



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2IUC  
Title : Structure of alkaline phosphatase from the Antarctic bacterium TAB5  
Authors : Wang, E.; Koutsioulis, D.; Leiros, H.K.S.; Andersen, O.A.; Bouriotis, V.;  
Hough, E.; Heikinheimo, P.  
Deposited on : 2006-06-01  
Resolution : 1.95 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : **NOT EXECUTED**  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : **NOT EXECUTED**  
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

PERCENTILES INFOmissingINFO

# 1 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5544 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 ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2536	1601	414	514	7	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	SER	LYS	conflict	UNP Q9KQY4
A	225	SER	LYS	conflict	UNP Q9KQY4
A	327	SER	GLU	conflict	UNP Q9KQY4
A	331	SER	THR	conflict	UNP Q9KQY4

- Molecule 2 is a protein called ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	342	2553	1611	415	520	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	58	SER	GLU	conflict	UNP Q9KQY4
B	122	SER	ASN	conflict	UNP Q9KQY4
B	176	SER	LYS	conflict	UNP Q9KQY4
B	178	SER	LYS	conflict	UNP Q9KQY4
B	180	SER	LYS	conflict	UNP Q9KQY4
B	290	SER	LYS	conflict	UNP Q9KQY4
B	313	SER	LYS	conflict	UNP Q9KQY4

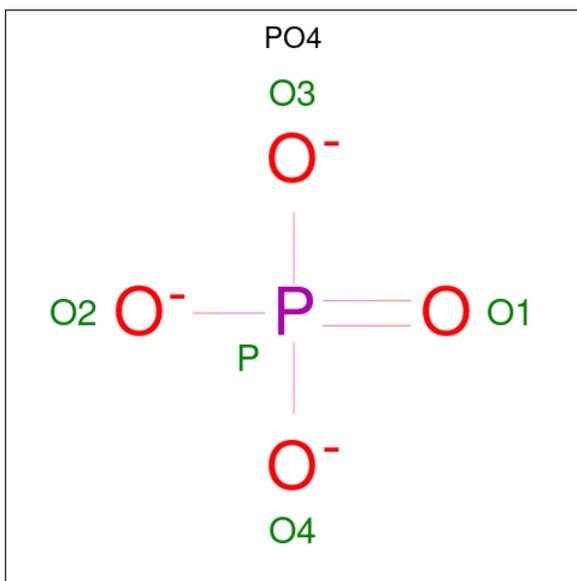
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

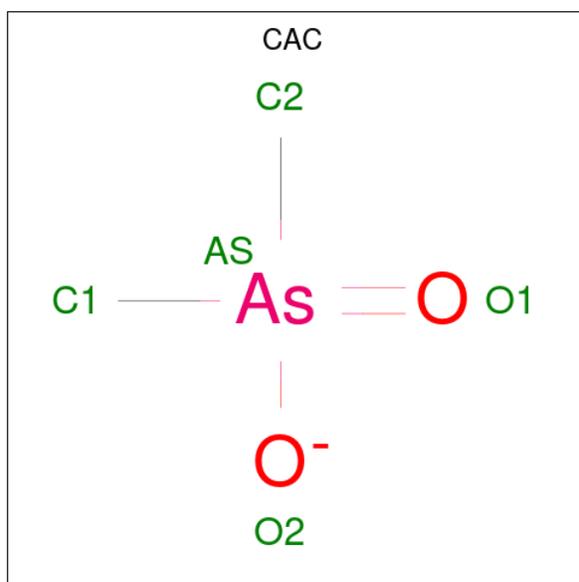
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
6	B	1	5	1	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	252	Total	O	0	0
			252	252		
7	B	186	Total	O	0	0
			186	186		

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.04Å 173.18Å 55.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.74 – 1.95 8.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.2 (8.74-1.95) 97.2 (8.72-1.95)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.162 , 0.225 0.164 , 0.226	Depositor DCC
$R_{free}$ test set	2433 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtrriage
Anisotropy	0.221	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

