



# wwPDB EM Validation Summary Report ⓘ

May 12, 2024 – 08:44 am BST

PDB ID : 6R7N  
EMDB ID : EMD-4744  
Title : Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome  
Authors : Faull, S.V.; Lau, A.M.C.; Martens, C.; Ahdash, Z.; Yebenes, H.; Schmidt, C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.  
Deposited on : 2019-03-29  
Resolution : 6.50 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

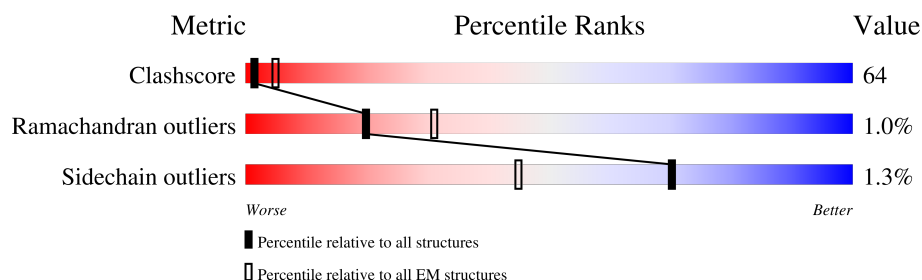
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*





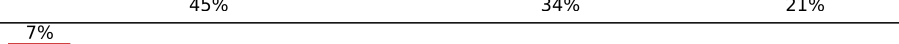
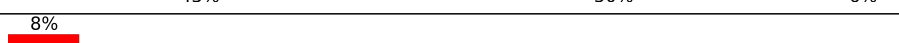
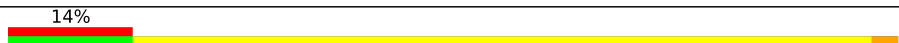

The reported resolution of this entry is 6.50 Å.

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	491	
2	D	406	
3	H	199	
4	P	104	
5	Q	112	
6	R	86	
7	C	401	
8	G	215	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	O	745	<div><div></div><div>7%</div><div>30%</div><div>65%</div><div></div><div>.</div><div>.</div></div>
10	B	443	<div><div></div><div>.</div><div>25%</div><div>70%</div><div></div><div>.</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24672 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	419	Total	C	N	O	S	0	0
			3348	2113	588	625	22		

- Molecule 2 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	406	Total	C	N	O	S	0	0
			3251	2047	566	622	16		

- Molecule 3 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	169	Total	C	N	O	S	0	0
			1347	866	233	244	4		

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	104	Total	C	N	O	S	0	0
			822	520	138	159	5		

- Molecule 5 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	88	Total	C	N	O	S	0	0
			698	450	112	130	6		

- Molecule 6 is a protein called RBX1 E3 ubiquitin-protein ligase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	86	Total	C	N	O	S	0	0
			690	433	128	120	9		

- Molecule 7 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	401	Total	C	N	O	S	0	0
			3191	2032	535	598	26		

- Molecule 8 is a protein called CSN7B\_HUMAN.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	215	Total	C	N	O	S	0	0
			1678	1060	283	328	7		

- Molecule 9 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	734	Total	C	N	O	S	0	0
			6020	3824	1021	1129	46		

- Molecule 10 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	443	Total	C	N	O	S	0	0
			3624	2287	610	708	19		

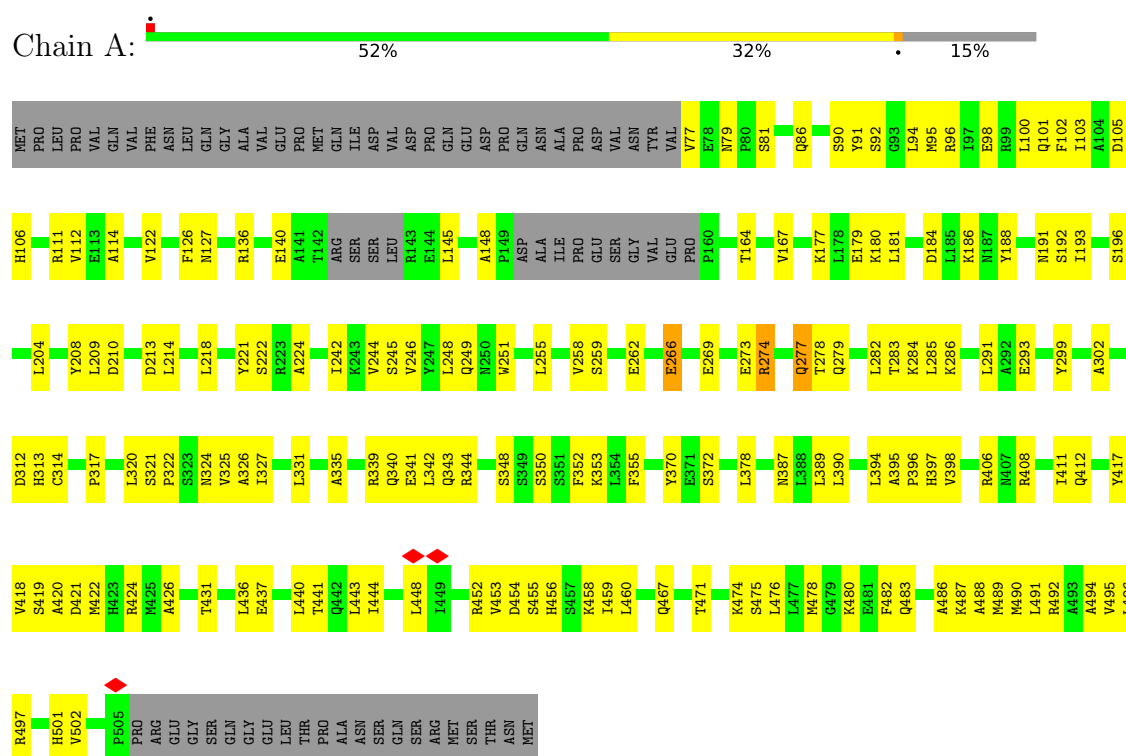
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	R	3	Total	Zn	0
			3	3	

