



## Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 08:23 AM JST

PDB ID : 6KRE  
EMDB ID : EMD-0757  
Title : TRiC at 0.05 mM ADP-AlFx, Conformation 2, 0.05-C2  
Authors : Jin, M.; Cong, Y.  
Deposited on : 2019-08-21  
Resolution : 4.45 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](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.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

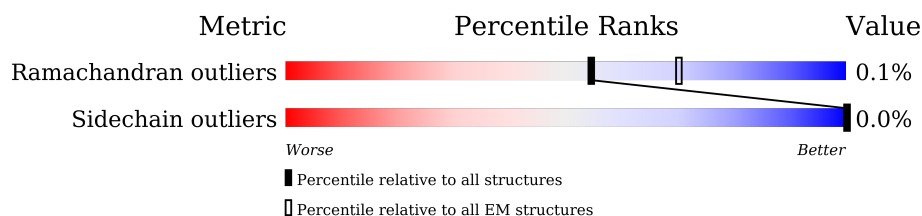
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.45 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  $\geq 3$ , 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	559	
1	a	559	
2	B	527	
2	b	527	
3	D	528	
3	d	528	
4	E	562	
4	e	562	
5	G	534	

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Mol	Chain	Length	Quality of chain
5	g	534	<div> <div>56%</div> <div>92%</div> <div>8%</div> </div>
6	H	550	<div> <div>60%</div> <div>89%</div> <div>11%</div> </div>
6	h	550	<div> <div>58%</div> <div>87%</div> <div>13%</div> </div>
7	Q	568	<div> <div>48%</div> <div>91%</div> <div>9%</div> </div>
7	q	568	<div> <div>53%</div> <div>92%</div> <div>8%</div> </div>
8	Z	546	<div> <div>44%</div> <div>96%</div> <div>• •</div> </div>
8	z	546	<div> <div>48%</div> <div>97%</div> <div>•</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 60321 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	506	Total	C	N	O	S	0	0
			3807	2386	661	742	18		
1	A	509	Total	C	N	O	S	0	0
			3832	2400	667	747	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			3833	2397	662	760	14		
2	b	444	Total	C	N	O	S	0	0
			3358	2098	582	666	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	479	Total	C	N	O	S	0	0
			3646	2278	645	707	16		
3	D	465	Total	C	N	O	S	0	0
			3531	2201	625	690	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	497	Total	C	N	O	S	0	0
			3804	2389	651	743	21		
4	E	502	Total	C	N	O	S	0	0
			3847	2415	655	756	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	493	Total	C	N	O	S	0	0
			3765	2365	659	715	26		
5	G	460	Total	C	N	O	S	0	0
			3506	2205	616	661	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	479	Total	C	N	O	S	0	0
			3650	2302	625	704	19		
6	H	488	Total	C	N	O	S	0	0
			3729	2353	637	720	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	524	Total	C	N	O	S	0	0
			3978	2508	677	767	26		
7	Q	515	Total	C	N	O	S	0	0
			3909	2466	664	754	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	529	Total	C	N	O	S	0	0
			4070	2555	705	793	17		
8	Z	527	Total	C	N	O	S	0	0
			4056	2547	703	789	17		

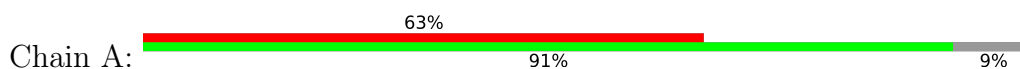
### 3 Residue-property plots

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

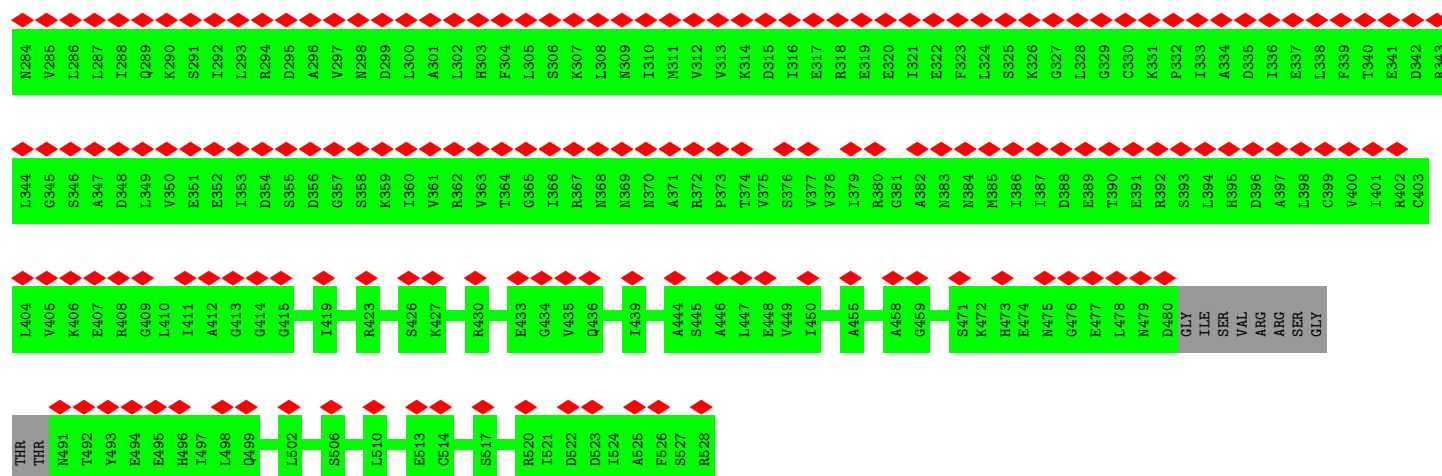




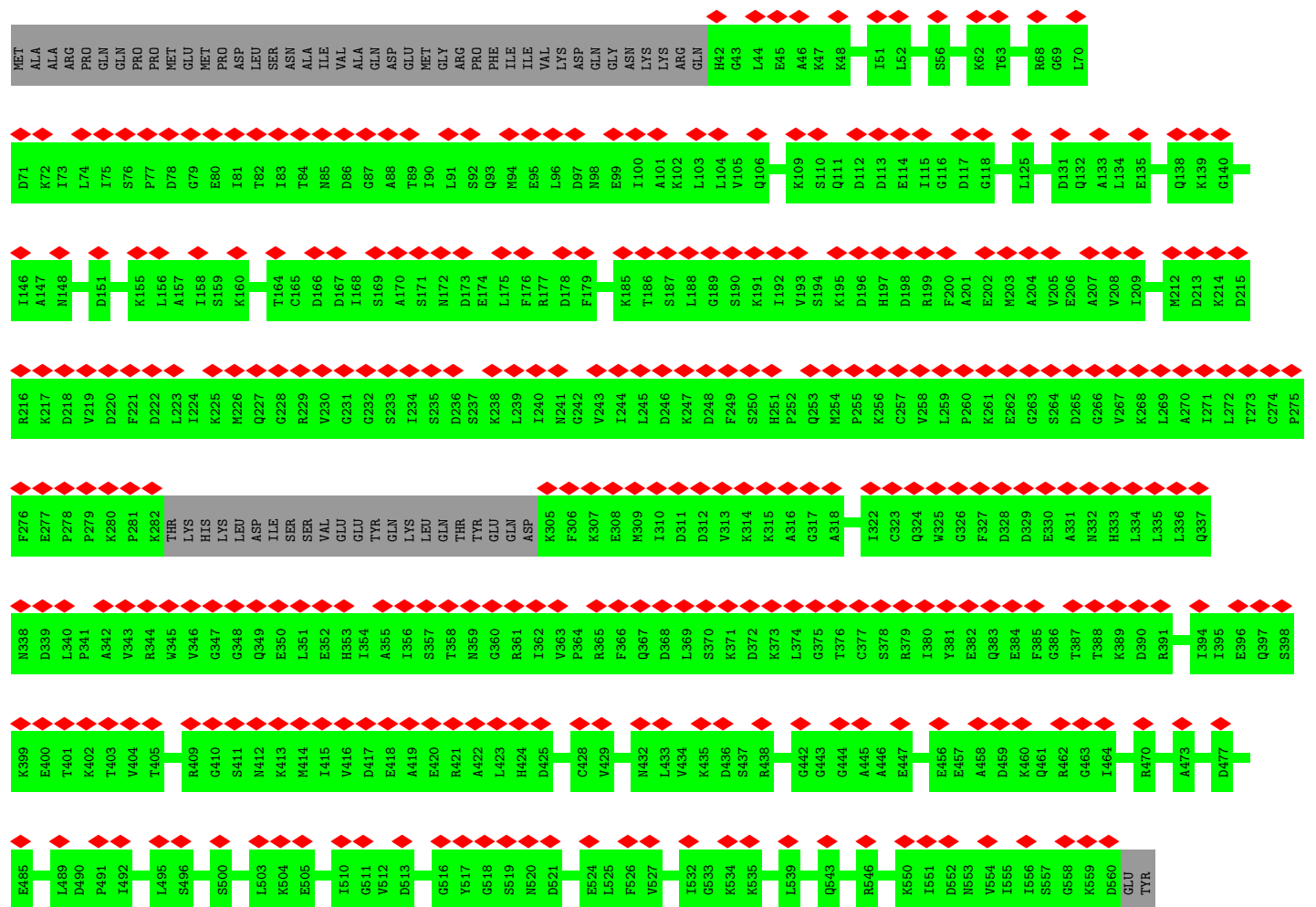
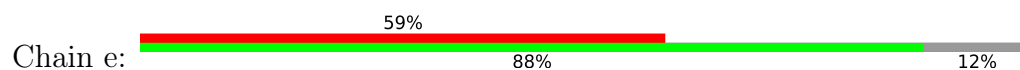




