



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 03:00 PM EDT

PDB ID : 5TB3
EMDB ID: : EMD-8394
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-11
Resolution : 4.70 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 : 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) : rb-20027939

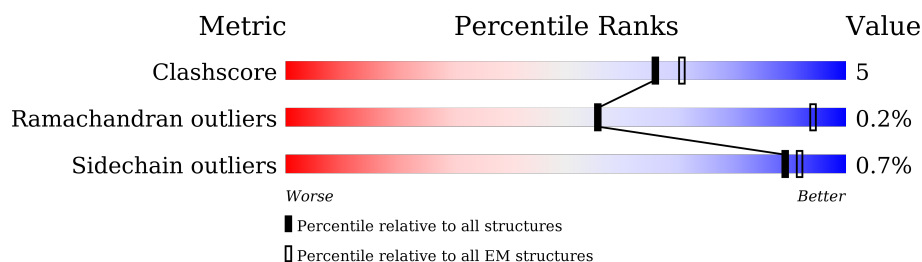
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	81% 18% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 121312 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	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		


- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)


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.

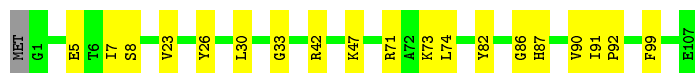
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




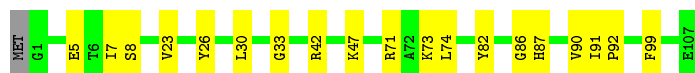
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




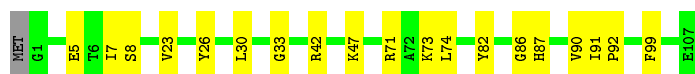
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




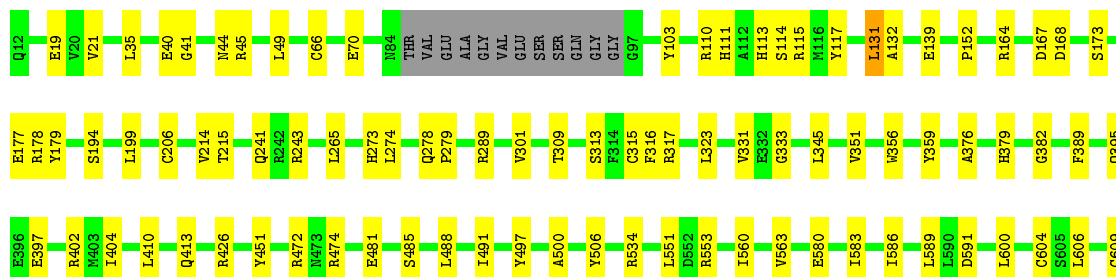
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 

