



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 12:59 am GMT

PDB ID : 8PQL
EMDB ID : EMD-17822
Title : K48-linked ubiquitin chain formation with a cullin-RING E3 ligase and Cdc34:
NEDD8-CUL2-RBX1-ELOB/C-FEM1C with trapped UBE2R2-donor UB-
acceptor UB-SIL1 peptide
Authors : Liwocha, J.; Prabu, J.R.; Kleiger, G.; Schulman, B.A.
Deposited on : 2023-07-11
Resolution : 3.76 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

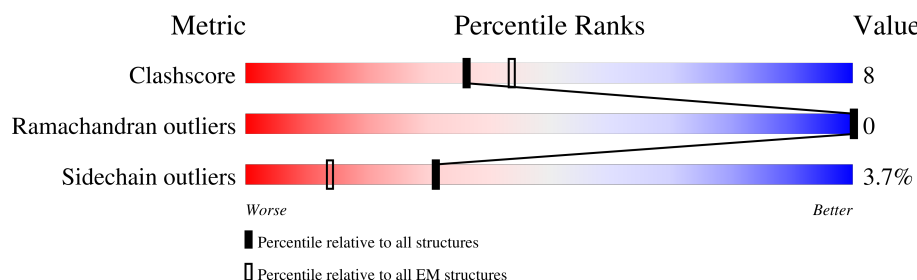
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.76 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	238	63% 15% 21%
2	E	704	9% 88%
3	H	617	79% 17% . .
4	K	108	54% 19% 28%
5	U	685	8% 89%
6	A	745	70% 14% 16%
7	D	112	67% 12% 21%
8	G	118	69% 12% . 18%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13553 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 Ubiquitin-conjugating enzyme E2 R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	187	Total	C	N	O	S	0	0
			1396	896	233	261	6		

- Molecule 2 is a protein called Polyubiquitin-C,Nucleotide exchange factor SIL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	85	Total	C	N	O	S	0	0
			592	372	108	111	1		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	48	CYS	LYS	engineered mutation	UNP P0CG48
E	698	PRO	SER	engineered mutation	UNP Q9H173
E	699	THR	LEU	engineered mutation	UNP Q9H173
E	700	GLN	LEU	engineered mutation	UNP Q9H173
E	701	GLY	LYS	engineered mutation	UNP Q9H173
E	702	ARG	GLU	engineered mutation	UNP Q9H173
E	703	ALA	LEU	engineered mutation	UNP Q9H173

- Molecule 3 is a protein called Protein fem-1 homolog C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	597	Total	C	N	O	S	0	0
			4249	2697	747	781	24		

- Molecule 4 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	78	Total	C	N	O	S	0	0
			563	356	104	94	9		

- Molecule 5 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	75	Total	C	N	O	0	0
			546	344	100	102		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-28	CYS	LYS	engineered mutation	UNP P0CG48

- Molecule 6 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	629	Total	C	N	O	S	0	0
			4820	3083	821	882	34		

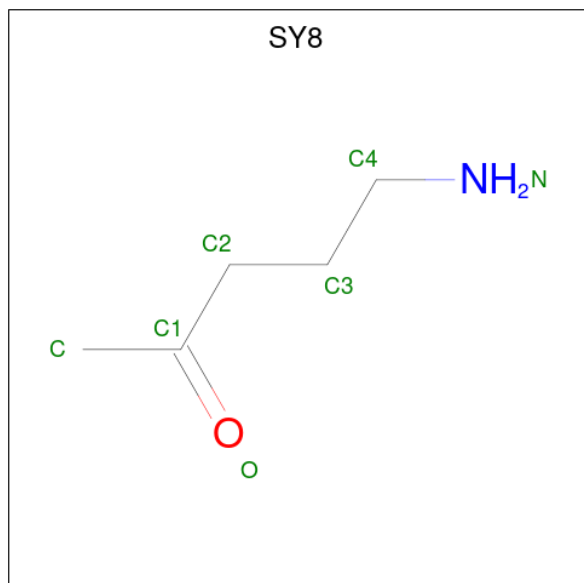
- Molecule 7 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	89	Total	C	N	O	S	0	0
			680	441	113	122	4		

- Molecule 8 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	97	Total	C	N	O	S	0	0
			697	444	120	130	3		

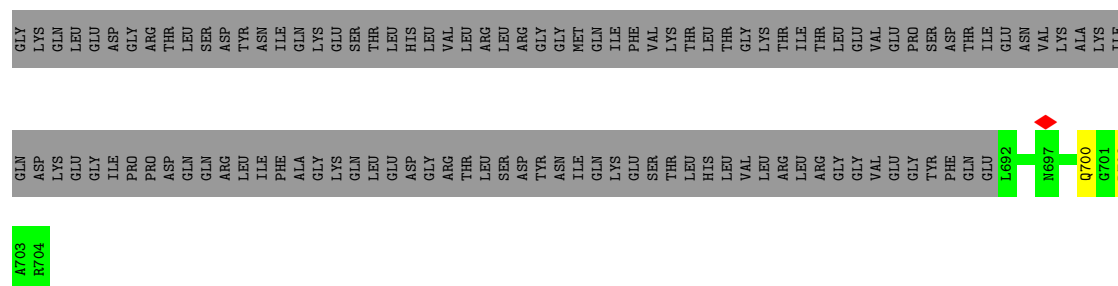
- Molecule 9 is 5-azanylpentan-2-one (three-letter code: SY8) (formula: C₅H₁₁NO).



