



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

Dec 4, 2017 – 11:49 AM EST

PDB ID : 5GW5  
EMDB ID: : EMD-9541  
Title : Structure of TRiC-AMP-PNP  
Authors : Zang, Y.; Jin, M.; Wang, H.; Cong, Y.  
Deposited on : unknown  
Resolution : 4.60 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-20030345

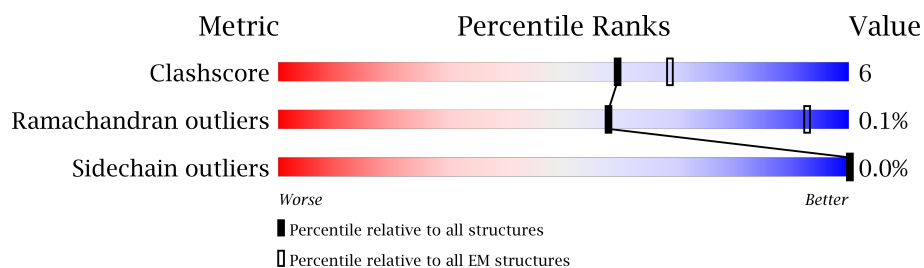
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 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	559	67% 31% .
1	a	559	97% .
2	B	527	76% 23% .
2	b	527	98% .
3	D	528	71% 27% .
3	d	528	98% .
4	E	562	68% 26% 6%
4	e	562	94% 6%
5	G	534	73% 24% .

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Mol	Chain	Length	Quality of chain
5	g	534	<div><div></div><div>97%</div><div></div></div>
6	H	550	<div><div></div><div>69%</div><div>25%</div><div>6%</div></div>
6	h	550	<div><div></div><div>94%</div><div>6%</div></div>
7	Q	568	<div><div></div><div>70%</div><div>25%</div><div></div></div>
7	q	568	<div><div></div><div>95%</div><div></div><div></div></div>
8	Z	546	<div><div></div><div>72%</div><div>26%</div><div></div></div>
8	z	546	<div><div></div><div>98%</div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 64544 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		
1	A	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		
2	B	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		
3	D	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		
4	E	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		
5	G	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		
6	H	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		

- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		
7	Q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		
8	Z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		

### 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.

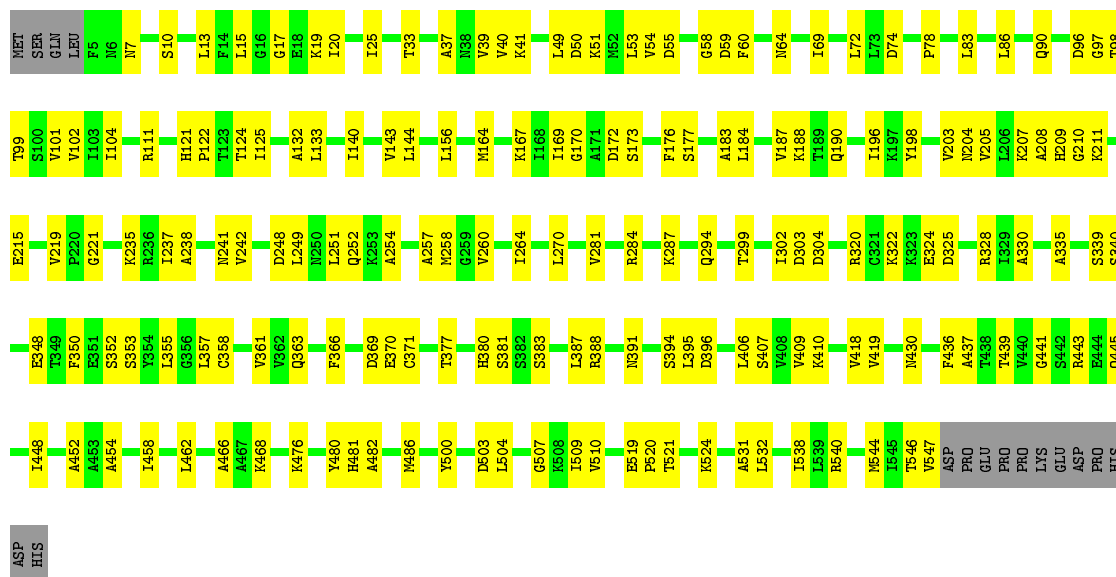
- Molecule 1: T-complex protein 1 subunit alpha

