



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Apr 12, 2017 – 03:01 PM EDT

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/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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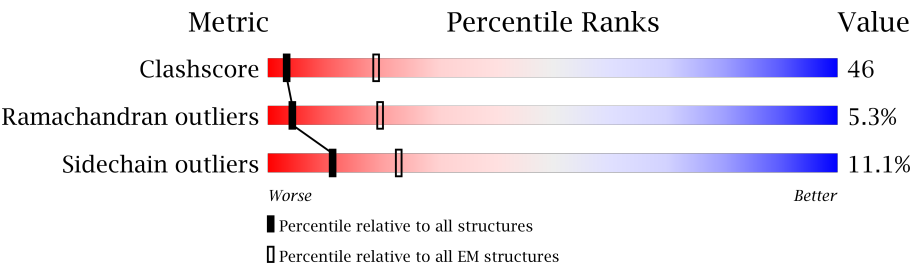
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

# 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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>37%</div><div>47%</div><div>10%</div><div>.</div><div>.</div></div>
1	B	513	<div><div>37%</div><div>47%</div><div>8%</div><div>.</div><div>6%</div></div>
1	C	513	<div><div>39%</div><div>51%</div><div>9%</div><div>.</div></div>
1	D	513	<div><div>38%</div><div>51%</div><div>9%</div><div>.</div></div>
1	E	513	<div><div>38%</div><div>52%</div><div>9%</div><div>.</div></div>
1	F	513	<div><div>36%</div><div>49%</div><div>9%</div><div>.</div><div>5%</div></div>
1	G	513	<div><div>38%</div><div>52%</div><div>9%</div><div>.</div></div>
1	H	513	<div><div>34%</div><div>51%</div><div>9%</div><div>.</div><div>5%</div></div>
1	I	513	<div><div>39%</div><div>44%</div><div>10%</div><div>7%</div></div>

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

## 2 Entry composition

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.

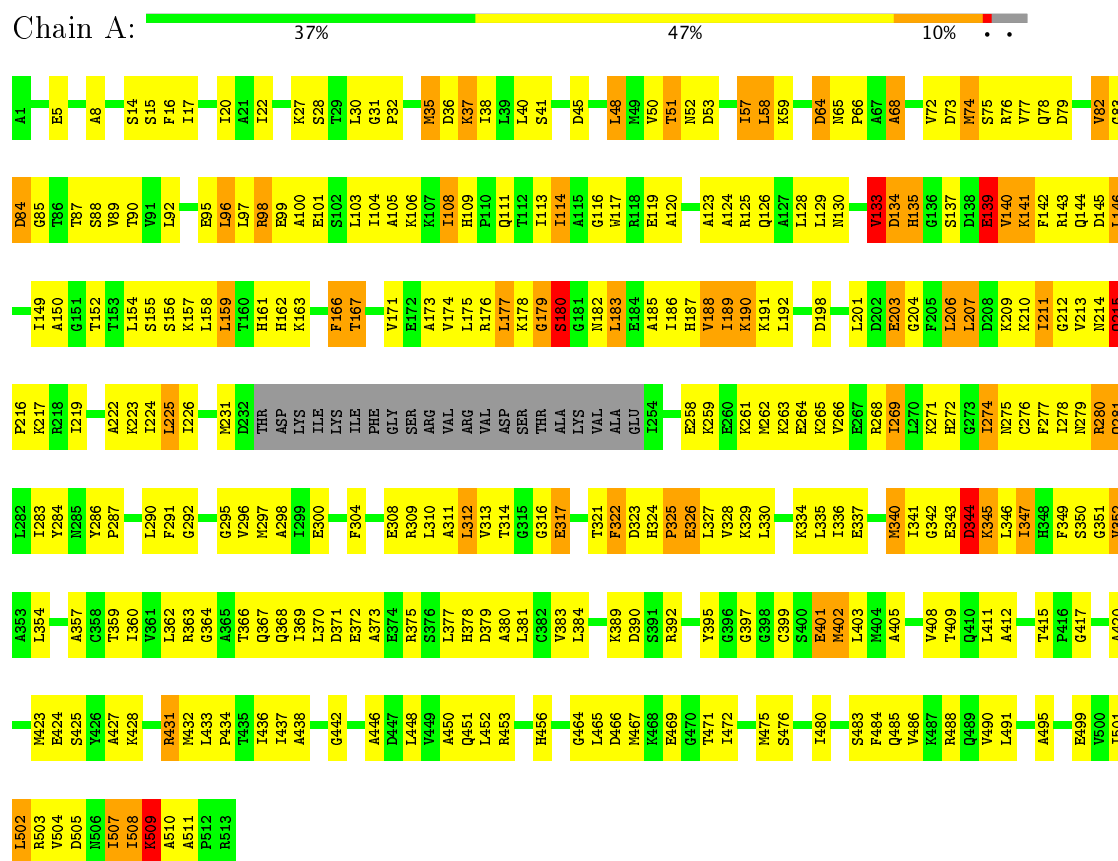
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

