



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:31 pm GMT

PDB ID : 4A00
EMDB ID : EMD-1960
Title : Symmetry-free cryo-EM map of TRiC in the nucleotide-free (apo) state
Authors : Cong, Y.; Schroder, G.F.; Meyer, A.S.; Jakana, J.; Ma, B.; Dougherty, M.T.; Schmid, M.F.; Reissmann, S.; Levitt, M.; Ludtke, S.L.; Frydman, J.; Chiu, W.
Deposited on : 2011-09-10
Resolution : 10.50 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.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

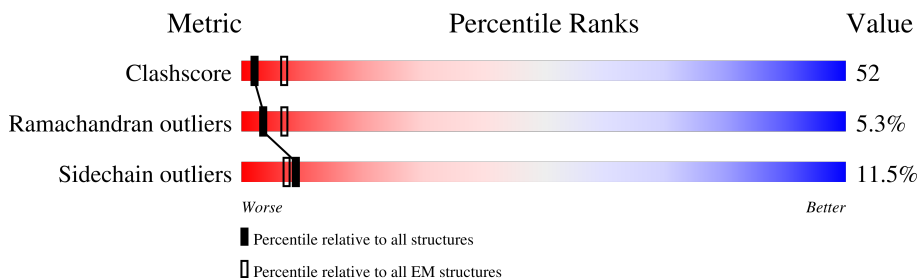
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.50 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 ≥ 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	513	
1	B	513	
1	C	513	
1	D	513	
1	E	513	
1	F	513	
1	G	513	
1	H	513	

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Mol	Chain	Length	Quality of chain
1	I	513	
1	J	513	
1	K	513	
1	L	513	
1	M	513	
1	N	513	
1	O	513	
1	P	513	

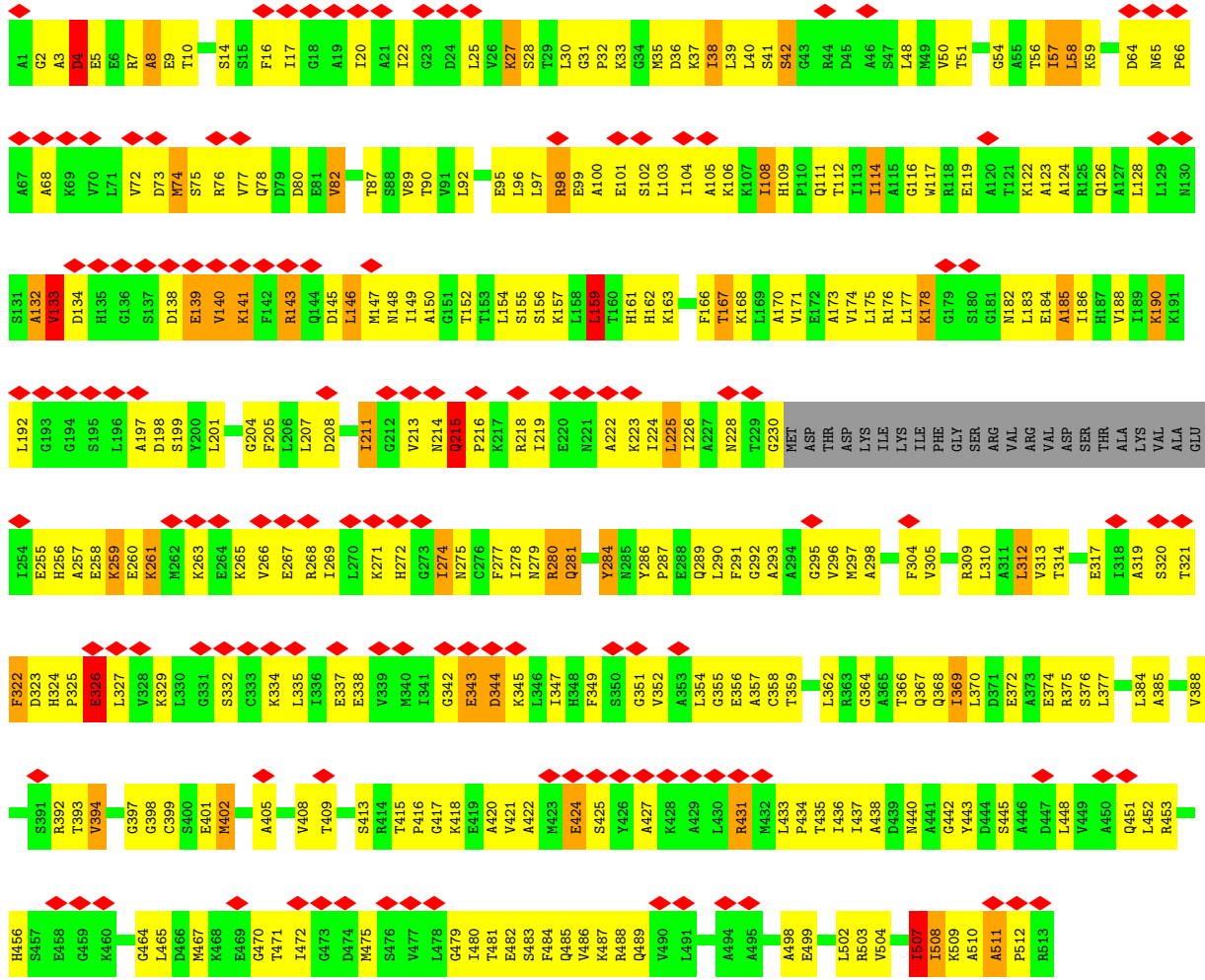
2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 56830 atoms, of which 0 are hydrogens and 0 are deuteriums.

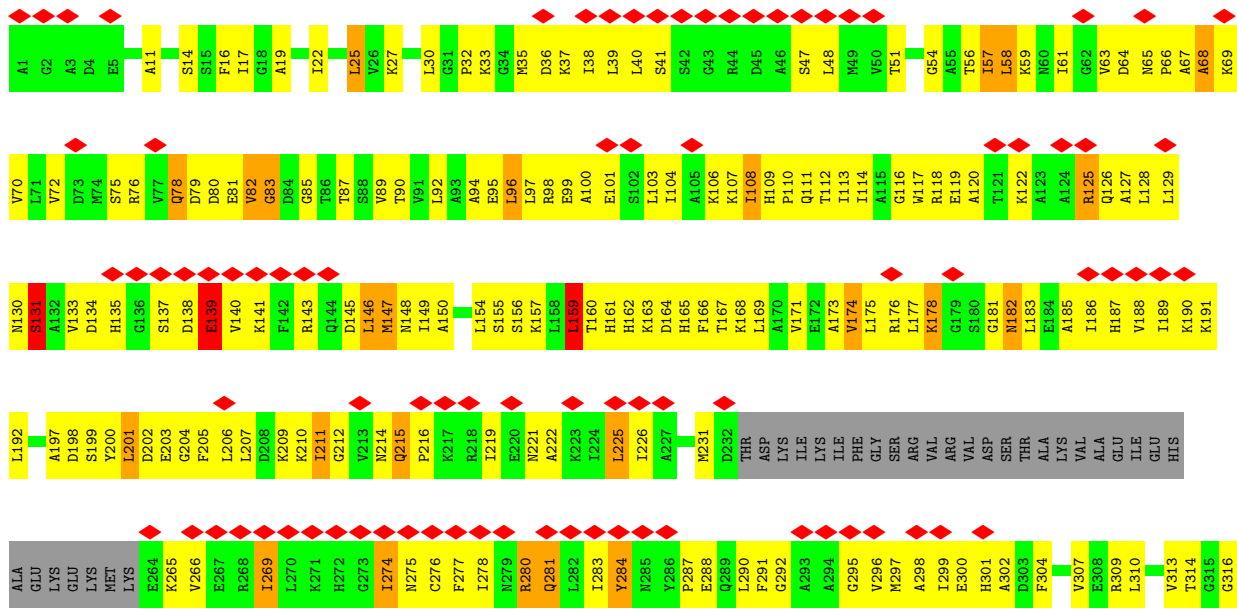
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

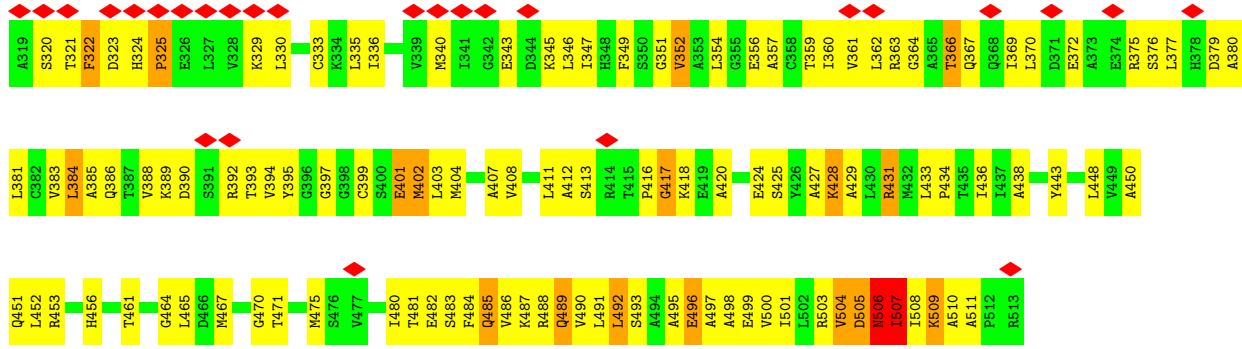
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	339	Total 2510	C 1552	N 449	O 496	S 13	0	0
1	B	490	Total 3677	C 2299	N 647	O 713	S 18	0	0
1	C	482	Total 3608	C 2255	N 634	O 701	S 18	0	0
1	D	489	Total 3666	C 2291	N 644	O 712	S 19	0	0
1	E	492	Total 3693	C 2308	N 649	O 717	S 19	0	0
1	F	488	Total 3661	C 2288	N 643	O 711	S 19	0	0
1	G	513	Total 3855	C 2409	N 679	O 748	S 19	0	0
1	H	493	Total 3702	C 2313	N 650	O 720	S 19	0	0
1	I	473	Total 3530	C 2206	N 620	O 686	S 18	0	0
1	J	490	Total 3673	C 2295	N 645	O 714	S 19	0	0
1	K	496	Total 3723	C 2327	N 654	O 723	S 19	0	0
1	L	491	Total 3685	C 2304	N 648	O 714	S 19	0	0
1	M	388	Total 2881	C 1792	N 506	O 569	S 14	0	0
1	N	486	Total 3643	C 2277	N 640	O 707	S 19	0	0
1	O	481	Total 3600	C 2251	N 633	O 698	S 18	0	0
1	P	496	Total 3723	C 2327	N 654	O 723	S 19	0	0

