



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:03 PM BST

PDB ID : 4A0O
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 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>

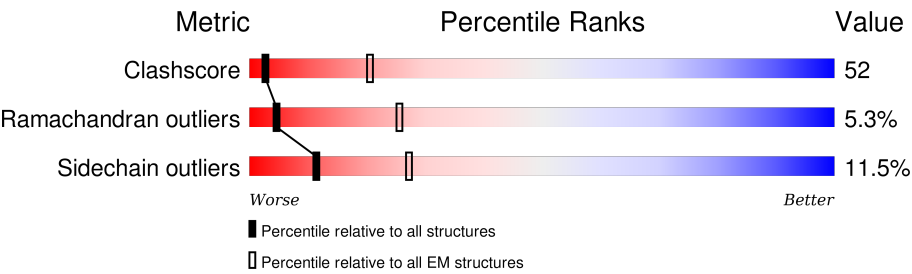
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 10.50 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	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	27% 33% 6% • 34%
1	B	513	38% 49% 8% • •
1	C	513	35% 50% 8% • 6%
1	D	513	35% 50% 9% • 5%
1	E	513	41% 45% 9% • •
1	F	513	37% 48% 10% 5%
1	G	513	36% 50% 14%
1	H	513	33% 52% 11% • •
1	I	513	33% 50% 8% • 8%

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Mol	Chain	Length	Quality of chain
1	J	513	<div><div></div><div>34%52%8%••</div></div>
1	K	513	<div><div></div><div>35%51%10%•</div></div>
1	L	513	<div><div></div><div>31%55%10%•</div></div>
1	M	513	<div><div></div><div>29%40%6%24%</div></div>
1	N	513	<div><div></div><div>38%47%8%•5%</div></div>
1	O	513	<div><div></div><div>36%46%11%•6%</div></div>
1	P	513	<div><div></div><div>35%50%11%•</div></div>

2 Entry composition

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.

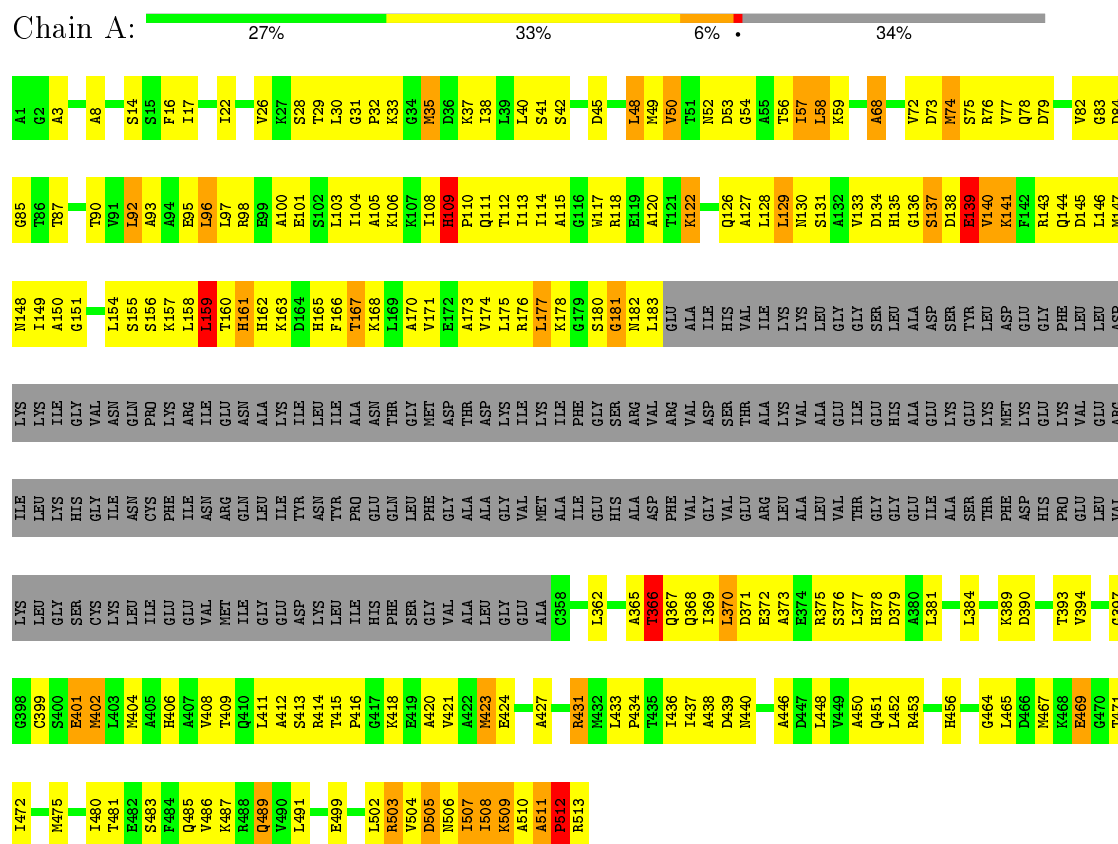
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

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

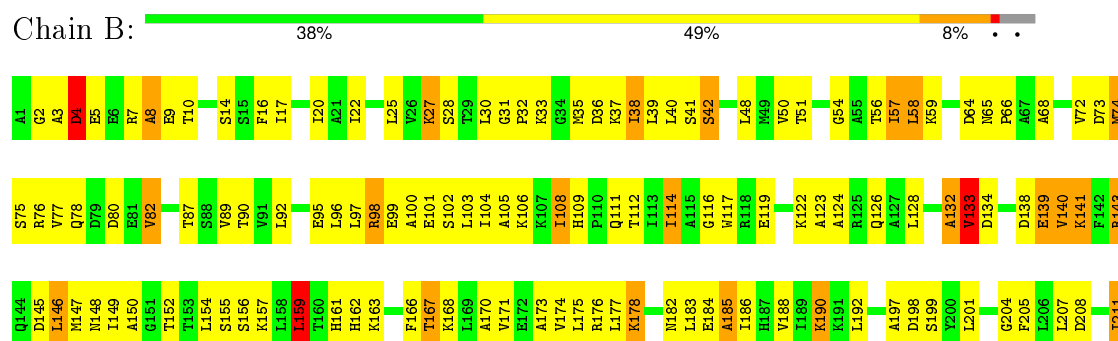
3 Residue-property plots

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.