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		

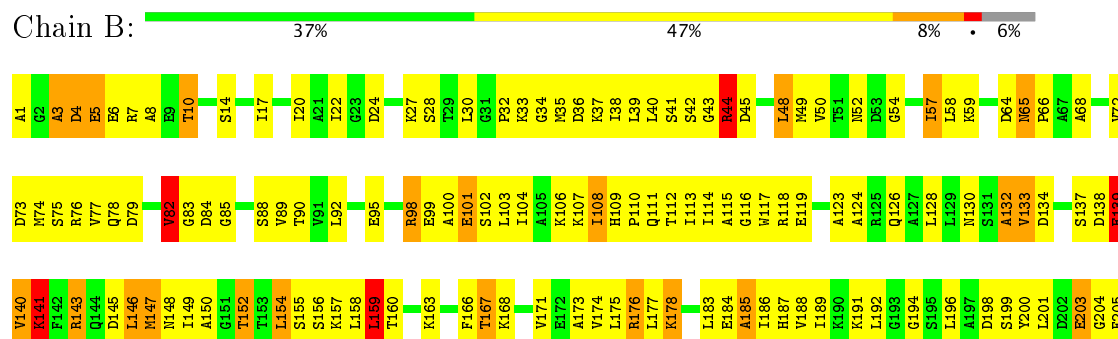
### 3 Residue-property plots

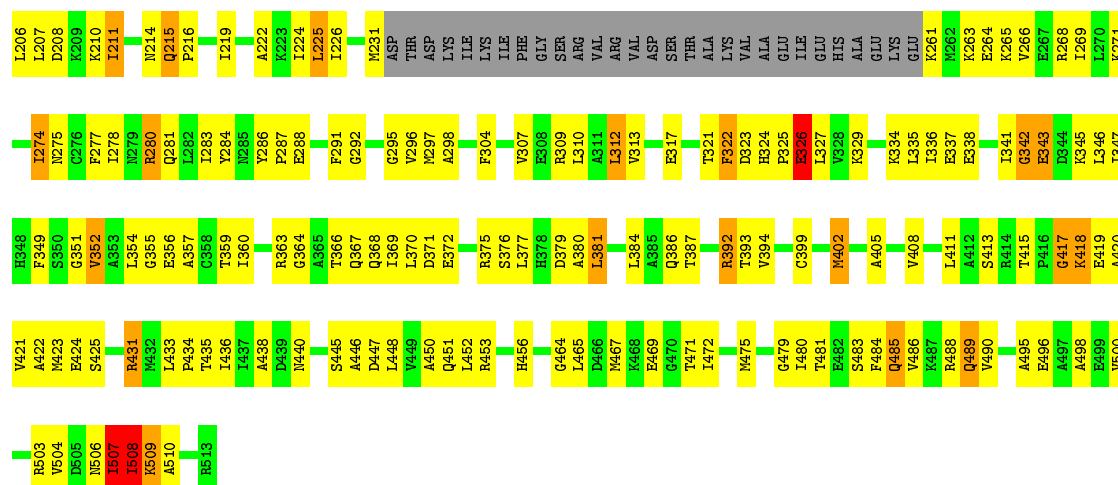
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



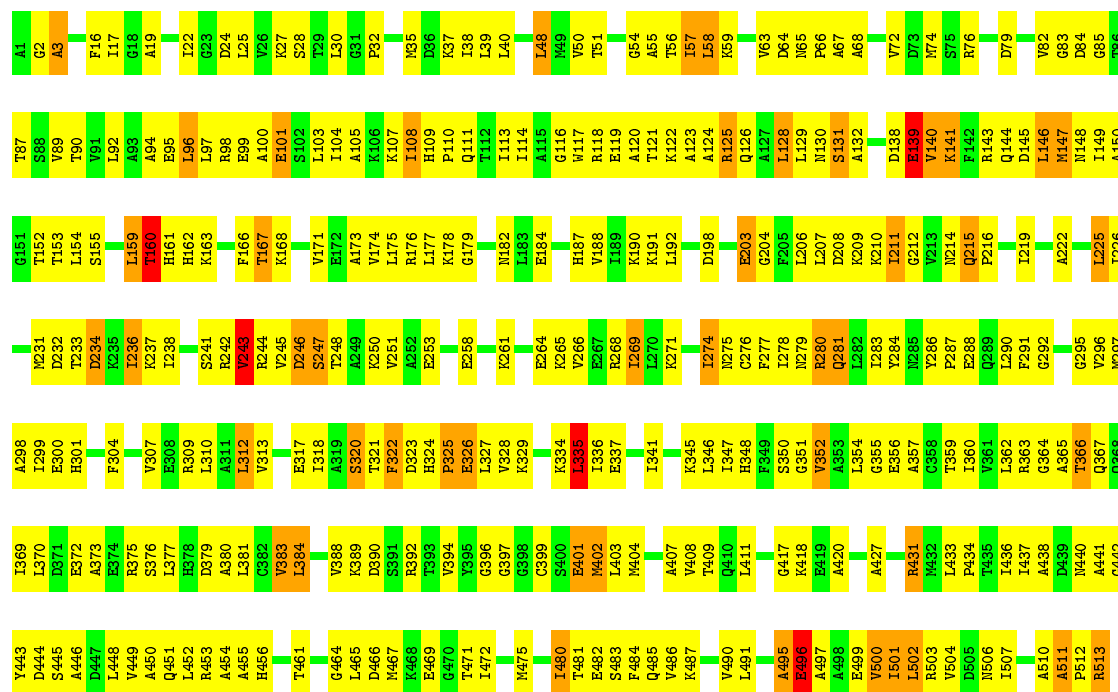
#### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

