



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:09 pm GMT

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/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

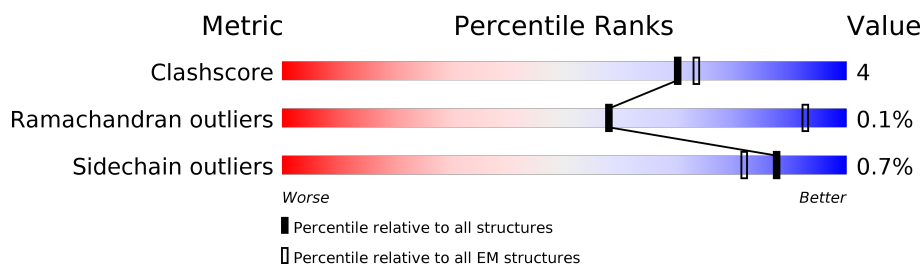
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	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	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		

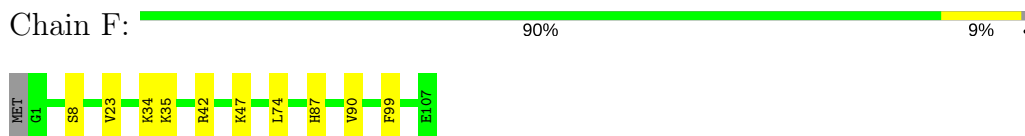
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

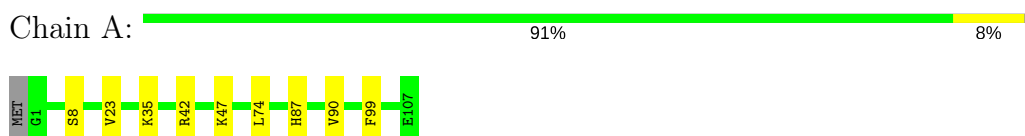
3 Residue-property plots

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

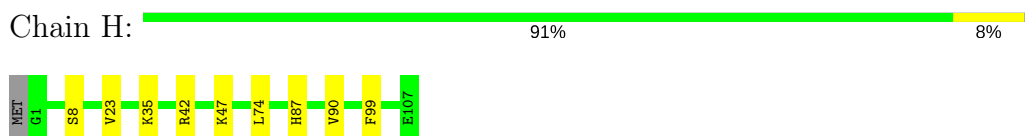
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



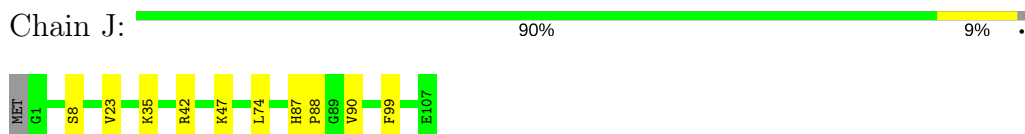
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



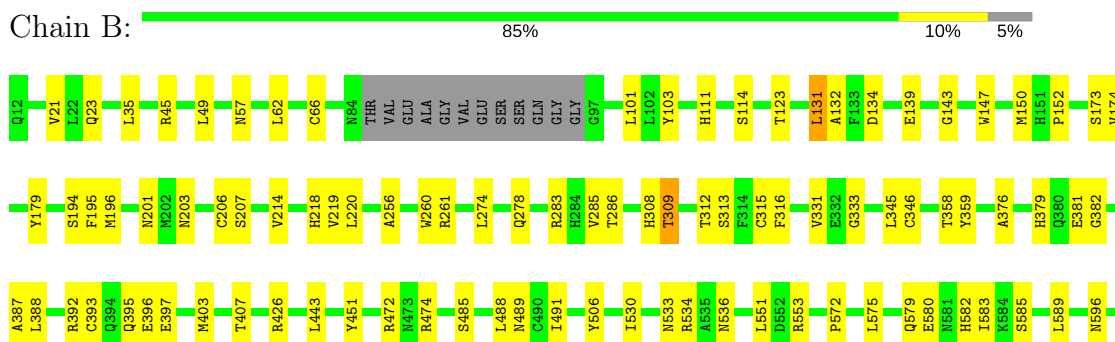
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

