



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 11:19 AM JST

PDB ID : 5GW5
EMDB ID : EMD-9541
Title : Structure of TRiC-AMP-PNP
Authors : Zang, Y.; Jin, M.; Wang, H.; Cong, Y.
Deposited on : 2016-09-08
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

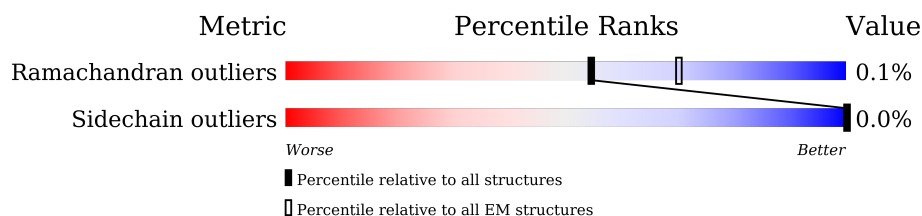
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	559	<div> <div>40%</div> <div>97%</div> </div>
1	a	559	<div> <div>40%</div> <div>97%</div> </div>
2	B	527	<div> <div>31%</div> <div>98%</div> </div>
2	b	527	<div> <div>35%</div> <div>98%</div> </div>
3	D	528	<div> <div>40%</div> <div>99%</div> </div>
3	d	528	<div> <div>46%</div> <div>98%</div> </div>
4	E	562	<div> <div>37%</div> <div>94%</div> <div>6%</div> </div>
4	e	562	<div> <div>35%</div> <div>94%</div> <div>6%</div> </div>
5	G	534	<div> <div>41%</div> <div>97%</div> </div>

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Mol	Chain	Length	Quality of chain
5	g	534	<div> <div>42%</div> <div>97%</div> <div>.</div> </div>
6	H	550	<div> <div>31%</div> <div>94%</div> <div>6%</div> </div>
6	h	550	<div> <div>30%</div> <div>94%</div> <div>6%</div> </div>
7	Q	568	<div> <div>37%</div> <div>95%</div> <div>.</div> </div>
7	q	568	<div> <div>34%</div> <div>95%</div> <div>.</div> </div>
8	Z	546	<div> <div>26%</div> <div>98%</div> <div>.</div> </div>
8	z	546	<div> <div>27%</div> <div>98%</div> <div>.</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 64544 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	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		
1	A	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		
2	B	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		
3	D	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		
4	E	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		
5	G	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		

- 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
			3969	2501	678	771	19		
6	H	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		
7	Q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		

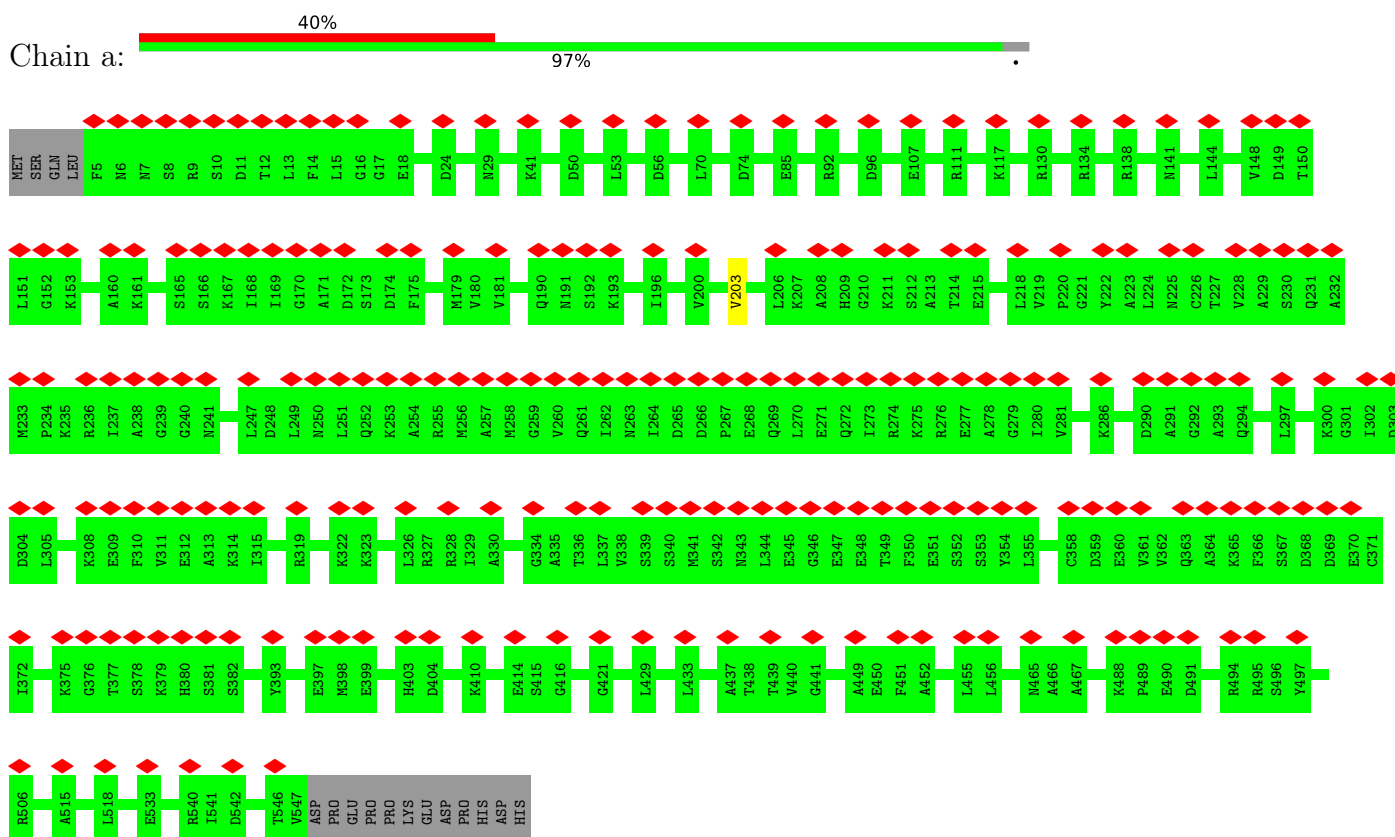
- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		
8	Z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		

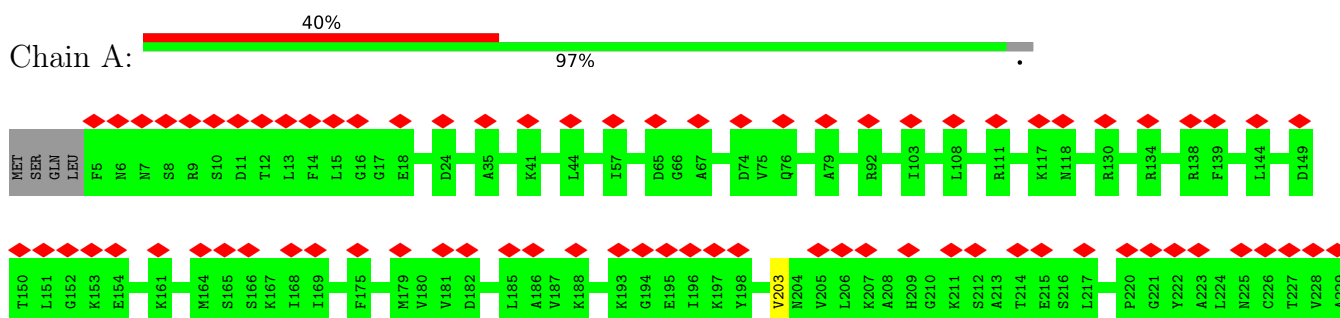
3 Residue-property plots

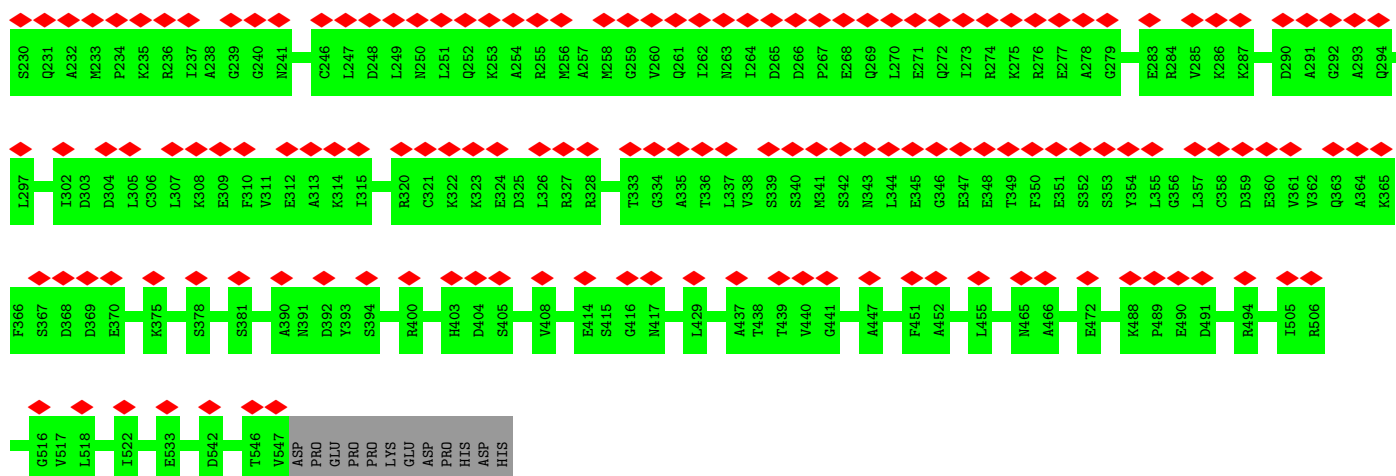
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

