



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:14 PM BST

PDB ID : 4A13
EMDB ID: : EMD-1963
Title : model refined against symmetry-free cryo-EM map of TRiC-ADP
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 : 11.30 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>

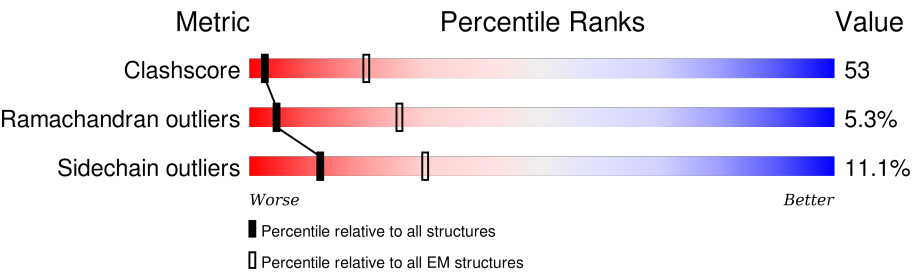
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 11.30 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	513	<div><div>41%</div><div>48%</div><div>10%</div></div>
1	B	513	<div><div>40%</div><div>47%</div><div>7%</div><div>5%</div></div>
1	C	513	<div><div>35%</div><div>53%</div><div>12%</div><div></div></div>
1	D	513	<div><div>36%</div><div>48%</div><div>11%</div><div>5%</div></div>
1	E	513	<div><div>39%</div><div>51%</div><div>8%</div><div></div></div>
1	F	513	<div><div>43%</div><div>48%</div><div>9%</div><div></div></div>
1	G	513	<div><div>32%</div><div>52%</div><div>10%</div><div>5%</div></div>
1	H	513	<div><div>34%</div><div>50%</div><div>10%</div><div>5%</div></div>
1	I	513	<div><div>38%</div><div>53%</div><div>8%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	513	<div><div></div><div>34%51%9%5%</div></div>
1	K	513	<div><div></div><div>34%50%10%••</div></div>
1	L	513	<div><div></div><div>31%56%9%•</div></div>
1	M	513	<div><div></div><div>38%51%10%•</div></div>
1	N	513	<div><div></div><div>32%53%9%5%</div></div>
1	O	513	<div><div></div><div>35%52%11%•</div></div>
1	P	513	<div><div></div><div>39%47%9%•5%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60012 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.

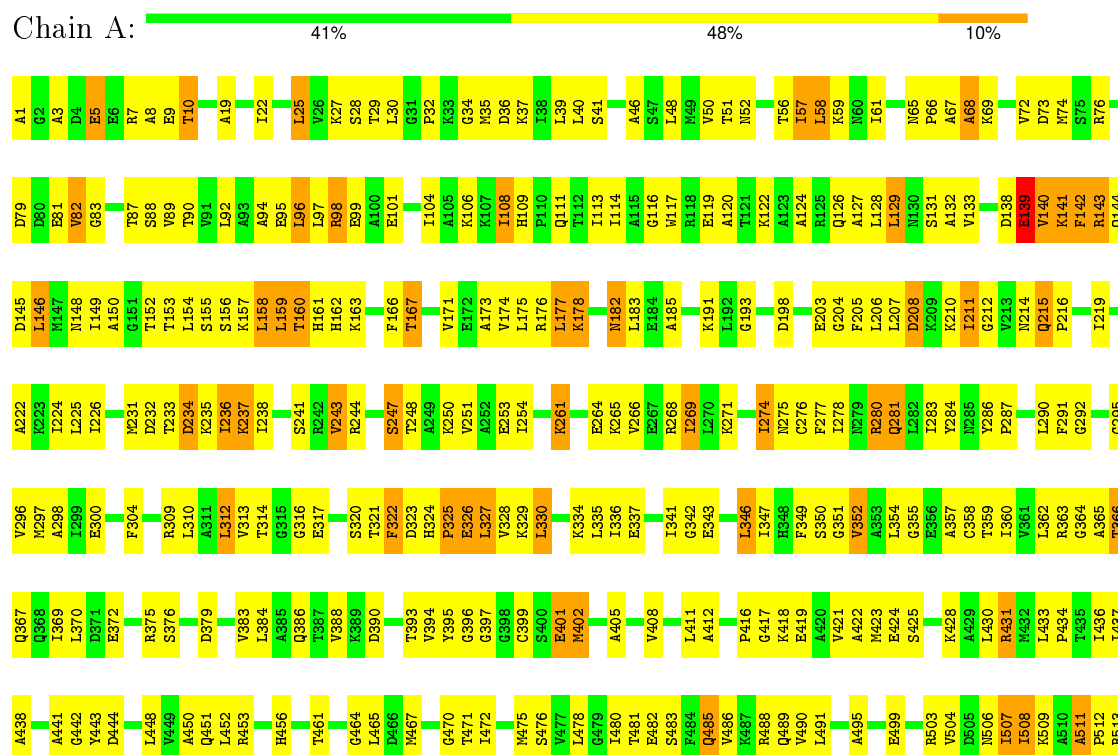
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	B	488	Total	C	N	O	S	0	0
			3666	2293	645	710	18		
1	C	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	D	489	Total	C	N	O	S	0	0
			3675	2298	646	713	18		
1	E	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	F	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	G	487	Total	C	N	O	S	0	0
			3658	2289	643	708	18		
1	H	489	Total	C	N	O	S	0	0
			3675	2298	646	713	18		
1	I	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	J	485	Total	C	N	O	S	0	0
			3634	2272	639	704	19		
1	K	490	Total	C	N	O	S	0	0
			3673	2295	645	714	19		
1	L	494	Total	C	N	O	S	0	0
			3707	2318	652	719	18		
1	M	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	N	488	Total	C	N	O	S	0	0
			3666	2293	645	710	18		
1	O	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	P	489	Total	C	N	O	S	0	0
			3673	2297	646	712	18		

