



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 03:06 PM EST

PDB ID : 6NRB  
EMDB ID : EMD-0493  
Title : hTRiC-hPFD Class2  
Authors : Gestaut, D.R.; Roh, S.H.; Ma, B.; Pintilie, G.; Joachimiak, L.A.; Leitner, A.; Walzthoeni, T.; Aebersold, R.; Chiu, W.; Frydman, J.  
Deposited on : 2019-01-23  
Resolution : 8.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

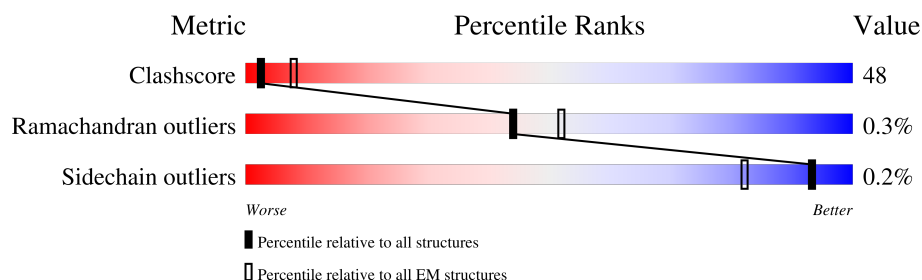
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	534	
1	I	534	
2	B	509	
2	J	509	
3	C	513	
3	K	513	
4	D	514	
4	L	514	

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Mol	Chain	Length	Quality of chain
5	E	517	 22% 76% .
5	M	517	 31% 68% .
6	F	515	 31% 68% .
6	N	515	 31% 68% .
7	G	514	 27% 71% .
7	O	514	 34% 65% .
8	H	514	 27% 71% ..
8	P	514	 33% 65% .
9	1	107	 37% 58% 41% .
10	2	103	 43% 64% 36% .
11	3	132	 24% 46% 54% .
12	4	104	 17% 40% 60% .
13	5	127	 17% 34% 66% .
14	6	102	 7% 33% 66% .

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 68284 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	521	Total	C	N	O	S	0	0
			3956	2479	691	763	23		
1	I	534	Total	C	N	O	S	0	0
			4056	2540	709	783	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	509	Total	C	N	O	S	0	0
			3829	2392	673	745	19		
2	J	508	Total	C	N	O	S	0	0
			3823	2389	672	743	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	509	Total	C	N	O	S	0	0
			3956	2465	697	764	30		
3	K	513	Total	C	N	O	S	0	0
			3985	2481	703	771	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	508	Total	C	N	O	S	0	0
			3832	2398	665	746	23		
4	L	513	Total	C	N	O	S	0	0
			3873	2422	674	754	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		
5	M	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	514	Total	C	N	O	S	0	0
			3945	2478	690	757	20		
6	N	513	Total	C	N	O	S	0	0
			3940	2476	689	755	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	512	Total	C	N	O	S	0	0
			3936	2485	682	746	23		
7	O	514	Total	C	N	O	S	0	0
			3947	2490	684	750	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	510	Total	C	N	O	S	0	0
			3892	2451	661	754	26		
8	P	509	Total	C	N	O	S	0	0
			3884	2447	659	752	26		

- Molecule 9 is a protein called Prefoldin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	107	Total	C	N	O	S	0	0
			874	546	150	173	5		

- Molecule 10 is a protein called Prefoldin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	103	Total	C	N	O	S	0	0
			830	513	151	163	3		

- Molecule 11 is a protein called Prefoldin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	132	Total	C	N	O	S	0	0
			1087	690	179	210	8		

- Molecule 12 is a protein called Prefoldin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	104	Total	C	N	O	S	0	0
			847	523	142	177	5		

- Molecule 13 is a protein called Prefoldin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	127	Total	C	N	O	S	0	0
			1018	647	166	197	8		

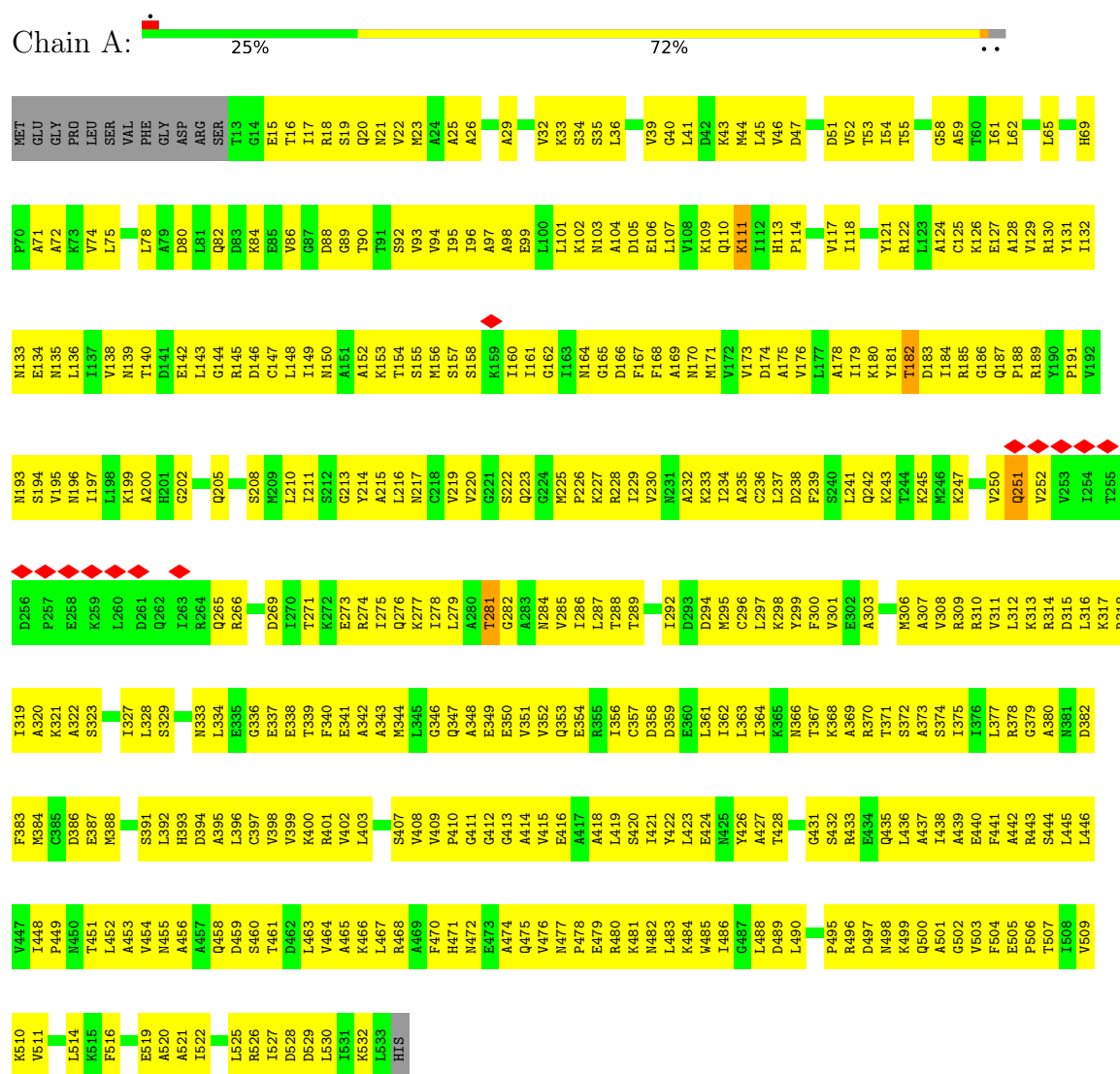
- Molecule 14 is a protein called Prefoldin subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6	102	Total	C	N	O	S	0	0
			826	511	148	166	1		

### 3 Residue-property plots

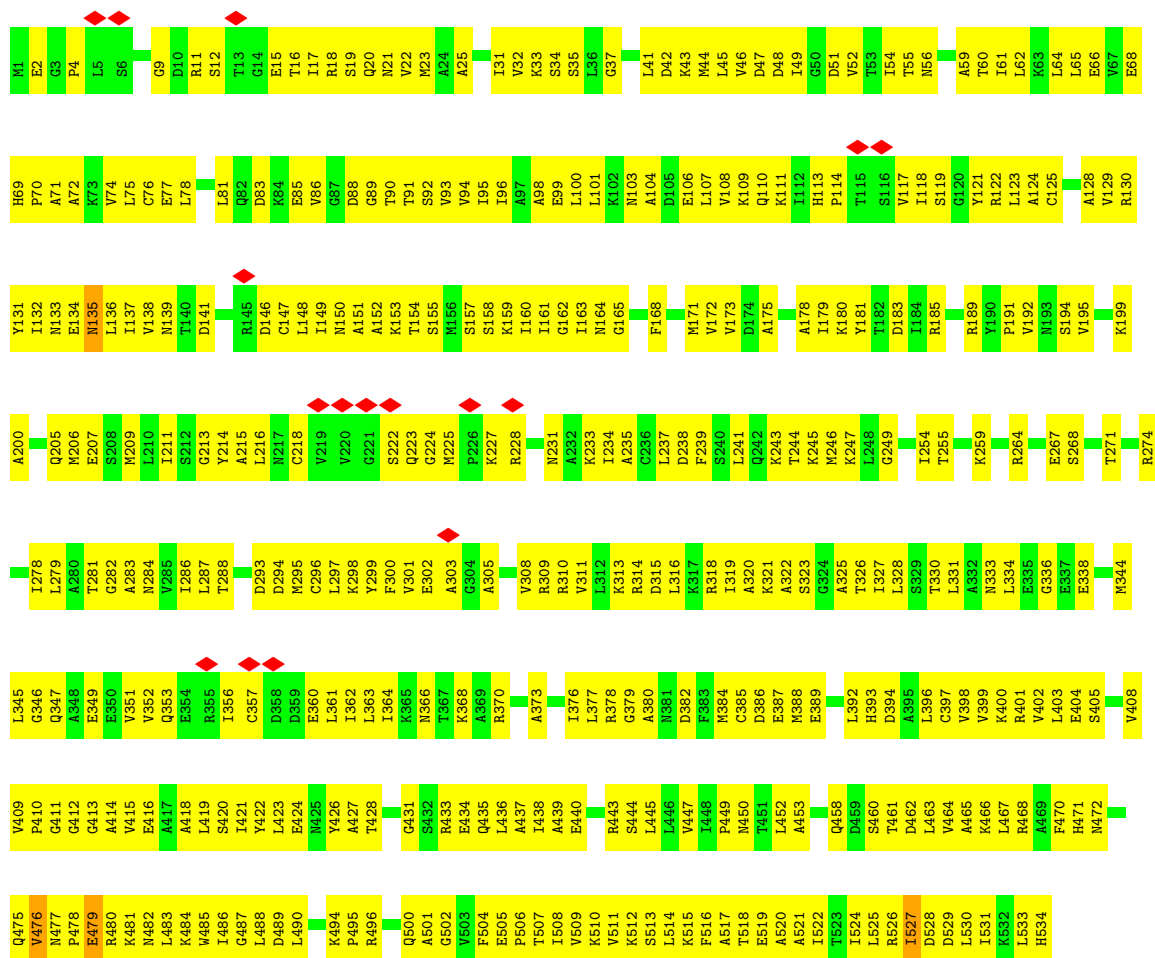
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

