



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

May 18, 2017 – 02:00 PM EDT

PDB ID : 5L1D  
EMDB ID: : EMD-8303  
Title : Structure of rabbit RyR2 in complex with FKBP12.6 in a closed state (conformation C1)  
Authors : Dhindwal, S.; Lobo, J.J.; Samso, M.  
Deposited on : 2016-07-29  
Resolution : 10.50 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



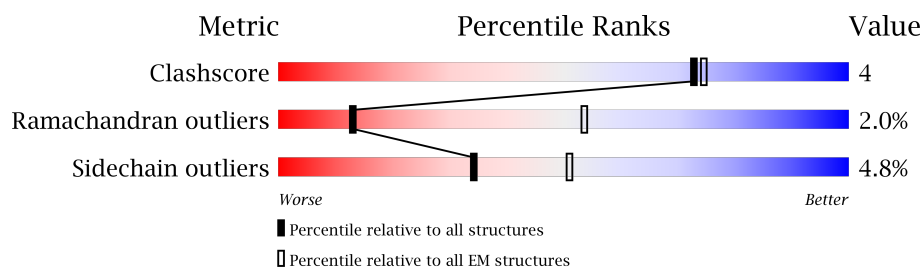
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.50 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	4387	
1	C	4387	
1	E	4387	
1	G	4387	
2	B	158	
2	D	158	
2	F	158	
2	H	158	



