



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2025 – 08:08 AM EDT

PDB ID : 9B48  
Title : Asp324Glu variant of phosphate transporter PiPT from Piriformospora indica  
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Deposited on : 2024-03-20  
Resolution : 4.00 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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

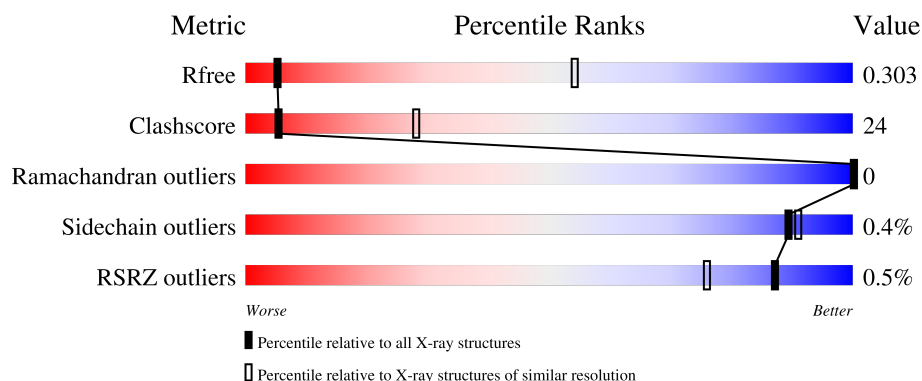
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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  $\geq 3$ , 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	530	<div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>51%</span> <span>30%</span> <span>19%</span> </div> </div>
1	B	530	<div> <div style="display: flex; justify-content: space-between;"> <span>48%</span> <span>33%</span> <span>19%</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13266 atoms, of which 6648 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 Phosphate transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	429	Total	C	H	N	O	S	0	0	0
			6633	2186	3324	543	564	16			
1	A	429	Total	C	H	N	O	S	0	0	0
			6633	2186	3324	543	564	16			

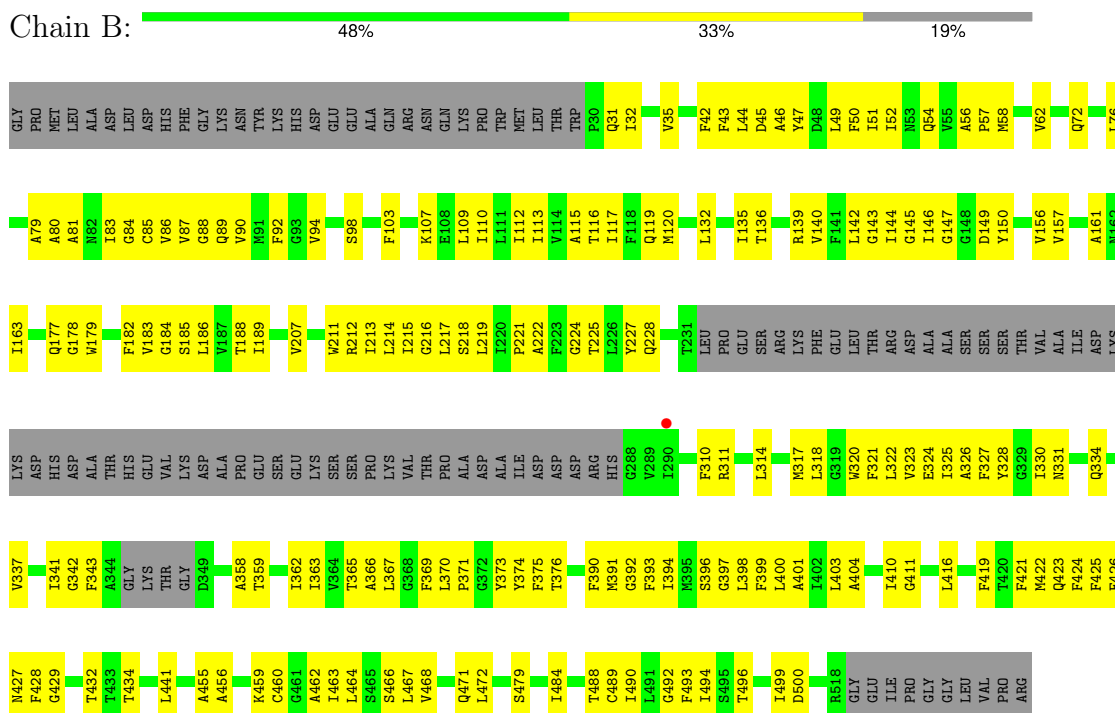
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A8N031
B	0	PRO	-	expression tag	UNP A8N031
B	324	GLU	ASP	engineered mutation	UNP A8N031
B	523	GLY	-	expression tag	UNP A8N031
B	524	GLY	-	expression tag	UNP A8N031
B	525	LEU	-	expression tag	UNP A8N031
B	526	VAL	-	expression tag	UNP A8N031
B	527	PRO	-	expression tag	UNP A8N031
B	528	ARG	-	expression tag	UNP A8N031
A	-1	GLY	-	expression tag	UNP A8N031
A	0	PRO	-	expression tag	UNP A8N031
A	324	GLU	ASP	engineered mutation	UNP A8N031
A	523	GLY	-	expression tag	UNP A8N031
A	524	GLY	-	expression tag	UNP A8N031
A	525	LEU	-	expression tag	UNP A8N031
A	526	VAL	-	expression tag	UNP A8N031
A	527	PRO	-	expression tag	UNP A8N031
A	528	ARG	-	expression tag	UNP A8N031

