



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 03:18 AM EDT

PDB ID : 4UWE  
EMDB ID: : EMD-2752  
Title : Structure of the ryanodine receptor at resolution of 8.5 Å in partially open state  
Authors : Efremov, R.G.; Leitner, A.; Aebersold, R.; Raunser, S.  
Deposited on : unknown  
Resolution : 8.50 Å(reported)  
Based on PDB ID : 2UWA

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](mailto: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.

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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) : rb-20029824

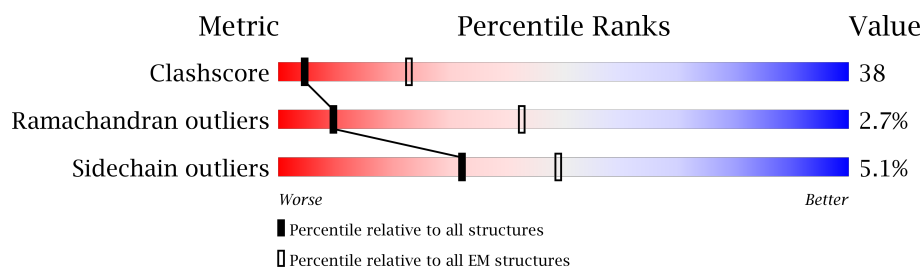
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 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  $\geq 3$ , 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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 81600 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.

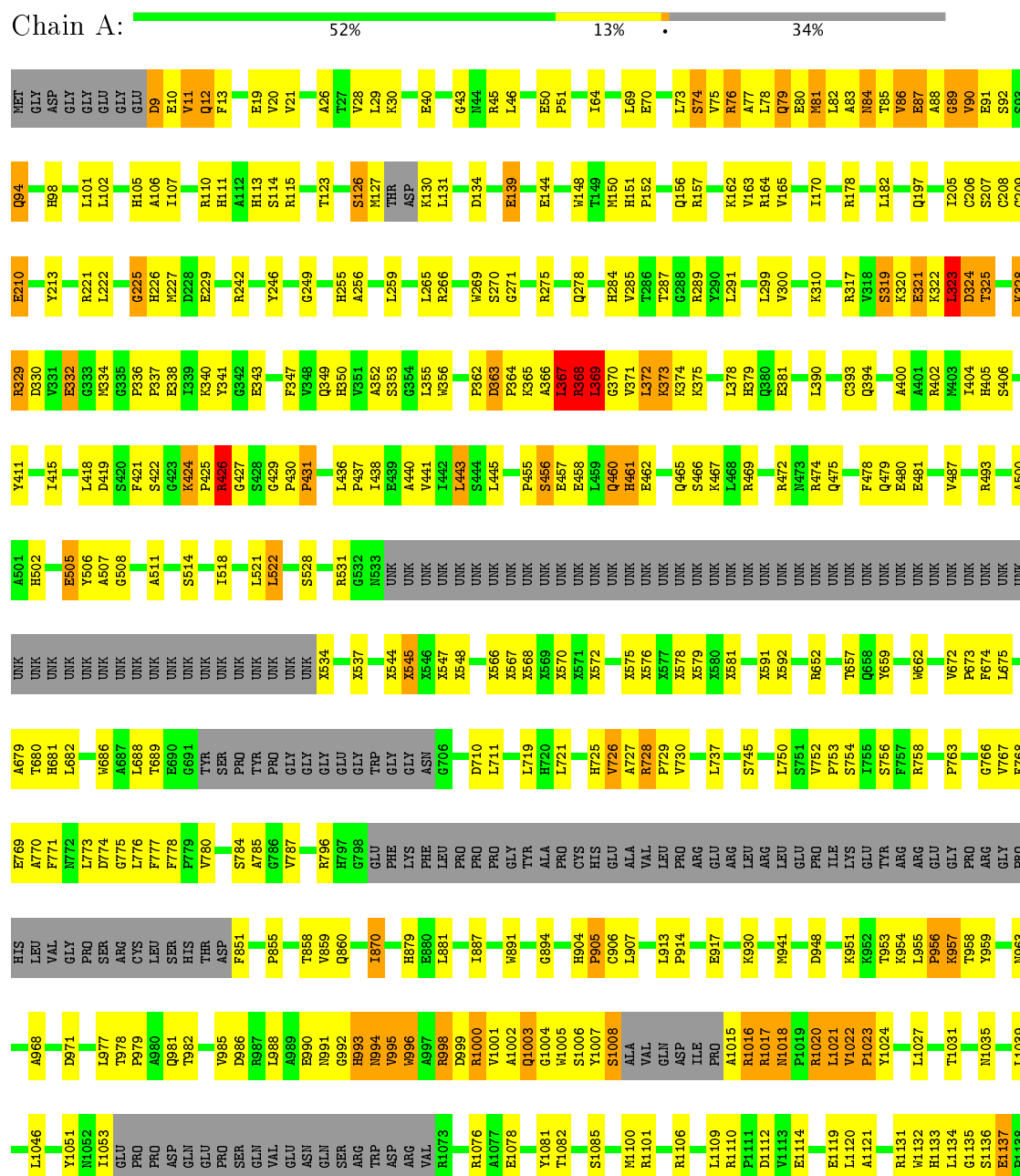
- Molecule 1 is a protein called RYANODINE RECEPTOR 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	B	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	C	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	D	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		

