



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:57 AM UTC

PDB ID : 6NEO / pdb_00006neo
Title : Crystal structure of PprA filament from *Deinococcus radiodurans*
Authors : Szabla, R.; Junop, M.S.; Rok, M.
Deposited on : 2018-12-18
Resolution : 5.94 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

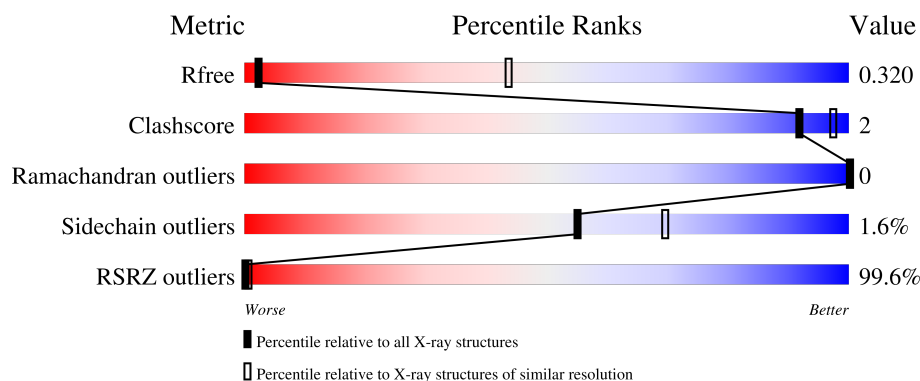
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.94 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	1137 (7.88-4.00)
Clashscore	190562	1203 (7.88-4.00)
Ramachandran outliers	187476	1028 (7.88-4.00)
Sidechain outliers	187428	1018 (7.88-3.98)
RSRZ outliers	180081	1130 (7.88-4.00)

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	B	278	92% 90% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1473 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 DNA repair protein PprA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	258	Total	C	N	O	0	0	0
			1473	870	287	316			

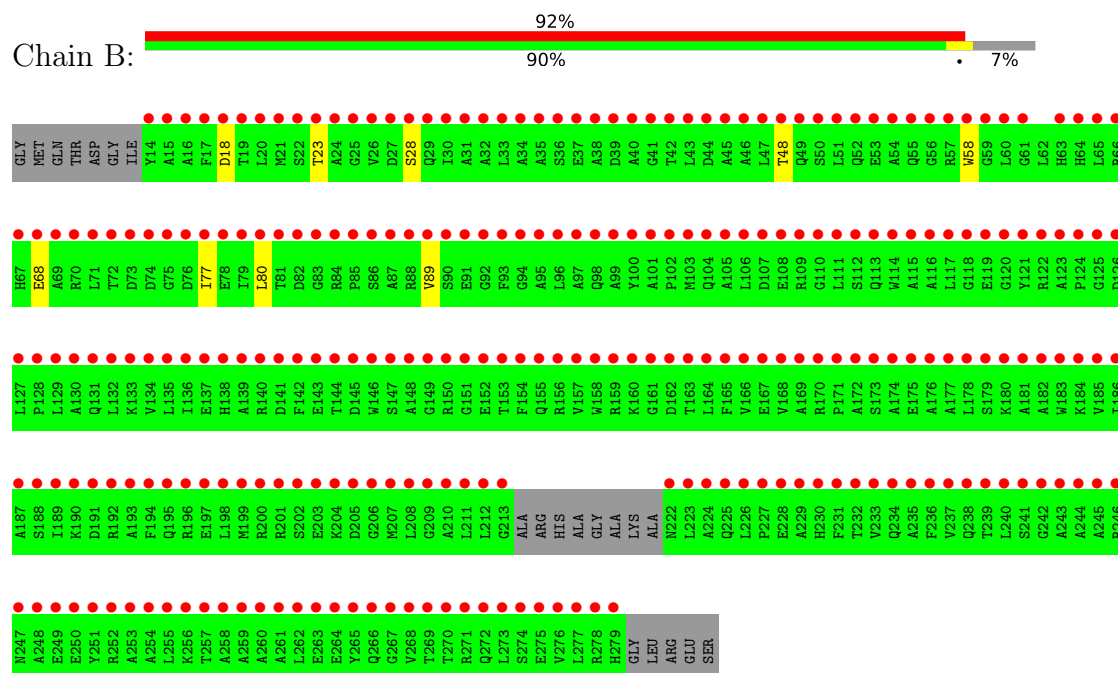
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	GLY	-	expression tag	UNP O32504
B	8	MET	-	expression tag	UNP O32504
B	180	LYS	ASP	engineered mutation	UNP O32504
B	184	LYS	ASP	engineered mutation	UNP O32504

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	148.98Å 148.98Å 79.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.03 – 5.94 50.03 – 5.94	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.03-5.94) 98.3 (50.03-5.94)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 6.15Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.287 , 0.309 0.288 , 0.320	Depositor DCC
R_{free} test set	74 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	247.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	1473	wwPDB-VP
Average B, all atoms (Å ²)	267.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	B	0.08	0/1489	0.25	0/2056

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	B	1473	0	988	4	0
All	All	1473	0	988	4	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 2.