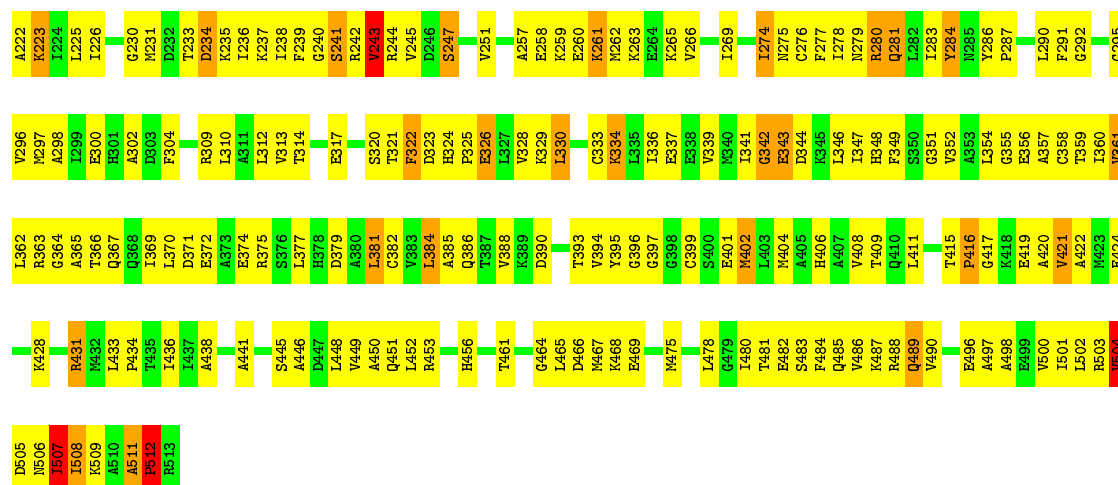
Chain C: 39% 51% 9% .



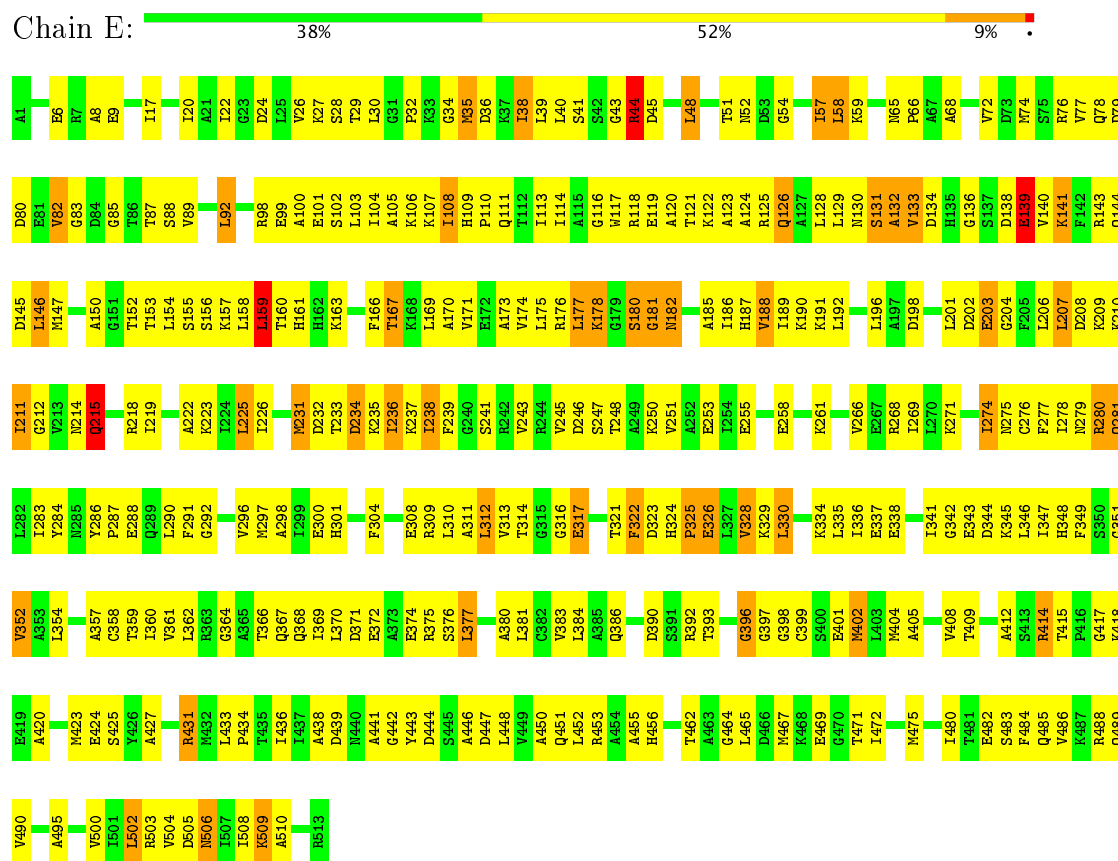
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain D: 38% 51% 9% .