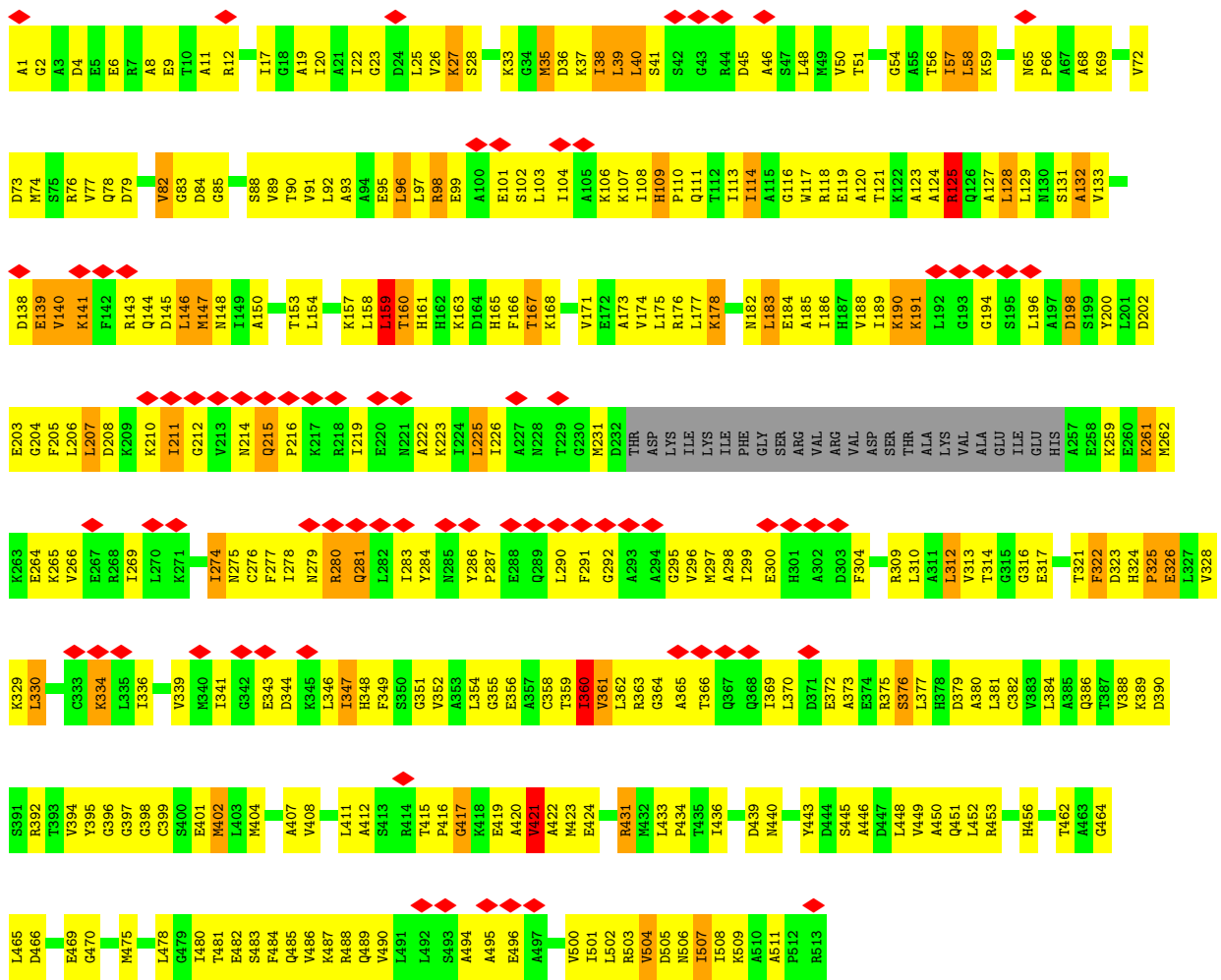


● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

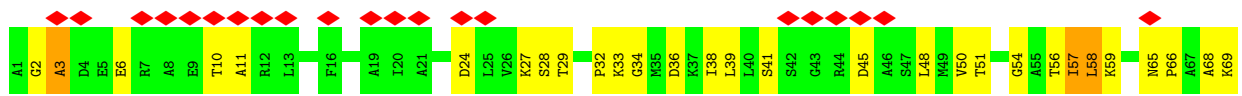
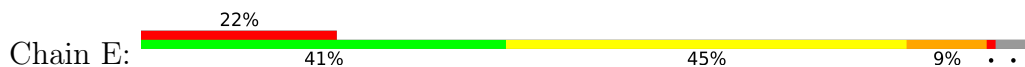


