



wwPDB EM Validation Summary Report ⓘ

Dec 4, 2023 – 12:19 PM JST

PDB ID : 8HKI
EMDB ID : EMD-34852
Title : Human TRiC open state
Authors : Cong, Y.; Liu, C.X.
Deposited on : 2022-11-27
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:

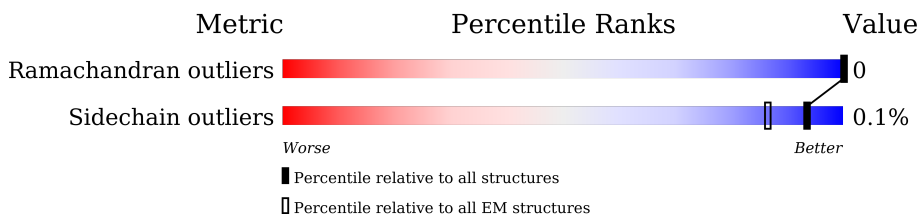
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 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.




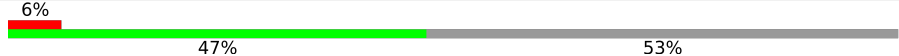

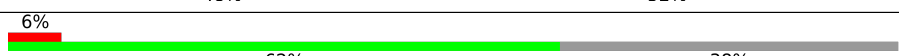

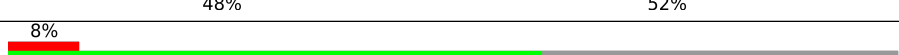
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	g	545	 44% 56%
6	H	543	 6% 47% 53%
6	h	543	 10% 62% 38%
7	Q	548	 6% 48% 52%
7	q	548	 6% 62% 38%
8	Z	531	 5% 48% 52%
8	z	531	 8% 60% 40%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 33926 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
			Total	C	N	O	S		
1	a	291	Total	C	N	O	S	0	0
			2182	1369	377	429	7		
1	A	255	Total	C	N	O	S	0	0
			1918	1210	330	373	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	327	Total	C	N	O	S	0	0
			2407	1482	430	483	12		
2	B	250	Total	C	N	O	S	0	0
			1842	1141	326	365	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	250	Total	C	N	O	S	0	0
			1870	1164	328	369	9		
3	d	278	Total	C	N	O	S	0	0
			2086	1295	366	416	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	254	Total	C	N	O	S	0	0
			1916	1180	338	379	19		
4	e	321	Total	C	N	O	S	0	0
			2433	1494	436	481	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	239	1822	1137	320	350	15	0	0
5	G	257	1946	1215	339	377	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	h	339	2585	1631	454	488	12	0	0
6	H	255	1929	1216	337	370	6	0	0

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

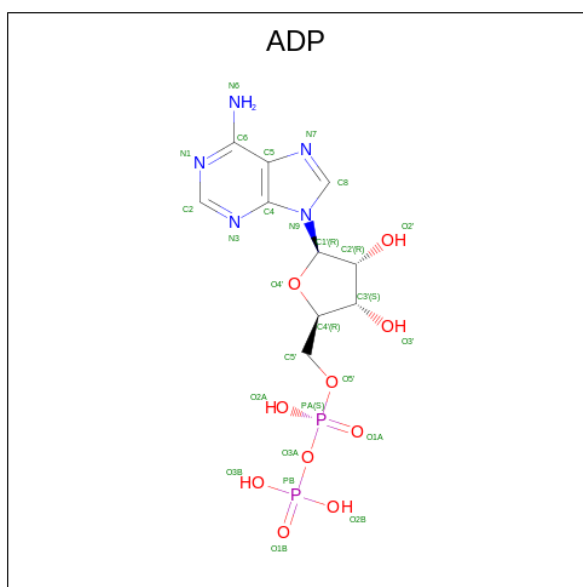
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	262	1998	1272	336	379	11	0	0
7	q	338	2574	1622	438	498	16	0	0

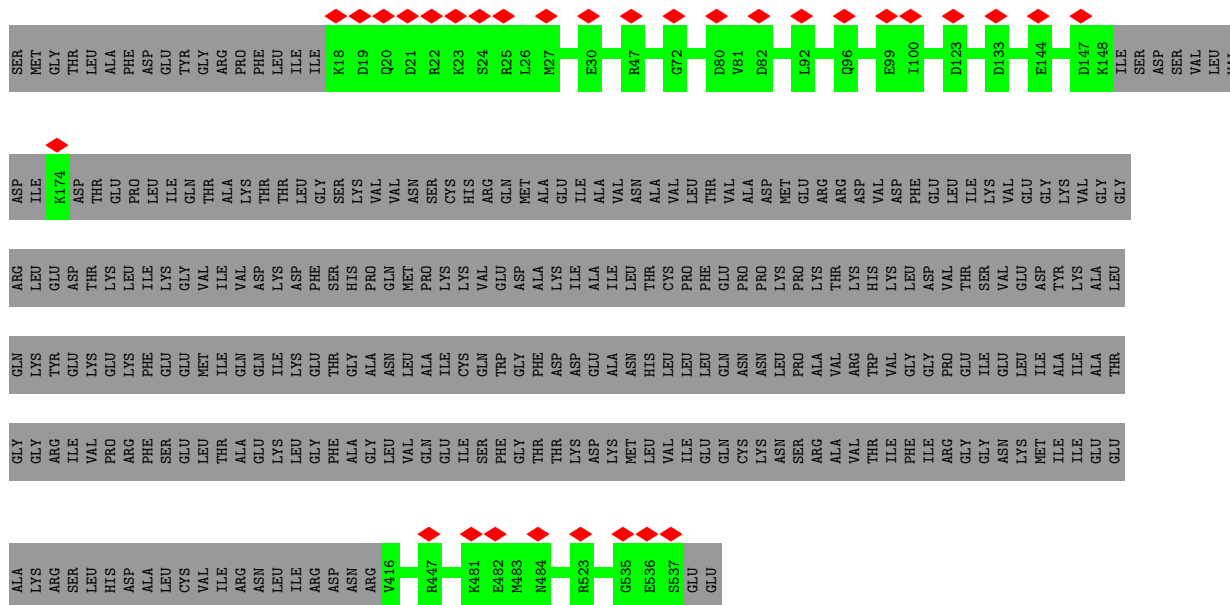
- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	255	1887	1188	325	364	10	0	0
8	z	316	2369	1480	420	458	11	0	0

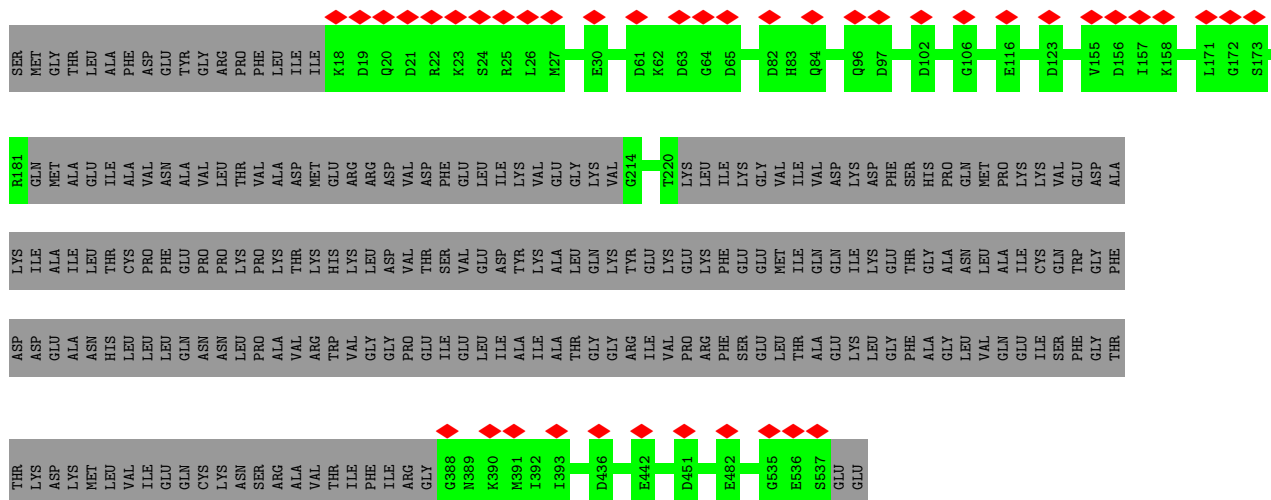
- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



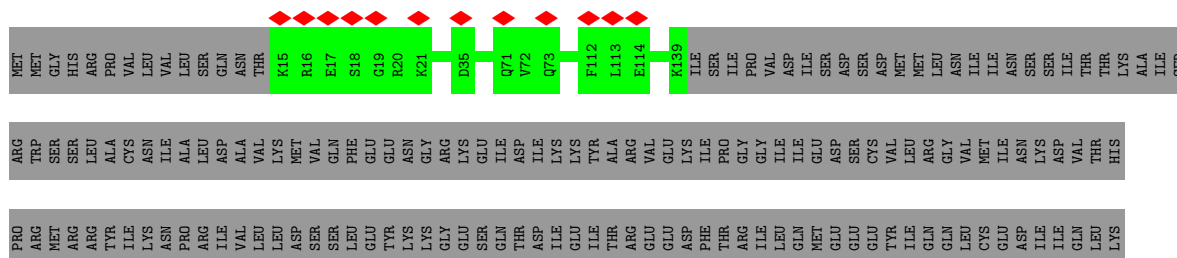
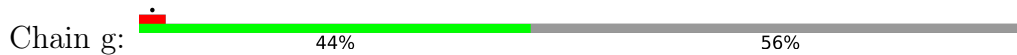
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