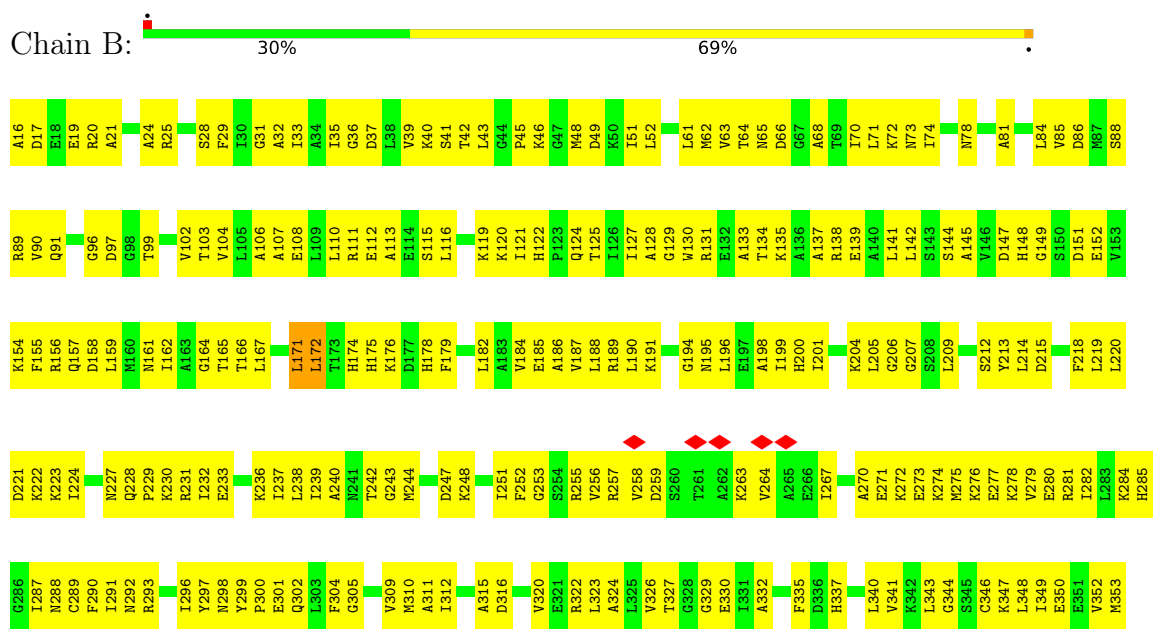


#### • Molecule 1: T-complex protein 1 subunit alpha

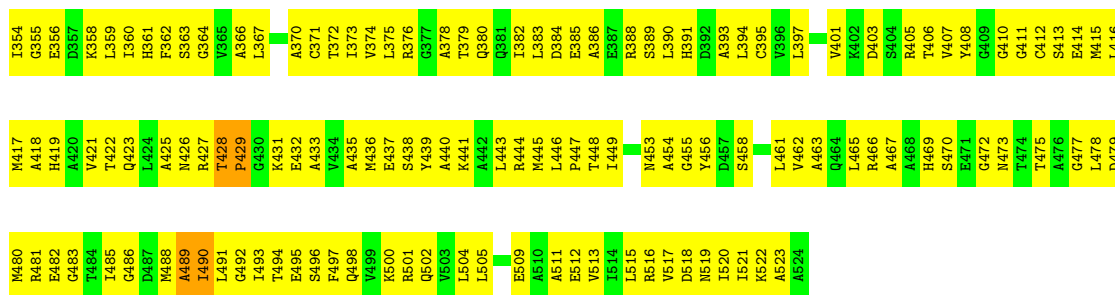




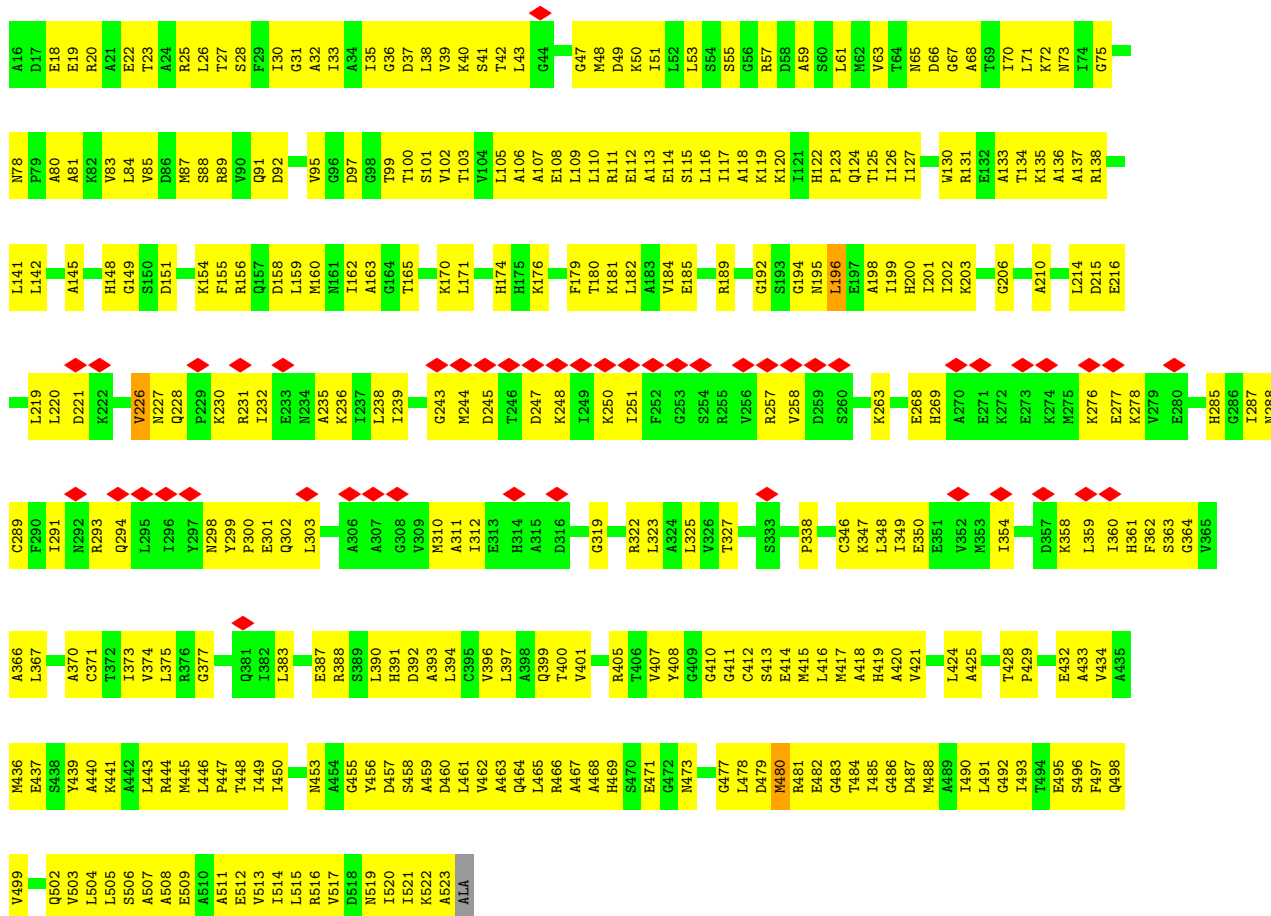
• Molecule 2: T-complex protein 1 subunit beta



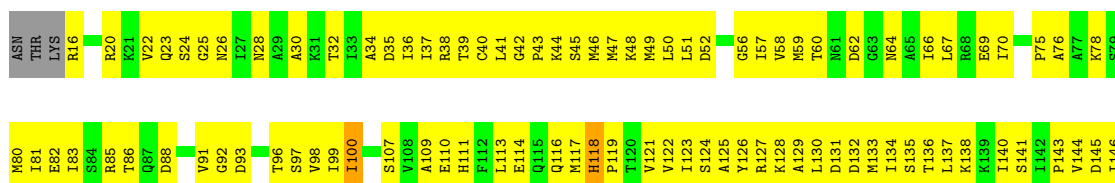




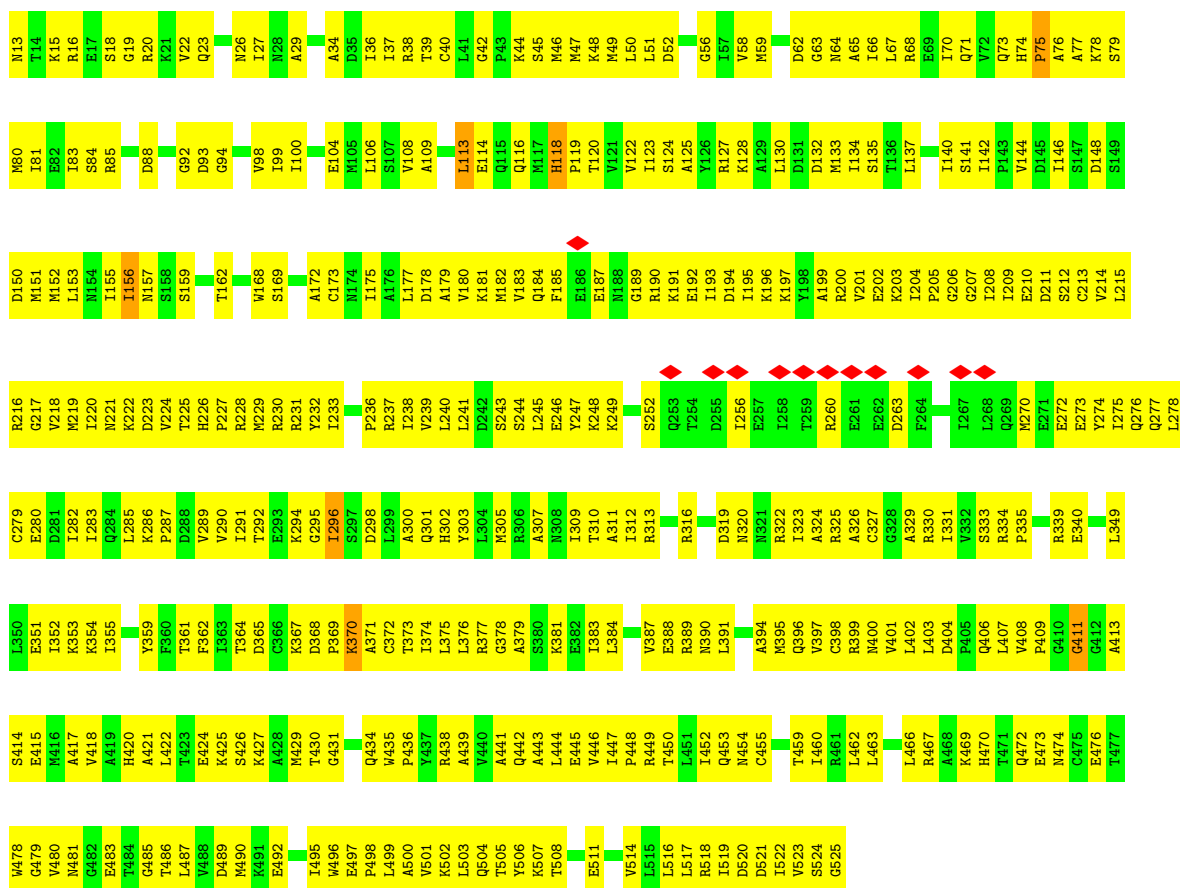
• Molecule 2: T-complex protein 1 subunit beta



