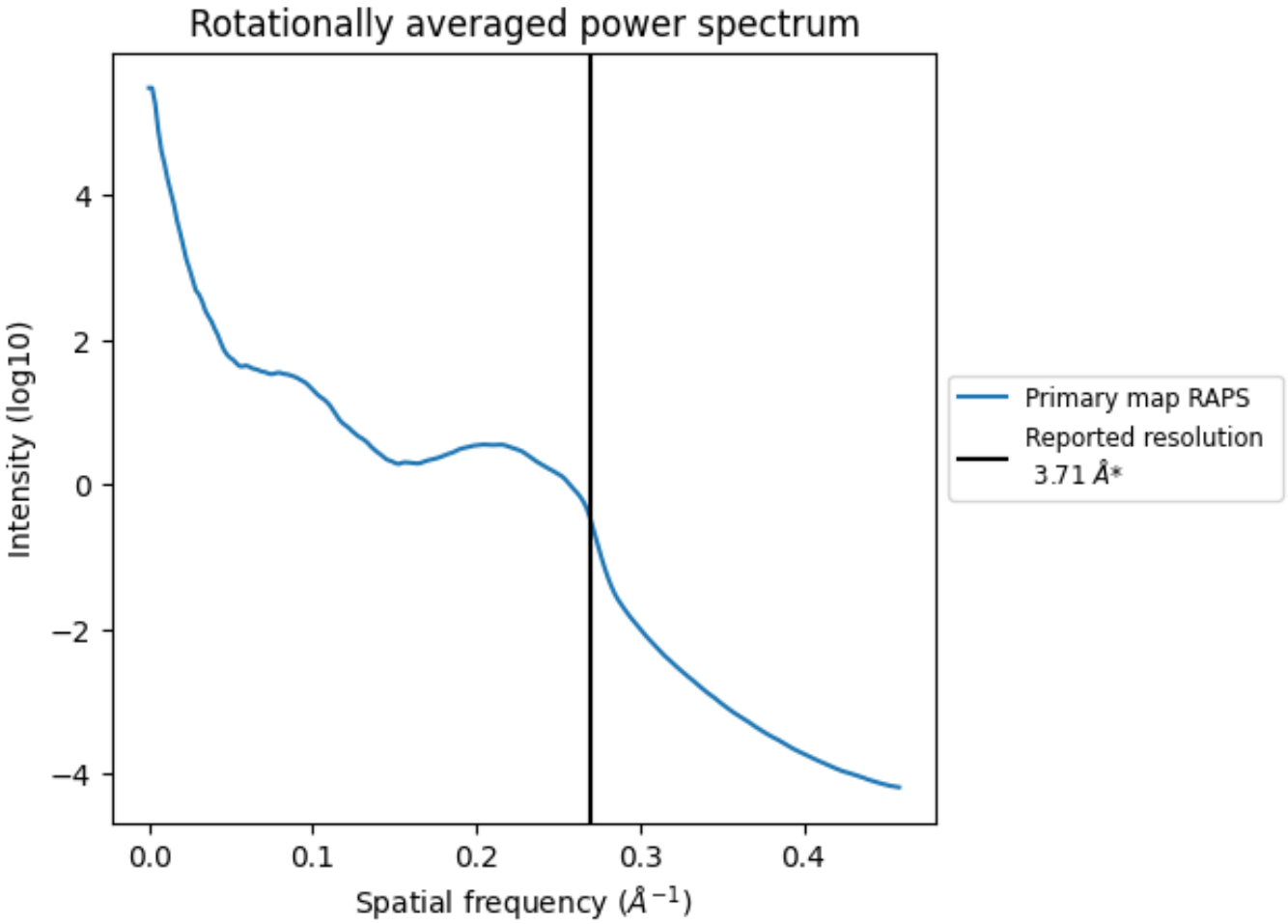
7.2 Volume estimate (i)



The volume at the recommended contour level is 430 nm^3; this corresponds to an approximate mass of 389 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)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

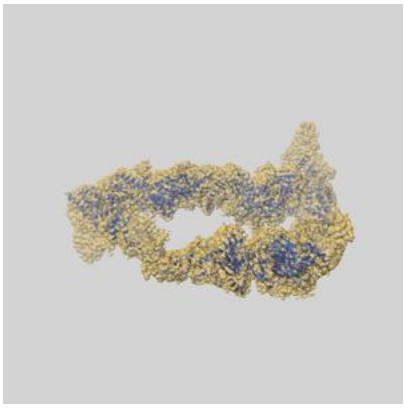
8 Fourier-Shell correlation (i)

