



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 03:33 AM JST

PDB ID : 7X0A
EMDB ID : EMD-32922
Title : Cryo-EM structure of human TRiC-NPP state
Authors : Cong, Y.; Liu, C.X.
Deposited on : 2022-02-21
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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) : 2.37.1

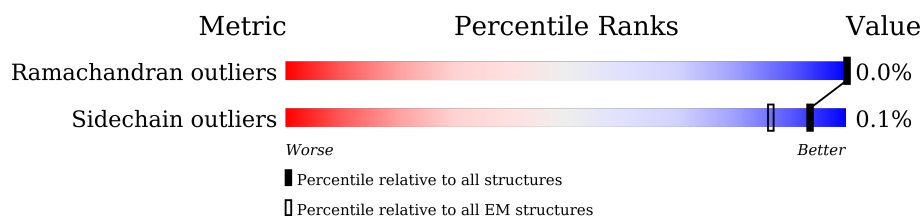
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	
1	a	556	
2	B	535	
2	b	535	
3	D	539	
3	d	539	
4	E	539	
4	e	539	
5	G	545	

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Mol	Chain	Length	Quality of chain
5	g	545	<div> <div>24%</div> <div>94%</div> <div>6%</div> </div>
6	H	543	<div> <div>36%</div> <div>96%</div> <div>.</div> </div>
6	h	543	<div> <div>27%</div> <div>96%</div> <div>.</div> </div>
7	Q	548	<div> <div>22%</div> <div>95%</div> <div>5%</div> </div>
7	q	548	<div> <div>15%</div> <div>95%</div> <div>5%</div> </div>
8	Z	531	<div> <div>23%</div> <div>98%</div> <div>.</div> </div>
8	z	531	<div> <div>18%</div> <div>98%</div> <div>.</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 61215 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	529	Total	C	N	O	S	0	0
			4017	2517	702	775	23		
1	A	470	Total	C	N	O	S	0	0
			3548	2230	618	679	21		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	446	Total	C	N	O	S	0	0
			3341	2090	588	647	16		
2	B	429	Total	C	N	O	S	0	0
			3213	2014	564	620	15		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	465	Total	C	N	O	S	0	0
			3512	2201	611	681	19		
3	d	516	Total	C	N	O	S	0	0
			3902	2440	678	761	23		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	520	Total	C	N	O	S	0	0
			4000	2498	700	772	30		
4	e	520	Total	C	N	O	S	0	0
			4000	2498	700	772	30		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	512	Total	C	N	O	S	0	0
			3979	2479	703	767	30		
5	G	486	Total	C	N	O	S	0	0
			3763	2348	668	717	30		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	519	Total	C	N	O	S	0	0
			3987	2518	690	756	23		
6	H	519	Total	C	N	O	S	0	0
			3987	2518	690	756	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	290	SER	LEU	engineered mutation	UNP Q99832
H	290	SER	LEU	engineered mutation	UNP Q99832

- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	523	Total	C	N	O	S	0	0
			3987	2515	677	768	27		
7	q	523	Total	C	N	O	S	0	0
			3987	2515	677	768	27		

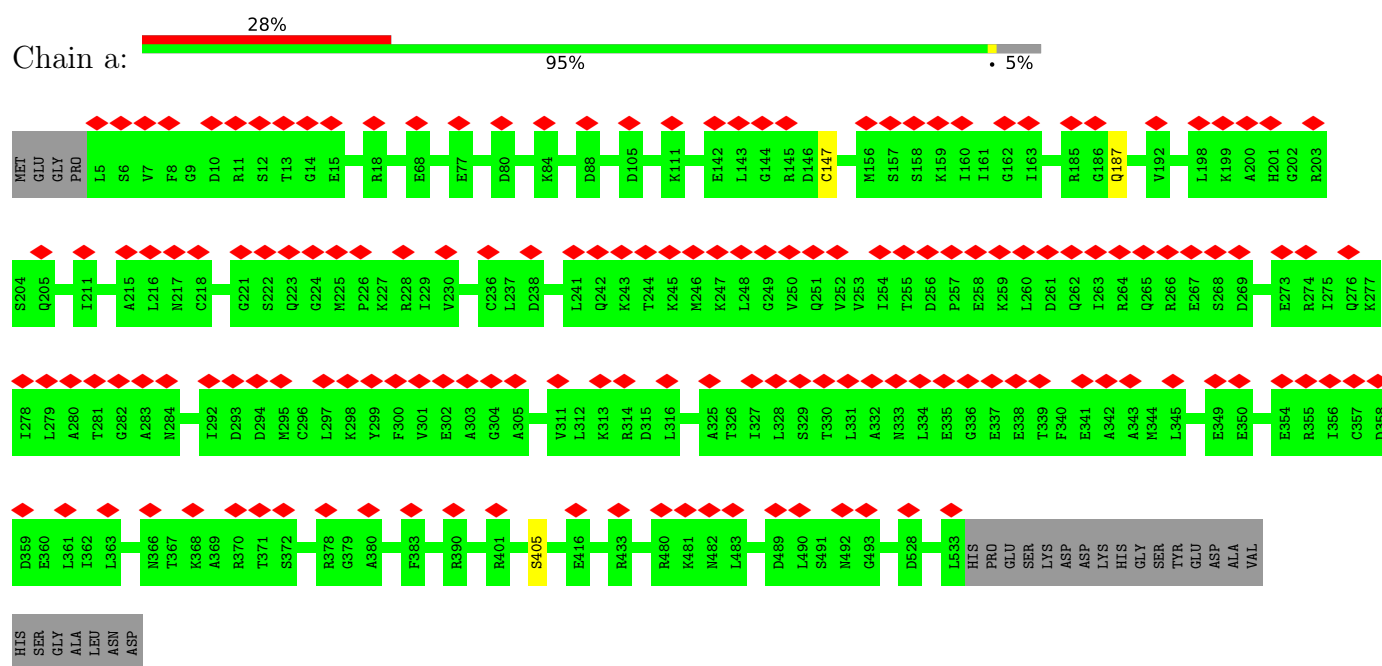
- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	521	Total	C	N	O	S	0	0
			3996	2511	699	765	21		
8	z	521	Total	C	N	O	S	0	0
			3996	2511	699	765	21		