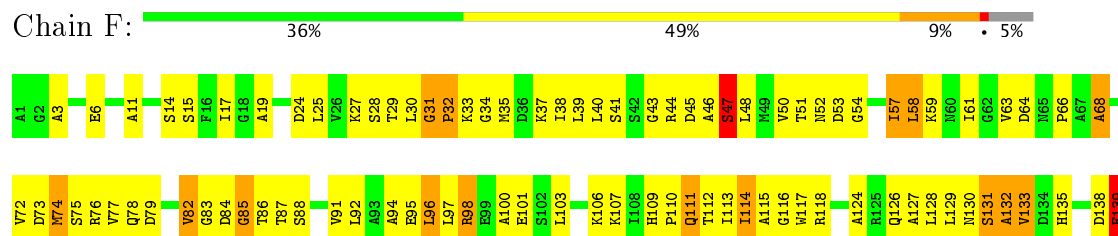


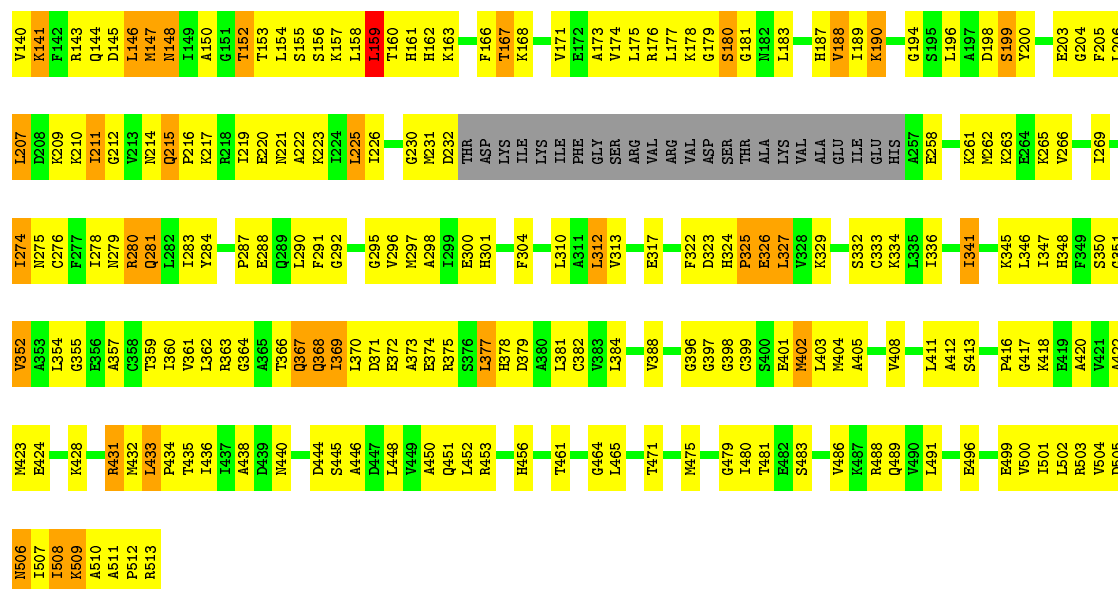


- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



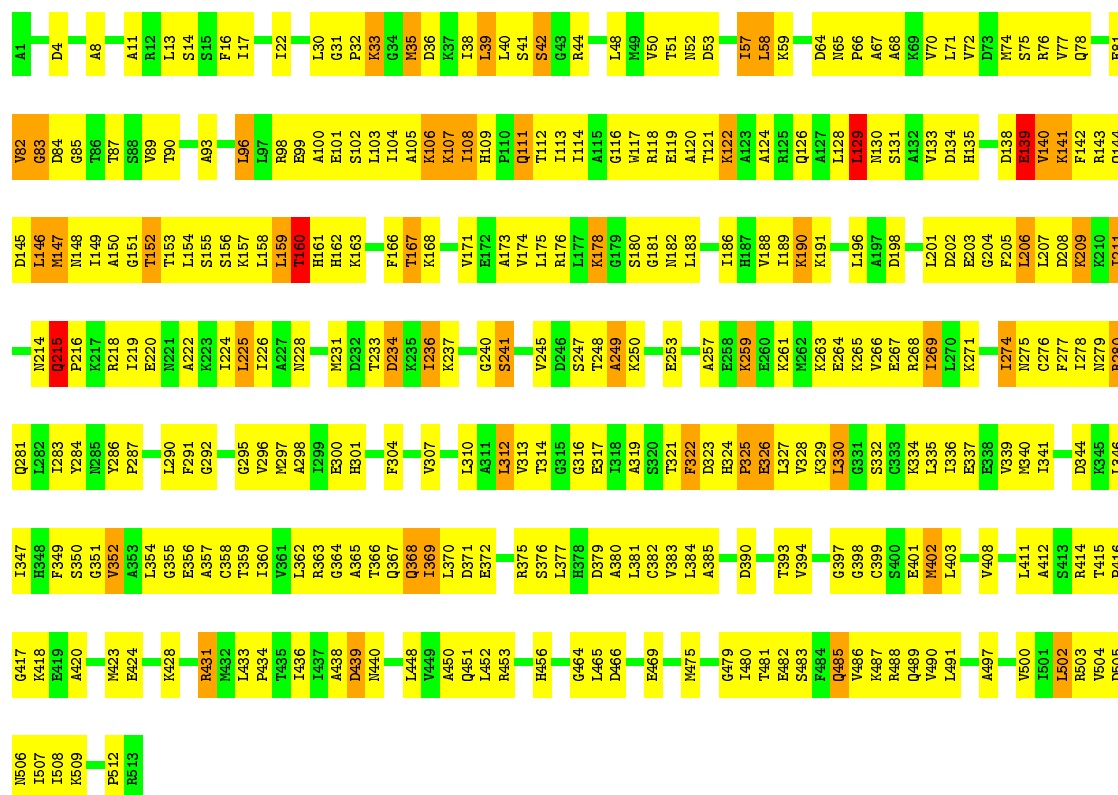
- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain G: 38% 52% 9% •

