



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:42 am BST

PDB ID : 4NCH
Title : Crystal Structure of Pyrococcus furiosus Rad50 L802W mutation
Authors : Classen, S.; Williams, G.J.; Arvai, A.S.; Williams, R.S.
Deposited on : 2013-10-24
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

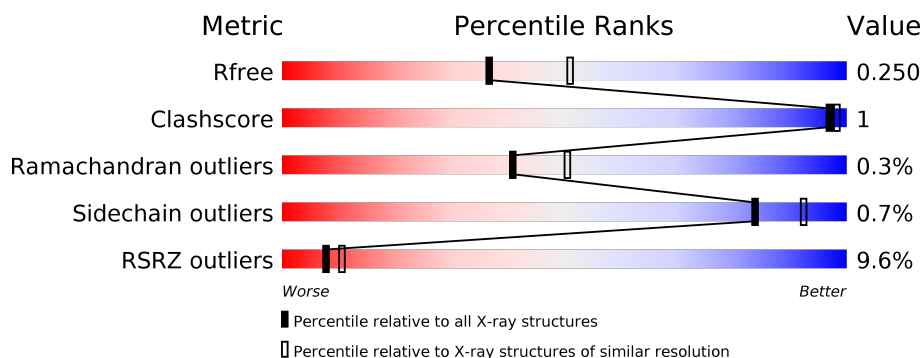
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	339	<div> <div>7%</div> <div>87%</div> <div>11%</div> </div>
1	B	339	<div> <div>10%</div> <div>87%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9441 atoms, of which 4502 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 DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	H	N	O	S	0	1	0
			4666	1500	2331	395	435	5			
1	B	304	Total	C	H	N	O	S	0	3	0
			4431	1459	2171	373	423	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	721	GLY	-	LINKER	UNP P58301
A	722	GLY	-	LINKER	UNP P58301
A	723	SER	-	LINKER	UNP P58301
A	724	GLY	-	LINKER	UNP P58301
A	725	GLY	-	LINKER	UNP P58301
A	802	TRP	LEU	ENGINEERED MUTATION	UNP P58301
B	721	GLY	-	LINKER	UNP P58301
B	722	GLY	-	LINKER	UNP P58301
B	723	SER	-	LINKER	UNP P58301
B	724	GLY	-	LINKER	UNP P58301
B	725	GLY	-	LINKER	UNP P58301
B	802	TRP	LEU	ENGINEERED MUTATION	UNP P58301

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

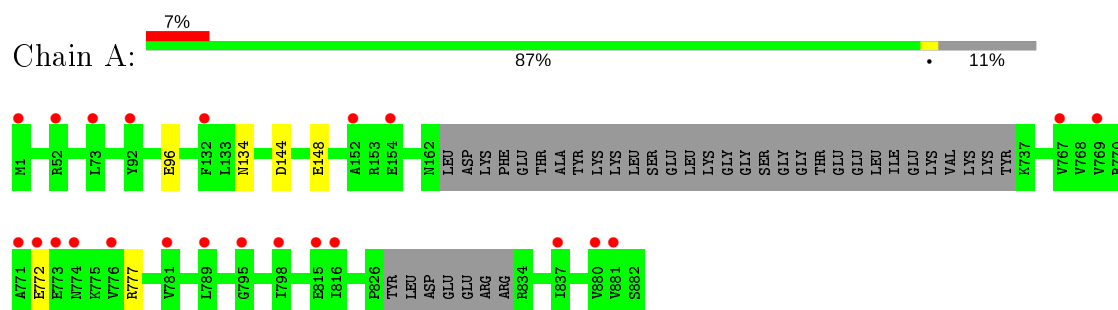
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	154	Total	O	0	0
			154	154		

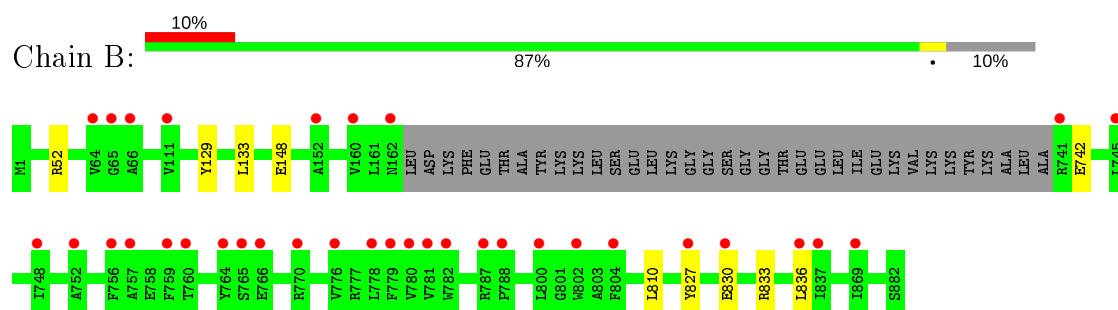
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA double-strand break repair Rad50 ATPase