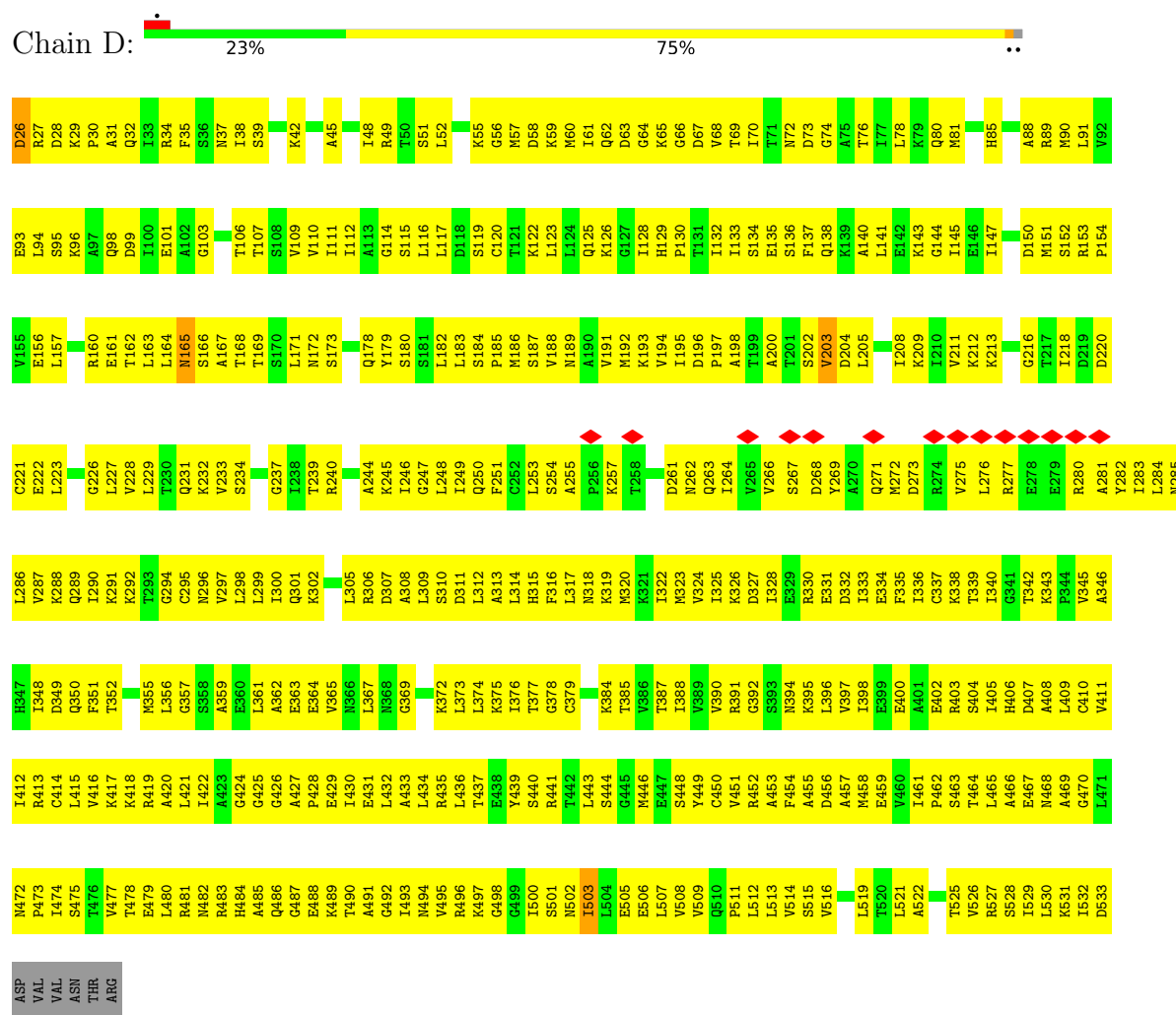
• Molecule 3: T-complex protein 1 subunit gamma



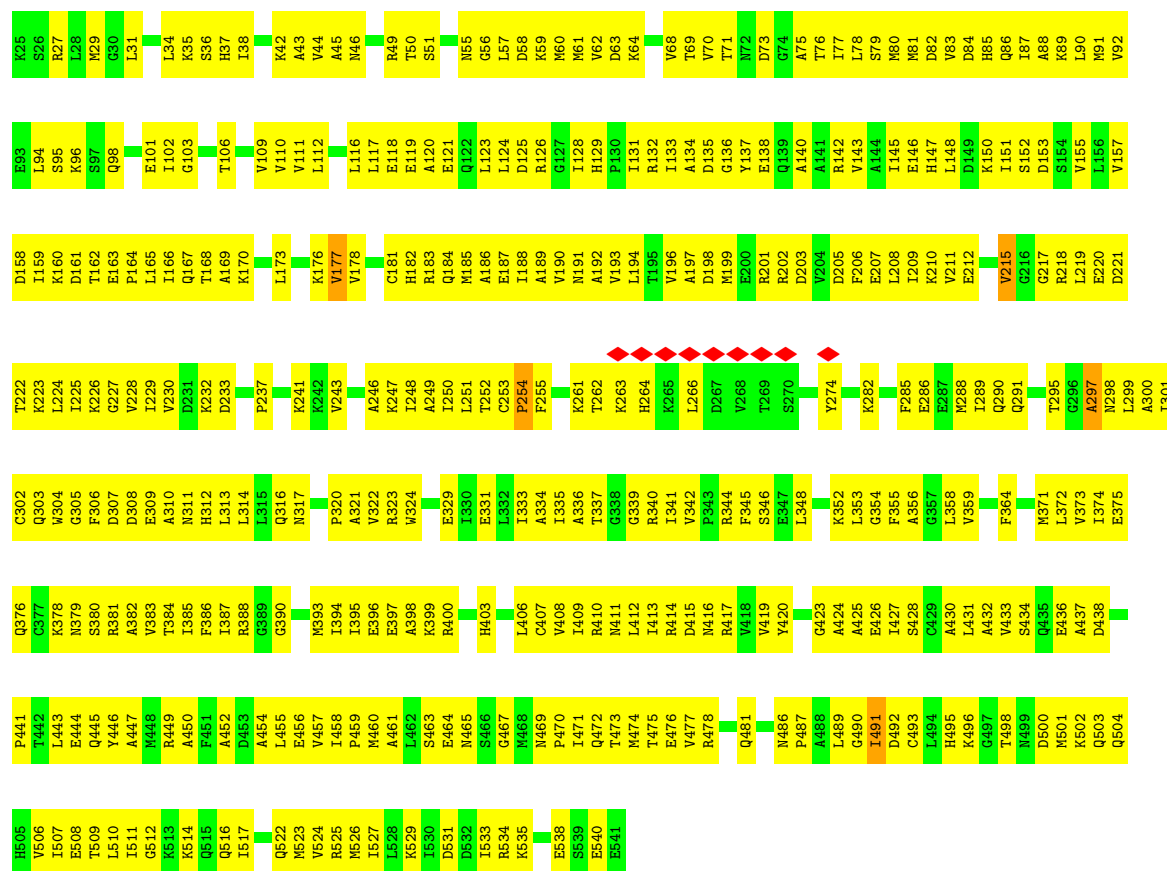
- Molecule 3: T-complex protein 1 subunit gamma



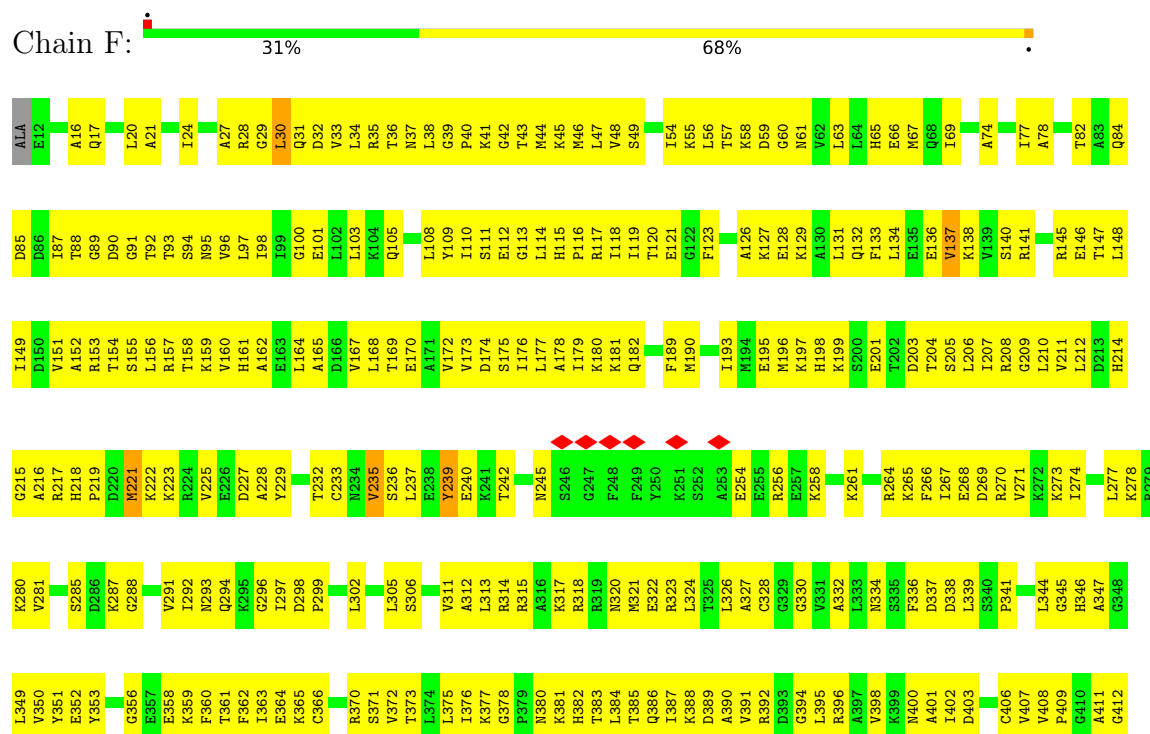
• Molecule 4: T-complex protein 1 subunit delta

