



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 4I6I / pdb_00004i6i
Title : Crystal structure of rabbit ryanodine receptor 1 (residues 1-559) disease mutant R45C
Authors : Kimlicka, L.; Van Petegem, F.
Deposited on : 2012-11-29
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

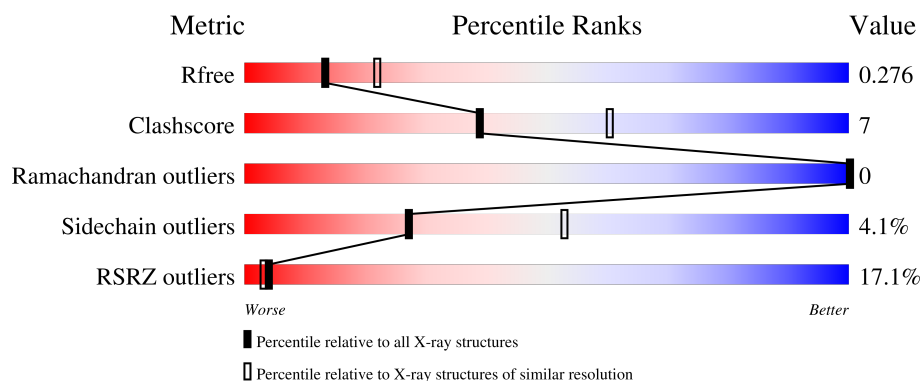
1 Overall quality at a glance

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of 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	559	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3356 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	451	Total	C	N	O	S	0	1	0
			3300	2088	583	603	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	CYS	ARG	engineered mutation	UNP P11716

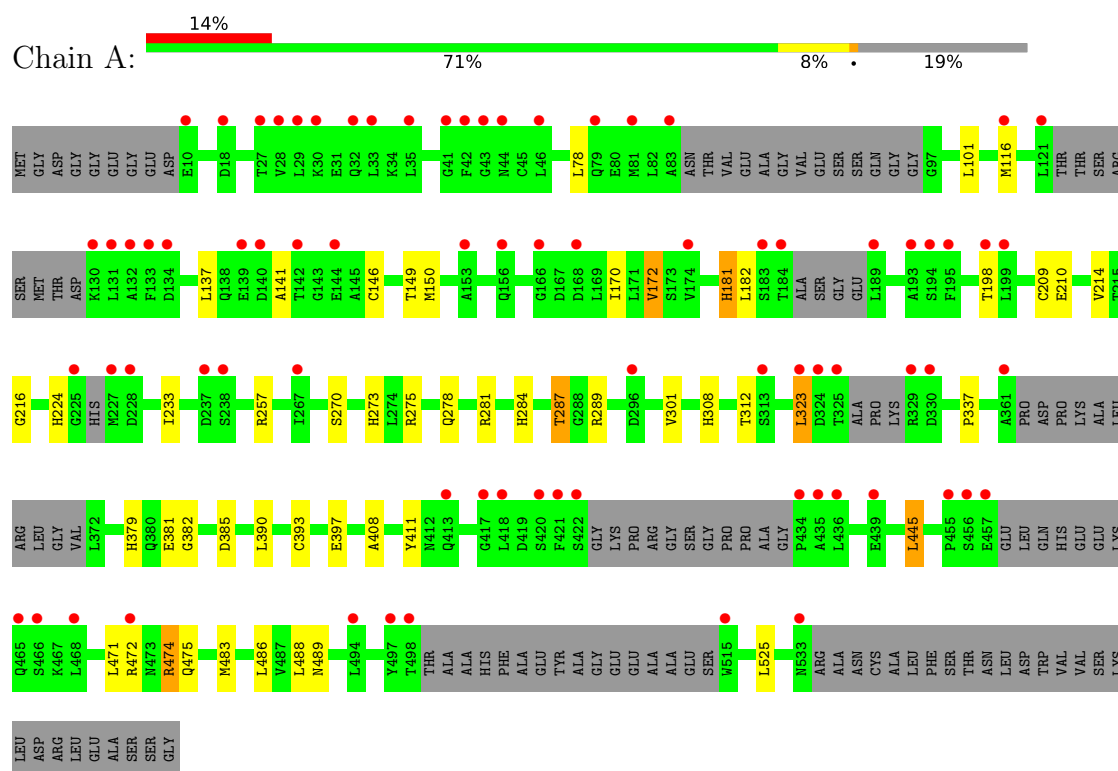
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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 ($RSRZ > 2$). 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	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.16Å 118.16Å 246.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.50 48.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.50) 100.0 (48.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.260 , 0.277 0.260 , 0.276	Depositor DCC
R_{free} test set	1804 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3356	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, 0.333 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	0.38	0/3364	0.73	0/4574