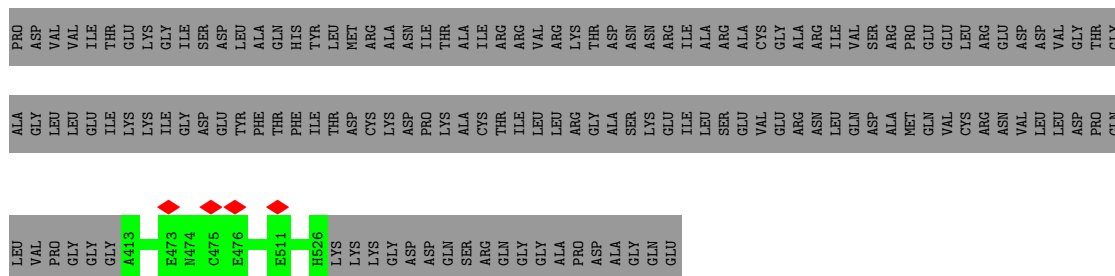


• Molecule 4: T-complex protein 1 subunit epsilon

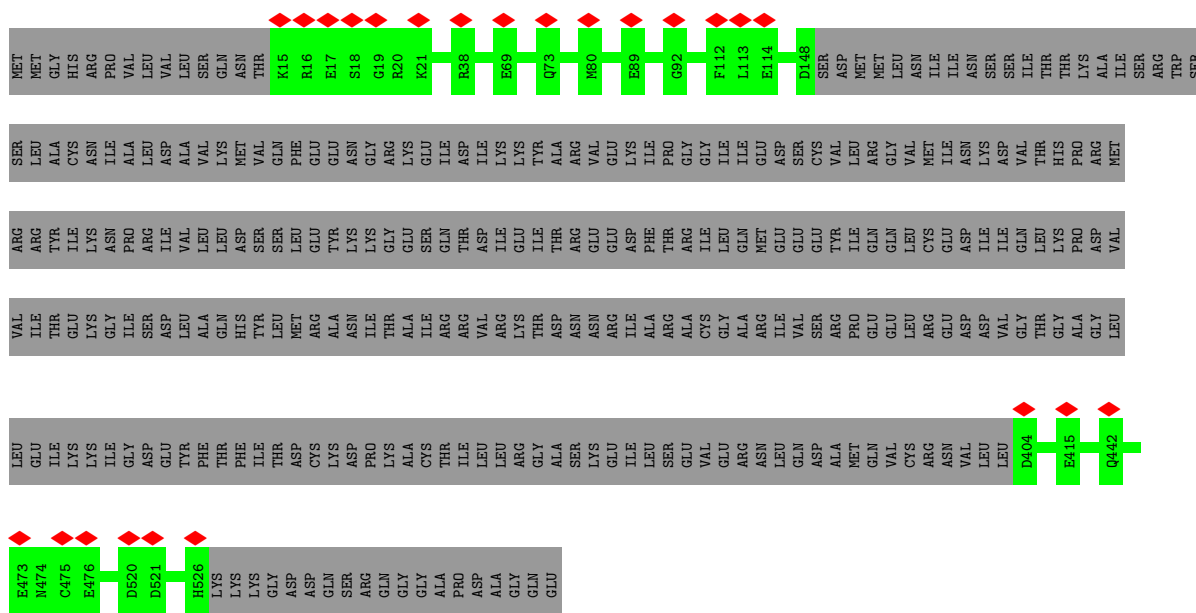


• Molecule 5: T-complex protein 1 subunit gamma

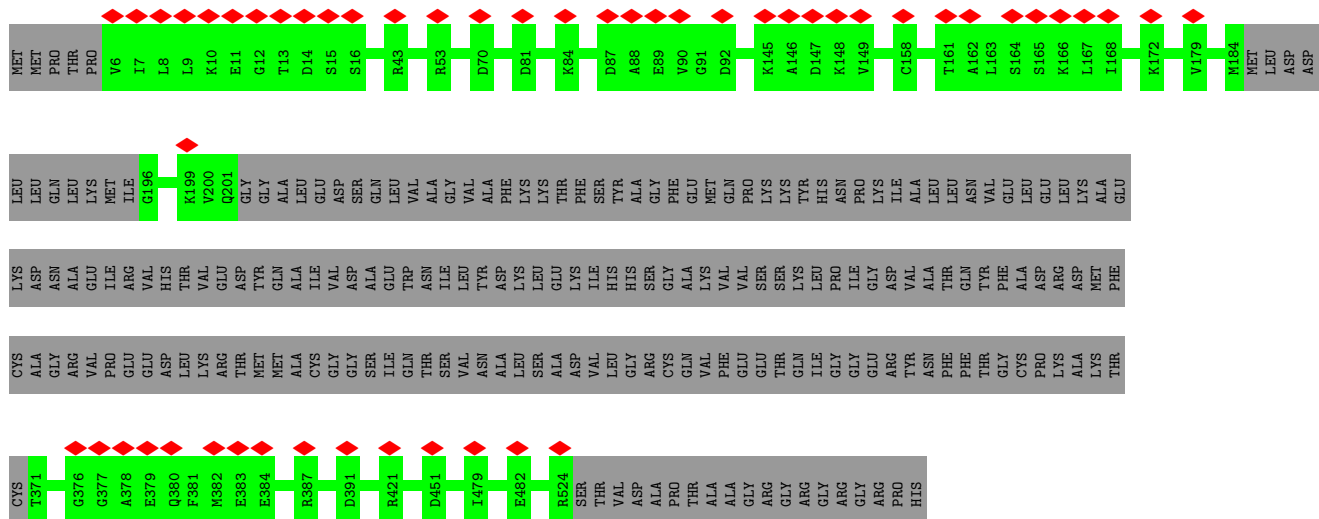




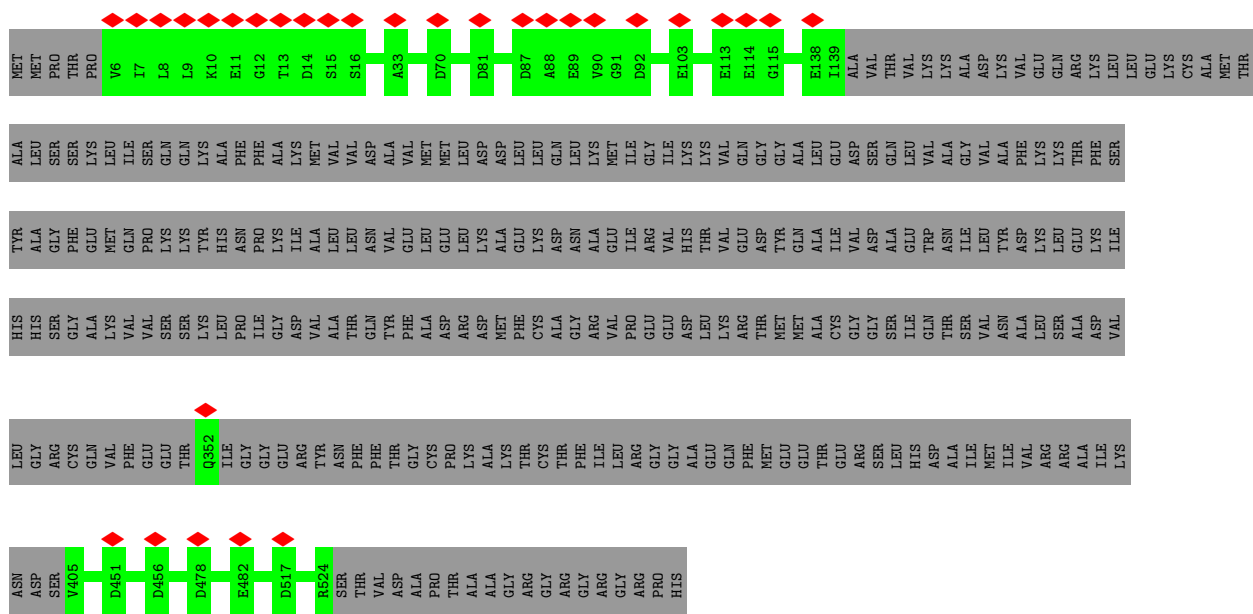
• Molecule 5: T-complex protein 1 subunit gamma



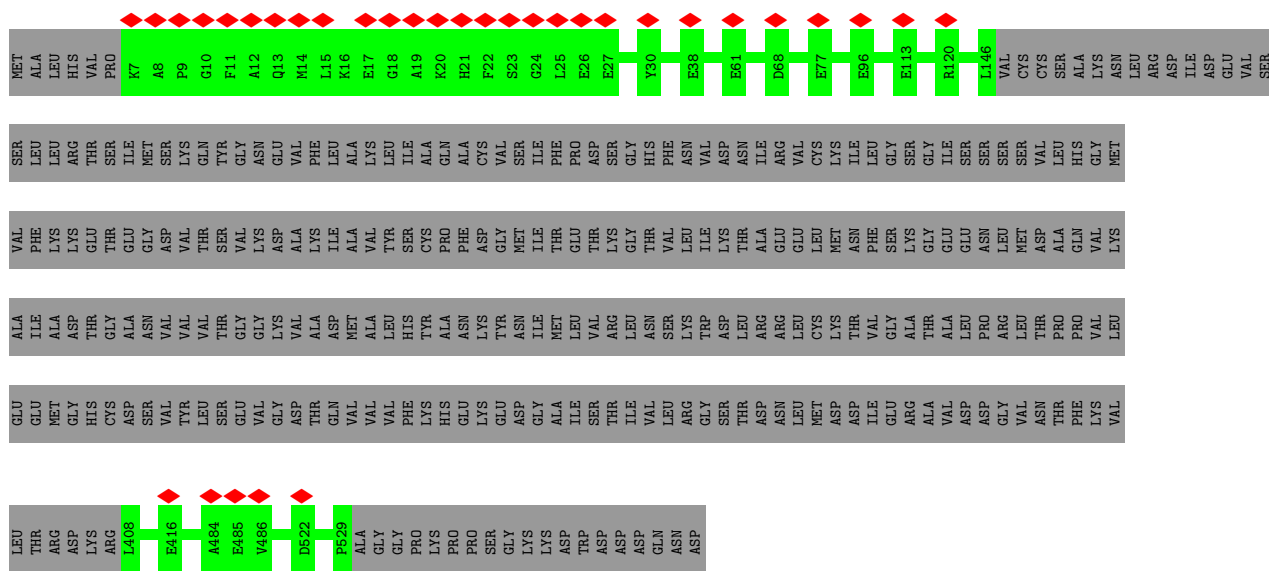
• Molecule 6: T-complex protein 1 subunit eta



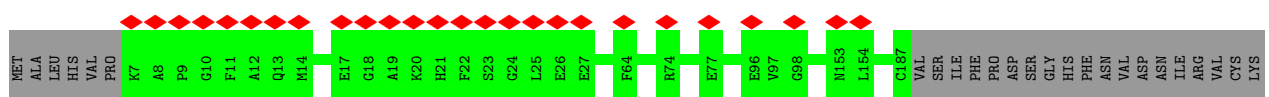
● Molecule 6: T-complex protein 1 subunit eta