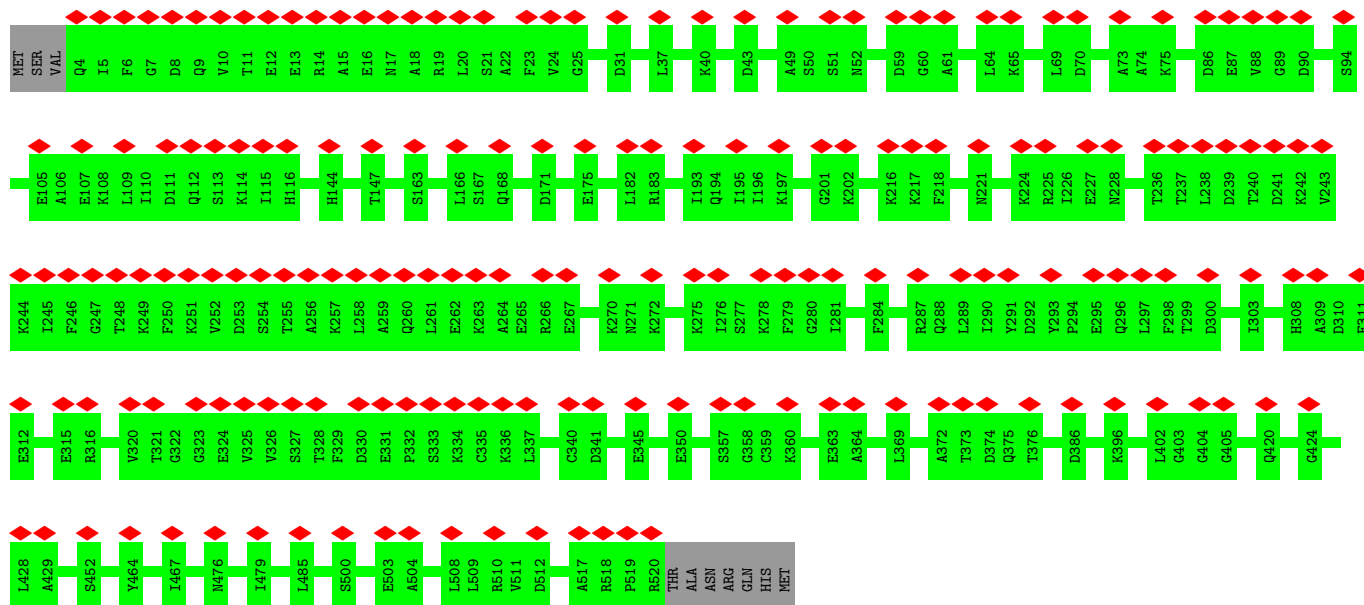


- Molecule 1: T-complex protein 1 subunit alpha

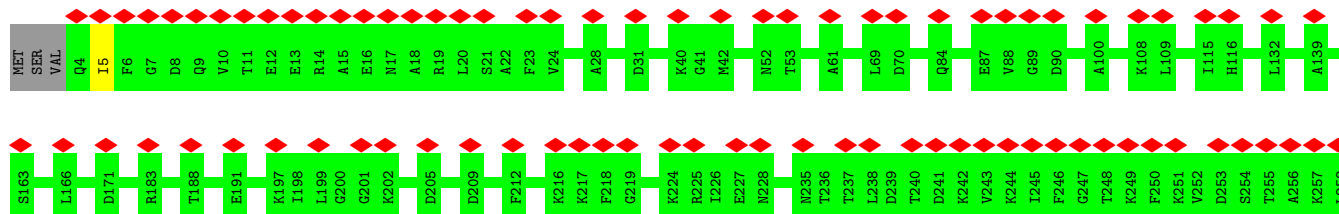




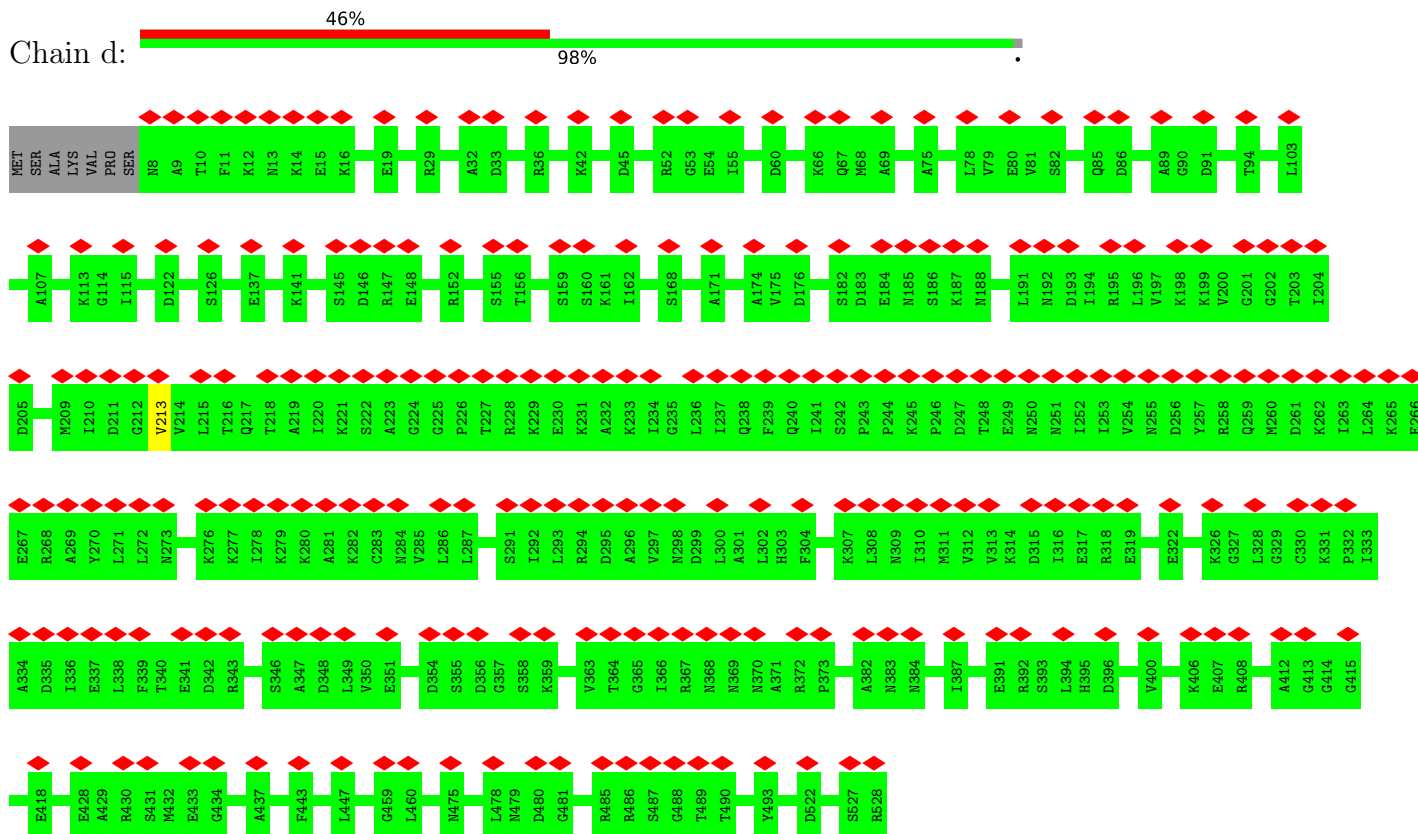
• Molecule 2: T-complex protein 1 subunit beta