- Molecule 1: DNA double-strand break repair Rad50 ATPase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.44Å 70.44Å 281.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.13 – 2.30 46.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.13-2.30) 99.8 (46.13-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1233	Depositor
R, R_{free}	0.207 , 0.246 0.210 , 0.250	Depositor DCC
R_{free} test set	1871 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9441	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 4.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.23	0/2373	0.41	0/3207
1	B	0.22	0/2307	0.40	0/3133
All	All	0.23	0/4680	0.41	0/6340

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

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	2335	2331	2325	4	0
1	B	2260	2171	2164	4	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	175	0	0	2	0
3	B	154	0	0	1	0
All	All	4939	4502	4489	8	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 1.

All (8) 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:144:ASP:O	1:A:148:GLU:N	2.44	0.50
1:A:772:GLU:OE1	1:A:777:ARG:NH2	2.44	0.50
1:B:52:ARG:O	1:B:129:TYR:OH	2.22	0.49
1:A:96:GLU:OE2	3:A:1080:HOH:O	2.20	0.42
1:B:830:GLU:OE2	1:B:833:ARG:NH1	2.53	0.42
1:B:129:TYR:CZ	1:B:133:LEU:HD12	2.55	0.41
1:B:833:ARG:NH2	3:B:1127:HOH:O	2.52	0.41
1:A:134:ASN:ND2	3:A:1064:HOH:O	2.52	0.41

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	296/339 (87%)	286 (97%)	10 (3%)	0	100	100
1	B	303/339 (89%)	289 (95%)	12 (4%)	2 (1%)	22	26
All	All	599/678 (88%)	575 (96%)	22 (4%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	GLU
1	B	742	GLU

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	241/294 (82%)	241 (100%)	0	100	100
1	B	218/294 (74%)	215 (99%)	3 (1%)	67	81
All	All	459/588 (78%)	456 (99%)	3 (1%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	810	LEU
1	B	827	TYR
1	B	836	LEU

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	SO4	A	902	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	901	-	4,4,4	0.16	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

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

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	301/339 (88%)	0.50	23 (7%) 13 18	25, 47, 100, 132	0
1	B	304/339 (89%)	0.60	35 (11%) 4 7	21, 55, 123, 162	0
All	All	605/678 (89%)	0.55	58 (9%) 8 10	21, 50, 115, 162	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	781	VAL	8.6
1	B	764	TYR	6.8
1	B	152	ALA	6.4
1	B	760	THR	5.5
1	B	780	VAL	5.4
1	B	782	TRP	4.8
1	A	880	VAL	4.7
1	B	756	PHE	4.4
1	A	776	VAL	4.3
1	A	798	ILE	4.3
1	B	836	LEU	4.2
1	B	741	ARG	4.1
1	A	781	VAL	4.0
1	A	774	ASN	3.8
1	A	771	ALA	3.8
1	B	800	LEU	3.6
1	B	779	PHE	3.5
1	A	73	LEU	3.4
1	B	776	VAL	3.4
1	B	778	LEU	3.4
1	A	837	ILE	3.3
1	B	765	SER	3.3
1	B	745	LEU	3.1
1	A	773	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	788	PRO	3.0
1	B	787	ARG	3.0
1	A	772	GLU	2.9
1	B	752	ALA	2.9
1	B	65	GLY	2.9
1	B	827	TYR	2.9
1	B	759	PHE	2.9
1	B	804	PHE	2.8
1	B	748	ILE	2.8
1	B	837	ILE	2.8
1	B	766	GLU	2.7
1	A	1	MET	2.7
1	A	152	ALA	2.6
1	B	869[A]	ILE	2.6
1	B	111	VAL	2.6
1	A	52	ARG	2.5
1	B	757	ALA	2.5
1	A	789	LEU	2.4
1	A	815	GLU	2.4
1	A	769	VAL	2.4
1	B	160	VAL	2.3
1	A	767	VAL	2.2
1	A	816	ILE	2.2
1	A	132	PHE	2.2
1	B	162	ASN	2.2
1	B	64	VAL	2.2
1	A	154	GLU	2.2
1	A	92	TYR	2.1
1	A	881	VAL	2.1
1	B	66	ALA	2.1
1	A	795	GLY	2.1
1	B	770	ARG	2.1
1	B	830	GLU	2.1
1	B	802	TRP	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 [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. 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	B-factors(\AA^2)	Q<0.9
2	SO4	A	902	5/5	0.87	0.32	49,49,54,71	0
2	SO4	B	901	5/5	0.89	0.28	32,36,43,84	0
2	SO4	A	901	5/5	0.99	0.12	23,24,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.