wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 02:25 AM JST

PDB ID	:	7WU7
EMDB ID	:	EMD-32823
Title	:	Prefoldin-tubulin-TRiC complex
Authors	:	Gestaut, D.; Zhao, Y.; Park, J.; Ma, B.; Leitner, A.; Collier, M.; Pintilie, G.; Roh, S.-H.; Chiu, W.; Frydman, J.
Deposited on	:	2022-02-07
Resolution	:	3.85 Å(reported)
Based on initial model	:	6NR8

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

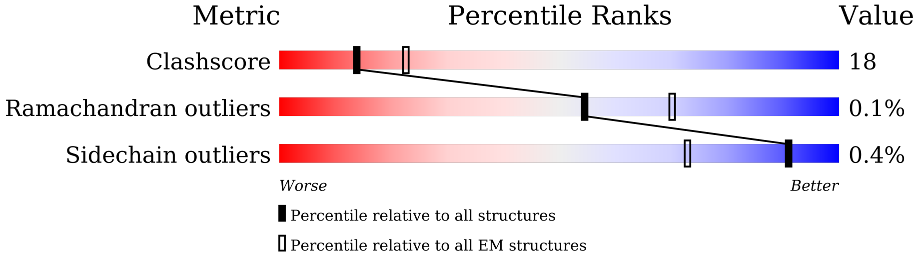
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

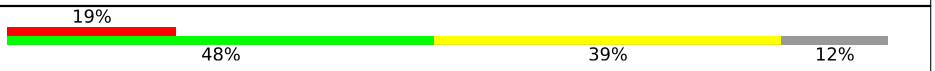
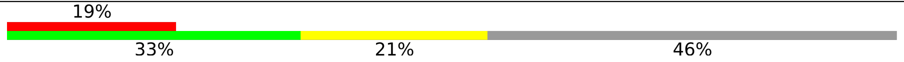
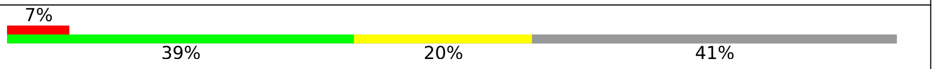
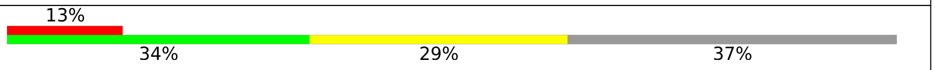
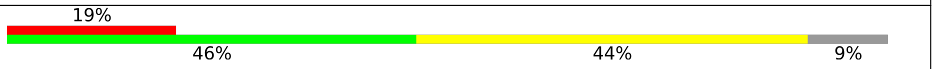
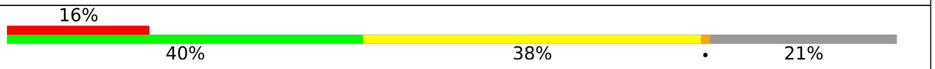
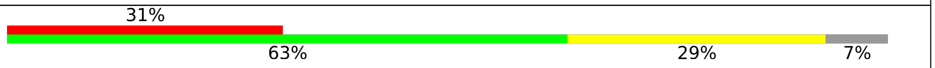
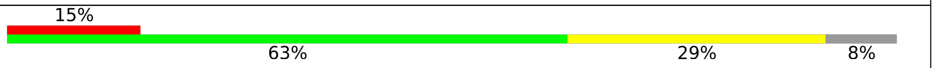
The reported resolution of this entry is 3.85 Å.

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.



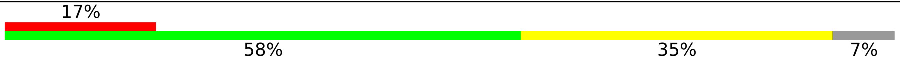
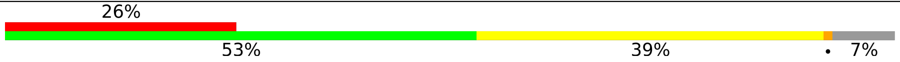
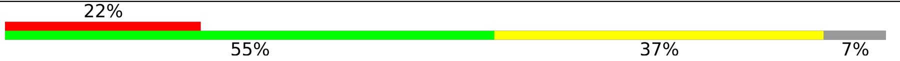
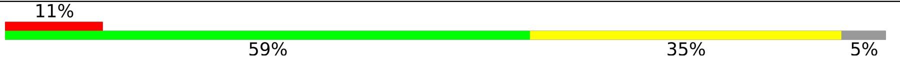
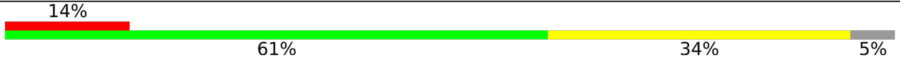
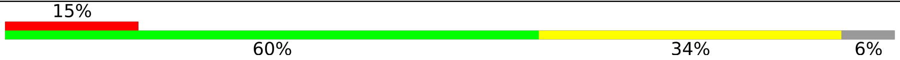
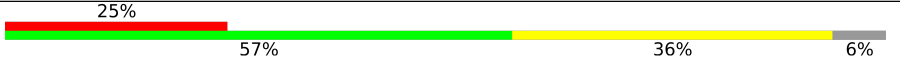
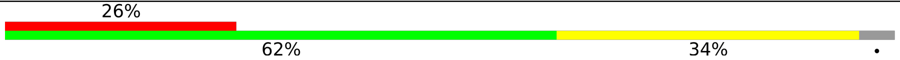
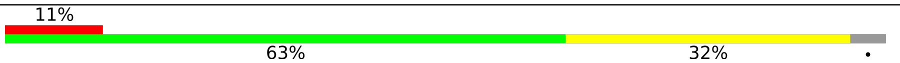
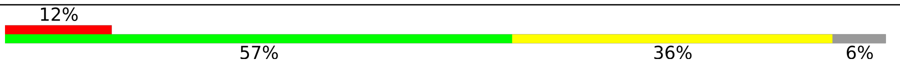
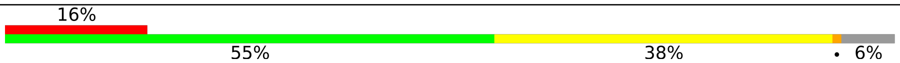
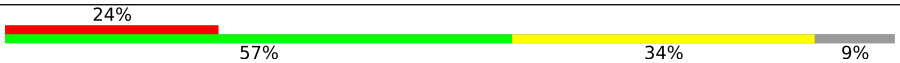
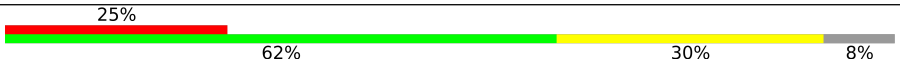
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1	122	
2	2	154	
3	3	197	
4	4	140	
5	5	140	
6	6	129	
7	A	556	
7	I	556	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	B	535	 28% 64% 29% 7%
8	J	535	 17% 58% 35% 7%
9	C	545	 26% 53% 39% • 7%
9	K	545	 22% 55% 37% 7%
10	D	539	 11% 59% 35% 5%
10	L	539	 14% 61% 34% 5%
11	E	541	 15% 60% 34% 6%
11	M	541	 25% 57% 36% 6%
12	F	531	 26% 62% 34% •
12	N	531	 11% 63% 32% •
13	G	543	 12% 57% 36% 6%
13	O	543	 16% 55% 38% • 6%
14	H	547	 24% 57% 34% 9%
14	P	547	 25% 62% 30% 8%

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 67031 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 Prefoldin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	107	873	546	150	172	5	0	0

- Molecule 2 is a protein called Prefoldin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	83	667	413	121	130	3	0	0

- Molecule 3 is a protein called Prefoldin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	116	956	607	157	186	6	0	0

- Molecule 4 is a protein called Prefoldin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	88	711	437	118	151	5	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	135	HIS	-	expression tag	UNP Q9NQP4
4	136	HIS	-	expression tag	UNP Q9NQP4
4	137	HIS	-	expression tag	UNP Q9NQP4
4	138	HIS	-	expression tag	UNP Q9NQP4
4	139	HIS	-	expression tag	UNP Q9NQP4
4	140	HIS	-	expression tag	UNP Q9NQP4

- Molecule 5 is a protein called Prefoldin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	127	Total	C	N	O	S	0	0
			1017	647	166	196	8		

- Molecule 6 is a protein called Prefoldin subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	102	Total	C	N	O	S	0	0
			825	511	148	165	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	516	Total	C	N	O	S	0	0
			3919	2456	685	755	23		
7	I	514	Total	C	N	O	S	0	0
			3903	2444	683	753	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	497	Total	C	N	O	S	0	0
			3736	2339	655	723	19		
8	J	497	Total	C	N	O	S	0	0
			3736	2339	655	723	19		

- Molecule 9 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	505	Total	C	N	O	S	0	0
			3924	2448	690	756	30		
9	K	505	Total	C	N	O	S	0	0
			3924	2448	690	756	30		

- Molecule 10 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	511	Total	C	N	O	S	0	0
			3847	2409	665	750	23		
10	L	511	Total	C	N	O	S	0	0
			3847	2407	666	751	23		

- Molecule 11 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	506	Total	C	N	O	S	0	0
			3883	2431	673	749	30		
11	M	506	Total	C	N	O	S	0	0
			3883	2431	673	749	30		

- Molecule 12 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	508	Total	C	N	O	S	0	0
			3903	2454	681	748	20		
12	N	508	Total	C	N	O	S	0	0
			3903	2454	681	748	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	528	PHE	SER	conflict	UNP P40227
N	528	PHE	SER	conflict	UNP P40227

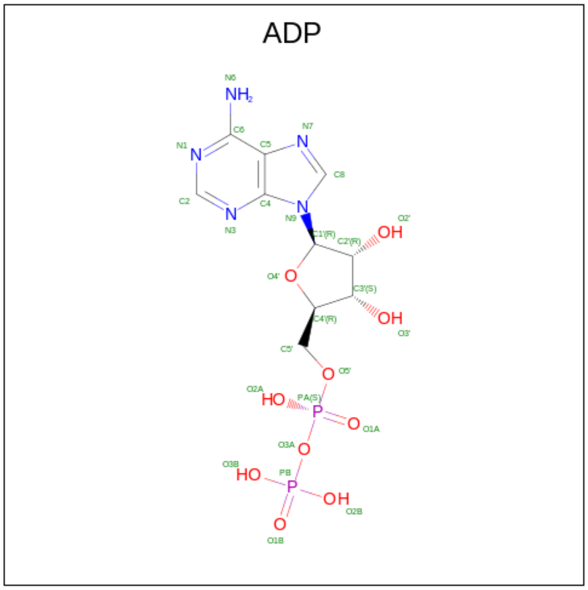
- Molecule 13 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	509	Total	C	N	O	S	0	0
			3910	2471	676	740	23		
13	O	509	Total	C	N	O	S	0	0
			3910	2471	676	740	23		

- Molecule 14 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	500	Total	C	N	O	S	0	0
			3816	2404	647	739	26		
14	P	502	Total	C	N	O	S	0	0
			3830	2413	650	741	26		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

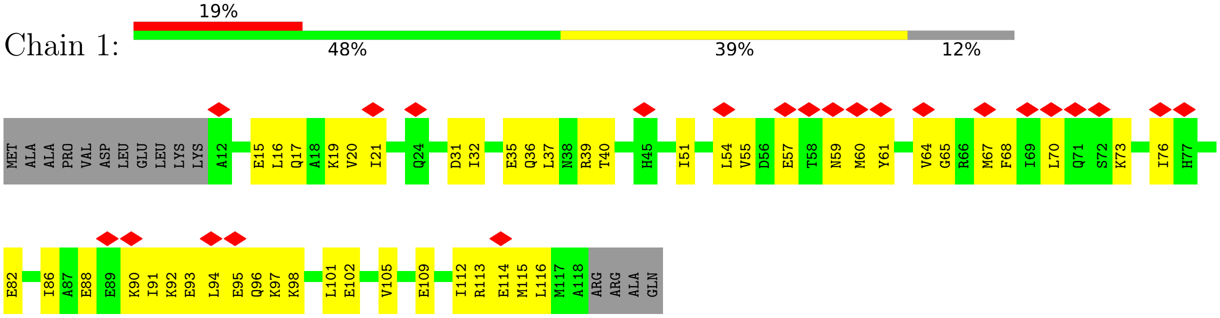


Mol	Chain	Residues	Atoms	AltConf
15	F	1	Total C N O P 27 10 5 10 2	0
15	H	1	Total C N O P 27 10 5 10 2	0
15	N	1	Total C N O P 27 10 5 10 2	0
15	P	1	Total C N O P 27 10 5 10 2	0

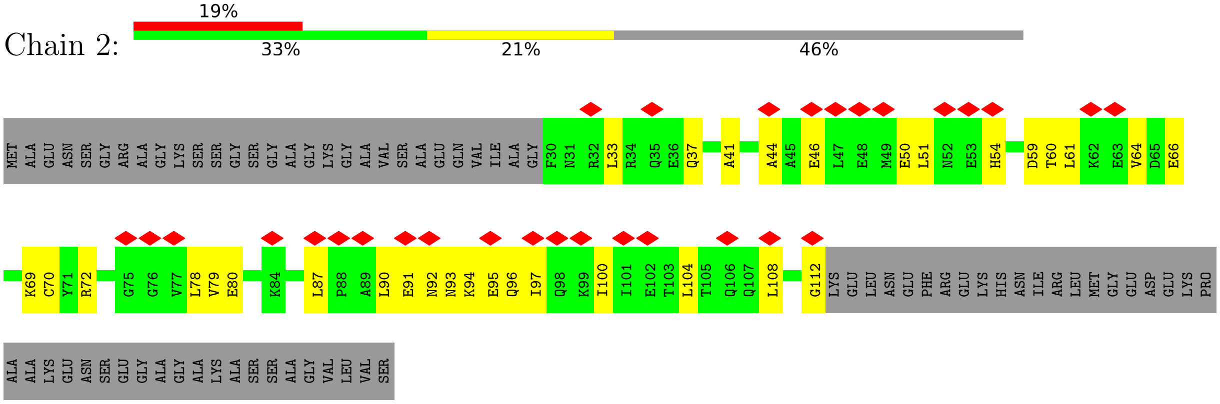
3 Residue-property plots ⓘ

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.

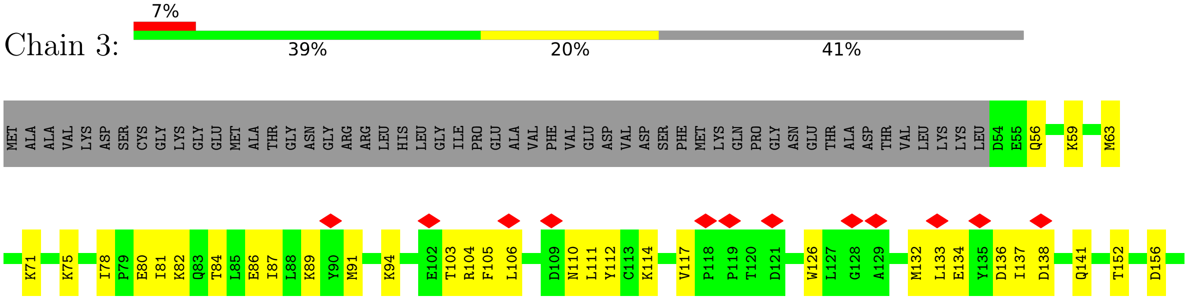
- Molecule 1: Prefoldin subunit 1

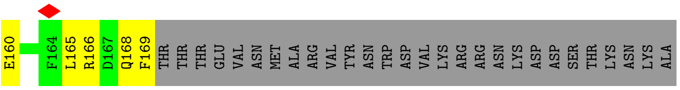


- Molecule 2: Prefoldin subunit 2



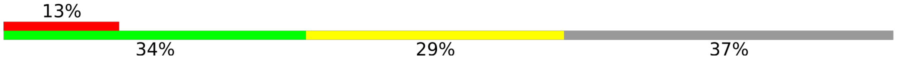
- Molecule 3: Prefoldin subunit 3

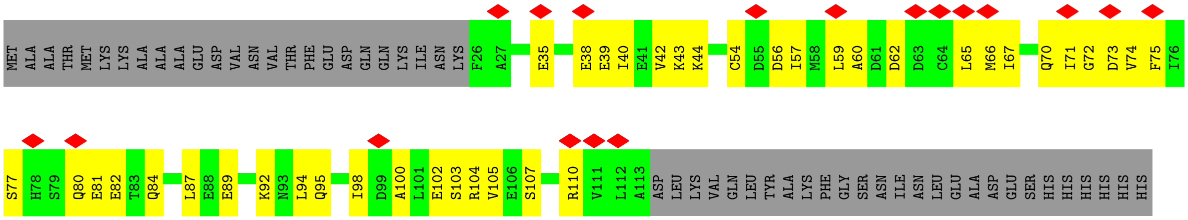




- Molecule 4: Prefoldin subunit 4

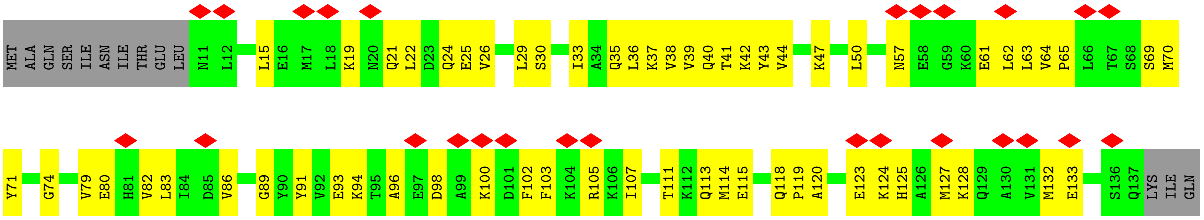
Chain 4:





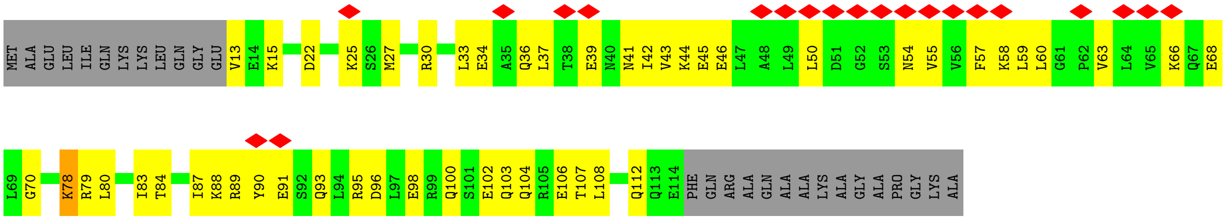
- Molecule 5: Prefoldin subunit 5

Chain 5:



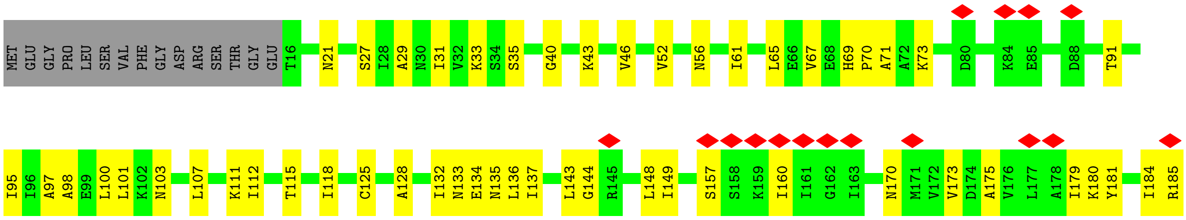
- Molecule 6: Prefoldin subunit 6

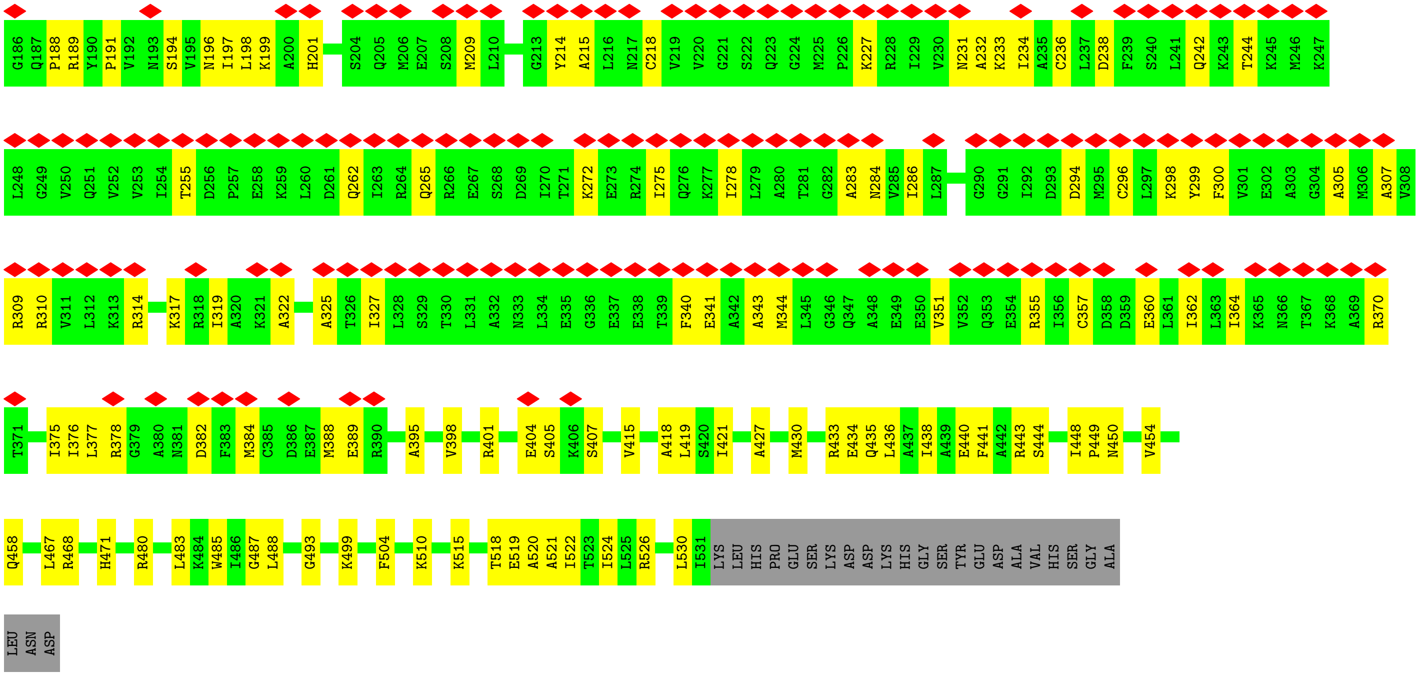
Chain 6:



- Molecule 7: T-complex protein 1 subunit alpha

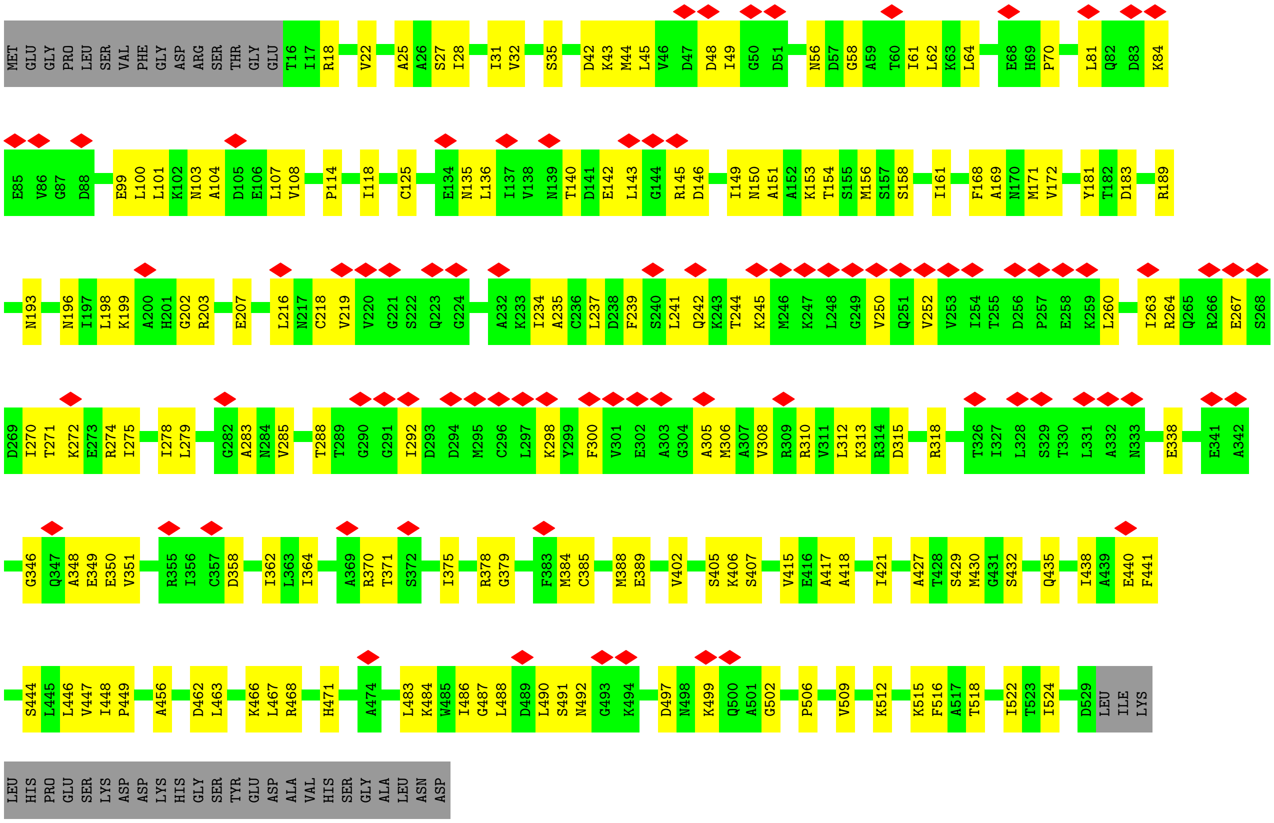
Chain A:



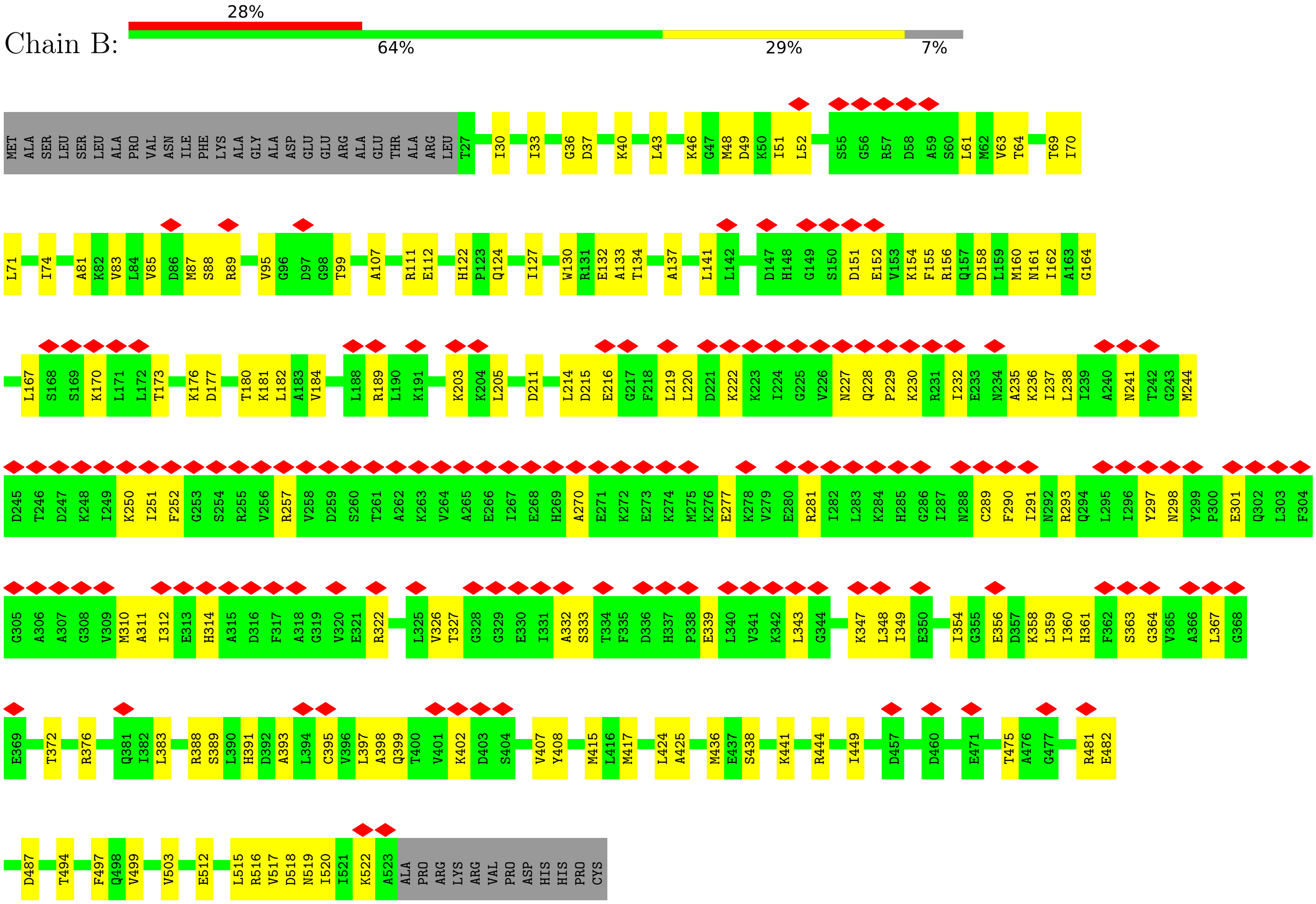


- Molecule 7: T-complex protein 1 subunit alpha

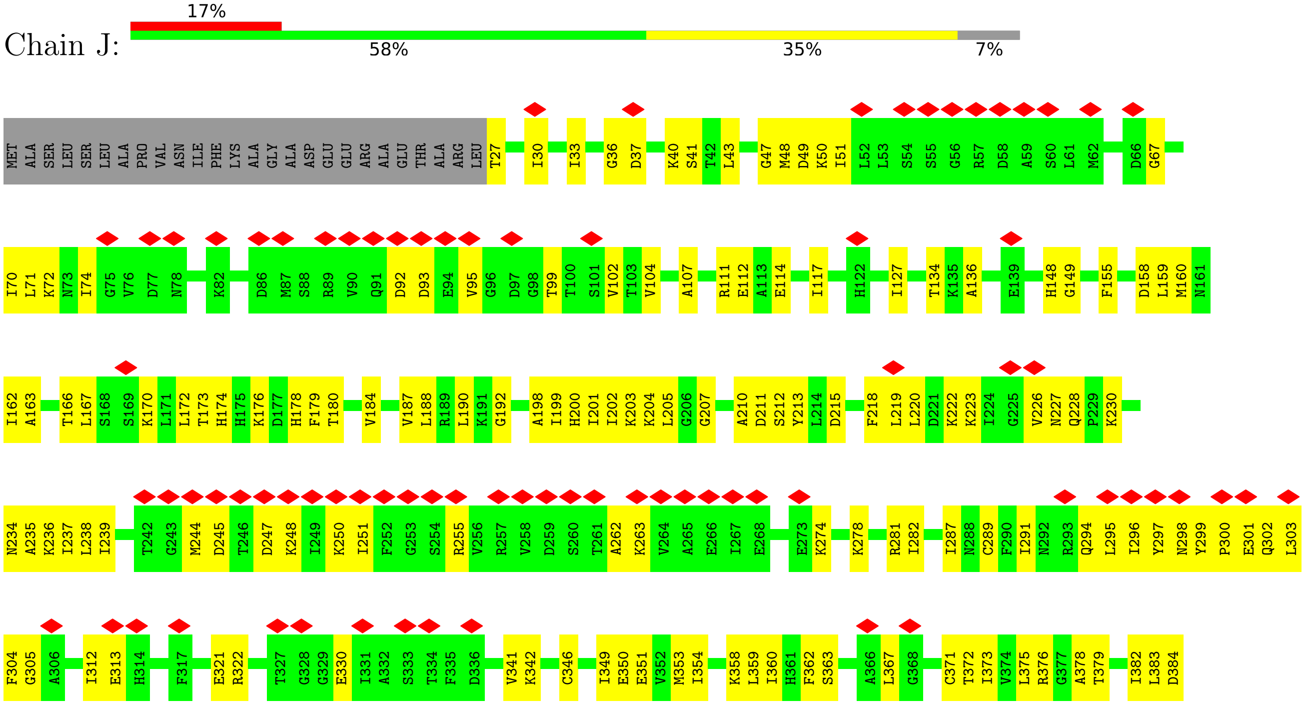
Chain I:

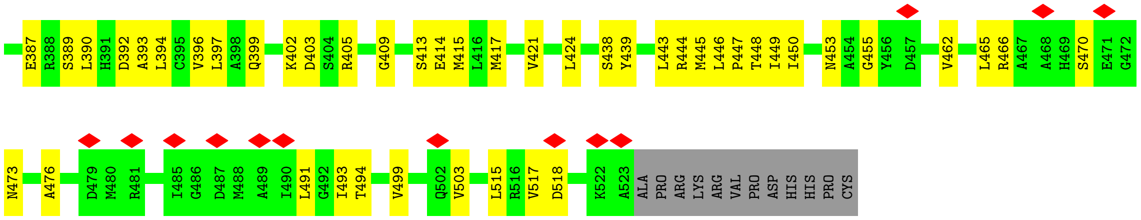


- Molecule 8: T-complex protein 1 subunit beta



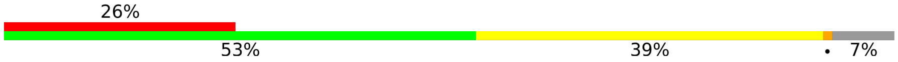
- Molecule 8: T-complex protein 1 subunit beta