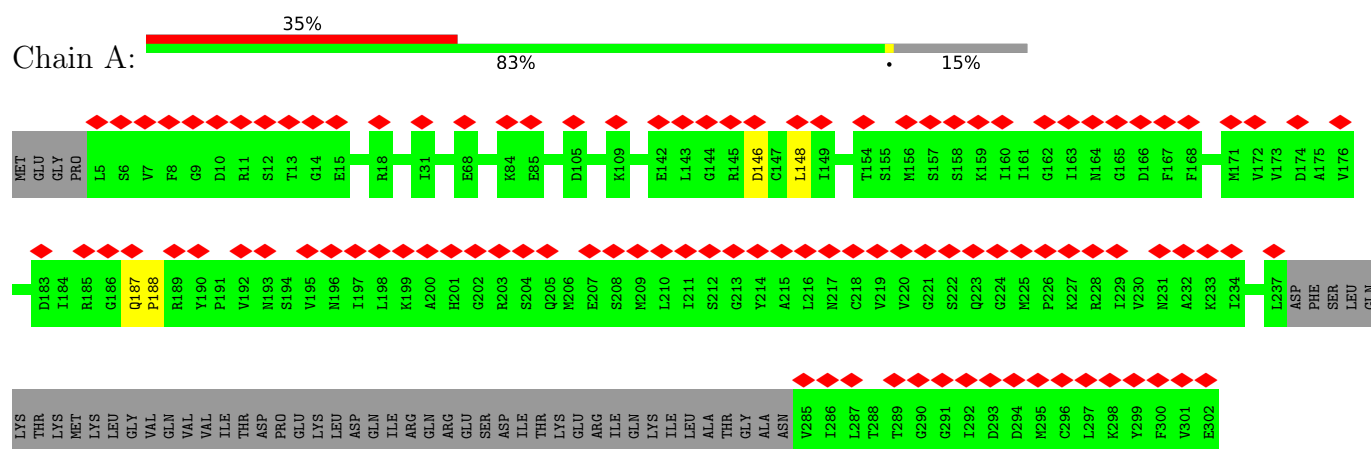
3 Residue-property plots

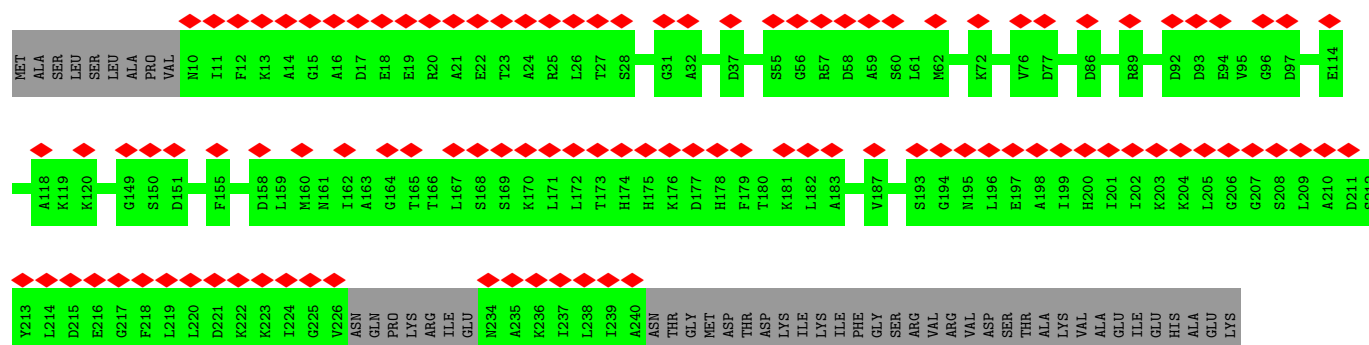
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

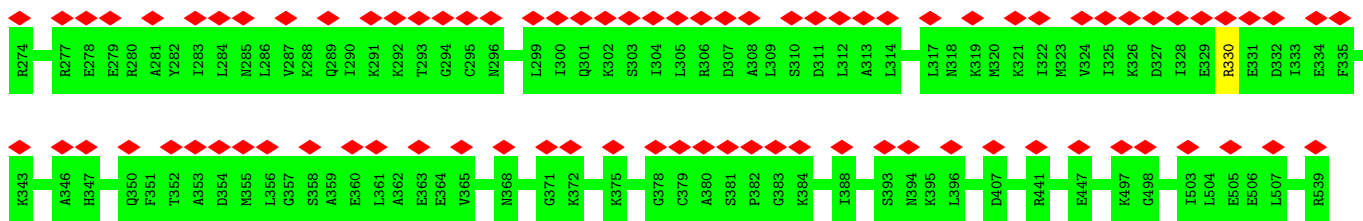
- Molecule 1: T-complex protein 1 subunit alpha



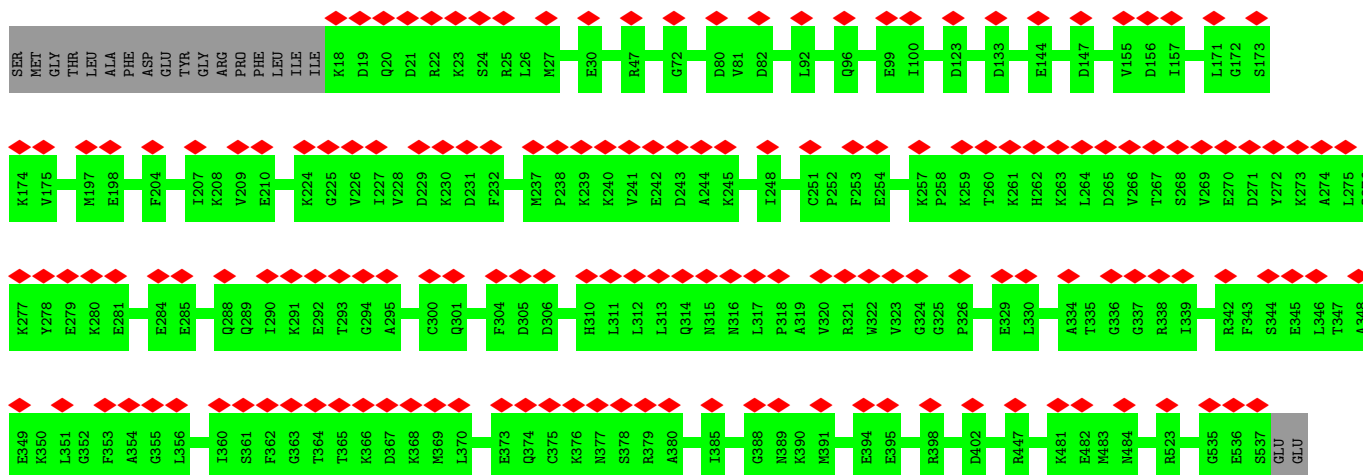
- Molecule 1: T-complex protein 1 subunit alpha



