



wwPDB X-ray Structure Validation Summary Report i

Aug 26, 2023 – 07:50 am BST

PDB ID : 8ACK
Title : Structure of *Pseudomonas aeruginosa* aminopeptidase, PaAP
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Deposited on : 2022-07-05
Resolution : 1.78 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 i 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](#) ①) were used in the production of this report:

MolProbity	: FAILED
Mogul	: 1.8.4, CSD as541be (2020)
Xtriage (Phenix)	: 1.13
EDS	: 2.35
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

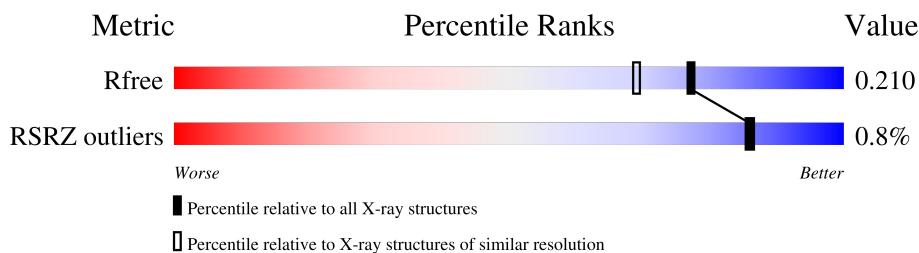
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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

2 Entry composition [\(i\)](#)

There are 6 unique types of molecules in this entry. The entry contains 8052 atoms, of which 12 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 Keratinase KP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	468	Total	C 3529	N 2224	O 593	S 702	10	0	0
1	A	468	Total	C 3529	N 2224	O 593	S 702	10	0	0

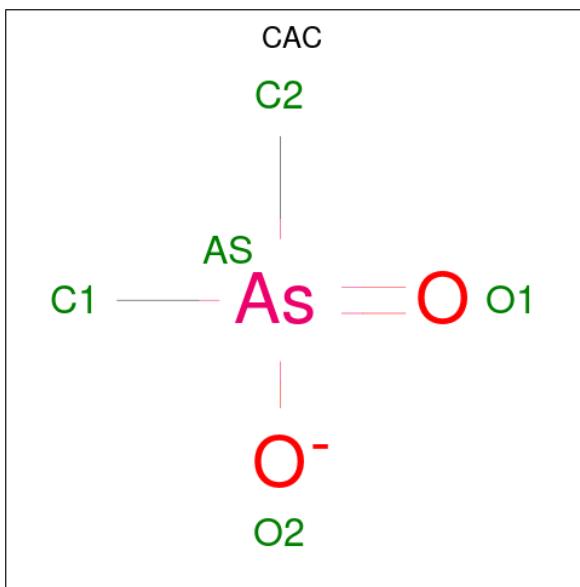
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	513	LEU	-	expression tag	UNP E3ULB5
B	514	VAL	-	expression tag	UNP E3ULB5
B	515	PRO	-	expression tag	UNP E3ULB5
B	516	ARG	-	expression tag	UNP E3ULB5
A	513	LEU	-	expression tag	UNP E3ULB5
A	514	VAL	-	expression tag	UNP E3ULB5
A	515	PRO	-	expression tag	UNP E3ULB5
A	516	ARG	-	expression tag	UNP E3ULB5

- Molecule 2 is a protein called PCP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total	C 83	N 55	O 16	12	0	0
2	C	9	Total	C 83	N 55	O 16	12	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total As C H O					0	0
			11	1	2	6	2		
3	A	1	Total As C H O					0	0
			11	1	2	6	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total Zn		0	0
			5	5		
4	A	5	Total Zn		0	0
			5	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total Na		0	0
			5	5		
5	A	2	Total Na		0	0
			2	2		
5	P	1	Total Na		0	0
			1	1		
5	C	1	Total Na		0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	415	Total O 415 415	0	0
6	A	356	Total O 356 356	0	0
6	P	8	Total O 8 8	0	0
6	C	8	Total O 8 8	0	0

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

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.29 Å 85.66 Å 98.10 Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	42.83 – 1.78 64.46 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.83-1.78) 98.7 (64.46-1.78)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.45 (at 1.78 Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R , R_{free}	0.171 , 0.210 0.173 , 0.210	Depositor DCC
R_{free} test set	4754 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

4.1 Standard geometry [\(i\)](#)

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

4.2 Too-close contacts [\(i\)](#)

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

4.3 Torsion angles [\(i\)](#)

4.3.1 Protein backbone [\(i\)](#)

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

4.3.2 Protein sidechains [\(i\)](#)

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

4.3.3 RNA [\(i\)](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

4.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [\(i\)](#)

Of 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 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
3	CAC	B	601	4	0,4,4	-	-	0,6,6	-	-
3	CAC	A	601	4	0,4,4	-	-	0,6,6	-	-

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 [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data [\(i\)](#)

5.1 Protein, DNA and RNA chains [\(i\)](#)

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	468/490 (95%)	0.03	5 (1%)	80	81	23, 35, 54, 91	0
1	B	468/490 (95%)	0.04	3 (0%)	89	89	22, 32, 49, 83	0
2	C	9/9 (100%)	0.34	0	100	100	31, 38, 53, 62	0
2	P	9/9 (100%)	0.18	0	100	100	28, 35, 47, 61	0
All	All	954/998 (95%)	0.04	8 (0%)	86	86	22, 34, 52, 91	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	TYR	3.7
1	A	121	TYR	3.3
1	B	301	PHE	3.3
1	B	511	GLN	3.1
1	A	301	PHE	3.0

5.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.4 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(Å ²)	Q<0.9
5	NA	C	101	1/1	0.87	0.14	42,42,42,42	0
5	NA	A	608	1/1	0.92	0.15	32,32,32,32	0
5	NA	B	607	1/1	0.92	0.25	28,28,28,28	0
4	ZN	A	606	1/1	0.93	0.04	94,94,94,94	0
5	NA	B	609	1/1	0.93	0.14	30,30,30,30	0
5	NA	B	611	1/1	0.96	0.23	27,27,27,27	0
5	NA	B	608	1/1	0.96	0.20	25,25,25,25	0
5	NA	B	610	1/1	0.96	0.10	35,35,35,35	0
3	CAC	B	601	5/5	0.97	0.14	35,71,85,85	0
5	NA	P	101	1/1	0.97	0.22	34,34,34,34	0
3	CAC	A	601	5/5	0.97	0.17	32,66,79,79	0
5	NA	A	607	1/1	0.98	0.23	25,25,25,25	0
4	ZN	B	606	1/1	0.98	0.07	44,44,44,44	0
4	ZN	A	604	1/1	0.99	0.12	31,31,31,31	0
4	ZN	A	605	1/1	0.99	0.07	39,39,39,39	0
4	ZN	B	603	1/1	0.99	0.10	29,29,29,29	0
4	ZN	B	604	1/1	0.99	0.09	37,37,37,37	0
4	ZN	B	602	1/1	0.99	0.13	31,31,31,31	0
4	ZN	A	602	1/1	0.99	0.10	33,33,33,33	0
4	ZN	B	605	1/1	1.00	0.08	31,31,31,31	0
4	ZN	A	603	1/1	1.00	0.10	30,30,30,30	0

5.5 Other polymers [\(i\)](#)

There are no such residues in this entry.