



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XOA
Title : CRYSTAL STRUCTURE OF THE N-TERMINAL THREE DOMAINS OF
THE SKELETAL MUSCLE RYANODINE RECEPTOR (RYR1)
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Deposited on : 2010-08-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

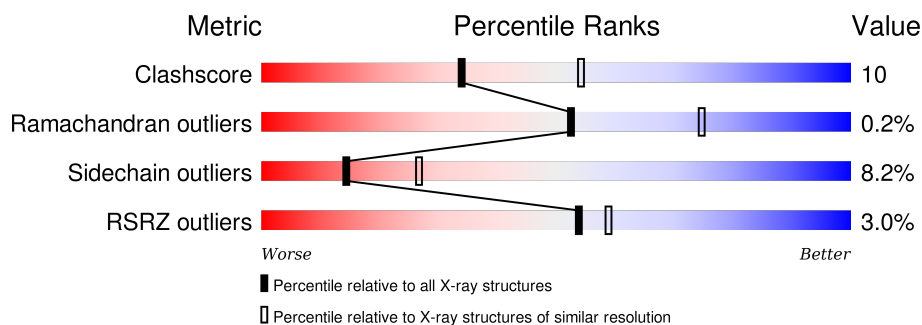
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	559	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3679 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3558	2254	622	655	27			

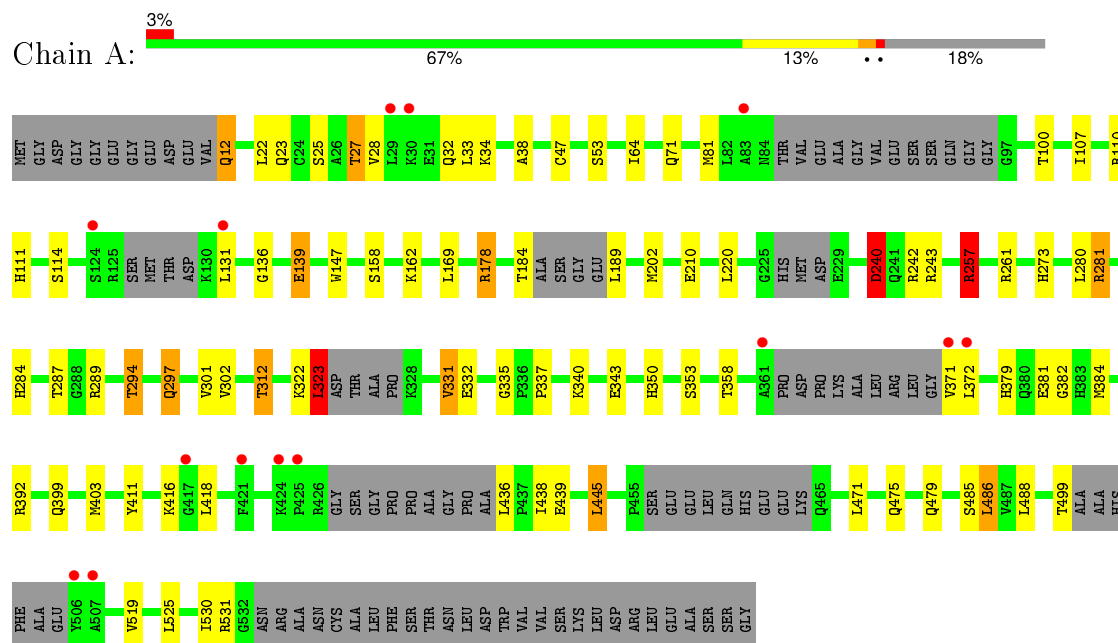
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	170.80 Å 170.80 Å 301.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 2.50 49.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.45-2.50) 99.6 (49.31-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.234 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 656411 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3679	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.88	2/3625 (0.1%)	0.91	7/4904 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CB-CG	5.26	1.62	1.52
1	A	139	GLU	CG-CD	5.11	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ARG	NE-CZ-NH2	-13.53	113.53	120.30
1	A	281	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	323	LEU	CA-CB-CG	7.13	131.71	115.30
1	A	261	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	257	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	257	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	384	MET	CG-SD-CE	-6.30	90.12	100.20

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	3558	0	3485	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	121	0	0	6	0
All	All	3679	0	3485	71	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 10.

