



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 07:14 PM EDT

PDB ID : 5TAU
EMDB ID: : EMD-8385
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 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 : 1.7.1 (RC1), CSD as537be (2016)
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) : rb-20027939

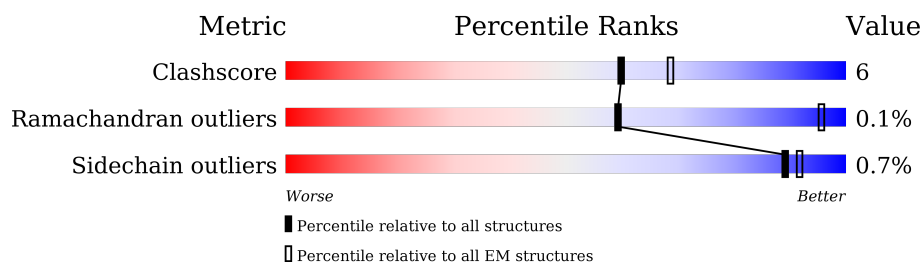
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121436 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.

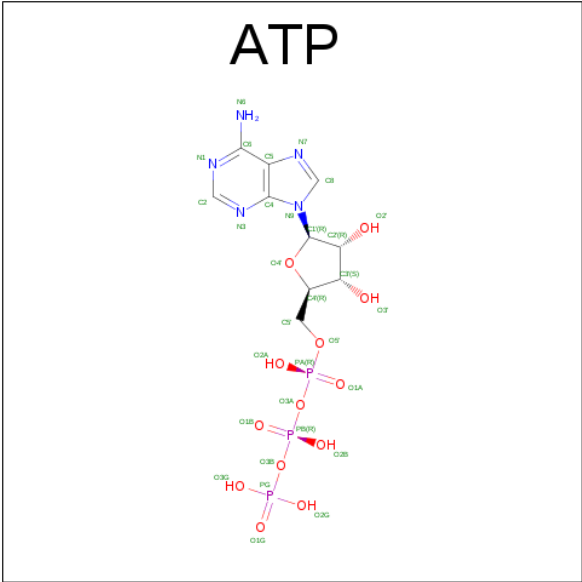
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

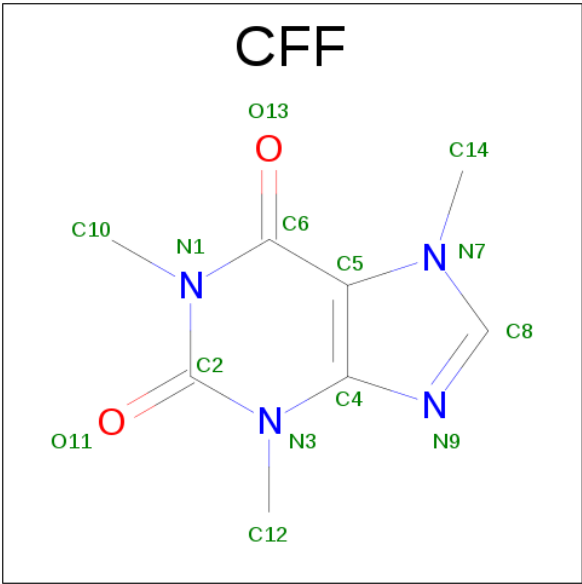
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

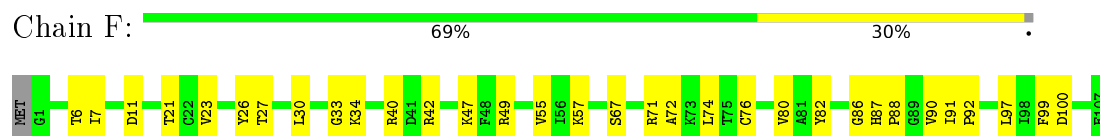
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

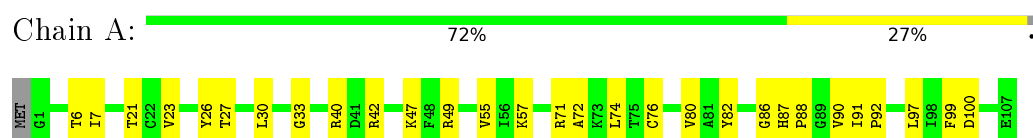
3 Residue-property plots

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.

