



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 02:34 AM EDT

PDB ID : 5T9S  
EMDB ID : EMD-8375  
Title : Structure of rabbit RyR1 (Ca<sup>2+</sup>-only dataset, class 4)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-09  
Resolution : 4.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

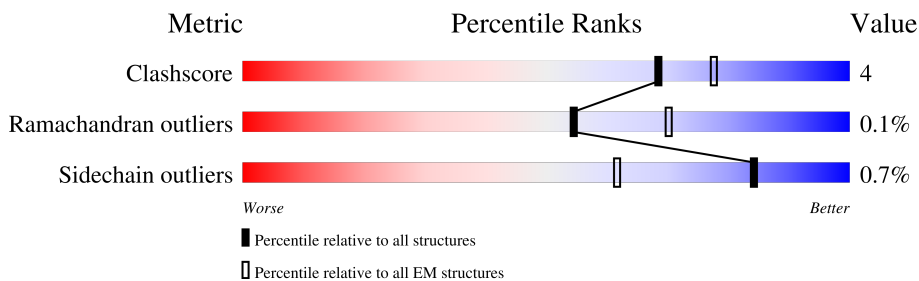
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	4676	
2	E	4676	
2	G	4676	
2	I	4676	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 120756 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
			Total	C	N	O	S		
1	F	107	818	516	144	154	4	0	0
1	A	107	818	516	144	154	4	0	0
1	H	107	818	516	144	154	4	0	0
1	J	107	818	516	144	154	4	0	0

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4168	29369	18608	5202	5402	157	0	0
2	E	4168	29369	18608	5202	5402	157	0	0
2	I	4168	29369	18608	5202	5402	157	0	0
2	G	4168	29369	18608	5202	5402	157	0	0

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

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


- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

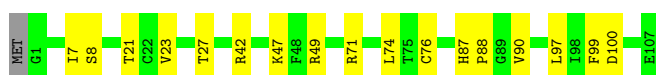
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

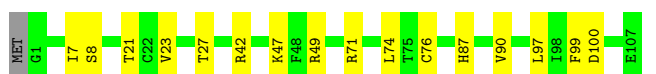
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




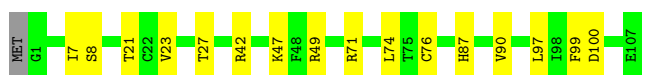
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




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

Chain H: 




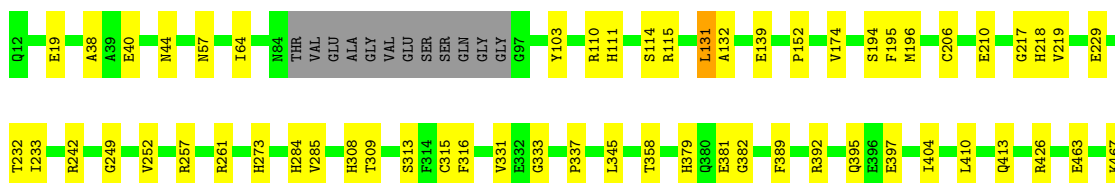
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 