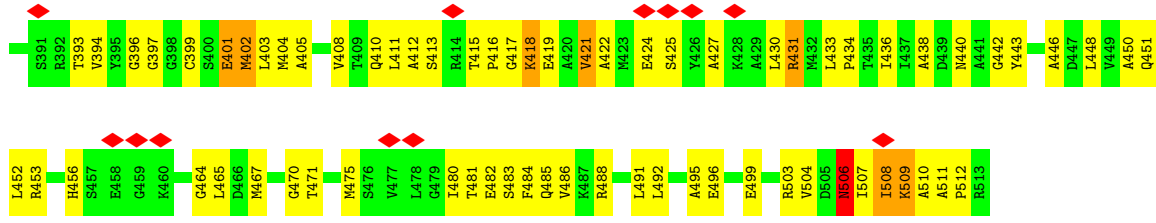


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

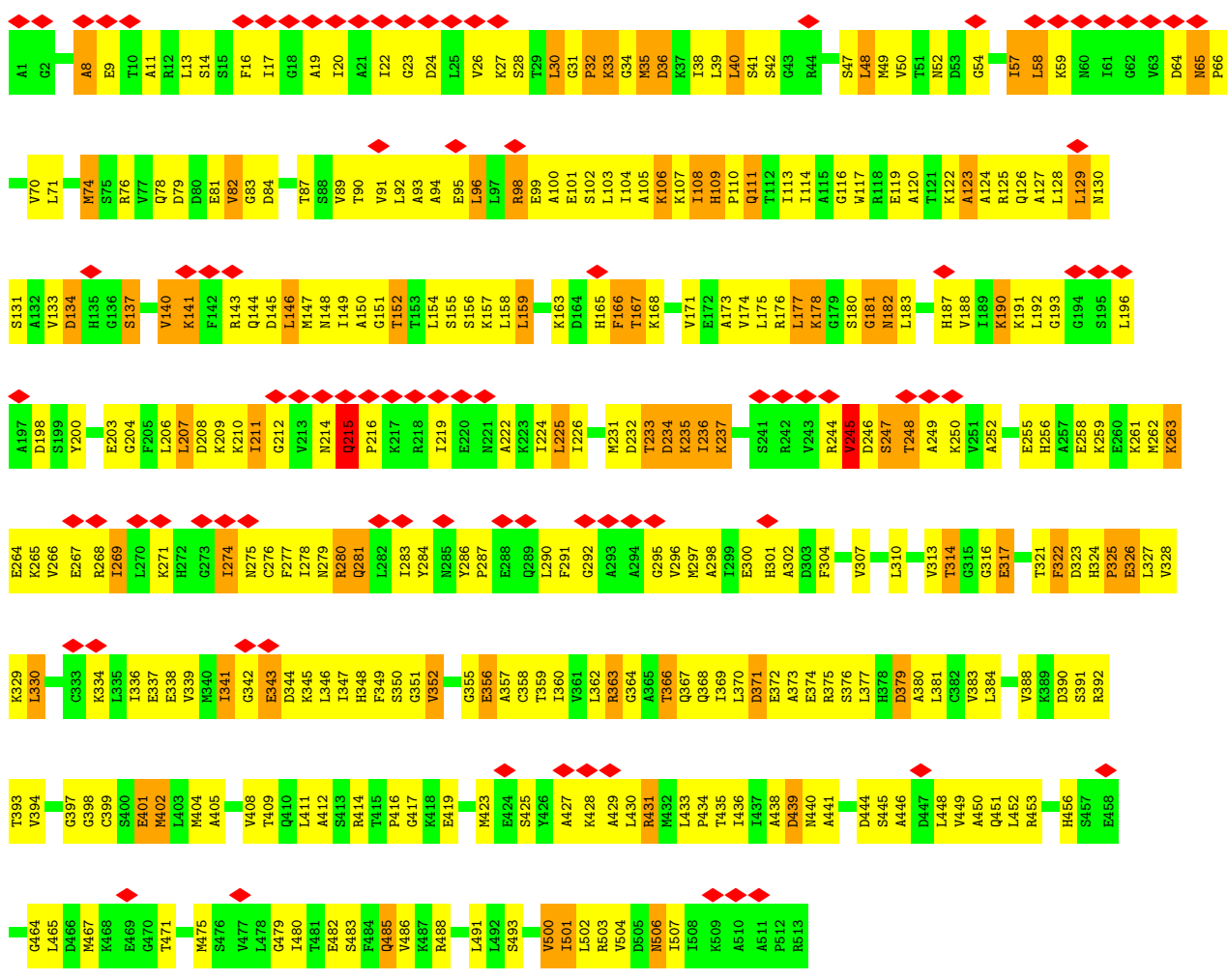


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



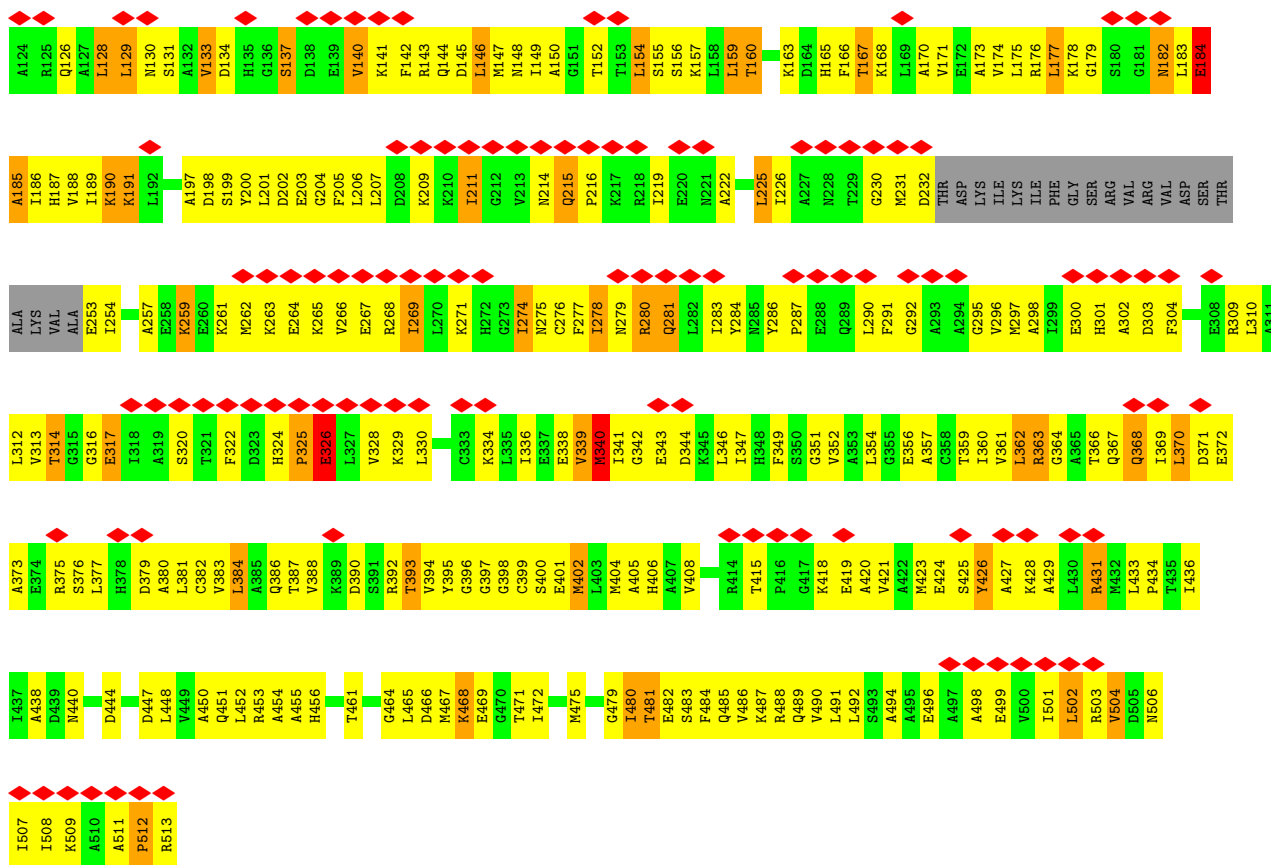


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

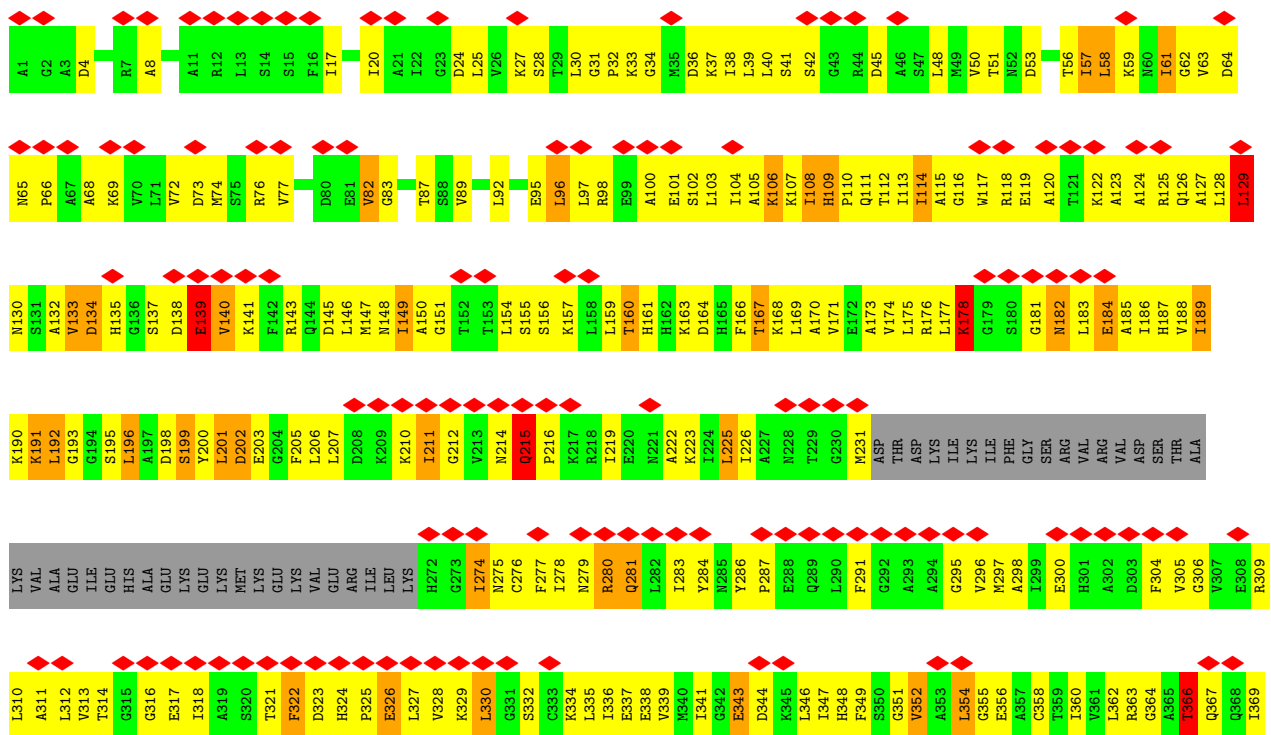


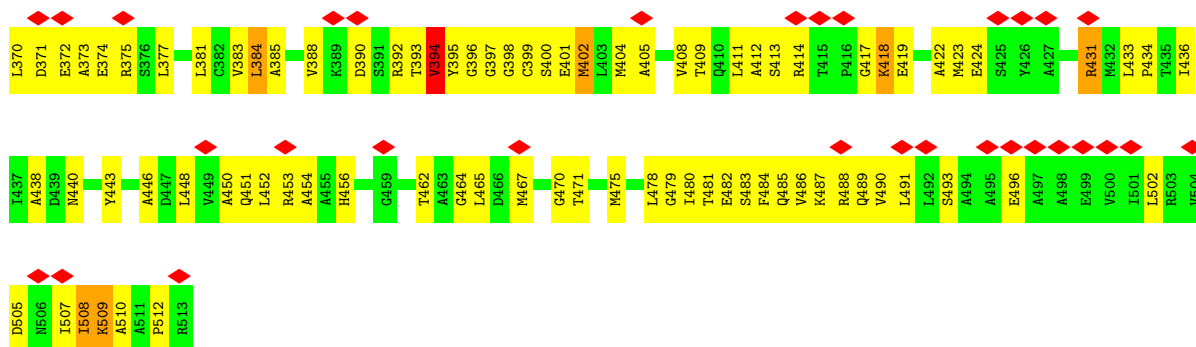
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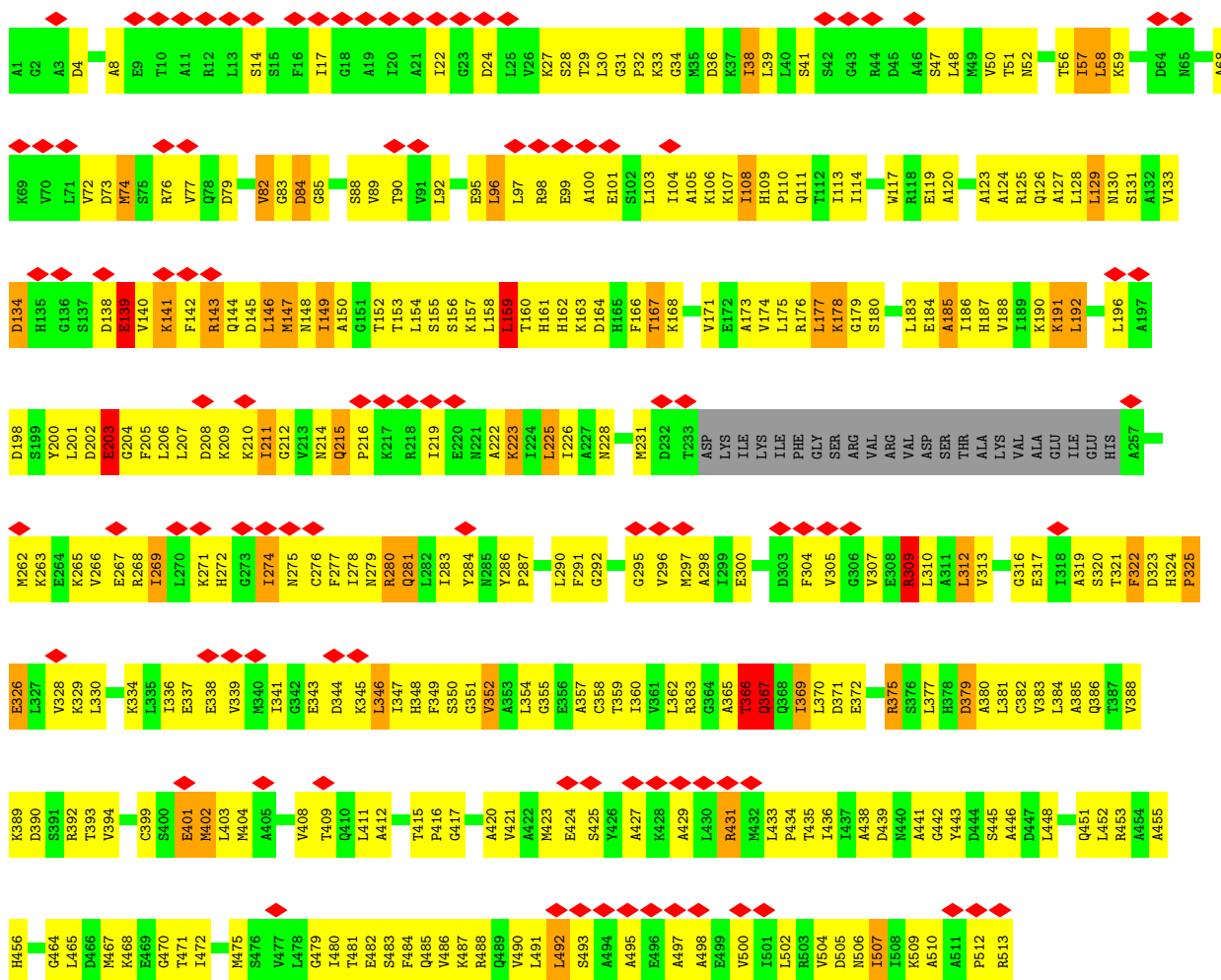


● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



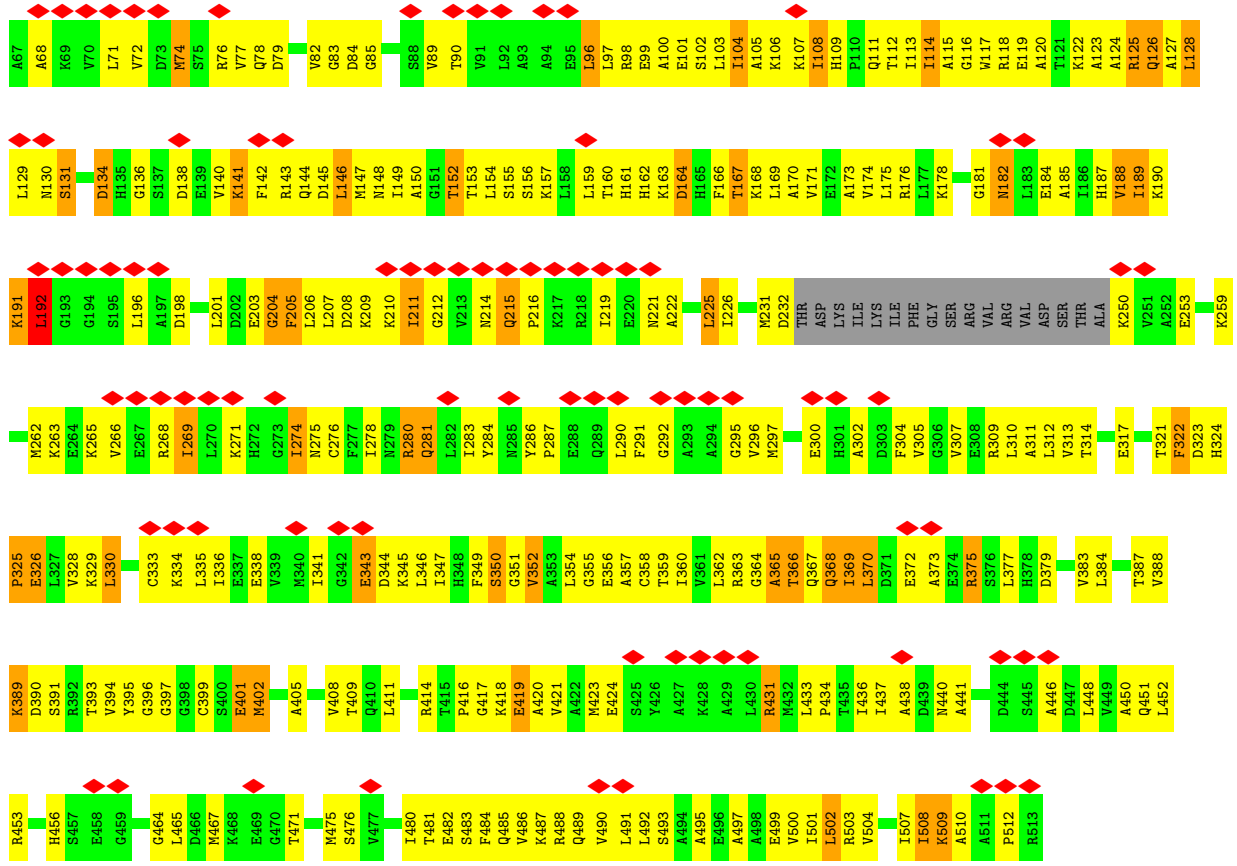


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

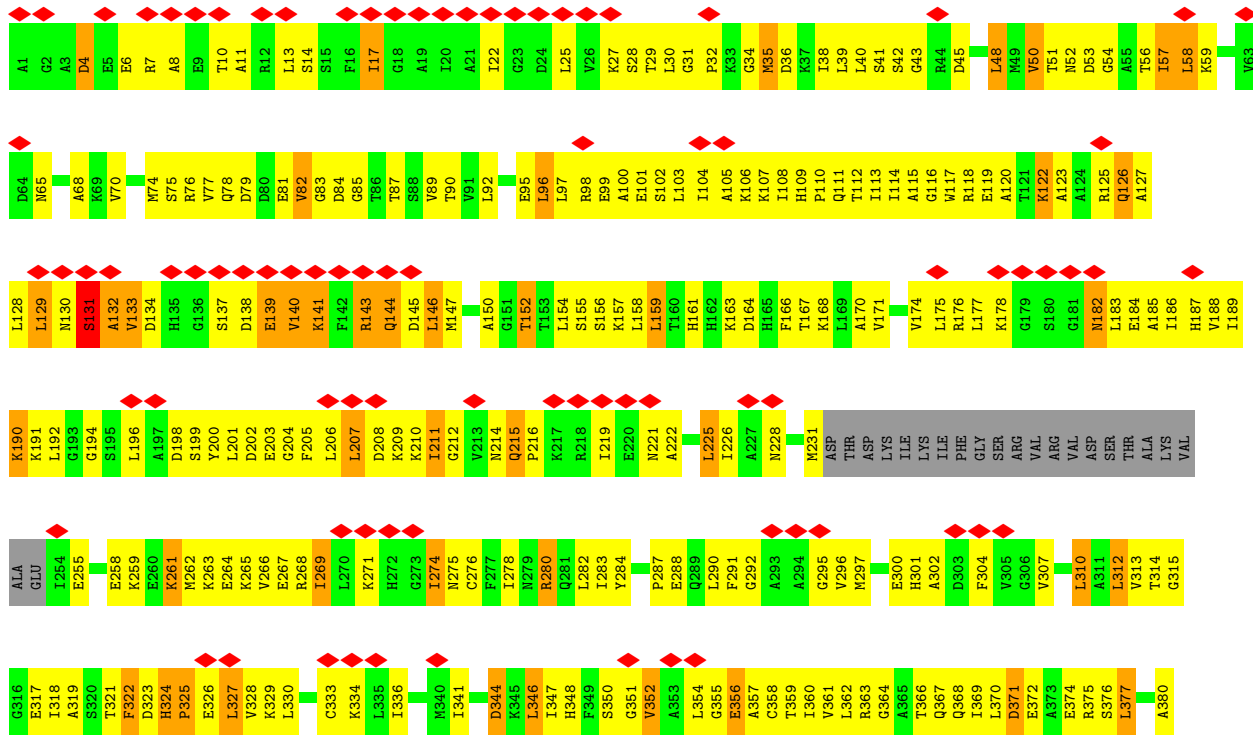


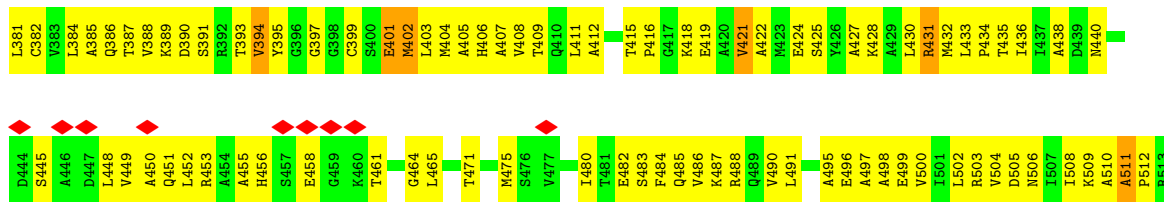
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