Chain a:  97%



- Molecule 1: T-complex protein 1 subunit alpha

Chain A:  67% 31%




- Molecule 2: T-complex protein 1 subunit beta

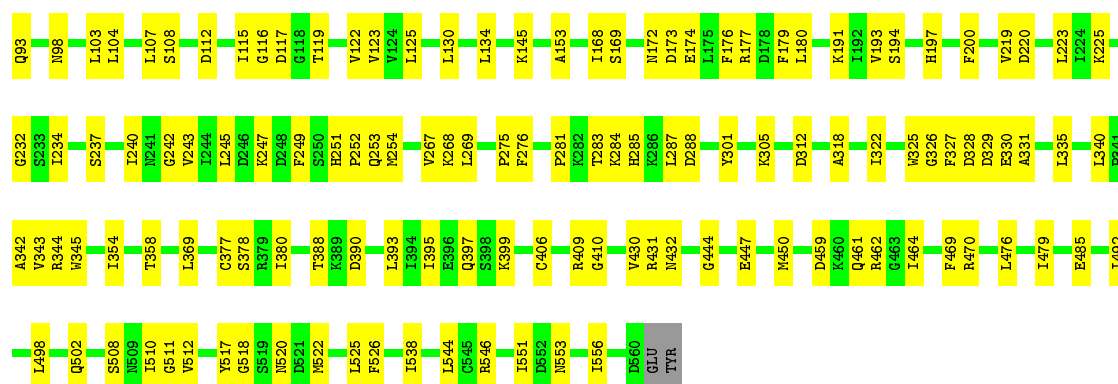
Chain b:  98%



- Molecule 2: T-complex protein 1 subunit beta

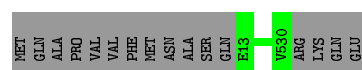
Chain B:  76% 23%





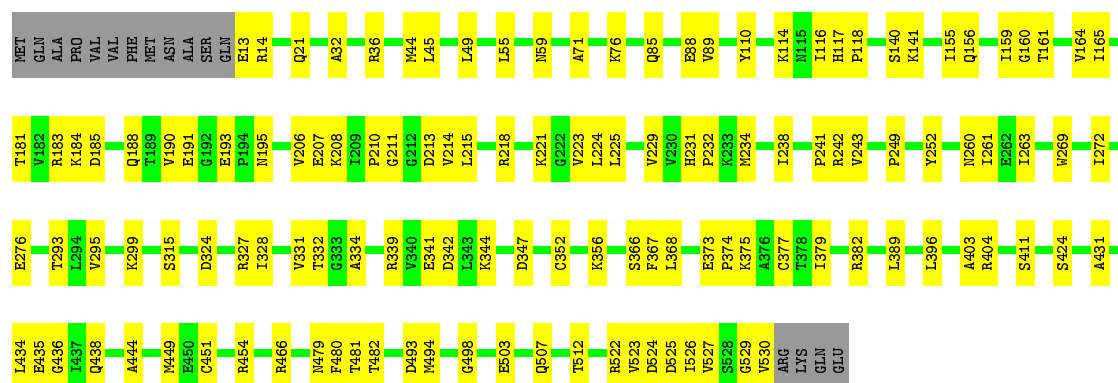
- Molecule 5: T-complex protein 1 subunit gamma

Chain g: 97%



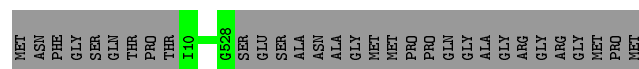
- Molecule 5: T-complex protein 1 subunit gamma

Chain G: 73%



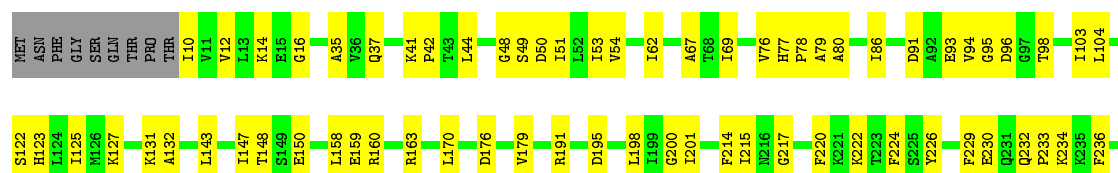
- Molecule 6: T-complex protein 1 subunit eta