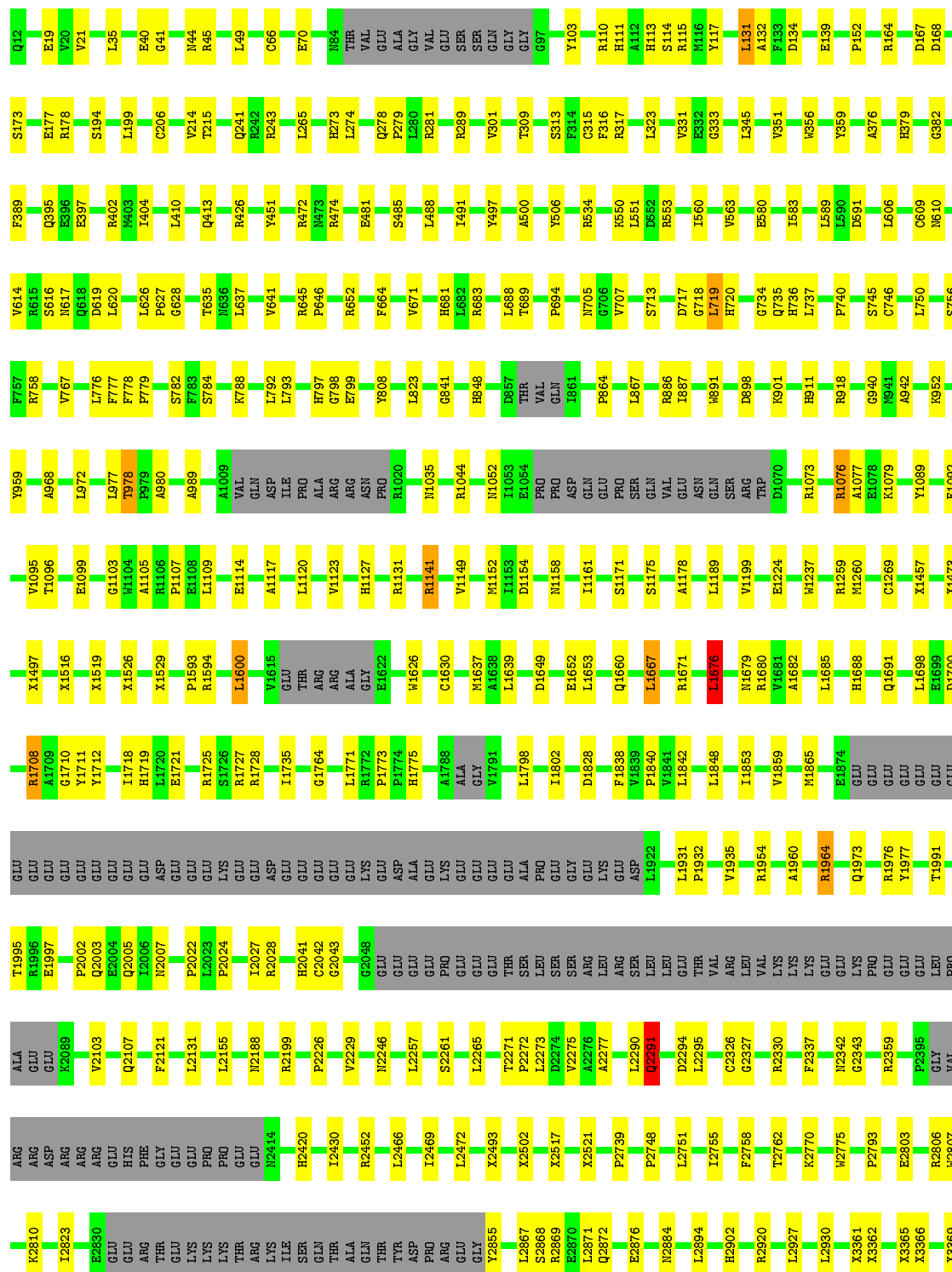


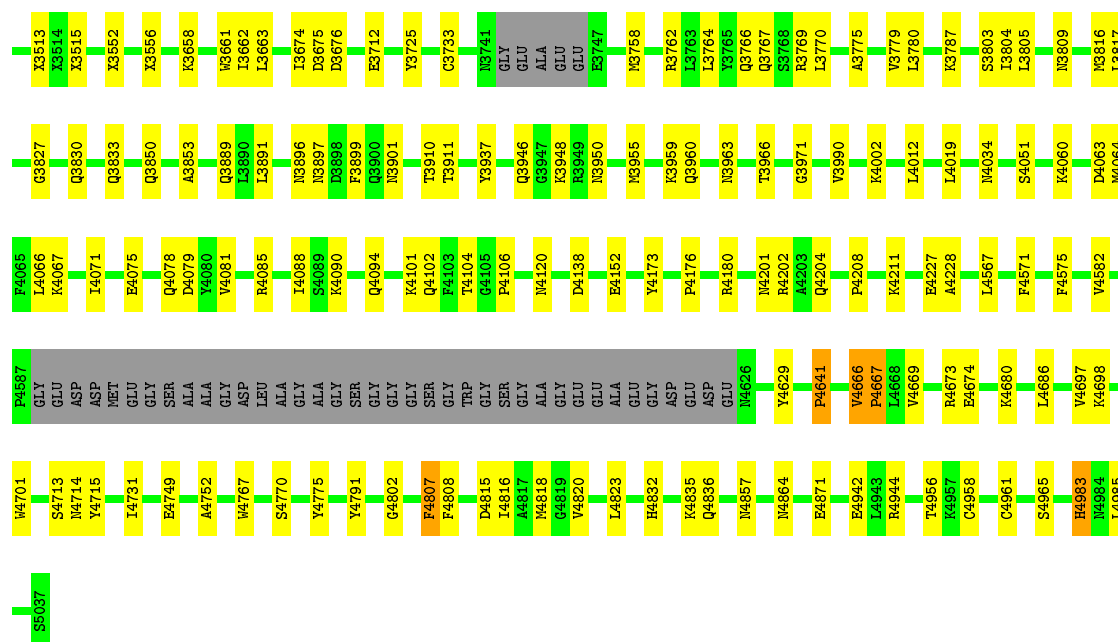
ASP	R4180	K3959	L3764	E2876	P2748	G2327	LYS	R1964	M1865	L1685	C1269	Y1089	A942	S756	H610
GLU	N4626	Q3960	Y3765	N2884	L2751	R2330	GLU	R1964	E1874	H1688	X1457	F1092	K952	R757	V614
N4201	N3963	Q3766	Q3767	L2894	L2751	F2337	LYS	Q1973	GLU	Q1691	X1473	F1092	Y959	R758	R615
R4202	T3966	S3768	S3769	L2894	I2755	F2337	PRO	R1976	GLU	Q1691	X1497	V1095	Y959	V767	S616
Q4204	T3966	R3769	L3770	H2902	F2758	N2342	GLU	Y1977	GLU	L1698	X1516	T1096	A968	P768	N617
A3775	G3971	A3775	A3775	R2920	T2762	G2343	LEU	T1991	GLU	E1699	X1516	E1099	L972	E769	N618
V3990	V3990	V3779	L3780	L2927	K2770	R2359	PRO	T1995	GLU	D1700	X1519	G1103	L977	L776	L626
K4002	K4002	L3780	L3780	L2927	K2770	R2359	ALA	R1996	GLU	R1708	X1526	W1104	T978	F777	P627
L4012	L4012	K3787	K3787	L2930	W2775	P2395	GLU	E1997	GLU	R1708	X1526	A1105	P979	P779	G628
L4019	L4019	S3803	S3803	X3361	P2793	VAL	GLU	P2002	GLU	G1710	X1529	P1107	A980	S782	T635
L3804	L3804	L3804	L3804	X3362	E2803	ARG	GLU	Q2003	GLU	Y1711	P1593	E1108	A989	F783	N636
L3805	L3805	L3805	L3805	X3365	E2803	ASP	GLU	Q2005	GLU	Y1712	R1594	L1109	A989	S784	L637
N3809	N3809	N3809	N3809	X3366	R2806	ARG	GLU	Q2006	GLU	I1718	L1600	E1114	A1009	K788	V641
M3816	M3816	L3817	L3817	X3369	W2807	ARG	ASP	N2007	ASP	H1719	L1600	E1114	VAL	K788	V641
L3817	L3817	L3817	L3817	X3369	W2807	GLU	GLU	N2007	ASP	H1720	L1600	E1114	GLN	K788	V641
Q3830	Q3830	Q3830	Q3830	X3514	E2811	GLU	GLU	P2022	GLU	R1725	M1608	A1117	ASP	L792	R645
Q3833	Q3833	Q3833	Q3833	X3514	E2811	GLU	GLU	P2022	GLU	R1725	M1608	A1117	ILE	L793	P646
Q3850	Q3850	Q3850	Q3850	X3514	E2811	GLU	GLU	P2022	GLU	R1725	M1608	A1117	PRO	L793	P646
A3853	A3853	A3853	A3853	X3518	L2823	GLU	GLU	P2024	GLU	S1726	V1615	V1123	ALA	H797	R652
Q3889	Q3889	Q3889	Q3889	X3552	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
