



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 02:55 AM JST

PDB ID : 6K15
EMDB ID : EMD-9905
Title : RSC substrate-recruitment module
Authors : Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on : 2019-05-09
Resolution : 3.40 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.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) : 2.31.2

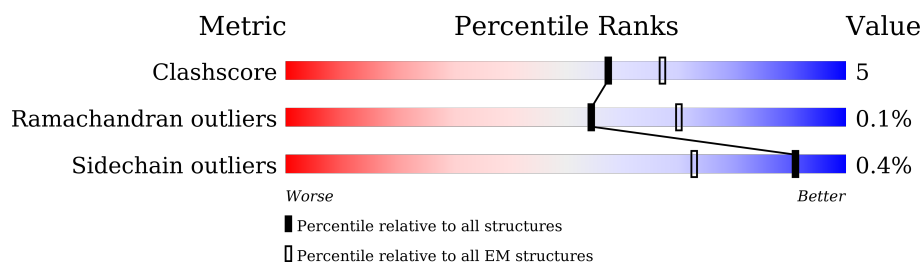
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 $\leq 5\%$. 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	F	435	
2	D	557	
2	H	557	
3	M	581	
4	I	483	
5	G	426	
6	A	502	
7	J	1359	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	E	78	<div><div><div></div><div></div><div></div><div></div></div><div>17%64%10%26%</div></div>
9	C	883	<div><div><div></div><div></div><div></div><div></div></div><div>96%</div></div>
10	K	885	<div><div><div></div><div></div><div></div><div></div></div><div>5%95%</div></div>
11	X	625	<div><div><div></div><div></div><div></div><div></div></div><div>9%19%76%</div></div>
12	L	889	<div><div><div></div><div></div><div></div><div></div></div><div>8%90%</div></div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21486 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 Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 2 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
2	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 3 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 4 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 5 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	246	Total	C	N	O	S	0	0
			1991	1268	335	380	8		

- Molecule 6 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 7 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		

- Molecule 8 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 10 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 11 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

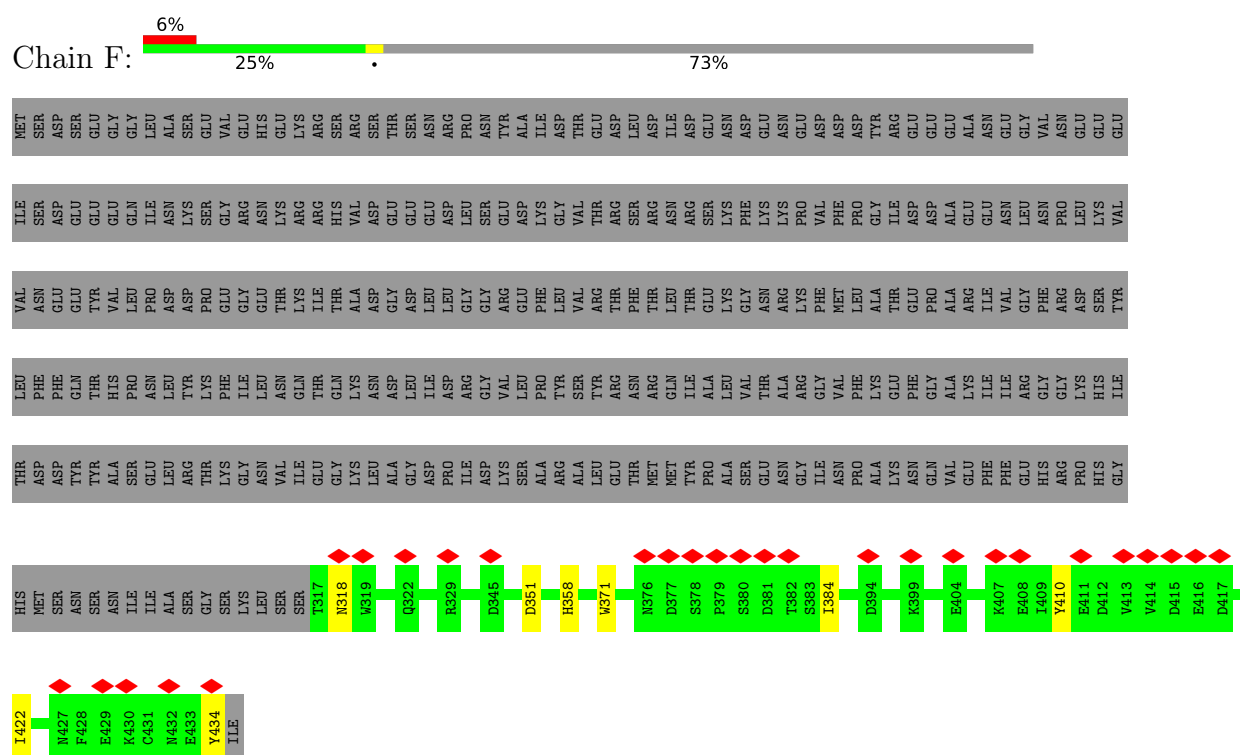
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	H	1	Total	Zn	0
			1	1	

