



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2021 – 11:04 am BST

PDB ID : 6FEI
Title : Phosphotriesterase PTE_A53_1
Authors : Dym, O.; Aggarwal, N.; Albeck, S.; Unger, T.; Hamer Rogotner, S.; Silman, I.; Leader, H.; Ashani, Y.; Goldsmith, M.; Greisen, P.; Tawfik, D.; Sussman, L.J.
Deposited on : 2018-01-02
Resolution : 1.70 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) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

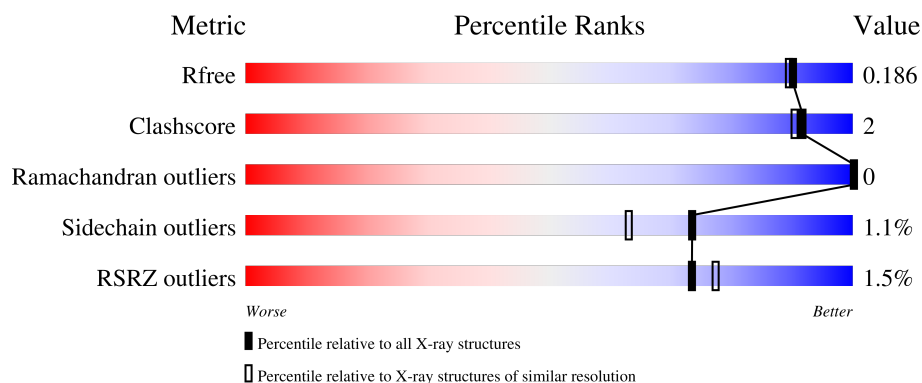
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	337	<div> <div>%</div> <div>94%</div> <div>• •</div> </div>
1	B	337	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>

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
2	FMT	B	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5590 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	2	0
			2489	1573	439	470	7			
1	B	337	Total	C	N	O	S	0	2	0
			2563	1620	449	487	7			

There are 30 discrepancies between the modelled and reference sequences:

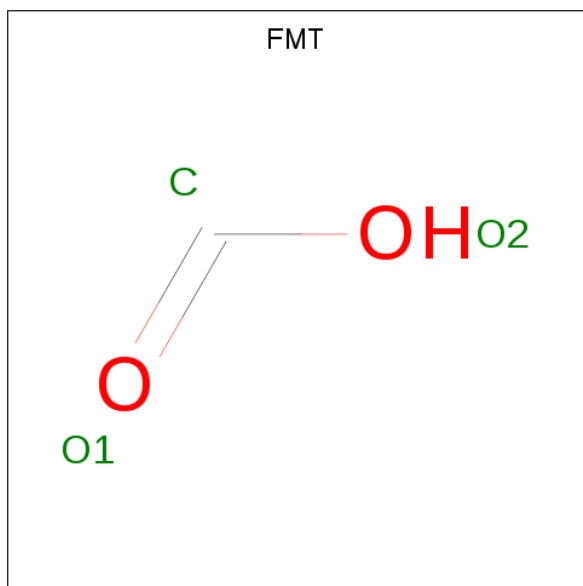
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ILE	-	expression tag	UNP P0A434
A	30	SER	-	expression tag	UNP P0A434
A	31	GLU	-	expression tag	UNP P0A434
A	32	PHE	-	expression tag	UNP P0A434
A	33	ILE	-	expression tag	UNP P0A434
A	77	ALA	LYS	conflict	UNP P0A434
A	80	VAL	ALA	conflict	UNP P0A434
A	106	ALA	ILE	conflict	UNP P0A434
A	132	GLU	PHE	conflict	UNP P0A434
A	173	GLN	THR	conflict	UNP P0A434
A	185	ARG	LYS	conflict	UNP P0A434
A	203	PHE	ALA	conflict	UNP P0A434
A	254	GLY	HIS	conflict	UNP P0A434
A	274	ASN	ILE	conflict	UNP P0A434
A	319	SER	ARG	conflict	UNP P0A434
B	26	ILE	-	expression tag	UNP P0A434
B	27	SER	-	expression tag	UNP P0A434
B	28	GLU	-	expression tag	UNP P0A434
B	29	PHE	-	expression tag	UNP P0A434
B	30	ILE	-	expression tag	UNP P0A434
B	77	ALA	LYS	conflict	UNP P0A434
B	80	VAL	ALA	conflict	UNP P0A434
B	106	ALA	ILE	conflict	UNP P0A434
B	132	GLU	PHE	conflict	UNP P0A434
B	173	GLN	THR	conflict	UNP P0A434

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	185	ARG	LYS	conflict	UNP P0A434
B	203	PHE	ALA	conflict	UNP P0A434
B	254	GLY	HIS	conflict	UNP P0A434
B	274	ASN	ILE	conflict	UNP P0A434
B	319	SER	ARG	conflict	UNP P0A434

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).