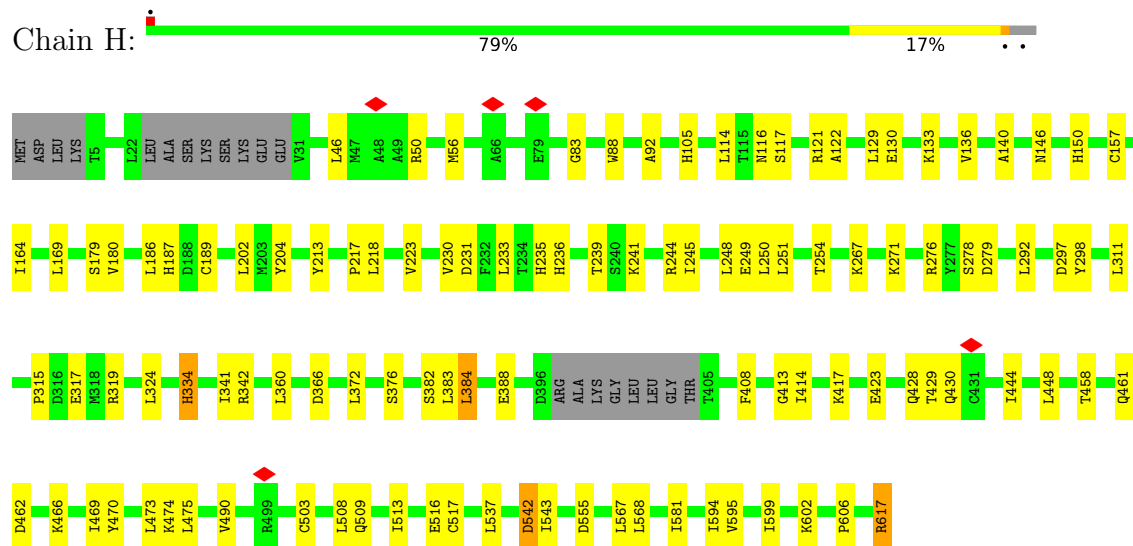
Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

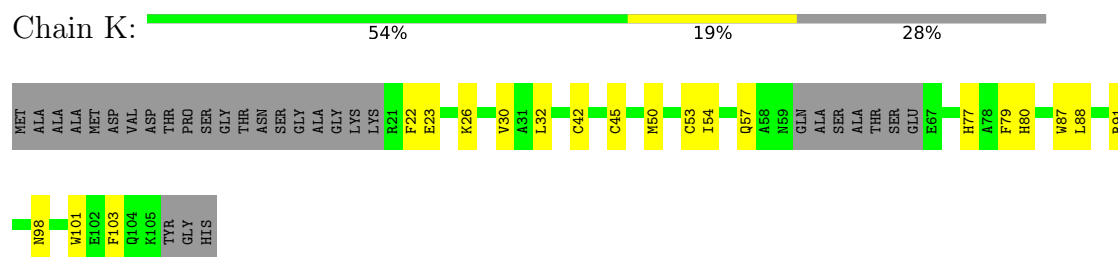
Mol	Chain	Residues	Atoms		AltConf
10	K	3	Total	Zn	0
			3	3	