GLY ASP	GLN PRO	LEU LEU	ALA GLY	R4137 D4138	L3805	ALA GLN	L2457	P2286	G2048	GLU GLU	G1710 Y1711	P1243	R1044	C811	V651 T642
ASP	MET	TRP	THR	N4138	K3815	THR	L2460	V2229	GLU	GLU	Y1712	R1259	N1052	R820	T646
MET	GLY	ALA	GLY	M4142	M3816	TYR	L2466	Q2247	GLU	GLU	I1718	X1519	I1053	L821	N647
GLY	ASP	VAL	ALA	L4152	L3817	PRO	L2469	L2287	PRO	ASP	L1720	X1520	E1054	D857	T648
THR	THR	ALA	GLY	P4155	S3831	ARG	L2472	A2276	GLU	GLU	E1721	X1526	PRO	THR	F649
PRO	ALA	ARG	ALA	R4159	Q3850	GLY	A2277	A2277	GLU	GLU	R1725	L1595	GLN	VAL	W662
ALA	ALA	GLY	ALA	R4167	M2856	M2856	A2277	A2277	THR	THR	S1726	L1595	PRO	GLN	Y663
GLU	PRO	ALA	ALA	A4168	Q2857	Q2857	P2739	A2277	SER	GLU	R1727	L1595	SER	PRO	F664
THR	THR	GLY	GLY	E4168	Q2858	Q2858	P2748	E2285	SER	GLU	R1728	L1595	GLN	GLN	V671
PRO	PRO	ALA	THR	S4169	P2859	P2859	L2751	L2286	SER	GLU	S1729	L1600	VAL	VAL	V671
GLY	GLY	GLY	VAL	E4172	S2868	S2868	L2755	A2287	ARG	GLU	R1743	L1613	GLU	GLU	W891
ALA	ALA	ALA	ALA	R4175	Q3900	Q3900	L2755	L2290	LEU	ALA	H1760	Q1614	ASN	ASN	A679
ALA	PRO	ALA	ALA	P4176	M3901	M3901	F2758	Q2291	ARG	GLU	H1775	V1615	GLN	GLN	R663
ALA	ALA	GLY	ALA	R4180	R3904	R3904	T2762	C2326	LEU	GLU	H1775	GLY	ARG	ARG	T689
ALA	ALA	ARG	ALA	T3910	T3905	T3905	H2763	G2327	GLU	GLU	A1788	ALA	THR	THR	N705
ALA	ALA	ARG	ARG	Y4194	T3911	T3911	E2764	F2337	THR	GLU	ALA	ALA	GLY	GLY	G706
ALA	ALA	LEU	LEU	R4202	T3912	T3912	K2765	F2340	ARG	GLU	PRO	GLY	PRO	PRO	V707
ALA	ALA	ALA	ALA	P4208	R2920	R2920	K2770	V2341	VAL	GLY	VAL	E1622	E1078	K1079	D717
ALA	ALA	ARG	ALA	R4211	L2927	L2927	W2775	N2342	LYS	GLU	A1793	A1627	E1093	A968	G718
ALA	ALA	ARG	ARG	Y4228	L2930	L2930	G2778	G2343	LYS	LYS	A1794	Q1630	E1094	L972	L719
ALA	ALA	GLY	ALA	E4232	L2937	L2937	T2787	E2347	LYS	GLU	P1795	Q1631	V1095	L972	H720
ALA	ALA	GLY	ALA	L4233	L2937	L2937	E2803	E2347	GLY	GLU	ALA	E1637	G1103	L977	Q735
ALA	ALA	GLY	ALA	S4236	L2937	L2937	R2806	E2347	LYS	GLU	VAL	A1638	G1103	L977	H736
ALA	ALA	GLY	ALA	I4251	L2937	L2937	W2807	E2347	LYS	GLU	VAL	L1639	G1103	L977	Q735
ALA	ALA	GLY	ALA	E4252	L2937	L2937	K2810	P2395	GLY	GLU	ALA	M1637	G1103	L977	H736
ALA	ALA	GLY	ALA	L4253	L2937	L2937	A2815	GLY	VAL	PRO	ALA	A1638	G1103	L977	Q735
ALA	ALA	GLY	ALA	PRO	L2937	L2937	A2815	ARG	ARG	GLU	GLU	L1639	G1103	L977	H736
ALA	ALA	GLY	ALA	GLY	L2937	L2937	L2823	ASP	ASP	GLU	GLU	E1662	G1103	L977	H736
ALA	ALA	GLY	ALA	PRO	L2937	L2937	E2830	ARG	ARG	GLU	GLU	R1671	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	L1676	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	M1679	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	R1680	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	Y1681	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	A1682	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	L1685	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	H1688	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	Y1689	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	D1690	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	L1698	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	L1703	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	R1708	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	A1709	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	W1237	G1103	L977	H736
ALA	ALA	GLY	ALA	ALA	L2937	L2937	GLY	ARG	ARG	GLU	GLU	W1237	G1103	L977	H736





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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  >5	RMSZ	# Z  >5
1	A	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.30	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	68

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	I	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	B	131	LEU	CA-CB-CG	8.10	133.94	115.30
2	E	1600	LEU	CA-CB-CG	7.05	131.51	115.30

There are no chirality outliers.

5 of 68 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 [i](#)

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	8	0
1	F	818	0	824	9	0
1	H	818	0	824	8	0
1	J	818	0	824	9	0
2	B	29369	0	24721	212	0
2	E	29369	0	24721	206	0
2	G	29369	0	24719	205	0
2	I	29369	0	24721	208	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
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102178	849	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 849 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:426:ARG:HB2	2:B:506:TYR:HA	1.78	0.66
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.78	0.66
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.78	0.66
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.78	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.77	0.64

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	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	47	80
2	E	3235/4676 (69%)	2896 (90%)	334 (10%)	5 (0%)	47	80
2	G	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	47	80
2	I	3235/4676 (69%)	2895 (90%)	335 (10%)	5 (0%)	47	80
All	All	13360/19136 (70%)	11959 (90%)	1381 (10%)	20 (0%)	54	85

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	1708	ARG
2	I	1708	ARG
2	G	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	2493/3202 (78%)	2475 (99%)	18 (1%)	84	90
2	E	2493/3202 (78%)	2475 (99%)	18 (1%)	84	90
2	G	2493/3202 (78%)	2475 (99%)	18 (1%)	84	90
2	I	2493/3202 (78%)	2475 (99%)	18 (1%)	84	90
All	All	10324/13164 (78%)	10252 (99%)	72 (1%)	84	90

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

Mol	Chain	Res	Type
2	G	978	THR
2	G	4995	LEU
2	G	1141	ARG
2	G	3805	LEU
2	E	1600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4054	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	G	3896	ASN
2	I	413	GLN
2	G	3781	GLN
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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	B	12
2	G	12
2	I	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.23
1	G	3613:UNK	C	3639:THR	N	43.95
1	I	3613:UNK	C	3639:THR	N	43.88
1	E	3613:UNK	C	3639:THR	N	43.84
1	E	3163:UNK	C	3170:UNK	N	16.60

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8375. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.