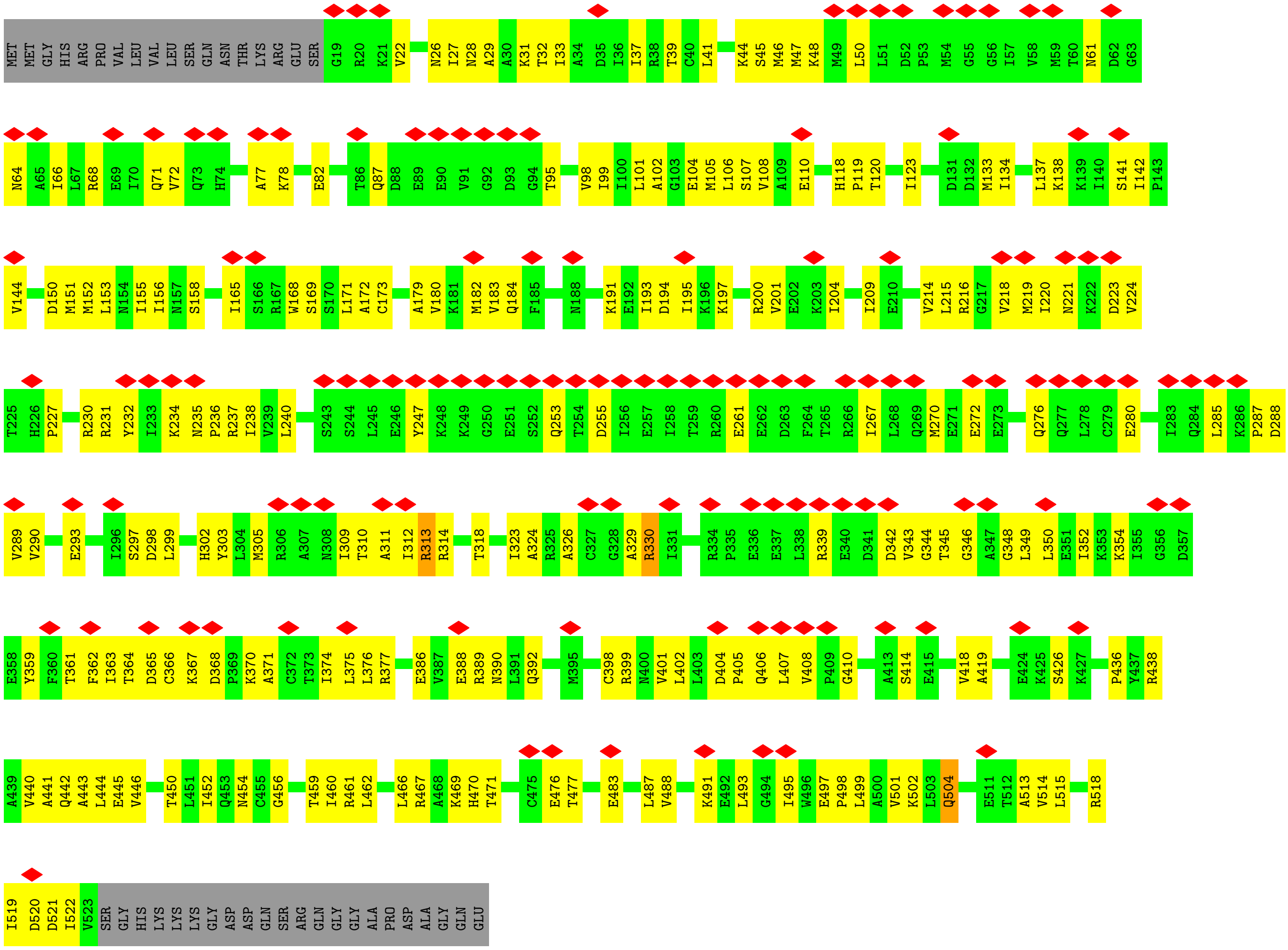




- Molecule 9: T-complex protein 1 subunit gamma

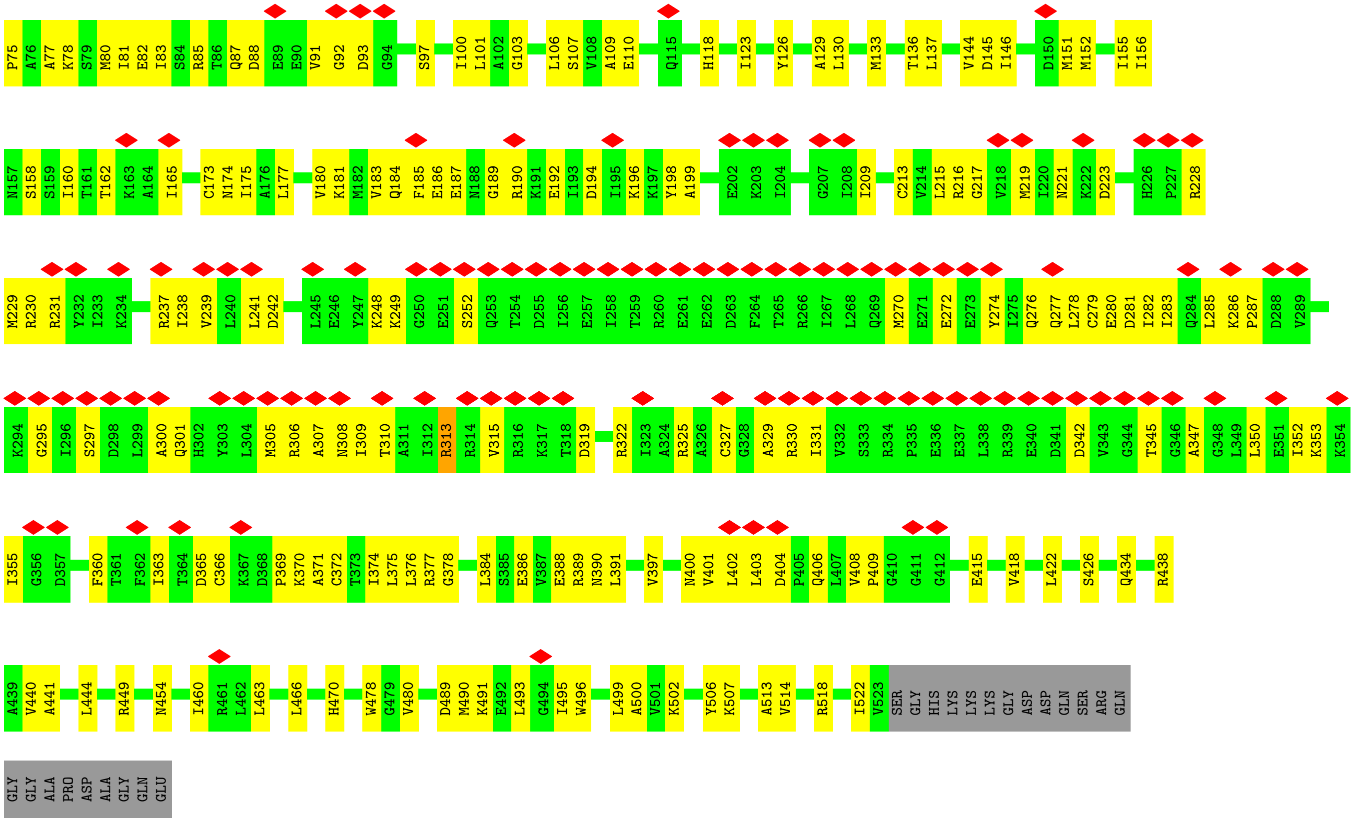
Chain C:



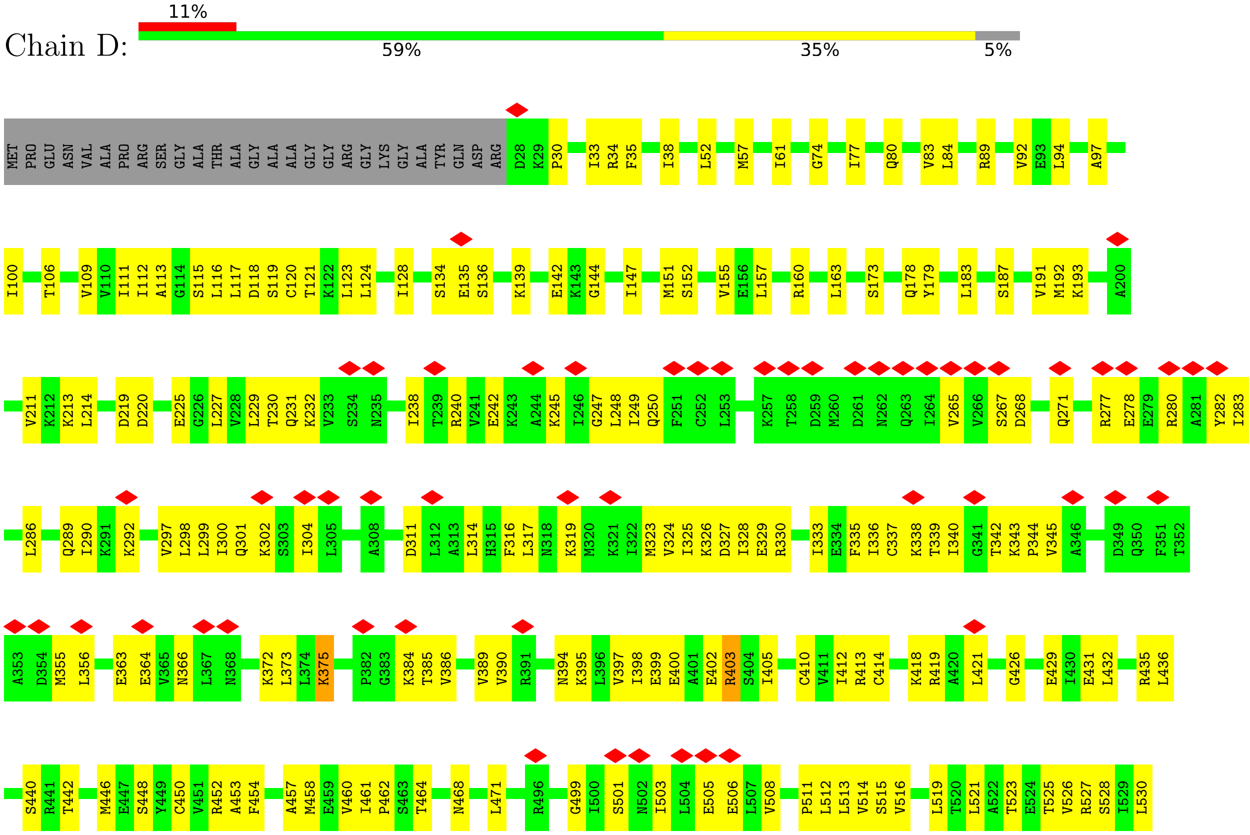


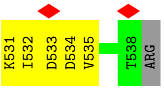
- Molecule 9: T-complex protein 1 subunit gamma

Chain K:



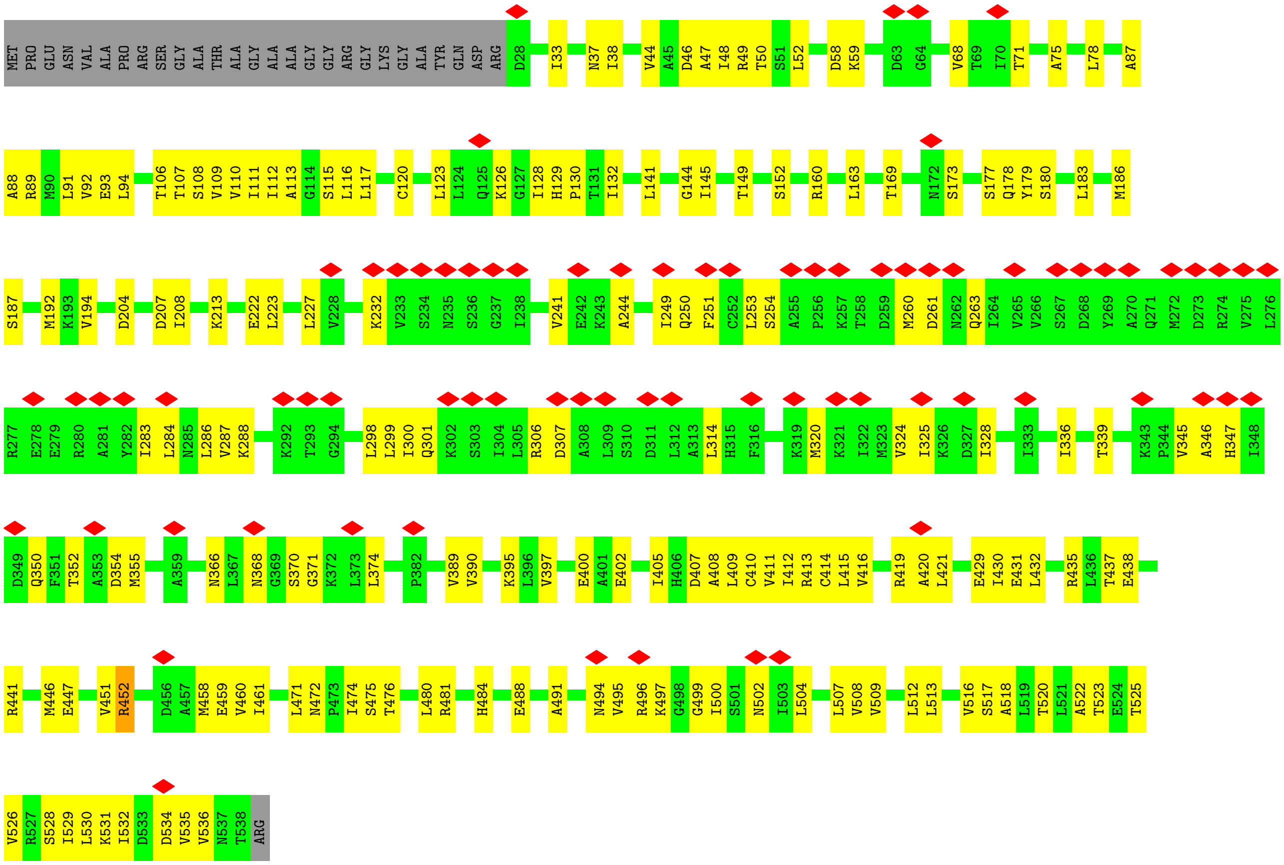
- Molecule 10: T-complex protein 1 subunit delta





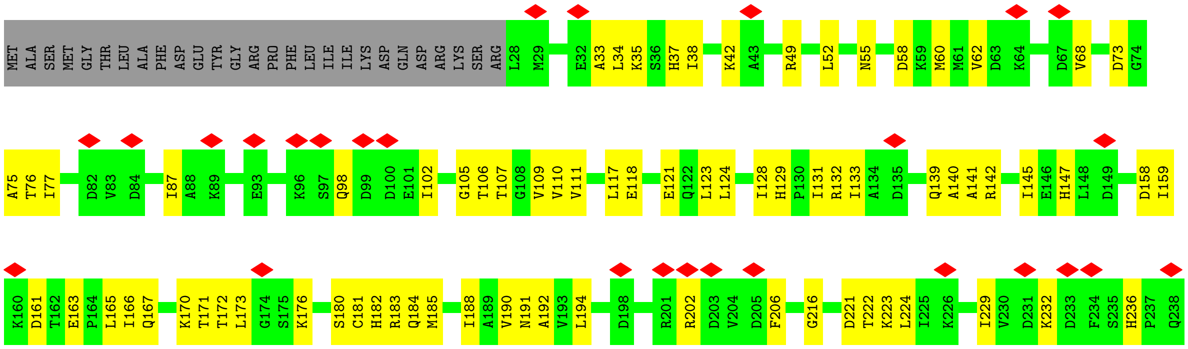
- Molecule 10: T-complex protein 1 subunit delta

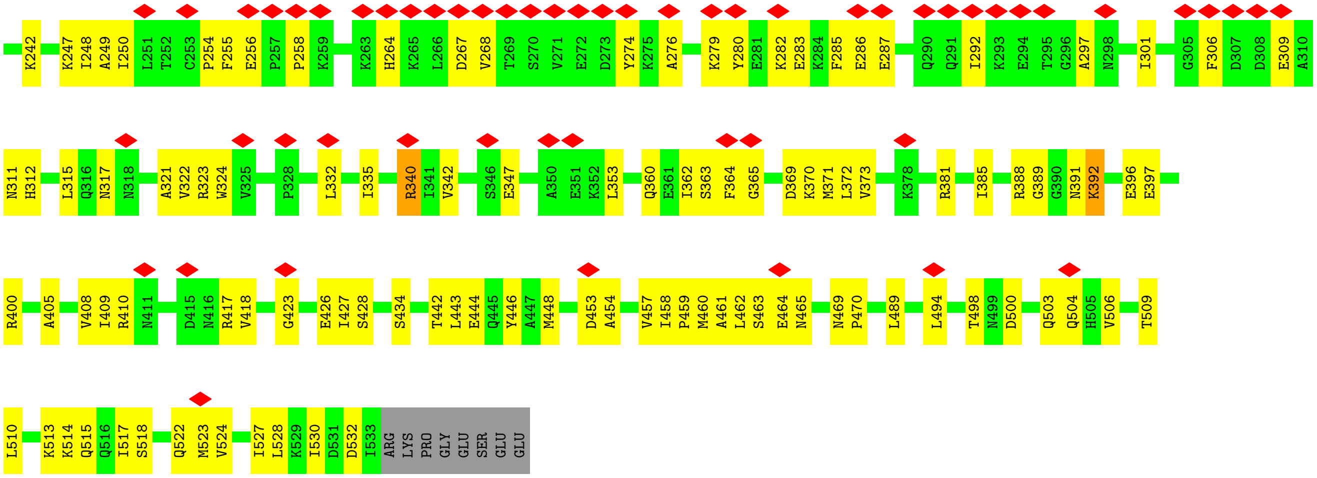
Chain L:



- Molecule 11: T-complex protein 1 subunit epsilon

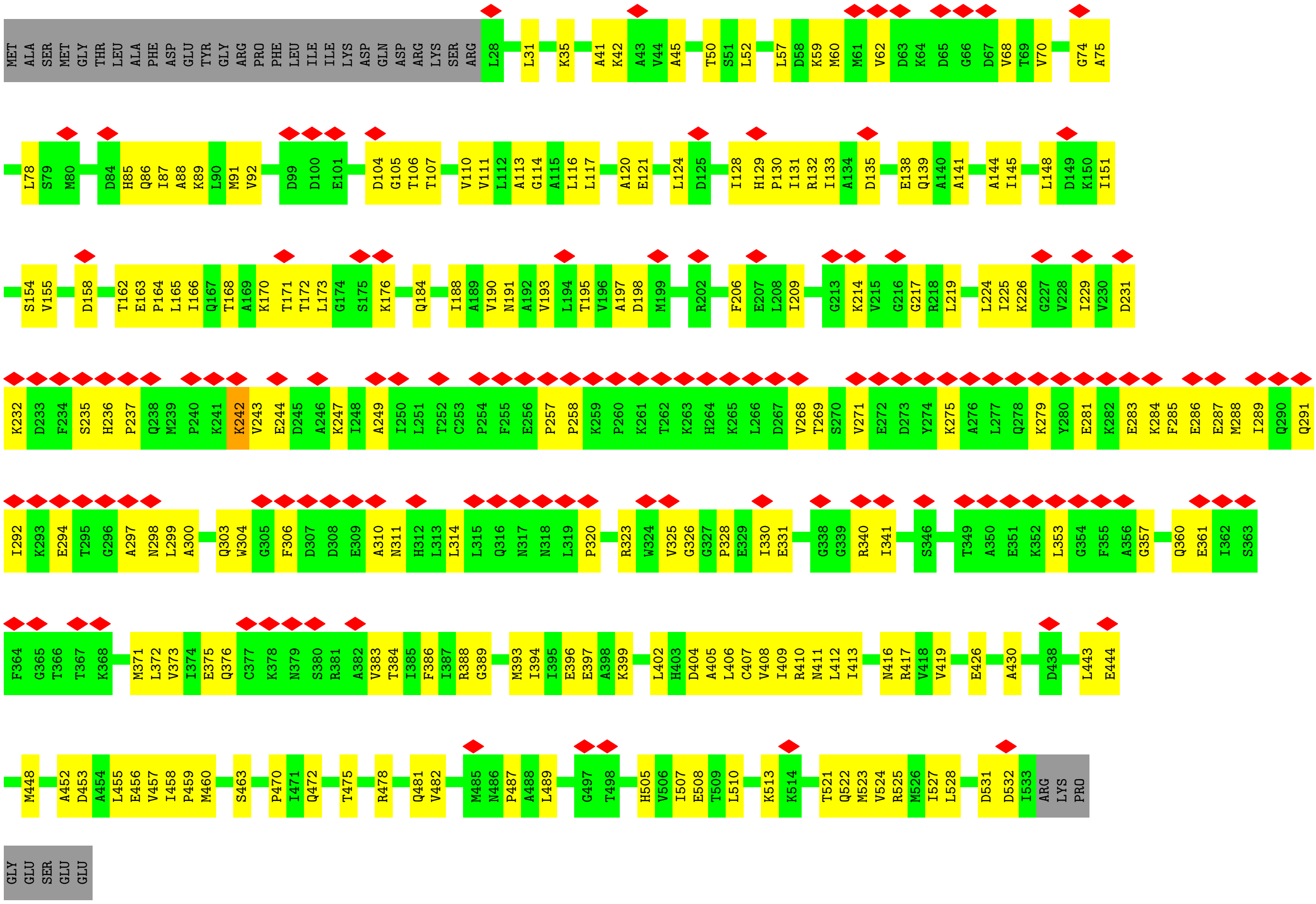
Chain E:





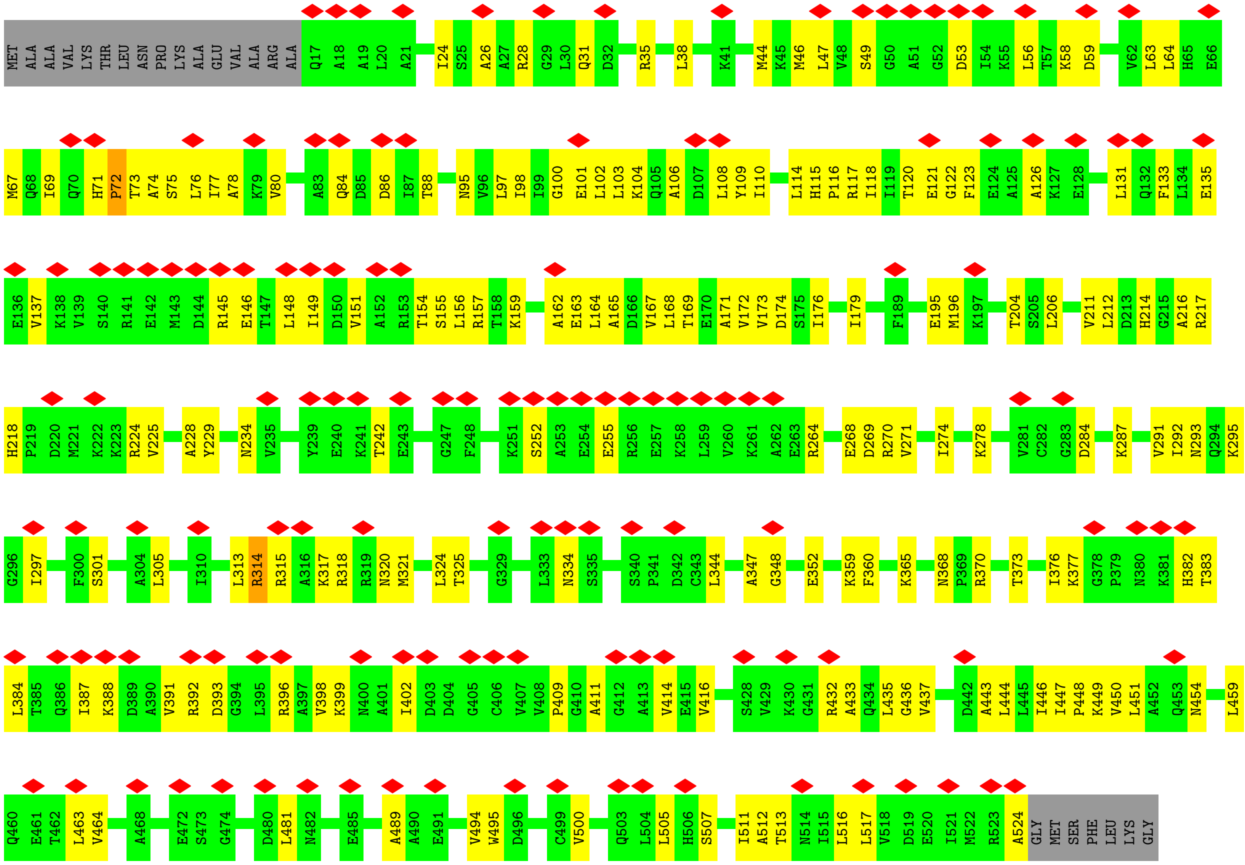
- Molecule 11: T-complex protein 1 subunit epsilon

Chain M:



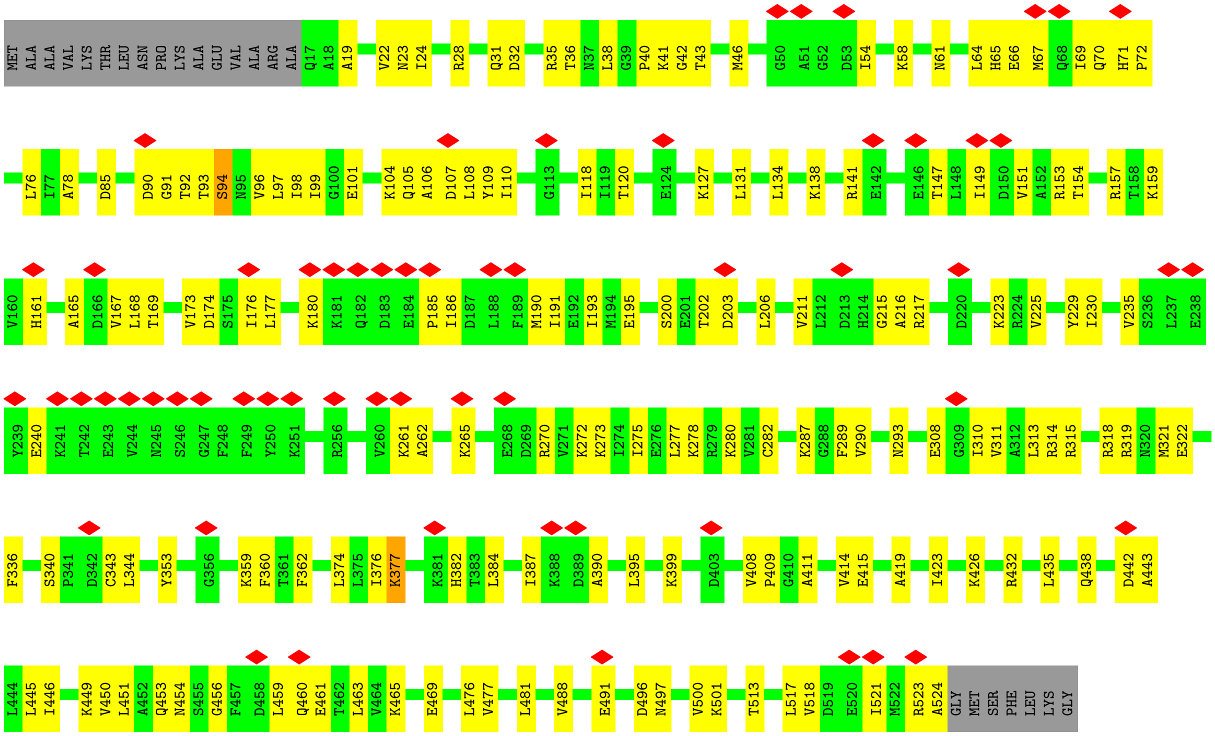
- Molecule 12: T-complex protein 1 subunit zeta

Chain F:



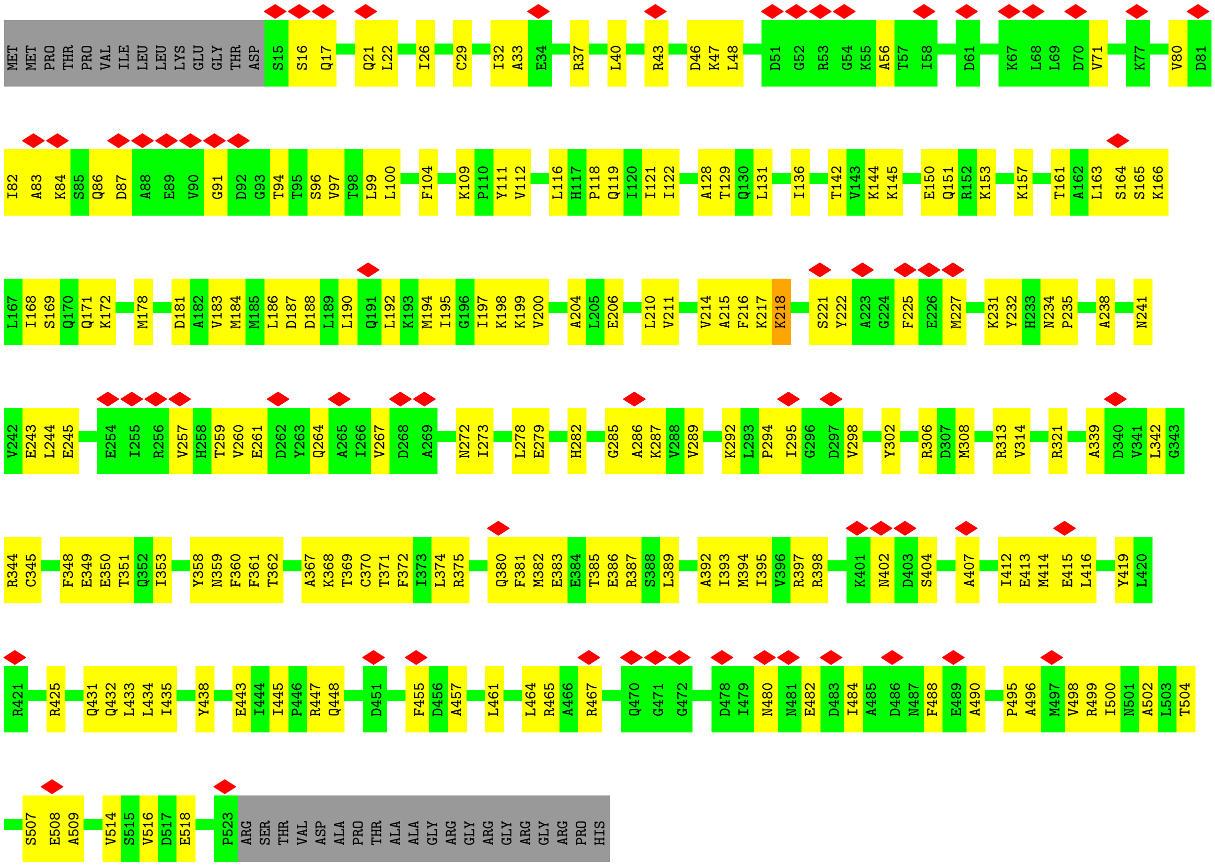
- Molecule 12: T-complex protein 1 subunit zeta

Chain N:



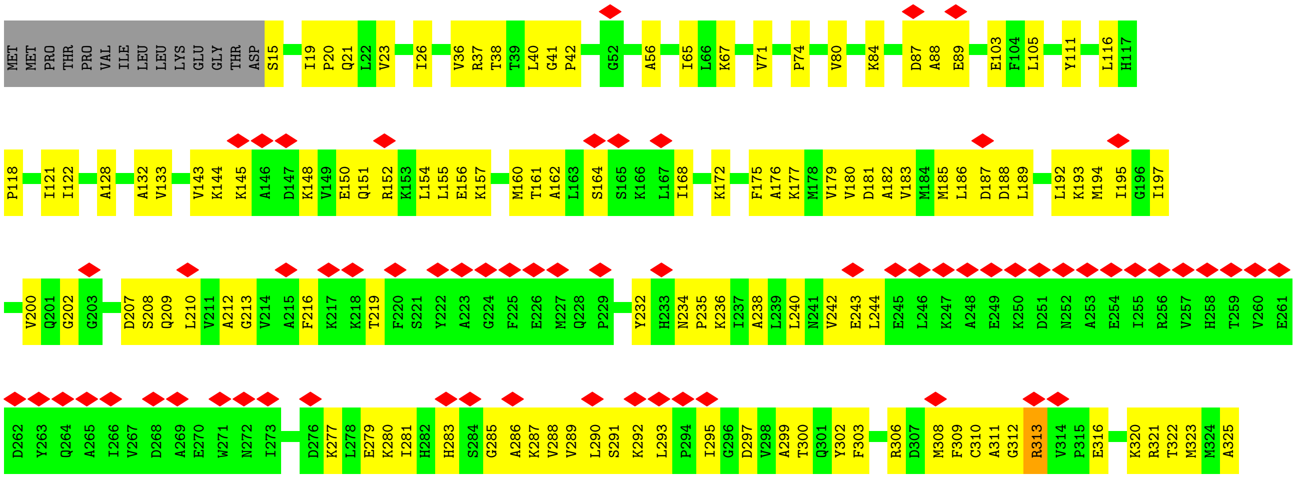
- Molecule 13: T-complex protein 1 subunit eta

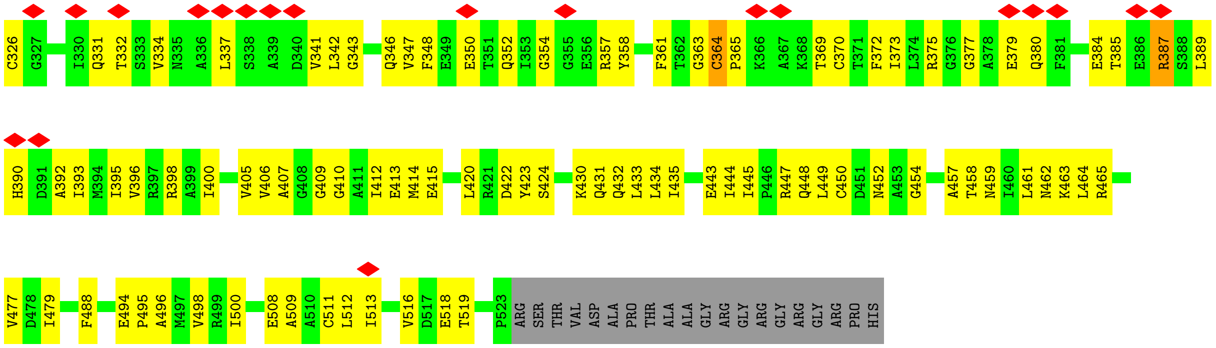
Chain G:



- Molecule 13: T-complex protein 1 subunit eta

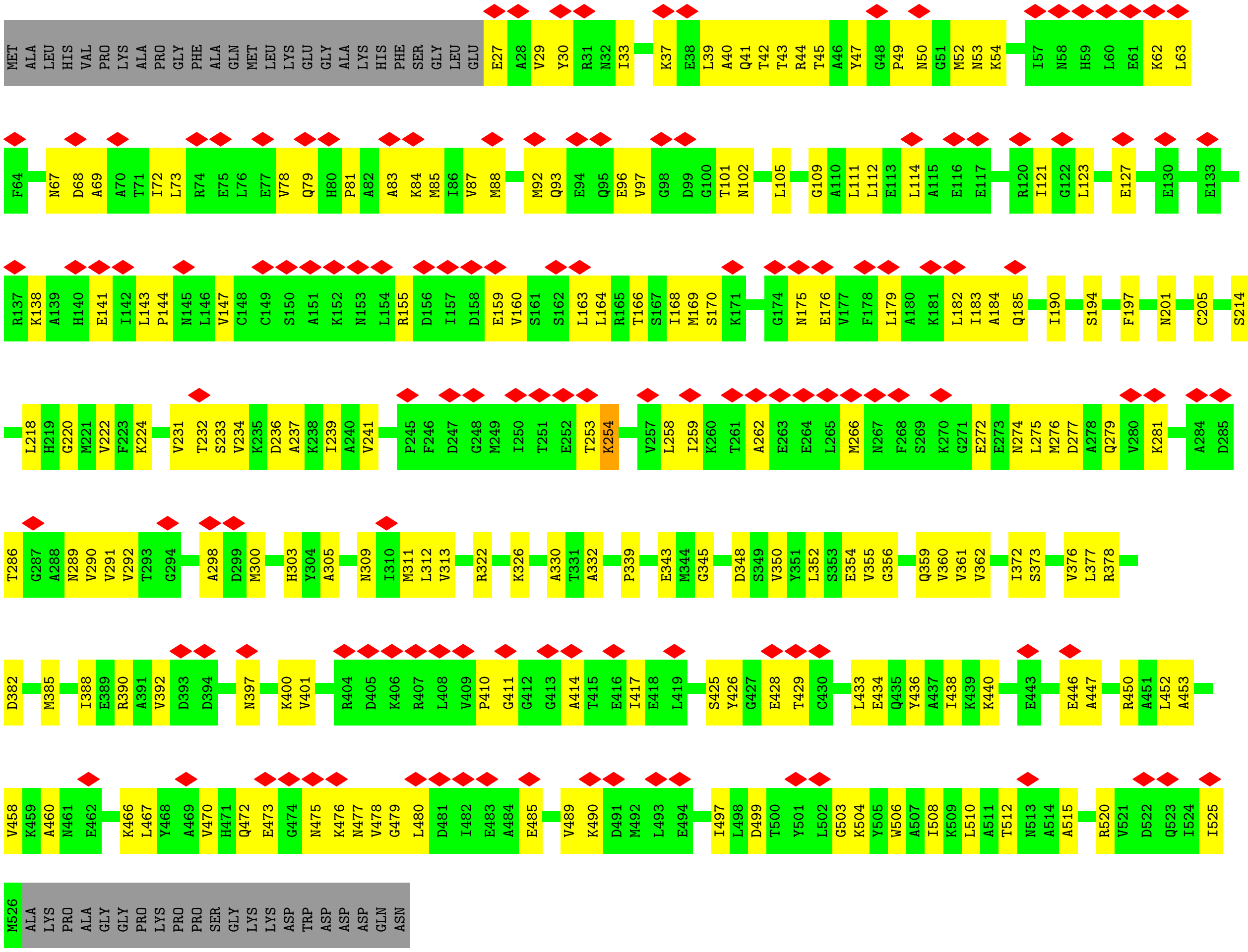
Chain O:





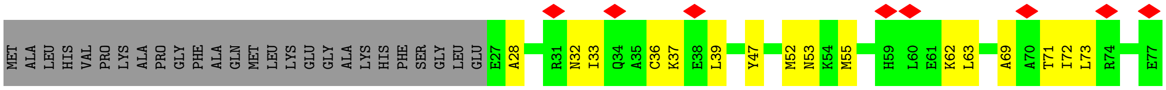
- Molecule 14: T-complex protein 1 subunit theta

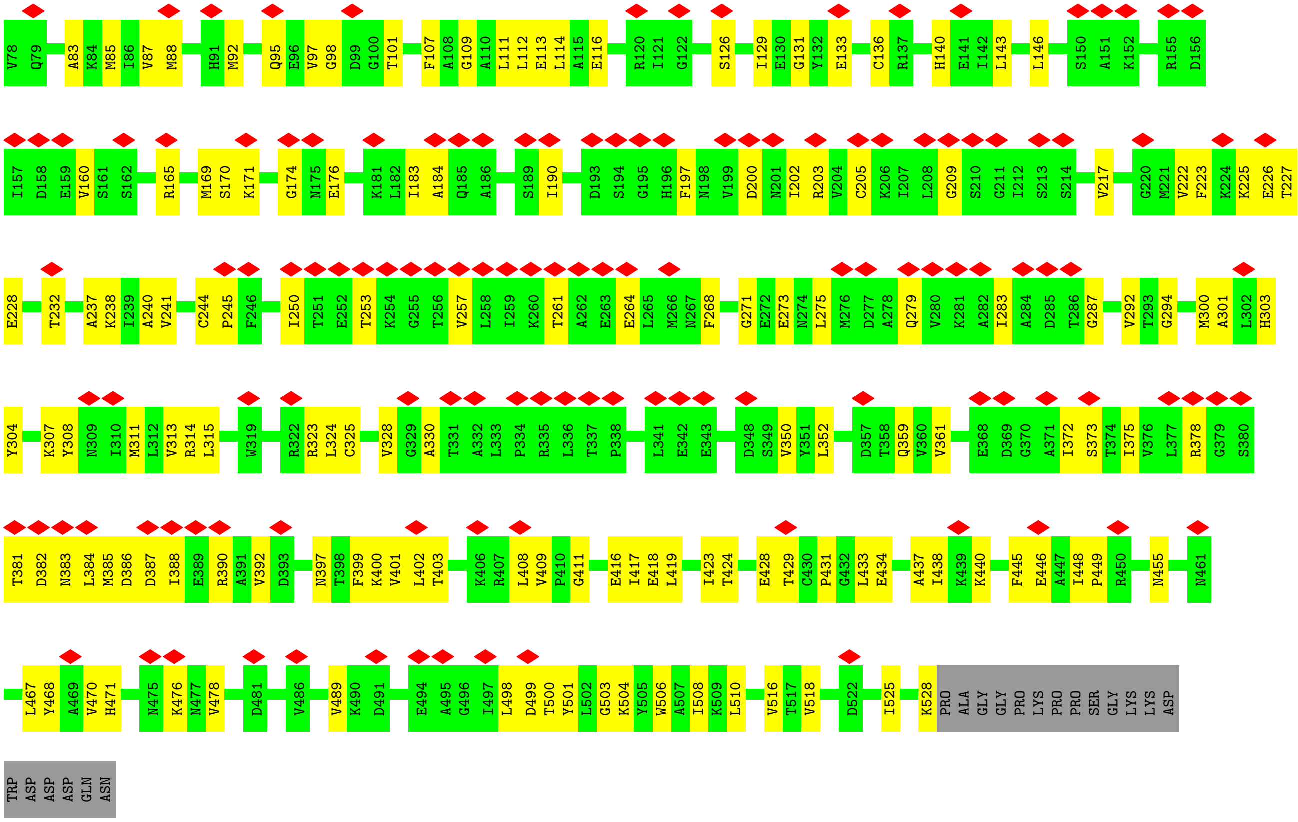
Chain H:



- Molecule 14: T-complex protein 1 subunit theta

Chain P:




V78 Q79 A83 K84 M85 I86 V87 M88 H91 M92 Q95 E96 V97 G98 D99 G100 T101 F107 A108 G109 A110 L111 L112 E113 L114 A115 E116 R120 I121 G122 S126 I129 E130 G131 Y132 E133 C136 R137 H140 E141 I142 L143 L146 S150 A151 K152 R155 D156
I157 D158 E159 V160 S161 S162 R165 M169 S170 K171 G174 N175 E176 K181 L182 I183 A184 Q185 A186 S189 I190 D193 S194 G195 H196 F197 N198 V199 D200 N201 I202 R203 V204 C205 K206 I207 L208 G209 S210 G211 I212 S213 S214 V217 G220 M221 V222 F223 K224 K225 E226 T227
E228 T232 A237 K238 I239 A240 V241 C244 P245 F246 I250 T251 E252 T253 K254 G255 T256 V257 L258 I259 K260 T261 A262 E263 E264 L265 M266 N267 F268 G271 E272 E273 N274 L275 M276 D277 A278 Q279 V280 K281 A282 I283 A284 D285 T286 G287 V292 T293 G294 M300 A301 L302 H303
Y304 K307 Y308 N309 I310 M311 L312 V313 R314 L315 W319 R322 R323 L324 G325 V328 G329 A330 T331 A332 L333 P334 R335 L336 T337 P338 L341 E342 E343 D348 S349 V350 Y351 L352 D357 T358 Q359 V360 V361 E368 D369 G370 A371 I372 S373 T374 I375 V376 L377 R378 G379 S380
T381 D382 N383 L384 M385 D386 D387 I388 E389 R390 A391 V392 D393 N397 T398 F399 K400 V401 L402 T403 K406 R407 L408 V409 P410 G411 E416 I417 E418 L419 I423 T424 E428 T429 C430 P431 G432 L433 E434 A437 I438 K439 K440 F445 E446 A447 I448 P449 R450 N455 N461
L467 Y468 A469 V470 H471 N475 K476 N477 V478 D481 V486 V489 K490 D491 E494 A495 G496 I497 L498 D499 T500 Y501 L502 G503 K504 Y505 W506 A507 I508 K509 L510 V516 T517 V518 D522 I525 K528 PRO ALA GLY GLY PRO LYS PRO PRO SER GLY LYS LYS ASP
TRP ASP ASP ASP GLN ASN

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed for every micrographs	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.117	Depositor
Minimum map value	-7.622	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.246	Depositor
Recommended contour level	0.943	Depositor
Map size (Å)	326.4, 326.4, 326.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1	0.30	0/879	0.62	0/1173
2	2	0.26	0/670	0.58	0/897
3	3	0.27	0/969	0.59	0/1300
4	4	0.25	0/715	0.57	0/959
5	5	0.28	0/1031	0.63	0/1385
6	6	0.26	0/829	0.59	0/1109
7	A	0.25	0/3955	0.56	0/5340
7	I	0.25	0/3939	0.56	0/5318
8	B	0.25	0/3776	0.54	0/5090
8	J	0.25	0/3776	0.55	0/5090
9	C	0.25	0/3968	0.59	0/5355
9	K	0.27	0/3968	0.58	0/5355
10	D	0.26	0/3878	0.57	0/5237
10	L	0.26	0/3878	0.57	0/5237
11	E	0.25	0/3928	0.54	0/5295
11	M	0.26	0/3928	0.56	0/5295
12	F	0.25	0/3949	0.55	0/5324
12	N	0.26	0/3949	0.58	0/5324
13	G	0.26	0/3965	0.54	0/5351
13	O	0.27	0/3965	0.57	0/5351
14	H	0.25	0/3867	0.53	0/5229
14	P	0.26	0/3881	0.52	0/5247
All	All	0.26	0/67663	0.56	0/91261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1	873	0	902	46	0
2	2	667	0	693	26	0
3	3	956	0	970	34	0
4	4	711	0	699	35	0
5	5	1017	0	1042	72	0
6	6	825	0	850	48	0
7	A	3919	0	4084	125	0
7	I	3903	0	4062	125	0
8	B	3736	0	3846	120	0
8	J	3736	0	3846	130	0
9	C	3924	0	4050	176	0
9	K	3924	0	4050	172	0
10	D	3847	0	4056	148	0
10	L	3847	0	4051	135	0
11	E	3883	0	3994	151	0
11	M	3883	0	3994	148	0
12	F	3903	0	4030	160	0
12	N	3903	0	4030	137	0
13	G	3910	0	4005	154	0
13	O	3910	0	4005	169	0
14	H	3816	0	3879	138	0
14	P	3830	0	3897	117	0
15	F	27	0	11	1	0
15	H	27	0	11	4	0
15	N	27	0	11	1	0
15	P	27	0	11	2	0
All	All	67031	0	69079	2413	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 18.

The worst 5 of 2413 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)
12:F:71:HIS:ND1	12:F:72:PRO:HD2	1.39	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:186:LEU:HD12	13:O:186:LEU:O	1.42	1.15
7:I:168:PHE:HZ	7:I:388:MET:HE1	1.14	1.08
7:I:161:ILE:HD12	7:I:388:MET:SD	1.98	1.03
11:M:154:SER:HB3	11:M:417:ARG:HG2	1.40	1.01

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	1	105/122 (86%)	103 (98%)	2 (2%)	0	100	100
2	2	81/154 (53%)	80 (99%)	1 (1%)	0	100	100
3	3	114/197 (58%)	108 (95%)	6 (5%)	0	100	100
4	4	86/140 (61%)	82 (95%)	4 (5%)	0	100	100
5	5	125/140 (89%)	118 (94%)	7 (6%)	0	100	100
6	6	100/129 (78%)	97 (97%)	3 (3%)	0	100	100
7	A	514/556 (92%)	495 (96%)	19 (4%)	0	100	100
7	I	512/556 (92%)	474 (93%)	38 (7%)	0	100	100
8	B	495/535 (92%)	472 (95%)	23 (5%)	0	100	100
8	J	495/535 (92%)	470 (95%)	25 (5%)	0	100	100
9	C	503/545 (92%)	477 (95%)	25 (5%)	1 (0%)	47	78
9	K	503/545 (92%)	466 (93%)	36 (7%)	1 (0%)	47	78
10	D	509/539 (94%)	486 (96%)	22 (4%)	1 (0%)	47	78
10	L	509/539 (94%)	479 (94%)	30 (6%)	0	100	100
11	E	504/541 (93%)	472 (94%)	32 (6%)	0	100	100
11	M	504/541 (93%)	478 (95%)	26 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	506/531 (95%)	484 (96%)	21 (4%)	1 (0%)	47	78
12	N	506/531 (95%)	471 (93%)	34 (7%)	1 (0%)	47	78
13	G	507/543 (93%)	477 (94%)	29 (6%)	1 (0%)	47	78
13	O	507/543 (93%)	472 (93%)	33 (6%)	2 (0%)	34	70
14	H	498/547 (91%)	482 (97%)	16 (3%)	0	100	100
14	P	500/547 (91%)	476 (95%)	24 (5%)	0	100	100
All	All	8683/9556 (91%)	8219 (95%)	456 (5%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	365	ASP
12	F	72	PRO
12	N	94	SER
13	O	364	CYS
13	G	144	LYS

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	1	97/109 (89%)	97 (100%)	0	100	100
2	2	74/122 (61%)	74 (100%)	0	100	100
3	3	107/175 (61%)	107 (100%)	0	100	100
4	4	81/125 (65%)	81 (100%)	0	100	100
5	5	116/128 (91%)	116 (100%)	0	100	100
6	6	91/108 (84%)	90 (99%)	1 (1%)	73	84
7	A	430/463 (93%)	428 (100%)	2 (0%)	88	93
7	I	428/463 (92%)	426 (100%)	2 (0%)	88	93
8	B	397/427 (93%)	396 (100%)	1 (0%)	92	95
8	J	397/427 (93%)	396 (100%)	1 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	437/469 (93%)	432 (99%)	5 (1%)	73	84
9	K	437/469 (93%)	435 (100%)	2 (0%)	88	93
10	D	435/452 (96%)	433 (100%)	2 (0%)	88	93
10	L	435/452 (96%)	433 (100%)	2 (0%)	88	93
11	E	426/456 (93%)	423 (99%)	3 (1%)	84	90
11	M	426/456 (93%)	425 (100%)	1 (0%)	93	96
12	F	426/442 (96%)	425 (100%)	1 (0%)	93	96
12	N	426/442 (96%)	423 (99%)	3 (1%)	84	90
13	G	417/443 (94%)	415 (100%)	2 (0%)	88	93
13	O	417/443 (94%)	415 (100%)	2 (0%)	88	93
14	H	416/451 (92%)	415 (100%)	1 (0%)	93	96
14	P	417/451 (92%)	417 (100%)	0	100	100
All	All	7333/7973 (92%)	7302 (100%)	31 (0%)	91	94

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	F	314	ARG
12	N	223	LYS
14	H	254	LYS
13	O	313	ARG
10	L	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	I	103	ASN
10	L	350	GLN
10	L	271	GLN
11	M	129	HIS
9	C	87	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	ADP	H	5000	-	24,29,29	3.30	7 (29%)	29,45,45	1.45	4 (13%)
15	ADP	N	601	-	24,29,29	3.29	8 (33%)	29,45,45	1.31	3 (10%)
15	ADP	P	601	-	24,29,29	3.27	7 (29%)	29,45,45	1.40	4 (13%)
15	ADP	F	601	-	24,29,29	3.29	7 (29%)	29,45,45	1.49	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	H	5000	-	-	6/12/32/32	0/3/3/3
15	ADP	N	601	-	-	1/12/32/32	0/3/3/3
15	ADP	P	601	-	-	6/12/32/32	0/3/3/3
15	ADP	F	601	-	-	5/12/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	5000	ADP	O4'-C1'	-9.24	1.28	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	601	ADP	O4'-C1'	-9.20	1.28	1.41
15	P	601	ADP	O4'-C1'	-8.92	1.28	1.41
15	N	601	ADP	O4'-C1'	-8.80	1.28	1.41
15	N	601	ADP	O4'-C4'	7.74	1.62	1.45

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	601	ADP	N3-C2-N1	-4.51	121.62	128.68
15	H	5000	ADP	N3-C2-N1	-4.45	121.72	128.68
15	F	601	ADP	N3-C2-N1	-4.42	121.77	128.68
15	P	601	ADP	N3-C2-N1	-4.33	121.90	128.68
15	P	601	ADP	PA-O3A-PB	-3.17	121.94	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	601	ADP	C5'-O5'-PA-O1A
15	F	601	ADP	C5'-O5'-PA-O2A
15	F	601	ADP	O4'-C4'-C5'-O5'
15	F	601	ADP	C3'-C4'-C5'-O5'
15	H	5000	ADP	PA-O3A-PB-O2B