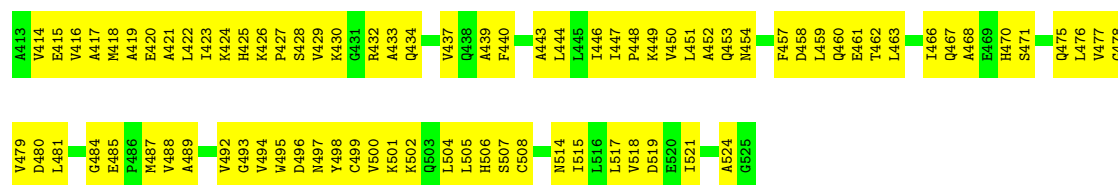




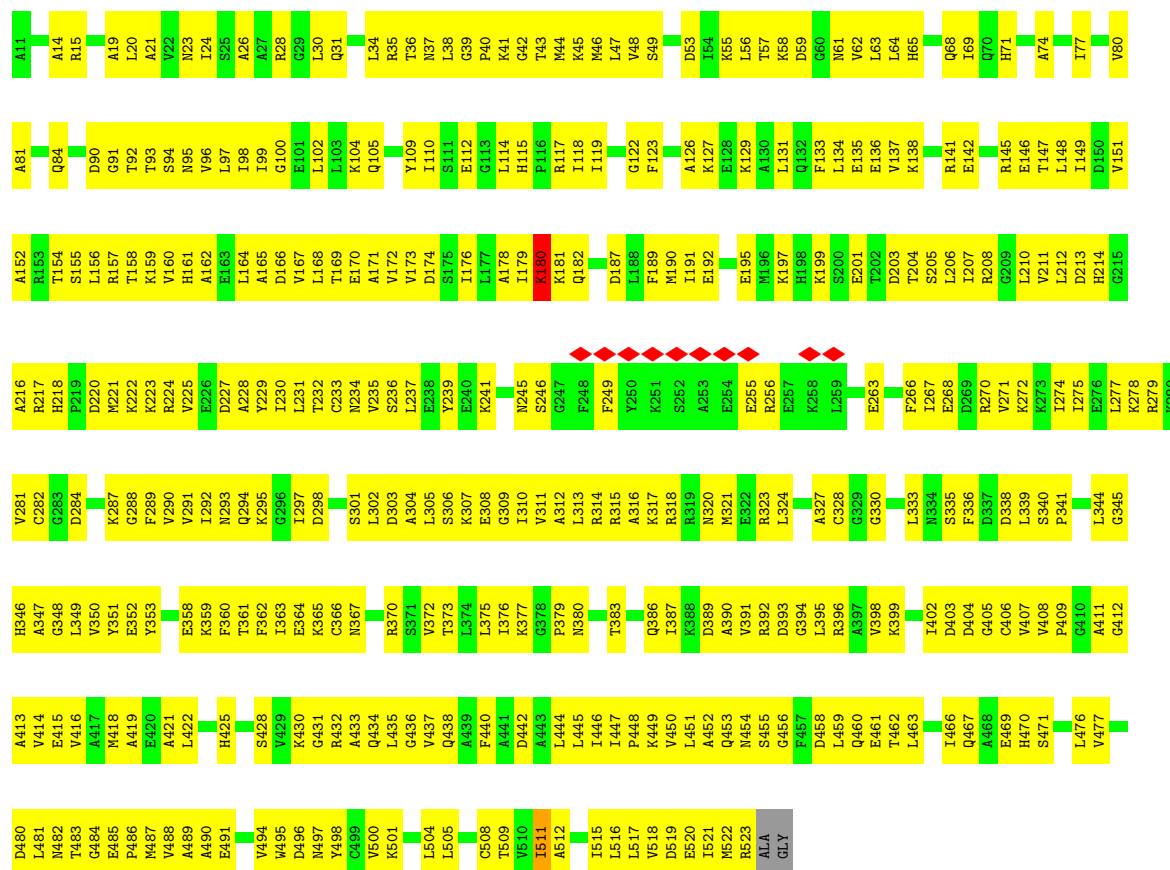


• Molecule 6: T-complex protein 1 subunit zeta

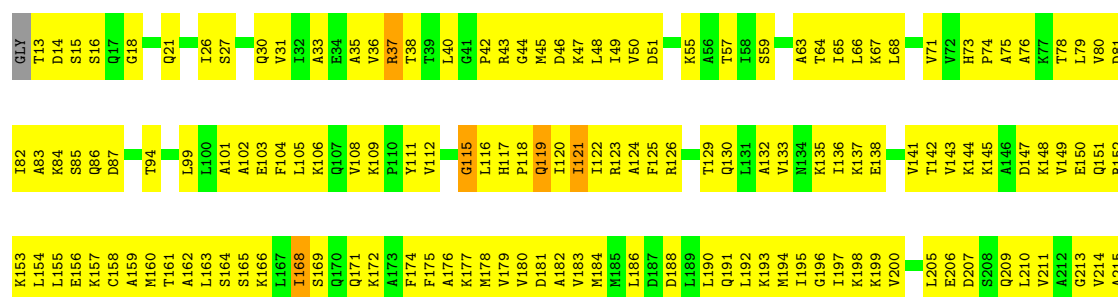




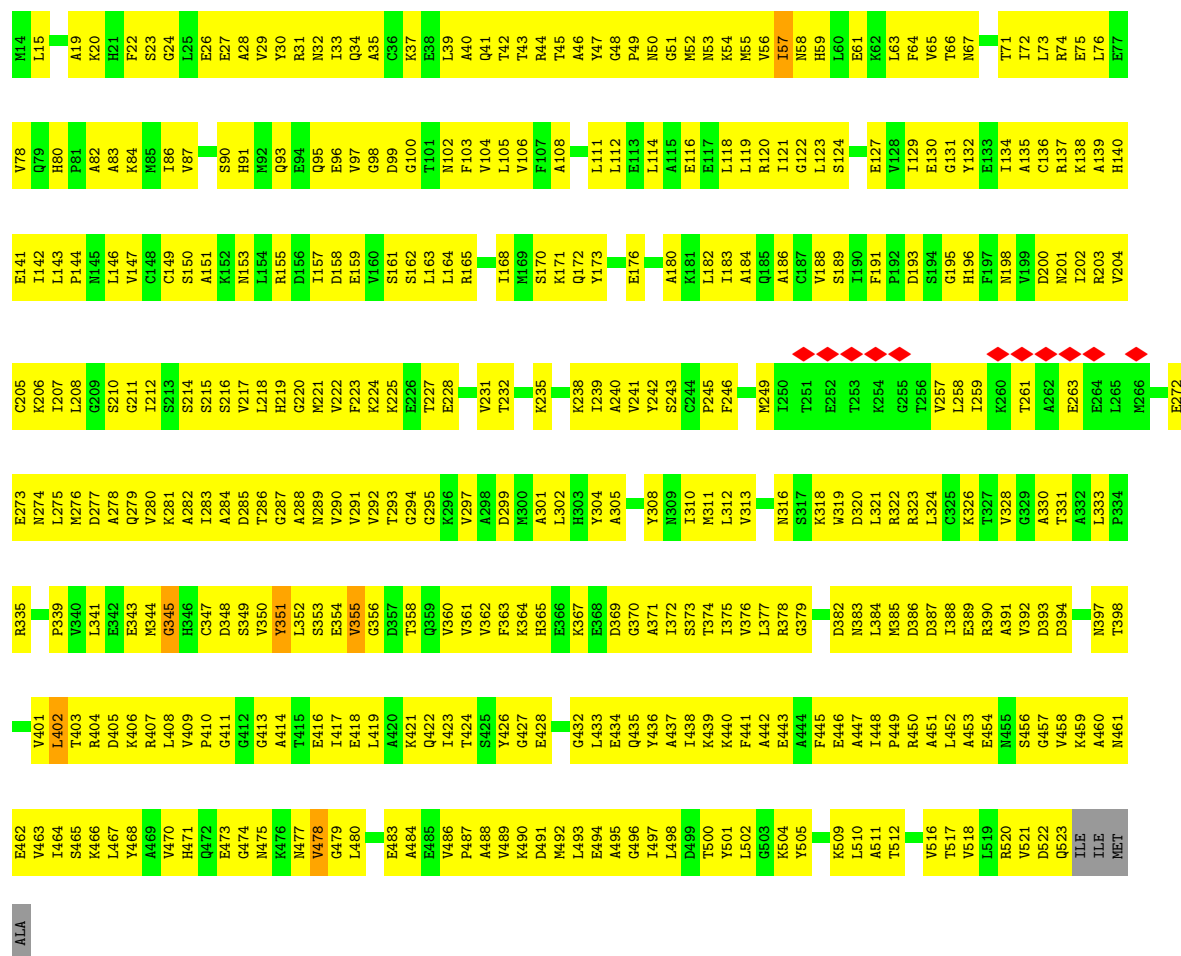
• Molecule 6: T-complex protein 1 subunit zeta



• Molecule 7: T-complex protein 1 subunit eta

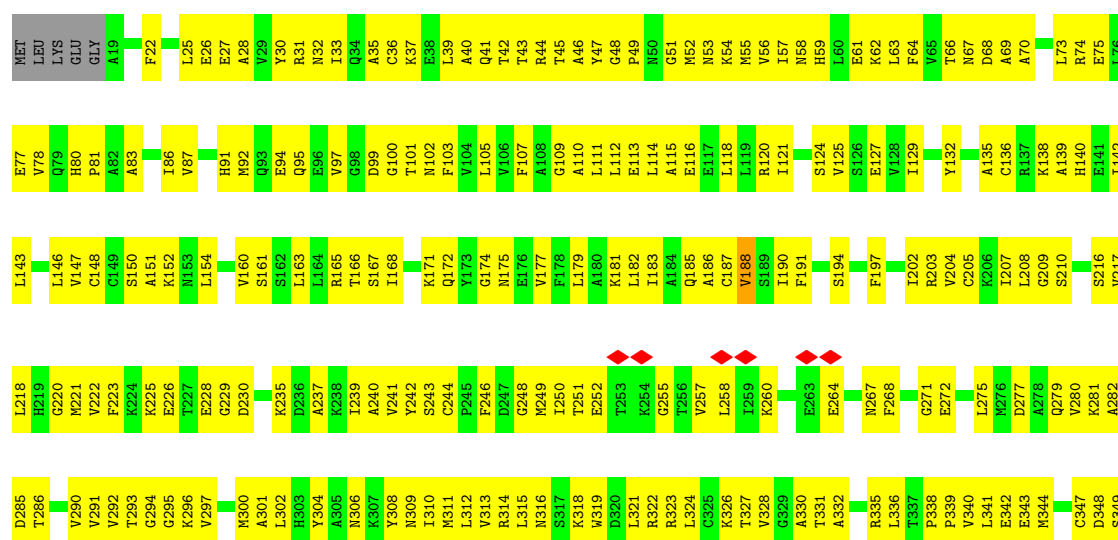




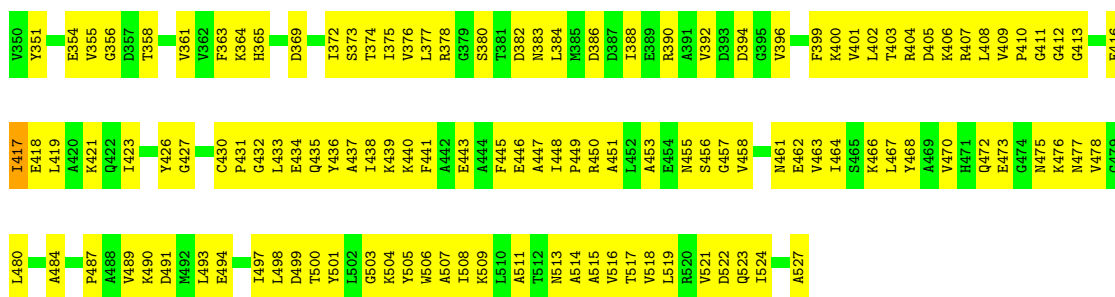


• Molecule 8: T-complex protein 1 subunit theta

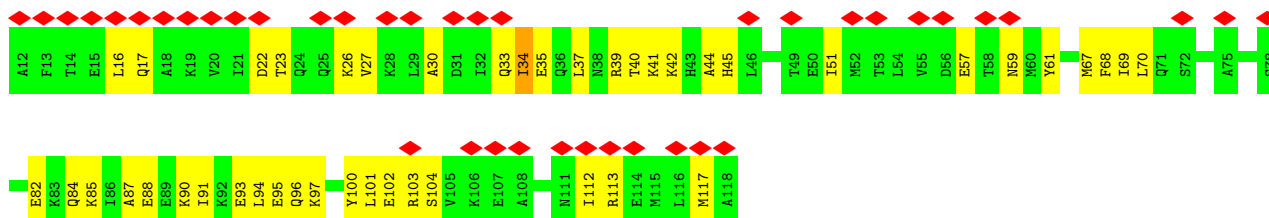
Chain P: 33% 65%



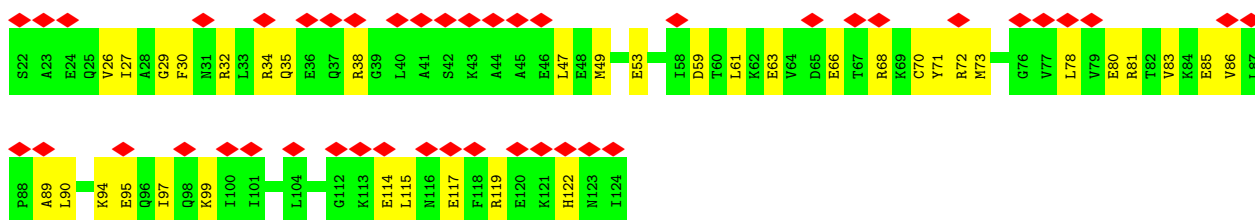
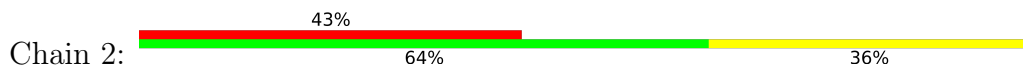




