

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 16, 2023 – 07:22 PM EST

PDB ID : 8TN2

Title: Structure of S. hygroscopicus aminotransferase MppQ complexed with pyrido

xal-5'-phosphate (PLP)

Authors : Silvaggi, N.R.; Vuksanovic, N.

Deposited on : 2023-08-01

Resolution : 1.75 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

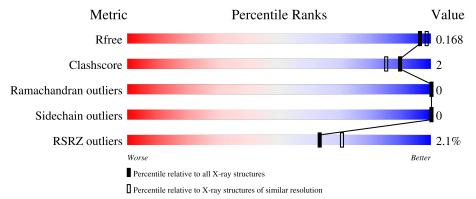
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.75 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 of 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 <=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	415	89%	•	6%
1	В	415	90%	•	7%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12791 atoms, of which 5970 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 PLP-dependent aminotransferase MppQ.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	1 A 389	Total	С	Н	N	О	Р	S	0	15	0
1 A	369	6005	1880	2999	556	561	1	8	0	15	U
1	D 206	Total	С	Н	N	О	Р	S	0	10	0
	386	5940	1859	2971	554	548	1	7		10	U

• Molecule 2 is water.

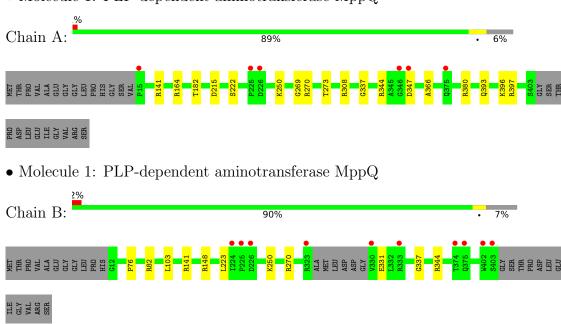
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	441	Total O 441 441	0	0
2	В	405	Total O 405 405	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PLP-dependent aminotransferase MppQ





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	47.73Å 114.50Å 133.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 - 1.75	Depositor
rtesolution (A)	41.43 - 1.75	EDS
% Data completeness	97.4 (35.10-1.75)	Depositor
(in resolution range)	98.0 (41.43-1.75)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.29 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D.D.	0.144 , 0.170	Depositor
$R, R_{free}$	0.140 , 0.168	DCC
$R_{free}$ test set	3587 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.42, 51.6	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12791	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: LLP

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.39	0/3094	0.65	0/4207	
1	В	0.36	0/3042	0.64	0/4136	
All	All	0.38	0/6136	0.64	0/8343	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	148	ARG	Sidechain

## 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	3006	2999	2947	13	0
1	В	2969	2971	2936	8	0
2	A	441	0	0	6	1
2	В	405	0	0	5	1
All	All	6821	5970	5883	21	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 2.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:344:ARG:NH1	2:A:502:HOH:O	2.25	0.56
1:A:164:ARG:NH2	2:A:505:HOH:O	2.40	0.54
1:A:347:ASP:HB2	2:A:661:HOH:O	2.10	0.51
1:A:270:ARG:NH2	2:A:508:HOH:O	2.41	0.46
1:B:141:ARG:NH2	2:B:509:HOH:O	2.47	0.46

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		$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \mathring{A}}) \end{array}$	Clash overlap (Å)	
2:A:776:HOH:O	2:B:788:HOH:O[2_554]	2.17	0.03	

### 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		Allowed	Outliers	Perce	ntiles	
1	A	401/415 (97%)	389 (97%)	12 (3%)	0	100	100
1	В	391/415 (94%)	382 (98%)	9 (2%)	0	100	100
All	All	792/830 (95%)	771 (97%)	21 (3%)	0	100	100



There are no Ramachandran outliers to report.

#### 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	303/310 (98%)	303 (100%)	0	100	100	
1	В	298/310~(96%)	298 (100%)	0	100	100	
All	All	601/620 (97%)	601 (100%)	0	100	100	

There are no protein residues with a non-rotameric sidechain to report.

Sometimes 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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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		nain Res	les Link Bond lengths		$ ag{ths}$	В	ond ang	les	
	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	A	250	1	23,24,25	2.73	7 (30%)	25,32,34	1.27	2 (8%)
1	LLP	В	250	1	23,24,25	2.76	7 (30%)	25,32,34	1.38	3 (12%)

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.

$\mathbf{Mol}$	$\mathbf{Type}$	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
1	LLP	A	250	1	-	7/16/17/19	0/1/1/1
1	LLP	В	250	1	-	6/16/17/19	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
1	В	250	LLP	C4-C4'	8.62	1.63	1.46
1	A	250	LLP	C4-C4'	8.28	1.62	1.46
1	В	250	LLP	C4-C5	-5.29	1.35	1.42
1	A	250	LLP	C4-C5	-5.27	1.35	1.42
1	A	250	LLP	C4'-NZ	5.17	1.44	1.27

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	В	250	LLP	C4-C4'-NZ	-3.97	106.09	124.31
1	A	250	LLP	C4-C4'-NZ	-3.51	108.18	124.31
1	В	250	LLP	C5-C6-N1	-3.08	118.69	123.82
1	A	250	LLP	C5-C6-N1	-2.41	119.81	123.82
1	В	250	LLP	C3-C4-C5	2.15	119.91	118.26

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	250	LLP	C4-C4'-NZ-CE
1	A	250	LLP	C5'-OP4-P-OP2
1	A	250	LLP	C5'-OP4-P-OP3
1	В	250	LLP	C3-C4-C4'-NZ
1	В	250	LLP	C5'-OP4-P-OP2

There are no ring outliers.

No monomer is involved in short contacts.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	388/415 (93%)	-0.24	6 (1%) 73 80	7, 12, 32, 62	0
1	В	385/415~(92%)	-0.05	10 (2%) 56 62	7, 13, 34, 54	0
All	All	773/830 (93%)	-0.14	16 (2%) 63 71	7, 13, 33, 62	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASP	6.4
1	A	375	GLN	5.8
1	A	346	GLY	5.2
1	В	375	GLN	4.4
1	A	15	PRO	4.4

### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	LLP	A	250	24/25	0.98	0.12	6,14,33,36	0
1	LLP	В	250	24/25	0.98	0.12	7,16,34,38	0

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



# 6.4 Ligands (i)

There are no ligands in this entry.

# 6.5 Other polymers (i)

There are no such residues in this entry.

