



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:12 PM BST

PDB ID : 4A0W  
EMDB ID: : EMD-1962  
Title : model built against symmetry-free cryo-EM map of TRiC-ADP-ATFx  
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 : 13.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

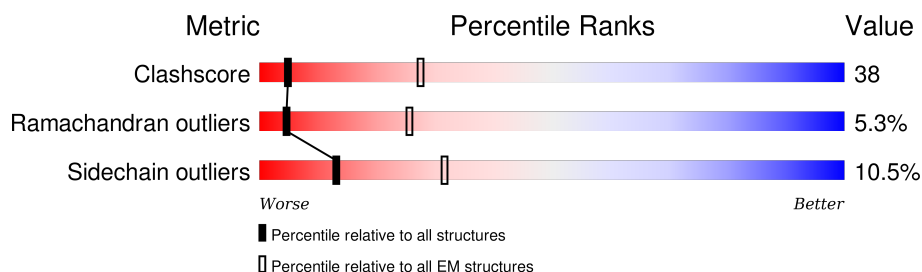
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.90 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  $\geq 3$ , 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	44% 46% 9% .
1	B	513	49% 41% 10% .
1	C	513	44% 43% 7% . .
1	D	513	43% 46% 10% .
1	E	513	48% 41% 10% .
1	F	513	45% 44% 10% .
1	G	513	46% 46% 8%
1	H	513	45% 41% 10% . .
1	I	513	46% 44% 9% .

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Mol	Chain	Length	Quality of chain
1	J	513	<div><div></div><div>48%44%7%.</div></div>
1	K	513	<div><div></div><div>41%47%8%. .</div></div>
1	L	513	<div><div></div><div>45%42%8%. .</div></div>
1	M	513	<div><div></div><div>49%43%7%.</div></div>
1	N	513	<div><div></div><div>43%44%9%. .</div></div>
1	O	513	<div><div></div><div>42%44%9%. .</div></div>
1	P	513	<div><div></div><div>47%44%8%.</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60649 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.

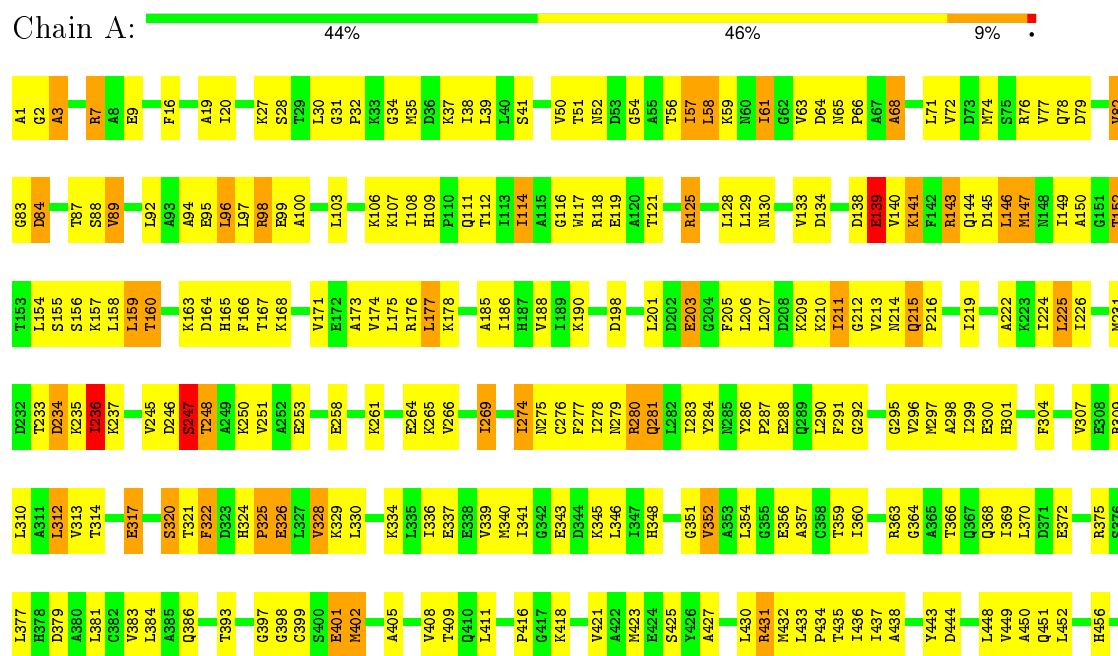
- Molecule 1 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	B	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	C	490	Total	C	N	O	S	0	0
			3673	2295	645	714	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	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	G	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	H	492	Total	C	N	O	S	0	0
			3693	2308	649	717	19		
1	I	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	J	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	K	491	Total	C	N	O	S	0	0
			3681	2299	646	717	19		
1	L	490	Total	C	N	O	S	0	0
			3676	2296	645	716	19		
1	M	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		
1	N	493	Total	C	N	O	S	0	0
			3700	2312	650	719	19		
1	O	490	Total	C	N	O	S	0	0
			3676	2296	645	716	19		
1	P	513	Total	C	N	O	S	0	0
			3855	2409	679	748	19		

