



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:16 PM GMT

PDB ID : 4L4I
Title : Crystal structure of mouse Ryanodine Receptor isoform 2 (RyR2) 1-547 disease mutant R420Q
Authors : Kimlicka, L.; Van Petegem, F.
Deposited on : 2013-06-07
Resolution : 2.15 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
<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

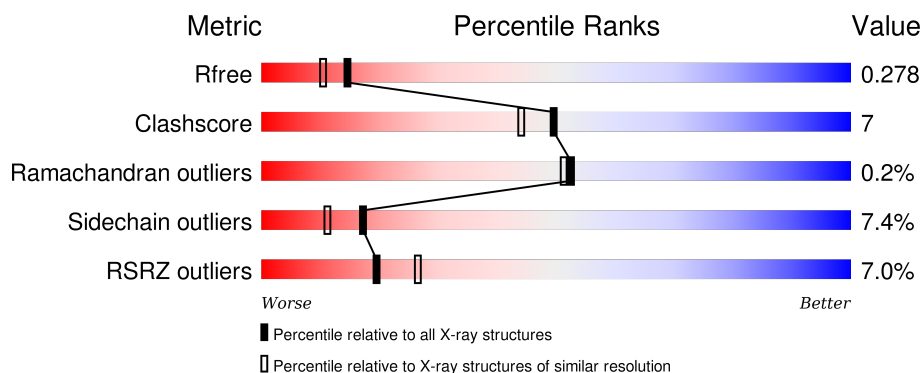
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	547	<div> <div>6%</div> <div>71%</div> <div>15%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	601	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3623 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3553	2243	625	667	18	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	ENGINEERED MUTATION	UNP E9Q401

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		

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.

Chain A:

6% 71% 15% 14%

MET ASP VAL GLU LYS TRP LYS PHE MET MET LYS THR VAL GLN LYS MET LEU ALA ASN THR VAL GLU LYS GLU GLN VAL

ASP VAL GLU LYS TRP LYS PHE MET MET LYS THR ALA GLN GLY GLY ASP GLU THR VAL GLN LYS MET LEU ALA ASN THR VAL GLU LYS GLU GLN VAL