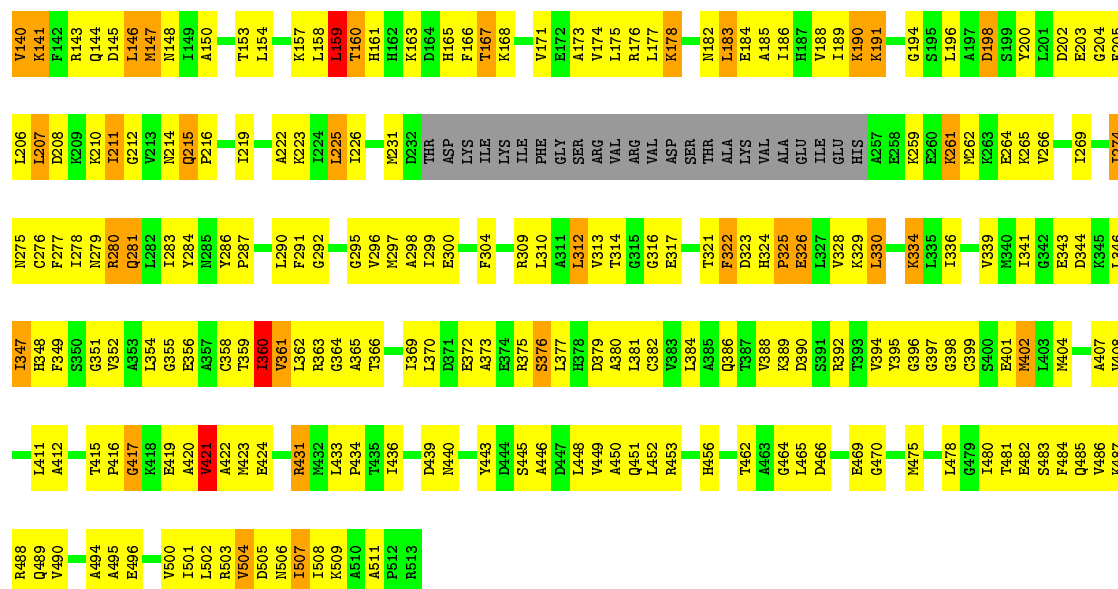
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

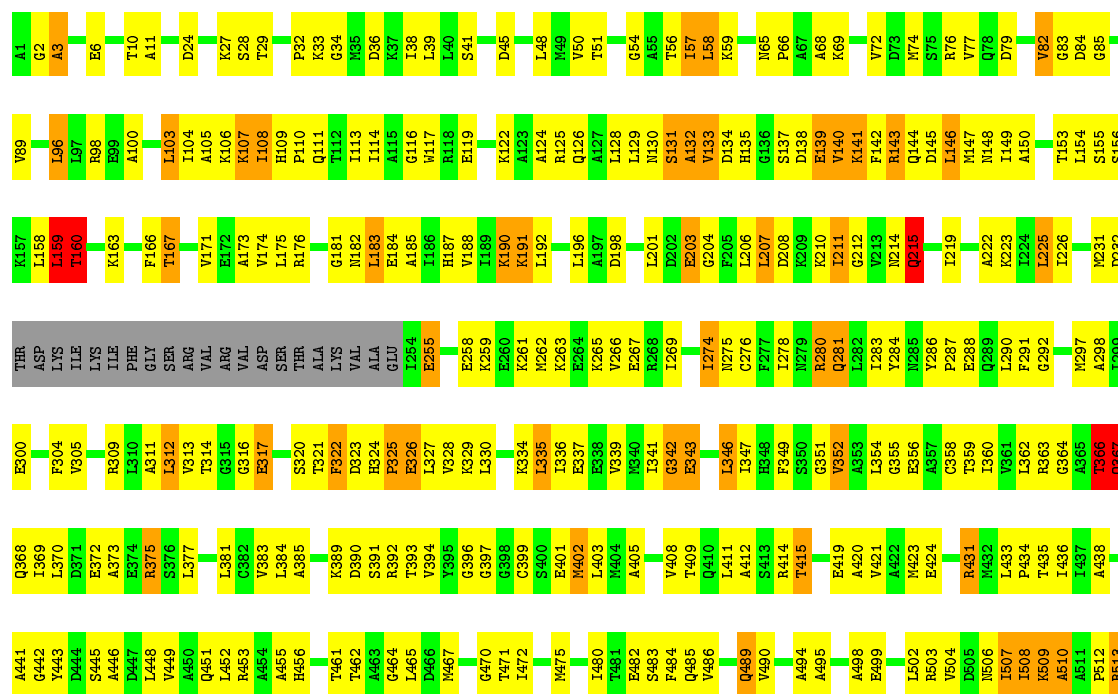






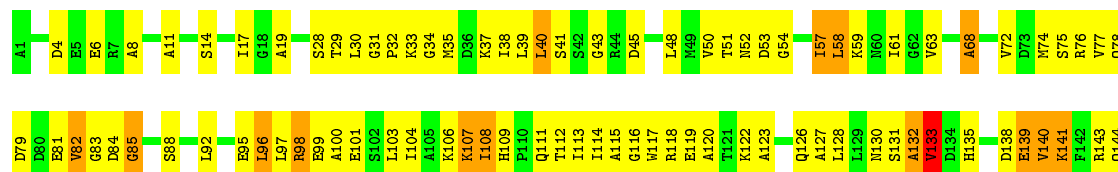
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