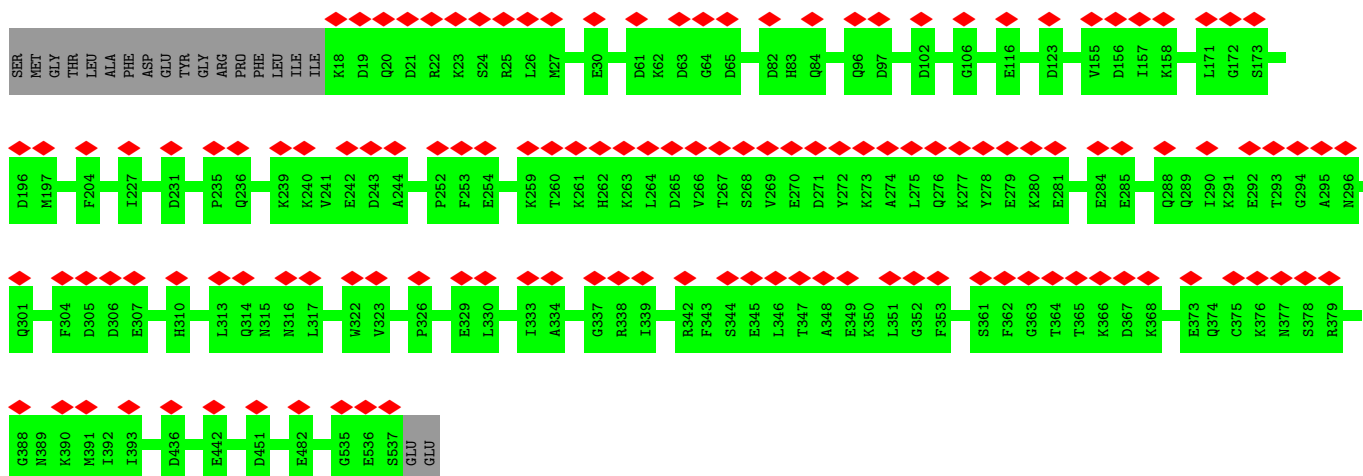




• Molecule 4: T-complex protein 1 subunit epsilon

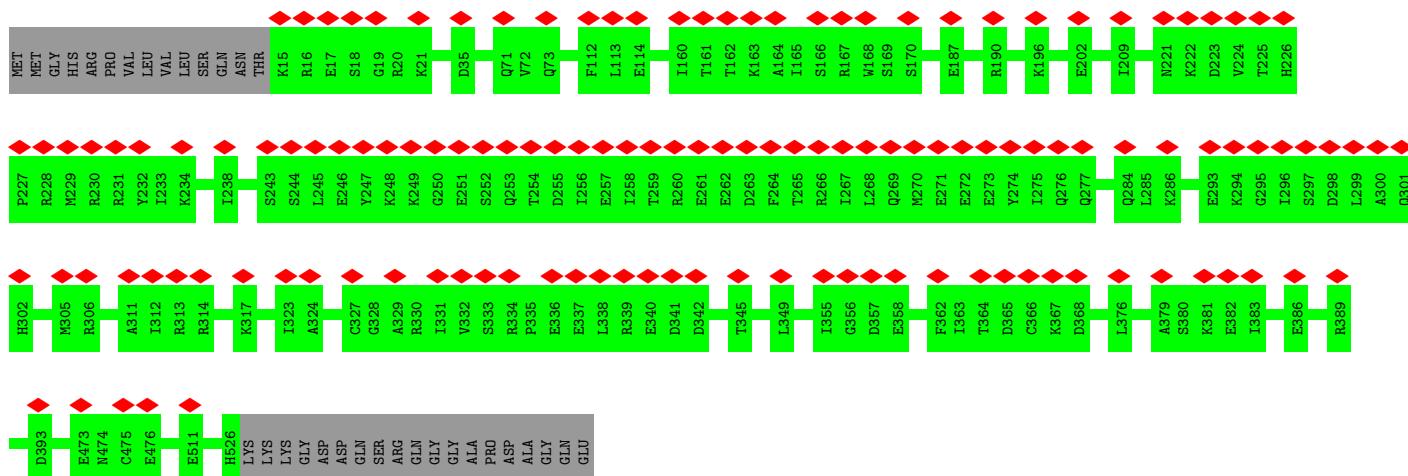


• Molecule 4: T-complex protein 1 subunit epsilon

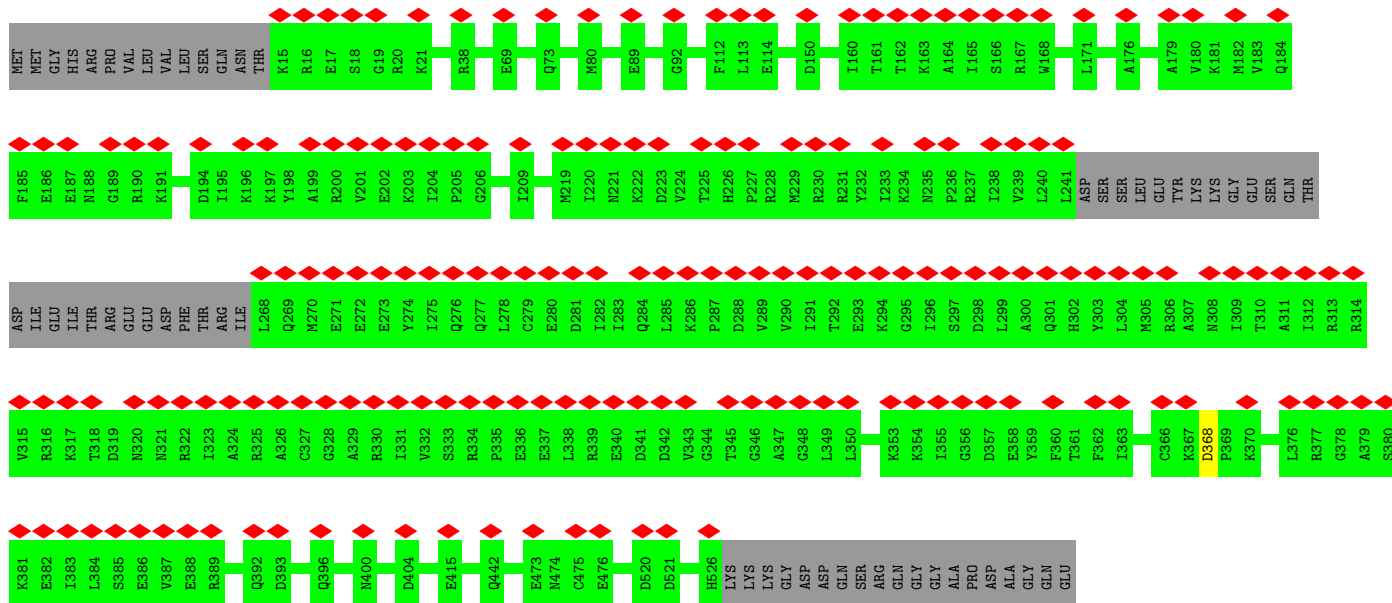
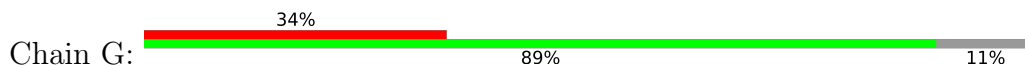


• Molecule 5: T-complex protein 1 subunit gamma

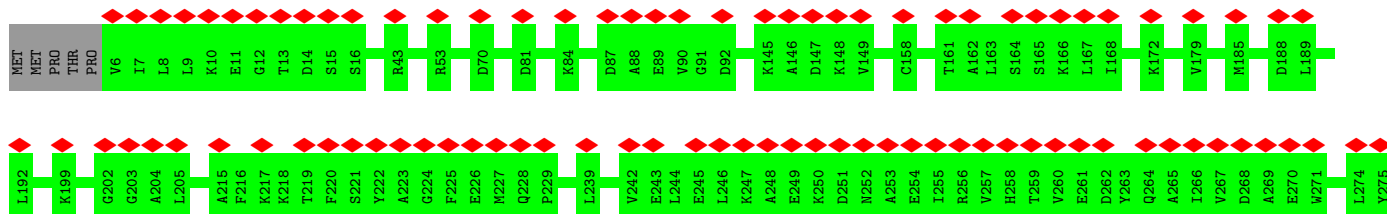


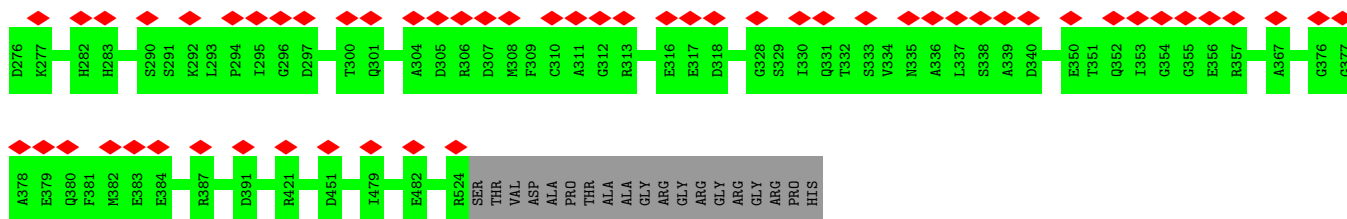


• Molecule 5: T-complex protein 1 subunit gamma



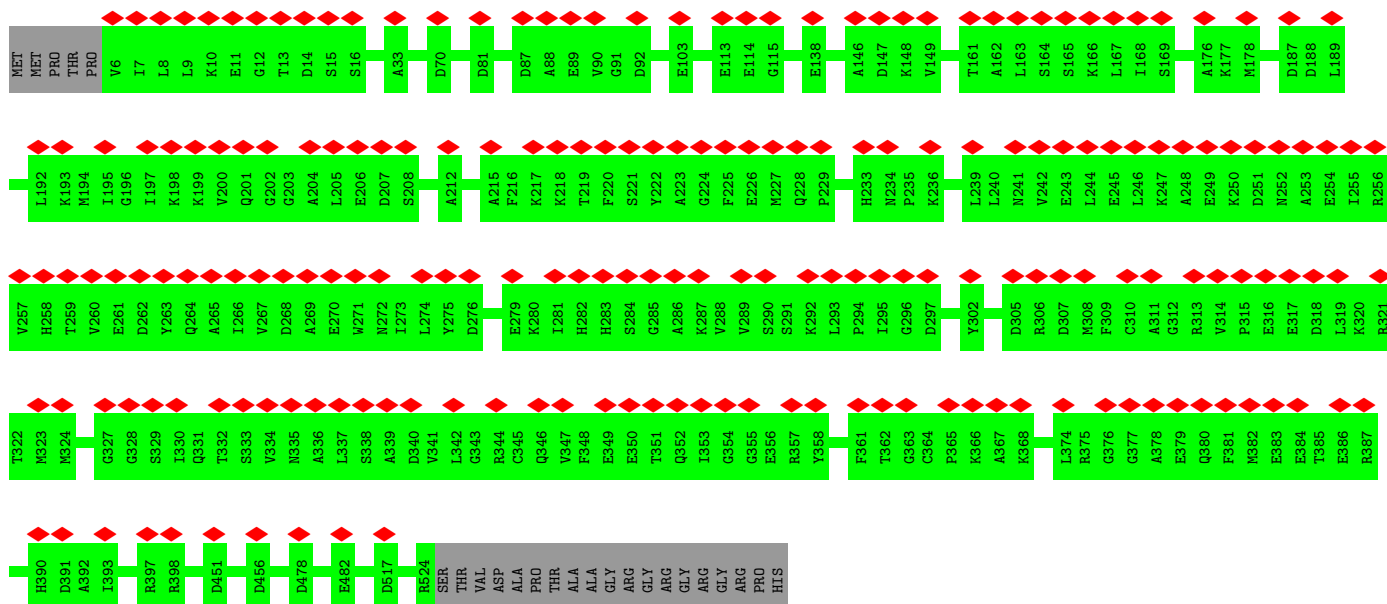
• Molecule 6: T-complex protein 1 subunit eta