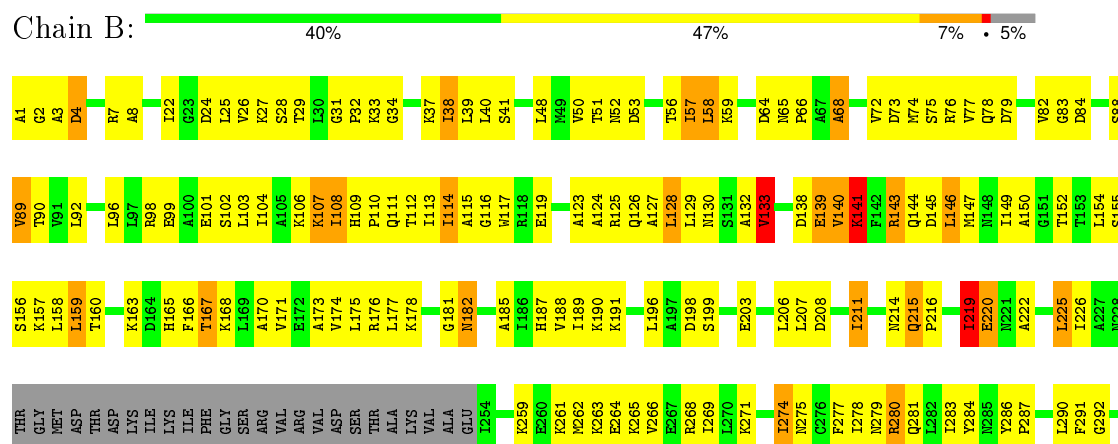
3 Residue-property plots

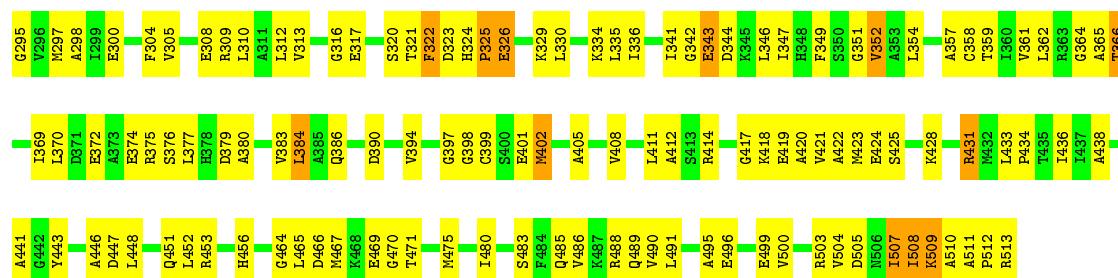
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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



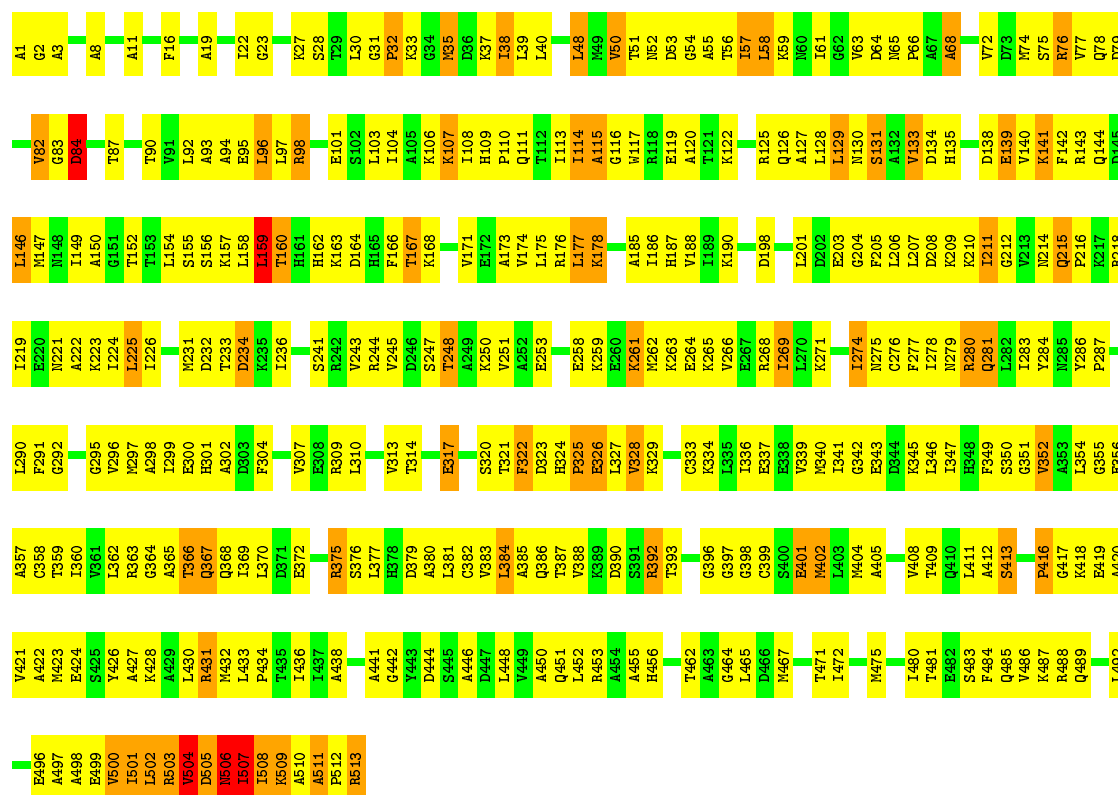
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





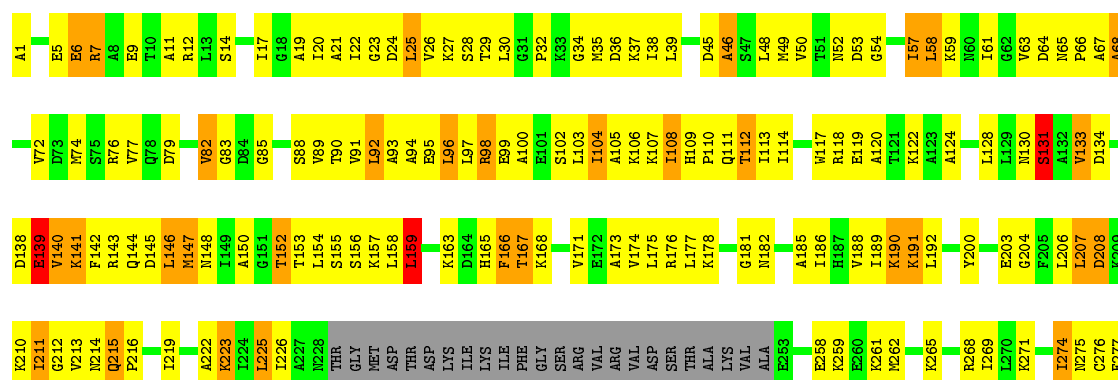
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