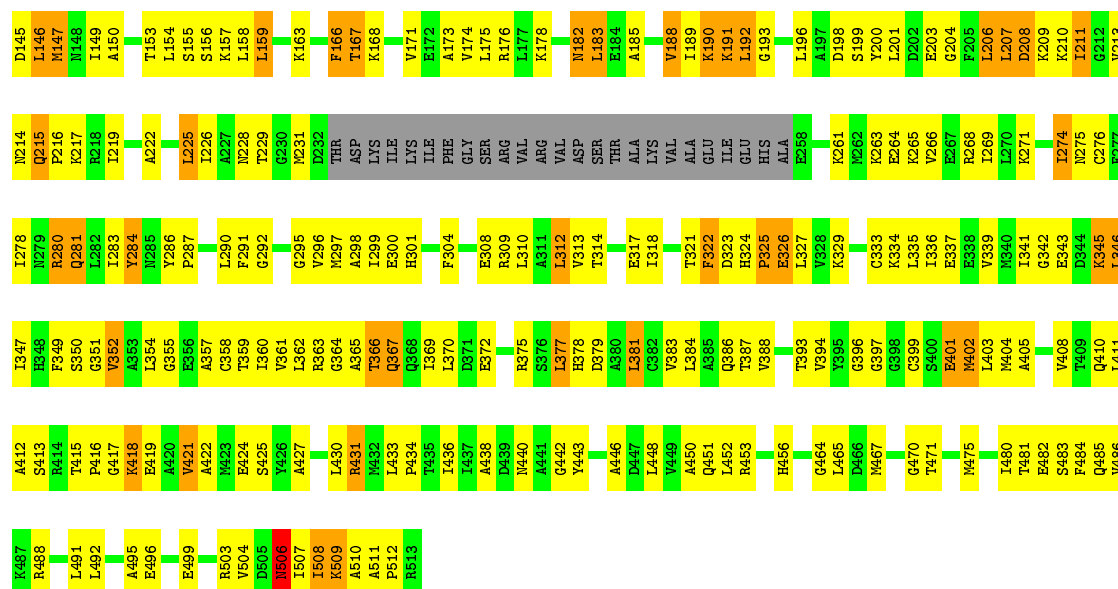
Chain E: 41% 45% 9% . .



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

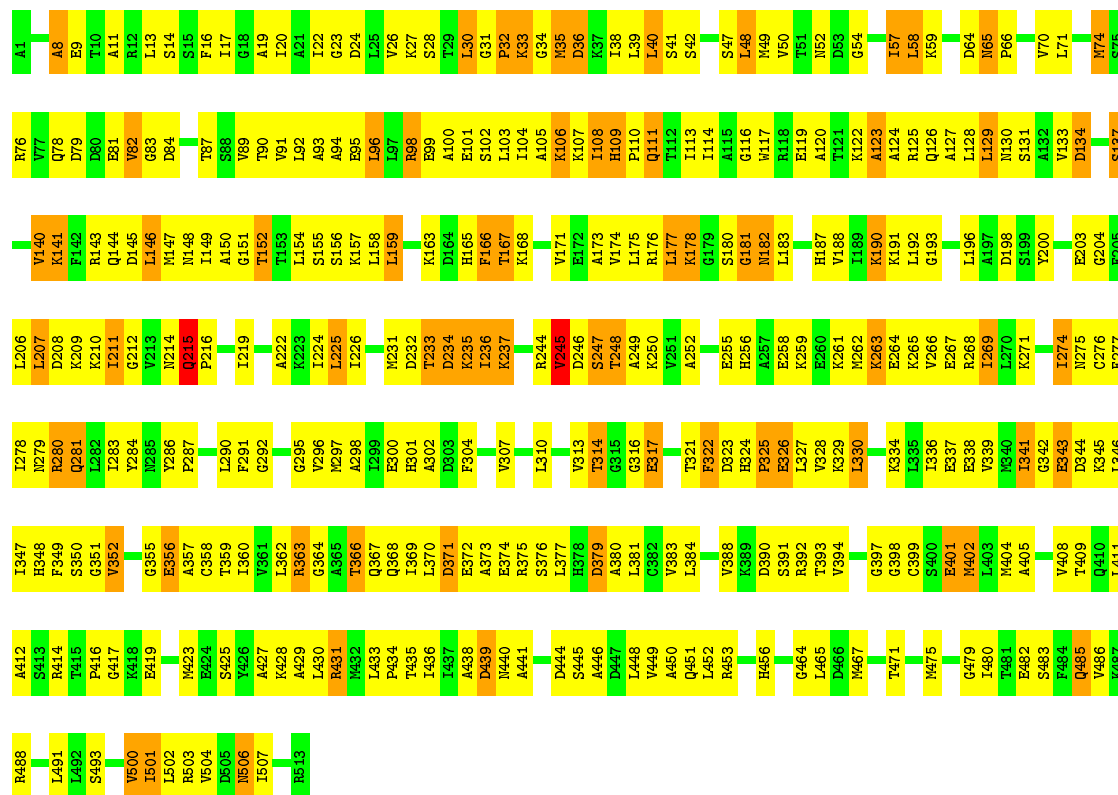
Chain F: 37% 48% 10% 5%





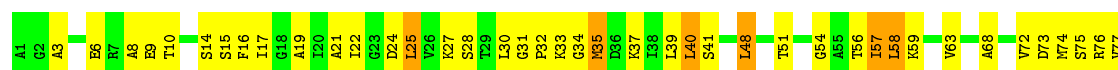
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