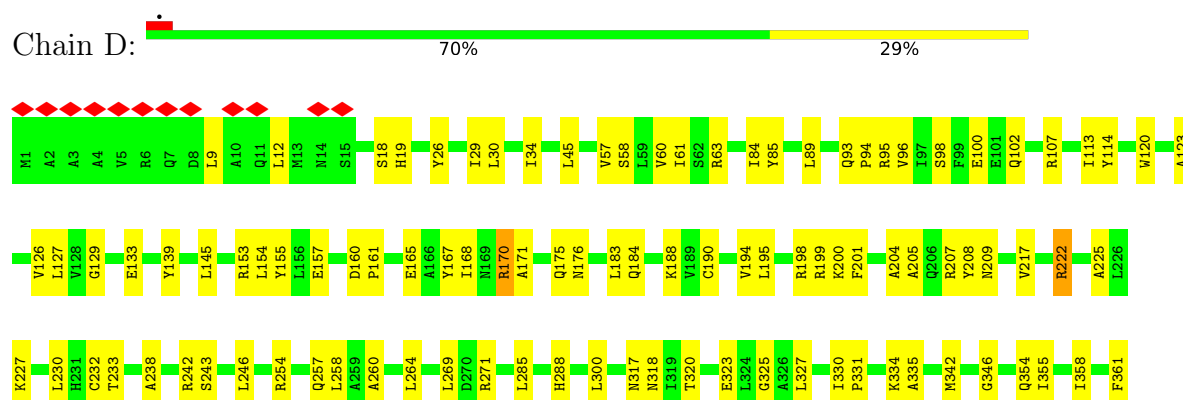
### 3 Residue-property plots

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: COP9 signalosome complex subunit 1



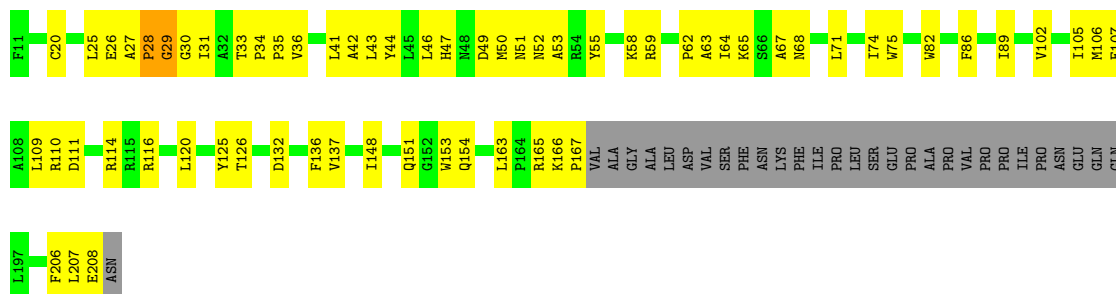
#### • Molecule 2: COP9 signalosome complex subunit 4





• Molecule 3: COP9 signalosome complex subunit 8

Chain H: 53% 31% 15%



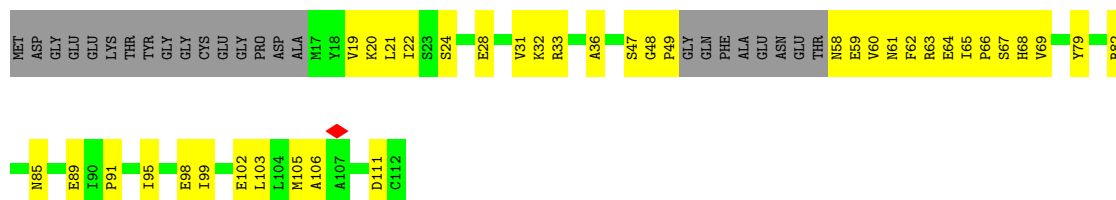
• Molecule 4: Elongin-B

Chain P: 74% 25%



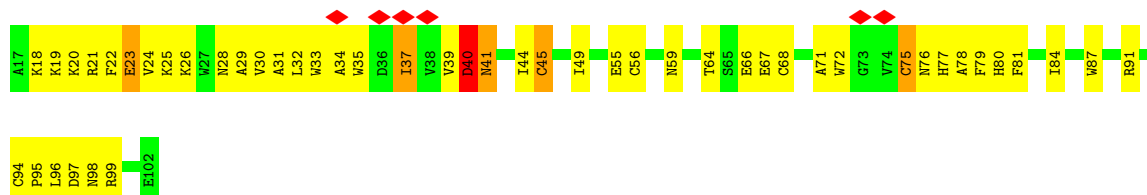
• Molecule 5: Elongin-C

Chain Q: 45% 34% 21%



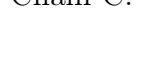
• Molecule 6: RBX1 E3 ubiquitin-protein ligase