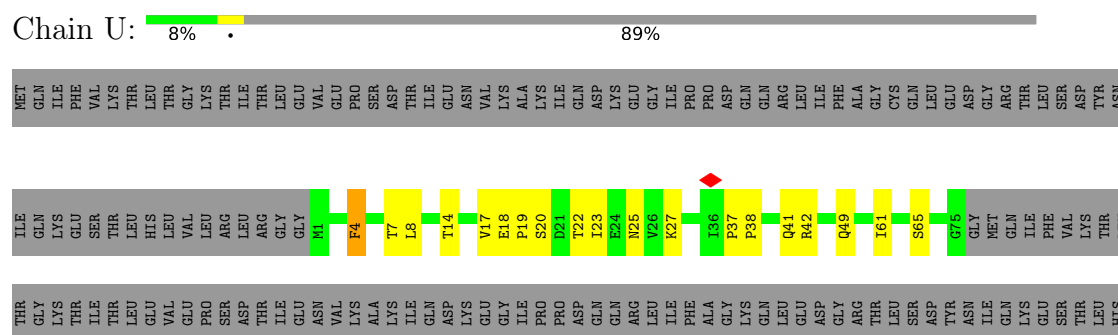
• Molecule 3: Protein fem-1 homolog C

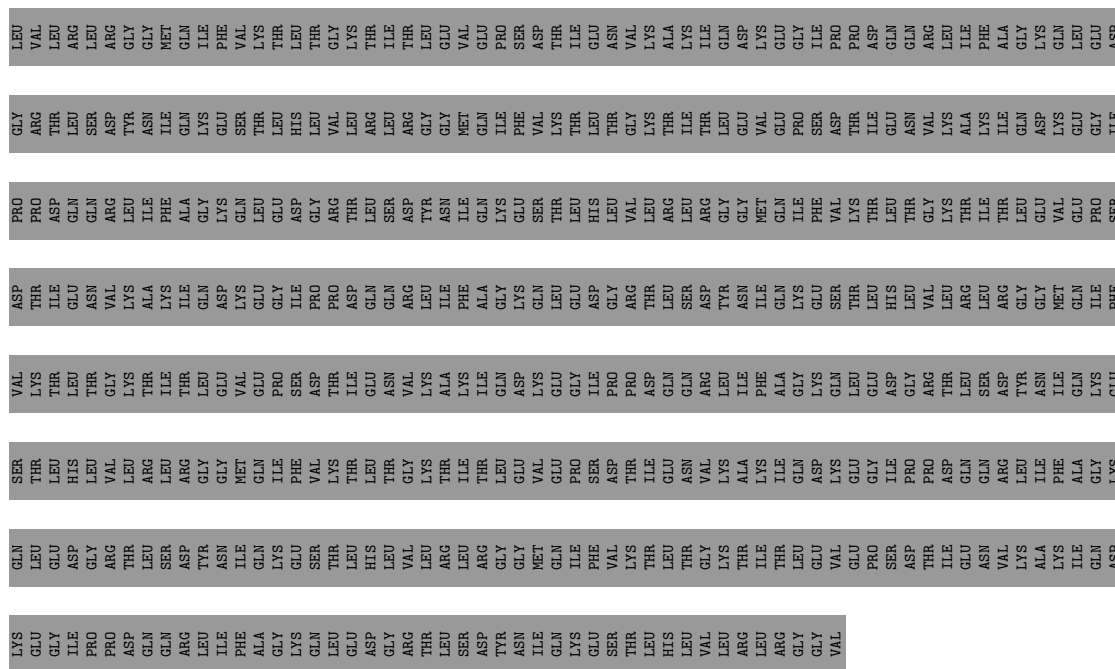


• Molecule 4: E3 ubiquitin-protein ligase RBX1

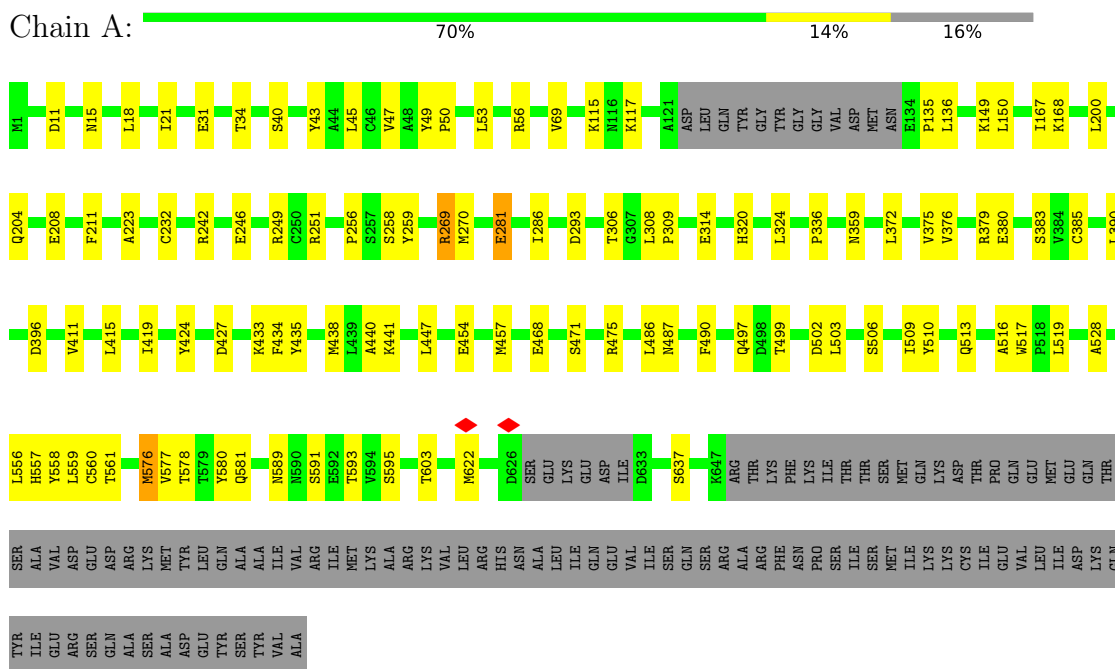


• Molecule 5: Ubiquitin

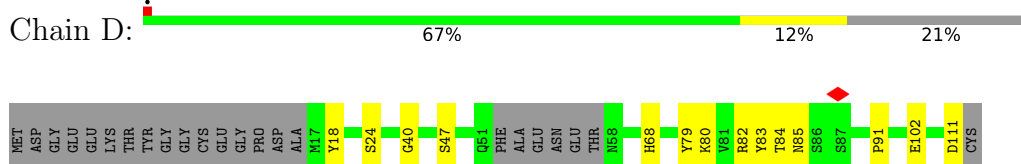




- Molecule 6: Cullin-2



- Molecule 7: Elongin-C



- Molecule 8: Elongin-B

Chain G:

69%

12%

•

18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	10.271	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.151	Depositor
Map size (\AA)	323.38, 323.38, 323.38	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.851, 0.851, 0.851	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SY8

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	C	0.28	0/1436	0.54	0/1973
2	E	0.24	0/598	0.53	0/814
3	H	0.26	0/4331	0.48	0/5916
4	K	0.26	0/580	0.56	0/795
5	U	0.26	0/552	0.57	0/751
6	A	0.27	0/4919	0.52	0/6681
7	D	0.26	0/695	0.46	0/941
8	G	0.26	0/711	0.56	0/970
All	All	0.26	0/13822	0.51	0/18841

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	1396	0	1268	21	0
2	E	592	0	556	10	0
3	H	4249	0	3903	63	0
4	K	563	0	435	14	0
5	U	546	0	533	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4820	0	4558	63	0
7	D	680	0	664	10	0
8	G	697	0	644	12	0
9	C	7	0	0	0	0
10	K	3	0	0	0	0
All	All	13553	0	12561	196	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 8.

