



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:45 PM EDT

PDB ID : 5TB0
EMDB ID: : EMD-8391
Title : Structure of rabbit RyR1 (EGTA-only 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 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

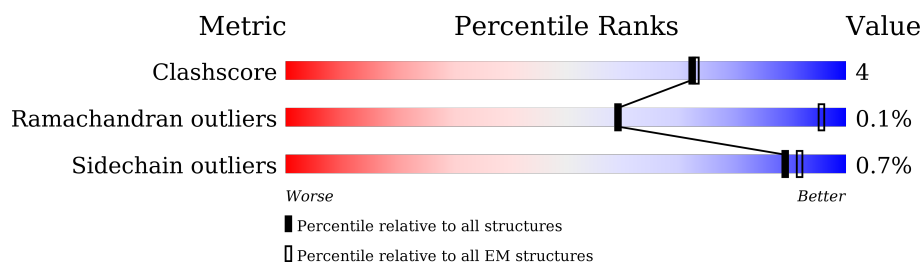
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	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	91% 8% .
1	F	108	90% 9% .
1	H	108	91% 8% .
1	J	108	90% 9% .
2	B	4416	85% 10% 5%
2	E	4416	85% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	85% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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	G	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		


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

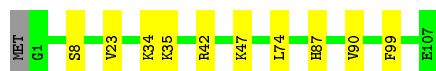
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

3 Residue-property plots

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.

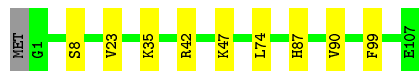
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



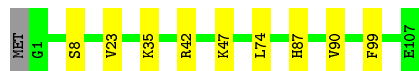
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



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

Chain H: 




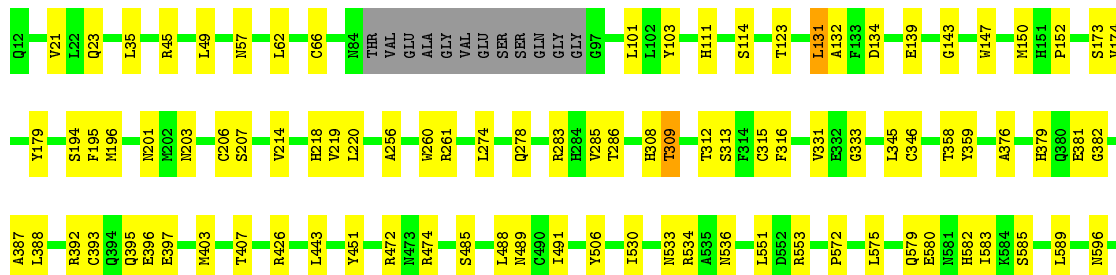
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



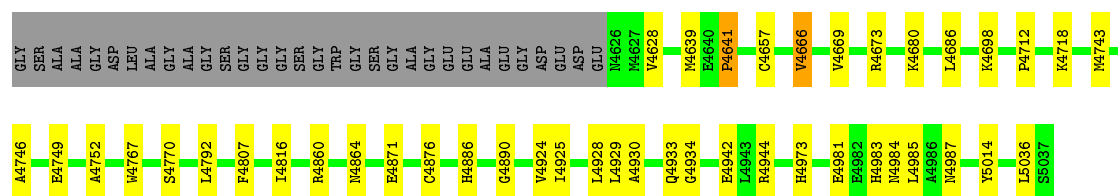
- Molecule 2: Ryanodine receptor 1

Chain B: 