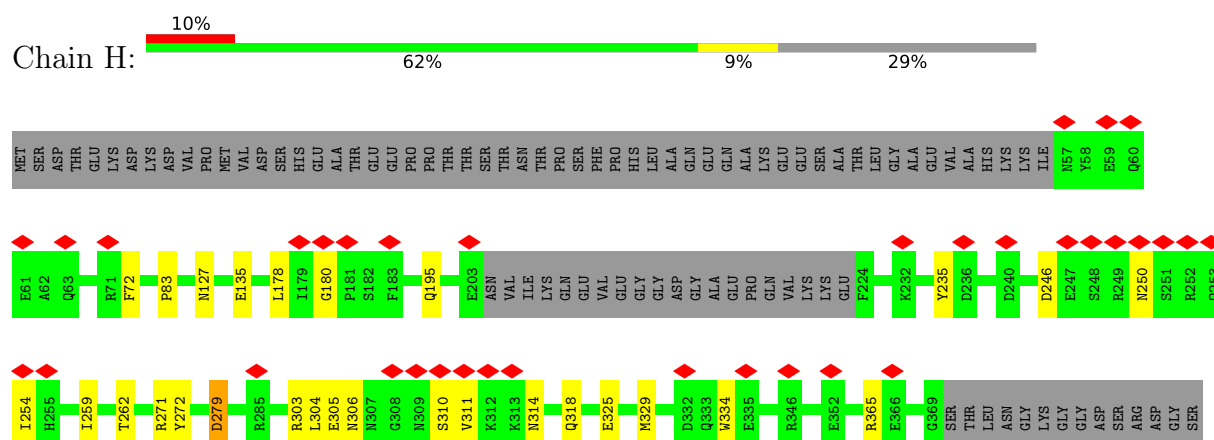
3 Residue-property plots

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.

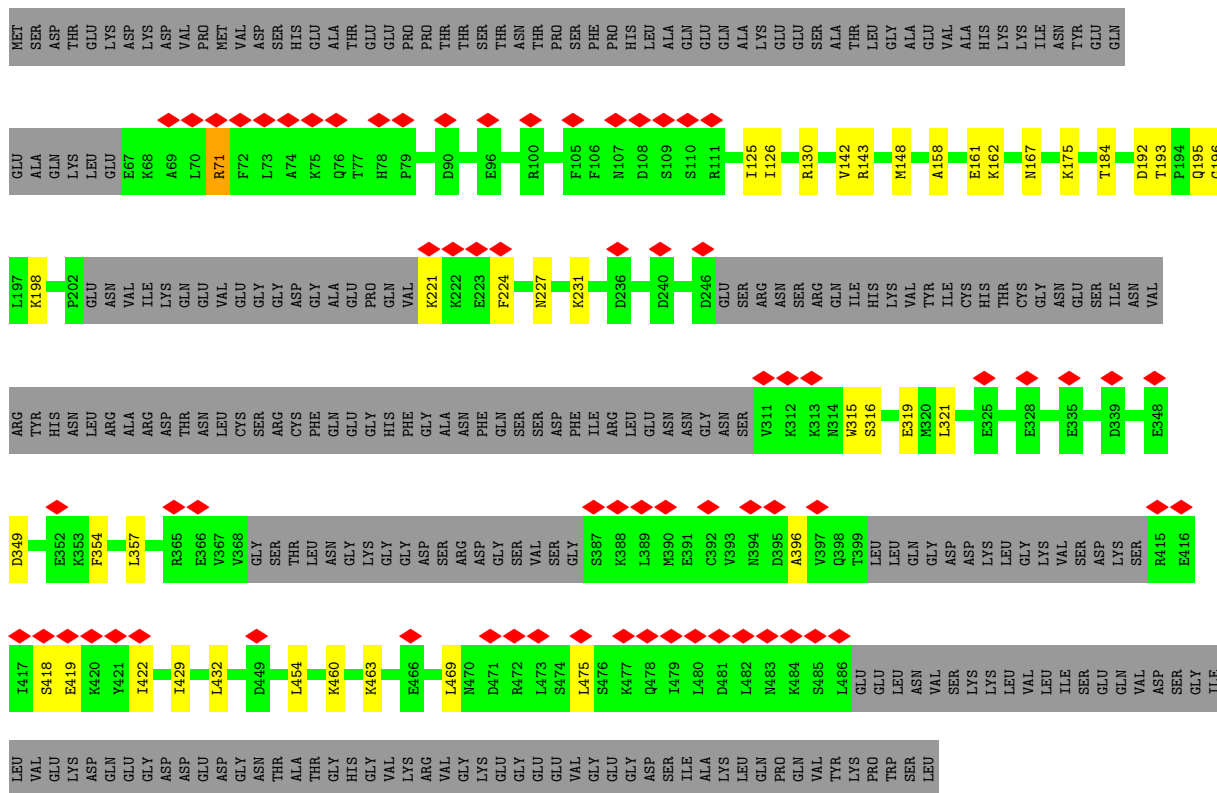
• Molecule 1: Chromatin structure-remodeling complex subunit RSC7



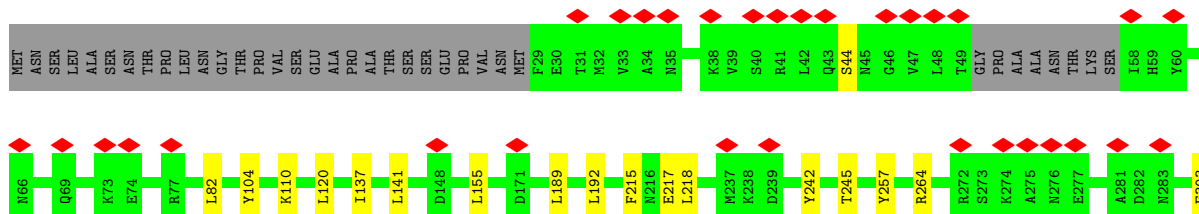
• Molecule 2: Chromatin structure-remodeling complex protein RSC8