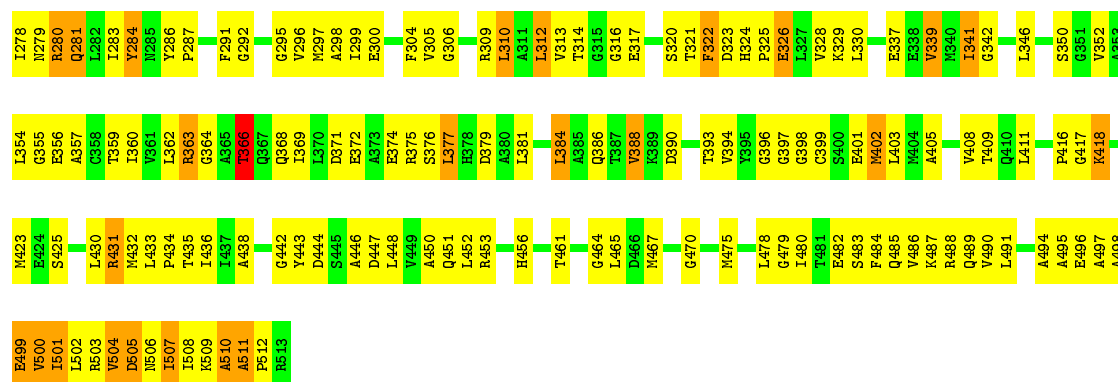
Chain C: 35% 53% 12%



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

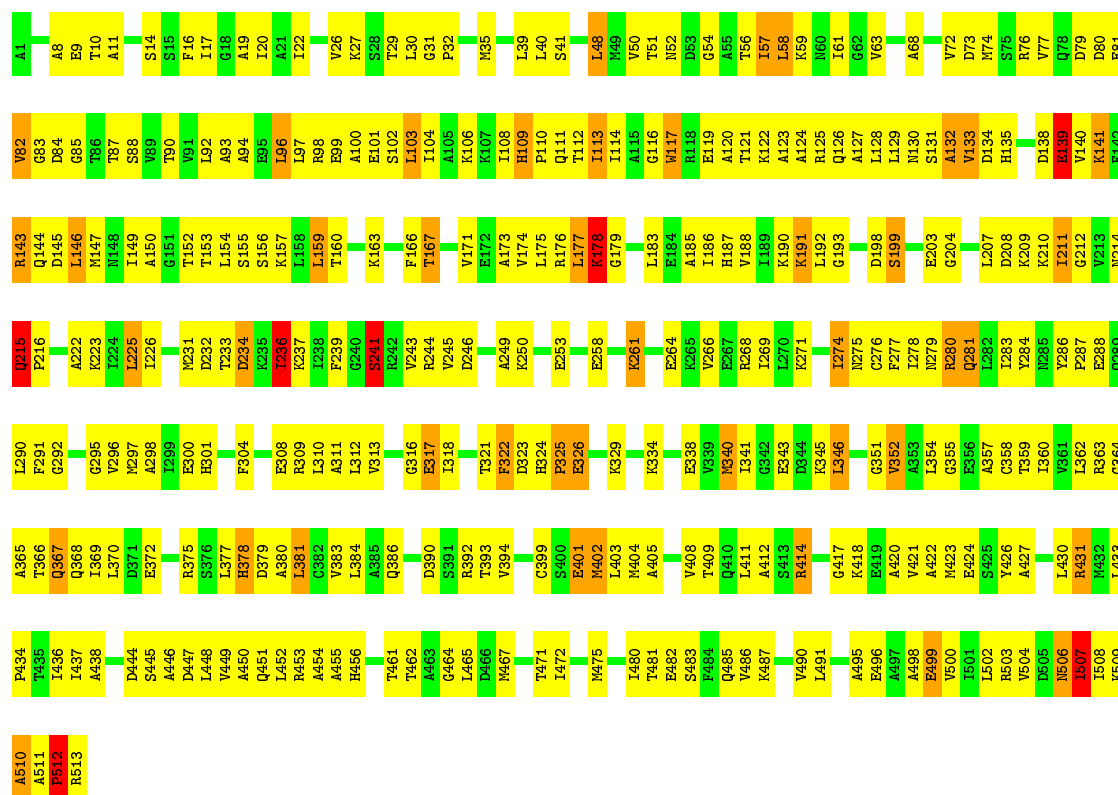
Chain D: 36% 48% 11% 5%





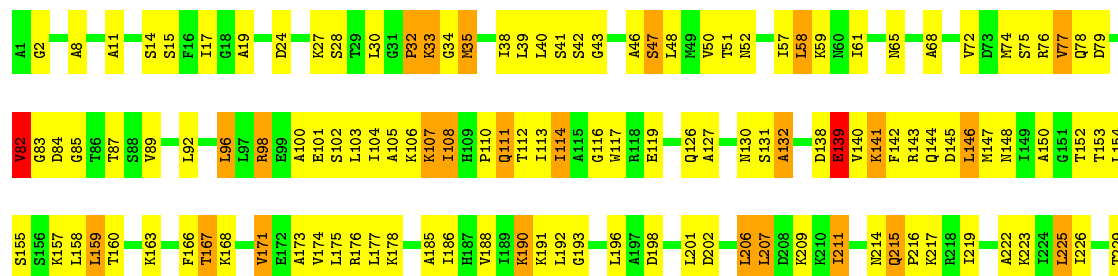
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