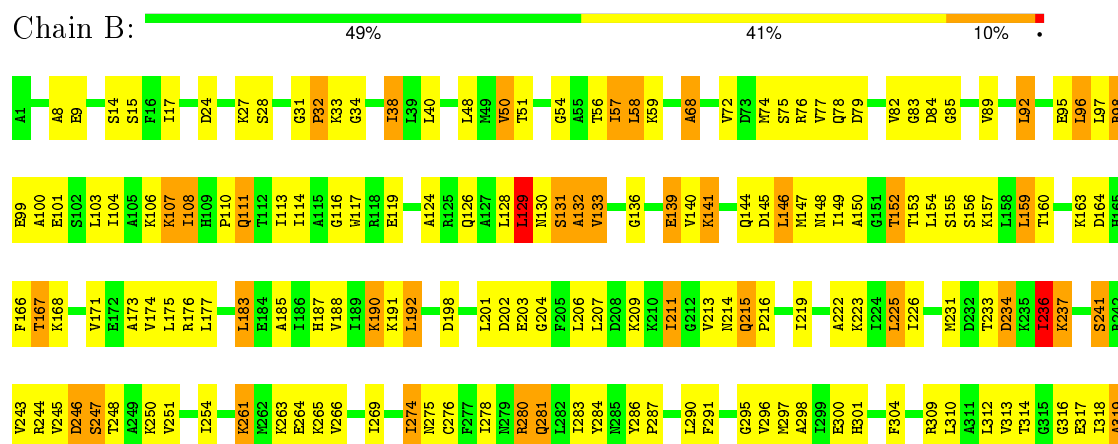
### 3 Residue-property plots

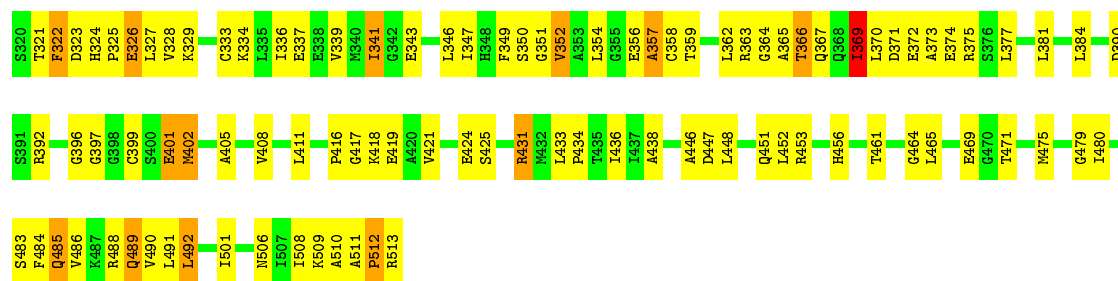
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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



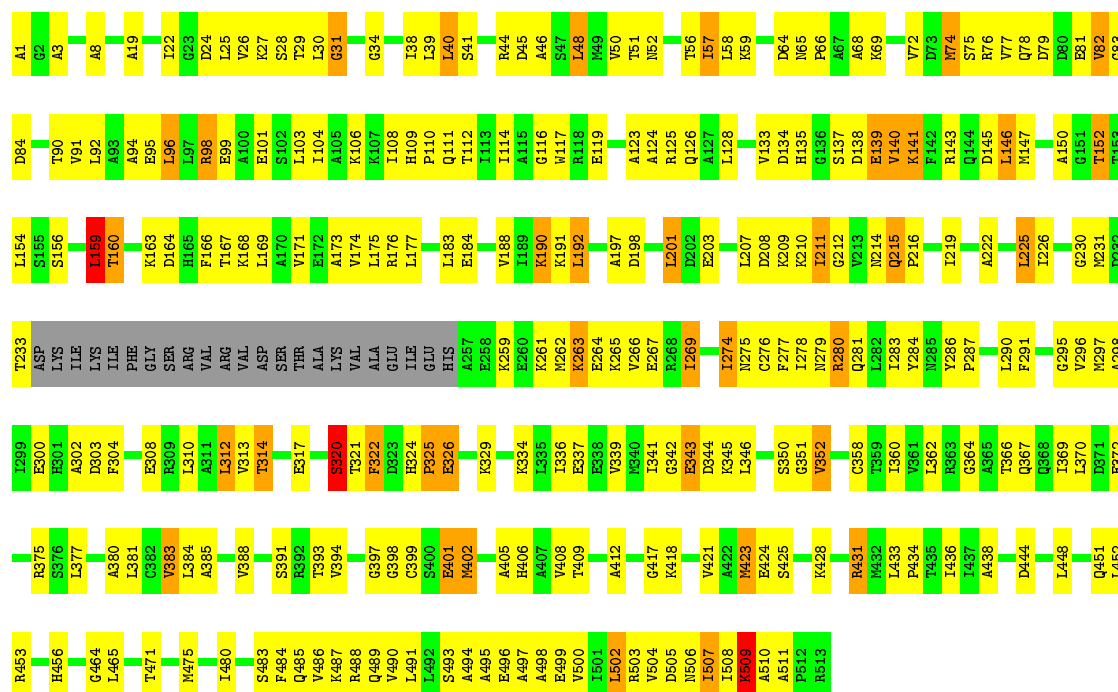
#### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





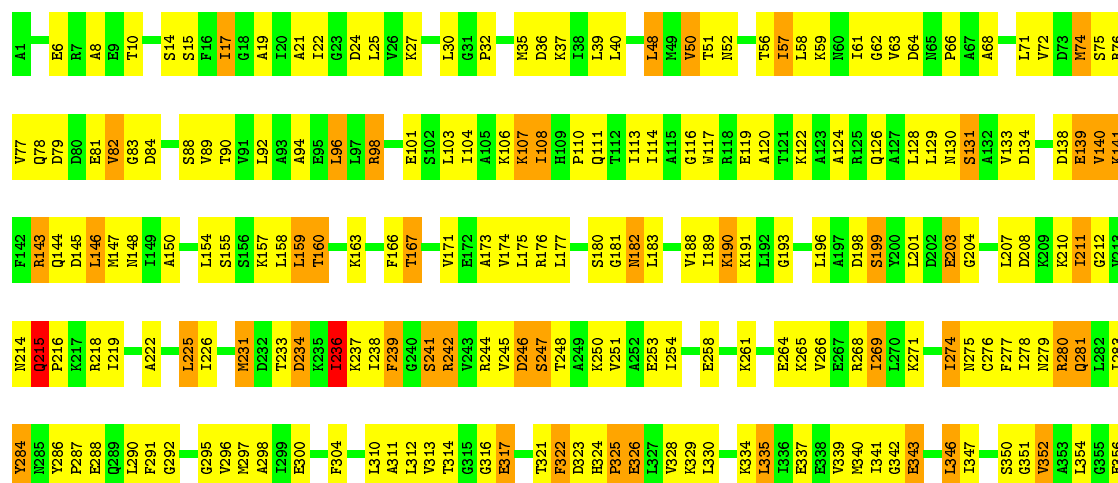
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