### 3 Model quality [i](#)

#### 3.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, MG, PO4

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	1.29	7/2583 (0.3%)	0.96	4/3499 (0.1%)
2	B	1.27	2/2600 (0.1%)	0.94	5/3523 (0.1%)
All	All	1.28	9/5183 (0.2%)	0.95	9/7022 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	CA-CB	-6.07	1.40	1.53
1	A	346	ALA	CA-CB	5.96	1.65	1.52
1	A	141	PHE	CE1-CZ	5.56	1.48	1.37
1	A	153	GLU	CG-CD	5.24	1.59	1.51
2	B	238	ALA	CA-CB	5.24	1.63	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	LEU	CB-CG-CD2	6.69	122.36	111.00
2	B	199	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	A	83	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	301	ASP	CB-CG-OD1	5.66	123.39	118.30
2	B	111	VAL	CG1-CB-CG2	-5.47	102.15	110.90

There are no chirality outliers.

There are no planarity outliers.

#### 3.2 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	2536	0	2434	23	0
2	B	2553	0	2453	37	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	2	0
5	B	1	0	0	1	0
6	B	5	0	0	0	0
7	A	252	0	0	6	0
7	B	186	0	0	6	0
All	All	5544	0	4887	59	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 6.

The worst 5 of 59 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:84:SER:OG	5:A:1006:PO4:P	2.08	1.11
2:B:84:SER:OG	5:B:1757:PO4:P	2.08	1.11
2:B:184:LEU:HB3	7:B:2096:HOH:O	1.59	1.00
1:A:198:GLY:HA3	7:A:2136:HOH:O	1.62	0.97
2:B:198:GLY:HA3	7:B:2102:HOH:O	1.65	0.96

There are no symmetry-related clashes.

### 3.3 Torsion angles [i](#)

#### 3.3.1 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	336/375 (90%)	322 (96%)	14 (4%)	0	100	100
2	B	338/375 (90%)	326 (96%)	11 (3%)	1 (0%)	41	30
All	All	674/750 (90%)	648 (96%)	25 (4%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	180	SER

### 3.3.2 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	268/307 (87%)	263 (98%)	5 (2%)	57	50
2	B	272/307 (89%)	266 (98%)	6 (2%)	52	44
All	All	540/614 (88%)	529 (98%)	11 (2%)	55	48

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	163	LEU
2	B	204	SER
2	B	304	THR
2	B	229	ASN
1	A	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	240	GLN
1	A	265	ASN
2	B	68	ASN
2	B	229	ASN

### 3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Mogul was not executed - this section is therefore empty.

### 3.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

### 3.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

### 3.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

### 3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 4 Fit of model and data [i](#)

### 4.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	340/375 (90%)	-0.27	2 (0%) 89 93	9, 15, 28, 51	1 (0%)
2	B	342/375 (91%)	-0.10	11 (3%) 47 57	10, 17, 34, 49	0
All	All	682/750 (90%)	-0.19	13 (1%) 66 74	9, 16, 32, 51	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	59	GLY	4.1
2	B	322	TYR	3.2
2	B	245	ASP	3.0
2	B	246	ASN	3.0
2	B	207	SER	2.7

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

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

### 4.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.4 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	PO4	B	1757	1/5	0.95	0.18	28,28,28,28	0
5	PO4	A	1006	1/5	0.96	0.15	24,24,24,24	0
4	MG	B	1010	1/1	0.97	0.09	29,29,29,29	0
6	CAC	B	1756	5/5	0.97	0.12	17,22,25,28	5
4	MG	A	1003	1/1	0.98	0.05	15,15,15,15	0
4	MG	B	1008	1/1	0.98	0.05	19,19,19,19	0
4	MG	A	1004	1/1	0.99	0.03	22,22,22,22	0
4	MG	B	1009	1/1	0.99	0.05	13,13,13,13	0
4	MG	A	1005	1/1	0.99	0.12	23,23,23,23	0
3	ZN	A	1002	1/1	1.00	0.03	18,18,18,18	0
3	ZN	B	1006	1/1	1.00	0.04	25,25,25,25	0
3	ZN	B	1007	1/1	1.00	0.04	18,18,18,18	0
3	ZN	A	1001	1/1	1.00	0.08	28,28,28,28	0

#### 4.5 Other polymers [i](#)

There are no such residues in this entry.