### 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: RYANODINE RECEPTOR 1



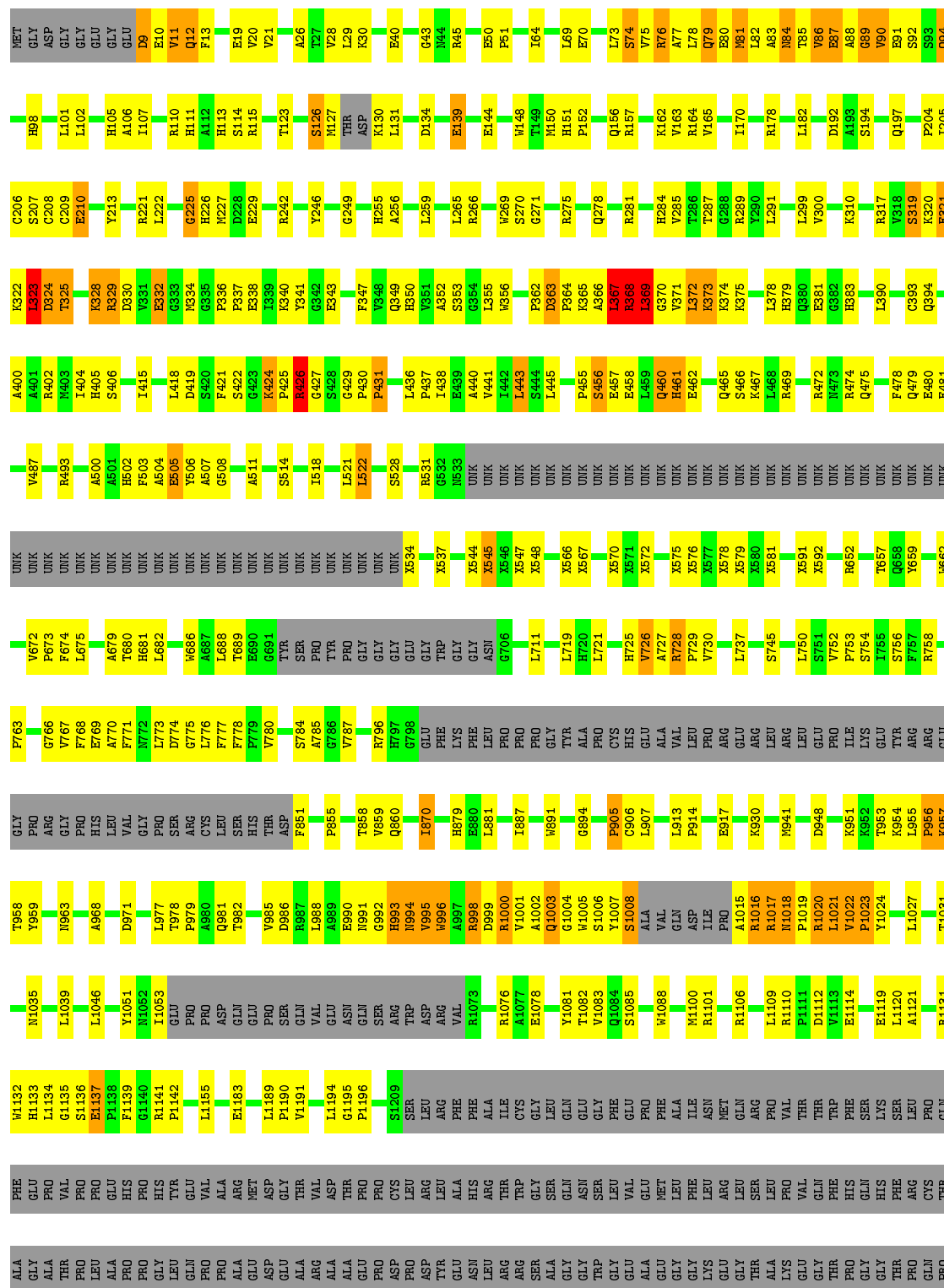






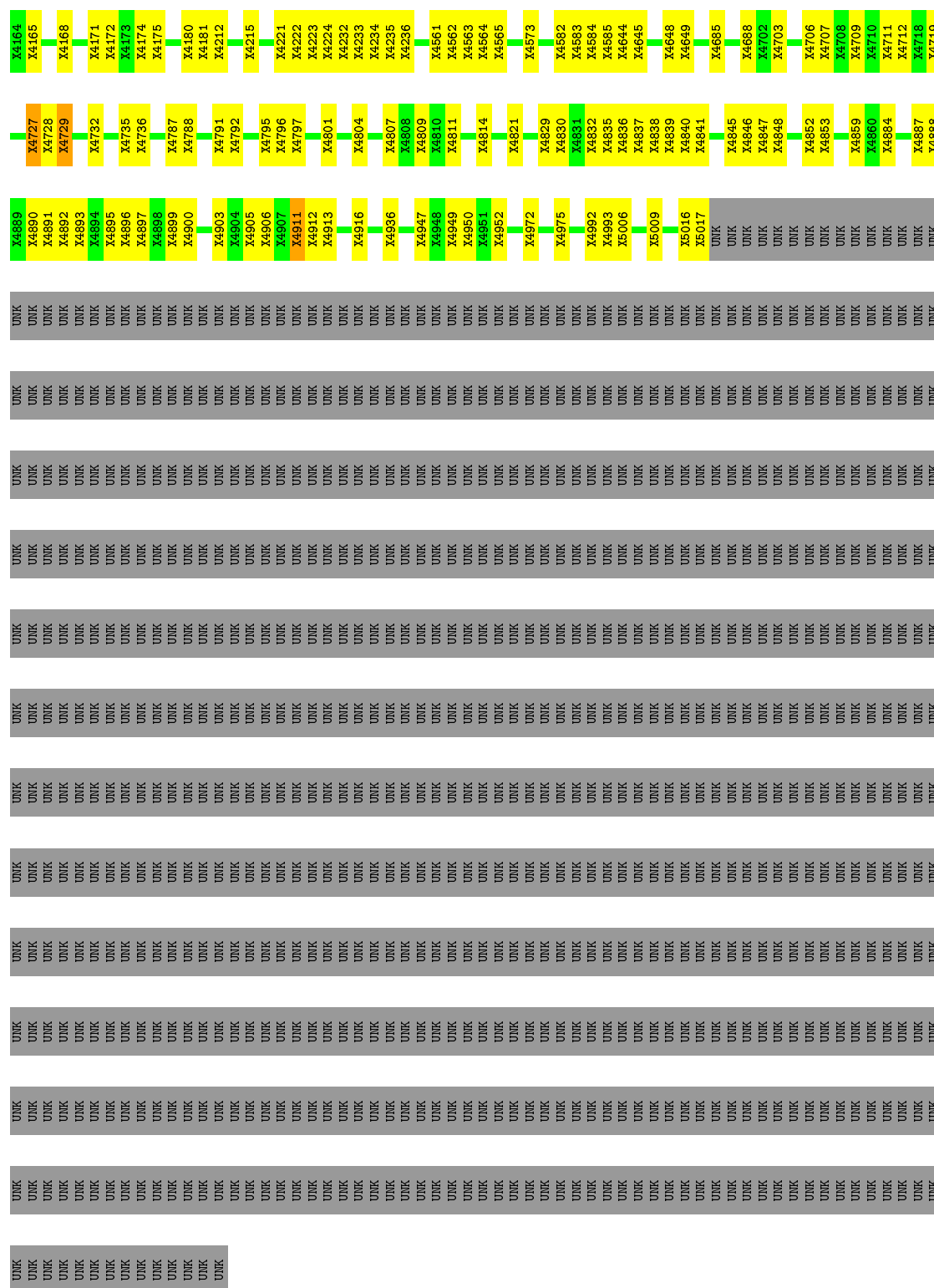
- Molecule 1: RYANODINE RECEPTOR 1

Chain B:  51% 13% 34%

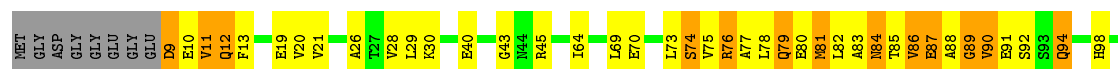






- Molecule 1: RYANODINE RECEPTOR 1



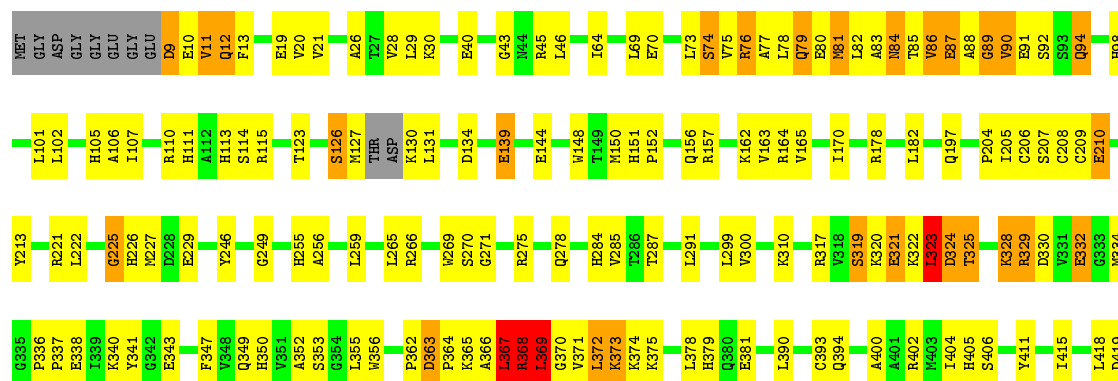
GLN	F1440	ASN	LEU	TYR	E1137	L1046	A968	PRO	E769	H681	UNK	A504	UNK	6333	R221	L101
GLN	A1441	GLU	GLN	GLU	E1137	L1046	A968	HIS	A770	L682	UNK	E505	UNK	R334	L222	H105
ARG	G1442	LYS	PRO	VAL	L1155	Y1051	D971	LEU	M772	R683	UNK	Y506	UNK	G335	G225	A106
GLY	Q1443	ASP	PRO	ALA	ARG	Y1051	D971	VAL	M772	R683	UNK	A507	UNK	P336	M227	I107
I1509	E1444	ALA	ALA	ARG	E1183	N1052	L977	GLY	L773	G685	UNK	G508	UNK	P337	M227	R110
S1510	P1445	THR	GLU	MET	E1183	N1052	L977	PRO	L773	G685	UNK	A511	UNK	P338	D228	H111
D1513	Y1480	THR	ASP	ASP	L1189	P1189	T978	SER	G775	M686	UNK	A511	UNK	P339	E229	A112
L1514	G1481	GLU	GLU	GLY	P1190	Q979	T978	ARG	L776	L688	UNK	S514	UNK	R340	R242	H113
V1515	W1482	LYS	ALA	THR	V1191	A980	A980	CYS	F777	T689	UNK	S514	UNK	Y341	Y246	R115