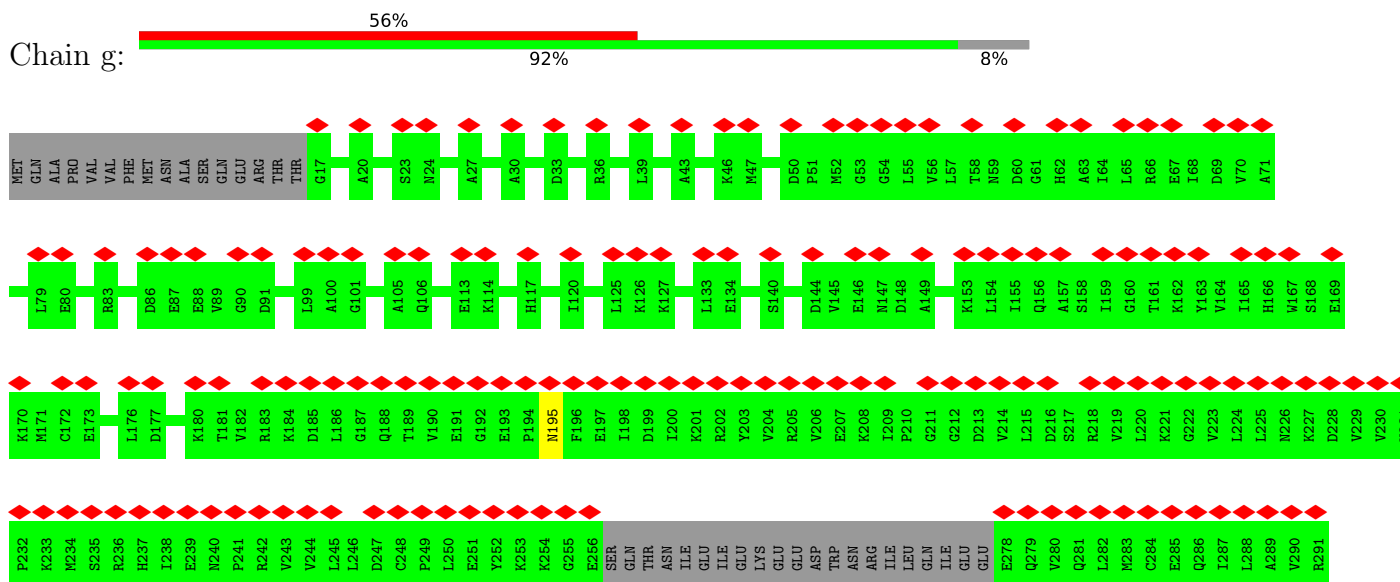
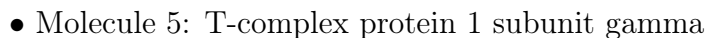


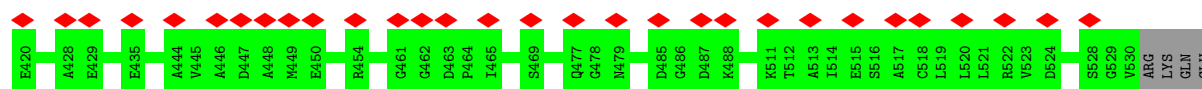
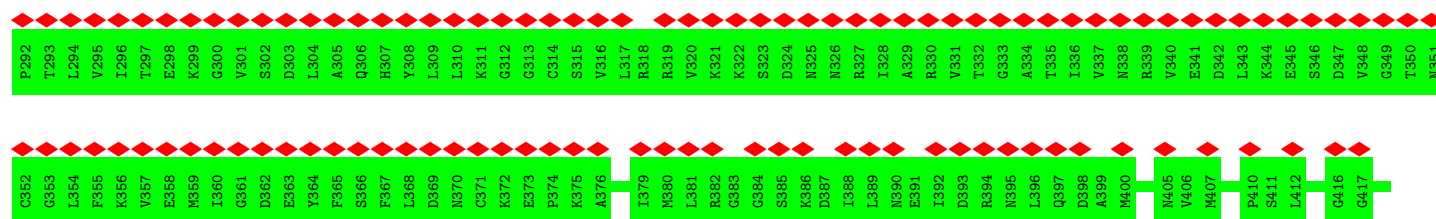


• Molecule 4: T-complex protein 1 subunit epsilon

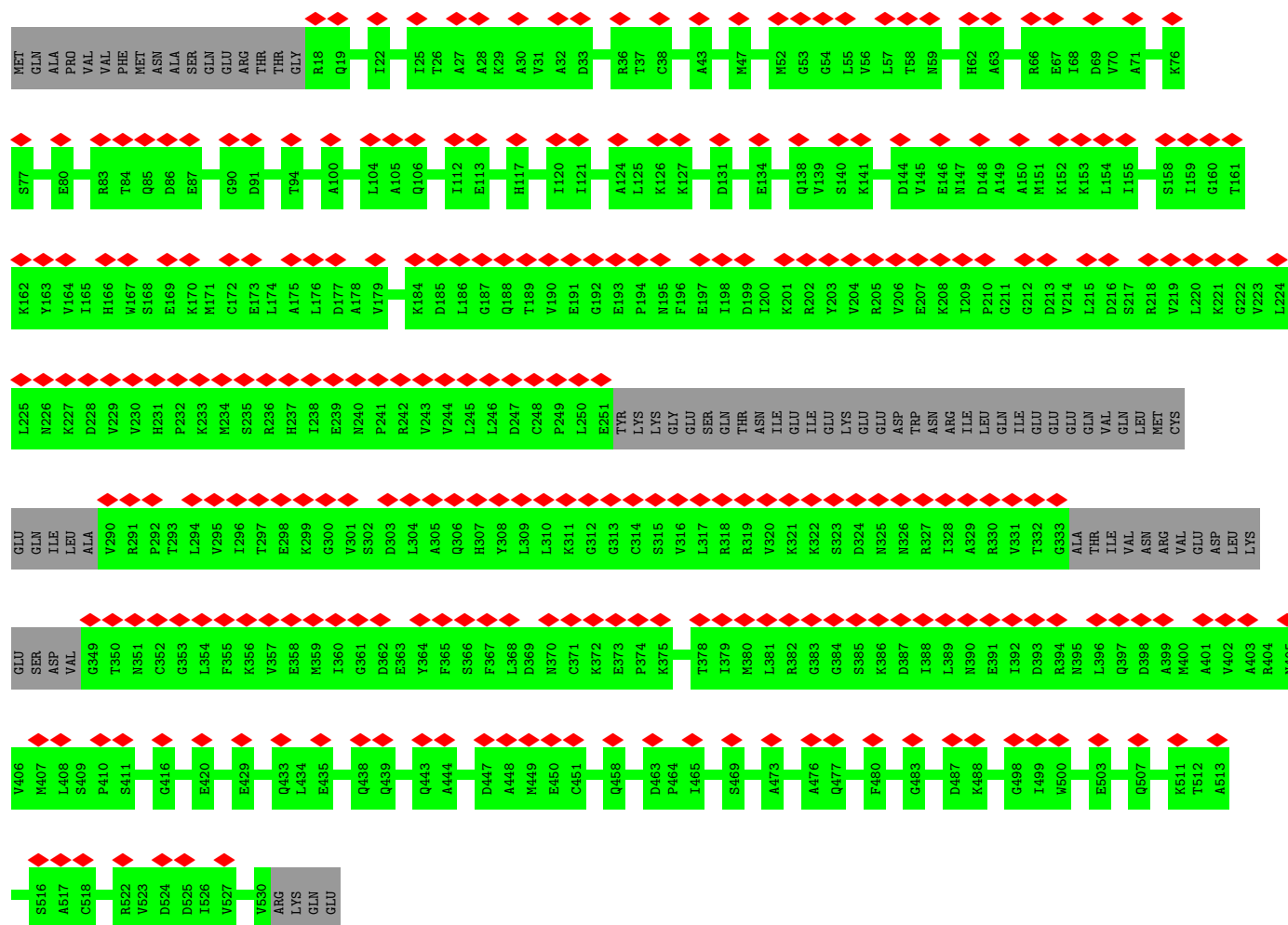
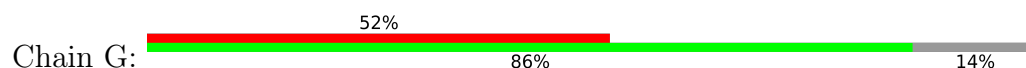