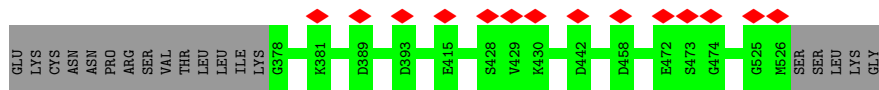


● Molecule 7: T-complex protein 1 subunit theta



● Molecule 7: T-complex protein 1 subunit theta





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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/1938	0.42	0/2626
1	a	0.23	0/2201	0.43	0/2978
2	B	0.24	0/1856	0.43	0/2507
2	b	0.23	0/2425	0.43	0/3271
3	D	0.24	0/1885	0.45	0/2544
3	d	0.24	0/2103	0.46	0/2841
4	E	0.24	0/1930	0.45	0/2592
4	e	0.24	0/2450	0.45	0/3293
5	G	0.23	0/1970	0.44	0/2665
5	g	0.23	0/1843	0.43	0/2489
6	H	0.24	0/1952	0.45	0/2645
6	h	0.24	0/2613	0.44	0/3525
7	Q	0.24	0/2028	0.42	0/2741
7	q	0.25	0/2606	0.43	0/3516
8	Z	0.24	0/1907	0.43	0/2582
8	z	0.23	0/2392	0.43	0/3232
All	All	0.24	0/34099	0.44	0/46047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	251/556 (45%)	250 (100%)	1 (0%)	0	100	100
1	a	285/556 (51%)	273 (96%)	12 (4%)	0	100	100
2	B	246/535 (46%)	239 (97%)	7 (3%)	0	100	100
2	b	319/535 (60%)	311 (98%)	8 (2%)	0	100	100
3	D	246/539 (46%)	245 (100%)	1 (0%)	0	100	100
3	d	274/539 (51%)	270 (98%)	4 (2%)	0	100	100
4	E	249/539 (46%)	243 (98%)	6 (2%)	0	100	100
4	e	315/539 (58%)	305 (97%)	10 (3%)	0	100	100
5	G	253/545 (46%)	244 (96%)	9 (4%)	0	100	100
5	g	235/545 (43%)	228 (97%)	7 (3%)	0	100	100
6	H	250/543 (46%)	245 (98%)	5 (2%)	0	100	100
6	h	333/543 (61%)	326 (98%)	7 (2%)	0	100	100
7	Q	258/548 (47%)	248 (96%)	10 (4%)	0	100	100
7	q	332/548 (61%)	320 (96%)	12 (4%)	0	100	100
8	Z	251/531 (47%)	248 (99%)	3 (1%)	0	100	100
8	z	310/531 (58%)	305 (98%)	5 (2%)	0	100	100
All	All	4407/8672 (51%)	4300 (98%)	107 (2%)	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	209/463 (45%)	209 (100%)	0	100	100
1	a	240/463 (52%)	238 (99%)	2 (1%)	81	92
2	B	192/427 (45%)	192 (100%)	0	100	100
2	b	253/427 (59%)	253 (100%)	0	100	100
3	D	205/452 (45%)	205 (100%)	0	100	100
3	d	232/452 (51%)	232 (100%)	0	100	100
4	E	208/455 (46%)	208 (100%)	0	100	100
4	e	268/455 (59%)	268 (100%)	0	100	100
5	G	215/469 (46%)	215 (100%)	0	100	100
5	g	200/469 (43%)	200 (100%)	0	100	100
6	H	205/443 (46%)	205 (100%)	0	100	100
6	h	276/443 (62%)	276 (100%)	0	100	100
7	Q	207/452 (46%)	207 (100%)	0	100	100
7	q	274/452 (61%)	274 (100%)	0	100	100
8	Z	201/442 (46%)	201 (100%)	0	100	100
8	z	255/442 (58%)	255 (100%)	0	100	100
All	All	3640/7206 (50%)	3638 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	147	CYS
1	a	405	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	133	ASN
1	a	435	GLN
3	d	129	HIS
4	e	520	GLN
7	q	523	GLN

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	q	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	g	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.41	4 (13%)
9	ADP	Z	601	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	Q	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	G	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
9	ADP	z	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	q	601	-	-	2/12/32/32	0/3/3/3
9	ADP	g	601	-	-	2/12/32/32	0/3/3/3
9	ADP	Z	601	-	-	2/12/32/32	0/3/3/3
9	ADP	Q	601	-	-	2/12/32/32	0/3/3/3
9	ADP	G	601	-	-	2/12/32/32	0/3/3/3
9	ADP	z	601	-	-	2/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	601	ADP	C5-C4	2.53	1.47	1.40
9	G	601	ADP	C5-C4	2.52	1.47	1.40
9	q	601	ADP	C5-C4	2.51	1.47	1.40
9	g	601	ADP	C5-C4	2.50	1.47	1.40
9	z	601	ADP	C5-C4	2.50	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	601	ADP	PA-O3A-PB	-3.28	121.56	132.83
9	q	601	ADP	PA-O3A-PB	-3.26	121.63	132.83
9	z	601	ADP	N3-C2-N1	-3.25	123.60	128.68
9	g	601	ADP	PA-O3A-PB	-3.24	121.70	132.83
9	Z	601	ADP	PA-O3A-PB	-3.24	121.71	132.83

There are no chirality outliers.

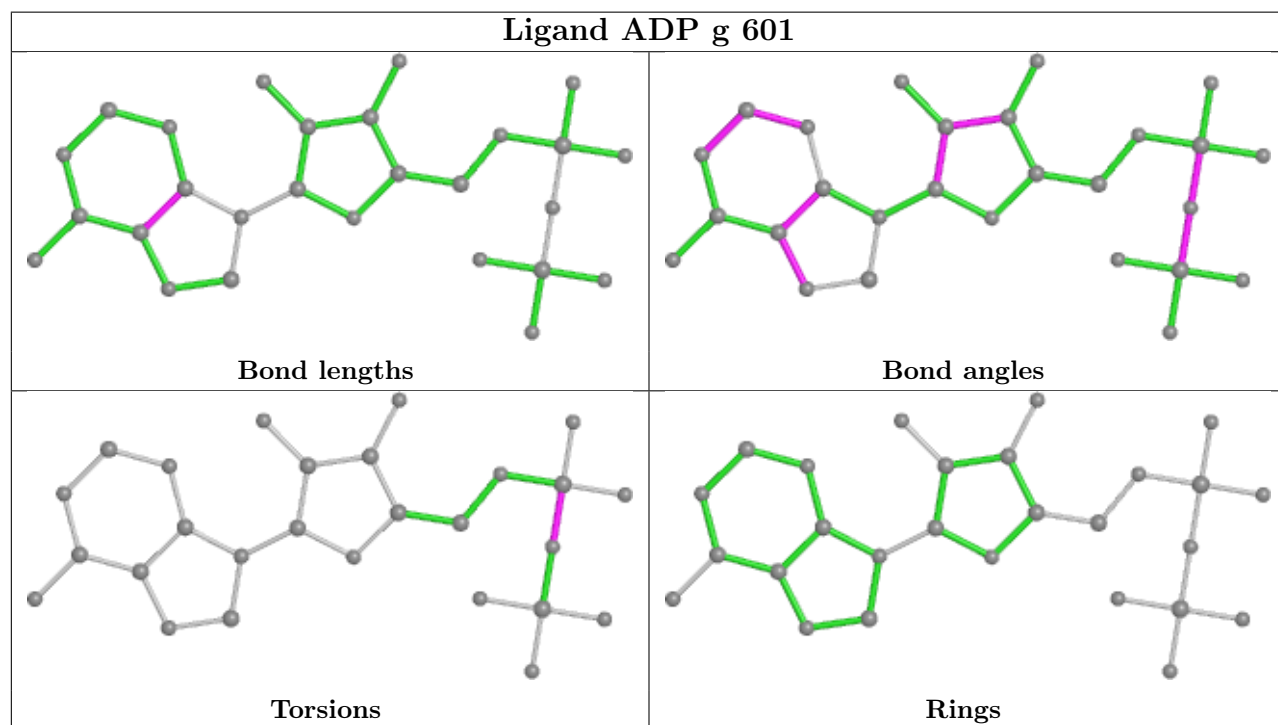
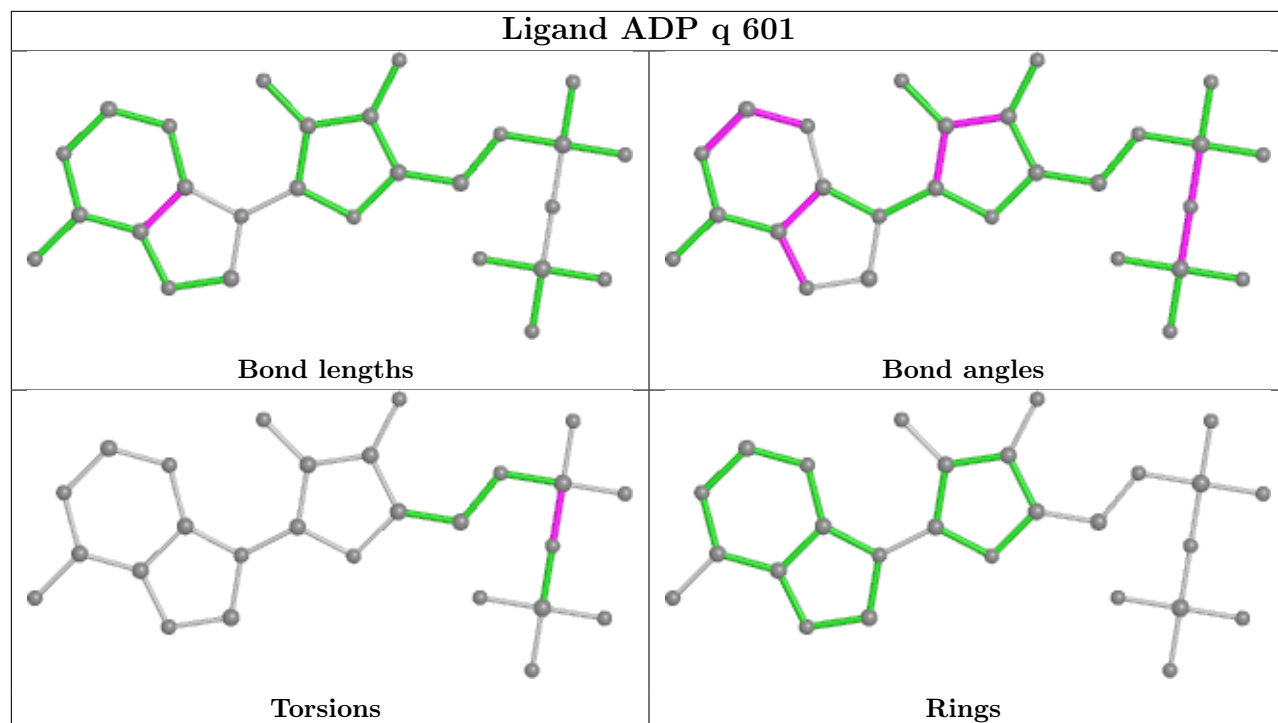
5 of 12 torsion outliers are listed below:

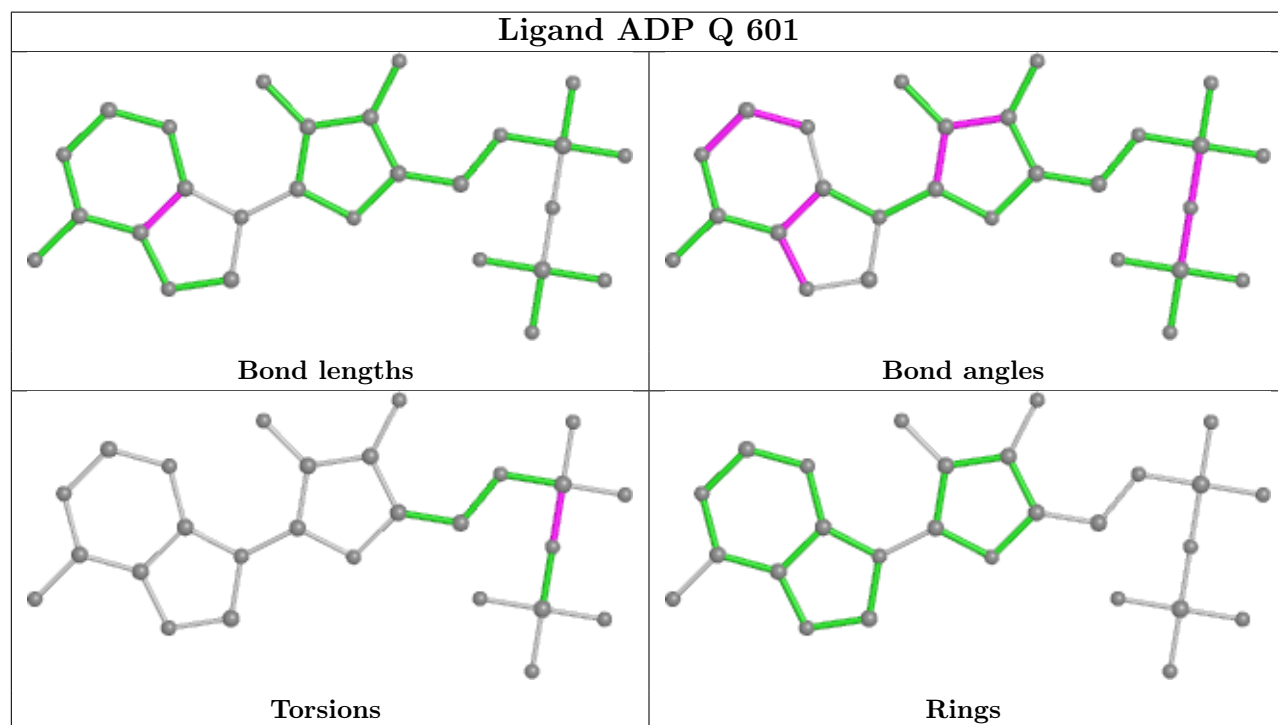
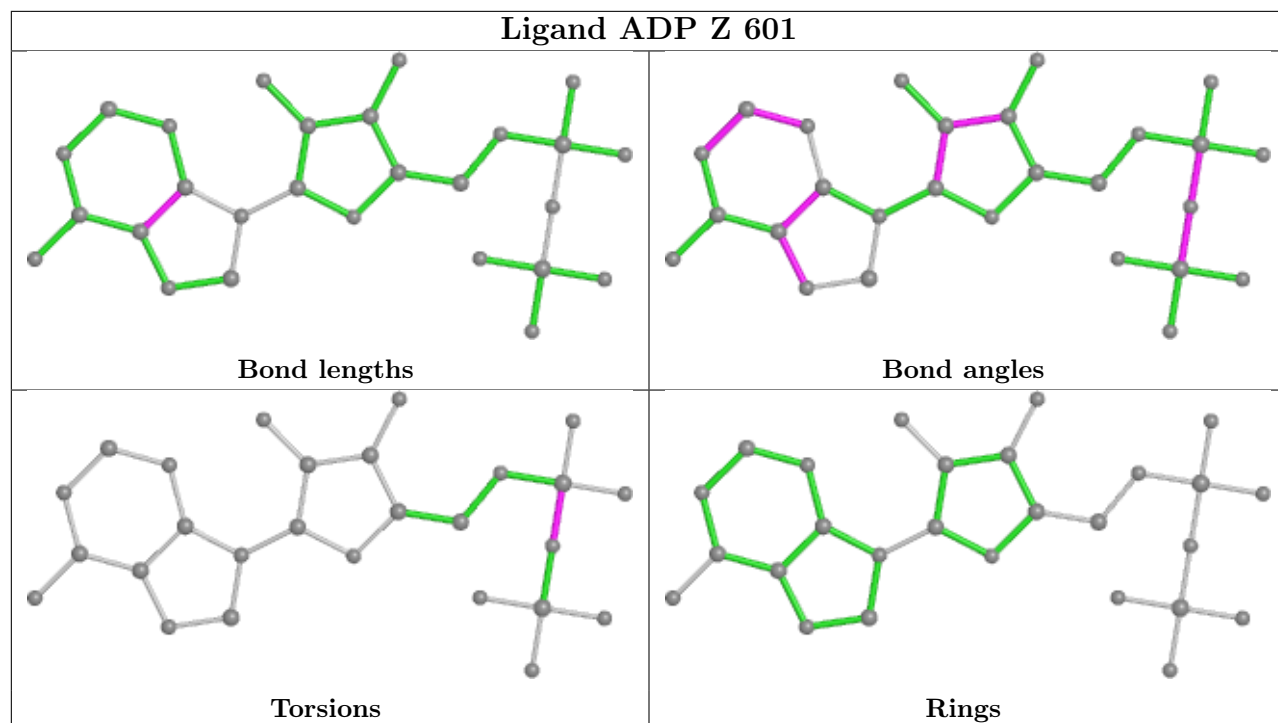
Mol	Chain	Res	Type	Atoms
9	g	601	ADP	PB-O3A-PA-O1A
9	g	601	ADP	PB-O3A-PA-O2A
9	G	601	ADP	PB-O3A-PA-O1A
9	G	601	ADP	PB-O3A-PA-O2A
9	Q	601	ADP	PB-O3A-PA-O1A

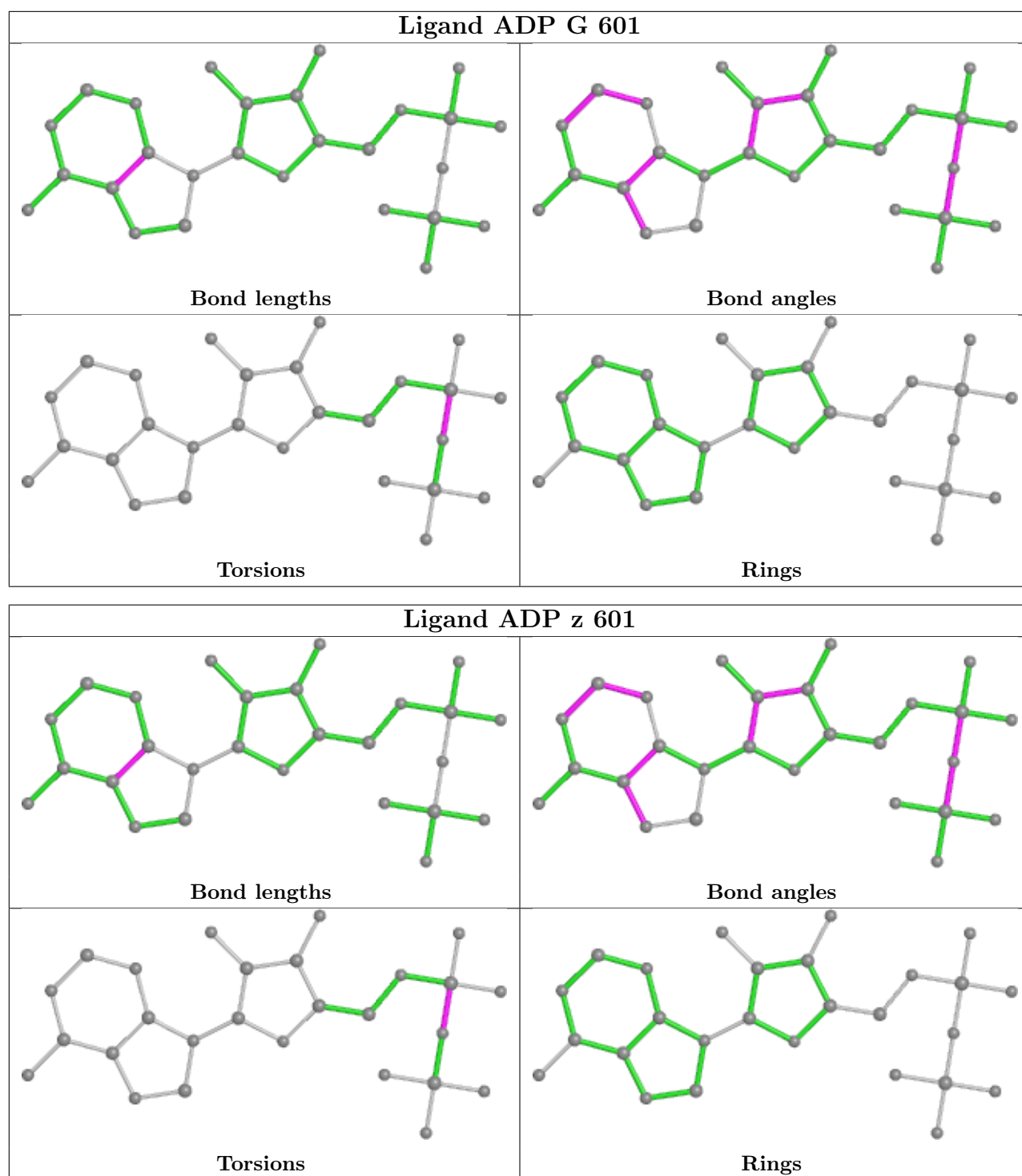
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

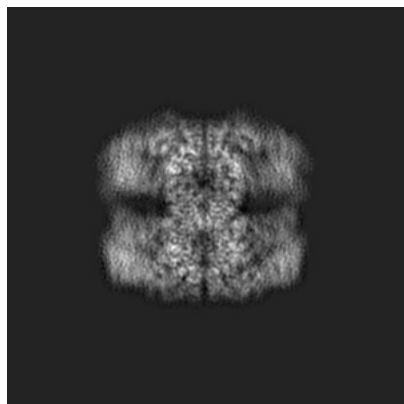
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34852. These allow visual inspection of the internal detail of the map and identification of artifacts.