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112936 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 Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	C	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	E	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	G	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-50	MET	-	expression tag	UNP P68106
B	-49	ASN	-	expression tag	UNP P68106
B	-48	HIS	-	expression tag	UNP P68106
B	-47	LYS	-	expression tag	UNP P68106
B	-46	VAL	-	expression tag	UNP P68106
B	-45	HIS	-	expression tag	UNP P68106
B	-44	HIS	-	expression tag	UNP P68106
B	-43	HIS	-	expression tag	UNP P68106
B	-42	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	HIS	-	expression tag	UNP P68106
B	-40	HIS	-	expression tag	UNP P68106
B	-39	MET	-	expression tag	UNP P68106
B	-38	ASP	-	expression tag	UNP P68106
B	-37	GLU	-	expression tag	UNP P68106
B	-36	LYS	-	expression tag	UNP P68106
B	-35	THR	-	expression tag	UNP P68106
B	-34	THR	-	expression tag	UNP P68106
B	-33	GLY	-	expression tag	UNP P68106
B	-32	TRP	-	expression tag	UNP P68106
B	-31	ARG	-	expression tag	UNP P68106
B	-30	GLY	-	expression tag	UNP P68106
B	-29	GLY	-	expression tag	UNP P68106
B	-28	HIS	-	expression tag	UNP P68106
B	-27	VAL	-	expression tag	UNP P68106
B	-26	VAL	-	expression tag	UNP P68106
B	-25	GLU	-	expression tag	UNP P68106
B	-24	GLY	-	expression tag	UNP P68106
B	-23	LEU	-	expression tag	UNP P68106
B	-22	ALA	-	expression tag	UNP P68106
B	-21	GLY	-	expression tag	UNP P68106
B	-20	GLU	-	expression tag	UNP P68106
B	-19	LEU	-	expression tag	UNP P68106
B	-18	GLU	-	expression tag	UNP P68106
B	-17	GLN	-	expression tag	UNP P68106
B	-16	LEU	-	expression tag	UNP P68106
B	-15	ARG	-	expression tag	UNP P68106
B	-14	ALA	-	expression tag	UNP P68106
B	-13	ARG	-	expression tag	UNP P68106
B	-12	LEU	-	expression tag	UNP P68106
B	-11	GLU	-	expression tag	UNP P68106
B	-10	HIS	-	expression tag	UNP P68106
B	-9	HIS	-	expression tag	UNP P68106
B	-8	PRO	-	expression tag	UNP P68106
B	-7	GLN	-	expression tag	UNP P68106
B	-6	GLY	-	expression tag	UNP P68106
B	-5	GLN	-	expression tag	UNP P68106
B	-4	ARG	-	expression tag	UNP P68106
B	-3	GLU	-	expression tag	UNP P68106
B	-2	PRO	-	expression tag	UNP P68106
B	-1	GLU	-	expression tag	UNP P68106
B	0	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	MET	-	expression tag	UNP P68106
D	-49	ASN	-	expression tag	UNP P68106
D	-48	HIS	-	expression tag	UNP P68106
D	-47	LYS	-	expression tag	UNP P68106
D	-46	VAL	-	expression tag	UNP P68106
D	-45	HIS	-	expression tag	UNP P68106
D	-44	HIS	-	expression tag	UNP P68106
D	-43	HIS	-	expression tag	UNP P68106
D	-42	HIS	-	expression tag	UNP P68106
D	-41	HIS	-	expression tag	UNP P68106
D	-40	HIS	-	expression tag	UNP P68106
D	-39	MET	-	expression tag	UNP P68106
D	-38	ASP	-	expression tag	UNP P68106
D	-37	GLU	-	expression tag	UNP P68106
D	-36	LYS	-	expression tag	UNP P68106
D	-35	THR	-	expression tag	UNP P68106
D	-34	THR	-	expression tag	UNP P68106
D	-33	GLY	-	expression tag	UNP P68106
D	-32	TRP	-	expression tag	UNP P68106
D	-31	ARG	-	expression tag	UNP P68106
D	-30	GLY	-	expression tag	UNP P68106
D	-29	GLY	-	expression tag	UNP P68106
D	-28	HIS	-	expression tag	UNP P68106
D	-27	VAL	-	expression tag	UNP P68106
D	-26	VAL	-	expression tag	UNP P68106
D	-25	GLU	-	expression tag	UNP P68106
D	-24	GLY	-	expression tag	UNP P68106
D	-23	LEU	-	expression tag	UNP P68106
D	-22	ALA	-	expression tag	UNP P68106
D	-21	GLY	-	expression tag	UNP P68106
D	-20	GLU	-	expression tag	UNP P68106
D	-19	LEU	-	expression tag	UNP P68106
D	-18	GLU	-	expression tag	UNP P68106
D	-17	GLN	-	expression tag	UNP P68106
D	-16	LEU	-	expression tag	UNP P68106
D	-15	ARG	-	expression tag	UNP P68106
D	-14	ALA	-	expression tag	UNP P68106
D	-13	ARG	-	expression tag	UNP P68106
D	-12	LEU	-	expression tag	UNP P68106
D	-11	GLU	-	expression tag	UNP P68106
D	-10	HIS	-	expression tag	UNP P68106
D	-9	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	PRO	-	expression tag	UNP P68106
D	-7	GLN	-	expression tag	UNP P68106
D	-6	GLY	-	expression tag	UNP P68106
D	-5	GLN	-	expression tag	UNP P68106