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

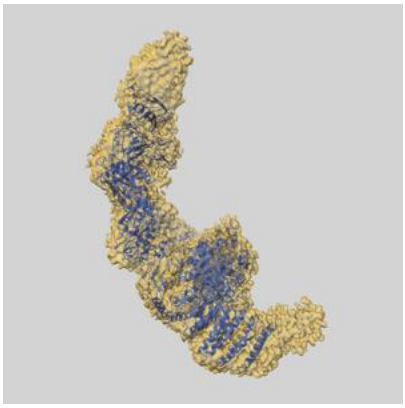
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30955 and PDB model 7E2D. Per-residue inclusion information can be found in section 3 on page 6.

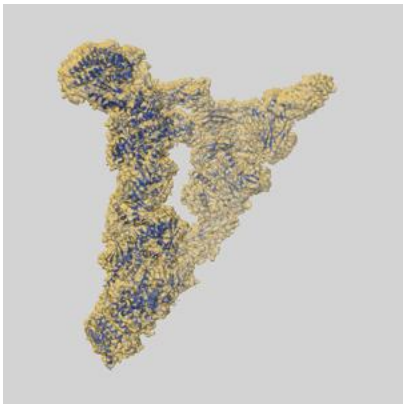
9.1 Map-model overlay



X



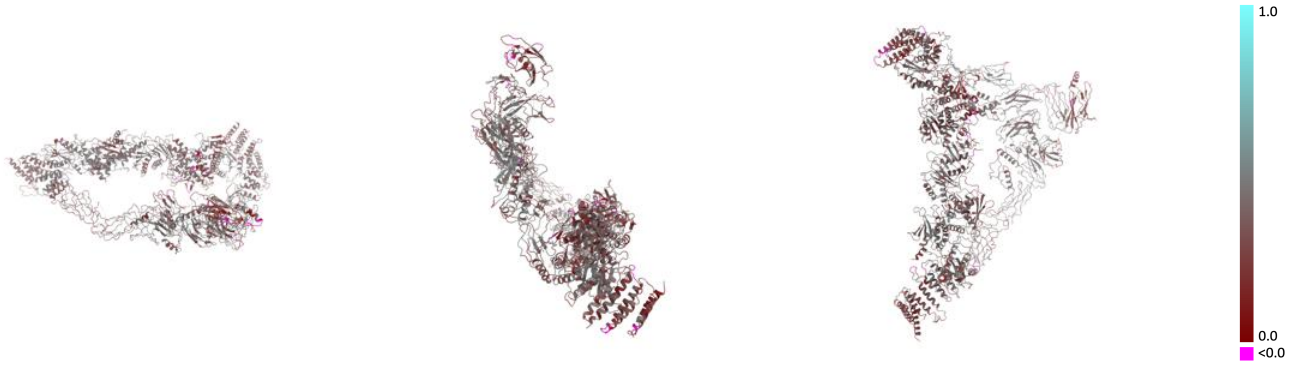
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

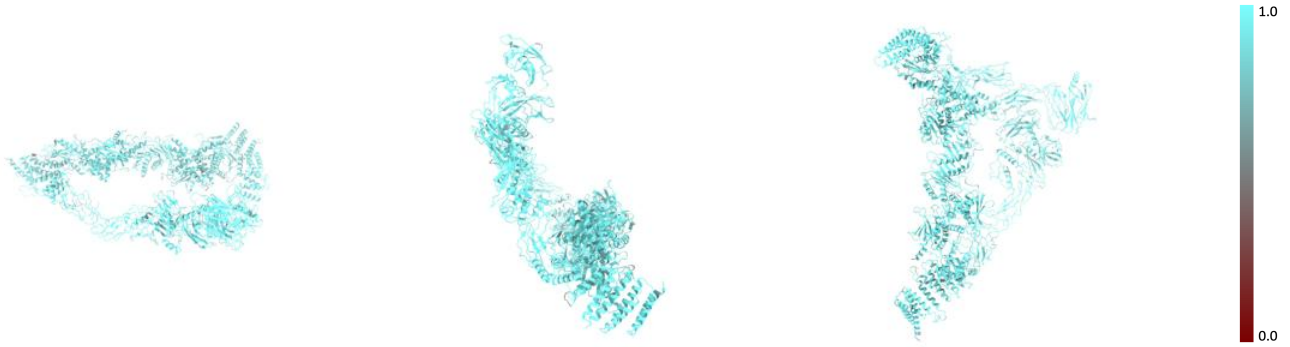
9.2 Q-score mapped to coordinate model



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.

