



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:20 am BST

PDB ID : 1LOK
Title : The 1.20 Angstrom Resolution Crystal Structure of the Aminopeptidase from *Aeromonas proteolytica* Complexed with Tris: A Tale of Buffer Inhibition
Authors : Desmarais, W.T.; Bienvenue, D.L.; Bzymek, K.P.; Holz, R.C.; Petsko, G.A.; Ringe, D.
Deposited on : 2002-05-06
Resolution : 1.20 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

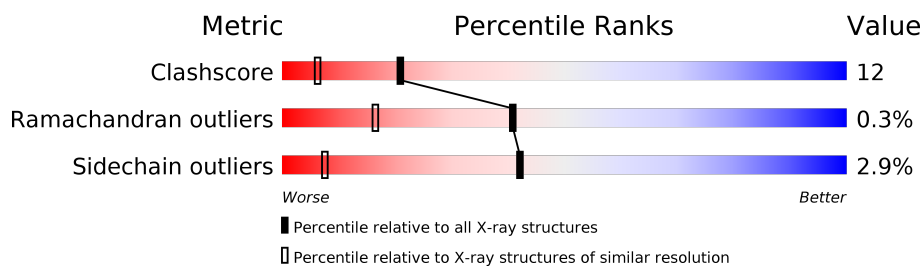
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	291	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2613 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 Bacterial leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	15	0
			2251	1397	372	470	12			

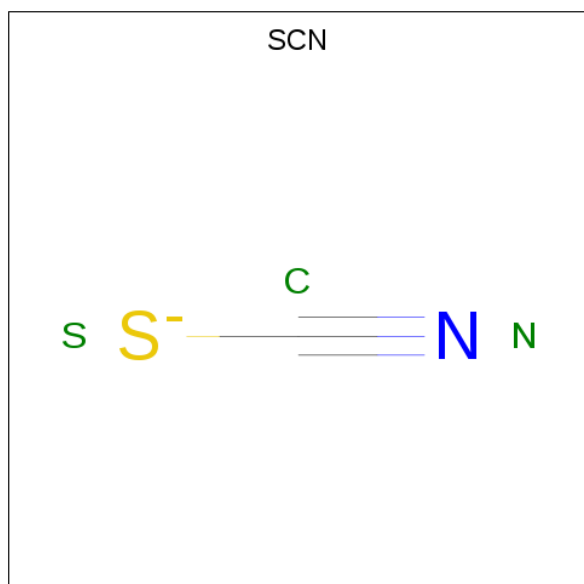
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

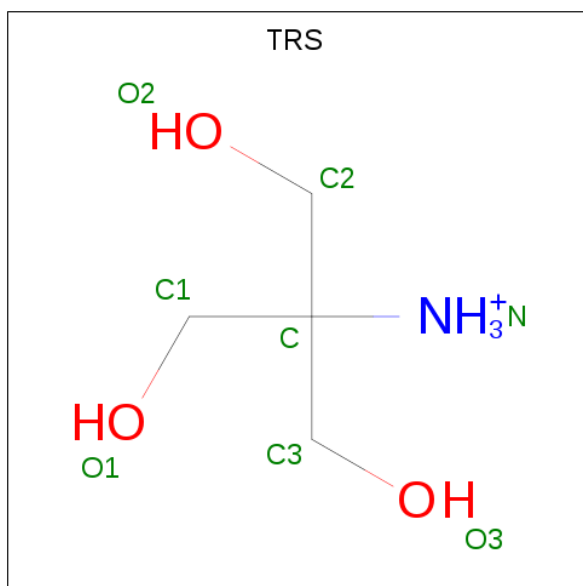
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

