



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:09 pm GMT

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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
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

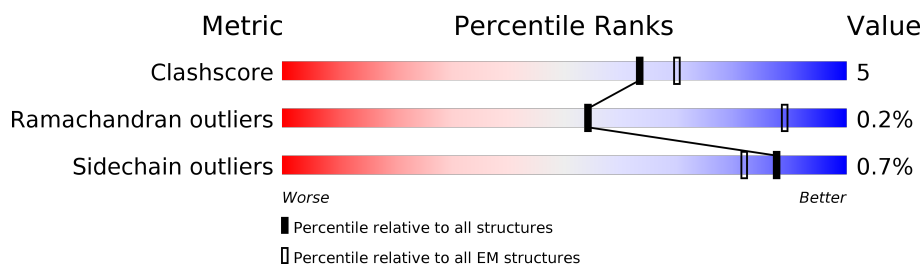
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	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: 




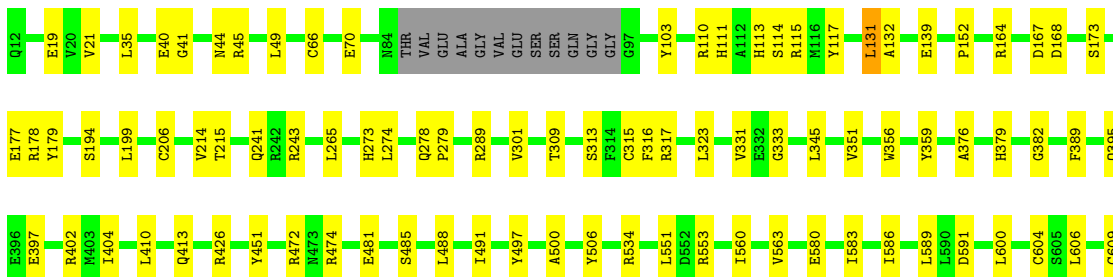
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 

