



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:57 PM UTC

PDB ID : 4G26 / pdb_00004g26
Title : Crystal Structure of proteinaceous RNase P 1 (PRORP1) from *A. thaliana* with Ca
Authors : Koutmos, M.; Howard, M.J.; Fierke, C.A.
Deposited on : 2012-07-11
Resolution : 1.75 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

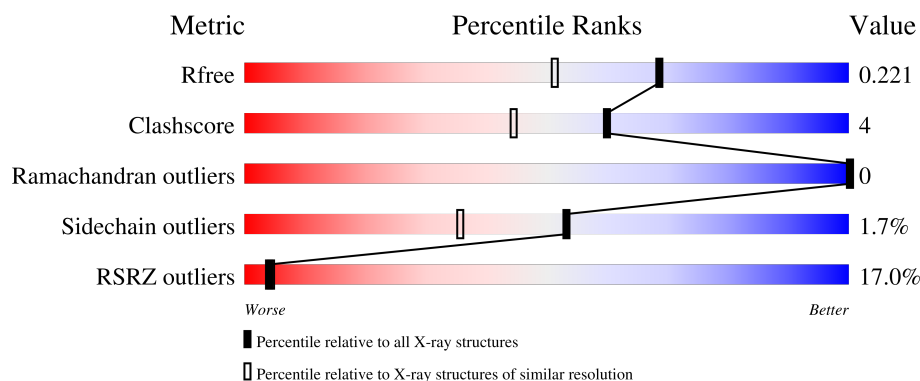
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	501	16% 85% 9% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4221 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 Pentatricopeptide repeat-containing protein At2g32230, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	5	7	0
			3831	2422	675	709	25			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLY	-	expression tag	UNP Q66GI4
A	73	ALA	-	expression tag	UNP Q66GI4
A	74	GLY	-	expression tag	UNP Q66GI4
A	75	HIS	-	expression tag	UNP Q66GI4
A	76	MET	-	expression tag	UNP Q66GI4

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

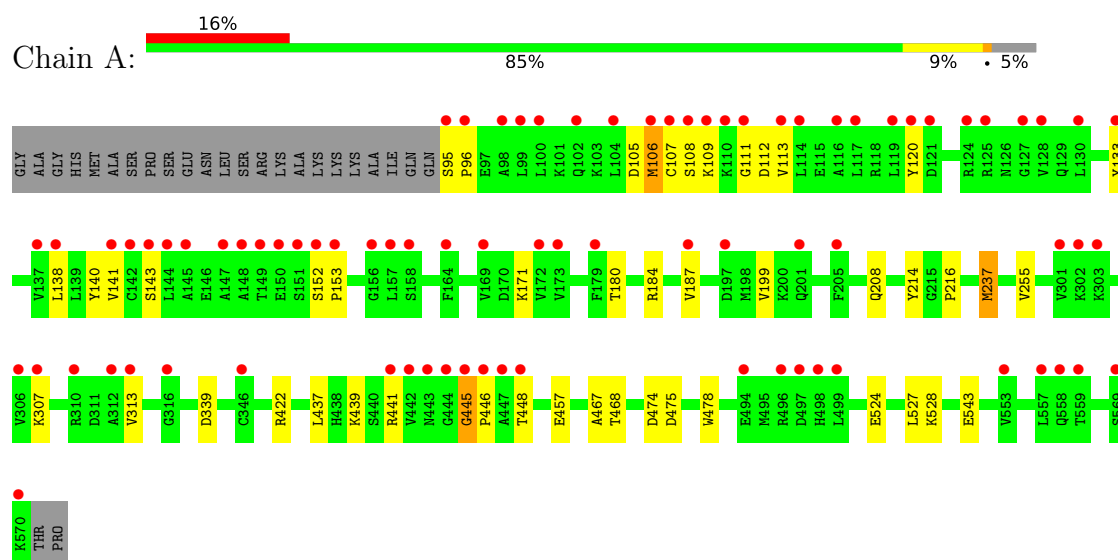
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	384	Total	O	0	0
			384	384		

- Molecule 1: Pentatricopeptide repeat-containing protein At2g32230, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.79Å 111.88Å 140.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.09 – 1.75 43.09 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.09-1.75) 98.1 (43.09-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.209 0.172 , 0.221	Depositor DCC
R_{free} test set	3319 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	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	0.96	EDS
Total number of atoms	4221	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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](#)

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

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	0.96	2/3936 (0.1%)	0.87	1/5317 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	MET	SD-CE	-6.78	1.62	1.79
1	A	445	GLY	CA-C	5.13	1.55	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LYS	N-CA-C	-5.37	105.98	112.54

