



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 09:43 am GMT

PDB ID : 7NHT  
EMDB ID : EMD-12341  
Title : Akirin2 bound human proteasome  
Authors : Singh, K.; Brunner, H.; Grishkovskaya, I.; de Almeida, M.; Hinterndorfer, M.; Zuber, J.; Haselbach, D.  
Deposited on : 2021-02-11  
Resolution : 2.80 Å (reported)  
Based on initial model : 5LE5

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) : 2.31.3

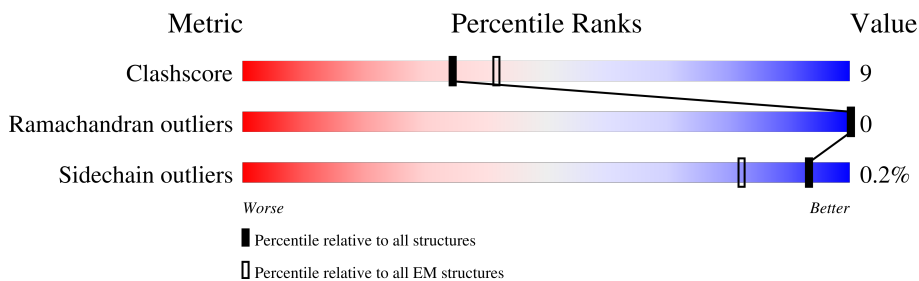
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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	234	
2	B	261	
3	C	248	
4	D	241	
5	E	263	
6	F	255	
7	G	246	
8	H	277	

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Mol	Chain	Length	Quality of chain
9	I	205	 80% 20%
10	J	201	 85% 13%
11	K	263	 60% 16% 24%
12	L	241	 69% 19% 12%
13	M	264	 63% 19% 18%
14	N	239	 73% 12% 15%
15	c	203	 24% 76%
15	d	203	 22% 78%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 24915 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	231	1799	1151	306	336	6	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	248	1945	1228	334	373	10	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	237	1846	1160	328	353	5	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	241	1841	1157	303	369	12	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	236	1846	1159	332	345	10	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	242	1889	1199	323	356	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	242	1882	1194	314	361	13	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	220	1659	1044	283	320	12	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	204	1591	1013	265	294	19	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	196	1561	1001	264	287	9	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	201	1555	980	273	293	9	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	213	1650	1044	283	313	10	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	216	1687	1064	291	320	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	203	1517	952	259	294	12	0	0

- Molecule 15 is a protein called Akirin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	c	48	332	207	60	64	1	0	0
15	d	44	312	195	56	60	1	0	0

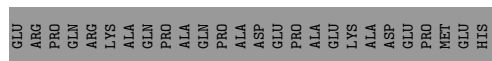
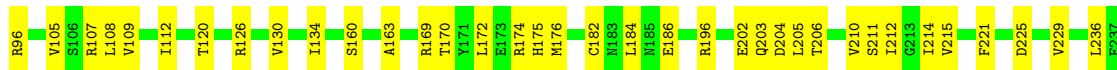
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
16	G	1	Total 1	K 1	0
16	L	1	Total 1	K 1	0
16	N	1	Total 1	K 1	0





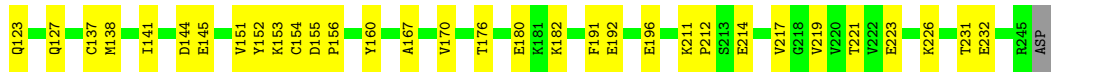
• Molecule 5: Proteasome subunit alpha type-1



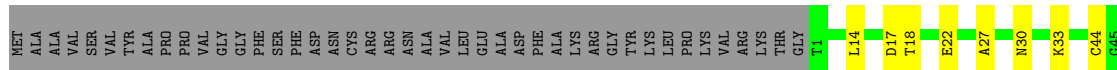
• Molecule 6: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-6