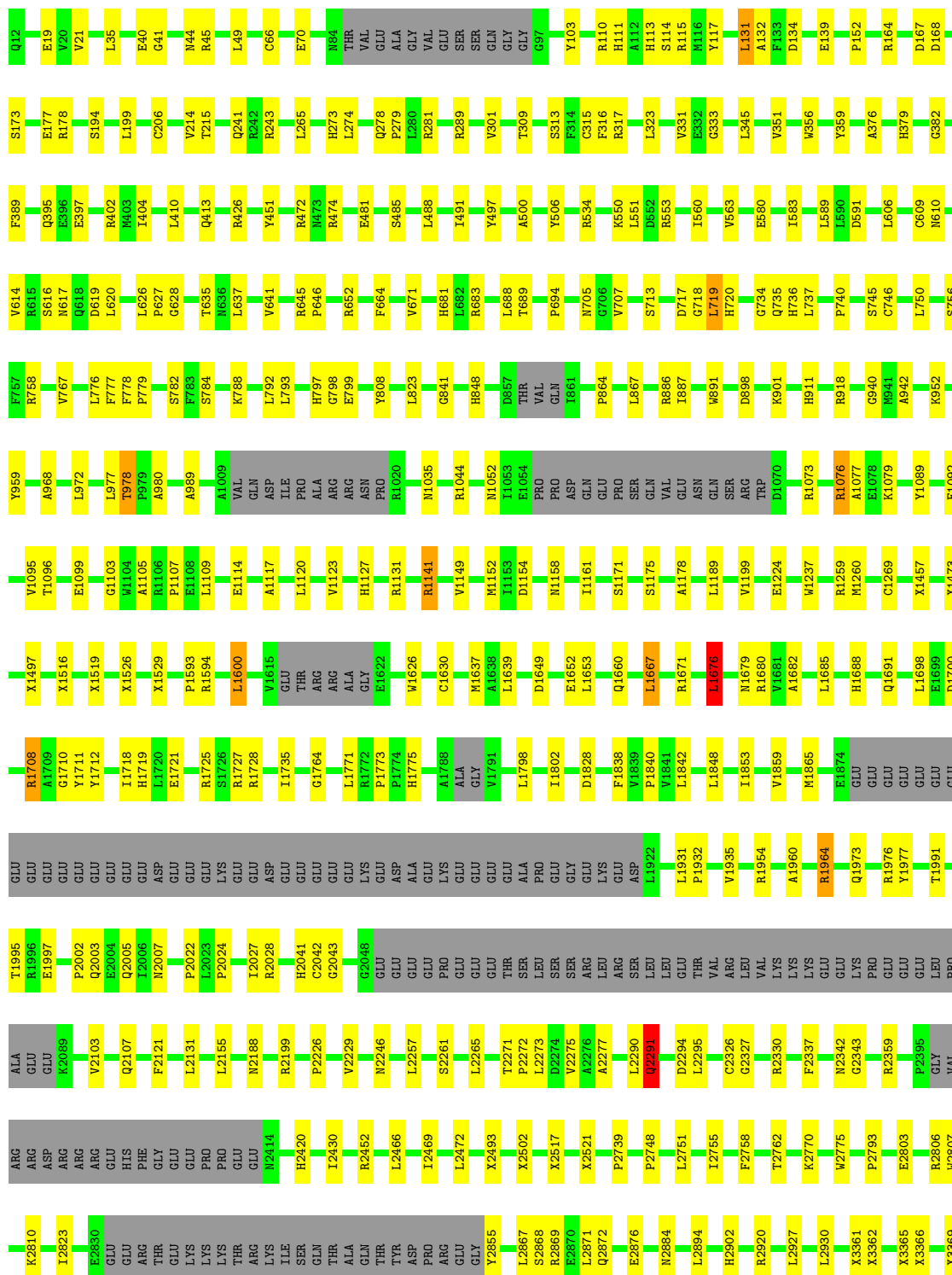


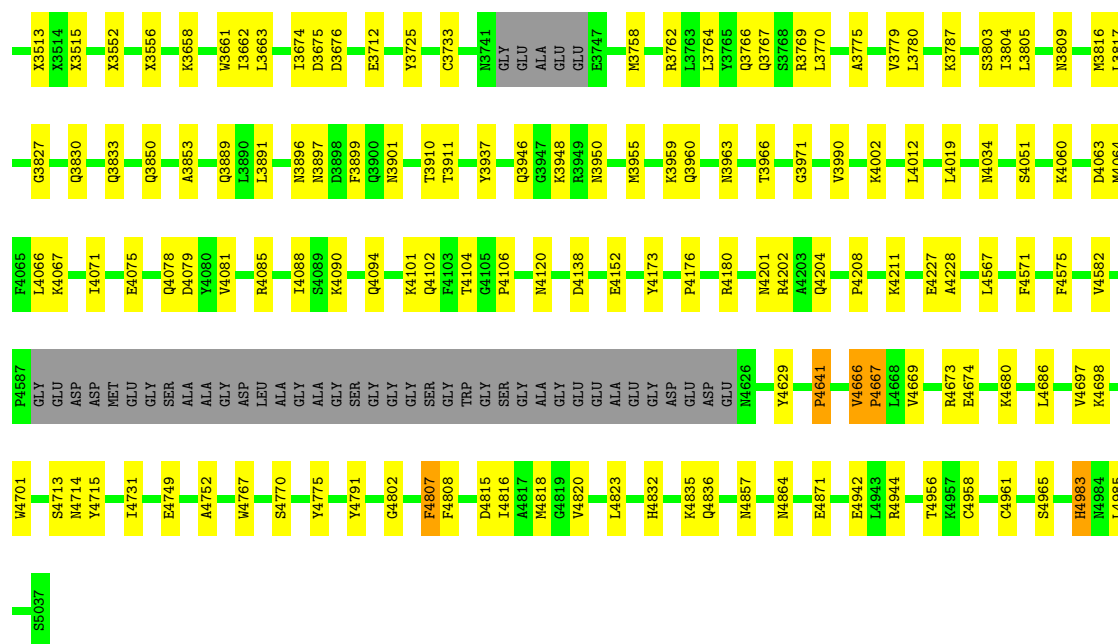
ASP	GLU	N4180	K3959	L3764	E2876	P2748	G2327	LYS	R1964	M1865	L1685	C1269	Y1089	A942	S756	H610
N4626	Y4629	N4201	N3963	Y3765	N2884	L2751	R2330	GLU	Q1973	E1874	H1688	X1457	F1092	K952	R757	V614
L4667	R4202	R3769	T3966	Q3767	L2894	I2755	F2337	LYS	R1976	GLU	Q1691	X1473	V1095	Y959	F758	S616
V4669	Q4204	L3770	H2902	S3768	H2902	F2758	G2343	GLU	Y1977	GLU	L1698	X1497	T1096	A968	V767	N617
P4641	A3775	A3779	R2920	K3787	R2920	T2762	P2395	LEU	T1991	GLU	E1699	X1516	E1099	L972	E769	D619
V4666	V3990	V3779	L2927	V3780	L2927	K2770	GLY	ALA	T1995	GLU	D1700	X1519	G1103	L977	L776	L626
L4668	K4002	L3780	L2930	Q2089	Q2089	Q2775	VAL	GLU	R1996	GLU	R1708	X1526	W1104	L977	F777	P627
V4669	L4012	K3787	X3361	Q2089	Q2089	Q2775	ARG	GLU	E1997	GLU	G1710	X1529	A1105	P979	F778	G628
R4673	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	T635
E4674	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	N636
K4680	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	L637
L4686	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	V641
V4697	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	R645
K4698	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	P646
V4701	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	R652
N4714	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	F664
Y4715	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	V671
I4731	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	R681
E4749	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	L682
A4752	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	R683
V4767	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	L688
S4770	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	T689
Y4791	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	P694
G4802	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	N705
F4807	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	V707
F4808	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	S713
D4815	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	D717
I4816	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	G718
A4817	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	L719
M4818	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	H720
G4819	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	G734
V4820	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	Q735
L4823	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	H736
H4832	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	L737
K4835	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	P740
Q4836	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	S745
N4857	L4019	S3803	X3362	Q2089	Q2089	Q2775	ARG	GLU	R1996	GLU	Y1711	X1529	R1106	A980	S782	C746