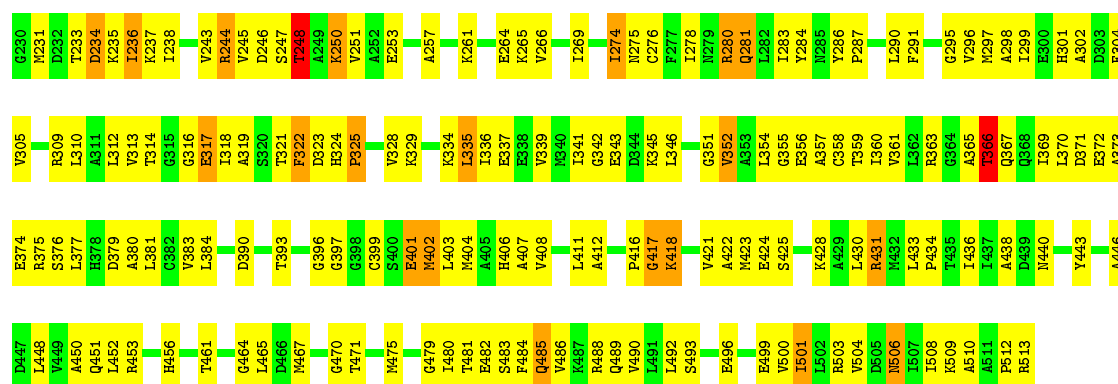
Chain E: 39% 51% 8% •



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

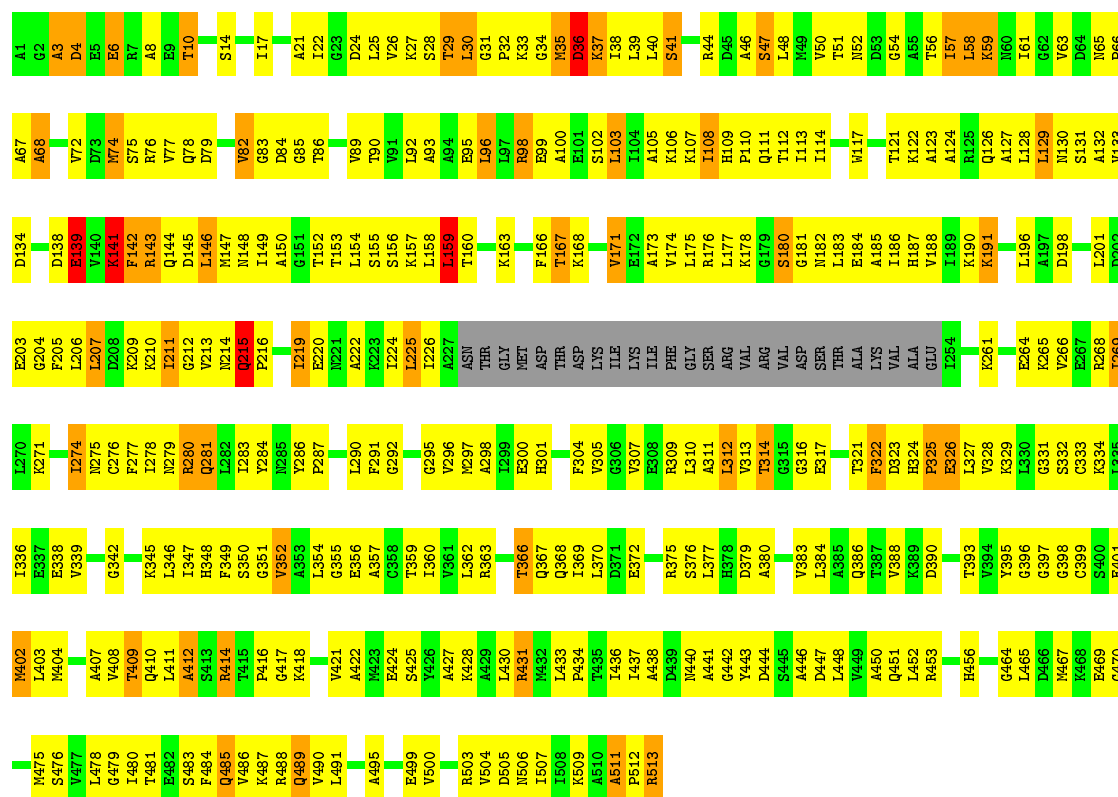
Chain F: 43% 48% 9% •





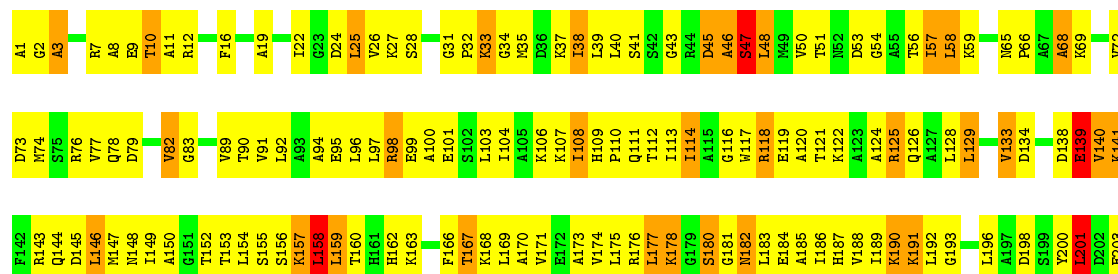
Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