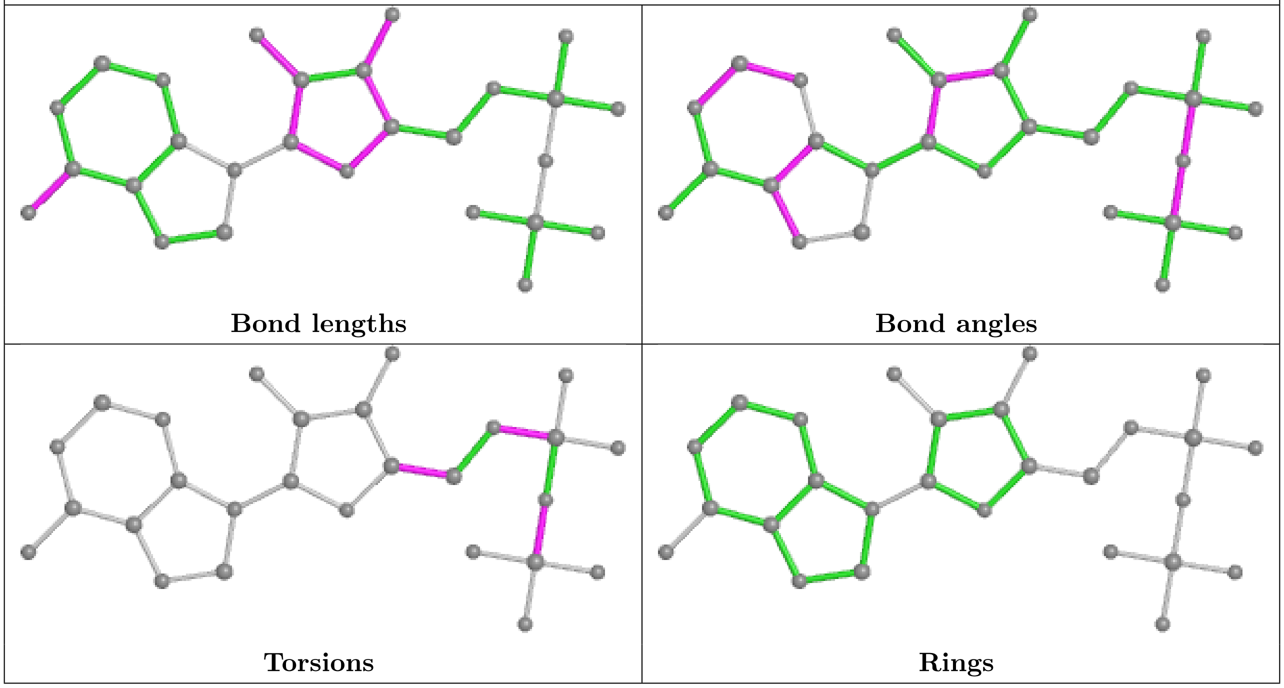
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	5000	ADP	4	0
15	N	601	ADP	1	0
15	P	601	ADP	2	0
15	F	601	ADP	1	0

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

Ligand ADP H 5000



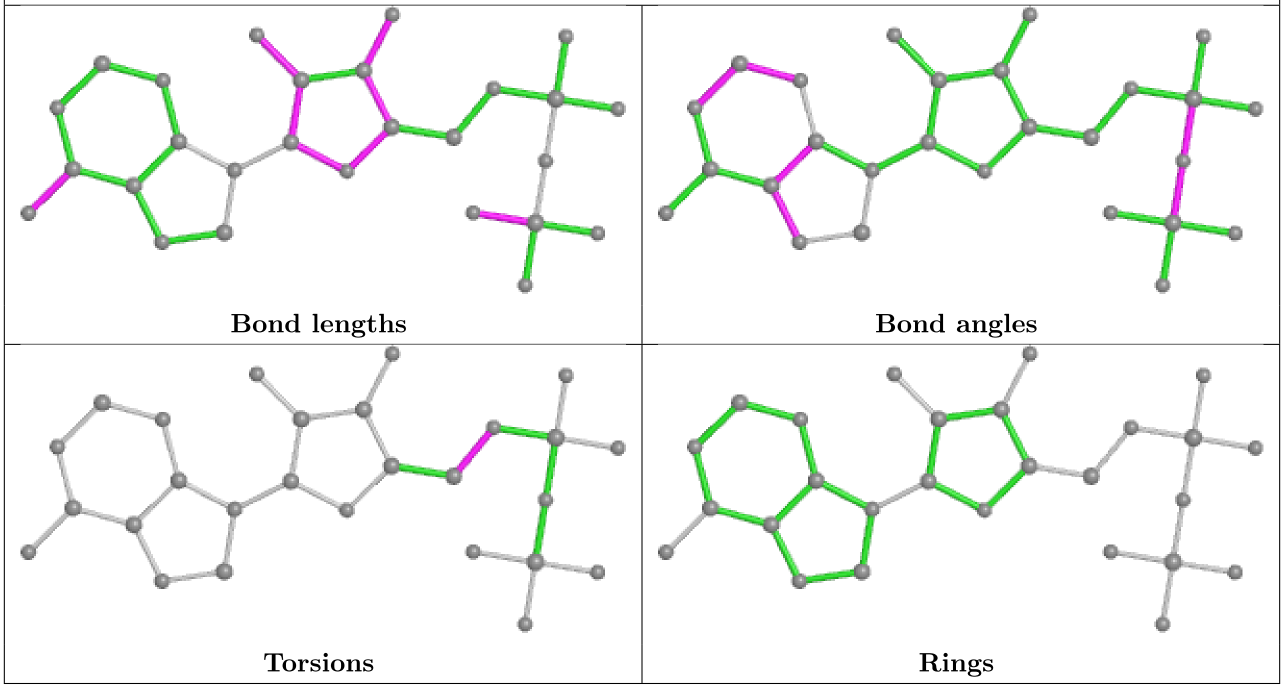
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP N 601



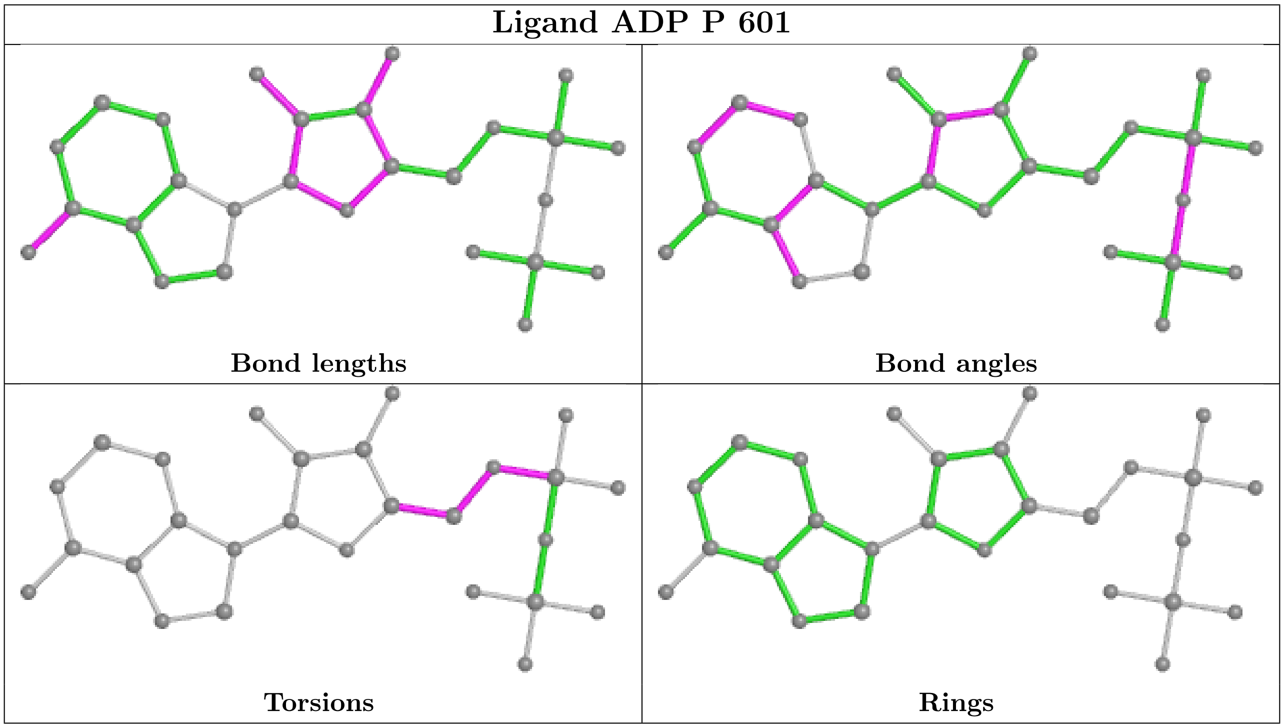
Bond lengths

Bond angles

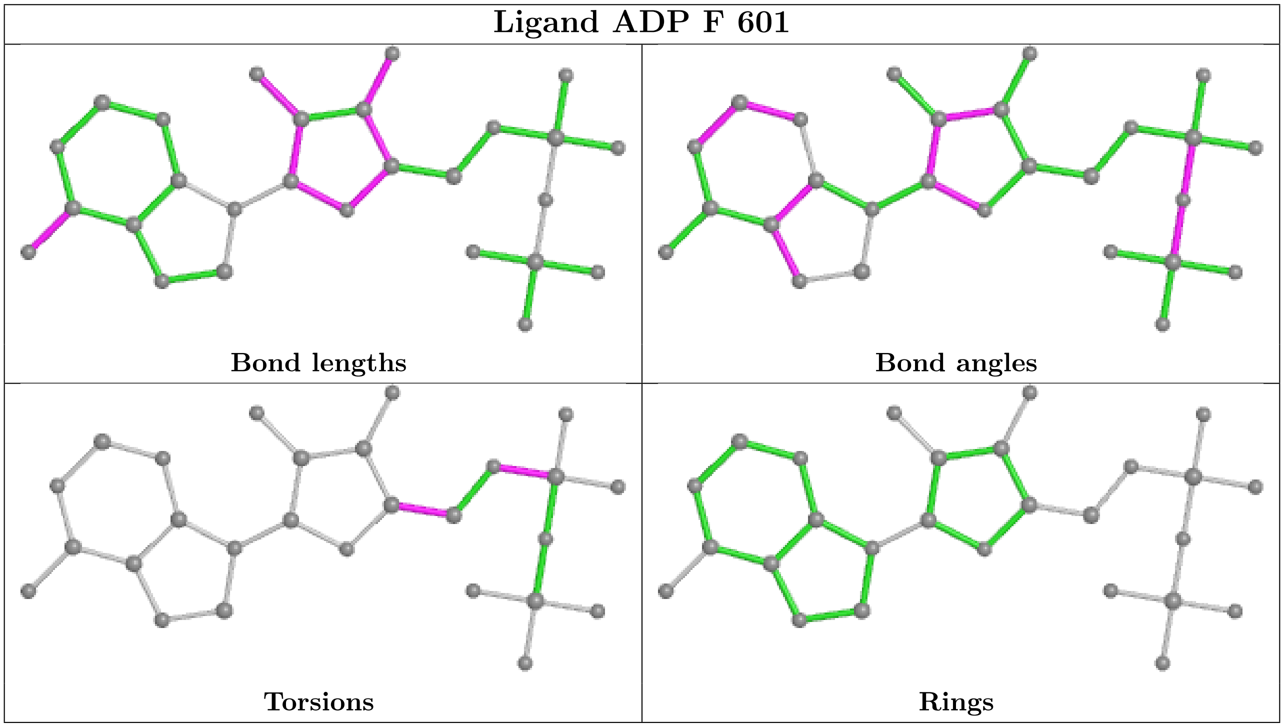
Torsions

Rings

Ligand ADP P 601



Ligand ADP F 601



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

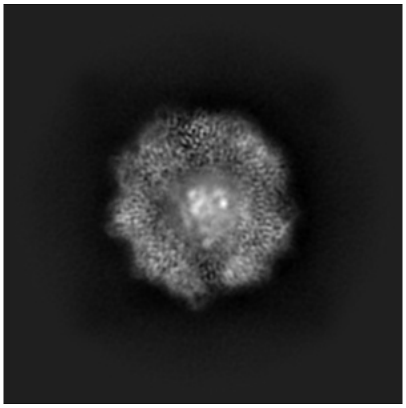
6 Map visualisation

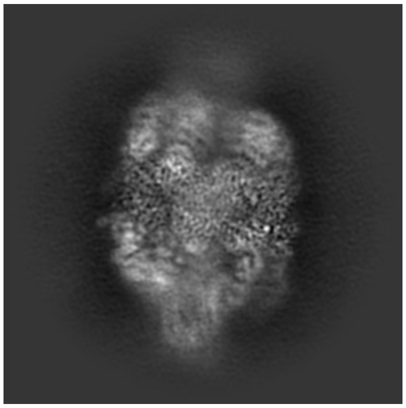
This section contains visualisations of the EMDB entry EMD-32823. These allow visual inspection of the internal detail of the map and identification of artifacts.

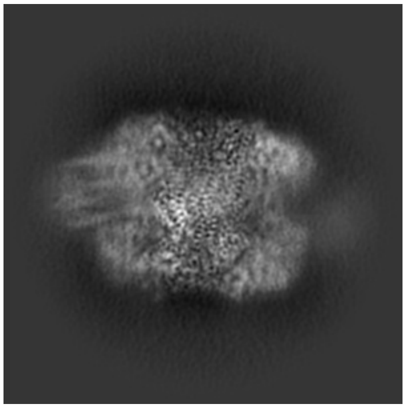
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

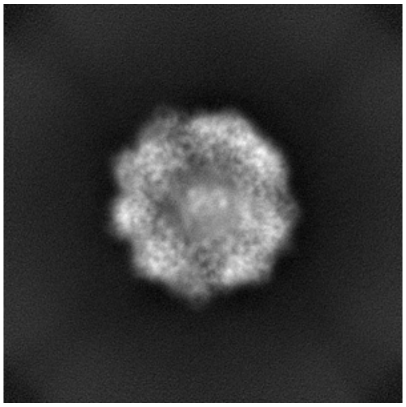
6.1.1 Primary map

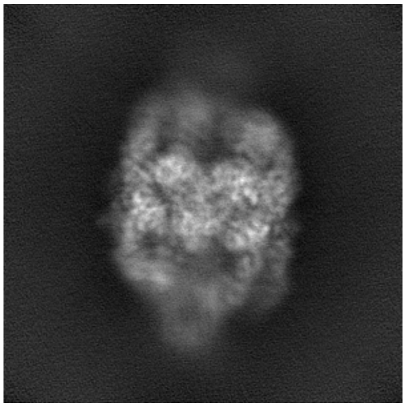

X

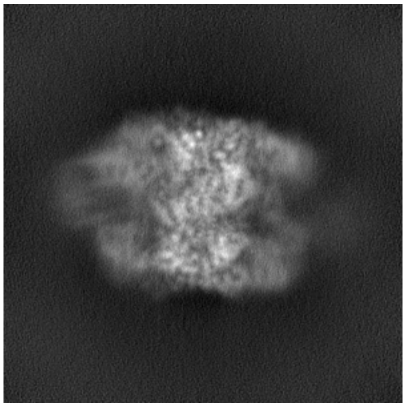

Y


Z

6.1.2 Raw map


X

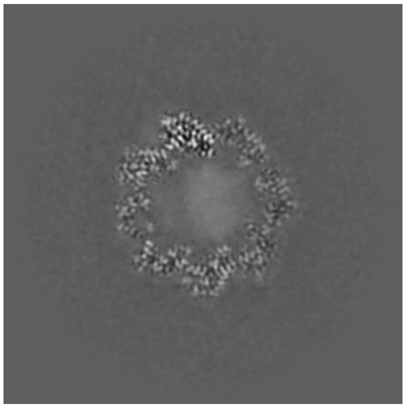

Y


Z

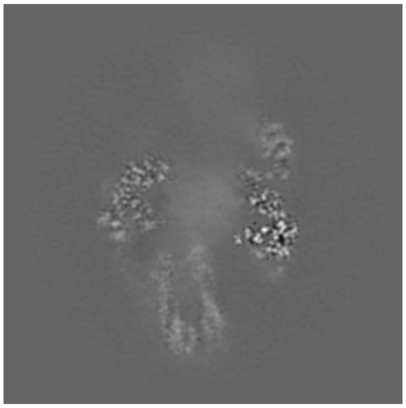
The images above show the map projected in three orthogonal directions.