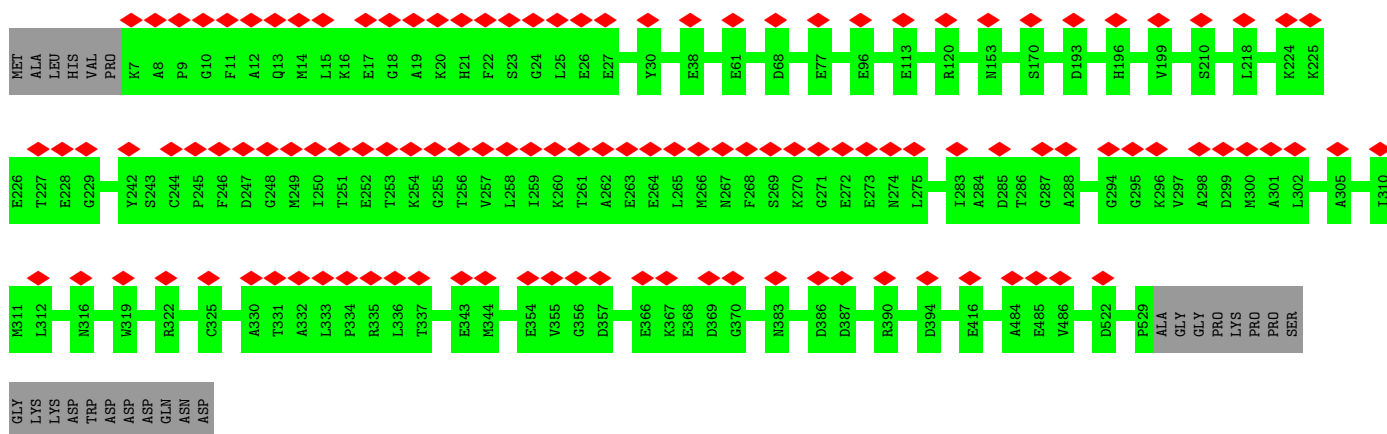
• Molecule 6: T-complex protein 1 subunit eta

Chain H: 36% 96%



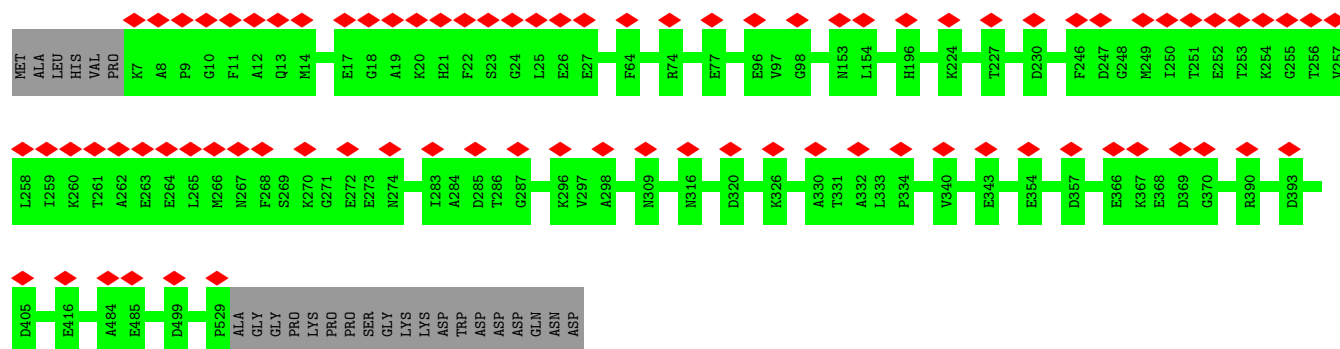
• Molecule 7: T-complex protein 1 subunit theta

Chain Q: 22% 95% 5%

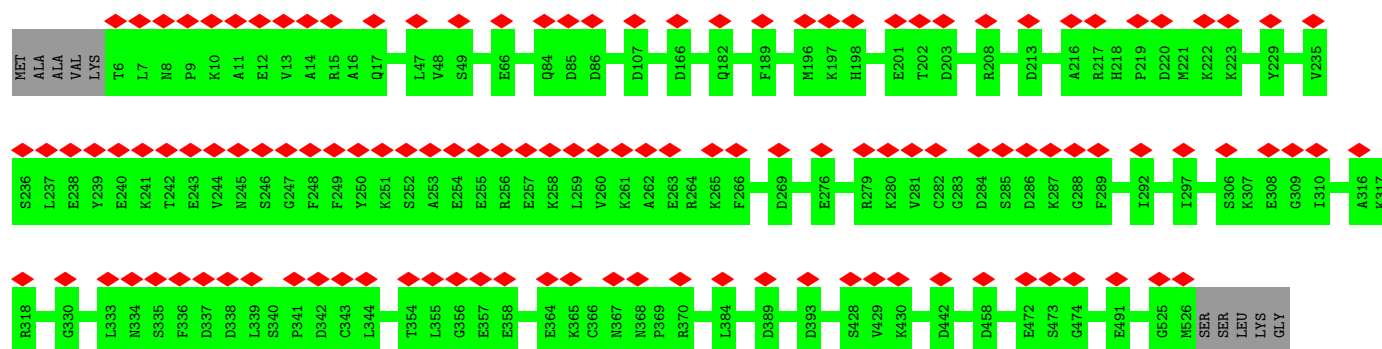


• Molecule 7: T-complex protein 1 subunit theta

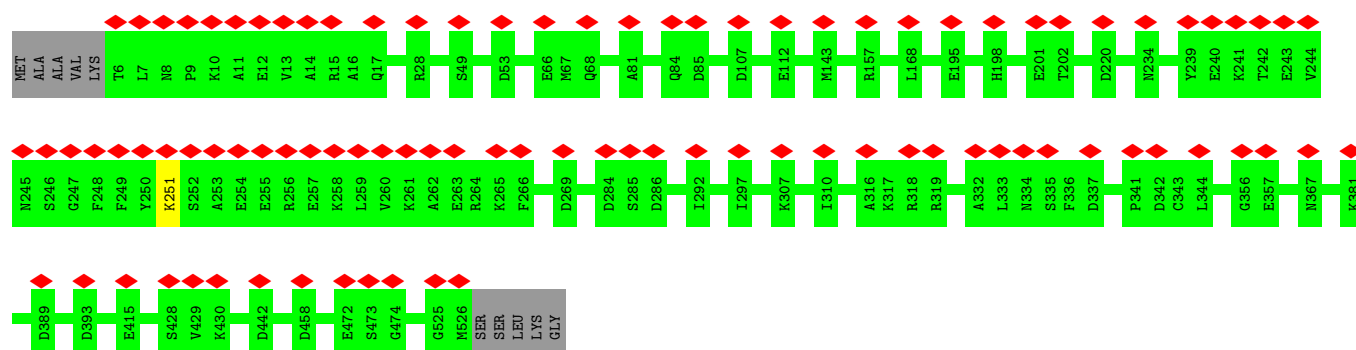
Chain q: 15% 95% 5%



• Molecule 8: T-complex protein 1 subunit zeta



• Molecule 8: T-complex protein 1 subunit zeta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185216	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.892	Depositor
Minimum map value	-1.544	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.124	Depositor
Recommended contour level	0.663	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3580	0.46	0/4832
1	a	0.24	0/4054	0.46	0/5472
2	B	0.24	0/3242	0.44	0/4370
2	b	0.24	0/3375	0.44	0/4553
3	D	0.24	0/3535	0.46	0/4764
3	d	0.24	0/3934	0.46	0/5310
4	E	0.24	0/4046	0.46	0/5449
4	e	0.24	0/4046	0.45	0/5449
5	G	0.24	0/3805	0.46	0/5133
5	g	0.24	0/4024	0.46	0/5428
6	H	0.25	0/4042	0.45	0/5454
6	h	0.24	0/4042	0.44	0/5454
7	Q	0.25	0/4043	0.43	0/5463
7	q	0.25	0/4043	0.44	0/5463
8	Z	0.24	0/4043	0.45	0/5451
8	z	0.24	0/4043	0.44	0/5451
All	All	0.24	0/61897	0.45	0/83496