I1516	W1483	ASN	ARG	VAL	Q981	ASN	A980	LEU	F778	E690	UNK	S514	UNK	P342	G249	T123
G1517	W1483	LYS	ALA	ASP	Q981	ASN	A980	LEU	F778	E690	UNK	S514	UNK	P343	H255	S126
C1518	T1484	ASP	ALA	ASP	T982	GLN	T982	SER	F779	G691	UNK	S514	UNK	E343	A256	THR
L1519	Y1487	ARG	GLU	THR	Y985	GLU	Y985	HIS	W780	T781	UNK	S514	UNK	E344	L259	ASP
L1520	H1488	GLY	PRO	PRO	D986	PRO	D986	ASP	W781	SER	UNK	S514	UNK	E345	L265	L130
D1522	H1488	ASP	ASP	CYS	R987	GLN	R987	ASP	S784	PRO	UNK	S514	UNK	E346	R266	L131
L1523	M1462	LEU	ASP	THR	A988	VAL	A988	VAL	A785	T787	UNK	S514	UNK	E347	G271	D134
M1527	N1463	LYS	ASP	ARG	E990	ASN	E990	GLY	G786	GLY	UNK	S514	UNK	E348	W269	E139
T1528	F1464	ALA	GLU	ALA	N991	GLN	N991	GLY	G787	GLY	UNK	S514	UNK	E349	R275	E144
F1529	D1465	LYS	ASN	HIS	G992	SER	G992	THR	R796	GLU	UNK	S514	UNK	E350	Q278	W148
S1467	S1467	ALA	LEU	ARG	H993	ARG	H993	ARG	R797	GLY	UNK	S514	UNK	E351	R281	T149
T1537	T1537	ALA	ARG	THR	N994	TRP	N994	TRP	G798	TRP	UNK	S514	UNK	E352	H284	M150
W1468	W1468	ALA	ARG	THR	Y995	ILE	Y995	ILE	G798	TRP	UNK	S514	UNK	E353	V285	P152
R1470	R1470	MET	SER	GLY	N996	ASP	N996	ASP	PHE	GLY	UNK	S514	UNK	E354	L291	V165