- Molecule 2: Chromatin structure-remodeling complex protein RSC8



- Molecule 3: Chromatin structure-remodeling complex subunit RSC9





- Molecule 10: Chromatin structure-remodeling complex protein RSC3

[illegible]

Chain X: 9% 19% 76%

[illegible]

P858
S859
L860
P861
G862
P863
P864
G867
L868
R869
P870
R878
R883
PRO
PRO
SER
SER
SER
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	280000	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	F	0.28	0/983	0.57	0/1337
2	D	0.29	0/2557	0.50	0/3442
2	H	0.30	0/3275	0.53	1/4409 (0.0%)
3	M	0.31	0/3113	0.58	0/4215
4	I	0.28	0/1976	0.56	0/2685
5	G	0.29	0/2033	0.57	0/2761
6	A	0.30	0/3077	0.54	0/4169
7	J	0.29	0/1836	0.55	1/2480 (0.0%)
8	E	0.27	0/480	0.56	0/643
9	C	0.28	0/272	0.44	0/366
10	K	0.27	0/356	0.50	0/483
11	X	0.31	0/1243	0.57	0/1672
12	L	0.28	0/681	0.62	1/921 (0.1%)
All	All	0.29	0/21882	0.55	3/29583 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	J	17	PRO	N-CA-CB	5.80	110.26	103.30
12	L	766	ASP	CB-CG-OD2	5.20	122.98	118.30
2	H	279	ASP	CB-CG-OD2	5.19	122.97	118.30

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	F	964	0	919	5	0
2	D	2510	0	2542	33	0
2	H	3215	0	3195	45	0
3	M	3058	0	3127	16	0
4	I	1944	0	1964	22	0
5	G	1991	0	1943	29	0
6	A	3007	0	3045	51	0
7	J	1814	0	1777	23	0
8	E	477	0	491	6	0
9	C	269	0	279	2	0
10	K	347	0	342	2	0
11	X	1220	0	1192	31	0
12	L	669	0	693	17	0
13	H	1	0	0	0	0
All	All	21486	0	21509	213	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 5.

The worst 5 of 213 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)
11:X:439:GLU:OE1	11:X:490:GLU:CG	1.64	1.46
6:A:238:GLU:OE2	7:J:212:ASN:ND2	1.71	1.21
12:L:765:THR:HG22	12:L:790:LEU:HD21	1.23	1.16
11:X:439:GLU:OE1	11:X:490:GLU:HG2	0.91	1.07
6:A:187:TYR:OH	6:A:235:THR:HG21	1.56	1.04

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	F	116/435 (27%)	102 (88%)	14 (12%)	0	100	100
2	D	295/557 (53%)	280 (95%)	15 (5%)	0	100	100
2	H	387/557 (70%)	356 (92%)	31 (8%)	0	100	100
3	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
4	I	236/483 (49%)	218 (92%)	18 (8%)	0	100	100
5	G	238/426 (56%)	213 (90%)	25 (10%)	0	100	100
6	A	357/502 (71%)	321 (90%)	36 (10%)	0	100	100
7	J	229/1359 (17%)	201 (88%)	27 (12%)	1 (0%)	34	67
8	E	56/78 (72%)	53 (95%)	3 (5%)	0	100	100
9	C	31/883 (4%)	31 (100%)	0	0	100	100
10	K	40/885 (4%)	38 (95%)	2 (5%)	0	100	100
11	X	139/625 (22%)	126 (91%)	13 (9%)	0	100	100
12	L	79/889 (9%)	69 (87%)	9 (11%)	1 (1%)	12	39
All	All	2581/8260 (31%)	2357 (91%)	222 (9%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	J	17	PRO
12	L	809	PRO

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	F	111/388 (29%)	111 (100%)	0	100	100
2	D	285/500 (57%)	284 (100%)	1 (0%)	91	95
2	H	363/500 (73%)	361 (99%)	2 (1%)	86	94
3	M	349/521 (67%)	348 (100%)	1 (0%)	92	97
4	I	223/435 (51%)	223 (100%)	0	100	100
5	G	225/384 (59%)	224 (100%)	1 (0%)	91	95
6	A	343/462 (74%)	342 (100%)	1 (0%)	92	97
7	J	187/1228 (15%)	186 (100%)	1 (0%)	88	94
8	E	56/75 (75%)	56 (100%)	0	100	100
9	C	32/824 (4%)	32 (100%)	0	100	100
10	K	39/832 (5%)	39 (100%)	0	100	100
11	X	141/578 (24%)	139 (99%)	2 (1%)	67	83
12	L	77/810 (10%)	77 (100%)	0	100	100
All	All	2431/7537 (32%)	2422 (100%)	9 (0%)	91	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	X	437	LEU
11	X	438	SER
3	M	104	TYR
5	G	172	ARG
6	A	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	352	HIS
7	J	90	GLN
11	X	494	ASN
6	A	484	ASN
7	J	259	GLN

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

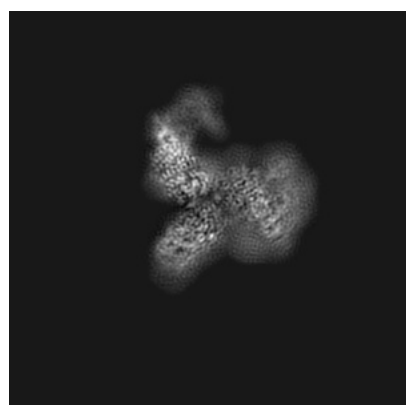
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9905. These allow visual inspection of the internal detail of the map and identification of artifacts.

