



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 11, 2018 – 11:45 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/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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

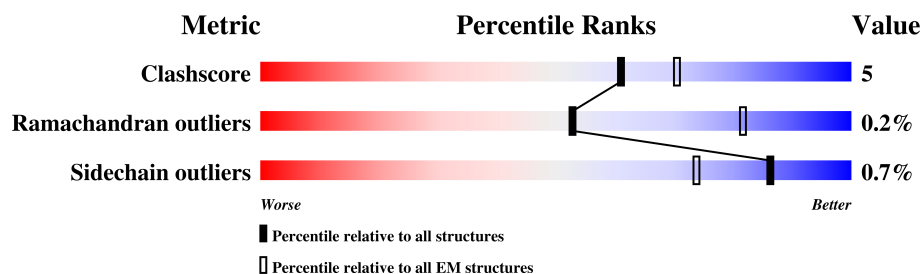
1 Overall quality at a glance

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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

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 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

Chain F: 




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

Chain A: 




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

Chain H: 




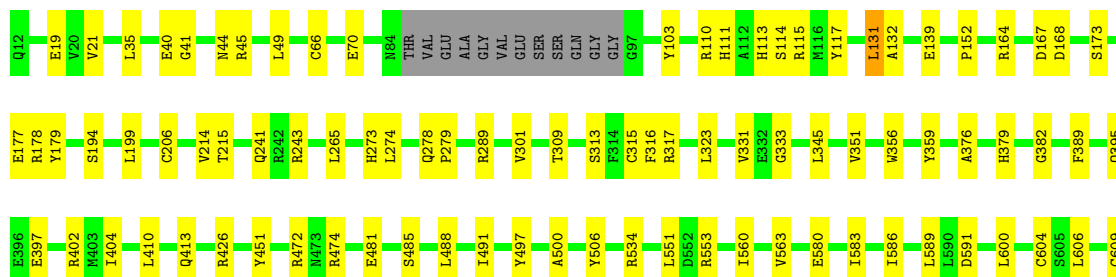
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 