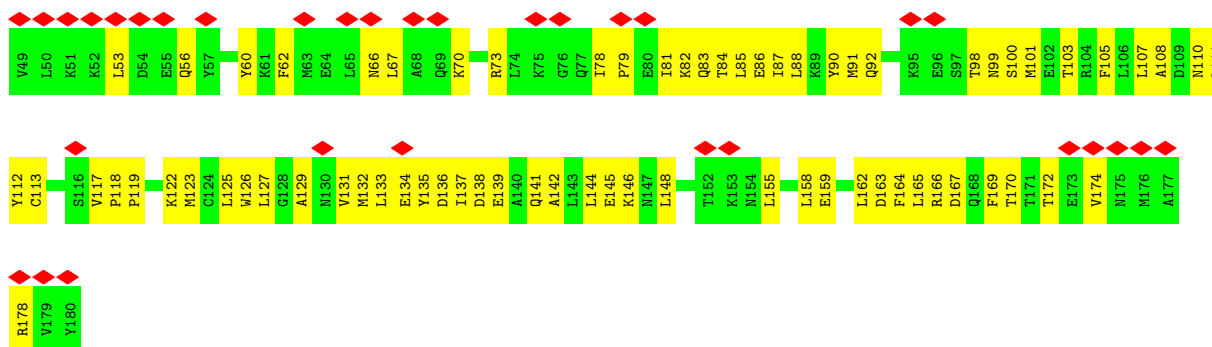
• Molecule 9: Prefoldin subunit 1



• Molecule 10: Prefoldin subunit 2

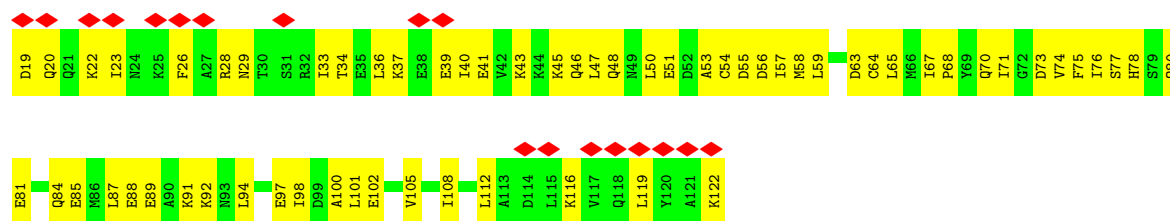


• Molecule 11: Prefoldin subunit 3



• Molecule 12: Prefoldin subunit 4

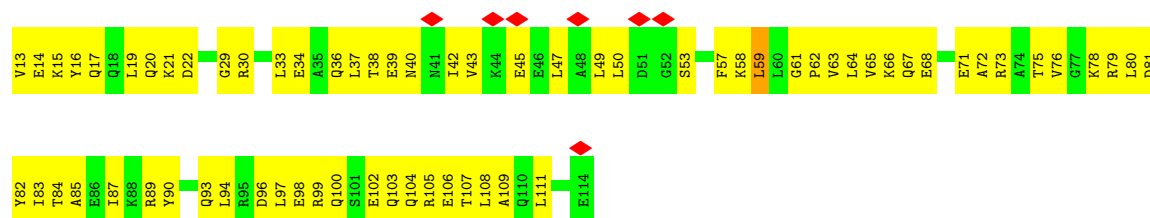




• Molecule 13: Prefoldin subunit 5



• Molecule 14: Prefoldin subunit 6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	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	0.133	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	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	0.30	0/3992	0.57	0/5389
1	I	0.29	0/4095	0.52	0/5526
2	B	0.30	0/3869	0.55	0/5214
2	J	0.27	0/3863	0.50	0/5207
3	C	0.31	0/4000	0.54	1/5397 (0.0%)
3	K	0.29	0/4029	0.54	1/5434 (0.0%)
4	D	0.31	0/3863	0.56	0/5214
4	L	0.28	0/3904	0.53	0/5269
5	E	0.31	0/4020	0.56	2/5414 (0.0%)
5	M	0.29	0/4020	0.53	0/5414
6	F	0.31	0/3991	0.55	2/5379 (0.0%)
6	N	0.29	0/3986	0.52	0/5374
7	G	0.31	0/3990	0.56	0/5383
7	O	0.29	0/4001	0.50	0/5396
8	H	0.32	0/3945	0.55	0/5331
8	P	0.30	0/3937	0.54	0/5321
9	1	0.24	0/880	0.39	0/1173
10	2	0.24	0/835	0.41	0/1116
11	3	0.27	0/1101	0.52	0/1476
12	4	0.27	0/852	0.48	0/1140
13	5	0.27	0/1032	0.48	0/1385
14	6	0.30	0/830	0.55	0/1109
All	All	0.30	0/69035	0.53	6/93061 (0.0%)

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	6
1	I	0	3
2	B	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	2
3	C	0	11
3	K	0	4
4	D	0	1
4	L	0	6
5	E	0	6
5	M	0	3
6	F	0	4
6	N	0	1
7	G	0	7
7	O	0	2
8	H	0	5
8	P	0	1
14	6	0	1
All	All	0	66

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	256	GLU	N-CA-C	-6.47	93.54	111.00
6	F	30	LEU	CB-CG-CD2	-5.62	101.45	111.00
3	C	368	ASP	CB-CG-OD1	5.42	123.17	118.30
6	F	30	LEU	CA-CB-CG	5.38	127.68	115.30
3	K	113	LEU	CA-CB-CG	-5.13	103.51	115.30

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	LYS	Peptide
1	A	242	GLN	Peptide
1	A	252	VAL	Peptide
1	A	281	THR	Peptide
1	A	282	GLY	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	4124	451	0
1	I	4056	0	4217	414	0
2	B	3829	0	3932	408	0
2	J	3823	0	3927	316	0
3	C	3956	0	4079	423	0
3	K	3985	0	4108	401	0
4	D	3832	0	4042	500	0
4	L	3873	0	4086	412	0
5	E	3974	0	4084	534	0
5	M	3974	0	4084	418	0
6	F	3945	0	4071	421	0
6	N	3940	0	4068	396	0
7	G	3936	0	4028	483	0
7	O	3947	0	4036	358	0
8	H	3892	0	3949	432	0
8	P	3884	0	3943	356	0
9	1	874	0	902	37	0
10	2	830	0	852	39	0
11	3	1087	0	1114	71	0
12	4	847	0	845	74	0
13	5	1018	0	1042	89	0
14	6	826	0	850	75	0
All	All	68284	0	70383	6618	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 6618 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:327:ALA:HA	6:F:370:ARG:H	1.23	1.04
4:D:247:GLY:HA2	4:D:356:LEU:HD22	1.45	0.99
8:P:187:CYS:HA	8:P:202:ILE:HD11	1.47	0.97
3:K:241:LEU:HA	3:K:245:LEU:HB2	1.43	0.96
6:N:31:GLN:HE22	6:N:100:GLY:H	1.12	0.96

There are no symmetry-related clashes.

## 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	519/534 (97%)	455 (88%)	63 (12%)	1 (0%)	47	81
1	I	532/534 (100%)	494 (93%)	37 (7%)	1 (0%)	47	81
2	B	507/509 (100%)	450 (89%)	54 (11%)	3 (1%)	25	66
2	J	506/509 (99%)	466 (92%)	39 (8%)	1 (0%)	47	81
3	C	507/513 (99%)	445 (88%)	61 (12%)	1 (0%)	47	81
3	K	511/513 (100%)	454 (89%)	55 (11%)	2 (0%)	34	72
4	D	506/514 (98%)	448 (88%)	56 (11%)	2 (0%)	34	72
4	L	511/514 (99%)	457 (89%)	54 (11%)	0	100	100
5	E	515/517 (100%)	456 (88%)	57 (11%)	2 (0%)	34	72
5	M	515/517 (100%)	477 (93%)	35 (7%)	3 (1%)	25	66
6	F	512/515 (99%)	456 (89%)	55 (11%)	1 (0%)	47	81
6	N	511/515 (99%)	464 (91%)	45 (9%)	2 (0%)	34	72
7	G	508/514 (99%)	449 (88%)	55 (11%)	4 (1%)	19	60
7	O	510/514 (99%)	462 (91%)	47 (9%)	1 (0%)	47	81
8	H	508/514 (99%)	443 (87%)	63 (12%)	2 (0%)	34	72
8	P	507/514 (99%)	455 (90%)	51 (10%)	1 (0%)	47	81
9	1	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
10	2	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
11	3	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
12	4	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
13	5	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	19	60
14	6	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
All	All	8848/8935 (99%)	7962 (90%)	858 (10%)	28 (0%)	44	77

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	441	PRO
2	J	226	VAL
1	A	251	GLN
7	G	284	SER
1	I	281	THR

### 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	434/445 (98%)	433 (100%)	1 (0%)	93	96
1	I	445/445 (100%)	443 (100%)	2 (0%)	91	94
2	B	405/405 (100%)	405 (100%)	0	100	100
2	J	405/405 (100%)	405 (100%)	0	100	100
3	C	441/444 (99%)	440 (100%)	1 (0%)	93	96
3	K	444/444 (100%)	442 (100%)	2 (0%)	88	93
4	D	433/439 (99%)	432 (100%)	1 (0%)	93	96
4	L	438/439 (100%)	436 (100%)	2 (0%)	88	93
5	E	436/436 (100%)	435 (100%)	1 (0%)	93	96
5	M	436/436 (100%)	436 (100%)	0	100	100
6	F	429/429 (100%)	429 (100%)	0	100	100
6	N	429/429 (100%)	428 (100%)	1 (0%)	93	96
7	G	420/421 (100%)	419 (100%)	1 (0%)	93	96
7	O	421/421 (100%)	420 (100%)	1 (0%)	93	96
8	H	423/426 (99%)	423 (100%)	0	100	100
8	P	422/426 (99%)	421 (100%)	1 (0%)	93	96
9	1	97/97 (100%)	96 (99%)	1 (1%)	76	86
10	2	91/91 (100%)	91 (100%)	0	100	100
11	3	122/122 (100%)	122 (100%)	0	100	100
12	4	96/96 (100%)	96 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	5	116/116 (100%)	116 (100%)	0	100	100
14	6	91/91 (100%)	91 (100%)	0	100	100
All	All	7474/7503 (100%)	7459 (100%)	15 (0%)	93	96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	156	ILE
8	P	417	ILE
3	K	296	ILE
9	1	34	ILE
6	N	511	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
6	N	467	GLN
11	3	110	ASN
7	O	151	GLN
8	P	316	ASN
13	5	54	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	O	1
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	258:HIS	C	259:THR	N	5.28
1	G	166:LYS	C	167:LEU	N	3.01

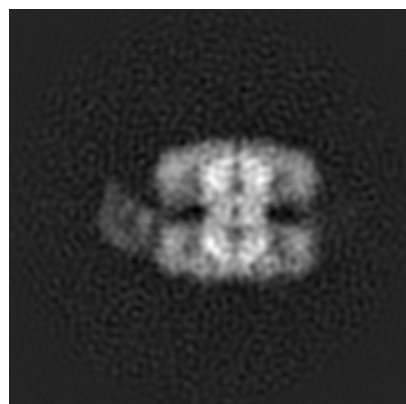
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0493. These allow visual inspection of the internal detail of the map and identification of artifacts.