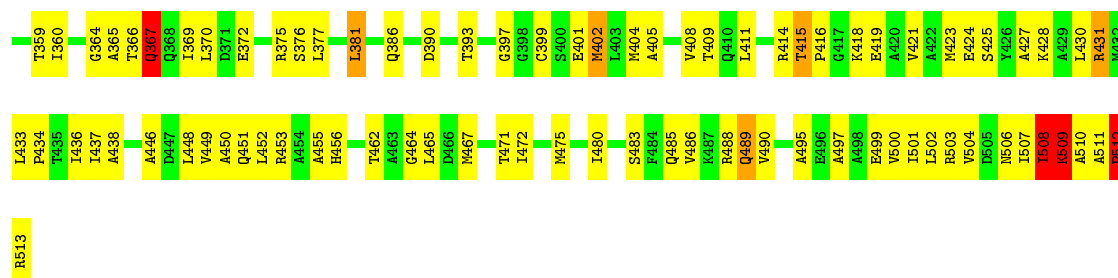
Chain C: 44% 43% 7%



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

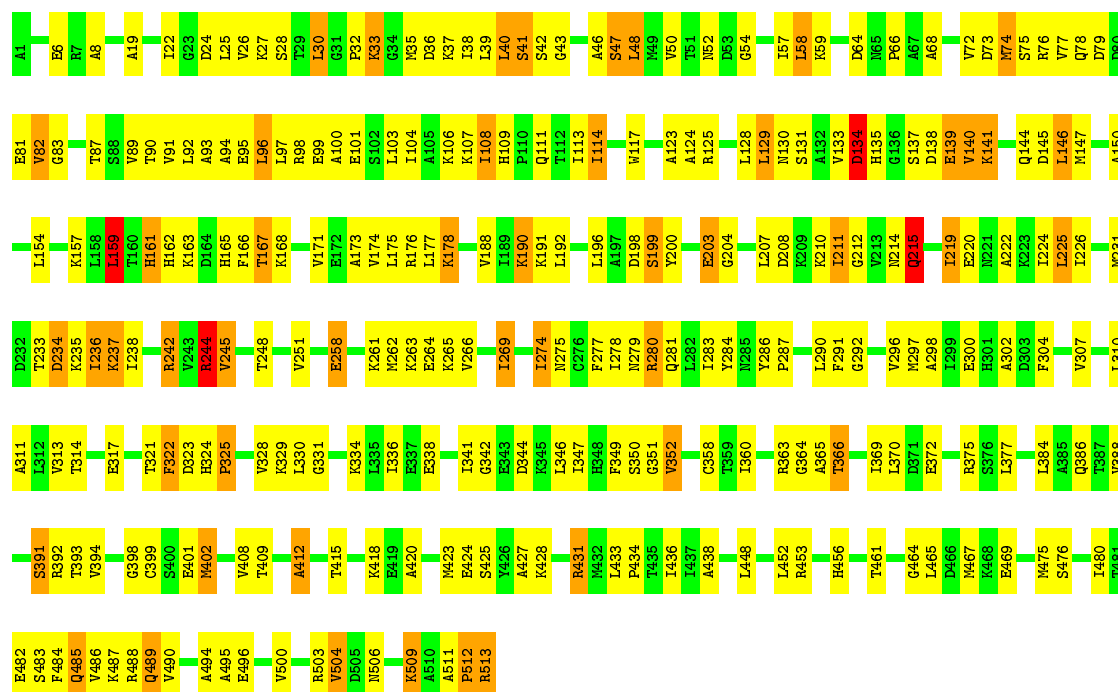
Chain D: 43% 46% 10%





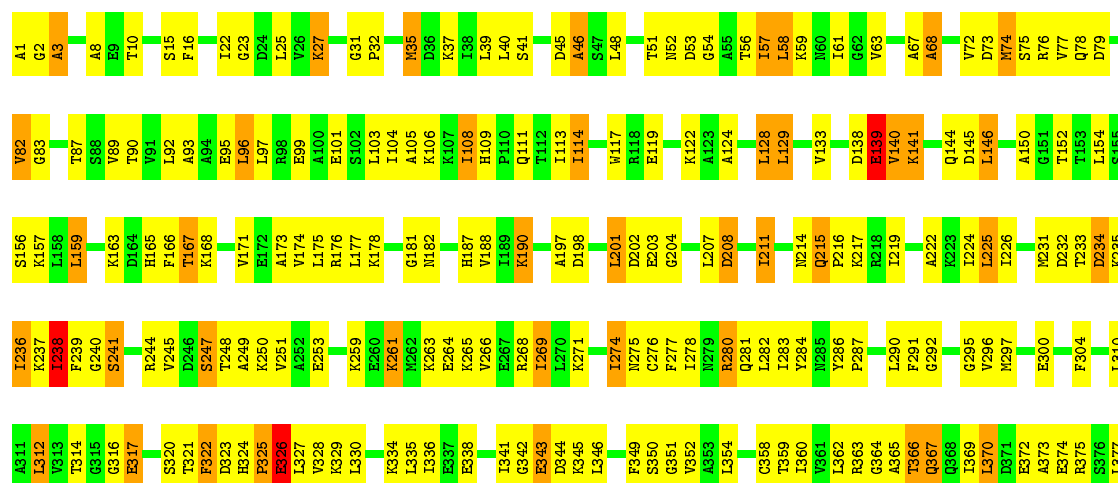
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