• Molecule 2: Ryanodine receptor 1

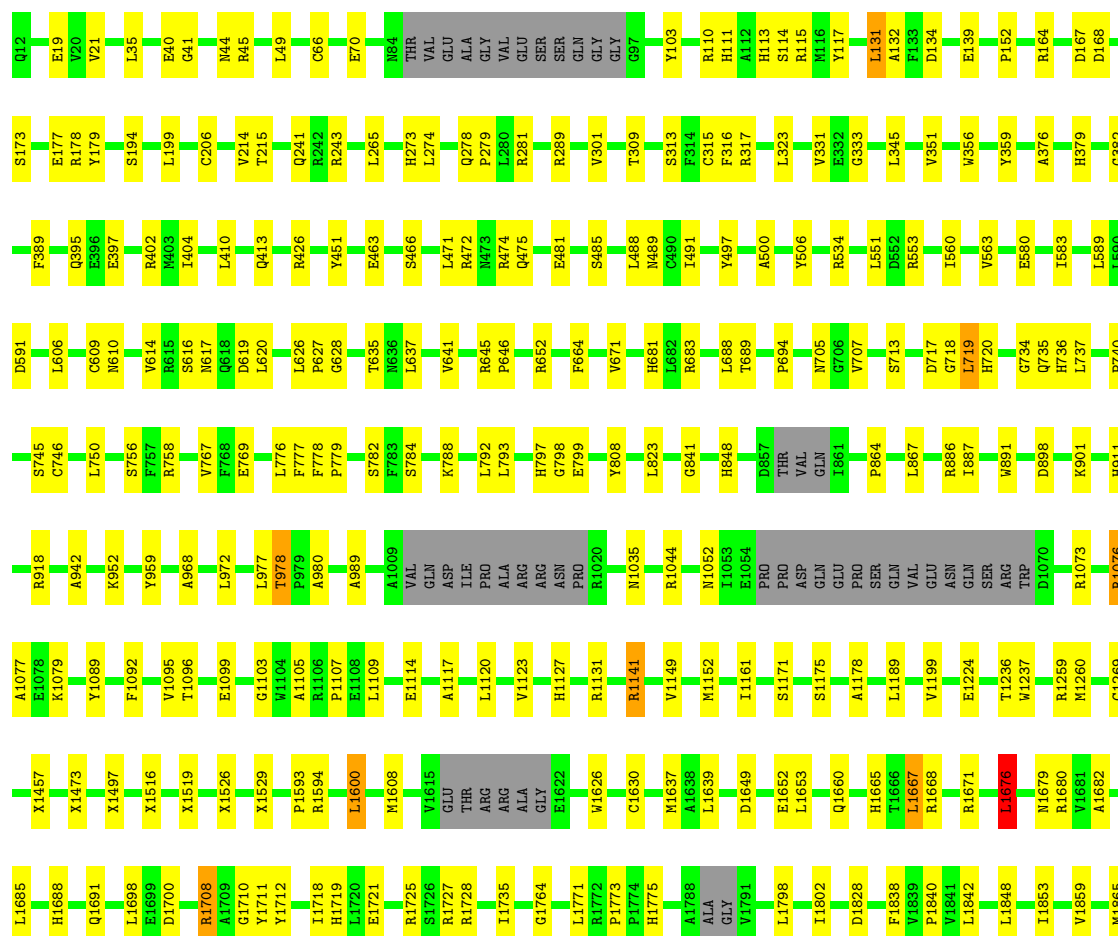
Chain E: 84% 11% 5%

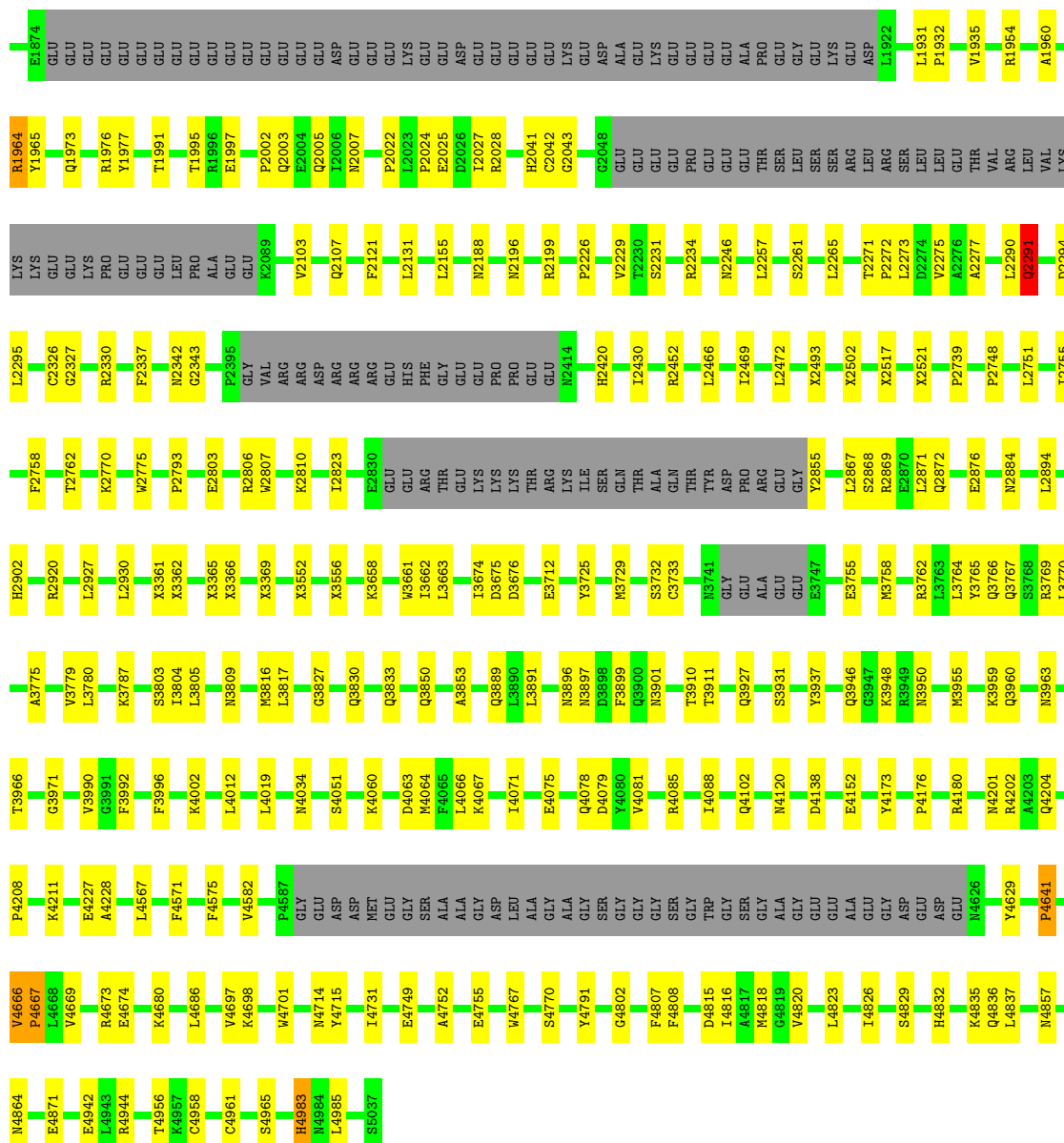




• Molecule 2: Ryanodine receptor 1

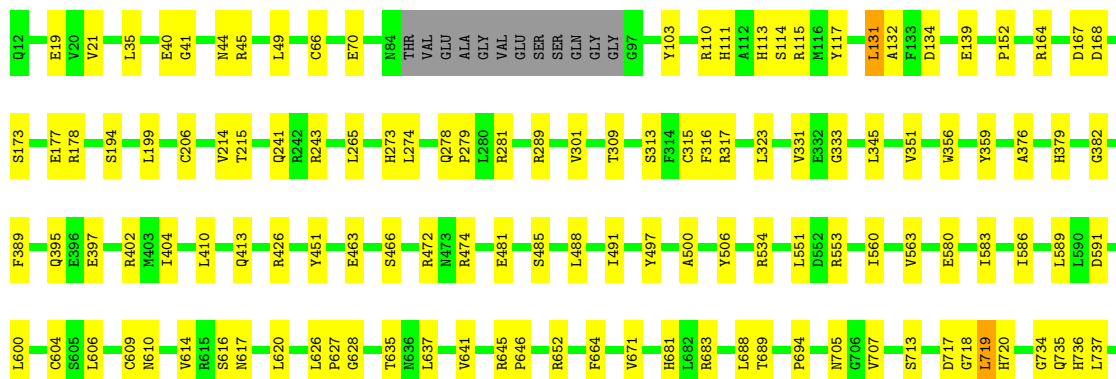
Chain I: 84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain G: 84% 11% 5%






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.30	0/25438	0.54	8/34548 (0.0%)
2	E	0.30	0/25438	0.54	8/34548 (0.0%)
2	G	0.30	0/25438	0.54	8/34548 (0.0%)
2	I	0.30	0/25438	0.54	8/34548 (0.0%)
All	All	0.30	0/105088	0.54	32/142684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

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

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

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29509	0	24752	277	0
2	E	29509	0	24753	269	0
2	G	29509	0	24753	269	0
2	I	29509	0	24753	276	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121312	0	102307	1111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1111 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4983:HIS:H	2:B:4983:HIS:CD2	2.10	0.70
2:E:4983:HIS:H	2:E:4983:HIS:CD2	2.10	0.70
2:G:4983:HIS:H	2:G:4983:HIS:CD2	2.10	0.69
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	51	85
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	51	85
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	51	85
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	51	85
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	54	85

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%)	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	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