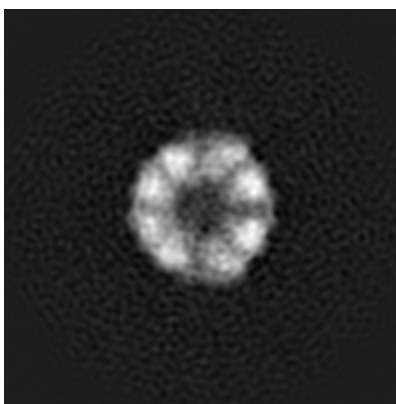
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

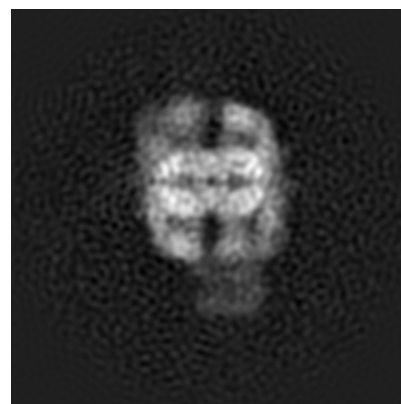
#### 6.1.1 Primary map



X

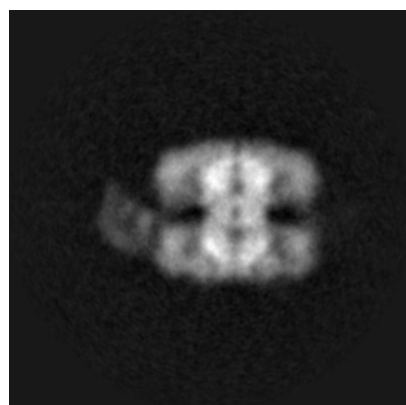


Y

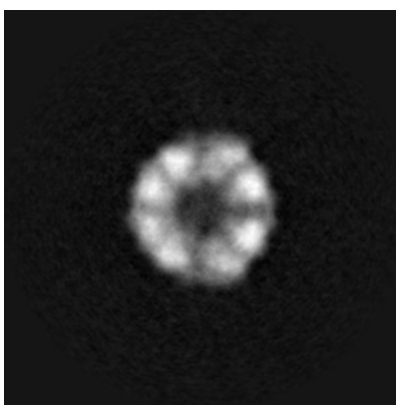


Z

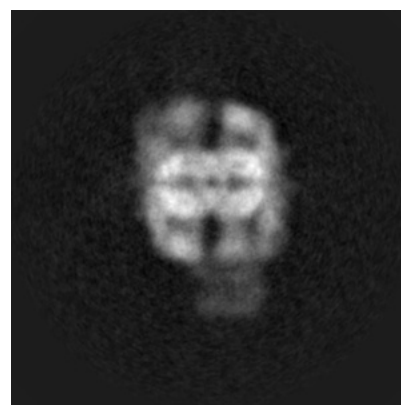
#### 6.1.2 Raw map



X



Y

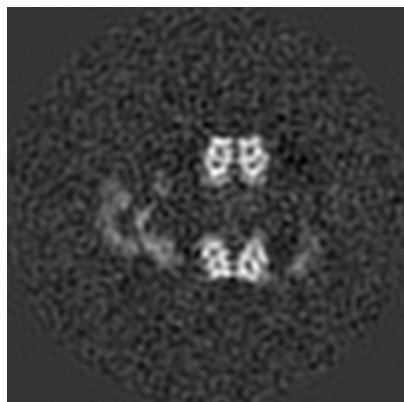


Z

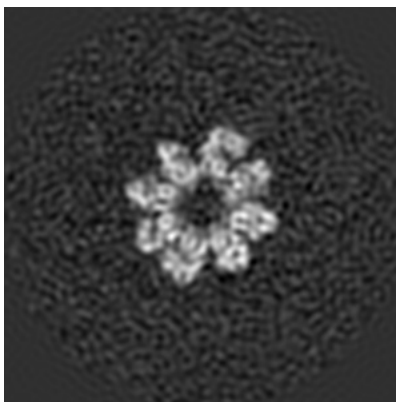
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

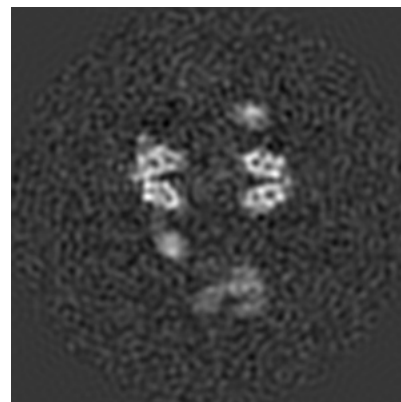
### 6.2.1 Primary map



X Index: 120

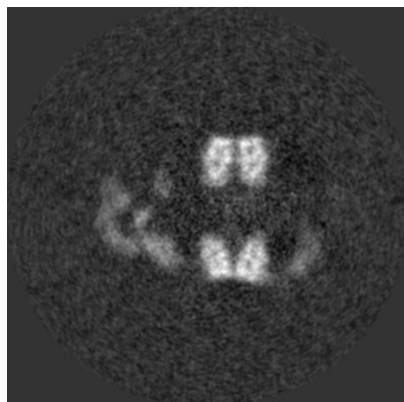


Y Index: 120

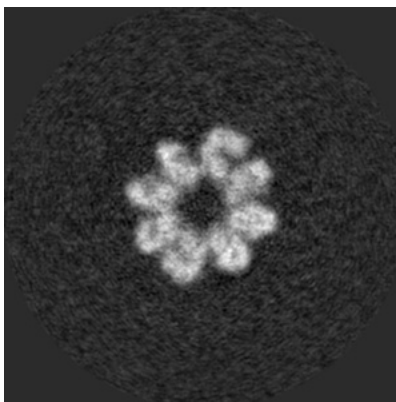


Z Index: 120

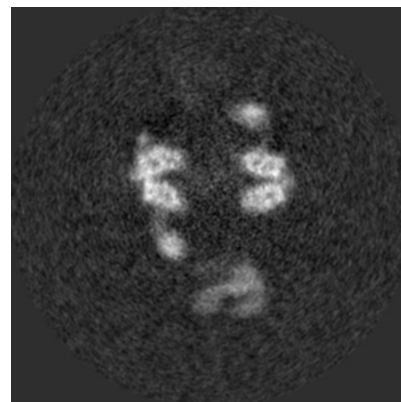
### 6.2.2 Raw map



X Index: 120



Y Index: 120

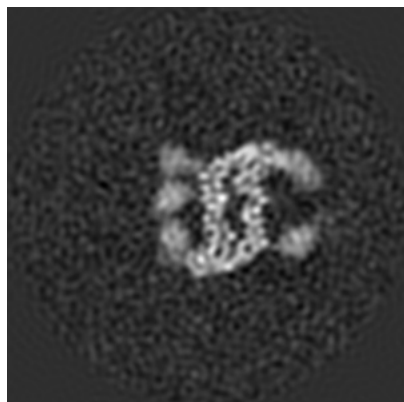


Z Index: 120

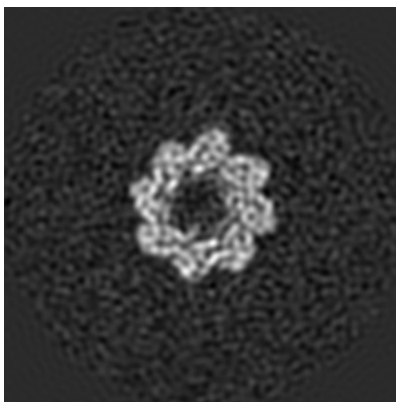
The images above show central slices of the map in three orthogonal directions.

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

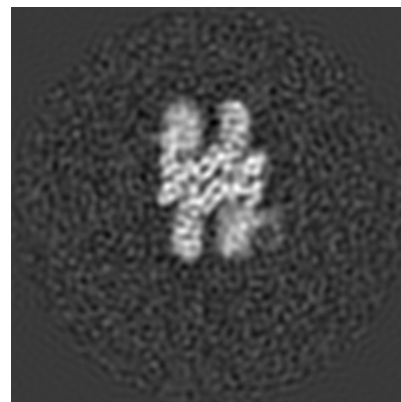
### 6.3.1 Primary map



X Index: 98

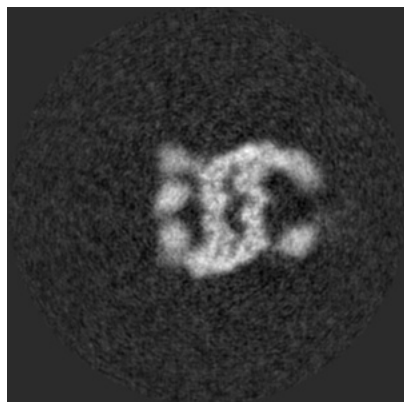


Y Index: 128

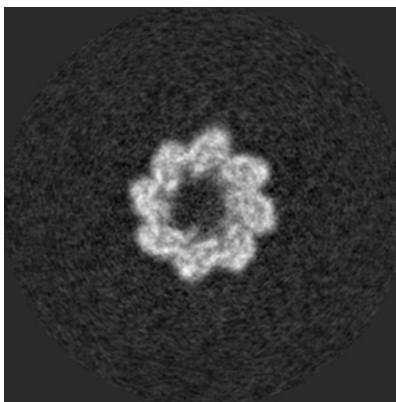


Z Index: 148

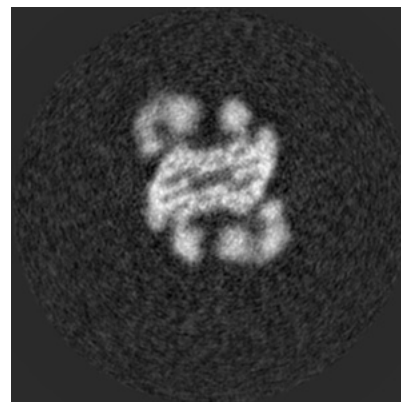
### 6.3.2 Raw map



X Index: 98



Y Index: 128



Z Index: 142

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

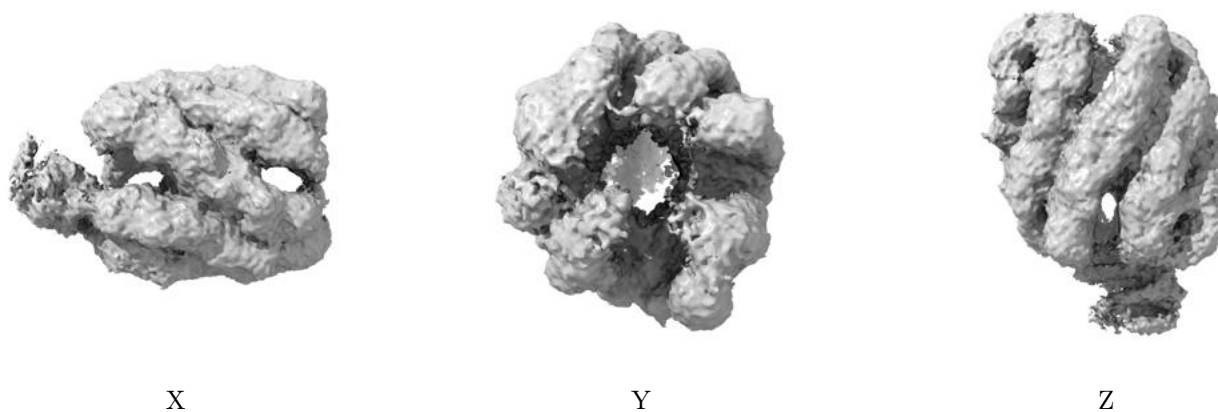
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