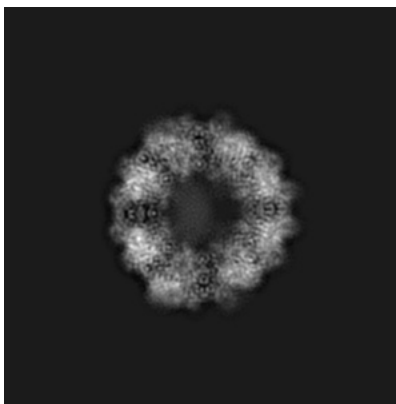
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

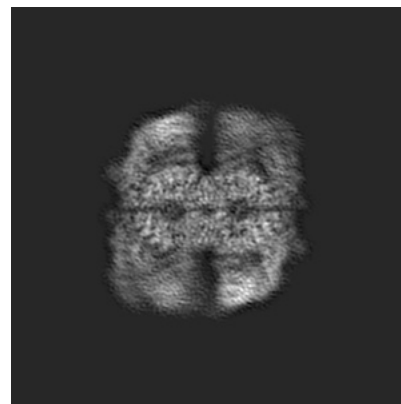
6.1.1 Primary map



X

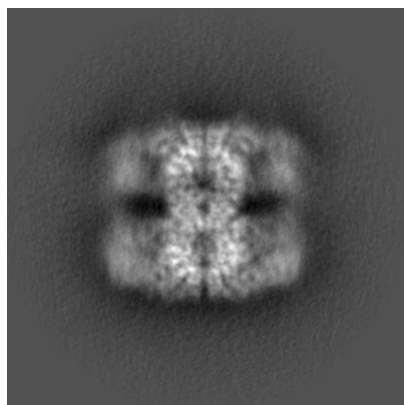


Y

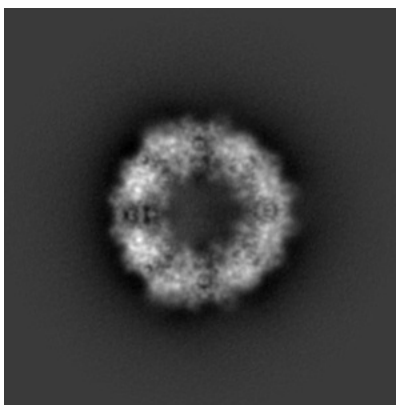


Z

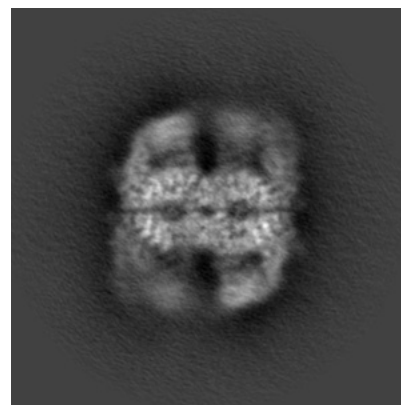
6.1.2 Raw map



X



Y

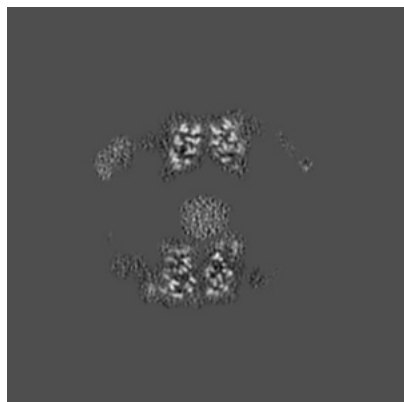


Z

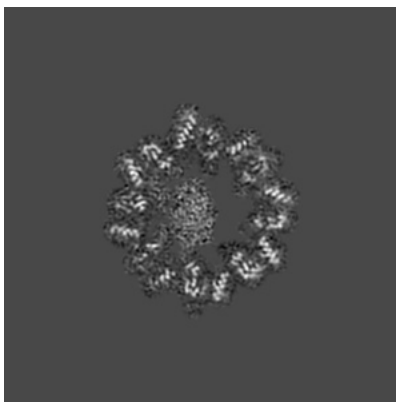
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

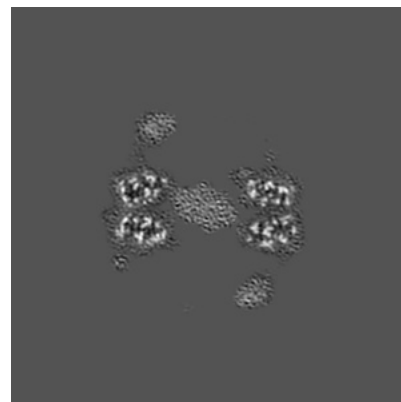
6.2.1 Primary map



X Index: 128

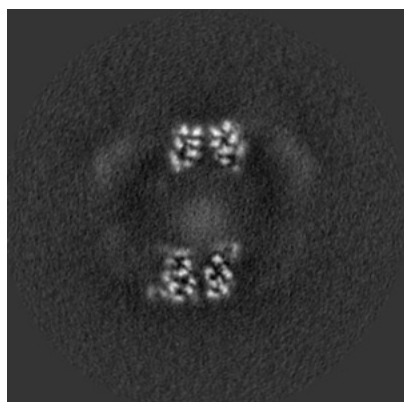


Y Index: 128

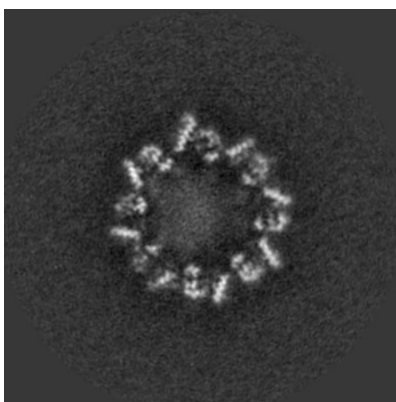


Z Index: 128

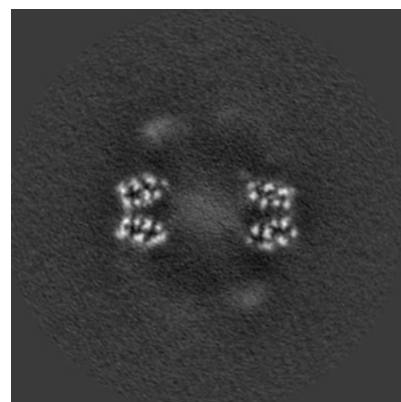
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

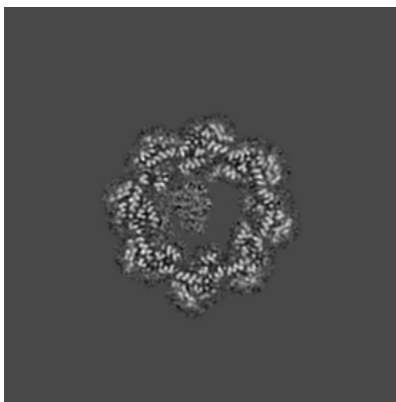
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

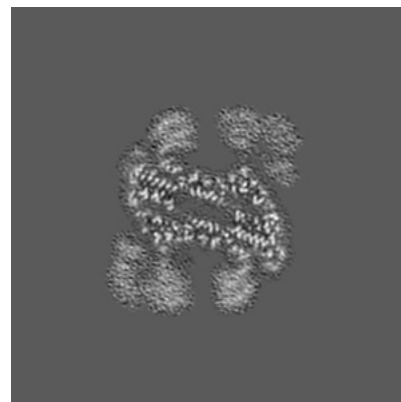
6.3.1 Primary map



X Index: 94

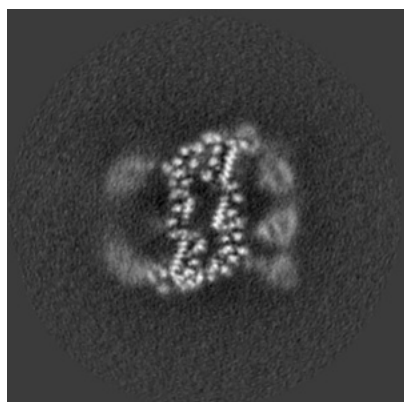


Y Index: 117

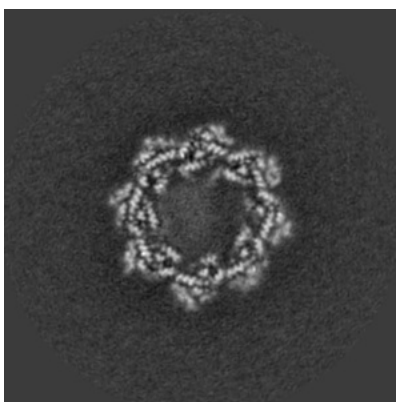


Z Index: 94

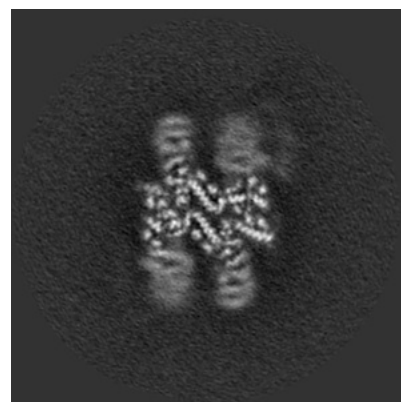
6.3.2 Raw map



X Index: 94



Y Index: 117

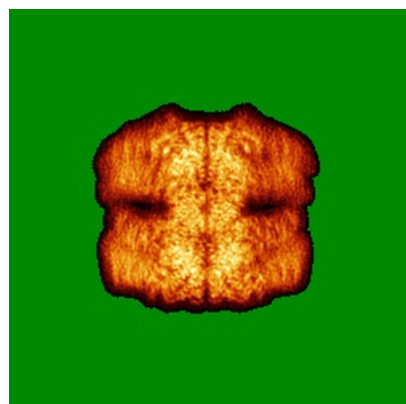


Z Index: 87

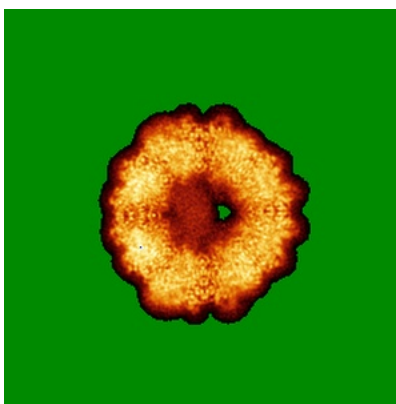
The images above show the largest variance slices of the map in three orthogonal directions.