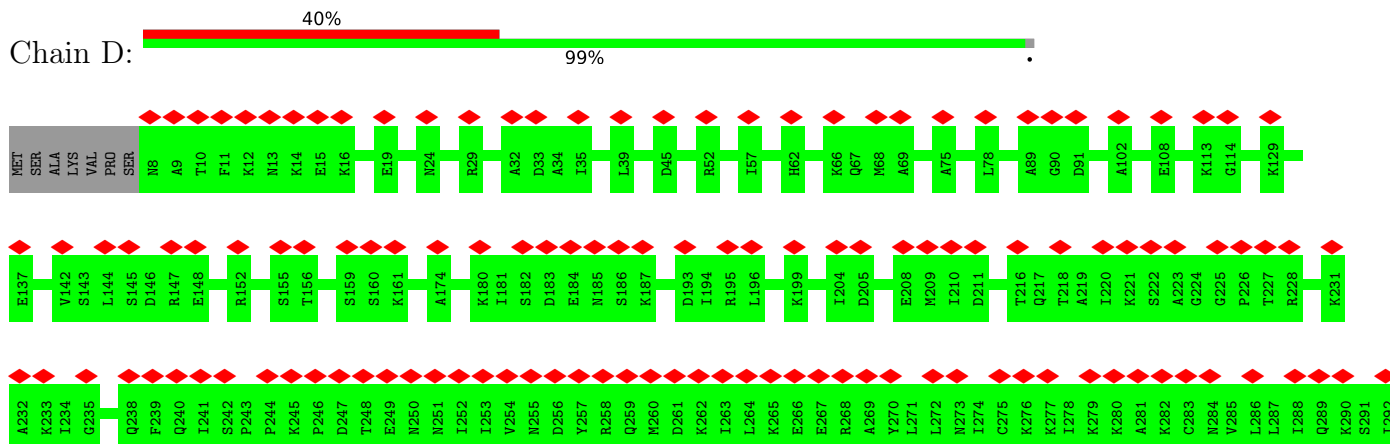
• Molecule 2: T-complex protein 1 subunit beta

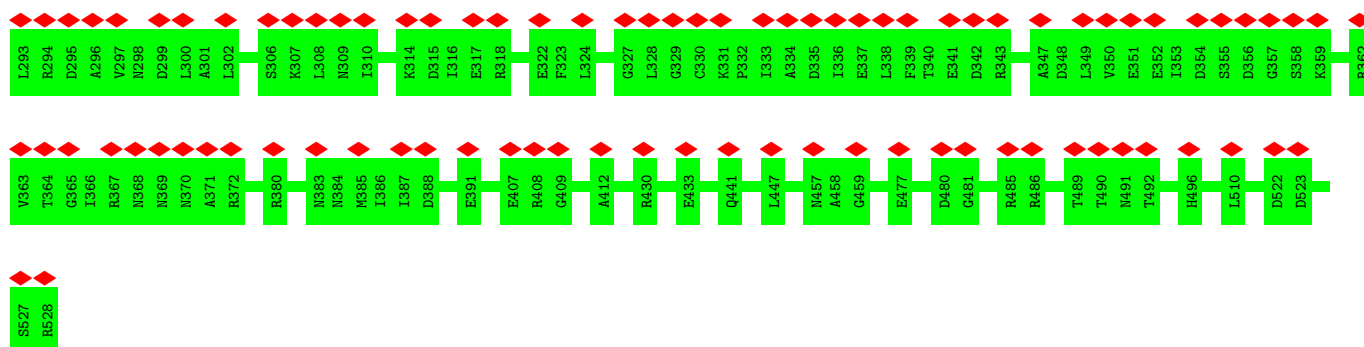


- Molecule 3: T-complex protein 1 subunit delta



- Molecule 3: T-complex protein 1 subunit delta





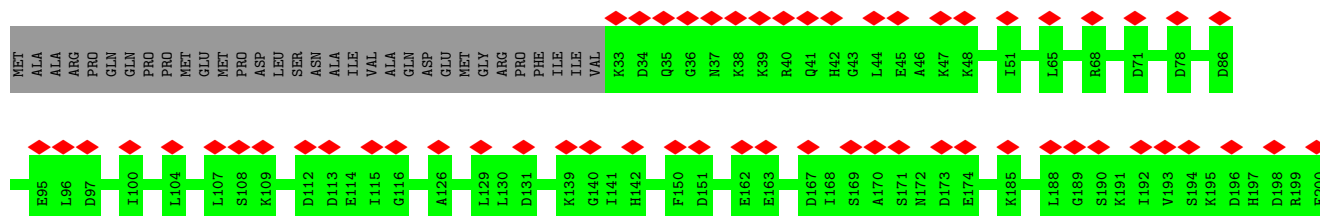
• Molecule 4: T-complex protein 1 subunit epsilon

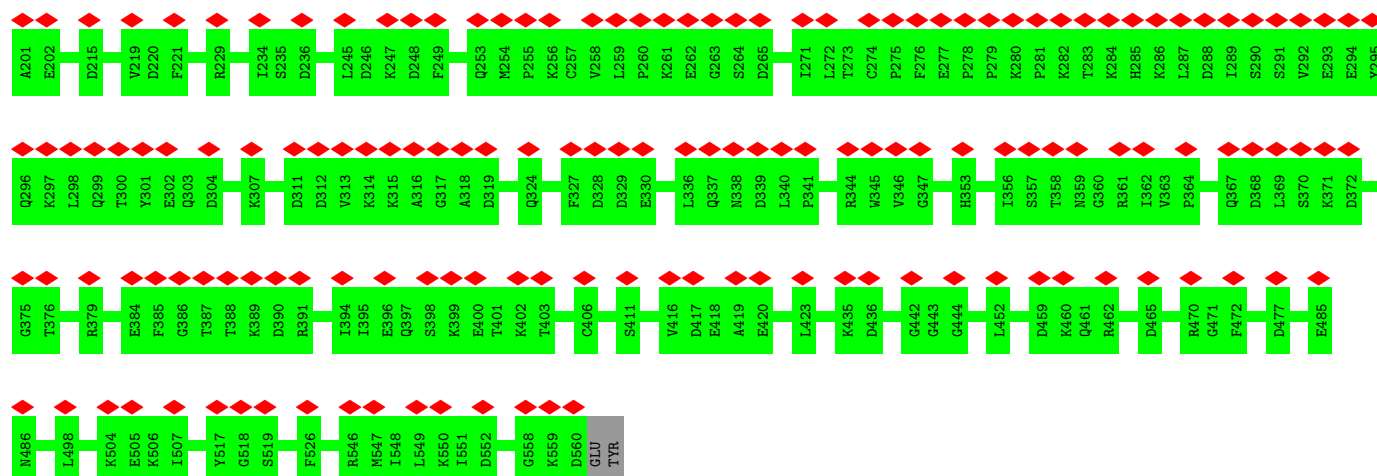
Chain e: 35% 94% 6%



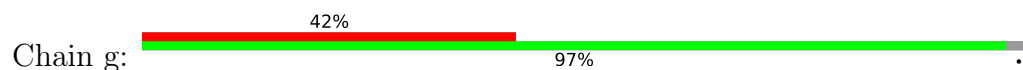
• Molecule 4: T-complex protein 1 subunit epsilon

Chain E: 37% 94% 6%

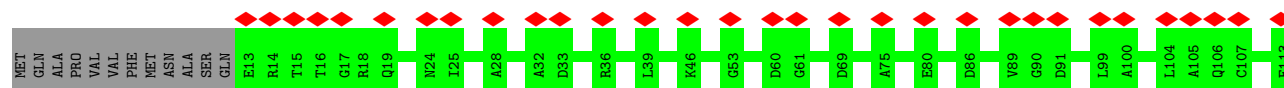
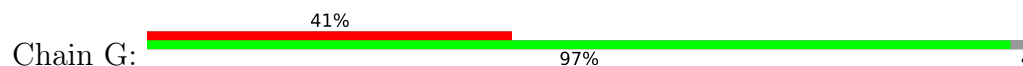