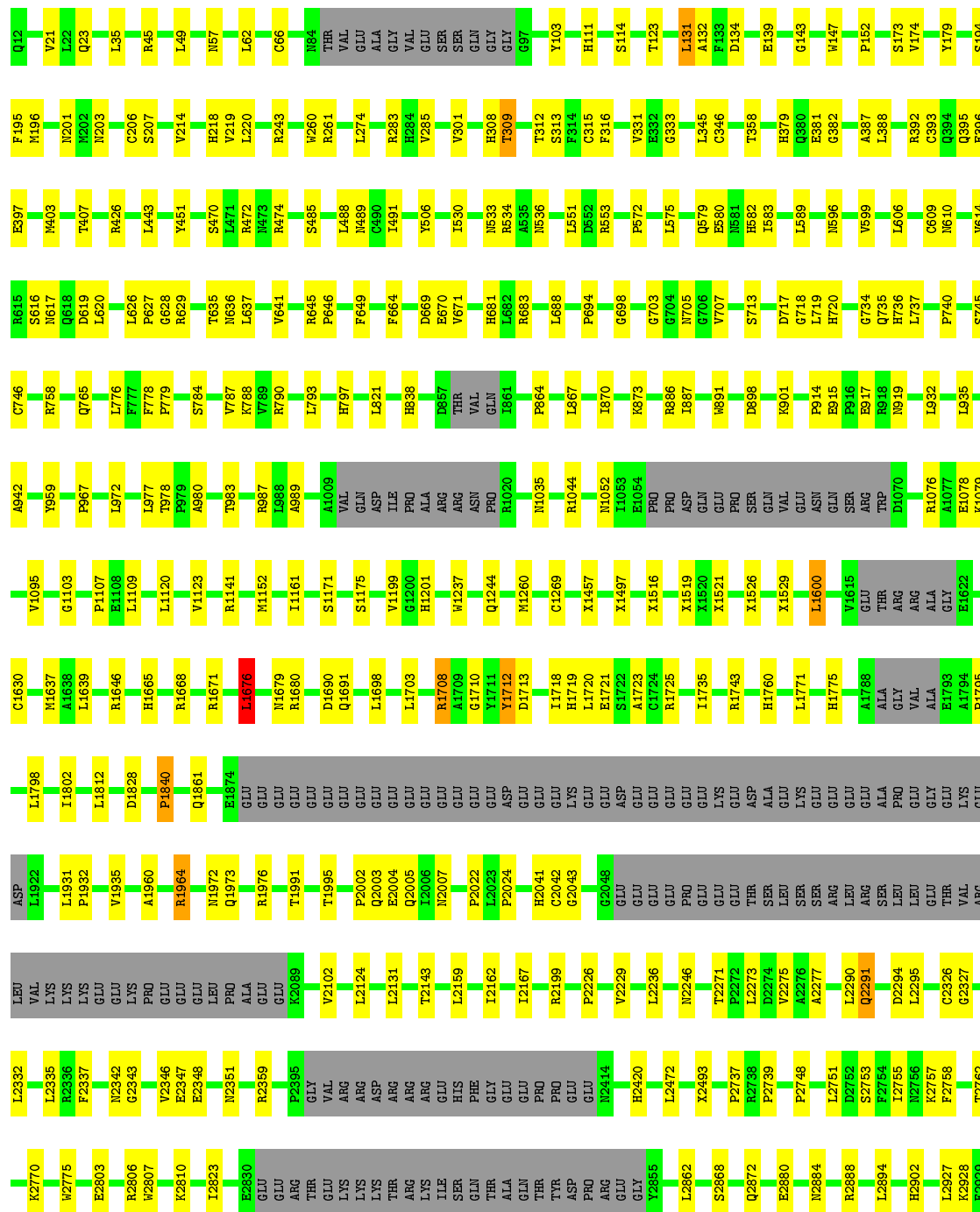
T4766	Q4078	K3787	L2862	X2674	V2275	X2674	X2675	X2676	A2276	V2275	LEU	ALA	VAL	V4615	R1076	L932	G734	V599
W4767	R4085	I3804	E2880	X2676	A2277	X2676	X2676	A2277	A2277	A2277	ARG	PRO	ALA	GLU	A1077	L935	Q735	L606
S4770	K4090	L3805	E2884	R2737	Q2290	R2737	R2737	R2737	Q2291	Q2291	LEU	GLY	ARG	ARG	K1079	L936	L737	C609
L4792	Q4094	N3809	R2888	P2739	D2294	P2739	P2739	P2739	Q2291	Q2291	GLU	LYS	ALA	ALA	V1095	G940	P740	N610
F4807	E4107	V3812	R2888	P2748	D2294	P2748	P2748	P2748	D2294	D2294	THR	ASP	L1798	GLY	V4615	S745	S745	V614
I4816	N4120	L3817	R2894	L2751	L2295	L2751	L2751	L2751	L2295	L2295	ARG	ASP	I1802	E1622	G1103	C746	C746	R615
V4848	N4142	L3842	H2902	D2752	Y2318	D2752	D2752	D2752	Y2318	Y2318	LEU	LYS	L1812	C1630	P1107	R758	R758	S616
T4852	L2927	Q3850	L2927	S2753	P2319	S2753	S2753	S2753	P2319	P2319	LYS	LYS	D1828	M1637	E1108	Q765	Q765	N617
R4860	K2928	F2929	F2929	F2754	C2326	F2754	F2754	F2754	C2326	C2326	LYS	LYS	D1828	A1638	R1110	L1109	L1109	N618
N4864	V4145	L2930	L2930	F2755	G2327	F2755	F2755	F2755	G2327	G2327	GLU	GLU	P1840	L1639	P1111	L1120	L1120	L620
E4871	P4155	X3362	X3362	F2756	L2332	F2756	F2756	F2756	L2332	L2332	LYS	PRO	Q1861	R1646	V1123	L972	L972	L626
C4876	L4166	X3365	X3365	F2757	L2335	F2757	F2757	F2757	L2335	L2335	GLU	GLU	Q1861	H1665	R1141	L977	L977	P627
H4886	A4167	X3366	X3366	F2758	R2336	F2758	F2758	F2758	R2336	R2336	GLU	GLU	M1865	R1668	R1141	T978	T978	P628
G4890	E4227	K3658	K3658	E2803	E2347	E2803	E2803	E2803	E2347	E2347	GLU	GLU	E1874	R1671	M1152	S784	S784	R629
I4925	A4228	W2807	W2807	R2806	E2348	R2806	R2806	R2806	E2348	E2348	LEU	LEU	GLU	R1671	M1152	K788	K788	T635
L4928	E4229	K3948	K3948	K2810	N2342	K3948	K3948	K3948	N2342	N2342	ALA	ALA	GLU	L1676	M1152	V789	V789	N636
A4930	E4232	M3955	M3955	L2823	G2343	M3955	M3955	M3955	G2343	G2343	GLU	GLU	GLU	L1676	M1152	R790	R790	L637
Q4933	E4239	V3961	V3961	E2830	P2395	V3961	V3961	V3961	P2395	P2395	GLU	GLU	GLU	L1676	M1152	S784	S784	T635
G4934	N4558	E3967	E3967	E2830	VAL	E3967	E3967	E3967	VAL	VAL	GLU	GLU	GLU	L1676	M1152	K788	K788	N636
E4942	L4567	G3971	G3971	E2830	ARG	L4567	L4567	L4567	ARG	ARG	GLU	GLU	GLU	L1676	M1152	V789	V789	L637
L4944	F4571	K4002	K4002	E2830	ASP	F4571	F4571	F4571	ASP	ASP	GLU	GLU	GLU	L1676	M1152	R790	R790	V641