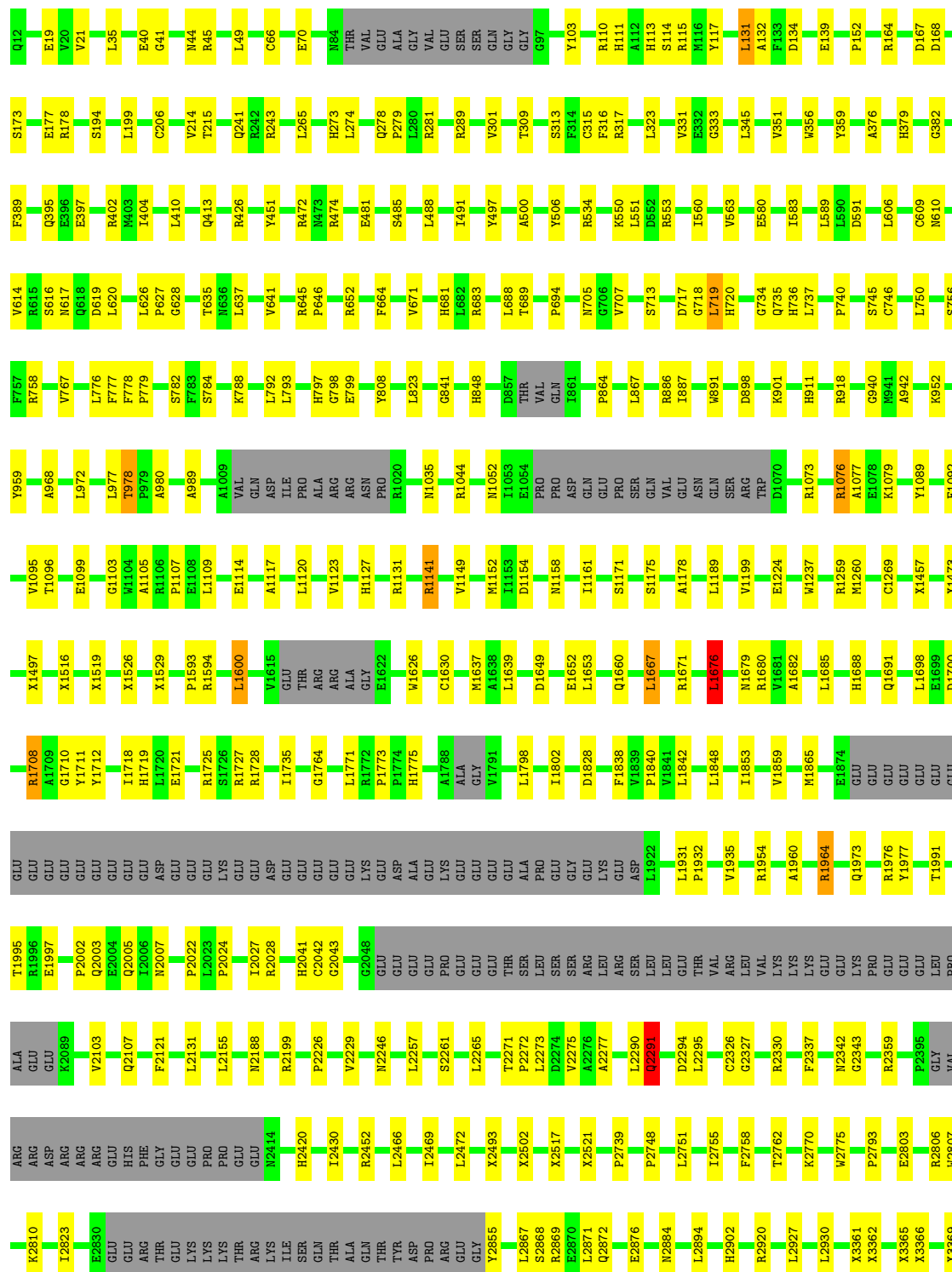


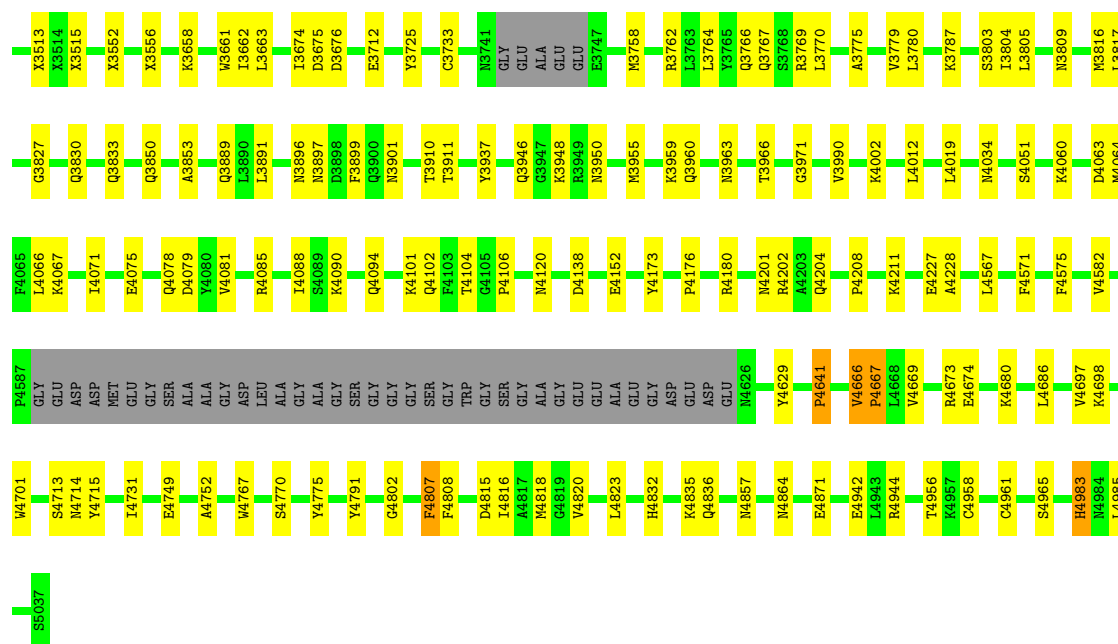
ASP	GLU	N4180	K3959	L3764	E2876	P2748	G2327	LYS	R1964	M1865	L1685	C1269	Y1089	A942	S756	H610
N4201	N3963	Q3767	N3963	Q3766	N2884	L2751	R2330	GLU	Q1973	E1874	H1688	X1457	F1092	K952	R757	V614
R4202	T3966	S3768	L2894	Q3767	L2894	I2755	F2337	PRO	R1976	GLU	Q1691	X1497	V1095	Y959	F758	S616
Q4204	L3770	R3769	H2902	L3770	H2902	F2758	G2343	GLU	Y1977	GLU	L1698	X1497	T1096	A968	P767	N617
A3775	A3775	A3775	R2920	A3775	R2920	T2762	R2359	LEU	T1991	GLU	E1699	X1516	E1099	L972	E769	D619
V3779	V3779	V3779	L2927	V3779	L2927	K2770	R2359	PRO	T1995	GLU	D1700	X1519	G1103	L977	L776	L626
L3780	L3780	L3780	L2930	L3780	L2930	Q2775	P2395	ALA	R1996	GLU	R1708	X1526	A1104	L977	F777	P627
K3787	K3787	K3787	X3361	K3787	X3361	P2793	P2395	GLY	E1997	GLU	A1709	X1526	A1105	P979	P779	G628
S3803	S3803	S3803	X3362	S3803	X3362	E2803	ARG	VAL	P2002	GLU	G1710	X1529	R1106	A980	S782	T635
L3804	L3804	L3804	X3365	L3804	X3365	E2803	ASP	ARG	Q2003	GLU	Y1711	P1593	E1108	A989	F783	N636
L3805	L3805	L3805	X3366	L3805	X3366	Q2107	ARG	ARG	E2004	GLU	Y1712	R1594	A1109	S784	L637	L637
N3809	N3809	N3809	X3369	N3809	X3369	F2121	ARG	ARG	Q2005	GLU	I1718	L1600	E1114	A1009	K788	V641
M3816	M3816	M3816	X3514	M3816	X3514	L2131	GLU	GLU	L2006	ASP	H1719	L1600	E1117	VAL	L792	R645
