



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:13 pm GMT

PDB ID : 5TAP
EMDB ID: : EMD-8381
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc29047

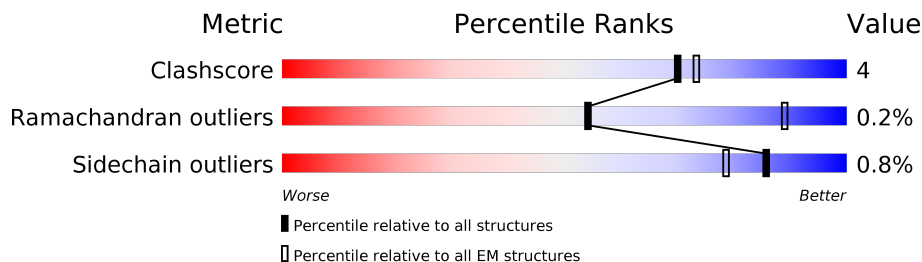
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 ≥ 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	85% 14% .
1	F	108	85% 14% .
1	H	108	83% 16% .
1	J	108	84% 15% .
2	B	4416	85% 9% 5%
2	E	4416	85% 9% 5%
2	G	4416	86% 9% 5%
2	I	4416	86% 9% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

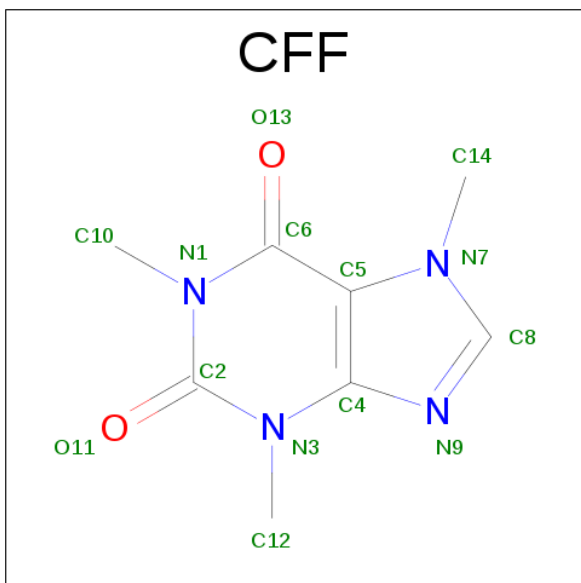
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



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

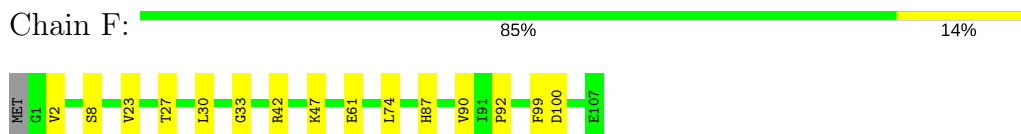
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

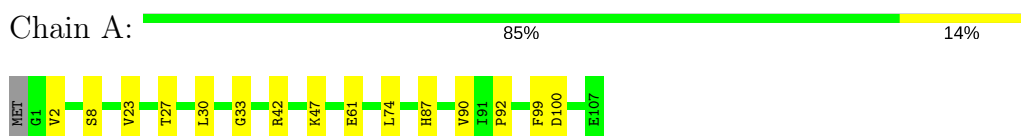
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

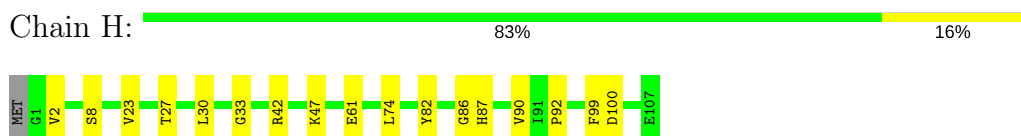
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



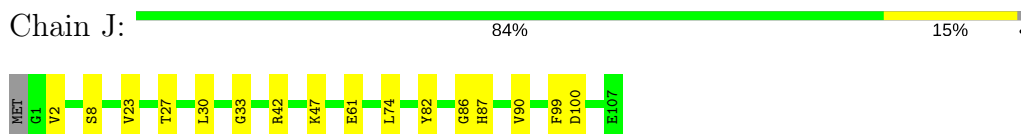
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