L3890	L3890	L3890	L3890	X3552	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
L3891	L3891	L3891	L3891	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N3896	N3896	N3896	N3896	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N3897	N3897	N3897	N3897	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
D3898	D3898	D3898	D3898	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N3900	N3900	N3900	N3900	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Q3900	Q3900	Q3900	Q3900	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N3901	N3901	N3901	N3901	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
T3910	T3910	T3910	T3910	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
T3911	T3911	T3911	T3911	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Q3927	Q3927	Q3927	Q3927	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
F4103	F4103	F4103	F4103	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
T4104	T4104	T4104	T4104	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
G4105	G4105	G4105	G4105	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
P4106	P4106	P4106	P4106	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Y3937	Y3937	Y3937	Y3937	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Q3946	Q3946	Q3946	Q3946	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
G3947	G3947	G3947	G3947	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
K3948	K3948	K3948	K3948	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
R3949	R3949	R3949	R3949	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N3950	N3950	N3950	N3950	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
M3955	M3955	M3955	M3955	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
P4176	P4176	P4176	P4176	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
R4701	R4701	R4701	R4701	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N4714	N4714	N4714	N4714	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Y4715	Y4715	Y4715	Y4715	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
I4731	I4731	I4731	I4731	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
E4749	E4749	E4749	E4749	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
A4752	A4752	A4752	A4752	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
W4767	W4767	W4767	W4767	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
S4770	S4770	S4770	S4770	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Y4791	Y4791	Y4791	Y4791	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
G4802	G4802	G4802	G4802	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
F4807	F4807	F4807	F4807	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
F4808	F4808	F4808	F4808	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
D4815	D4815	D4815	D4815	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
I4816	I4816	I4816	I4816	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
A4817	A4817	A4817	A4817	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N4818	N4818	N4818	N4818	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
G4819	G4819	G4819	G4819	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
V4820	V4820	V4820	V4820	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
L4823	L4823	L4823	L4823	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
H4832	H4832	H4832	H4832	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
K4835	K4835	K4835	K4835	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
Q4836	Q4836	Q4836	Q4836	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652
N4857	N4857	N4857	N4857	X3556	E2830	GLU	GLU	P2027	GLU	R1727	GLU	H1127	ARG	G798	R652