The worst 5 of 196 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:K:53:CYS:SG	4:K:80:HIS:NE2	2.50	0.83
7:D:40:GLY:H	7:D:111:ASP:HB2	1.51	0.75
2:E:36:ILE:HD12	2:E:37:PRO:HD2	1.70	0.73
4:K:26:LYS:HB2	6:A:506:SER:HB3	1.71	0.72
5:U:61:ILE:O	5:U:65:SER:OG	2.12	0.68

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	C	185/238 (78%)	155 (84%)	30 (16%)	0	100	100
2	E	81/704 (12%)	78 (96%)	3 (4%)	0	100	100
3	H	591/617 (96%)	543 (92%)	48 (8%)	0	100	100
4	K	74/108 (68%)	64 (86%)	10 (14%)	0	100	100
5	U	73/685 (11%)	64 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	623/745 (84%)	582 (93%)	41 (7%)	0	100	100
7	D	85/112 (76%)	77 (91%)	8 (9%)	0	100	100
8	G	95/118 (80%)	76 (80%)	19 (20%)	0	100	100
All	All	1807/3327 (54%)	1639 (91%)	168 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	C	138/217 (64%)	132 (96%)	6 (4%)	25	50
2	E	55/628 (9%)	53 (96%)	2 (4%)	30	55
3	H	390/532 (73%)	378 (97%)	12 (3%)	35	58
4	K	45/90 (50%)	40 (89%)	5 (11%)	5	23
5	U	54/613 (9%)	53 (98%)	1 (2%)	52	70
6	A	487/681 (72%)	469 (96%)	18 (4%)	29	54
7	D	71/96 (74%)	69 (97%)	2 (3%)	38	60
8	G	65/103 (63%)	63 (97%)	2 (3%)	35	58
All	All	1305/2960 (44%)	1257 (96%)	48 (4%)	31	54

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	149	LYS
6	A	447	LEU
6	A	242	ARG
6	A	293	ASP
6	A	513	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	K	77	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SY8	C	701	1,2,5	6,6,6	0.28	0	6,6,6	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SY8	C	701	1,2,5	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

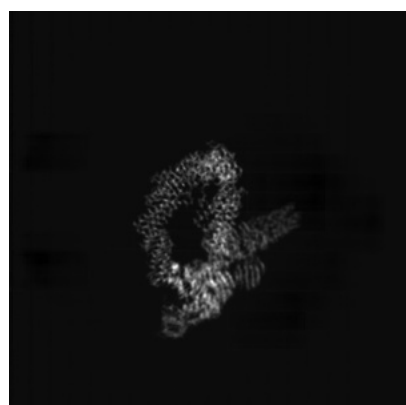
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17822. These allow visual inspection of the internal detail of the map and identification of artifacts.

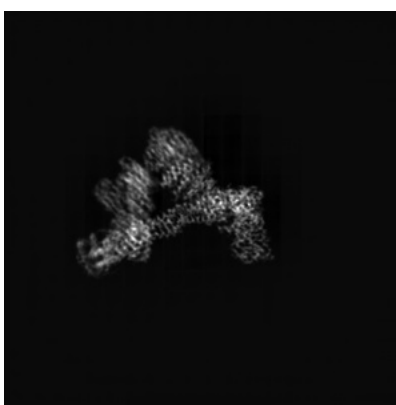
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

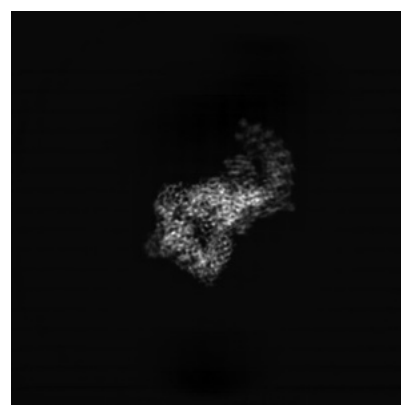
6.1.1 Primary map



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: 190



Y Index: 190



Z Index: 190

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: 197



Y Index: 203

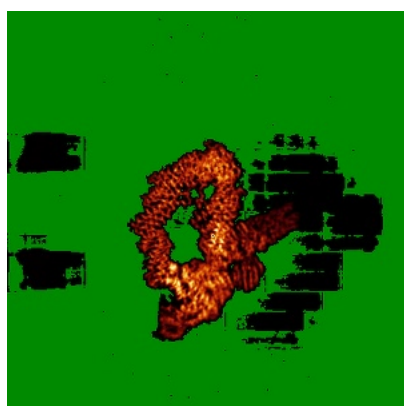


Z Index: 122

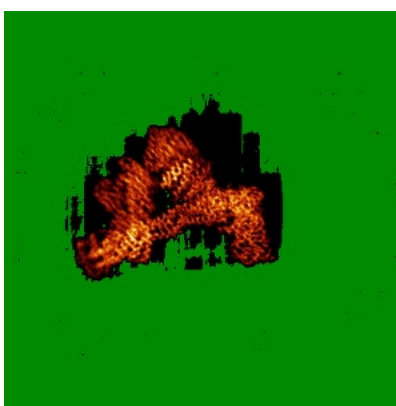
The images above show the largest variance slices of the map in three orthogonal directions.