D	-4	ARG	-	expression tag	UNP P68106
D	-3	GLU	-	expression tag	UNP P68106
D	-2	PRO	-	expression tag	UNP P68106
D	-1	GLU	-	expression tag	UNP P68106
D	0	LEU	-	expression tag	UNP P68106
F	-50	MET	-	expression tag	UNP P68106
F	-49	ASN	-	expression tag	UNP P68106
F	-48	HIS	-	expression tag	UNP P68106
F	-47	LYS	-	expression tag	UNP P68106
F	-46	VAL	-	expression tag	UNP P68106
F	-45	HIS	-	expression tag	UNP P68106
F	-44	HIS	-	expression tag	UNP P68106
F	-43	HIS	-	expression tag	UNP P68106
F	-42	HIS	-	expression tag	UNP P68106
F	-41	HIS	-	expression tag	UNP P68106
F	-40	HIS	-	expression tag	UNP P68106
F	-39	MET	-	expression tag	UNP P68106
F	-38	ASP	-	expression tag	UNP P68106
F	-37	GLU	-	expression tag	UNP P68106
F	-36	LYS	-	expression tag	UNP P68106
F	-35	THR	-	expression tag	UNP P68106
F	-34	THR	-	expression tag	UNP P68106
F	-33	GLY	-	expression tag	UNP P68106
F	-32	TRP	-	expression tag	UNP P68106
F	-31	ARG	-	expression tag	UNP P68106
F	-30	GLY	-	expression tag	UNP P68106
F	-29	GLY	-	expression tag	UNP P68106
F	-28	HIS	-	expression tag	UNP P68106
F	-27	VAL	-	expression tag	UNP P68106
F	-26	VAL	-	expression tag	UNP P68106
F	-25	GLU	-	expression tag	UNP P68106
F	-24	GLY	-	expression tag	UNP P68106
F	-23	LEU	-	expression tag	UNP P68106
F	-22	ALA	-	expression tag	UNP P68106
F	-21	GLY	-	expression tag	UNP P68106
F	-20	GLU	-	expression tag	UNP P68106
F	-19	LEU	-	expression tag	UNP P68106
F	-18	GLU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	GLN	-	expression tag	UNP P68106
F	-16	LEU	-	expression tag	UNP P68106
F	-15	ARG	-	expression tag	UNP P68106
F	-14	ALA	-	expression tag	UNP P68106
F	-13	ARG	-	expression tag	UNP P68106
F	-12	LEU	-	expression tag	UNP P68106
F	-11	GLU	-	expression tag	UNP P68106
F	-10	HIS	-	expression tag	UNP P68106
F	-9	HIS	-	expression tag	UNP P68106
F	-8	PRO	-	expression tag	UNP P68106
F	-7	GLN	-	expression tag	UNP P68106
F	-6	GLY	-	expression tag	UNP P68106
F	-5	GLN	-	expression tag	UNP P68106
F	-4	ARG	-	expression tag	UNP P68106
F	-3	GLU	-	expression tag	UNP P68106
F	-2	PRO	-	expression tag	UNP P68106
F	-1	GLU	-	expression tag	UNP P68106
F	0	LEU	-	expression tag	UNP P68106
H	-50	MET	-	expression tag	UNP P68106
H	-49	ASN	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	LYS	-	expression tag	UNP P68106
H	-46	VAL	-	expression tag	UNP P68106
H	-45	HIS	-	expression tag	UNP P68106
H	-44	HIS	-	expression tag	UNP P68106
H	-43	HIS	-	expression tag	UNP P68106
H	-42	HIS	-	expression tag	UNP P68106
H	-41	HIS	-	expression tag	UNP P68106
H	-40	HIS	-	expression tag	UNP P68106
H	-39	MET	-	expression tag	UNP P68106
H	-38	ASP	-	expression tag	UNP P68106
H	-37	GLU	-	expression tag	UNP P68106
H	-36	LYS	-	expression tag	UNP P68106
H	-35	THR	-	expression tag	UNP P68106
H	-34	THR	-	expression tag	UNP P68106
H	-33	GLY	-	expression tag	UNP P68106
H	-32	TRP	-	expression tag	UNP P68106
H	-31	ARG	-	expression tag	UNP P68106
H	-30	GLY	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	HIS	-	expression tag	UNP P68106
H	-27	VAL	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-26	VAL	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	GLY	-	expression tag	UNP P68106
H	-23	LEU	-	expression tag	UNP P68106
H	-22	ALA	-	expression tag	UNP P68106
H	-21	GLY	-	expression tag	UNP P68106
H	-20	GLU	-	expression tag	UNP P68106
H	-19	LEU	-	expression tag	UNP P68106
H	-18	GLU	-	expression tag	UNP P68106
H	-17	GLN	-	expression tag	UNP P68106
H	-16	LEU	-	expression tag	UNP P68106
H	-15	ARG	-	expression tag	UNP P68106
H	-14	ALA	-	expression tag	UNP P68106
H	-13	ARG	-	expression tag	UNP P68106
H	-12	LEU	-	expression tag	UNP P68106
H	-11	GLU	-	expression tag	UNP P68106
H	-10	HIS	-	expression tag	UNP P68106
H	-9	HIS	-	expression tag	UNP P68106
H	-8	PRO	-	expression tag	UNP P68106
H	-7	GLN	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	GLN	-	expression tag	UNP P68106
H	-4	ARG	-	expression tag	UNP P68106
H	-3	GLU	-	expression tag	UNP P68106
H	-2	PRO	-	expression tag	UNP P68106
H	-1	GLU	-	expression tag	UNP P68106
H	0	LEU	-	expression tag	UNP P68106







