



## wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:30 AM EST

PDB ID : 6CIJ  
EMDB ID : EMD-7480  
Title : Cryo-EM structure of mouse RAG1/2 HFC complex containing partial HMGB1 linker(3.9 Å)  
Authors : Chen, X.; Kim, M.; Chuenchor, W.; Cui, Y.; Zhang, X.; Zhou, Z.H.; Gellert, M.; Yang, W.  
Deposited on : 2018-02-24  
Resolution : 3.90 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](mailto: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>.

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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

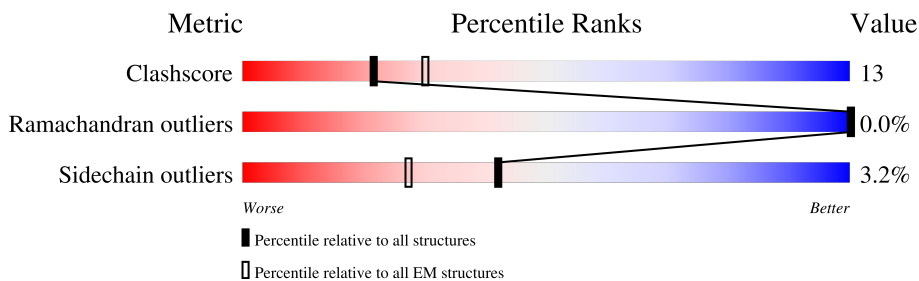
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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  $\geq 3$ , 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	776	
1	C	776	
2	F	46	
3	I	16	
4	J	20	
5	G	61	
6	N	163	
7	L	30	

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Mol	Chain	Length	Quality of chain
8	B	520	 49% 16% • 34%
8	D	520	 51% 14% • 35%
9	M	41	 39% 61%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20413 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4921	3097	876	914	34		
1	C	616	Total	C	N	O	S	0	0
			4946	3115	880	917	34		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	962	GLN	GLU	conflict	UNP P15919
C	962	GLN	GLU	conflict	UNP P15919

- Molecule 2 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	46	Total	C	N	O	P	0	0
			947	452	172	278	45		

- Molecule 3 is a DNA chain called DNA (5'-D(\*GP\*AP\*TP\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	16	Total	C	N	O	P	0	0
			323	156	54	98	15		

- Molecule 4 is a DNA chain called DNA (5'-D(P\*CP\*TP\*GP\*GP\*AP\*TP\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	19	Total	C	N	O	P	0	0
			387	185	64	119	19		

- Molecule 5 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	60	Total	C	N	O	P	0	0
			1225	586	215	365	59		

- Molecule 6 is a protein called High mobility group protein B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	133	Total	C	N	O	S	0	0
			910	577	158	170	5		

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	30	Total	C	N	O	P	0	0
			610	290	118	172	30		

- Molecule 8 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	340	Total	C	N	O	S	0	0
			2643	1689	447	489	18		
8	B	342	Total	C	N	O	S	0	0
			2652	1694	448	492	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	490	ALA	THR	conflict	UNP P21784
B	490	ALA	THR	conflict	UNP P21784

- Molecule 9 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	41	Total	C	N	O	P	0	0
			845	400	170	234	41		

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

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Zn	0
			1	1	
10	C	1	Total	Zn	0
			1	1	

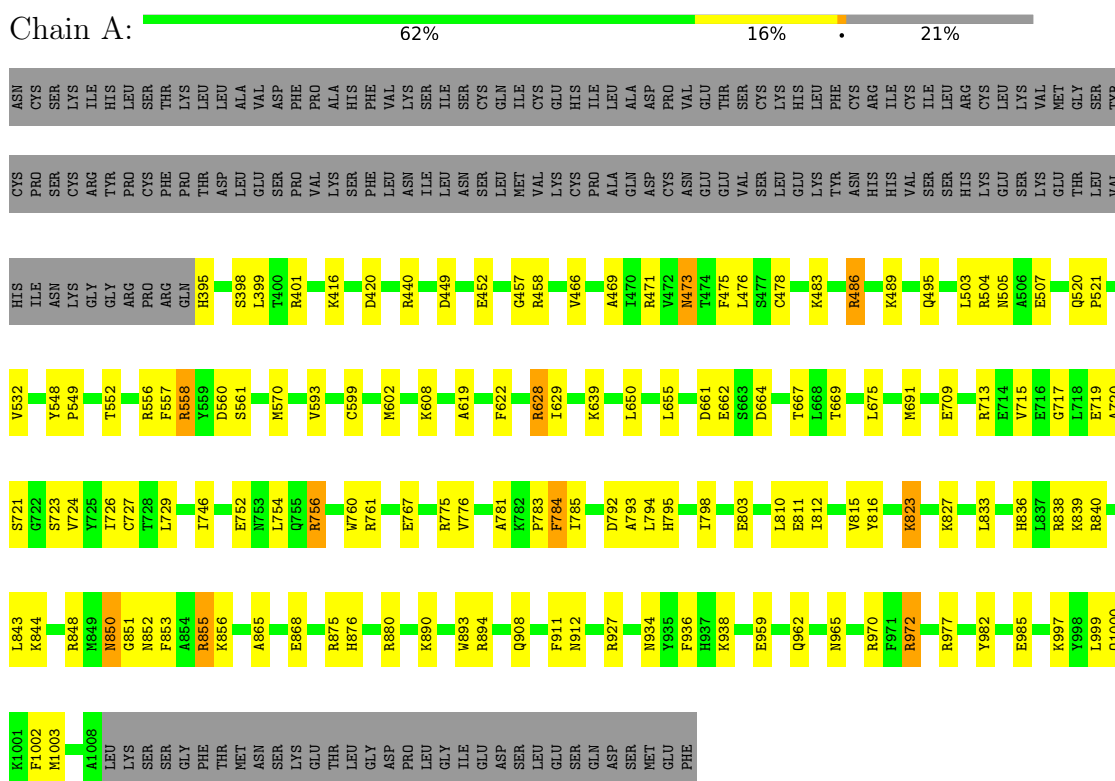
- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total 1	Ca 1	0
11	C	1	Total 1	Ca 1	0

