



## wwPDB EM Validation Summary Report ⓘ

Feb 25, 2024 – 04:51 PM EST

PDB ID : 5KHU  
EMDB ID : EMD-4021  
Title : Model of human Anaphase-promoting complex/Cyclosome (APC15 deletion mutant), in complex with the Mitotic checkpoint complex (APC/C-CDC20-MCC) based on cryo EM data at 4.8 Angstrom resolution  
Authors : Yamaguchi, M.; VanderLinden, R.; Dube, P.; Stark, H.; Schulman, B.  
Deposited on : 2016-06-15  
Resolution : 4.80 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.dev70  
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

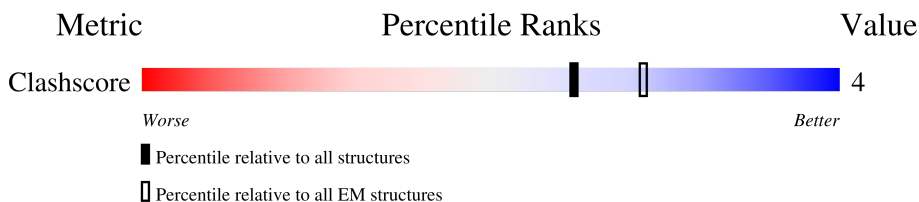
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


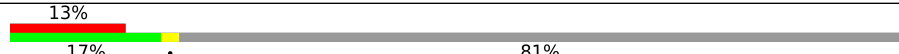

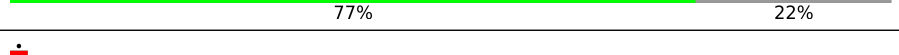


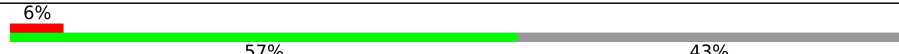



The reported resolution of this entry is 4.80 Å.

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.








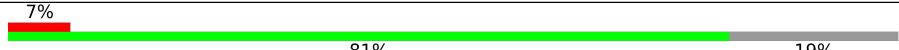
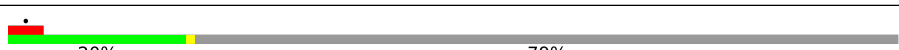
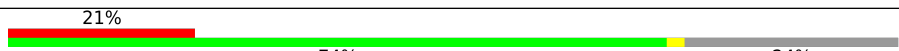
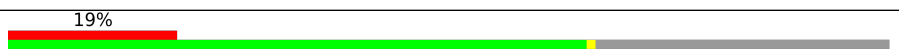

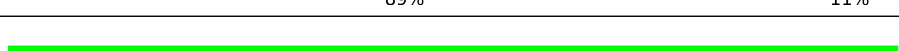
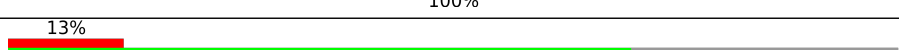
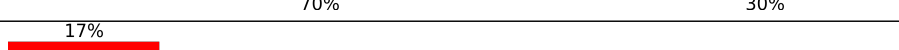
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297

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	1944	 70% 29%
2	B	84	 17% 81% 13%
3	C	597	 77% 22% 6%
3	P	597	 74% 26% 6%
4	E	110	 10% 51% 49%
5	F	824	 6% 57% 43%
5	H	824	 58% 42% 6%
6	G	85	 29% 71%
6	W	85	 29% 71%
7	I	808	 16% 87% 13%

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Mol	Chain	Length	Quality of chain
8	J	620	 81% 19%
8	K	620	 80% 20%
9	L	185	 89% 9% 6%
10	M	74	 58% 42% 7%
11	N	822	 74% 24% 30%
12	O	755	 81% 19% 7%
13	Q	1050	 79% 20% 20%
14	R	499	 74% 24% 21%
14	S	499	 65% 33% 19%
15	T	205	 89% 11% 49%
16	U	9	 100%
17	X	565	 70% 30% 13%
17	Y	565	 76% 24% 17%

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 8453 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	1374	Total C 1374 1374	0	1374

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLU	SER	engineered mutation	UNP Q9H1A4
A	286	GLU	SER	engineered mutation	UNP Q9H1A4
A	291	GLU	THR	engineered mutation	UNP Q9H1A4
A	313	GLU	SER	engineered mutation	UNP Q9H1A4
A	316	GLU	THR	engineered mutation	UNP Q9H1A4
A	317	GLU	SER	engineered mutation	UNP Q9H1A4
A	334	GLU	SER	engineered mutation	UNP Q9H1A4
A	341	GLU	SER	engineered mutation	UNP Q9H1A4
A	343	GLU	SER	engineered mutation	UNP Q9H1A4
A	355	GLU	SER	engineered mutation	UNP Q9H1A4
A	362	GLU	SER	engineered mutation	UNP Q9H1A4
A	372	GLU	SER	engineered mutation	UNP Q9H1A4
A	377	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	THR	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	671	GLN	ASN	conflict	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	?	GLU	SER	engineered mutation	UNP Q9H1A4
A	916	GLU	SER	engineered mutation	UNP Q9H1A4
A	1347	GLU	SER	engineered mutation	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B	16	Total C 16 16	0	16

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	C	463	Total C 463 463	0	463
3	P	442	Total C 442 442	0	442

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLU	THR	engineered mutation	UNP Q9UJX2
C	562	GLU	THR	engineered mutation	UNP Q9UJX2
C	582	GLU	THR	engineered mutation	UNP Q9UJX2
C	588	GLU	SER	engineered mutation	UNP Q9UJX2
C	596	GLU	THR	engineered mutation	UNP Q9UJX2
P	542	GLU	THR	engineered mutation	UNP Q9UJX2
P	562	GLU	THR	engineered mutation	UNP Q9UJX2
P	582	GLU	THR	engineered mutation	UNP Q9UJX2
P	588	GLU	SER	engineered mutation	UNP Q9UJX2
P	596	GLU	THR	engineered mutation	UNP Q9UJX2

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	E	56	Total C 56 56	0	56

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	F	473	Total C 473 473	0	473
5	H	479	Total C 479 479	0	479

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	200	GLU	THR	engineered mutation	UNP P30260
F	205	GLU	THR	engineered mutation	UNP P30260
F	220	GLU	SER	engineered mutation	UNP P30260
F	241	GLU	SER	engineered mutation	UNP P30260
F	276	GLU	SER	engineered mutation	UNP P30260
F	320	GLU	SER	engineered mutation	UNP P30260
F	336	GLU	SER	engineered mutation	UNP P30260
F	339	GLU	SER	engineered mutation	UNP P30260
F	386	GLU	SER	engineered mutation	UNP P30260
F	387	GLU	SER	engineered mutation	UNP P30260
F	393	GLU	SER	engineered mutation	UNP P30260
F	426	GLU	SER	engineered mutation	UNP P30260
F	435	GLU	SER	engineered mutation	UNP P30260
F	446	GLU	THR	engineered mutation	UNP P30260
H	200	GLU	THR	engineered mutation	UNP P30260
H	205	GLU	THR	engineered mutation	UNP P30260
H	220	GLU	SER	engineered mutation	UNP P30260
H	241	GLU	SER	engineered mutation	UNP P30260
H	276	GLU	SER	engineered mutation	UNP P30260
H	320	GLU	SER	engineered mutation	UNP P30260
H	336	GLU	SER	engineered mutation	UNP P30260
H	339	GLU	SER	engineered mutation	UNP P30260
H	386	GLU	SER	engineered mutation	UNP P30260
H	387	GLU	SER	engineered mutation	UNP P30260
H	393	GLU	SER	engineered mutation	UNP P30260
H	426	GLU	SER	engineered mutation	UNP P30260
H	435	GLU	SER	engineered mutation	UNP P30260
H	446	GLU	THR	engineered mutation	UNP P30260

- Molecule 6 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	G	25	Total C 25 25	0	25
6	W	25	Total C 25 25	0	25