• Molecule 5: T-complex protein 1 subunit gamma

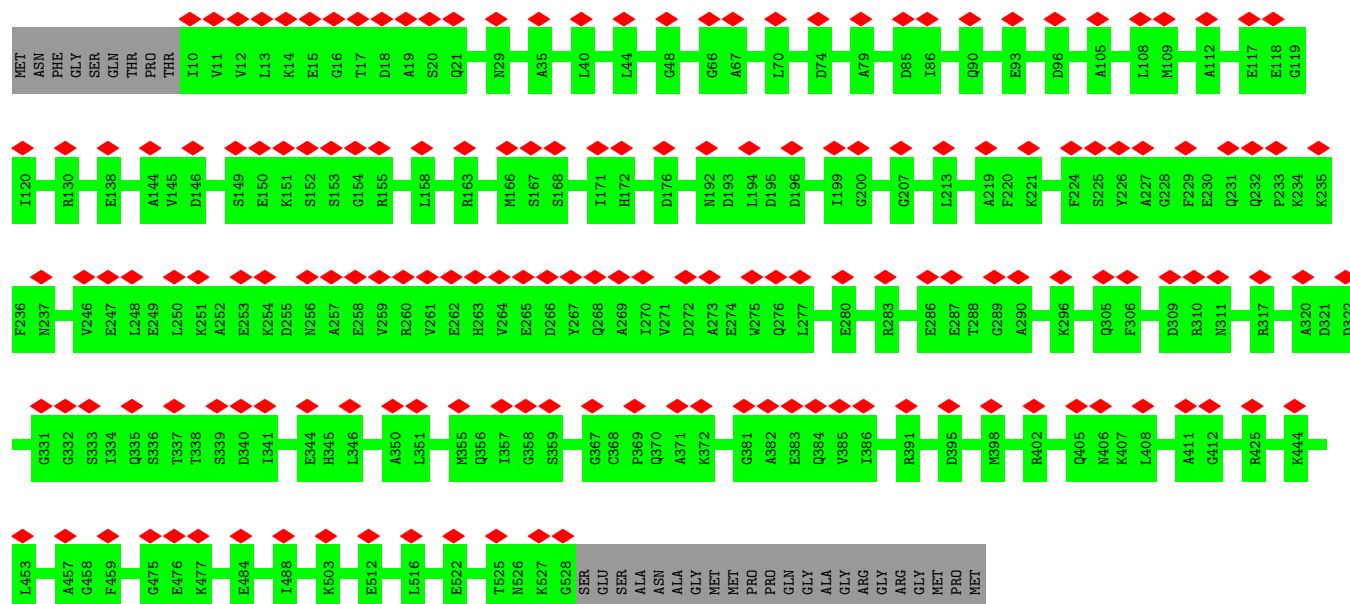


• Molecule 5: T-complex protein 1 subunit gamma

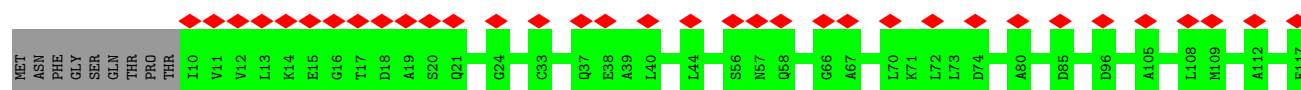


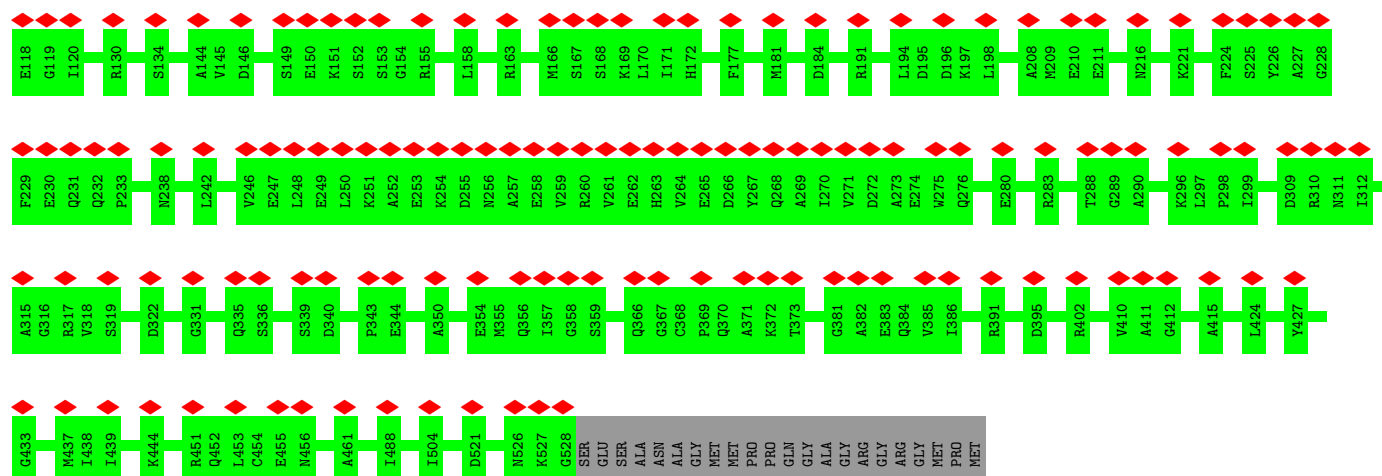


• Molecule 6: T-complex protein 1 subunit eta

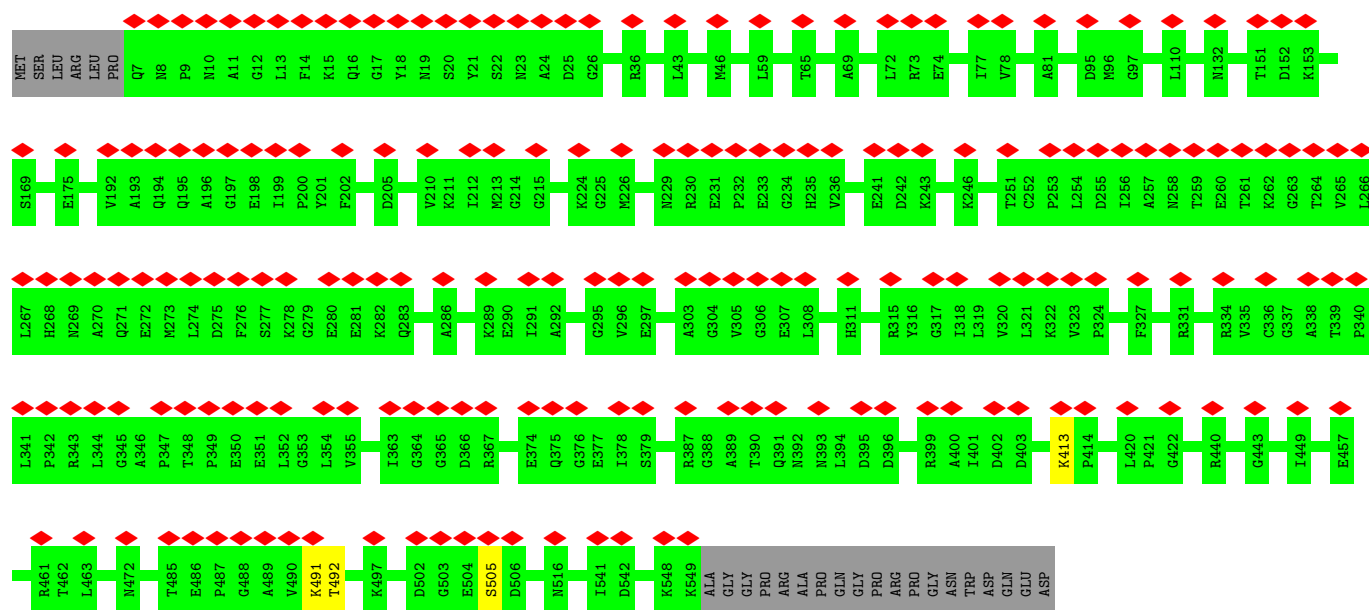


• Molecule 6: T-complex protein 1 subunit eta

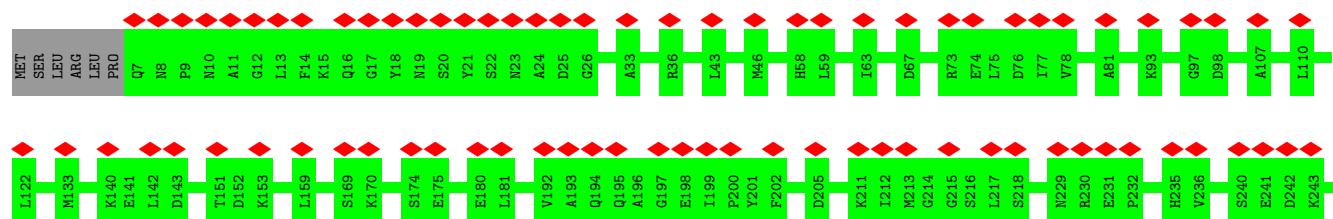


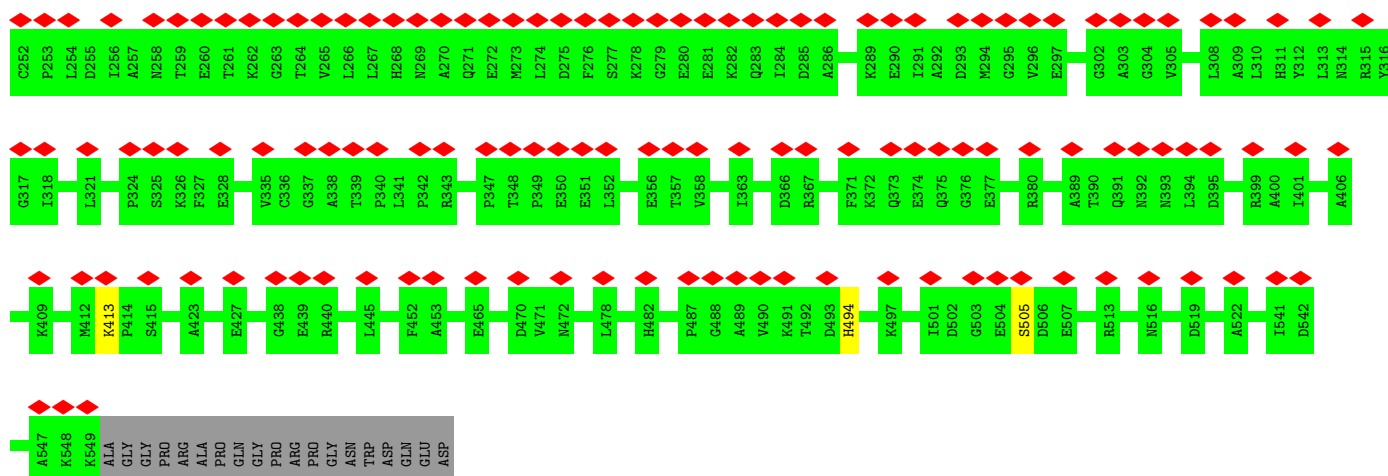


• Molecule 7: T-complex protein 1 subunit theta

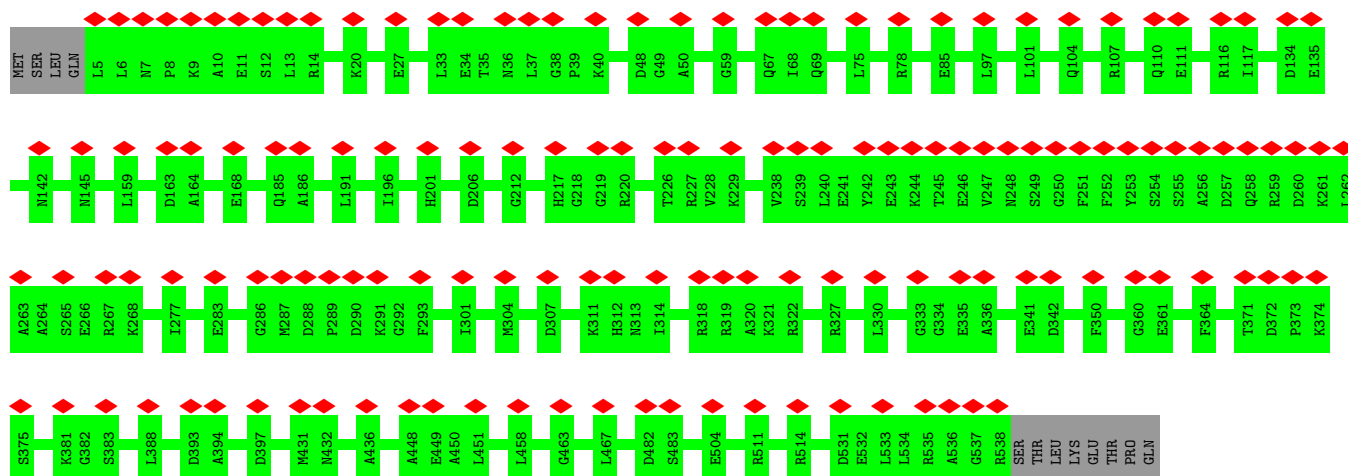


• Molecule 7: T-complex protein 1 subunit theta

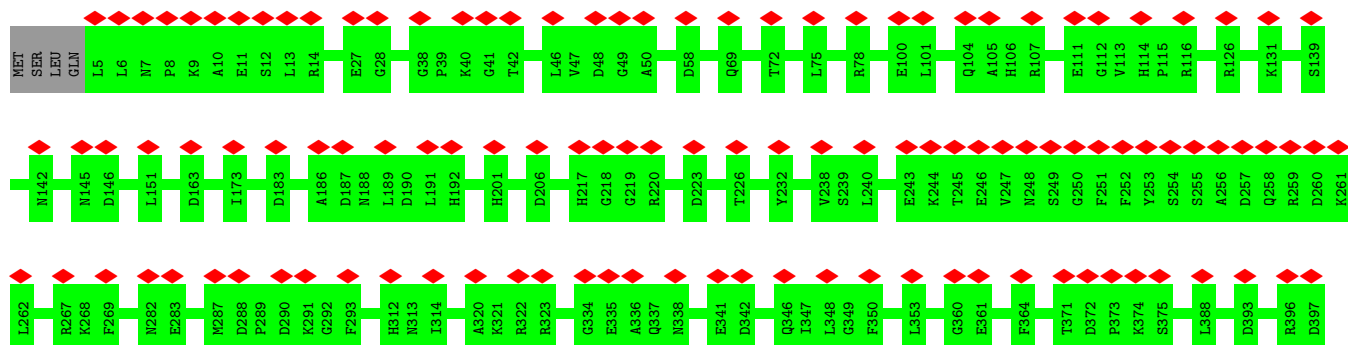




• Molecule 8: T-complex protein 1 subunit zeta



• Molecule 8: T-complex protein 1 subunit zeta



G598	L399	D408	A415	L422	A429	R430	M431	R432	K433	L434	I444	F447	F464	D465	P466	L467	D475	D479	A480	Q481	D482	S483	D484	E485	T486	R487	L493	R494	I495	E504	N526	E532	G537	R538	SER	THR	LEU	LYS	GLU	THR	PRO	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67990	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)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.336	Depositor
Minimum map value	-1.585	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.921	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	0.23	0/4140	0.41	0/5585
1	a	0.23	0/4140	0.41	0/5585
2	B	0.23	0/3969	0.39	0/5348
2	b	0.23	0/3969	0.40	0/5348
3	D	0.23	0/4022	0.39	0/5421
3	d	0.23	0/4022	0.39	0/5421
4	E	0.23	0/4117	0.40	0/5539
4	e	0.23	0/4117	0.39	0/5539
5	G	0.22	0/4029	0.39	0/5442
5	g	0.22	0/4029	0.40	0/5442
6	H	0.23	0/4018	0.39	0/5422
6	h	0.23	0/4018	0.40	0/5422
7	Q	0.29	1/4175 (0.0%)	0.40	0/5636
7	q	0.29	1/4175 (0.0%)	0.41	0/5636
8	Z	0.23	0/4162	0.41	0/5624
8	z	0.23	0/4162	0.39	0/5624
All	All	0.24	2/65264 (0.0%)	0.40	0/88034

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
7	q	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	q	413	LYS	C-N	11.30	1.55	1.34
7	Q	413	LYS	C-N	11.25	1.55	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	q	491	LYS	Peptide
7	q	505	SER	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	541/559 (97%)	507 (94%)	33 (6%)	1 (0%)	47	81
1	a	541/559 (97%)	501 (93%)	39 (7%)	1 (0%)	47	81
2	B	515/527 (98%)	490 (95%)	23 (4%)	2 (0%)	34	72
2	b	515/527 (98%)	486 (94%)	29 (6%)	0	100	100
