



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:12 am BST

PDB ID : 5TOO
Title : Crystal structure of alkaline phosphatase PafA T79S, N100A, K162A, R164A mutant
Authors : Lyubimov, A.Y.; Sunden, F.; AlSadhan, I.; Herschlag, D.
Deposited on : 2016-10-18
Resolution : 2.03 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

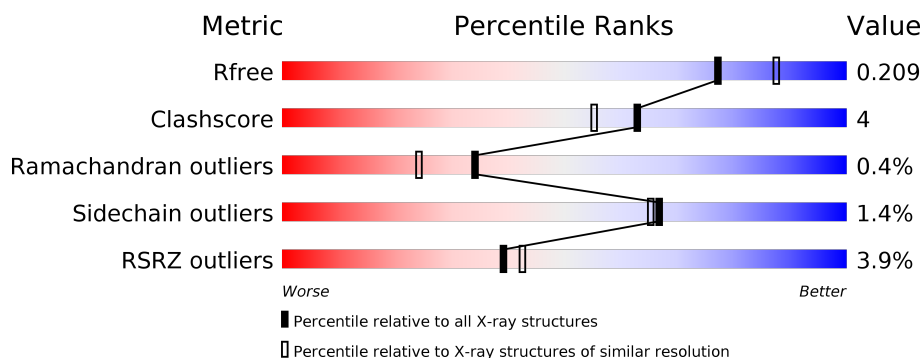
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div>4%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	605	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8108 atoms, of which 3869 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 PafA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	517	Total	C	H	N	O	S	0	0	0
			7887	2563	3869	663	779	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP Q9KJX5
A	13	ASP	-	expression tag	UNP Q9KJX5
A	14	ILE	-	expression tag	UNP Q9KJX5
A	15	GLY	-	expression tag	UNP Q9KJX5
A	16	ILE	-	expression tag	UNP Q9KJX5
A	17	ASP	-	expression tag	UNP Q9KJX5
A	18	SER	-	expression tag	UNP Q9KJX5
A	19	ASP	-	expression tag	UNP Q9KJX5
A	20	PRO	-	expression tag	UNP Q9KJX5
A	79	SER	THR	engineered mutation	UNP Q9KJX5
A	100	ALA	ASN	engineered mutation	UNP Q9KJX5
A	162	ALA	LYS	engineered mutation	UNP Q9KJX5
A	164	ALA	ARG	engineered mutation	UNP Q9KJX5
A	547	ILE	-	expression tag	UNP Q9KJX5
A	548	GLU	-	expression tag	UNP Q9KJX5
A	549	GLY	-	expression tag	UNP Q9KJX5
A	550	ARG	-	expression tag	UNP Q9KJX5
A	551	SER	-	expression tag	UNP Q9KJX5
A	552	ALA	-	expression tag	UNP Q9KJX5
A	553	TRP	-	expression tag	UNP Q9KJX5
A	554	SER	-	expression tag	UNP Q9KJX5
A	555	HIS	-	expression tag	UNP Q9KJX5
A	556	PRO	-	expression tag	UNP Q9KJX5
A	557	GLN	-	expression tag	UNP Q9KJX5
A	558	PHE	-	expression tag	UNP Q9KJX5
A	559	GLU	-	expression tag	UNP Q9KJX5
A	560	LYS	-	expression tag	UNP Q9KJX5

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Zn 4	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

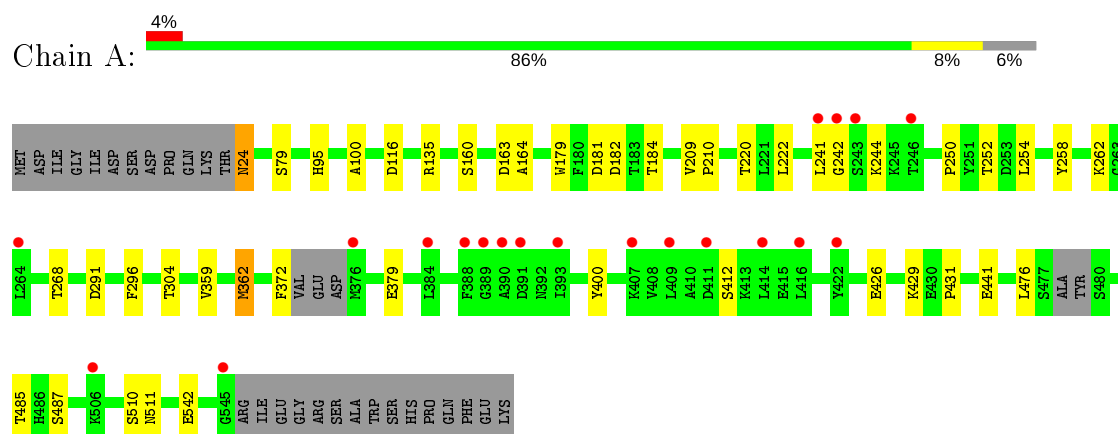
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total 216	O 216	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Alkaline phosphatase PafA



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	113.33Å 113.33Å 69.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.01 – 2.03 41.01 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.01-2.03) 96.9 (41.01-2.03)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.170 , 0.209 0.171 , 0.209	Depositor DCC
R_{free} test set	1494 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8108	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	1/4119 (0.0%)	0.71	0/5609

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	TYR	CD1-CE1	-7.63	1.27	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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	4018	3869	3868	34	0
2	A	4	0	0	0	0
3	A	1	0	0	3	0
4	A	216	0	0	15	1
All	All	4239	3869	3868	34	1

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 4.