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	GLU	SER	engineered mutation	UNP Q8NHZ8
G	52	GLU	SER	engineered mutation	UNP Q8NHZ8
G	82	GLU	SER	engineered mutation	UNP Q8NHZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	51	GLU	SER	engineered mutation	UNP Q8NHZ8
W	52	GLU	SER	engineered mutation	UNP Q8NHZ8
W	82	GLU	SER	engineered mutation	UNP Q8NHZ8

- Molecule 7 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	I	706	Total C 706 706	0	706

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	777	GLU	SER	engineered mutation	UNP Q9UJX5
I	779	GLU	SER	engineered mutation	UNP Q9UJX5

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	J	504	Total C 504 504	0	504
8	K	493	Total C 493 493	0	493

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	112	GLU	SER	engineered mutation	UNP Q13042
J	560	GLU	SER	engineered mutation	UNP Q13042
J	581	GLU	THR	engineered mutation	UNP Q13042
J	585	GLU	THR	engineered mutation	UNP Q13042
J	586	GLU	SER	engineered mutation	UNP Q13042
K	112	GLU	SER	engineered mutation	UNP Q13042
K	560	GLU	SER	engineered mutation	UNP Q13042
K	581	GLU	THR	engineered mutation	UNP Q13042
K	585	GLU	THR	engineered mutation	UNP Q13042
K	586	GLU	SER	engineered mutation	UNP Q13042

- Molecule 9 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	L	169	Total C 169 169	0	169

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLU	THR	engineered mutation	UNP Q9UM13

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	M	43	Total C 43 43	0	43

- Molecule 11 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	N	627	Total C 627 627	0	627

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	218	GLU	SER	engineered mutation	UNP Q9UJX6
N	314	GLU	SER	engineered mutation	UNP Q9UJX6
N	470	GLU	SER	engineered mutation	UNP Q9UJX6
N	534	GLU	SER	engineered mutation	UNP Q9UJX6
N	811	GLU	SER	engineered mutation	UNP Q9UJX6

- Molecule 12 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	O	608	Total C 608 608	0	608

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	178	GLU	THR	engineered mutation	UNP Q9UJX4
O	179	GLU	SER	engineered mutation	UNP Q9UJX4
O	195	GLU	SER	engineered mutation	UNP Q9UJX4
O	202	GLU	SER	engineered mutation	UNP Q9UJX4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	221	GLU	SER	engineered mutation	UNP Q9UJX4
O	232	GLU	THR	engineered mutation	UNP Q9UJX4
O	364	GLU	SER	engineered mutation	UNP Q9UJX4

- Molecule 13 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	Q	219	Total C 219 219	0	219

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	367	GLU	SER	engineered mutation	UNP O60566
Q	435	GLU	SER	engineered mutation	UNP O60566
Q	543	GLU	SER	engineered mutation	UNP O60566
Q	600	GLU	THR	engineered mutation	UNP O60566
Q	665	GLU	SER	engineered mutation	UNP O60566
Q	670	GLU	SER	engineered mutation	UNP O60566
Q	720	GLU	SER	engineered mutation	UNP O60566
Q	1043	GLU	SER	engineered mutation	UNP O60566

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	R	378	Total C 378 378	0	378
14	S	333	Total C 333 333	0	333

- Molecule 15 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	T	183	Total C 183 183	0	183

- Molecule 16 is a protein called unknown.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	U	9	Total C 9 9	0	9

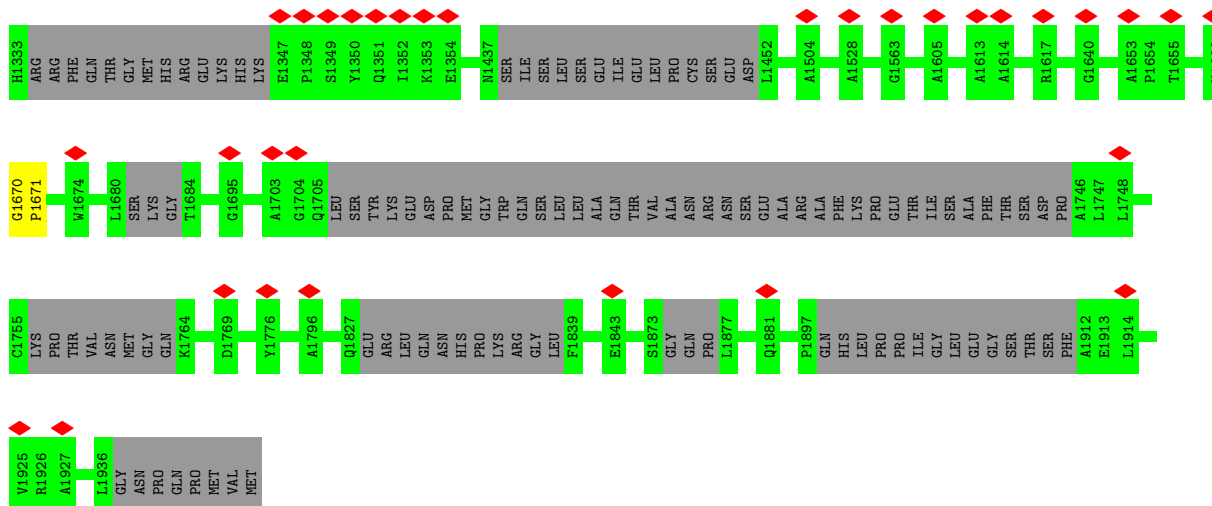
- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	X	396	Total C 396 396	0	396
17	Y	432	Total C 432 432	0	432

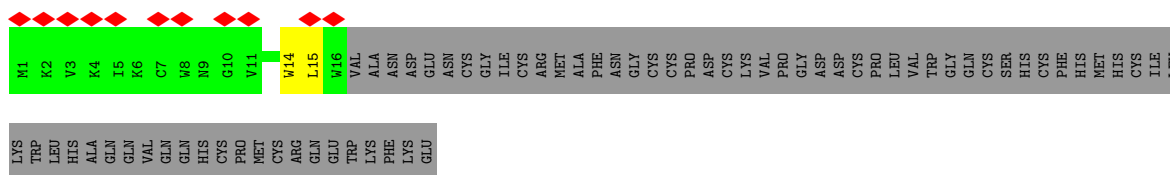
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	119	GLU	SER	engineered mutation	UNP Q9UJX3
X	120	GLU	THR	engineered mutation	UNP Q9UJX3
X	123	GLU	SER	engineered mutation	UNP Q9UJX3
X	125	GLU	SER	engineered mutation	UNP Q9UJX3
X	126	GLU	THR	engineered mutation	UNP Q9UJX3
Y	119	GLU	SER	engineered mutation	UNP Q9UJX3
Y	120	GLU	THR	engineered mutation	UNP Q9UJX3
Y	123	GLU	SER	engineered mutation	UNP Q9UJX3
Y	125	GLU	SER	engineered mutation	UNP Q9UJX3
Y	126	GLU	THR	engineered mutation	UNP Q9UJX3

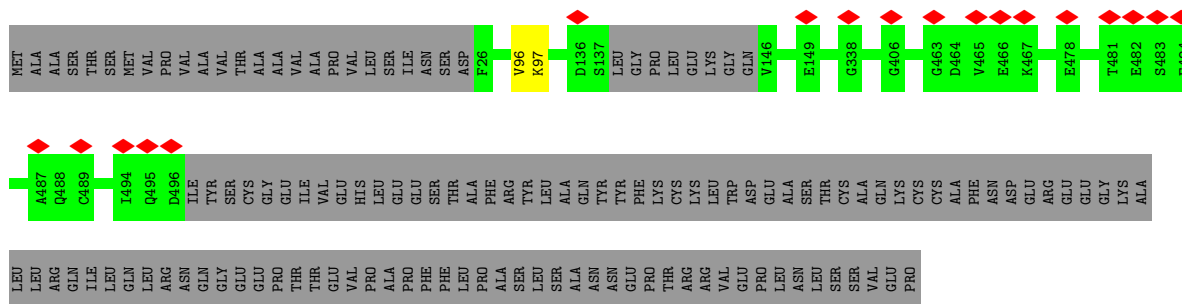
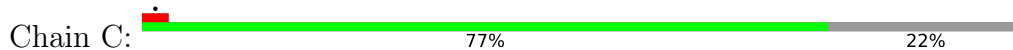