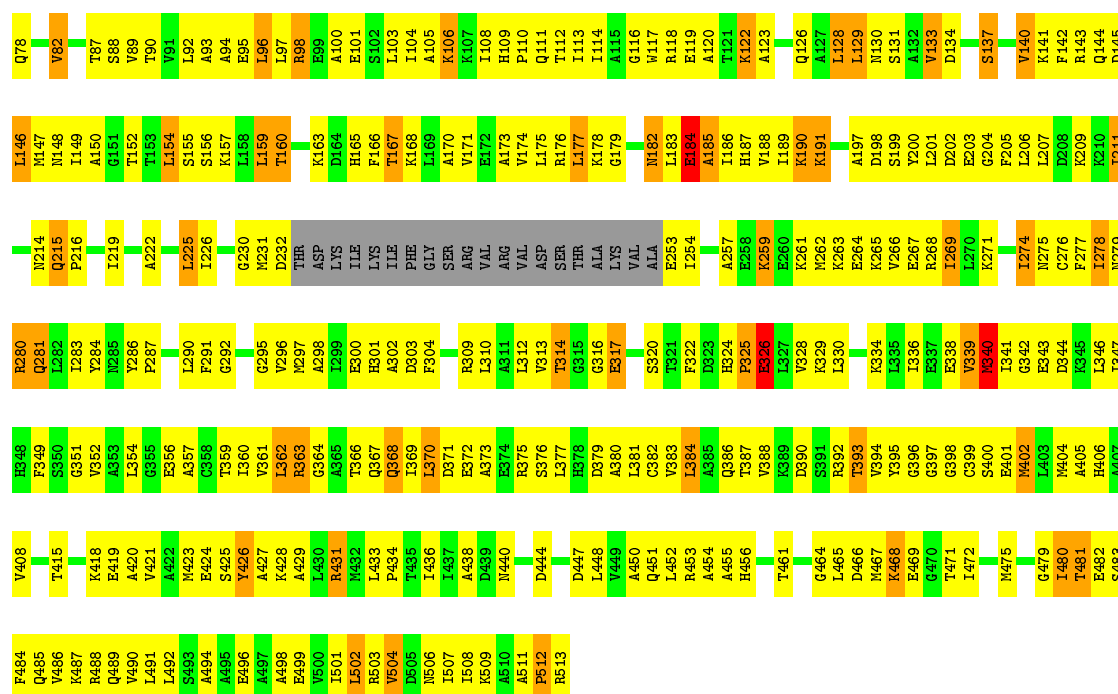
Chain G: 36% 50% 14%



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

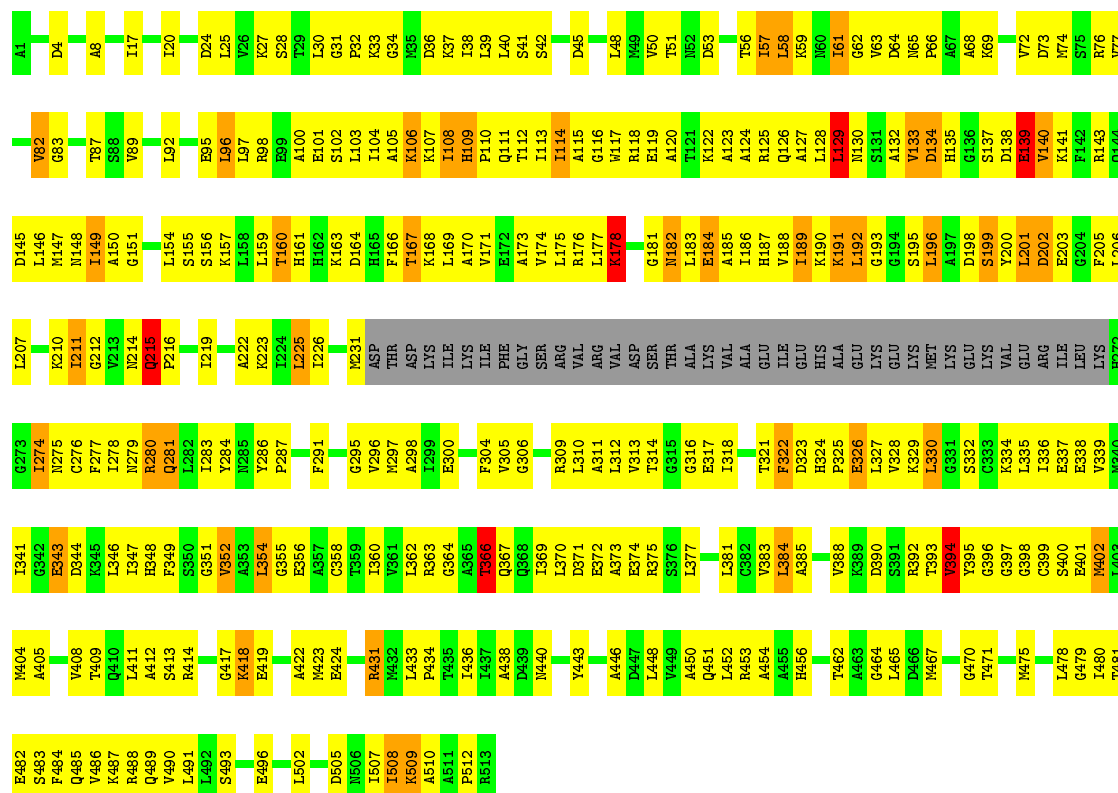
Chain H: 33% 52% 11%





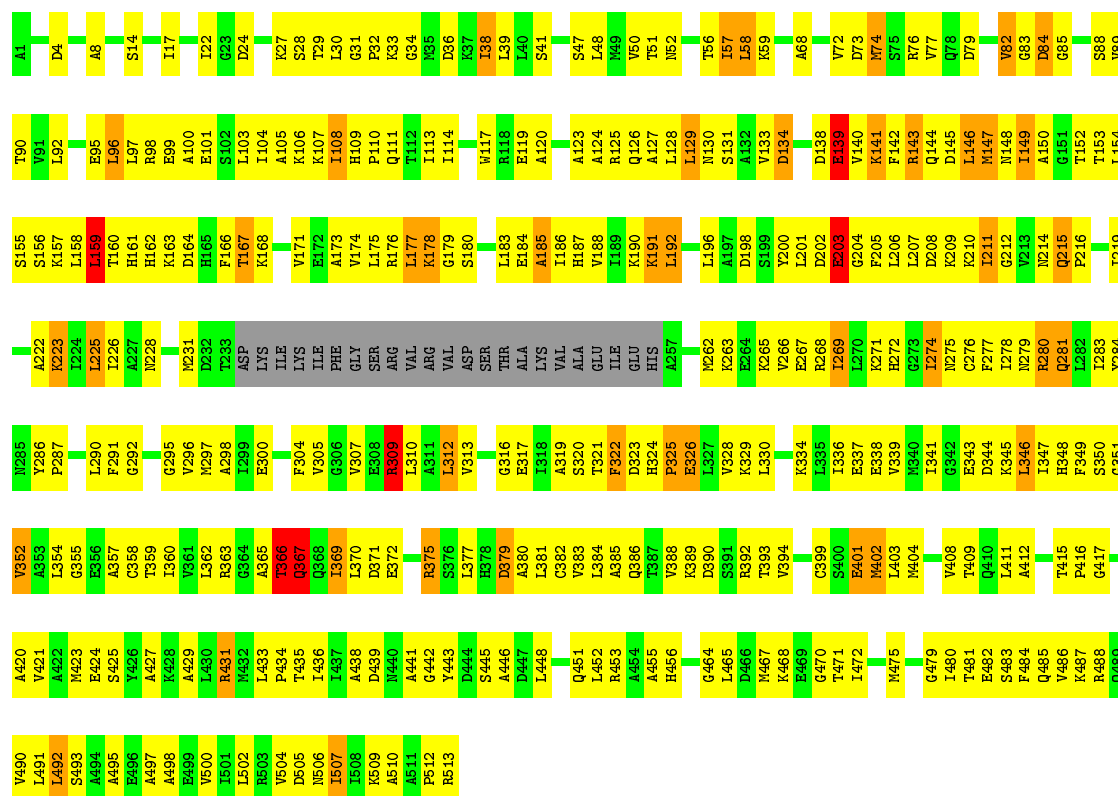
Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain I: 33% 50% 8% 8%



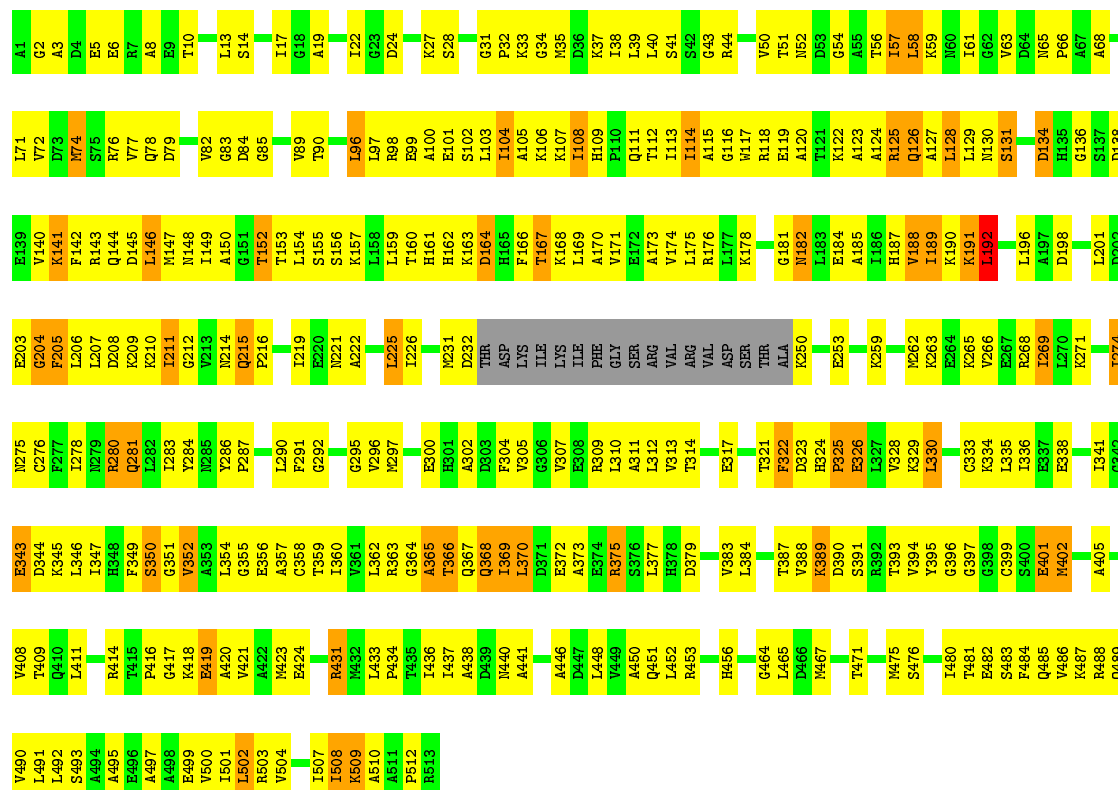
Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain J: 34% 52% 8% . .