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
1	a	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Peptide
1	A	187	GLN	Peptide
1	a	187	GLN	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	462/556 (83%)	444 (96%)	15 (3%)	3 (1%)	25	59
1	a	527/556 (95%)	493 (94%)	34 (6%)	0	100	100
2	B	417/535 (78%)	405 (97%)	12 (3%)	0	100	100
2	b	440/535 (82%)	428 (97%)	12 (3%)	0	100	100
3	D	453/539 (84%)	446 (98%)	7 (2%)	0	100	100
3	d	514/539 (95%)	501 (98%)	13 (2%)	0	100	100
4	E	518/539 (96%)	496 (96%)	22 (4%)	0	100	100
4	e	518/539 (96%)	499 (96%)	19 (4%)	0	100	100
5	G	482/545 (88%)	462 (96%)	20 (4%)	0	100	100
5	g	510/545 (94%)	494 (97%)	16 (3%)	0	100	100
6	H	517/543 (95%)	500 (97%)	17 (3%)	0	100	100
6	h	517/543 (95%)	501 (97%)	16 (3%)	0	100	100
7	Q	521/548 (95%)	506 (97%)	15 (3%)	0	100	100
7	q	521/548 (95%)	505 (97%)	16 (3%)	0	100	100
8	Z	519/531 (98%)	500 (96%)	19 (4%)	0	100	100
8	z	519/531 (98%)	501 (96%)	18 (4%)	0	100	100
All	All	7955/8672 (92%)	7681 (97%)	271 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	SER
1	A	404	GLU
1	A	188	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/463 (84%)	386 (100%)	2 (0%)	88	94
1	a	441/463 (95%)	439 (100%)	2 (0%)	88	94
2	B	338/427 (79%)	338 (100%)	0	100	100
2	b	350/427 (82%)	350 (100%)	0	100	100
3	D	396/452 (88%)	396 (100%)	0	100	100
3	d	441/452 (98%)	440 (100%)	1 (0%)	93	97
4	E	439/455 (96%)	439 (100%)	0	100	100
4	e	439/455 (96%)	439 (100%)	0	100	100
5	G	418/469 (89%)	417 (100%)	1 (0%)	93	97
5	g	443/469 (94%)	443 (100%)	0	100	100
6	H	426/443 (96%)	426 (100%)	0	100	100
6	h	426/443 (96%)	426 (100%)	0	100	100
7	Q	432/452 (96%)	432 (100%)	0	100	100
7	q	432/452 (96%)	432 (100%)	0	100	100
8	Z	435/442 (98%)	435 (100%)	0	100	100
8	z	435/442 (98%)	434 (100%)	1 (0%)	93	97
All	All	6679/7206 (93%)	6672 (100%)	7 (0%)	93	98

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	SER

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Mol	Chain	Res	Type
3	d	330	ARG
8	z	251	LYS
5	G	368	ASP
1	A	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	276	GLN
6	h	233	HIS
7	q	523	GLN
6	H	480	ASN
7	q	289	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](#)

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.

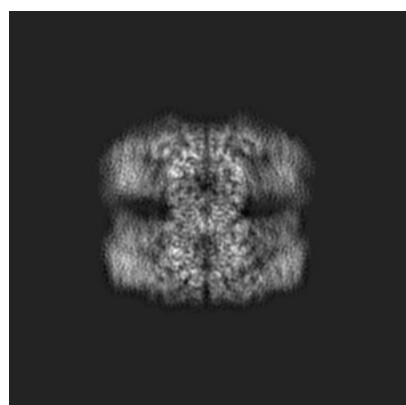
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32922. These allow visual inspection of the internal detail of the map and identification of artifacts.

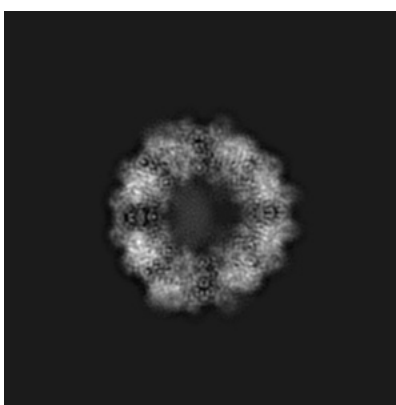
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

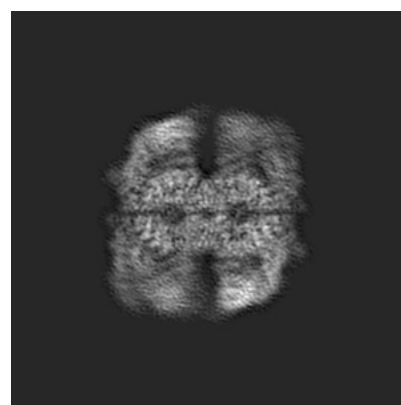
6.1.1 Primary map



X



Y

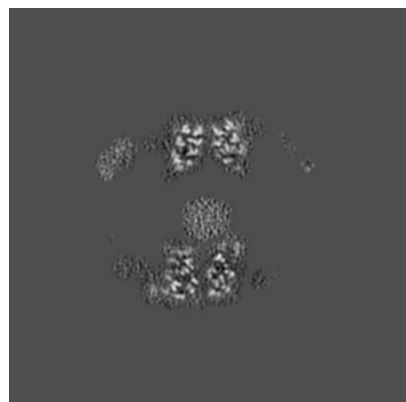


Z

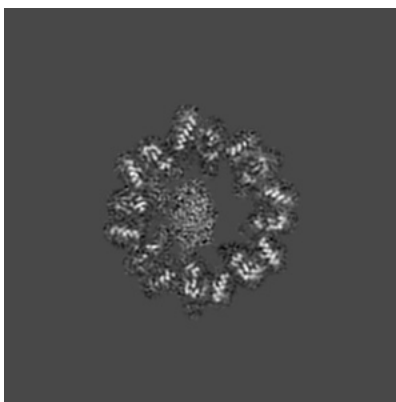
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

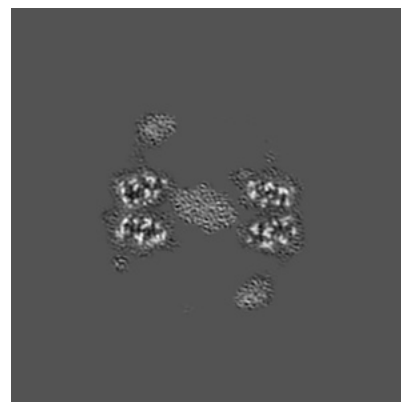
6.2.1 Primary map



X Index: 128



Y Index: 128

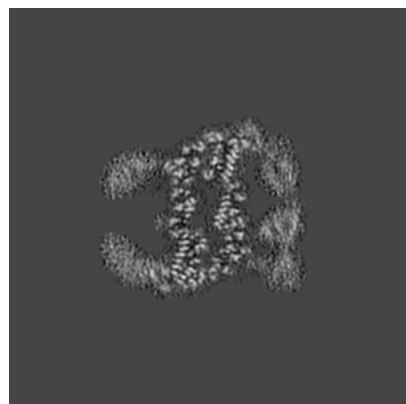


Z Index: 128

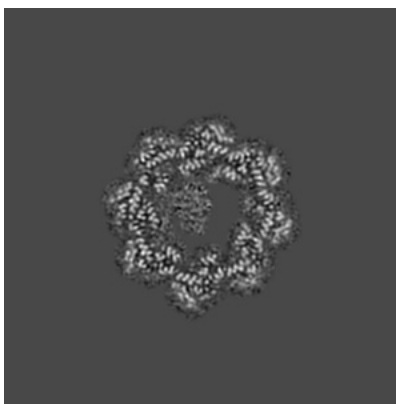
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

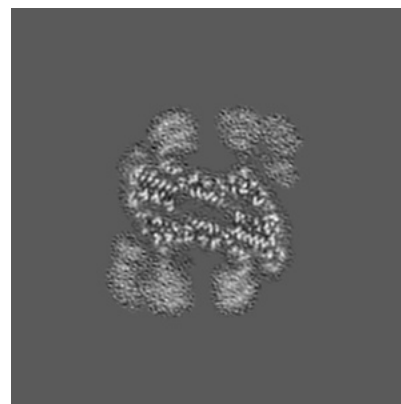
6.3.1 Primary map



X Index: 94



Y Index: 117

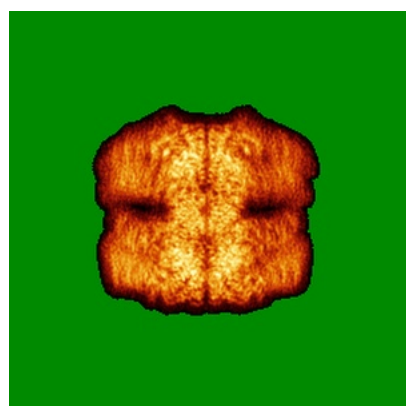


Z Index: 94

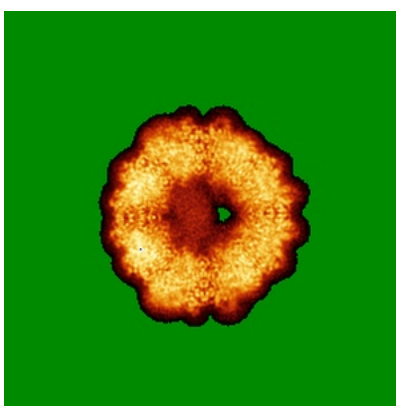
The images above show the largest variance slices of the map in three orthogonal directions.