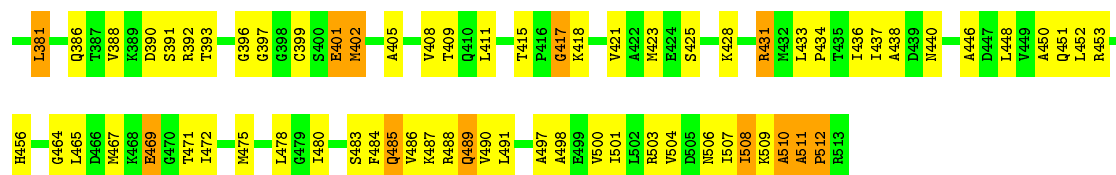
Chain E: 48% 41% 10%



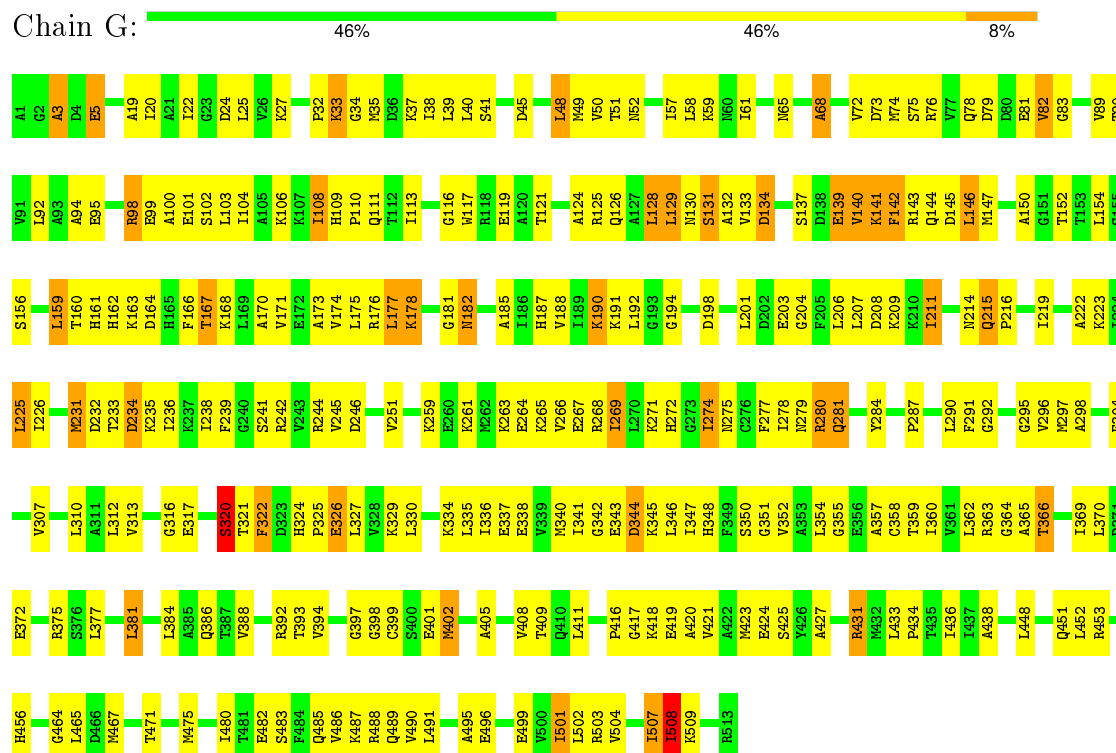
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain F: 45% 44% 10%

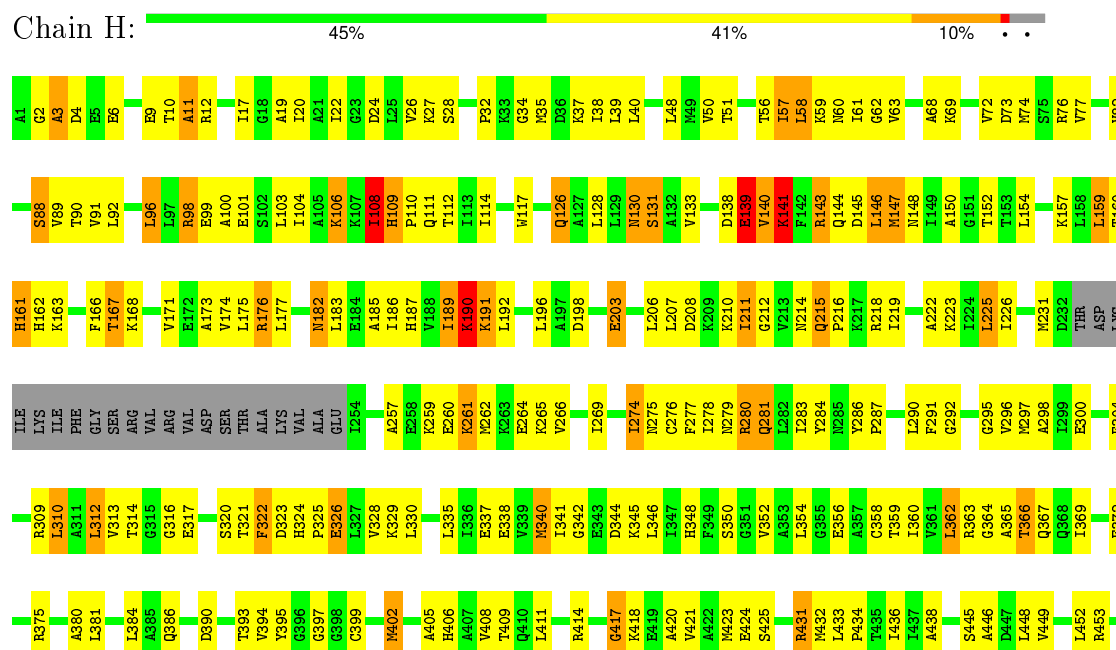




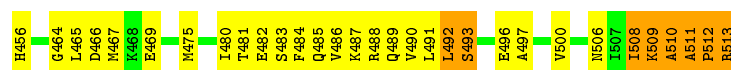
### • Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



