



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:29 PM GMT

PDB ID : 1VHS  
Title : Crystal structure of a putative phosphinothricin N-acetyltransferase  
Authors : Structural GenomiX  
Deposited on : 2003-12-01  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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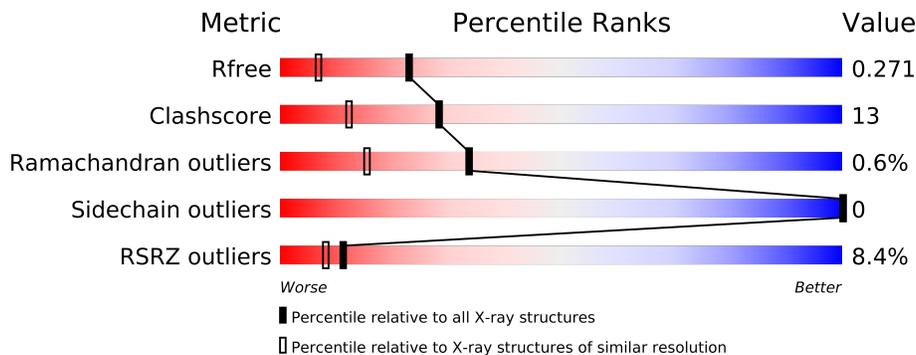
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2776 atoms, of which 0 are hydrogen and 0 are deuterium.

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 similar to phosphinothricin acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	165	1293	824	218	246	1	4	0	5	0
1	B	158	1239	798	210	227	1	3	0	6	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P71043
A	0	SER	-	cloning artifact	UNP P71043
A	1	LEU	-	cloning artifact	UNP P71043
A	26	MSE	MET	modified residue	UNP P71043
A	40	MSE	MET	modified residue	UNP P71043
A	117	MSE	MET	modified residue	UNP P71043
A	148	MSE	MET	modified residue	UNP P71043
A	164	GLU	-	cloning artifact	UNP P71043
A	165	GLY	-	cloning artifact	UNP P71043
A	166	GLY	-	cloning artifact	UNP P71043
A	167	SER	-	cloning artifact	UNP P71043
A	168	HIS	-	cloning artifact	UNP P71043
A	169	HIS	-	cloning artifact	UNP P71043
A	170	HIS	-	cloning artifact	UNP P71043
A	171	HIS	-	cloning artifact	UNP P71043
A	172	HIS	-	cloning artifact	UNP P71043
A	173	HIS	-	cloning artifact	UNP P71043
B	-1	MSE	-	cloning artifact	UNP P71043
B	0	SER	-	cloning artifact	UNP P71043
B	1	LEU	-	cloning artifact	UNP P71043
B	26	MSE	MET	modified residue	UNP P71043
B	40	MSE	MET	modified residue	UNP P71043
B	117	MSE	MET	modified residue	UNP P71043
B	148	MSE	MET	modified residue	UNP P71043
B	164	GLU	-	cloning artifact	UNP P71043

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Chain	Residue	Modelled	Actual	Comment	Reference
B	165	GLY	-	cloning artifact	UNP P71043
B	166	GLY	-	cloning artifact	UNP P71043
B	167	SER	-	cloning artifact	UNP P71043
B	168	HIS	-	cloning artifact	UNP P71043
B	169	HIS	-	cloning artifact	UNP P71043
B	170	HIS	-	cloning artifact	UNP P71043
B	171	HIS	-	cloning artifact	UNP P71043
B	172	HIS	-	cloning artifact	UNP P71043
B	173	HIS	-	cloning artifact	UNP P71043

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	116	Total 116	O 116	0	0
2	B	128	Total 128	O 128	0	0