Chain R: 7% 43% 50% 6%



• Molecule 7: COP9 signalosome complex subunit 3

Chain C: 8% 82% 17%









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22471	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.607	Depositor
Minimum map value	-7.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.65	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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

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	0.32	0/3404	0.60	0/4588
2	D	0.33	0/3302	0.59	0/4457
3	H	0.32	0/1380	0.58	0/1877
4	P	0.31	0/838	0.62	1/1132 (0.1%)
5	Q	0.31	0/713	0.63	0/962
6	R	1.08	1/706 (0.1%)	0.92	2/955 (0.2%)
7	C	0.44	1/3249 (0.0%)	0.54	0/4387
8	G	0.32	0/1697	0.60	2/2293 (0.1%)
9	O	0.89	0/6135	1.12	8/8258 (0.1%)
10	B	0.90	1/3685 (0.0%)	1.14	11/4958 (0.2%)
All	All	0.64	3/25109 (0.0%)	0.85	24/33867 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	D	0	2
3	H	0	1
4	P	0	1
6	R	0	4
7	C	0	2
8	G	0	2
10	B	0	2
All	All	0	16

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	40	ASP	C-N	27.24	1.96	1.34
10	B	413	HIS	C-N	7.49	1.51	1.34
7	C	387	ASP	C-N	6.79	1.49	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	67	TRP	CA-CB-CG	-15.59	84.08	113.70
6	R	40	ASP	CA-C-N	-13.57	87.34	117.20
6	R	40	ASP	C-N-CA	10.80	148.71	121.70
10	B	84	ASN	C-N-CA	9.79	146.17	121.70
9	O	694	LEU	CB-CA-C	-7.47	96.01	110.20

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	GLU	Peptide
1	A	277	GLN	Peptide
2	D	133	GLU	Peptide
2	D	58	SER	Peptide
3	H	28	PRO	Peptide

## 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	3348	0	3384	292	0
2	D	3251	0	3246	224	0
3	H	1347	0	1337	177	0
4	P	822	0	824	20	0
5	Q	698	0	697	209	0
6	R	690	0	655	176	0
7	C	3191	0	3206	292	0
8	G	1678	0	1708	526	0
9	O	6020	0	6008	1377	0
10	B	3624	0	3599	793	0
11	R	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24672	0	24664	3143	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 64.

The worst 5 of 3143 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)
6:R:35:TRP:CE3	9:O:514:ALA:HB1	1.16	1.66
9:O:163:LEU:HD13	9:O:185:ILE:CD1	1.20	1.63
9:O:155:LEU:CD1	9:O:187:SER:HB3	1.25	1.60
1:A:495:VAL:HG12	7:C:169:ILE:CD1	1.18	1.60
9:O:456:ALA:CB	10:B:188:LEU:HD12	1.18	1.59

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	415/491 (84%)	381 (92%)	34 (8%)	0	100	100
2	D	402/406 (99%)	387 (96%)	15 (4%)	0	100	100
3	H	165/199 (83%)	154 (93%)	10 (6%)	1 (1%)	25	66
4	P	102/104 (98%)	88 (86%)	14 (14%)	0	100	100
5	Q	84/112 (75%)	75 (89%)	9 (11%)	0	100	100
6	R	82/86 (95%)	64 (78%)	16 (20%)	2 (2%)	6	33
7	C	397/401 (99%)	360 (91%)	24 (6%)	13 (3%)	4	26
8	G	213/215 (99%)	184 (86%)	28 (13%)	1 (0%)	29	69
9	O	728/745 (98%)	671 (92%)	50 (7%)	7 (1%)	15	54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	B	439/443 (99%)	408 (93%)	25 (6%)	6 (1%)	11	46
All	All	3027/3202 (94%)	2772 (92%)	225 (7%)	30 (1%)	20	54

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	41	ASN
7	C	51	VAL
7	C	68	MET
9	O	27	LEU
10	B	30	VAL

### 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	365/429 (85%)	364 (100%)	1 (0%)	92	95
2	D	347/347 (100%)	344 (99%)	3 (1%)	78	88
3	H	140/166 (84%)	139 (99%)	1 (1%)	84	90
4	P	92/92 (100%)	92 (100%)	0	100	100
5	Q	79/96 (82%)	79 (100%)	0	100	100
6	R	73/75 (97%)	72 (99%)	1 (1%)	67	80
7	C	358/358 (100%)	351 (98%)	7 (2%)	55	74
8	G	184/184 (100%)	182 (99%)	2 (1%)	73	84
9	O	674/681 (99%)	664 (98%)	10 (2%)	65	80
10	B	405/405 (100%)	395 (98%)	10 (2%)	47	68
All	All	2717/2833 (96%)	2682 (99%)	35 (1%)	70	82

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	B	140	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	B	143	LYS
10	B	325	GLU
7	C	396	GLU
7	C	321	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
9	O	606	ASN
10	B	313	ASN
9	O	667	GLN
10	B	74	GLN
10	B	396	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	R	2
2	D	1
7	C	1
10	B	1
9	O	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	33:TRP	C	34:ALA	N	5.88
1	D	315:LEU	C	316:TYR	N	3.54
1	C	399:VAL	C	400:ASN	N	3.46
1	B	416:ARG	C	417:GLY	N	3.16
1	O	175:ASP	C	176:PRO	N	2.97