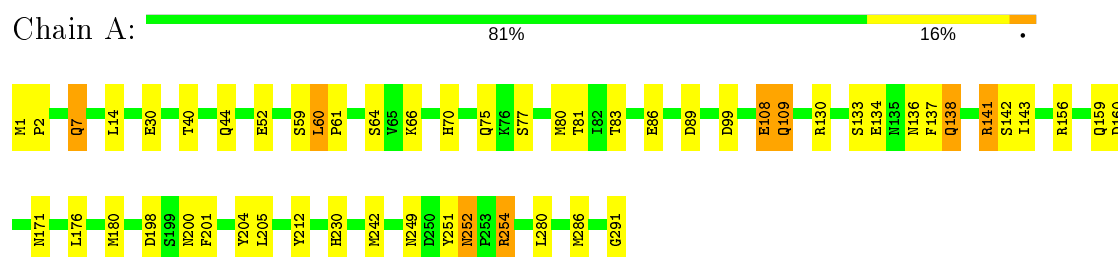
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	348	Total	O	0	0
			348	348		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Bacterial leucyl aminopeptidase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.34Å 108.34Å 93.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.08 – 1.20	Depositor
% Data completeness (in resolution range)	(Not available) (27.08-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.158 , 0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2613	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.84	1/2376 (0.0%)	1.20	18/3236 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	GLY	C-OXT	82.90	2.80	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	A	251	TYR	CB-CG-CD1	8.31	125.99	121.00
1	A	201	PHE	CB-CG-CD1	7.44	126.01	120.80
1	A	251	TYR	CG-CD1-CE1	6.88	126.81	121.30
1	A	242	MET	CA-CB-CG	-6.84	101.67	113.30
1	A	201	PHE	CB-CG-CD2	-6.81	116.03	120.80
1	A	212	TYR	CB-CG-CD2	6.36	124.81	121.00
1	A	89	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	254	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	254	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	30	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	A	130	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	108[A]	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	A	108[B]	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	A	59	SER	C-N-CA	5.47	135.38	121.70
1	A	198	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	156[A]	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	156[B]	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2251	0	2113	53	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	8	0	9	0	0
6	A	348	0	0	14	0
All	All	2613	0	2122	53	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 12.

