



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 09:22 PM EDT

PDB ID : 5TA3
EMDB ID: : EMD-8377
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-09
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 : 1.7.1 (RC1), CSD as537be (2016)
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

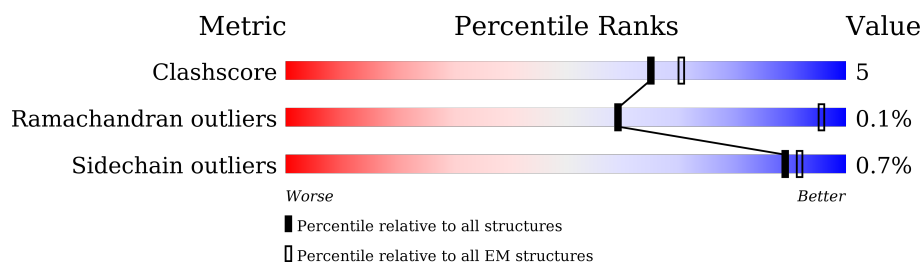
1 Overall quality at a glance

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	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

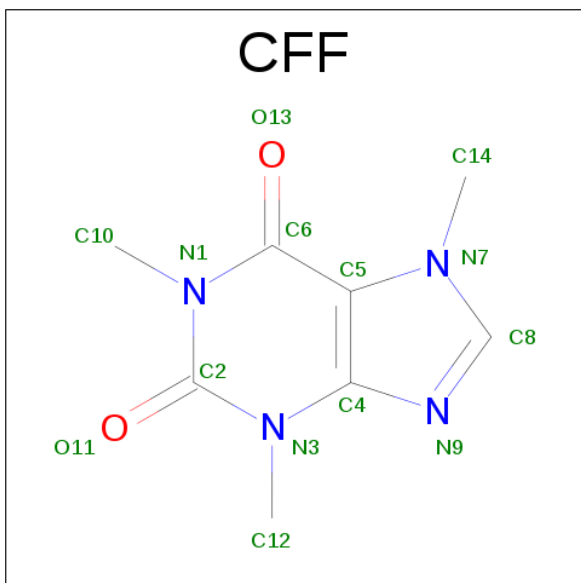
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	G	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	E	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	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

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

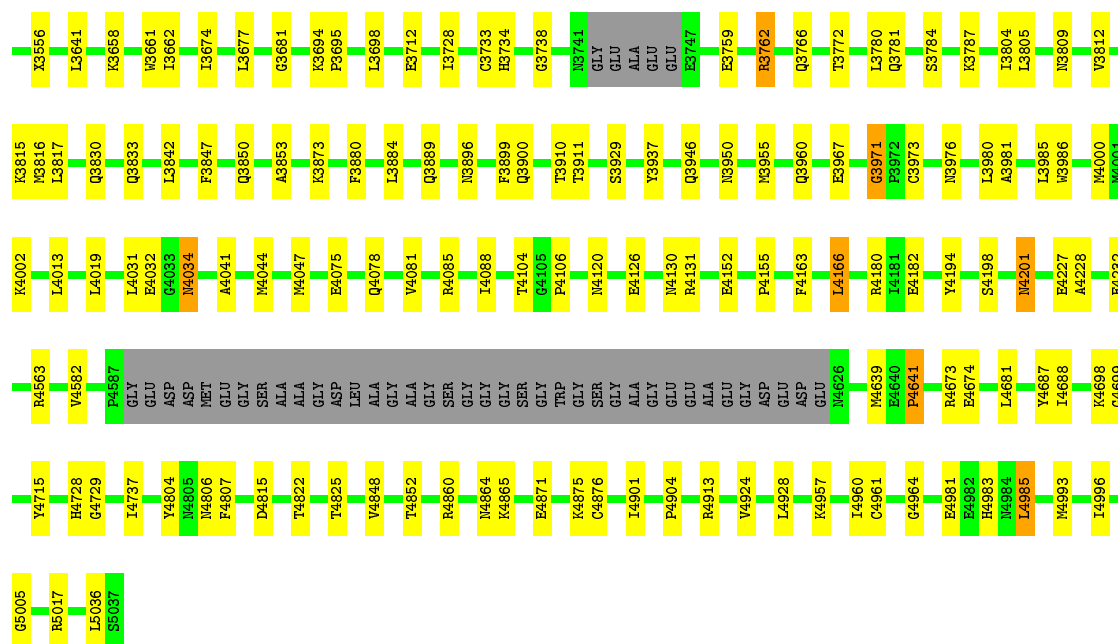
Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

