



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 01:45 am BST

PDB ID : 1EI6
Title : CRYSTAL STRUCTURE OF PHOSPHONOACETATE HYDROLASE
COMPLEXED WITH PHOSPHONOFORMATE
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Deposited on : 2000-02-24
Resolution : 2.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

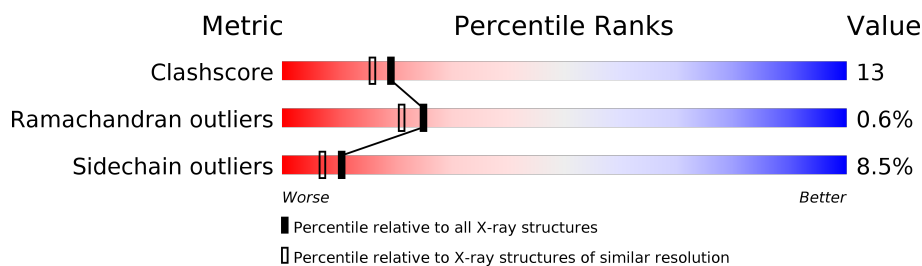
1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 ≥ 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	406	63% 32% .
1	B	406	62% 30% 6% ..
1	C	406	63% 28% 8% .
1	D	406	64% 28% 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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PPF	C	413	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12751 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 PHOSPHONOACETATE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3087	1953	535	586	13			
1	B	403	Total	C	N	O	S	0	0	0
			3068	1941	534	580	13			
1	C	401	Total	C	N	O	S	0	0	0
			3047	1928	529	577	13			
1	D	395	Total	C	N	O	S	0	0	0
			3011	1906	522	570	13			

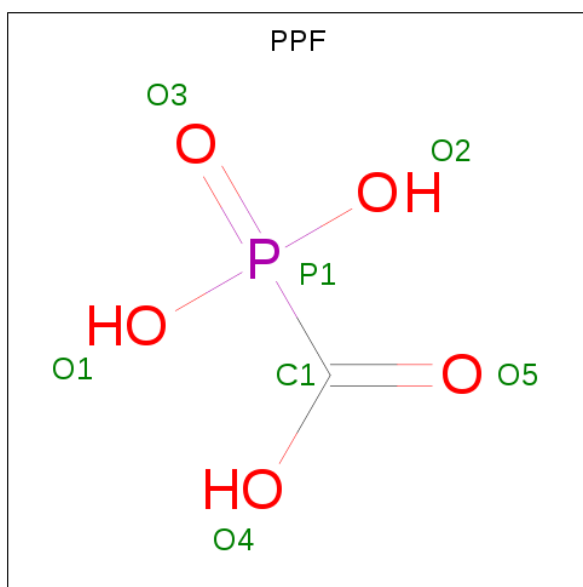
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	GLN	CONFLICT	UNP Q51782
B	3	ASN	GLN	CONFLICT	UNP Q51782
C	3	ASN	GLN	CONFLICT	UNP Q51782
D	3	ASN	GLN	CONFLICT	UNP Q51782

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

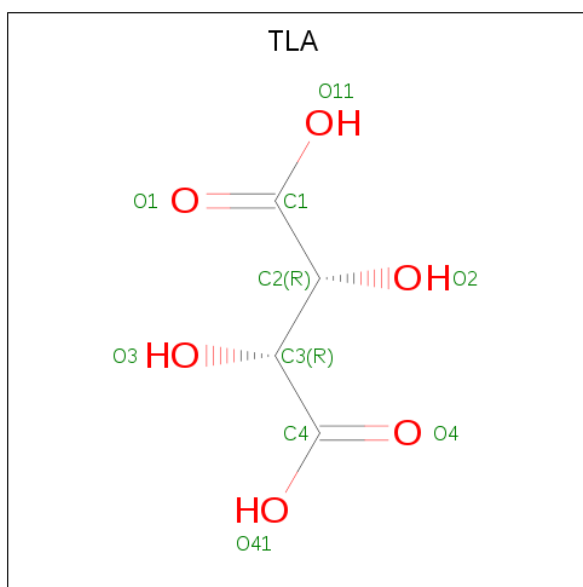
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHONOFORMIC ACID (three-letter code: PPF) (formula: CH₃O₅P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			7	1	5	1		
3	C	1	Total	C	O	P	0	0
			7	1	5	1		
3	D	1	Total	C	O	P	0	0
			7	1	5	1		