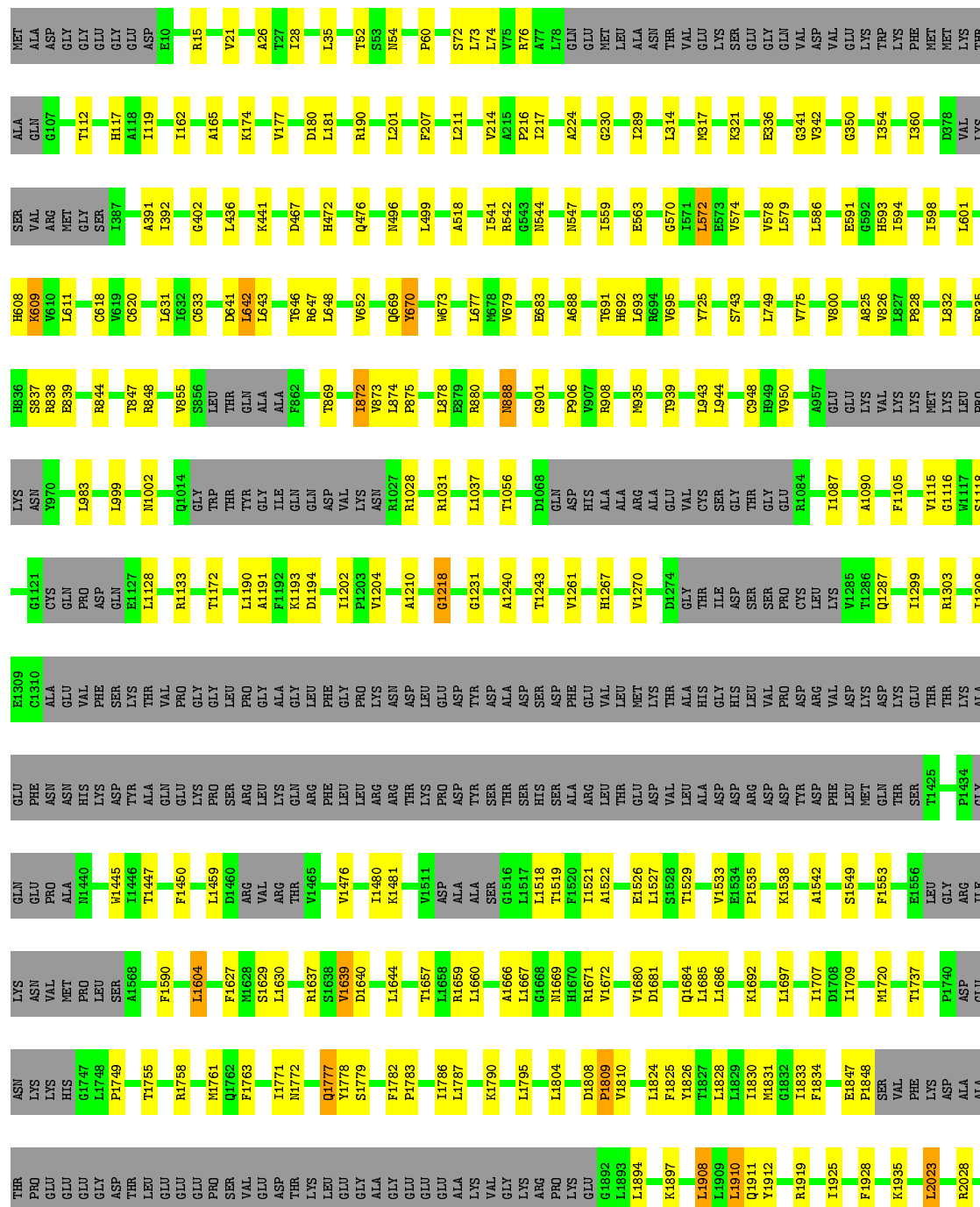







• Molecule 1: Ryanodine Receptor

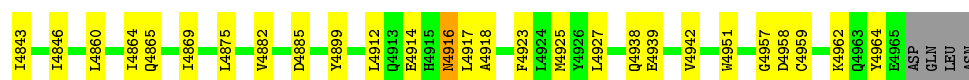
Chain C: 70% 11% 19%





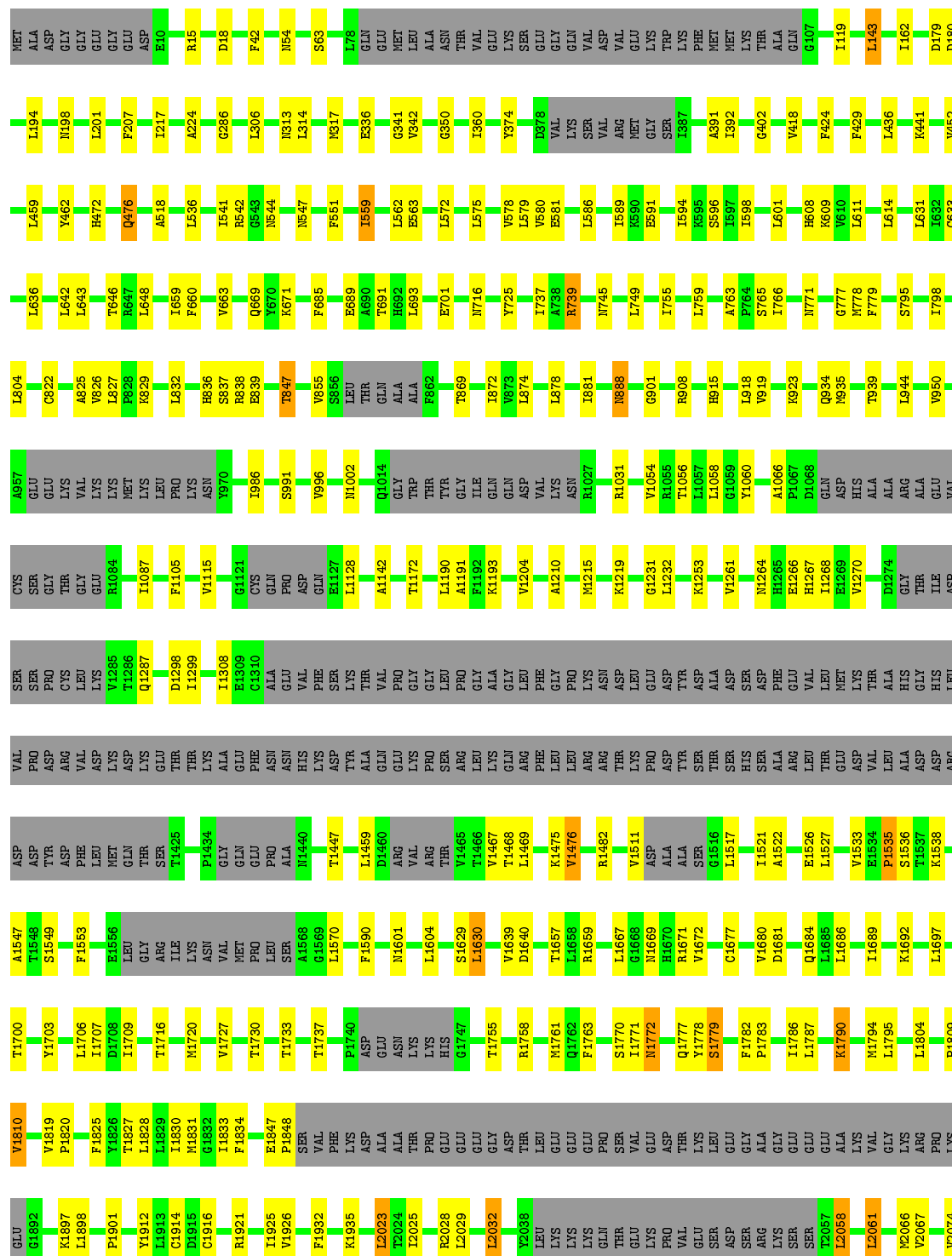
[illegible]





