



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 10:12 PM EDT

PDB ID : 2J82  
Title : Structural analysis of the PP2C Family Phosphatase tPphA from *Thermosynechococcus elongatus*  
Authors : Schlicker, C.; Kloft, N.; Forchhammer, K.; Becker, S.  
Deposited on : unknown  
Resolution : 1.28 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

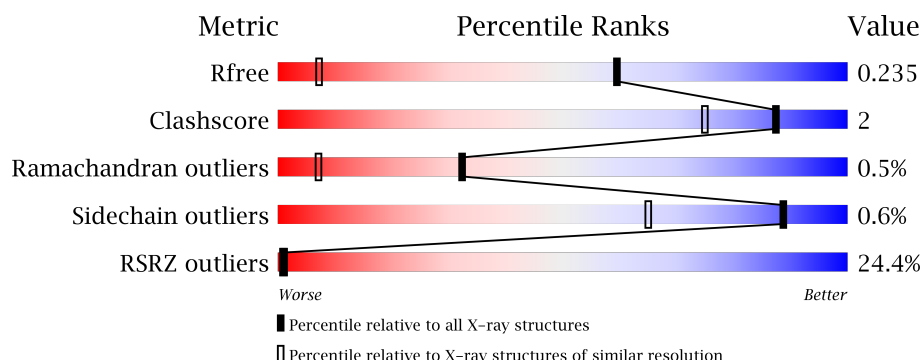
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.28 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))
$R_{free}$	100719	1367 (1.30-1.26)
Clashscore	112137	1447 (1.30-1.26)
Ramachandran outliers	110173	1392 (1.30-1.26)
Sidechain outliers	110143	1391 (1.30-1.26)
RSRZ outliers	101464	1370 (1.30-1.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	240	<div> <div>23%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1822 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 PROTEIN SERINE-THREONINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	36	0
			1682	1041	302	331	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	1
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	1
			2	2		

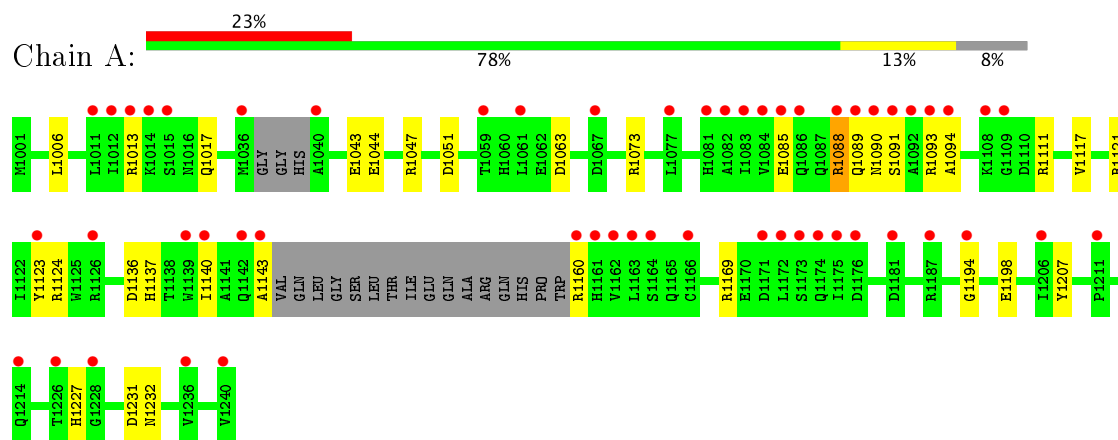
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		

### 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 ( $\text{RSRZ} > 2$ ). 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: PROTEIN SERINE-THREONINE PHOSPHATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.22Å 151.80Å 82.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.81 – 1.28 41.25 – 1.28	Depositor EDS
% Data completeness (in resolution range)	99.2 (75.81-1.28) 96.8 (41.25-1.28)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.28Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.165 , 0.204 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	2983 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1822	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% 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.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.66	0/1730	1.45	31/2341 (1.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1169	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	1063	ASP	CB-CG-OD1	-8.34	110.80	118.30
1	A	1169	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	1013[A]	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	1090	ASN	C-N-CA	7.93	141.53	121.70
1	A	1093[A]	ARG	C-N-CA	7.82	141.25	121.70
1	A	1091	SER	O-C-N	-7.76	110.28	122.70
1	A	1169	ARG	CD-NE-CZ	7.01	133.42	123.60
1	A	1124	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	1088	ARG	C-N-CA	6.49	137.93	121.70
1	A	1047	ARG	CD-NE-CZ	6.47	132.65	123.60
1	A	1088	ARG	O-C-N	-6.30	112.62	122.70
1	A	1231	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	1044	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	A	1006	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	1089	GLN	C-N-CA	5.92	136.51	121.70
1	A	1207	TYR	CG-CD1-CE1	5.86	125.99	121.30
1	A	1091	SER	C-N-CA	-5.72	107.41	121.70
1	A	1073	ARG	CD-NE-CZ	5.70	131.59	123.60
1	A	1117	VAL	C-N-CA	5.68	134.23	122.30
1	A	1160	ARG	C-N-CA	5.63	135.79	121.70
1	A	1063	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	1121	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	1051	ASP	CB-CG-OD1	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1123[A]	TYR	CA-CB-CG	5.26	123.40	113.40
1	A	1207	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
1	A	1136	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	1117	VAL	O-C-N	-5.07	114.58	123.20
1	A	1137	HIS	CG-ND1-CE1	5.06	115.29	108.20
1	A	1207	TYR	CZ-CE2-CD2	5.03	124.33	119.80
1	A	1111	ARG	NE-CZ-NH2	-5.01	117.80	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	1682	0	1562	8	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	136	0	0	2	0
All	All	1822	0	1562	8	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 2.