F1539	F1539	THR	ALA	GLN	A997	VAL	A997	VAL	LYS	ASN	UNK	S514	UNK	E355	L299	I170
F1540	A1471	THR	GLY	GLN	R998	R1073	R998	GLN	PHE	G706	UNK	S514	UNK	E356	V300	R178
E1543	T1472	PRO	GLY	ASN	D999	R1076	D999	GLY	LEU	D710	UNK	S514	UNK	E357	R317	L182
T1546	K1547	PRO	TRP	SER	R1000	A1077	R1000	GLY	PRO	L711	UNK	S514	UNK	E358	G388	Q197
K1547	G1477	ALA	GLY	LEU	T1001	E1078	T1001	GLY	PRO	L711	UNK	S514	UNK	E359	R289	P204
P1550	D1478	LEU	GLY	VAL	Q1003	Q1084	Q1003	VAL	TYR	H719	UNK	S514	UNK	E360	V163	C206
V1552	V1552	GLN	GLY	MET	W1005	Q1084	W1005	GLN	ALA	L721	UNK	S514	UNK	E361	R164	C208
F1553	F1553	LEU	GLY	LEU	S1085	S1085	S1085	GLN	HIS	H725	UNK	S514	UNK	E362	V165	C209
V1554	V1554	PRO	GLY	THR	W1088	W1088	W1088	VAL	ALA	A727	UNK	S514	UNK	E363	I170	E210
P1556	P1556	ASP	ALA	LEU	M1100	M1100	M1100	GLN	VAL	R728	UNK	S514	UNK	E364	L299	Y213
T1557	T1557	VAL	GLY	GLN	R1101	R1101	R1101	ILE	LEU	V730	UNK	S514	UNK	E365	V300	
H1558	H1558	VAL	GLY	GLN	THR	THR	THR	THR	PRO	L737	UNK	S514	UNK	E366	R317	
Q1559	Q1559	ALA	THR	PHE	R1106	R1106	R1106	THR	ARG	L737	UNK	S514	UNK	E367	G388	
E1565	E1565	ASP	GLY	HIS	L1109	L1109	L1109	THR	GLU	S745	UNK	S514	UNK	E368	R317	