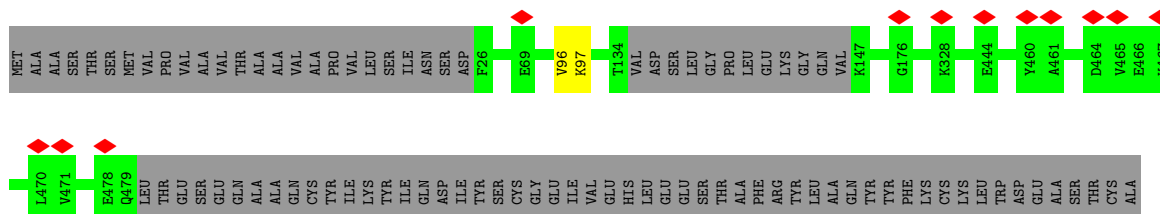
- Molecule 2: Anaphase-promoting complex subunit 11



- Molecule 3: Cell division cycle protein 23 homolog



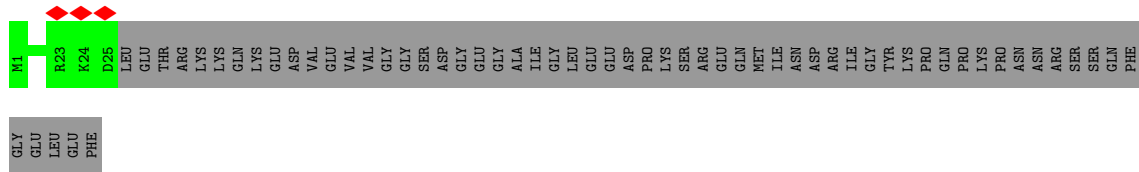
- Molecule 3: Cell division cycle protein 23 homolog



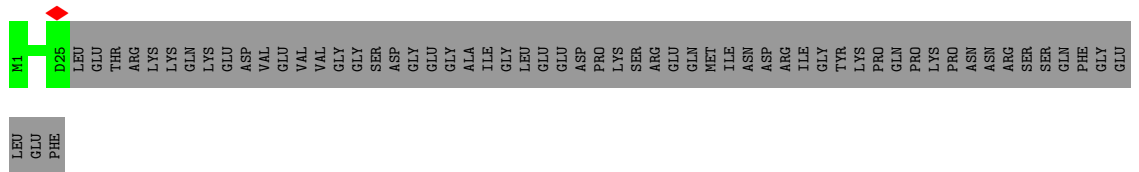




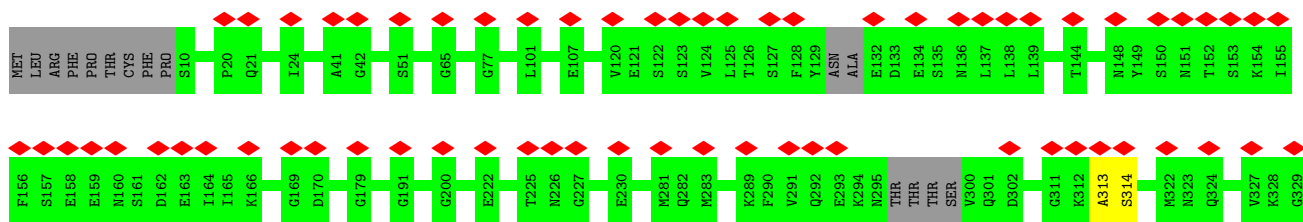
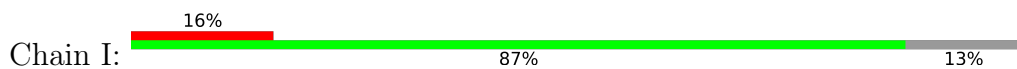
• Molecule 6: Anaphase-promoting complex subunit CDC26



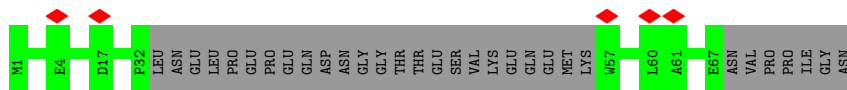
• Molecule 6: Anaphase-promoting complex subunit CDC26



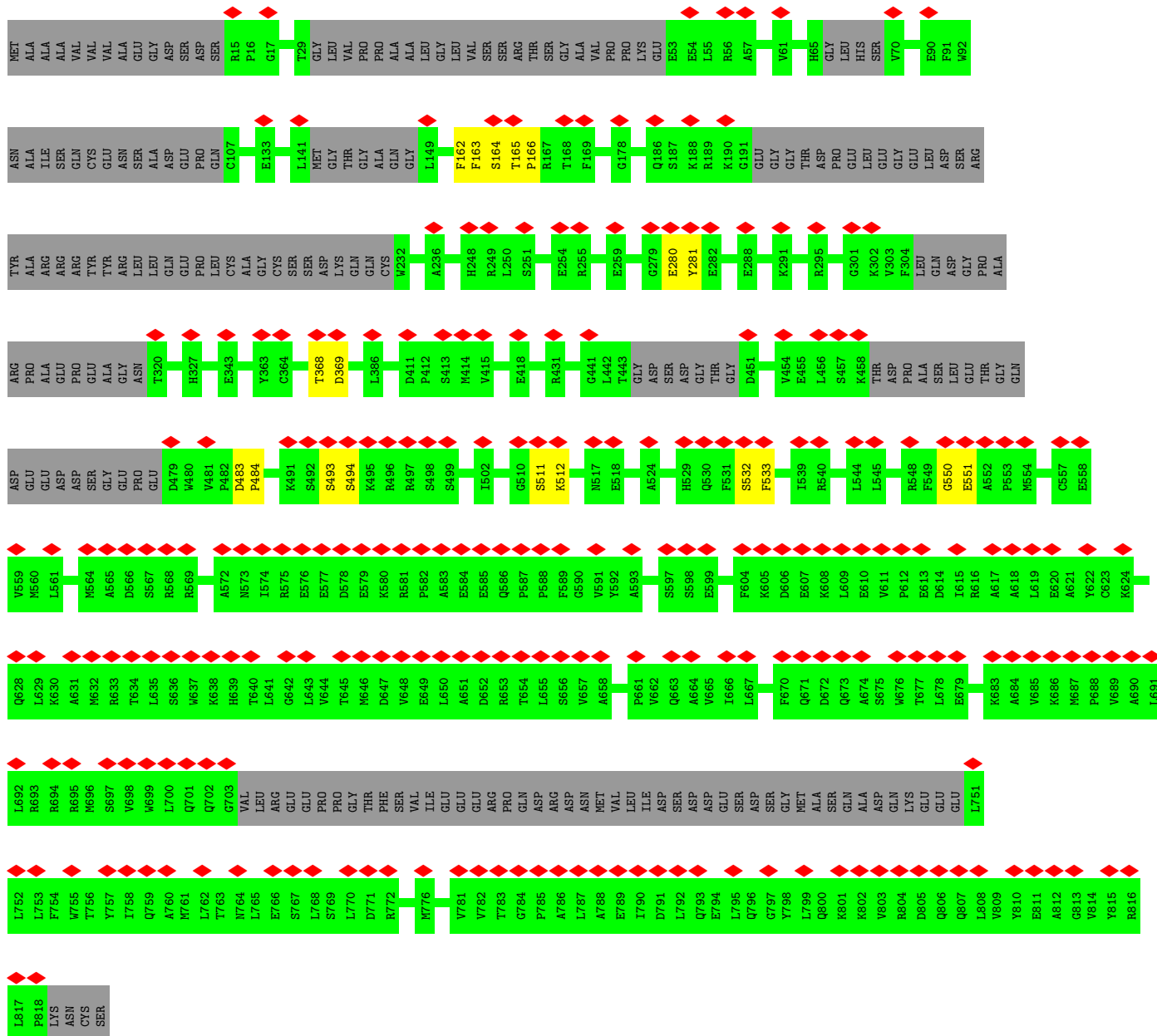
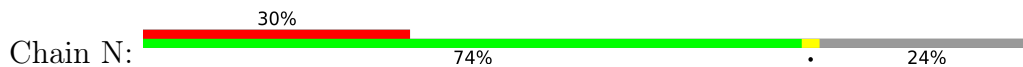
• Molecule 7: Anaphase-promoting complex subunit 4