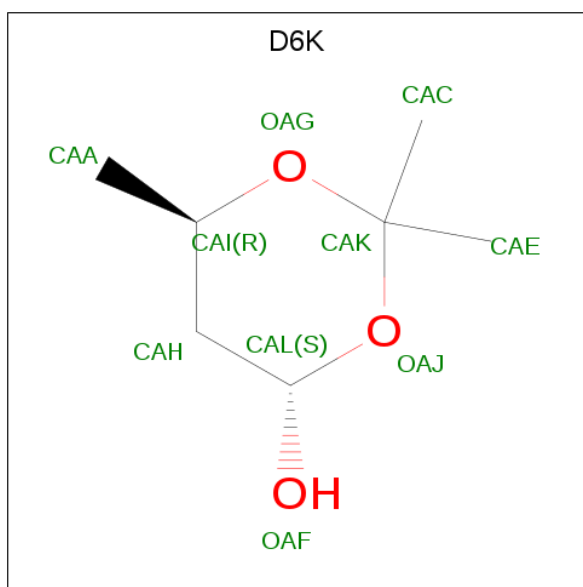


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is (4 {S},6 {R})-2,2,6-trimethyl-1,3-dioxan-4-ol (three-letter code: D6K) (formula: C₇H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	7	3		

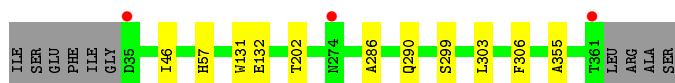
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	271	Total	O	0	0
			271	271		
5	B	247	Total	O	0	0
			247	247		

3 Residue-property plots [i](#)

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 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.

- Molecule 1: Parathion hydrolase



- Molecule 1: Parathion hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.23Å 81.25Å 70.67Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	39.17 – 1.70 39.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.17-1.70) 99.7 (39.18-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1692: ???)	Depositor
R, R_{free}	0.155 , 0.185 0.156 , 0.186	Depositor DCC
R_{free} test set	3397 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5590	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, FMT, D6K

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	0.34	0/2536	0.56	0/3447
1	B	0.34	0/2615	0.54	0/3552
All	All	0.34	0/5151	0.55	0/6999

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	THR	Peptide

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	2489	0	2483	5	0
1	B	2563	0	2560	11	0
2	A	3	0	0	0	0
2	B	3	0	0	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	10	0	0	0	0
5	A	271	0	0	1	0
5	B	247	0	0	1	0
All	All	5590	0	5043	16	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 2.

The worst 5 of 16 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:B:169:LYS:NZ	2:B:401:FMT:C	1.69	1.49
1:B:169:LYS:HZ2	2:B:401:FMT:C	1.20	1.47
1:B:207:ARG:HE	1:B:239:TYR:HB2	1.49	0.77
1:B:169:LYS:CE	2:B:401:FMT:C	2.71	0.69
1:B:274:ASN:OD1	5:B:501:HOH:O	2.20	0.49

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	327/337 (97%)	320 (98%)	7 (2%)	0	100	100
1	B	335/337 (99%)	328 (98%)	7 (2%)	0	100	100
All	All	662/674 (98%)	648 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	259/270 (96%)	257 (99%)	2 (1%)	81	74
1	B	269/270 (100%)	265 (98%)	4 (2%)	65	51
All	All	528/540 (98%)	522 (99%)	6 (1%)	73	63

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	PHE
1	B	299	SER
1	B	306	PHE
1	A	306	PHE
1	A	299	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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$
2	FMT	A	401	3	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B	401	3	0,2,2	0.00	-	0,1,1	0.00	-
4	D6K	A	404	3	10,10,10	1.47	1 (10%)	13,15,15	2.89	7 (53%)

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	D6K	A	404	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	D6K	OAJ-CAL	2.48	1.47	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	D6K	OAG-CAI-CAH	-5.35	103.82	109.36
4	A	404	D6K	CAE-CAK-CAC	-4.35	107.64	112.92
4	A	404	D6K	CAA-CAI-CAH	-4.11	106.95	113.40
4	A	404	D6K	OAJ-CAK-CAE	3.37	119.27	108.59
4	A	404	D6K	OAJ-CAK-OAG	-3.16	106.74	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FMT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	30:ILE	C	34:GLY	N	6.79

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, 95th 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 ²)	Q<0.9
1	A	327/337 (97%)	-0.14	3 (0%) 84 87	17, 21, 30, 54	0
1	B	337/337 (100%)	-0.12	7 (2%) 63 67	18, 24, 36, 53	0
All	All	664/674 (98%)	-0.13	10 (1%) 73 77	17, 23, 33, 54	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	PHE	5.6
1	B	365	SER	3.8
1	A	35	ASP	3.5
1	B	34	GLY	3.4
1	B	30	ILE	3.1

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 monosaccharides 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, 95th 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(\AA^2)	Q<0.9
4	D6K	A	404	10/10	0.74	0.19	21,27,33,38	0
2	FMT	B	401	3/3	0.92	0.09	21,21,22,24	0
2	FMT	A	401	3/3	0.94	0.08	17,17,17,19	0
3	ZN	B	403	1/1	0.99	0.04	24,24,24,24	0
3	ZN	B	402	1/1	1.00	0.06	23,23,23,23	0
3	ZN	A	402	1/1	1.00	0.05	20,20,20,20	0
3	ZN	A	403	1/1	1.00	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.