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

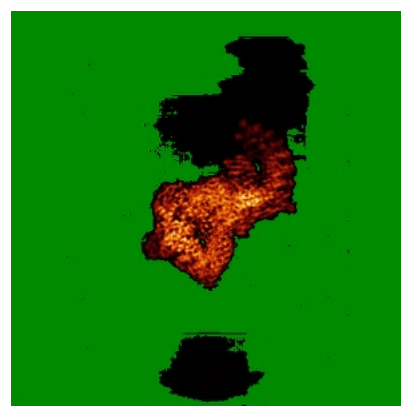
6.4.1 Primary map



X



Y

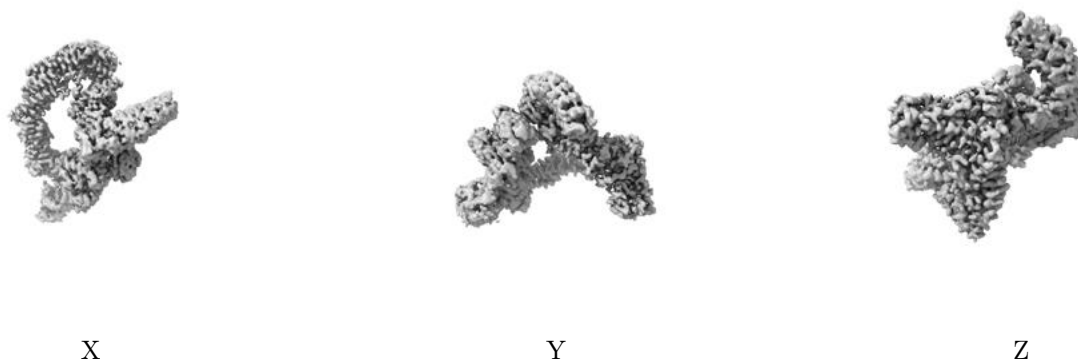


Z

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 0.151. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

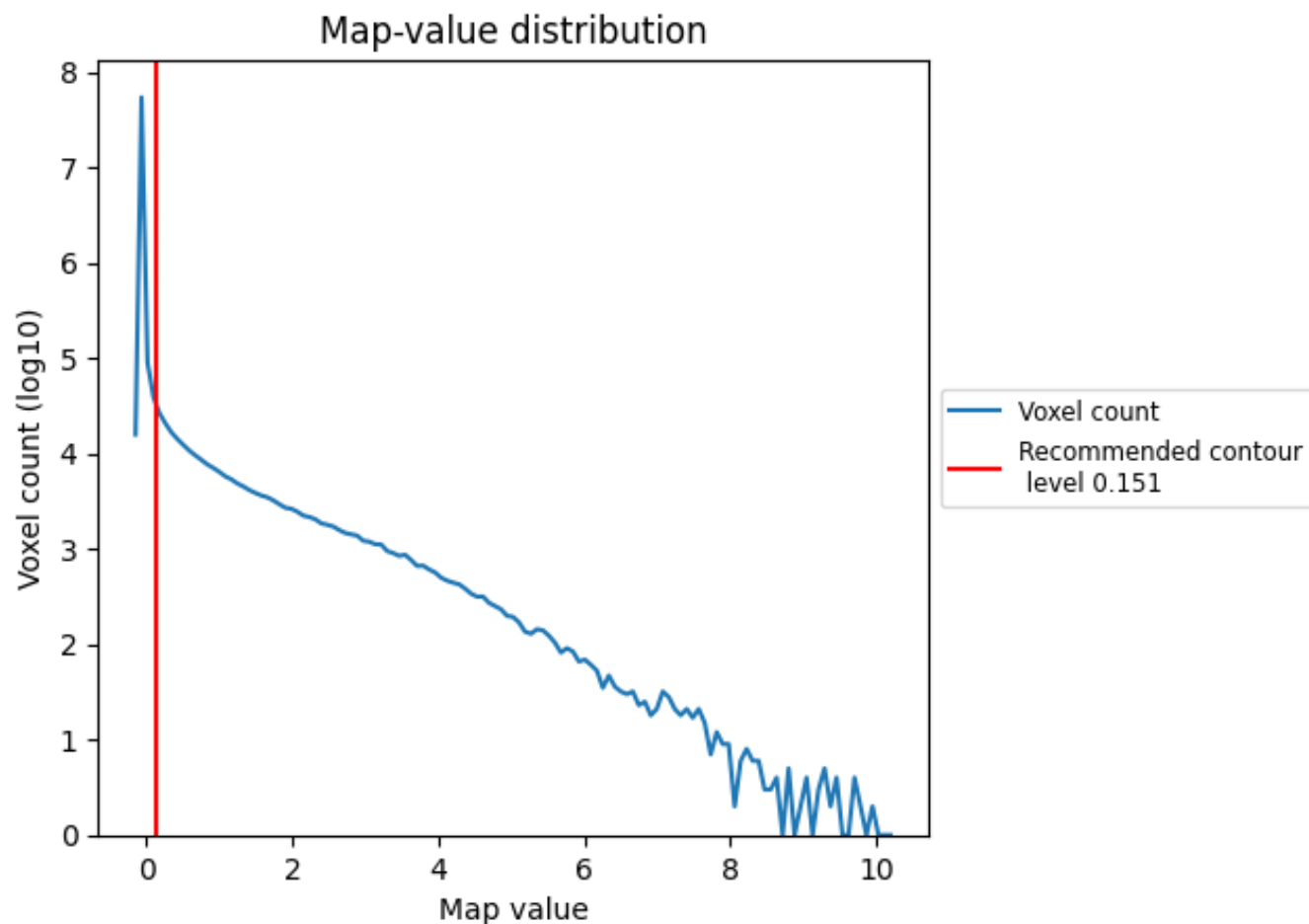
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