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

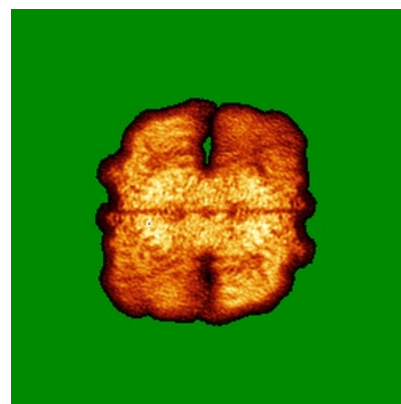
6.4.1 Primary map



X

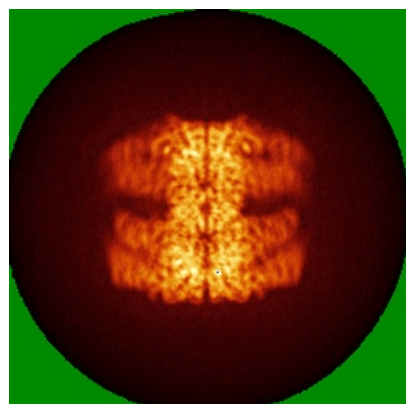


Y

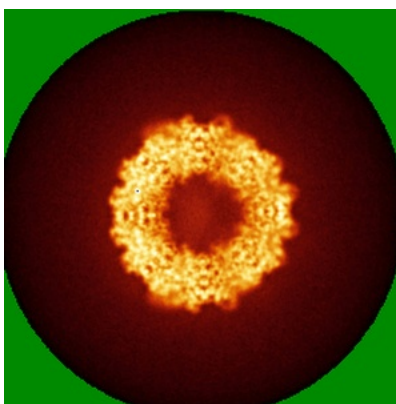


Z

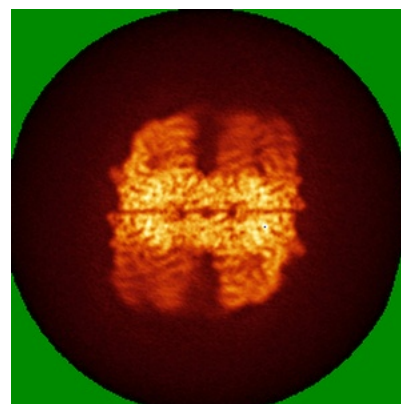
6.4.2 Raw map



X



Y

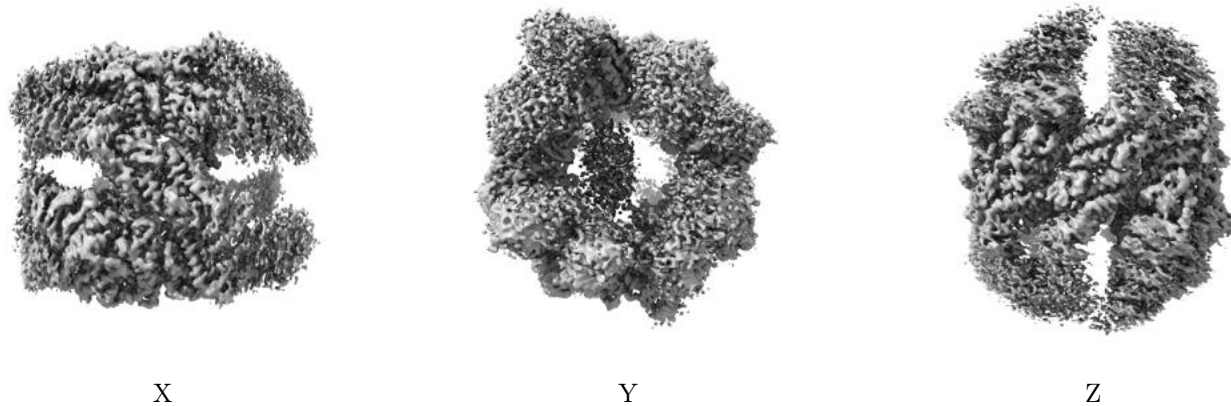


Z

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.

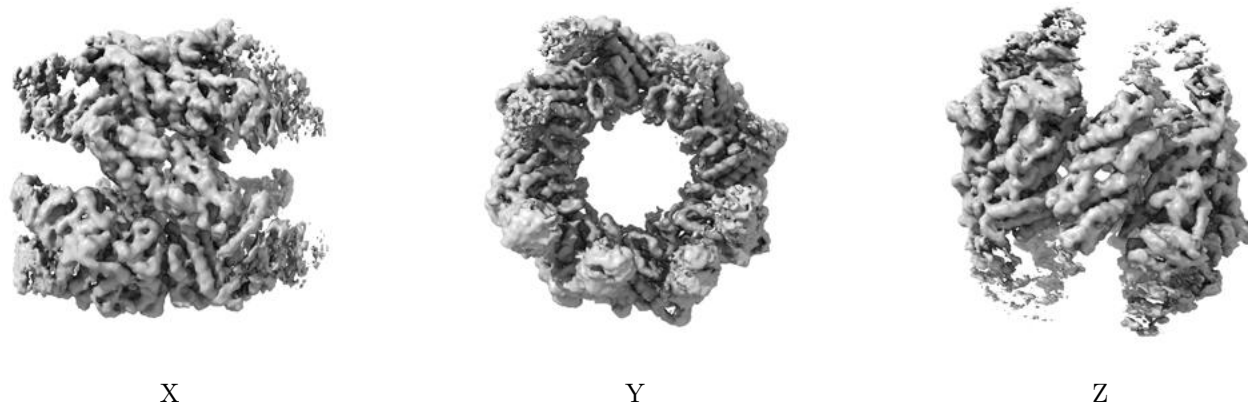
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

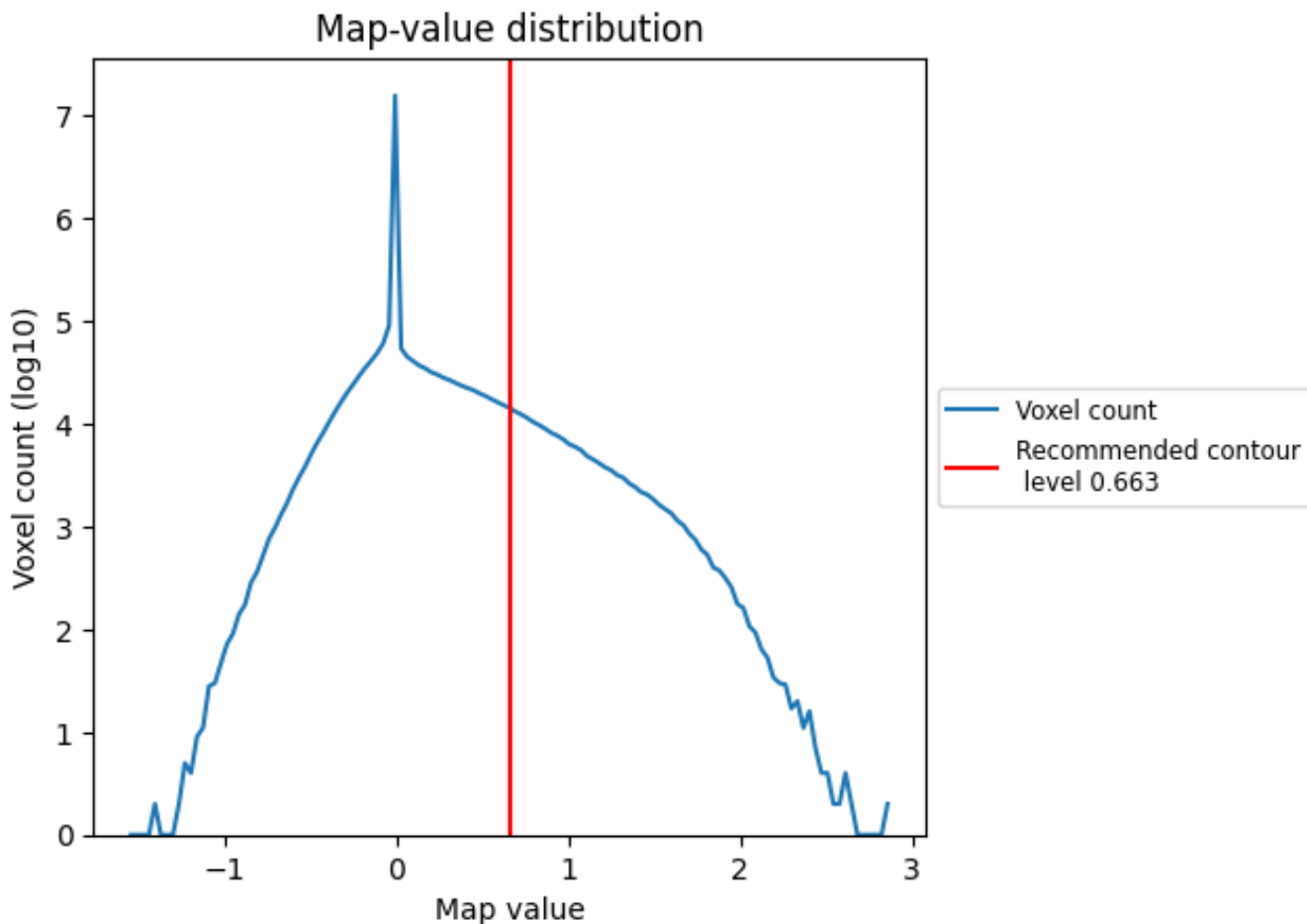
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