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

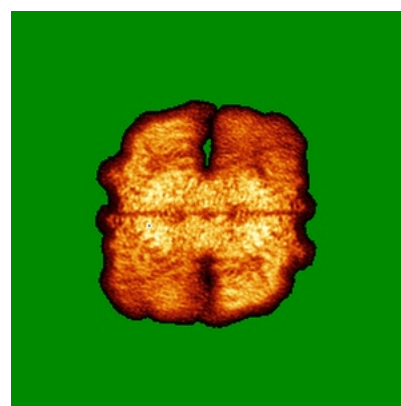
6.4.1 Primary map



X



Y

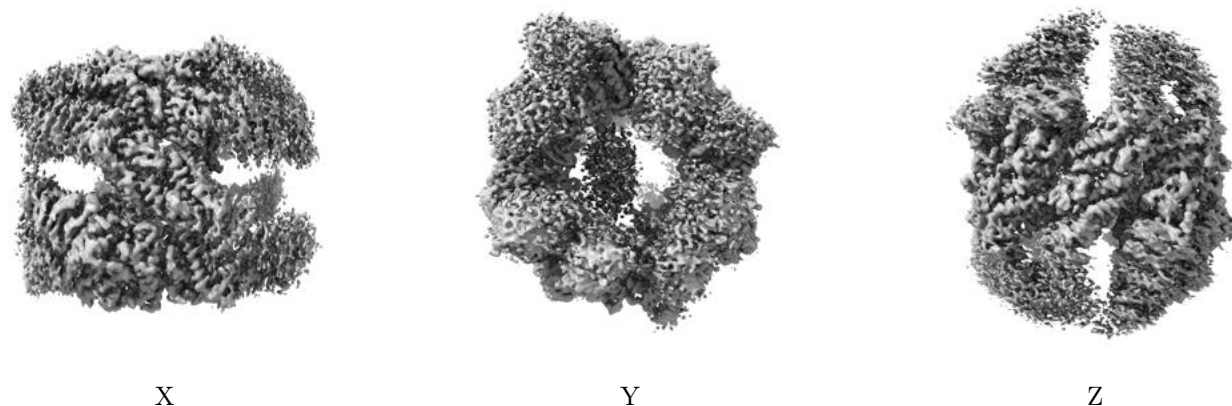


Z

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

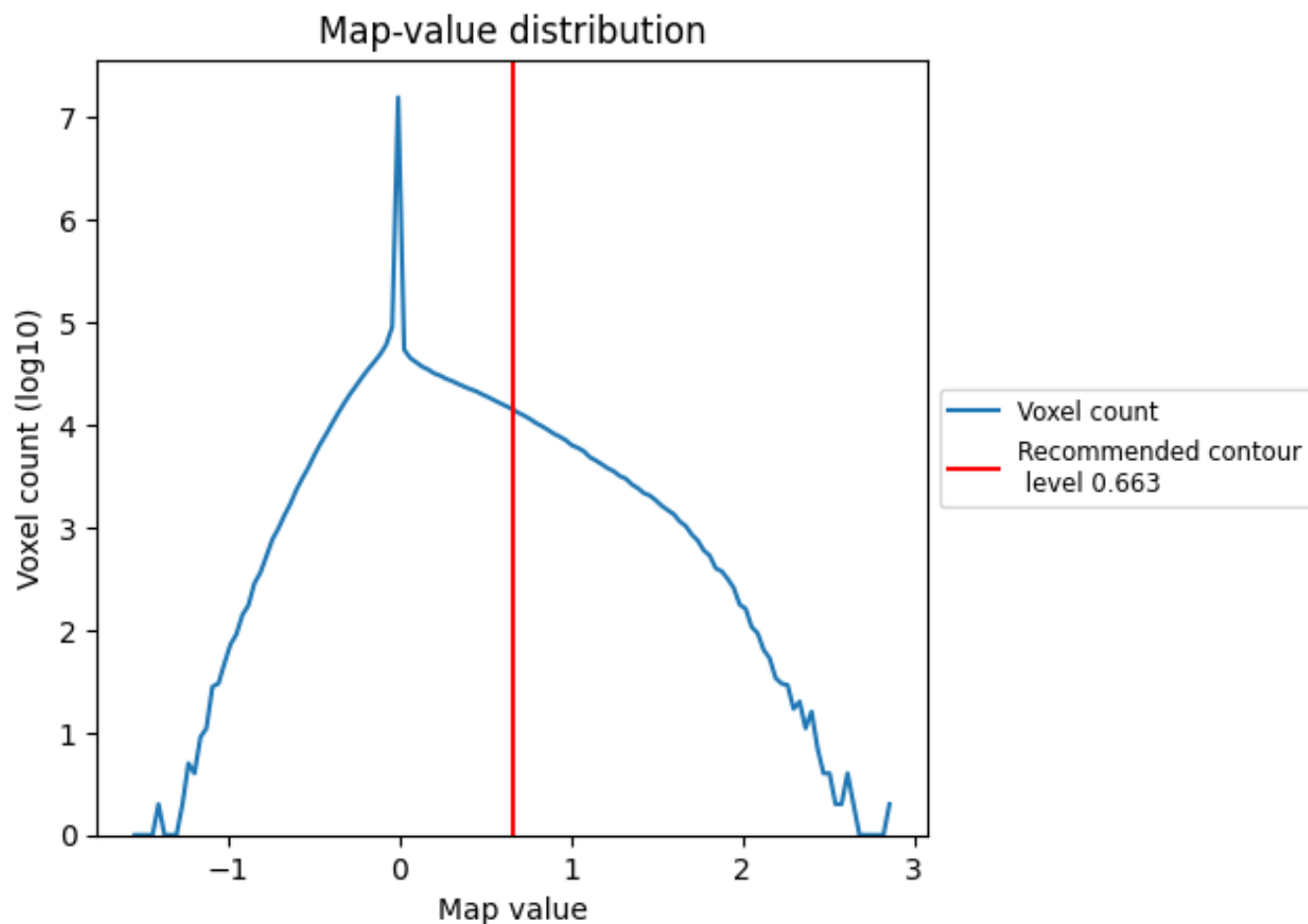
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