6.2 Central slices

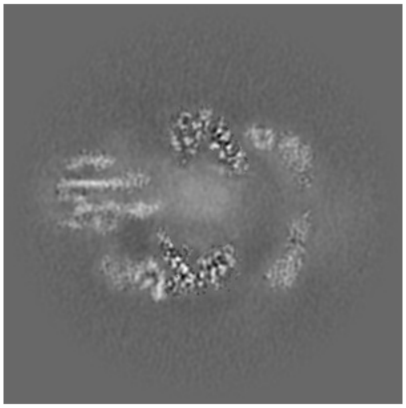
6.2.1 Primary map



X Index: 160

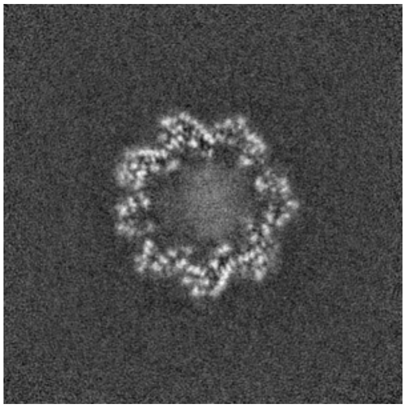


Y Index: 160

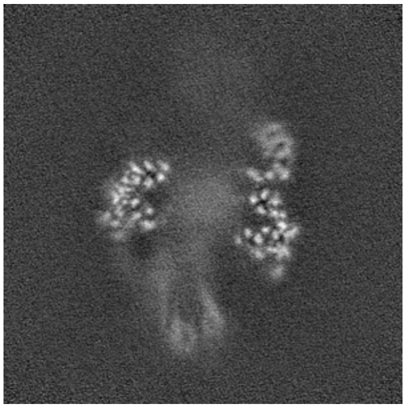


Z Index: 160

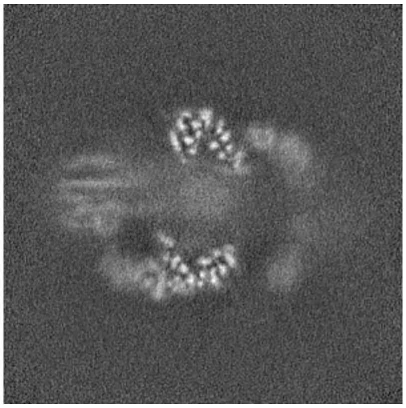
6.2.2 Raw map



X Index: 160



Y Index: 160

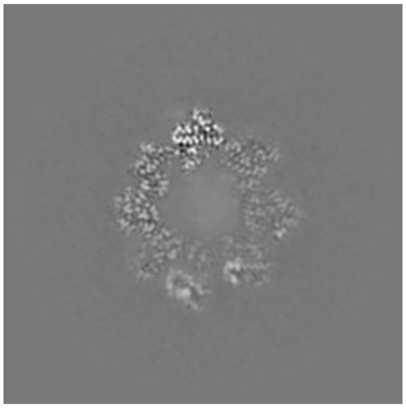


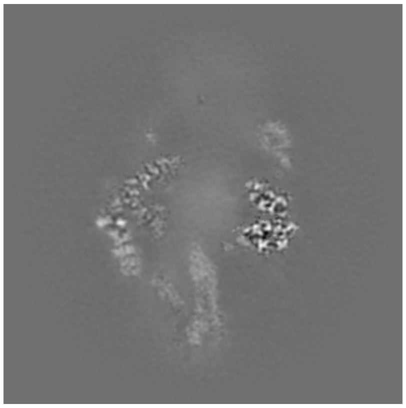
Z Index: 160

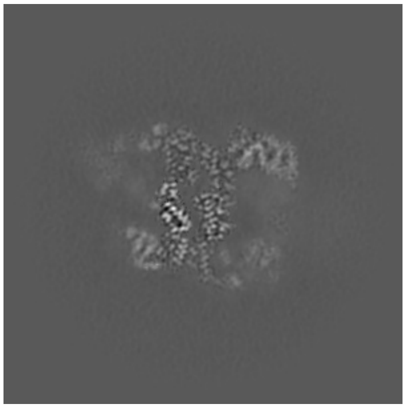
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

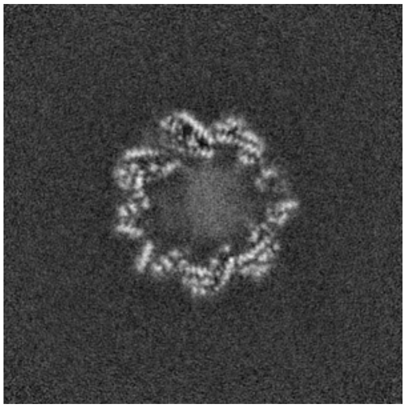
6.3.1 Primary map

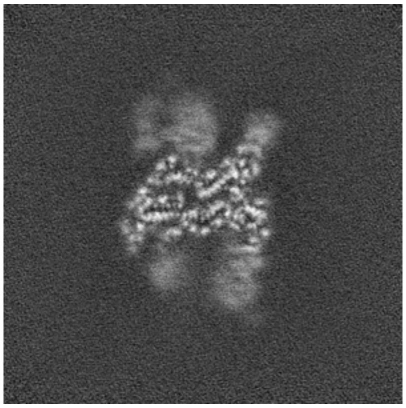

X Index: 141

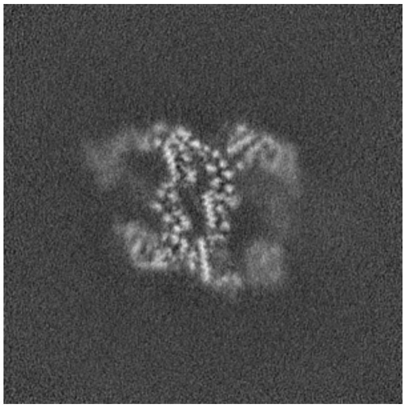

Y Index: 153


Z Index: 202

6.3.2 Raw map


X Index: 162

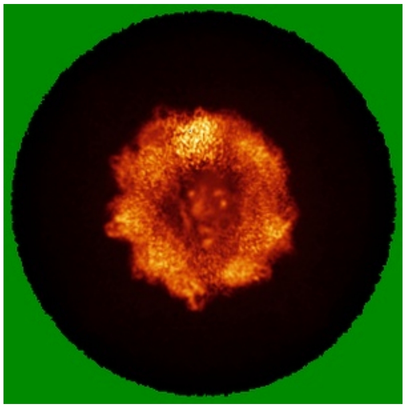

Y Index: 207


Z Index: 200

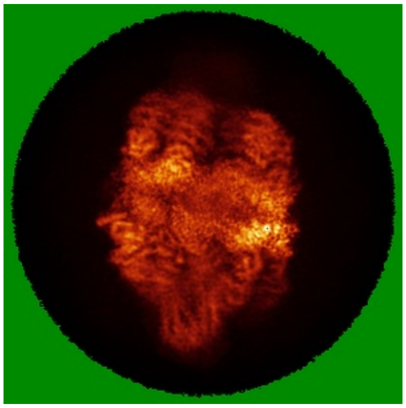
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

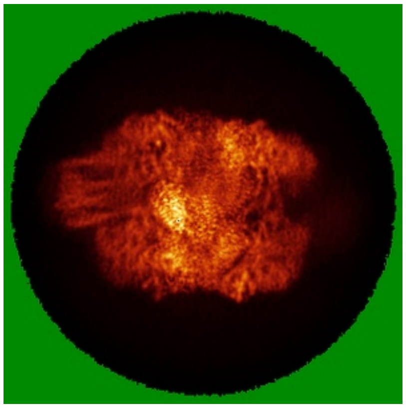
6.4.1 Primary map



X

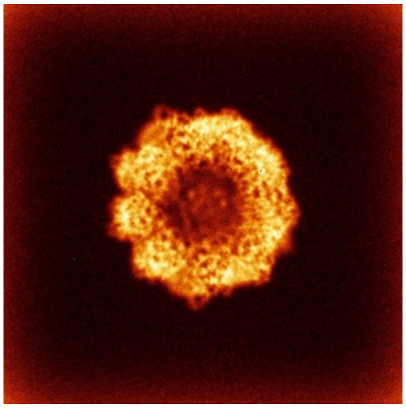


Y

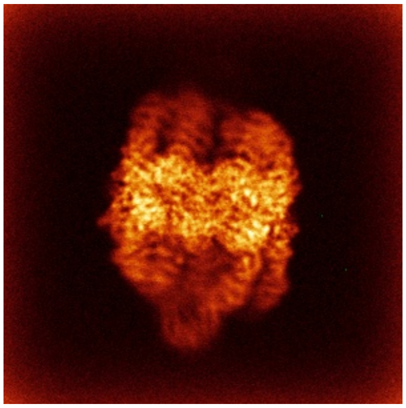


Z

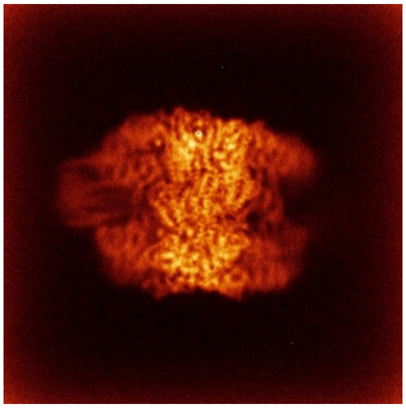
6.4.2 Raw map



X



Y

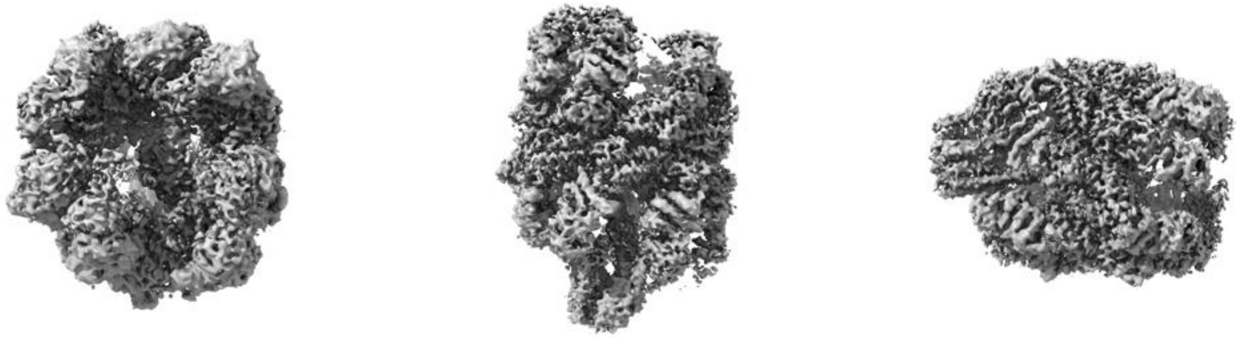


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

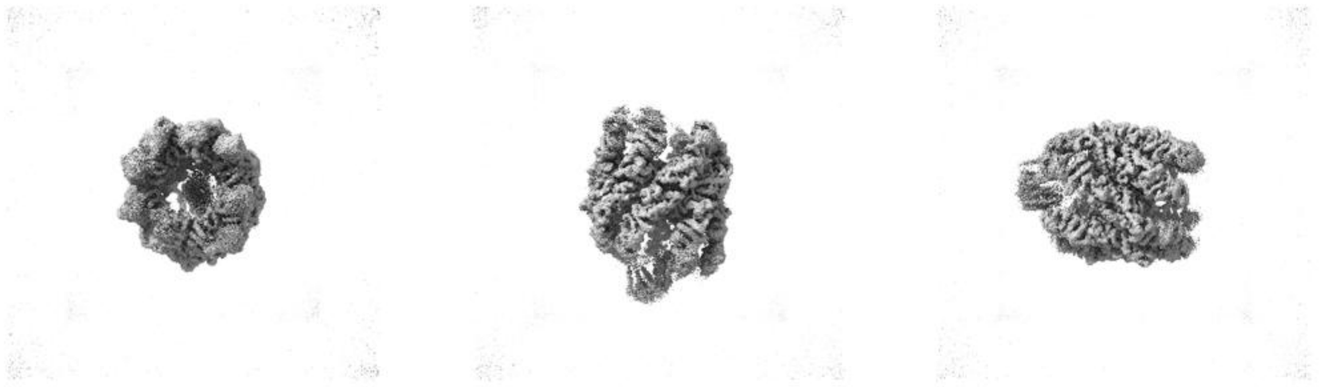
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.943. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

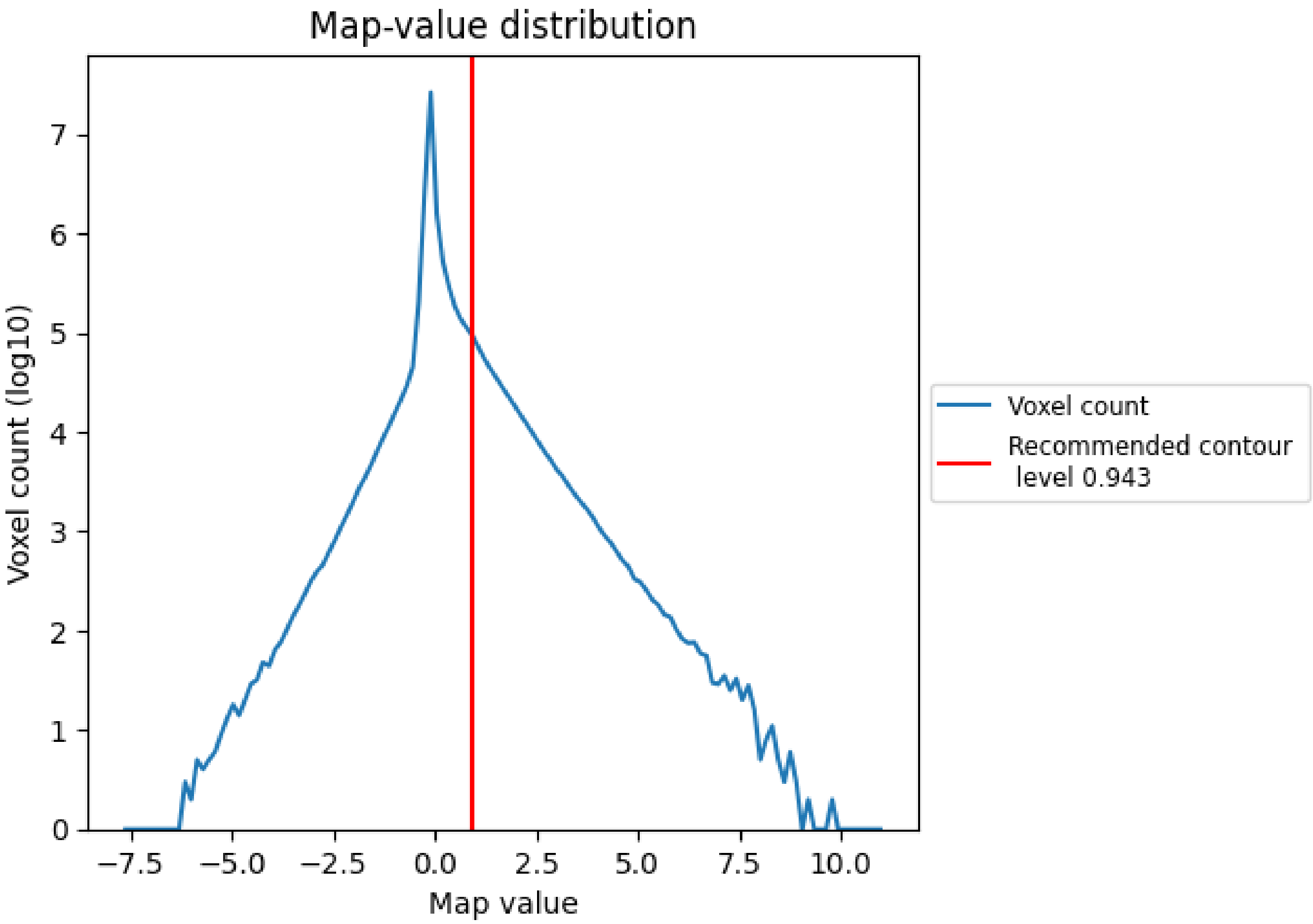
6.6 Mask visualisation

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

7 Map analysis ⓘ

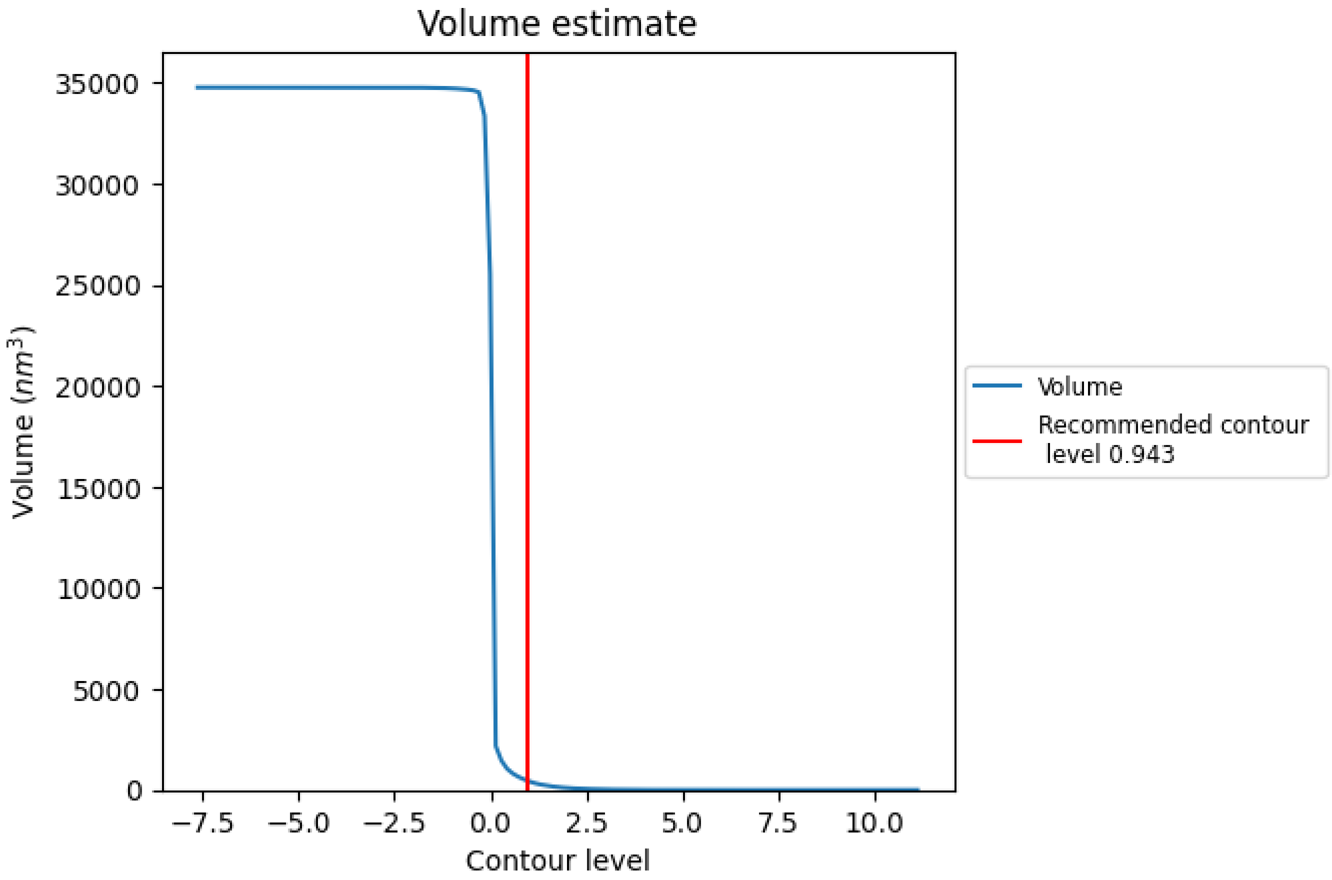
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