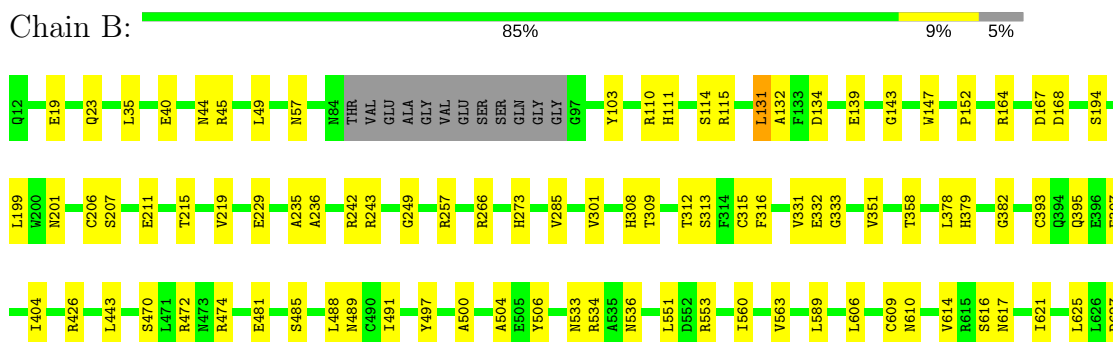
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