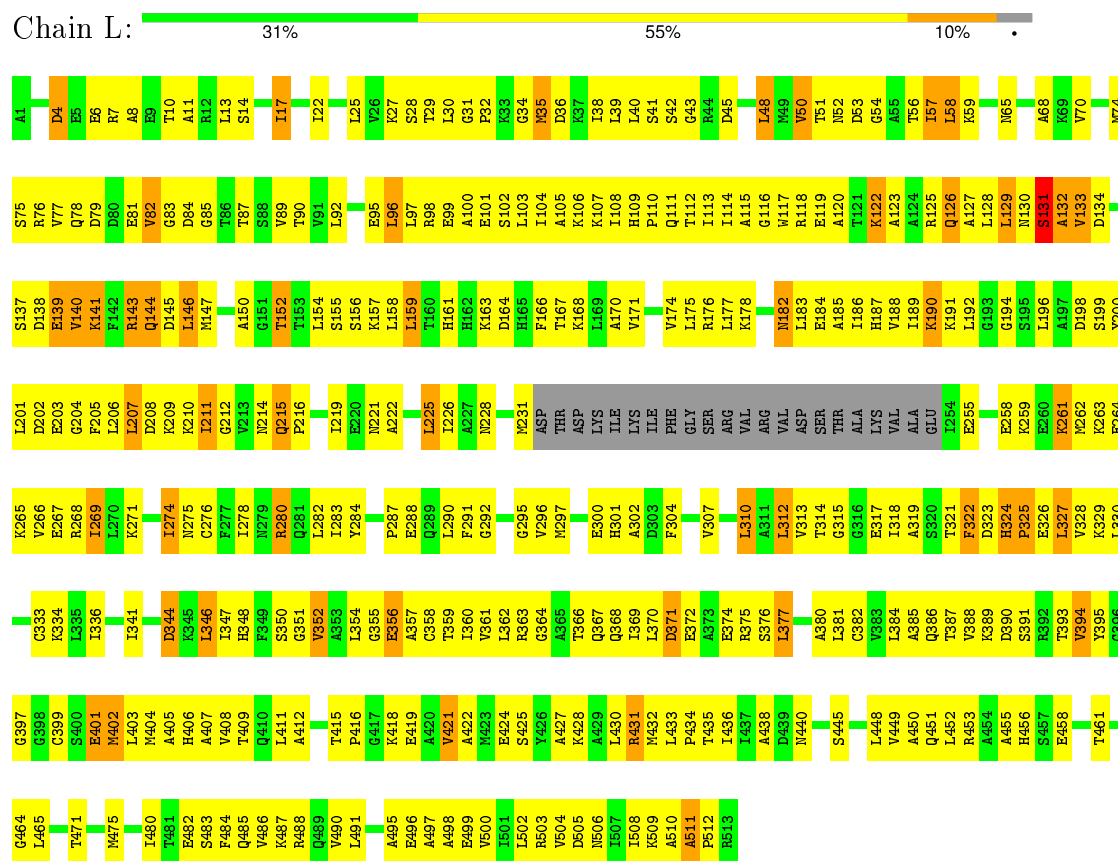


● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

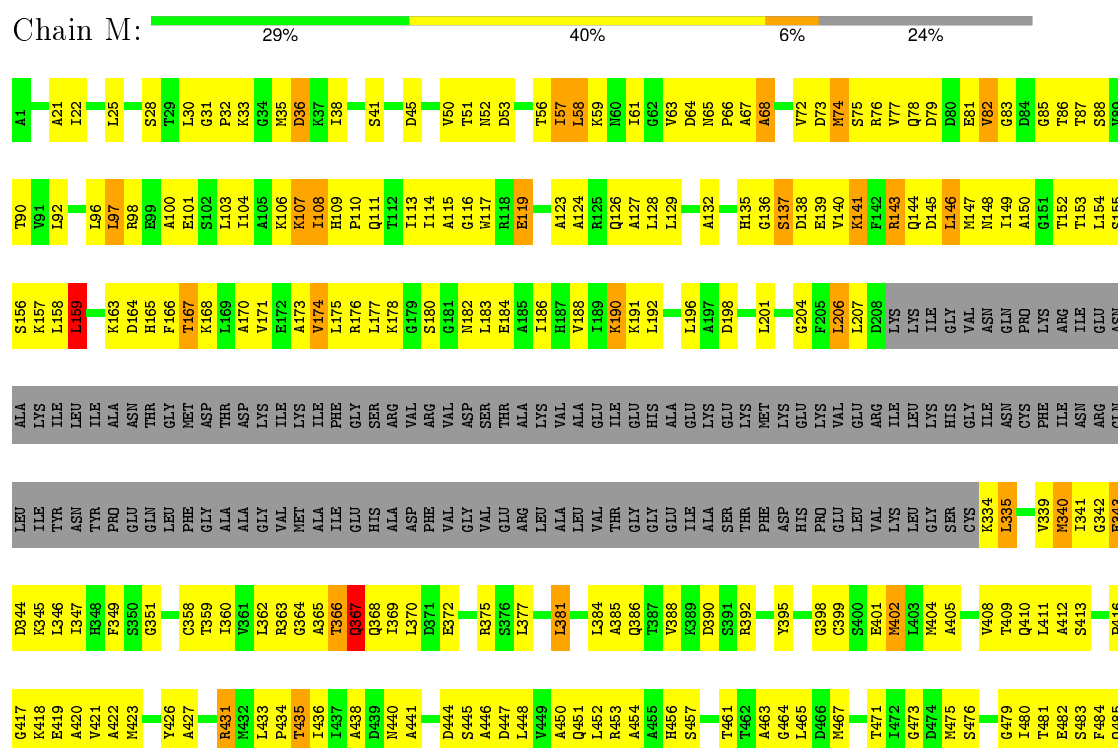
Chain K: 35% 51% 10%

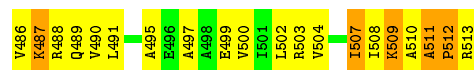