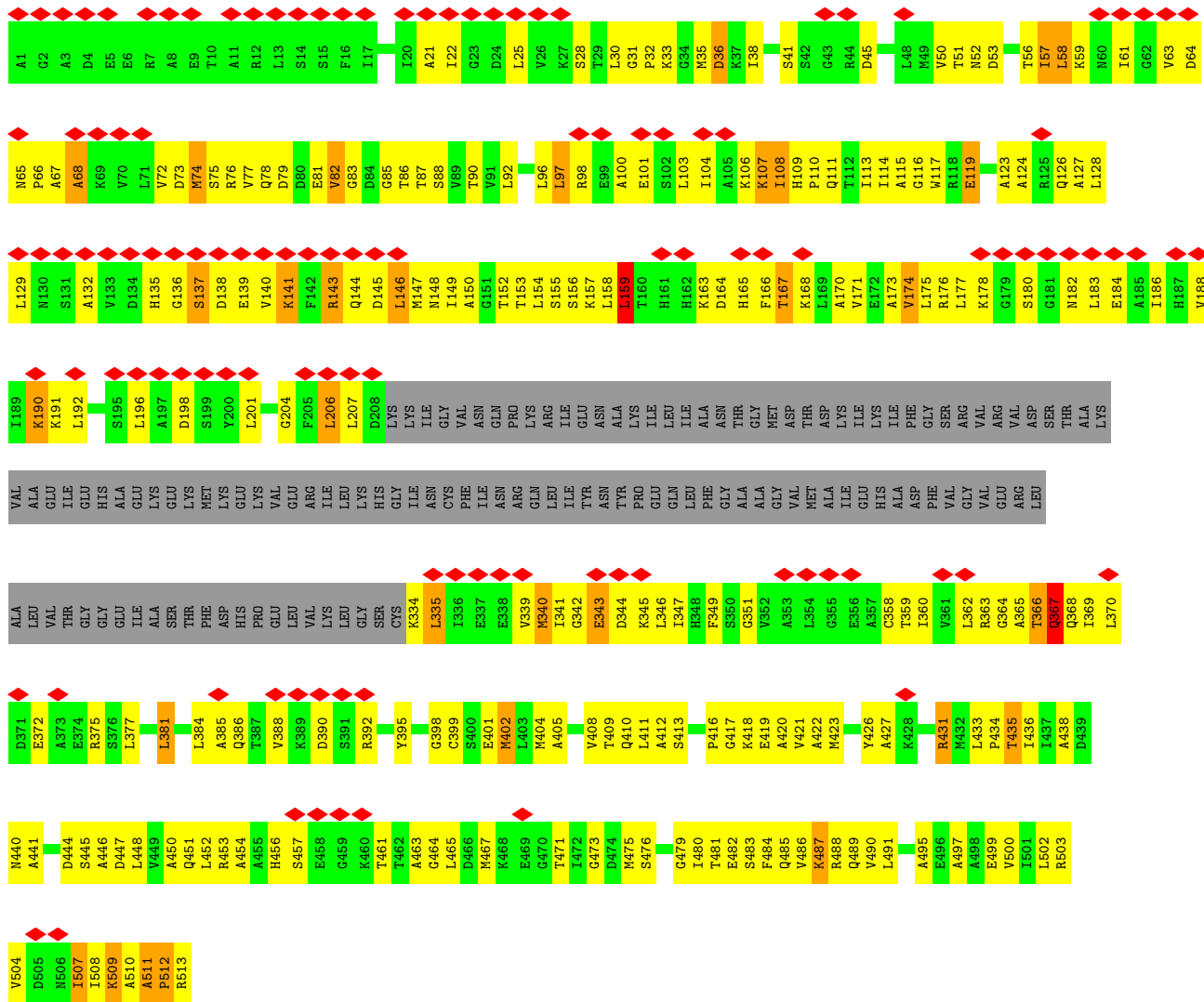


● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



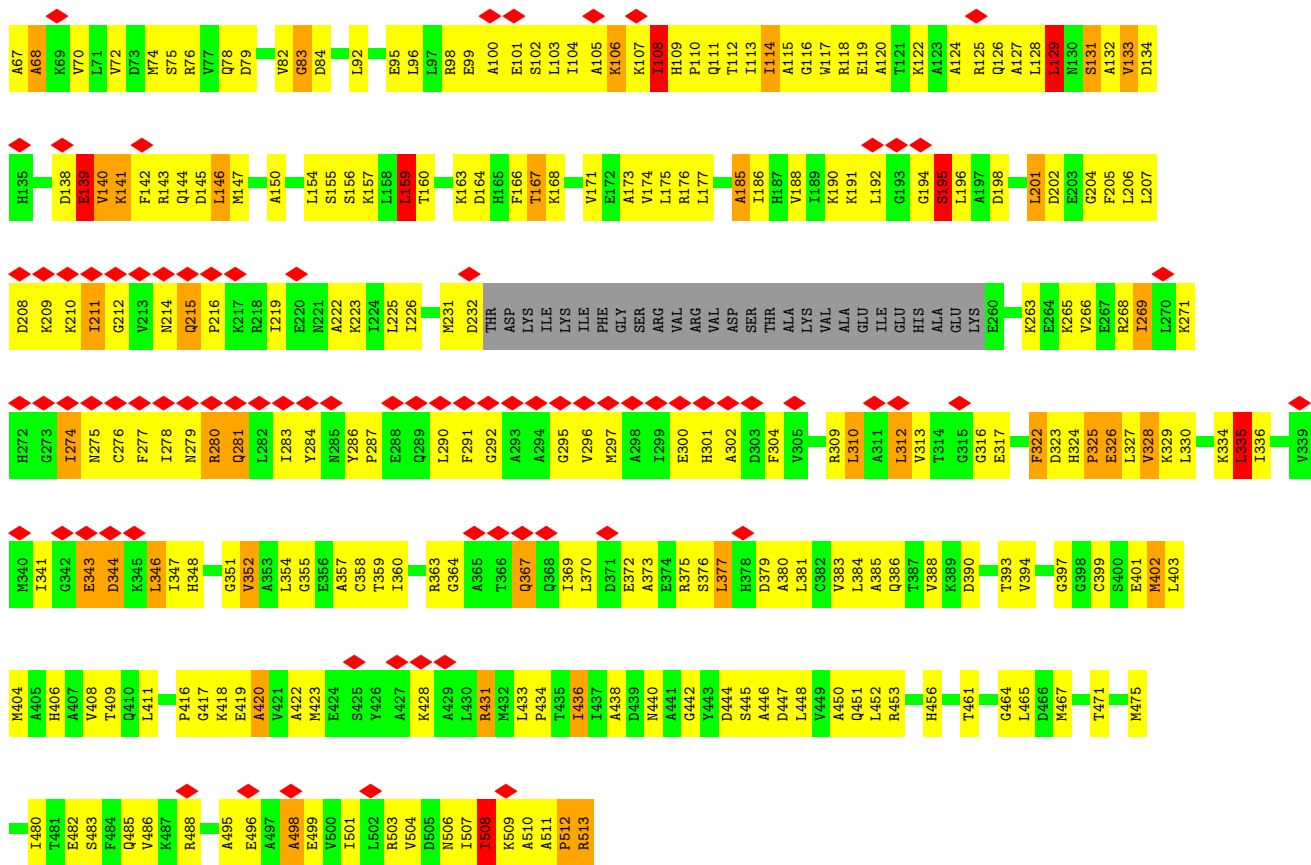


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

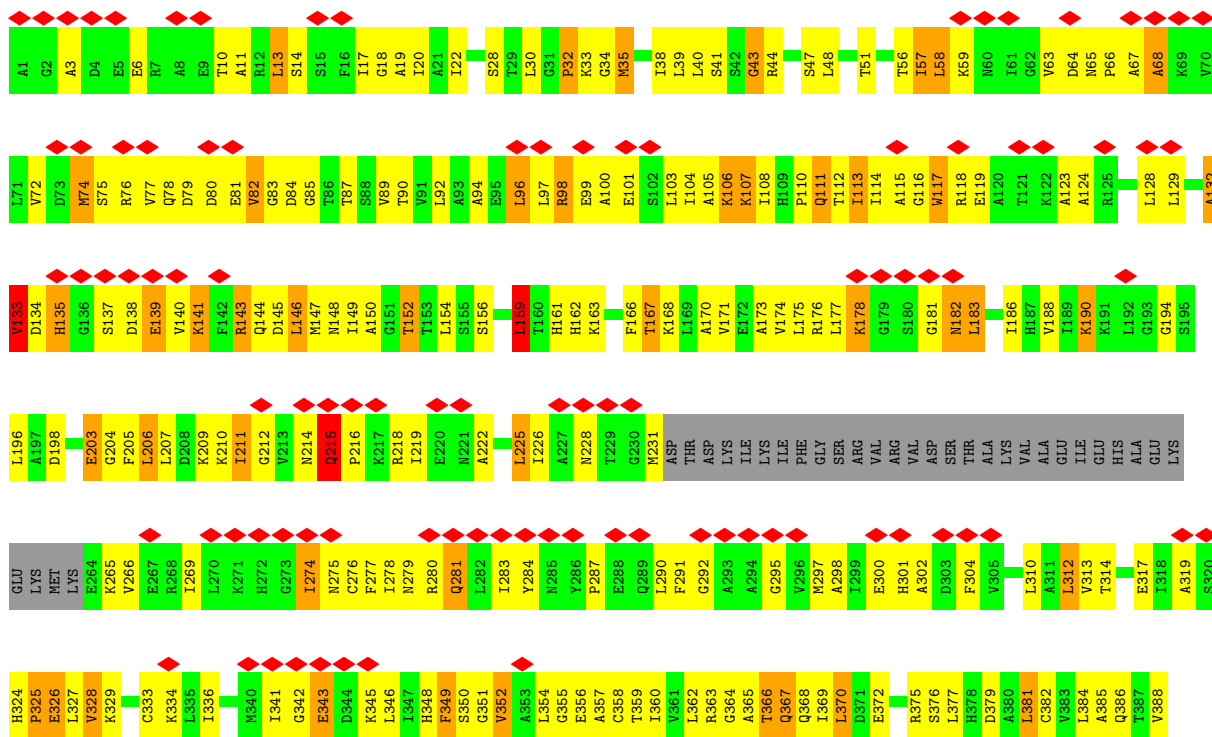


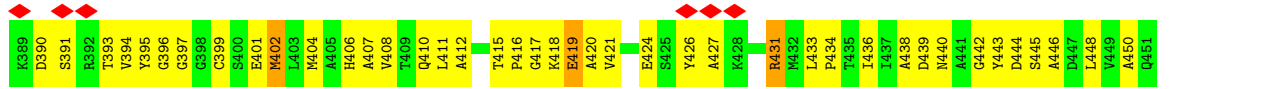
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



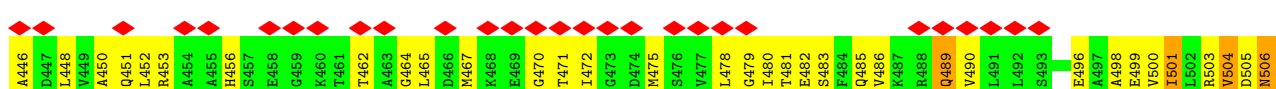
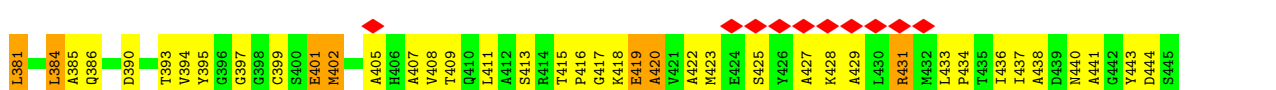
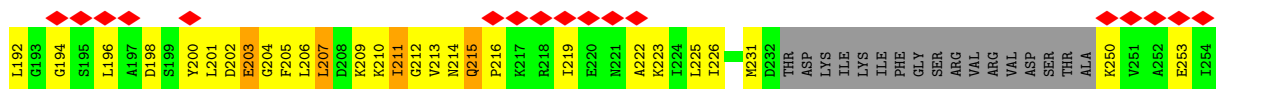
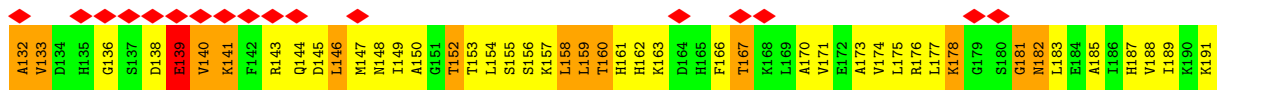
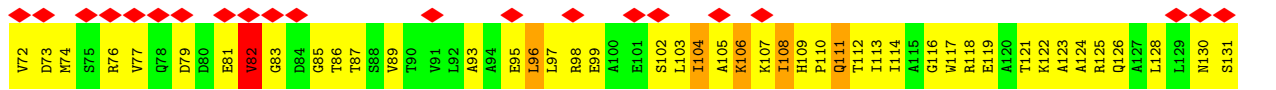
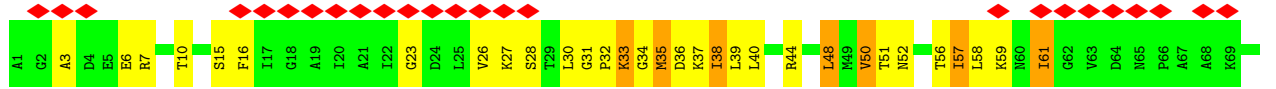


● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47151	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	2.515	Depositor
Minimum map value	-0.425	Depositor
Average map value	0.075	Depositor
Map value standard deviation	0.283	Depositor
Recommended contour level	1.13	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.4, 2.4, 2.4	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	0.51	0/2531	0.81	1/3415 (0.0%)
1	B	0.46	0/3716	0.77	1/5007 (0.0%)
1	C	0.46	0/3646	0.80	2/4916 (0.0%)
1	D	0.47	0/3704	0.80	3/4990 (0.1%)
1	E	0.44	0/3732	0.75	0/5028
1	F	0.45	0/3699	0.80	3/4983 (0.1%)
1	G	0.48	0/3896	0.80	0/5249
1	H	0.46	0/3741	0.83	1/5040 (0.0%)
1	I	0.47	0/3568	0.79	1/4813 (0.0%)
1	J	0.45	0/3711	0.76	1/5000 (0.0%)
1	K	0.47	0/3762	0.77	0/5068
1	L	0.45	0/3724	0.80	1/5017 (0.0%)
1	M	0.47	0/2907	0.79	0/3920
1	N	0.45	0/3681	0.77	0/4960
1	O	0.48	0/3638	0.79	2/4905 (0.0%)
1	P	0.48	0/3762	0.80	2/5068 (0.0%)
All	All	0.46	0/57418	0.79	18/77379 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	309	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	125	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	512	PRO	CA-N-CD	-6.87	101.88	111.50
1	B	326	GLU	N-CA-CB	6.65	122.56	110.60
1	C	125	ARG	CB-CA-C	-6.35	97.70	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2510	0	2583	272	0
1	B	3677	0	3782	401	0
1	C	3608	0	3706	388	0
1	D	3666	0	3771	394	0
1	E	3693	0	3795	373	0
1	F	3661	0	3766	436	0
1	G	3855	0	3970	419	0
1	H	3702	0	3801	405	0
1	I	3530	0	3620	431	0
1	J	3673	0	3778	410	0
1	K	3723	0	3828	437	0
1	L	3685	0	3791	434	0
1	M	2881	0	2960	316	0
1	N	3643	0	3747	395	0
1	O	3600	0	3702	447	0
1	P	3723	0	3828	445	0
All	All	56830	0	58428	6005	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 52.