• Molecule 4: T-complex protein 1 subunit epsilon

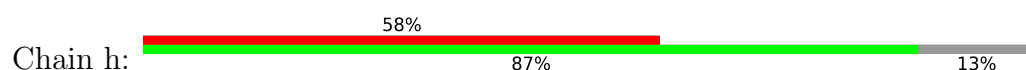


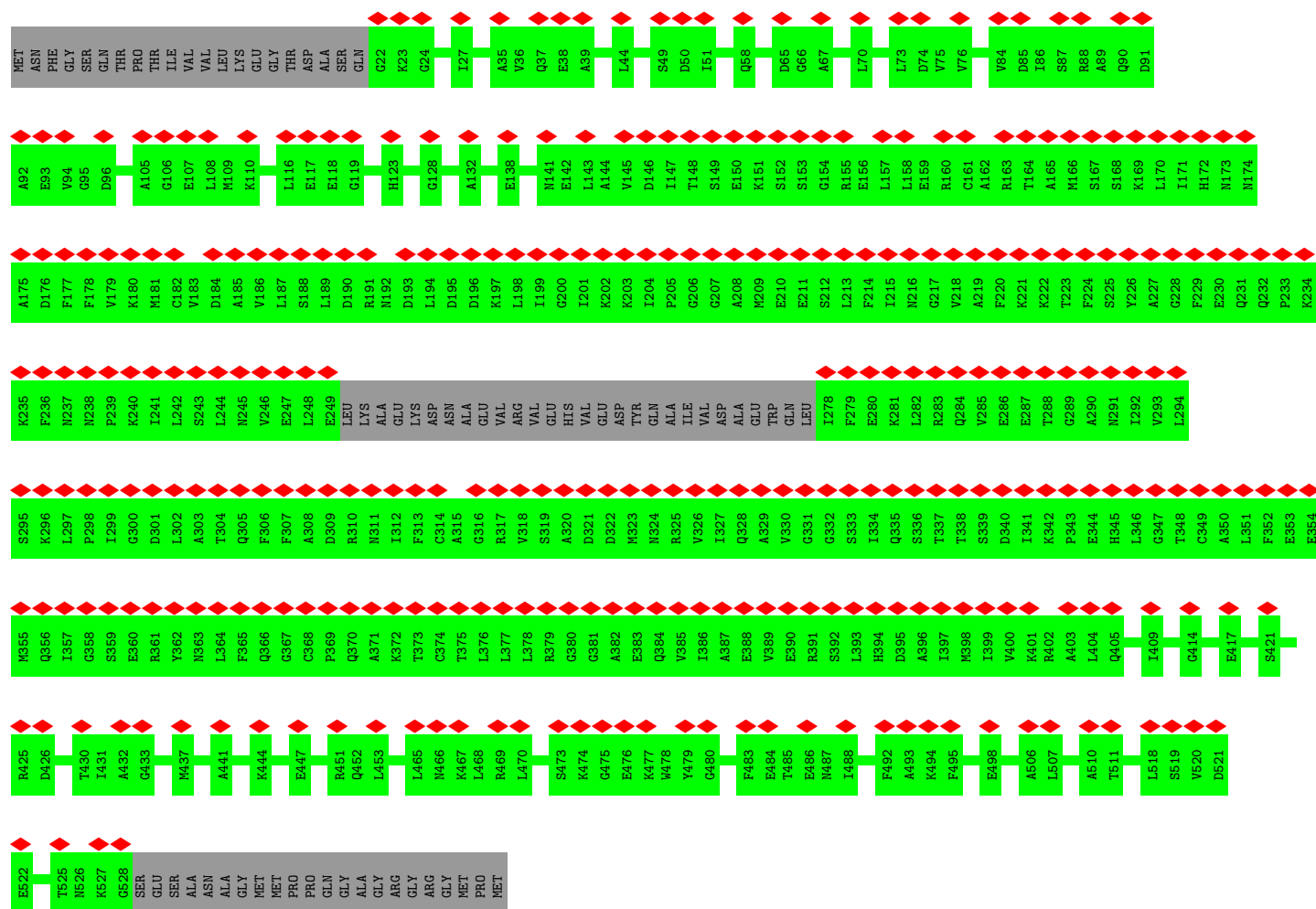


• Molecule 5: T-complex protein 1 subunit gamma

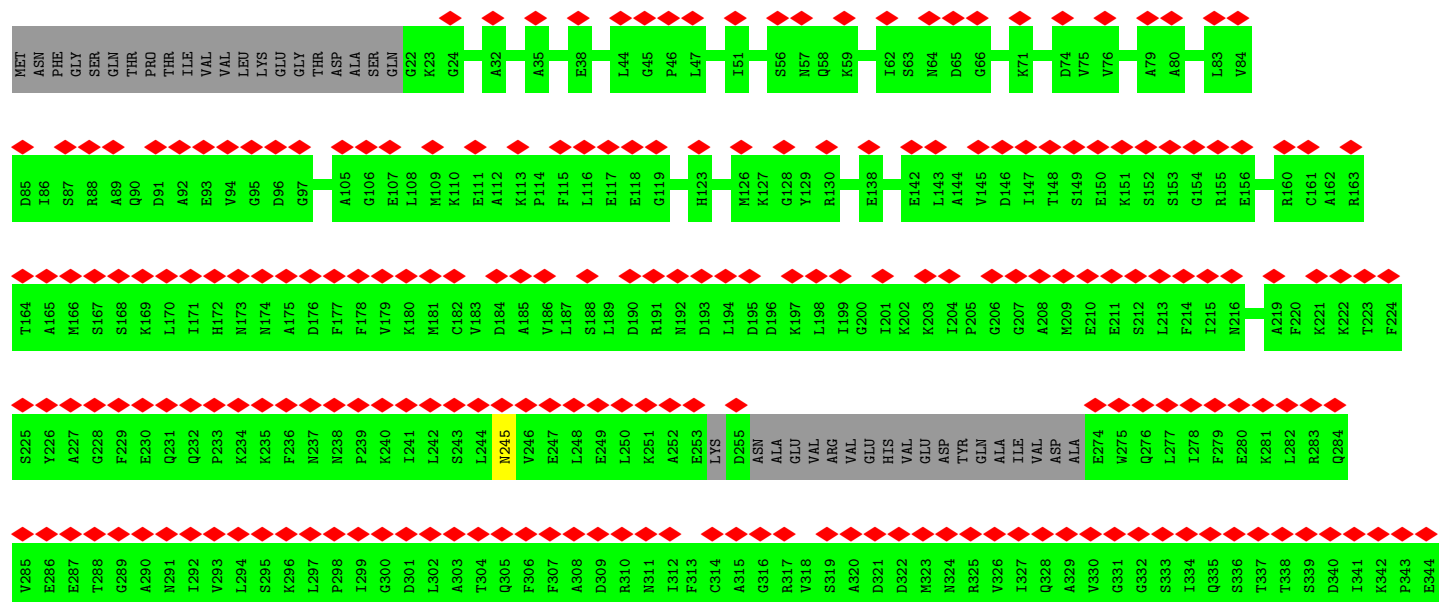
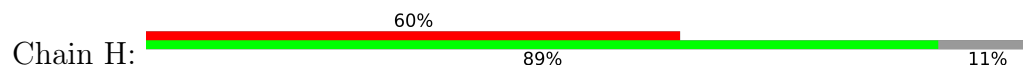


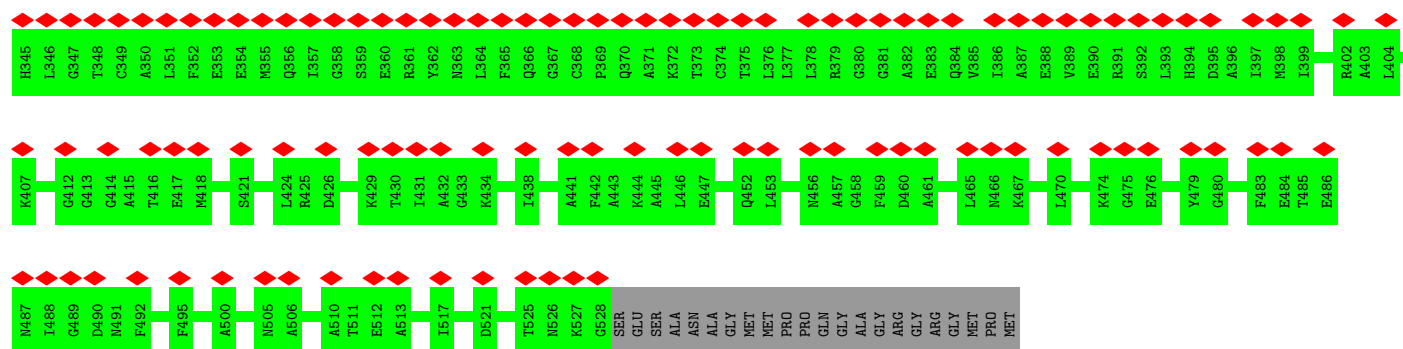
• Molecule 6: T-complex protein 1 subunit eta