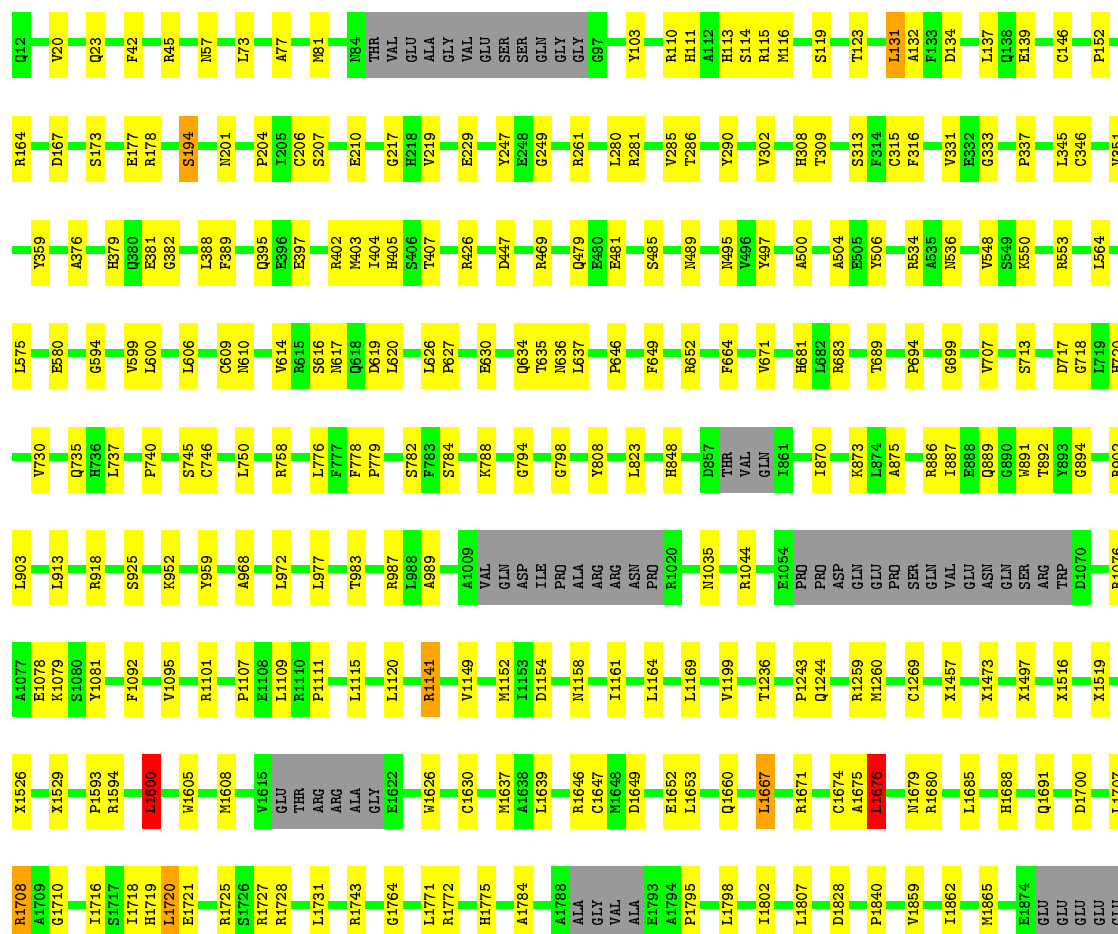
G4685	E4227	M4000	X3362	H2126	F2034	GLU	R1725	W1605	R1101	K952	V730	R553
I4686	A4228	M4001	X3365	R2127	L2038	GLU	S1726	M1608	A1105	VAL	V730	L564
I4687	E4232	K4002	X3366	Q2128	L2038	LYS	R1727	M1608	R1106	GLN	Q735	L575
T4688	E4232	M3816	X3369	D2129	C2042	GLU	R1728	V1615	P1107	ASP	H736	L575
T4689	R4563	L4013	X3369	G2130	G2043	ASP	L1731	GLU	E1108	ARG	L737	E580
K4698	V4582	L4019	X3552	G2132	G2048	GLU	L1731	THR	L1109	LYS	P740	E580
G4699	V4582	E4031	X3556	E2133	G2048	GLU	R1743	ARG	R1110	ALA	C746	E594
Y4715	P4587	E4032	L3641	I2144	GLU	GLU	G1764	ALA	L1115	LYS	S745	V599
H4728	GLU	G4033	X3658	M2153	GLU	GLU	L1771	GLY	L1120	GLU	L750	L600
G4729	ASP	M4034	X3658	S2154	PRO	ASP	R1772	E1622	L1120	VAL	L750	L606
I4737	ASP	A4041	W3661	L2155	GLU	ASP	H1775	W1626	R1141	GLN	R758	C609
G4763	GLU	M4044	I3662	N2188	GLU	GLU	H1775	C1630	V1149	ASP	L776	M610
T4766	SER	M4047	L3674	S2243	THR	THR	A1788	M1637	M1152	ILE	F777	V614
Y4804	ALA	E4075	D3675	N2246	SER	LEU	GLY	A1638	I1152	PRO	F778	R615
M4805	GLY	F3880	D3676	L2265	SER	SER	VAL	L1639	D1154	ALA	P779	S616
M4806	ASP	G3681	G3681	G2266	ARG	GLU	ALA	R1646	N1158	ARG	S782	M617
F4807	LEU	L3884	E3712	G2266	LEU	PRO	E1793	C1647	N1158	ASN	K788	D619
ALA	ALA	V4081	E3712	G2266	ARG	GLU	A1794	M1648	L1161	PRO	K788	L620
GLY	GLY	Q3889	E3712	L2273	SER	GLY	P1795	D1649	R1020	GLU	G794	L626
ALA	ALA	T3728	R2452	A2277	LEU	GLU	L1798	E1652	R1025	LYS	G798	E630
T4822	GLY	C3733	L2472	L2290	GLU	LYS	I1802	L1653	K1032	GLU	L803	E630
T4825	GLY	H3734	Q2291	Q2291	VAL	THR	L1807	Q1660	M1035	PRO	P804	T635