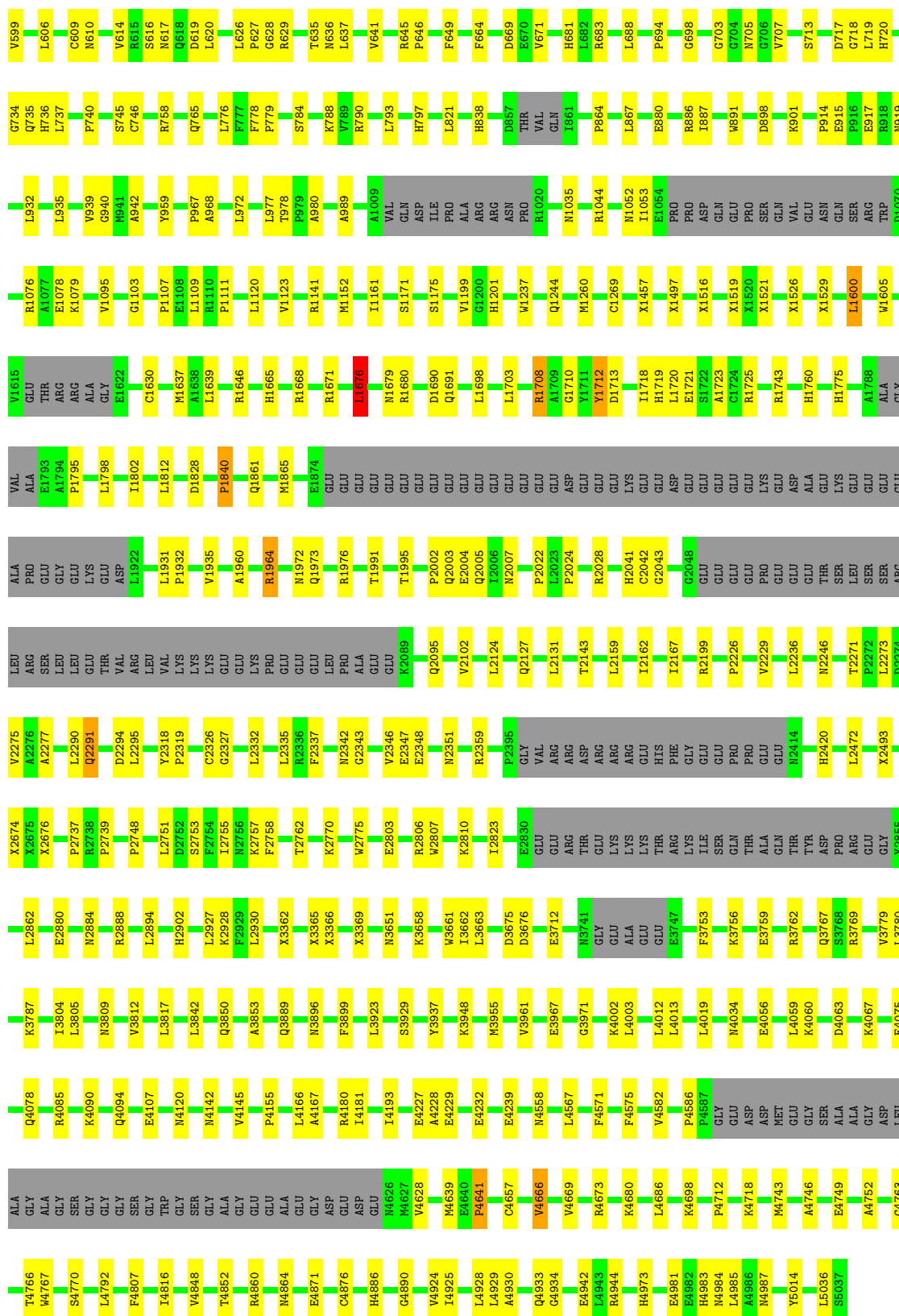


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

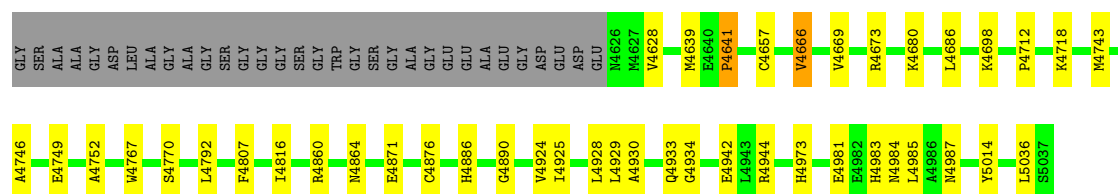




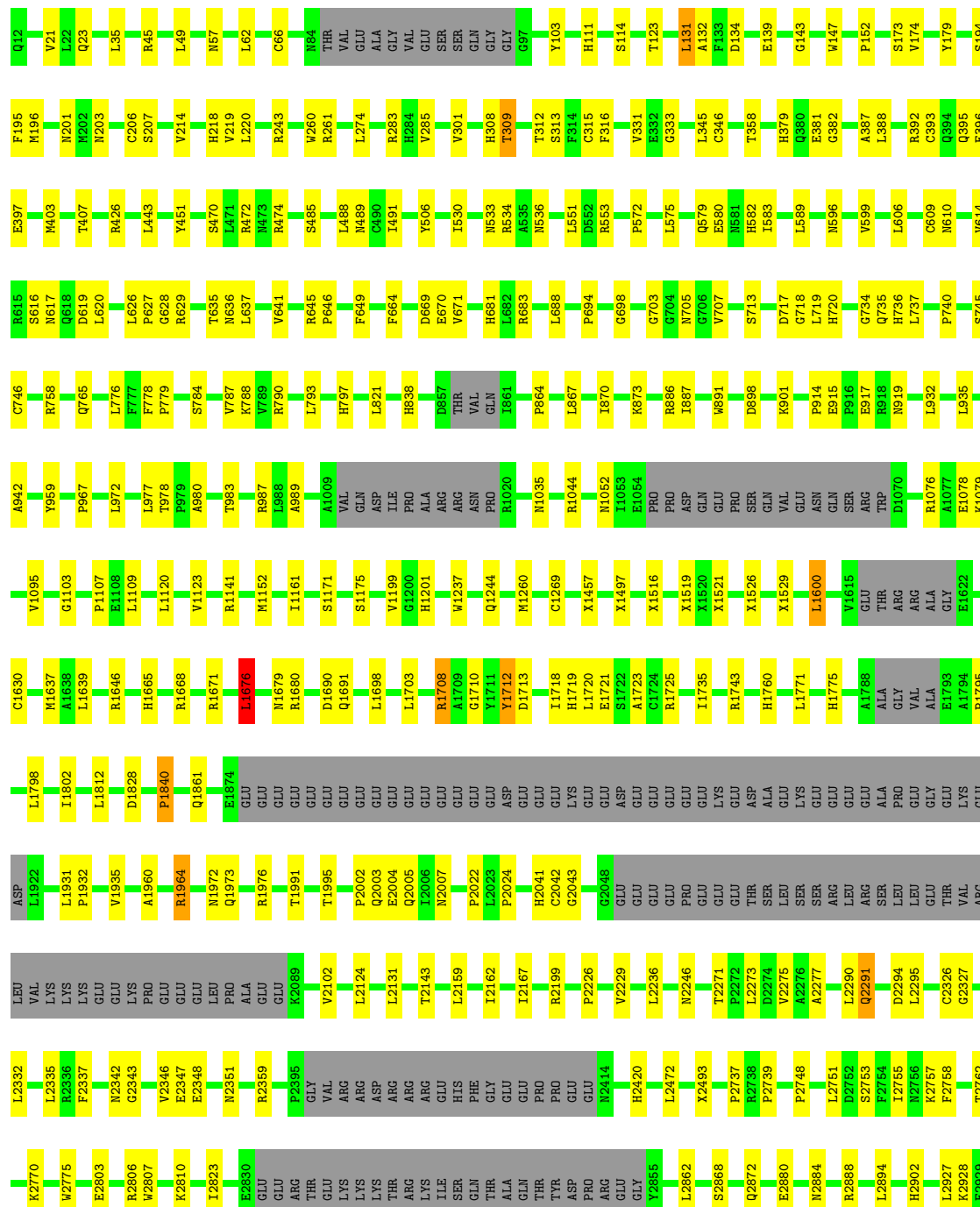
• Molecule 2: Ryanodine receptor 1

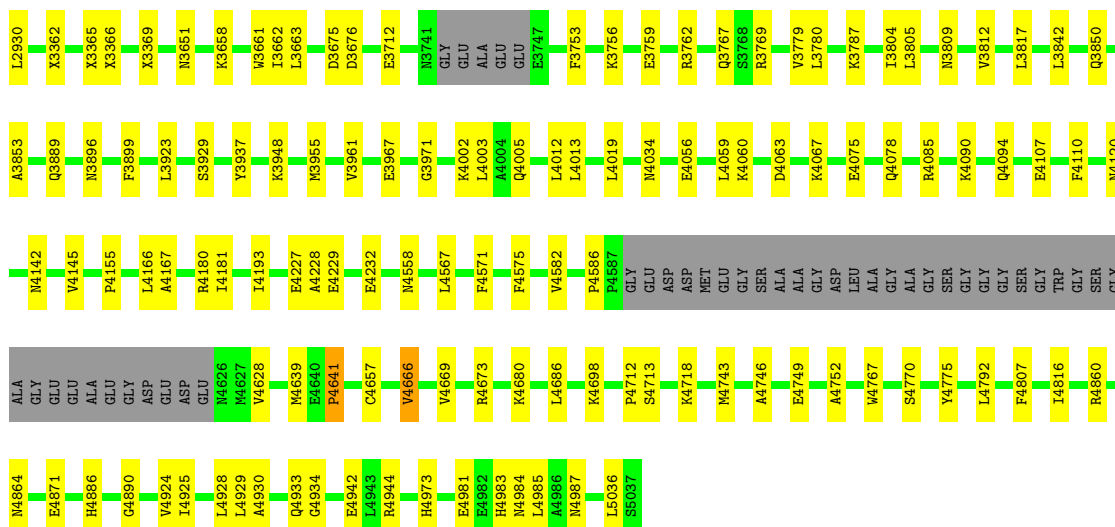
Chain G: 85% 10% 5%



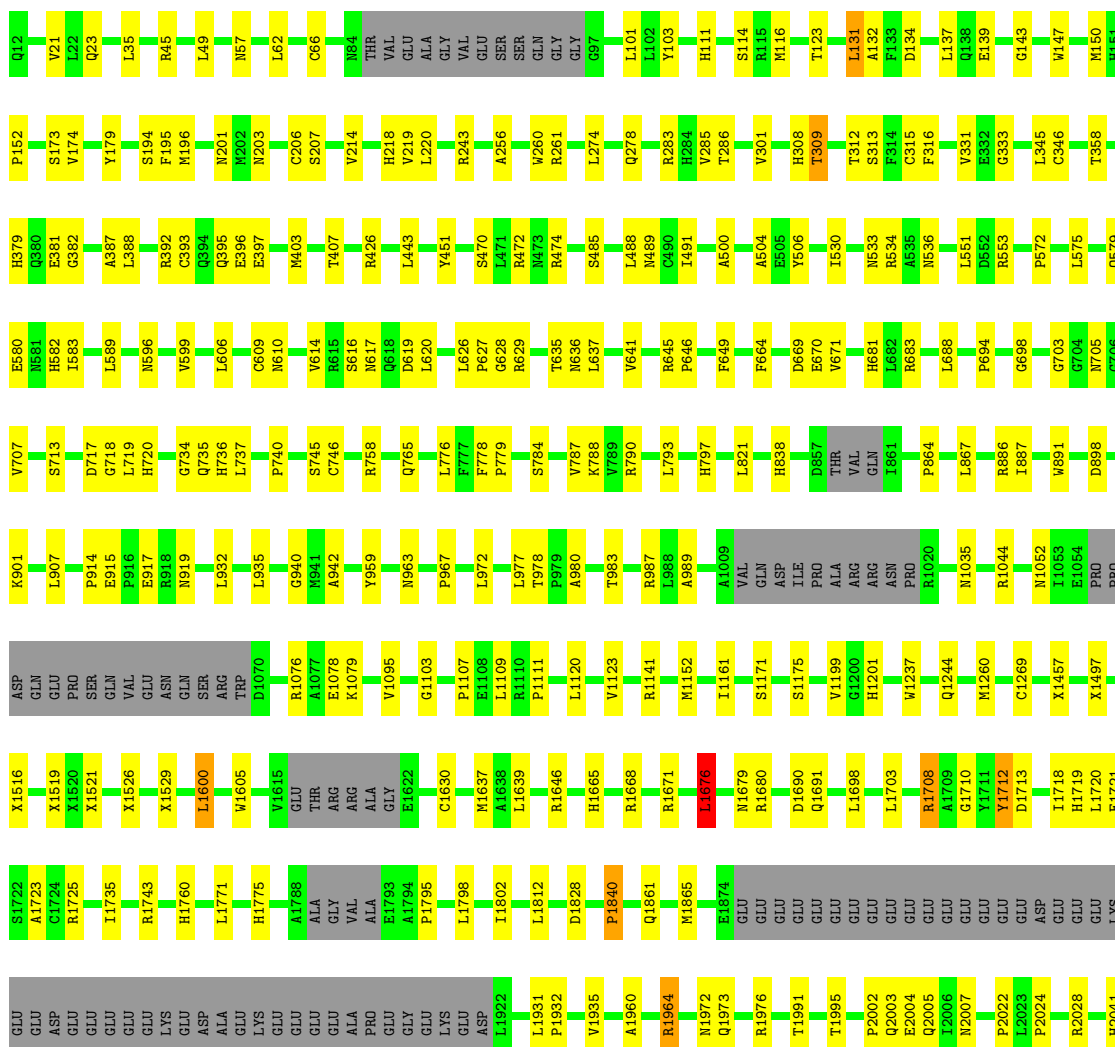
- Molecule 2: Ryanodine receptor 1





- Molecule 2: Ryanodine receptor 1

Chain I:



N4984	P4712	GLY	F3753	SER	GLU	C2042
L4985	K4718	GLU	K3756	GLN	PRO	C2043
A4986	M4743	ASP	E3759	THR	PRO	G2048
N4987	A4746	ASP	R3762	ALA	GLU	GLU
L5036	E4749	MET	Q3767	GLN	GLU	GLU
S5037	A4752	GLY	S3768	THR	GLU	GLU