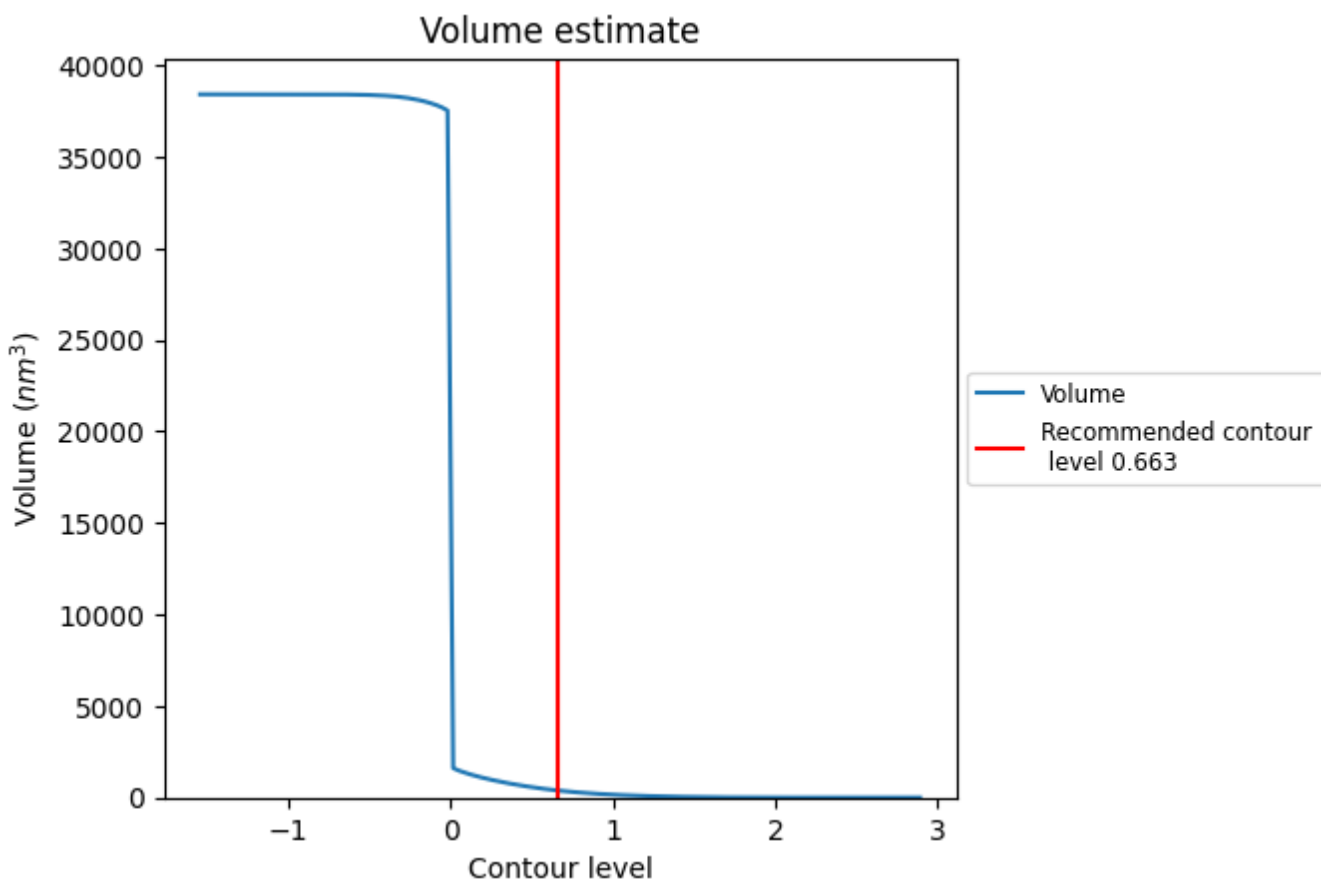
This section contains the results of statistical analysis of the map.

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.

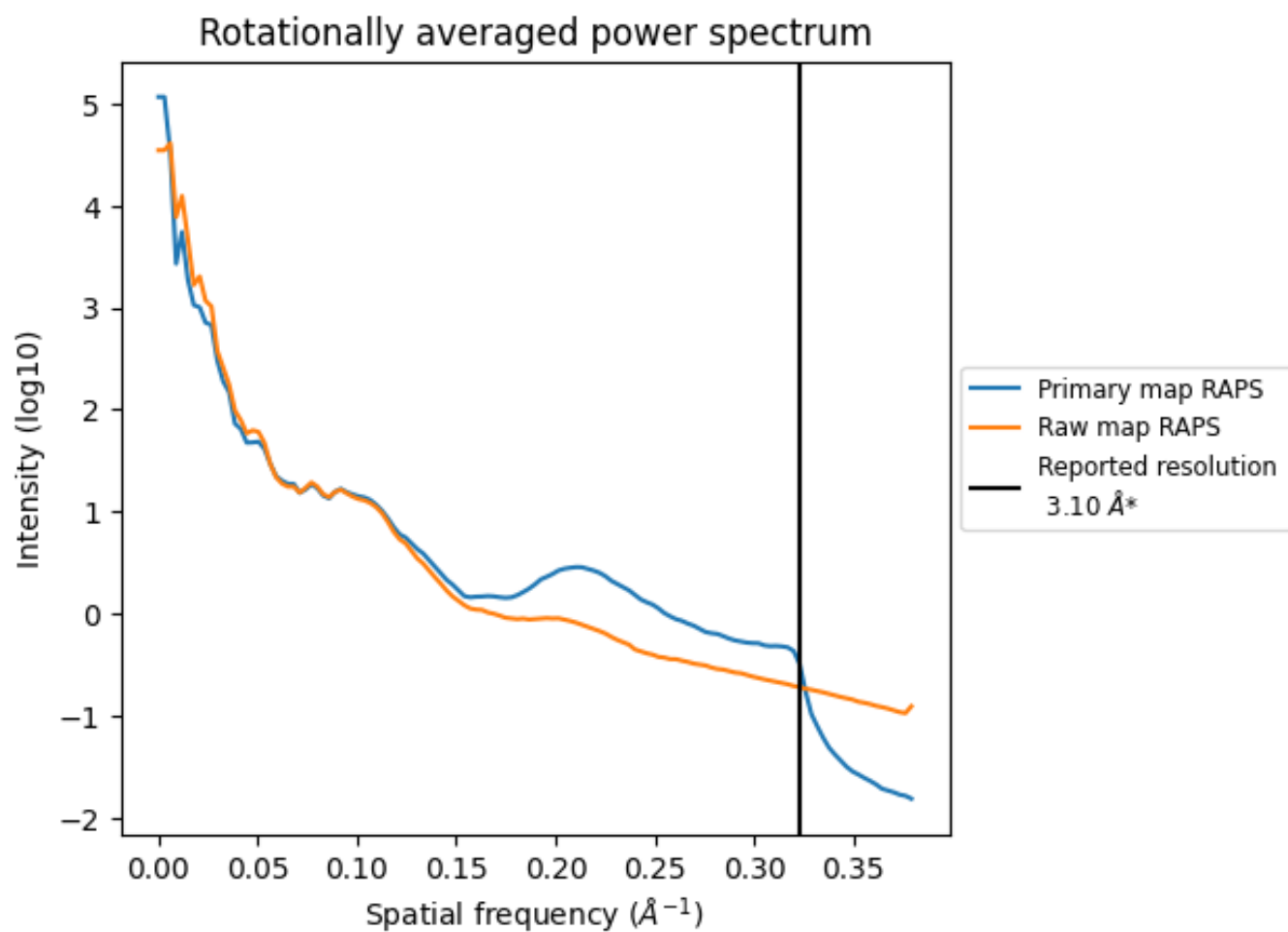
7.2 Volume estimate [i](#)