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.51Å 50.83Å 87.61Å 90.00° 116.67° 90.00°	Depositor
Resolution (Å)	42.22 – 1.80 42.22 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.22-1.80) 97.9 (42.22-1.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.79Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, $R_{free}$	0.238 , 0.280 0.225 , 0.271	Depositor DCC
$R_{free}$ test set	1528 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 30362 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0912e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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	0.31	0/1353	0.55	0/1829
1	B	0.31	0/1299	0.54	0/1755
All	All	0.31	0/2652	0.54	0/3584

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1293	0	1234	26	1
1	B	1239	0	1188	38	0
2	A	116	0	0	5	0
2	B	128	0	0	9	0
All	All	2776	0	2422	63	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:PRO:HG3	1:B:162[A]:LEU:HD23	1.46	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:GLU:HG3	2:B:196:HOH:O	1.82	0.78
1:B:40[B]:MSE:HE3	1:B:44:SER:OG	1.92	0.68
1:B:134:HIS:HD2	2:B:195:HOH:O	1.79	0.65
1:A:51:PRO:HG2	1:A:53:TYR:CE1	2.31	0.64
1:A:25:ARG:HA	2:A:245:HOH:O	1.98	0.63
1:A:67:SER:HB3	1:A:84[A]:SER:OG	1.99	0.61
1:B:125:LYS:HE3	2:B:263:HOH:O	2.02	0.59
1:B:1:LEU:HD11	1:B:96:VAL:HG13	1.85	0.58
1:B:119:PHE:HD2	1:B:155:LEU:HD21	1.67	0.58
1:B:22:ILE:HD12	1:B:23:ALA:N	2.20	0.56
1:B:51:PRO:HG2	1:B:53:TYR:CE1	2.41	0.56
1:A:162:LEU:HD12	1:A:162:LEU:N	2.21	0.56
1:A:28:THR:HG22	2:A:232:HOH:O	2.06	0.56
1:A:114:ARG:HG3	1:A:163:SER:HB2	1.88	0.55
1:A:25:ARG:HH21	1:A:31:THR:HB	1.70	0.55
1:B:72:TYR:CE2	1:B:74:ARG:HG3	2.42	0.55
1:B:22:ILE:HD11	2:B:275:HOH:O	2.07	0.55
1:B:41:GLU:HG2	2:B:217:HOH:O	2.07	0.54
1:B:110:ASN:HA	2:B:252:HOH:O	2.07	0.54
1:B:62:VAL:HG23	2:B:243:HOH:O	2.09	0.53
1:B:22:ILE:C	1:B:22:ILE:HD12	2.30	0.52
1:B:119:PHE:HB3	1:B:155:LEU:HD11	1.91	0.52
1:A:22:ILE:HG23	1:A:30:ASP:O	2.10	0.52
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.93	0.51
1:B:98:SER:HA	1:B:130:LEU:HD11	1.93	0.51
1:A:121:PHE:HB3	1:A:123:HIS:CE1	2.45	0.51
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.93	0.50
1:A:125:LYS:HB2	1:A:126:PRO:HD3	1.94	0.50
1:A:40:MSE:HE3	1:A:44:SER:OG	2.12	0.50
1:A:22:ILE:HG12	1:A:28:THR:HG21	1.93	0.50
1:B:121:PHE:HB3	1:B:123[A]:HIS:CD2	2.47	0.49
1:B:57:ASP:OD2	1:B:61:ASN:HB2	2.14	0.48
1:A:134:HIS:HE1	2:A:207:HOH:O	1.95	0.48
1:A:75:PRO:HA	1:A:78:ASN:ND2	2.29	0.48
1:A:25:ARG:NH2	2:A:243:HOH:O	2.44	0.47
1:A:119:PHE:HD2	1:A:155:LEU:HD21	1.79	0.47
1:B:19:ASN:O	1:B:22:ILE:HG13	2.14	0.47
1:B:74:ARG:NH1	2:B:209:HOH:O	2.35	0.47
1:B:59:ASN:HB2	1:B:61:ASN:ND2	2.30	0.47
1:B:124:ASN:O	1:B:128[A]:LEU:HG	2.14	0.46
1:A:71:PHE:HA	1:A:82[A]:GLU:OE2	2.15	0.46
1:A:162:LEU:N	1:A:162:LEU:CD1	2.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:39:ARG:HA	2:B:204:HOH:O	2.16	0.45
1:A:25:ARG:HH11	1:A:25:ARG:HG3	1.81	0.44
1:A:57:ASP:OD2	1:A:61:ASN:HB2	2.18	0.44
1:A:84[C]:SER:OG	1:A:86:TYR:HE1	2.01	0.44
1:B:125:LYS:HD3	1:B:128[A]:LEU:HD12	1.99	0.43
1:A:150:GLY:O	1:B:164:GLU:HA	2.19	0.43
1:B:1:LEU:CD1	1:B:96:VAL:HG13	2.48	0.43
1:B:125:LYS:N	1:B:126:PRO:CD	2.82	0.43
1:B:67:SER:HB3	1:B:84:SER:OG	2.19	0.42
1:B:72:TYR:CE2	1:B:74:ARG:NH1	2.87	0.42
1:B:39:ARG:HH11	1:B:39:ARG:HG2	1.85	0.42
1:B:141:LEU:C	1:B:141:LEU:HD23	2.41	0.41
1:B:56:GLU:HA	1:B:61:ASN:O	2.21	0.41
1:B:80:THR:CG2	1:B:117:MSE:HE2	2.51	0.41
1:A:41:GLU:HG2	2:A:266:HOH:O	2.20	0.41
1:A:80:THR:CG2	1:A:117:MSE:HE2	2.51	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	Distance(Å)	Clash(Å)
1:A:59:ASN:OD1	1:A:59:ASN:OD1[2_555]	2.02	0.18