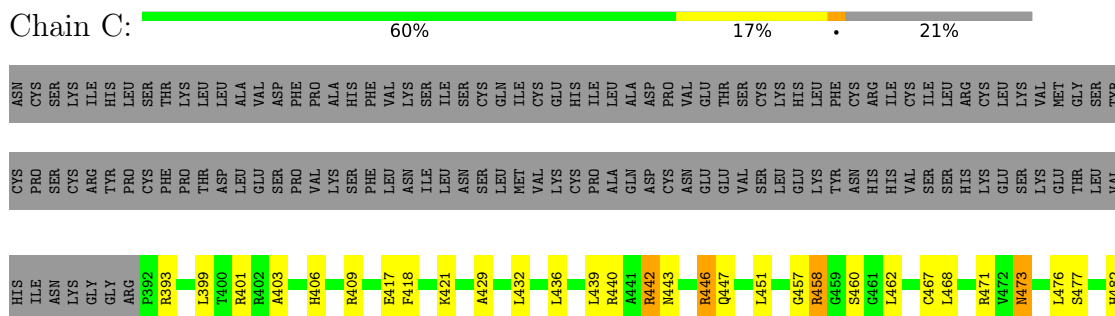
### 3 Residue-property plots

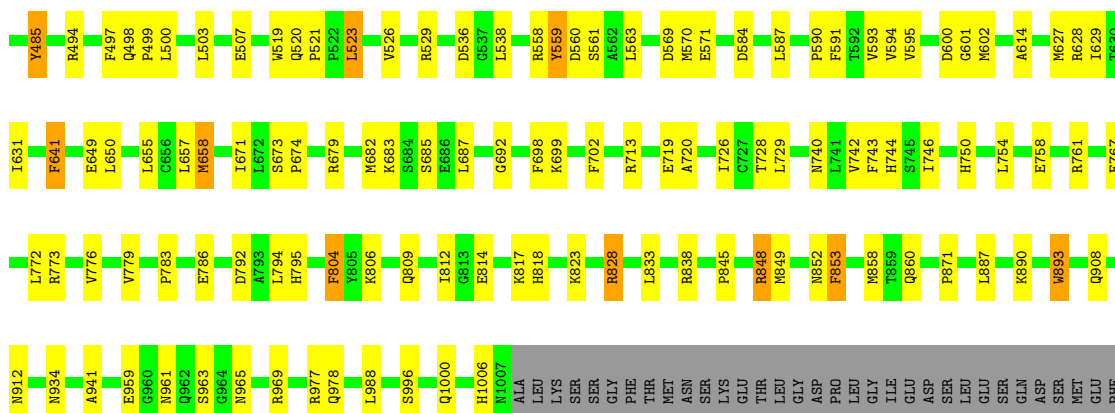
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: V(D)J recombination-activating protein 1



- Molecule 1: V(D)J recombination-activating protein 1





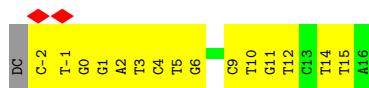
• Molecule 2: DNA (46-MER)



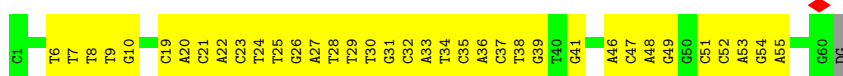
• Molecule 3: DNA (5'-D(\*GP\*AP\*TP\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*TP\*A)-3')



• Molecule 4: DNA (5'-D(P\*CP\*TP\*GP\*GP\*AP\*TP\*CP\*TP\*GP\*GP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*TP\*A)-3')



• Molecule 5: DNA (60-MER)

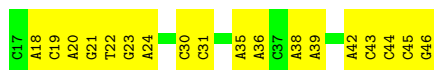


• Molecule 6: High mobility group protein B1

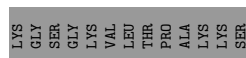
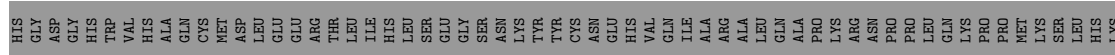
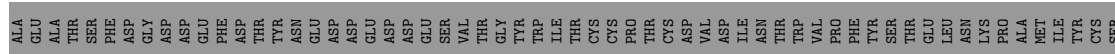
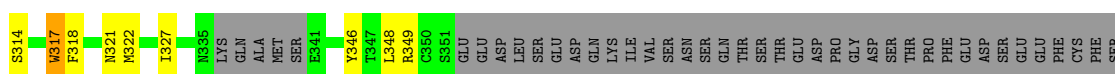
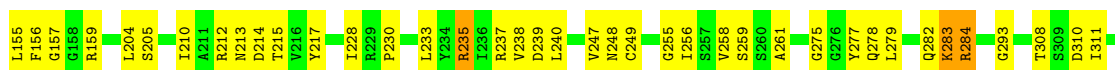
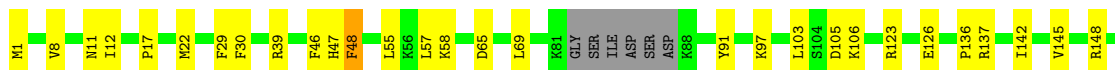