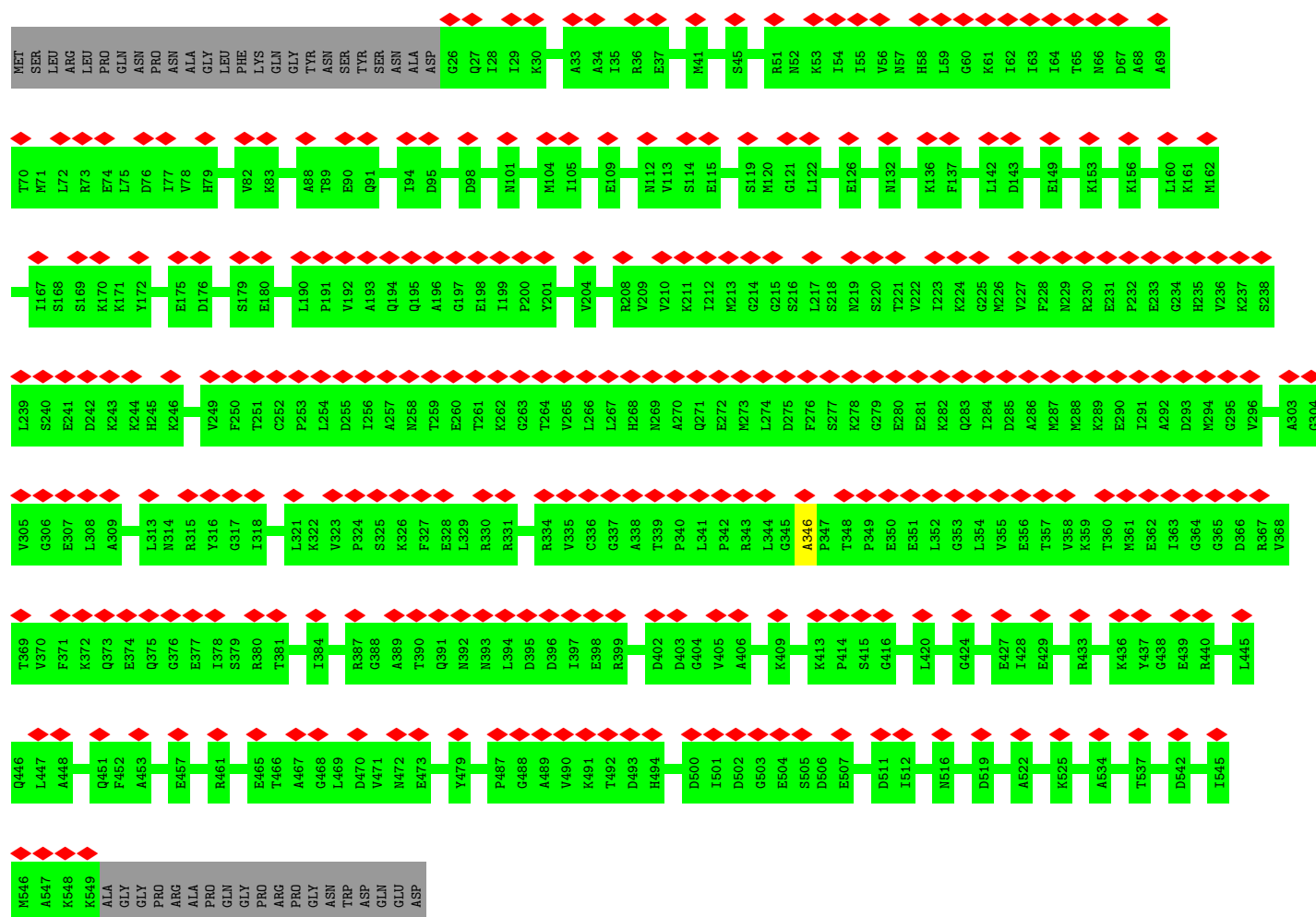
• Molecule 6: T-complex protein 1 subunit eta





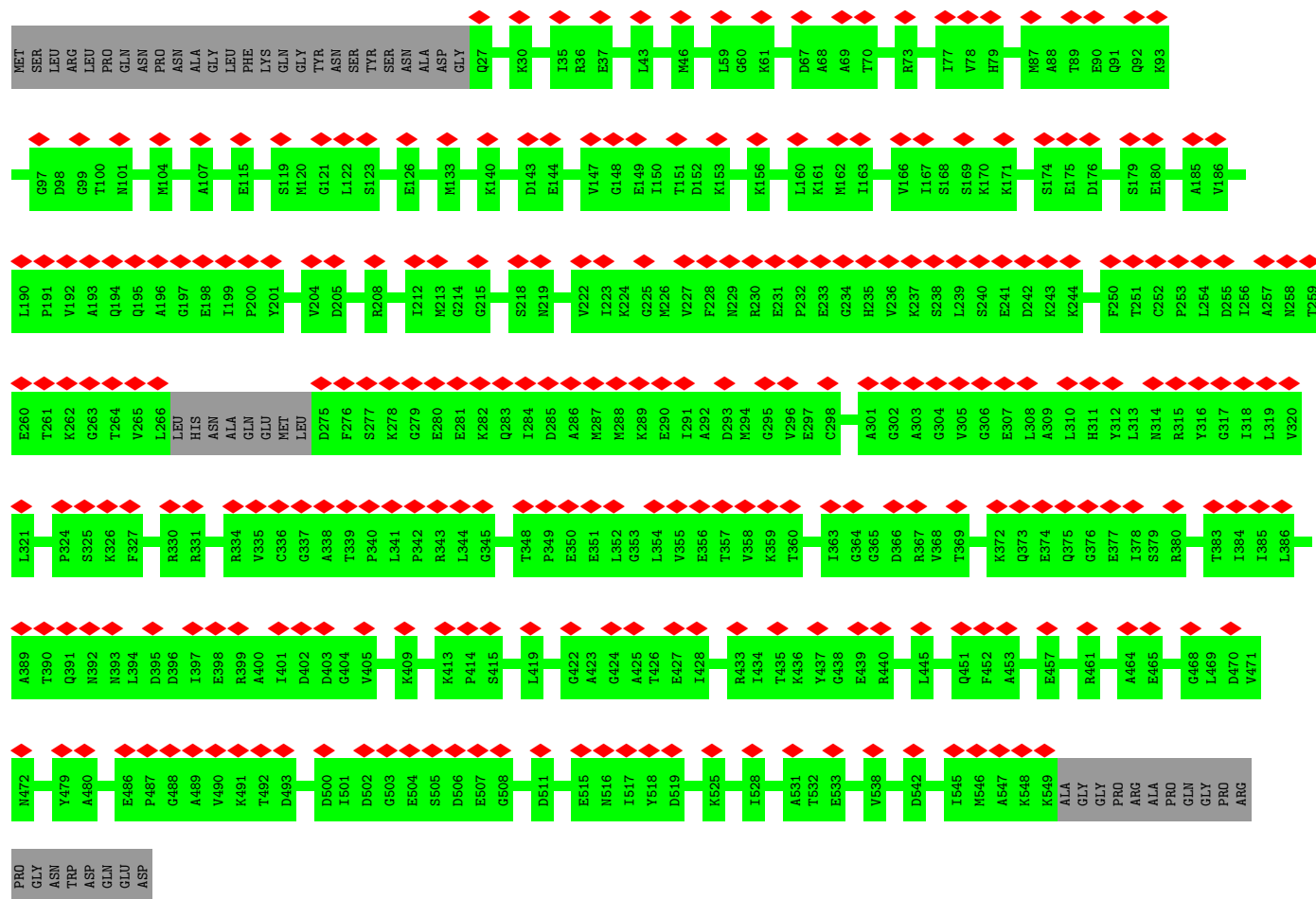
• Molecule 7: T-complex protein 1 subunit theta

Chain q: 53% 92% 8%



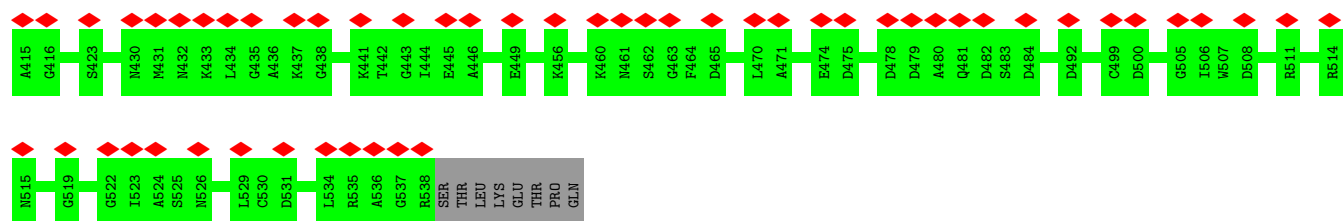
• Molecule 7: T-complex protein 1 subunit theta

