



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2023 – 05:34 PM EDT

PDB ID : 4PVB
Title : Crystal structure of Aminopeptidase N in complex with the phosphonic acid analogue of leucine (D-(S)-LeuP)
Authors : Nocek, B.; Vassiliou, S.; Berlicki, L.; Mulligan, R.; Mucha, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2014-03-16
Resolution : 2.10 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 ⓘ 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

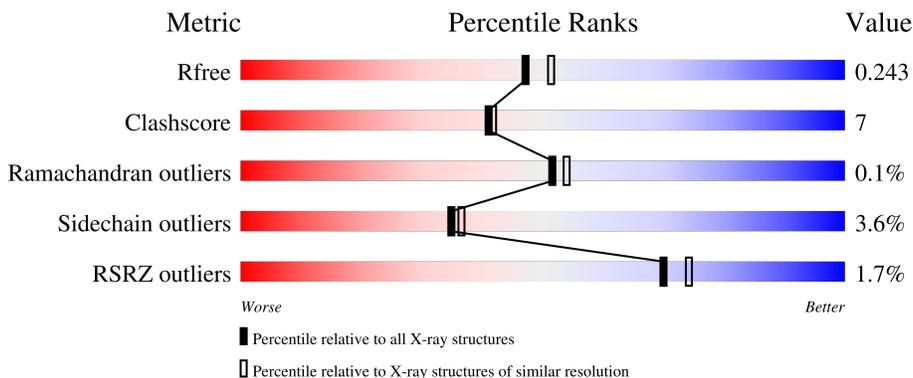
1 Overall quality at a glance

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)

2 Entry composition [i](#)

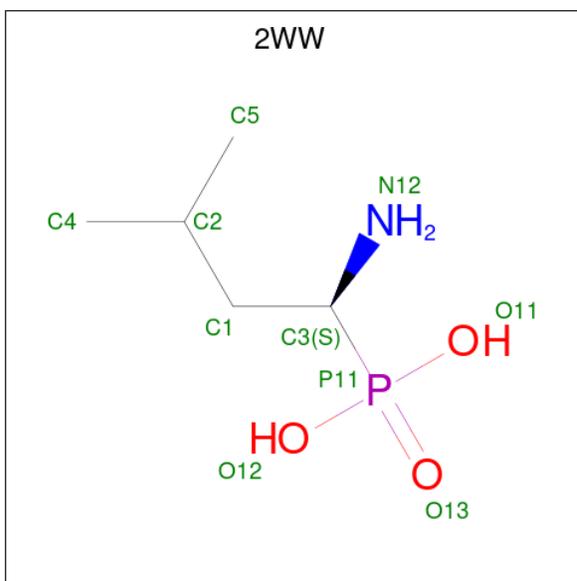
There are 6 unique types of molecules in this entry. The entry contains 7259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminopeptidase N.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	864	6864	4352	1186	1303	5	18	0	1	0

- Molecule 2 is [(1S)-1-amino-3-methylbutyl]phosphonic acid (three-letter code: 2WW) (formula: C₅H₁₄NO₃P).

