



# Full wwPDB X-ray Structure Validation Report

Nov 4, 2014 – 05:17 PM EST

PDB ID : 4JKQ  
Title : Crystal structure of the N-terminal region of the human ryanodine receptor 2  
Authors : Baueroва, V.; Sevcik, J.  
Deposited on : 2013-03-11  
Resolution : 2.39 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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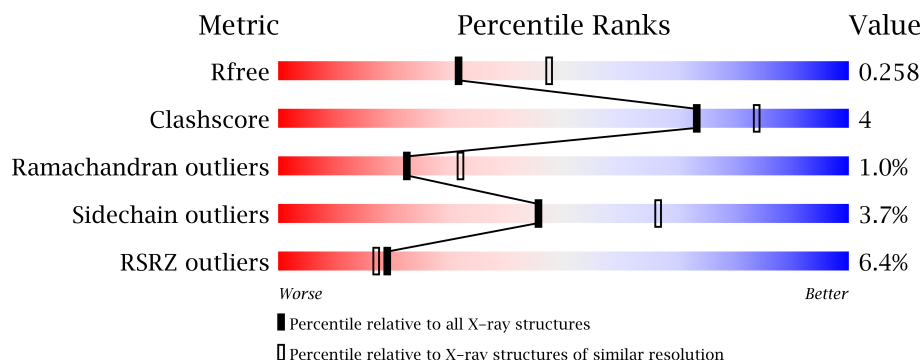
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 2.39 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	606	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4013 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3934	2460	708	748	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.45Å 75.45Å 248.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 2.39 48.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.77-2.39) 100.0 (48.00-2.39)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.224 , 0.261 0.223 , 0.258	Depositor DCC
$R_{free}$ test set	1444 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29402 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	5/4009 (0.1%)	0.61	0/5411

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	GLU	CD-OE2	6.15	1.32	1.25
1	A	284	TRP	CD2-CE2	5.64	1.48	1.41
1	A	212	TRP	CD2-CE2	5.42	1.47	1.41
1	A	526	TRP	CD2-CE2	5.23	1.47	1.41
1	A	291	TRP	CD2-CE2	5.09	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3934	0	3870	33	0
2	A	79	0	0	0	0
All	All	4013	0	3870	33	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:CYS:SG	1:A:158:CYS:HB3	2.17	0.84
1:A:308:LEU:HD13	1:A:393:MET:HG3	1.61	0.82
1:A:373:THR:HG22	1:A:374:TYR:H	1.49	0.77
1:A:223:ALA:HB3	1:A:225:GLN:HE21	1.56	0.70
1:A:237:LEU:HD23	1:A:244:CYS:HB3	1.74	0.70
1:A:373:THR:HG23	1:A:401:ASP:OD1	1.92	0.69
1:A:36:CYS:HB3	1:A:65:CYS:SG	2.37	0.65
1:A:36:CYS:CB	1:A:65:CYS:SG	2.94	0.56
1:A:123:HIS:O	1:A:126:SER:O	2.27	0.52
1:A:253:GLY:HA3	1:A:256:GLN:HB3	1.94	0.50
1:A:27:THR:HG22	1:A:32:GLN:OE1	2.13	0.49
1:A:409:GLN:HB2	1:A:412:GLU:HG2	1.94	0.49
1:A:301:THR:HG21	1:A:492:GLU:OE1	2.13	0.47
1:A:51:SER:O	1:A:60:PRO:HB3	2.14	0.47
1:A:125:TYR:CZ	1:A:417:ARG:HD2	2.50	0.46
1:A:336:GLU:HB3	1:A:337:LYS:H	1.51	0.46
1:A:43:GLY:O	1:A:44:ASN:HB2	2.16	0.46
1:A:143:LEU:O	1:A:190:ARG:NH1	2.49	0.44
1:A:419:ILE:O	1:A:423:VAL:HG23	2.17	0.44
1:A:224:ALA:HA	1:A:229:ILE:HD11	1.98	0.44
1:A:22:LEU:HD23	1:A:214:VAL:HG22	2.00	0.43
1:A:35:LEU:HD23	1:A:49:LEU:HB3	2.00	0.42
1:A:23:GLN:HA	1:A:35:LEU:O	2.19	0.42
1:A:16:THR:O	1:A:17:ASP:HB2	2.19	0.42
1:A:248:PRO:O	1:A:257:ARG:HD2	2.20	0.42
1:A:246:THR:OG1	1:A:247:VAL:N	2.53	0.42
1:A:191:TYR:O	1:A:205:ALA:HA	2.19	0.42
1:A:34:LYS:H	1:A:53:SER:HB3	1.85	0.42
1:A:363:ILE:CD1	1:A:403:ILE:HG13	2.51	0.41
1:A:25:THR:HG22	1:A:34:LYS:HG2	2.03	0.41
1:A:373:THR:HG22	1:A:374:TYR:N	2.25	0.41
1:A:375:GLN:HB3	1:A:392:ILE:HG12	2.03	0.41
1:A:249:SER:O	1:A:251:GLU:N	2.48	0.40

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 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	493/606 (81%)	457 (93%)	31 (6%)	5 (1%)	22	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	250	GLY
1	A	336	GLU
1	A	41	GLY
1	A	199	GLY

### 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 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	430/522 (82%)	414 (96%)	16 (4%)	45	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	158	CYS
1	A	190	ARG
1	A	211	LEU
1	A	241	MET
1	A	257	ARG
1	A	301	THR
1	A	313	ASN

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Mol	Chain	Res	Type
1	A	336	GLU
1	A	342	VAL
1	A	351	THR
1	A	375	GLN
1	A	417	ARG
1	A	441	LYS
1	A	454	LEU
1	A	527	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	33	GLN
1	A	209	GLN
1	A	225	GLN
1	A	261	HIS
1	A	365	HIS
1	A	388	GLN
1	A	490	GLN
1	A	544	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	499/606 (82%)	0.45	32 (6%) 19 17	28, 56, 114, 165	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	VAL	9.9
1	A	342	VAL	8.0
1	A	140	THR	7.9
1	A	76	ARG	7.8
1	A	338	LEU	7.5
1	A	339	ASP	7.1
1	A	78	LEU	6.0
1	A	252	HIS	5.9
1	A	198	ASN	5.9
1	A	75	VAL	5.8
1	A	341	GLY	5.2
1	A	377	VAL	5.0
1	A	378	ASP	4.6
1	A	469	HIS	4.5
1	A	77	ALA	4.2
1	A	11	ILE	3.6
1	A	199	GLY	3.4
1	A	348	GLY	3.3
1	A	240	HIS	3.3
1	A	223	ALA	3.2
1	A	349	MET	3.1
1	A	107	GLY	2.9
1	A	253	GLY	2.7
1	A	224	ALA	2.5
1	A	108	GLY	2.5
1	A	351	THR	2.4
1	A	309	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.2
1	A	350	GLY	2.1
1	A	141	ASP	2.1
1	A	343	ARG	2.0
1	A	113	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.