3	D	519/528 (98%)	494 (95%)	25 (5%)	0	100	100
3	d	519/528 (98%)	494 (95%)	24 (5%)	1 (0%)	47	81
4	E	526/562 (94%)	502 (95%)	24 (5%)	0	100	100
4	e	526/562 (94%)	503 (96%)	23 (4%)	0	100	100
5	G	516/534 (97%)	496 (96%)	20 (4%)	0	100	100
5	g	516/534 (97%)	491 (95%)	25 (5%)	0	100	100
6	H	517/550 (94%)	497 (96%)	20 (4%)	0	100	100
6	h	517/550 (94%)	497 (96%)	20 (4%)	0	100	100
7	Q	541/568 (95%)	520 (96%)	19 (4%)	2 (0%)	34	72
7	q	541/568 (95%)	516 (95%)	25 (5%)	0	100	100
8	Z	532/546 (97%)	513 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	z	532/546 (97%)	518 (97%)	14 (3%)	0	100	100
All	All	8414/8748 (96%)	8025 (95%)	382 (4%)	7 (0%)	54	85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Q	505	SER
7	Q	494	HIS
2	B	5	ILE
3	d	213	VAL
2	B	467	ILE
1	a	203	VAL
1	A	203	VAL

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	455/471 (97%)	455 (100%)	0	100	100
1	a	455/471 (97%)	455 (100%)	0	100	100
2	B	432/441 (98%)	432 (100%)	0	100	100
2	b	432/441 (98%)	432 (100%)	0	100	100
3	D	447/453 (99%)	447 (100%)	0	100	100
3	d	447/453 (99%)	447 (100%)	0	100	100
4	E	454/483 (94%)	454 (100%)	0	100	100
4	e	454/483 (94%)	454 (100%)	0	100	100
5	G	441/455 (97%)	441 (100%)	0	100	100
5	g	441/455 (97%)	441 (100%)	0	100	100
6	H	432/454 (95%)	432 (100%)	0	100	100
6	h	432/454 (95%)	432 (100%)	0	100	100
7	Q	454/473 (96%)	454 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	q	454/473 (96%)	453 (100%)	1 (0%)	93	96
8	Z	451/463 (97%)	451 (100%)	0	100	100
8	z	451/463 (97%)	451 (100%)	0	100	100
All	All	7132/7386 (97%)	7131 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	q	492	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	417	ASN
1	A	190	GLN
2	b	192	HIS
2	b	304	ASN
2	b	420	GLN
2	B	420	GLN
3	d	250	ASN
3	d	284	ASN
3	D	250	ASN
3	D	284	ASN
3	D	395	HIS
4	e	111	GLN
4	e	397	GLN
4	e	432	ASN
4	e	502	GLN
4	E	42	HIS
4	E	241	ASN
4	E	466	GLN
4	E	502	GLN
5	g	85	GLN
5	g	188	GLN
5	g	479	ASN
5	G	85	GLN
5	G	188	GLN
5	G	438	GLN
6	H	232	GLN
6	H	435	GLN

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Mol	Chain	Res	Type
6	H	526	ASN
7	q	373	GLN
7	q	494	HIS
7	Q	91	GLN
7	Q	129	GLN
7	Q	314	ASN
7	Q	373	GLN
7	Q	494	HIS
8	z	230	ASN
8	z	237	ASN
8	z	356	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](#)

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.