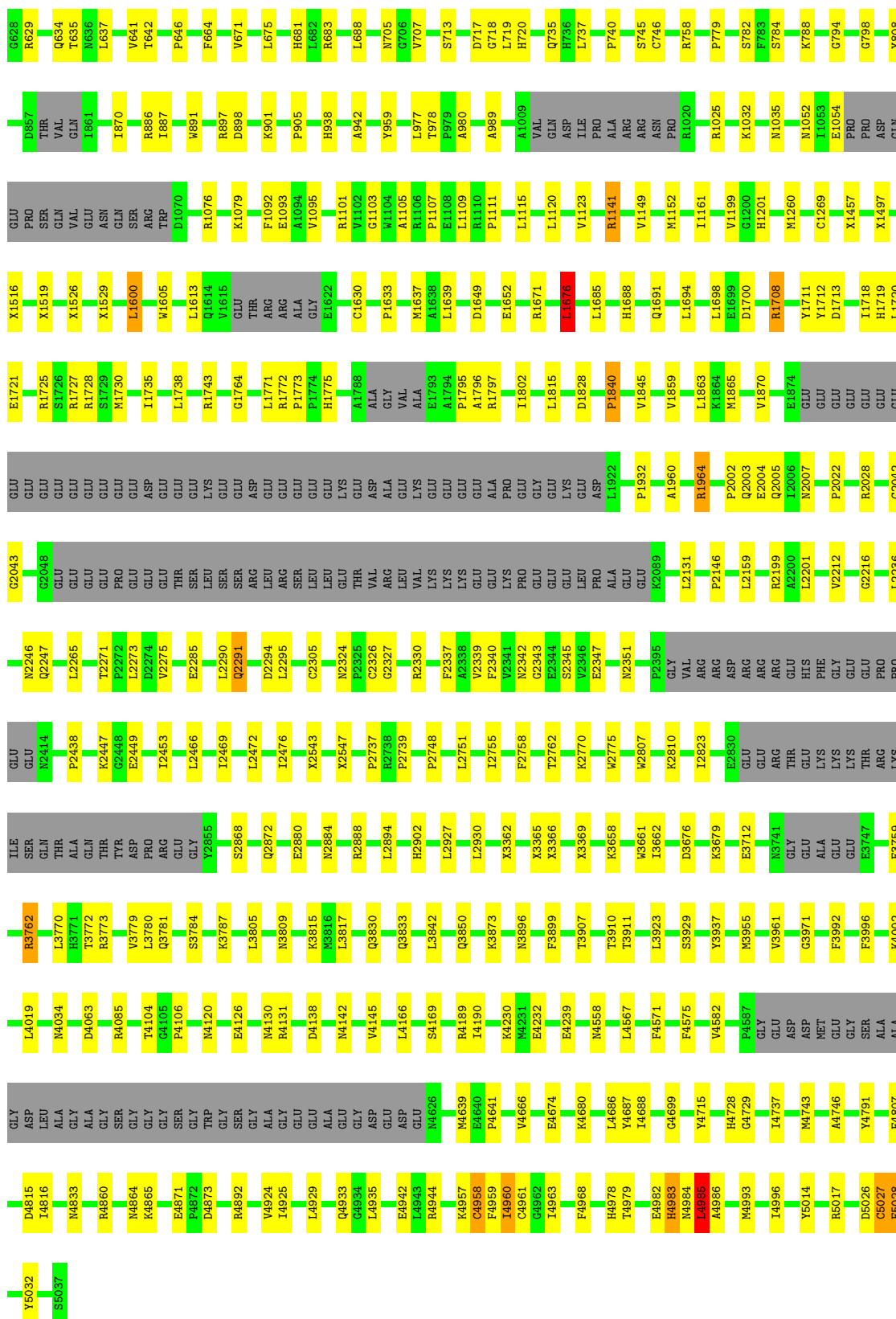


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1



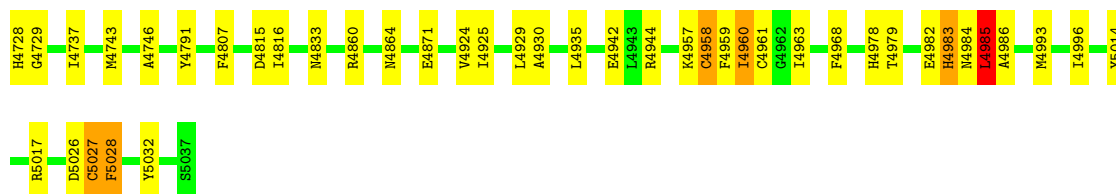


- Molecule 2: Ryanodine receptor 1

Chain E:

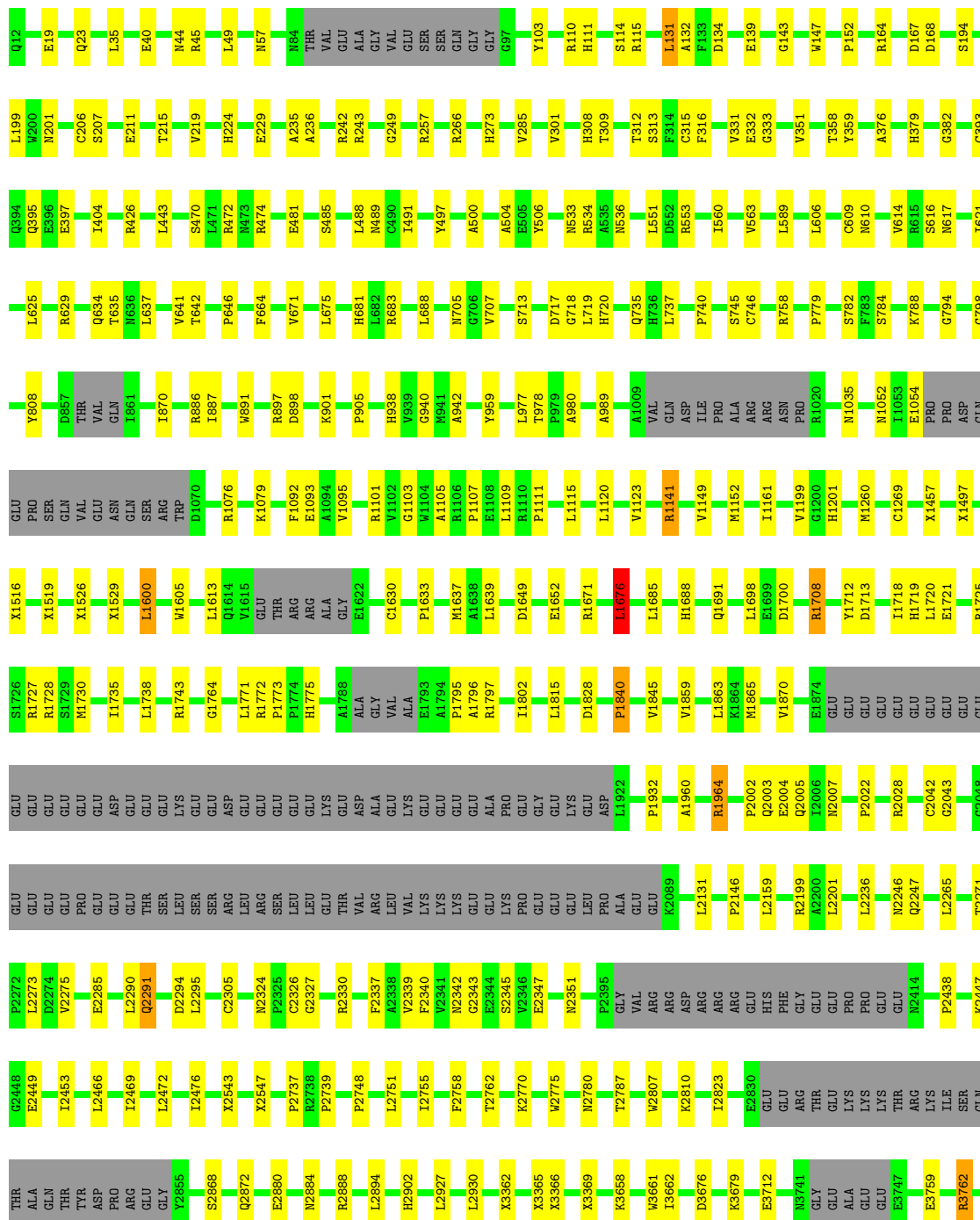


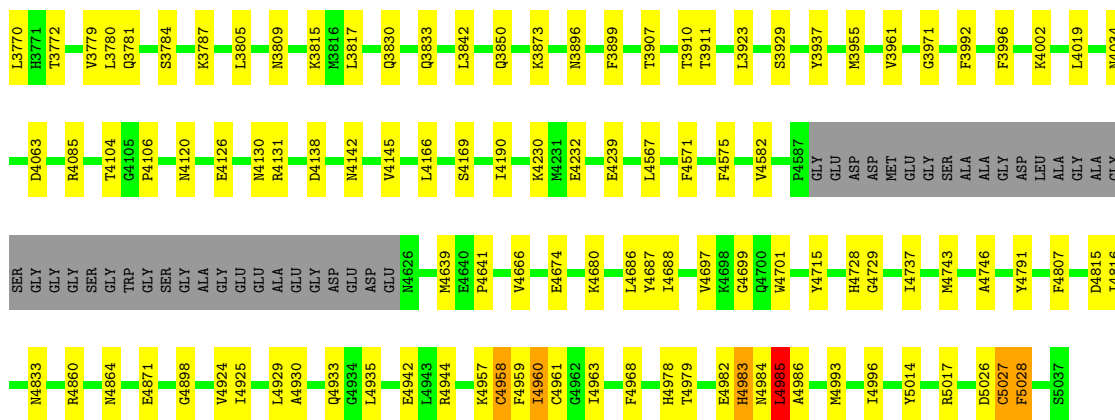
ASP	F3992	GLU	GLU	HIS	G2216	G2048	GLU	L1720	PRO	Y808	P627	C393	L199	Q12
ASP	F3992	ALA	LYS	PHE	G2216	GLU	GLU	E1721	ASP	G941	G628	Q394	W200	Q12
GLU	F3996	GLU	LYS	GLU	L2236	GLU	GLU	R1725	GLU	G941	R629	Q395	N201	E19
GLY		THR	THR	GLU	L2236	GLU	GLU	R1726	PRO	D857	G634	E396	C206	Q23
SER	K4002	ARG	ARG	PRO	N2246	GLU	PRO	R1727	SER	THR	T635	E397	S207	
ALA	L4019	LIE	LIE	PRO	Q2247	GLU	GLU	R1728	GLM	VAL	R636	I404	E211	L35
ALA		GLU	GLU	GLU	L2257	GLU	GLU	I1735	VAL	GLN	L637	I404	E211	
GLY		SER	SER	GLU	L2257	GLU	GLU	I1735	GLU	GLU	L637	R426	E40	E40
ASP	M4034	GLN	GLN	N2414	L2265	GLU	GLU	L1738	ASN	ASN	V641	R426	T215	
LEU		THR	THR	SER	L2265	THR	LYS	L1738	GLM	R886	T642	L443	V219	N44
ALA	D4063	ALA	ALA	P2438	T2271	GLU	GLU	R1743	GLM	I887	T642	L443	V219	R45
GLY		GLN	LEU	P2438	T2271	GLU	GLU	R1743	SER	I887	T642	L443	V219	
ALA	R4085	THR	SER	K2447	P2272	SER	ASP	G1764	ARG	W891	P646	S470	H224	L49
GLY		THR	SER	G2448	L2273	SER	GLU	G1764	ARG	W891	P646	L471	H224	
SER	T4104	ASP	ARG	E2449	D2274	ARG	GLU	L1771	THR	R897	V671	N473	E229	N57
GLY	G4105	PRO	LEU	D2274	V2275	LEU	GLU	L1771	GLU	D898	V671	R474	E229	
GLY	P4106	ARG	ARG	A2276	A2276	ARG	GLU	R1772	GLU	D898	V671	R474	E229	
