



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:39 PM UTC

PDB ID : 9YI3 / pdb_00009yi3
Title : Crystal structure of PprA S-F filament from *Deinococcus radiodurans*
Authors : Szabla, R.; Junop, M.S.
Deposited on : 2025-10-01
Resolution : 1.82 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

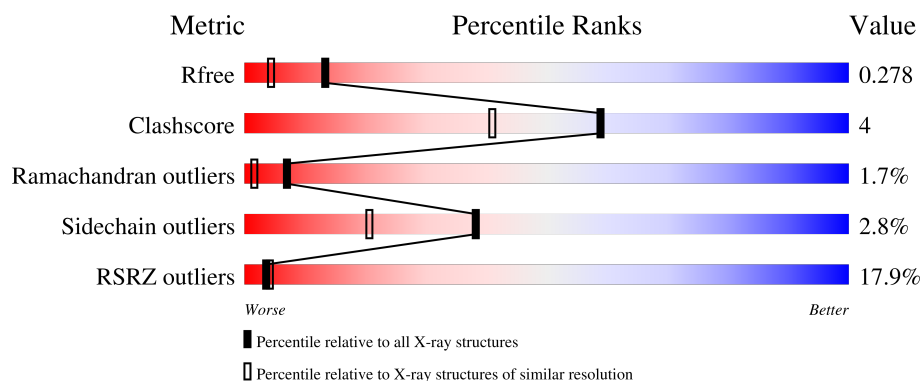
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	276	
1	B	276	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8430 atoms, of which 4112 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 repair protein PprA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	H	N	O	Se	588	0	0
			4150	1299	2056	387	404	4			
1	B	276	Total	C	H	N	O	Se	944	0	0
			4150	1299	2056	387	404	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LYS	ASP	engineered mutation	UNP O32504
A	184	LYS	ASP	engineered mutation	UNP O32504
B	180	LYS	ASP	engineered mutation	UNP O32504
B	184	LYS	ASP	engineered mutation	UNP O32504

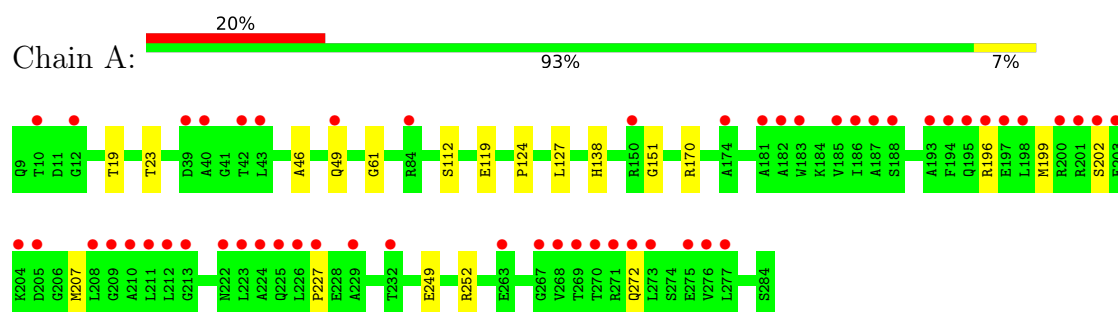
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	62	Total	O	0	0
			62	62		

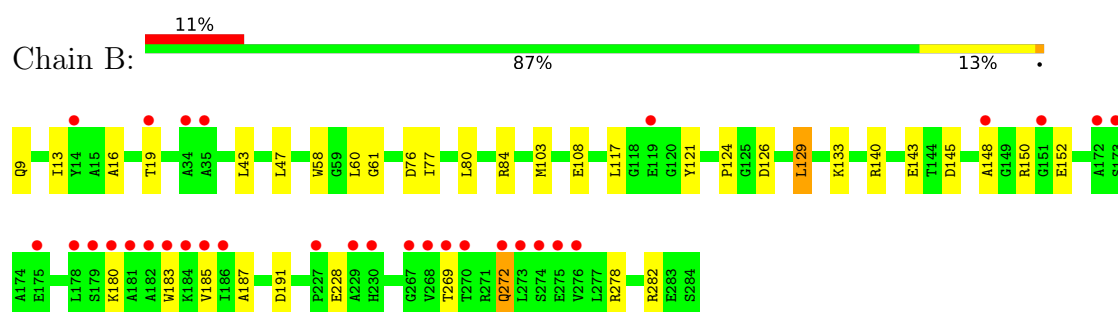
3 Residue-property plots [i](#)