- Molecule 1: Ryanodine Receptor

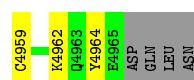
Chain E:  70% 11% 1% 19%





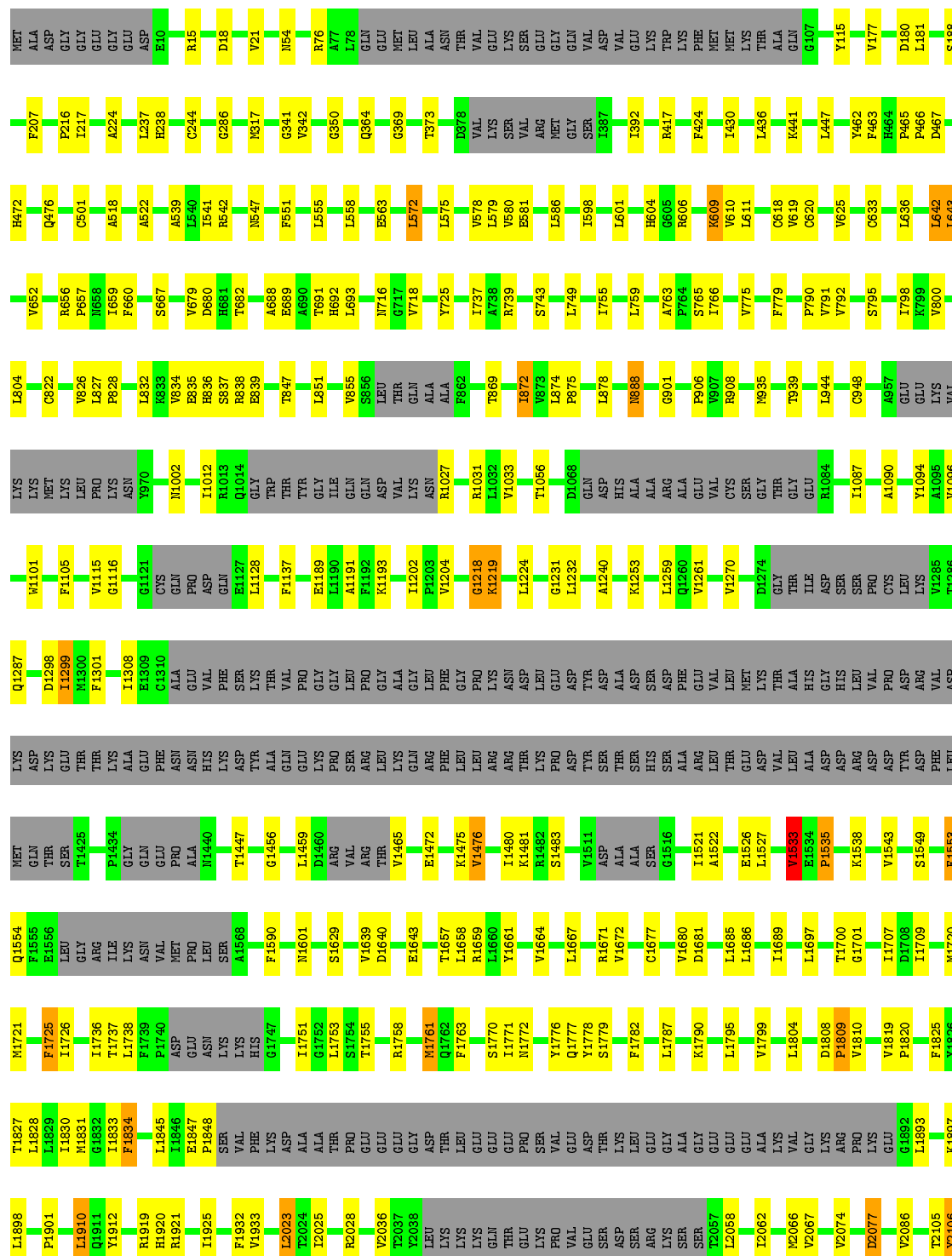
L4722	L4595	GLU	GLU	THR	PHE	SER	F4130	N4010	T3861	ASP	F2493	PRO	SER	D2077
M4730	K4596	ALA	SER	LEU	VAL	VAL	L4134	V4011	Q3862	ASP	M2841	THR	T2238	V2081
A4742	F4602	PHE	GLN	SER	SER	THR	I4137	M4013	N3865	GLU	K2858	GLY	E2259	Q2091
A4743	E4607	THR	GLN	ASP	PHE	ARG	I4137	I4014	Q3883	GLU	L2861	SER	P2260	V2099
F4752	K4611	LYS	LYS	LEU	ARG	SER	I4146	F4018	Q3883	GLU	L2861	LYS	V2266	
Y4781	G4616	ILE	ILE	THR	ARG	ALA	F4018	F4018	F3889	THR	K2864	THR	L2275	Y2106
T4784	L4617	LYS	LYS	ASP	PHE	PHE	F4150	M4020	M3890	Q3728	L2872	ASP	GLN	T2107
K4807	L4618	GLU	GLU	LYS	ARG	ALA	F4151	LEU	M3891	A3737	L2873	THR	SER	I2126
E4821	L4619	GLU	LYS	GLU	ILE	LEU	E4152	LYS	D3897	M3740	P2874	GLU	CYS	L2129
E4821	T4620	GLU	GLU	THR	CYS	ARG	P4164	LEU	V3898	L3899	L2894	GLU	GLN	L2130
M4816	E4621	GLU	GLU	THR	GLU	ASN	K4170	LYS	I3899	L3742	L2894	GLU	VAL	S2131
	Q4622	LYS	LYS	GLU	ILE	LEU	G4181	ASP	F3907	T3752	L2897	ASP	SER	V2132
	P4623	THR	GLU	SER	LEU	LEU	G4181	L4027	F3907	T3752	L2897	THR	LYS	ARG
	D4633	SER	GLU	ASP	LEU	THR	K4186	F4033	I3911	A3758	V2904	ILE	GLY	GLY
G4830	I4637	THR	THR	LEU	GLY	LEU	K4186	F4033	Q3912	A3758	V2904	ILE	GLY	GLY
I4833	M4638	VAL	SER	LEU	SER	ARG	V4191	P4038	Q3916	Q3775	K3614	HIS	TYR	NET
T4839	T4639	GLU	GLU	ASP	LEU	LEU	M4192	F4049	Q3916	Q3775	V3618	GLY	PRO	GLY
Q4840	Q4640	GLY	GLU	ILE	VAL	LEU	F4193	H4056	T3920	M3778	E2111	ASP	ASP	LYS
E4840	S4641	LYS	LYS	PHE	GLU	SER	G4194	H4056	Q3926	M3778	E2111	ILE	ILE	E2137
	V4651	GLU	GLU	GLY	GLY	LEU	E4195	E4065	Q3926	V3788	N2723	GLY	GLY	P2159
R4845	K4652	PRO	LEU	ASP	LYS	SER	I4198	F4067	C3929	L3797	E2746	PRO	ASN	T2170
Q4865	V4655	SER	GLU	LYS	ILE	LYS	I4207	M4076	V3945	C3801	GLY	MET	GLY	