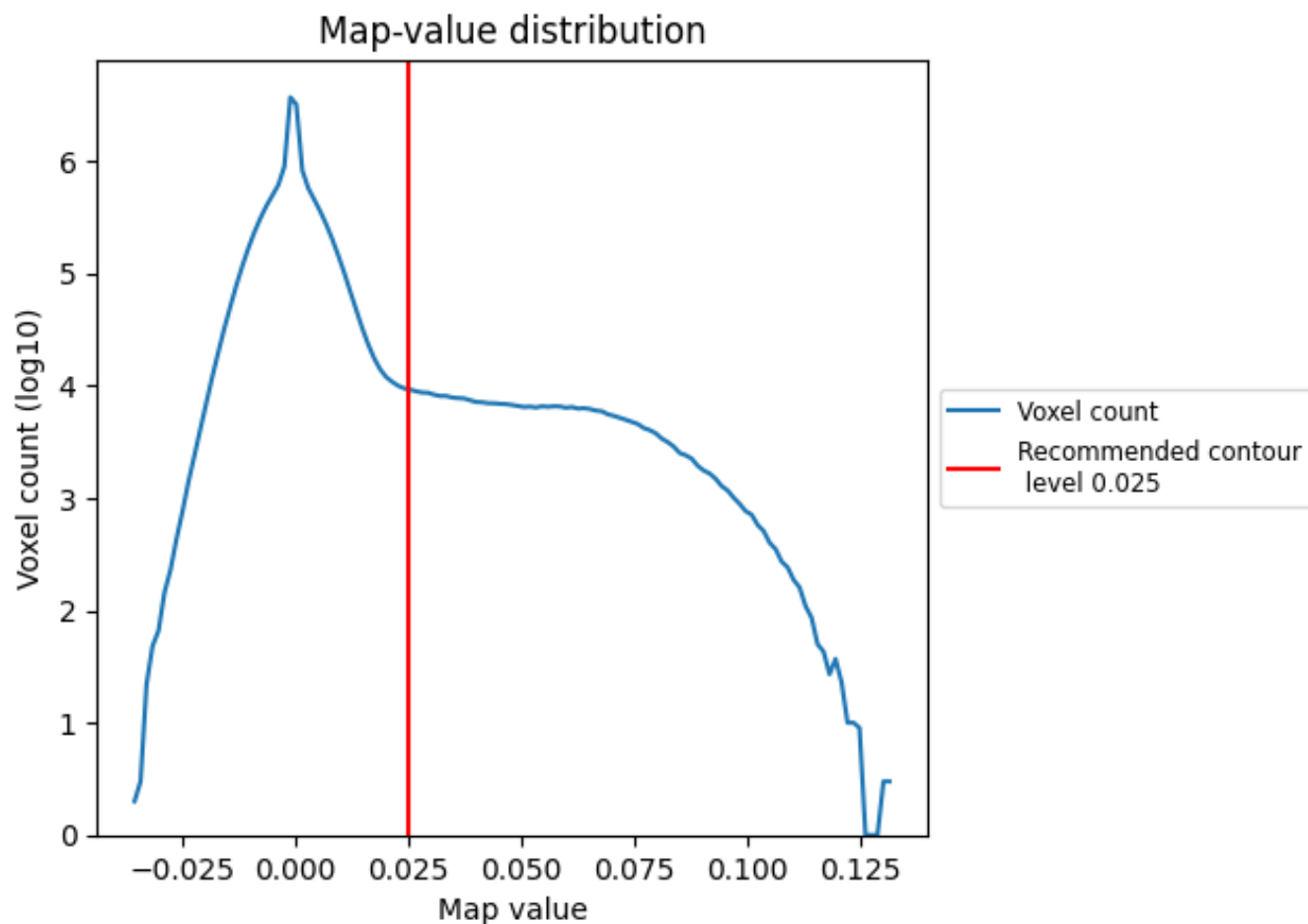
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

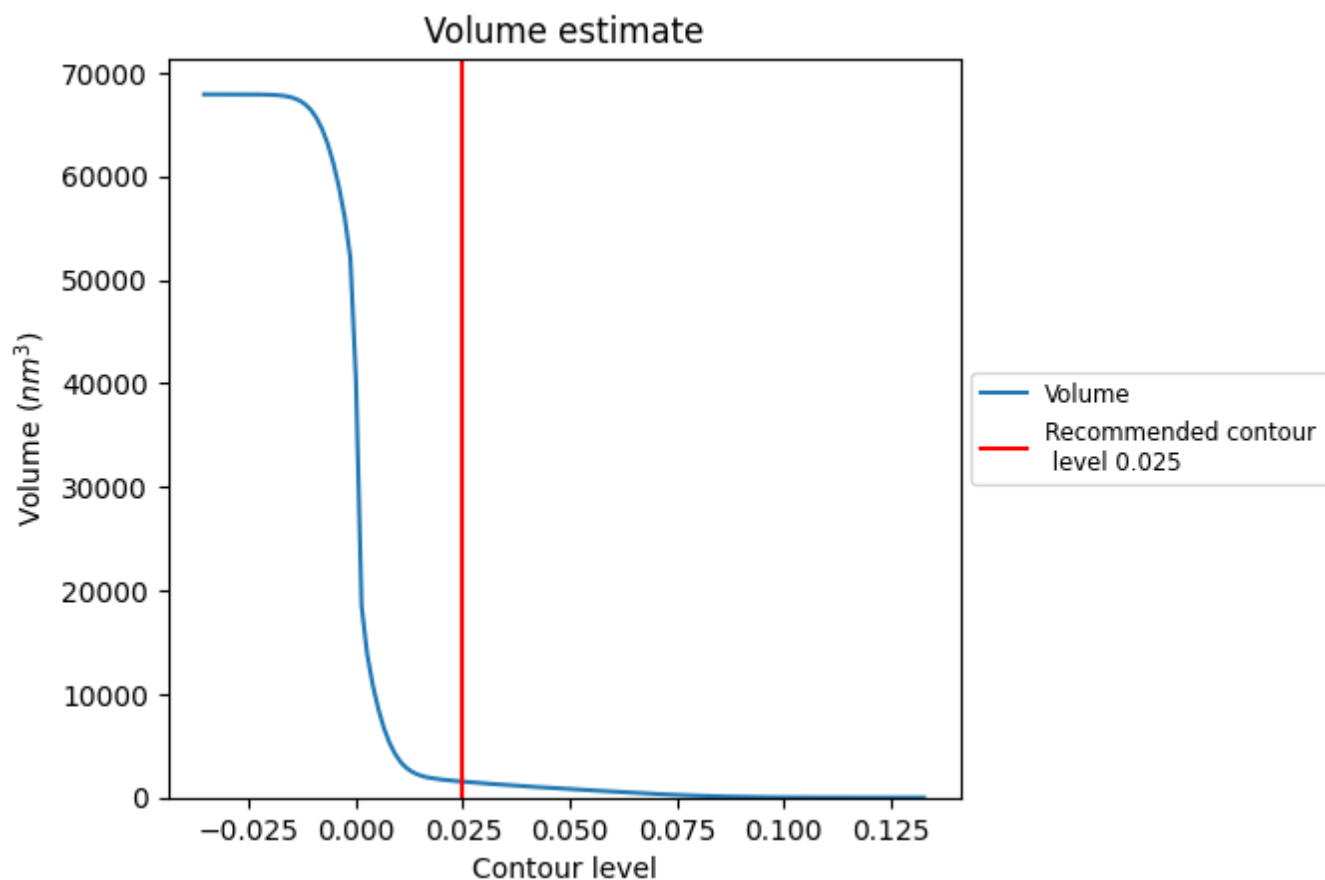
This section contains the results of statistical analysis of the map.

### 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](#)

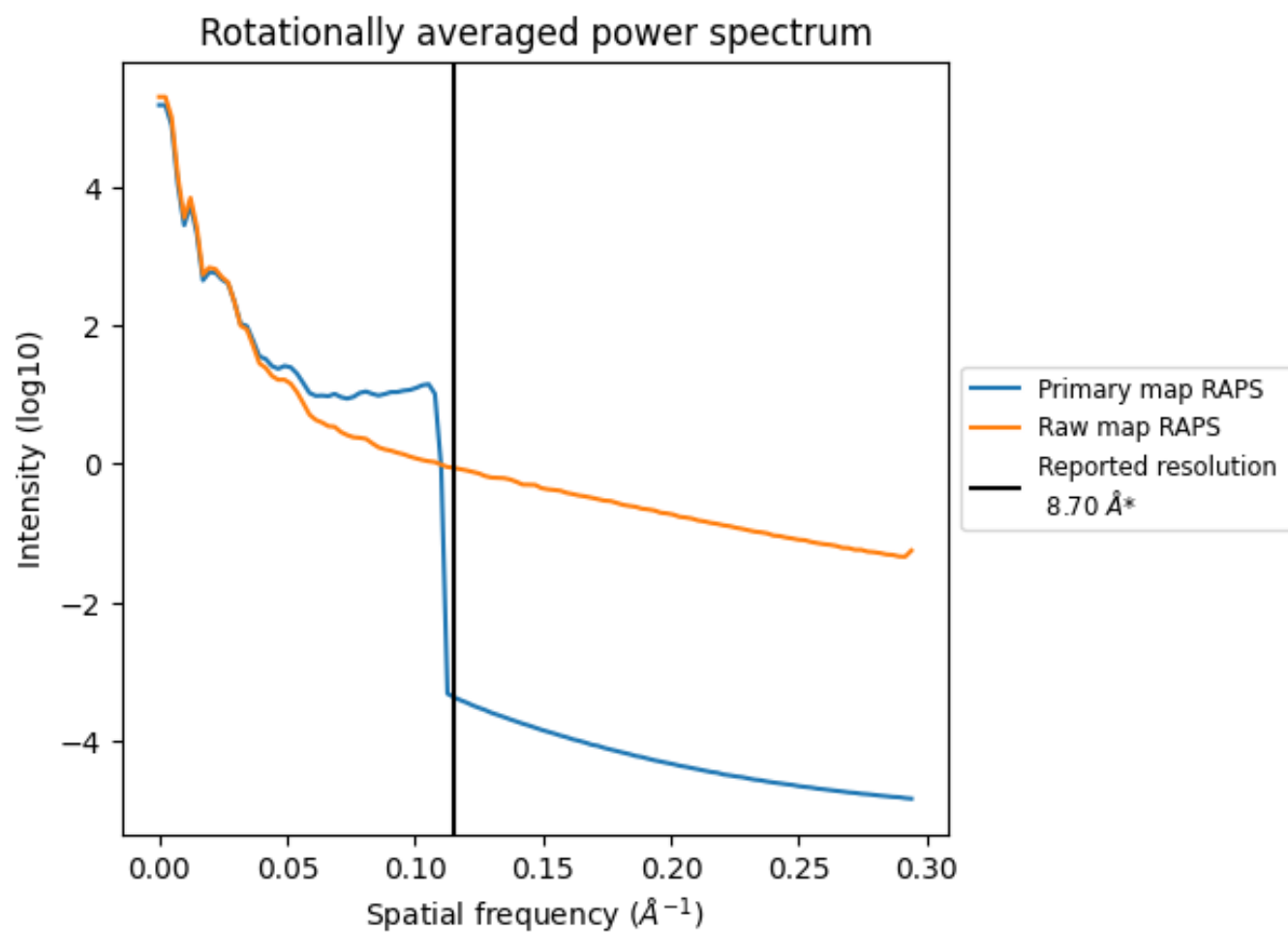


The volume at the recommended contour level is 1539 nm<sup>3</sup>; this corresponds to an approximate mass of 1390 kDa.

