wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:03 PM BST

PDB ID	:	4A0V
EMDB ID:	:	EMD-1961
Title	:	model refined against the Symmetry-free cryo-EM map of TRiC-AMP-PNP
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	:	2011-09-13
Resolution	:	10.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

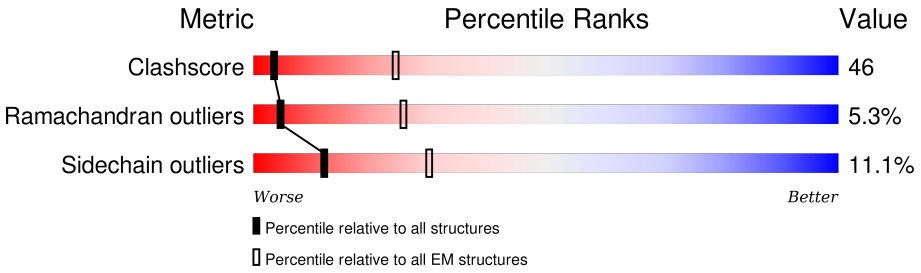
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.70 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	513	37% 47% 10% • •
1	B	513	37% 47% 8% • 6%
1	C	513	39% 51% 9% •
1	D	513	38% 51% 9% •
1	E	513	38% 52% 9% •
1	F	513	36% 49% 9% • 5%
1	G	513	38% 52% 9% •
1	H	513	34% 51% 9% • 5%
1	I	513	39% 44% 10% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	513	44% 45% 10%
1	K	513	41% 49% 10%
1	L	513	40% 47% 8% 6%
1	M	513	38% 48% 8% 5%
1	N	513	43% 44% 7%
1	O	513	36% 48% 9% 6%
1	P	513	41% 49% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 59707 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.

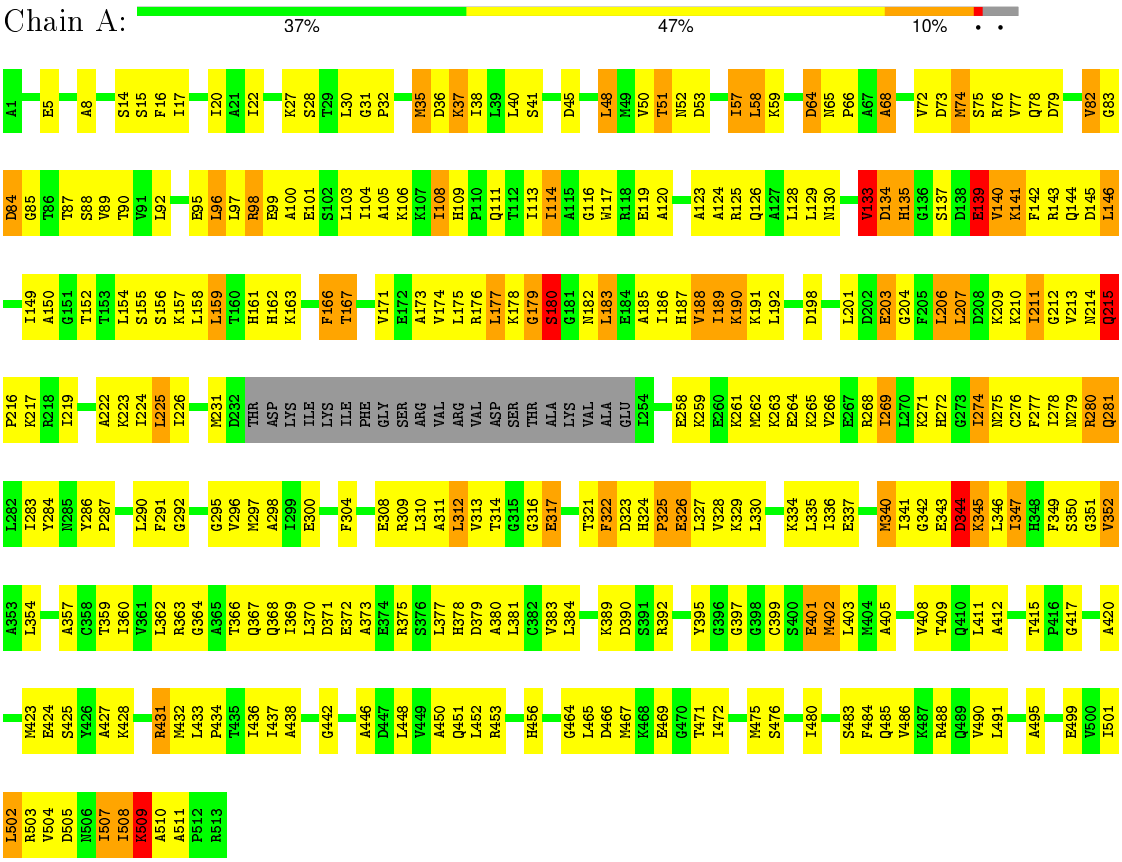
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	492	Total	C	N	O	S	0	0
			3693	2308	649	717	19		
1	B	484	Total	C	N	O	S	0	0
			3626	2268	638	701	19		
1	C	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	D	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	E	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	F	489	Total	C	N	O	S	0	0
			3666	2291	644	712	19		
1	G	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	H	485	Total	C	N	O	S	0	0
			3634	2272	639	704	19		
1	I	476	Total	C	N	O	S	0	0
			3555	2224	624	689	18		
1	J	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	K	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	L	484	Total	C	N	O	S	0	0
			3626	2268	638	701	19		
1	M	486	Total	C	N	O	S	0	0
			3641	2276	640	706	19		
1	N	490	Total	C	N	O	S	0	0
			3673	2295	645	714	19		
1	O	482	Total	C	N	O	S	0	0
			3608	2255	634	701	18		
1	P	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		

3 Residue-property plots (i)

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

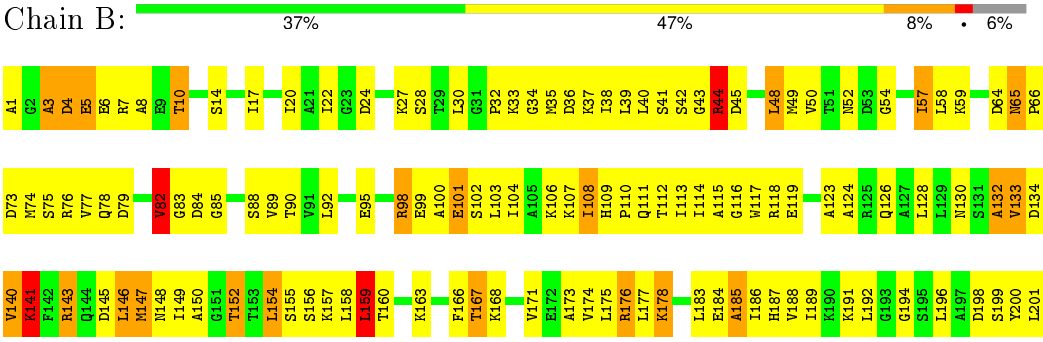
- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

