



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5TAS
EMDB ID: : EMD-8383
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc29047

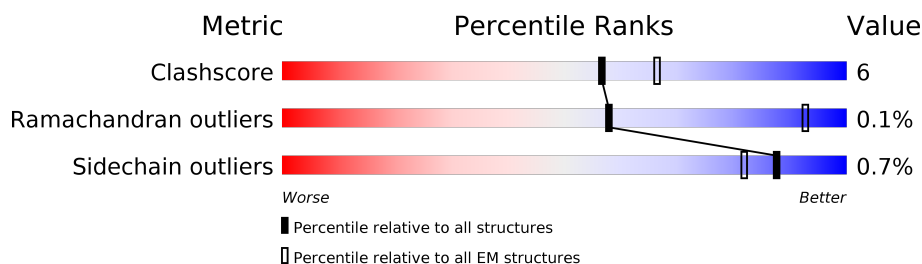
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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 ≥ 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	69% 31% .
1	F	108	70% 29% .
1	H	108	71% 28% .
1	J	108	72% 27% .
2	B	4416	82% 12% 5%
2	E	4416	82% 12% 5%
2	G	4416	82% 12% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

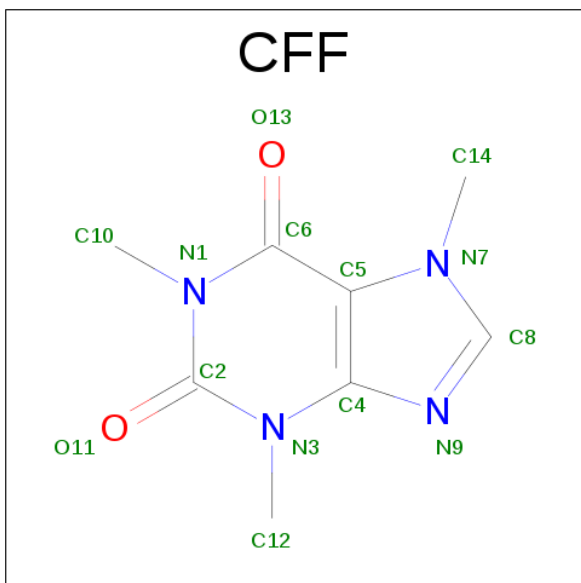
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

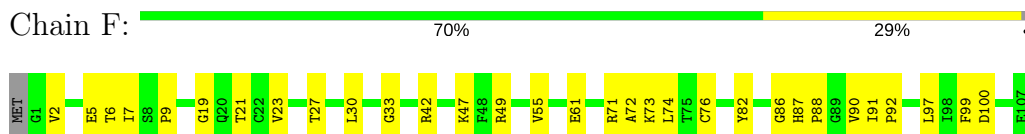
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

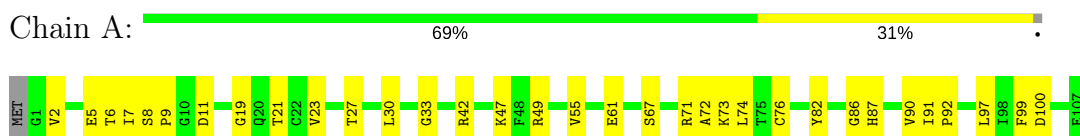
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

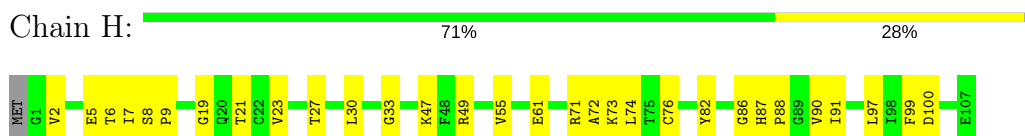
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



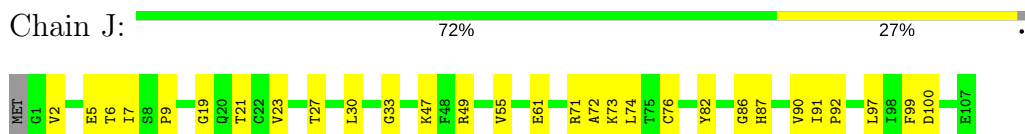
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