I4869	I4668	THR	SER	GLY	VAL	LYS	SER	E4077	V3946		ALA	HIS		V2174
R4876	L4672	GLU	GLU	GLY	ALA	NET	GLU	T4078	G3947	L3806	GLU	LEU		M2175
D4885	M4673	ASN	GLU	GLY	GLU	LYS	ASP	R4087	H3950	K3814	PRO	ILE	L2325	L2179
	MET	ALA	ASN	THR	LEU	LEU	LEU	PHE	F3952	ALA	GLU	ALA	L2326	G2180
C4893	ASP	LYS	VAL	LYS	ALA	LYS	ASN	GLU	Q3956	GLY	ASP	LYS	CYS	GLY
T4911	L4917	LYS	VAL	ILE	ASN	NET	ARG	H4091	L3959	GLY	VAL	GLY	PHE	GLY
L4912	ALA	THR	THR	PRO	PRO	THR	SER	P4091		MET	THR	PRO	GLY	LYS
	LEU	SER	ASN	HIS	ASP	VAL	ALA	F4097	D3962	VAL	LYS	ILE	LEU	ILE
H4915	ASP	LEU	LYS	PRO	THR	ASP	LYS	M4098		THR	K3661	THR	ALA	THR
M4916	PHE	ASP	LYS	ASN	THR	ASP	LYS	V4099	I3966	GLU	L2423	ARG	ARG	PHE
A4918	SER	SER	GLN	ALA	ASP	VAL	GLU	A4100	T3867	GLY	L2424	GLY	GLY	P2190
	ALA	SER	LYS	GLY	GLU	THR	SER	L4101	Q3969	SER	ARG	GLU	GLY	R2191
F4923	ARG	HIS	ARG	LEU	VAL	ALA	GLU	L4103	K3970	GLY	THR	C2462	GLY	M2192
F4923	GLU	ARG	ASN	SER	ARG	PHE	LYS	F3971	F3971	GLY	ARG	L2473	ASN	I2206
L4924	LYS	ILE	GLN	ASP	GLY	PHE	GLU	N4112	L3972	LYS	ILE			
M4925	LYS	ILE	LEU	LEU	ASP	ASP	ARG	R4115	D3866	VAL	SER	T2477	G2343	Y2220
Y4926	LYS	ALA	THR	SER	GLY	TYR	GLU	L4116	L3975	LEU	GLN	GLY	T2354	V2227
L4927	PRO	V4559	HIS	ASN	GLY	TRP	GLU	Q4117	M3979	D3833	GLN	GLU	ALA	GLY
	LYS	LYS	ARG	PRO	GLY	SER	GLU		Y3983	F3836	VAL	ASP	PRO	LEU
E4939	LYS	T4573	TTR	VAL	GLU	ILE	GLY	L4120	Y3983	F3836	GLN	V2481	ASP	ALA
	ASP	R4574	GLY	LEU	ARG	PHE	PRO	E4121	HIS	F3841	SER	F2484	SER	PRO
V4942	SER	L4575	ILE	ILE	LYS	THR	LYS	L4122	V3991	F3841	VAL	L2489	ARG	ALA
M4951	LEU	I4576	PRO	PRO	PRO	THR	MET	A4123	V3992	ASP	GLU	L2489	ASP	NET
			GLU	GLU	NET	LEU	GLY	L3847	GLU	L3847	GLU	V2491	GLY	GLY
	S4697	I4584	VAL	VAL	GLU	THR	PHE	L4127	V4005	P3840	GLU	V2491	PRO	ARG
			THR	GLN	THR	LYS	PHE							