The worst 5 of 6005 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)
1:E:11:ALA:HB1	1:E:506:ASN:HB3	1.23	1.18
1:G:146:LEU:HD12	1:G:171:VAL:HG13	1.25	1.17
1:C:146:LEU:HD12	1:C:171:VAL:HG13	1.24	1.17
1:H:146:LEU:HD12	1:H:171:VAL:HG13	1.14	1.14
1:P:146:LEU:HD12	1:P:171:VAL:HG13	1.23	1.13

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	335/513 (65%)	299 (89%)	14 (4%)	22 (7%)	1	16
1	B	486/513 (95%)	441 (91%)	18 (4%)	27 (6%)	2	19
1	C	478/513 (93%)	425 (89%)	28 (6%)	25 (5%)	2	19
1	D	485/513 (94%)	439 (90%)	21 (4%)	25 (5%)	2	19
1	E	488/513 (95%)	443 (91%)	16 (3%)	29 (6%)	1	17
1	F	484/513 (94%)	439 (91%)	22 (4%)	23 (5%)	2	21
1	G	511/513 (100%)	450 (88%)	31 (6%)	30 (6%)	1	17
1	H	489/513 (95%)	434 (89%)	31 (6%)	24 (5%)	2	20
1	I	469/513 (91%)	421 (90%)	18 (4%)	30 (6%)	1	16
1	J	486/513 (95%)	438 (90%)	25 (5%)	23 (5%)	2	21
1	K	492/513 (96%)	438 (89%)	25 (5%)	29 (6%)	1	17
1	L	487/513 (95%)	450 (92%)	21 (4%)	16 (3%)	4	26
1	M	384/513 (75%)	347 (90%)	17 (4%)	20 (5%)	2	19
1	N	482/513 (94%)	429 (89%)	26 (5%)	27 (6%)	2	19
1	O	477/513 (93%)	422 (88%)	28 (6%)	27 (6%)	1	18
1	P	492/513 (96%)	449 (91%)	21 (4%)	22 (4%)	2	22
All	All	7525/8208 (92%)	6764 (90%)	362 (5%)	399 (5%)	3	19

5 of 399 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	37	LYS
1	A	68	ALA
1	A	139	GLU
1	A	180	SER

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	266/409 (65%)	238 (90%)	28 (10%)	7	24
1	B	389/409 (95%)	351 (90%)	38 (10%)	8	26
1	C	382/409 (93%)	339 (89%)	43 (11%)	6	21
1	D	388/409 (95%)	346 (89%)	42 (11%)	6	23
1	E	391/409 (96%)	347 (89%)	44 (11%)	6	21
1	F	388/409 (95%)	348 (90%)	40 (10%)	7	25
1	G	409/409 (100%)	349 (85%)	60 (15%)	3	15
1	H	392/409 (96%)	335 (86%)	57 (14%)	3	15
1	I	373/409 (91%)	327 (88%)	46 (12%)	4	19
1	J	389/409 (95%)	344 (88%)	45 (12%)	5	21
1	K	394/409 (96%)	354 (90%)	40 (10%)	7	25
1	L	390/409 (95%)	343 (88%)	47 (12%)	5	20
1	M	305/409 (75%)	276 (90%)	29 (10%)	8	27
1	N	386/409 (94%)	344 (89%)	42 (11%)	6	23
1	O	381/409 (93%)	337 (88%)	44 (12%)	5	21
1	P	394/409 (96%)	347 (88%)	47 (12%)	5	20
All	All	6017/6544 (92%)	5325 (88%)	692 (12%)	9	21

5 of 692 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	225	LEU
1	N	146	LEU
1	K	401	GLU
1	K	211	ILE
1	L	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	126	GLN
1	L	111	GLN
1	P	148	ASN
1	J	348	HIS
1	K	161	HIS

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.

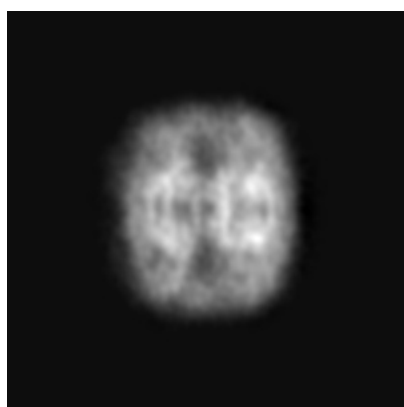
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1960. These allow visual inspection of the internal detail of the map and identification of artifacts.

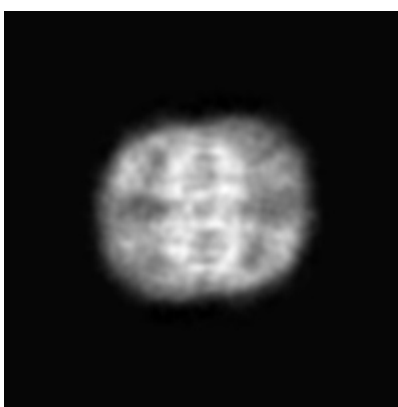
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

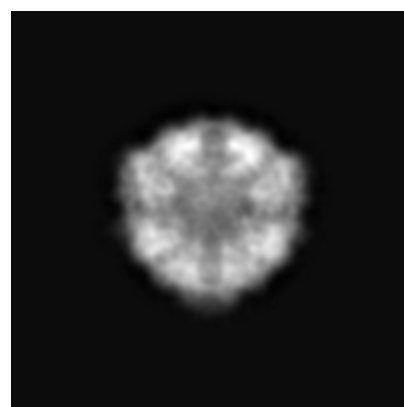
6.1.1 Primary map



X



Y

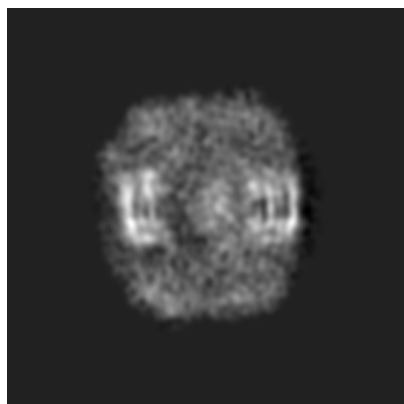


Z

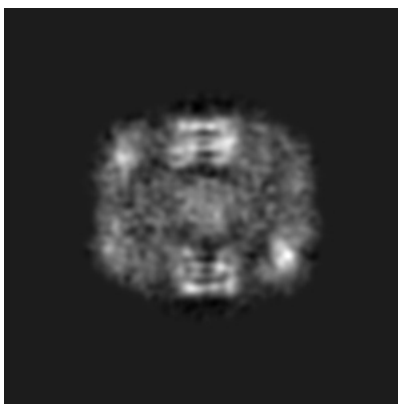
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

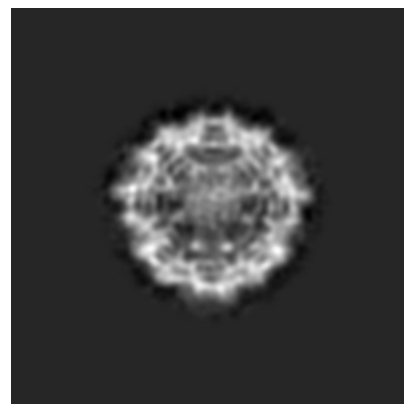
6.2.1 Primary map



X Index: 72



Y Index: 72

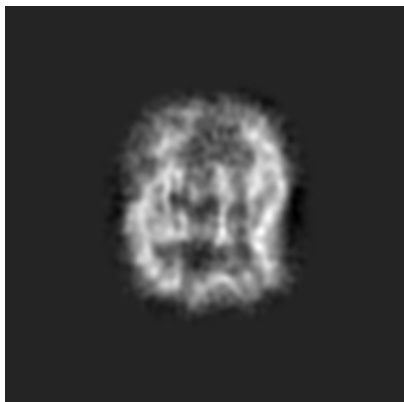


Z Index: 72

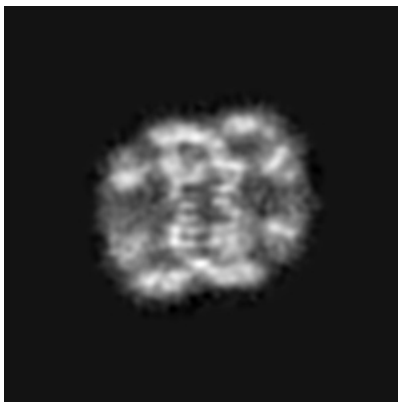
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

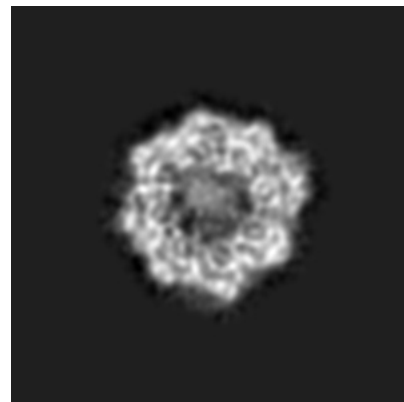
6.3.1 Primary map



X Index: 87



Y Index: 89

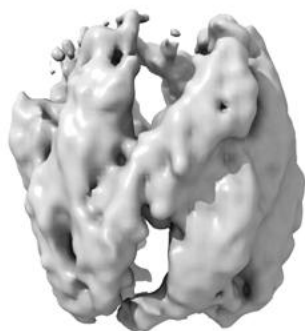


Z Index: 78

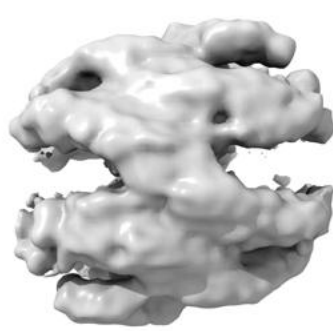
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

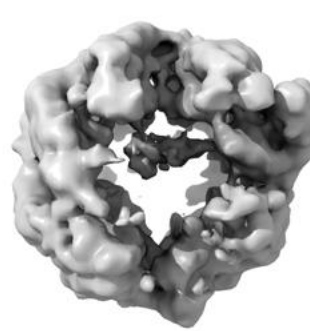
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