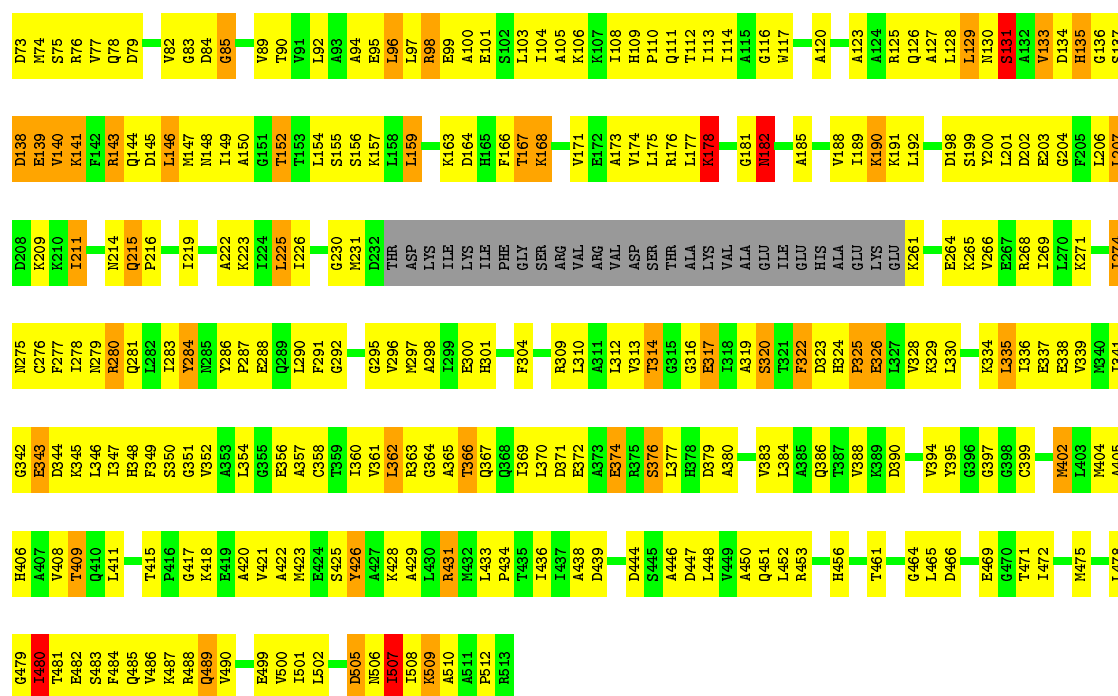


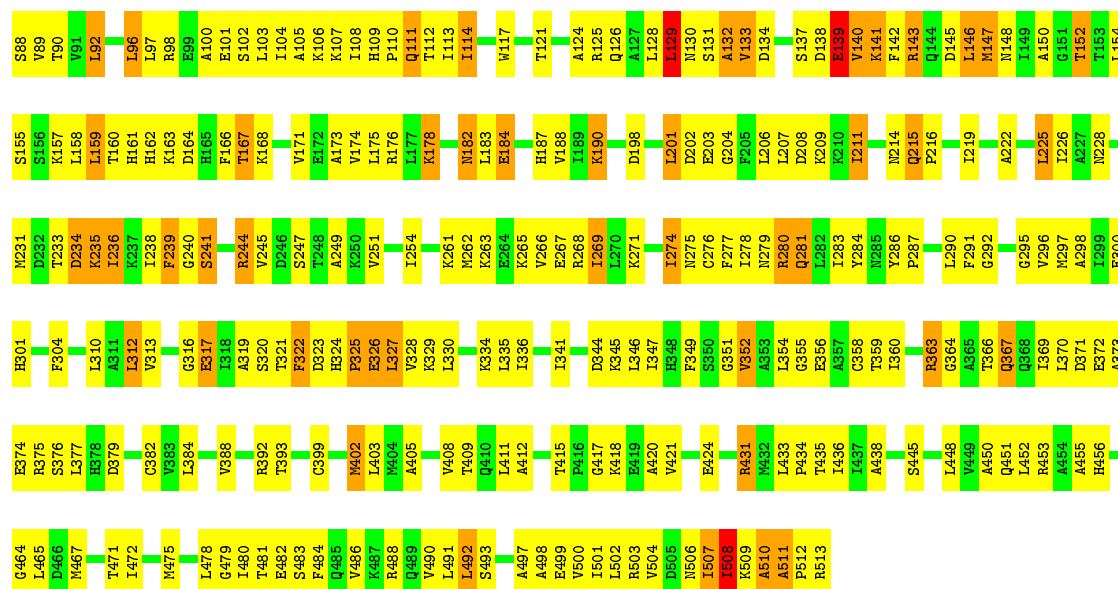
### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain H: 34% 51% 9% 5% •