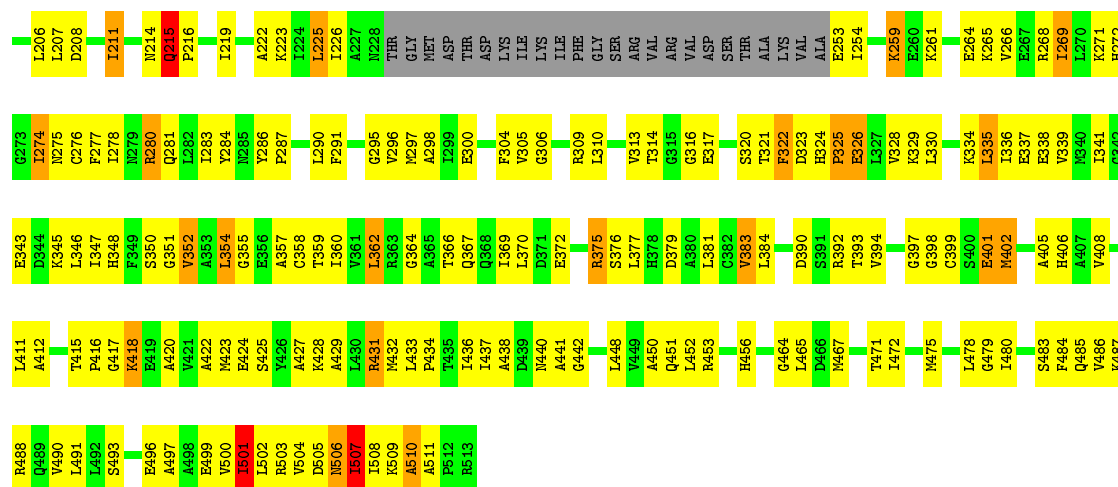
Chain G: 32% 52% 10% 5%



Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

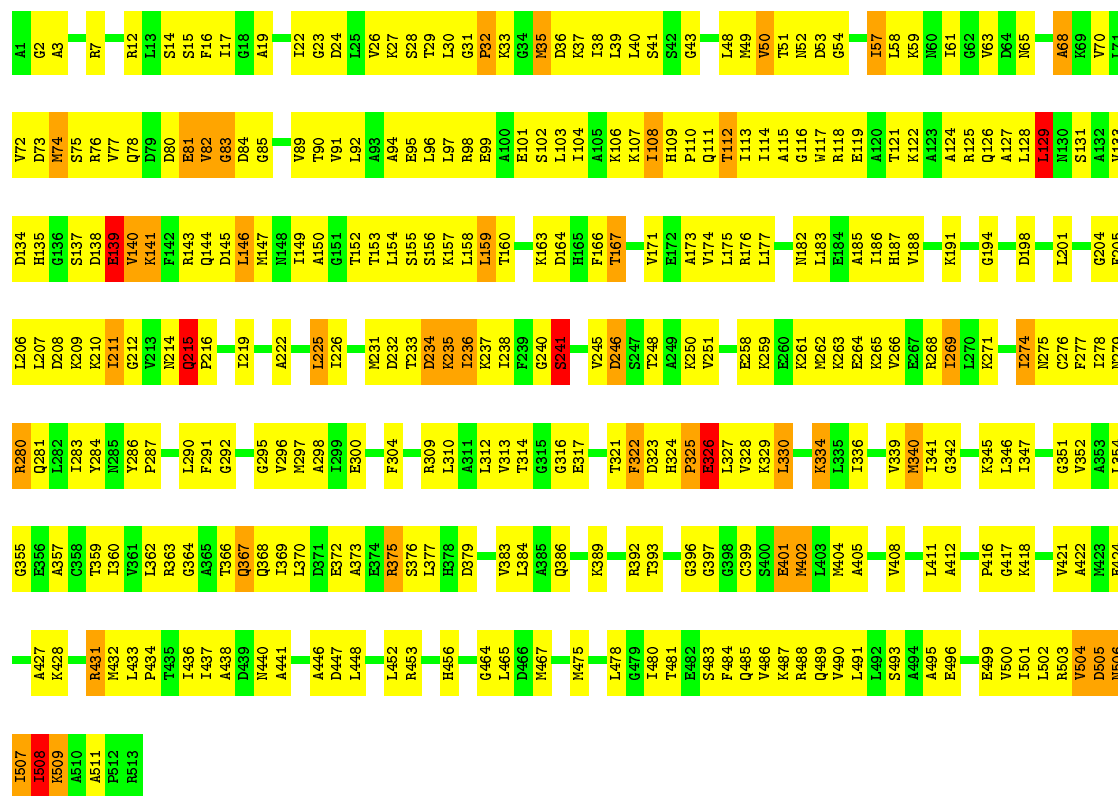
Chain H: 34% 50% 10% 5%





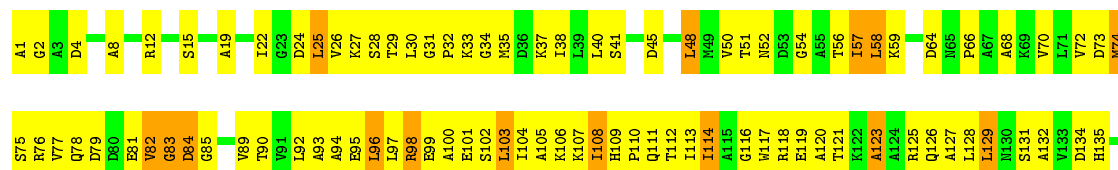
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

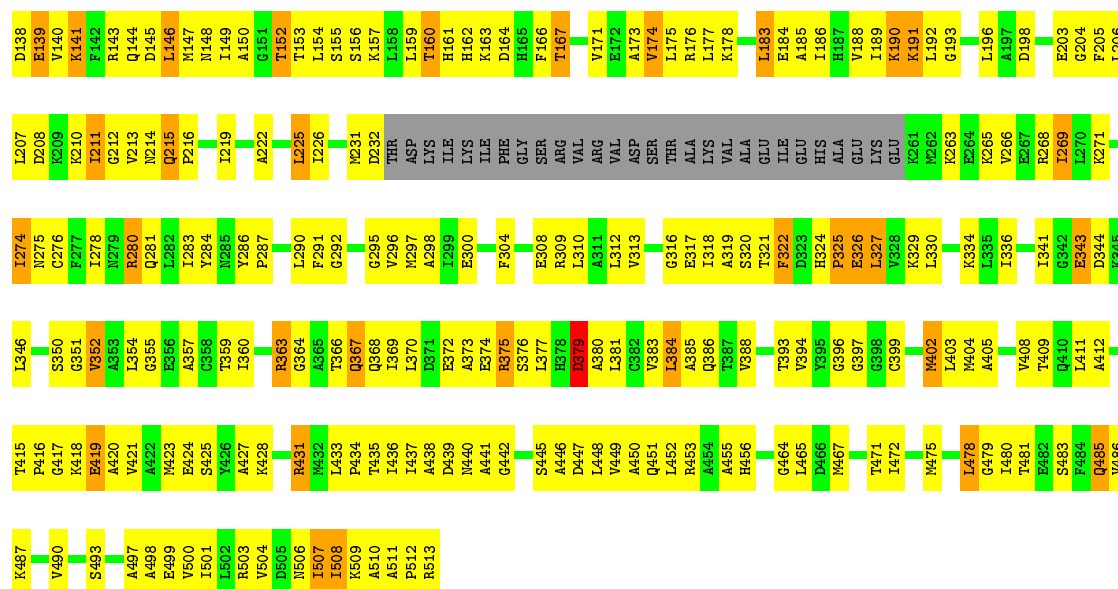
Chain I: 38% 53% 8% •



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

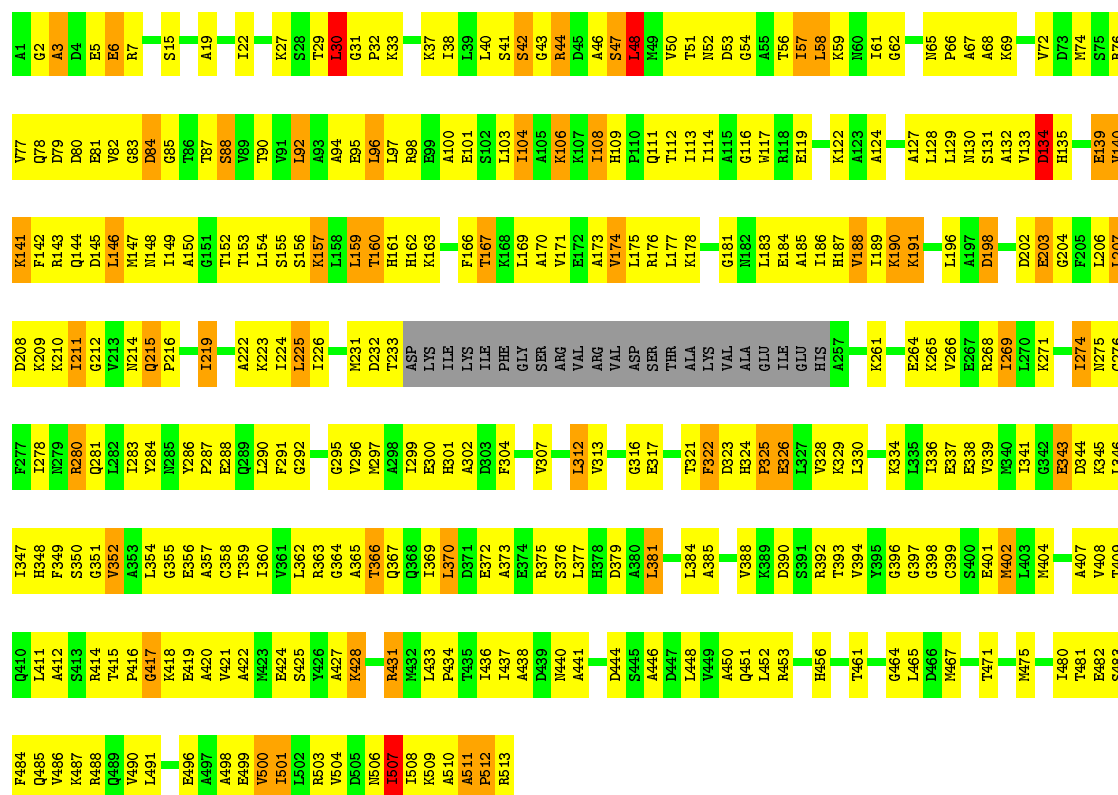
Chain J: 34% 51% 9% 5%





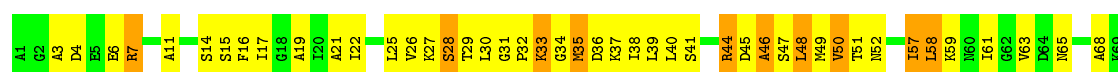
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