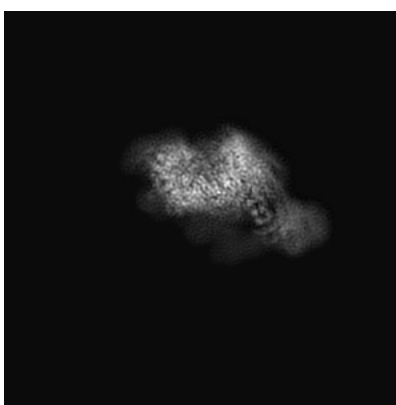
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

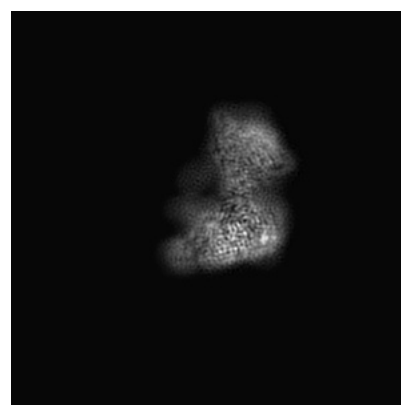
6.1.1 Primary map



X



Y



Z

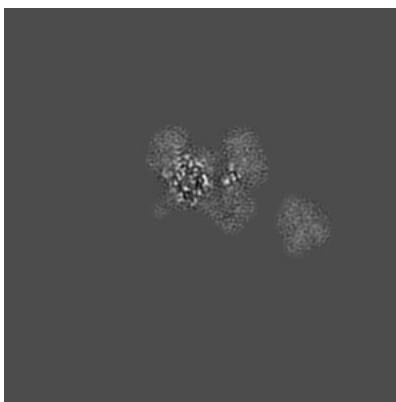
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

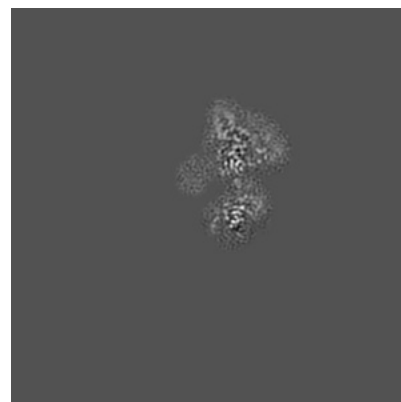
6.2.1 Primary map



X Index: 180



Y Index: 180

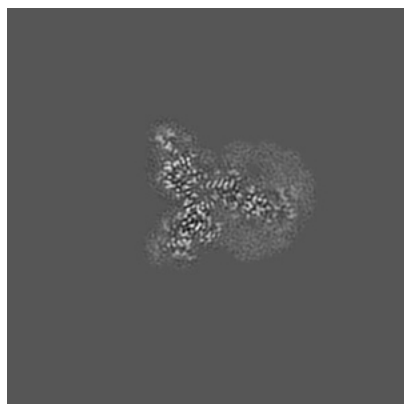


Z Index: 180

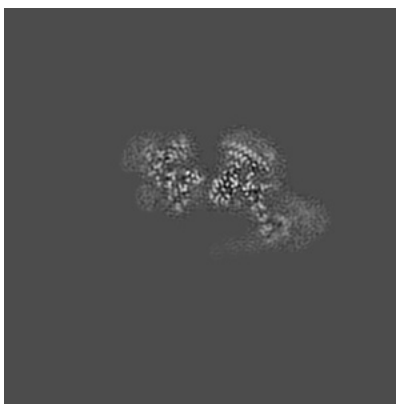
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