H4973	F4575	L4003	L4003	E2830	ARG	F4575	F4575	F4575	ARG	ARG	GLU	GLU	GLU	L1676	M1152	L793	L793	R645
E4981	V4582	L4012	L4012	E2830	GLU	V4582	V4582	V4582	GLU	GLU	GLU	GLU	GLU	L1676	M1152	H797	H797	P646
E4982	P4587	L4013	L4013	E2830	THR	P4587	P4587	P4587	THR	THR	GLU	GLU	GLU	L1676	M1152	I161	I161	H681
H4983	GLY	L4019	L4019	E2830	ARG	GLY	GLY	GLY	ARG	ARG	GLU	GLU	GLU	L1676	M1152	VAL	VAL	L682
N4984	GLY	L4019	L4019	E2830	ASP	GLY	GLY	GLY	ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	V671
L4985	P4712	L4034	L4034	E2830	GLU	P4712	P4712	P4712	GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	H681
A4986	K4718	E4056	E4056	E2830	THR	K4718	K4718	K4718	THR	THR	GLU	GLU	GLU	L1676	M1152	L867	L867	L688
N4987	ASP	E4056	E4056	E2830	ARG	ASP	ASP	ASP	ARG	ARG	GLU	GLU	GLU	L1676	M1152	E880	E880	P694
Y5014	M4743	L4059	L4059	E2830	ALA	M4743	M4743	M4743	ALA	ALA	GLU	GLU	GLU	L1676	M1152	PRO	PRO	P698
L5036	A4746	K4060	K4060	E2830	THR	A4746	A4746	A4746	THR	THR	GLU	GLU	GLU	L1676	M1152	ASP	ASP	G698
S5037	E4749	D4063	D4063	E2830	ASP	E4749	E4749	E4749	ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	G703
	A4752	K4067	K4067	E2830	PRO	A4752	A4752	A4752	PRO	PRO	GLU	GLU	GLU	L1676	M1152	GLU	GLU	G704
	G4763	E4075	E4075	E2830	ARG	G4763	G4763	G4763	ARG	ARG	GLU	GLU	GLU	L1676	M1152	PRO	PRO	N705
				E2830	GLY				GLY	GLY	GLU	GLU	GLU	L1676	M1152	SER	SER	G706
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	VAL	VAL	V707
				E2830	ILE				ILE	ILE	GLU	GLU	GLU	L1676	M1152	ASN	ASN	S713
				E2830	SER				SER	SER	GLU	GLU	GLU	L1676	M1152	GLN	GLN	D717
				E2830	GLN				GLN	GLN	GLU	GLU	GLU	L1676	M1152	GLN	GLN	G718
				E2830	ALA				ALA	ALA	GLU	GLU	GLU	L1676	M1152	GLN	GLN	L719
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	H720
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	PRO				PRO	PRO	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLY				GLY	GLY	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ASP				ASP	ASP	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	GLU				GLU	GLU	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	THR				THR	THR	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830	ARG				ARG	ARG	GLU	GLU	GLU	L1676	M1152	GLN	GLN	
				E2830														