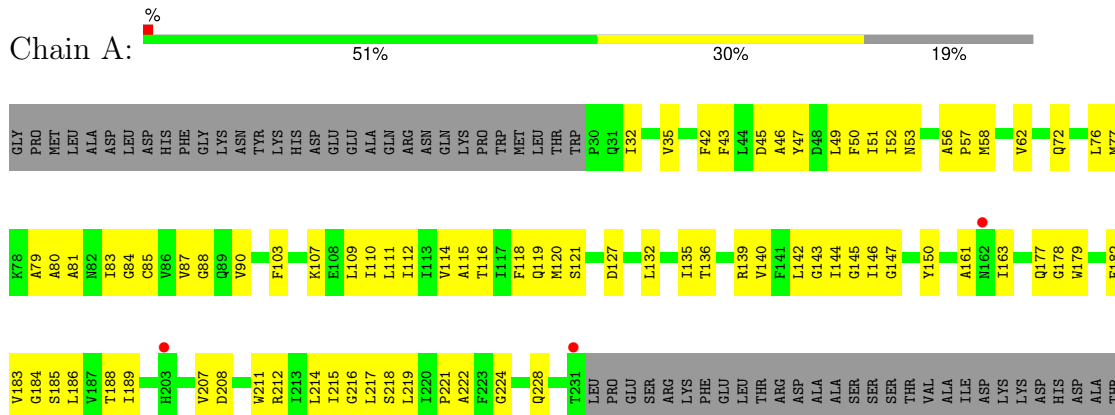
### 3 Residue-property plots [i](#)

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: Phosphate transporter



#### • Molecule 1: Phosphate transporter



HIS	GLU	VAL	LYS	ASP	PRO	ALA	GLU	SER	GLU	LYS	SER	SER	PRO	LYS	VAL	THR	PRO	ALA	ASP	ALA	ILE	ASP	ASP	ASP	ARG	HIS	G288	F310	R311	L314	G315	S316	W320	F321	L322	V323	E324	I325	A326	F327	I330	N331	Q334	V337	I341	G342	F343	A344	GLY	LYS	THR	GLY
D349	A358	T359	I362	I363	V364	T365	A366	L367	G368	F369	L370	P371	G372	Y373	Y374	F375	T376	F390	M391	G392	F393	I394	M395	S396	L400	L403	A404	I407	I410	G411	L416	F419	T420	F421	M422	Q423	F424	F425	F426	N427	F428	T434	F435	I436	E440	L441	A455					
K459	G460	G461	A462	I463	L464	S465	S466	L467	V468	Q471	L472	S479	I484	T488	C489	G492	F493	T496	F497	L498	I499	D500	R518	GLY	GLU	ILE	PRO	GLY	GLY	LEU	VAL	PRO	ARG																			

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.39Å 173.39Å 169.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.69 – 4.00 86.69 – 4.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.69-4.00) 86.1 (86.69-4.00)	Depositor EDS
$R_{merge}$	0.53	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.261 , 0.266 0.289 , 0.303	Depositor DCC
$R_{free}$ test set	1372 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.0	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 176.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

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	0.32	0/3391	0.52	0/4595
1	B	0.32	0/3391	0.53	0/4595
All	All	0.32	0/6782	0.53	0/9190

There are no bond length outliers.

There are no bond angle outliers.

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	3309	3324	3324	152	0
1	B	3309	3324	3324	162	0
All	All	6618	6648	6648	312	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 24.

The worst 5 of 312 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:85:CYS:SG	1:A:459:LYS:NZ	2.52	0.81
1:B:392:GLY:O	1:B:396:SER:OG	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:O	1:B:147:GLY:N	2.15	0.79
1:A:376:THR:OG1	1:A:427:ASN:O	2.03	0.77
1:B:119:GLN:HE22	1:B:142:LEU:HD22	1.51	0.75

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	423/530 (80%)	411 (97%)	12 (3%)	0	100	100
1	B	423/530 (80%)	413 (98%)	10 (2%)	0	100	100
All	All	846/1060 (80%)	824 (97%)	22 (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	338/433 (78%)	337 (100%)	1 (0%)	91	92
1	B	338/433 (78%)	336 (99%)	2 (1%)	84	88
All	All	676/866 (78%)	673 (100%)	3 (0%)	89	91

All (3) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	31	GLN
1	B	42	PHE
1	A	127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	423	GLN
1	B	423	GLN
1	B	431	ASN
1	A	177	GLN

### 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 oligosaccharides 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<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	429/530 (80%)	-0.63	3 (0%) 84 71	127, 174, 284, 372	0
1	B	429/530 (80%)	-0.69	1 (0%) 92 85	124, 177, 284, 374	0
All	All	858/1060 (80%)	-0.66	4 (0%) 87 76	124, 175, 284, 374	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	HIS	3.8
1	B	290	ILE	2.8
1	A	231	THR	2.2
1	A	162	ASN	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 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.