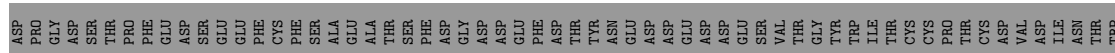
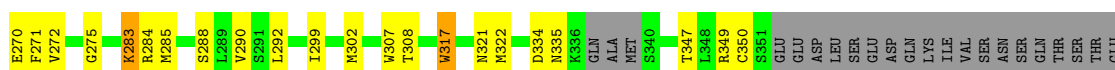
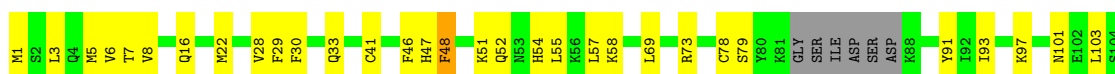
- Molecule 7: DNA (30-MER)



- Molecule 8: V(D)J recombination-activating protein 2



- Molecule 8: V(D)J recombination-activating protein 2



VAL  
PRO  
PHE  
TYR  
SER  
THR  
GLU  
LEU  
ASN  
LYS  
LYS  
ALA  
MET  
ILE  
TYR  
CYS  
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● Molecule 9: DNA (41-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49624	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 ( $e^-/\text{\AA}^2$ )	57.6	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	0.117	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	308.16, 308.16, 308.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: CA, 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	A	0.24	0/5022	0.40	0/6767
1	C	0.24	0/5049	0.41	0/6802
2	F	0.53	0/1062	0.94	0/1640
3	I	0.51	0/360	0.98	0/554
4	J	0.53	0/431	1.03	0/663
5	G	0.50	0/1371	0.94	0/2115
6	N	0.25	0/934	0.40	0/1270
7	L	0.50	0/685	0.83	0/1052
8	B	0.24	0/2719	0.42	0/3690
8	D	0.24	0/2710	0.42	0/3678
9	M	0.48	0/952	0.81	0/1466
All	All	0.32	0/21295	0.58	0/29697

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	A	4921	0	4887	124	0
1	C	4946	0	4919	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	947	0	522	24	0
3	I	323	0	184	4	0
4	J	387	0	217	10	0
5	G	1225	0	681	41	0
6	N	910	0	726	23	0
7	L	610	0	335	18	0
8	B	2652	0	2577	65	0
8	D	2643	0	2571	62	0
9	M	845	0	457	50	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
All	All	20413	0	18076	498	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 13.

The worst 5 of 498 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:HG22	1:A:784:PHE:CE2	1.90	1.05
8:D:235:ARG:NH1	8:D:237:ARG:HH22	1.56	1.04
1:C:761:ARG:HH12	8:D:106:LYS:NZ	1.61	0.96
1:A:504:ARG:HG3	1:A:504:ARG:HH11	1.34	0.92
8:D:235:ARG:HH11	8:D:237:ARG:HH22	1.17	0.92

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	612/776 (79%)	590 (96%)	21 (3%)	1 (0%)	47	79
1	C	614/776 (79%)	588 (96%)	26 (4%)	0	100	100
6	N	125/163 (77%)	117 (94%)	8 (6%)	0	100	100
8	B	336/520 (65%)	331 (98%)	5 (2%)	0	100	100
8	D	334/520 (64%)	322 (96%)	12 (4%)	0	100	100
All	All	2021/2755 (73%)	1948 (96%)	72 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	GLY

### 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	A	536/692 (78%)	516 (96%)	20 (4%)	34	60
1	C	540/692 (78%)	522 (97%)	18 (3%)	38	63
6	N	71/139 (51%)	67 (94%)	4 (6%)	21	51
8	B	293/461 (64%)	287 (98%)	6 (2%)	55	74
8	D	292/461 (63%)	285 (98%)	7 (2%)	49	69
All	All	1732/2445 (71%)	1677 (97%)	55 (3%)	42	63

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	641	PHE
1	C	853	PHE
8	B	317	TRP
8	B	5	MET
1	C	658	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	934	ASN
8	B	47	HIS
1	C	978	GLN
8	B	222	HIS
8	D	94	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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.

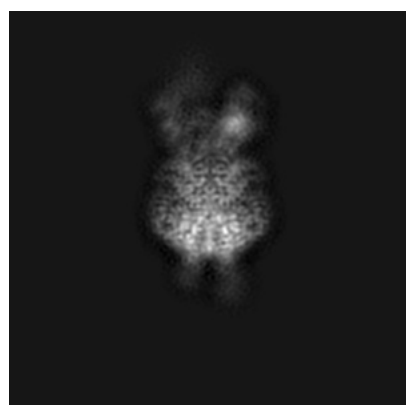
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7480. These allow visual inspection of the internal detail of the map and identification of artifacts.