GLY		GLU	GLU	L2466	E2285	SER	GLU	P1773	GLU	K901	L675	E481	A235	N84
SER		GLY	LEU	L2466	E2285	LEU	LYS	P1773	GLU	K901	L675	E481	A236	THR
GLY		GLY	LEU	L2466	E2285	LEU	LYS	H1775	GLU	P905	H681	S485	R242	VAL
GLY		GLY	LEU	L2469	L2290	THR	ASP	V1615	GLU	P905	H681	S485	R242	GLU
TRP	E4126	TRP	GLU	L2469	L2290	THR	ALA	V1615	GLU	P905	H681	S485	R243	ALA
GLY		GLY	THR	L2472	Q2281	VAL	GLU	A1788	F1092	H838	R683	L488	R249	GLY
SER	N4130	SER	VAL	L2472	D2294	GLU	LYS	ALA	E1093	V939	R683	L488	R249	VAL
GLY	R4131	GLY	VAL	L2476	L2295	GLU	LYS	GLY	A1094	G940	L688	N489	G249	GLU
ALA		GLY	LEU	L2476	L2295	GLU	GLU	VAL	ARG	N941	L688	N489	G249	GLU
GLY	D4138	GLY	LEU	L2476	L2295	VAL	GLU	ALA	V1095	A942	N705	I491	R257	SER
GLU		GLY	VAL	L2476	L2295	VAL	GLU	ALA	ALA	A942	N705	I491	R257	SER
GLU		GLY	LYS	L2543	C2305	LYS	GLU	E1793	GLY	R1101	G706	Y497	R266	GLN
GLU		GLY	LYS	L2543	C2305	LYS	GLU	A1794	GLY	R1101	G706	Y497	R266	GLY
ALA		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
ALA		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
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GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS	ALA	E1794	G1103	Y959	V707	A800	H273	GLY
GLY		GLY	LYS	L2547	N2324	LYS</								