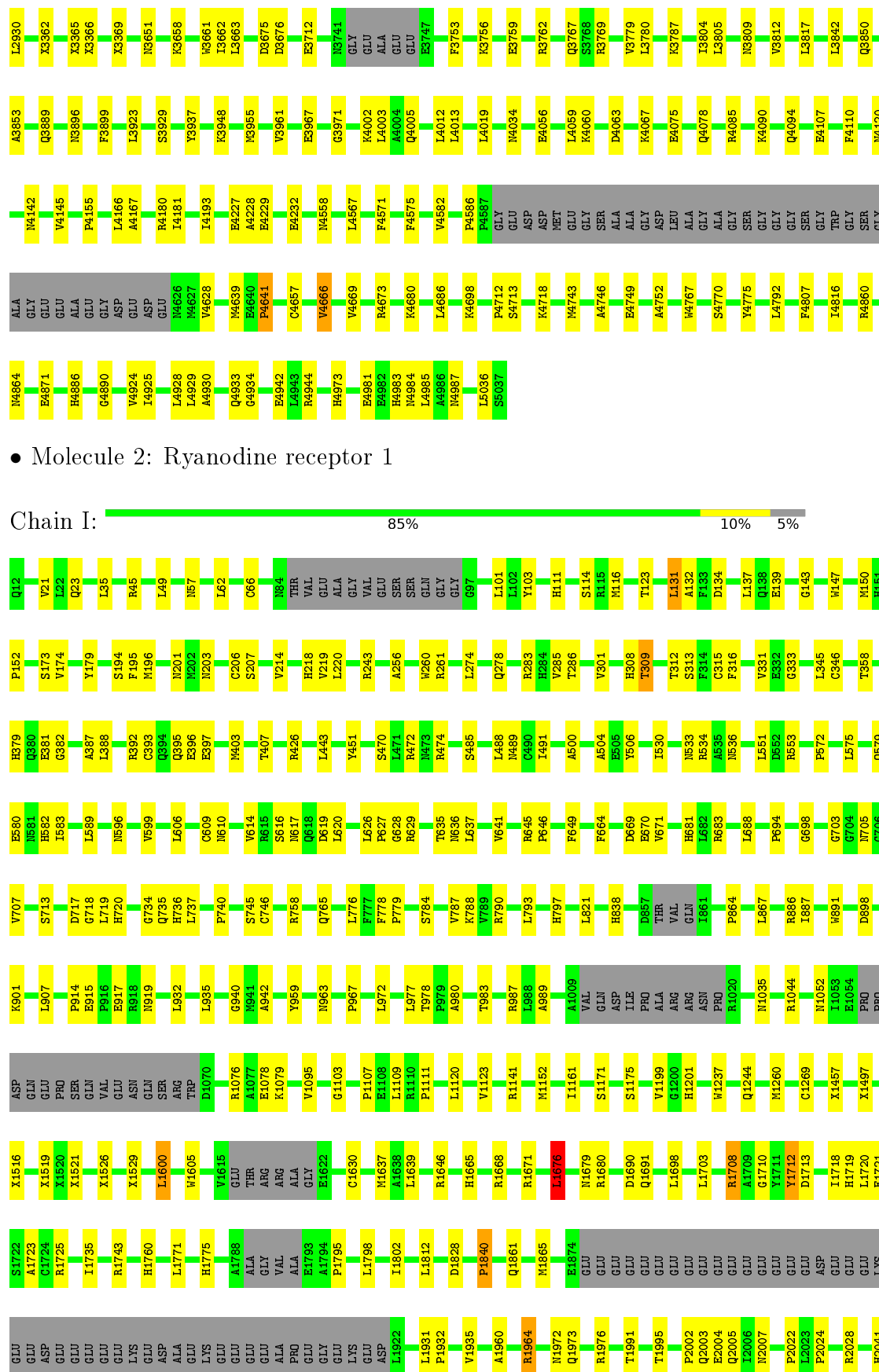
D4063	R3769	Q2872	V2275	LEU	ALA	ALA	R1076	L932	Q735	L606	L388	Y179	Q12
K4067	V3779	A2373	A2276	ARG	GLY	GLY	A1077	L932	H736	L606	L388	Y179	Q12
L3780	P2737	A2374	A2277	LEU	VAL	ALA	E1078	L935	L737	C609	R392	S194	V21
E4075	P2739	L2378	L2290	LEU	GLY	ALA	K1079	L935	P740	N610	C393	F195	Q23
Q4078	P2748	A2379	L2291	THR	GLY	P1795	V1095	V939	S745	V614	Q395	M196	L35
S3803	L2751	D2294	Q2291	VAL	GLY	P1795	G1103	G940	C746	R615	E396	M201	L45
R4085	D2752	L2295	L2295	ARG	GLY	L1798	G1103	G940	R758	S616	E397	M202	R45
L3805	S2753	VAL	C2326	LEU	ASP	H1640	P1107	A942	Q765	N617	M403	M203	L49
K4090	R2888	VAL	Q2327	LYS	L1802	P1642	E1108	V959	Q765	Q618	T407	C206	L49
Q4094	L2894	LYS	Q2327	LYS	L1802	P1642	L1109	P967	Q765	D619	T407	S207	H57
K4101	H2902	LYS	L2332	LYS	L1842	R1646	L1120	L972	L776	L626	R426	V214	L62
E4107	L2927	GLU	L2335	GLU	D1828	H1665	V1123	L972	F777	P627	L443	V214	L62
L3842	L2927	LYS	R2336	LYS	P1840	H1665	V1123	L977	F778	G628	L443	H218	C66
L3842	L2927	PRO	R2337	PRO	P1840	H1668	R1141	L977	P779	R629	Y451	V219	L62
Q3850	L2930	GLU	Q1861	GLU	Q1861	R1671	M1152	P979	S784	V641	R474	L220	H84
A3853	X3362	GLU	M1865	GLU	M1865	R1671	M1152	A980	V787	T635	S470	R243	THR
N3896	X3365	LEU	E1874	ALA	E1874	L1676	I1161	A989	K788	N636	L471	R243	VAL
P4155	X3366	PRO	GLU	GLU	GLU	R1679	S1171	A989	V789	L637	R472	A256	GLU
L4166	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	ALA
A4167	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLY
R4180	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	VAL
L4181	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
L4193	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	VAL
E4227	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
A4228	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
E4229	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
E4232	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
E4239	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
N4558	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
L4567	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
F4571	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
F4575	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
V4582	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
P4586	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
P4587	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
G1Y	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
ASP	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
NET	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU
GLU	X3369	GLU	GLU	GLU	GLU	R1680	S1171	A989	R790	V641	R474	A256	GLU