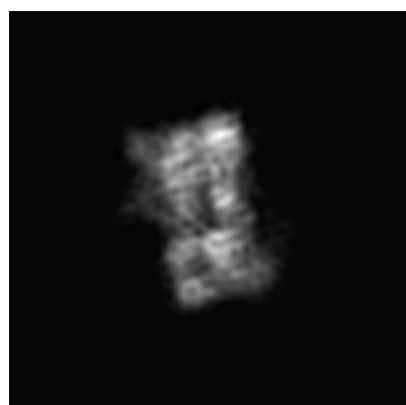
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4744. These allow visual inspection of the internal detail of the map and identification of artifacts.

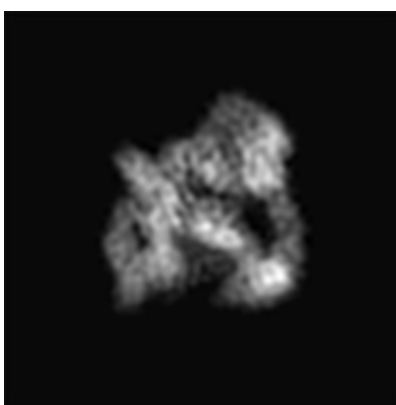
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

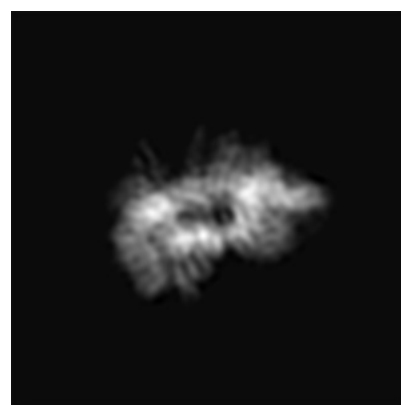
#### 6.1.1 Primary map



X



Y



Z

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

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

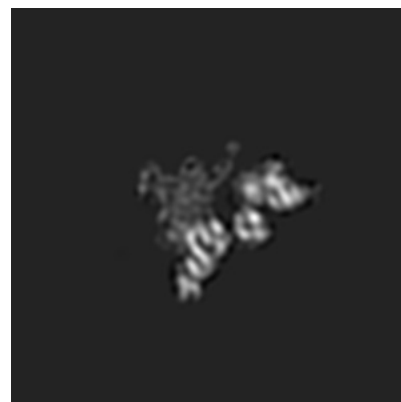
#### 6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 178



Y Index: 159



Z Index: 199

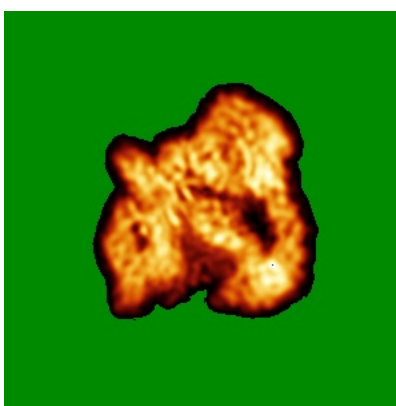
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

