



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 AM UTC

PDB ID : 1PTA / pdb_00001pta
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

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

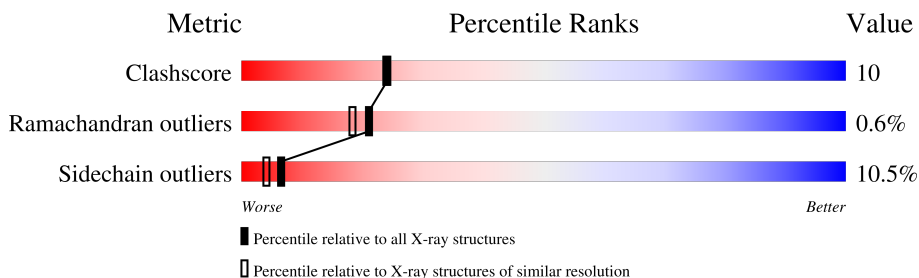
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	 68% 23% 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.

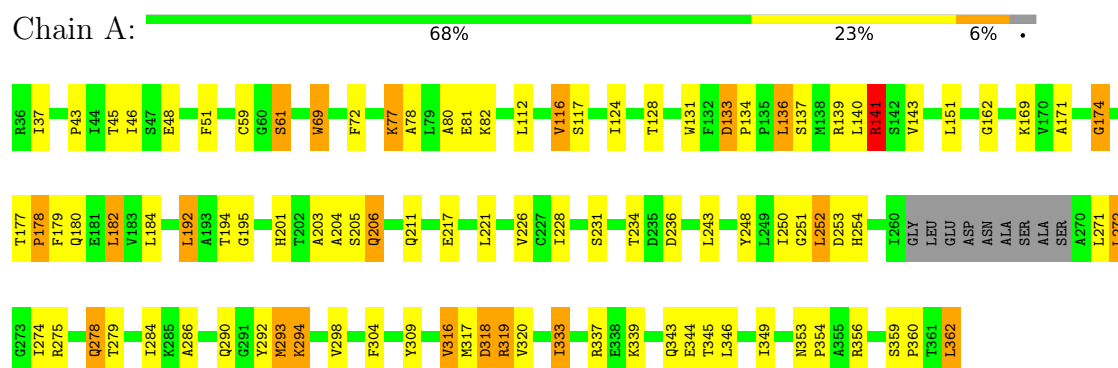
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	129	Total	O	0	0
			129	129		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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 is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	35.0	wwPDB-VP

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	1.25	2/2486 (0.1%)	1.61	25/3375 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ILE	CA-CB	-5.76	1.50	1.53
1	A	251	GLY	CA-C	-5.52	1.48	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ILE	CA-C-N	-10.51	112.96	122.73
1	A	250	ILE	C-N-CA	-10.51	112.96	122.73
1	A	226	VAL	N-CA-C	7.73	118.93	108.11
1	A	320	VAL	N-CA-C	7.45	119.19	109.58
1	A	252	LEU	N-CA-C	-7.39	94.43	107.73
1	A	253	ASP	N-CA-C	7.39	125.56	113.89
1	A	304	PHE	CA-CB-CG	-6.76	107.04	113.80
1	A	128	THR	N-CA-CB	6.57	120.91	111.05
1	A	292	TYR	N-CA-C	6.05	119.62	112.72
1	A	344	GLU	CB-CG-CD	-5.86	102.64	112.60
1	A	116	VAL	N-CA-CB	5.83	118.47	110.54
1	A	162	GLY	N-CA-C	-5.63	107.87	115.36
1	A	316	VAL	N-CA-C	5.50	116.65	108.23
1	A	141	ARG	O-C-N	-5.49	116.76	122.96
1	A	141	ARG	N-CA-CB	-5.49	101.95	110.29
1	A	151	LEU	CA-C-O	5.47	126.34	120.55
1	A	178	PRO	N-CA-C	-5.46	106.42	113.57
1	A	128	THR	N-CA-C	-5.46	101.46	109.81
1	A	349	ILE	N-CA-C	5.44	116.22	110.72
1	A	69	TRP	O-C-N	5.36	125.11	121.19
1	A	253	ASP	N-CA-CB	-5.29	103.33	110.95
1	A	194	THR	N-CA-C	5.28	120.00	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	MET	CA-CB-CG	-5.24	103.62	114.10
1	A	274	ILE	N-CA-C	5.20	115.98	107.24
1	A	182	LEU	CB-CA-C	-5.15	102.80	110.88

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:HE21	1:A:278:GLN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	1:A:343:GLN:HA	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:HE21	1:A:206:GLN:HB2	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:51:PHE:C	1:A:51:PHE:CD1	2.94	0.46
1:A:293:MET:HE3	1:A:345:THR:HG23	1.98	0.45
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:HD3	1:A:339:LYS:HA	1.74	0.45
1:A:137:SER:O	1:A:141:ARG:HD2	2.17	0.44
1:A:294:LYS:O	1:A:356:ARG:NH2	2.49	0.44
1:A:275:ARG:HB3	1:A:279:THR:OG1	2.17	0.43
1:A:117:SER:HB2	1:A:124:ILE:HD12	2.01	0.43
1:A:284:ILE:HD11	1:A:298:VAL:HG21	2.00	0.43
1:A:77:LYS:HG2	1:A:78:ALA:N	2.33	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:234:THR:HG21	1:A:272:LEU:CD2	2.51	0.41
1:A:353:ASN:N	1:A:354:PRO:HD2	2.36	0.41
1:A:51:PHE:C	1:A:51:PHE:HD1	2.29	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

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	314/327 (96%)	307 (98%)	5 (2%)	2 (1%)	21	18

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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%)	6	4

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

Mol	Chain	Res	Type
1	A	59	CYS
1	A	61	SER
1	A	77	LYS
1	A	81	GLU
1	A	82	LYS
1	A	116	VAL
1	A	133	ASP
1	A	136	LEU
1	A	139	ARG

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Mol	Chain	Res	Type
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	294	LYS
1	A	317	MET
1	A	318	ASP
1	A	319	ARG
1	A	337	ARG
1	A	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	211	GLN
1	A	278	GLN
1	A	295	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.