GLY	GLY	G3738	L2479	Q2292	ARG	VAL	L1807	Q1660	M1035	PRO	Y808	R636
SER	SER	N3741	X2587	Q2293	LEU	LEU	D1828	L1667	R1044	PRO	L823	P646
TRP	GLY	GLU	S2868	D2294	VAL	LYS	P1840	R1671	E1054	PRO	H848	F649
GLY	GLY	ALA	R2869	L2295	VAL	LYS	V1859	C1674	ASP	GLN	D857	R652
GLY	GLY	ALA	Q2872	L2302	LYS	LYS	I1862	A1675	GLU	PRO	THR	F664
ALA	ALA	GLU	N2884	C2305	GLU	GLU	M1865	L1676	C1269	GLU	VAL	F664
GLU	GLU	GLU	E3759	Y2318	PRO	GLU	E1874	N1679	R1680	SER	GLN	V671
ALA	ALA	N3950	R2888	N2324	GLU	GLU	GLU	R1685	X1457	GLN	I861	V671
GLU	GLU	M3955	L2911	P2325	LEU	LEU	GLU	L1685	X1473	VAL	I870	R683
GLY	GLY	Q3960	K2916	C2326	ALA	ALA	GLU	H1688	X1497	ASN	K873	T689
ASP	ASP	E3967	L2927	G2327	ALA	ALA	GLU	D1700	X1516	SER	R856	P694
ASP	ASP	T3772	L2927	R2330	GLU	GLU	GLU	L1707	X1519	ARG	I887	P694
GLU	GLU	R3762	L2930	Y2331	GLU	GLU	GLU	R1708	E1070	TRP	E888	G699
GLY	GLY	Q3766	K2916	L2335	GLU	GLU	GLU	A1709	R1076	GLU	Q889	V707
GLU	GLU	E3766	K2916	R2336	ALA	ALA	GLU	G1710	X1526	GLU	W891	S713
GLU	GLU	T3772	L2927	F2337	GLU	GLU	GLU	I1716	K1079	GLU	T892	S713
GLU	GLU	L3780	L2930	G2340	GLU	GLU	GLU	S1717	X1529	GLU	Y893	S713
GLU	GLU	Q3781	X2950	F2340	GLU	GLU	GLU	I1718	F1092	GLU	G894	D717
GLU	GLU	S3784	X2954	V2102	GLU	GLU	GLU	H1719	R1594	GLU	L1720	L718
GLU	GLU	K3787	X2959	R2104	GLU	GLU	GLU	L1720	V1095	GLU	R902	L718
GLU	GLU	L3804	X2963	Q2107	GLU	GLU	GLU	E1721	L1600	GLU	L903	H720
GLU	GLU	L3805	X2963	L2124	GLU	GLU	GLU	E1721	L1600	GLU	L903	H720
GLU	GLU	N3809	X3361	L2124	GLU	GLU	GLU	E1721	L1600	GLU	L903	H720
GLU	GLU	N3809	X3361	L2124	GLU	GLU	GLU	E1721	L1600	GLU	L903	H720