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	169/175 (97%)	166 (98%)	3 (2%)	0	100 100
1	B	160/175 (91%)	155 (97%)	3 (2%)	2 (1%)	18 4
All	All	329/350 (94%)	321 (98%)	6 (2%)	2 (1%)	33 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	LYS
1	B	73	GLY

### 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	134/139 (96%)	134 (100%)	0	100	100
1	B	127/139 (91%)	127 (100%)	0	100	100
All	All	261/278 (94%)	261 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	B	19	ASN
1	B	61	ASN
1	B	110	ASN
1	B	134	HIS

### 5.3.3 RNA [i](#)

There are no RNA chains 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

There are no ligands in this entry.

## 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 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	165/175 (94%)	0.39	10 (6%) <span style="border: 1px solid red; padding: 2px;">21</span> <span style="border: 1px solid red; padding: 2px;">15</span>	12, 26, 49, 54	0
1	B	158/175 (90%)	0.58	17 (10%) <span style="border: 1px solid red; padding: 2px;">6</span> <span style="border: 1px solid red; padding: 2px;">5</span>	13, 28, 66, 75	0
All	All	323/350 (92%)	0.48	27 (8%) <span style="border: 1px solid red; padding: 2px;">11</span> <span style="border: 1px solid red; padding: 2px;">8</span>	12, 27, 59, 75	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ALA	5.9
1	B	88	ASP	3.9
1	A	93	GLY	3.7
1	B	123[A]	HIS	3.7
1	A	29	ALA	3.5
1	B	90	ALA	3.5
1	B	92	ARG	3.2
1	B	122	GLY	3.2
1	A	96	VAL	3.1
1	B	121	PHE	3.1
1	A	23	ALA	2.9
1	A	92	ARG	2.9
1	A	59	ASN	2.8
1	B	18	TYR	2.7
1	A	26	MSE	2.7
1	B	163	SER	2.6
1	B	36	PRO	2.6
1	A	27	VAL	2.6
1	A	89	GLU	2.5
1	B	93	GLY	2.4
1	B	0	SER	2.3
1	B	40[A]	MSE	2.3
1	B	43	PHE	2.3
1	A	163	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	59	ASN	2.2
1	B	24	SER	2.2
1	B	16	ALA	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.