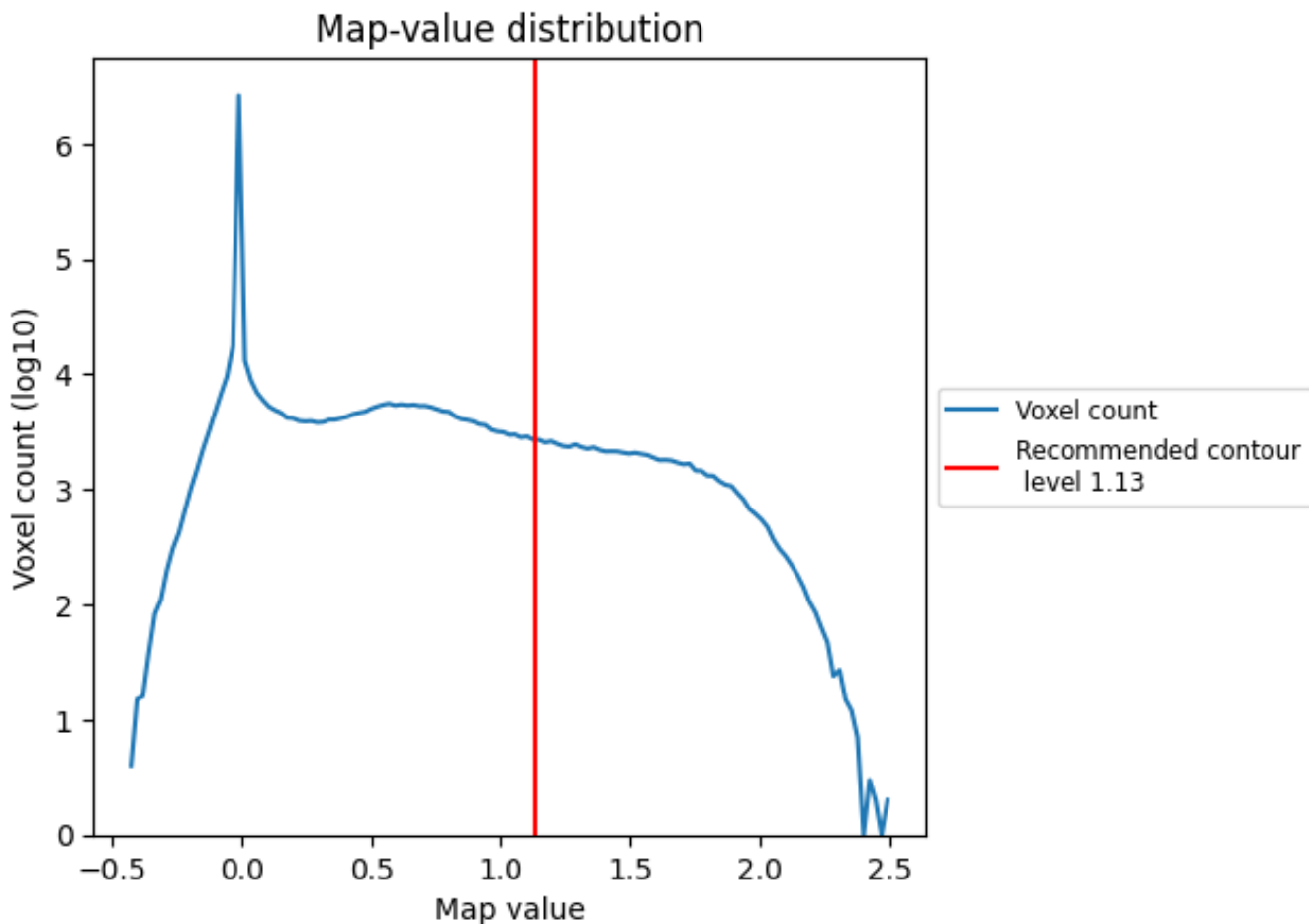
6.5 Mask visualisation

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

7 Map analysis [i](#)

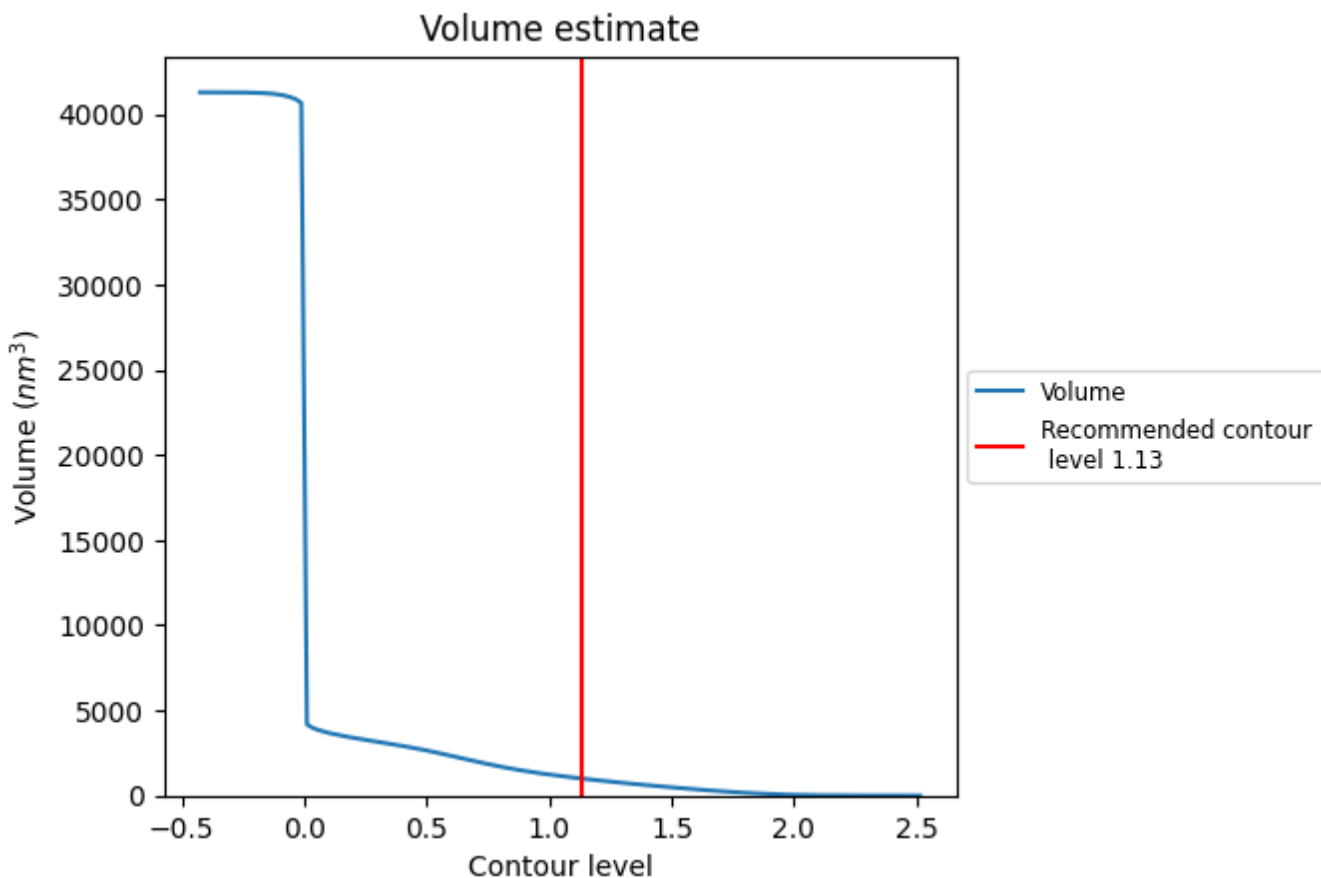
This section contains the results of statistical analysis of the map.

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.

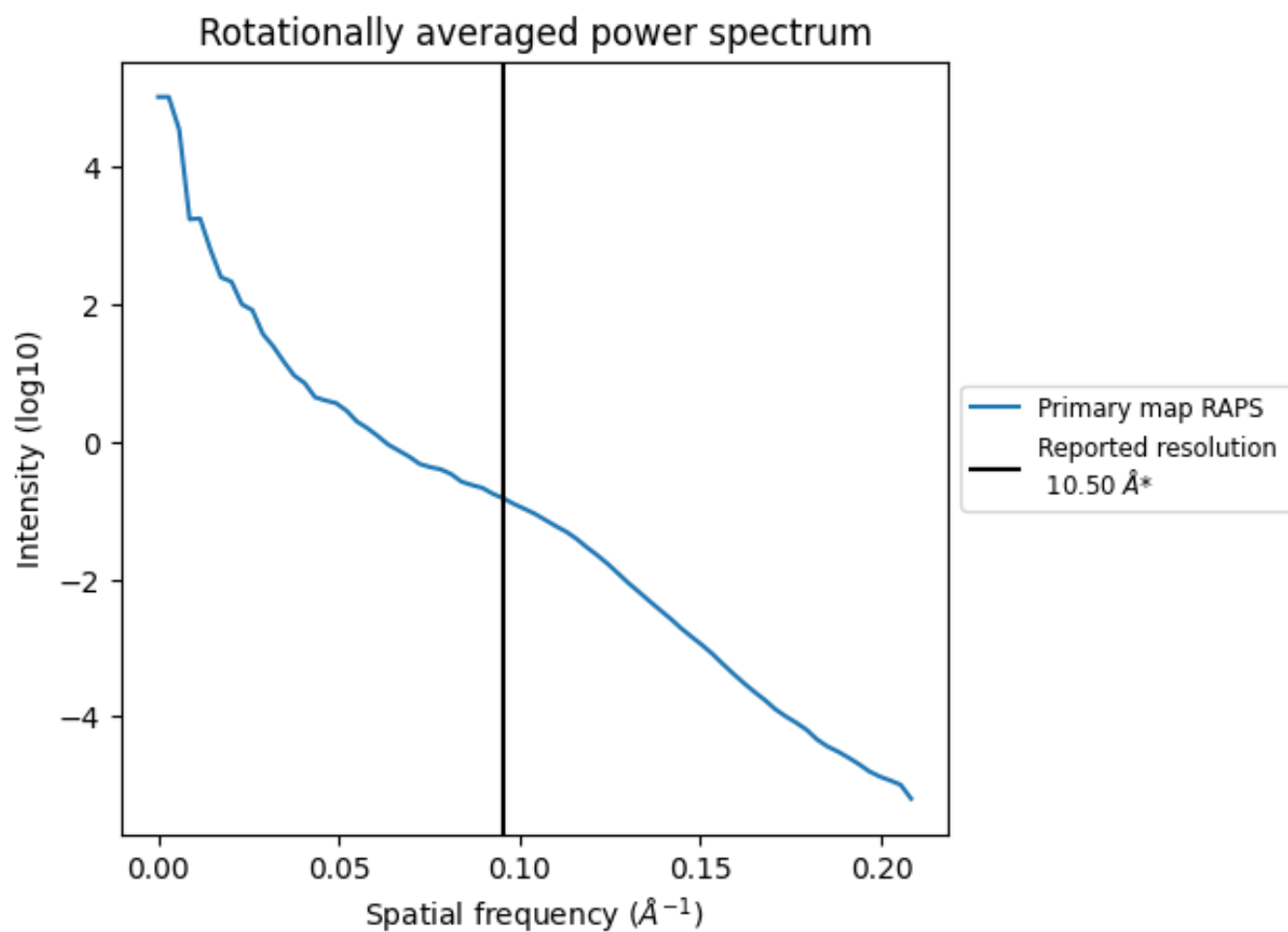
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1005 nm³; this corresponds to an approximate mass of 908 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 0.095 \AA^{-1}