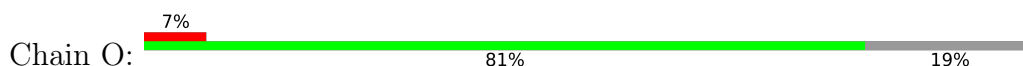




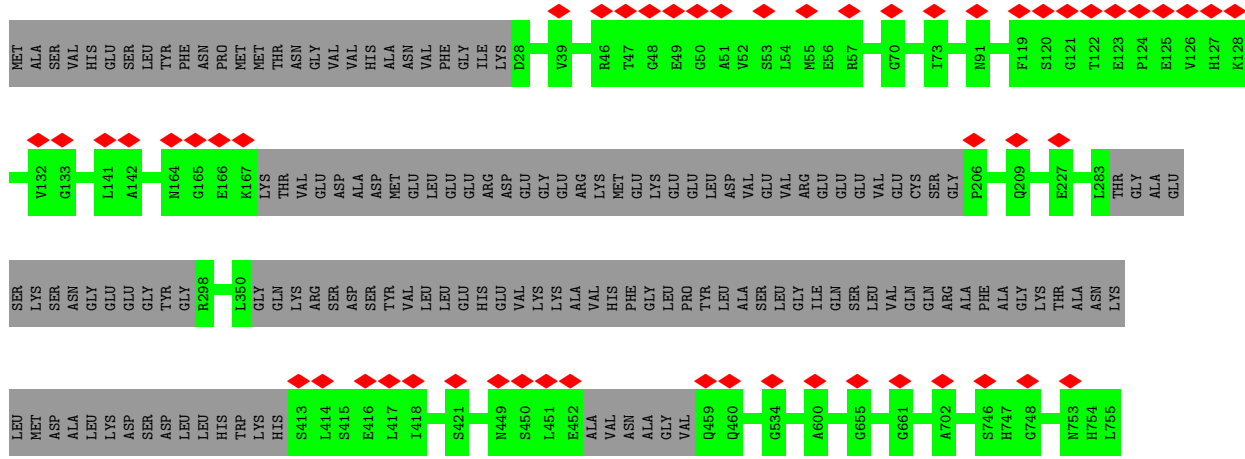
• Molecule 11: Anaphase-promoting complex subunit 2



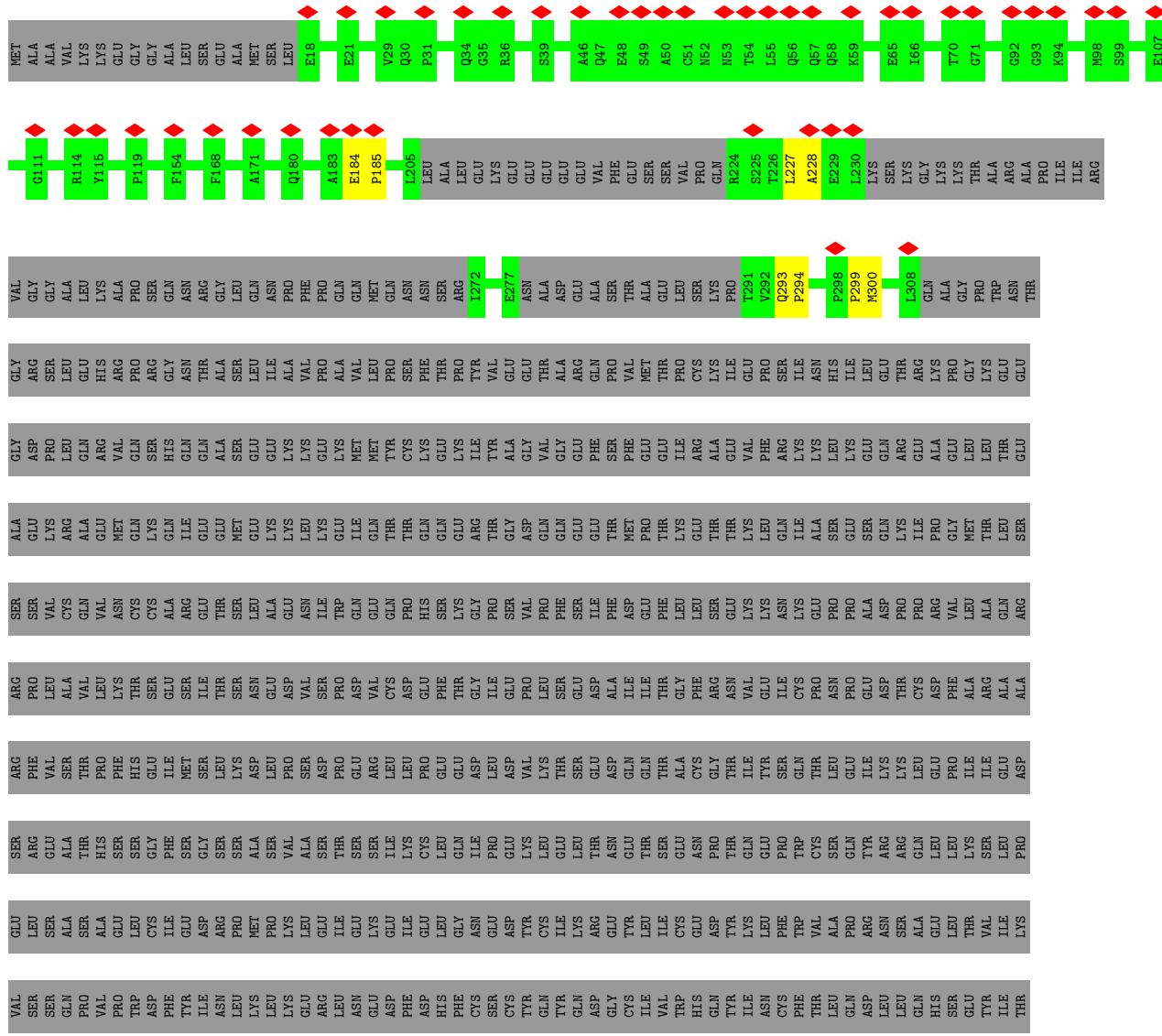
• Molecule 12: Anaphase-promoting complex subunit 5





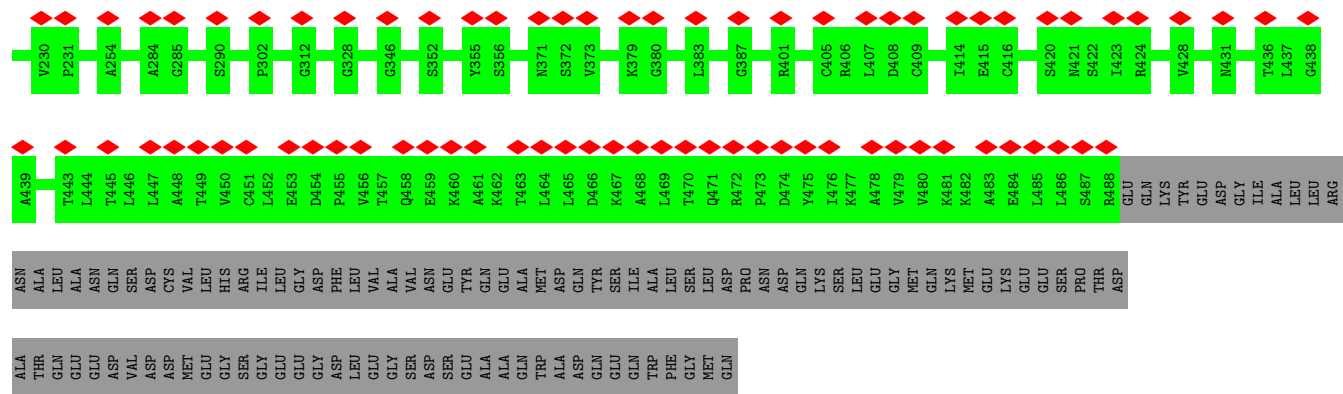


• Molecule 13: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	268851	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.480	Depositor
Minimum map value	-0.255	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.072	Depositor
Map size (Å)	406.4, 406.4, 406.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

## 5 Model quality

### 5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	1374	0	0	6	0
2	B	16	0	0	1	0
3	C	463	0	0	1	0
3	P	442	0	0	1	0
4	E	56	0	0	0	0
5	F	473	0	0	1	0
5	H	479	0	0	0	0
6	G	25	0	0	0	0
6	W	25	0	0	0	0
7	I	706	0	0	2	0
8	J	504	0	0	0	0
8	K	493	0	0	0	0
9	L	169	0	0	2	0
10	M	43	0	0	0	0
11	N	627	0	0	10	0
12	O	608	0	0	0	0
13	Q	219	0	0	4	0
14	R	378	0	0	6	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	333	0	0	4	0
15	T	183	0	0	0	0
16	U	9	0	0	0	0
17	X	396	0	0	0	0
17	Y	432	0	0	0	0
All	All	8453	0	0	38	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 4.