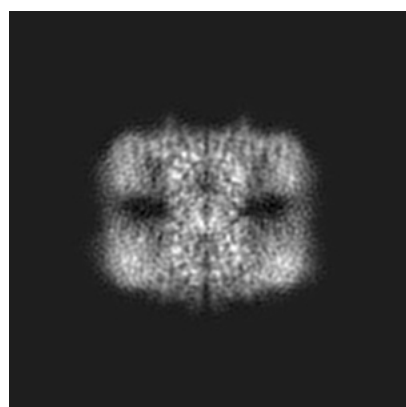
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9541. These allow visual inspection of the internal detail of the map and identification of artifacts.

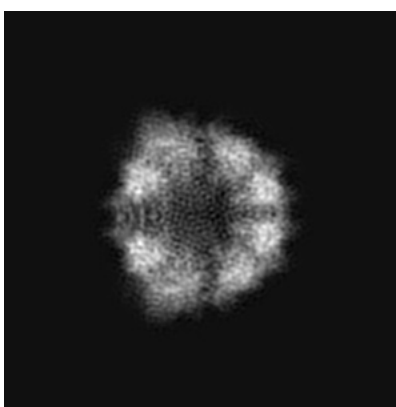
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

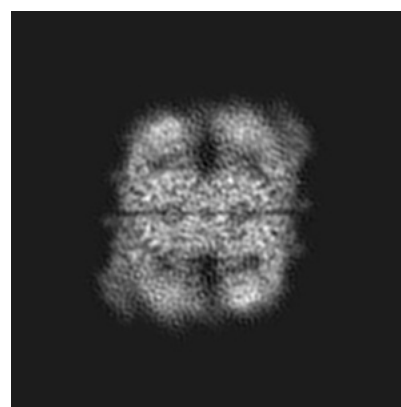
6.1.1 Primary map



X



Y

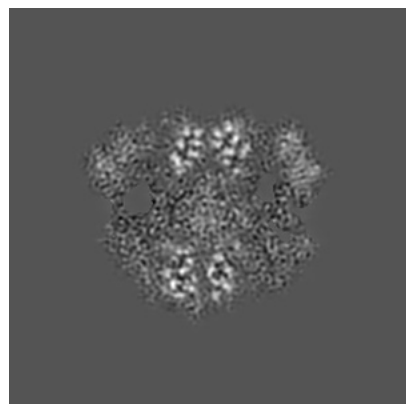


Z

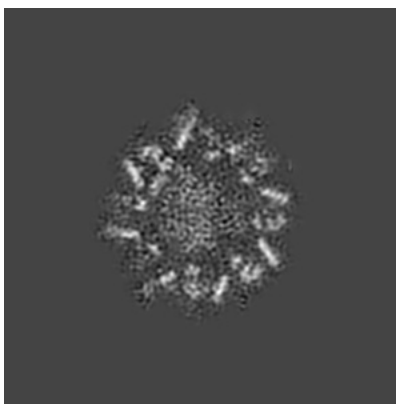
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

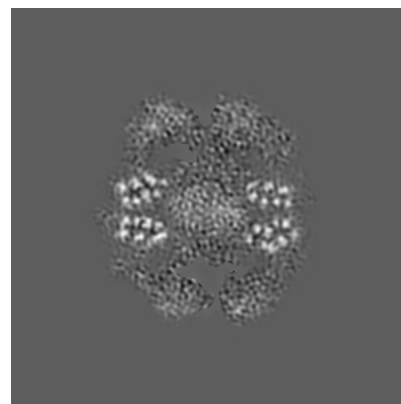
6.2.1 Primary map



X Index: 128



Y Index: 128

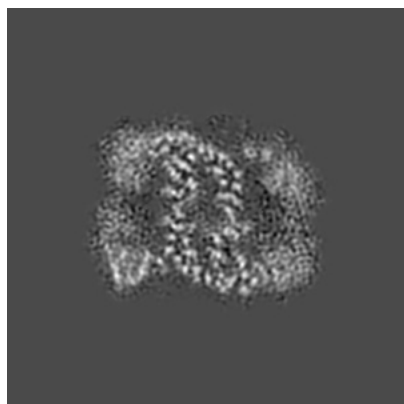


Z Index: 128

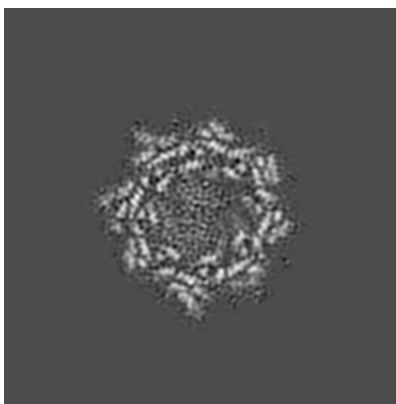
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

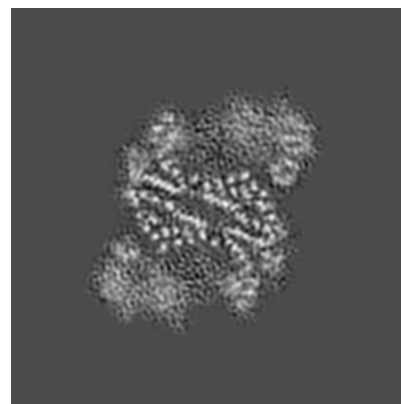
6.3.1 Primary map



X Index: 151



Y Index: 117



Z Index: 96

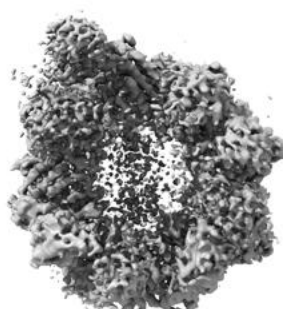
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

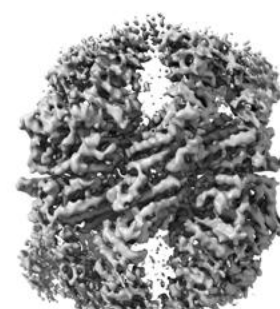
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.921. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