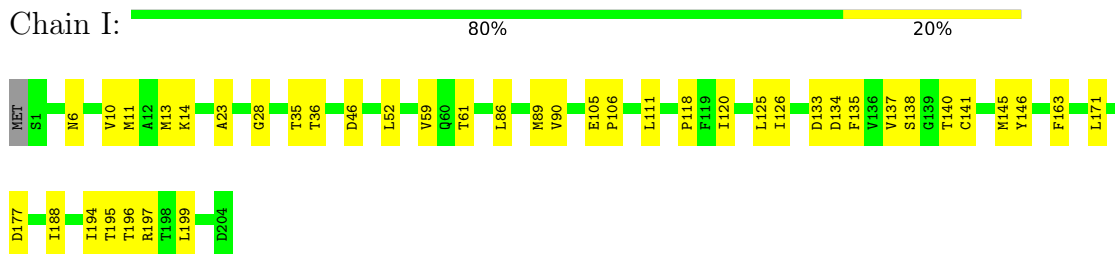


• Molecule 8: Proteasome subunit beta type-7

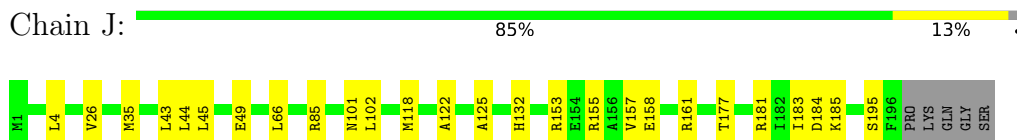


• Molecule 9: Proteasome subunit beta type-3

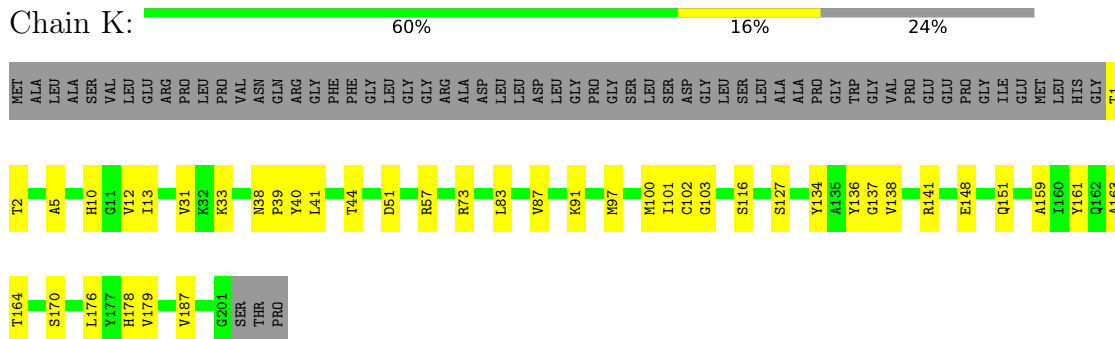




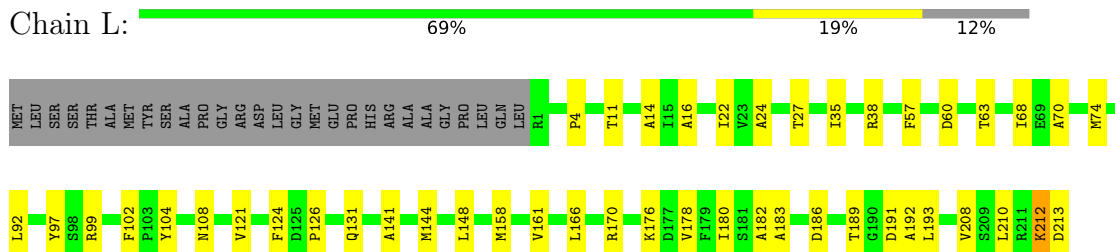
- Molecule 10: Proteasome subunit beta type-2



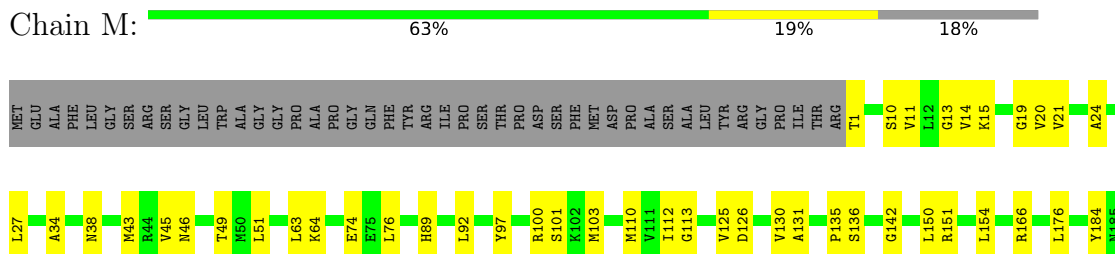
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1

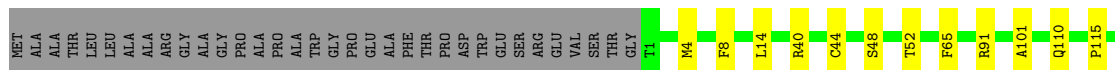


- Molecule 13: Proteasome subunit beta type-4

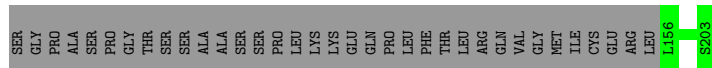




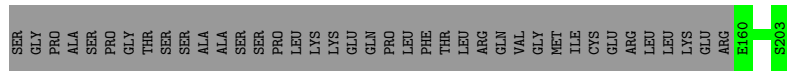
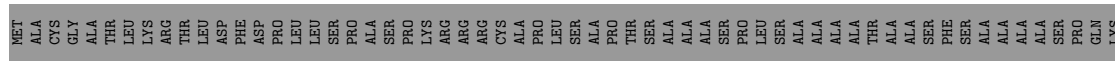
• Molecule 14: Proteasome subunit beta type-6