All (4) 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:23:THR:HG23	1:B:58:TRP:HE1	1.56	0.70
1:B:48:THR:HG23	1:B:68:GLU:HA	1.95	0.48
1:B:18:ASP:OD1	1:B:28:SER:OG	2.32	0.47
1:B:77:ILE:O	1:B:89:VAL:N	2.48	0.43

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	B	254/278 (91%)	248 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	63/201 (31%)	62 (98%)	1 (2%)	55	69

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	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 [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	B	258/278 (92%)	16.26	257 (99%) 0 1	190, 263, 331, 351	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	GLU	90.3
1	B	267	GLY	79.4
1	B	120	GLY	60.7
1	B	239	THR	59.7
1	B	264	GLU	58.5
1	B	270	THR	55.5
1	B	268	VAL	48.8
1	B	119	GLU	47.5
1	B	222	ASN	46.9
1	B	271	ARG	44.9
1	B	22	SER	43.7
1	B	195	GLN	41.8
1	B	272	GLN	40.7
1	B	180	LYS	40.4
1	B	225	GLN	38.4
1	B	266	GLN	33.4
1	B	77	ILE	33.2
1	B	126	ASP	32.0
1	B	52	GLN	31.6
1	B	36	SER	31.0
1	B	241	SER	29.7
1	B	53	GLU	29.4
1	B	91	GLU	29.0
1	B	25	GLY	28.3
1	B	252	ARG	27.6
1	B	58	TRP	27.5
1	B	55	GLN	27.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	ARG	27.4
1	B	184	LYS	27.4
1	B	224	ALA	26.9
1	B	19	THR	26.5
1	B	237	VAL	26.3
1	B	30	ILE	25.9
1	B	145	ASP	25.8
1	B	82	ASP	25.6
1	B	112	SER	25.5
1	B	73	ASP	25.2
1	B	37	GLU	25.1
1	B	202	SER	25.0
1	B	56	GLY	25.0
1	B	147	SER	24.8
1	B	157	VAL	24.5
1	B	243	ALA	24.1
1	B	34	ALA	23.7
1	B	238	GLN	23.0
1	B	85	PRO	22.9
1	B	16	ALA	22.8
1	B	90	SER	22.3
1	B	190	LYS	22.3
1	B	226	LEU	22.1
1	B	230	HIS	22.0
1	B	155	GLN	22.0
1	B	183	TRP	21.8
1	B	86	SER	21.6
1	B	161	GLY	21.5
1	B	256	LYS	21.5
1	B	175	GLU	21.3
1	B	223	LEU	21.2
1	B	148	ALA	21.1
1	B	75	GLY	21.0
1	B	47	LEU	20.6
1	B	160	LYS	20.4
1	B	27	ASP	20.0
1	B	192	ARG	19.7
1	B	131	GLN	19.7
1	B	228	GLU	19.7
1	B	14	TYR	19.6
1	B	150	ARG	19.4
1	B	33	LEU	19.0

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Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	18.9
1	B	152	GLU	18.6
1	B	80	LEU	18.4
1	B	102	PRO	18.2
1	B	23	THR	18.0
1	B	188	SER	18.0
1	B	208	LEU	17.9
1	B	227	PRO	17.9
1	B	64	HIS	17.8
1	B	249	GLU	17.6
1	B	117	LEU	17.6
1	B	32	ALA	17.5
1	B	57	ARG	17.4
1	B	173	SER	17.4
1	B	205	ASP	17.2
1	B	206	GLY	17.1
1	B	151	GLY	17.1
1	B	121	TYR	17.1
1	B	277	LEU	17.1
1	B	83	GLY	17.1
1	B	43	LEU	17.1
1	B	109	ARG	16.9
1	B	189	ILE	16.9
1	B	154	PHE	16.8
1	B	207	MET	16.6
1	B	276	VAL	16.6
1	B	212	LEU	16.6
1	B	178	LEU	16.5
1	B	71	LEU	16.0
1	B	111	LEU	15.8
1	B	54	ALA	15.7
1	B	63	HIS	15.5
1	B	242	GLY	15.4
1	B	162	ASP	15.3
1	B	49	GLN	15.2
1	B	137	GLU	15.1
1	B	199	MET	15.0
1	B	144	THR	15.0
1	B	279	HIS	14.9
1	B	229	ALA	14.8
1	B	68	GLU	14.8
1	B	171	PRO	14.7