• Molecule 2: Ryanodine receptor 1

Chain I: 84% 11% 5%



GLU	Q2003	GLU	L2335	GLU	W2775	GLU	L2930	GLU	H3771	GLU	N3950	GLU	E4152	GLU	D4899	GLU	Y4626	GLU	E4900	GLU	D4899
GLU	E2004	GLU	L2336	GLU	W2776	GLU	L2931	GLU	T3772	GLU	E4901	GLU	P4155	GLU	E4902	GLU	Y4627	GLU	I4901	GLU	E4903
GLU	Q2005	GLU	F2337	GLU	G2778	GLU	X2950	GLU	G3773	GLU	M3955	GLU	F4163	GLU	P4904	GLU	Y4628	GLU	P4905	GLU	E4904
GLU	N2007	GLU	F2340	GLU	T2787	GLU	X2954	GLU	G3774	GLU	Q3960	GLU	L4166	GLU	R4913	GLU	Y4629	GLU	P4906	GLU	E4905
GLU	P2022	GLU	V2346	GLU	W2807	GLU	X2959	GLU	Q3781	GLU	E3967	GLU	R4180	GLU	V4924	GLU	Y4630	GLU	P4907	GLU	E4906
GLU	L2023	GLU	E2347	GLU	P2810	GLU	X2963	GLU	S3784	GLU	G3971	GLU	I4181	GLU	L4928	GLU	Y4631	GLU	P4908	GLU	E4907
GLU	P2024	GLU	E2348	GLU	K2814	GLU	X3361	GLU	K3787	GLU	C3973	GLU	E4182	GLU	K4957	GLU	Y4632	GLU	P4909	GLU	E4908
GLU	T2027	GLU	V2353	GLU	L2823	GLU	X3362	GLU	I3804	GLU	N3976	GLU	Y4194	GLU	K4958	GLU	Y4633	GLU	P4910	GLU	E4909
GLU	R2028	GLU	L2357	GLU	E2830	GLU	X3366	GLU	I3805	GLU	L3980	GLU	S4198	GLU	K4959	GLU	Y4634	GLU	P4911	GLU	E4910
GLU	F2034	GLU	P2395	GLU	GLU	GLU	X3369	GLU	N3809	GLU	A3981	GLU	N4201	GLU	K4960	GLU	Y4635	GLU	P4912	GLU	E4911
GLU	L2038	GLU	VAL	GLU	GLU	GLU	X3582	GLU	V3812	GLU	L3985	GLU	E4227	GLU	K4961	GLU	Y4636	GLU	P4913	GLU	E4912
GLU	C2042	GLU	ARG	GLU	THR	GLU	X3586	GLU	K3815	GLU	W3986	GLU	A4228	GLU	K4962	GLU	Y4637	GLU	P4914	GLU	E4913
GLU	G2043	GLU	ASP	GLU	GLU	GLU	X3556	GLU	M3816	GLU	M4000	GLU	E4232	GLU	K4963	GLU	Y4638	GLU	P4915	GLU	E4914
GLU	G2048	GLU	ARG	GLU	LYS	GLU	L3641	GLU	L3817	GLU	K4002	GLU	R4563	GLU	K4964	GLU	Y4639	GLU	P4916	GLU	E4915
GLU	GLU	GLU	GLU	GLU	THR	GLU	X3658	GLU	Q3830	GLU	L4013	GLU	V4582	GLU	K4965	GLU	Y4640	GLU	P4917	GLU	E4916
GLU	PRO	GLU	HIS	GLU	ARG	GLU	X3661	GLU	Q3833	GLU	L4019	GLU	P4587	GLU	K4966	GLU	Y4641	GLU	P4918	GLU	E4917
GLU	GLU	GLU	PHE	GLU	ILE	GLU	X3662	GLU	L3842	GLU	L4031	GLU	GLU	GLU	K4967	GLU	Y4642	GLU	P4919	GLU	E4918
GLU	GLU	GLU	GLU	GLU	GLU	GLU	X3674	GLU	F3847	GLU	M4044	GLU	ASP	GLU	K4968	GLU	Y4643	GLU	P4920	GLU	E4919
GLU	THR	GLU	GLU	GLU	THR	GLU	L3677	GLU	R3849	GLU	A4041	GLU	MET	GLU	K4969	GLU	Y4644	GLU	P4921	GLU	E4920