Chain Q: 48% 91% 9%



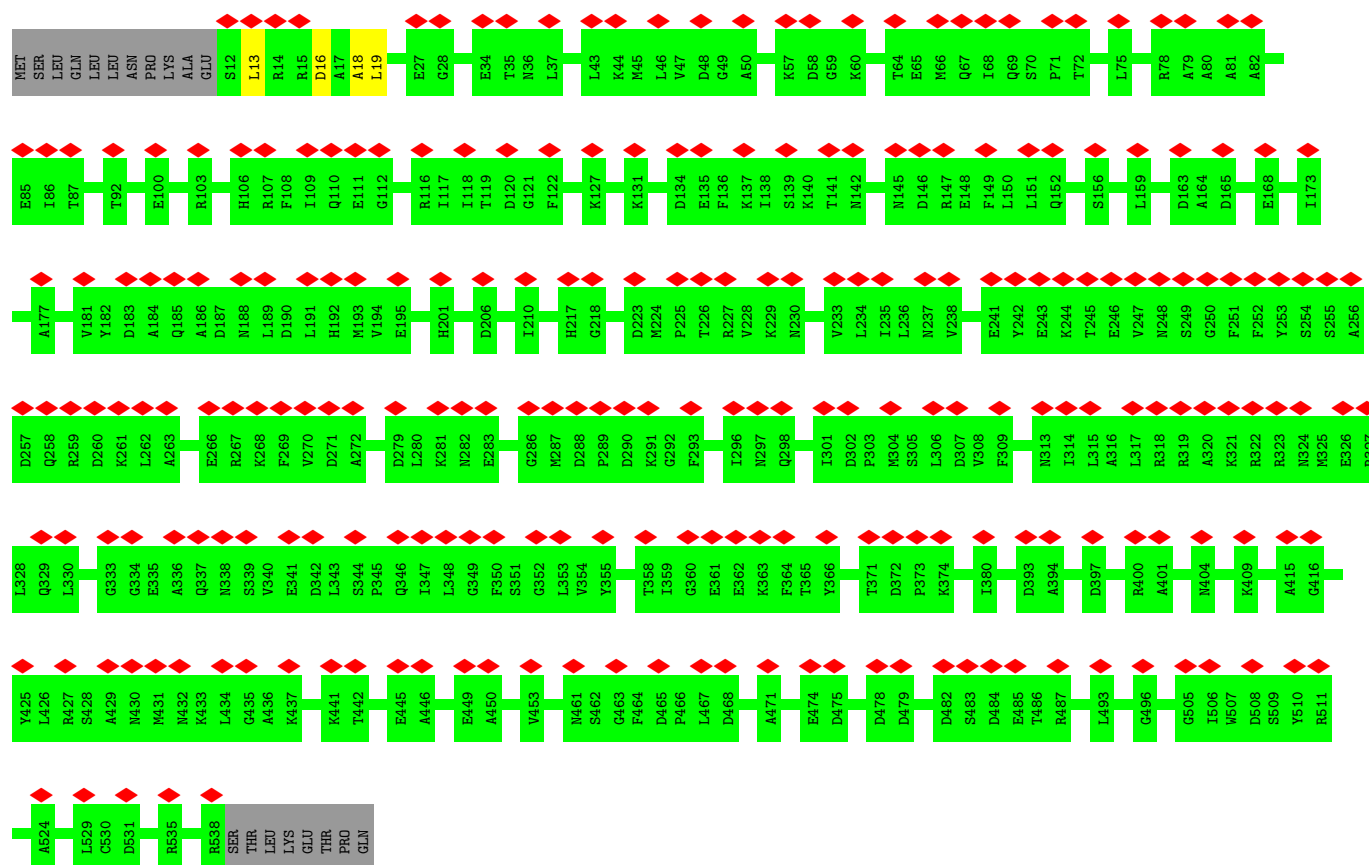
• Molecule 8: T-complex protein 1 subunit zeta





• Molecule 8: T-complex protein 1 subunit zeta

Chain Z: 44% 96%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.258	Depositor
Minimum map value	-1.848	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.195	Depositor
Recommended contour level	0.85	Depositor
Map size ( $\text{\AA}$ )	258.328, 258.328, 258.328	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.318, 1.318, 1.318	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0/3865	0.40	0/5215
1	a	0.23	0/3840	0.40	0/5182
2	B	0.23	0/3871	0.39	0/5216
2	b	0.23	0/3390	0.39	0/4573
3	D	0.23	0/3561	0.40	0/4801
3	d	0.23	0/3678	0.39	0/4956
4	E	0.23	0/3892	0.39	0/5241
4	e	0.23	0/3849	0.39	0/5181
5	G	0.23	0/3548	0.39	0/4791
5	g	0.23	0/3809	0.38	0/5143
6	H	0.23	0/3774	0.39	0/5087
6	h	0.23	0/3694	0.38	0/4980
7	Q	0.24	0/3953	0.40	0/5334
7	q	0.25	1/4024 (0.0%)	0.40	0/5431
8	Z	0.23	0/4107	0.40	0/5549
8	z	0.23	0/4121	0.40	0/5568
All	All	0.23	1/60976 (0.0%)	0.39	0/82248

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	q	346	ALA	C-N	5.08	1.43	1.34

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

### 5.3.1 Protein backbone

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	505/559 (90%)	476 (94%)	29 (6%)	0	100	100
1	a	502/559 (90%)	477 (95%)	24 (5%)	1 (0%)	47	81
2	B	503/527 (95%)	480 (95%)	23 (5%)	0	100	100
2	b	438/527 (83%)	419 (96%)	19 (4%)	0	100	100
3	D	459/528 (87%)	440 (96%)	18 (4%)	1 (0%)	47	81
3	d	473/528 (90%)	450 (95%)	22 (5%)	1 (0%)	47	81
4	E	498/562 (89%)	479 (96%)	19 (4%)	0	100	100
4	e	493/562 (88%)	476 (97%)	17 (3%)	0	100	100
5	G	454/534 (85%)	437 (96%)	17 (4%)	0	100	100
5	g	489/534 (92%)	469 (96%)	19 (4%)	1 (0%)	47	81
6	H	483/550 (88%)	469 (97%)	13 (3%)	1 (0%)	47	81
6	h	475/550 (86%)	461 (97%)	14 (3%)	0	100	100
7	Q	511/568 (90%)	490 (96%)	21 (4%)	0	100	100
7	q	522/568 (92%)	498 (95%)	24 (5%)	0	100	100
8	Z	525/546 (96%)	501 (95%)	22 (4%)	2 (0%)	34	72
8	z	527/546 (96%)	508 (96%)	19 (4%)	0	100	100
All	All	7857/8748 (90%)	7530 (96%)	320 (4%)	7 (0%)	54	85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	g	195	ASN
6	H	245	ASN
8	Z	18	ALA
8	Z	16	ASP
3	d	213	VAL
3	D	213	VAL

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Mol	Chain	Res	Type
1	a	203	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	425/471 (90%)	425 (100%)	0	100	100
1	a	423/471 (90%)	423 (100%)	0	100	100
2	B	422/441 (96%)	422 (100%)	0	100	100
2	b	368/441 (83%)	368 (100%)	0	100	100
3	D	396/453 (87%)	396 (100%)	0	100	100
3	d	408/453 (90%)	408 (100%)	0	100	100
4	E	429/483 (89%)	429 (100%)	0	100	100
4	e	424/483 (88%)	424 (100%)	0	100	100
5	G	387/455 (85%)	387 (100%)	0	100	100
5	g	416/455 (91%)	416 (100%)	0	100	100
6	H	406/454 (89%)	406 (100%)	0	100	100
6	h	398/454 (88%)	398 (100%)	0	100	100
7	Q	432/473 (91%)	432 (100%)	0	100	100
7	q	439/473 (93%)	439 (100%)	0	100	100
8	Z	445/463 (96%)	443 (100%)	2 (0%)	91	94
8	z	446/463 (96%)	446 (100%)	0	100	100
All	All	6664/7386 (90%)	6662 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
8	Z	13	LEU
8	Z	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	89	GLN
1	a	90	GLN
1	a	209	HIS
3	d	240	GLN
3	d	289	GLN
3	D	284	ASN
3	D	289	GLN
4	e	142	HIS
4	e	432	ASN
4	e	509	ASN
4	e	536	GLN
4	E	241	ASN
4	E	332	ASN
4	E	353	HIS
4	E	536	GLN
5	G	85	GLN
5	G	188	GLN
6	h	216	ASN
6	H	37	GLN
6	H	356	GLN
6	H	394	HIS
6	H	491	ASN
7	Q	27	GLN
7	Q	91	GLN
7	Q	92	GLN
8	z	385	HIS
8	Z	185	GLN
8	Z	356	GLN
2	b	192	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

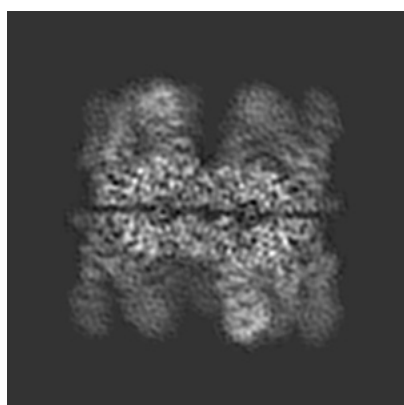
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0757. These allow visual inspection of the internal detail of the map and identification of artifacts.