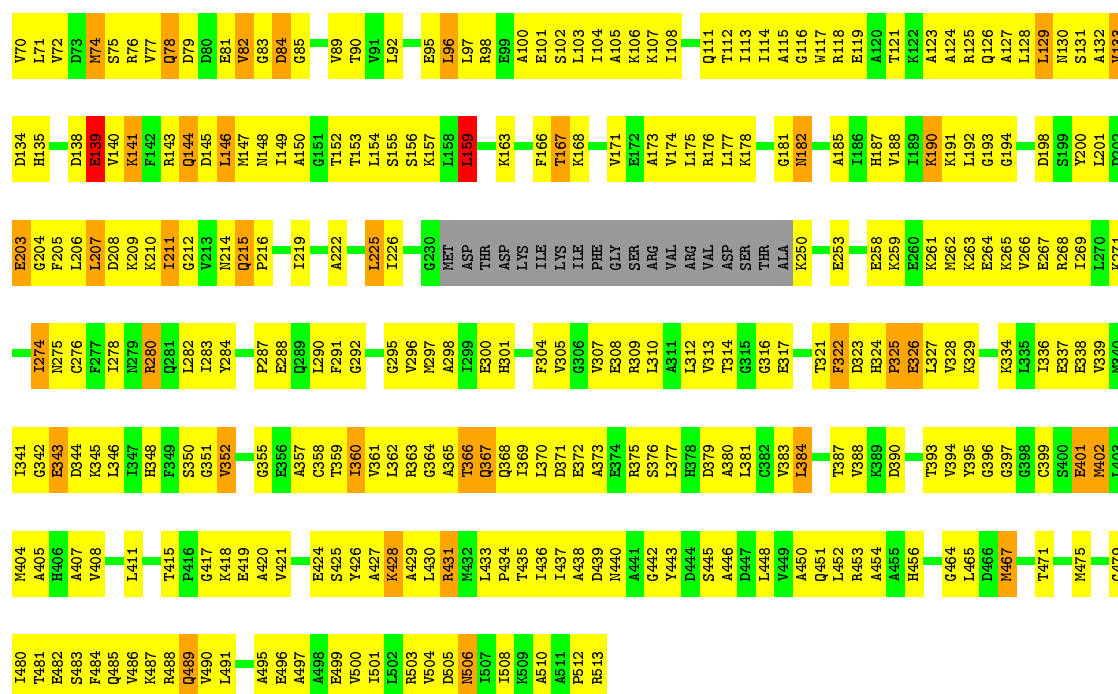
Chain K: 34% 50% 10% . .



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

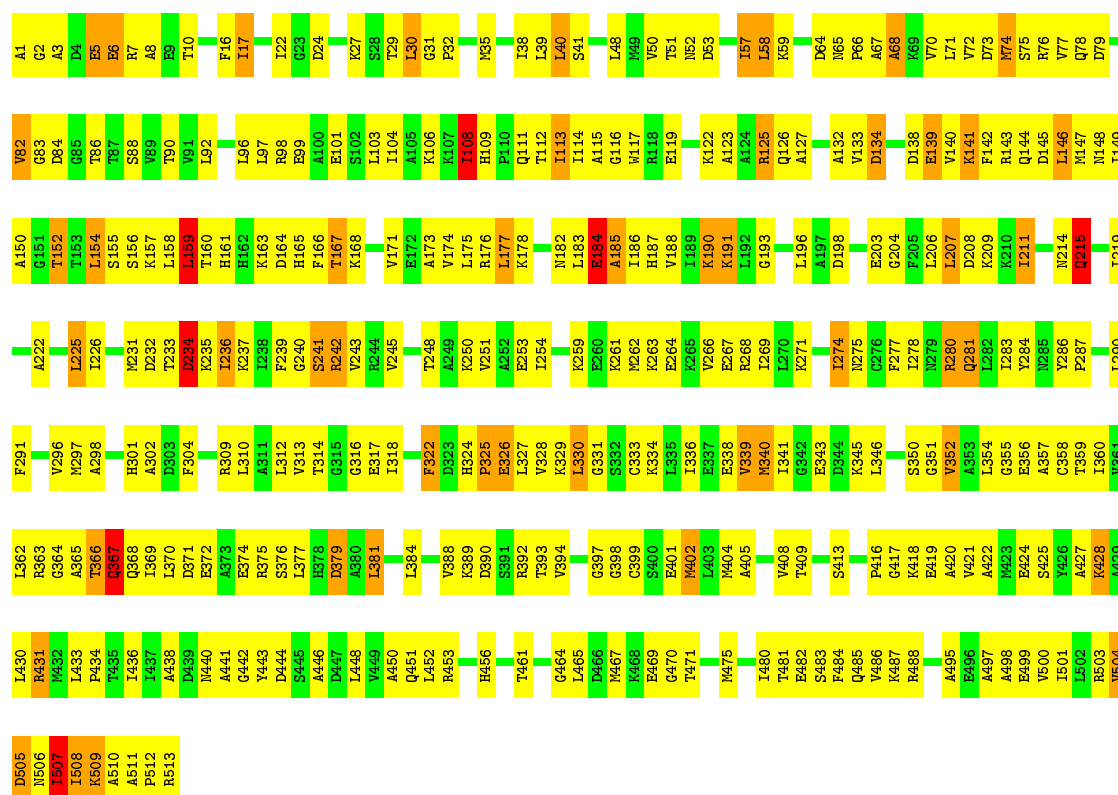
Chain L: 31% 56% 9% .