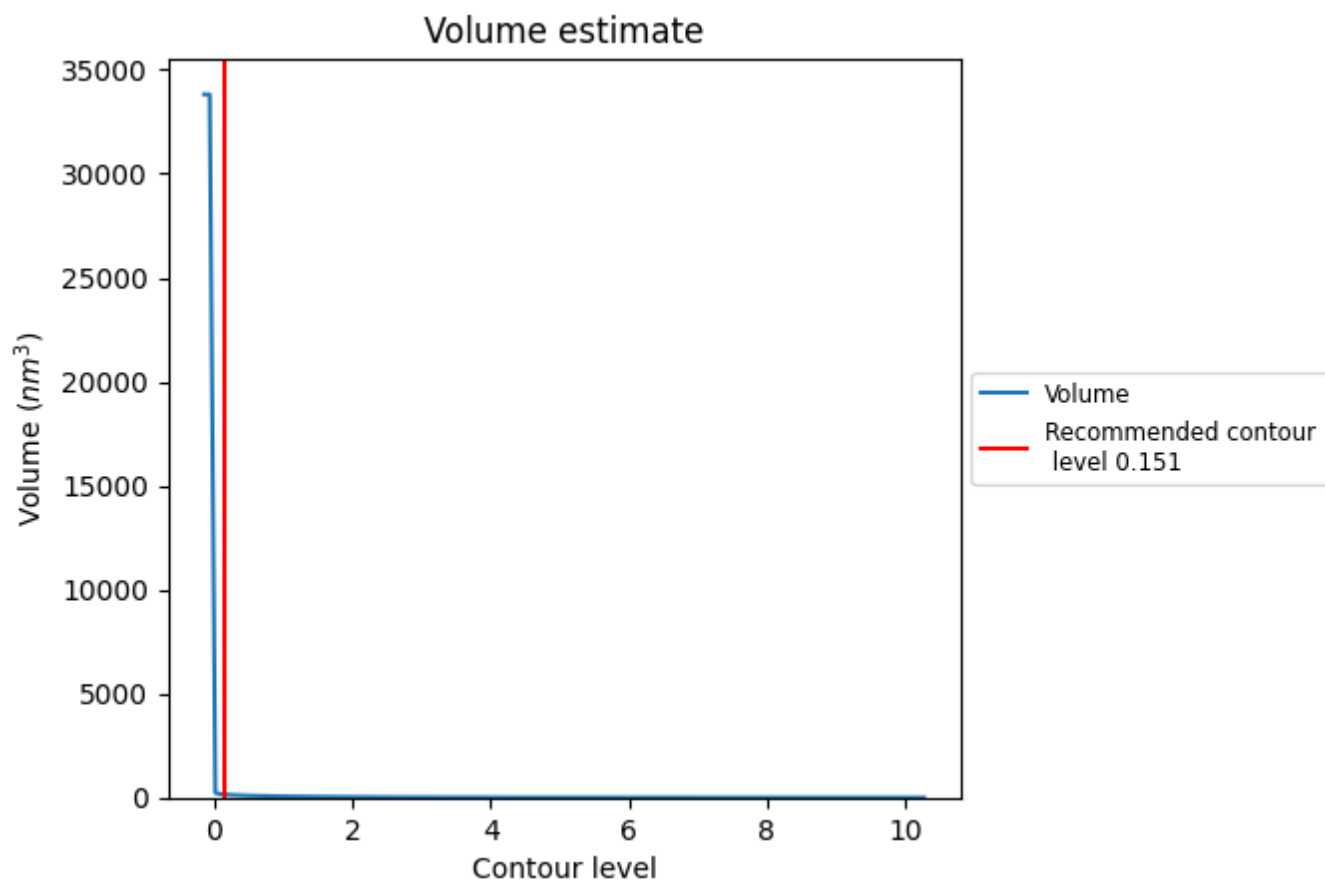
This section contains the results of statistical analysis of the map.

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.

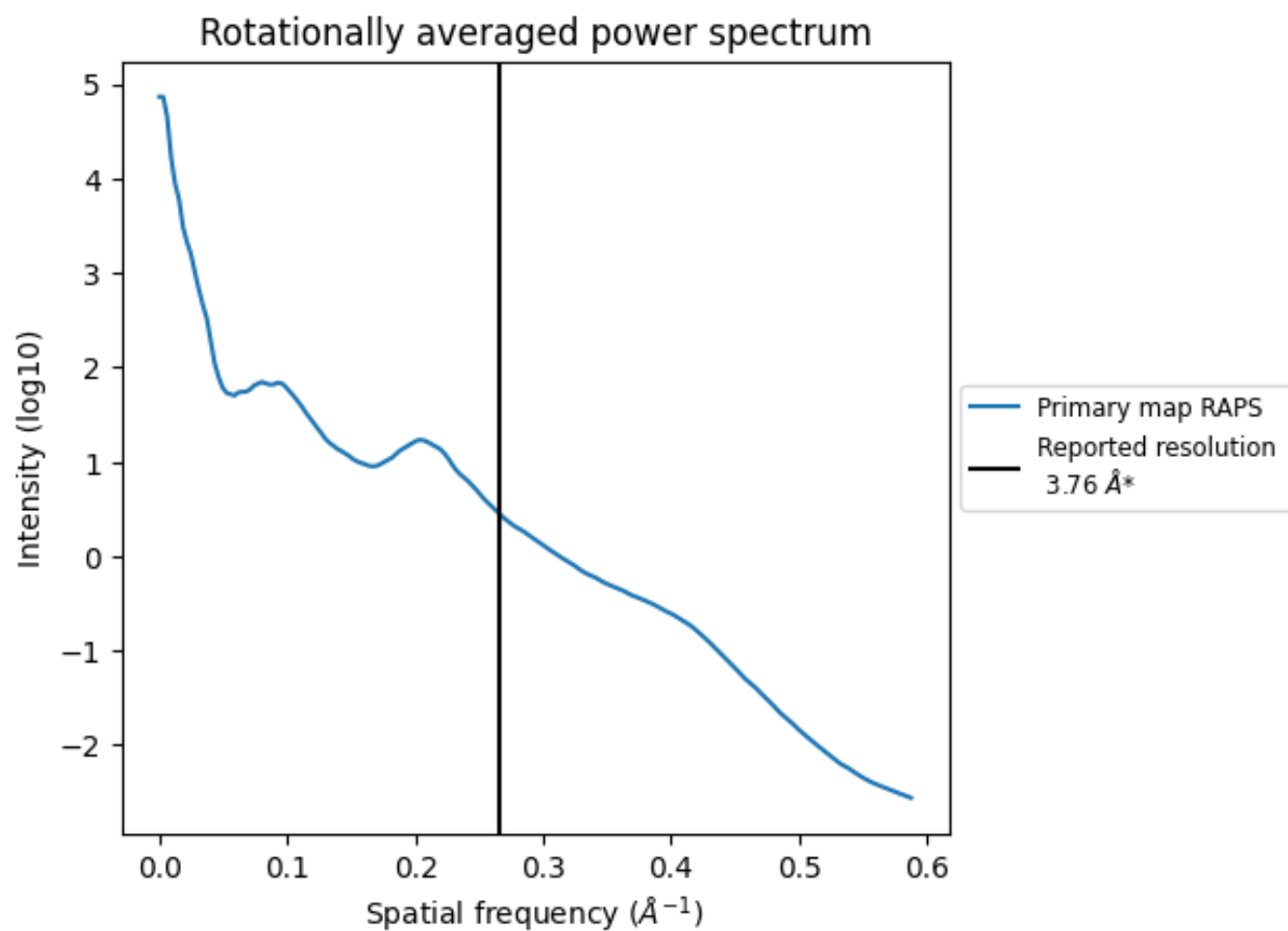
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 135 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 0.266 Å⁻¹