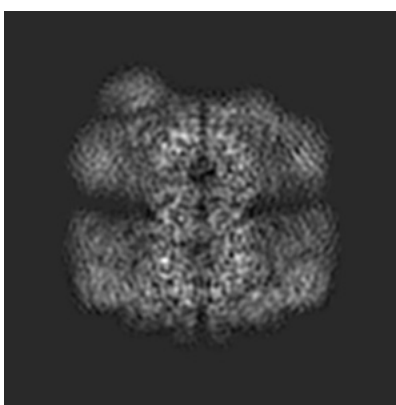
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

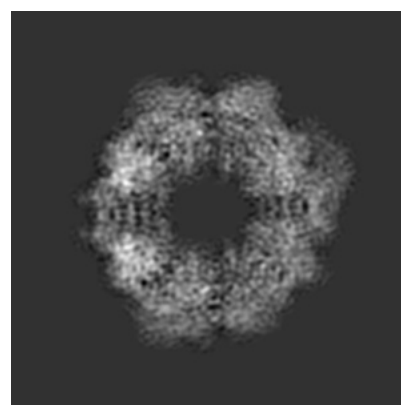
#### 6.1.1 Primary map



X



Y

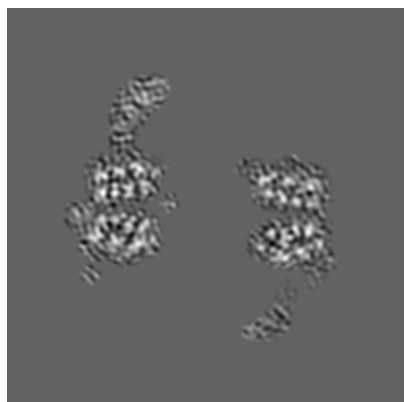


Z

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

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

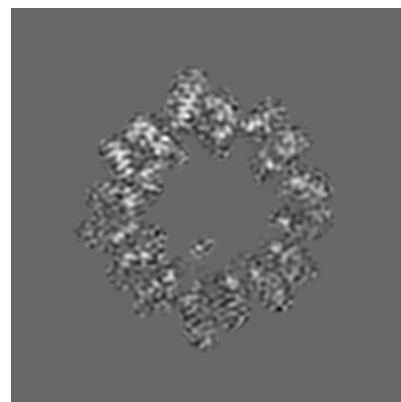
#### 6.2.1 Primary map



X Index: 98



Y Index: 98

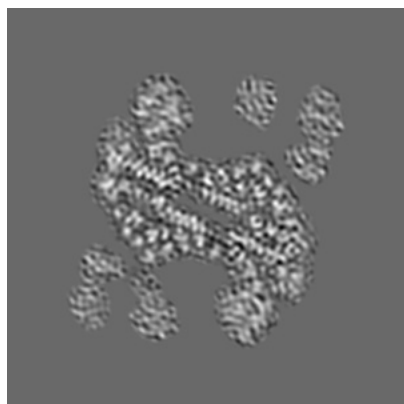


Z Index: 98

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

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

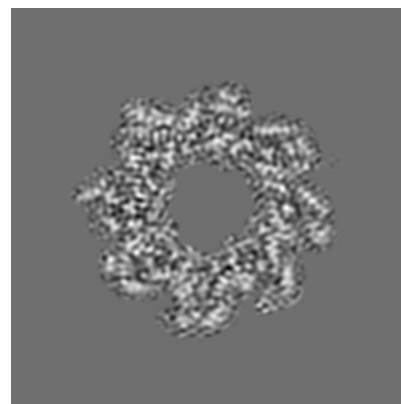
### 6.3.1 Primary map



X Index: 67



Y Index: 122



Z Index: 84

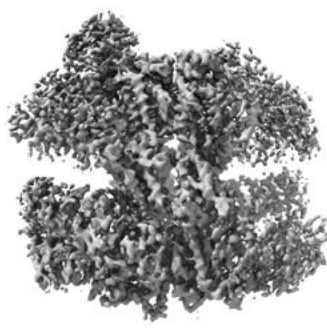
The images above show the largest variance slices of the map in three orthogonal directions.

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



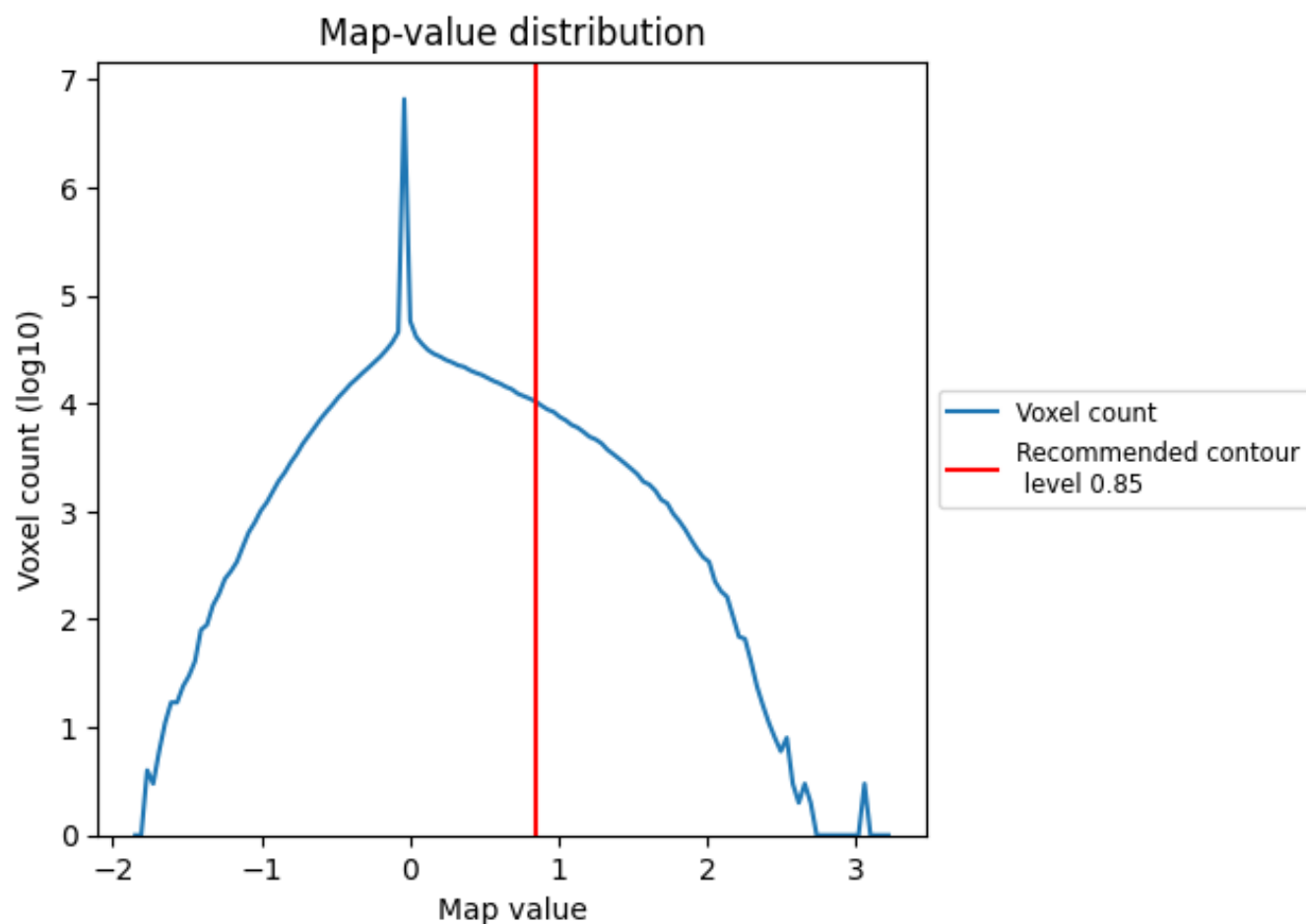
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