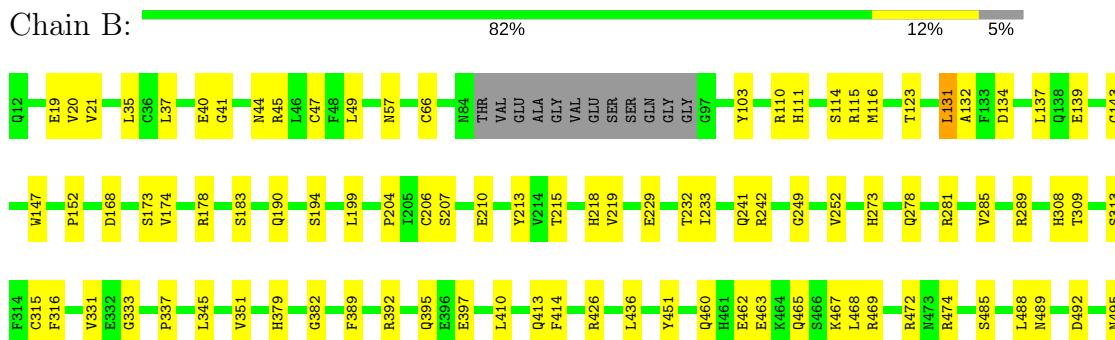
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



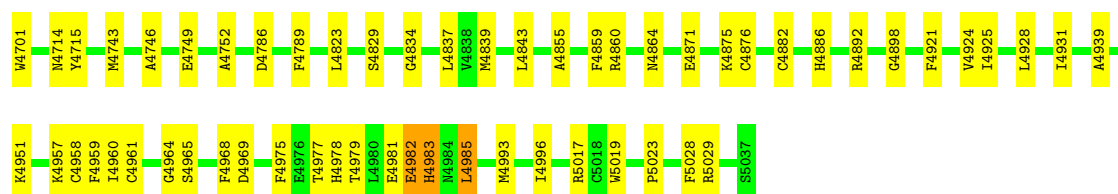
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

