WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 09:44 pm GMT

PDB ID	:	1H71
Title	:	Psychrophilic Protease from Pseudoalteromonas 'TAC II 18'
Authors	:	Villeret, V.; Van Petegem, F.; Aghajari, N.; Chessa, J.-P.; Gerday, C.; Haser, R.; Van Beeumen, J.
Deposited on	:	2001-07-02
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

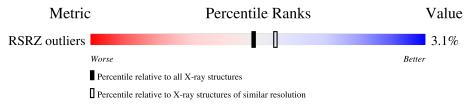|		
MolProbity	:	**FAILED**
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
RSRZ outliers		3.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
RSRZ outliers	127900	5083 (2.10-2.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3696 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 SERRALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	456	Total 3403	C 2131	N 569	O 701	S 2	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	22	ASP	GLU	conflict	UNP O69771
P	117	GLN	MET	conflict	UNP O69771

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	8	Total 8	Ca 8	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	284	Total 284	O 284	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.00Å 57.55Å 161.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.10) 96.7 (14.99-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.221 0.147 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.3	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3696	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	P	456/463 (98%)	-0.42	14 (3%)	49	55	20, 28, 47, 68	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	222	THR	7.6
1	P	127	GLY	6.3
1	P	443	GLN	4.3
1	P	224	GLU	3.7
1	P	68	VAL	3.6
1	P	111	ARG	3.1
1	P	189	ASN	3.1
1	P	3	GLY	3.0
1	P	128	GLY	2.8
1	P	126	ASN	2.7
1	P	419	HIS	2.3
1	P	384	LYS	2.2
1	P	223	GLY	2.1
1	P	225	GLY	2.1

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 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, 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(Å^2)	Q<0.9
2	CA	P	500	1/1	0.98	0.10	39,39,39,39	0
2	CA	P	506	1/1	0.99	0.08	24,24,24,24	0
2	CA	P	507	1/1	0.99	0.08	26,26,26,26	0
2	CA	P	503	1/1	1.00	0.11	24,24,24,24	0
2	CA	P	504	1/1	1.00	0.11	25,25,25,25	0
2	CA	P	505	1/1	1.00	0.08	25,25,25,25	0
2	CA	P	501	1/1	1.00	0.09	24,24,24,24	0
2	CA	P	502	1/1	1.00	0.15	23,23,23,23	0
3	ZN	P	600	1/1	1.00	0.06	28,28,28,28	0

5.5 Other polymers ⓘ

There are no such residues in this entry.