• Molecule 15: Akirin-2



• Molecule 15: Akirin-2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37447	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 ( $e^-/\text{\AA}^2$ )	33	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.719	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.33	0/1838	0.44	0/2490
2	B	0.32	0/1975	0.49	0/2663
3	C	0.32	0/1872	0.46	0/2530
4	D	0.29	0/1870	0.45	0/2528
5	E	0.31	0/1881	0.47	0/2544
6	F	0.32	0/1924	0.47	0/2591
7	G	0.33	0/1916	0.46	0/2591
8	H	0.30	0/1686	0.47	0/2282
9	I	0.31	0/1620	0.47	0/2184
10	J	0.32	0/1593	0.47	0/2156
11	K	0.34	0/1586	0.48	0/2142
12	L	0.31	0/1680	0.49	0/2264
13	M	0.32	0/1720	0.45	0/2328
14	N	0.32	0/1544	0.46	0/2092
15	c	0.27	0/338	0.40	0/459
15	d	0.27	0/318	0.34	0/431
All	All	0.32	0/25361	0.46	0/34275

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

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	1799	0	1793	40	0
2	B	1945	0	1951	42	0
3	C	1846	0	1853	32	0
4	D	1841	0	1814	40	0
5	E	1846	0	1824	46	0
6	F	1889	0	1878	42	0
7	G	1882	0	1881	46	0
8	H	1659	0	1681	20	0
9	I	1591	0	1612	29	0
10	J	1561	0	1558	21	0
11	K	1555	0	1517	28	0
12	L	1650	0	1645	33	0
13	M	1687	0	1666	37	0
14	N	1517	0	1490	17	0
15	c	332	0	250	0	0
15	d	312	0	242	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
All	All	24915	0	24655	430	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 9.

The worst 5 of 430 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)
2:B:136:TYR:HE1	2:B:150:SER:HG	0.97	0.91
7:G:231:THR:HG22	7:G:232:GLU:H	1.40	0.86
8:H:163:ILE:HG12	8:H:170:GLY:HA2	1.58	0.85
7:G:231:THR:HG22	7:G:232:GLU:N	1.93	0.84
4:D:121:LEU:HD12	5:E:79:ALA:HB3	1.67	0.77

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	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
2	B	246/261 (94%)	242 (98%)	4 (2%)	0	100	100
3	C	235/248 (95%)	230 (98%)	5 (2%)	0	100	100
4	D	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
5	E	234/263 (89%)	225 (96%)	9 (4%)	0	100	100
6	F	240/255 (94%)	234 (98%)	6 (2%)	0	100	100
7	G	240/246 (98%)	232 (97%)	8 (3%)	0	100	100
8	H	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
11	K	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
12	L	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
13	M	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
14	N	201/239 (84%)	195 (97%)	6 (3%)	0	100	100
15	c	46/203 (23%)	44 (96%)	2 (4%)	0	100	100
15	d	42/203 (21%)	42 (100%)	0	0	100	100
All	All	3190/3844 (83%)	3101 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	188/191 (98%)	188 (100%)	0	100	100
2	B	206/221 (93%)	204 (99%)	2 (1%)	76	93
3	C	195/211 (92%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	201/203 (99%)	201 (100%)	0	100	100
5	E	198/224 (88%)	198 (100%)	0	100	100
6	F	198/212 (93%)	198 (100%)	0	100	100
7	G	205/210 (98%)	205 (100%)	0	100	100
8	H	181/228 (79%)	180 (99%)	1 (1%)	86	96
9	I	173/174 (99%)	173 (100%)	0	100	100
10	J	165/171 (96%)	165 (100%)	0	100	100
11	K	155/202 (77%)	155 (100%)	0	100	100
12	L	177/199 (89%)	176 (99%)	1 (1%)	86	96
13	M	179/215 (83%)	179 (100%)	0	100	100
14	N	157/181 (87%)	156 (99%)	1 (1%)	86	96
15	c	23/171 (14%)	23 (100%)	0	100	100
15	d	23/171 (14%)	23 (100%)	0	100	100
All	All	2624/3184 (82%)	2619 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	50	ARG
2	B	51	ASN
8	H	182	LYS
12	L	212	LYS
14	N	144	ARG

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

Mol	Chain	Res	Type
4	D	155	HIS
7	G	24	GLN
12	L	108	ASN
9	I	6	ASN
3	C	154	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 3 ligands modelled in this entry, 3 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.



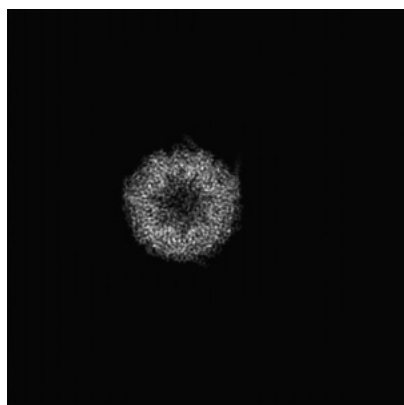
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12341. These allow visual inspection of the internal detail of the map and identification of artifacts.