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



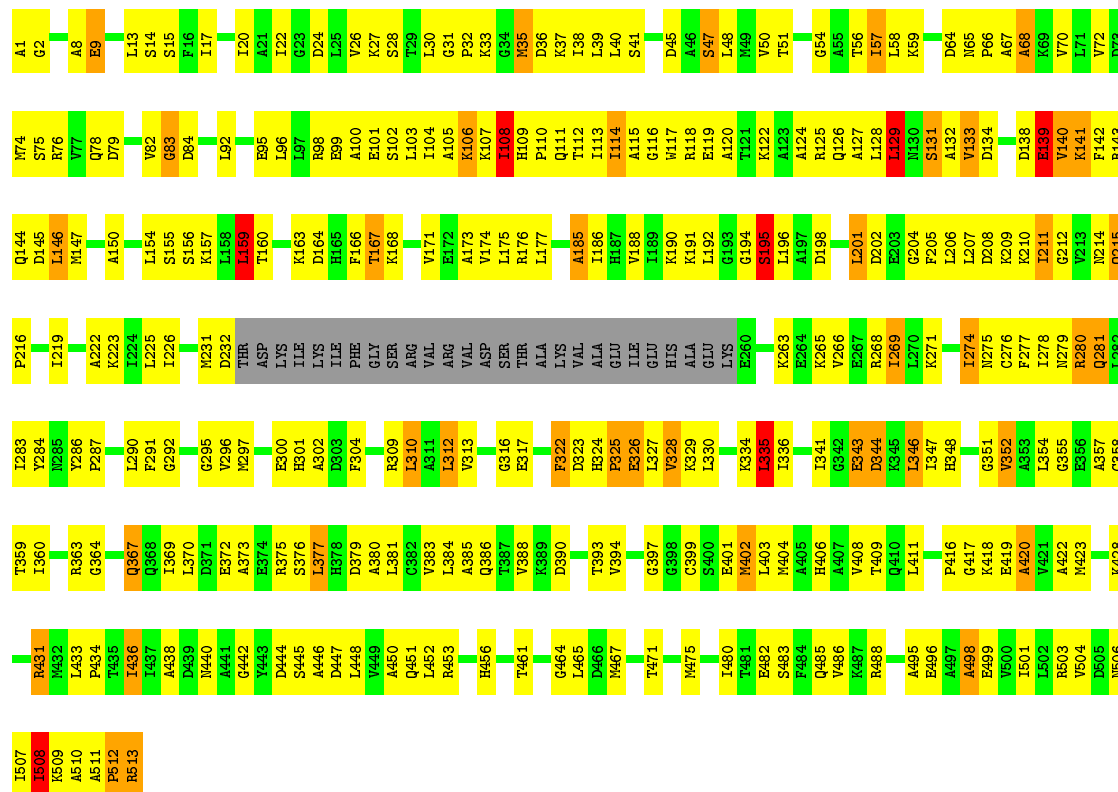
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





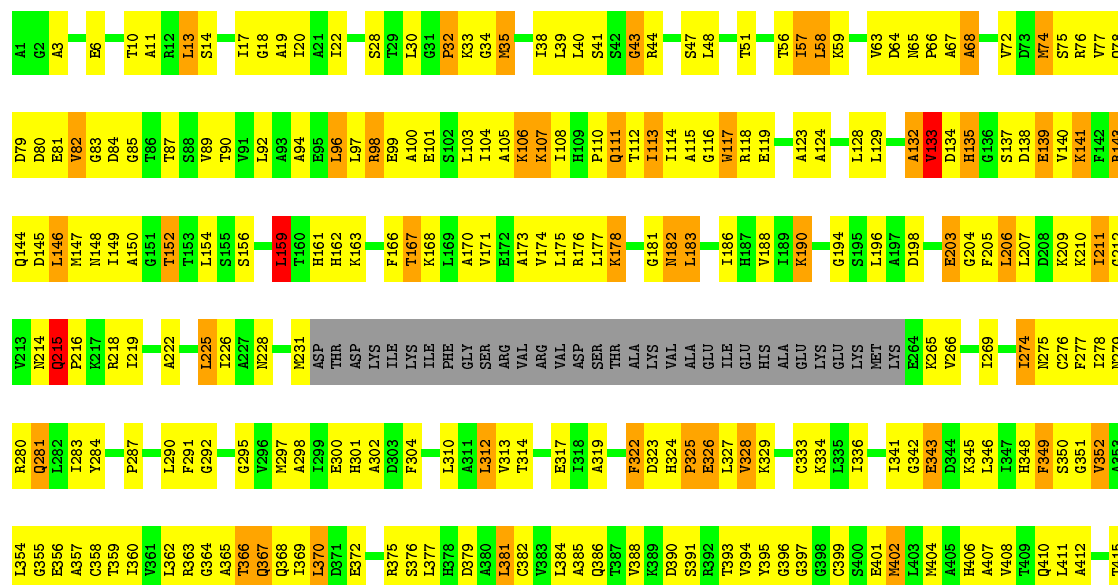
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