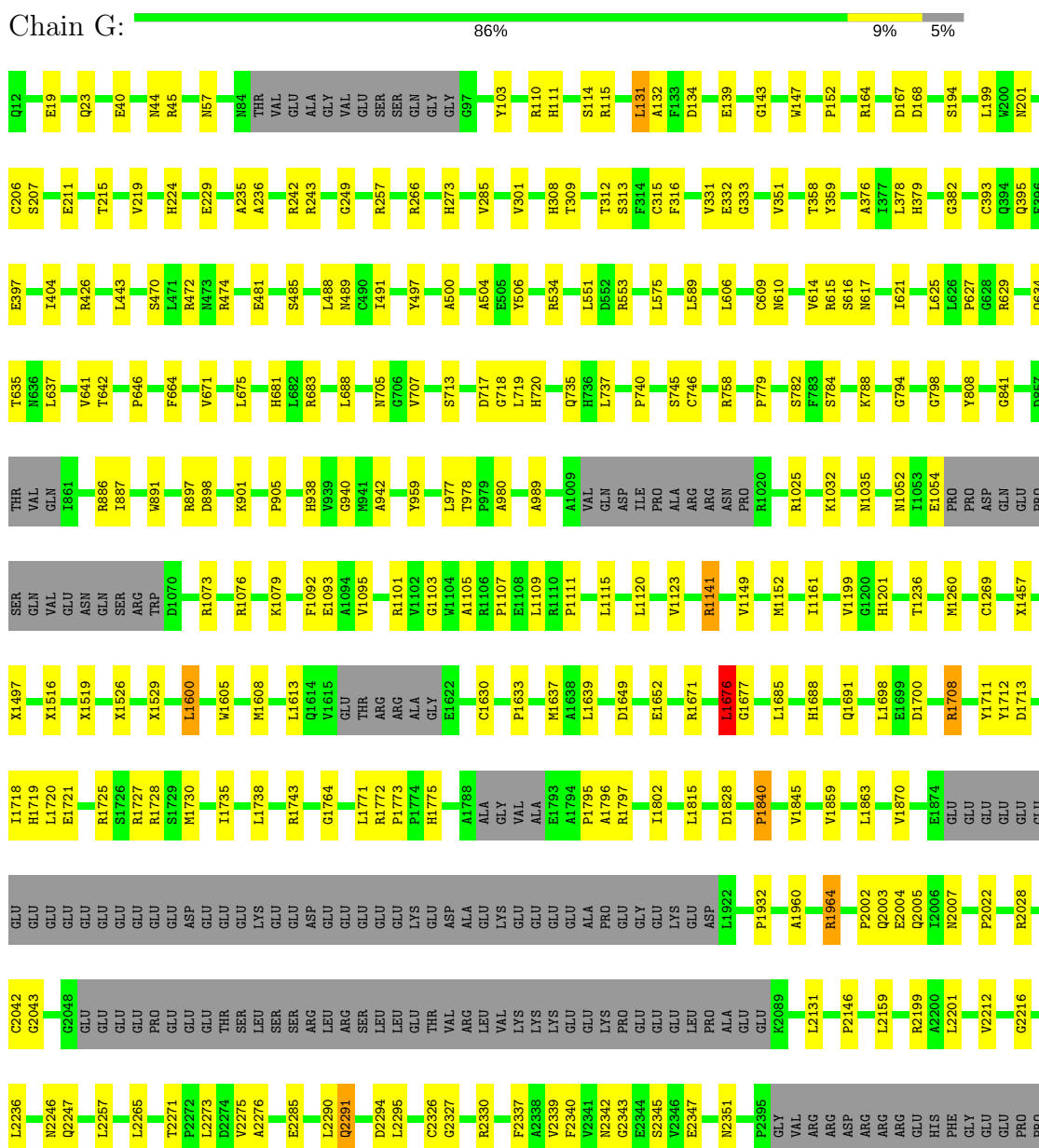
• Molecule 2: Ryanodine receptor 1

Chain I: 86% 9% 5%





- Molecule 2: Ryanodine receptor 1



D4873	ALA	P4106	GLU	GLN	SER	GLU
V4924	GLU	M4120	V3779	L3780	THR	L2414
I4925	GLU	E4126	Q3781	ALA	GLN	P2438
L4929	GLU	E4130	S3784	THR	THR	
A4930	GLY	M4130	K3787	TYR	TYR	K2447
Q4933	ASP	R4131	K3787	ASP	ASP	G2448
G4934	GLU	R4131	K3787	PRO	PRO	E2449
L4935	ASP	D4138	L3805	ARG	ARG	
	GLU	M4142	M3809	GLY	GLY	I2453
E4942	M4639	V4145	K3815	GLY	GLY	L2466
L4943	E4640	K3815	K3815	S2868		I2469
R4944	P4641	L3817	L3817			
K4951	V4666	Q3830	Q3830	Q2872		L2472
K4957	E4674	R4189	Q3833	N2884		I2476
F4959	K4680	I4190	L3942	R2888		P2737
I4960	L4886	K4230	Q3850	L2927		R2738
C4961	Y4687	L4567	K3873	L2930		P2739
G4962	I4688	F4571	T3907	X3362		T2742
L4963	V4697	F4575	T3910	X3365		P2748
F4968	K4698	F4575	T3911	X3366		L2761
H4978	G4699	V4582	F3899	X3369		I2755
T4979	Q4700	P4587	T3907			F2758
	W4701	GLU	T3910	K3658		T2762
E4982	Y4715	GLU	T3911			
H4983	H4728	ASP	L3923	W3661		K2770
L4985	G4729	ASP	L3923	I3662		
A4986	GLU	MET	S3929	D3676		W2775
M4993	I4737	GLU	S3929			
L4996	GLY	GLY	Y3937	X3679		W2807
D5026	M4743	SER	Y3937			
C5027	ALA	ALA	M3955	E3712		K2810
F5028	A4746	ALA	M3955			E2811
	Y4791	GLY	V3961	M3741		
Y5032	ASP	LEU	V3961	GLY		I2823
	F4807	ALA	G3971	GLU		
S5037	D4815	GLY	K4002	ALA		E2830
	I4816	GLY	K4002	GLU		GLU
	M4833	SER	L4019	E3747		ARG
	R4860	GLY	M4034	E3759		THR
	M4864	SER	D4063	R3762		LYS
	K4865	TRP	R4085	L3770		LYS
		GLY		H3771		THR
		GLY		T4104		ARG
	E4871	SER	T4104	P3772		LYS
	P4873	GLY	L4105	P3772		THR

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	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	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	818	0	824	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	31	0	12	2	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	121452	0	102380	949	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 4.