GLU	THR	GLU	PRO	GLU	ALA	GLU	G3681	GLU	Q3850	GLU	M4047	GLU	GLY	GLU	K4970	GLU	Y4645	GLU	P4922	GLU	E4921
GLU	LEU	GLU	PRO	GLU	ASP	GLU	L3698	GLU	A3853	GLU	M4048	GLU	ALA	GLU	K4971	GLU	Y4646	GLU	P4923	GLU	E4922
GLU	LEU	GLU	ARG	GLU	PRO	GLU	E3712	GLU	K3873	GLU	M4049	GLU	ALA	GLU	K4972	GLU	Y4647	GLU	P4924	GLU	E4923
GLU	LEU	GLU	LEU	GLU	ARG	GLU	E3728	GLU	F3880	GLU	E4075	GLU	GLY	GLU	K4973	GLU	Y4648	GLU	P4925	GLU	E4924
GLU	GLU	GLU	L2290	GLU	GLY	GLU	L3728	GLU	L3884	GLU	Q4078	GLU	ALA	GLU	K4974	GLU	Y4649	GLU	P4926	GLU	E4925
GLU	GLU	GLU	L2291	GLU	Y2855	GLU	C3733	GLU	Q3889	GLU	V4081	GLU	GLY	GLU	K4975	GLU	Y4650	GLU	P4927	GLU	E4926
GLU	GLU	GLU	L2292	GLU	S2868	GLU	H3734	GLU	L3890	GLU	R4085	GLU	GLY	GLU	K4976	GLU	Y4651	GLU	P4928	GLU	E4927
GLU	GLU	GLU	L2293	GLU	R2869	GLU	G3738	GLU	L3891	GLU	R4086	GLU	GLY	GLU	K4977	GLU	Y4652	GLU	P4929	GLU	E4928
GLU	GLU	GLU	L2294	GLU	Q2872	GLU	N3741	GLU	N3896	GLU	I4088	GLU	GLY	GLU	K4978	GLU	Y4653	GLU	P4930	GLU	E4929
GLU	GLU	GLU	L2295	GLU	M2874	GLU	GLY	GLU	N3897	GLU	T4104	GLU	GLY	GLU	K4979	GLU	Y4654	GLU	P4931	GLU	E4930
GLU	GLU	GLU	L2302	GLU	L2878	GLU	ALA	GLU	Q3900	GLU	G4105	GLU	GLY	GLU	K4980	GLU	Y4655	GLU	P4932	GLU	E4931
GLU	GLU	GLU	L2305	GLU	N2884	GLU	GLU	GLU	T3910	GLU	P4106	GLU	GLY	GLU	K4981	GLU	Y4656	GLU	P4933	GLU	E4932
GLU	GLU	GLU	L2318	GLU	R2888	GLU	E3747	GLU	T3911	GLU	N4120	GLU	GLY	GLU	K4982	GLU	Y4657	GLU	P4934	GLU	E4933
GLU	GLU	GLU	N2324	GLU	R2888	GLU	E3759	GLU	S3929	GLU	E4126	GLU	ALA	GLU	K4983	GLU	Y4658	GLU	P4935	GLU	E4934
GLU	GLU	GLU	P2325	GLU	L2911	GLU	R3762	GLU	Y3937	GLU	N4130	GLU	GLY	GLU	K4984	GLU	Y4659	GLU	P4936	GLU	E4935
GLU	GLU	GLU	C2326	GLU	K2916	GLU	Q3766	GLU	Q3946	GLU	R4131	GLU	GLU	GLU	K4985	GLU	Y4660	GLU	P4937	GLU	E4936
GLU	GLU	GLU	G2327	GLU	L2927	GLU		GLU		GLU		GLU	GLU	GLU	K4986	GLU	Y4661	GLU	P4938	GLU	E4937
GLU	GLU	GLU	R2330	GLU		GLU		GLU		GLU		GLU	GLU	GLU	K4987	GLU	Y4662	GLU	P4939	GLU	E4938
GLU	GLU	GLU	Y2331	GLU		GLU		GLU		GLU		GLU	GLU	GLU	K4988	GLU	Y4663	GLU	P4940	GLU	E4939
GLU	GLU	GLU	L2332	GLU		GLU		GLU		GLU		GLU	GLU	GLU	K4989	GLU	Y4664	GLU	P4941	GLU	E4940