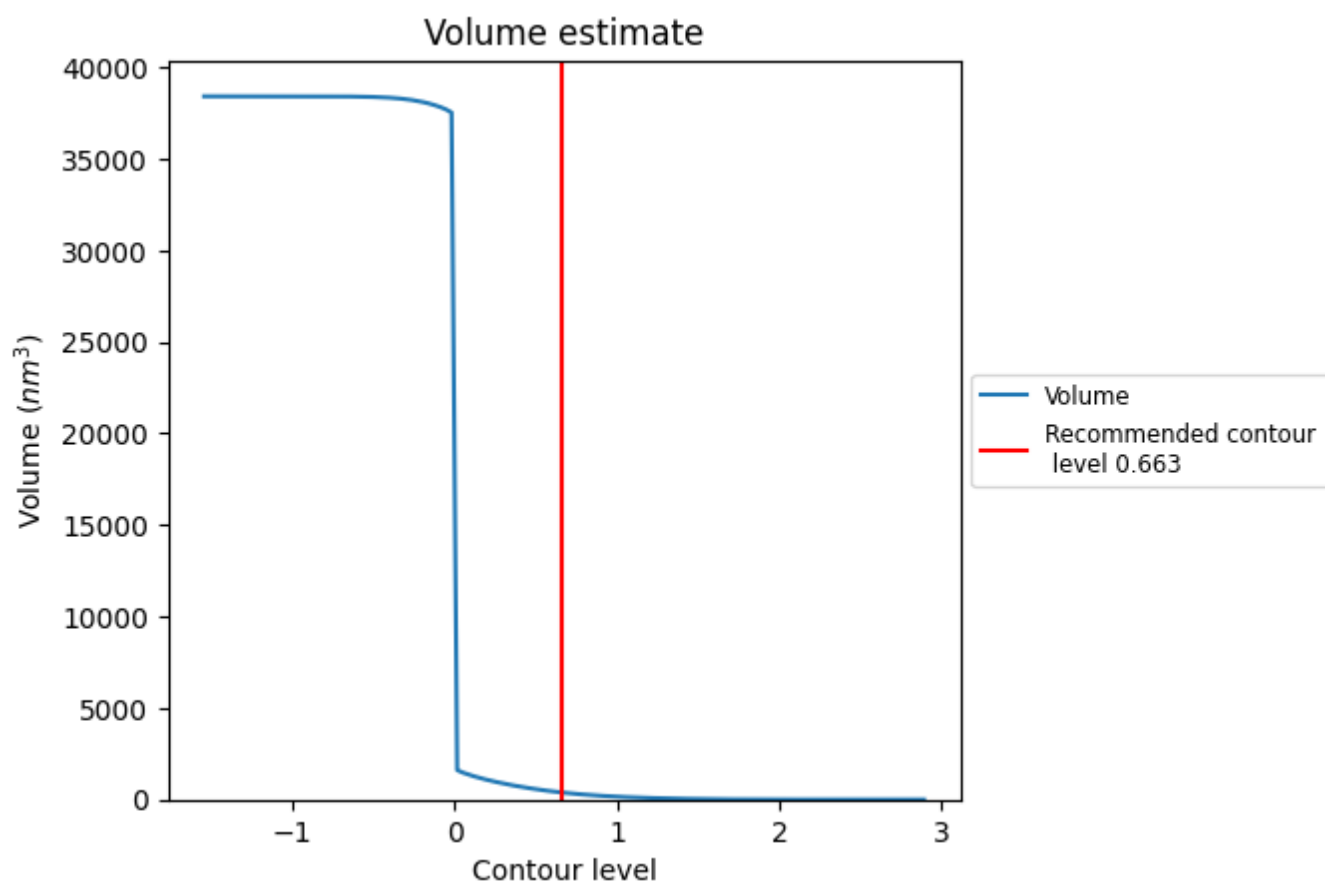
This section contains the results of statistical analysis of the map.

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.

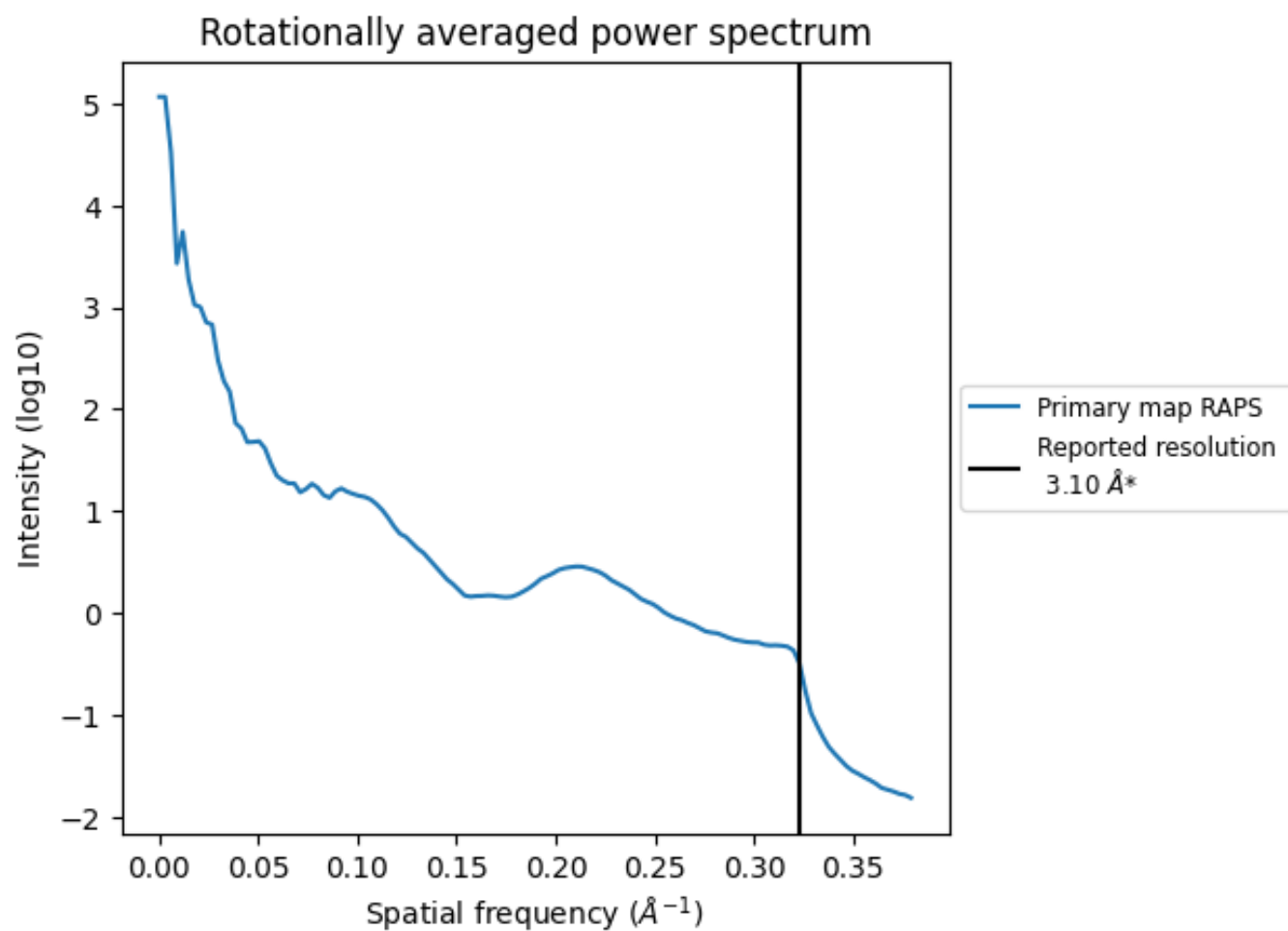
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 0.323 Å⁻¹

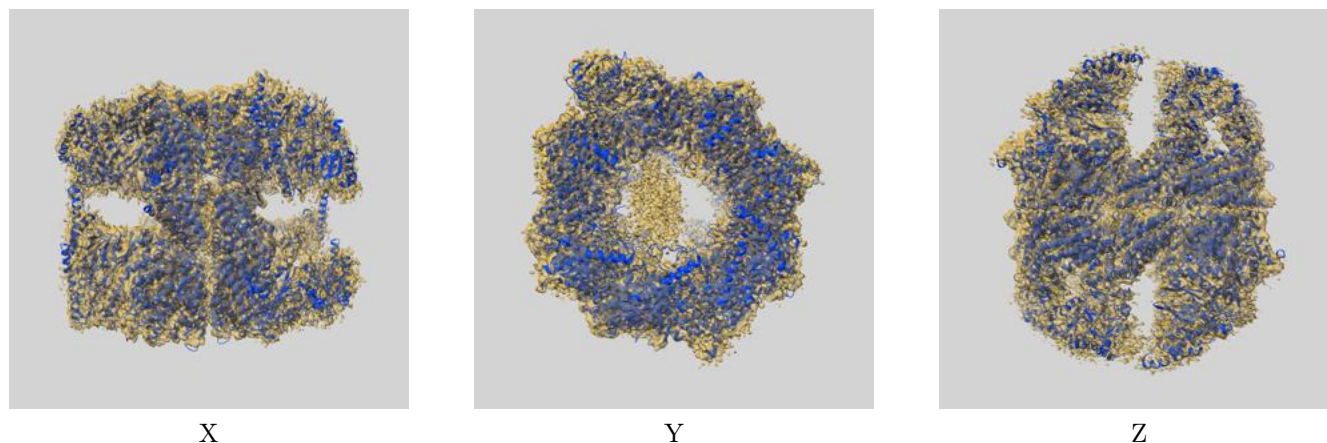
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

