



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 11:36 PM BST

PDB ID : 6UHE
Title : Closed-form Crystal Structure of Human RYR Receptor 3 (848-1055)
Authors : Wu, R.; Kim, Y.; Jedrzejczak, R.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2019-09-27
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

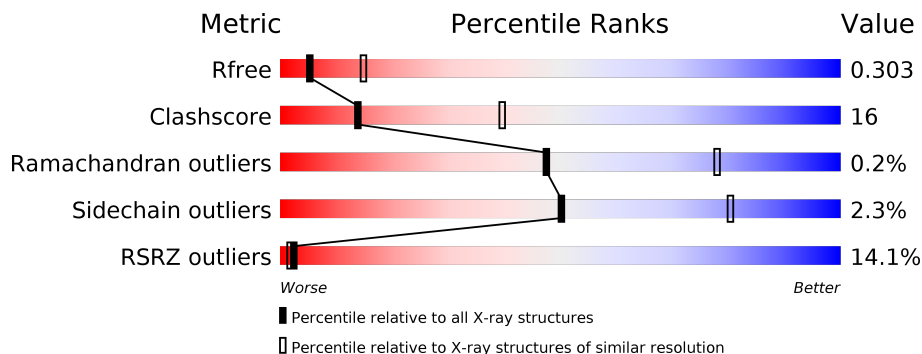
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	
1	B	211	
1	C	211	
1	D	211	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6710 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1679	C 1068	N 297	O 307	S 7	0	0	0
1	B	204	Total 1656	C 1055	N 292	O 302	S 7	0	0	0
1	C	208	Total 1684	C 1071	N 298	O 308	S 7	0	0	0
1	D	206	Total 1670	C 1062	N 294	O 307	S 7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	845	SER	-	expression tag	UNP Q15413
A	846	ASN	-	expression tag	UNP Q15413
A	847	ALA	-	expression tag	UNP Q15413
B	845	SER	-	expression tag	UNP Q15413
B	846	ASN	-	expression tag	UNP Q15413
B	847	ALA	-	expression tag	UNP Q15413
C	845	SER	-	expression tag	UNP Q15413
C	846	ASN	-	expression tag	UNP Q15413
C	847	ALA	-	expression tag	UNP Q15413
D	845	SER	-	expression tag	UNP Q15413
D	846	ASN	-	expression tag	UNP Q15413
D	847	ALA	-	expression tag	UNP Q15413

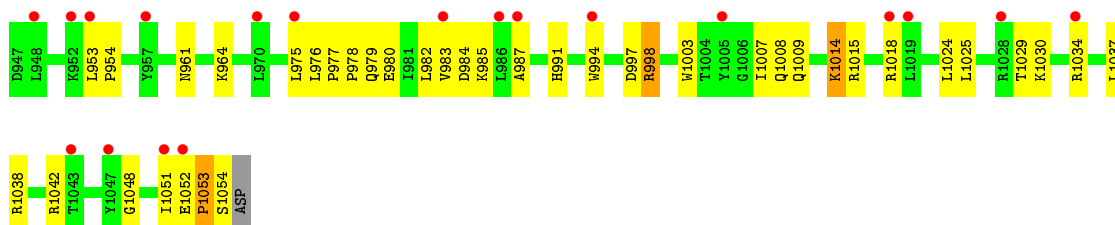
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	O 3	0	0
2	B	10	Total 10	O 10	0	0

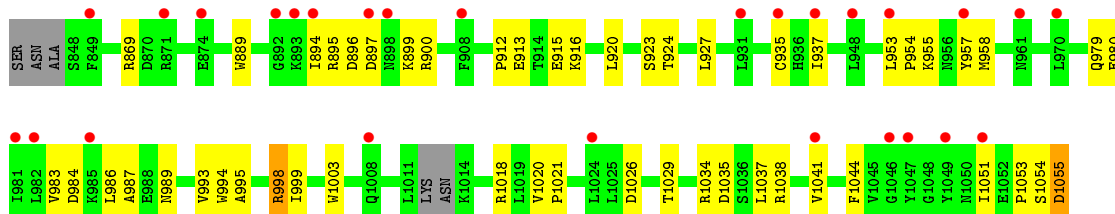
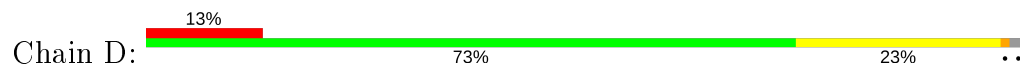
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	4	Total O 4 4	0	0
2	D	4	Total O 4 4	0	0