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 i

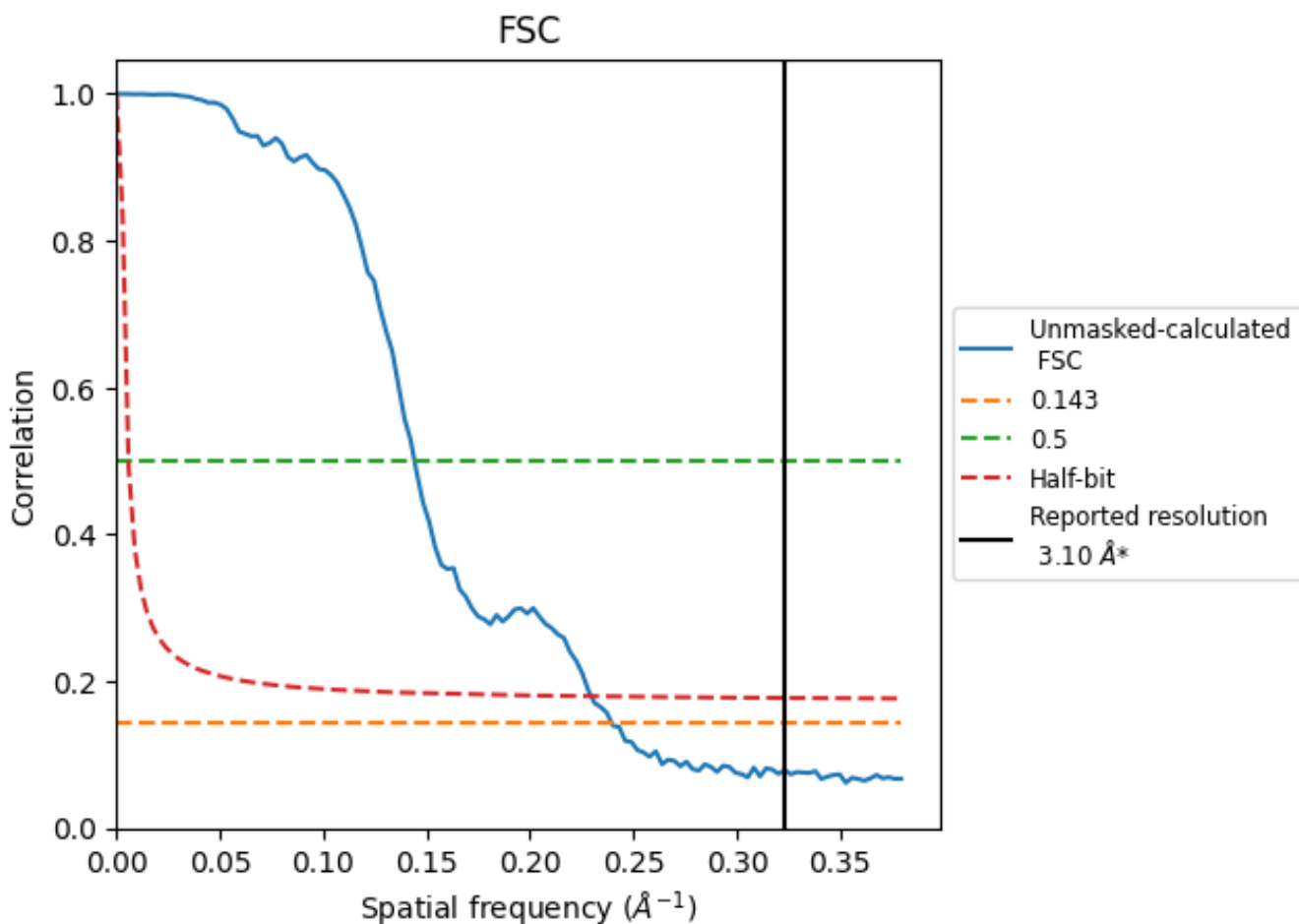


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

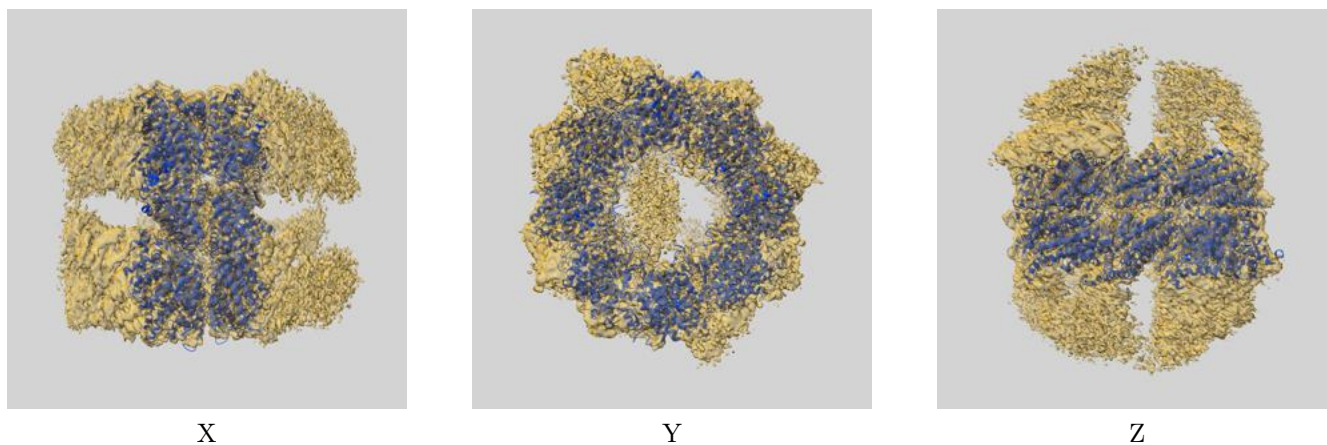
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.94	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

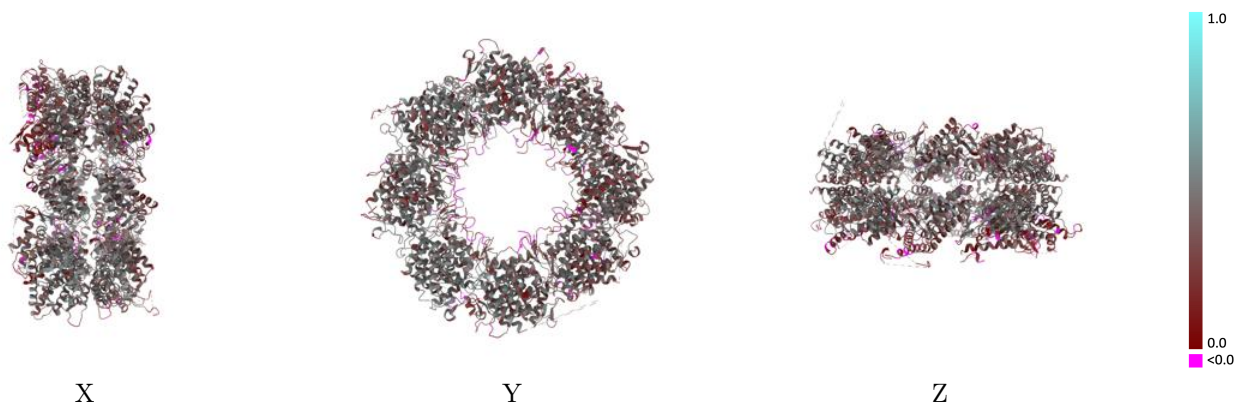
This section contains information regarding the fit between EMDB map EMD-34852 and PDB model 8HKI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



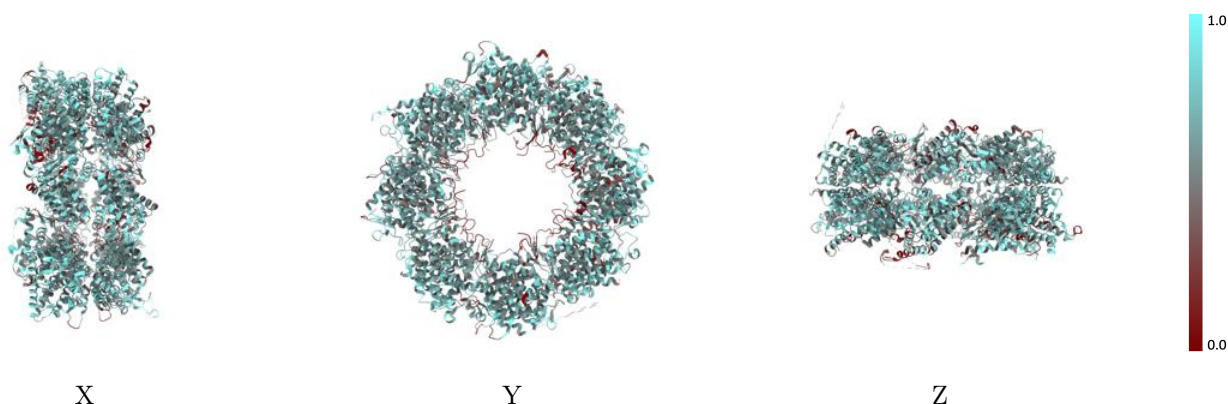
The images above show the 3D surface view of the map at the recommended contour level 0.663 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



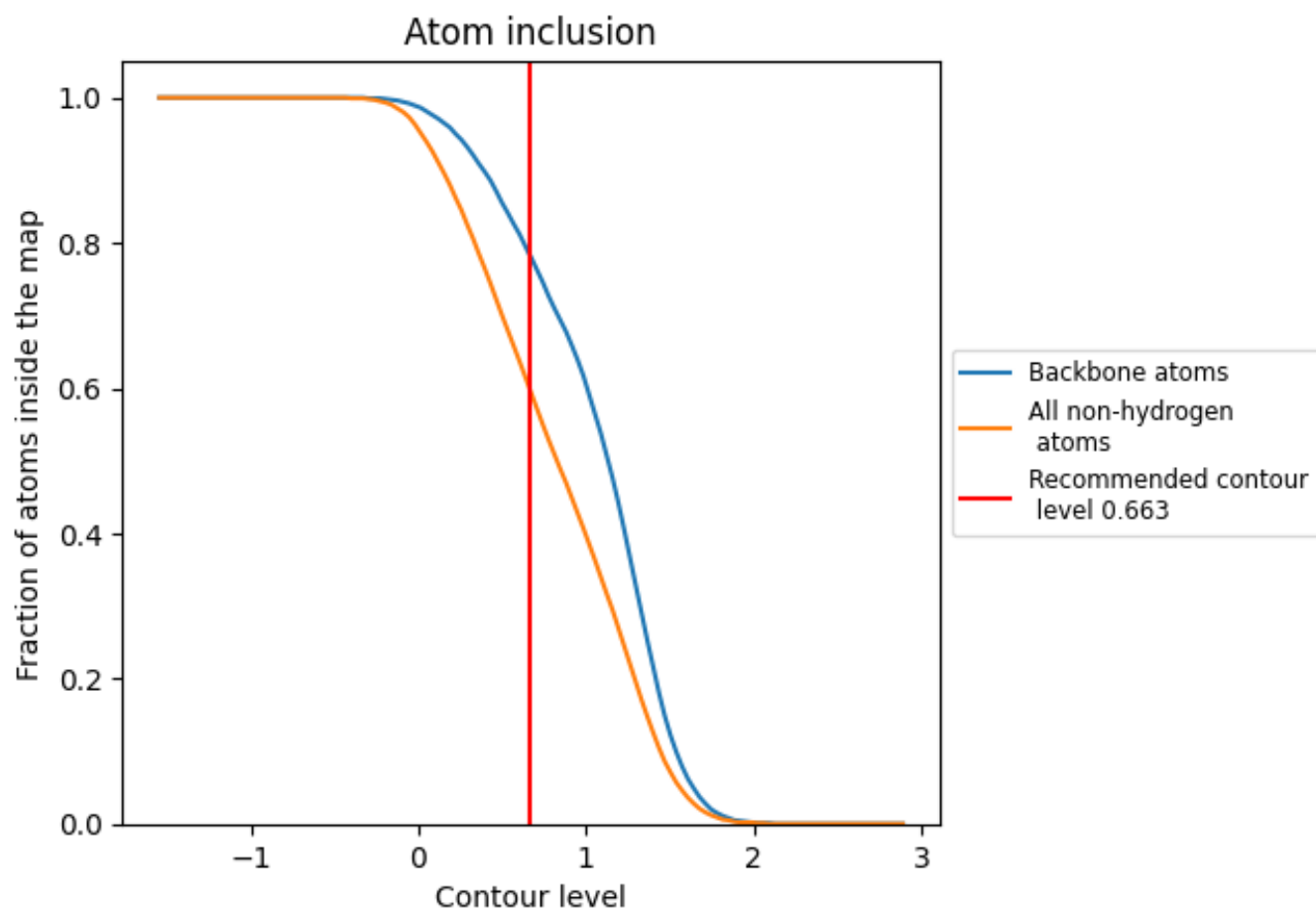
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 60% 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 (0.663) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6000	 0.3660
A	 0.6010	 0.3690
B	 0.5630	 0.3360
D	 0.5920	 0.3570
E	 0.6050	 0.3490
G	 0.6180	 0.3920
H	 0.6120	 0.3850
Q	 0.6000	 0.4040
Z	 0.5940	 0.3800
a	 0.5980	 0.3490
b	 0.5590	 0.3170
d	 0.6080	 0.3630
e	 0.6110	 0.3280
g	 0.6250	 0.4250
h	 0.5940	 0.3400
q	 0.6180	 0.3900
z	 0.6110	 0.3920