L3817	L3817	L3817	X3518	L3817	X3518	L2155	GLY	GLU	N2007	GLU	L1720	L1600	A1117	GLN	L793	P646
Q3830	Q3830	Q3830	X3552	Q3830	X3552	L2823	GLU	PRO	P2022	GLU	E1721	M1608	L1120	ASP	L797	R652
Q3833	Q3833	Q3833	X3556	Q3833	X3556	E2830	PRO	PRO	L2023	GLU	R1725	M1608	L1123	ILE	H797	R652
Q3850	Q3850	Q3850	X3558	Q3850	X3558	L2823	GLU	GLU	P2024	GLU	R1727	M1608	V1127	PRO	G798	F664
A3853	A3853	A3853	X3558	A3853	X3558	L2823	GLU	GLU	P2027	GLU	R1728	M1608	H1127	ARG	E799	V671
Q3889	Q3889	Q3889	X3661	Q3889	X3661	E2830	GLU	GLU	L2028	GLU	R1735	M1608	R1131	ARG	Y808	H681
L3890	L3890	L3890	X3662	L3890	X3662	E2830	GLU	GLU	H2041	GLU	G1764	M1637	R1141	PRO	L823	L682
L3891	L3891	L3891	X3663	L3891	X3663	E2830	GLU	GLU	C2042	GLU	G1764	M1637	M1035	R1020	G841	R683
N3896	N3896	N3896	X3674	N3896	X3674	L2823	GLU	GLU	C2043	GLU	L1771	M1637	R1044	M1035	G841	R683
N3897	N3897	N3897	X3675	N3897	X3675	E2830	GLU	GLU	G2046	GLU	R1772	M1637	V1149	R1044	H848	L688
F3899	F3899	F3899	X3676	F3899	X3676	E2830	GLU	GLU	GLU	GLU	P1773	M1637	M1152	N1052	D857	T689
Q3900	Q3900	Q3900	X3676	Q3900	X3676	E2830	GLU	GLU	GLU	GLU	H1775	M1637	I1153	I1053	THR	P694
N3901	N3901	N3901	X3676	N3901	X3676	E2830	GLU	GLU	GLU	GLU	A1788	M1637	D1154	E1054	VAL	P694
T3910	T3910	T3910	X3725	T3910	X3725	L2823	GLU	GLU	GLU	GLU	ALA	M1637	N1158	PRO	GLN	N705