All (8) 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:1085[A]:GLU:O	1:A:1088:ARG:O	2.30	0.49
1:A:1194[A]:GLY:HA3	1:A:1232:ASN:O	2.15	0.46
1:A:1140:ILE:O	1:A:1143:ALA:N	2.49	0.45
1:A:1140:ILE:HG12	4:A:2090:HOH:O	2.16	0.45
1:A:1198:GLU:OE1	1:A:1227[B]:HIS:HD2	1.99	0.45
1:A:1198:GLU:O	1:A:1227[B]:HIS:CD2	2.73	0.42
1:A:1227[B]:HIS:CD2	4:A:2109:HOH:O	2.73	0.40
1:A:1017:GLN:H	1:A:1232:ASN:ND2	2.19	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	221/240 (92%)	213 (96%)	7 (3%)	1 (0%)	32 7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1094[A]	ALA

### 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	175/200 (88%)	174 (99%)	1 (1%)	89 65

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1043	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1080	ASN

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Mol	Chain	Res	Type
1	A	1174	GLN
1	A	1232	ASN

### 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 4 ligands modelled in this entry, 4 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	221/240 (92%)	1.79	54 (24%) <b>1</b> <b>1</b>	17, 24, 52, 63	44 (19%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1161	HIS	12.7
1	A	1061[A]	LEU	12.2
1	A	1236[A]	VAL	11.6
1	A	1206[A]	ILE	11.4
1	A	1123[A]	TYR	10.7
1	A	1084[A]	VAL	10.1
1	A	1083[A]	ILE	9.4
1	A	1077[B]	LEU	9.4
1	A	1011[A]	LEU	9.0
1	A	1059[A]	THR	9.0
1	A	1160	ARG	7.9
1	A	1012[A]	ILE	7.7
1	A	1091	SER	7.7
1	A	1082[A]	ALA	7.4
1	A	1143	ALA	7.4
1	A	1162	VAL	7.2
1	A	1140	ILE	7.0
1	A	1089	GLN	6.8
1	A	1187[A]	ARG	6.8
1	A	1139[A]	TRP	6.3
1	A	1094[A]	ALA	6.2
1	A	1228[A]	GLY	6.2
1	A	1015[A]	SER	6.2
1	A	1092[A]	ALA	5.9
1	A	1214[A]	GLN	5.8
1	A	1174	GLN	5.8
1	A	1013[A]	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	1181[A]	ASP	5.3
1	A	1109[A]	GLY	5.3
1	A	1067[A]	ASP	5.1
1	A	1194[A]	GLY	4.9
1	A	1126[A]	ARG	4.8
1	A	1086[A]	GLN	4.5
1	A	1036	MET	4.2
1	A	1090	ASN	4.0
1	A	1088	ARG	3.9
1	A	1014[A]	LYS	3.8
1	A	1085[A]	GLU	3.8
1	A	1093[A]	ARG	3.8
1	A	1173	SER	3.7
1	A	1176[A]	ASP	3.7
1	A	1164[A]	SER	3.6
1	A	1040	ALA	3.4
1	A	1172	LEU	3.3
1	A	1211	PRO	3.2
1	A	1142	GLN	3.0
1	A	1240	VAL	2.6
1	A	1226	THR	2.5
1	A	1175	ILE	2.5
1	A	1081[A]	HIS	2.5
1	A	1163	LEU	2.4
1	A	1171	ASP	2.2
1	A	1108	LYS	2.1
1	A	1166[A]	CYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	2243[B]	1/1	1.00	0.06	-1.01	21,21,21,21	1
3	MG	A	2242[A]	1/1	1.00	0.06	-1.01	21,21,21,21	1
2	CA	A	2241	1/1	1.00	0.06	-1.25	22,22,22,22	0
3	MG	A	2244	1/1	0.98	0.07	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.