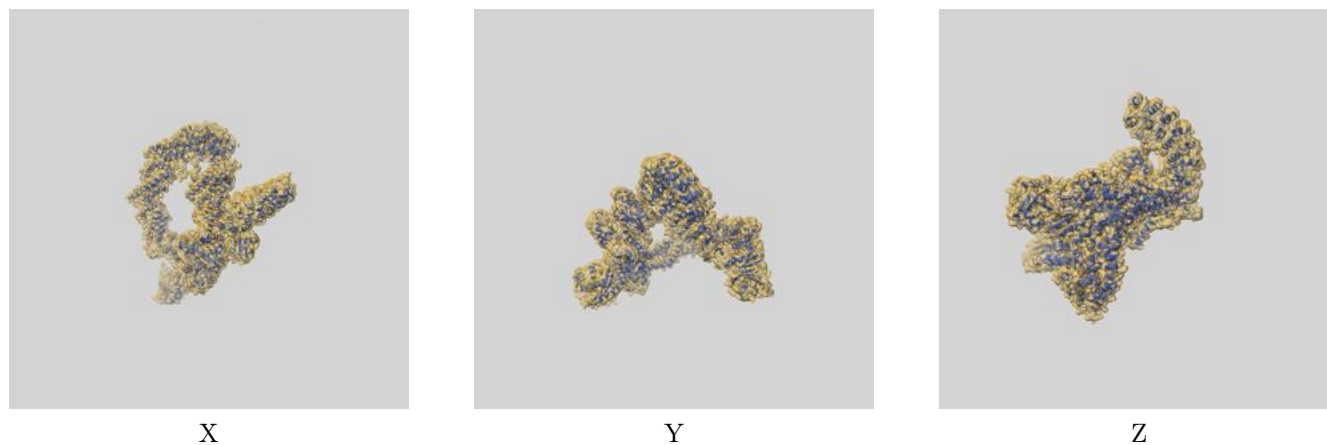
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

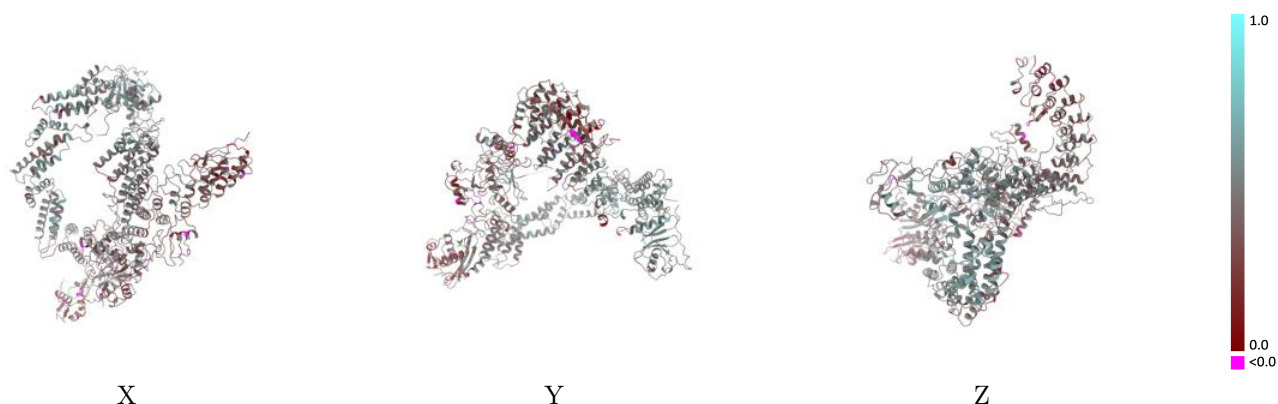
This section contains information regarding the fit between EMDB map EMD-17822 and PDB model 8PQL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