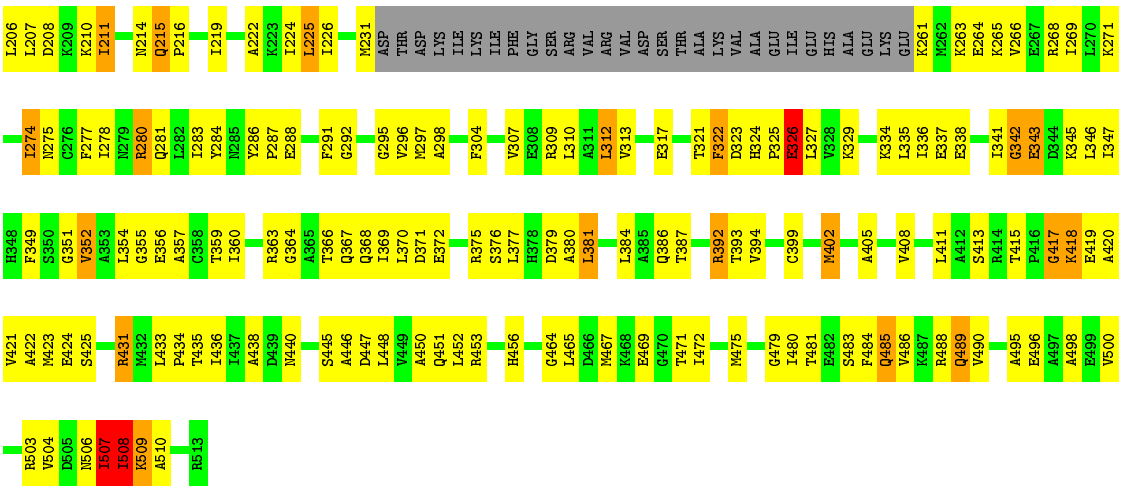
Chain A:



- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

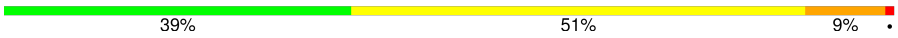
Chain B:

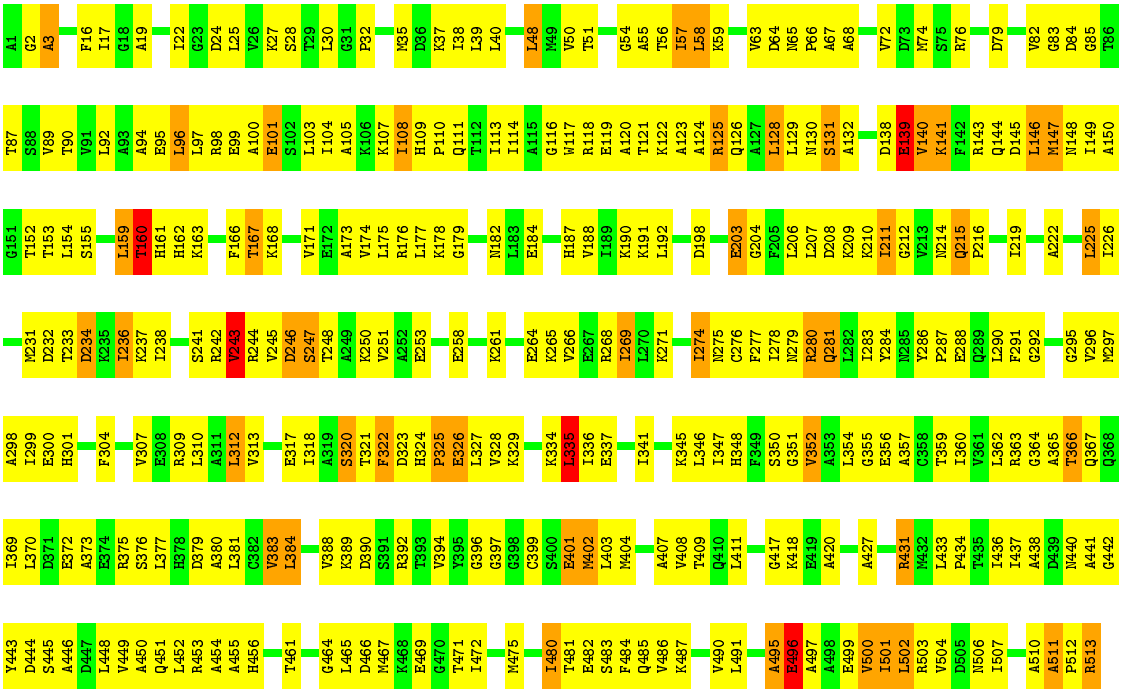




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

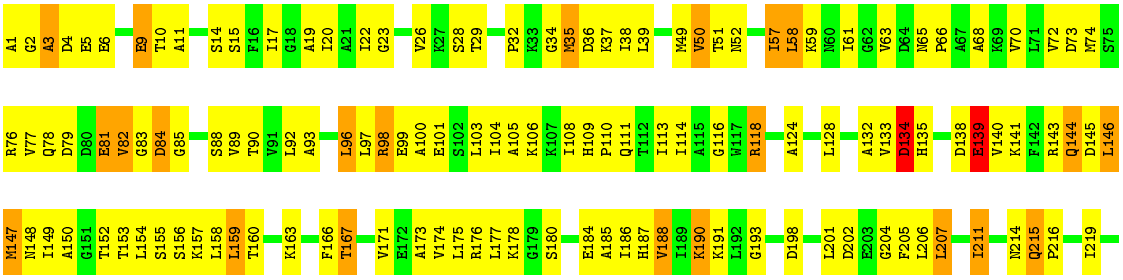
Chain C:

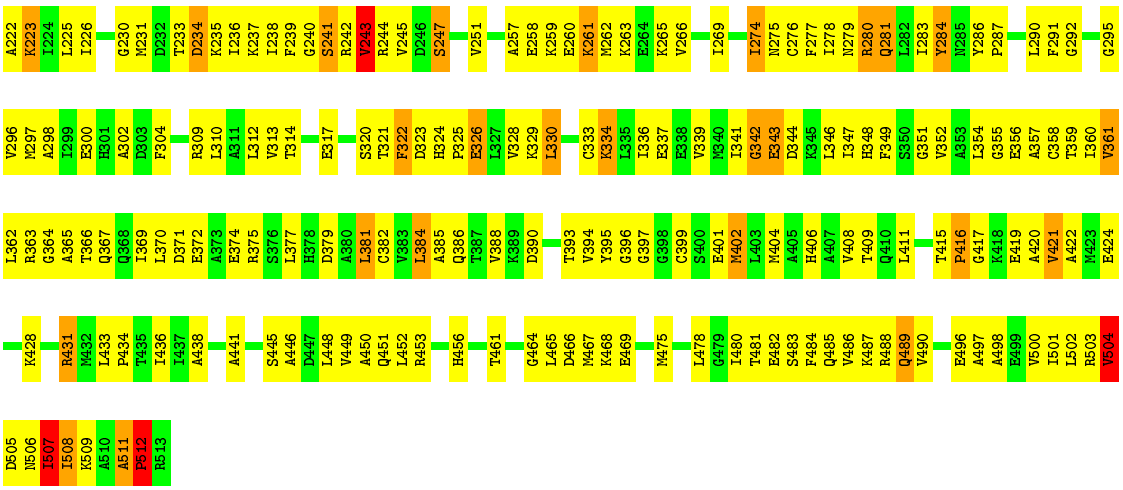




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

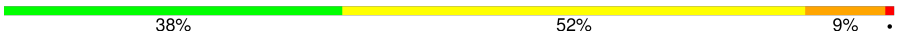
Chain D:

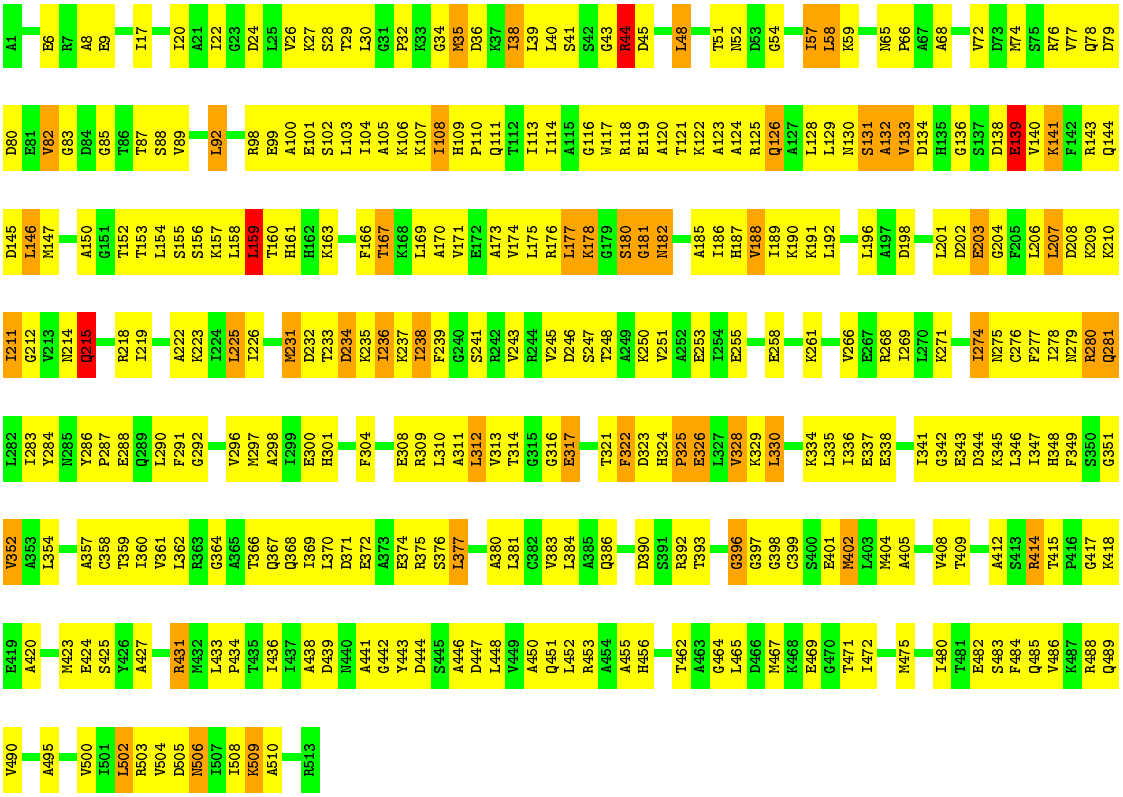




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

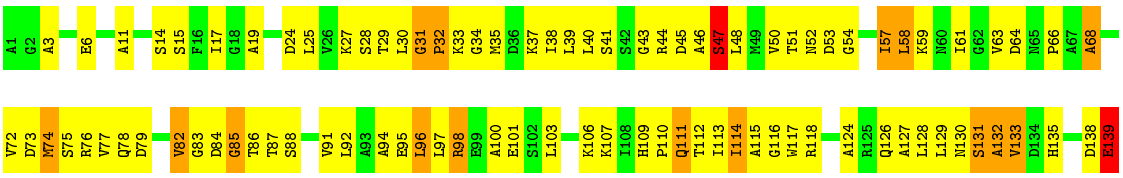
Chain E:

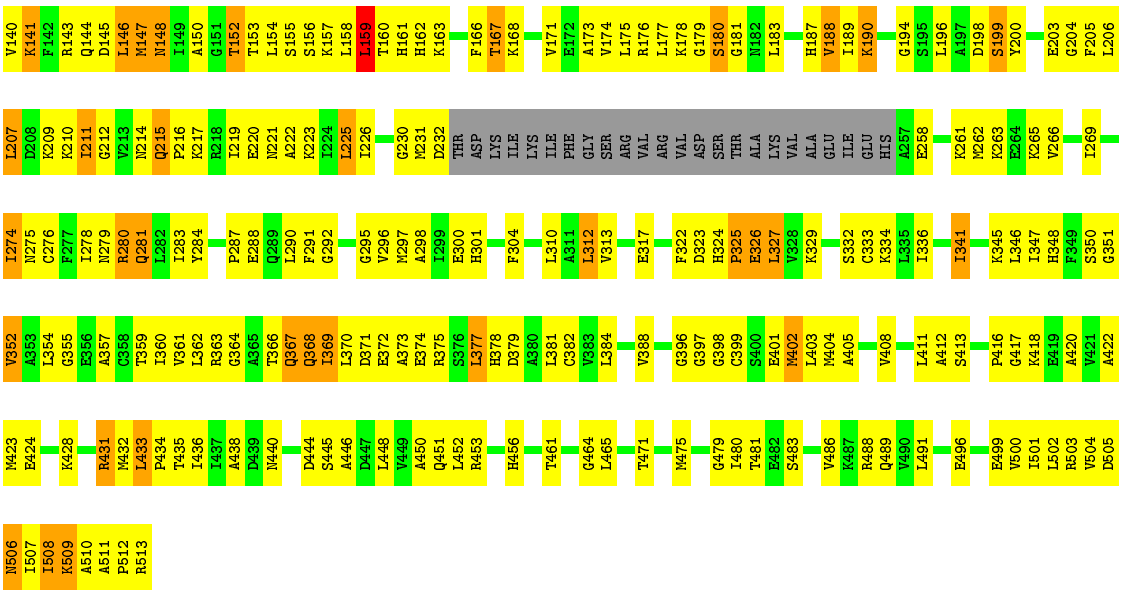




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

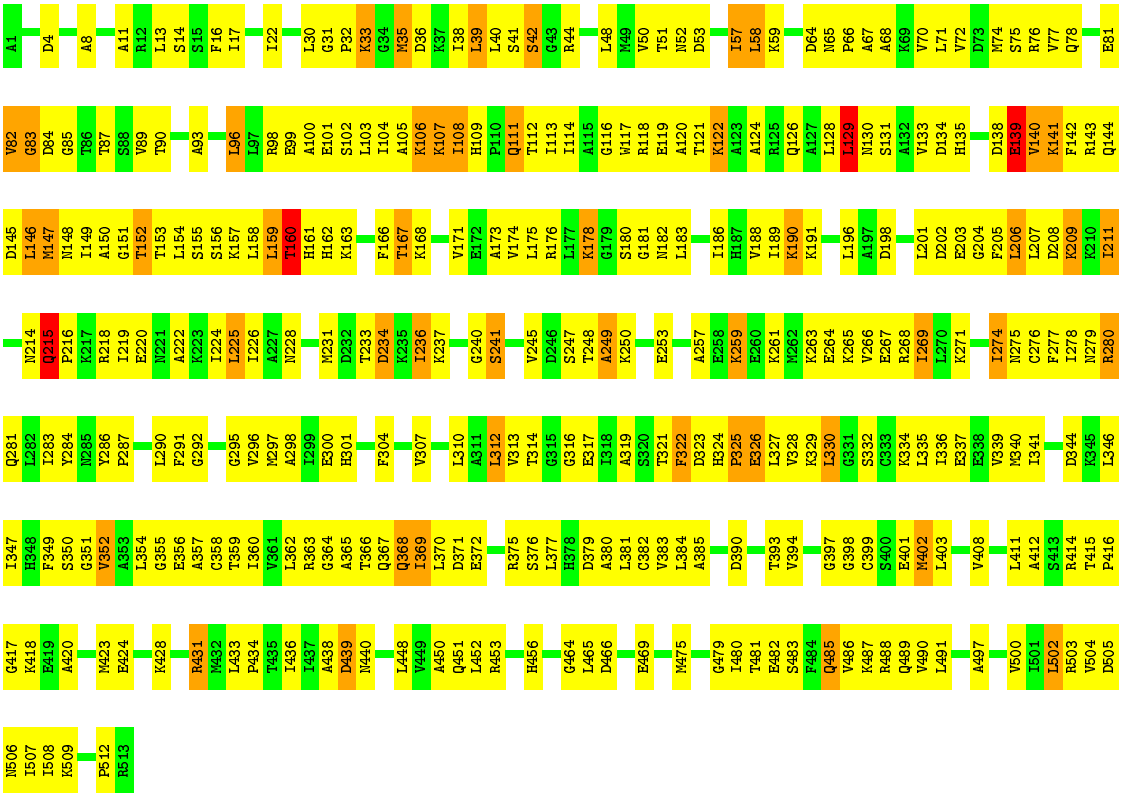
Chain F:





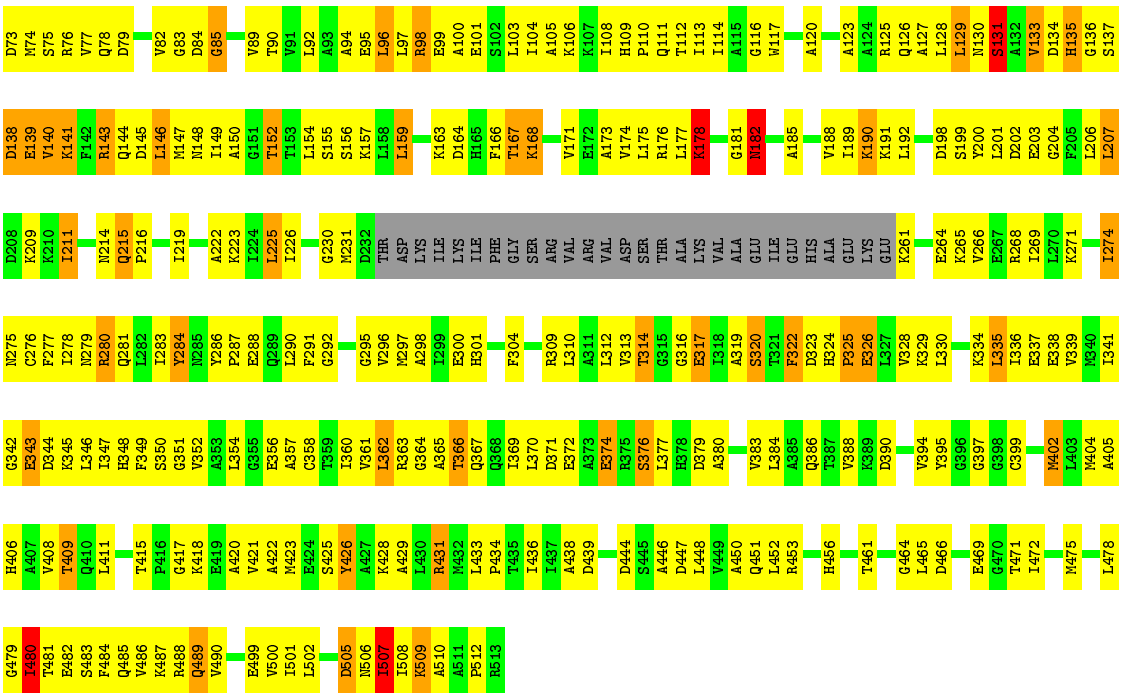
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain G:



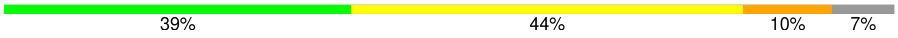
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

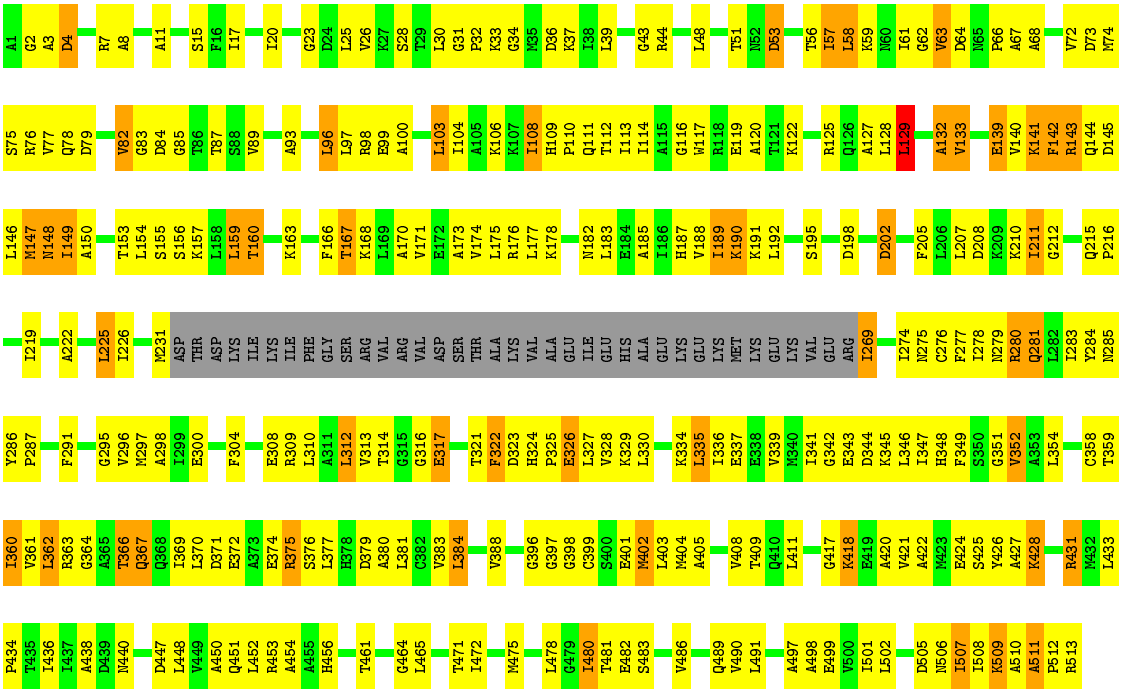
Chain H:



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

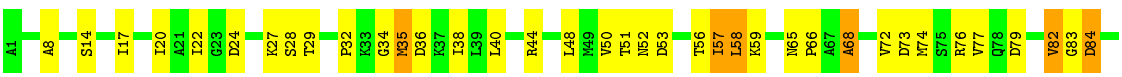
Chain I:

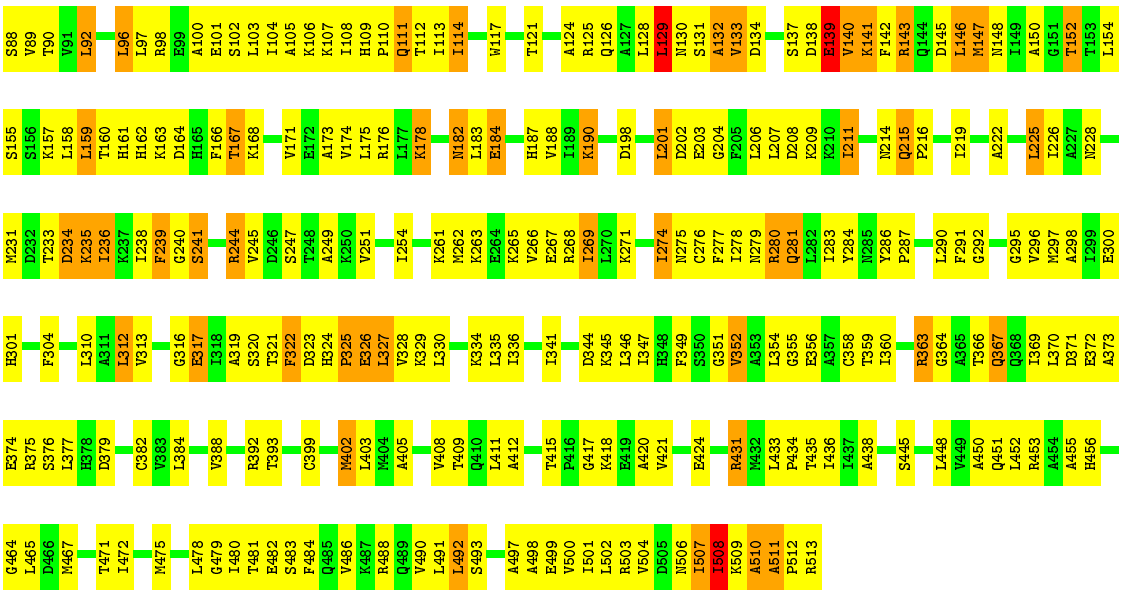




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

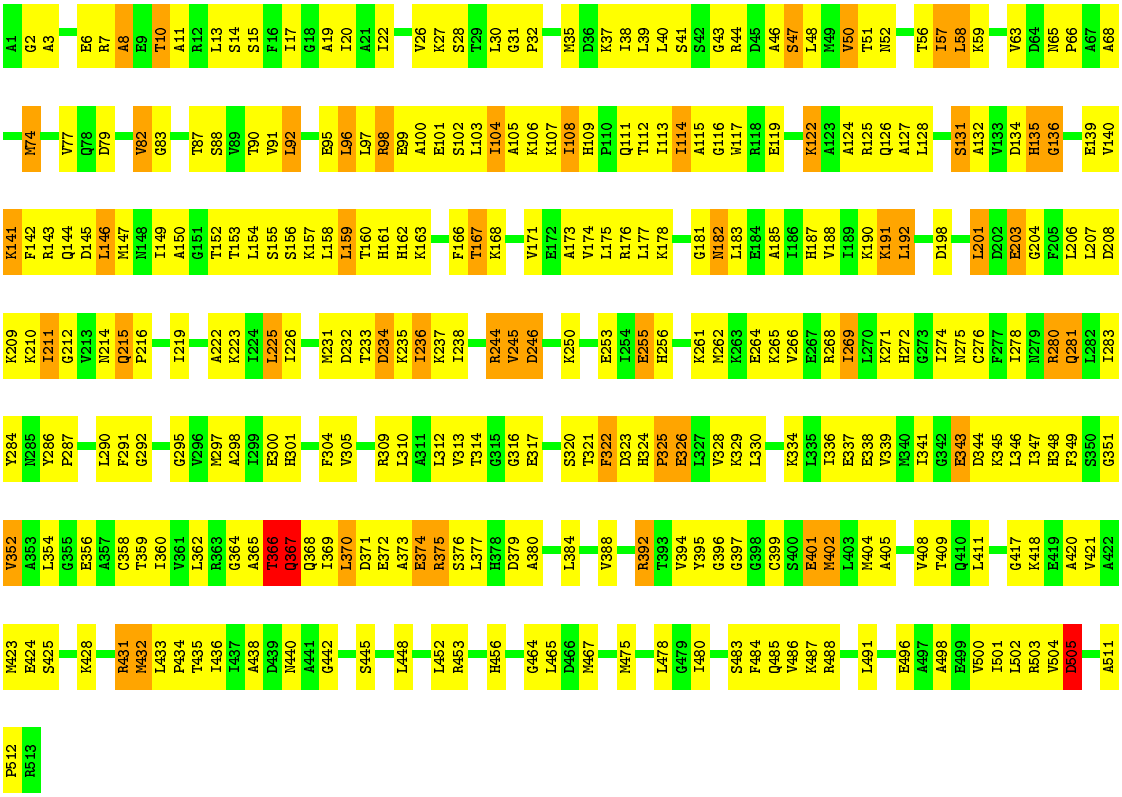
Chain J:





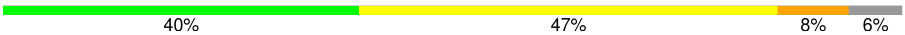
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

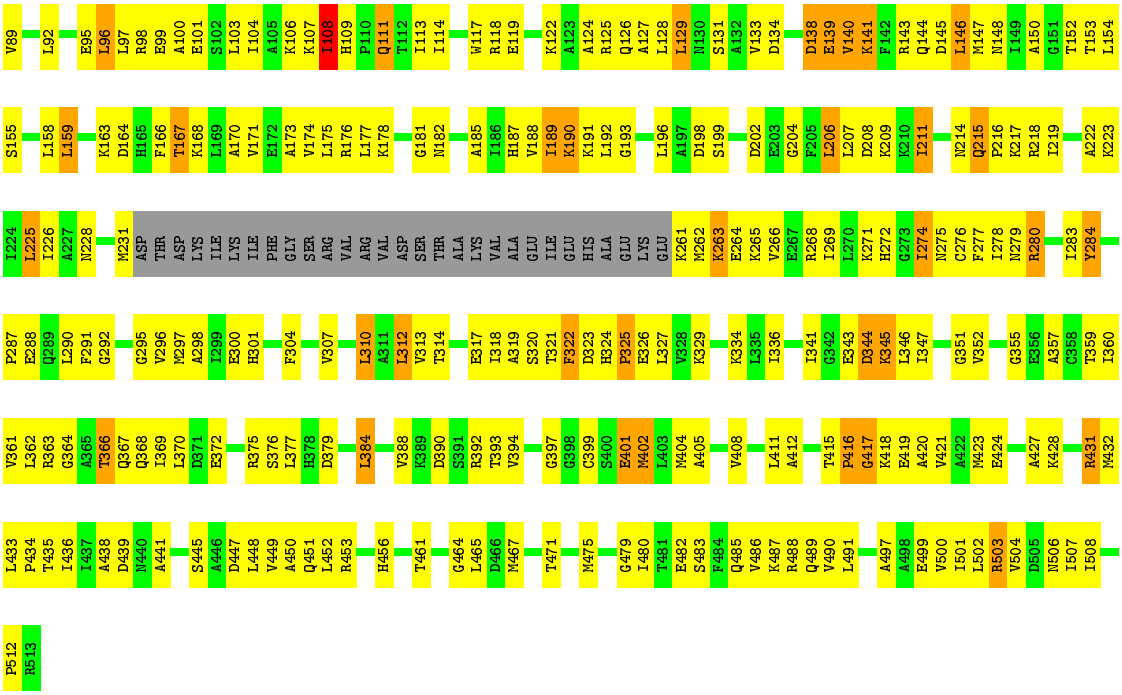
Chain K:



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

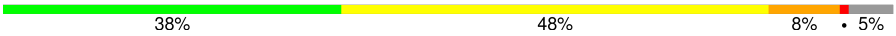
Chain L:

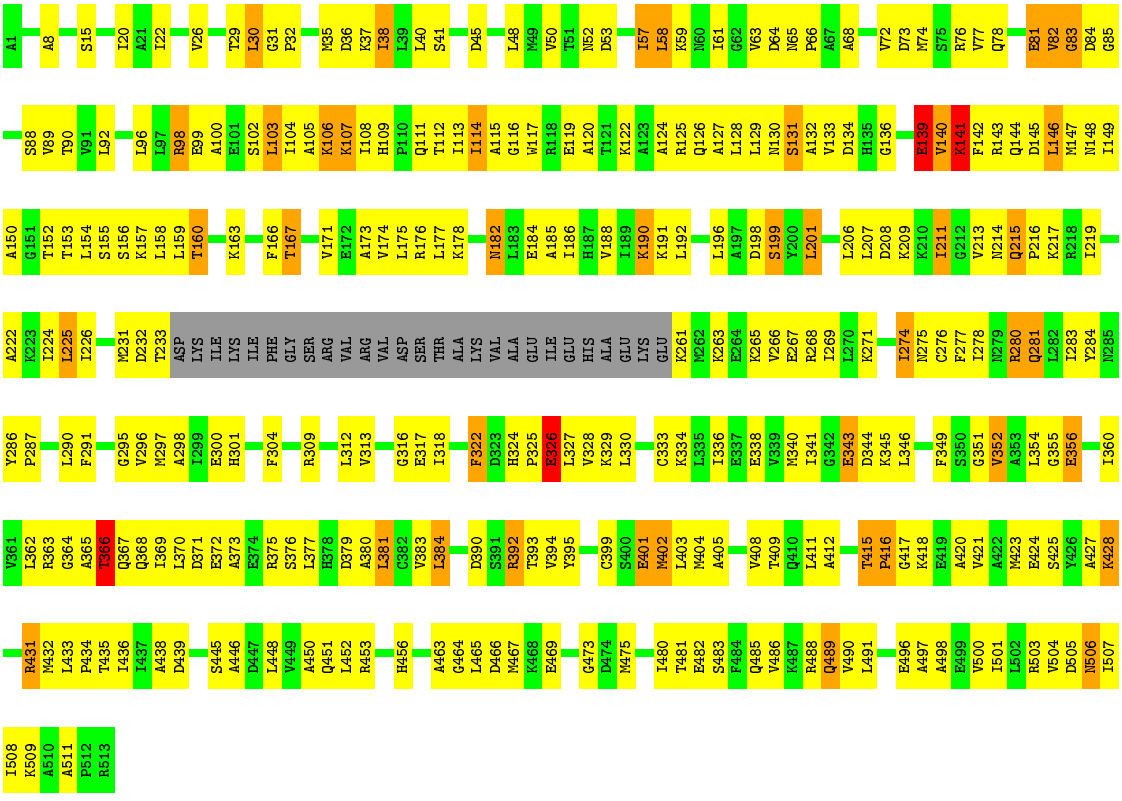




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

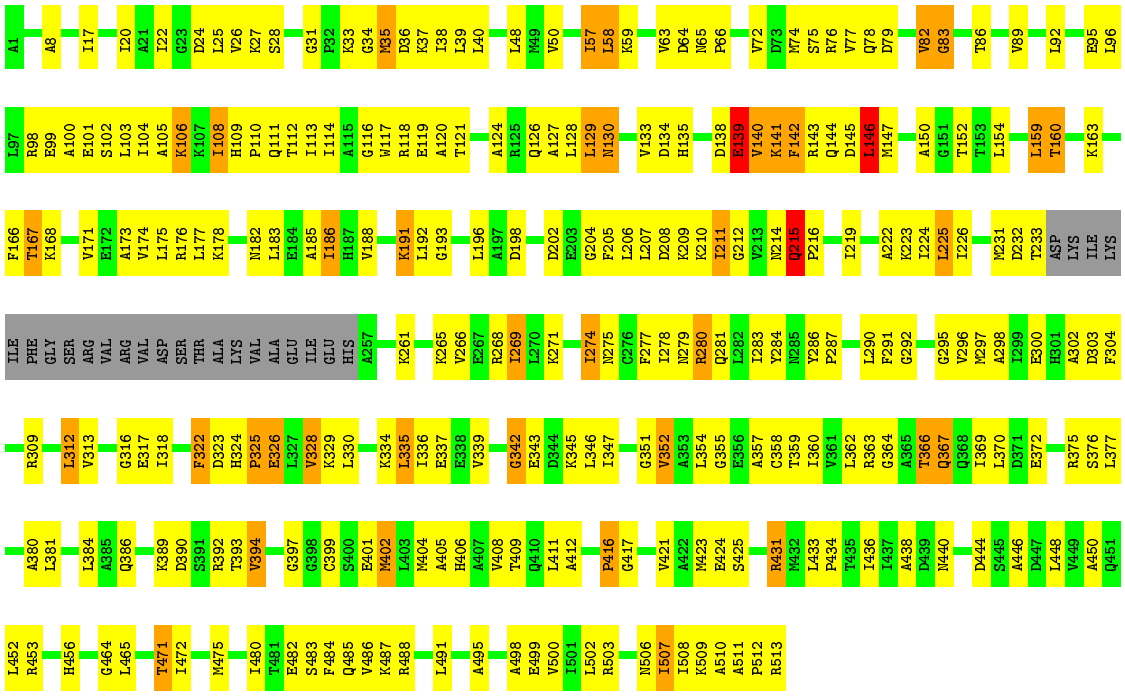
Chain M:





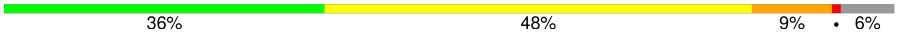
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