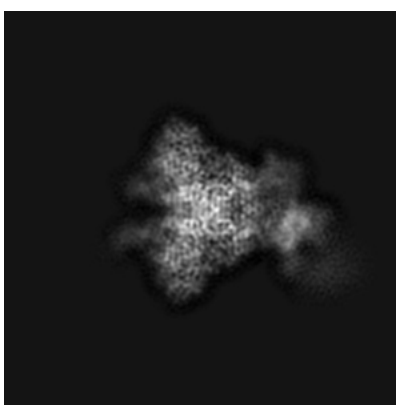
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

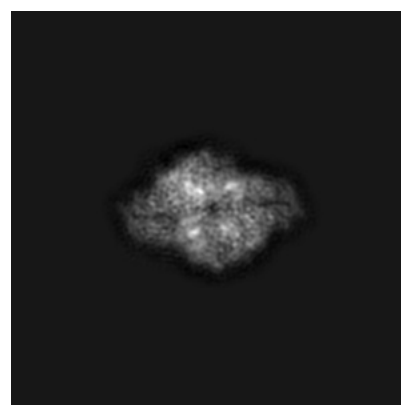
#### 6.1.1 Primary map



X



Y

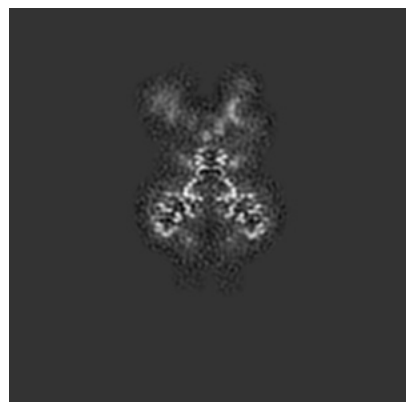


Z

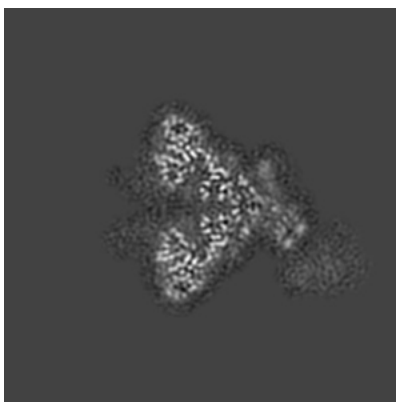
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

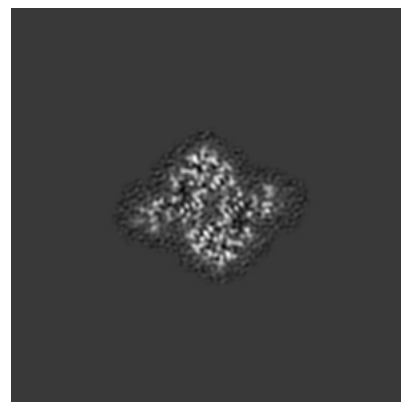
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

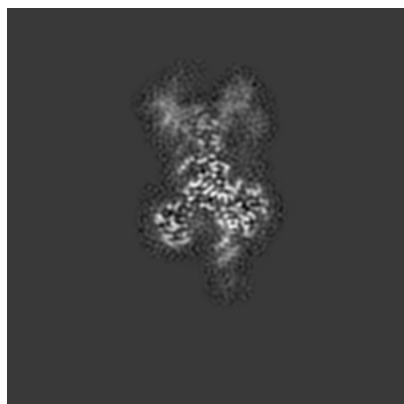


Z Index: 144

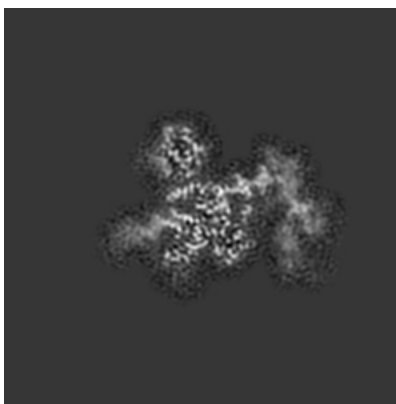
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