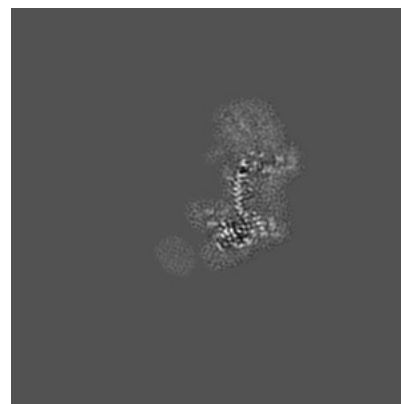
6.3.1 Primary map



X Index: 202



Y Index: 154



Z Index: 201

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

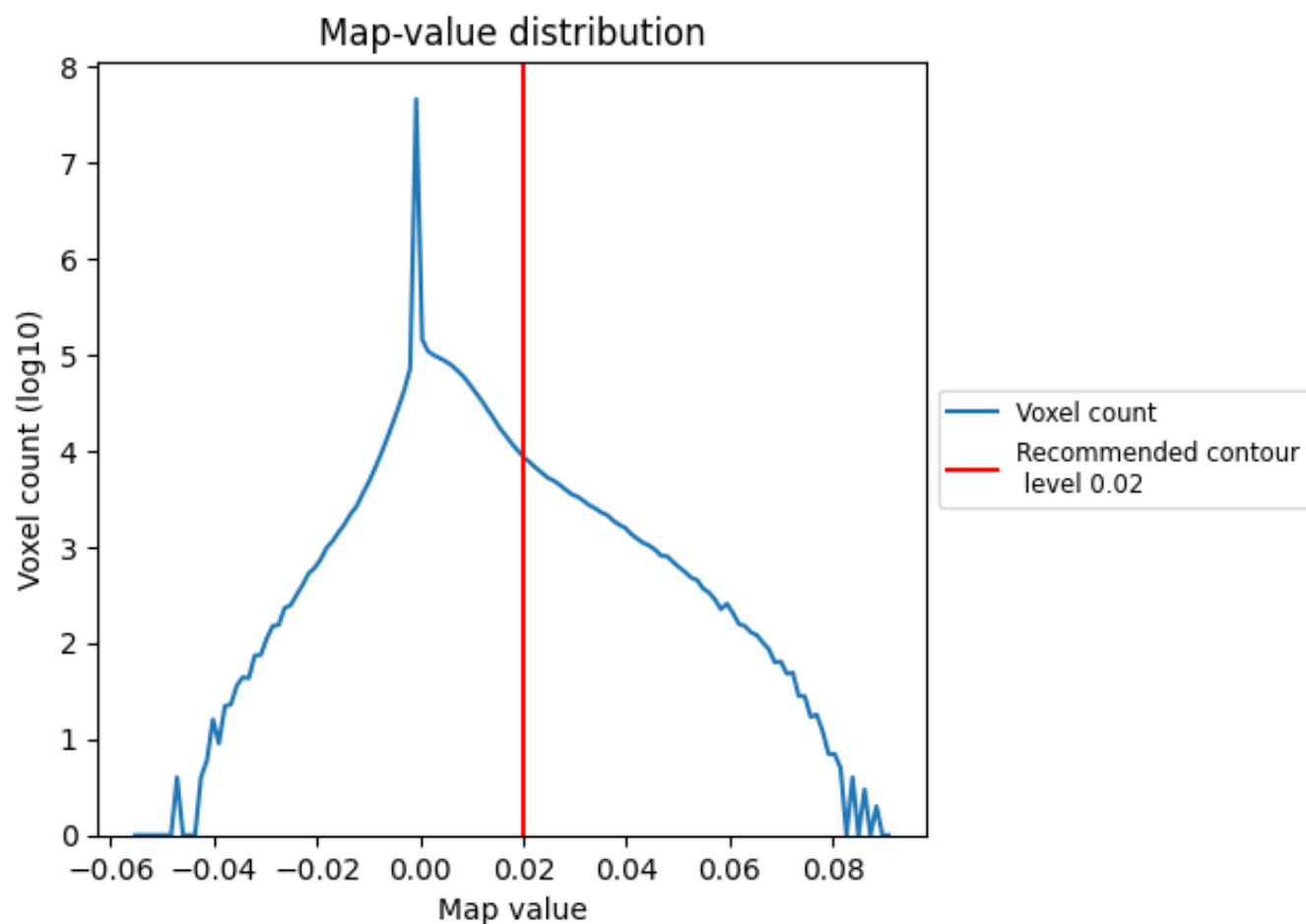
6.5 Mask visualisation

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