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	3831	0	3808	33	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	384	0	0	3	0
All	All	4221	0	3808	33	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 (33) 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:441:ARG:O	1:A:446:PRO:HG2	1.62	0.98
1:A:422[A]:ARG:HD2	4:A:1298:HOH:O	1.63	0.97
1:A:106:MET:O	1:A:108:SER:HA	1.84	0.78
1:A:140:TYR:O	1:A:143:SER:HB2	1.92	0.69
1:A:107:CYS:HA	1:A:108:SER:HB3	1.82	0.60
1:A:152:SER:HB2	1:A:153:PRO:HD2	1.82	0.59
1:A:106:MET:C	1:A:108:SER:HA	2.28	0.57
1:A:106:MET:HA	1:A:106:MET:HE2	1.88	0.55
1:A:187:VAL:HG23	1:A:216:PRO:HG3	1.89	0.53
1:A:108:SER:HB2	1:A:111:GLY:H	1.74	0.53
1:A:105:ASP:OD1	1:A:133:TYR:OH	2.23	0.52
1:A:143:SER:HB3	1:A:184:ARG:NH1	2.25	0.52
1:A:95:SER:N	4:A:1438:HOH:O	2.44	0.50
1:A:437:LEU:O	1:A:467:ALA:HA	2.12	0.50
1:A:457:GLU:HG2	4:A:1268:HOH:O	2.11	0.49
1:A:527:LEU:HD23	1:A:528:LYS:N	2.29	0.48
1:A:468:THR:OG1	1:A:474[B]:ASP:OD1	2.20	0.47
1:A:422[B]:ARG:HD3	1:A:422[B]:ARG:HA	1.61	0.47
1:A:527:LEU:HD23	1:A:527:LEU:C	2.40	0.47
1:A:184:ARG:HH11	1:A:184:ARG:HB3	1.81	0.46
1:A:113:VAL:HG22	1:A:141:VAL:HG12	1.96	0.46
1:A:120:TYR:HB2	1:A:138:LEU:HD21	1.97	0.46
1:A:180:THR:O	1:A:184:ARG:HG3	2.16	0.45
1:A:445:GLY:O	1:A:448:THR:OG1	2.24	0.45
1:A:108:SER:OG	1:A:112:ASP:N	2.51	0.44
1:A:199:VAL:HG11	1:A:214:TYR:CE1	2.51	0.44
1:A:108:SER:CB	1:A:111:GLY:H	2.30	0.43
1:A:313:VAL:HG21	1:A:543:GLU:HG2	2.00	0.43
1:A:339:ASP:OD1	1:A:339:ASP:C	2.63	0.42
1:A:475:ASP:HA	1:A:478:TRP:CE2	2.56	0.41
1:A:95:SER:HA	1:A:96:PRO:HD3	1.86	0.41
1:A:120:TYR:CD1	1:A:138:LEU:HD21	2.56	0.41
1:A:237:MET:HE2	1:A:237:MET:HB3	1.89	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	481/501 (96%)	471 (98%)	10 (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	417/431 (97%)	409 (98%)	8 (2%)	50	31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	MET
1	A	171	LYS
1	A	208	GLN
1	A	255	VAL
1	A	307	LYS
1	A	439	LYS
1	A	524[A]	GLU
1	A	524[B]	GLU

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	129	GLN
1	A	417	ASN
1	A	516	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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	476/501 (95%)	0.67	81 (17%) 4 4	16, 40, 82, 101	7 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	6.4
1	A	128	VAL	6.1
1	A	569	SER	5.9
1	A	107	CYS	5.5
1	A	144	LEU	5.3
1	A	96	PRO	4.6
1	A	95	SER	4.5
1	A	497	ASP	4.4
1	A	445	GLY	4.4
1	A	108	SER	4.4
1	A	444	GLY	4.3
1	A	446	PRO	4.2
1	A	148	ALA	4.2
1	A	559	THR	4.2
1	A	570	LYS	4.2
1	A	141	VAL	4.2
1	A	447	ALA	4.0
1	A	498	HIS	3.9
1	A	442	VAL	3.9
1	A	145	ALA	3.9
1	A	499	LEU	3.7
1	A	149	THR	3.7
1	A	164	PHE	3.5
1	A	496	ARG	3.5
1	A	130	LEU	3.4
1	A	157	LEU	3.4
1	A	152	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	310	ARG	3.3
1	A	448	THR	3.3
1	A	137	VAL	3.2
1	A	173	VAL	3.1
1	A	153	PRO	3.1
1	A	133	TYR	3.1
1	A	117	LEU	3.1
1	A	113	VAL	3.0
1	A	151	SER	3.0
1	A	106	MET	3.0
1	A	494	GLU	2.9
1	A	119	LEU	2.9
1	A	125	ARG	2.9
1	A	313	VAL	2.8
1	A	124	ARG	2.8
1	A	99	LEU	2.8
1	A	116	ALA	2.8
1	A	553	VAL	2.8
1	A	307	LYS	2.8
1	A	156	GLY	2.8
1	A	303	LYS	2.7
1	A	169	VAL	2.7
1	A	346	CYS	2.7
1	A	143	SER	2.7
1	A	98	ALA	2.7
1	A	557	LEU	2.6
1	A	187	VAL	2.6
1	A	306	VAL	2.6
1	A	147	ALA	2.6
1	A	104	LEU	2.5
1	A	127	GLY	2.5
1	A	443	ASN	2.4
1	A	197	ASP	2.4
1	A	109	LYS	2.4
1	A	100	LEU	2.4
1	A	142	CYS	2.4
1	A	121	ASP	2.4
1	A	441	ARG	2.4
1	A	110	LYS	2.3
1	A	179	PHE	2.3
1	A	111	GLY	2.3
1	A	102	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	TYR	2.3
1	A	205	PHE	2.2
1	A	302	LYS	2.2
1	A	201	GLN	2.1
1	A	312	ALA	2.1
1	A	316	GLY	2.1
1	A	172	VAL	2.1
1	A	301	VAL	2.1
1	A	138	LEU	2.1
1	A	150	GLU	2.0
1	A	558	GLN	2.0
1	A	158	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](#)

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($\text{\AA}^2$)	Q<0.9
3	CA	A	1003	1/1	0.85	0.29	75,75,75,75	0
3	CA	A	1005	1/1	0.89	0.29	65,65,65,65	0
3	CA	A	1002	1/1	0.99	0.09	48,48,48,48	1
3	CA	A	1006	1/1	0.99	0.07	29,29,29,29	0
2	ZN	A	1001	1/1	1.00	0.01	38,38,38,38	0
3	CA	A	1004	1/1	1.00	0.09	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.