Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 05:50 AM EDT

PDB ID	:	6BV8
Title	:	Structure of proteinaceous RNase P 1 (PRORP1) from A. thaliana complexed with Mn after 3-hour soak with juglone
Authors	:	Karasik, A.; Wu, N.; Fierke, C.A.; Koutmos, M.
Deposited on	:	2017-12-12
Resolution	:	2.10 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:

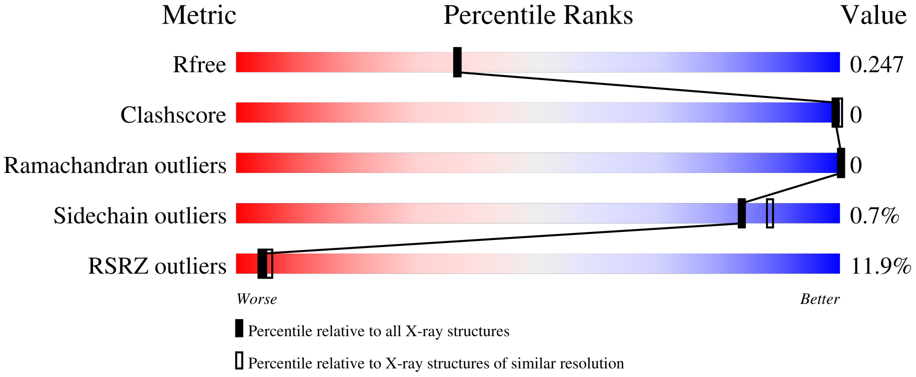
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

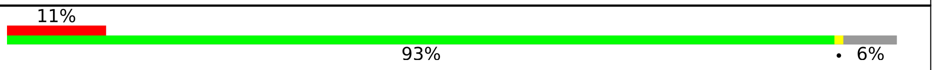
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7787 atoms, of which 3759 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.

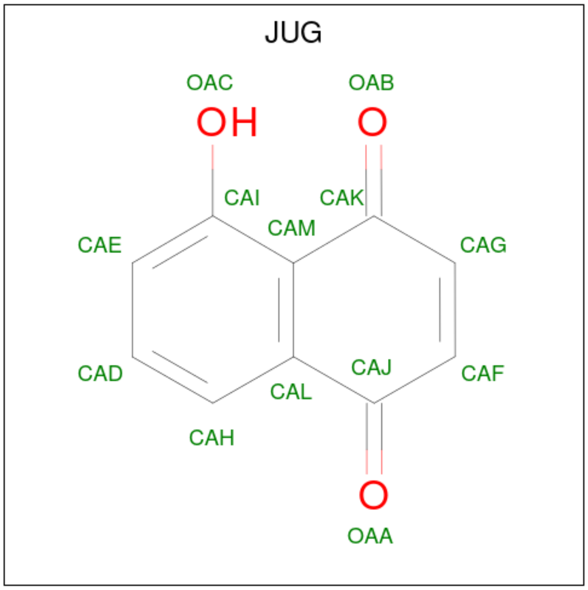
- Molecule 1 is a protein called Proteinaceous RNase P 1, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	472	7529	2388	3754	665	697	25	0	1	0

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 5-hydroxynaphthalene-1,4-dione (three-letter code: JUG) (formula: $C_{10}H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 18 10 5 3	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0

- Molecule 6 is water.

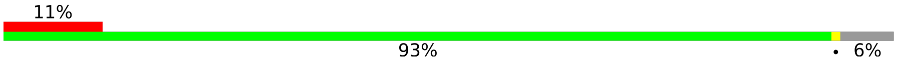
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	236	Total O 236 236	0	0

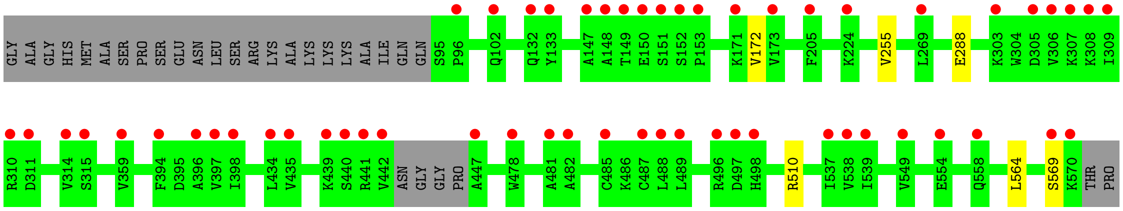
3 Residue-property plots

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: Proteinaceous RNase P 1, chloroplastic/mitochondrial

