



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:08 PM BST

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 : 2014-08-11
Resolution : 8.50 Å(reported)
Based on PDB ID : 2UWA

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

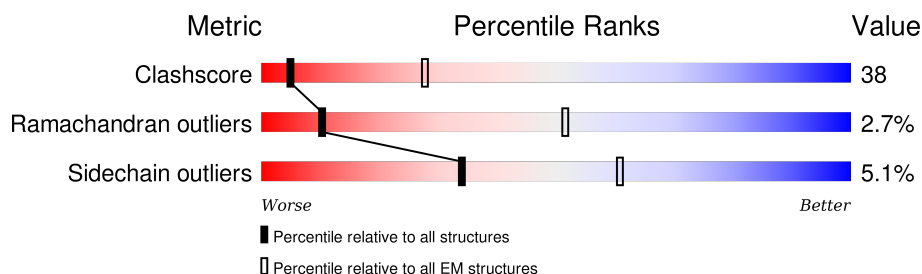
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	5037	<div> <div>52%</div> <div>13%</div> <div>•</div> <div>34%</div> </div>
1	B	5037	<div> <div>51%</div> <div>13%</div> <div>•</div> <div>34%</div> </div>
1	C	5037	<div> <div>52%</div> <div>13%</div> <div>•</div> <div>34%</div> </div>
1	D	5037	<div> <div>52%</div> <div>13%</div> <div>•</div> <div>34%</div> </div>

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.

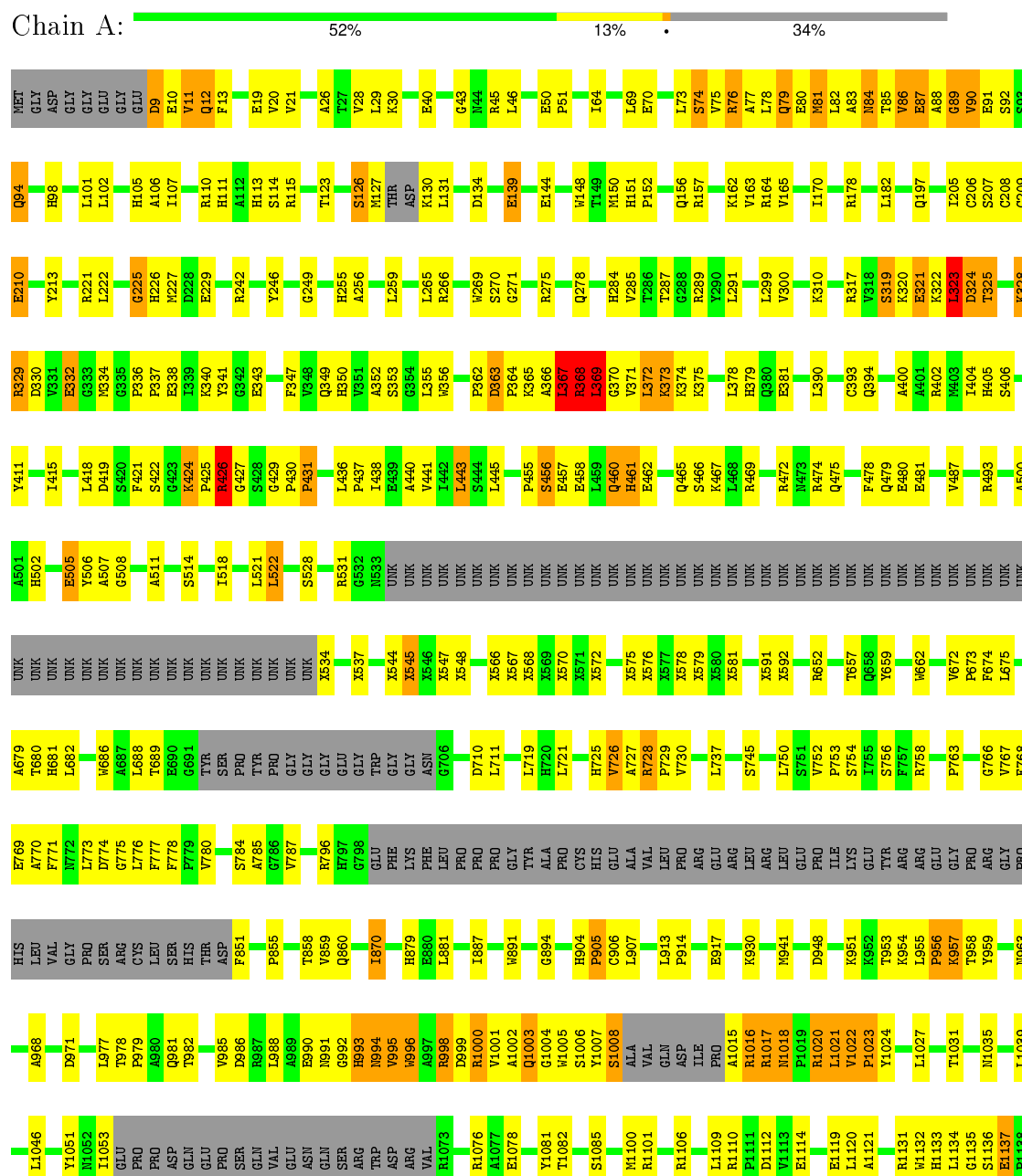
- Molecule 1 is a protein called RYANODINE RECEPTOR 1.