- Molecule 1: Ryanodine Receptor

Chain G:  70% 10% 19%





[illegible]

- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

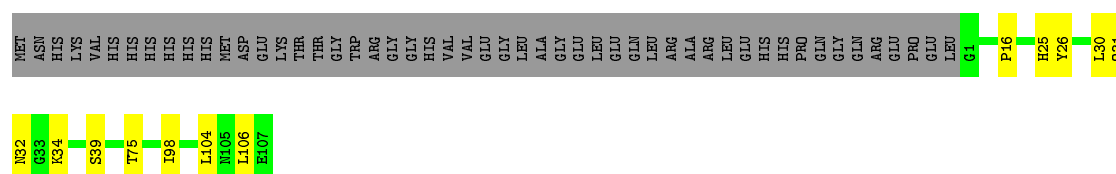


Chain B:  58% 10% 32%



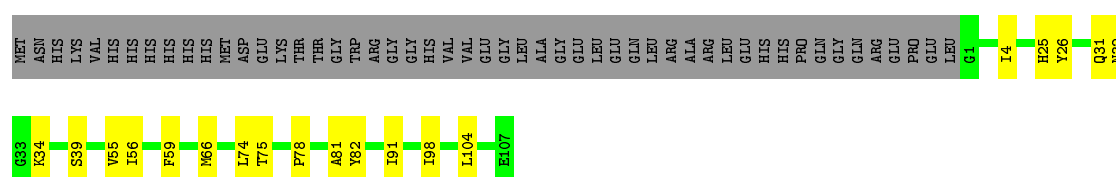
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:  60% 8% 32%