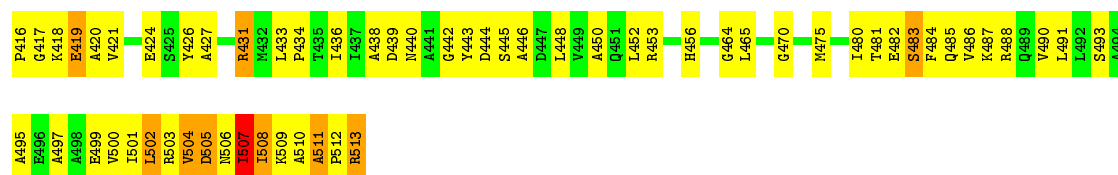
Chain N: 38% 47% 8% 5%



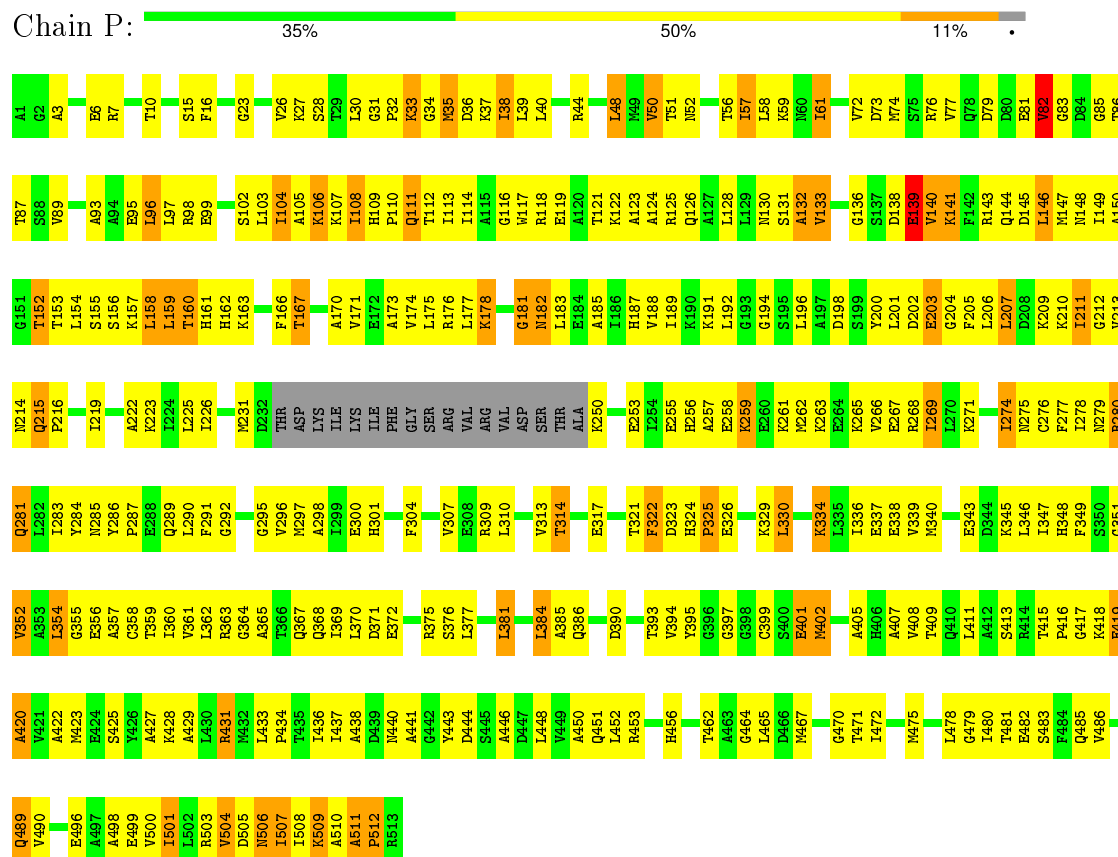
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain O: 36% 46% 11% 6%





• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



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	Not provided, Not provided	Depositor
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	Not provided	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	0.51	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 ⓘ

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	24
1	B	486/513 (95%)	441 (91%)	18 (4%)	27 (6%)	2	28
1	C	478/513 (93%)	425 (89%)	28 (6%)	25 (5%)	2	30
1	D	485/513 (94%)	439 (90%)	21 (4%)	25 (5%)	2	30
1	E	488/513 (95%)	443 (91%)	16 (3%)	29 (6%)	2	27
1	F	484/513 (94%)	439 (91%)	22 (4%)	23 (5%)	3	32
1	G	511/513 (100%)	450 (88%)	31 (6%)	30 (6%)	2	27
1	H	489/513 (95%)	434 (89%)	31 (6%)	24 (5%)	3	31
1	I	469/513 (91%)	421 (90%)	18 (4%)	30 (6%)	2	25
1	J	486/513 (95%)	438 (90%)	25 (5%)	23 (5%)	3	32
1	K	492/513 (96%)	438 (89%)	25 (5%)	29 (6%)	2	27
1	L	487/513 (95%)	450 (92%)	21 (4%)	16 (3%)	5	40
1	M	384/513 (75%)	347 (90%)	17 (4%)	20 (5%)	2	30
1	N	482/513 (94%)	429 (89%)	26 (5%)	27 (6%)	2	28
1	O	477/513 (93%)	422 (88%)	28 (6%)	27 (6%)	2	28
1	P	492/513 (96%)	449 (91%)	21 (4%)	22 (4%)	3	33
All	All	7525/8208 (92%)	6764 (90%)	362 (5%)	399 (5%)	4	29

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 ⓘ

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%)	8	36
1	B	389/409 (95%)	351 (90%)	38 (10%)	10	39
1	C	382/409 (93%)	339 (89%)	43 (11%)	7	33
1	D	388/409 (95%)	346 (89%)	42 (11%)	8	35
1	E	391/409 (96%)	347 (89%)	44 (11%)	7	33
1	F	388/409 (95%)	348 (90%)	40 (10%)	9	37
1	G	409/409 (100%)	349 (85%)	60 (15%)	4	24
1	H	392/409 (96%)	335 (86%)	57 (14%)	4	24
1	I	373/409 (91%)	327 (88%)	46 (12%)	6	30
1	J	389/409 (95%)	344 (88%)	45 (12%)	7	32
1	K	394/409 (96%)	354 (90%)	40 (10%)	9	37
1	L	390/409 (95%)	343 (88%)	47 (12%)	6	31
1	M	305/409 (75%)	276 (90%)	29 (10%)	11	41
1	N	386/409 (94%)	344 (89%)	42 (11%)	8	35
1	O	381/409 (93%)	337 (88%)	44 (12%)	7	32
1	P	394/409 (96%)	347 (88%)	47 (12%)	6	31
All	All	6017/6544 (92%)	5325 (88%)	692 (12%)	11	32

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

Mol	Chain	Res	Type
1	H	152	THR
1	I	409	THR
1	O	431	ARG
1	H	203	GLU
1	H	507	ILE

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

Mol	Chain	Res	Type
1	H	410	GLN
1	J	161	HIS
1	O	386	GLN
1	H	451	GLN
1	I	451	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.