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 ⓘ

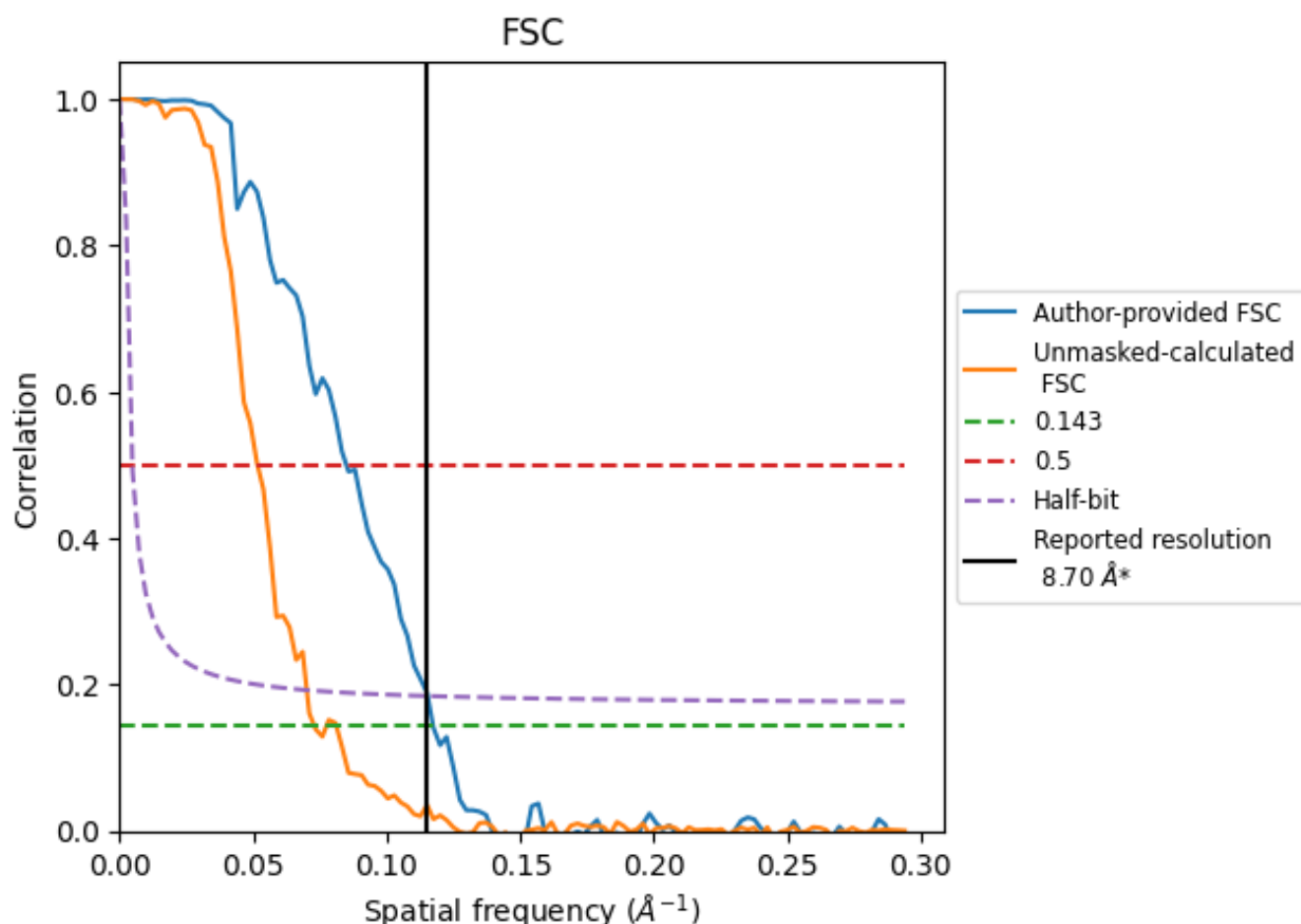


\*Reported resolution corresponds to spatial frequency of 0.115  $\text{\AA}^{-1}$

## 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 0.115 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

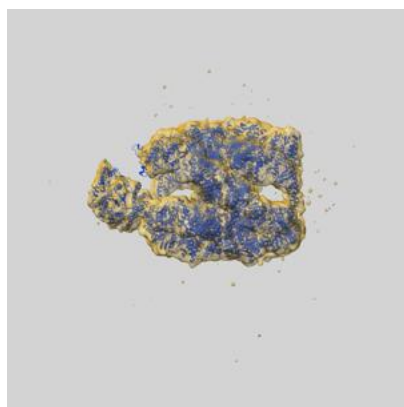
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.51	11.76	8.67
Unmasked-calculated*	13.70	19.34	14.25

\*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 13.70 differs from the reported value 8.7 by more than 10 %

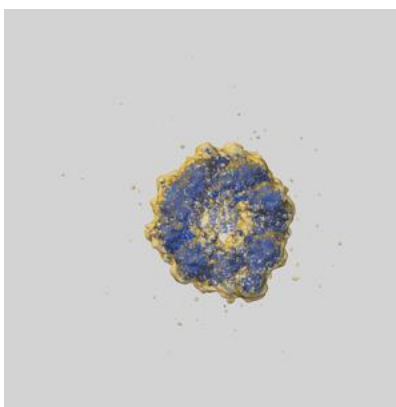
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0493 and PDB model 6NRB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

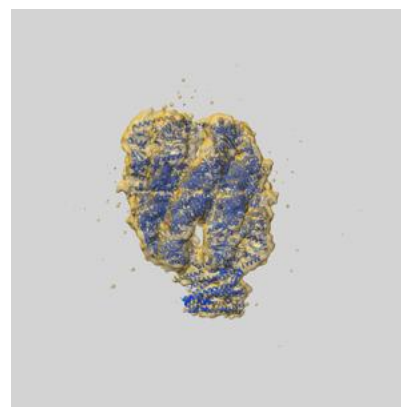
### 9.1 Map-model overlay [i](#)



X



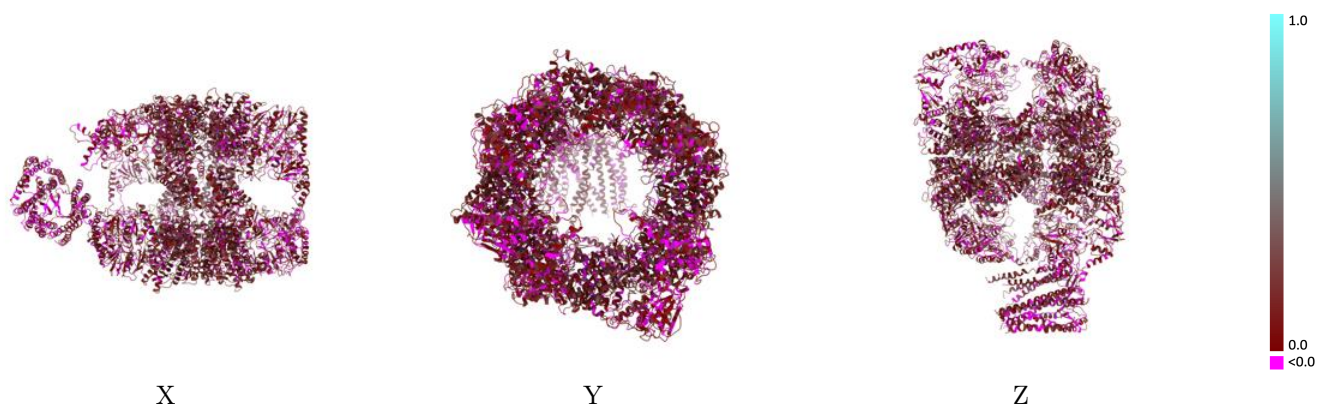
Y



Z

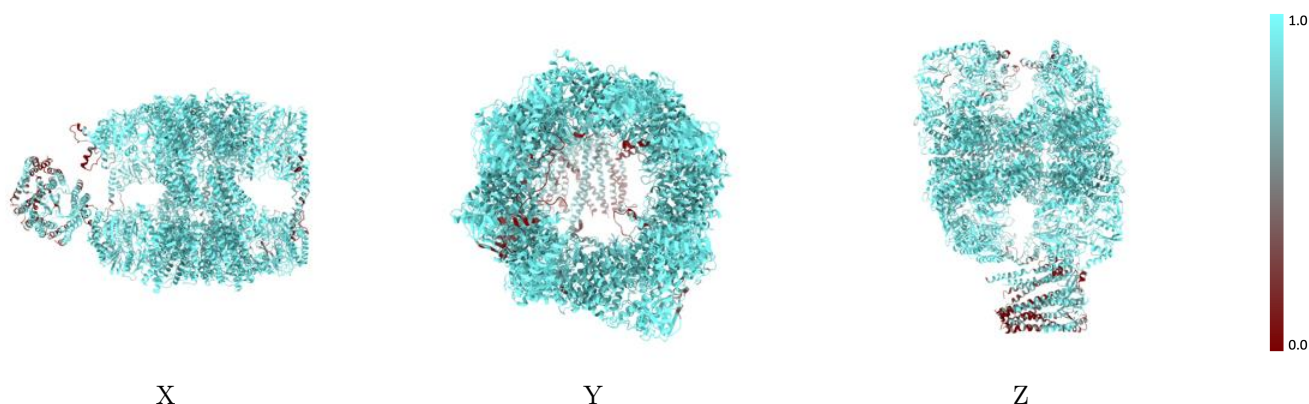
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



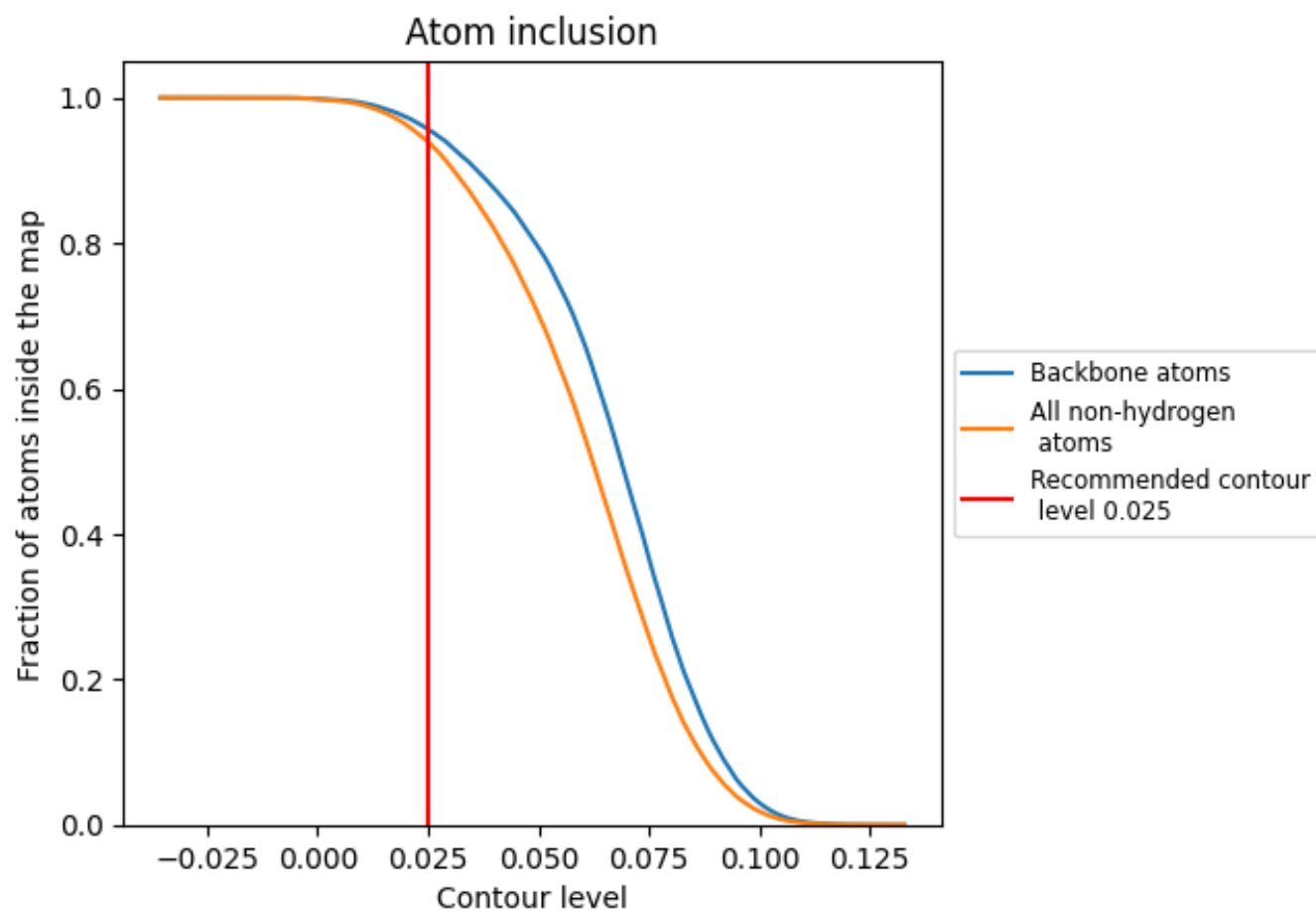
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9392	 0.1090
1	 0.5440	 0.0680
2	 0.5018	 0.0370
3	 0.7131	 0.0610
4	 0.7897	 0.0970
5	 0.7421	 0.0880
6	 0.8591	 0.1050
A	 0.9638	 0.1160
B	 0.9756	 0.1190
C	 0.9438	 0.1110
D	 0.9592	 0.1230
E	 0.9862	 0.1190
F	 0.9784	 0.1220
G	 0.9856	 0.1220
H	 0.9680	 0.1180
I	 0.9529	 0.0800
J	 0.8785	 0.0920
K	 0.9514	 0.1040
L	 0.9665	 0.1180
M	 0.9679	 0.1120
N	 0.9657	 0.1150
O	 0.9552	 0.1060
P	 0.9708	 0.1120