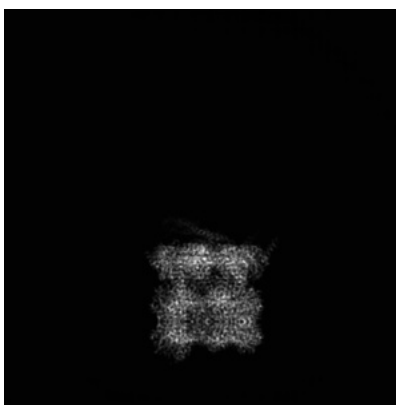
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

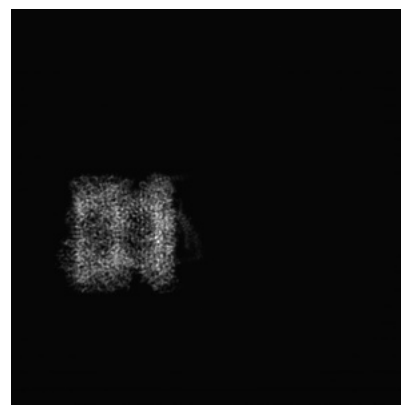
#### 6.1.1 Primary map



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](#)

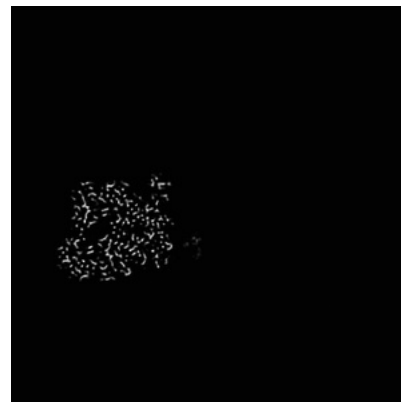
### 6.3.1 Primary map



X Index: 131



Y Index: 180

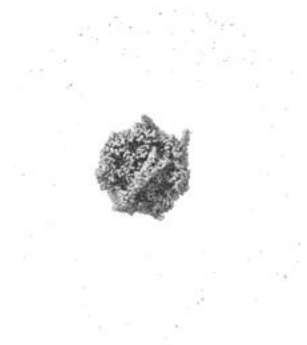


Z Index: 159

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

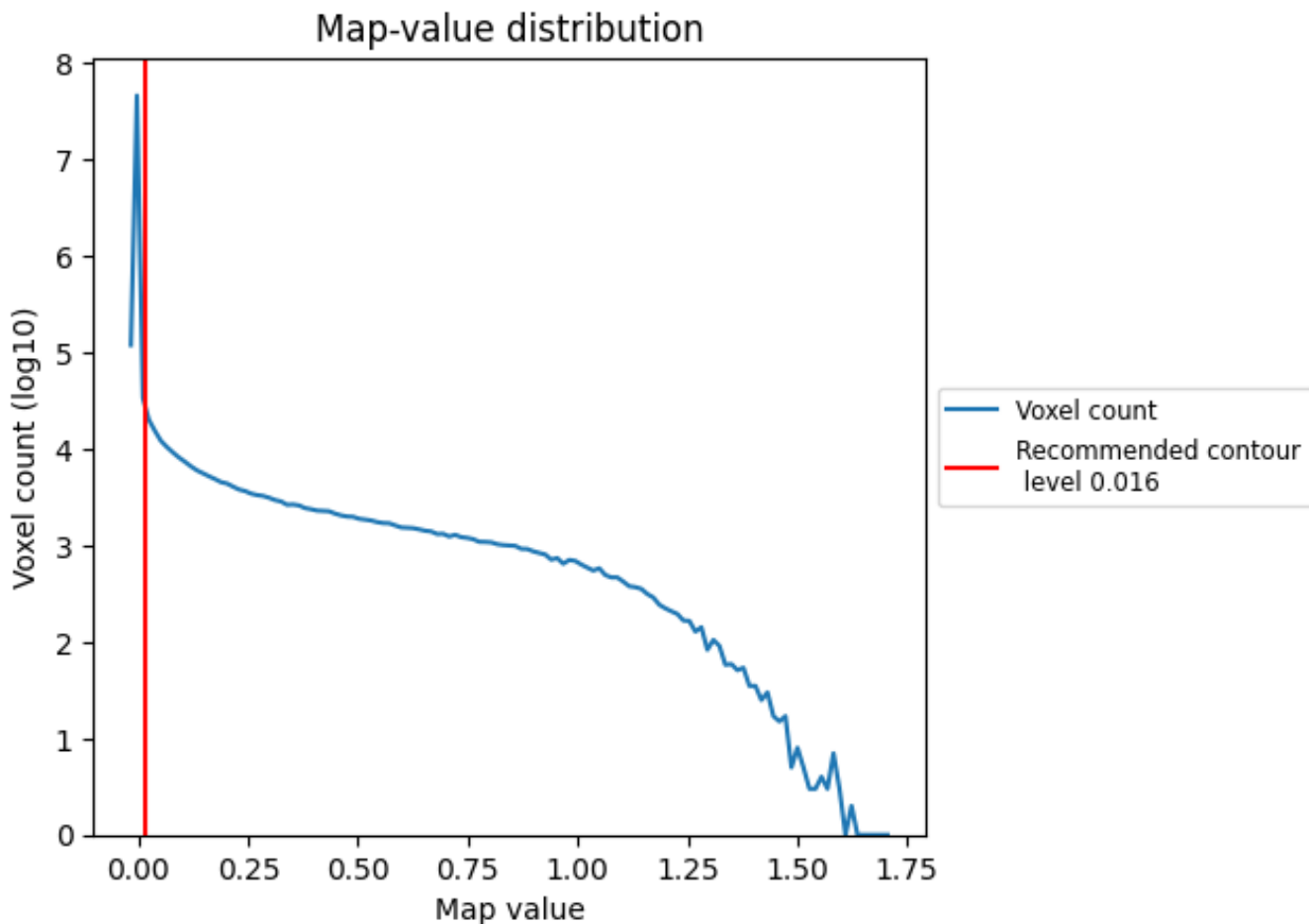
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