There are no bond length outliers.

There are no bond angle outliers.

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	3300	0	3050	43	0
2	A	56	0	0	1	0
All	All	3356	0	3050	43	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 7.

All (43) 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:474:ARG:HG2	1:A:474:ARG:HH11	1.40	0.85
1:A:379:HIS:HD2	1:A:382:GLY:H	1.32	0.77
1:A:210:GLU:HG3	1:A:337:PRO:HG3	1.72	0.71
1:A:224:HIS:HE1	1:A:385:ASP:O	1.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:HIS:CD2	1:A:382:GLY:H	2.16	0.63
1:A:281:ARG:HD3	1:A:312:THR:HG21	1.80	0.63
1:A:284:HIS:CD2	1:A:287:THR:HB	2.34	0.62
1:A:323:LEU:H	1:A:323:LEU:HD23	1.63	0.62
1:A:210:GLU:H	1:A:273:HIS:HE1	1.50	0.60
1:A:289:ARG:CB	1:A:301:VAL:CG1	2.82	0.58
1:A:257:ARG:O	1:A:284:HIS:HE1	1.88	0.57
1:A:181:HIS:HA	1:A:198:THR:OG1	2.04	0.57
1:A:284:HIS:HD2	1:A:287:THR:H	1.54	0.56
1:A:281:ARG:HD3	1:A:312:THR:CG2	2.36	0.55
1:A:472:ARG:HA	1:A:475:GLN:HE21	1.72	0.55
1:A:275:ARG:H	1:A:278:GLN:HE21	1.55	0.54
1:A:289:ARG:CB	1:A:301:VAL:HG12	2.38	0.54
1:A:289:ARG:HB3	1:A:301:VAL:CG1	2.37	0.53
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.16	0.53
1:A:289:ARG:HB2	1:A:301:VAL:CG1	2.37	0.53
1:A:210:GLU:H	1:A:273:HIS:CE1	2.27	0.52
1:A:289:ARG:HB3	1:A:301:VAL:HG12	1.90	0.52
1:A:224:HIS:CE1	1:A:385:ASP:O	2.59	0.51
1:A:275:ARG:H	1:A:278:GLN:NE2	2.10	0.50
1:A:308:HIS:O	1:A:312:THR:HG22	2.13	0.49
1:A:116:MET:HE3	1:A:137:LEU:HB3	1.95	0.48
1:A:411:TYR:HB2	1:A:486:LEU:HD11	1.97	0.47
1:A:379:HIS:CD2	1:A:381:GLU:H	2.34	0.46
1:A:284:HIS:HD2	1:A:287:THR:HB	1.79	0.46
1:A:141:ALA:HA	1:A:146:CYS:SG	2.57	0.45
1:A:393:CYS:SG	1:A:397:GLU:HB3	2.57	0.45
1:A:474:ARG:HH11	1:A:474:ARG:CG	2.19	0.45
1:A:411:TYR:OH	1:A:445:LEU:HD13	2.18	0.43
1:A:233:ILE:HG12	1:A:284:HIS:CE1	2.54	0.43
1:A:214:VAL:HG21	1:A:390:LEU:HD12	2.00	0.43
1:A:474:ARG:NH1	1:A:474:ARG:CG	2.81	0.43
1:A:323:LEU:H	1:A:323:LEU:CD2	2.32	0.42
1:A:101:LEU:HB3	1:A:150:MET:HE1	2.02	0.42
1:A:257:ARG:HD3	2:A:631:HOH:O	2.19	0.42
1:A:149:THR:OG1	1:A:172:VAL:HG22	2.20	0.41
1:A:182:LEU:H	1:A:198:THR:HG21	1.85	0.41
1:A:216:GLY:HA3	1:A:270:SER:O	2.21	0.41
1:A:408:ALA:HB2	1:A:483:MET:HE1	2.03	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	432/559 (77%)	424 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	319/469 (68%)	306 (96%)	13 (4%)	27	53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	170	ILE
1	A	172	VAL
1	A	181	HIS
1	A	209	CYS
1	A	287	THR
1	A	323	LEU
1	A	445	LEU
1	A	471	LEU
1	A	474	ARG
1	A	488	LEU
1	A	489	ASN
1	A	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	54	ASN
1	A	57	ASN
1	A	98	HIS
1	A	203	ASN
1	A	224	HIS
1	A	273	HIS
1	A	278	GLN
1	A	284	HIS
1	A	308	HIS
1	A	379	HIS
1	A	383	HIS
1	A	405	HIS
1	A	412	ASN
1	A	475	GLN
1	A	495	ASN
1	A	533	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 oligosaccharides 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.