Chain h: 94%

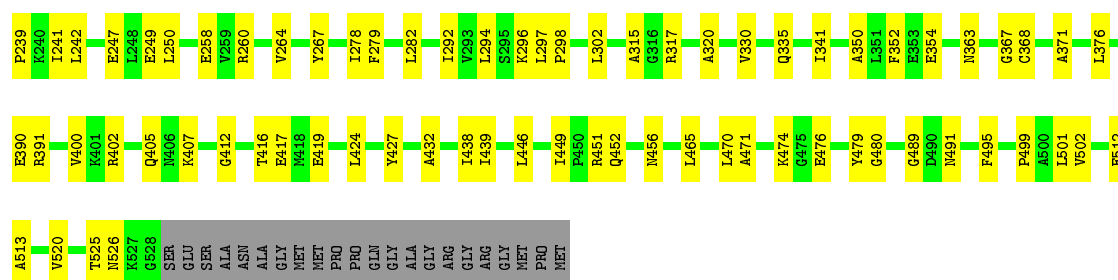


- Molecule 6: T-complex protein 1 subunit eta

Chain H: 69%

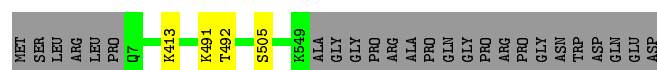






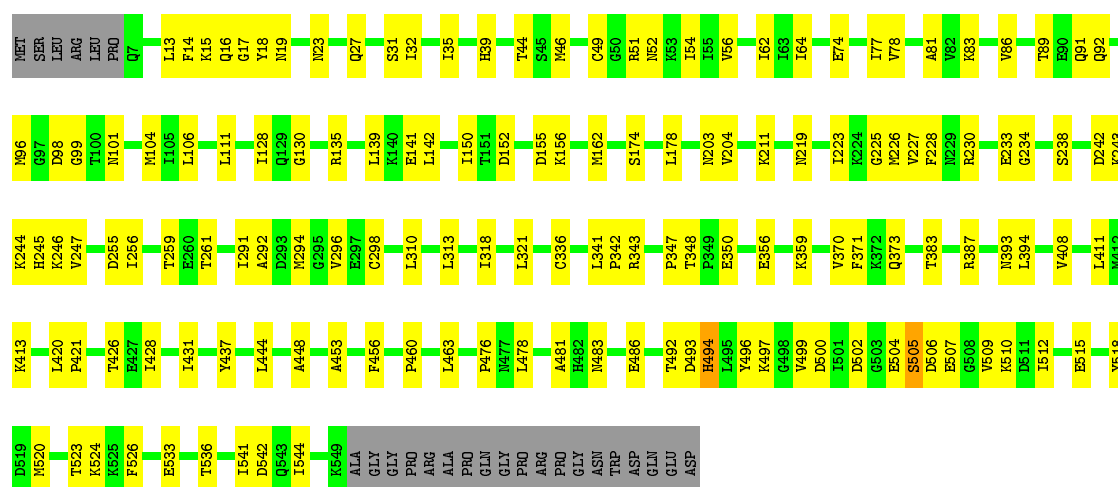
- Molecule 7: T-complex protein 1 subunit theta

Chain q: 95%



- Molecule 7: T-complex protein 1 subunit theta

Chain Q: 70%



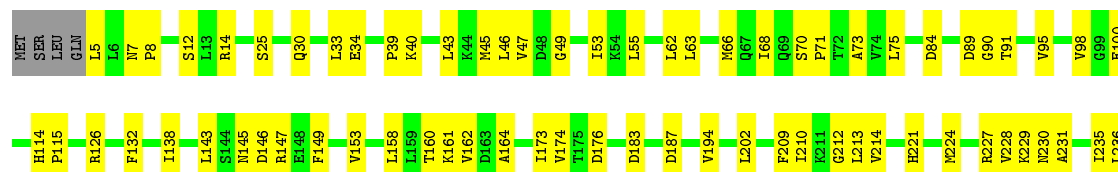
- Molecule 8: T-complex protein 1 subunit zeta

Chain z: 98%



- Molecule 8: T-complex protein 1 subunit zeta

Chain Z: 72%



L529	L348	I237
E532	I353	Y238
R538	V354	S239
SER	Y355	L240
THR	T358	E241
LEU	I359	Y242
LYS	E362	T245
GLU	K363	E246
THR	K367	V247
PRO	V367	Y253
GLN	T368	R259
	E369	
	N370	R267
		K268
	P373	D271
	K374	D271
	S375	L272
	C376	K273
	T377	L280
	K381	
	G382	C285
	S383	
	D393	D290
		K291
	R396	E292
	D397	F293
	G398	V294
	L399	I295
	V405	I296
		N297
	I411	Q298
		I301
	L422	A316
		L317
	V453	R318
	L458	
	V459	R322
	S462	K325
	V469	
	E476	L328
		V331
	E485	E335
	T486	A336
	R487	Q337
	L493	N338
		S339
		V340
		E341
		D342
		T518
		A524
		I347