• Molecule 2: Ryanodine receptor 1

Chain E:  84% 11% 5%

Q12	R164	Y359	E580	Q12	R164	Y359	E580
V20	D167	A376	G594	V20	D167	A376	G594
Q23	S173	H379	V599	Q23	S173	H379	V599
F42	E177	Q380	L606	F42	E177	Q380	L606
R45	R178	E381	G609	R45	R178	E381	G609
N57	S194	L388	N610	N57	S194	L388	N610
L73	H201	F389	V614	L73	H201	F389	V614
A77	P204	Q395	R615	A77	P204	Q395	R615
M81	I205	E396	S616	M81	I205	E396	S616
N84	C206	E397	N617	N84	C206	E397	N617
THR	S207	R402	G618	THR	S207	R402	G618
VAL	E210	M403	D619	VAL	E210	M403	D619
GLU	G217	I404	L620	GLU	G217	I404	L620
SER	H218	H405	L626	SER	H218	H405	L626
GLN	V219	R426	P627	GLN	V219	R426	P627
GLY	E229	D447	G628	GLY	E229	D447	G628
GLU	Y247	R469	R629	GLU	Y247	R469	R629
SER	E248	Q479	B630	SER	E248	Q479	B630
GLN	G249	E480	Q634	GLN	G249	E480	Q634
GLY	R261	E481	T635	GLY	R261	E481	T635
G97	L280	S485	P646	G97	L280	S485	P646
Y103	R281	N489	F649	Y103	R281	N489	F649
R110	V285	N495	R652	R110	V285	N495	R652
H111	T286	V496	F664	H111	T286	V496	F664
A112	Y290	Y497	V671	A112	Y290	Y497	V671
H113	S302	A500	H681	H113	S302	A500	H681
S114	H308	A504	L682	S114	H308	A504	L682
R115	T309	E505	R683	R115	T309	E505	R683
M116	S313	Y506	T689	M116	S313	Y506	T689
S119	F314	R534	P694	S119	F314	R534	P694
T123	C315	A535	G699	T123	C315	A535	G699
L131	F316	N536	V707	L131	F316	N536	V707
F133	V331	V548	S713	F133	V331	V548	S713
D134	E332	S549	D717	D134	E332	S549	D717
L137	G333	K550	G718	L137	G333	K550	G718
Q138	P337	R553	H720	Q138	P337	R553	H720
E139	L345	L564		E139	L345	L564	
C146	C346	L575		C146	C346	L575	
P152	V351			P152	V351		

