



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:36 PM GMT

PDB ID : 1PTA  
Title : THREE-DIMENSIONAL STRUCTURE OF PHOSPHOTRIESTERASE: AN ENZYME CAPABLE OF DETOXIFYING ORGANOPHOSPHATE NERVE AGENTS  
Authors : Benning, M.; Holden, H.M.  
Deposited on : 1994-07-07  
Resolution : 2.10 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

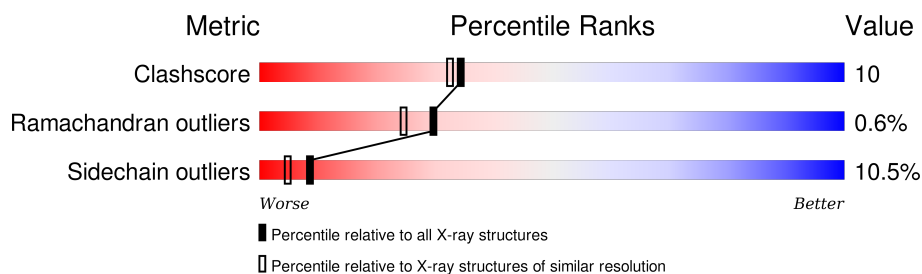
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	 63% 27% 6% ••

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2568 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 PHOSPHOTRIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2439	1550	434	448	7			

- Molecule 2 is water.

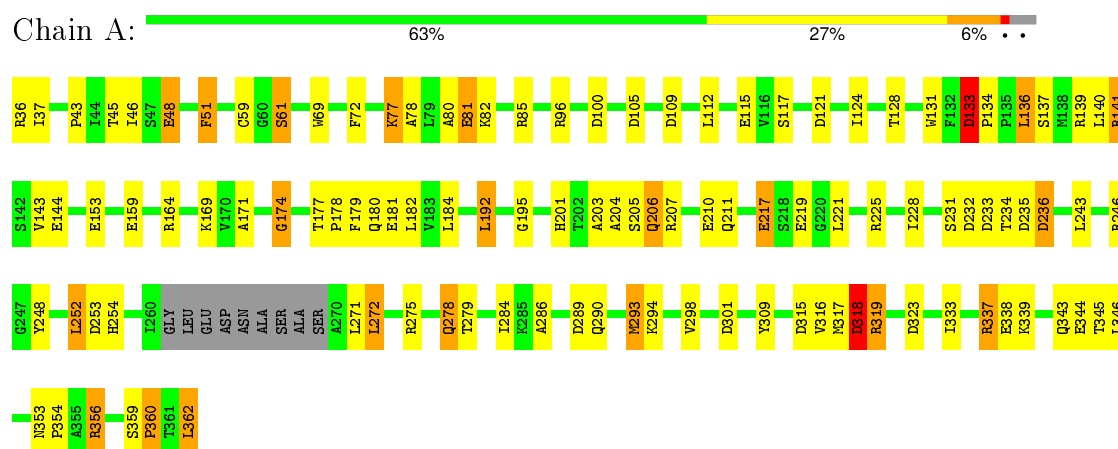
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	129	Total	O	0	0
			129	129		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: PHOSPHOTRIESTERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.20 Å 93.70 Å 45.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.10 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.10-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 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	1.00	12/2486 (0.5%)	1.41	37/3375 (1.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLU	CD-OE2	7.13	1.33	1.25
1	A	144	GLU	CD-OE1	6.93	1.33	1.25
1	A	81	GLU	CD-OE1	6.53	1.32	1.25
1	A	344	GLU	CD-OE1	6.44	1.32	1.25
1	A	159	GLU	CD-OE1	5.73	1.31	1.25
1	A	338	GLU	CD-OE2	5.66	1.31	1.25
1	A	210	GLU	CD-OE1	5.55	1.31	1.25
1	A	181	GLU	CD-OE2	5.52	1.31	1.25
1	A	217	GLU	CD-OE1	5.42	1.31	1.25
1	A	219	GLU	CD-OE1	5.36	1.31	1.25
1	A	153	GLU	CD-OE1	5.31	1.31	1.25
1	A	48	GLU	CD-OE2	5.28	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	96	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	133	ASP	CB-CG-OD1	-8.37	110.77	118.30
1	A	315	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	A	337	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	253	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	109	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	164	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	164	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	207	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	246	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	356	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	109	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	100	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	96	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	323	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	A	252	LEU	N-CA-C	-6.14	94.43	111.00
1	A	235	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	235	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	105	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	236	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	105	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	100	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	A	232	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	293	MET	CA-CB-CG	-5.70	103.62	113.30
1	A	225	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	318	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	128	THR	N-CA-CB	5.58	120.91	110.30
1	A	36	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	289	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	323	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	253	ASP	N-CA-C	5.39	125.56	111.00
1	A	121	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	233	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	315	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	301	ASP	CB-CG-OD1	-5.09	113.72	118.30

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	2439	0	2475	49	0
2	A	129	0	0	2	0
All	All	2568	0	2475	49	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 10.