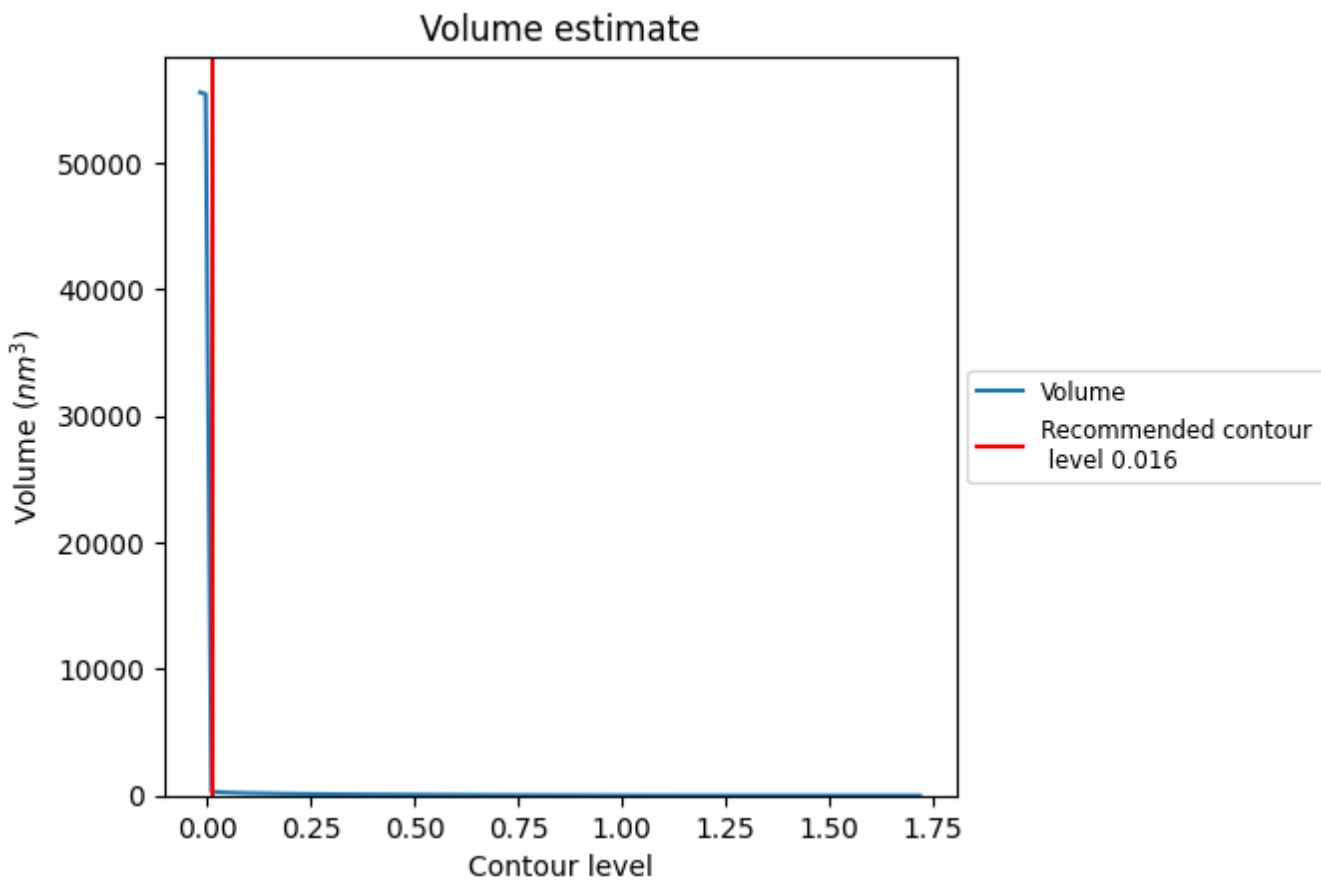
This section contains the results of statistical analysis of the map.