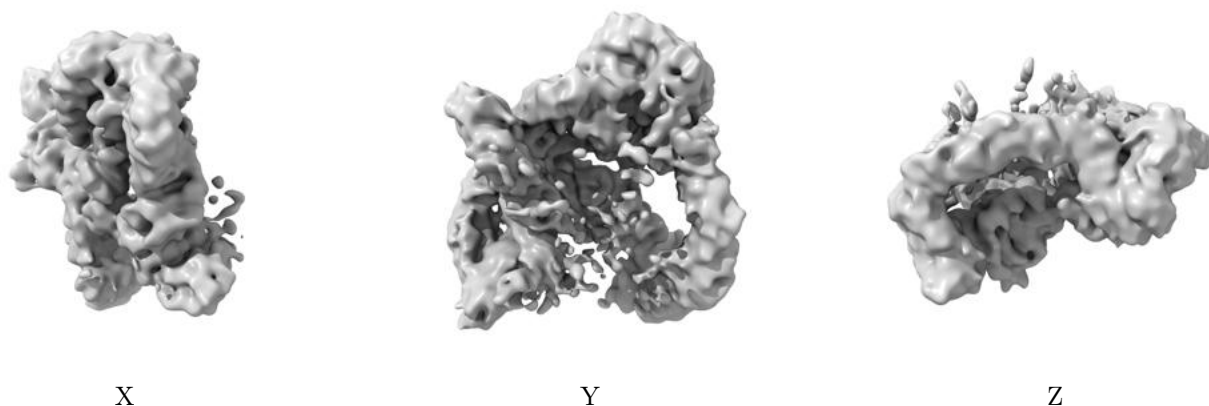


Z

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

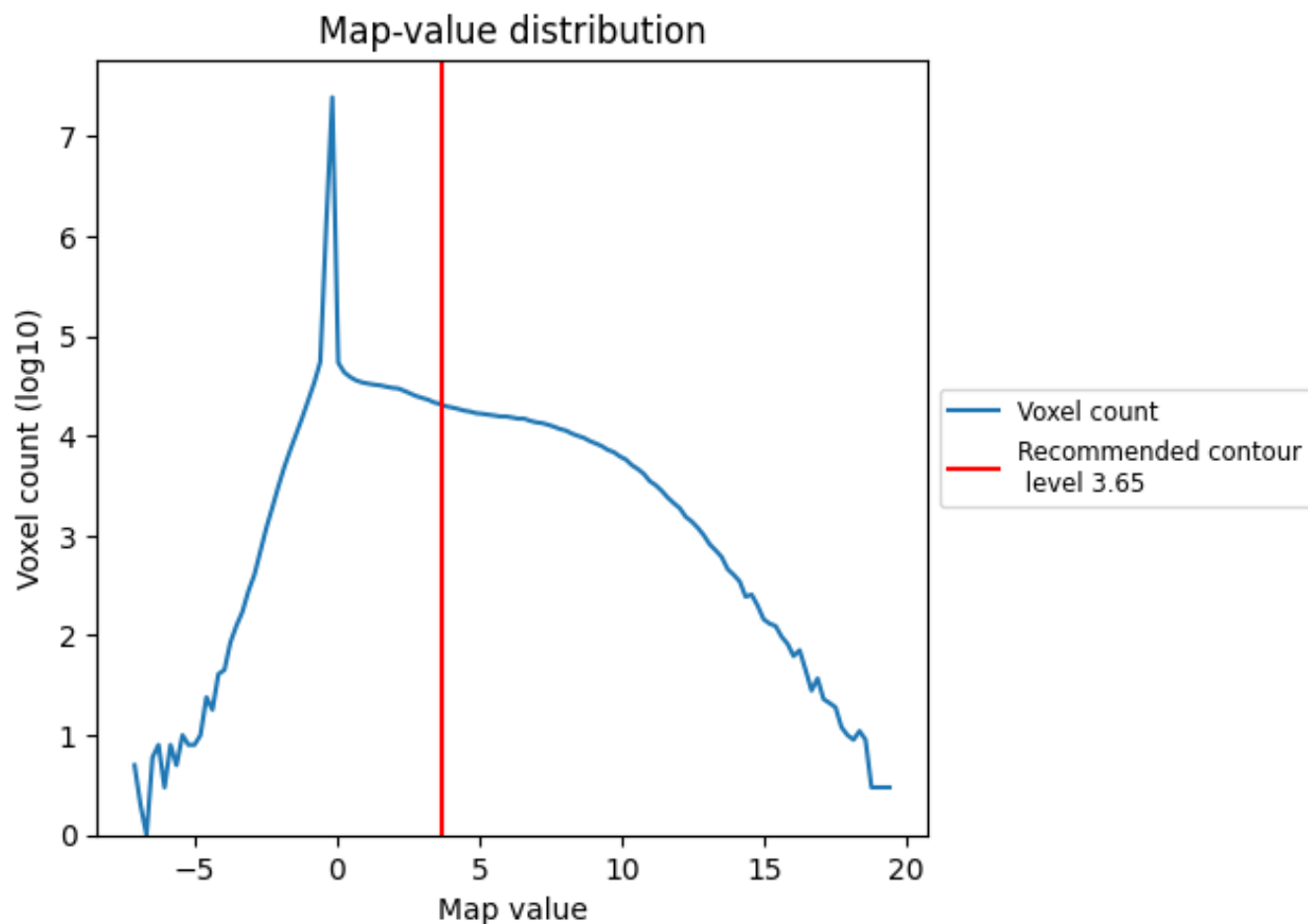
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