• Molecule 2: Ryanodine receptor 1

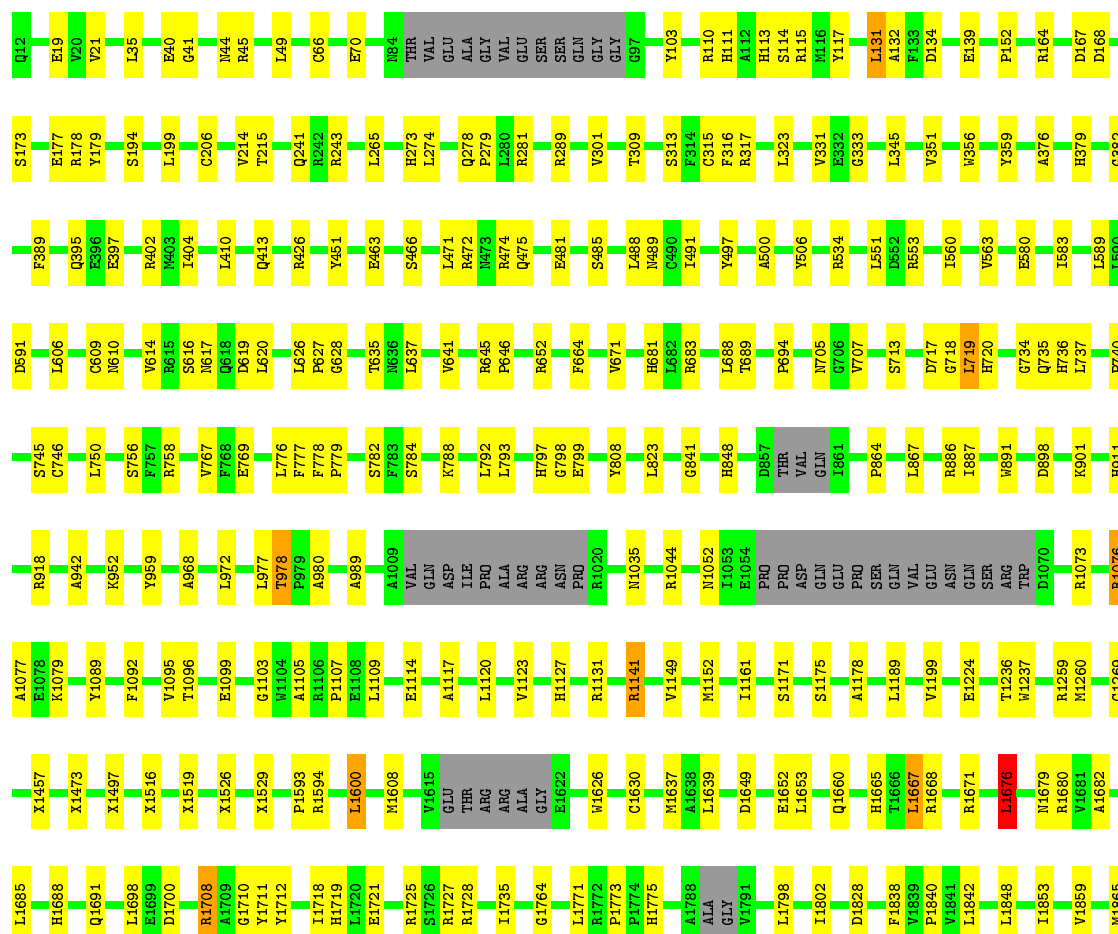
Chain E: 84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain I: 84% 11% 5%





L600	F389	S173	Q12
C604	Q395	E177	E19
S605	E396	R178	V20
L606	E397	S194	V21
C609	R402	L199	L35
M610	M403	L199	E40
V614	I404	C206	G41
S616	L410	V214	M44
M617	Q413	T215	R45
L620	R426	Q241	L49
L626	Y451	R242	C66
P227	E463	R243	E70
G628	S466	L265	E70
T635	R472	H273	N84
M636	R473	L274	T88
L637	R474	Q278	VAL
V641	R474	P279	GLJ
R645	E481	L280	ALA
P646	S485	R281	GLY
R652	L488	R289	GLU
F664	I491	V301	SER
V671	Y497	T309	SER
H681	A500	S313	GLY
L682	R506	C315	GLY
R683	Y506	F316	GLY
L688	R534	R317	G97
T689	L551	L323	Y103
P694	D552	V331	R110
N705	R553	E332	H111
G706	I560	G333	A112
V707	V663	L345	H113
S713	E580	V351	S114
D717	L583	R356	R115
R718	L586	Y359	M116
L719	S689	A376	Y117
H720	L590	H379	L131
G734	D591	G382	A132
R736			F133
L737			D134
			E139
			P152
			R164
			D167
			D168