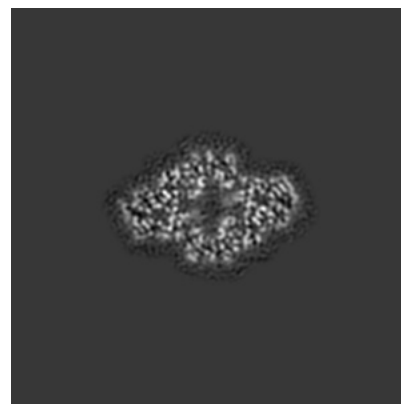
### 6.3.1 Primary map



X Index: 136



Y Index: 160



Z Index: 130

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

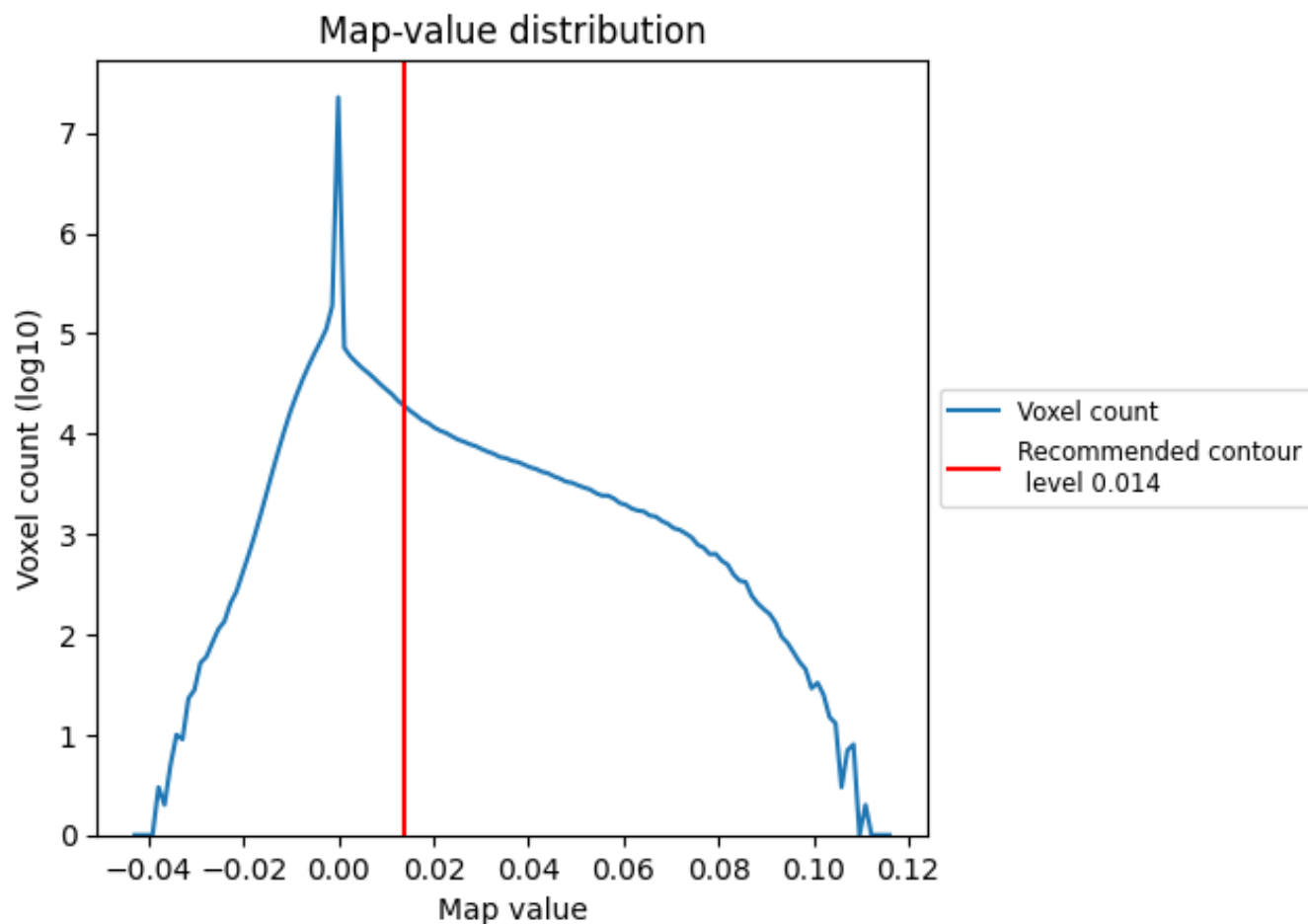
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