### 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.

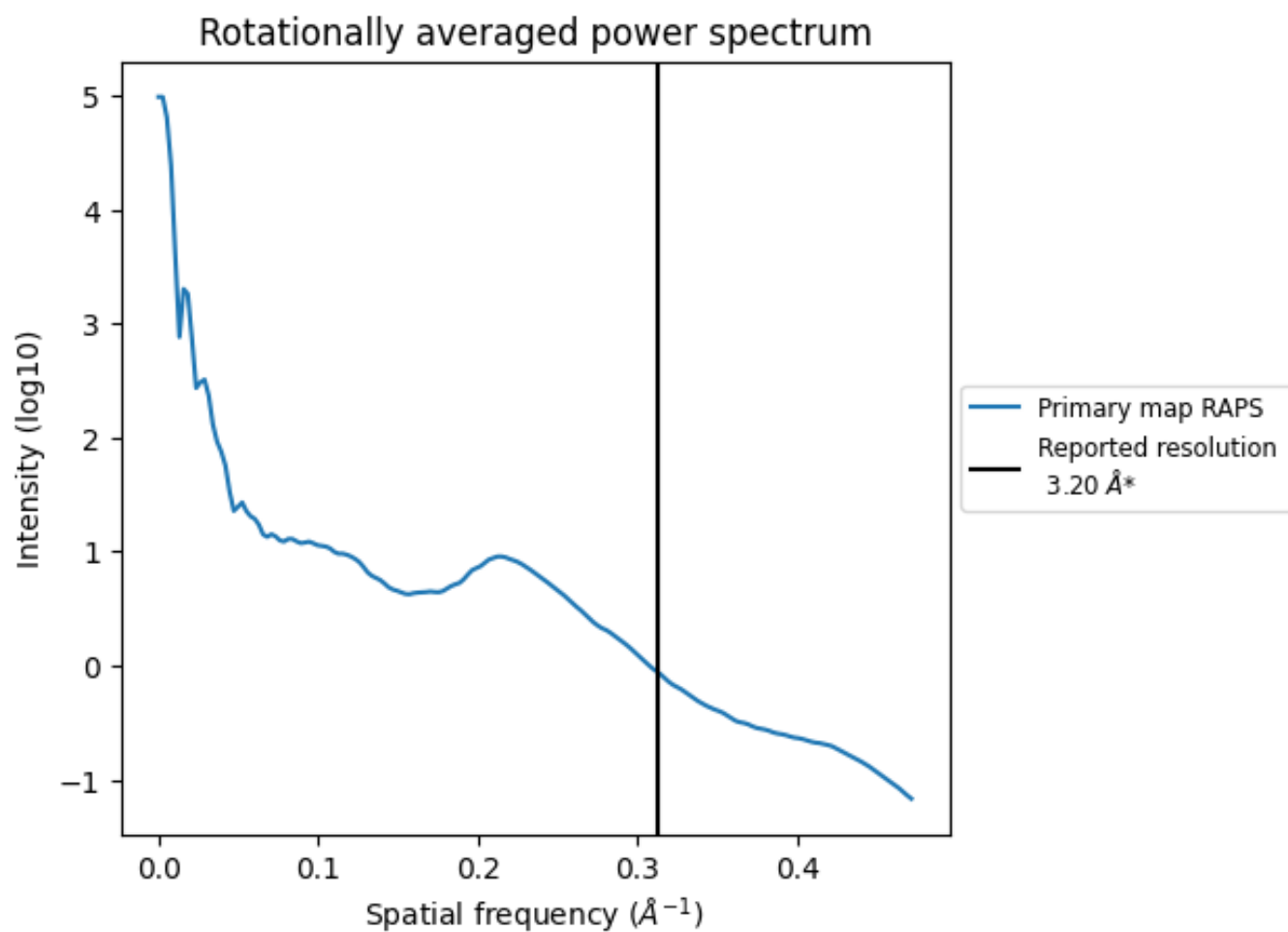
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 302  $\text{nm}^3$ ; this corresponds to an approximate mass of 273 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 0.312 Å<sup>-1</sup>