7 Map analysis [i](#)

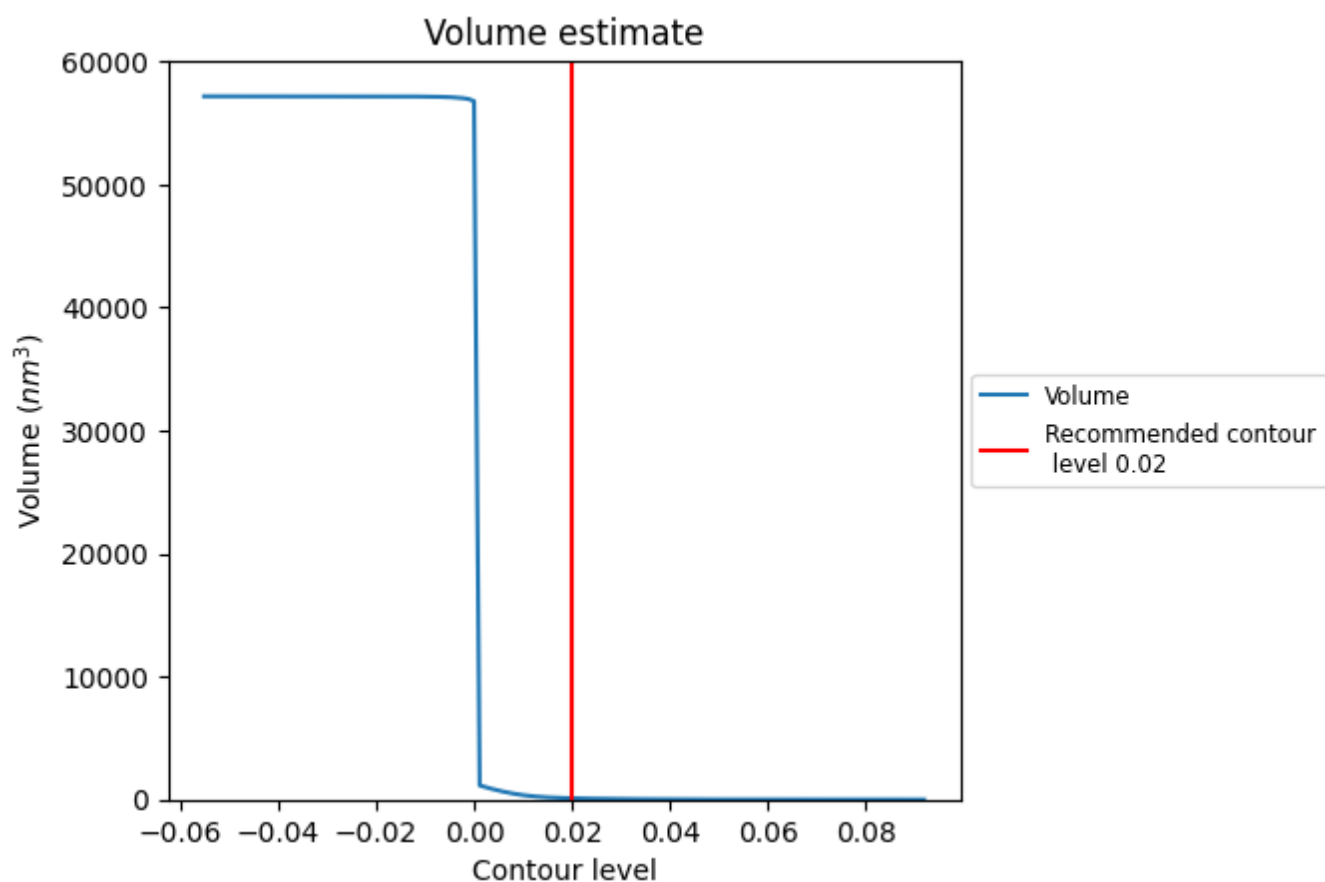
This section contains the results of statistical analysis of the map.

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.

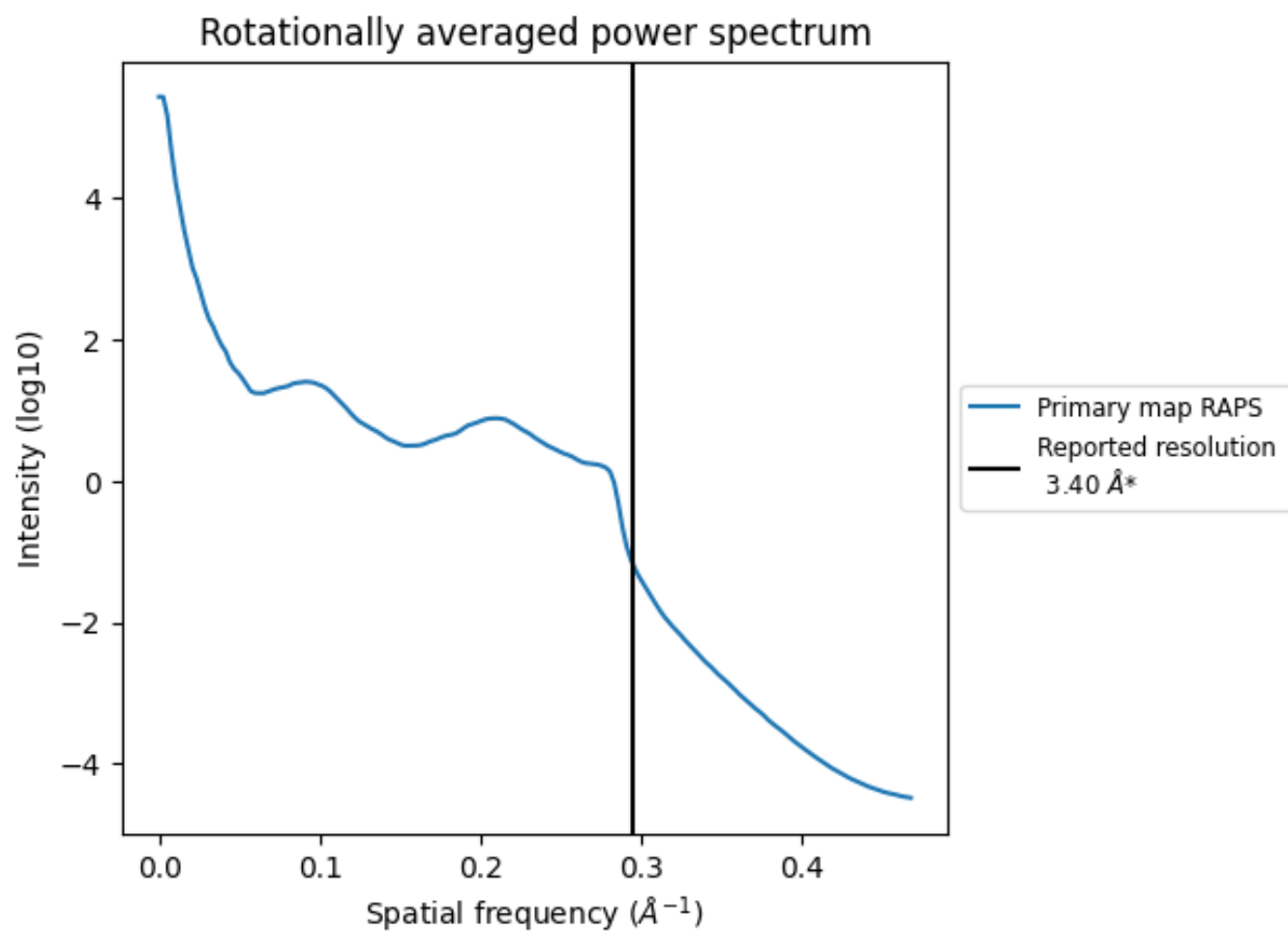
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 0.294 Å⁻¹