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 errors 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.

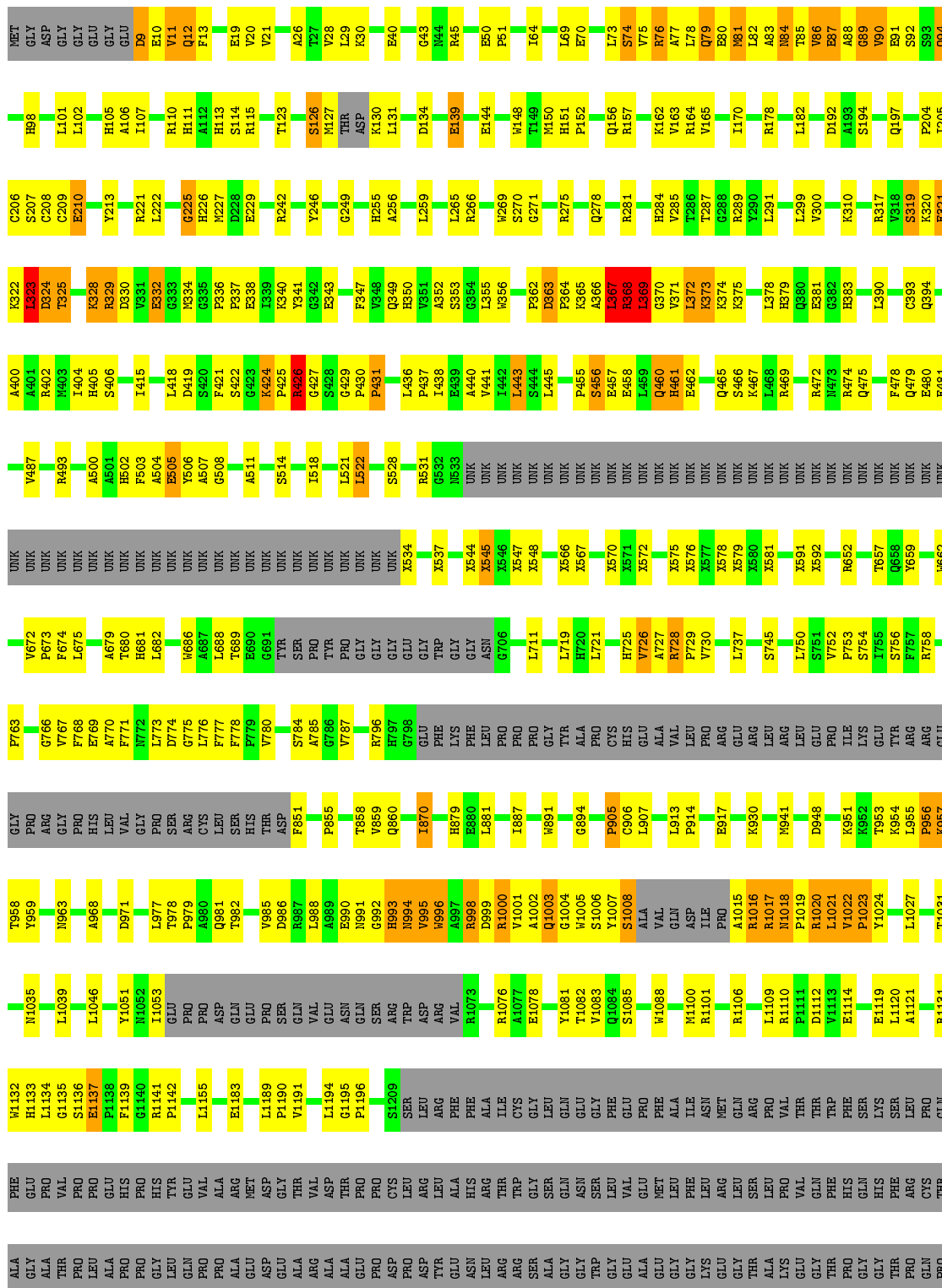
• Molecule 1: RYANODINE RECEPTOR 1















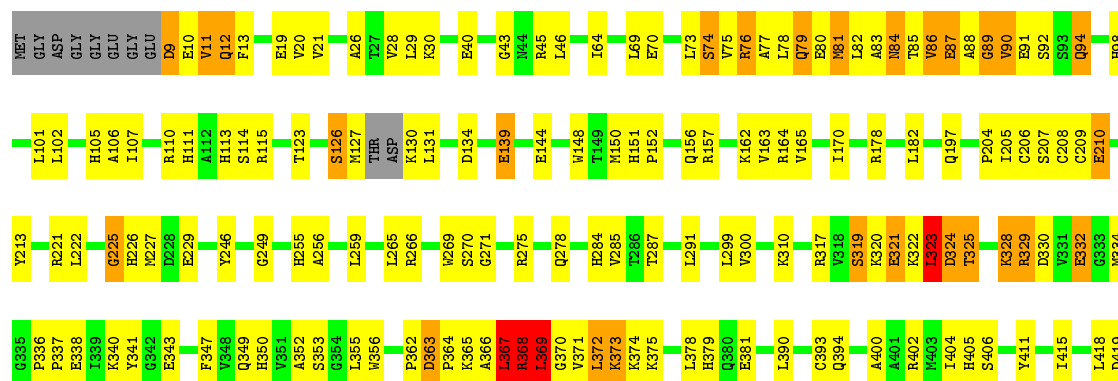





[illegible]

- Molecule 1: RYANODINE RECEPTOR 1

Chain D:  52% 13% 34%









[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL CORRECTION, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	0.9	Depositor
Maximum defocus (nm)	3.9	Depositor
Magnification	60000	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

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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	45
1	B	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	45
1	C	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	45
1	D	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	6	45
All	All	5120/20148 (25%)	4700 (92%)	284 (6%)	136 (3%)	10	45

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%)	29	66
1	B	1112/1410 (79%)	1055 (95%)	57 (5%)	29	66
1	C	1112/1410 (79%)	1055 (95%)	57 (5%)	29	66
1	D	1112/1410 (79%)	1055 (95%)	57 (5%)	29	66
All	All	4448/5640 (79%)	4220 (95%)	228 (5%)	34	66

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 ⓘ

There are no chain breaks in this entry.