Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:38 PM JST

PDB ID	:	5YFE
Title	:	Enzymatic and structural characterization of the poly (ethylene terephthalate) hydrolase PETase from I. sakaiensis
Authors	:	Bao, R.; He, L.H.; Liu, B.
Deposited on	:	2017-09-21
Resolution	:	1.39 Å(reported)

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

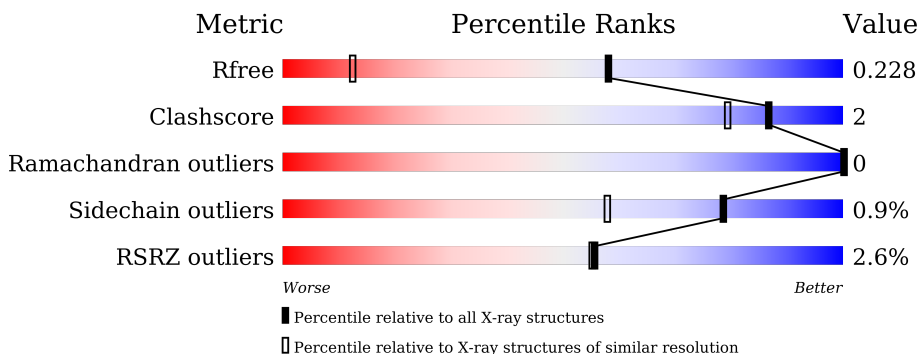|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.39 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.9%
RSRZ outliers		2.6%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 <=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	272	3% ... 85% ... 13% ··

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3971 atoms, of which 1906 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 Poly(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	268	3865	1218	1891	354	391	11	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	THR	engineered mutation	UNP A0A0K8P6T7
A	198	ALA	ARG	engineered mutation	UNP A0A0K8P6T7
A	261	ASN	ALA	engineered mutation	UNP A0A0K8P6T7
A	265	LEU	-	expression tag	UNP A0A0K8P6T7
A	266	GLU	-	expression tag	UNP A0A0K8P6T7
A	267	HIS	-	expression tag	UNP A0A0K8P6T7
A	268	HIS	-	expression tag	UNP A0A0K8P6T7
A	269	HIS	-	expression tag	UNP A0A0K8P6T7
A	270	HIS	-	expression tag	UNP A0A0K8P6T7
A	271	HIS	-	expression tag	UNP A0A0K8P6T7
A	272	HIS	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO   OH

O1   O2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	A	1	Total 13	C 3	H 7	O 3	0	0