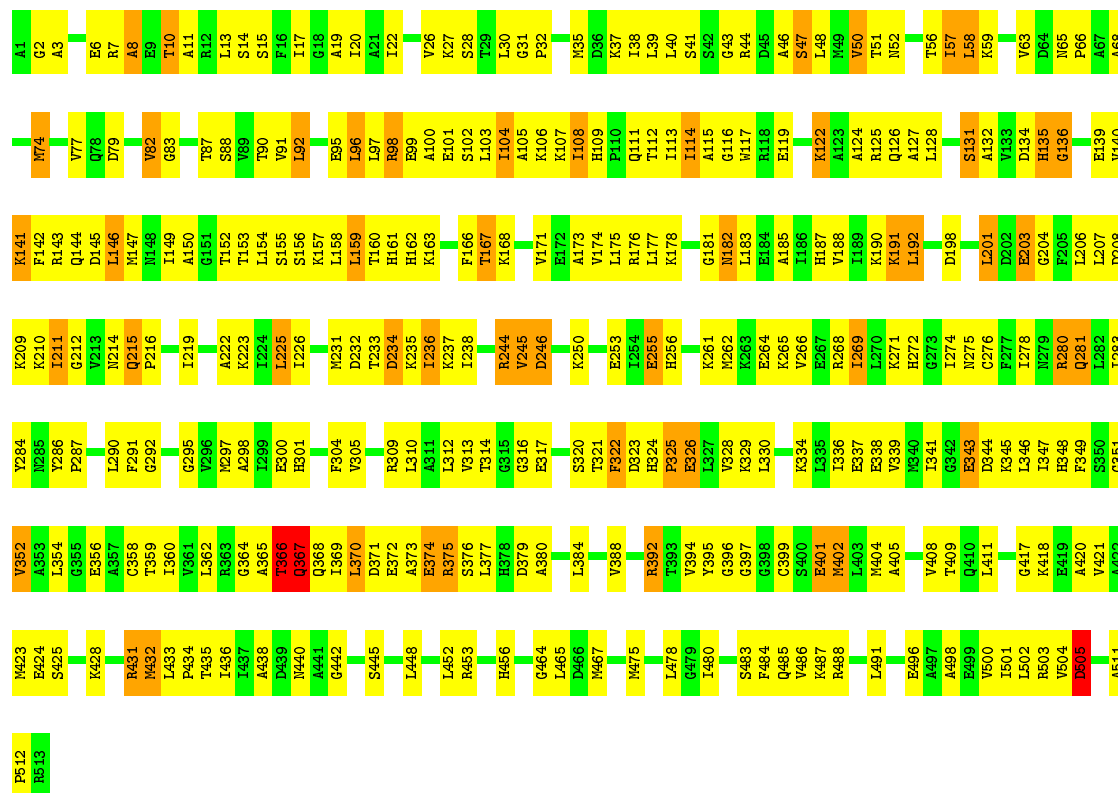






### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

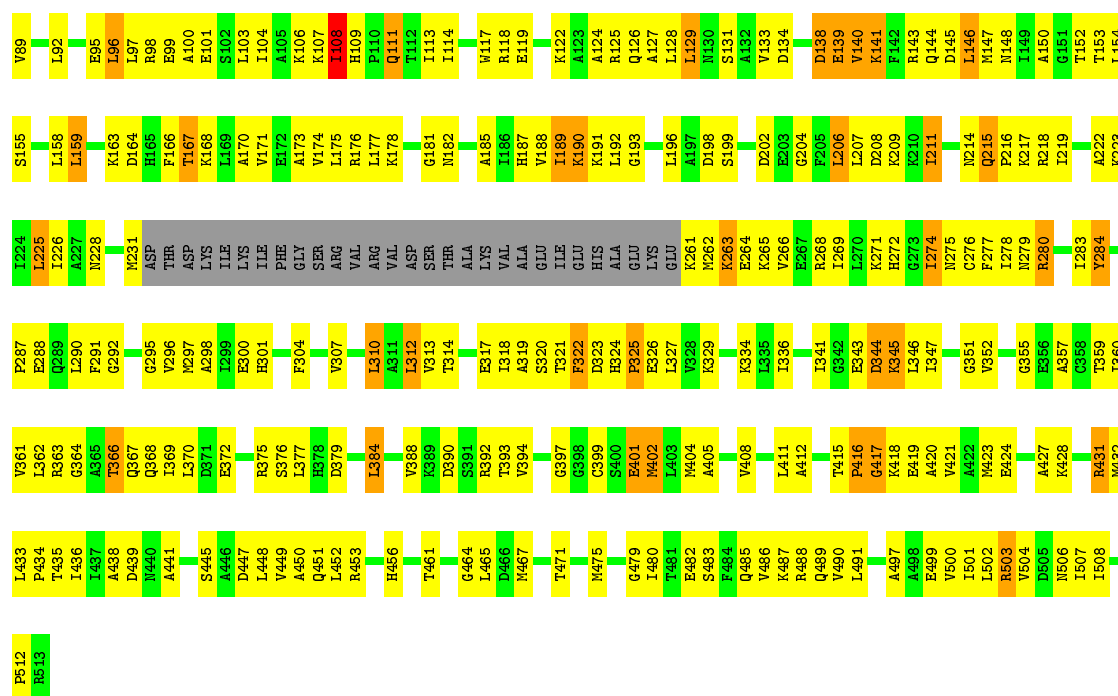
Chain K: 41% 49% 10% •



### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

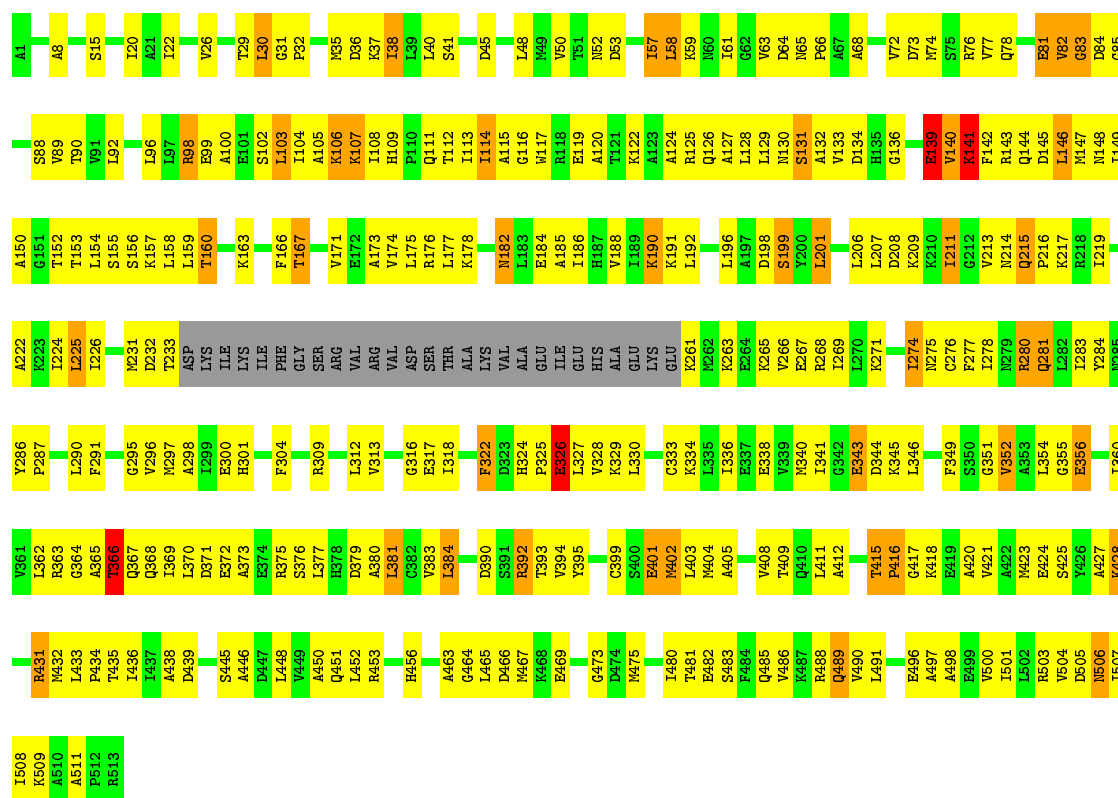