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, 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	451/559 (80%)	0.98	77 (17%) 4 3	23, 60, 109, 138	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	THR	6.8
1	A	131	LEU	6.7
1	A	130	LYS	5.7
1	A	83	ALA	5.7
1	A	457	GLU	5.4
1	A	325	THR	5.4
1	A	324	ASP	5.4
1	A	466	SER	5.4
1	A	422	SER	4.9
1	A	27	THR	4.5
1	A	168	ASP	4.4
1	A	237	ASP	4.3
1	A	30	LYS	4.3
1	A	434	PRO	4.2
1	A	133	PHE	4.1
1	A	132	ALA	4.1
1	A	81	MET	4.0
1	A	468	LEU	3.9
1	A	46	LEU	3.8
1	A	421	PHE	3.8
1	A	42	PHE	3.7
1	A	32	GLN	3.7
1	A	515	TRP	3.6
1	A	497	TYR	3.6
1	A	227	MET	3.4
1	A	144	GLU	3.3
1	A	330	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	329	ARG	3.1
1	A	184	THR	3.1
1	A	455	PRO	3.1
1	A	41	GLY	3.0
1	A	28	VAL	3.0
1	A	323	LEU	3.0
1	A	29	LEU	3.0
1	A	44	ASN	3.0
1	A	436	LEU	2.9
1	A	10	GLU	2.9
1	A	238	SER	2.8
1	A	228	ASP	2.8
1	A	313	SER	2.8
1	A	413	GLN	2.7
1	A	420	SER	2.7
1	A	79	GLN	2.7
1	A	121	LEU	2.7
1	A	18	ASP	2.6
1	A	418	LEU	2.6
1	A	465	GLN	2.6
1	A	296	ASP	2.6
1	A	439	GLU	2.6
1	A	198	THR	2.5
1	A	472	ARG	2.5
1	A	199	LEU	2.5
1	A	361	ALA	2.5
1	A	33	LEU	2.4
1	A	194	SER	2.4
1	A	195	PHE	2.4
1	A	174	VAL	2.4
1	A	417	GLY	2.4
1	A	153	ALA	2.4
1	A	142	THR	2.3
1	A	166	GLY	2.3
1	A	267	ILE	2.3
1	A	225	GLY	2.2
1	A	140	ASP	2.2
1	A	189	LEU	2.2
1	A	193	ALA	2.1
1	A	134	ASP	2.1
1	A	533	ASN	2.1
1	A	35	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	2.1
1	A	494	LEU	2.1
1	A	435	ALA	2.1
1	A	116	MET	2.1
1	A	456	SER	2.0
1	A	156	GLN	2.0
1	A	139	GLU	2.0
1	A	183	SER	2.0

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 oligosaccharides 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.