WORLDWIDE
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PROTEIN DATA BANK

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0

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: Poly(ethylene terephthalate) hydrolase
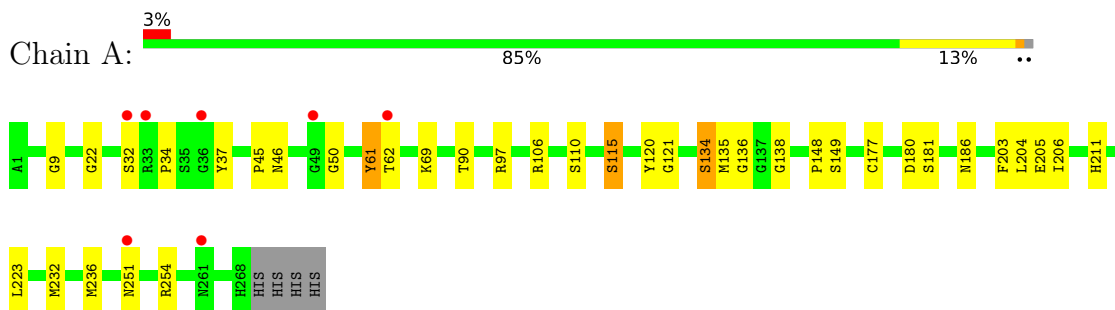
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.95Å 56.64Å 80.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 1.39 37.88 – 1.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.88-1.39) 100.0 (37.88-1.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.235 0.219 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å^2)	8.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 36.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3971	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	1.32	24/2021 (1.2%)	0.96	7/2754 (0.3%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE1	-8.30	1.16	1.25
1	A	115	SER	CB-OG	-7.62	1.32	1.42
1	A	120	TYR	CG-CD1	-7.44	1.29	1.39
1	A	181	SER	CB-OG	-7.19	1.32	1.42
1	A	61	TYR	CG-CD1	-6.49	1.30	1.39
1	A	110	SER	CB-OG	-6.08	1.34	1.42
1	A	45	PRO	C-O	-6.06	1.11	1.23
1	A	206	ILE	C-O	-5.97	1.12	1.23
1	A	22	GLY	N-CA	-5.67	1.37	1.46
1	A	50	GLY	C-O	-5.61	1.14	1.23
1	A	121	GLY	C-O	-5.53	1.14	1.23
1	A	148	PRO	C-O	-5.50	1.12	1.23
1	A	134	SER	C-O	-5.46	1.12	1.23
1	A	186	ASN	C-O	-5.35	1.13	1.23
1	A	136	GLY	C-O	-5.30	1.15	1.23
1	A	223	LEU	C-O	-5.29	1.13	1.23
1	A	135	MET	C-O	-5.28	1.13	1.23
1	A	46	ASN	C-O	-5.25	1.13	1.23
1	A	120	TYR	CE1-CZ	-5.24	1.31	1.38
1	A	149	SER	C-O	-5.23	1.13	1.23
1	A	97	ARG	CZ-NH2	-5.23	1.26	1.33
1	A	9	GLY	C-O	-5.22	1.15	1.23
1	A	203	PHE	CG-CD2	-5.08	1.31	1.38
1	A	138	GLY	C-O	-5.04	1.15	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	106	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	97	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	97	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	106	ARG	CD-NE-CZ	6.77	133.07	123.60
1	A	251	ASN	CB-CA-C	5.69	121.77	110.40
1	A	69	LYS	CD-CE-NZ	5.32	123.94	111.70

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	1974	1891	1891	8	0
2	A	10	0	0	0	0
3	A	12	15	16	0	0
4	A	69	0	0	0	0
All	All	2065	1906	1907	8	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.

All (8) 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:62:THR:HA	1:A:90:THR:HB	1.81	0.61
1:A:34:PRO:HB3	1:A:37:TYR:CZ	2.40	0.56
1:A:134:SER:OG	1:A:211:HIS:CE1	2.66	0.48
1:A:61:TYR:C	1:A:62:THR:HG23	2.36	0.46
1:A:204:LEU:C	1:A:204:LEU:HD23	2.36	0.45
1:A:232:MET:O	1:A:236:MET:HB2	2.19	0.43
1:A:254:ARG:HG3	1:A:254:ARG:HH11	1.84	0.41
1:A:177:CYS:O	1:A:180:ASP:HB2	2.22	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	266/272 (98%)	258 (97%)	8 (3%)	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	213/217 (98%)	211 (99%)	2 (1%)	78	58

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	261	ASN

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 ⓘ

4 ligands are modelled in this entry.

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	$\#|Z| > 2$
3	GOL	A	303	-	5,5,5	0.75	0	5,5,5	0.59	0
2	SO4	A	302	-	4,4,4	0.29	0	6,6,6	0.63	0
3	GOL	A	304	-	5,5,5	0.63	0	5,5,5	1.01	0
2	SO4	A	301	-	4,4,4	0.35	0	6,6,6	1.03	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
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	A	304	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	268/272 (98%)	0.35	7 (2%)	56	55	4, 10, 21, 42	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	ASN	3.2
1	A	36	GLY	2.6
1	A	49	GLY	2.6
1	A	33	ARG	2.5
1	A	32	SER	2.3
1	A	62	THR	2.3
1	A	261	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	SO4	A	302	5/5	0.82	0.24	30,54,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	301	5/5	0.85	0.15	10,20,23,36	5
3	GOL	A	304	6/6	0.91	0.14	17,20,25,28	0
3	GOL	A	303	6/6	0.93	0.17	16,37,49,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.