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

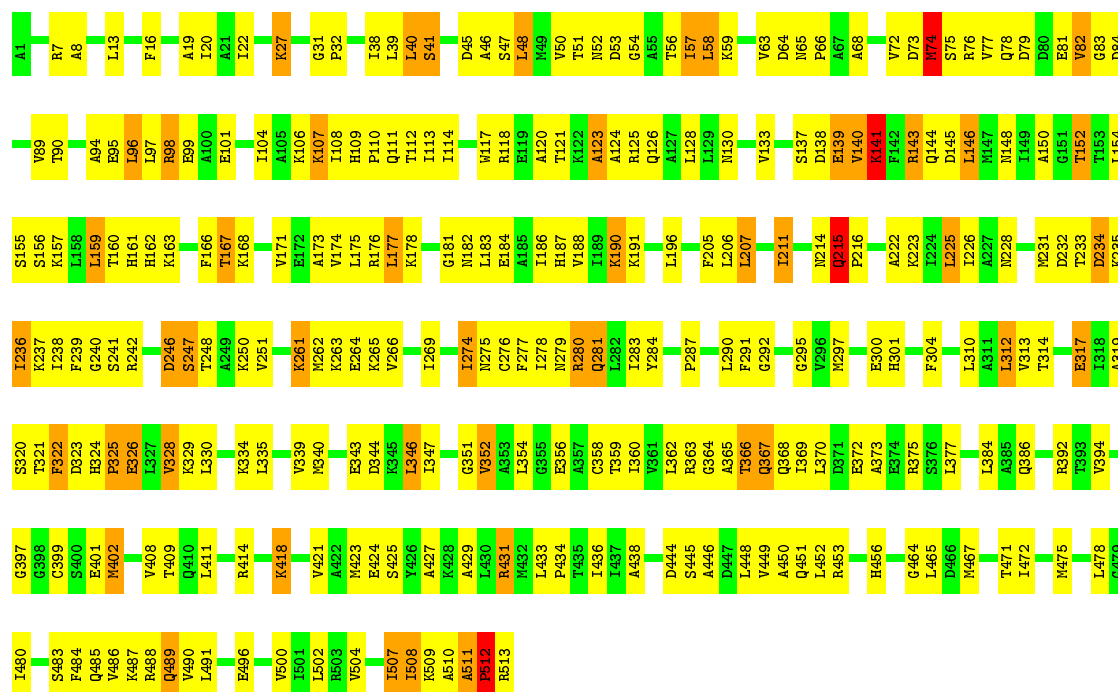






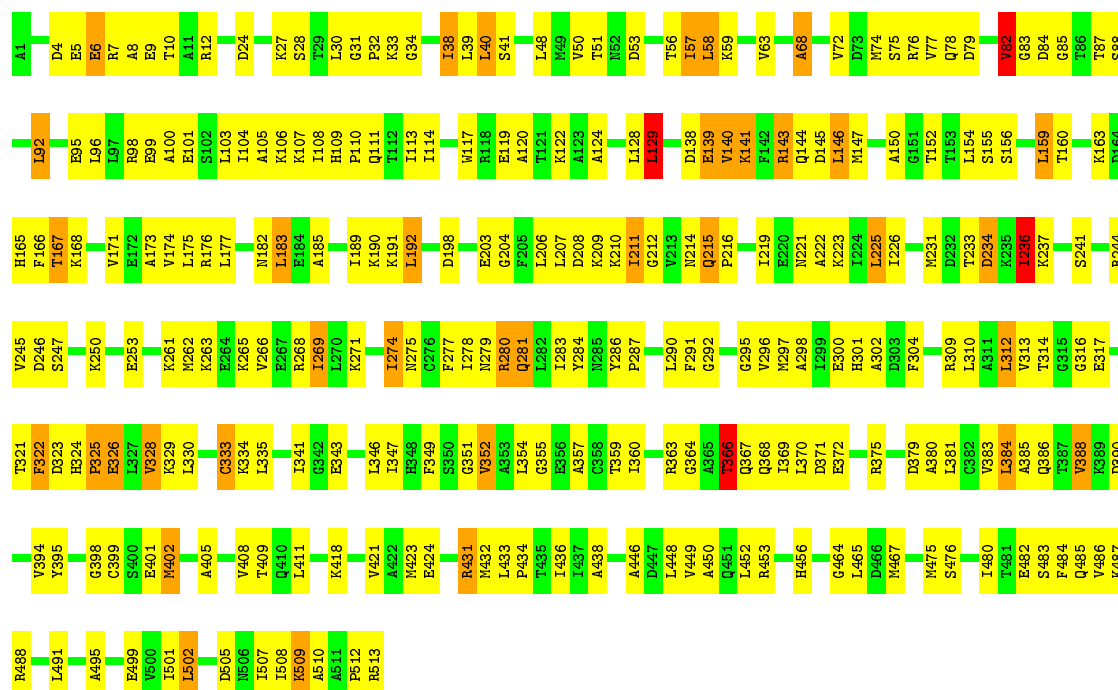
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain I: 46% 44% 9%



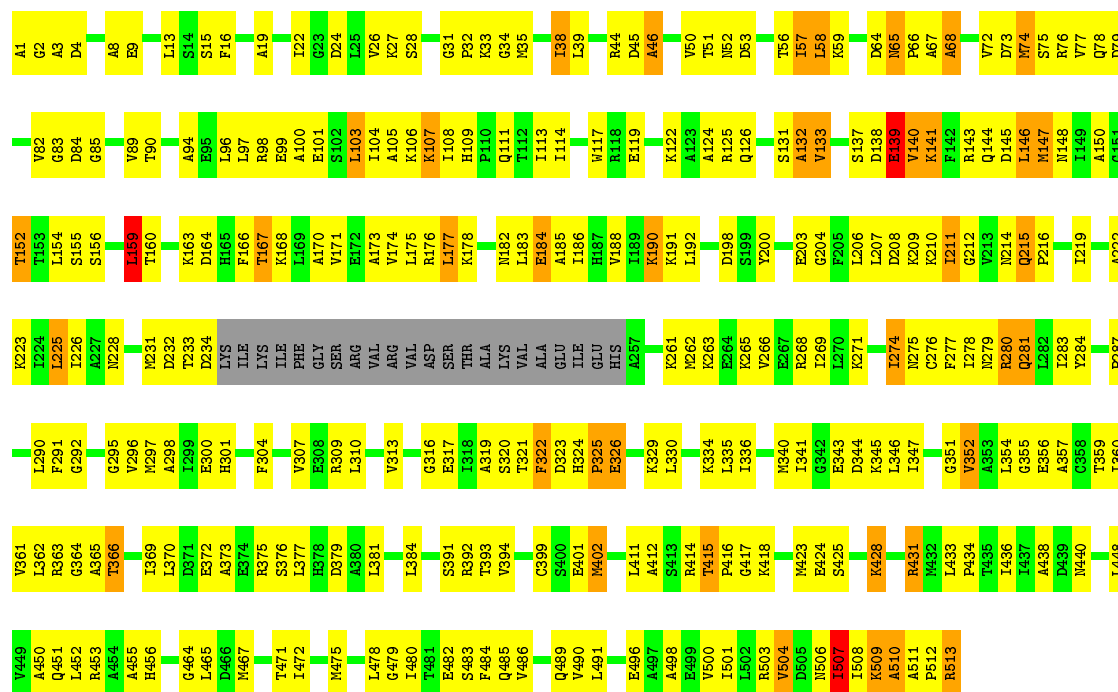
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain J: 48% 44% 7%