The worst 5 of 949 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:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:H	2:B:4983:HIS:CD2	1.94	0.86

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	51	85
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	51	85
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	54	85

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
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	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	86	92

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4957	LYS
2	I	1600	LEU
2	G	4131	ARG
2	E	4960	ILE
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3896	ASN
2	I	379	HIS
2	G	3896	ASN
2	E	3946	GLN
2	E	4806	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](#)

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	-	27,33,33	0.90	1 (3%)	25,52,52	1.60	3 (12%)
4	CFF	B	5102	-	7,15,15	1.99	2 (28%)	8,23,23	1.37	2 (25%)
3	ATP	E	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.61	3 (12%)
4	CFF	E	5102	-	7,15,15	1.99	2 (28%)	8,23,23	1.38	2 (25%)
3	ATP	G	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.62	3 (12%)
4	CFF	G	5102	-	7,15,15	2.00	2 (28%)	8,23,23	1.38	2 (25%)
3	ATP	I	5101	-	27,33,33	0.90	1 (3%)	25,52,52	1.60	3 (12%)
4	CFF	I	5102	-	7,15,15	2.01	2 (28%)	8,23,23	1.37	2 (25%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C6-N1	-4.07	1.32	1.38
4	G	5102	CFF	C6-N1	-4.02	1.32	1.38
4	B	5102	CFF	C6-N1	-4.02	1.32	1.38
4	E	5102	CFF	C6-N1	-4.01	1.32	1.38
4	G	5102	CFF	O13-C6	-2.42	1.18	1.24

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-6.04	123.60	128.86
3	E	5101	ATP	N3-C2-N1	-6.01	123.62	128.86
3	B	5101	ATP	N3-C2-N1	-5.99	123.64	128.86
3	I	5101	ATP	N3-C2-N1	-5.94	123.69	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5102	CFF	C14-N7-C8	-2.81	112.09	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	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	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80