The worst 5 of 38 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)
14:R:97:LYS:CA	14:R:98:GLU:CA	2.65	0.74
14:R:420:PHE:CA	14:R:421:ALA:CA	2.75	0.65
14:R:99:ASN:CA	14:R:100:GLN:CA	2.77	0.62
11:N:164:SER:CA	11:N:165:THR:CA	2.78	0.60
11:N:280:GLU:CA	11:N:281:TYR:CA	2.82	0.57

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

There are no ligands in this entry.

## 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.



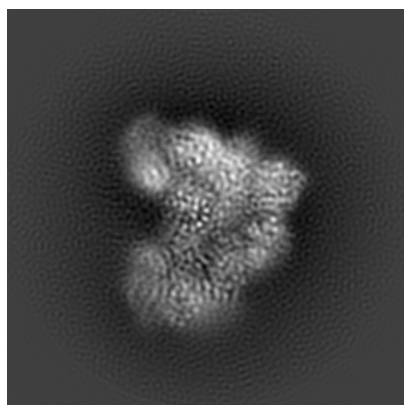
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4021. These allow visual inspection of the internal detail of the map and identification of artifacts.

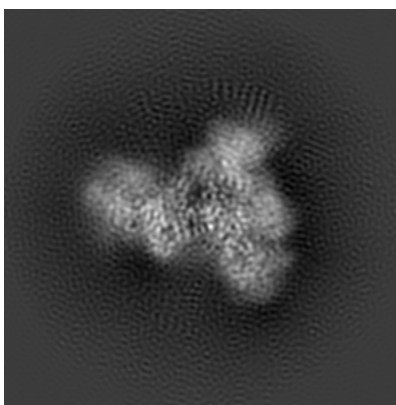
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

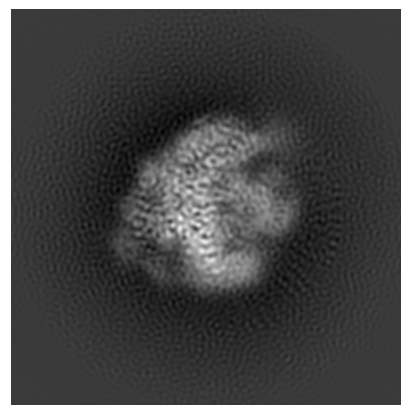
#### 6.1.1 Primary map



X



Y

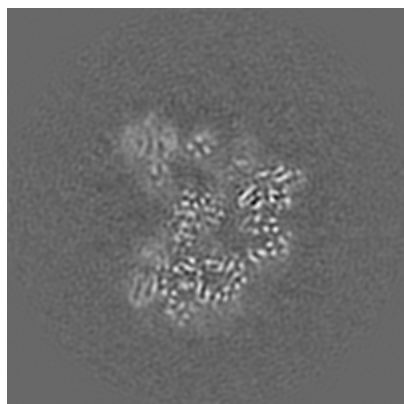


Z

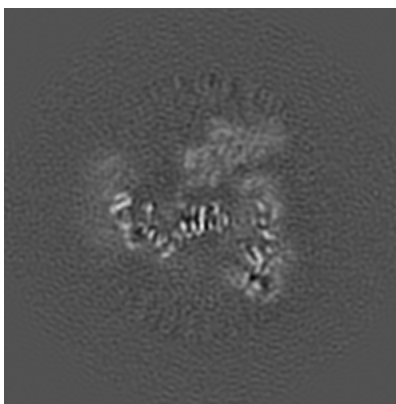
The images above show the map projected in three orthogonal directions.

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

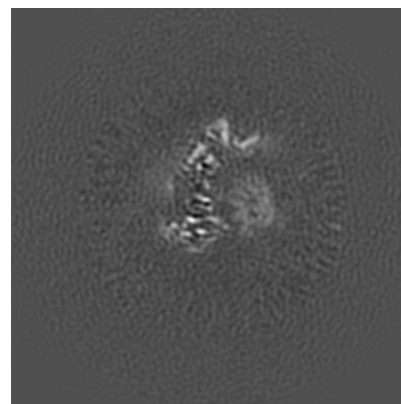
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

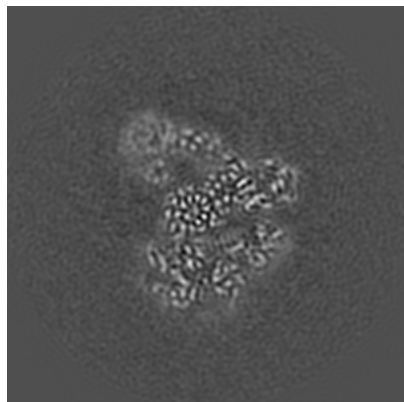


Z Index: 160

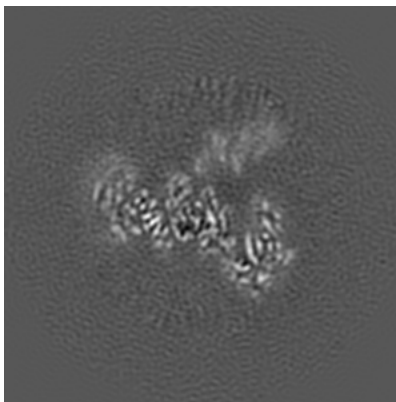
The images above show central slices of the map in three orthogonal directions.

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

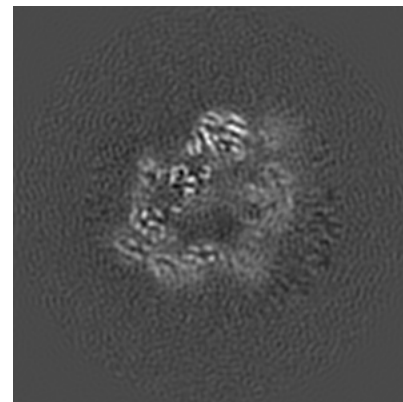
### 6.3.1 Primary map



X Index: 151



Y Index: 146

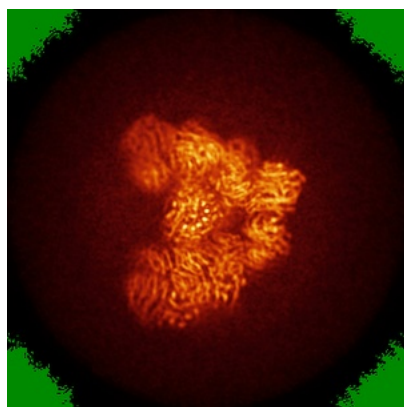


Z Index: 188

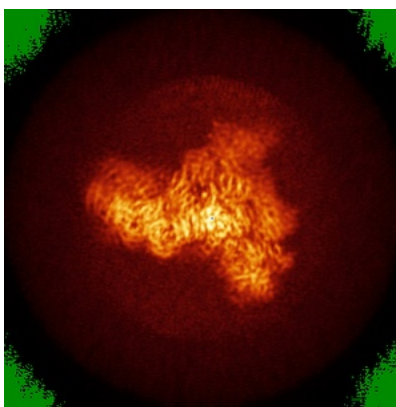
The images above show the largest variance slices of the map in three orthogonal directions.

