



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:54 PM UTC

PDB ID : 2AKC / pdb\_00002akc  
Title : Crystal structure of tungstate complex of the PhoN protein from *S. typhimurium*  
Authors : Makde, R.D.; Kumar, V.  
Deposited on : 2005-08-03  
Resolution : 2.30 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

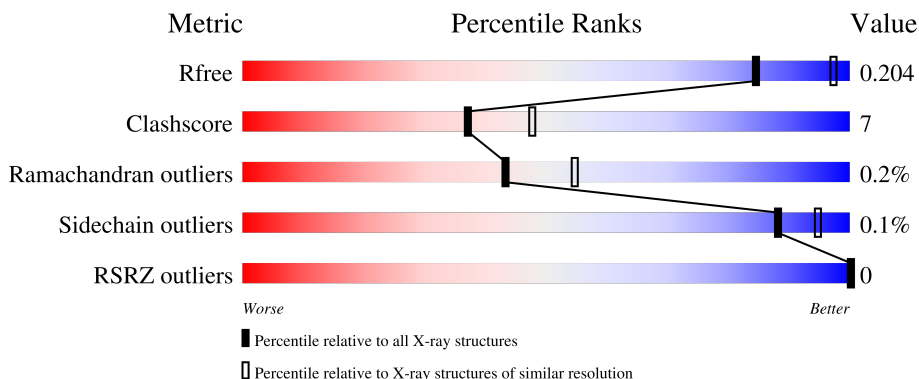
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


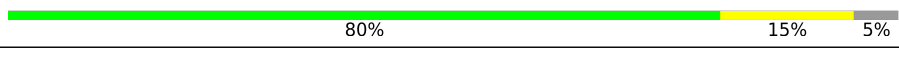
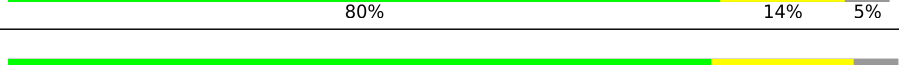

The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	230	 76% 19% 5%
1	B	230	 80% 15% 5%
1	C	230	 80% 14% 5%
1	D	230	 79% 16% 5%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	WO4	A	501	-	-	X	-
2	WO4	D	504	-	-	X	-

## 2 Entry composition [i](#)

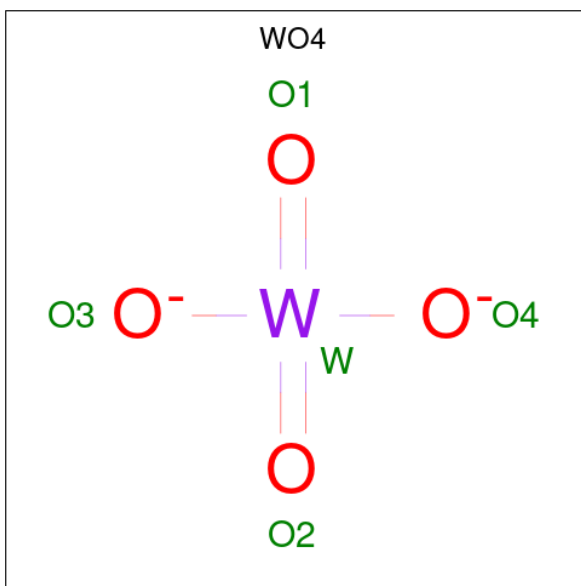
There are 3 unique types of molecules in this entry. The entry contains 7328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 class A nonspecific acid phosphatase PhoN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1741	C 1104	N 308	O 324	S 5	0	0	0
1	B	219	Total 1747	C 1107	N 309	O 326	S 5	0	0	0
1	C	219	Total 1747	C 1107	N 309	O 326	S 5	0	0	0
1	D	219	Total 1747	C 1107	N 309	O 326	S 5	0	0	0

- Molecule 2 is TUNGSTATE(VI)ION (CCD ID: WO4) (formula: O<sub>4</sub>W).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	W		
2	A	1	Total 5	O 4	W 1	0	0
2	B	1	Total 5	O 4	W 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	W	0	0
			5	4	1		
2	D	1	Total	O	W	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	75	Total	O	0	0
			75	75		
3	C	86	Total	O	0	0
			86	86		
3	D	87	Total	O	0	0
			87	87		