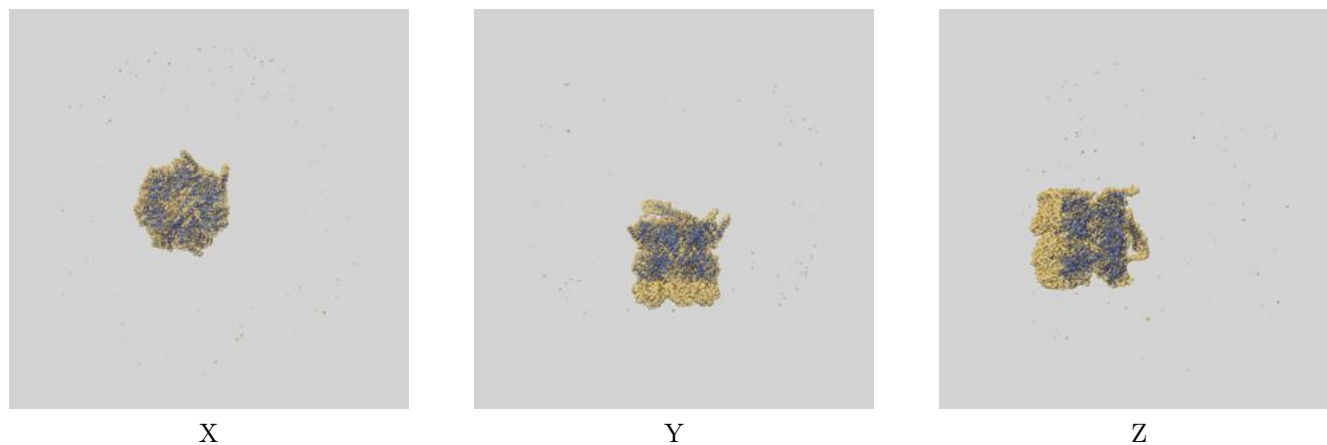
## 8 Fourier-Shell correlation

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-12341 and PDB model 7NHT. Per-residue inclusion information can be found in section 3 on page 7.

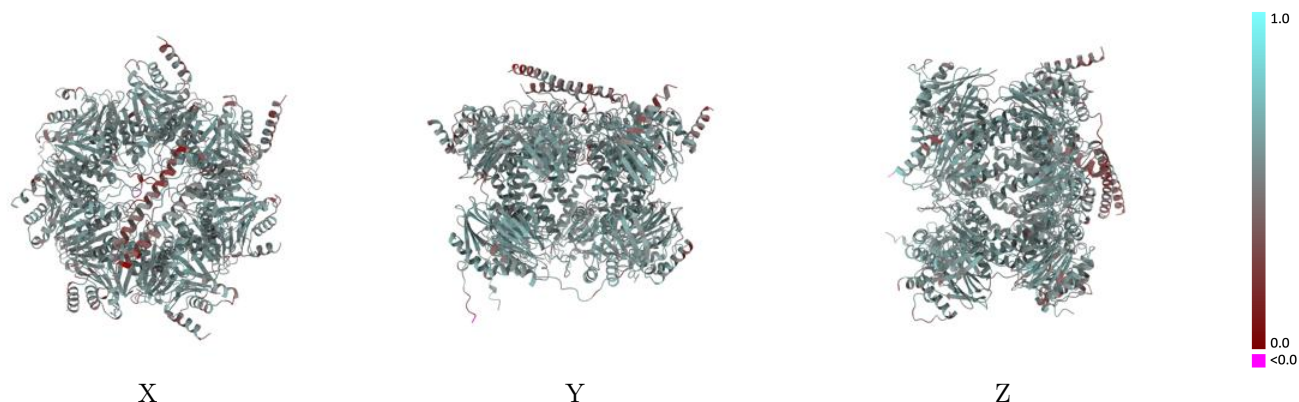
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