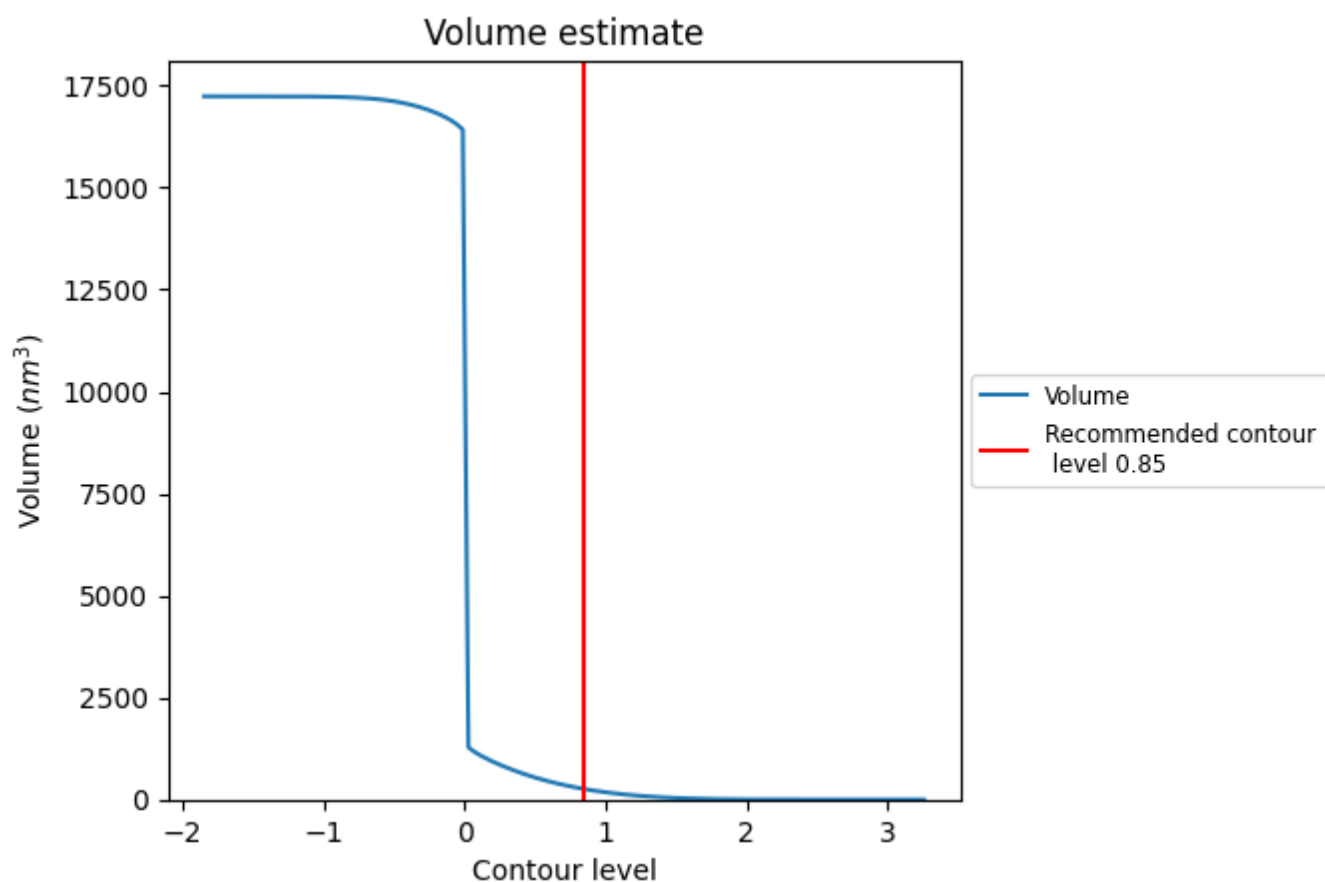
This section contains the results of statistical analysis of the map.

### 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.

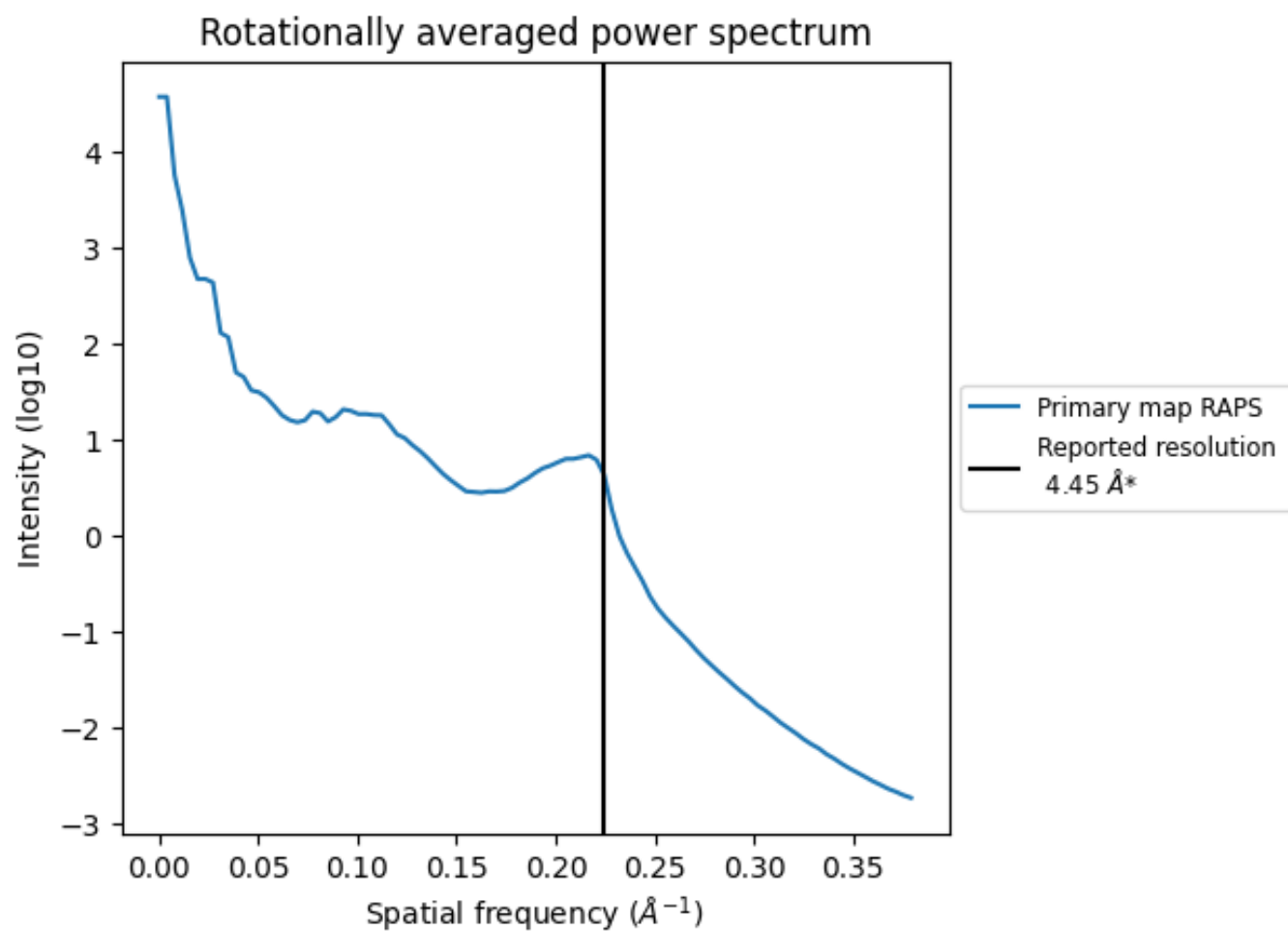
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm<sup>3</sup>; this corresponds to an approximate mass of 232 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 0.225 Å<sup>-1</sup>

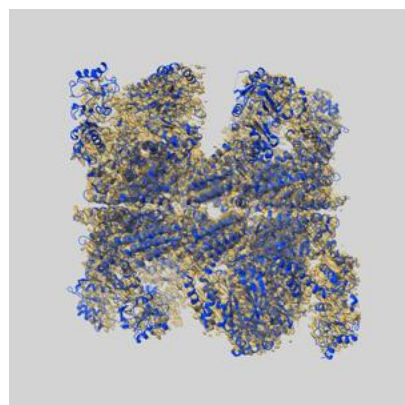
## 8 Fourier-Shell correlation ⓘ

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

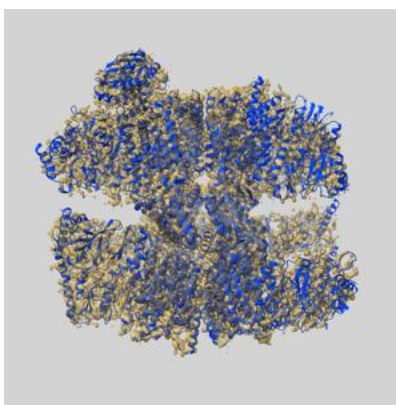
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0757 and PDB model 6KRE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