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

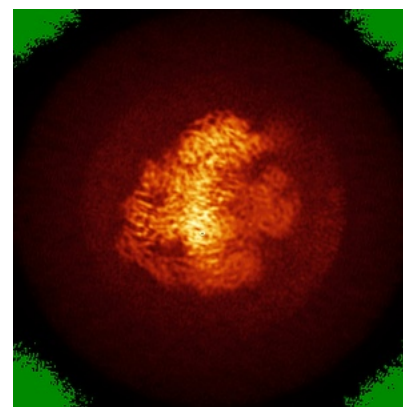
### 6.4.1 Primary map



X



Y

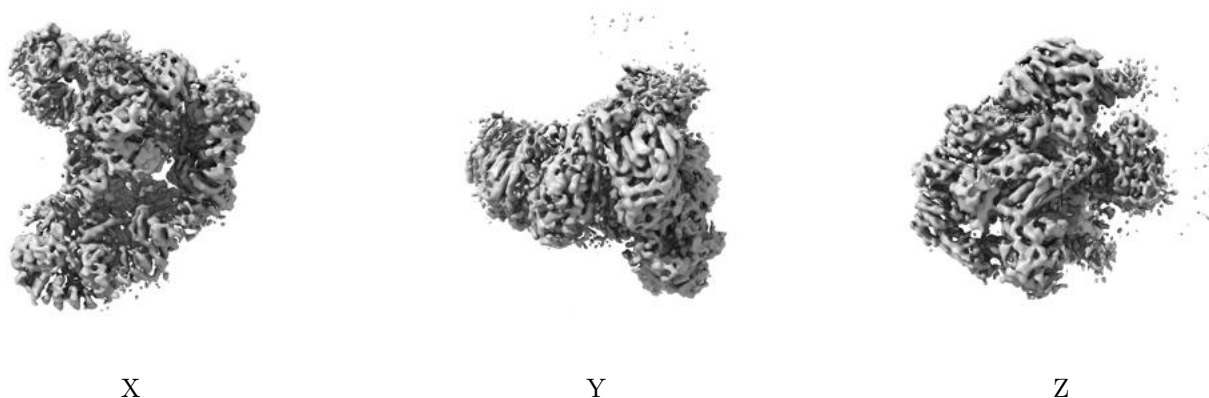


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

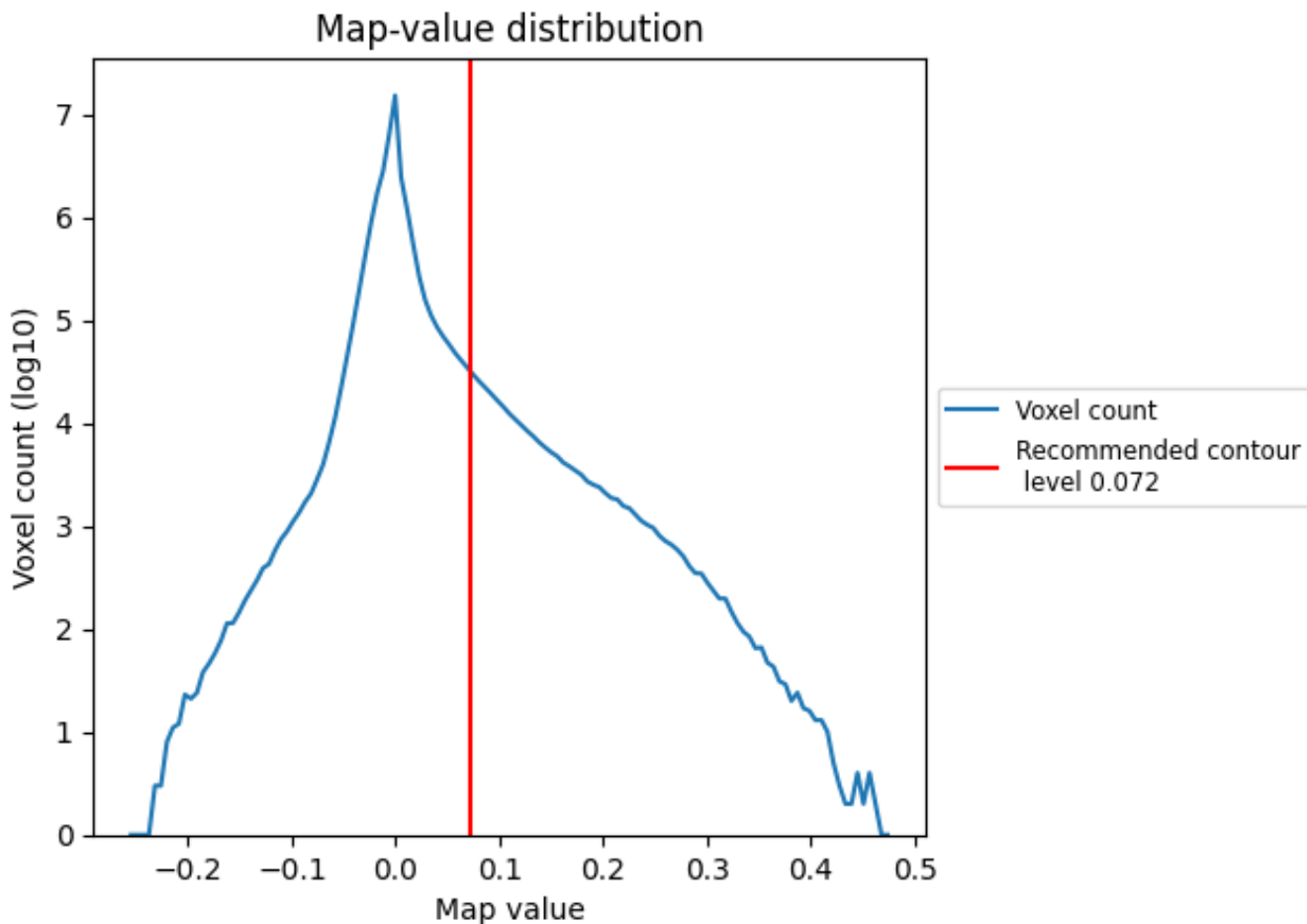
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