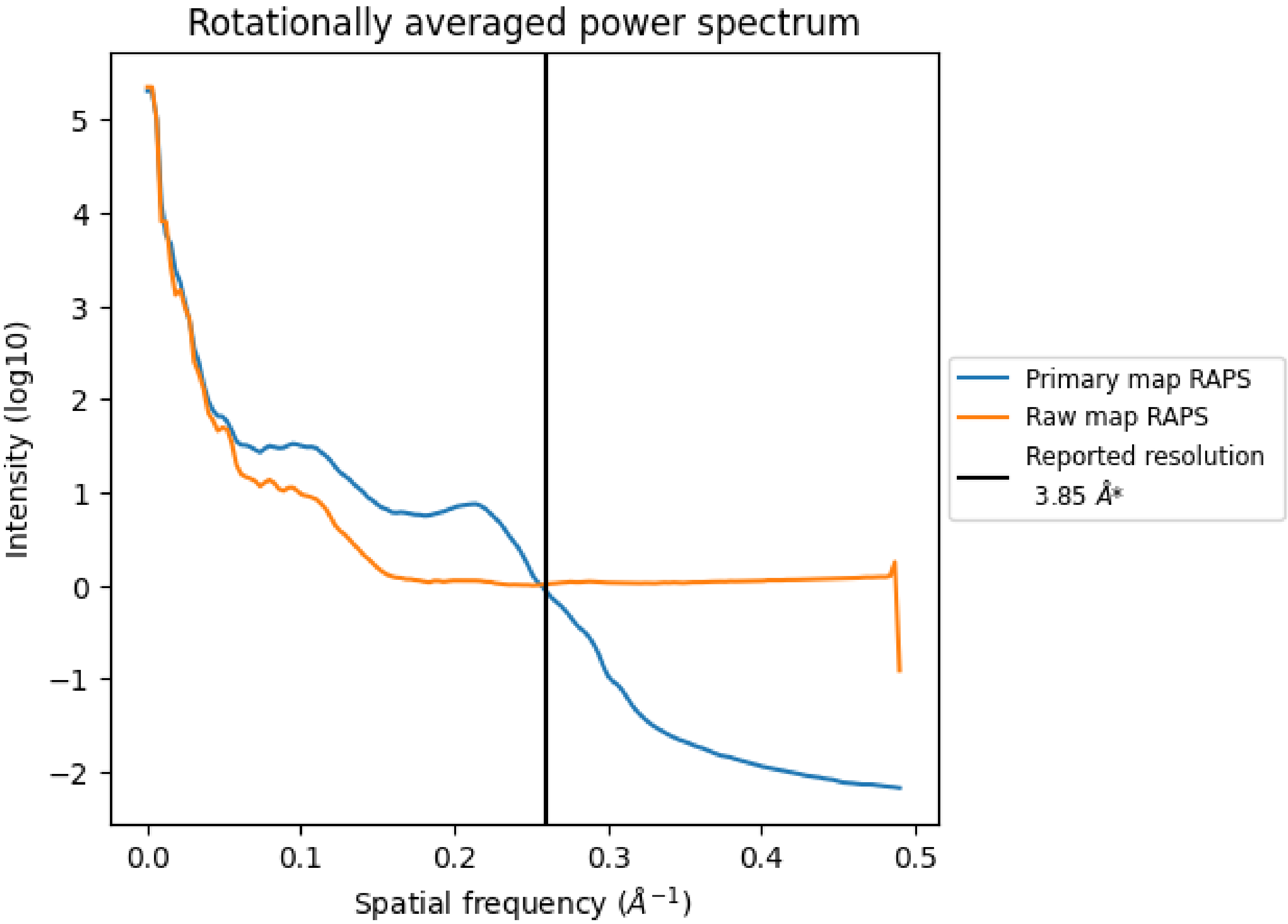
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 423 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 ⓘ

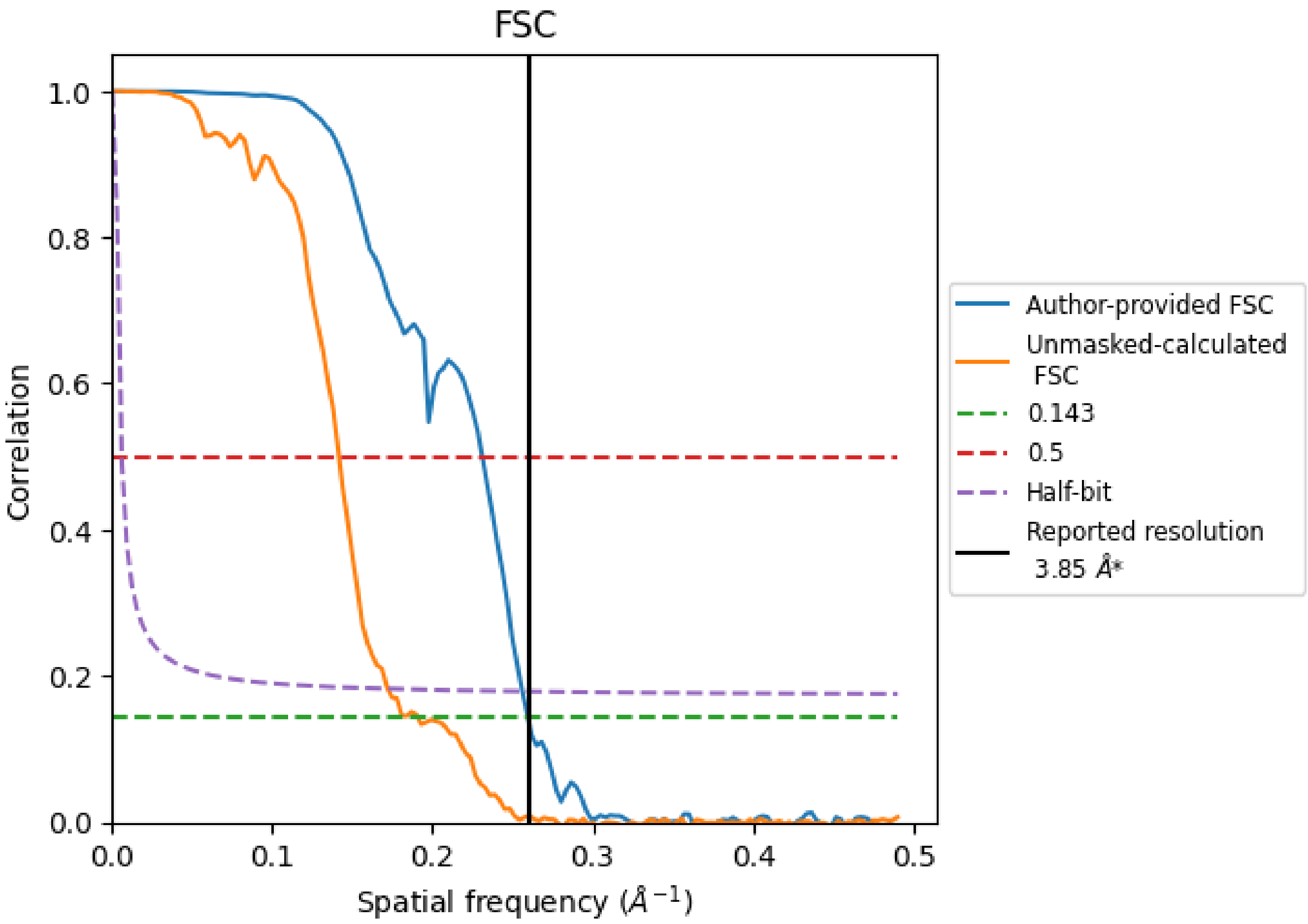


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

8.2 Resolution estimates ⓘ

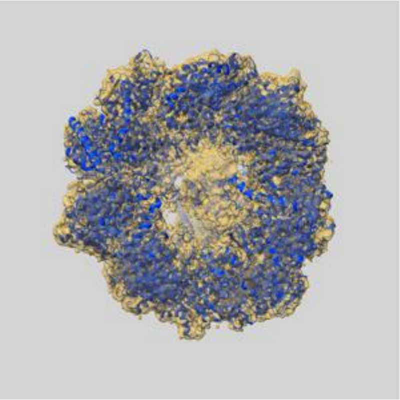
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.85	4.33	3.90
Unmasked-calculated*	5.24	7.06	5.81

*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 5.24 differs from the reported value 3.85 by more than 10 %

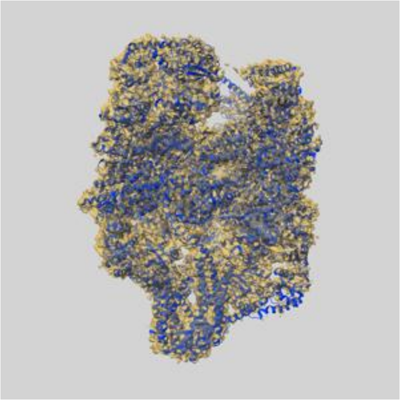
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32823 and PDB model 7WU7. Per-residue inclusion information can be found in section 3 on page 8.

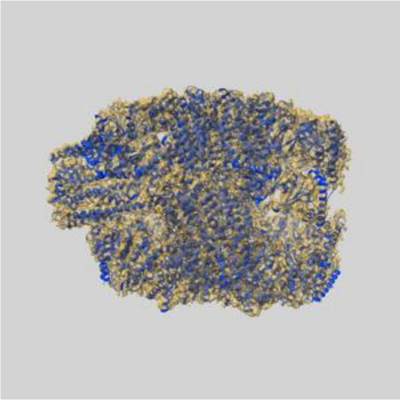
9.1 Map-model overlay ⓘ



X



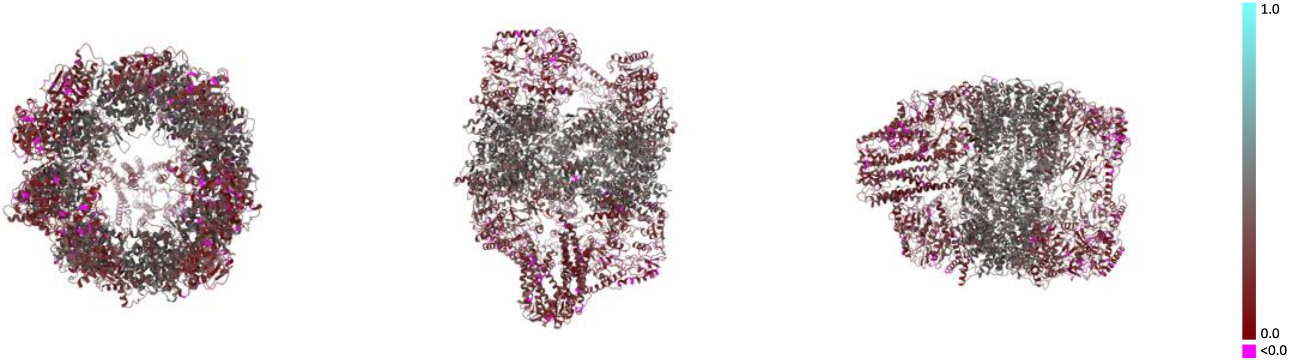
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.943 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.

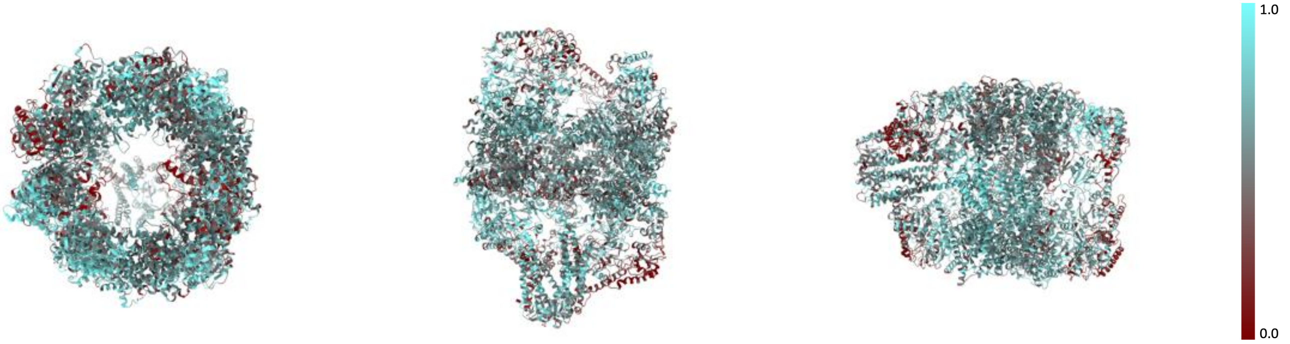
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

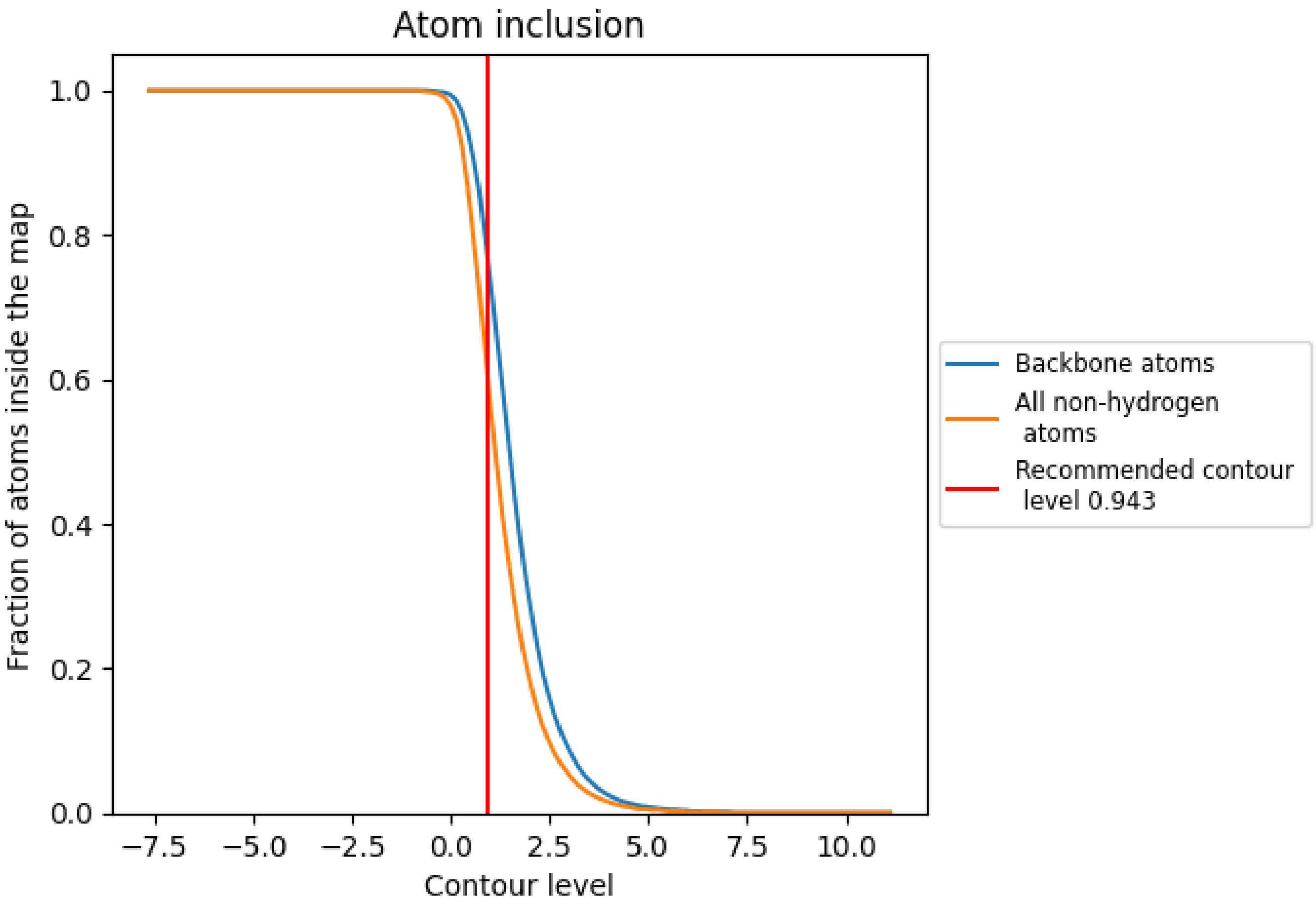
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.943).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 60% 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 (0.943) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.3020
1	0.6210	0.2070
2	0.5150	0.2520
3	0.7030	0.2300
4	0.6210	0.2110
5	0.5870	0.2020
6	0.6670	0.1780
A	0.5600	0.3060
B	0.5440	0.2970
C	0.5200	0.2900
D	0.6580	0.3150
E	0.6120	0.2960
F	0.5590	0.3300
G	0.6570	0.3030
H	0.5600	0.3370
I	0.6230	0.3000
J	0.6330	0.2930
K	0.5880	0.2820
L	0.6630	0.3070
M	0.5130	0.2970
N	0.6710	0.3480
O	0.6380	0.3080
P	0.5310	0.3480