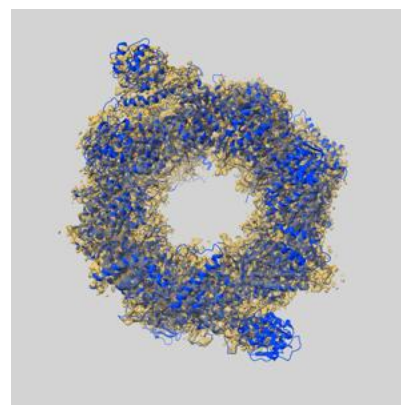
### 9.1 Map-model overlay [i](#)



X



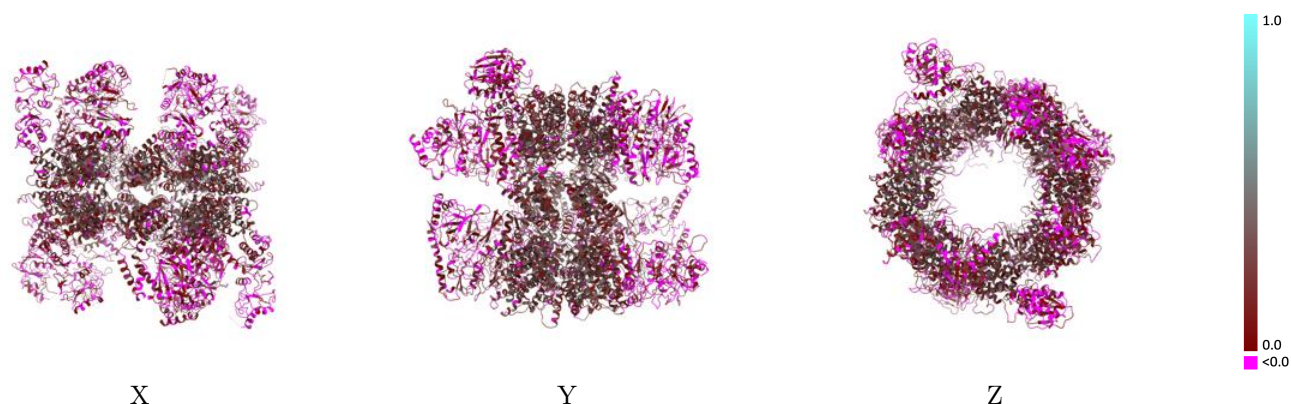
Y



Z

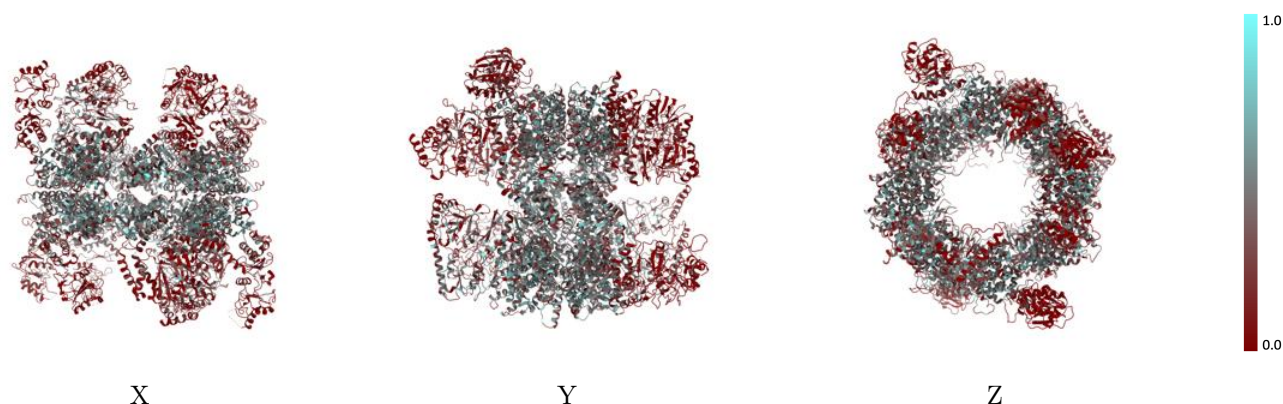
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



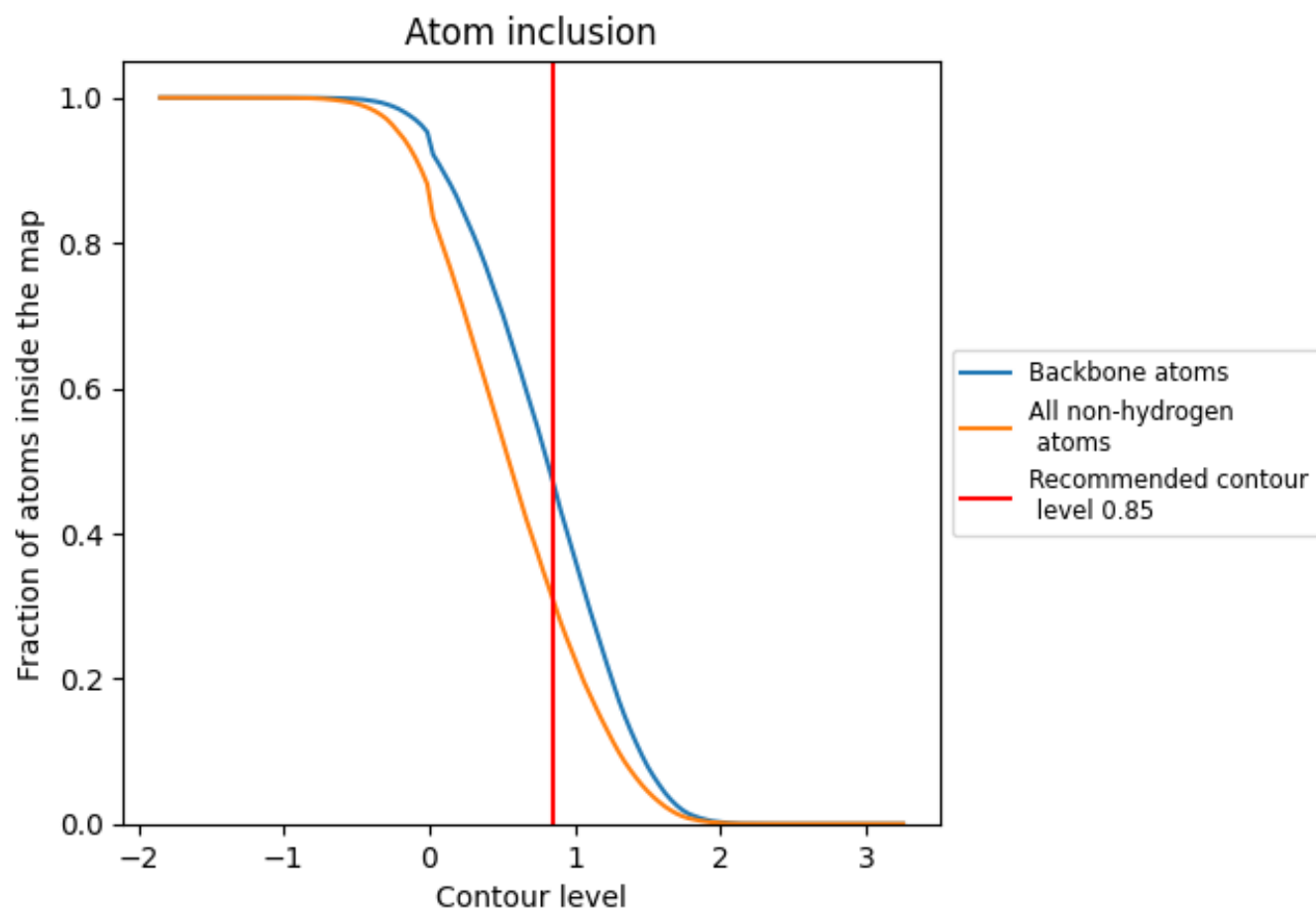
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).

## 9.4 Atom inclusion [i](#)





































At the recommended contour level, 47% of all backbone atoms, 31% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3092	 0.1480
A	 0.2805	 0.1380
B	 0.2686	 0.1110
D	 0.2666	 0.1430
E	 0.3201	 0.1510
G	 0.3178	 0.1490
H	 0.2826	 0.1190
Q	 0.3615	 0.1740
Z	 0.4193	 0.1980
a	 0.2974	 0.1440
b	 0.2451	 0.1310
d	 0.2566	 0.1150
e	 0.2899	 0.1400
g	 0.3042	 0.1430
h	 0.2497	 0.1210
q	 0.3528	 0.1700
z	 0.4038	 0.2000