	G4763	GLY	R3769	TYR	GLU	GLU
	T4766	SER	Q3779	ASP	GLU	GLU
	W4767	ALA	L3780	PRO	GLU	GLU
	S4770	ALA	K3787	ARG	GLU	GLU
	L4792	GLY	S3803	GLY	GLU	GLU
	F4807	SER	I3804	GLY	GLU	THR
	I4816	GLY	L3805	E2880	THR	SER
	V4848	GLY	K4090	L2884	LEU	LEU
	T4852	SER	Q4094	R2888	LEU	LEU
	R4860	TRP	E4107	L2894	GLU	THR
N4864		SER	M4120	L2751	THR	VAL
E4871		GLY	N4142	D2752	ARG	ARG
C4876		ALA	V4145	S2753	LEU	VAL
H4886		GLY	P4155	F2754	LEU	VAL
G4890		ASP	L4166	N2756	LYS	LYS
V4924		GLU	A4167	K2757	LYS	LYS
I4925		ASP	V4180	F2758	LYS	LYS
L4928		GLU	I4181	T2762	GLU	GLU
L4929		M4626	I4193	K2770	GLU	GLU
A4930		M4627	E4227	W2775	PRO	GLU
		E4640	A4228	E2803	GLU	GLU
		P4641	E4229	R2806	LEU	LEU
		C4657	E4232	W2807	PRO	PRO
		V4666	M4558	K2810	ALA	ALA
Q4933		V4669	L4567	I2823	GLU	GLU
G4934		R4673	F4571	E2830	GLY	R2089
E4942		K4680	F4575	GLU	VAL	Q2095
L4943		L4686	V4582	THR	ARG	V2102
R4944		K4698	P4586	ARG	ARG	L2124
H4973			P4587	ASP	ASP	Q2127
E4981				GLY	ARG	L2131
E4982				THR	GLU	L2159
H4983				ARG	HTS	L2162
				LYS	PHE	
				GLY	GLU	
				ILE		

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(°)	Ideal(°)
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%)	55	89
2	E	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	55	89
2	G	3235/4416 (73%)	2875 (89%)	356 (11%)	4 (0%)	55	89
2	I	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	55	89
All	All	13360/18096 (74%)	11875 (89%)	1469 (11%)	16 (0%)	58	89

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 [i](#)

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%)	87	93
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	87	93
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	87	93

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 [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 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	46.34