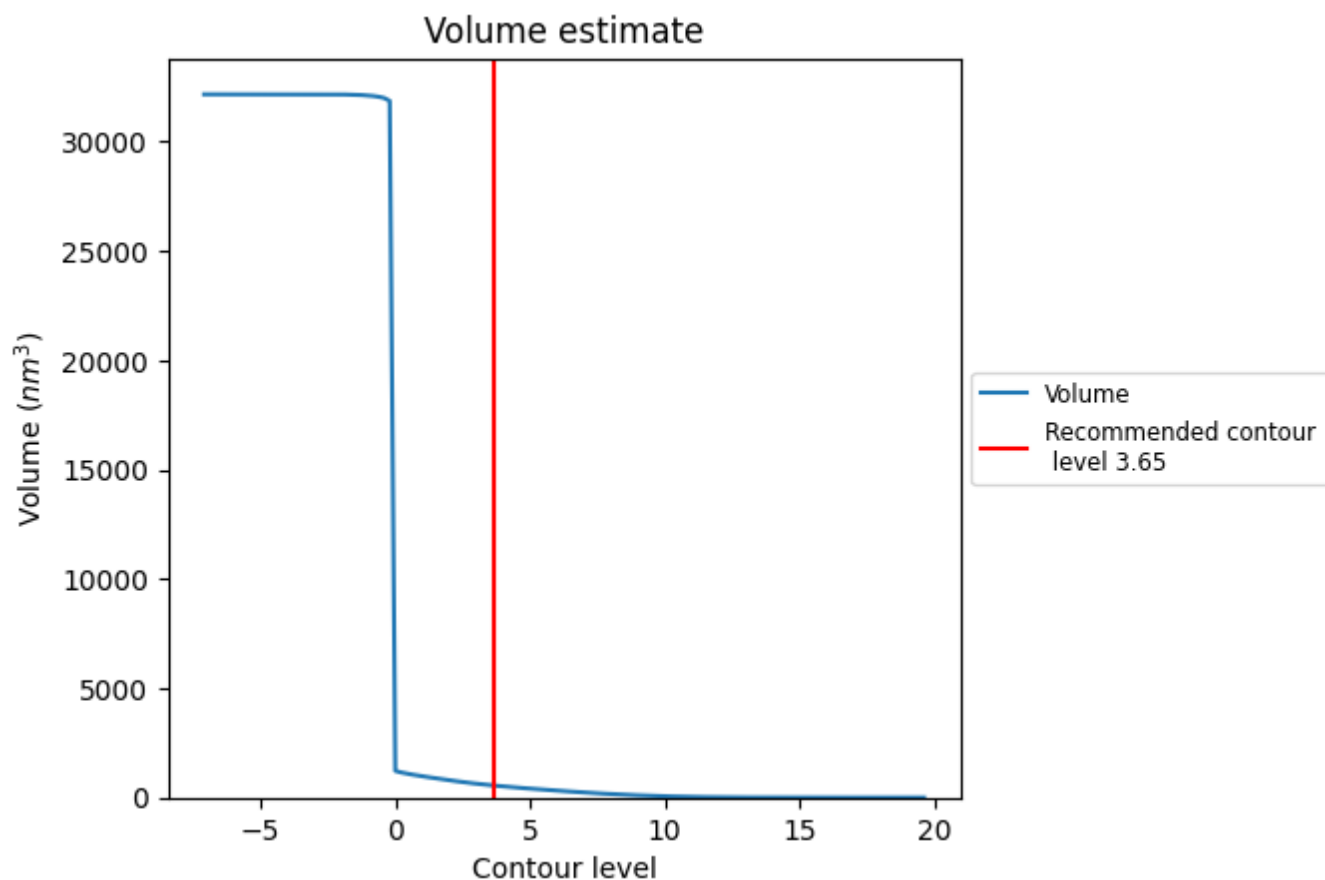
This section contains the results of statistical analysis of the map.

### 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.

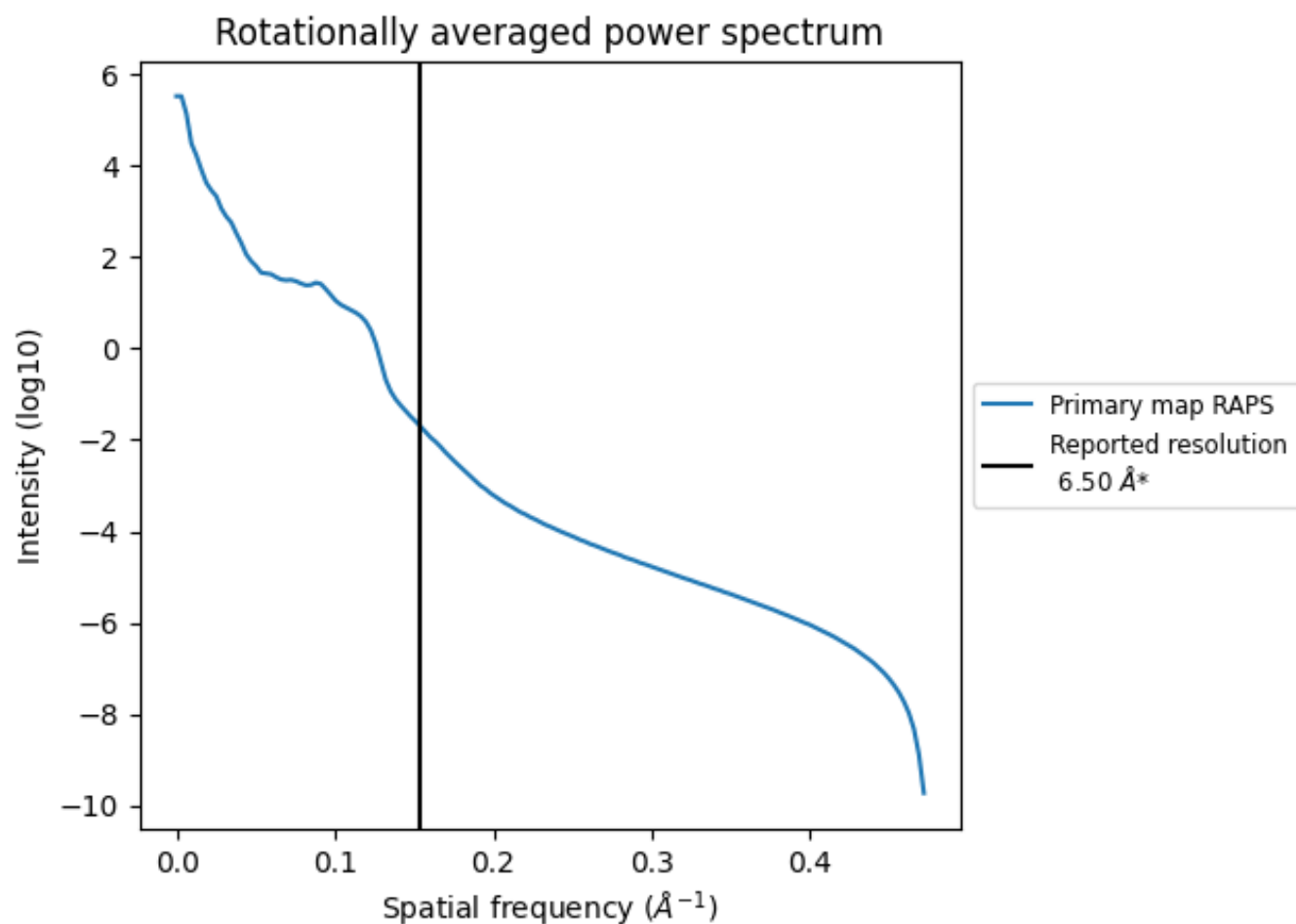
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 551 nm<sup>3</sup>; this corresponds to an approximate mass of 498 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 0.154 Å<sup>-1</sup>