Q3927	Q3927	Q3927	X3733	Q3927	X3733	E2830	GLU	GLU	GLU	GLU	V1791	M1637	I1161	ASP	G706	V707
F4103	F4103	F4103	X3741	F4103	X3741	E2830	GLU	GLU	GLU	GLU	L1798	M1637	S1171	GLU	P864	S713
T4104	T4104	T4104	GLY	T4104	GLY	E2830	GLU	GLU	GLU	GLU	I1802	M1637	S1175	PRO	L867	D717
G4105	G4105	G4105	ALA	G4105	ALA	E2830	GLU	GLU	GLU	GLU	D1828	M1637	A1178	VAL	R886	G718
P4106	P4106	P4106	ALA	P4106	ALA	E2830	GLU	GLU	GLU	GLU	F1838	M1637	L1189	GLU	I887	L719
N4120	N4120	N4120	GLU	N4120	GLU	E2830	GLU	GLU	GLU	GLU	P1840	M1637	V1199	ASN	W891	H720
Q3946	Q3946	Q3946	GLU	Q3946	GLU	E2830	GLU	GLU	GLU	GLU	V1841	M1637	E1224	GLN	D898	G734
K3948	K3948	K3948	GLU	K3948	GLU	E2830	GLU	GLU	GLU	GLU	L1842	M1637	E1236	ARG	Q735	Q735
P3949	P3949	P3949	GLU	P3949	GLU	E2830	GLU	GLU	GLU	GLU	L1848	M1637	T1237	TRP	H736	H736
N3950	N3950	N3950	GLU	N3950	GLU	E2830	GLU	GLU	GLU	GLU	L1853	M1637	W1237	D1070	L737	L737
M3955	M3955	M3955	GLU	M3955	GLU	E2830	GLU	GLU	GLU	GLU	I1859	M1637	R1073	ARG	P740	P740
P4176	P4176	P4176	GLU	P4176	GLU	E2830	GLU	GLU	GLU	GLU	I1859	M1637	R1076	TRP	S745	S745
N4857	N4857	N4857	GLU	N4857	GLU	E2830	GLU	GLU	GLU	GLU	I1859	M1637	A1077	ARG	C746	C746
N4857	N4857	N4857	GLU	N4857	GLU	E2830	GLU	GLU	GLU	GLU	I1859	M1637	E1078	TRP	G940	G940
N4857	N4857	N4857	GLU	N4857	GLU	E2830	GLU	GLU	GLU	GLU	I1859	M1637	K1079	TRP	M941	M941