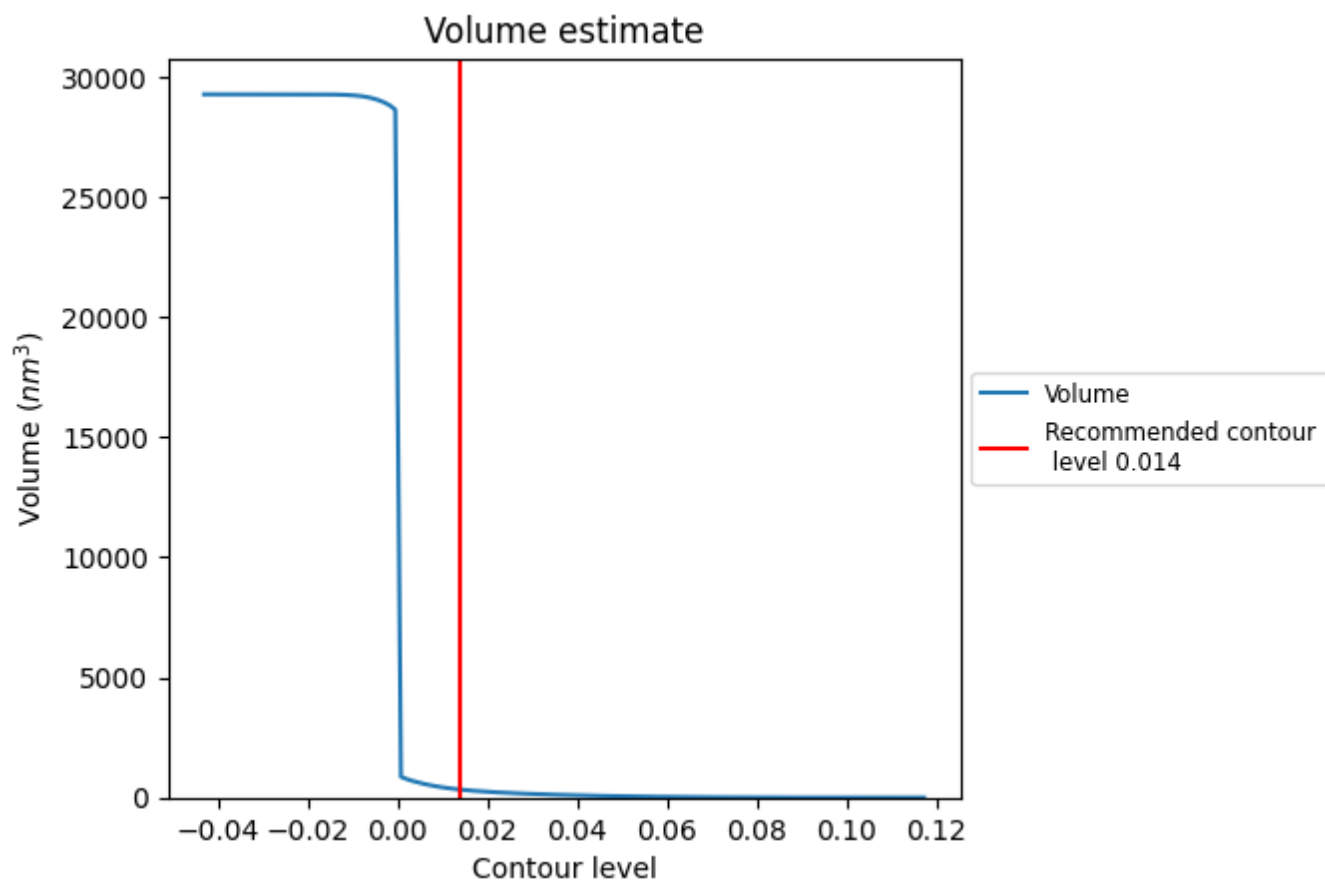
This section contains the results of statistical analysis of the map.

### 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.

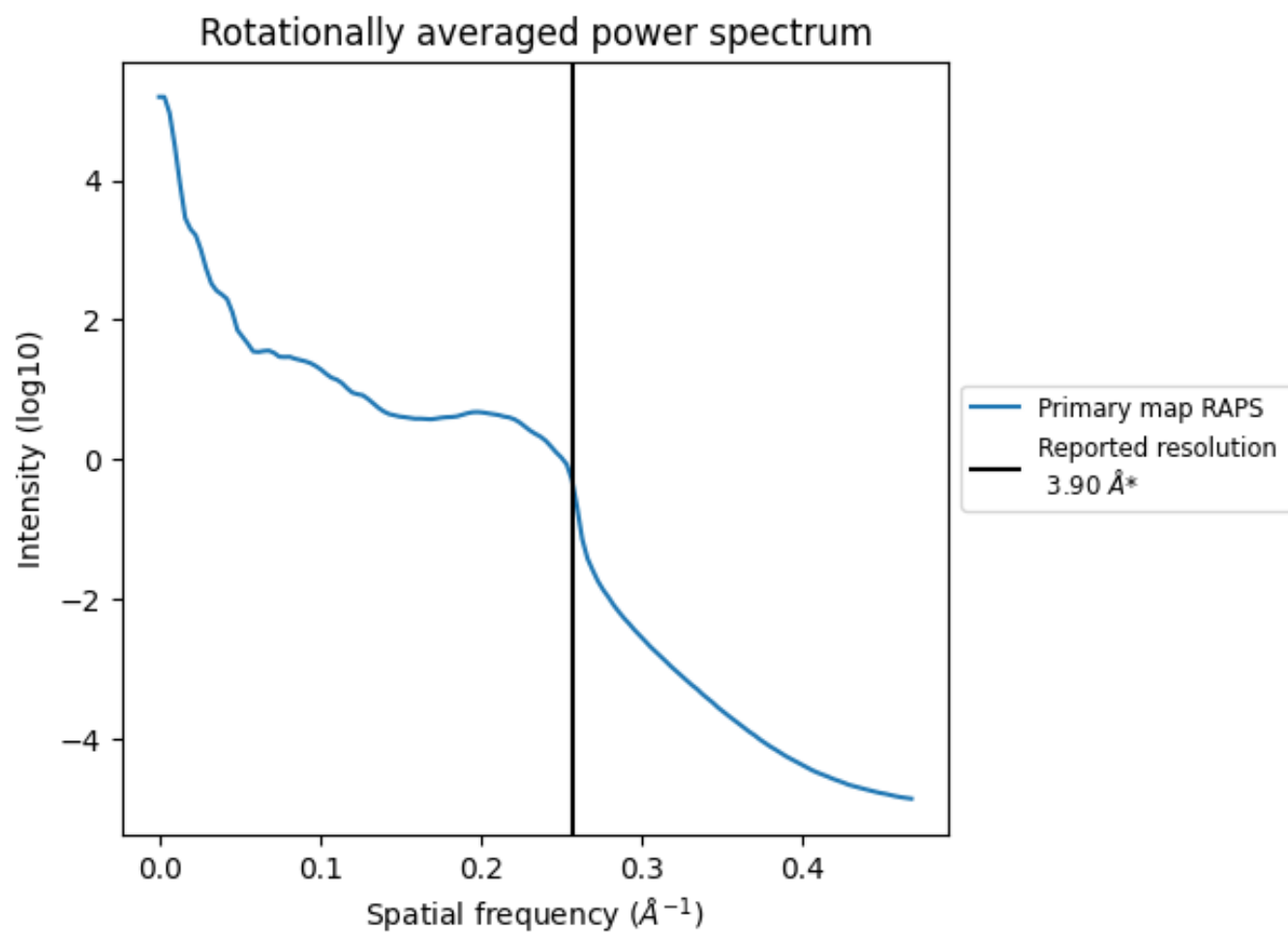
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $332 \text{ nm}^3$ ; this corresponds to an approximate mass of 300 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 0.256 Å<sup>-1</sup>