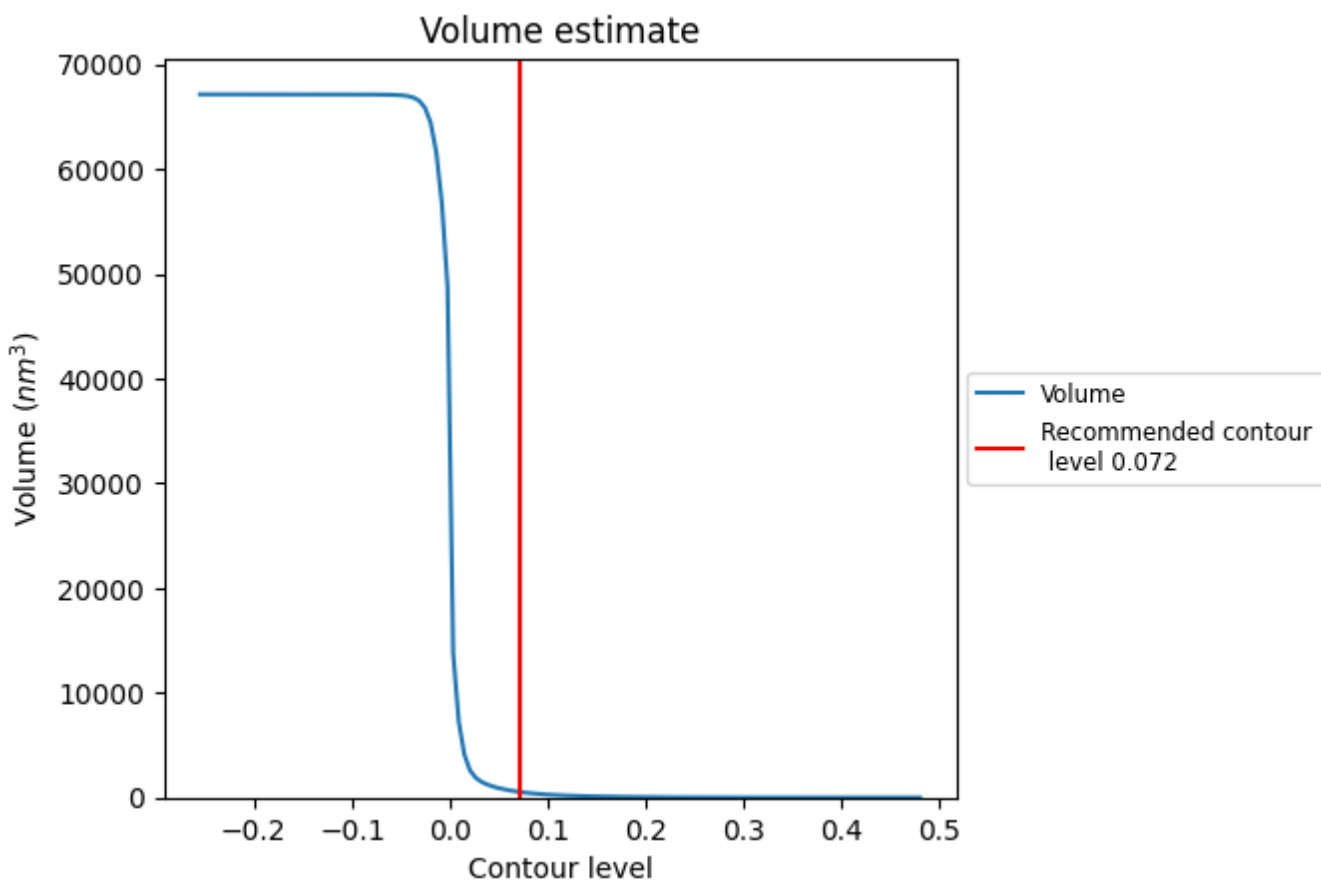
This section contains the results of statistical analysis of the map.

### 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.

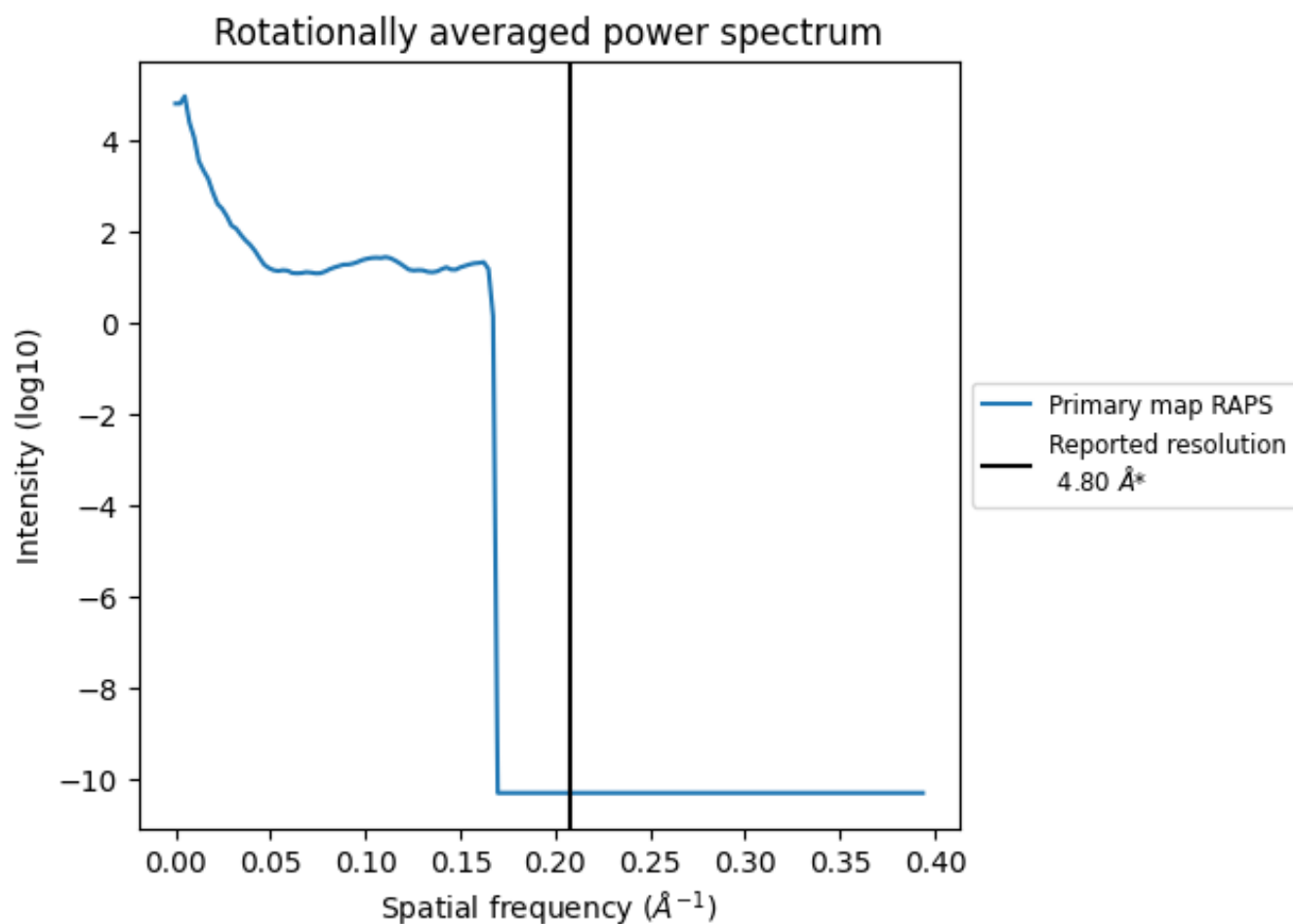
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 525 nm<sup>3</sup>; this corresponds to an approximate mass of 474 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  $0.208 \text{\AA}^{-1}$

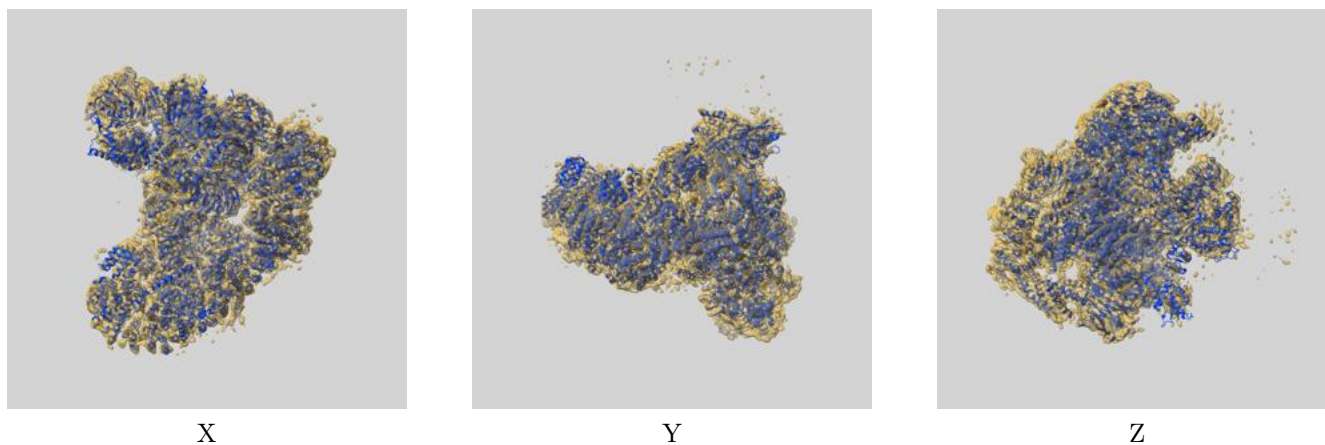
## 8 Fourier-Shell correlation

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-4021 and PDB model 5KHU. Per-residue inclusion information can be found in section [3](#) on page [11](#).