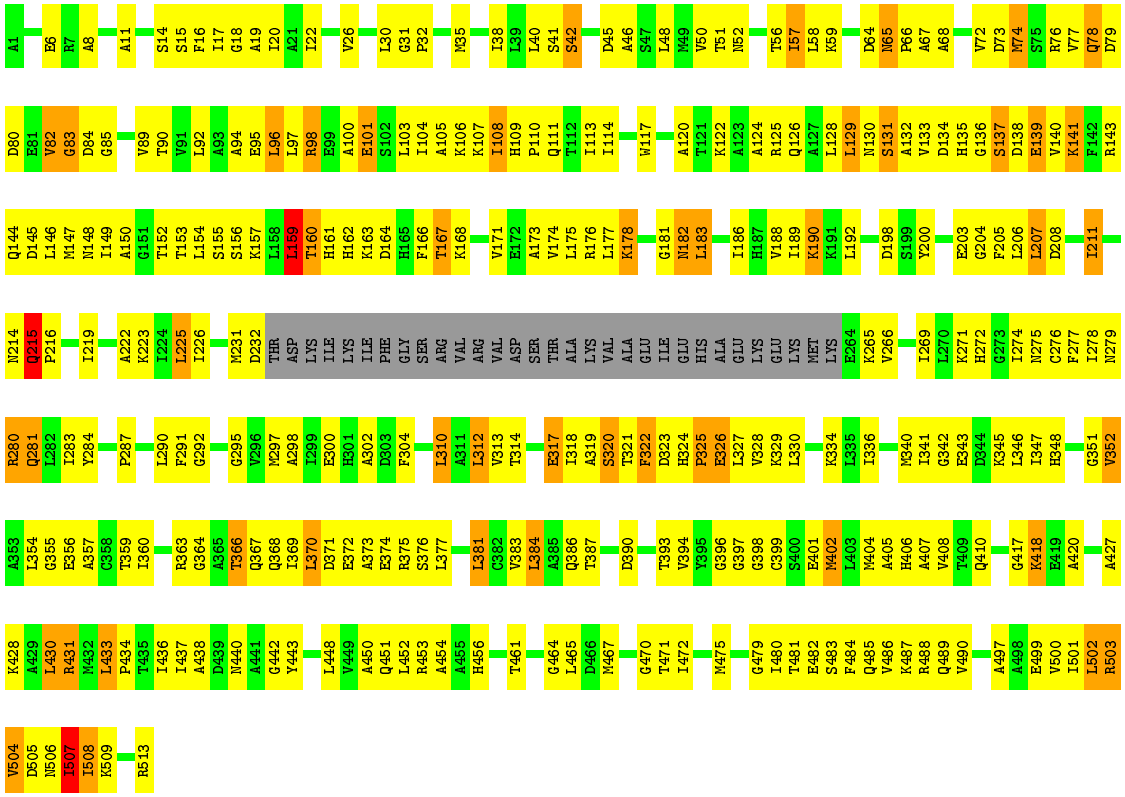
Chain N:



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

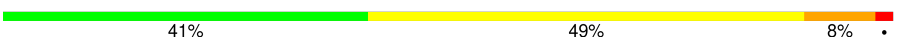
Chain O:

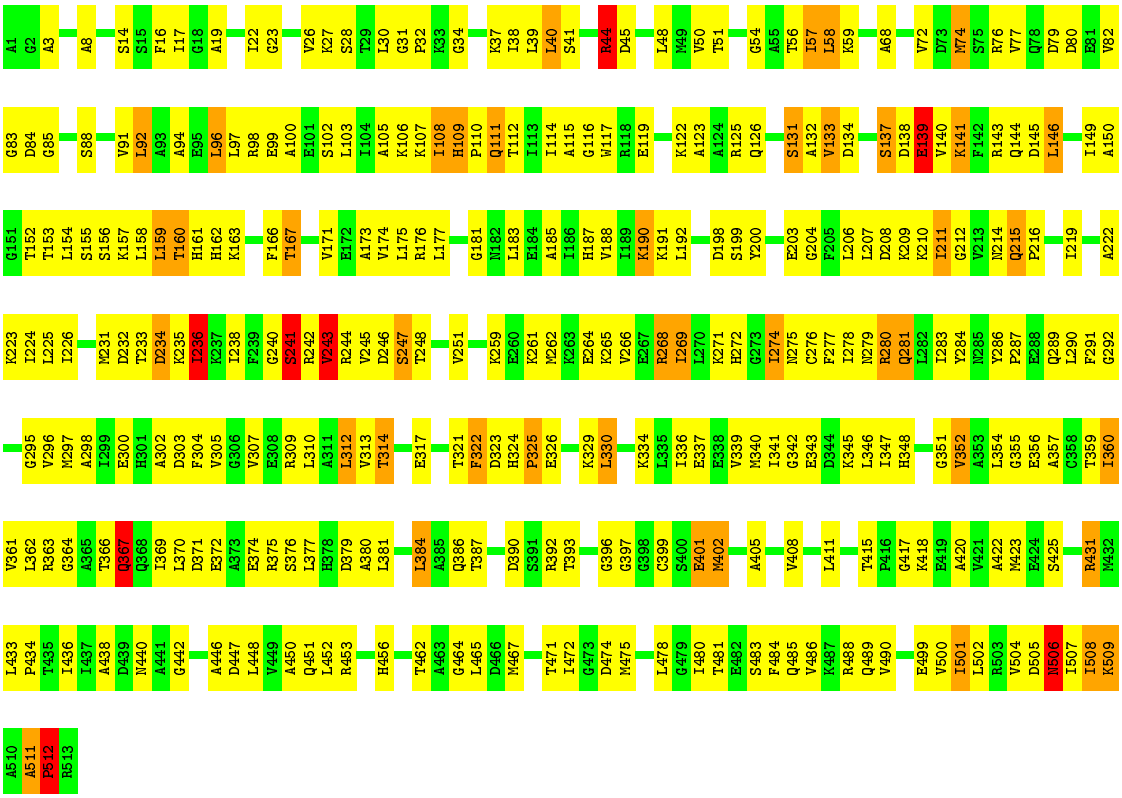




• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain P:




A1 G2 A3 A8 S14 S15 F16 I17 G18 A19 I22 G23 V26 K27 S28 T29 I30 G31 P32 K33 G34 K37 I38 L39 L40 S41 R44 D45 L48 M49 V50 T51 G54 A55 T56 I57 L58 K59 A68 V72 D73 M74 S75 R76 V77 Q78 D79 D80 E81 V82
G83 D84 G85 S88 V91 L92 A93 A94 E95 L96 L97 R98 E99 A100 E101 S102 L103 I104 A105 K106 K107 I108 H109 P110 Q111 T112 I113 I114 A115 G116 W117 R118 E119 K122 A123 A124 R125 Q126 S131 A132 V133 D134 S137 D138 E139 V140 K141 F142 R143 Q144 D145 L146 I149 A150
G151 T152 T153 L154 S155 S156 K157 L158 L159 T160 H161 H162 K163 F166 T167 V171 E172 A173 V174 L175 R176 L177 G181 N182 L183 E184 A185 I186 H187 V188 I189 K190 K191 L192 D198 S199 Y200 E203 G204 F205 L206 L207 D208 K209 K210 I211 G212 V213 N214 Q215 P216 I219 A222
K223 I224 L225 I226 M231 D232 T233 D234 K235 I236 K237 I238 F239 G240 S241 R242 V243 R244 V245 D246 S247 T248 V251 K259 E260 K261 M262 K263 E264 K265 V266 E267 R268 I269 L270 K271 H272 G273 I274 N275 C276 F277 I278 N279 R280 Q281 L282 I283 Y284 N285 Y286 P287 E288 Q289 L290 F291 G292
G295 V296 M297 A298 I299 E300 H301 A302 D303 F304 V305 G306 V307 E308 R309 L310 A311 L312 V313 T314 E317 T321 F322 D323 H324 P325 E326 K329 L330 K334 L335 I336 E337 E338 V339 M340 I341 G342 E343 D344 K345 L346 I347 H348 G351 V352 A353 L354 G355 E356 A357 C358 T359 I360
V361 L362 R363 G364 A365 T366 Q367 Q368 I369 L370 D371 E372 A373 E374 R375 S376 L377 H378 D379 A380 L381 I384 A385 Q386 T387 D390 S391 R392 T393 G396 G397 G398 C399 S400 E401 M402 A405 V408 L411 T415 P416 G417 K418 E419 A420 V421 A422 M423 E424 S425 R431 M432
L433 P434 T435 I436 I437 A438 D439 N440 A441 G442 A446 D447 L448 V449 A450 Q451 L452 R453 H456 T462 A463 G464 L465 D466 M467 T471 I472 G473 D474 M475 L478 G479 I480 T481 E482 S483 F484 Q485 V486 K487 R488 Q489 V490 E499 V500 I501 L502 R503 V504 D505 N506 I507 I508 K509
A510 A511 P512 R513

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.45	0/3732	0.80	2/5028 (0.0%)
1	B	0.46	0/3664	0.75	1/4937 (0.0%)
1	C	0.45	0/3896	0.76	0/5249
1	D	0.46	0/3896	0.78	1/5249 (0.0%)
1	E	0.45	0/3896	0.78	1/5249 (0.0%)
1	F	0.46	0/3704	0.76	1/4990 (0.0%)
1	G	0.47	0/3896	0.78	1/5249 (0.0%)
1	H	0.45	0/3672	0.77	0/4948
1	I	0.46	0/3593	0.77	1/4846 (0.0%)
1	J	0.44	0/3896	0.78	0/5249
1	K	0.46	0/3896	0.77	1/5249 (0.0%)
1	L	0.45	0/3664	0.74	0/4937
1	M	0.44	0/3679	0.75	1/4958 (0.0%)
1	N	0.44	0/3711	0.73	0/5000
1	O	0.46	0/3646	0.78	1/4916 (0.0%)
1	P	0.45	0/3896	0.81	3/5249 (0.1%)
All	All	0.45	0/60337	0.77	14/81303 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	44	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	P	44	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	P	268	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	M	392	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	I	63	VAL	CB-CA-C	-5.92	100.16	111.40

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	3693	0	3795	393	0
1	B	3626	0	3737	373	0
1	C	3855	0	3970	369	0
1	D	3855	0	3970	358	0
1	E	3855	0	3970	373	0
1	F	3666	0	3771	378	0
1	G	3855	0	3970	396	0
1	H	3634	0	3741	375	0
1	I	3555	0	3655	334	0
1	J	3855	0	3970	337	0
1	K	3855	0	3970	380	0
1	L	3626	0	3737	337	0
1	M	3641	0	3748	339	0
1	N	3673	0	3778	301	0
1	O	3608	0	3706	379	0
1	P	3855	0	3970	382	0
All	All	59707	0	61458	5516	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 46.

The worst 5 of 5516 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:C:450:ALA:HB2	1:L:418:LYS:HG2	1.30	1.13
1:B:146:LEU:HD12	1:B:171:VAL:HG13	1.31	1.12
1:K:146:LEU:HD12	1:K:171:VAL:HG13	1.30	1.11
1:M:82:VAL:HG21	1:M:486:VAL:HG12	1.29	1.10
1:A:159:LEU:HD12	1:A:369:ILE:HG23	1.33	1.09

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	488/513 (95%)	432 (88%)	24 (5%)	32 (7%)	1	24
1	B	480/513 (94%)	430 (90%)	23 (5%)	27 (6%)	2	28
1	C	511/513 (100%)	456 (89%)	25 (5%)	30 (6%)	2	27
1	D	511/513 (100%)	456 (89%)	25 (5%)	30 (6%)	2	27
1	E	511/513 (100%)	458 (90%)	24 (5%)	29 (6%)	2	28
1	F	485/513 (94%)	429 (88%)	31 (6%)	25 (5%)	2	30
1	G	511/513 (100%)	456 (89%)	29 (6%)	26 (5%)	2	30
1	H	481/513 (94%)	427 (89%)	25 (5%)	29 (6%)	2	26
1	I	472/513 (92%)	433 (92%)	15 (3%)	24 (5%)	2	30
1	J	511/513 (100%)	457 (89%)	26 (5%)	28 (6%)	2	29
1	K	511/513 (100%)	462 (90%)	23 (4%)	26 (5%)	2	30
1	L	480/513 (94%)	437 (91%)	22 (5%)	21 (4%)	3	33
1	M	482/513 (94%)	437 (91%)	23 (5%)	22 (5%)	3	33
1	N	486/513 (95%)	439 (90%)	27 (6%)	20 (4%)	3	35
1	O	478/513 (93%)	427 (89%)	27 (6%)	24 (5%)	3	31
1	P	511/513 (100%)	453 (89%)	29 (6%)	29 (6%)	2	28
All	All	7909/8208 (96%)	7089 (90%)	398 (5%)	422 (5%)	4	29

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	37	LYS
1	A	68	ALA
1	A	84	ASP
1	A	133	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	391/409 (96%)	341 (87%)	50 (13%)	5 29
1	B	384/409 (94%)	343 (89%)	41 (11%)	8 36
1	C	409/409 (100%)	362 (88%)	47 (12%)	7 32
1	D	409/409 (100%)	362 (88%)	47 (12%)	7 32
1	E	409/409 (100%)	359 (88%)	50 (12%)	6 31
1	F	388/409 (95%)	338 (87%)	50 (13%)	5 28
1	G	409/409 (100%)	364 (89%)	45 (11%)	8 34
1	H	385/409 (94%)	340 (88%)	45 (12%)	7 32
1	I	376/409 (92%)	336 (89%)	40 (11%)	8 36
1	J	409/409 (100%)	363 (89%)	46 (11%)	7 33
1	K	409/409 (100%)	366 (90%)	43 (10%)	8 36
1	L	384/409 (94%)	341 (89%)	43 (11%)	7 33
1	M	386/409 (94%)	347 (90%)	39 (10%)	9 38
1	N	389/409 (95%)	353 (91%)	36 (9%)	11 42
1	O	382/409 (93%)	343 (90%)	39 (10%)	9 37
1	P	409/409 (100%)	366 (90%)	43 (10%)	8 36
All	All	6328/6544 (97%)	5624 (89%)	704 (11%)	12 34

5 of 704 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	326	GLU
1	I	202	ASP
1	O	352	VAL
1	G	485	GLN
1	H	317	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	182	ASN
1	I	489	GLN
1	O	506	ASN
1	H	367	GLN
1	I	285	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.