- Molecule 1: Ryanodine receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	64.67Å 64.67Å 469.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.34 – 2.89 48.11 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.34-2.89) 99.2 (48.11-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.11.1-2575_1309	Depositor
R, R_{free}	0.254 , 0.302 0.257 , 0.303	Depositor DCC
R_{free} test set	1243 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtrriage
Anisotropy	0.481	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.457 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6710	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1/1718 (0.1%)	0.44	0/2327
1	B	0.34	1/1694 (0.1%)	0.50	0/2294
1	C	0.30	1/1723 (0.1%)	0.49	1/2334 (0.0%)
1	D	0.26	0/1708	0.47	1/2313 (0.0%)
All	All	0.30	3/6843 (0.0%)	0.48	2/9268 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1053	PRO	N-CD	5.92	1.56	1.47
1	C	1053	PRO	N-CD	5.15	1.55	1.47
1	B	1021	PRO	N-CD	-5.00	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1052	GLU	C-N-CD	5.70	140.38	128.40
1	D	1055	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1679	0	1701	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1656	0	1676	56	0
1	C	1684	0	1707	43	0
1	D	1670	0	1686	55	0
2	A	3	0	0	0	0
2	B	10	0	0	2	0
2	C	4	0	0	2	0
2	D	4	0	0	0	0
All	All	6710	0	6770	212	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 16.

The worst 5 of 212 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:B:1020:VAL:CG1	1:B:1021:PRO:HD2	1.74	1.17
1:B:1020:VAL:HG13	1:B:1021:PRO:HD2	1.22	1.15
1:B:868:ILE:HG22	2:B:1103:HOH:O	1.71	0.88
1:D:869:ARG:HD3	1:D:924:THR:HG23	1.54	0.87
1:D:869:ARG:HG3	1:D:924:THR:HG22	1.56	0.87

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 X-ray entries followed by that with respect to entries of similar resolution.

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	205/211 (97%)	201 (98%)	3 (2%)	1 (0%)	29 61
1	B	200/211 (95%)	191 (96%)	8 (4%)	1 (0%)	29 61
1	C	206/211 (98%)	202 (98%)	4 (2%)	0	100 100
1	D	202/211 (96%)	196 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	813/844 (96%)	790 (97%)	21 (3%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1053	PRO
1	B	906	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	187/190 (98%)	183 (98%)	4 (2%)	53 81
1	B	184/190 (97%)	178 (97%)	6 (3%)	38 72
1	C	187/190 (98%)	183 (98%)	4 (2%)	53 81
1	D	186/190 (98%)	183 (98%)	3 (2%)	62 86
All	All	744/760 (98%)	727 (98%)	17 (2%)	50 80

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	956	ASN
1	B	964	LYS
1	C	1014	LYS
1	B	941	ASN
1	D	900	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/211 (98%)	0.84	27 (13%) 3 2	87, 115, 157, 177	0
1	B	204/211 (96%)	0.81	28 (13%) 3 2	77, 112, 161, 192	0
1	C	208/211 (98%)	0.85	34 (16%) 1 1	85, 113, 168, 202	0
1	D	206/211 (97%)	0.78	27 (13%) 3 2	76, 112, 160, 215	0
All	All	825/844 (97%)	0.82	116 (14%) 2 2	76, 114, 162, 215	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	948	LEU	8.1
1	D	898	ASN	7.7
1	D	892	GLY	7.0
1	A	1019	LEU	6.1
1	D	897	ASP	6.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.