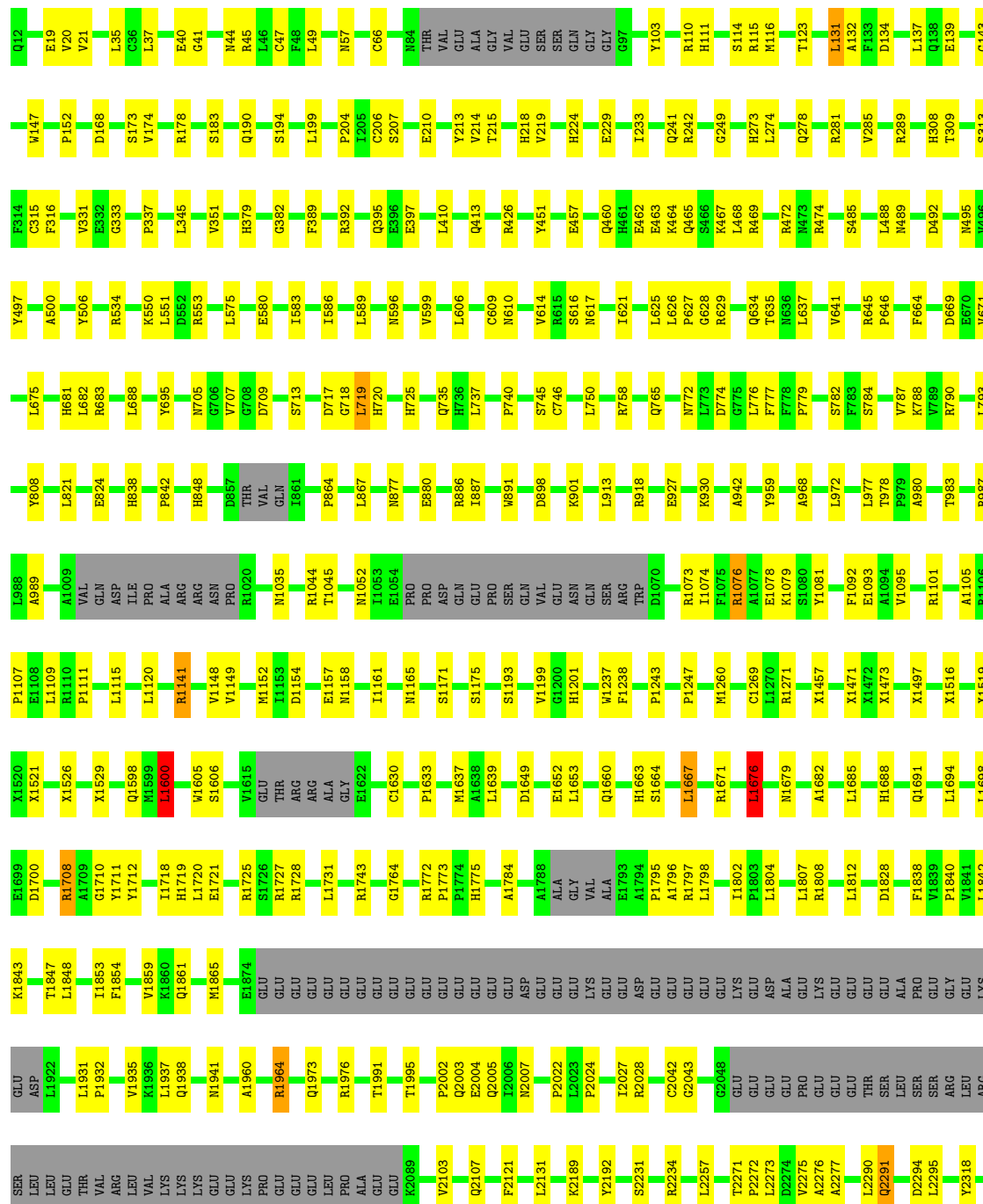


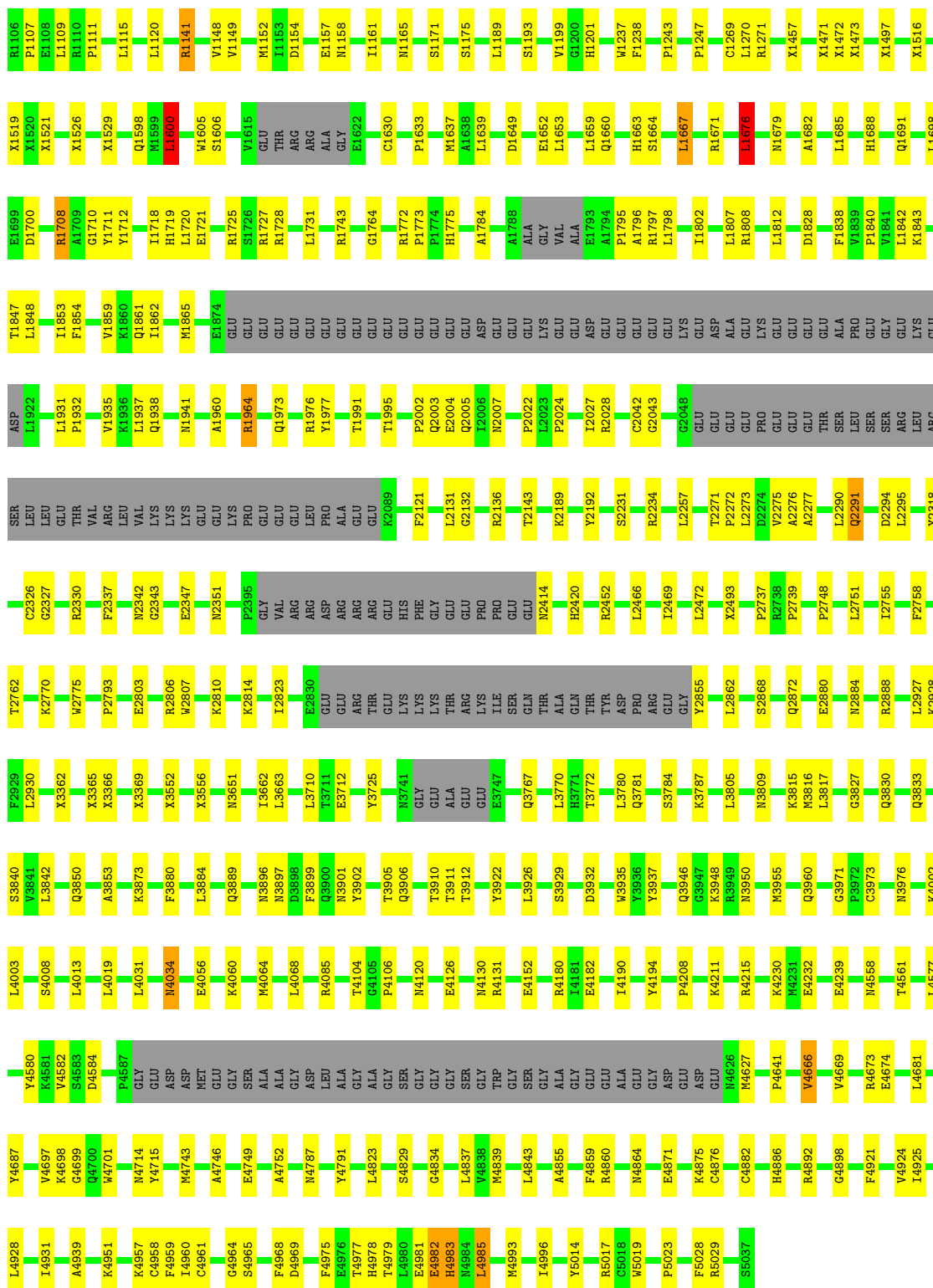
V496	V671	L793	A989	A1105	X1497	Q1691	V1839	GLU	LEU	C2326	T2762	X3362	Q3850	L4013	P4587
Y497	L675	Y808	A1009	R1106	X1516	L1694	P1840	GLY	ARG	G2327	K2770	X3365	A3853	L4019	GLY
A500	H681	L821	VAL	E1108	X1519	L1842	V1841	LEU	LEU	X1843	V2775	X3366	X3873	L4031	ASP
A504	L682	E824	GLN	R1110	X1521	L1698	K1843	GLU	THR	R2330	P2793	X3369	F3880	M4034	ASP
E505	R683	E824	ASP	R1111	X1526	E1699	T1847	ASP	VAL	F2337	E2803	X3369	F3880	M4034	WET
Y506	L688	E838	ILE	P1111	X1526	D1700	L1848	ASP	VAL	P2337	P2793	X3369	F3880	M4034	WET
R534	Y695	H838	ALA	L1115	X1526	D1700	L1848	ASP	VAL	P2337	P2793	X3369	F3880	M4034	WET
R534	Y695	H838	ALA	L1115	X1526	D1700	L1848	ASP	VAL	P2337	P2793	X3369	F3880	M4034	WET
K550	N705	H848	ARG	L1120	X1529	X1708	F1854	ARG	VAL	E2342	E2803	X3369	F3880	M4034	WET
L551	N705	H848	ASN	Q1130	Q1598	Y1711	V1859	LYS	LYS	E2347	E2803	X3369	F3880	M4034	WET
E552	G766	H848	PRD	Q1138	Q1599	Y1712	K1860	LYS	LYS	E2347	E2803	X3369	F3880	M4034	WET
R553	G766	H848	PRD	P1138	Q1599	Y1712	K1860	LYS	LYS	E2347	E2803	X3369	F3880	M4034	WET
L575	G766	H848	PRD	P1138	Q1599	Y1712	K1860	LYS	LYS	E2347	E2803	X3369	F3880	M4034	WET
L575	G766	H848	PRD	P1138	Q1599	Y1712	K1860	LYS	LYS	E2347	E2803	X3369	F3880	M4034	WET
E580	S713	L861	VAL	R1141	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L683	D717	P864	GLN	V1148	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L589	L719	P865	GLN	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
N596	H720	P865	GLN	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
N596	H720	P865	GLN	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
V699	H725	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L606	H736	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
C609	H740	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
N610	H740	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
V614	S745	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
R615	C746	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
S616	L750	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
N617	L750	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L621	R758	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L625	Q765	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L626	N772	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
P627	L773	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
G628	D774	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
R629	G775	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
Q634	L776	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
T635	F777	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
N638	F778	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
L637	P779	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
V641	S782	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
R645	S784	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
P646	V787	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
F664	K788	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
D669	V789	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET
E670	X1473	P865	PRD	V1149	W1605	H719	M1865	PRO	PRO	E2347	E2803	X3369	F3880	M4034	WET