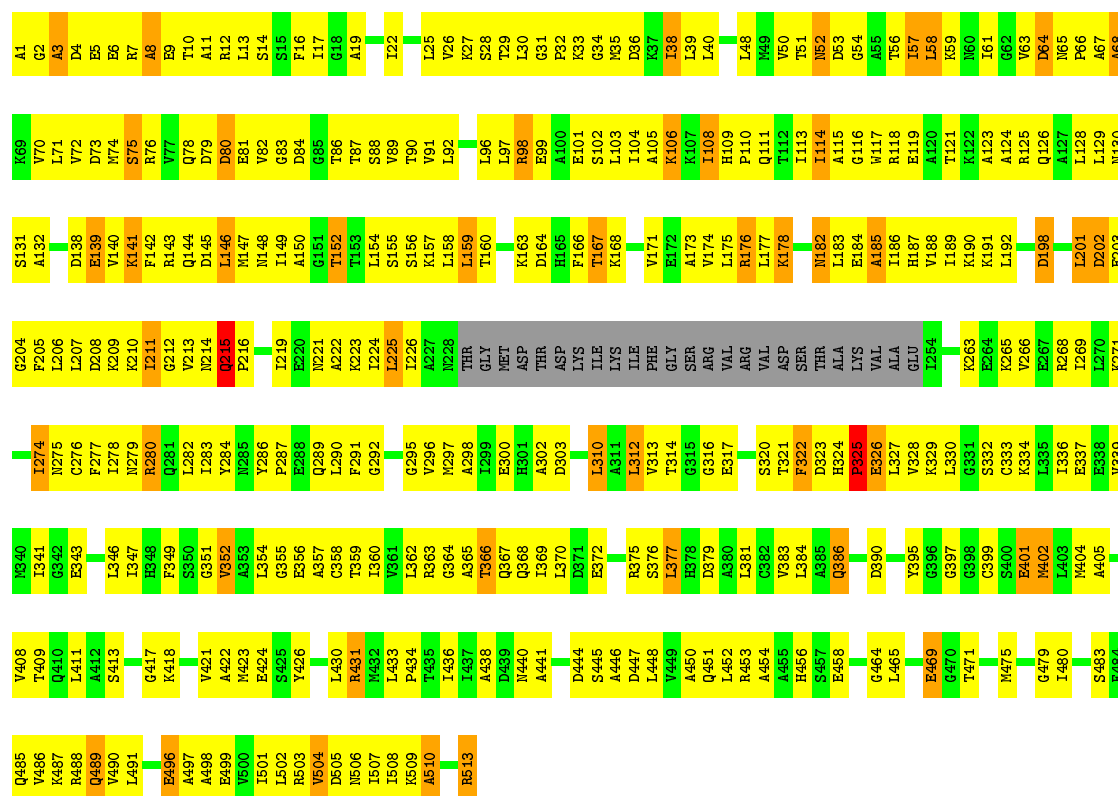
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain M: 38% 51% 10%



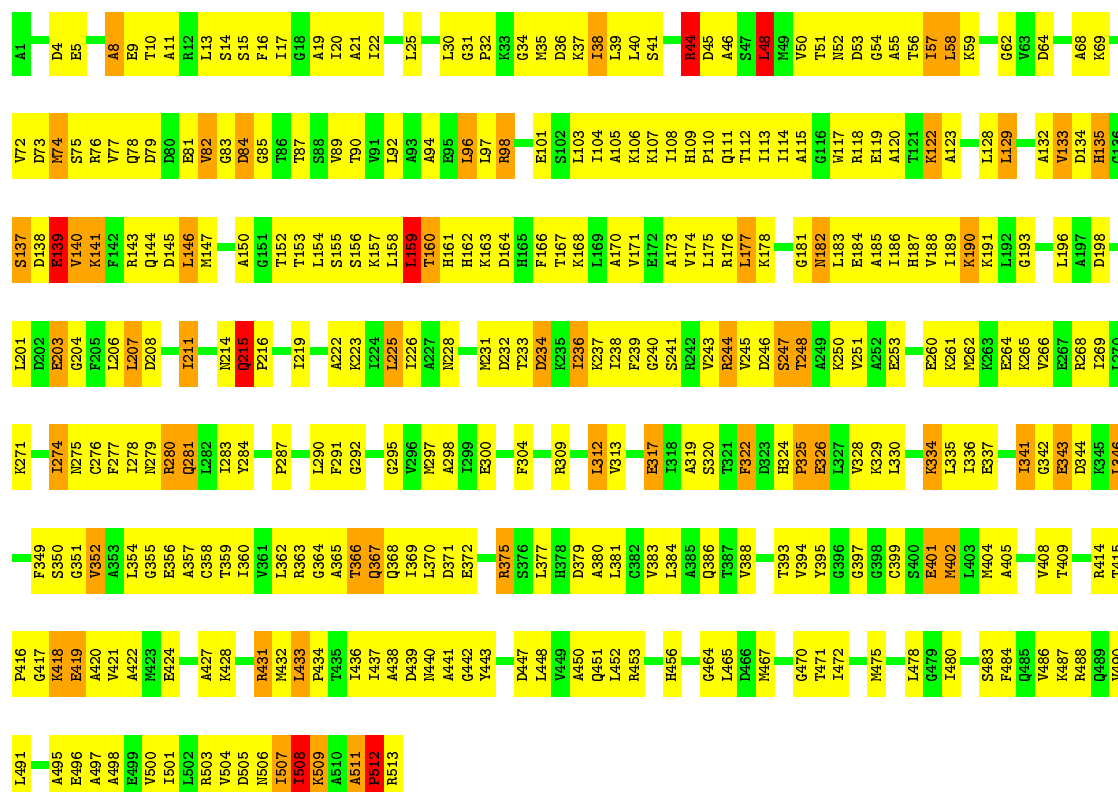
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain N: 32% 53% 9% 5%



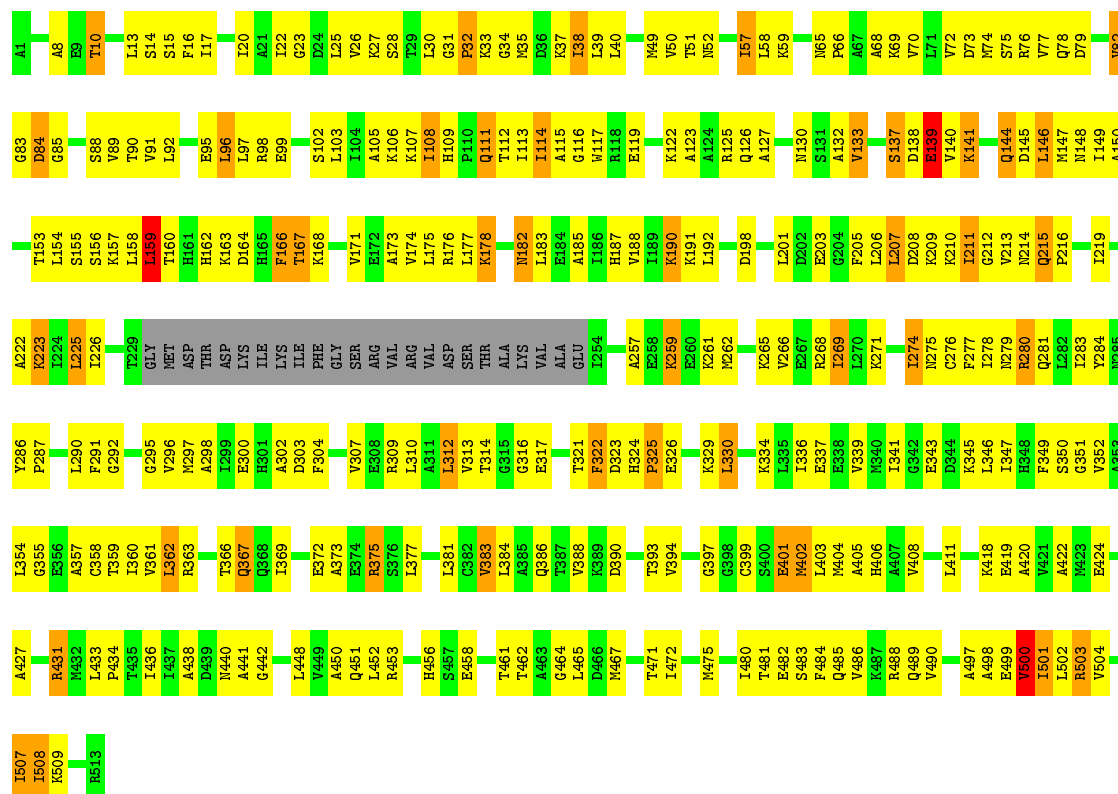
● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain O: 35% 52% 11%



● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain P:  39% 47% 9% 5%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality [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 >2	RMSZ	# Z >2
1	A	0.47	0/3896	0.80	1/5249 (0.0%)
1	B	0.47	0/3705	0.74	0/4992
1	C	0.52	1/3896 (0.0%)	0.84	5/5249 (0.1%)
1	D	0.45	0/3714	0.75	0/5004
1	E	0.47	0/3896	0.80	2/5249 (0.0%)
1	F	0.44	0/3896	0.75	0/5249
1	G	0.47	0/3697	0.78	1/4981 (0.0%)
1	H	0.46	0/3714	0.80	5/5004 (0.1%)
1	I	0.47	0/3896	0.80	0/5249
1	J	0.46	0/3672	0.76	1/4948 (0.0%)
1	K	0.48	0/3711	0.81	2/5000 (0.0%)
1	L	0.47	0/3746	0.80	1/5047 (0.0%)
1	M	0.46	0/3896	0.78	0/5249
1	N	0.46	0/3705	0.79	0/4992
1	O	0.47	0/3896	0.80	3/5249 (0.1%)
1	P	0.47	0/3712	0.80	2/5002 (0.0%)
All	All	0.47	1/60648 (0.0%)	0.79	23/81713 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	505	ASP	N-CA	5.51	1.57	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	512	PRO	N-CA-CB	-7.26	94.59	103.30
1	H	508	ILE	N-CA-C	7.21	130.46	111.00
1	O	509	LYS	N-CA-CB	-6.72	98.51	110.60
1	C	504	VAL	CB-CA-C	6.53	123.81	111.40
1	K	157	LYS	N-CA-CB	-6.51	98.88	110.60

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	A	3855	0	3970	432	0
1	B	3666	0	3772	369	0
1	C	3855	0	3970	524	0
1	D	3675	0	3778	422	0
1	E	3855	0	3970	456	0
1	F	3855	0	3970	339	0
1	G	3658	0	3766	429	0
1	H	3675	0	3778	425	0
1	I	3855	0	3970	453	0
1	J	3634	0	3741	434	0
1	K	3673	0	3778	440	0
1	L	3707	0	3815	479	0
1	M	3855	0	3970	432	0
1	N	3666	0	3772	486	0
1	O	3855	0	3970	451	0
1	P	3673	0	3779	414	0
All	All	60012	0	61769	6493	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 53.

The worst 5 of 6493 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:117:TRP:CE3	1:C:505:ASP:HA	1.82	1.15
1:K:146:LEU:HD12	1:K:171:VAL:HG13	1.14	1.13
1:N:146:LEU:HD12	1:N:171:VAL:HG13	1.26	1.12
1:P:146:LEU:HD12	1:P:171:VAL:HG13	1.31	1.12
1:E:146:LEU:HD12	1:E:171:VAL:HG13	1.24	1.11

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	511/513 (100%)	455 (89%)	30 (6%)	26 (5%)	2	30
1	B	484/513 (94%)	432 (89%)	30 (6%)	22 (4%)	3	33
1	C	511/513 (100%)	449 (88%)	25 (5%)	37 (7%)	1	22
1	D	485/513 (94%)	438 (90%)	23 (5%)	24 (5%)	3	31
1	E	511/513 (100%)	458 (90%)	29 (6%)	24 (5%)	3	32
1	F	511/513 (100%)	449 (88%)	32 (6%)	30 (6%)	2	27
1	G	483/513 (94%)	424 (88%)	31 (6%)	28 (6%)	2	27
1	H	485/513 (94%)	436 (90%)	22 (4%)	27 (6%)	2	28
1	I	511/513 (100%)	454 (89%)	25 (5%)	32 (6%)	2	25
1	J	481/513 (94%)	435 (90%)	21 (4%)	25 (5%)	2	30
1	K	486/513 (95%)	435 (90%)	26 (5%)	25 (5%)	2	30
1	L	490/513 (96%)	439 (90%)	30 (6%)	21 (4%)	3	34
1	M	511/513 (100%)	463 (91%)	17 (3%)	31 (6%)	2	26
1	N	484/513 (94%)	441 (91%)	27 (6%)	16 (3%)	5	40
1	O	511/513 (100%)	454 (89%)	26 (5%)	31 (6%)	2	26
1	P	485/513 (94%)	442 (91%)	22 (4%)	21 (4%)	3	34
All	All	7940/8208 (97%)	7104 (90%)	416 (5%)	420 (5%)	4	29

5 of 420 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	208	ASP
1	A	215	GLN
1	A	234	ASP
1	A	236	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/409 (100%)	366 (90%)	43 (10%)	8	36
1	B	388/409 (95%)	357 (92%)	31 (8%)	15	50
1	C	409/409 (100%)	363 (89%)	46 (11%)	7	33
1	D	389/409 (95%)	341 (88%)	48 (12%)	6	30
1	E	409/409 (100%)	361 (88%)	48 (12%)	7	32
1	F	409/409 (100%)	370 (90%)	39 (10%)	11	41
1	G	387/409 (95%)	342 (88%)	45 (12%)	7	32
1	H	389/409 (95%)	341 (88%)	48 (12%)	6	30
1	I	409/409 (100%)	370 (90%)	39 (10%)	11	41
1	J	385/409 (94%)	344 (89%)	41 (11%)	8	36
1	K	389/409 (95%)	343 (88%)	46 (12%)	6	32
1	L	392/409 (96%)	347 (88%)	45 (12%)	7	32
1	M	409/409 (100%)	366 (90%)	43 (10%)	8	36
1	N	388/409 (95%)	339 (87%)	49 (13%)	5	29
1	O	409/409 (100%)	355 (87%)	54 (13%)	5	28
1	P	389/409 (95%)	351 (90%)	38 (10%)	10	39
All	All	6359/6544 (97%)	5656 (89%)	703 (11%)	12	34

5 of 703 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	157	LYS
1	J	96	LEU
1	O	352	VAL
1	H	201	LEU
1	I	112	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	148	ASN
1	J	506	ASN
1	P	126	GLN
1	I	386	GLN
1	J	386	GLN

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 carbohydrates 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.