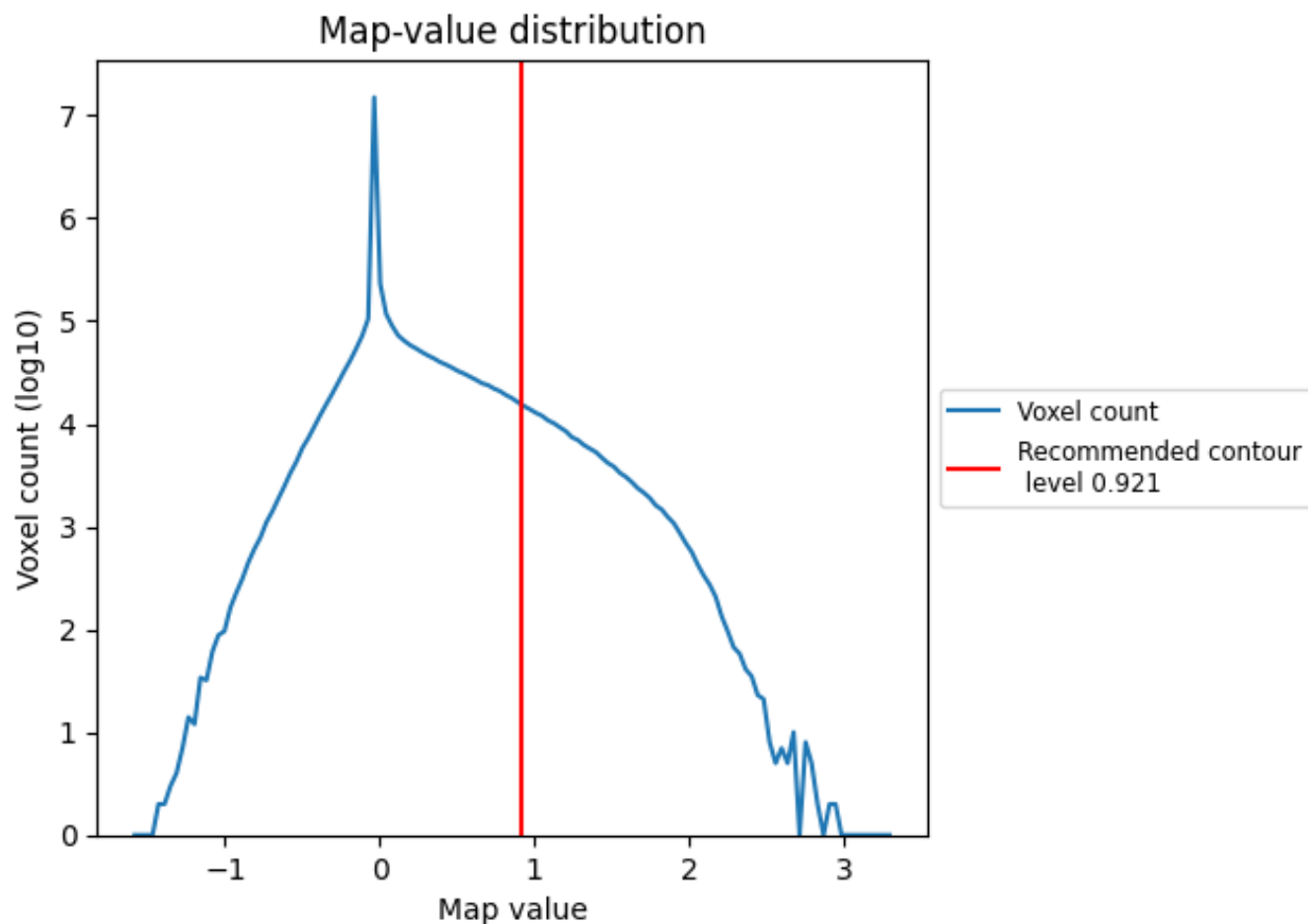
6.5 Mask visualisation

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

7 Map analysis [i](#)

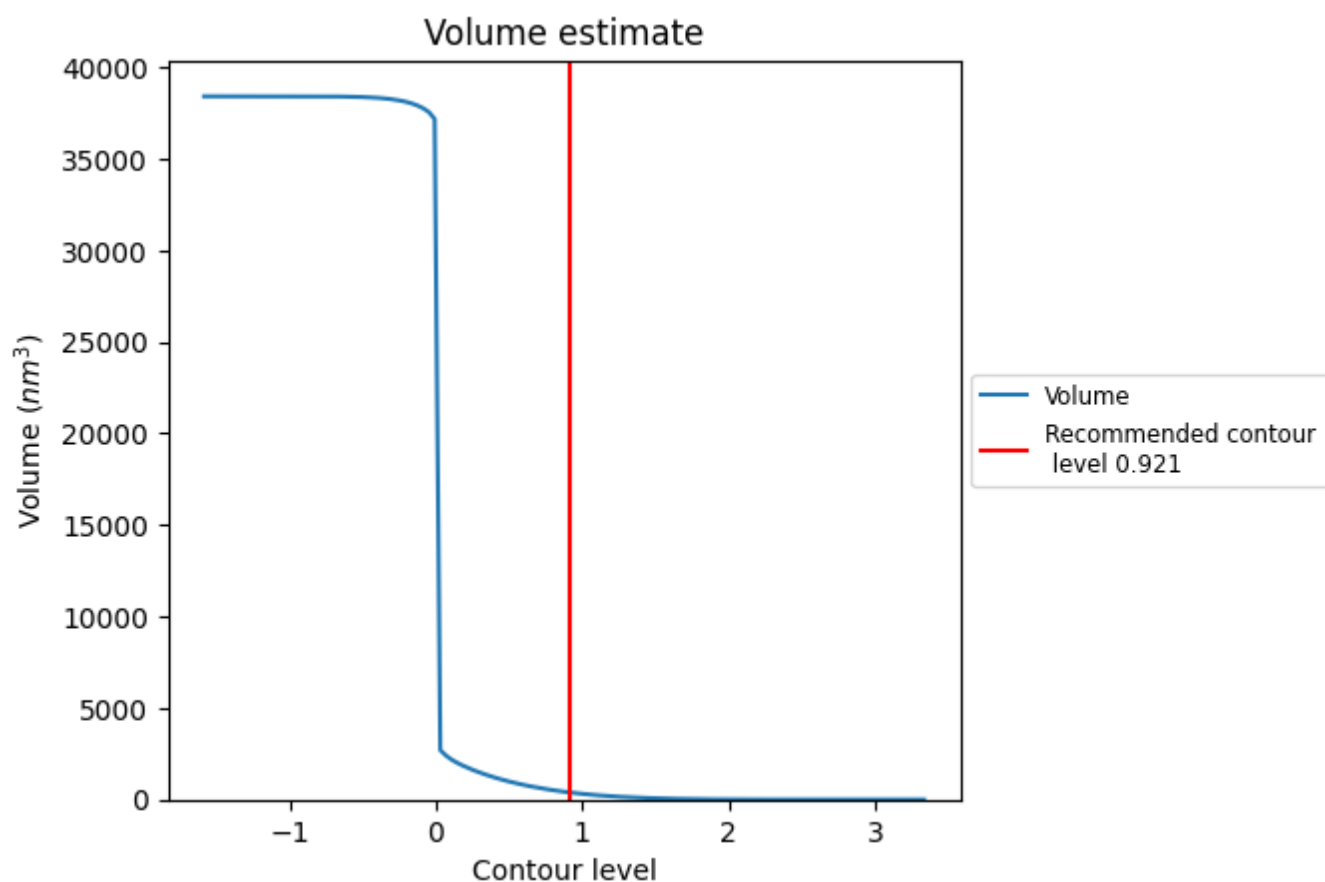
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

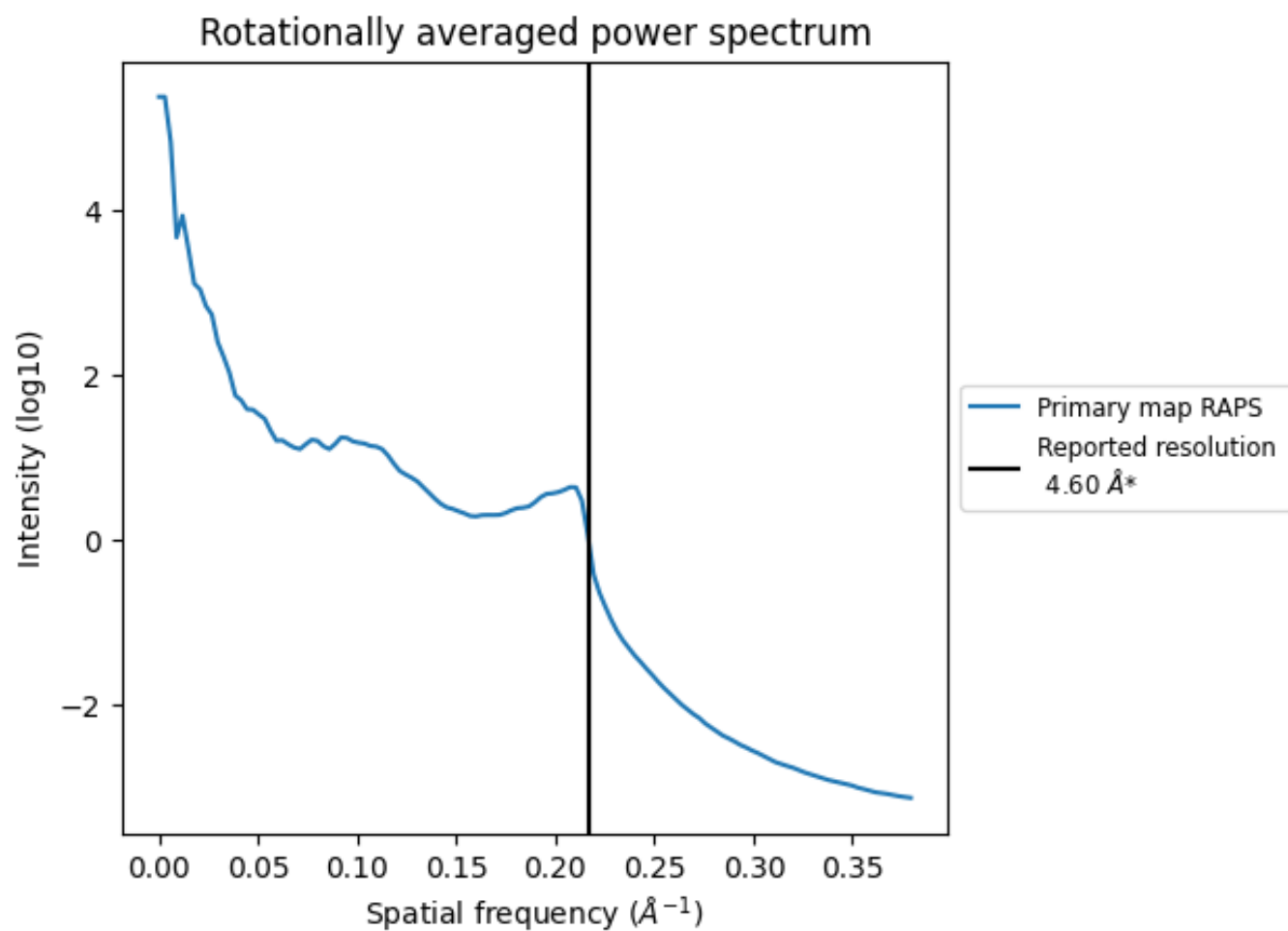
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 344 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 0.217 Å⁻¹

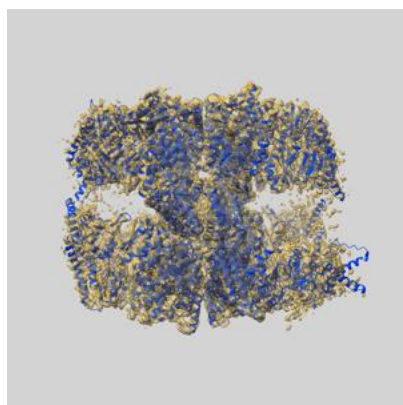
8 Fourier-Shell correlation

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

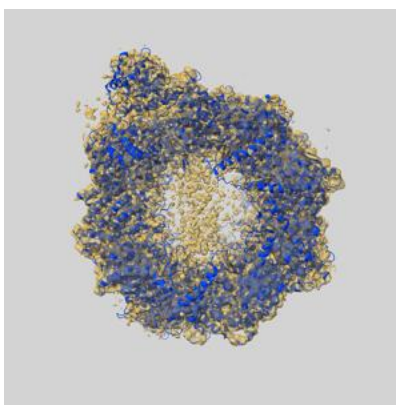
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9541 and PDB model 5GW5. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