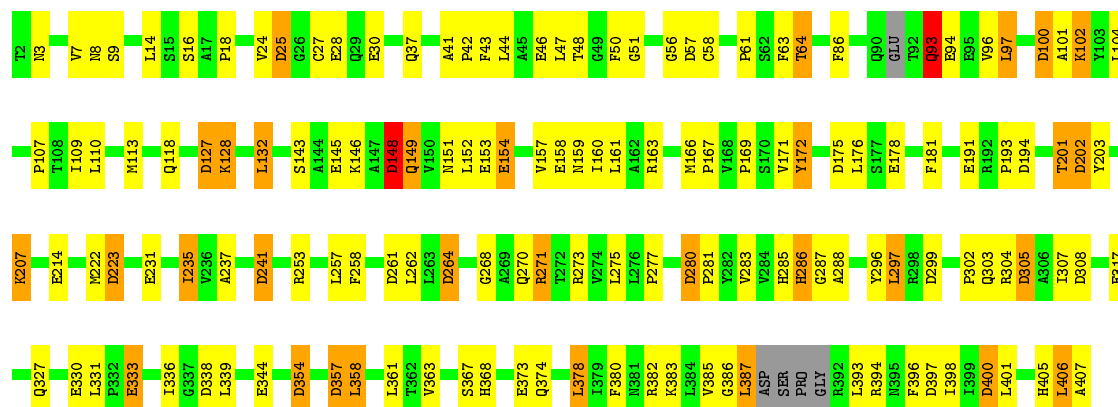
- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O		
			10	4	6	0	0

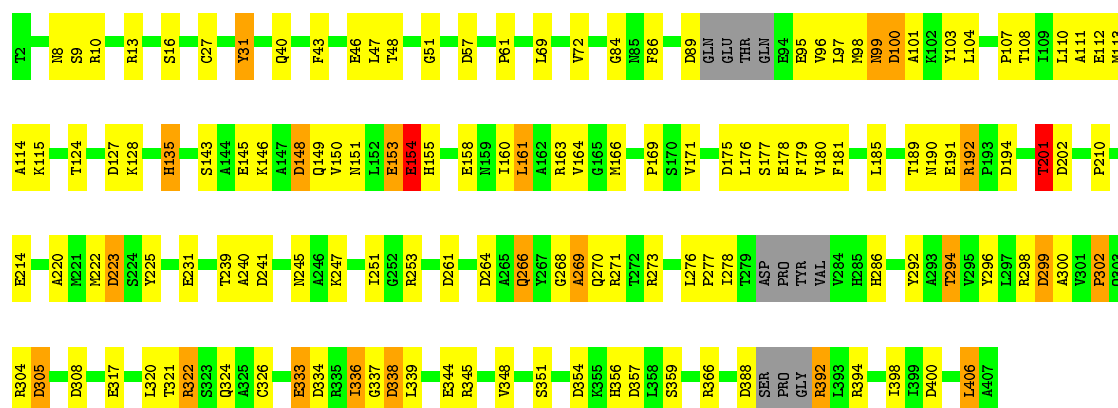
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total 137	O 137	0	0
5	B	137	Total 137	O 137	0	0
5	C	108	Total 108	O 108	0	0
5	D	117	Total 117	O 117	0	0



● Molecule 1: PHOSPHONOACETATE HYDROLASE

Chain D: 64% 28% 5% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.50 Å 129.54 Å 133.38 Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.0 (20.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.192 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12751	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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: ZN, TLA, PPF

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	0.98	18/3146 (0.6%)	1.27	40/4276 (0.9%)
1	B	0.94	13/3126 (0.4%)	1.27	44/4250 (1.0%)
1	C	0.96	15/3104 (0.5%)	1.25	46/4218 (1.1%)
1	D	0.95	15/3066 (0.5%)	1.23	45/4163 (1.1%)
All	All	0.96	61/12442 (0.5%)	1.26	175/16907 (1.0%)