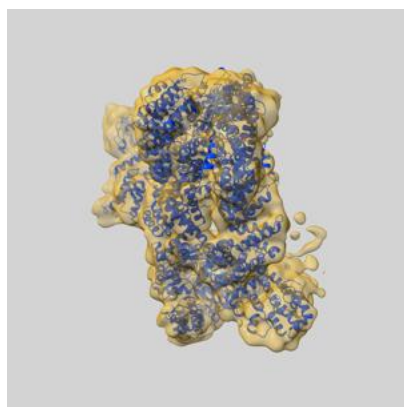
## 8 Fourier-Shell correlation

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

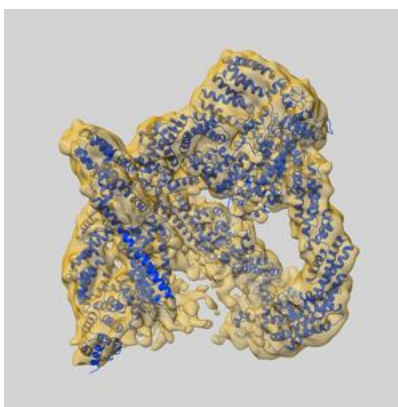
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4744 and PDB model 6R7N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

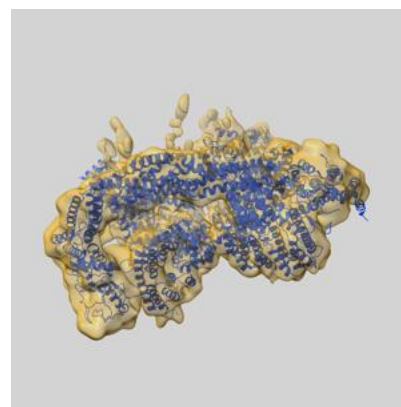
### 9.1 Map-model overlay [i](#)



X



Y

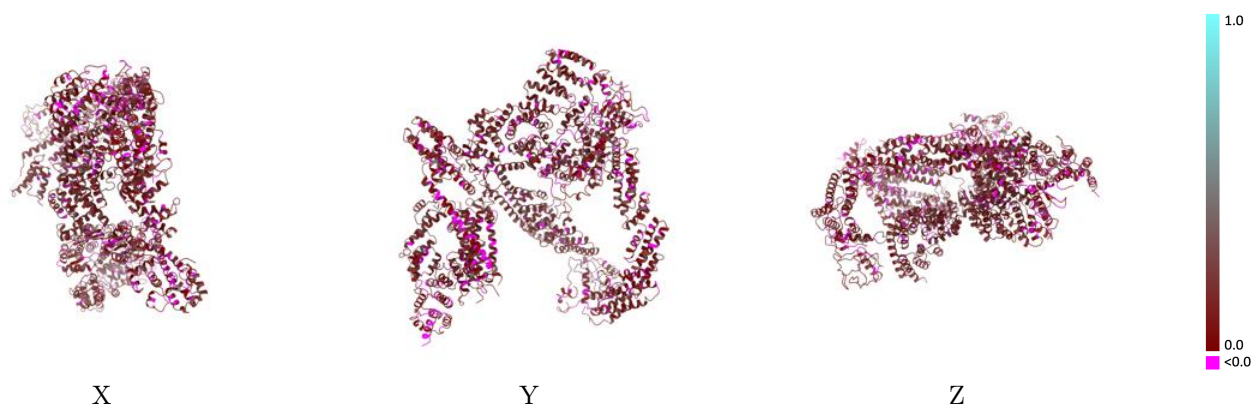


Z

The images above show the 3D surface view of the map at the recommended contour level 3.65 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.