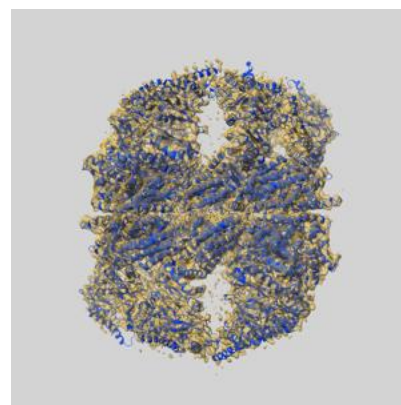
9.1 Map-model overlay [i](#)



X



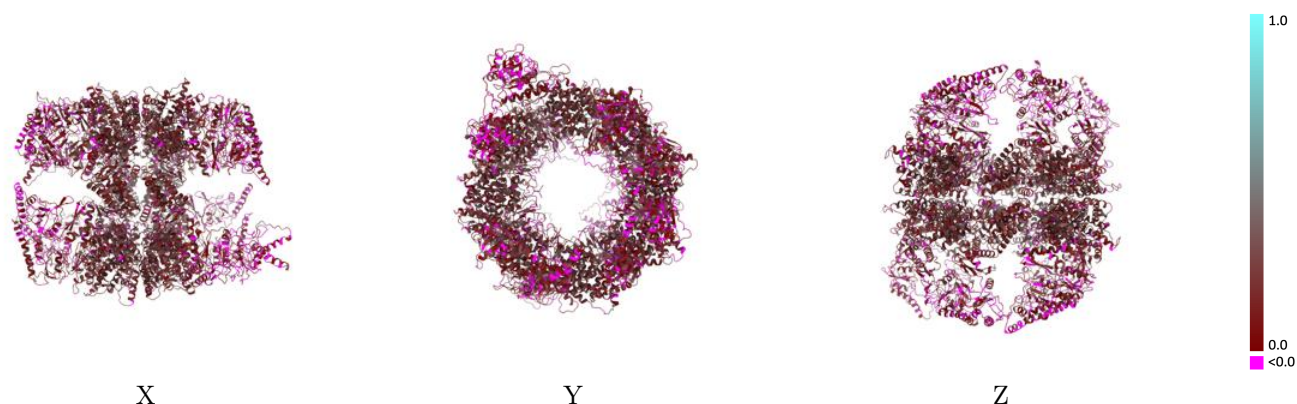
Y



Z

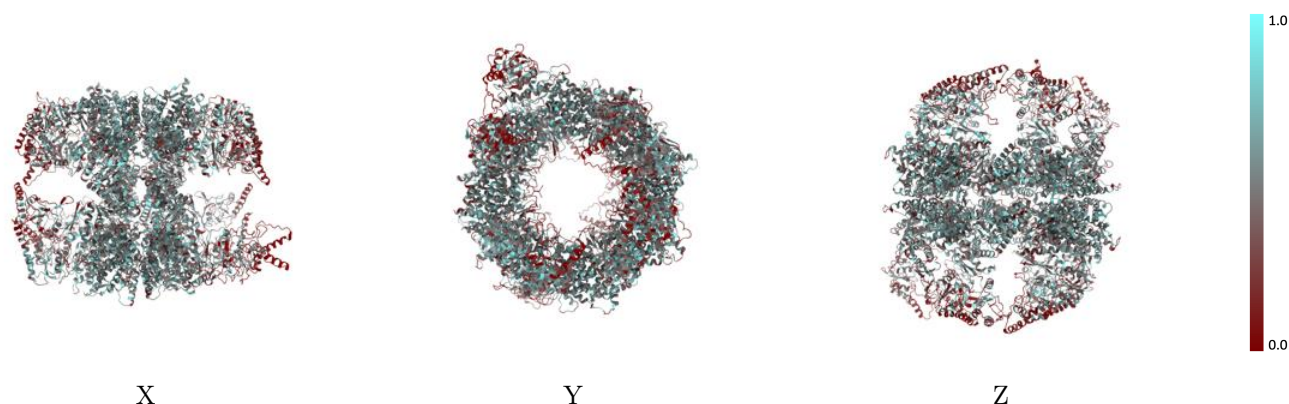
The images above show the 3D surface view of the map at the recommended contour level 0.921 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



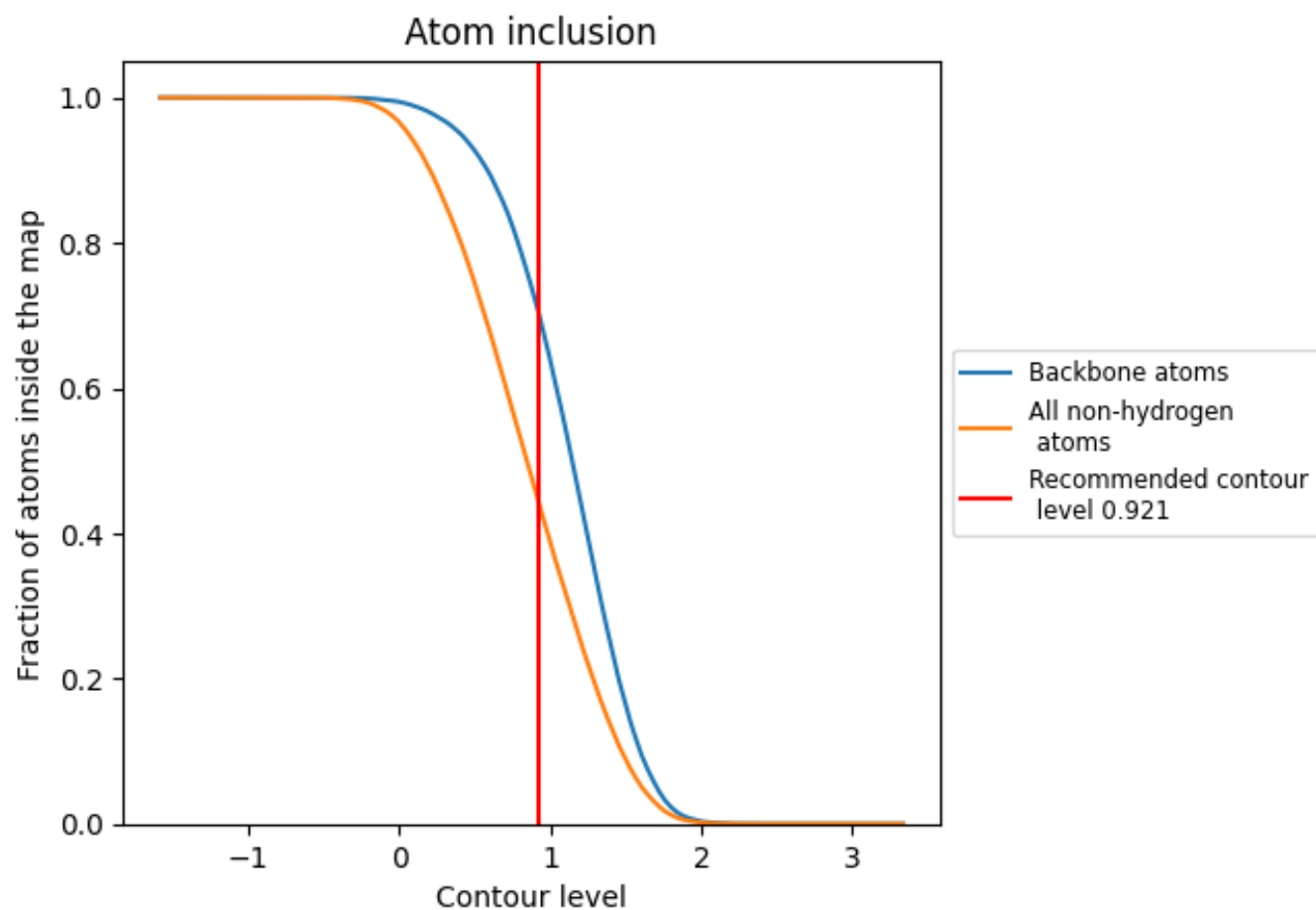
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.921).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 44% 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 (0.921) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4433	 0.1660
A	 0.4264	 0.1580
B	 0.4677	 0.1680
D	 0.4206	 0.1650
E	 0.4418	 0.1400
G	 0.4110	 0.1560
H	 0.4702	 0.1670
Q	 0.4355	 0.1650
Z	 0.4958	 0.1950
a	 0.4147	 0.1590
b	 0.4483	 0.1630
d	 0.3925	 0.1600
e	 0.4435	 0.1590
g	 0.4156	 0.1600
h	 0.4692	 0.1770
q	 0.4362	 0.1660
z	 0.5025	 0.2010