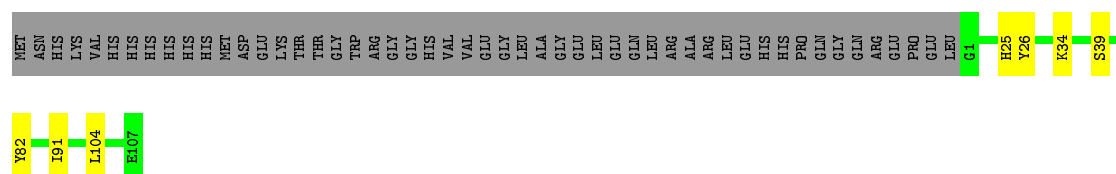
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:  56% 12% 32%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:  63% 0% 32%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13158	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	62000	Depositor
Image detector	Not provided	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	0.78	0/25831	0.64	1/34865 (0.0%)
1	C	0.78	0/25831	0.64	1/34865 (0.0%)
1	E	0.78	0/25831	0.64	1/34865 (0.0%)
1	G	0.78	0/25831	0.64	0/34865
2	B	0.85	0/834	0.64	0/1123
2	D	0.85	0/834	0.63	0/1123
2	F	0.84	0/834	0.64	0/1123
2	H	0.86	0/834	0.65	0/1123
All	All	0.78	0/106660	0.64	3/143952 (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	C	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1630	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	1630	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	1630	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	604	HIS	Peptide
1	C	3614	ARG	Peptide
1	G	3614	ARG	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	27416	0	25487	197	0
1	C	27416	0	25485	217	0
1	E	27416	0	25489	211	0
1	G	27416	0	25485	206	0
2	B	818	0	824	10	0
2	D	818	0	824	5	0
2	F	818	0	824	9	0
2	H	818	0	824	5	0
All	All	112936	0	105242	843	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 843 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:E:3945:VAL:HG11	1:E:3983:LEU:HD21	1.47	0.94
1:A:874:LEU:HD23	1:A:878:LEU:HD13	1.50	0.94
1:E:1172:THR:HG21	1:E:1190:LEU:HD13	1.58	0.86
1:G:874:LEU:HD23	1:G:878:LEU:HD13	1.60	0.82
1:E:1261:VAL:HG11	1:E:1270:VAL:HG11	1.63	0.78

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	3065/4387 (70%)	2784 (91%)	217 (7%)	64 (2%)	8	45
1	C	3065/4387 (70%)	2773 (90%)	236 (8%)	56 (2%)	10	49
1	E	3065/4387 (70%)	2765 (90%)	238 (8%)	62 (2%)	9	46
1	G	3065/4387 (70%)	2789 (91%)	211 (7%)	65 (2%)	8	45
2	B	105/158 (66%)	97 (92%)	7 (7%)	1 (1%)	18	61
2	D	105/158 (66%)	96 (91%)	8 (8%)	1 (1%)	18	61
2	F	105/158 (66%)	97 (92%)	6 (6%)	2 (2%)	9	47
2	H	105/158 (66%)	97 (92%)	8 (8%)	0	100	100
All	All	12680/18180 (70%)	11498 (91%)	931 (7%)	251 (2%)	13	46

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	HIS
1	A	1476	VAL
1	A	1549	SER
1	A	1779	SER
1	A	3897	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	2774/3480 (80%)	2648 (96%)	126 (4%)	32	63

*Continued on next page...*



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	2774/3480 (80%)	2639 (95%)	135 (5%)	29	61
1	E	2774/3480 (80%)	2624 (95%)	150 (5%)	26	58
1	G	2774/3480 (80%)	2642 (95%)	132 (5%)	30	61
2	B	88/131 (67%)	87 (99%)	1 (1%)	78	89
2	D	88/131 (67%)	87 (99%)	1 (1%)	78	89
2	F	88/131 (67%)	87 (99%)	1 (1%)	78	89
2	H	88/131 (67%)	87 (99%)	1 (1%)	78	89
All	All	11448/14444 (79%)	10901 (95%)	547 (5%)	34	61

5 of 547 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4200	GLU
1	E	1287	GLN
1	G	2747	ILE
1	C	4752	PHE
1	E	441	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4010	ASN
1	E	1147	GLN
1	G	3926	GLN
1	C	4644	ASN
1	E	476	GLN

### 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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	27
1	A	27
1	C	27
1	E	27

The worst 5 of 108 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3612:UNK	C	3613:PRO	N	76.52
1	G	3612:UNK	C	3613:PRO	N	75.29
1	E	3612:UNK	C	3613:PRO	N	74.52
1	A	3612:UNK	C	3613:PRO	N	74.10
1	E	2701:UNK	C	2702:PHE	N	43.29