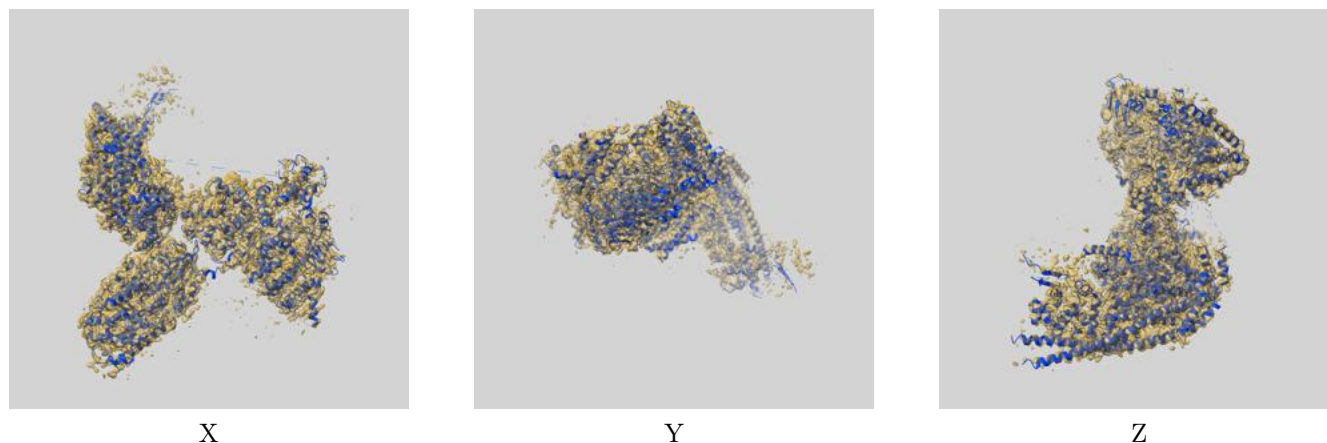
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

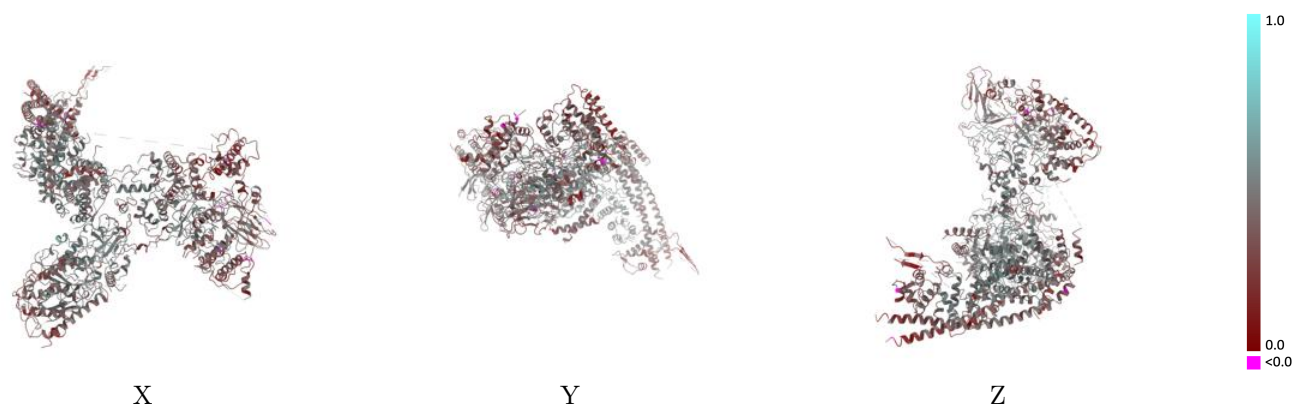
This section contains information regarding the fit between EMDB map EMD-9905 and PDB model 6K15. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