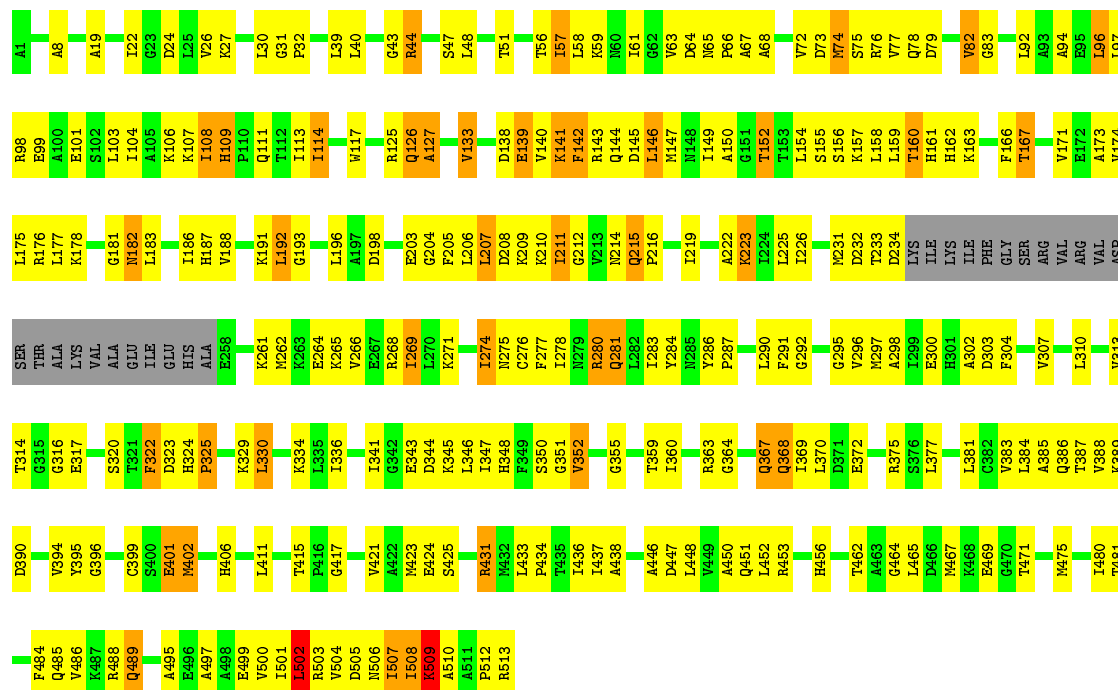
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain K: 