V4924	E4640	E4181	P3972	S3784	X3361	X2807	L2124	T2027	E1721	Y1615	P1107	Y959	V730
L4928	P4641	E4182	C3973	R3787	X3362	X2810	E2125	R2028	R1725	THR	E1108	Y959	Q735
K4957	E4674	Y4194	N3976	L3804	X3365	X2814	R2126	F2034	S1726	GLU	R1109	A968	H736
L4960	L4681	S4198	L3980	L3805	X3366	X2823	Y2128	L2038	R1727	ARG	P1111	L972	L737
C4961	L4681	S4198	A3981	N3809	X3369	X2823	Y2129	L2038	R1728	ALA	L1115	L972	P740
Q4964	Y4687	E4201	R3984	V3812	X3552	E2830	Y2130	C2042	L1731	GLY	L1120	L977	S745
E4981	L4688	E4227	L3985	V3812	X3552	GLU	Y2131	G2043	R1743	E1622	L1120	T983	C746
E4982	E4698	A4228	N3986	X3815	X3556	GLU	E2133	G2048	G1764	W1626	R1141	R987	L750
H4983	Q4699	E4232	X3556	X3816	L3641	THR	L2155	GLU	G1764	C1630	V1149	L988	R758
L4985	Y4715	R4563	L3641	X3658	L3641	GLU	L2188	GLU	R1772	M1637	M1152	Y989	L776
M4993	R4728	Y4582	L3658	X3658	L3658	GLU	S2243	GLU	H1775	A1638	D1153	VAL	F777
L4996	Q4729	Y4587	X3661	X3662	L3662	GLU	Y2246	GLU	A1784	L1639	D1154	GLN	F778
G5005	M4737	L4031	X3674	L3674	L3674	THR	L2265	THR	A1788	R1646	H1158	ASP	P779
R5017	M4743	E4032	X3675	L3675	L3675	GLU	G2266	SER	ALA	C1647	I1161	PRO	S782
L5036	A4746	Q4034	L3677	L3677	L3677	GLU	L2273	SER	VAL	D1649	L1164	ALA	F783
S5037	Y4804	M4044	L3681	L3681	L3681	THR	L2277	ARG	ALA	E1652	L1169	ASN	S784
	M4805	SER	L3698	L3698	L3698	ALA	L2290	LEU	A1794	L1653	P1199	PRO	K788
	F4807	ALA	L3712	L3712	L3712	GLU	Q2291	ARG	PY795	Q1660	V1236	R1020	G794
	D4815	ASP	E3712	L3728	L3728	GLU	Q2293	LEU	L1798	H1665	T1236	M1035	G798
	T4822	ALA	L3733	L3733	L3733	GLU	L2295	THR	I1802	L1667	P1243	R1044	Y808
	T4825	ALA	H3734	L3734	L3734	GLU	L2302	VAL	L1807	R1671	Q1244	E1084	L823
	Y4843	GLY	L3890	L3890	L3890	GLY	C2305	VAL	D1828	C1674	R1269	PRO	H848
	T4852	GLY	L3896	L3896	L3896	GLY	Y2318	LYS	P1840	A1675	C1269	ASP	D857
	R4860	SER	F3889	L3899	L3899	GLU	L2324	LYS	V1859	L1679	X1457	GLU	THR
	M4864	GLU	Q3900	L3900	L3900	GLU	Y2325	LYS	I1862	R1680	X1473	SER	VAL
	K4865	TRP	T3910	L3911	L3911	GLU	C2326	PRO	M1865	L1685	X1497	GLN	L861
	E4871	SER	S3929	L3929	L3929	GLU	Q2327	GLU	A1960	H1688	X1516	ASN	L870
	K4875	ALA	Y3937	L3937	L3937	GLU	R2330	GLU	E1874	GLU	X1519	SER	K873
	C4876	ALA	R3762	L3946	L3946	GLU	L2332	LEU	Q1970	Q1691	X1526	TRP	R886
	Y4888	ALA	Q3766	L3950	L3950	GLU	Y2335	ALA	D1700	D1700	X1529	R1076	L887
	L4901	GLY	H3771	L3955	L3955	GLU	F2337	GLU	L1707	R1708	X1593	K1079	Q889
	P4904	ASP	T3772	X3955	L3955	GLU	L2340	Q2095	A1709	G1710	P1594	F1092	G890
	R4913	ASP	G3774	X3954	L3954	GLU	Y2346	GLU	G1710	G1710	F1092	F1092	G894
	D4917	GLU	L3780	X3967	L3967	GLU	E2347	GLU	I1716	S1717	L1600	V1095	R902
			Q3781	X3963	L3963	GLU	E2348	R2104	I1718	I1718	H1605	R1101	L903
						GLU	Y2353	Q2107	L1720	L1720	M1608	K952	