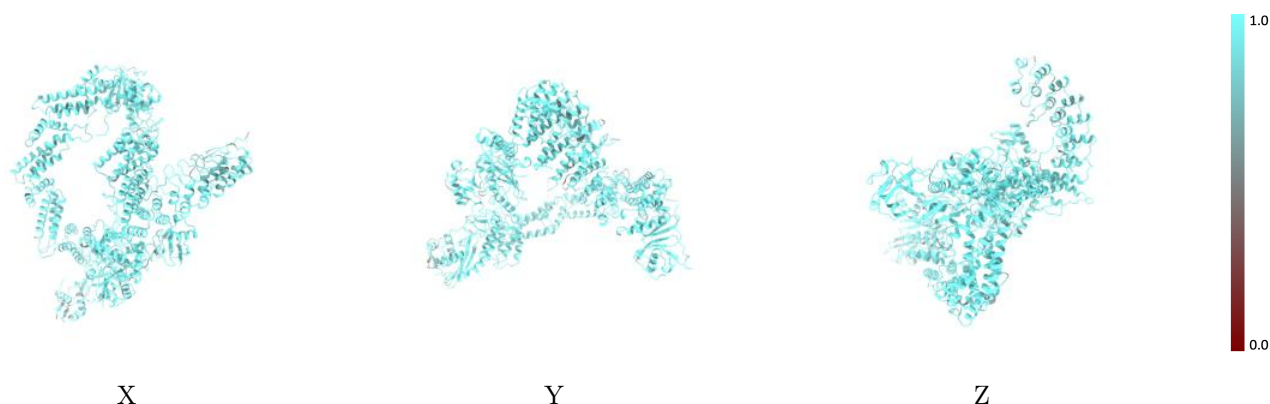
The images above show the 3D surface view of the map at the recommended contour level 0.151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



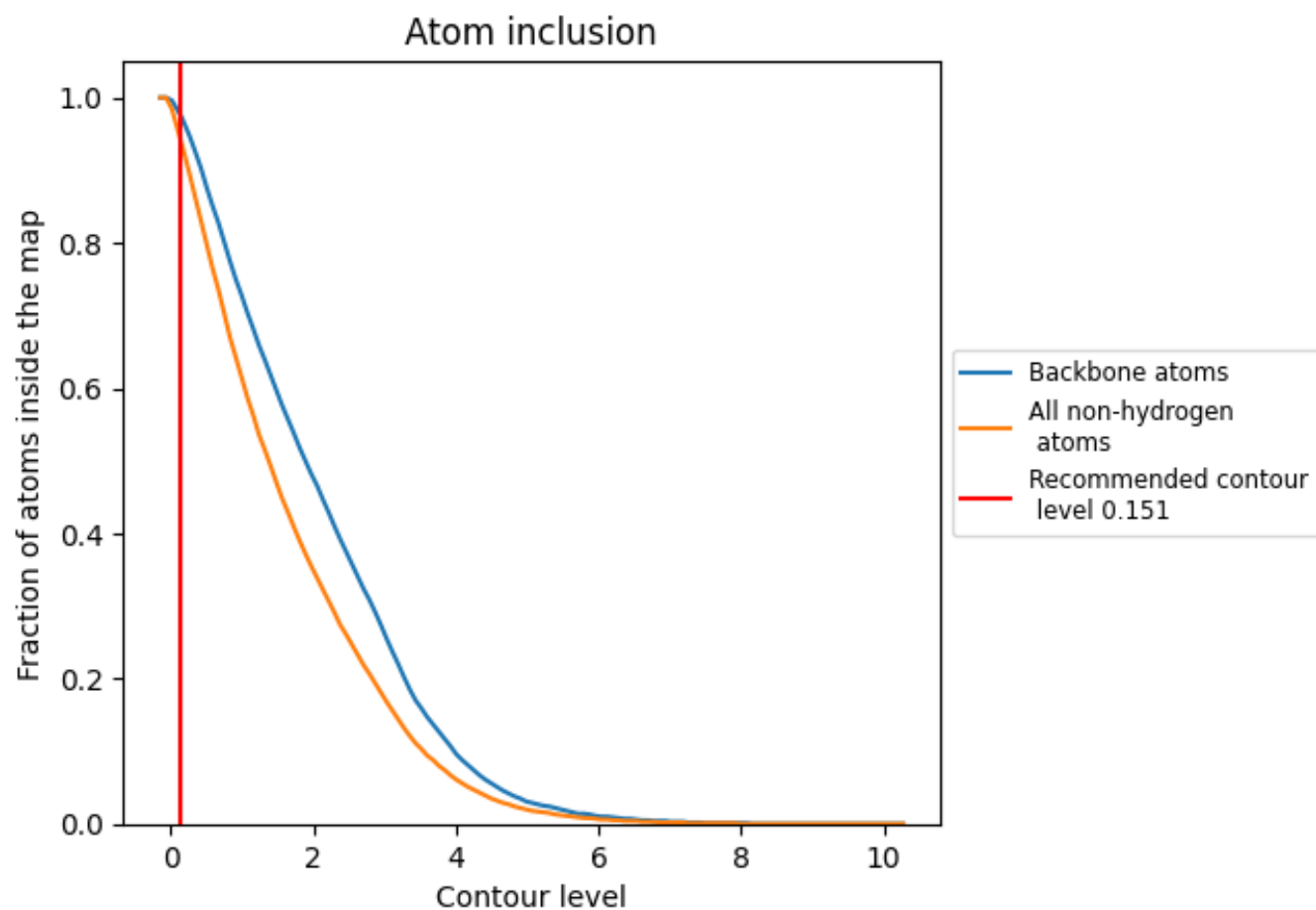
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.151).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9390	<div><div></div></div> 0.4310
A	<div><div></div></div> 0.9360	<div><div></div></div> 0.4430
C	<div><div></div></div> 0.9460	<div><div></div></div> 0.4080
D	<div><div></div></div> 0.9360	<div><div></div></div> 0.5050
E	<div><div></div></div> 0.9330	<div><div></div></div> 0.3830
G	<div><div></div></div> 0.9490	<div><div></div></div> 0.4670
H	<div><div></div></div> 0.9390	<div><div></div></div> 0.4310
K	<div><div></div></div> 0.9590	<div><div></div></div> 0.3860
U	<div><div></div></div> 0.9220	<div><div></div></div> 0.3510

1.0

0.0

<0.0