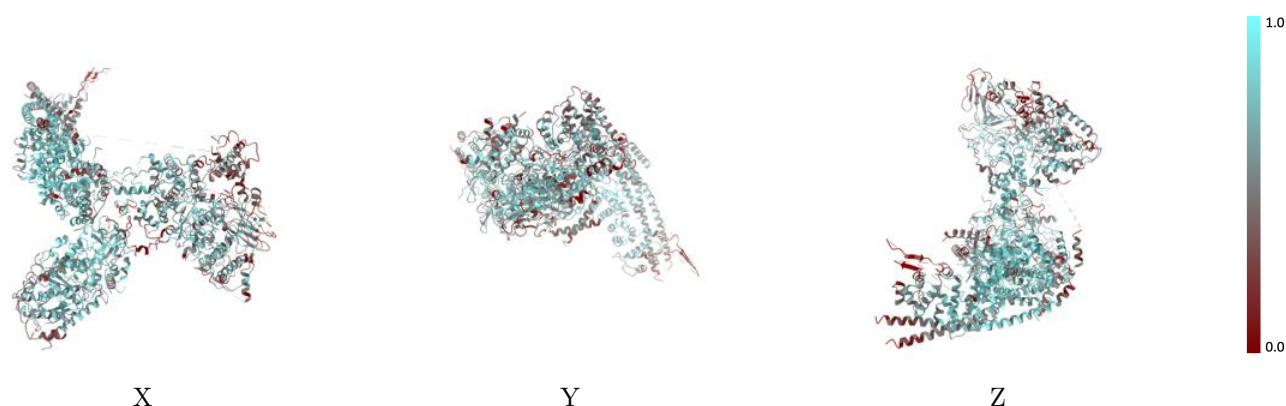
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



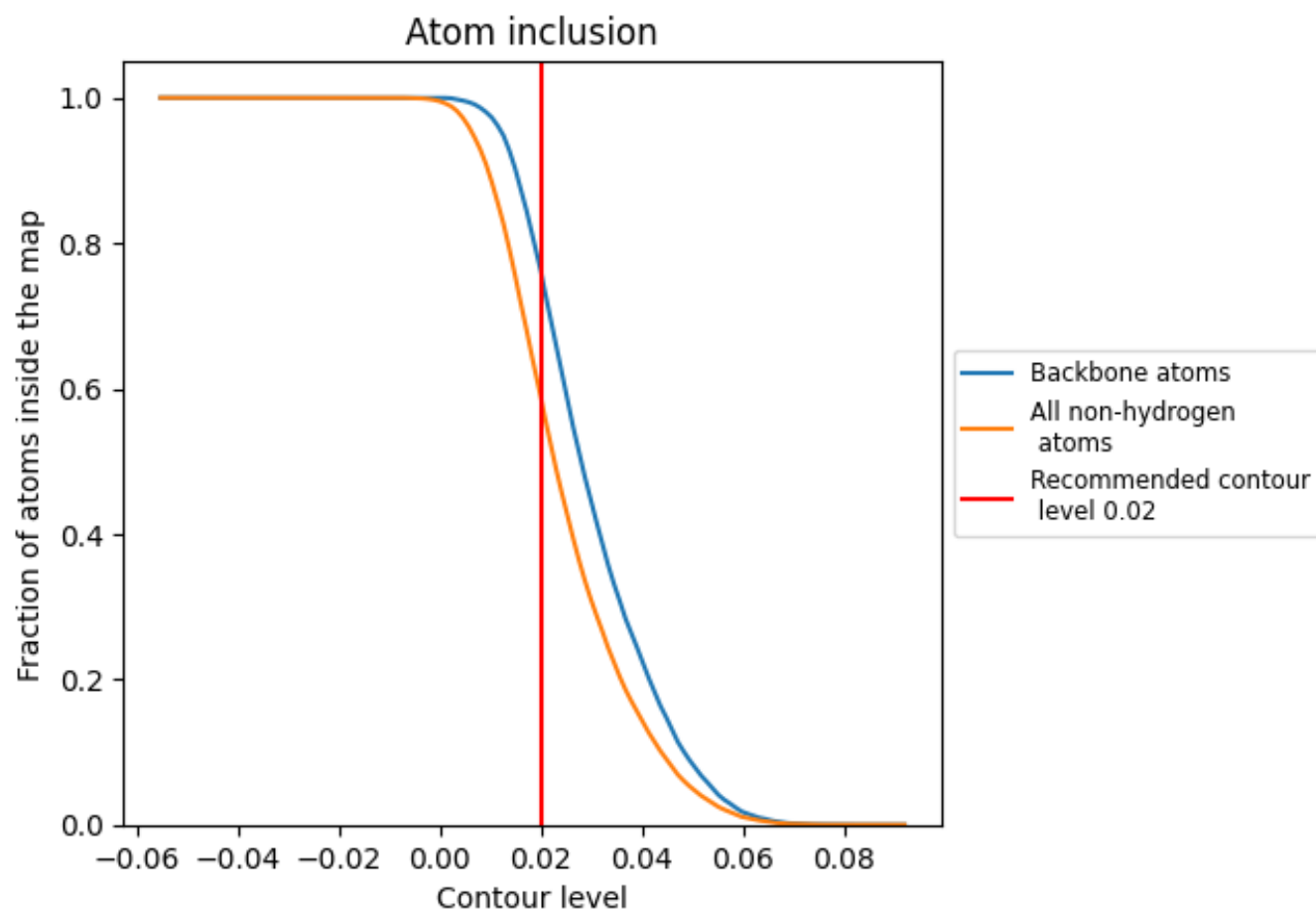
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 59% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5885	 0.4130
A	 0.5655	 0.3890
C	 0.3941	 0.3780
D	 0.5712	 0.3900
E	 0.5919	 0.4050
F	 0.5667	 0.4040
G	 0.6042	 0.4310
H	 0.6539	 0.4470
I	 0.5637	 0.3860
J	 0.5307	 0.3860
K	 0.4198	 0.4270
L	 0.5015	 0.3900
M	 0.7109	 0.4710
X	 0.4556	 0.3620