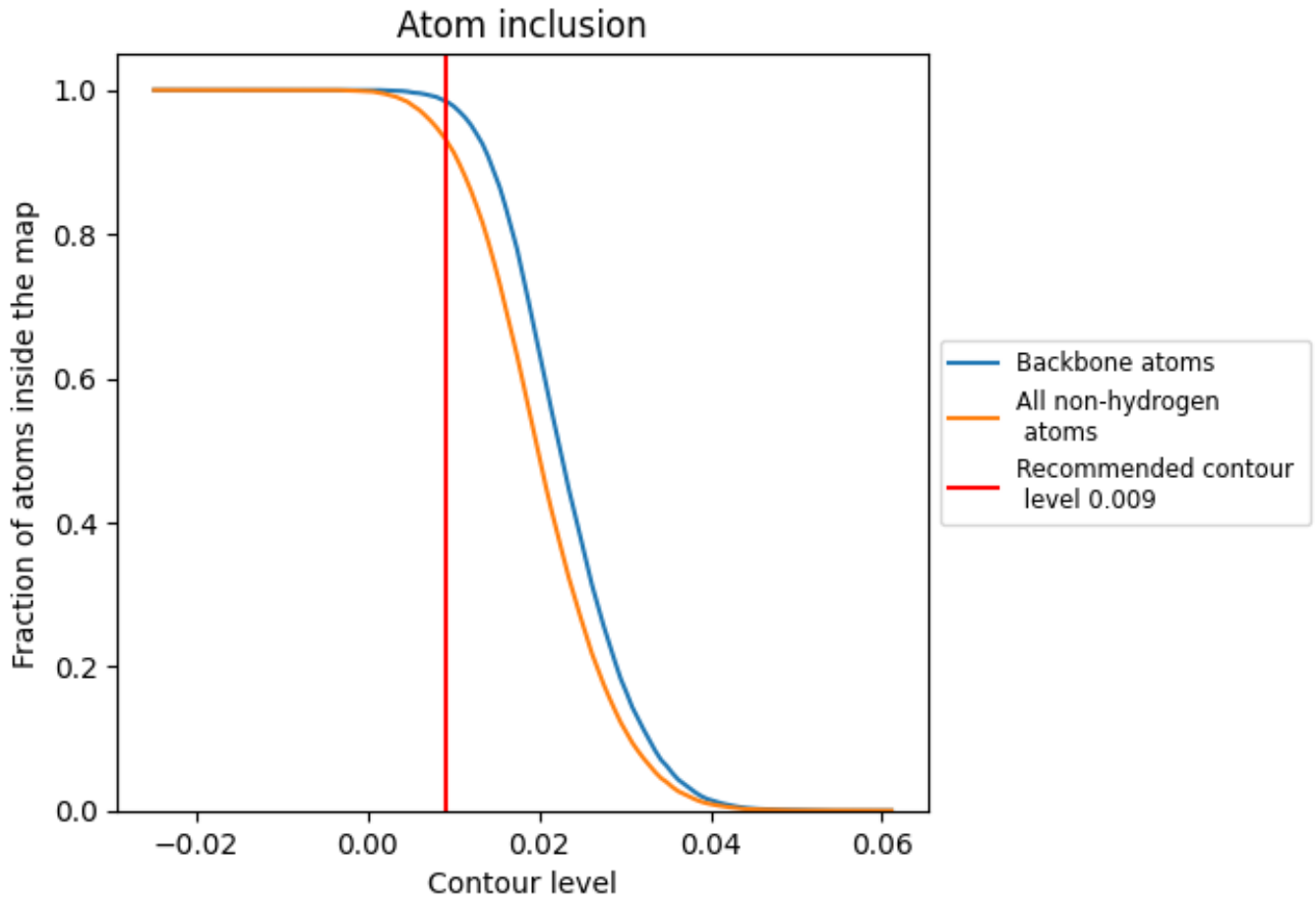
9.3 Atom inclusion mapped to coordinate model



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9331	0.3630
A	0.8727	0.3870
B	0.8953	0.2910
C	0.9191	0.3530
D	0.9254	0.3410
E	0.9433	0.3840
F	0.9295	0.3850
G	0.9336	0.3960
H	0.9233	0.3870
I	0.9795	0.3690
J	0.9264	0.3680
K	0.9382	0.3280