All (34) 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:241:LEU:C	4:A:701:HOH:O	1.94	1.05
1:A:79:SER:OG	3:A:605:CL:CL	2.16	0.98
1:A:242:GLY:N	4:A:701:HOH:O	1.95	0.98
1:A:242:GLY:CA	4:A:701:HOH:O	2.14	0.94
1:A:242:GLY:C	4:A:701:HOH:O	2.05	0.93
1:A:241:LEU:O	4:A:701:HOH:O	1.85	0.91
1:A:362:MET:SD	4:A:815:HOH:O	2.32	0.86
1:A:400:TYR:OH	4:A:702:HOH:O	2.06	0.73
1:A:412:SER:O	4:A:704:HOH:O	2.09	0.70
1:A:24:ASN:N	1:A:24:ASN:HD22	1.90	0.69
1:A:79:SER:CB	3:A:605:CL:CL	2.80	0.65
1:A:441:GLU:OE2	4:A:706:HOH:O	2.14	0.65
1:A:511:ASN:OD1	4:A:707:HOH:O	2.16	0.61
1:A:242:GLY:O	4:A:701:HOH:O	2.11	0.61
1:A:116:ASP:OD2	1:A:135:ARG:NH2	2.33	0.55
1:A:379:GLU:CB	4:A:703:HOH:O	2.56	0.53
1:A:163:ASP:OD1	1:A:164:ALA:N	2.40	0.52
1:A:182:ASP:O	1:A:262:LYS:HB2	2.11	0.51
1:A:379:GLU:N	4:A:703:HOH:O	2.09	0.49
1:A:254:LEU:HD21	1:A:268:THR:HG21	1.95	0.48
1:A:244:LYS:NZ	1:A:250:PRO:O	2.35	0.48
1:A:291:ASP:O	4:A:708:HOH:O	2.20	0.47
1:A:220:THR:OG1	1:A:222:LEU:O	2.22	0.47
1:A:79:SER:HB2	1:A:100:ALA:HB2	1.97	0.46
1:A:476:LEU:HD22	1:A:485:THR:HG22	1.99	0.44
1:A:160:SER:O	1:A:179:TRP:HA	2.18	0.44
1:A:542:GLU:HG2	4:A:719:HOH:O	2.18	0.42
1:A:426:GLU:O	1:A:429:LYS:HG2	2.20	0.42
1:A:372:PHE:C	1:A:372:PHE:CD2	2.93	0.42
1:A:79:SER:HB3	3:A:605:CL:CL	2.56	0.42
1:A:181:ASP:OD1	1:A:184:THR:HG23	2.21	0.41
1:A:359:VAL:HG23	1:A:476:LEU:HD12	2.02	0.41
1:A:209:VAL:N	1:A:210:PRO:CD	2.84	0.41
1:A:510:SER:HB2	1:A:542:GLU:OE2	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:783:HOH:O	4:A:869:HOH:O 8_474	1.73	0.47

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	511/549 (93%)	487 (95%)	22 (4%)	2 (0%)	34 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	SER
1	A	431	PRO

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	436/472 (92%)	430 (99%)	6 (1%)	67 65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	95	HIS
1	A	252	THR
1	A	296	PHE
1	A	304	THR
1	A	362	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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.

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 [i](#)

6.1 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	517/549 (94%)	0.13	20 (3%)	39 42	19, 34, 65, 80	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	PHE	6.5
1	A	241	LEU	5.2
1	A	407	LYS	3.6
1	A	242	GLY	3.5
1	A	390	ALA	3.4
1	A	389	GLY	3.4
1	A	409	LEU	3.4
1	A	545	GLY	3.2
1	A	243	SER	3.2
1	A	246	THR	3.2
1	A	384	LEU	3.1
1	A	376	MET	3.1
1	A	391	ASP	2.8
1	A	264	LEU	2.6
1	A	414	LEU	2.3
1	A	416	LEU	2.3
1	A	422	TYR	2.3
1	A	411	ASP	2.2
1	A	393	ILE	2.1
1	A	506	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 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(\AA^2)	Q<0.9
2	ZN	A	604	1/1	0.95	0.17	67,67,67,67	0
3	CL	A	605	1/1	0.96	0.24	38,38,38,38	0
2	ZN	A	603	1/1	0.97	0.10	69,69,69,69	0
2	ZN	A	602	1/1	0.99	0.09	35,35,35,35	0
2	ZN	A	601	1/1	0.99	0.08	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.