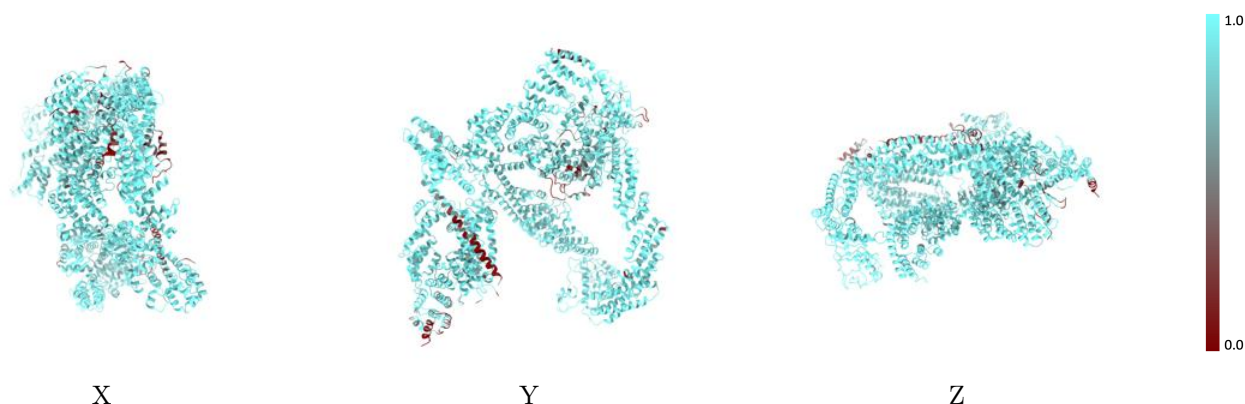


## 9.2 Q-score mapped to coordinate model [i](#)



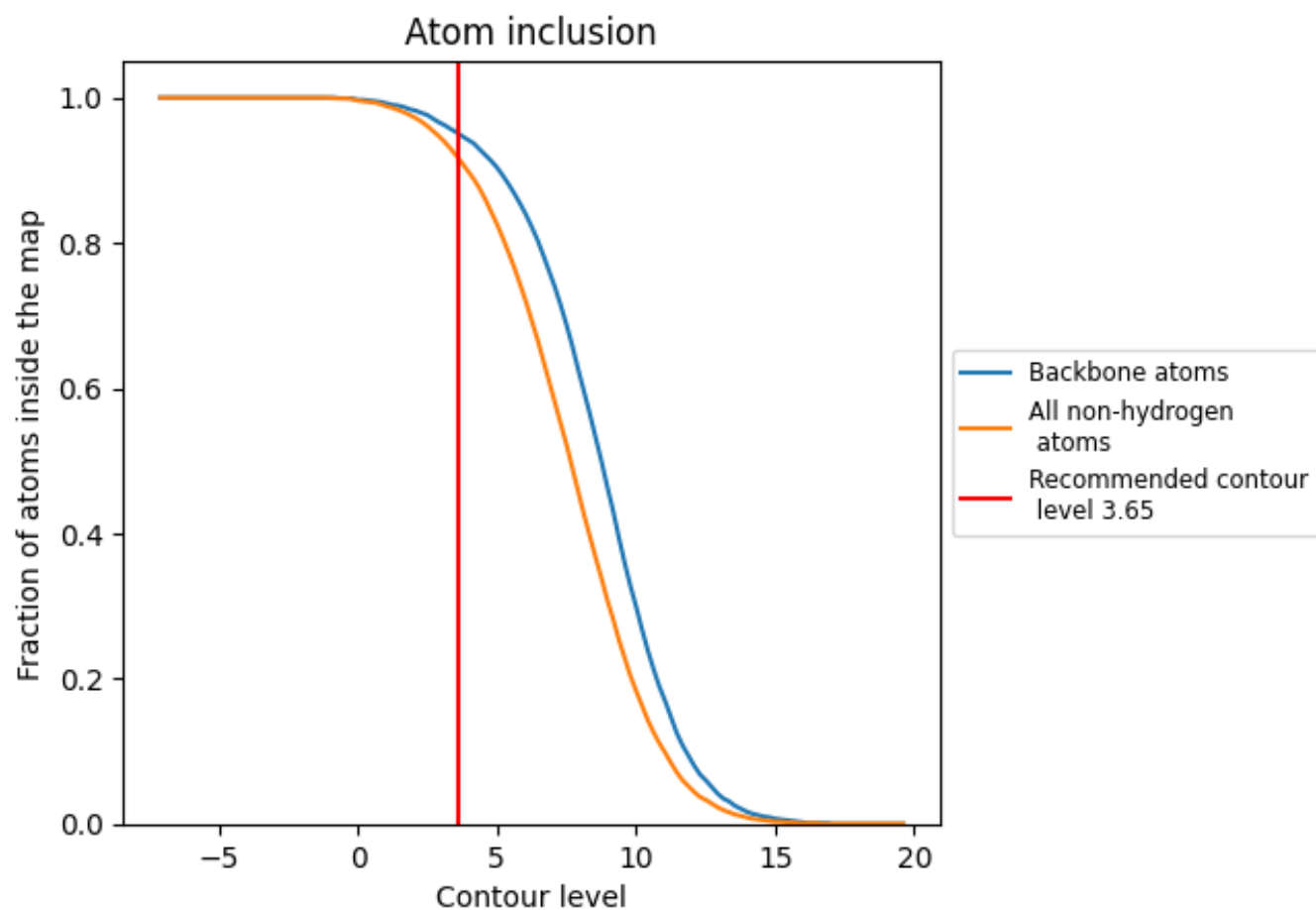
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.65).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (3.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.1360
A	 0.9570	 0.1650
B	 0.9350	 0.1500
C	 0.8650	 0.0990
D	 0.9500	 0.1570
G	 0.8050	 0.0980
H	 0.9840	 0.1510
O	 0.8880	 0.1310
P	 0.9950	 0.1410
Q	 0.9800	 0.1290
R	 0.9000	 0.0980