V202	D203	A204	V208	I219	K228	V229	E232	S241	LYS	GLU	GLU	ARG	PRO	GLU	LEU	ASN	TYR
------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.80Å 45.20Å 112.70Å 90.00° 111.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (20.00-2.30) 92.1 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.164 , 0.211 0.158 , 0.204	Depositor DCC
$R_{free}$ test set	1885 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.430	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: WO4

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	0.42	0/1789	0.91	4/2427 (0.2%)
1	B	0.41	0/1795	0.91	7/2435 (0.3%)
1	C	0.42	0/1795	0.89	1/2435 (0.0%)
1	D	0.42	0/1795	0.90	3/2435 (0.1%)
All	All	0.42	0/7174	0.90	15/9732 (0.2%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	GLU	N-CA-C	7.55	120.47	111.33
1	B	120	ALA	N-CA-C	7.40	120.05	111.02
1	A	120	ALA	N-CA-C	7.36	119.99	111.02
1	B	173	ARG	CA-C-N	7.08	127.68	119.47
1	B	173	ARG	C-N-CA	7.08	127.68	119.47

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	1741	0	1688	29	0
1	B	1747	0	1693	19	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1747	0	1693	25	0
1	D	1747	0	1693	25	0
2	A	5	0	0	3	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	2	0
3	A	78	0	0	1	0
3	B	75	0	0	0	0
3	C	86	0	0	3	0
3	D	87	0	0	4	0
All	All	7328	0	6767	98	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 7.

The worst 5 of 98 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:66:SER:HB2	1:A:67:PRO:HD2	1.66	0.78
1:C:45:ASN:ND2	1:C:46:ASP:H	1.85	0.74
1:A:88:SER:HB2	1:A:89:PRO:HD3	1.77	0.67
1:C:228:LYS:O	1:C:232:GLU:HG3	1.97	0.64
1:A:145:GLU:O	1:A:149:ARG:HG2	1.98	0.64

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	216/230 (94%)	211 (98%)	5 (2%)	0	100 100
1	B	217/230 (94%)	213 (98%)	3 (1%)	1 (0%)	24 31

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	D	217/230 (94%)	211 (97%)	5 (2%)	1 (0%)	24	31
All	All	867/920 (94%)	847 (98%)	18 (2%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	ASN
1	D	34	ASN

### 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	183/194 (94%)	183 (100%)	0	100	100
1	B	184/194 (95%)	184 (100%)	0	100	100
1	C	184/194 (95%)	183 (100%)	1 (0%)	81	90
1	D	184/194 (95%)	184 (100%)	0	100	100
All	All	735/776 (95%)	734 (100%)	1 (0%)	88	95

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

Mol	Chain	Res	Type
1	C	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	146	ASN
1	D	217	GLN
1	B	237	ASN
1	C	36	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	45	ASN

### 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](#)

4 ligands 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	WO4	D	504	1	2,4,4	1.57	0	-		
2	WO4	B	502	1	2,4,4	1.65	0	-		
2	WO4	A	501	1	2,4,4	1.40	0	-		
2	WO4	C	503	1	2,4,4	1.61	0	-		

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	504	WO4	2	0
2	B	502	WO4	1	0
2	A	501	WO4	3	0
2	C	503	WO4	1	0

## 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	218/230 (94%)	-0.44	0 100 100	14, 27, 45, 69	0
1	B	219/230 (95%)	-0.47	0 100 100	14, 27, 46, 66	0
1	C	219/230 (95%)	-0.48	0 100 100	13, 26, 45, 67	0
1	D	219/230 (95%)	-0.48	0 100 100	12, 26, 49, 64	0
All	All	875/920 (95%)	-0.47	0 100 100	12, 26, 46, 69	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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, 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(Å <sup>2</sup> )	Q<0.9
2	WO4	A	501	5/5	1.00	0.04	18,19,23,24	0
2	WO4	B	502	5/5	1.00	0.04	19,22,25,30	0
2	WO4	C	503	5/5	1.00	0.04	18,20,23,24	0
2	WO4	D	504	5/5	1.00	0.04	23,24,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.