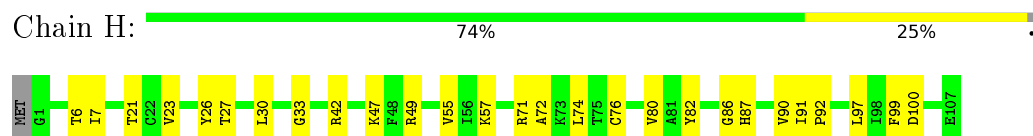
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



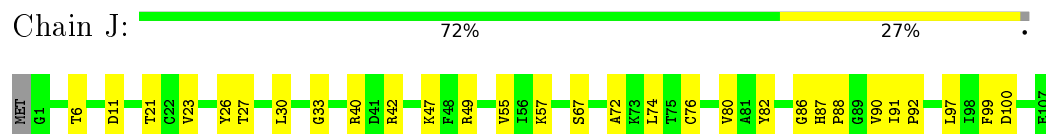
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



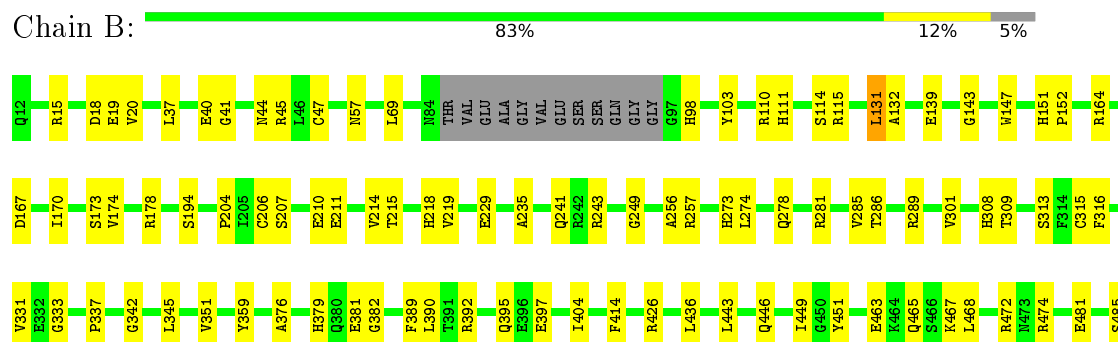
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1











Q4949	A4746	SER	L4089
K4957	E4749	ALA	D4063
C4958	A4752	GLY	R4085
F4959	G4763	ASP	T4104
I4960	T4766	LEU	G4105
C4961	W4778	ALA	P4106
G4964	D4786	GLY	M4120
S4965	F4789	GLY	D4138
D4966	S4799	SER	E4152
Y4967	L4800	TRP	R4159
F4968	H4803	GLY	A4167
D4969	H4812	ALA	E4168
H4973	I4826	GLY	S4169
G4974	S4829	GLU	E4172
F4975	M4839	ALA	Y4173
E4976	L4844	GLU	F4174
T4977	R4860	GLU	R4175
H4978	C4876	ASP	P4176
T4979	Y4888	GLU	Y4177
L4980	R4892	ASP	R4180
E4981	G4898	GLU	I4183
E4982	D4899	M4627	I4190
H4983	P4904	Y4666	E4191
M4984	R4913	V4669	R4192
L4985	T4919	R4673	I4193
A4986	F4922	E4674	Y4194
M4993	F4923	I4681	M4201
I4996	V4924	Y4687	Q4204
F5028	L4928	K4698	L4577
R5029	I4931	G4699	Y4580
Q5035	A4939	D4702	K4581
L5036	D4945	V4705	V4582
S5037		M4714	S4583
		M4743	D4584
			P4587
			GLY
			GLU
			ASP
			ASP
			MET
			GLU
			GLY