All (53) 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:61:PRO:CG	1:A:138:GLN:HE22	1.18	1.52
1:A:61:PRO:CG	1:A:138:GLN:NE2	1.79	1.42
1:A:61:PRO:HG3	1:A:138:GLN:CD	1.58	1.24
1:A:61:PRO:HG3	1:A:138:GLN:NE2	1.46	1.15
1:A:61:PRO:HG2	1:A:138:GLN:HE22	0.91	1.03
1:A:7:GLN:H	1:A:7:GLN:HE21	1.12	0.95
1:A:61:PRO:CB	1:A:138:GLN:HE22	1.83	0.91
1:A:61:PRO:CG	1:A:138:GLN:CD	2.28	0.86
1:A:1[B]:MET:HG3	1:A:2:PRO:HD2	1.56	0.85
1:A:61:PRO:HG3	1:A:138:GLN:OE1	1.80	0.81
1:A:61:PRO:HG2	1:A:138:GLN:NE2	1.60	0.77
1:A:60:LEU:HD13	1:A:133:SER:HA	1.66	0.77
1:A:61:PRO:CG	1:A:138:GLN:OE1	2.33	0.76
1:A:61:PRO:CB	1:A:138:GLN:NE2	2.47	0.73
1:A:137:PHE:O	1:A:138:GLN:OE1	2.10	0.69
1:A:83:THR:HA	1:A:142[B]:SER:OG	1.93	0.69
1:A:252:ASN:HD22	1:A:254:ARG:H	1.46	0.64
1:A:1[B]:MET:HG2	1:A:204:TYR:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108[A]:GLU:HG2	6:A:1297:HOH:O	1.98	0.63
1:A:52[B]:GLU:HG2	6:A:1157:HOH:O	1.98	0.62
1:A:83:THR:HB	6:A:1337:HOH:O	2.02	0.60
1:A:70:HIS:HE1	1:A:77:SER:OG	1.88	0.56
1:A:7:GLN:HE21	1:A:7:GLN:N	1.95	0.56
1:A:44:GLN:HG3	6:A:1107:HOH:O	2.04	0.55
1:A:60:LEU:CD1	1:A:133:SER:HA	2.35	0.54
1:A:109:GLN:HG2	6:A:1285:HOH:O	2.07	0.52
1:A:137:PHE:HE2	1:A:143:ILE:HD12	1.75	0.52
1:A:64[B]:SER:OG	1:A:66[B]:LYS:HE2	2.10	0.51
1:A:66[B]:LYS:NZ	1:A:81:THR:HG23	2.25	0.51
1:A:75:GLN:HE22	1:A:99:ASP:HB3	1.76	0.51
1:A:14:LEU:HD12	1:A:280:LEU:HD23	1.93	0.49
1:A:252:ASN:ND2	1:A:254:ARG:H	2.08	0.49
1:A:40[A]:THR:HG23	1:A:108[A]:GLU:OE2	2.12	0.49
1:A:176[A]:LEU:HD13	1:A:205:LEU:HD11	1.96	0.47
1:A:137:PHE:C	1:A:138:GLN:OE1	2.52	0.47
1:A:200:ASN:ND2	6:A:1006:HOH:O	2.48	0.47
1:A:60:LEU:HD12	1:A:61:PRO:HD2	1.97	0.46
1:A:136:ASN:ND2	6:A:1159:HOH:O	2.49	0.45
1:A:159:GLN:NE2	6:A:1278:HOH:O	2.50	0.45
1:A:70:HIS:HD2	1:A:160:ASP:OD2	1.99	0.45
1:A:1[A]:MET:HE2	6:A:1346:HOH:O	2.17	0.43
1:A:61:PRO:HB2	1:A:138:GLN:NE2	2.33	0.43
1:A:7:GLN:NE2	6:A:1242:HOH:O	2.51	0.43
1:A:230:HIS:HE1	6:A:1241:HOH:O	2.01	0.42
1:A:230:HIS:H	1:A:230:HIS:CD2	2.39	0.41
1:A:60:LEU:HD23	1:A:80:MET:CE	2.49	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.84	0.41
1:A:141:ARG:HD2	1:A:286:MET:O	2.20	0.41
1:A:134:GLU:HA	1:A:134:GLU:OE2	2.20	0.41
1:A:249:ASN:ND2	6:A:1163:HOH:O	2.54	0.40
1:A:2:PRO:HD3	6:A:1137:HOH:O	2.20	0.40
1:A:66[B]:LYS:HD2	6:A:1308:HOH:O	2.20	0.40

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	A	303/291 (104%)	297 (98%)	5 (2%)	1 (0%)	41 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	MET

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	A	254/239 (106%)	247 (97%)	7 (3%)	43 8

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	60	LEU
1	A	86	GLU
1	A	109	GLN
1	A	138	GLN
1	A	171	ASN
1	A	252	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	70	HIS
1	A	75	GLN
1	A	136	ASN
1	A	159	GLN
1	A	200	ASN
1	A	203	GLN
1	A	230	HIS
1	A	235	ASN
1	A	249	ASN
1	A	252	ASN
1	A	259	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 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	$\# Z > 2$
4	SCN	A	1973	-	1,2,2	0.29	0	0,1,1	0.00	-
5	TRS	A	800	2	7,7,7	2.48	4 (57%)	9,9,9	1.55	2 (22%)

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
5	TRS	A	800	2	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	TRS	C2-C	3.77	1.64	1.53
5	A	800	TRS	C-N	-3.42	1.37	1.49
5	A	800	TRS	C1-C	3.03	1.62	1.53
5	A	800	TRS	C3-C	2.80	1.61	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	TRS	O2-C2-C	-3.19	100.88	111.00
5	A	800	TRS	C2-C-N	-2.48	100.58	107.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	TRS	C1-C-C2-O2
5	A	800	TRS	C3-C-C2-O2
5	A	800	TRS	N-C-C2-O2

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.