C4961	V4869	A4228	F3996	I3809	X3365	E2803	G2343	LEU	GLU	Q1691	C1269	R1073	R918	P740
S4965	R4673	S4236	K4002	I3816	X3366	R2806	F2395	PRO	GLU	L1698	X1487	R1076	A942	S745
E4976	K4675	L4567	L4012	I3817	X3369	W2807	VAL	ALA	GLU	E1699	X1473	A1077	A946	C746
K4680	F4571	F4571	L4019	G3827	X3513	K2810	ARG	GLU	GLU	D1700	X1473	E1078	R949	L750
L4686	F4575	F4575	M4034	Q3830	X3514	I2823	ASP	VAL	GLU	A1709	X1497	Y1089	K952	S756
Y4687	F4582	F4582	S4051	Q3833	X3515	I2823	ARG	GLU	GLU	G1710	X1516	F1092	Y959	F757
V4697	F4587	F4587	K4060	L3842	X3552	E2830	ARG	GLU	GLU	Y1711	X1519	Y1095	Y959	R758
K4698	F4587	F4587	D4063	Q3850	X3556	E2830	HIS	GLU	GLU	Y1712	X1519	T1096	A968	V767
G4699	F4587	F4587	M4064	Q3853	X3558	E2830	PHE	GLU	GLU	H1718	X1526	T1096	A968	L776
Y4701	F4587	F4587	M4064	A3853	X3558	E2830	GLU	GLU	GLU	H1719	X1526	T1096	A968	L776
M4714	F4587	F4587	F4065	Q3889	X3661	E2830	GLU	GLU	GLU	E1720	X1529	E1099	L972	F777
Y4715	F4587	F4587	L4066	I3662	X3661	E2830	PRO	GLU	GLU	E1721	X1529	E1099	L972	F778
Y4715	F4587	F4587	K4067	I3663	X3663	E2830	PRO	GLU	GLU	E1721	X1529	E1099	L972	P779
E4749	F4587	F4587	I4071	I3674	X3674	E2830	GLU	GLU	GLU	R1725	P1593	G1103	L977	S782
A4752	F4587	F4587	E4075	D3675	X3675	E2830	GLU	GLU	GLU	R1726	P1594	G1103	L977	S782
V4767	F4587	F4587	F4078	D3676	X3676	E2830	GLU	GLU	GLU	R1727	P1594	G1103	L977	S782
S4770	F4587	F4587	D4079	D3676	X3676	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
Y4791	F4587	F4587	V4081	I3725	X3725	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
G4802	F4587	F4587	R4085	C3733	X3733	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
F4807	F4587	F4587	I4088	X3741	X3741	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
F4808	F4587	F4587	K4101	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
D4815	F4587	F4587	Q4102	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
I4816	F4587	F4587	I4120	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
A4817	F4587	F4587	D4138	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
I4818	F4587	F4587	E4152	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
V4820	F4587	F4587	S4169	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
L4823	F4587	F4587	Y4173	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
H4832	F4587	F4587	P4176	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
K4835	F4587	F4587	R4180	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
Q4836	F4587	F4587	I4201	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
I4864	F4587	F4587	R4202	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
E4871	F4587	F4587	Q4203	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
F4942	F4587	F4587	Q4204	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
L4943	F4587	F4587	P4208	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
R4944	F4587	F4587	K4211	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
T4956	F4587	F4587	F4227	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
K4957	F4587	F4587	F4227	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782
C4958	F4587	F4587	F4227	GLY	GLY	E2830	GLU	GLU	GLU	R1728	P1594	G1103	L977	S782

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: ZN

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	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.30	0/25438	0.54	8/34548 (0.0%)
2	E	0.30	0/25438	0.54	8/34548 (0.0%)
2	G	0.30	0/25438	0.54	8/34548 (0.0%)
2	I	0.30	0/25438	0.54	8/34548 (0.0%)
All	All	0.30	0/105088	0.54	32/142684 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.74	133.11	115.30
2	B	131	LEU	CA-CB-CG	7.73	133.09	115.30
2	I	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	G	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	E	1600	LEU	CA-CB-CG	7.38	132.27	115.30

There are no chirality outliers.

5 of 56 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	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29509	0	24752	277	0
2	E	29509	0	24753	269	0
2	G	29509	0	24753	269	0
2	I	29509	0	24753	276	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121312	0	102307	1111	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 5.

The worst 5 of 1111 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:4983:HIS:H	2:B:4983:HIS:CD2	2.10	0.70
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.10	0.70
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.10	0.69
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65

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	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	52	86
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	52	86
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	56	86

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

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%)	2475 (99%)	18 (1%)	88	94
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	88	94
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	89	94

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4085	ARG
2	I	978	THR
2	G	3896	ASN
2	E	4120	ASN
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	3950	ASN
2	I	413	GLN
2	G	3896	ASN
2	E	4034	ASN
2	E	4946	GLN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	48.21