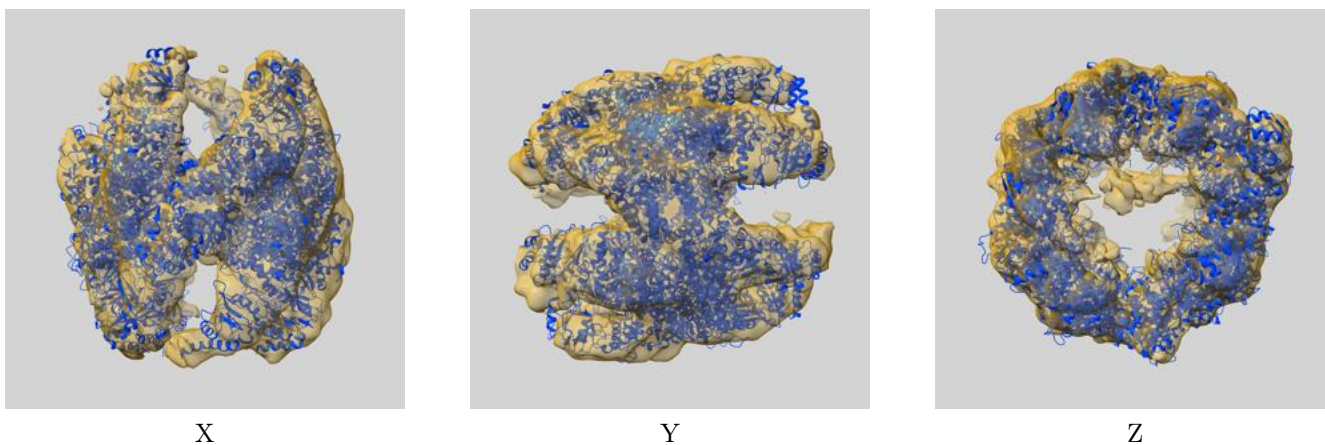
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

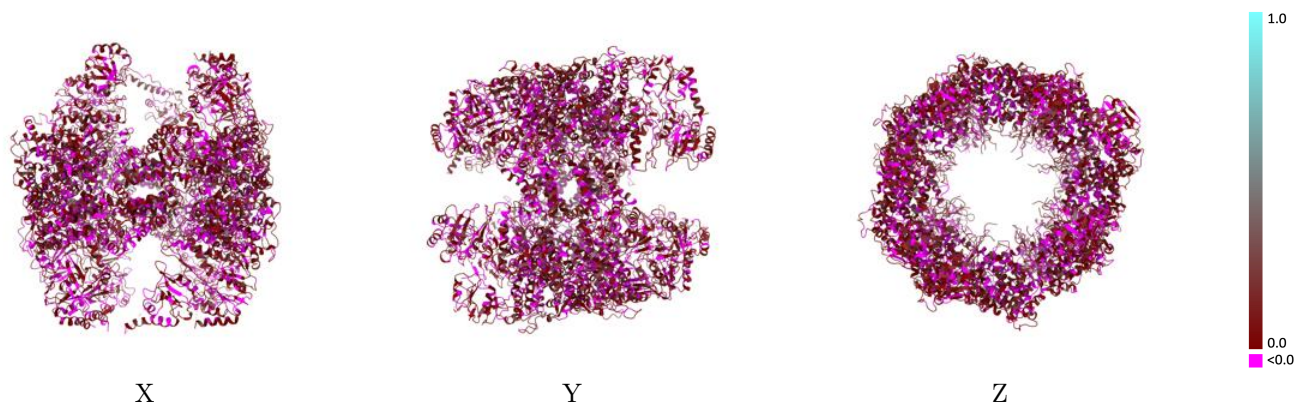
This section contains information regarding the fit between EMDB map EMD-1960 and PDB model 4A0O. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



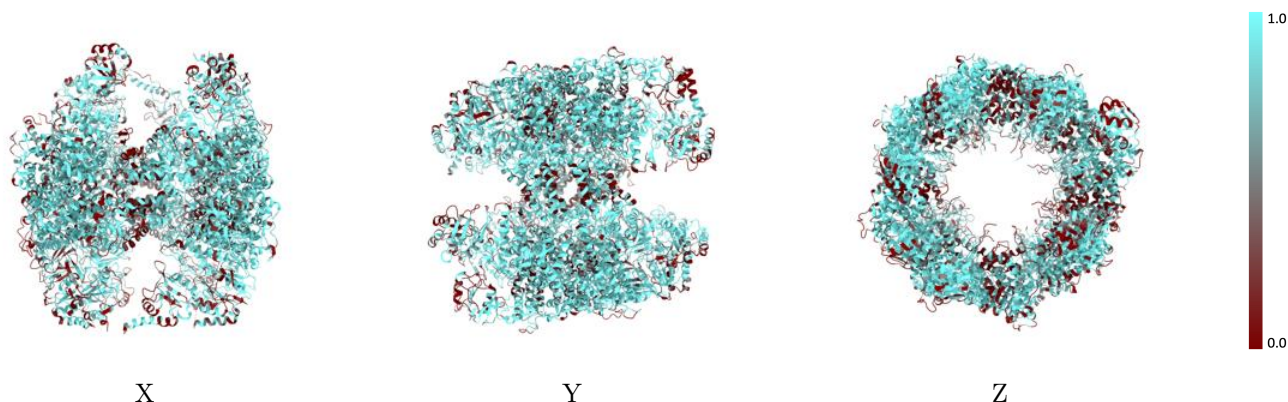
The images above show the 3D surface view of the map at the recommended contour level 1.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



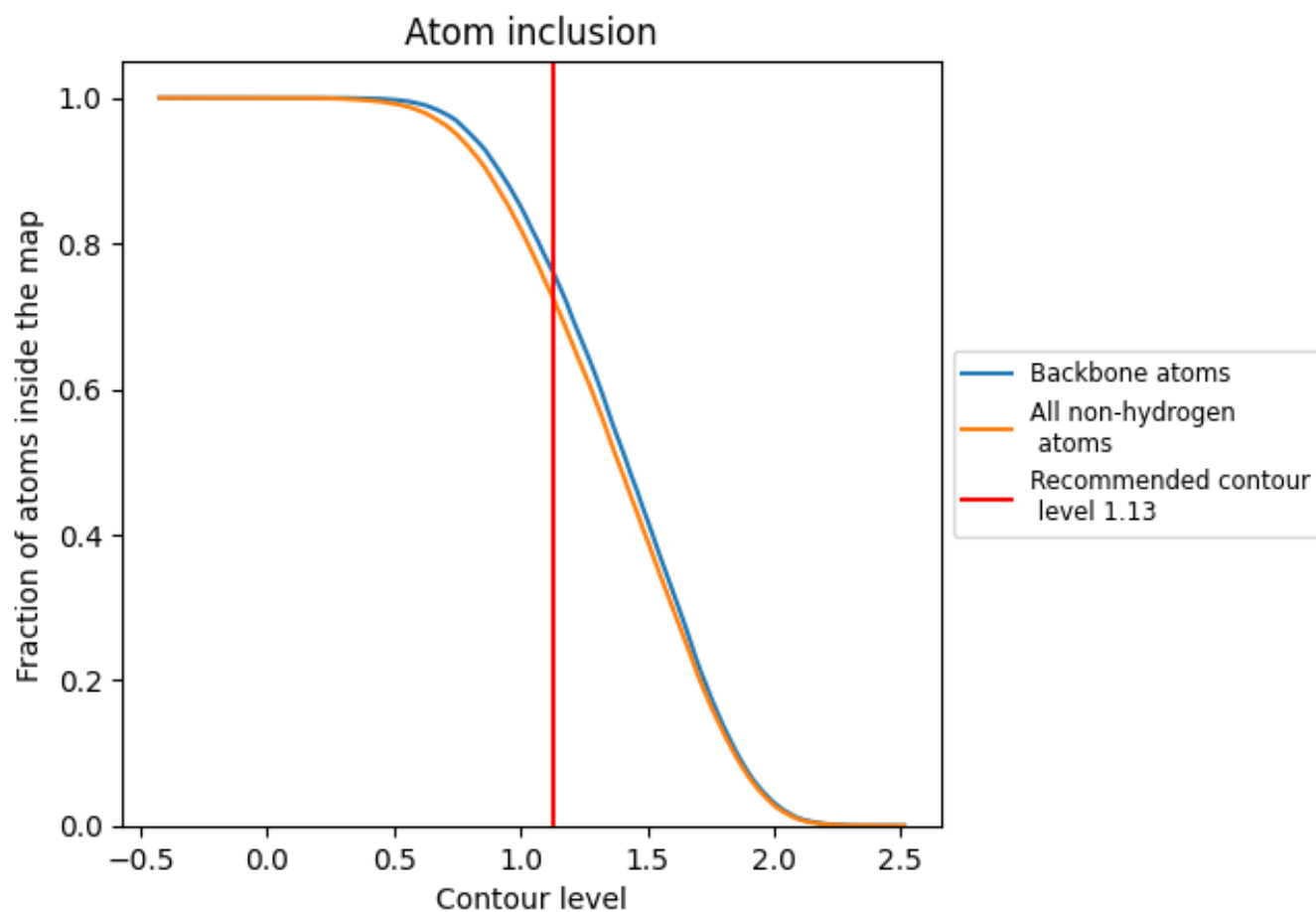
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.13).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (1.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7236	 0.0560
A	 0.6769	 0.0570
B	 0.6947	 0.0490
C	 0.7048	 0.0600
D	 0.7978	 0.0710
E	 0.7444	 0.0660
F	 0.7956	 0.0660
G	 0.7871	 0.0570
H	 0.6382	 0.0520
I	 0.6291	 0.0510
J	 0.7686	 0.0610
K	 0.7307	 0.0460
L	 0.7691	 0.0570
M	 0.6310	 0.0400
N	 0.7689	 0.0610
O	 0.7323	 0.0520
P	 0.6691	 0.0410