GLU V346 V347 V348 V349 V350 V351 V352 V353 V354 V355 V356 V357 V358 V359 V360 V361 V362 V363 V364 V365 V366 V367 V368 V369 V370 V371 V372 V373 V374 V375 V376 V377 V378 V379 V380 V381 V382 V383 V384 V385 V386 V387 V388 V389 V390 V391 V392 V393 V394 V395 V396 V397 V398 V399 V400 V401 V402 V403 V404 V405 V406 V407 V408 V409 V410 V411 V412 V413 V414 V415 V416 V417 V418 V419 V420 V421 V422 V423 V424 V425 V426 V427 V428 V429 V430 V431 V432 V433 V434 V435 V436 V437 V438 V439 V440 V441 V442 V443 V444 V445 V446 V447 V448 V449 V450 V451 V452 V453 V454 V455 V456 V457 V458 V459 V460 V461 V462 V463 V464 V465 V466 V467 V468 V469 V470 V471 V472 V473 V474 V475 V476 V477 V478 V479 V480 V481 V482 V483 V484 V485 V486 V487 V488 V489 V490 V491 V492 V493 V494 V495 V496 V497 V498 V499 V500 V501 V502 V503 V504 V505 V506 V507 V508 V509 V510 V511 V512 V513 V514 V515 V516 V517 V518 V519 V520 V521 V522 V523 V524 V525 V526 V527 V528 V529 V530 V531 V532 V533 V534 V535 V536 V537 V538 V539 V540 V541 V542 V543 V544 V545 V546 V547 V548 V549 V550 V551 V552 V553 V554 V555 V556 V557 V558 V559 V560 V561 V562 V563 V564 V565 V566 V567 V568 V569 V570 V571 V572 V573 V574 V575 V576 V577 V578 V579 V580 V581 V582 V583 V584 V585 V586 V587 V588 V589 V590 V591 V592 V593 V594 V595 V596 V597 V598 V599 V600 V601 V602 V603 V604 V605 V606 V607 V608 V609 V610 V611 V612 V613 V614 V615 V616 V617 V618 V619 V620 V621 V622 V623 V624 V625 V626 V627 V628 V629 V630 V631 V632 V633 V634 V635 V636 V637 V638 V639 V640 V641 V642 V643 V644 V645 V646 V647 V648 V649 V650 V651 V652 V653 V654 V655 V656 V657 V658 V659 V660 V661 V662 V663 V664 V665 V666 V667 V668 V669 V670 V671 V672 V673 V674 V675 V676 V677 V678 V679 V680 V681 V682 V683 V684 V685 V686 V687 V688 V689 V690 V691 V692 V693 V694 V695 V696 V697 V698 V699 V700 V701 V702 V703 V704 V705 V706 V707 V708 V709 V710 V711 V712 V713 V714 V715 V716 V717 V718 V719 V720 V721 V722 V723 V724 V725 V726 V727 V728 V729 V730 V731 V732 V733 V734 V735 V736 V737 V738 V739 V740 V741 V742 V743 V744 V745 V746 V747 V748 V749 V750 V751 V752 V753 V754 V755 V756 V757 V758 V759 V760 V761 V762 V763 V764 V765 V766 V767 V768 V769 V770 V771 V772 V773 V774 V775 V776 V777 V778 V779 V780 V781 V782 V783 V784 V785 V786 V787 V788 V789 V790 V791 V792 V793 V794 V795 V796 V797 V798 V799 V800 V801 V802 V803 V804 V805 V806 V807 V808 V809 V810 V811 V812 V813 V814 V815 V816 V817 V818 V819 V820 V821 V822 V823 V824 V825 V826 V827 V828 V829 V830 V831 V832 V833 V834 V835 V836 V837 V838 V839 V840 V841 V842 V843 V844 V845 V846 V847 V848 V849 V850 V851 V852 V853 V854 V855 V856 V857 V858 V859 V860 V861 V862 V863 V864 V865 V866 V867 V868 V869 V870 V871 V872 V873 V874 V875 V876 V877 V878 V879 V880 V881 V882 V883 V884 V885 V886 V887 V888 V889 V890 V891 V892 V893 V894 V895 V896 V897 V898 V899 V900 V901 V902 V903 V904 V905 V906 V907 V908 V909 V910 V911 V912 V913 V914 V915 V916 V917 V918 V919 V920 V921 V922 V923 V924 V925 V926 V927 V928 V929 V930 V931 V932 V933 V934 V935 V936 V937 V938 V939 V940 V941 V942 V943 V944 V945 V946 V947 V948 V949 V950 V951 V952 V953 V954 V955 V956 V957 V958 V959 V960 V961 V962 V963 V964 V965 V966 V967 V968 V969 V970 V971 V972 V973 V974 V975 V976 V977 V978 V979 V980 V981 V982 V983 V984 V985 V986 V987 V988 V989 V990 V991 V992 V993 V994 V995 V996 V997 V998 V999 V1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	78.05Å 78.05Å 248.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.89 – 2.15 41.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.89-2.15) 99.7 (41.87-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.228 , 0.263 0.242 , 0.278	Depositor DCC
R_{free} test set	2137 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 43007 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3623	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.65	1/3642 (0.0%)	0.72	2/4950 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	CYS	CB-SG	-5.97	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	VAL	CB-CA-C	-5.87	100.24	111.40
1	A	530	LEU	CB-CG-CD1	5.64	120.60	111.00

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	3553	0	3313	49	0
2	A	6	0	8	6	0
3	A	64	0	0	0	0
All	All	3623	0	3321	49	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.

The worst 5 of 49 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:258:ARG:HG2	1:A:258:ARG:HH11	1.22	1.05
1:A:42:PHE:HA	2:A:601:GOL:H12	1.53	0.88
1:A:394:HIS:HD2	1:A:397:GLY:H	1.33	0.76
1:A:458:ASP:HB3	2:A:601:GOL:H2	1.68	0.76
1:A:258:ARG:HG2	1:A:258:ARG:NH1	1.94	0.74

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	467/547 (85%)	454 (97%)	12 (3%)	1 (0%)	52 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ILE

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	358/470 (76%)	331 (92%)	27 (8%)	17	10

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	VAL
1	A	347	ASP
1	A	536	LEU
1	A	301	THR
1	A	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	HIS
1	A	394	HIS
1	A	484	ASN
1	A	193	HIS
1	A	427	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	601	-	5,5,5	0.58	0	5,5,5	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	601	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	6	0

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	473/547 (86%)	0.58	33 (6%)	19 26	25, 62, 105, 158	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	SER	4.7
1	A	75	VAL	4.4
1	A	347	ASP	3.9
1	A	197	GLY	3.7
1	A	201	TRP	3.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	601	6/6	0.92	0.19	0.45	56,57,60,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.