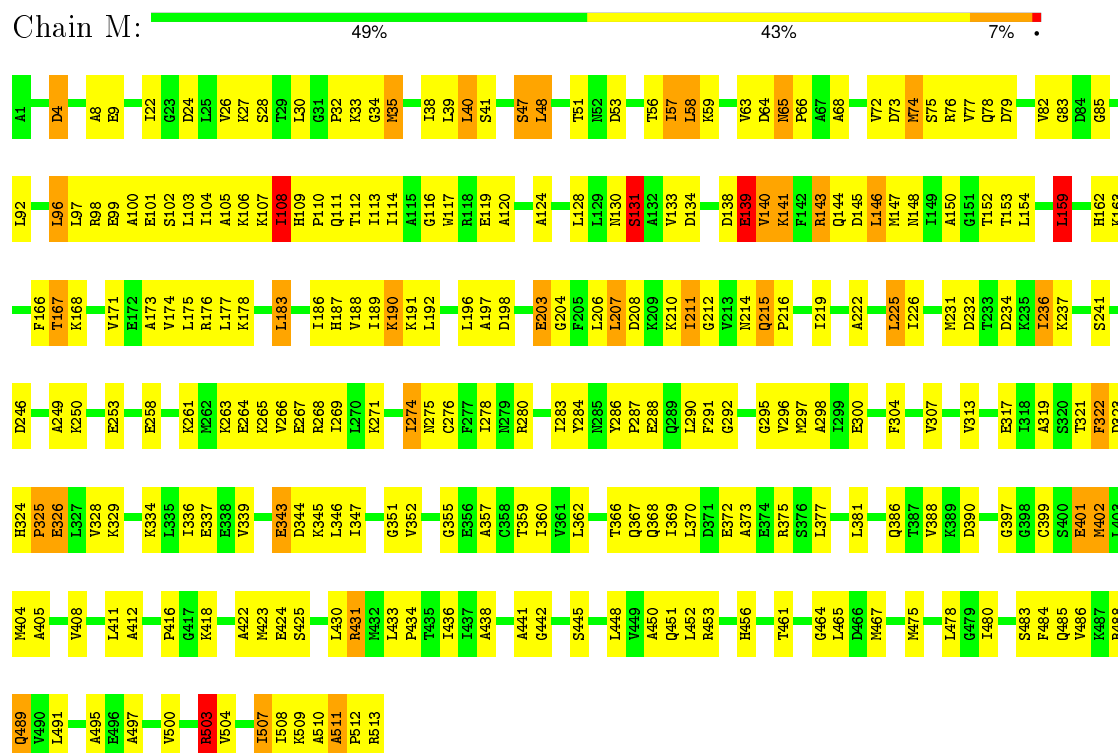


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

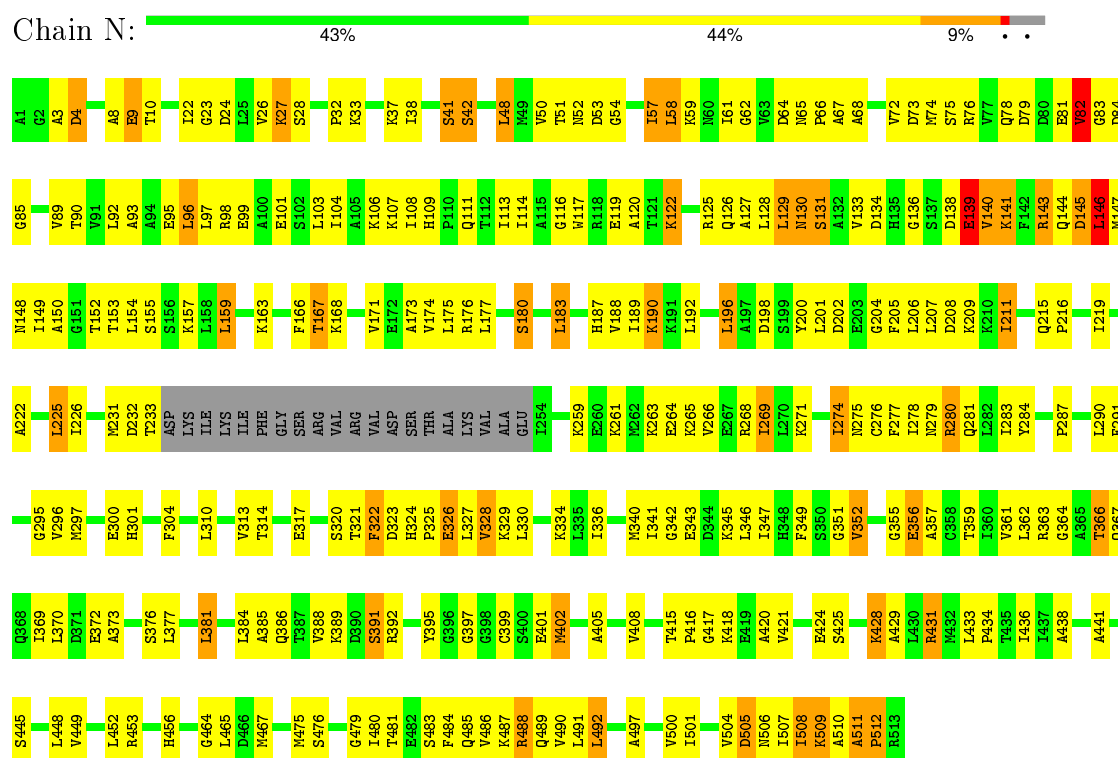
Chain L: 



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

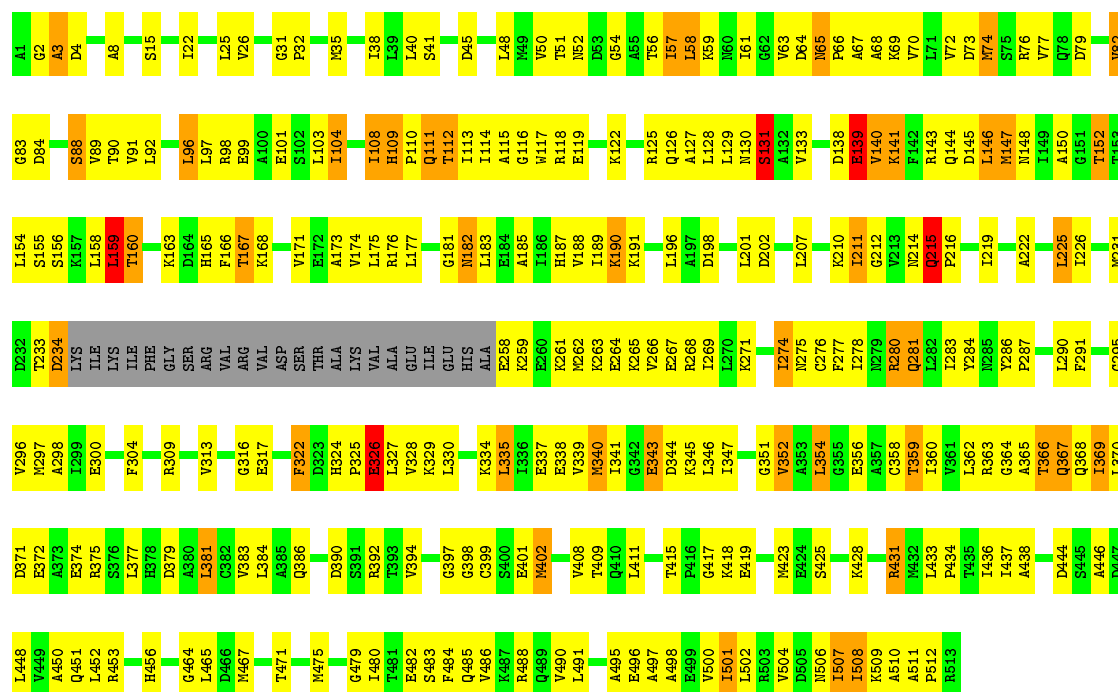


• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA



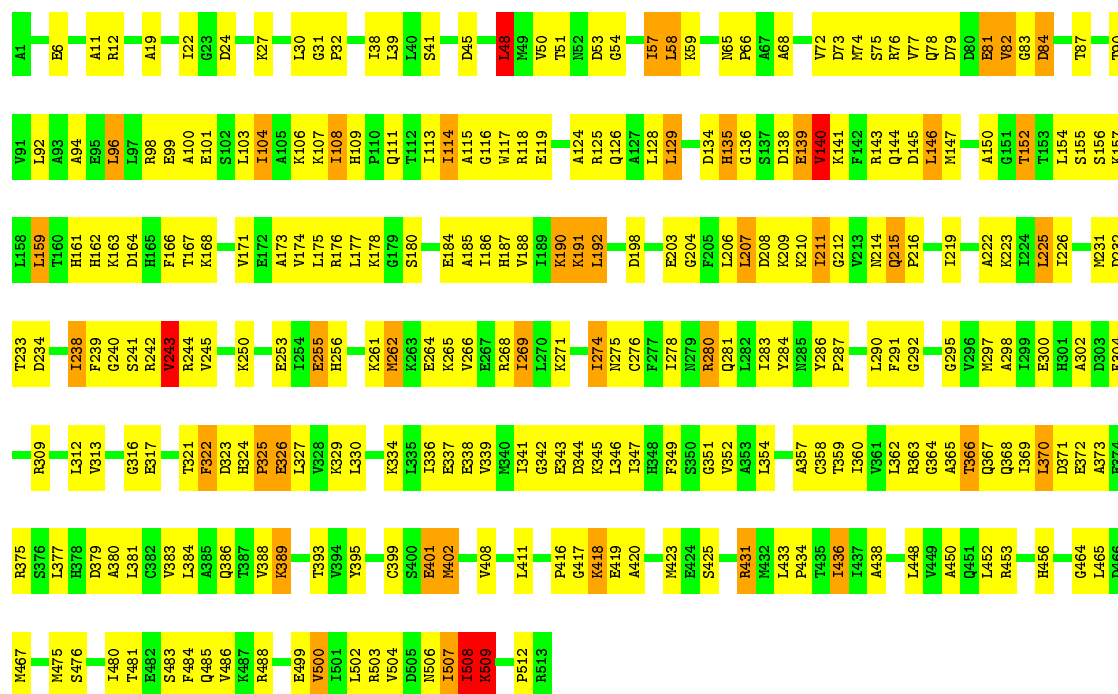
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA





• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain P: 47% 44% 8%



## 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, Not provided	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

### 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	0/3896	0.75	1/5249 (0.0%)
1	B	0.44	0/3896	0.74	0/5249
1	C	0.43	0/3711	0.72	0/5000
1	D	0.45	0/3896	0.73	3/5249 (0.1%)
1	E	0.45	0/3896	0.75	0/5249
1	F	0.46	0/3896	0.75	1/5249 (0.0%)
1	G	0.46	0/3896	0.76	1/5249 (0.0%)
1	H	0.45	0/3732	0.72	0/5028
1	I	0.45	0/3896	0.77	1/5249 (0.0%)
1	J	0.44	0/3896	0.71	0/5249
1	K	0.44	0/3719	0.71	0/5011
1	L	0.45	0/3714	0.71	0/5004
1	M	0.45	0/3896	0.73	1/5249 (0.0%)
1	N	0.43	0/3739	0.73	1/5038 (0.0%)
1	O	0.45	0/3714	0.75	0/5004
1	P	0.43	0/3896	0.76	1/5249 (0.0%)
All	All	0.45	0/61289	0.74	10/82575 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	PRO	N-CA-CB	-7.85	93.88	103.30
1	N	488	ARG	CB-CA-C	-6.44	97.51	110.40
1	P	508	ILE	CB-CA-C	-6.11	99.37	111.60
1	I	74	MET	CA-CB-CG	6.06	123.60	113.30
1	D	242	ARG	N-CA-CB	-5.80	100.16	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	311	0
1	B	3855	0	3970	315	0
1	C	3673	0	3778	314	0
1	D	3855	0	3970	311	0
1	E	3855	0	3970	285	0
1	F	3855	0	3970	330	0
1	G	3855	0	3970	321	0
1	H	3693	0	3795	306	0
1	I	3855	0	3970	322	0
1	J	3855	0	3970	293	0
1	K	3681	0	3782	313	0
1	L	3676	0	3777	298	0
1	M	3855	0	3970	282	0
1	N	3700	0	3802	303	0
1	O	3676	0	3777	307	0
1	P	3855	0	3970	291	0
All	All	60649	0	62411	4706	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 38.

The worst 5 of 4706 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:O:146:LEU:HD12	1:O:171:VAL:HG13	1.25	1.16
1:B:146:LEU:HD12	1:B:171:VAL:HG13	1.24	1.12
1:L:146:LEU:HD12	1:L:171:VAL:HG13	1.31	1.09
1:A:266:VAL:HB	1:A:290:LEU:HD21	1.35	1.08
1:D:266:VAL:HB	1:D:290:LEU:HD21	1.32	1.08

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%)	459 (90%)	30 (6%)	22 (4%)	3	34
1	B	511/513 (100%)	455 (89%)	27 (5%)	29 (6%)	2	28
1	C	486/513 (95%)	442 (91%)	22 (4%)	22 (4%)	3	33
1	D	511/513 (100%)	456 (89%)	22 (4%)	33 (6%)	1	25
1	E	511/513 (100%)	445 (87%)	26 (5%)	40 (8%)	1	20
1	F	511/513 (100%)	461 (90%)	19 (4%)	31 (6%)	2	26
1	G	511/513 (100%)	462 (90%)	25 (5%)	24 (5%)	3	32
1	H	488/513 (95%)	437 (90%)	24 (5%)	27 (6%)	2	29
1	I	511/513 (100%)	453 (89%)	27 (5%)	31 (6%)	2	26
1	J	511/513 (100%)	462 (90%)	27 (5%)	22 (4%)	3	34
1	K	487/513 (95%)	444 (91%)	20 (4%)	23 (5%)	3	32
1	L	486/513 (95%)	435 (90%)	28 (6%)	23 (5%)	3	32
1	M	511/513 (100%)	455 (89%)	33 (6%)	23 (4%)	3	33
1	N	489/513 (95%)	435 (89%)	30 (6%)	24 (5%)	3	31
1	O	486/513 (95%)	445 (92%)	18 (4%)	23 (5%)	3	32
1	P	511/513 (100%)	465 (91%)	21 (4%)	25 (5%)	3	31
All	All	8032/8208 (98%)	7211 (90%)	399 (5%)	422 (5%)	4	29

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	82	VAL
1	A	84	ASP
1	A	141	LYS
1	A	234	ASP



### 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%)	362 (88%)	47 (12%)	7	32
1	B	409/409 (100%)	367 (90%)	42 (10%)	9	37
1	C	389/409 (95%)	350 (90%)	39 (10%)	9	38
1	D	409/409 (100%)	362 (88%)	47 (12%)	7	32
1	E	409/409 (100%)	370 (90%)	39 (10%)	11	41
1	F	409/409 (100%)	364 (89%)	45 (11%)	8	34
1	G	409/409 (100%)	369 (90%)	40 (10%)	10	39
1	H	391/409 (96%)	349 (89%)	42 (11%)	8	36
1	I	409/409 (100%)	364 (89%)	45 (11%)	8	34
1	J	409/409 (100%)	372 (91%)	37 (9%)	12	44
1	K	390/409 (95%)	349 (90%)	41 (10%)	8	36
1	L	390/409 (95%)	354 (91%)	36 (9%)	11	43
1	M	409/409 (100%)	373 (91%)	36 (9%)	12	45
1	N	392/409 (96%)	344 (88%)	48 (12%)	6	31
1	O	390/409 (95%)	347 (89%)	43 (11%)	8	34
1	P	409/409 (100%)	360 (88%)	49 (12%)	6	31
All	All	6432/6544 (98%)	5756 (90%)	676 (10%)	13	36

5 of 676 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	108	ILE
1	I	409	THR
1	O	431	ARG
1	H	160	THR
1	I	40	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	489	GLN
1	J	130	ASN
1	O	451	GLN
1	I	126	GLN
1	I	410	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.