• Molecule 2: Ryanodine receptor 1

Chain E: 85% 10% 5%








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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.32	0/25428	0.56	9/34534 (0.0%)
2	E	0.32	0/25428	0.56	9/34534 (0.0%)
2	G	0.32	0/25428	0.56	9/34534 (0.0%)
2	I	0.32	0/25428	0.56	9/34534 (0.0%)
All	All	0.32	0/105048	0.56	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	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	G	131	LEU	CA-CB-CG	8.74	135.39	115.30
2	B	131	LEU	CA-CB-CG	8.73	135.38	115.30
2	I	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	E	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	I	1676	LEU	CA-CB-CG	6.26	129.70	115.30

There are no chirality outliers.

5 of 76 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	5	0
1	F	818	0	824	6	0
1	H	818	0	824	5	0
1	J	818	0	824	6	0
2	B	29499	0	24749	236	0
2	E	29499	0	24750	227	0
2	G	29499	0	24749	236	0
2	I	29499	0	24749	237	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	121272	0	102293	929	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 929 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:2291:GLN:HB3	2:I:2294:ASP:H	1.55	0.72
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.55	0.71
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.55	0.71
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.55	0.71
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.62	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	3235/4416 (73%)	2874 (89%)	357 (11%)	4 (0%)	56	90
2	E	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2875 (89%)	356 (11%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	56	90
All	All	13360/18096 (74%)	11875 (89%)	1469 (11%)	16 (0%)	59	90

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	I	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%)	2476 (99%)	17 (1%)	88	94
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	89	94

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	4034	ASN
2	E	1076	ARG
2	I	3805	LEU
2	G	4085	ARG
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3767	GLN
2	E	273	HIS
2	I	3767	GLN
2	G	3896	ASN
2	G	4553	ASN

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	73.03
1	G	4345:UNK	C	4540:PHE	N	73.03
1	E	4345:UNK	C	4540:PHE	N	73.03
1	I	4345:UNK	C	4540:PHE	N	73.03

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	46.34