• Molecule 2: Ryanodine receptor 1

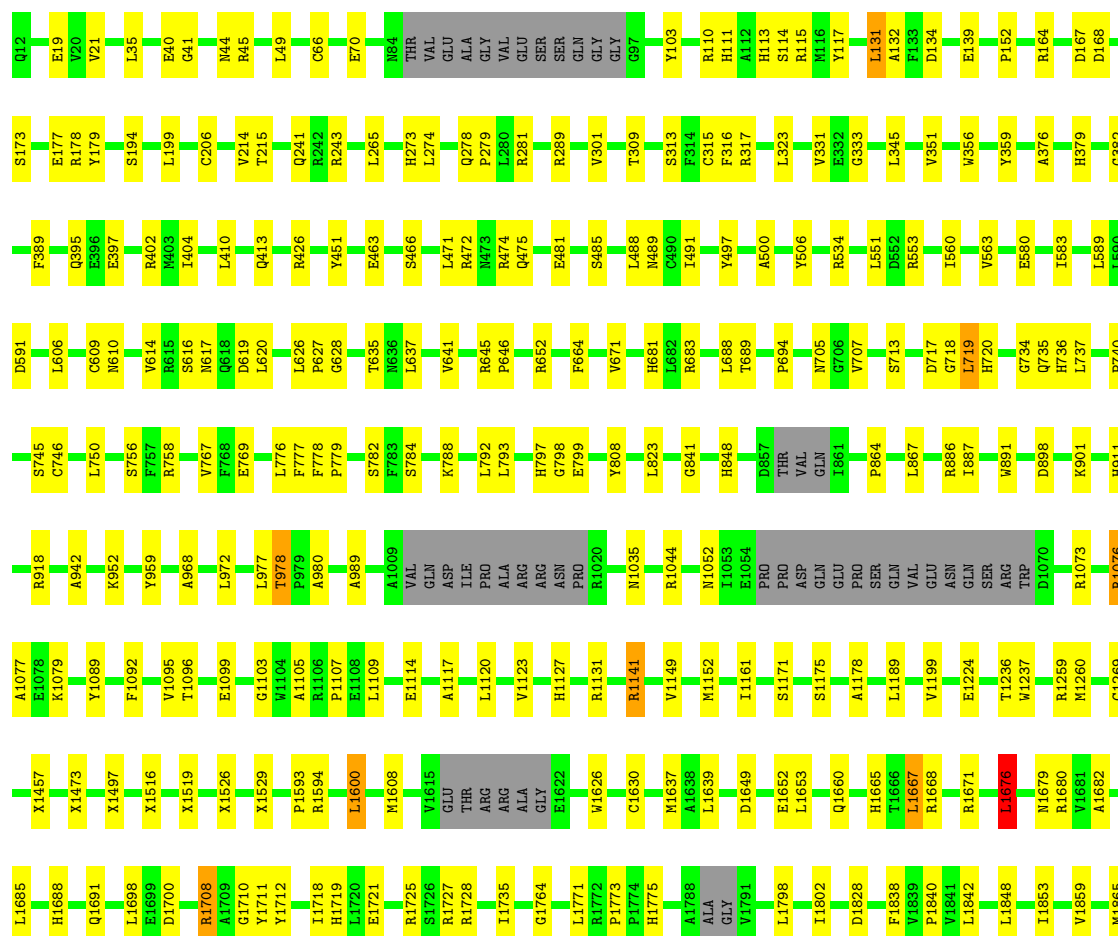
Chain E: 84% 11% 5%

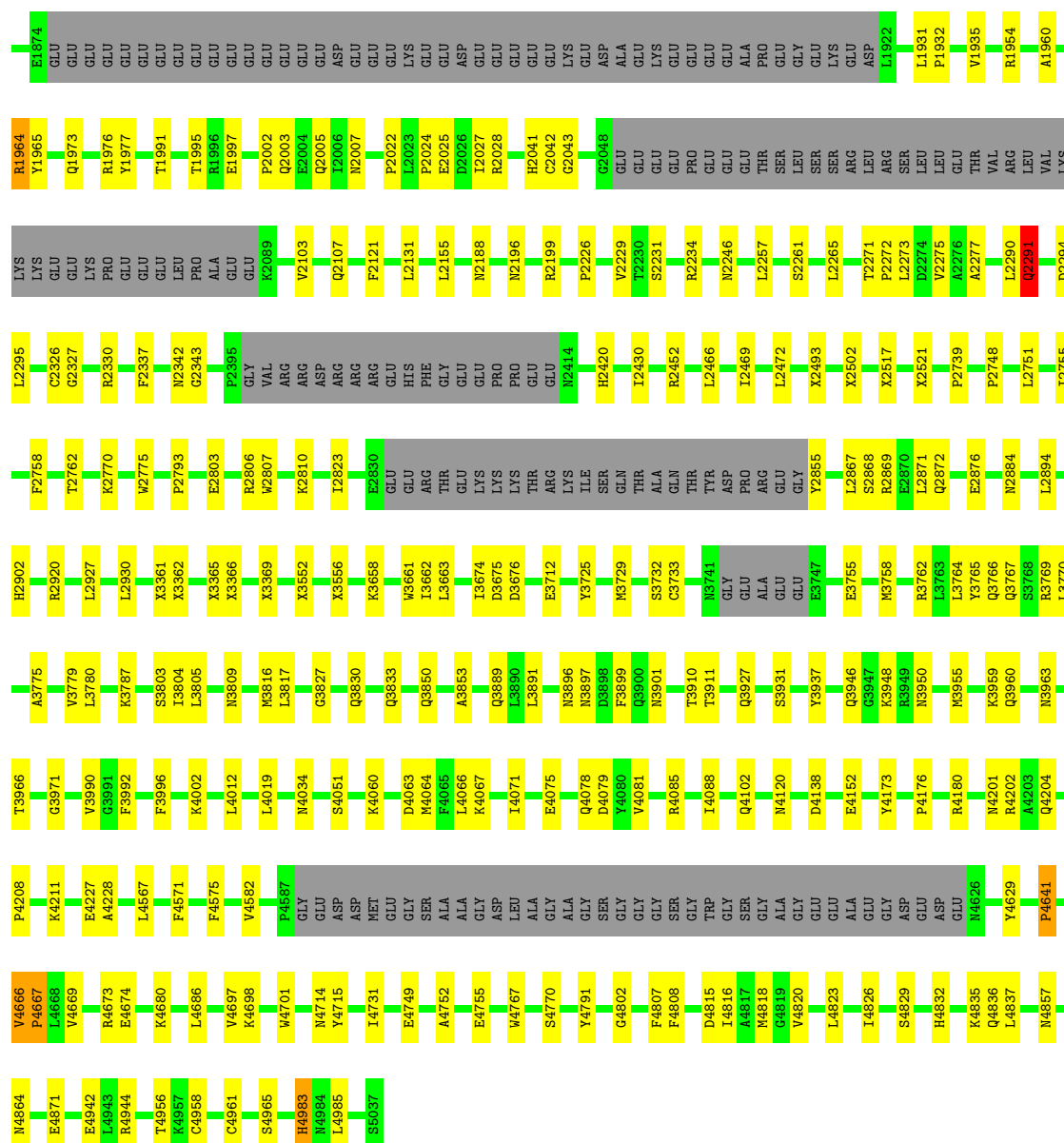




• Molecule 2: Ryanodine receptor 1

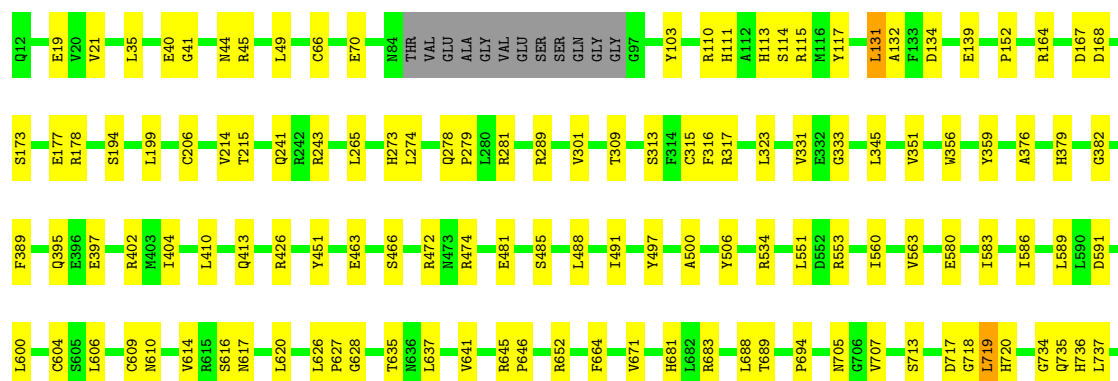
Chain I: 84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain G: 84% 11% 5%



C4961	V4669	A4228	I3809	X3365	E2803	G2343	LEU	T1991	GLU	Q1691	C1269	R1073	R918	P740
S4965	R4673	S4236	N3816	X3366	R2806	F2395	PRO	T1995	GLU	L1698	X1457	R1076	A942	S745
K4675	E4674	L4567	L3817	X3369	W2807	VAL	ALA	R1996	GLU	E1699	G1077	A1077	A946	C746
K4680	K4676	F4571	G3827	X3513	R2810	ARG	GLU	E1997	GLU	D1700	X1473	K1079	K949	L750
L4686	L4677	F4575	Q3830	X3514	K2814	ARG	VAL	P2002	GLU	R1708	X1497	Y1089	S756	S756
Y4687	L4686	F4575	Q3833	X3515	L2823	ARG	ARG	Q2003	GLU	A1709	X1516	F1092	K952	F757
V4697	Y4687	V4582	Q3833	X3552	E2830	ARG	ARG	Q2004	GLU	Y1711	X1519	Y959	R758	R758
K4698	L4686	F4587	L3842	X3556	GLU	GLU	F2121	Q2006	GLU	Y1712	X1519	V1095	V767	V767
G4699	Y4687	F4587	Q3850	X3558	ARG	HIS	L2131	Q2007	GLU	I1718	X1526	T1096	A968	V767
W4700	Y4701	F4587	Q3853	X3568	THR	PHE	L2131	P2022	ASP	H1719	X1526	E1099	L972	L776
N4714	Y4715	F4587	Q3853	X3661	GLU	GLU	L2155	P2022	GLU	E1721	X1529	G1103	L977	F777
Y4715	Y4715	F4587	Q3853	X3662	THR	GLU	L2155	P2024	GLU	E1721	X1529	G1103	L977	P779
E4749	Y4715	F4587	Q3853	X3663	LYS	PRO	N2188	R2028	GLU	R1725	P1593	Y1104	P979	S782
A4752	Y4715	F4587	Q3853	X3663	LYS	PRO	N2188	R2028	GLU	R1725	P1593	Y1104	P979	S782
K4767	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
S4770	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
Y4791	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
G4802	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
F4807	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
F4808	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
D4815	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
I4816	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
K4817	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
K4818	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
V4820	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
L4823	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
H4832	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
K4835	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
Q4836	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
H4864	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
E4871	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
E4942	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
L4943	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
R4944	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
T4956	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
K4957	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	S782
C4958	Y4715	F4587	Q3853	X3663	THR	GLU	N2196	R2028	GLU	R1725	P1593	Y1104	P979	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	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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%)	49	84
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	49	84
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	49	84
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	49	84
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	53	84

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%)	85	92
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	85	92
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	85	92
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	85	92
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	86	92

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

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