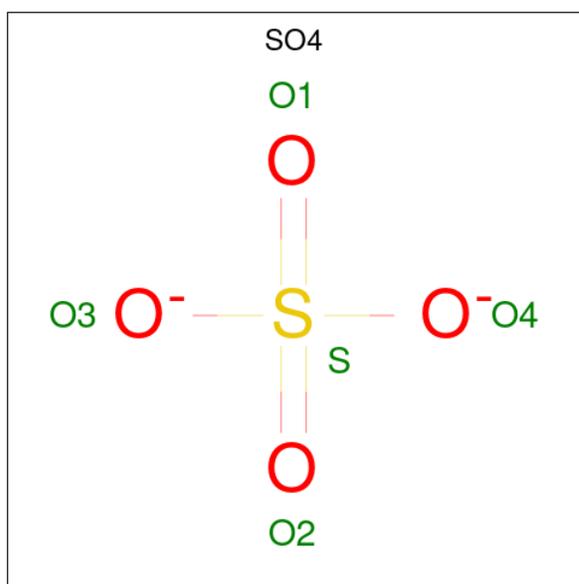


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	10	5	1	3	1	0	0

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

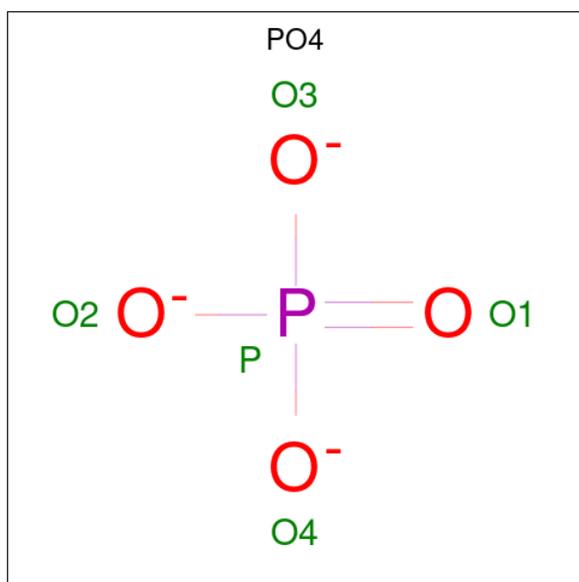
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	351	Total	O	0	3
			354	354		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	224.26Å 224.26Å 57.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.00 – 2.10 32.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (32.00-2.10) 85.9 (32.37-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.233 0.191 , 0.243	Depositor DCC
R_{free} test set	2753 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7259	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, 2WW, SO4

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	0.86	1/7001 (0.0%)	0.89	4/9463 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	GLU	CD-OE1	5.18	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	277	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	85	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	85	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	6864	0	6716	97	0
2	A	10	0	13	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	0	0	0
5	A	5	0	0	0	0
6	A	354	0	0	12	0
All	All	7259	0	6729	97	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 7.

The worst 5 of 97 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:453:ASN:HD21	1:A:520:THR:HG23	1.38	0.88
1:A:655:ASN:OD1	1:A:679:ARG:CD	2.28	0.82
1:A:508:THR:H	1:A:512:GLN:HE22	1.28	0.82
1:A:655:ASN:OD1	1:A:679:ARG:HD2	1.82	0.80
1:A:453:ASN:ND2	1:A:520:THR:HG23	1.98	0.77

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	863/867 (100%)	838 (97%)	24 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	830	CYS

4.3.2 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	730/715 (102%)	704 (96%)	26 (4%)	35 36

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	517	GLU
1	A	856	LYS
1	A	509	GLU
1	A	520	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	HIS
1	A	818	GLN
1	A	438	GLN
1	A	836	HIS
1	A	605	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	SO4	A	1005	-	4,4,4	0.31	0	6,6,6	0.51	0
4	SO4	A	1007	-	4,4,4	0.57	0	6,6,6	0.43	0
5	PO4	A	1008	-	4,4,4	0.70	0	6,6,6	1.12	0
4	SO4	A	1004	-	4,4,4	0.37	0	6,6,6	0.73	0
4	SO4	A	1003	-	4,4,4	0.22	0	6,6,6	0.75	0
2	2WW	A	1001	3	8,9,9	4.15	3 (37%)	8,13,13	2.69	3 (37%)
4	SO4	A	1006	-	4,4,4	0.47	0	6,6,6	0.38	0

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	2WW	A	1001	3	-	6/9/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	2WW	P11-C3	9.87	1.93	1.84
2	A	1001	2WW	P11-O11	-4.96	1.47	1.54
2	A	1001	2WW	P11-O12	-3.37	1.49	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	2WW	C1-C3-N12	5.07	122.15	110.17
2	A	1001	2WW	O12-P11-O11	3.85	118.00	107.64
2	A	1001	2WW	O12-P11-O13	3.22	121.54	113.45

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	2WW	C1-C3-P11-O11
2	A	1001	2WW	C1-C3-P11-O12
2	A	1001	2WW	C1-C3-P11-O13
2	A	1001	2WW	C2-C1-C3-N12
2	A	1001	2WW	C3-C1-C2-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	2WW	2	0

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	846/867 (97%)	-0.24	14 (1%) 70 74	18, 30, 56, 78	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	GLY	3.7
1	A	852	GLU	3.4
1	A	451	LYS	3.3
1	A	182	LEU	3.3
1	A	500	ALA	2.8

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
3	ZN	A	1002	1/1	0.93	0.05	34,34,34,34	1
4	SO4	A	1007	5/5	0.93	0.23	59,60,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	1006	5/5	0.94	0.21	61,65,73,74	0
4	SO4	A	1005	5/5	0.94	0.26	59,61,67,70	0
2	2WW	A	1001	10/10	0.96	0.14	27,30,34,39	0
4	SO4	A	1004	5/5	0.97	0.08	53,53,60,71	0
5	PO4	A	1008	5/5	0.97	0.06	40,47,55,58	0
4	SO4	A	1003	5/5	0.99	0.08	32,36,39,47	0

5.5 Other polymers [i](#)

There are no such residues in this entry.