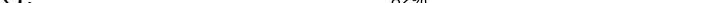
• Molecule 2: Ryanodine receptor 1

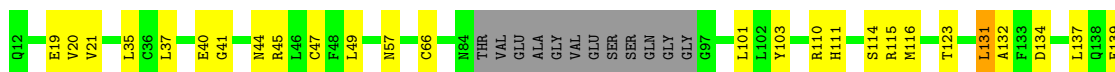
Chain I: 83% 12% 5%





- Molecule 2: Ryanodine receptor 1

Chain G:  82% 12% 5%



K3816	E2880	R2738	V2275	A1682	X1471	F1092	L972	S782	V641	S485	R289	G143
L3817	E2880	P2739	A2276	L1685	X1472	E1093	L977	F783	R645	L488	V301	W147
G3827	N2884	P2748	A2277	H1688	X1473	A1094	T978	S784	P646	N489	H308	M150
Q3830	R2888	L2751	L2290	Q1691	X1497	V1095	P979	V787	F664	D492	T309	H151
Q3833	L2927	L2755	D2294	L1698	X1516	A1105	T983	R790	D669	N495	S313	P152
K2928	K2928	L2758	L2295	L1699	X1519	P1107	R987	L793	E670	Y496	F314	E161
S3840	F2929	F2768	Y2318	D1700	X1520	E1108	L988	Y808	V671	Y497	C315	D168
V3841	L2930	T2762	Y2318	B1708	X1521	E1109	A989	Y808	L675	A500	F316	D168
L3842	X3362	K2770	C2326	A1709	X1526	R1110	A1009	L821	H681	Y506	V331	S173
Q3850	X3365	K2770	G2327	G1710	X1529	P1111	VAL	L821	L682	Y506	E332	V174
A3853	X3366	W2775	R2330	Y1711	X1529	L1115	GLN	E824	R683	R534	G333	R178
K3873	X3369	P2793	F2337	Y1712	Q1598	L1120	ASP	H838	L688	X550	P337	S183
F3880	X3552	E2803	N2342	I1718	N1599	L1120	PRO	P842	Y695	L551	L345	Q190
L3884	X3556	R2806	G2343	H1719	L1660	R1141	ALA	P842	N705	D852	V351	S194
Q3889	N3651	E2347	E2347	E1721	W1605	V1148	ARG	H848	G706	R553	H379	L199
K3896	L3662	N2351	N2351	R1725	V1615	V1149	PRO	D857	V707	L575	G382	L199
N3897	L3663	P2395	P2395	S1726	GLU	M1152	B1020	THR	D709	E580	G382	P204
D3898	L3710	GLY	GLY	R1727	THR	M1152	M1035	VAL	S713	L583	F389	L205
F3899	L3711	VAL	VAL	R1728	ARG	D1154	R1044	GLN	D717	L586	R392	C206
Q3900	T3711	ARG	ARG	L1731	ALA	E1157	T1045	ARG	G718	L589	Q395	E210
N3901	E3712	ARG	ARG	R1743	GLY	M1158	M1082	L867	L719	E396	E396	Y213
Y3902	Y3725	ASP	ASP	GL764	E1692	I1161	I1053	N877	H720	N596	E397	T215
T3905	N3741	ARG	ARG	G1772	C1630	M1165	I1054	E880	H725	V599	L410	T215
Q3906	GLY	GLU	GLU	P1773	P1633	S1171	PRO	P1773	Q735	L606	Q413	H218
T3910	GLY	GLU	GLU	P1774	M1637	S1175	ASP	E880	H736	L606	F414	V219
T3911	ALA	GLU	GLU	H1775	A1638	S1175	GLN	R886	L737	C609	R426	H224
T3912	GLU	GLU	GLU	H1775	L1639	L1189	PRO	R886	L737	N610	L436	E229
Y3922	E3747	ILE	ILE	A1784	L1639	L1189	SER	N891	P740	G614	Y451	T233
L3926	Q3767	PRO	PRO	A1788	D1649	S1193	GLN	D898	S745	R615	Q460	Q241
S3929	L3770	GLU	GLU	ALA	E1652	V1199	VAL	D898	C746	S616	E462	R242
D3932	H3771	GLN	GLU	VAL	L1653	GL200	ASN	K901	L750	N617	E463	R243
K3935	L3780	THR	THR	E1793	L1659	H1201	ARG	L913	R758	I621	K464	G249
Y3936	Q3781	TYR	TYR	A1794	Q1660	V1237	TRP	B918	Q765	L625	Q465	H273
Y3937	S3784	PRO	PRO	P1795	H1663	F1238	D1070	E927	N772	L626	P627	L274
Q3946	Q3947	GLY	GLY	A1796	S1664	P1243	R1073	K930	L773	G628	S466	R243
K3948	K3948	GLY	GLY	L1667	L1667	P1247	F1075	R930	D774	R629	K467	L274
K3949	K3949	ASP	ASP	L1671	R1671	P1247	R1076	A942	G775	Q634	L468	Q278
N3950	L3805	GLU	GLU	L1807	L1671	C1269	A1077	Y959	L776	T635	R469	Q278
K3955	N3809	GLU	GLU	R1808	L1676	L1270	E1078	F777	F777	R636	N472	R281
	K3815	PRO	PRO	L1812	N1679	R1271	S1080	A968	P779	L637	N473	Y285
		GLU	GLU			X1457	Y1081				R474	