Chain A:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.68Å 111.33Å 139.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.99 – 2.10 27.04 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (86.99-2.10) 98.8 (27.04-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.200 , 0.236 0.210 , 0.247	Depositor DCC
R_{free} test set	1900 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7787	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: JUG, CL, ZN, MN

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	0.53	0/3860	0.69	1/5213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	510	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	3775	3754	3754	1	0
2	A	13	5	5	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	236	0	0	0	0
All	All	4028	3759	3759	1	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 0.

All (1) 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:288:GLU:HA	1:A:564:LEU:HD21	1.98	0.46

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	469/501 (94%)	459 (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	411/431 (95%)	408 (99%)	3 (1%)	84 88

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

Mol	Chain	Res	Type
1	A	172	VAL
1	A	255	VAL
1	A	569	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	JUG	A	601	1	14,14,14	2.44	4 (28%)	20,20,20	1.21	2 (10%)

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	JUG	A	601	1	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JUG	CAL-CAM	5.62	1.49	1.41
2	A	601	JUG	CAM-CAI	4.66	1.49	1.41
2	A	601	JUG	CAG-CAK	-2.98	1.39	1.46
2	A	601	JUG	CAF-CAJ	-2.86	1.40	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	JUG	CAM-CAL-CAJ	-2.57	117.02	120.11
2	A	601	JUG	CAE-CAI-CAM	-2.00	117.59	120.17

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 ⓘ

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	472/501 (94%)	0.47	56 (11%)	4	5	25, 53, 81, 100	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	SER	6.2
1	A	149	THR	4.9
1	A	397	VAL	4.6
1	A	496	ARG	4.5
1	A	173	VAL	4.4
1	A	307	LYS	4.1
1	A	441	ARG	4.1
1	A	498	HIS	4.0
1	A	442	VAL	3.8
1	A	303	LYS	3.8
1	A	148	ALA	3.7
1	A	554	GLU	3.6
1	A	314	VAL	3.6
1	A	308	LYS	3.5
1	A	434	LEU	3.5
1	A	440	SER	3.4
1	A	102	GLN	3.4
1	A	396	ALA	3.3
1	A	558	GLN	3.2
1	A	150	GLU	3.0
1	A	487	CYS	3.0
1	A	152	SER	3.0
1	A	153	PRO	2.8
1	A	539	ILE	2.8
1	A	310	ARG	2.7
1	A	549	VAL	2.7
1	A	489	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	538	VAL	2.6
1	A	394	PHE	2.6
1	A	315	SER	2.5
1	A	398	ILE	2.5
1	A	132	GLN	2.5
1	A	482	ALA	2.5
1	A	205	PHE	2.5
1	A	447	ALA	2.4
1	A	435	VAL	2.4
1	A	147	ALA	2.4
1	A	171	LYS	2.4
1	A	497	ASP	2.4
1	A	311	ASP	2.4
1	A	306	VAL	2.4
1	A	481	ALA	2.3
1	A	305	ASP	2.3
1	A	359	VAL	2.3
1	A	485	CYS	2.3
1	A	309	ILE	2.3
1	A	570	LYS	2.2
1	A	96	PRO	2.2
1	A	478	TRP	2.2
1	A	439	LYS	2.2
1	A	269	LEU	2.1
1	A	488	LEU	2.1
1	A	133	TYR	2.1
1	A	537	ILE	2.0
1	A	224	LYS	2.0
1	A	151	SER	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95^{th} 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(Å^2)**	**Q<0.9**
2	JUG	A	601	13/13	0.92	0.11	46,56,61,61	0
4	ZN	A	603	1/1	0.99	0.10	48,48,48,48	0
5	CL	A	604	1/1	0.99	0.17	33,33,33,33	0
5	CL	A	605	1/1	0.99	0.12	33,33,33,33	0
3	MN	A	602	1/1	1.00	0.08	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.