All (71) 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:A:12:GLN:HE21	1:A:12:GLN:HA	1.05	1.14
1:A:281:ARG:HD3	1:A:312:THR:CG2	1.77	1.13
1:A:281:ARG:HD3	1:A:312:THR:HG21	1.42	0.97
1:A:110:ARG:HD3	2:A:2015:HOH:O	1.70	0.89
1:A:12:GLN:NE2	1:A:12:GLN:HA	1.87	0.89
1:A:399:GLN:HG2	1:A:403:MET:HE2	1.54	0.89
1:A:322:LYS:O	1:A:323:LEU:HD23	1.73	0.88
1:A:281:ARG:HD3	1:A:312:THR:HG23	1.59	0.83
1:A:257:ARG:HD3	2:A:2044:HOH:O	1.77	0.82
1:A:289:ARG:HB2	1:A:301:VAL:HG13	1.63	0.80
1:A:399:GLN:HG2	1:A:403:MET:CE	2.12	0.79
1:A:399:GLN:CG	1:A:403:MET:HE2	2.15	0.77
1:A:379:HIS:CD2	1:A:381:GLU:H	2.04	0.75
1:A:281:ARG:CD	1:A:312:THR:HG23	2.16	0.73
1:A:240:ASP:HB3	1:A:242:ARG:H	1.53	0.72
1:A:281:ARG:HG2	1:A:312:THR:HG23	1.71	0.72
1:A:210:GLU:HG3	1:A:337:PRO:HG3	1.74	0.70
1:A:281:ARG:CD	1:A:312:THR:CG2	2.63	0.70
1:A:131:LEU:O	1:A:178:ARG:NH2	2.22	0.70
1:A:379:HIS:HD2	1:A:382:GLY:H	1.38	0.69
1:A:289:ARG:CB	1:A:301:VAL:HG13	2.23	0.68
1:A:322:LYS:O	1:A:323:LEU:CD2	2.42	0.67
1:A:475:GLN:O	1:A:479:GLN:HG3	1.96	0.65
1:A:379:HIS:CD2	1:A:382:GLY:H	2.15	0.65
1:A:281:ARG:CG	1:A:312:THR:HG23	2.28	0.62
1:A:12:GLN:HE21	1:A:12:GLN:CA	1.93	0.61
1:A:411:TYR:HB2	1:A:486:LEU:HD11	1.82	0.61
1:A:379:HIS:HD2	1:A:381:GLU:H	1.46	0.60
1:A:71:GLN:HG2	1:A:147:TRP:HH2	1.67	0.60
1:A:289:ARG:HB2	1:A:301:VAL:CG1	2.31	0.60
1:A:340:LYS:HD3	2:A:2077:HOH:O	2.00	0.59
1:A:257:ARG:O	1:A:284:HIS:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD21	1:A:202:MET:HE2	1.86	0.58
1:A:294:THR:HG22	1:A:297:GLN:H	1.70	0.57
1:A:33:LEU:HD12	1:A:53:SER:HB2	1.86	0.57
1:A:243:ARG:HD2	2:A:2064:HOH:O	2.05	0.56
1:A:22:LEU:HD21	1:A:202:MET:CE	2.36	0.55
1:A:27:THR:HB	1:A:32:GLN:OE1	2.07	0.55
1:A:23:GLN:NE2	1:A:34:LYS:HD3	2.23	0.54
1:A:107:ILE:CD1	1:A:202:MET:HE1	2.38	0.53
1:A:411:TYR:OH	1:A:445:LEU:HD13	2.08	0.53
1:A:220:LEU:C	1:A:220:LEU:HD12	2.31	0.51
1:A:436:LEU:HB3	1:A:438:ILE:CD1	2.41	0.51
1:A:210:GLU:H	1:A:273:HIS:CE1	2.31	0.49
1:A:439:GLU:HB2	2:A:2102:HOH:O	2.13	0.48
1:A:210:GLU:H	1:A:273:HIS:HE1	1.62	0.48
1:A:107:ILE:HD11	1:A:202:MET:HE1	1.95	0.48
1:A:284:HIS:HD2	1:A:287:THR:H	1.60	0.48
1:A:331:VAL:HG12	1:A:332:GLU:H	1.80	0.47
1:A:358:THR:HG21	1:A:382:GLY:HA2	1.97	0.47
1:A:100:THR:HG21	1:A:162:LYS:HD3	1.96	0.47
1:A:340:LYS:HE2	1:A:343:GLU:OE1	2.16	0.46
1:A:399:GLN:HG2	1:A:403:MET:HE3	1.96	0.45
1:A:530:ILE:O	1:A:531:ARG:C	2.54	0.45
1:A:240:ASP:HB3	1:A:242:ARG:N	2.28	0.45
1:A:64:ILE:O	1:A:111:HIS:HE1	2.00	0.45
1:A:111:HIS:HD2	1:A:114:SER:OG	1.99	0.45
1:A:280:LEU:HD12	1:A:280:LEU:C	2.37	0.45
1:A:273:HIS:HD2	1:A:335:GLY:O	2.00	0.44
1:A:289:ARG:HD2	2:A:2060:HOH:O	2.17	0.44
1:A:38:ALA:O	1:A:47:CYS:HA	2.18	0.44
1:A:294:THR:CG2	1:A:297:GLN:H	2.31	0.44
1:A:399:GLN:CD	1:A:403:MET:HE2	2.38	0.43
1:A:411:TYR:HB2	1:A:486:LEU:CD1	2.45	0.43
1:A:436:LEU:HB3	1:A:438:ILE:HD12	2.00	0.43
1:A:111:HIS:CD2	1:A:114:SER:H	2.36	0.43
1:A:399:GLN:O	1:A:403:MET:HG3	2.21	0.41
1:A:350:HIS:HD2	1:A:353:SER:H	1.67	0.41
1:A:220:LEU:HD12	1:A:220:LEU:O	2.20	0.41
1:A:371:VAL:HG13	1:A:371:VAL:O	2.20	0.41
1:A:47:CYS:SG	1:A:136:GLY:HA2	2.61	0.40