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ZN, ATP

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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25424	0.53	8/34530 (0.0%)
2	E	0.29	0/25424	0.53	9/34530 (0.0%)
2	G	0.29	0/25424	0.53	8/34530 (0.0%)
2	I	0.29	0/25424	0.53	8/34530 (0.0%)
All	All	0.29	0/105032	0.53	33/142612 (0.0%)

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
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.24	134.26	115.30
2	E	131	LEU	CA-CB-CG	8.24	134.25	115.30
2	I	131	LEU	CA-CB-CG	8.23	134.24	115.30
2	G	131	LEU	CA-CB-CG	8.23	134.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4985	LEU	CA-CB-CG	7.85	133.36	115.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	818	0	824	18	0
1	F	818	0	824	20	0
1	H	818	0	824	15	0
1	J	818	0	824	17	0
2	B	29495	0	24734	313	0
2	E	29495	0	24734	312	0
2	G	29495	0	24734	310	0
2	I	29495	0	24734	314	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121436	0	102320	1289	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 1289 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)
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.60	0.90
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.60	0.90
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.60	0.89
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.60	0.89
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.86	0.76

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	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2926 (90%)	304 (9%)	5 (0%)	52	86
2	E	3235/4416 (73%)	2924 (90%)	306 (10%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2925 (90%)	305 (9%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2922 (90%)	308 (10%)	5 (0%)	52	86
All	All	13360/18096 (74%)	12077 (90%)	1263 (10%)	20 (0%)	59	90

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU

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Mol	Chain	Res	Type
2	I	4985	LEU
2	E	4985	LEU
2	G	4985	LEU
2	B	1708	ARG

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2492/3022 (82%)	2473 (99%)	19 (1%)	86	94
2	E	2492/3022 (82%)	2473 (99%)	19 (1%)	86	94
2	G	2492/3022 (82%)	2473 (99%)	19 (1%)	86	94
2	I	2492/3022 (82%)	2473 (99%)	19 (1%)	86	94
All	All	10320/12444 (83%)	10244 (99%)	76 (1%)	89	94

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4839	MET
2	E	1141	ARG
2	G	4085	ARG
2	I	4913	ARG
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3946	GLN

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Mol	Chain	Res	Type
2	E	273	HIS
2	G	3946	GLN
2	I	3960	GLN
2	I	4142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.61	1 (3%)
4	CFF	B	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	E	5101	-	26,33,33	0.93	1 (3%)	26,52,52	1.62	1 (3%)
4	CFF	E	5102	-	8,15,15	2.38	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	G	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.62	1 (3%)
4	CFF	G	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	I	5101	-	26,33,33	0.94	1 (3%)	26,52,52	1.61	1 (3%)
4	CFF	I	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.25	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C4-N3	-4.57	1.33	1.39
4	G	5102	CFF	C4-N3	-4.51	1.33	1.39
4	I	5102	CFF	C4-N3	-4.50	1.33	1.39
4	B	5102	CFF	C4-N3	-4.50	1.33	1.39
4	I	5102	CFF	C6-N1	-3.82	1.32	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-6.41	123.83	128.87
3	E	5101	ATP	N3-C2-N1	-6.37	123.87	128.87
3	I	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
3	B	5101	ATP	N3-C2-N1	-6.35	123.88	128.87
4	G	5102	CFF	C14-N7-C8	-2.54	112.07	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.97
1	I	4345:UNK	C	4540:PHE	N	72.97
1	E	4345:UNK	C	4540:PHE	N	72.97
1	G	4345:UNK	C	4540:PHE	N	72.97
1	B	3613:UNK	C	3639:THR	N	44.25