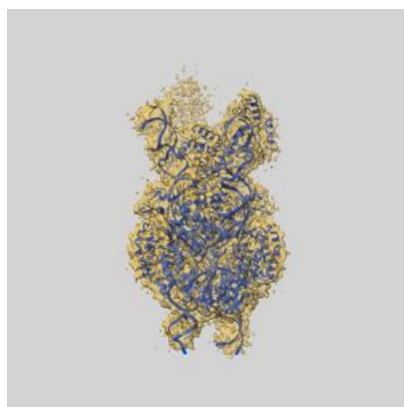
## 8 Fourier-Shell correlation ⓘ

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

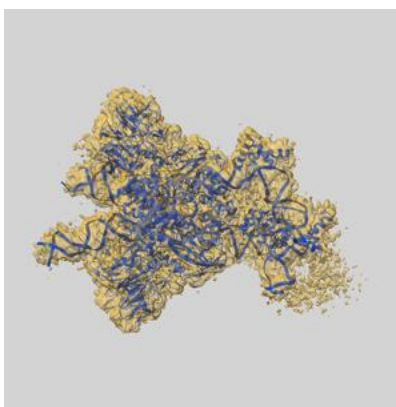
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7480 and PDB model 6CIJ. Per-residue inclusion information can be found in section 3 on page 7.

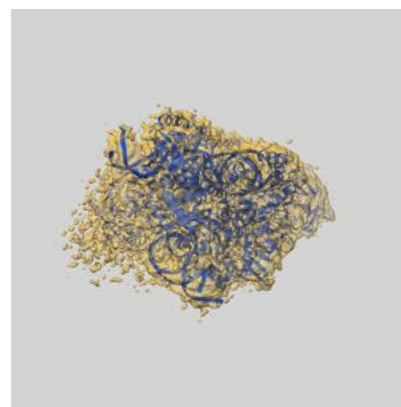
### 9.1 Map-model overlay [i](#)



X



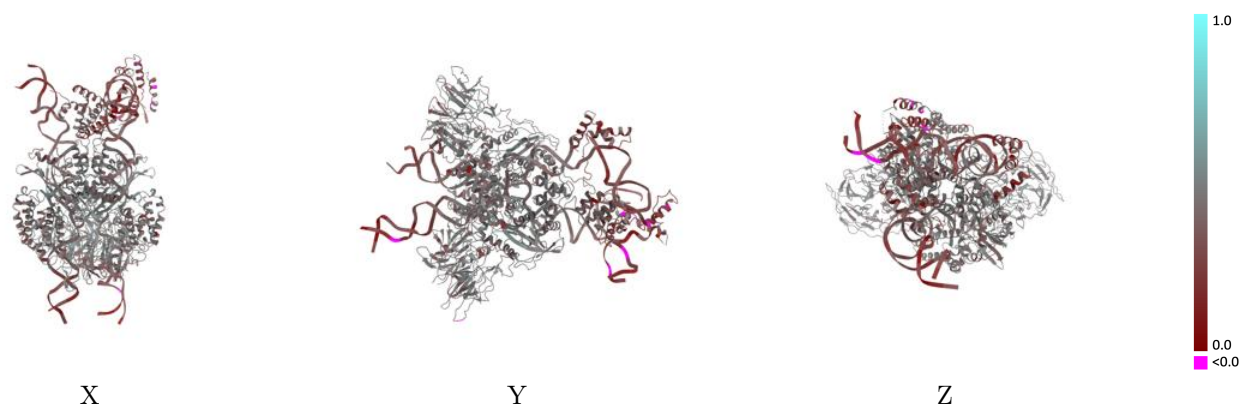
Y



Z

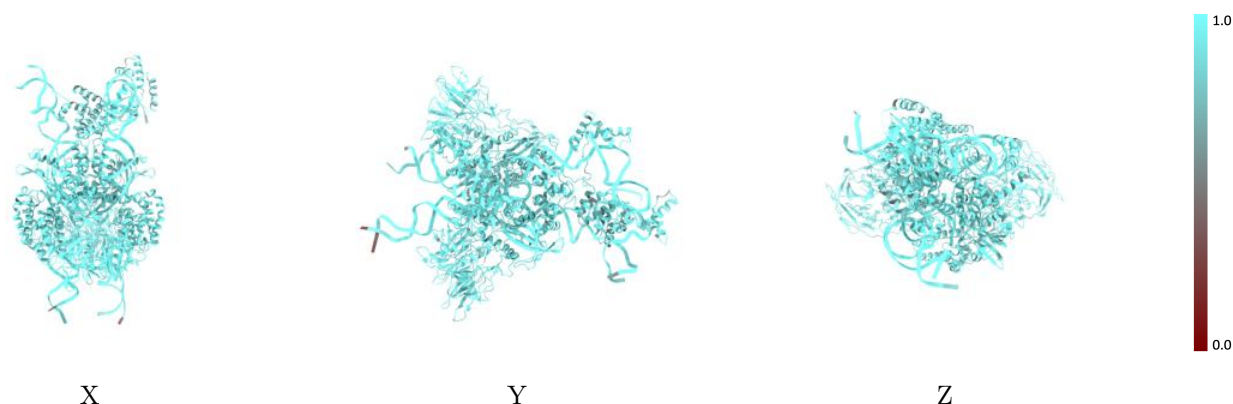
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