Chain L: 40% 47% 8% 6%





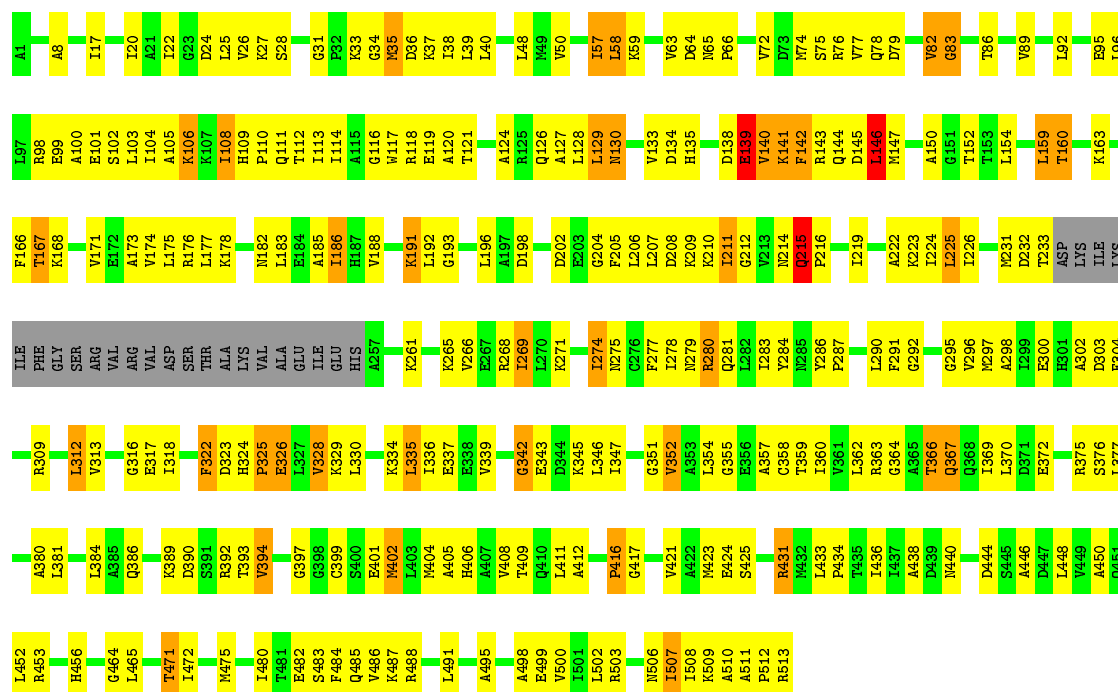
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain M:



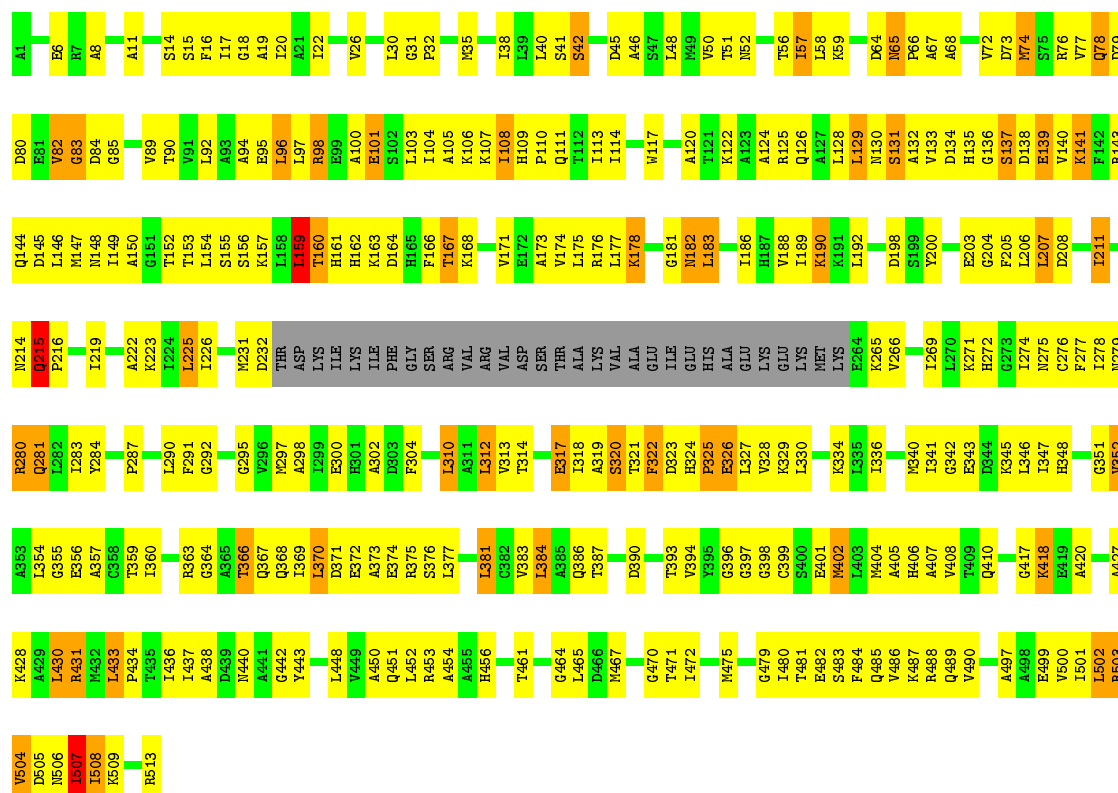
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain N:



- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

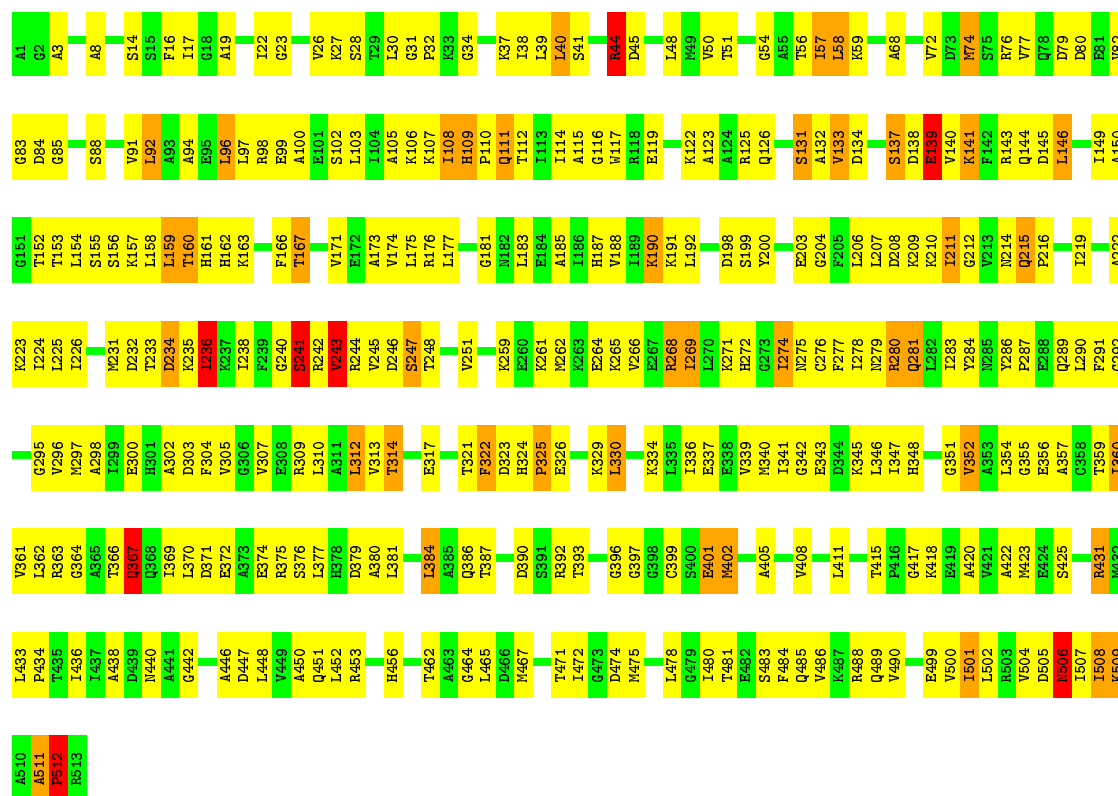
Chain O:



● Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain P:





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	29374	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	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	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(°)	Ideal(°)
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 ⓘ

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

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 ⓘ

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	25
1	B	384/409 (94%)	343 (89%)	41 (11%)	8	31
1	C	409/409 (100%)	362 (88%)	47 (12%)	6	28
1	D	409/409 (100%)	362 (88%)	47 (12%)	6	28
1	E	409/409 (100%)	359 (88%)	50 (12%)	6	26
1	F	388/409 (95%)	338 (87%)	50 (13%)	5	25
1	G	409/409 (100%)	364 (89%)	45 (11%)	7	30
1	H	385/409 (94%)	340 (88%)	45 (12%)	6	27
1	I	376/409 (92%)	336 (89%)	40 (11%)	8	31
1	J	409/409 (100%)	363 (89%)	46 (11%)	7	29
1	K	409/409 (100%)	366 (90%)	43 (10%)	8	32
1	L	384/409 (94%)	341 (89%)	43 (11%)	7	29
1	M	386/409 (94%)	347 (90%)	39 (10%)	9	33
1	N	389/409 (95%)	353 (91%)	36 (9%)	10	37
1	O	382/409 (93%)	343 (90%)	39 (10%)	8	33
1	P	409/409 (100%)	366 (90%)	43 (10%)	8	32
All	All	6328/6544 (97%)	5624 (89%)	704 (11%)	11	29

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 [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.