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Mol	Chain	Res	Type	RSRZ
1	B	66	ARG	14.5
1	B	209	GLY	14.4
1	B	163	THR	14.4
1	B	17	PHE	14.4
1	B	261	ALA	14.3
1	B	113	GLN	14.3
1	B	210	ALA	14.2
1	B	269	THR	14.2
1	B	116	ALA	14.2
1	B	129	LEU	14.0
1	B	15	ALA	14.0
1	B	44	ASP	13.8
1	B	186	ILE	13.6
1	B	203	GLU	13.6
1	B	92	GLY	13.6
1	B	38	ALA	13.6
1	B	84	ARG	13.4
1	B	141	ASP	13.3
1	B	247	ASN	13.3
1	B	28	SER	13.2
1	B	97	ALA	13.1
1	B	118	GLY	13.0
1	B	29	GLN	12.9
1	B	275	GLU	12.8
1	B	244	ALA	12.7
1	B	250	GLU	12.7
1	B	179	SER	12.7
1	B	51	LEU	12.6
1	B	273	LEU	12.6
1	B	98	GLN	12.5
1	B	197	GLU	12.2
1	B	231	PHE	12.2
1	B	198	LEU	12.2
1	B	174	ALA	12.1
1	B	146	TRP	12.0
1	B	149	GLY	11.9
1	B	191	ASP	11.9
1	B	245	ALA	11.9
1	B	40	ALA	11.7
1	B	255	LEU	11.7
1	B	94	GLY	11.7
1	B	79	ILE	11.6

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Mol	Chain	Res	Type	RSRZ
1	B	169	ALA	11.4
1	B	200	ARG	11.4
1	B	20	LEU	11.4
1	B	122	ARG	11.3
1	B	81	THR	11.3
1	B	99	ALA	11.3
1	B	46	ALA	11.2
1	B	153	THR	11.2
1	B	42	THR	11.1
1	B	240	LEU	10.9
1	B	31	ALA	10.8
1	B	201	ARG	10.8
1	B	265	TYR	10.8
1	B	70	ARG	10.8
1	B	24	ALA	10.7
1	B	158	TRP	10.6
1	B	95	ALA	10.6
1	B	204	LYS	10.5
1	B	61	GLY	10.4
1	B	134	VAL	10.3
1	B	138	HIS	10.3
1	B	125	GLY	10.1
1	B	101	ALA	10.1
1	B	89	VAL	10.0
1	B	170	ARG	9.8
1	B	128	PRO	9.8
1	B	232	THR	9.7
1	B	278	ARG	9.7
1	B	96	LEU	9.6
1	B	59	GLY	9.6
1	B	167	GLU	9.5
1	B	274	SER	9.5
1	B	76	ASP	9.4
1	B	107	ASP	9.4
1	B	253	ALA	9.4
1	B	123	ALA	9.2
1	B	182	ALA	9.2
1	B	39	ASP	9.1
1	B	100	TYR	9.0
1	B	35	ALA	8.9
1	B	74	ASP	8.8
1	B	166	VAL	8.8

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Mol	Chain	Res	Type	RSRZ
1	B	257	THR	8.6
1	B	110	GLY	8.4
1	B	260	ALA	8.3
1	B	78	GLU	8.2
1	B	172	ALA	8.2
1	B	176	ALA	8.2
1	B	259	ALA	8.1
1	B	159	ARG	8.1
1	B	130	ALA	8.1
1	B	236	PHE	8.1
1	B	26	VAL	8.0
1	B	181	ALA	8.0
1	B	196	ARG	8.0
1	B	88	ARG	8.0
1	B	124	PRO	7.9
1	B	69	ALA	7.9
1	B	235	ALA	7.7
1	B	114	TRP	7.6
1	B	18	ASP	7.5
1	B	127	LEU	7.5
1	B	168	VAL	7.5
1	B	106	LEU	7.4
1	B	177	ALA	7.4
1	B	194	PHE	7.3
1	B	140	ARG	7.3
1	B	67	HIS	6.9
1	B	60	LEU	6.9
1	B	136	ILE	6.6
1	B	142	PHE	6.6
1	B	164	LEU	6.6
1	B	41	GLY	6.5
1	B	132	LEU	6.5
1	B	213	GLY	6.5
1	B	105	ALA	6.4
1	B	187	ALA	6.4
1	B	185	VAL	6.4
1	B	87	ALA	6.3
1	B	65	LEU	6.2
1	B	72	THR	6.1
1	B	251	TYR	6.1
1	B	248	ALA	6.0
1	B	93	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLN	5.6
1	B	115	ALA	5.6
1	B	139	ALA	5.5
1	B	246	ARG	5.4
1	B	193	ALA	5.2
1	B	165	PHE	5.0
1	B	143	GLU	5.0
1	B	233	VAL	4.8
1	B	133	LYS	4.7
1	B	135	LEU	4.6
1	B	45	ALA	4.6
1	B	258	ALA	4.5
1	B	50	SER	4.4
1	B	21	MET	4.2
1	B	103	MET	4.1
1	B	48	THR	4.0
1	B	254	ALA	4.0
1	B	108	GLU	3.7
1	B	262	LEU	2.9
1	B	104	GLN	2.6

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.