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: DNA repair protein PprA



• Molecule 1: DNA repair protein PprA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.42Å 147.35Å 44.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.47 – 1.82 44.47 – 1.82	Depositor EDS
% Data completeness (in resolution range)	52.3 (44.47-1.82) 52.3 (44.47-1.82)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.82Å)	Xtriage
Refinement program	PHENIX 2.0_5824	Depositor
R, R_{free}	0.262 , 0.275 (Not available) , 0.278	Depositor DCC
R_{free} test set	1409 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8430	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.83% 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	0.39	0/2125	0.58	0/2866
1	B	0.53	0/2125	0.78	0/2866
All	All	0.46	0/4250	0.69	0/5732

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	278	ARG	Sidechain
1	B	282	ARG	Sidechain

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	2094	2056	2053	11	0
1	B	2094	2056	2053	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	68	0	0	1	0
2	B	62	0	0	2	0
All	All	4318	4112	4106	30	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 4.

All (30) 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:B:228:GLU:N	1:B:228:GLU:OE1	2.26	0.68
1:B:61:GLY:HA2	2:B:314:HOH:O	1.97	0.65
1:B:108:GLU:H	1:B:108:GLU:CD	2.06	0.63
1:A:124:PRO:HG2	1:A:127:LEU:HD13	1.81	0.62
1:B:58:TRP:HB3	1:B:60:LEU:HD13	1.87	0.56
1:A:61:GLY:HA3	1:A:112:SER:HB2	1.88	0.55
1:A:249:GLU:OE2	1:A:252:ARG:NH2	2.39	0.54
1:B:16:ALA:O	1:B:19:THR:HG22	2.09	0.53
1:A:19:THR:HG22	1:A:227:PRO:HG3	1.91	0.52
1:B:269:THR:HA	1:B:272:GLN:HG3	1.92	0.52
1:A:252:ARG:HD2	2:A:342:HOH:O	2.14	0.48
1:B:117:LEU:HD22	1:B:117:LEU:N	2.29	0.47
1:B:13:ILE:HD11	1:B:77:ILE:H	1.80	0.47
1:A:196:ARG:HA	1:A:199:MSE:CE	2.46	0.45
1:B:108:GLU:CD	1:B:108:GLU:N	2.72	0.45
1:B:13:ILE:CD1	1:B:76:ASP:HA	2.47	0.43
1:B:13:ILE:HD13	1:B:76:ASP:HA	1.99	0.43
1:B:80:LEU:HD23	1:B:84:ARG:C	2.43	0.43
1:A:138:HIS:HA	1:B:121:TYR:CE2	2.53	0.43
1:A:23:THR:HG21	1:A:227:PRO:HB2	2.01	0.42
1:B:129:LEU:O	1:B:129:LEU:HD22	2.19	0.42
1:B:43:LEU:O	1:B:47:LEU:HG	2.20	0.42
1:B:13:ILE:HG12	1:B:77:ILE:HD12	2.01	0.41
1:A:151:GLY:O	1:A:170:ARG:NH1	2.54	0.41
1:A:46:ALA:HA	1:A:49:GLN:HG2	2.02	0.40
1:B:84:ARG:HH22	1:B:103:MSE:CE	2.35	0.40
1:B:117:LEU:HD23	1:B:143:GLU:HB2	2.02	0.40
1:B:124:PRO:HB2	1:B:126:ASP:OD1	2.20	0.40
1:B:148:ALA:HB2	2:B:329:HOH:O	2.22	0.40
1:A:202:SER:CB	1:A:207:MSE:CE	3.00	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	28/276 (10%)	27 (96%)	1 (4%)	0	100	100
1	B	208/276 (75%)	192 (92%)	12 (6%)	4 (2%)	6	1
All	All	236/552 (43%)	219 (93%)	13 (6%)	4 (2%)	7	1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ARG
1	B	191	ASP
1	B	187	ALA
1	B	140	ARG