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, CA, 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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.30	0/25428	0.54	9/34534 (0.0%)
2	E	0.30	0/25428	0.54	9/34534 (0.0%)
2	G	0.30	0/25428	0.54	9/34534 (0.0%)
2	I	0.30	0/25428	0.54	9/34534 (0.0%)
All	All	0.30	0/105048	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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

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	B	131	LEU	CA-CB-CG	7.43	132.38	115.30
2	G	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	I	131	LEU	CA-CB-CG	7.42	132.36	115.30
2	E	131	LEU	CA-CB-CG	7.41	132.34	115.30
2	G	4985	LEU	CA-CB-CG	6.93	131.25	115.30

There are no chirality outliers.

5 of 60 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	13	0
1	F	818	0	824	18	0
1	H	818	0	824	17	0
1	J	818	0	824	19	0
2	B	29499	0	24746	271	0
2	E	29499	0	24745	276	0
2	G	29499	0	24745	266	0
2	I	29499	0	24745	278	0
3	B	31	0	12	2	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102365	1132	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 1132 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:4985:LEU:HB2	3:I:5101:ATP:HN61	1.52	0.74
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.73
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.71	0.73
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.52	0.73

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	52	86
2	G	3235/4416 (73%)	2881 (89%)	349 (11%)	5 (0%)	52	86
2	I	3235/4416 (73%)	2882 (89%)	348 (11%)	5 (0%)	52	86
All	All	13360/18096 (74%)	11903 (89%)	1437 (11%)	20 (0%)	59	90

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	B	4641	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	4120	ASN

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Mol	Chain	Res	Type
2	I	1141	ARG
2	E	4034	ASN
2	G	4131	ARG
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	G	3946	GLN
2	I	479	GLN
2	E	3889	GLN
2	G	3960	GLN
2	G	4806	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 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	-	26,33,33	0.91	1 (3%)	26,52,52	1.77	2 (7%)
4	CFF	B	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.19	1 (12%)
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.75	3 (11%)
4	CFF	E	5102	-	8,15,15	2.43	3 (37%)	8,23,23	1.19	1 (12%)
3	ATP	G	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.77	3 (11%)
4	CFF	G	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.18	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.76	3 (11%)
4	CFF	I	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.19	1 (12%)

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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C4-N3	-4.77	1.33	1.39
4	I	5102	CFF	C4-N3	-4.76	1.33	1.39
4	E	5102	CFF	C4-N3	-4.62	1.33	1.39
4	B	5102	CFF	C4-N3	-4.58	1.33	1.39
4	I	5102	CFF	C6-N1	-4.05	1.32	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	N3-C2-N1	-7.00	123.38	128.87
3	G	5101	ATP	N3-C2-N1	-6.97	123.40	128.87
3	I	5101	ATP	N3-C2-N1	-6.95	123.42	128.87
3	E	5101	ATP	N3-C2-N1	-6.89	123.46	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-2.63	111.56	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
4	B	5102	CFF	1	0
3	E	5101	ATP	1	0
4	E	5102	CFF	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0
4	I	5102	CFF	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	E	4345:UNK	C	4540:PHE	N	73.04
1	B	4345:UNK	C	4540:PHE	N	73.02
1	I	4345:UNK	C	4540:PHE	N	73.01
1	G	4345:UNK	C	4540:PHE	N	73.00
1	E	3613:UNK	C	3639:THR	N	45.97