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	442/559 (79%)	417 (94%)	24 (5%)	1 (0%)	52	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ASP

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	378/469 (81%)	347 (92%)	31 (8%)	14	27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	25	SER
1	A	27	THR
1	A	28	VAL
1	A	81	MET
1	A	139	GLU
1	A	158	SER
1	A	169	LEU
1	A	178	ARG
1	A	184	THR

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	240	ASP
1	A	257	ARG
1	A	294	THR
1	A	297	GLN
1	A	302	VAL
1	A	312	THR
1	A	323	LEU
1	A	331	VAL
1	A	372	LEU
1	A	392	ARG
1	A	416	LYS
1	A	418	LEU
1	A	445	LEU
1	A	471	LEU
1	A	485	SER
1	A	486	LEU
1	A	488	LEU
1	A	499	THR
1	A	519	VAL
1	A	525	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	GLN
1	A	54	ASN
1	A	57	ASN
1	A	111	HIS
1	A	151	HIS
1	A	224	HIS
1	A	273	HIS
1	A	284	HIS
1	A	350	HIS
1	A	379	HIS
1	A	383	HIS
1	A	489	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](#)

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	461/559 (82%)	0.12	14 (3%) 54 59	29, 51, 87, 115	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	VAL	5.9
1	A	29	LEU	4.2
1	A	361	ALA	3.7
1	A	417	GLY	3.2
1	A	506	TYR	3.1
1	A	421	PHE	2.7
1	A	124	SER	2.7
1	A	425	PRO	2.5
1	A	131	LEU	2.4
1	A	372	LEU	2.4
1	A	507	ALA	2.4
1	A	424	LYS	2.4
1	A	83	ALA	2.2
1	A	30	LYS	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.