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	GLU	CD-OE2	7.22	1.33	1.25
1	C	330	GLU	CD-OE2	7.01	1.33	1.25
1	D	231	GLU	CD-OE2	6.85	1.33	1.25
1	C	178	GLU	CD-OE2	6.50	1.32	1.25
1	A	112	GLU	CD-OE2	6.49	1.32	1.25

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	D	127	ASP	CB-CG-OD2	-8.51	110.65	118.30
1	A	194	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	B	354	ASP	CB-CG-OD2	-8.13	110.99	118.30
1	D	202	ASP	CB-CG-OD2	-7.94	111.16	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	3087	0	3065	72	0
1	B	3068	0	3046	90	0
1	C	3047	0	3013	88	0
1	D	3011	0	2989	67	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	0	2	0
3	C	7	0	0	6	0
3	D	7	0	0	0	0
4	B	10	0	1	0	0
5	A	137	0	0	3	0
5	B	137	0	0	2	0
5	C	108	0	0	3	0
5	D	117	0	0	3	0
All	All	12751	0	12114	313	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 13.

The worst 5 of 313 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:385:VAL:HG13	1:A:407:ALA:HB2	1.51	0.91
1:A:77:PRO:HG2	1:A:331:LEU:HD23	1.57	0.85
1:B:7:VAL:HG22	1:B:112:GLU:HG3	1.58	0.84
1:B:154:GLU:HG2	1:B:155:HIS:CE1	2.12	0.84
1:D:166:MET:HE2	1:D:179:PHE:HD1	1.42	0.83

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	400/406 (98%)	379 (95%)	21 (5%)	0	100	100
1	B	399/406 (98%)	381 (96%)	15 (4%)	3 (1%)	19	15
1	C	395/406 (97%)	373 (94%)	21 (5%)	1 (0%)	41	41
1	D	387/406 (95%)	366 (95%)	16 (4%)	5 (1%)	12	7
All	All	1581/1624 (97%)	1499 (95%)	73 (5%)	9 (1%)	25	21

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	ASP
1	D	299	ASP
1	D	269	ALA
1	D	277	PRO
1	B	330	GLU

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	330/333 (99%)	301 (91%)	29 (9%)	10	6
1	B	327/333 (98%)	300 (92%)	27 (8%)	11	7
1	C	323/333 (97%)	290 (90%)	33 (10%)	7	4
1	D	321/333 (96%)	300 (94%)	21 (6%)	17	14
All	All	1301/1332 (98%)	1191 (92%)	110 (8%)	10	7

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	339	LEU
1	C	97	LEU
1	D	266	GLN
1	B	383	LYS
1	B	406	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	85	ASN
1	C	286	HIS
1	D	327	GLN
1	C	93	GLN
1	C	266	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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
4	TLA	B	411	2	3,9,9	3.37	3 (100%)	6,12,12	3.83	3 (50%)
3	PPF	C	413	2	3,6,6	2.01	1 (33%)	5,9,9	1.14	0
3	PPF	A	410	2	3,6,6	1.59	1 (33%)	5,9,9	0.82	0
3	PPF	D	412	2	3,6,6	1.75	1 (33%)	5,9,9	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLA	B	411	2	-	0/4/12/12	-
3	PPF	C	413	2	-	0/0/6/6	-
3	PPF	A	410	2	-	0/0/6/6	-
3	PPF	D	412	2	-	0/0/6/6	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	411	TLA	C3-C2	-3.94	1.38	1.53
4	B	411	TLA	O2-C2	-3.46	1.35	1.42
4	B	411	TLA	O3-C3	-2.54	1.37	1.42
3	D	412	PPF	P1-O2	-2.32	1.48	1.54
3	C	413	PPF	P1-O2	-2.31	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	411	TLA	C4-C3-C2	-6.93	98.20	113.11
4	B	411	TLA	O2-C2-C3	5.21	126.31	108.90
4	B	411	TLA	C1-C2-C3	-3.26	106.10	113.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	413	PPF	6	0
3	A	410	PPF	2	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 ⓘ

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.