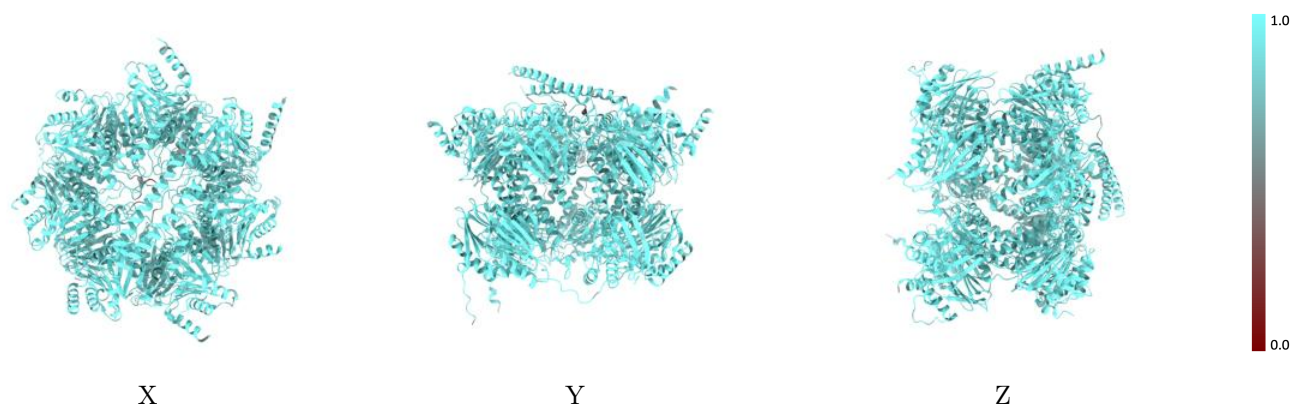


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



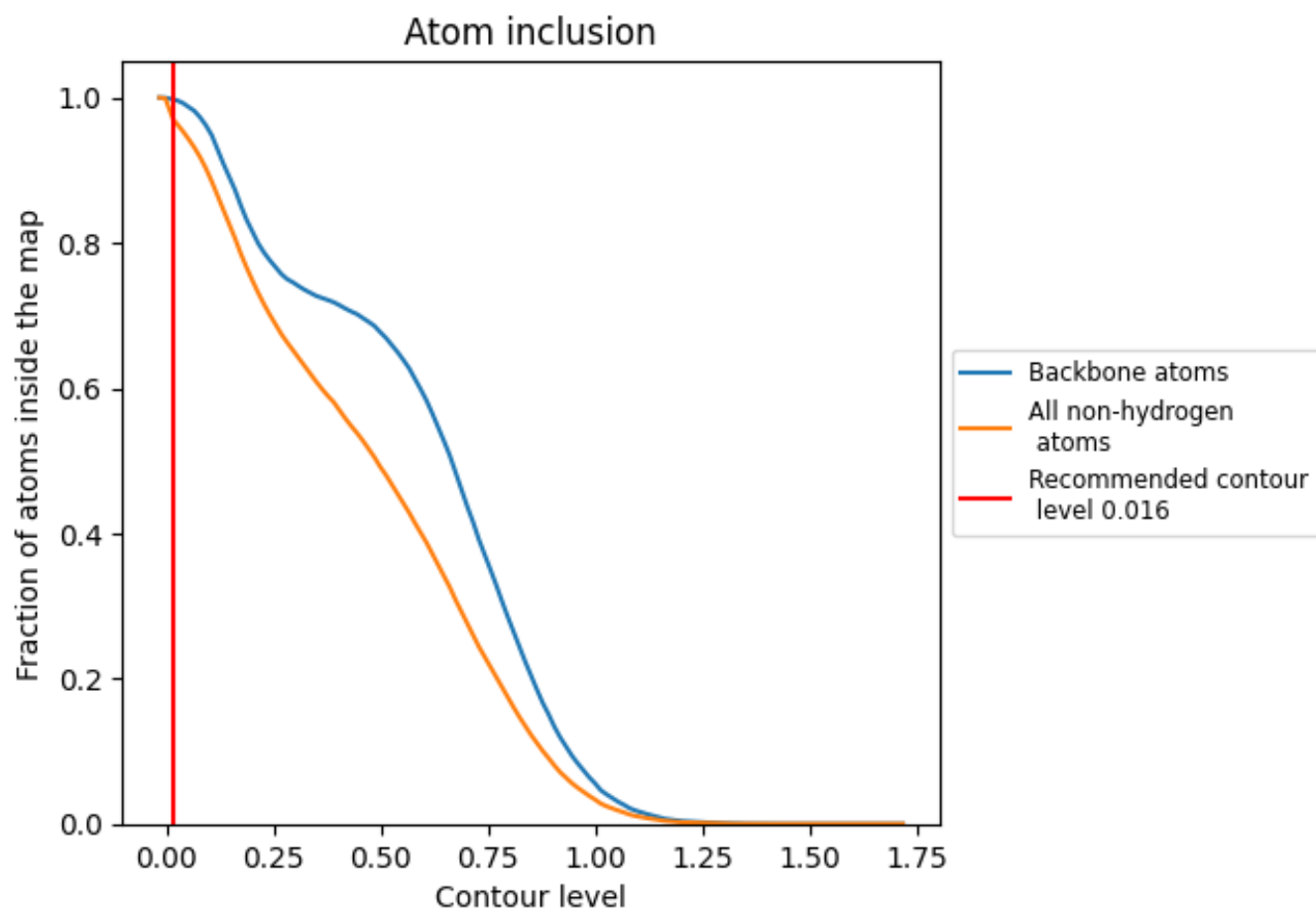
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9697	 0.5470
A	 0.9722	 0.5520
B	 0.9638	 0.5430
C	 0.9617	 0.5390
D	 0.9544	 0.5310
E	 0.9678	 0.5430
F	 0.9637	 0.5400
G	 0.9665	 0.5450
H	 0.9791	 0.5610
I	 0.9827	 0.5680
J	 0.9758	 0.5580
K	 0.9841	 0.5640
L	 0.9814	 0.5590
M	 0.9781	 0.5670
N	 0.9717	 0.5610
c	 0.9292	 0.3970
d	 0.9082	 0.3580