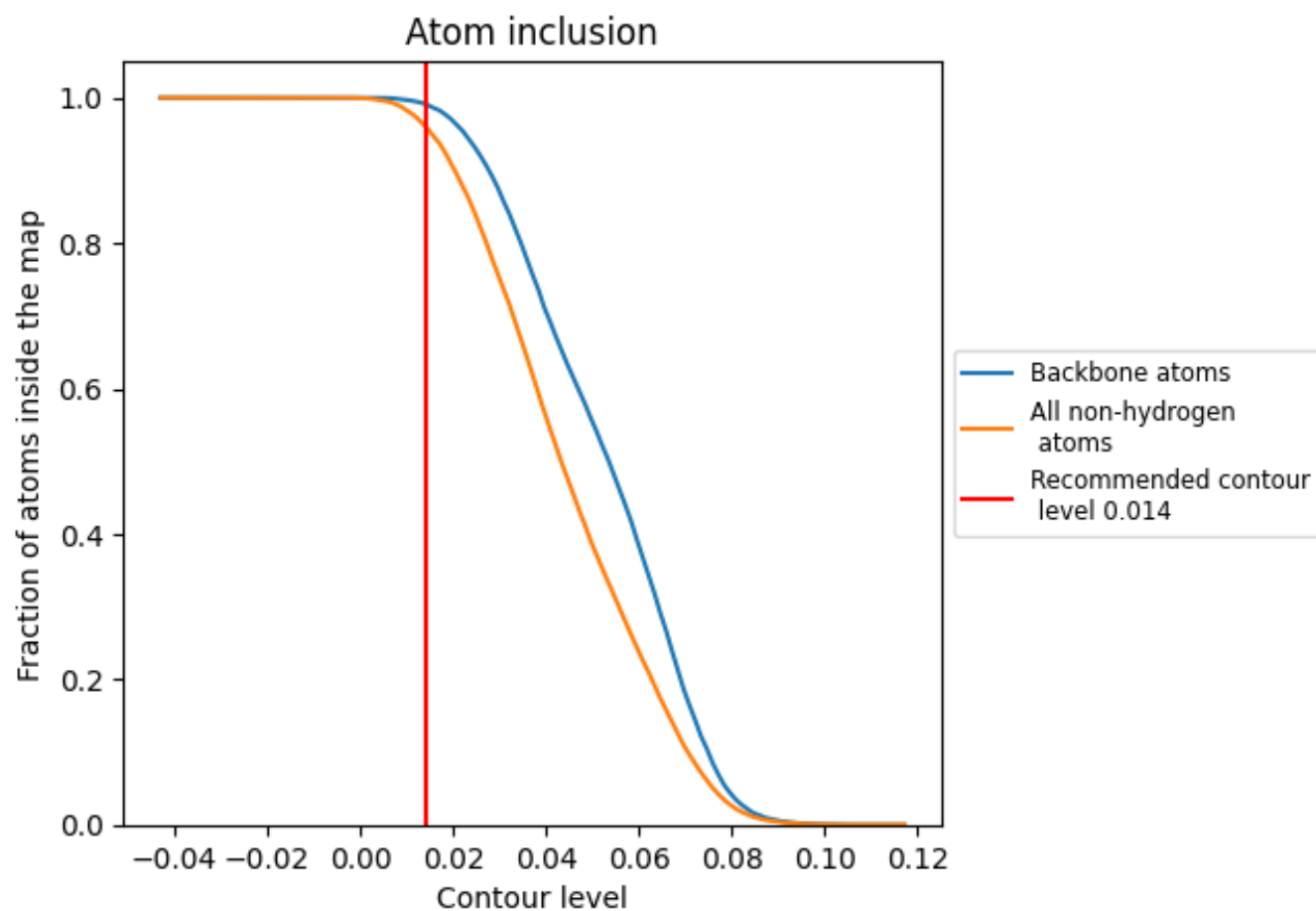
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9611	<div></div> 0.4090
A	<div></div> 0.9630	<div></div> 0.4390
B	<div></div> 0.9643	<div></div> 0.4520
C	<div></div> 0.9597	<div></div> 0.4370
D	<div></div> 0.9596	<div></div> 0.4520
F	<div></div> 0.9768	<div></div> 0.3300
G	<div></div> 0.9600	<div></div> 0.3030
I	<div></div> 0.9783	<div></div> 0.3350
J	<div></div> 0.9147	<div></div> 0.2810
L	<div></div> 0.9934	<div></div> 0.3470
M	<div></div> 0.9811	<div></div> 0.3220
N	<div></div> 0.9111	<div></div> 0.2700

1.0

0.0

<0.0