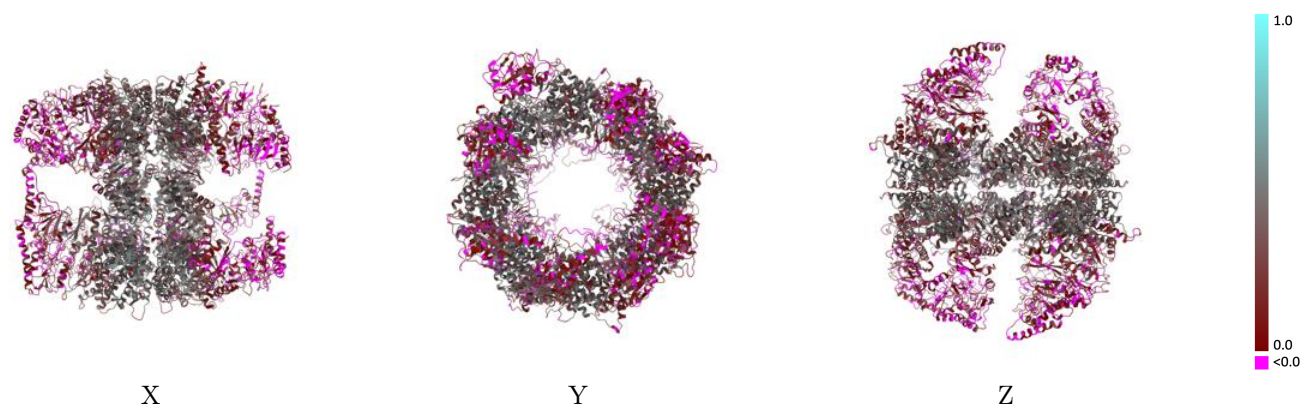
This section contains information regarding the fit between EMDB map EMD-32922 and PDB model 7X0A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



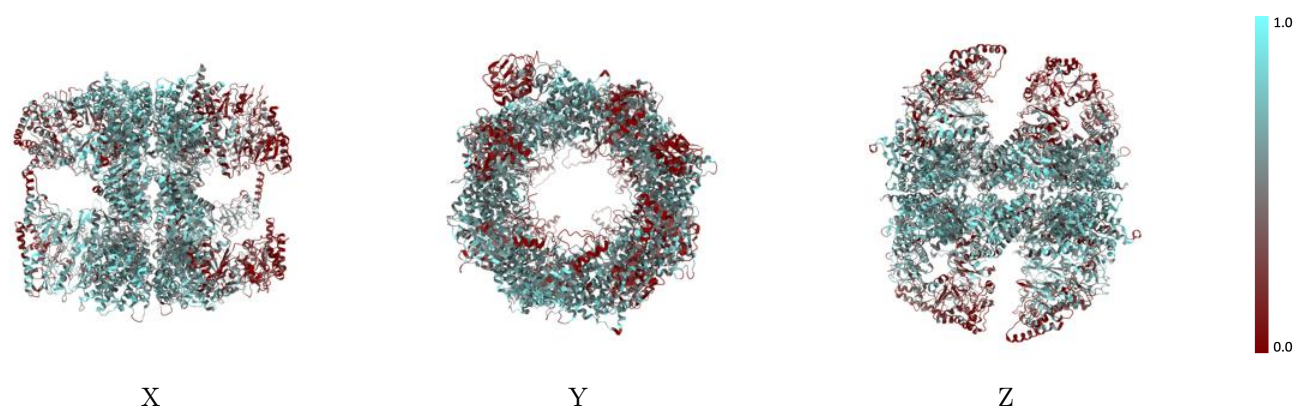
The images above show the 3D surface view of the map at the recommended contour level 0.663 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



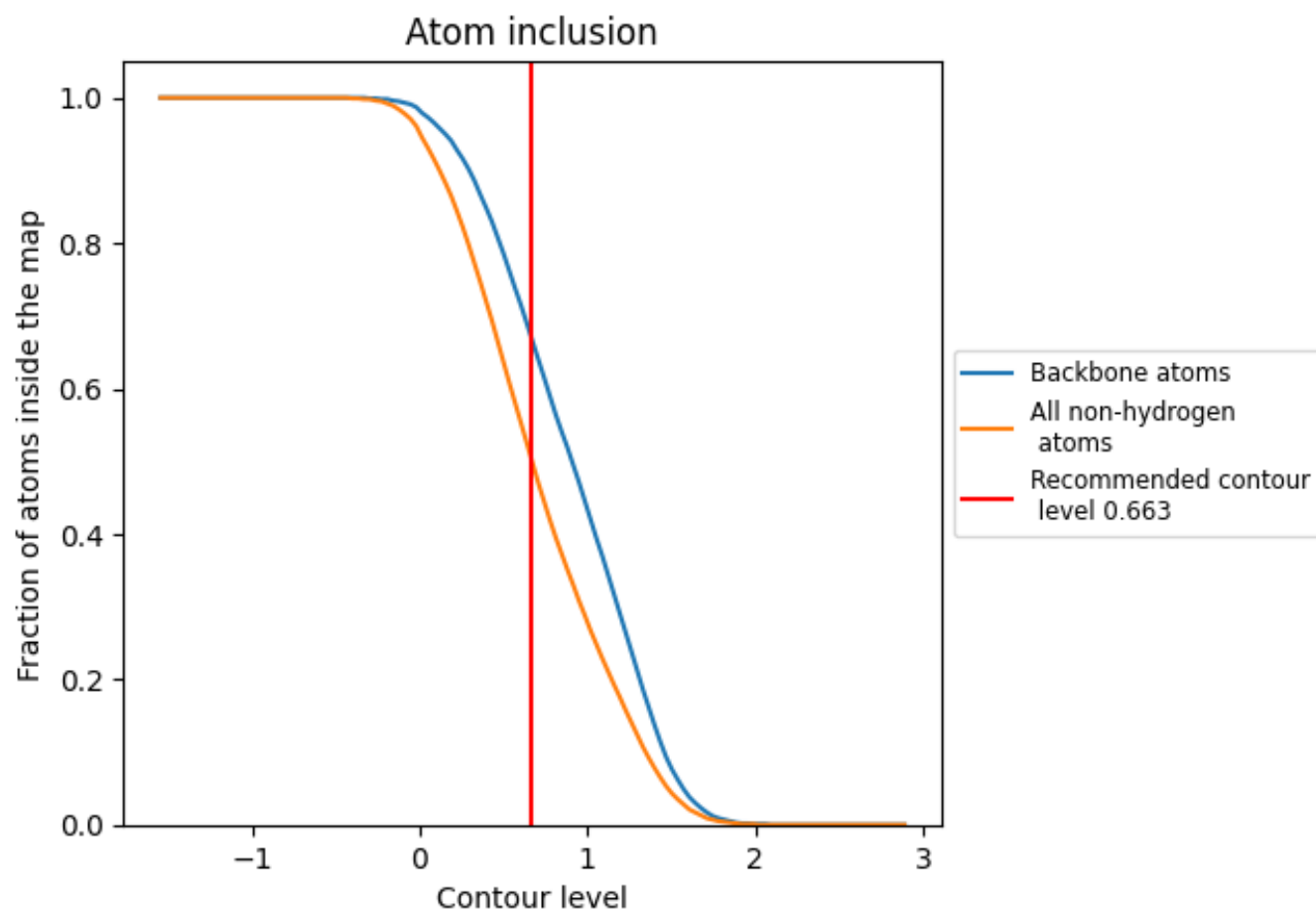
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.663).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 51% 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 (0.663) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5060	<div></div> 0.2560
A	<div></div> 0.4340	<div></div> 0.2320
B	<div></div> 0.4180	<div></div> 0.2400
D	<div></div> 0.4380	<div></div> 0.2290
E	<div></div> 0.4950	<div></div> 0.2310
G	<div></div> 0.4510	<div></div> 0.2530
H	<div></div> 0.4630	<div></div> 0.2480
Q	<div></div> 0.5590	<div></div> 0.3010
Z	<div></div> 0.5340	<div></div> 0.2750
a	<div></div> 0.5100	<div></div> 0.2360
b	<div></div> 0.4720	<div></div> 0.2470
d	<div></div> 0.5100	<div></div> 0.2370
e	<div></div> 0.5430	<div></div> 0.2360
g	<div></div> 0.5300	<div></div> 0.2650
h	<div></div> 0.5260	<div></div> 0.2480
q	<div></div> 0.5940	<div></div> 0.3100
z	<div></div> 0.5820	<div></div> 0.2950

1.0

0.0

<0.0