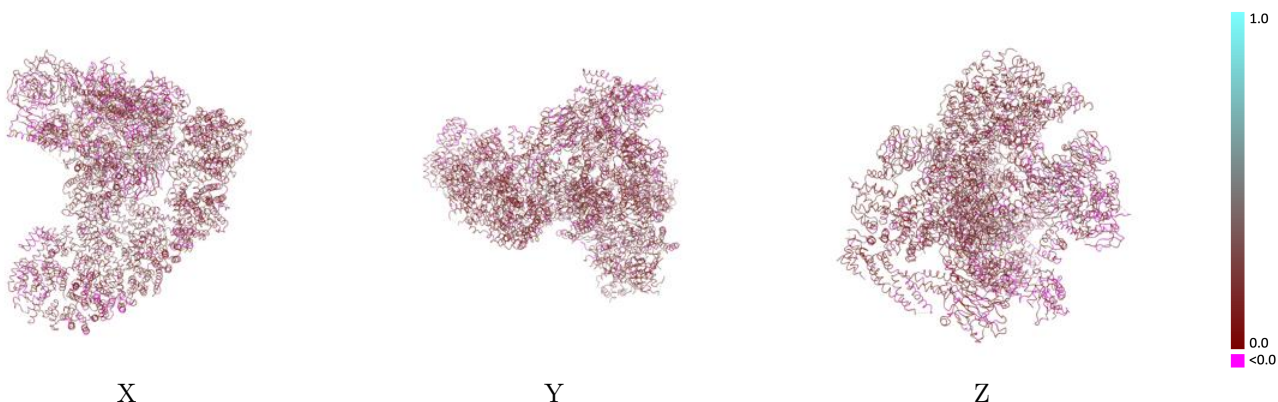
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.072 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.

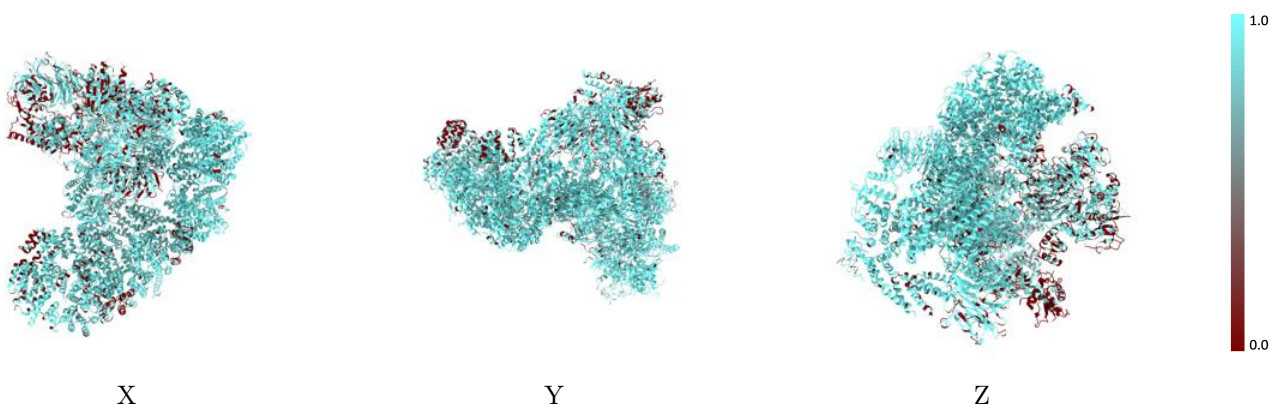


## 9.2 Q-score mapped to coordinate model [i](#)



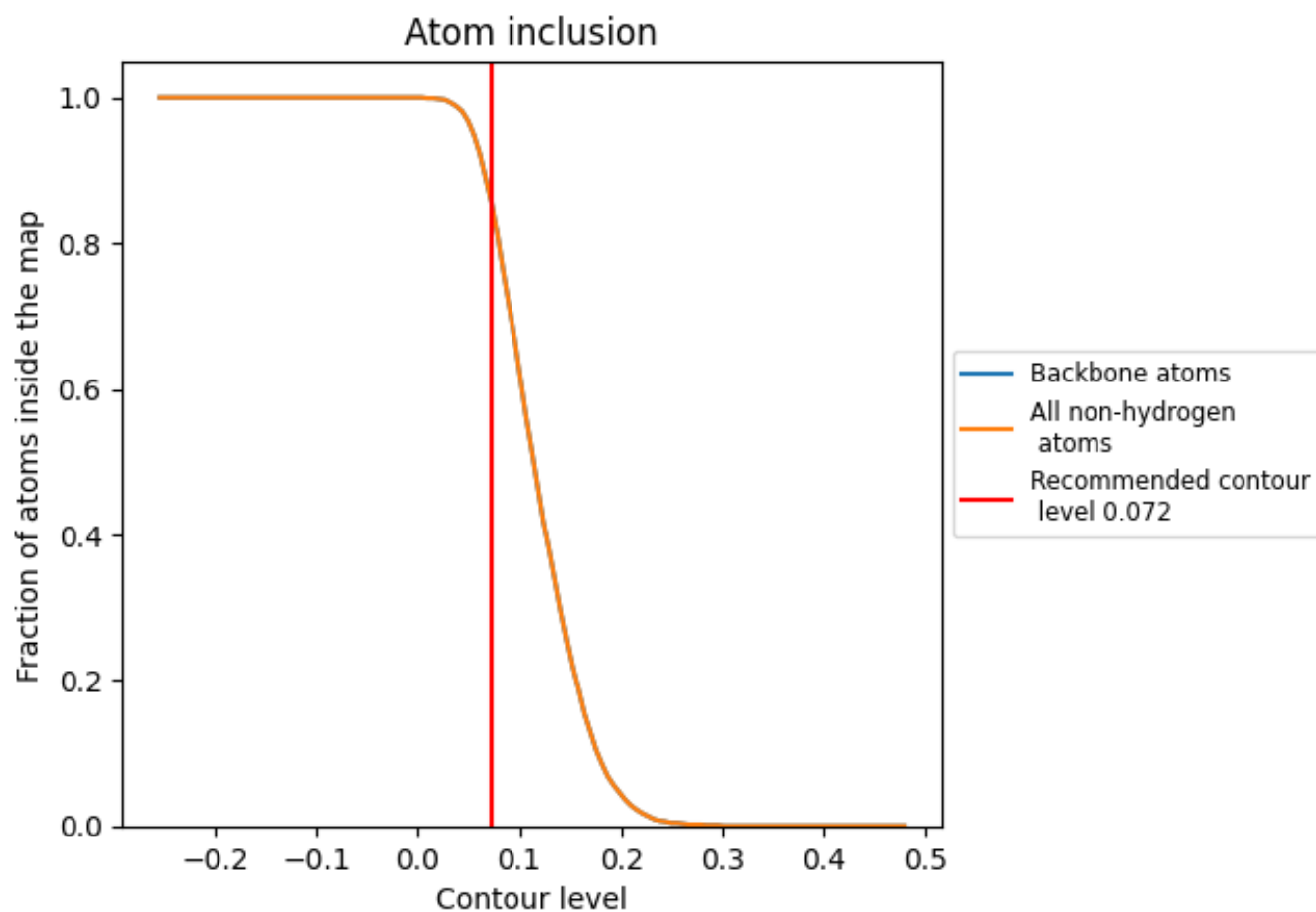
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.072).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.072) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.1670
A	 0.9410	 0.1980
B	 0.3120	 0.1400
C	 0.9610	 0.1720
E	 0.8040	 0.1410
F	 0.8920	 0.1540
G	 0.8800	 0.2150
H	 0.9770	 0.1650
I	 0.8220	 0.1620
J	 0.9720	 0.1580
K	 0.9620	 0.1610
L	 0.9290	 0.2280
M	 0.8840	 0.2270
N	 0.6050	 0.1390
O	 0.9110	 0.1570
P	 0.9730	 0.1690
Q	 0.7940	 0.1610
R	 0.7250	 0.1790
S	 0.7150	 0.1770
T	 0.4480	 0.1340
U	 1.0000	 0.3230
W	 0.9600	 0.3120
X	 0.8180	 0.1380
Y	 0.7800	 0.1380