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	67990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	0.23	0/4140	0.41	0/5585
1	a	0.23	0/4140	0.41	0/5585
2	B	0.23	0/3969	0.39	0/5348
2	b	0.23	0/3969	0.40	0/5348
3	D	0.23	0/4022	0.39	0/5421
3	d	0.23	0/4022	0.39	0/5421
4	E	0.23	0/4117	0.40	0/5539
4	e	0.23	0/4117	0.39	0/5539
5	G	0.22	0/4029	0.39	0/5442
5	g	0.22	0/4029	0.40	0/5442
6	H	0.23	0/4018	0.39	0/5422
6	h	0.23	0/4018	0.40	0/5422
7	Q	0.29	1/4175 (0.0%)	0.40	0/5636
7	q	0.29	1/4175 (0.0%)	0.41	0/5636
8	Z	0.23	0/4162	0.41	0/5624
8	z	0.23	0/4162	0.39	0/5624
All	All	0.24	2/65264 (0.0%)	0.40	0/88034

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	q	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	q	413	LYS	C-N	11.30	1.55	1.34
7	Q	413	LYS	C-N	11.25	1.55	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	q	491	LYS	Peptide
7	q	505	SER	Peptide

## 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	4103	0	4269	124	0
1	a	4103	0	4269	0	0
2	B	3930	0	4034	88	0
2	b	3930	0	4034	0	0
3	D	3985	0	4157	101	0
3	d	3985	0	4157	0	0
4	E	4068	0	4163	107	0
4	e	4068	0	4163	0	0
5	G	3982	0	4123	87	0
5	g	3982	0	4123	0	0
6	H	3969	0	4055	93	0
6	h	3969	0	4055	0	0
7	Q	4125	0	4260	104	0
7	q	4125	0	4260	0	0
8	Z	4110	0	4204	95	0
8	z	4110	0	4204	0	0
All	All	64544	0	66530	724	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 6.

The worst 5 of 724 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)
7:Q:493:ASP:O	7:Q:494:HIS:CG	2.14	1.00
1:A:252:GLN:HA	1:A:303:ASP:HB2	1.76	0.82
2:B:39:PRO:HB3	2:B:162:SER:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:193:VAL:HG13	4:E:200:PHE:HD2	1.77	0.78
7:Q:493:ASP:O	7:Q:494:HIS:CD2	2.36	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	541/559 (97%)	507 (94%)	33 (6%)	1 (0%)	51	85
1	a	541/559 (97%)	501 (93%)	39 (7%)	1 (0%)	51	85
2	B	515/527 (98%)	490 (95%)	23 (4%)	2 (0%)	38	77
2	b	515/527 (98%)	486 (94%)	29 (6%)	0	100	100
3	D	519/528 (98%)	494 (95%)	25 (5%)	0	100	100
3	d	519/528 (98%)	494 (95%)	24 (5%)	1 (0%)	51	85
4	E	526/562 (94%)	502 (95%)	24 (5%)	0	100	100
4	e	526/562 (94%)	503 (96%)	23 (4%)	0	100	100
5	G	516/534 (97%)	496 (96%)	20 (4%)	0	100	100
5	g	516/534 (97%)	491 (95%)	25 (5%)	0	100	100
6	H	517/550 (94%)	497 (96%)	20 (4%)	0	100	100
6	h	517/550 (94%)	497 (96%)	20 (4%)	0	100	100
7	Q	541/568 (95%)	520 (96%)	19 (4%)	2 (0%)	38	77
7	q	541/568 (95%)	516 (95%)	25 (5%)	0	100	100
8	Z	532/546 (97%)	513 (96%)	19 (4%)	0	100	100
8	z	532/546 (97%)	518 (97%)	14 (3%)	0	100	100
All	All	8414/8748 (96%)	8025 (95%)	382 (4%)	7 (0%)	58	89

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Q	505	SER
7	Q	494	HIS
2	B	5	ILE
3	d	213	VAL
2	B	467	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	455/471 (97%)	455 (100%)	0	100	100
1	a	455/471 (97%)	455 (100%)	0	100	100
2	B	432/441 (98%)	432 (100%)	0	100	100
2	b	432/441 (98%)	432 (100%)	0	100	100
3	D	447/453 (99%)	447 (100%)	0	100	100
3	d	447/453 (99%)	447 (100%)	0	100	100
4	E	454/483 (94%)	454 (100%)	0	100	100
4	e	454/483 (94%)	454 (100%)	0	100	100
5	G	441/455 (97%)	441 (100%)	0	100	100
5	g	441/455 (97%)	441 (100%)	0	100	100
6	H	432/454 (95%)	432 (100%)	0	100	100
6	h	432/454 (95%)	432 (100%)	0	100	100
7	Q	454/473 (96%)	454 (100%)	0	100	100
7	q	454/473 (96%)	453 (100%)	1 (0%)	94	96
8	Z	451/463 (97%)	451 (100%)	0	100	100
8	z	451/463 (97%)	451 (100%)	0	100	100
All	All	7132/7386 (97%)	7131 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	q	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	466	GLN
5	g	479	ASN
8	z	230	ASN
5	g	85	GLN
5	G	85	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.