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	200/196 (102%)	198 (99%)	2 (1%)	68	60
1	B	200/196 (102%)	191 (96%)	9 (4%)	24	8
All	All	400/392 (102%)	389 (97%)	11 (3%)	38	21

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	272	GLN
1	B	9	GLN
1	B	129	LEU
1	B	133	LYS
1	B	145	ASP
1	B	152	GLU
1	B	180	LYS
1	B	183	TRP
1	B	185	VAL
1	B	272	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	B	155	GLN
1	B	272	GLN

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	252/276 (91%)	0.99	54 (21%) 2 2	6, 20, 60, 92	24 (9%)
1	B	224/276 (81%)	0.87	31 (13%) 6 7	9, 23, 45, 59	14 (6%)
All	All	476/552 (86%)	0.94	85 (17%) 3 4	6, 22, 56, 92	38 (7%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ALA	6.7
1	A	194	PHE	6.4
1	B	182	ALA	6.3
1	B	183	TRP	6.1
1	B	276	VAL	5.3
1	A	222	ASN	5.3
1	A	277	LEU	5.3
1	B	186	ILE	4.9
1	A	276	VAL	4.8
1	A	186	ILE	4.7
1	B	185	VAL	4.7
1	A	223	LEU	4.6
1	A	212	LEU	4.2
1	A	202	SER	4.2
1	A	188	SER	4.1
1	A	198	LEU	4.0
1	B	181	ALA	4.0
1	A	10	THR	3.9
1	A	200	ARG	3.9
1	A	197	GLU	3.9
1	A	226	LEU	3.8
1	B	178	LEU	3.8
1	A	201	ARG	3.8
1	A	205	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	3.8
1	B	179	SER	3.8
1	A	196	ARG	3.7
1	A	224	ALA	3.6
1	A	185	VAL	3.6
1	A	203	GLU	3.6
1	A	42	THR	3.6
1	A	209	GLY	3.5
1	A	183	TRP	3.5
1	A	210	ALA	3.3
1	A	273	LEU	3.3
1	A	275	GLU	3.3
1	A	195	GLN	3.3
1	A	187	ALA	3.3
1	A	211	LEU	3.3
1	A	181	ALA	3.2
1	B	269	THR	3.2
1	B	267	GLY	3.2
1	B	274	SER	3.2
1	A	150	ARG	3.2
1	B	148	ALA	3.2
1	B	173	SER	3.2
1	A	204	LYS	3.1
1	B	270	THR	3.1
1	B	275	GLU	3.1
1	A	213	GLY	3.1
1	B	273	LEU	3.0
1	B	175	GLU	3.0
1	A	39	ASP	3.0
1	A	272	GLN	2.9
1	A	232	THR	2.9
1	A	267	GLY	2.8
1	B	268	VAL	2.8
1	B	172	ALA	2.8
1	B	151	GLY	2.8
1	A	227	PRO	2.8
1	A	40	ALA	2.8
1	A	12	GLY	2.7
1	B	119	GLU	2.6
1	B	229	ALA	2.6
1	A	270	THR	2.6
1	B	230	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	269	THR	2.4
1	B	184	LYS	2.4
1	A	271	ARG	2.4
1	A	43	LEU	2.3
1	A	268	VAL	2.3
1	B	272	GLN	2.3
1	B	34	ALA	2.3
1	A	263	GLU	2.3
1	B	35	ALA	2.2
1	A	225	GLN	2.2
1	A	208	LEU	2.2
1	A	174	ALA	2.2
1	B	14	TYR	2.2
1	B	180	LYS	2.1
1	B	227	PRO	2.1
1	A	49	GLN	2.1
1	A	84	ARG	2.0
1	A	229	ALA	2.0
1	B	19	THR	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.