V4924	Q3960	E4232	V4666
I4925	G3971	E4239	V4669
L4928	P3972	N4558	E4673
I4931	C3973	T4561	E4674
A4939	N3976	L4577	L4681
K4957	K4002	Y4580	Y4687
C4958	L4003	K4581	V4697
F4959	S4008	V4582	K4698
I4960	L4013	S4583	C4699
C4961	D4584	Q4700	V4700
G4964	L4019	W4701	M4714
S4965	L4031	GLY	Y4715
F4968	L4034	GLU	Y4743
D4969	E4056	ASP	A4746
F4975	K4060	ASP	E4749
E4976	M4064	MET	A4752
T4977	L4068	GLY	K4821
H4978	R4085	SER	T4822
T4979	T4104	ALA	L4823
L4980	G4105	GLY	S4829
E4981	P4106	ALA	G4834
E4982	N4120	SER	L4837
H4983	E4126	GLY	W4838
W4984	M4130	SER	M4839
L4985	R4131	TRP	A4855
M4993	E4152	SER	F4859
I4996	R4180	GLY	R4860
Y5014	I4181	ALA	M4864
R5017	E4182	GLY	E4871
C5018	I4190	ALA	K4875
W5019	Y4194	GLU	C4876
P5023	P4208	ASP	C4882
F5028	K4211	ASP	R4892
S5037	R4215	GLU	G4898
	K4230	M4626	F4921
	M4231	M4627	
		P4641	

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, 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	0.31	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	0.29	0/25428	0.53	9/34534 (0.0%)
2	E	0.29	0/25428	0.53	9/34534 (0.0%)
2	G	0.29	0/25428	0.53	9/34534 (0.0%)
2	I	0.29	0/25428	0.53	9/34534 (0.0%)
All	All	0.29	0/105048	0.53	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
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.04	133.78	115.30
2	B	131	LEU	CA-CB-CG	8.02	133.75	115.30
2	I	131	LEU	CA-CB-CG	8.01	133.73	115.30
2	E	131	LEU	CA-CB-CG	8.00	133.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1600	LEU	CA-CB-CG	7.20	131.87	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	808	TYR	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	21	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	316	0
2	E	29499	0	24746	322	0
2	G	29499	0	24746	319	0
2	I	29499	0	24746	317	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1324	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 6.

The worst 5 of 1324 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:G:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	55	88
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	55	88
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	55	88
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	55	88
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	58	88

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1840	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%)	87	93
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	87	93
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	87	93

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

Mol	Chain	Res	Type
2	I	4131	ARG
2	E	1141	ARG
2	G	4085	ARG
2	I	4839	MET
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3946	GLN

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Mol	Chain	Res	Type
2	E	379	HIS
2	G	3946	GLN
2	I	3960	GLN
2	I	4142	ASN

5.3.3 RNA [i](#)

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 12 ligands modelled in this entry, 4 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	-	27,33,33	0.92	1 (3%)	25,52,52	1.65	2 (8%)
4	CFF	B	5102	-	7,15,15	1.83	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	E	5101	-	27,33,33	0.92	1 (3%)	25,52,52	1.64	2 (8%)
4	CFF	E	5102	-	7,15,15	1.82	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	G	5101	-	27,33,33	0.93	1 (3%)	25,52,52	1.65	2 (8%)
4	CFF	G	5102	-	7,15,15	1.83	2 (28%)	8,23,23	1.30	1 (12%)
3	ATP	I	5101	-	27,33,33	0.93	1 (3%)	25,52,52	1.66	2 (8%)
4	CFF	I	5102	-	7,15,15	1.82	2 (28%)	8,23,23	1.30	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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C6-N1	-3.79	1.32	1.38
4	E	5102	CFF	C6-N1	-3.79	1.32	1.38
4	G	5102	CFF	C6-N1	-3.78	1.32	1.38
4	I	5102	CFF	C6-N1	-3.75	1.32	1.38
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5101	ATP	N3-C2-N1	-6.11	123.54	128.86
3	G	5101	ATP	N3-C2-N1	-6.06	123.58	128.86
3	B	5101	ATP	N3-C2-N1	-6.06	123.58	128.86
3	E	5101	ATP	N3-C2-N1	-6.02	123.61	128.86
3	I	5101	ATP	C4-C5-N7	-2.98	106.53	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 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	2	0
4	E	5102	CFF	1	0

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

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	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63