L1566	L1566	THR	GLY	GLN	L1110	L1110	L1110	SER	LEU	S745	UNK	S514	UNK	E369	V318	
G1567	G1567	THR	THR	PHE	P1111	P1111	P1111	THR	ARG	S745	UNK	S514	UNK	E370	S319	
K1568	K1568	PRO	PRO	ARG	D1112	D1112	D1112	ARG	LEU	S745	UNK	S514	UNK	E371	K320	
Q1569	Q1569	GLN	GLN	CYS	V1113	V1113	V1113	THR	PRO	S745	UNK	S514	UNK	E372	E321	
N1571	N1571	THR	GLY	THR	E1114	E1114	E1114	THR	ILE	S745	UNK	S514	UNK	E373	K322	
UNK	UNK	ALA	GLY	ALA	E1119	E1119	E1119	THR	LYS	S745	UNK	S514	UNK	E374	R402	
UNK	UNK	VAL	VAL	ALA	L1120	L1120	L1120	THR	GLU	S745	UNK	S514	UNK	E375	R402	
UNK	UNK	GLN	GLN	ALA	T1432	T1432	T1432	THR	TYR	S745	UNK	S514	UNK	E376	R402	
UNK	UNK	ASP	GLN	THR	Y1434	Y1434	Y1434	THR	ARG	S745	UNK	S514	UNK	E377	R402	
UNK	UNK	PHE	PRO	PRO	Y1435	Y1435	Y1435	THR	ARG	S745	UNK	S514	UNK	E378	R402	
UNK	UNK	VAL	VAL	VAL	S1436	S1436	S1436	THR	ARG	S745	UNK	S514	UNK	E379	R402	
UNK	UNK	SER	ARG	ARG	V1437	V1437	V1437	THR	ARG	S745	UNK	S514	UNK	E380	R402	
UNK	UNK	PRO	ALA	ALA	R1438	R1438	R1438	THR	ARG	S745	UNK	S514	UNK	E381	R402	
UNK	UNK	GLY	ALA	ALA	V1439	V1439	V1439	THR	ARG	S745	UNK	S514	UNK	E382	R402	