All (49) 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:169:LYS:NZ	1:A:201:HIS:NE2	2.12	0.97
1:A:177:THR:HB	1:A:178:PRO:HD2	1.62	0.81
1:A:192:LEU:HD12	1:A:221:LEU:HD13	1.68	0.75
1:A:46:ILE:HD11	1:A:359:SER:OG	1.87	0.74
1:A:278:GLN:H	1:A:278:GLN:HE21	1.35	0.74
1:A:192:LEU:HD12	1:A:221:LEU:CD1	2.26	0.65
1:A:177:THR:HB	1:A:178:PRO:CD	2.27	0.64
1:A:174:GLY:O	1:A:203:ALA:HB1	1.99	0.62
1:A:316:VAL:CG1	1:A:318:ASP:HB3	2.35	0.56
1:A:174:GLY:HA2	1:A:204:ALA:CB	2.36	0.55
1:A:217:GLU:HG3	1:A:248:TYR:OH	2.08	0.54
1:A:177:THR:OG1	1:A:180:GLN:HG3	2.08	0.53
1:A:61:SER:OG	1:A:309:TYR:O	2.26	0.53
1:A:319:ARG:NH1	2:A:487:HOH:O	2.41	0.53
1:A:319:ARG:NH2	2:A:487:HOH:O	2.36	0.51
1:A:169:LYS:CE	1:A:201:HIS:NE2	2.75	0.50
1:A:80:ALA:HB2	1:A:112:LEU:HD11	1.93	0.49
1:A:69:TRP:CE2	1:A:72:PHE:HB2	2.47	0.49
1:A:343:GLN:HA	1:A:343:GLN:NE2	2.26	0.49
1:A:133:ASP:N	1:A:134:PRO:HD3	2.28	0.48
1:A:174:GLY:HA2	1:A:204:ALA:HB2	1.95	0.48
1:A:316:VAL:HG13	1:A:318:ASP:HB3	1.95	0.48
1:A:195:GLY:O	1:A:360:PRO:HA	2.14	0.48
1:A:206:GLN:HB2	1:A:206:GLN:HE21	1.44	0.47
1:A:333:ILE:HG23	1:A:346:LEU:HD13	1.96	0.47
1:A:143:VAL:HG23	1:A:182:LEU:HG	1.98	0.46
1:A:37:ILE:O	1:A:43:PRO:HA	2.16	0.46
1:A:143:VAL:CG2	1:A:182:LEU:HG	2.46	0.45
1:A:192:LEU:O	1:A:362:LEU:HD21	2.17	0.45
1:A:286:ALA:O	1:A:290:GLN:HG2	2.17	0.45
1:A:178:PRO:CD	1:A:179:PHE:H	2.30	0.45
1:A:339:LYS:HA	1:A:339:LYS:HD3	1.74	0.45
1:A:77:LYS:CG	1:A:78:ALA:N	2.80	0.44
1:A:294:LYS:O	1:A:356:ARG:NH2	2.49	0.44
1:A:137:SER:O	1:A:141:ARG:HD2	2.17	0.44
1:A:77:LYS:HG2	1:A:78:ALA:N	2.33	0.44
1:A:275:ARG:HB3	1:A:279:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HD11	1:A:298:VAL:HG21	2.00	0.43
1:A:117:SER:HB2	1:A:124:ILE:HD12	2.01	0.43
1:A:136:LEU:HA	1:A:136:LEU:HD12	1.81	0.41
1:A:252:LEU:O	1:A:298:VAL:HA	2.20	0.41
1:A:45:THR:HG23	1:A:48:GLU:OE1	2.20	0.41
1:A:231:SER:HA	1:A:254:HIS:O	2.21	0.41
1:A:293:MET:HE1	1:A:345:THR:HA	2.03	0.41
1:A:353:ASN:N	1:A:354:PRO:HD2	2.36	0.41
1:A:234:THR:HG21	1:A:272:LEU:CD2	2.51	0.41
1:A:51:PHE:C	1:A:51:PHE:CD1	2.94	0.41
1:A:133:ASP:N	1:A:134:PRO:CD	2.84	0.40
1:A:131:TRP:HA	1:A:171:ALA:HB3	2.02	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	314/327 (96%)	307 (98%)	5 (2%)	2 (1%)	30	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLY
1	A	205	SER

### 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	257/263 (98%)	230 (90%)	27 (10%)	8 5

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	59	CYS
1	A	61	SER
1	A	77	LYS
1	A	81	GLU
1	A	82	LYS
1	A	133	ASP
1	A	136	LEU
1	A	139	ARG
1	A	140	LEU
1	A	141	ARG
1	A	184	LEU
1	A	192	LEU
1	A	206	GLN
1	A	211	GLN
1	A	228	ILE
1	A	236	ASP
1	A	243	LEU
1	A	271	LEU
1	A	272	LEU
1	A	278	GLN
1	A	317	MET
1	A	318	ASP
1	A	319	ARG
1	A	337	ARG
1	A	360	PRO
1	A	362	LEU

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	206	GLN
1	A	211	GLN
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	295	GLN
1	A	343	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 carbohydrates 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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.