[illegible]

- Molecule 1: RYANODINE RECEPTOR 1

Chain D:  52% 13% 34%



[illegible]

[illegible]

[illegible]

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	94354	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	58610	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	B	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	C	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	D	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
All	All	0.40	8/42224 (0.0%)	0.61	44/57252 (0.1%)

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	12
1	B	0	12
1	C	0	13
1	D	0	13
All	All	0	50

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	CYS	C-N	13.92	1.66	1.34
1	C	209	CYS	C-N	13.92	1.66	1.34
1	D	209	CYS	C-N	13.92	1.66	1.34
1	B	209	CYS	C-N	13.90	1.66	1.34
1	A	394	GLN	C-N	11.34	1.60	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	LEU	CA-CB-CG	11.70	142.21	115.30
1	A	367	LEU	CA-CB-CG	11.68	142.16	115.30
1	D	367	LEU	CA-CB-CG	11.68	142.16	115.30

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	CYS	O-C-N	-11.67	104.02	122.70
1	B	367	LEU	CA-CB-CG	11.66	142.11	115.30

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3055	UNK	Peptide
1	A	3205	UNK	Peptide
1	A	3265	UNK	Mainchain
1	A	545	UNK	Peptide
1	A	88	ALA	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	20400	0	12256	1263	0
1	B	20400	0	12257	1265	0
1	C	20400	0	12256	1268	0
1	D	20400	0	12255	1263	0
All	All	81600	0	49024	4945	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 38.

The worst 5 of 4945 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)
1:D:956:PRO:HG3	1:D:959:TYR:CZ	1.25	1.70
1:A:657:THR:HG21	1:A:662:TRP:CE3	1.15	1.68
1:C:956:PRO:HG3	1:C:959:TYR:CZ	1.25	1.65
1:D:657:THR:HG21	1:D:662:TRP:CD2	1.31	1.65
1:B:956:PRO:CD	1:B:959:TYR:CD2	1.74	1.64

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	40
1	B	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	40
1	C	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	40
1	D	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	40
All	All	5120/20148 (25%)	4700 (92%)	284 (6%)	136 (3%)	10	40

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	368	ARG
1	A	393	CYS
1	A	425	PRO
1	A	426	ARG

### 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	1112/1410 (79%)	1055 (95%)	57 (5%)	28	60
1	B	1112/1410 (79%)	1055 (95%)	57 (5%)	28	60
1	C	1112/1410 (79%)	1055 (95%)	57 (5%)	28	60
1	D	1112/1410 (79%)	1055 (95%)	57 (5%)	28	60
All	All	4448/5640 (79%)	4220 (95%)	228 (5%)	32	60

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1003	GLN
1	C	139	GLU
1	D	870	ILE
1	B	1016	ARG
1	C	10	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1035	ASN
1	C	151	HIS
1	D	879	HIS
1	B	1420	ASN
1	B	2877	GLN

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	96
1	A	96
1	D	96
1	C	96

The worst 5 of 384 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1863:UNK	C	1935:UNK	N	104.73
1	B	1863:UNK	C	1935:UNK	N	104.73
1	D	1863:UNK	C	1935:UNK	N	104.73
1	C	1863:UNK	C	1935:UNK	N	104.72
1	A	2939:ARG	C	2953:UNK	N	48.34