

# Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2022 – 08:14 am GMT

PDB ID : 7OSB

Title : Crystal Structure of a Double Mutant PETase (S238F/W159H) from Ideonella

sakaiensis

Authors: Shakespeare, T.J.; Zahn, M.; Allen, M.D.; McGeehan, J.E.

Deposited on : 2021-06-08

Resolution : 1.45 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.24

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

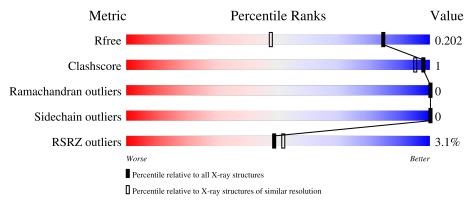
Validation Pipeline (wwPDB-VP) : 2.24

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.45 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	298	88%	• 11%
1	В	298	88%	11%
1	С	298	87%	• 11%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7047 atoms, of which 0 are hydrogens and 0 are deuteriums.

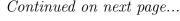
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Poly(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	266	Total	С	N	О	S	0	2	0
1	A	200	1973	1219	355	388	11	0		
1	В	264	Total	С	N	О	S	0	6	0
1	Ъ	204	1973	1220	355	387	11	U		
1	С	C 264	Total	С	N	О	S	0	2	0
1			1954	1208	351	384	11		2	U

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	HIS	TRP	engineered mutation	UNP A0A0K8P6T7
A	238	PHE	SER	engineered mutation	UNP A0A0K8P6T7
A	291	LEU	-	linker	UNP A0A0K8P6T7
A	292	GLU	-	linker	UNP A0A0K8P6T7
A	293	HIS	-	expression tag	UNP A0A0K8P6T7
A	294	HIS	-	expression tag	UNP A0A0K8P6T7
A	295	HIS	-	expression tag	UNP A0A0K8P6T7
A	296	HIS	-	expression tag	UNP A0A0K8P6T7
A	297	HIS	-	expression tag	UNP A0A0K8P6T7
A	298	HIS	-	expression tag	UNP A0A0K8P6T7
В	159	HIS	TRP	engineered mutation	UNP A0A0K8P6T7
В	238	PHE	SER	engineered mutation	UNP A0A0K8P6T7
В	291	LEU	-	linker	UNP A0A0K8P6T7
В	292	GLU	-	linker	UNP A0A0K8P6T7
В	293	HIS	-	expression tag	UNP A0A0K8P6T7
В	294	HIS	-	expression tag	UNP A0A0K8P6T7
В	295	HIS	-	expression tag	UNP A0A0K8P6T7
В	296	HIS	-	expression tag	UNP A0A0K8P6T7
В	297	HIS	-	expression tag	UNP A0A0K8P6T7
В	298	HIS	=	expression tag	UNP A0A0K8P6T7
С	159	HIS	TRP	engineered mutation	UNP A0A0K8P6T7
С	238	PHE	SER	engineered mutation	UNP A0A0K8P6T7
С	291	LEU	-	linker	UNP A0A0K8P6T7

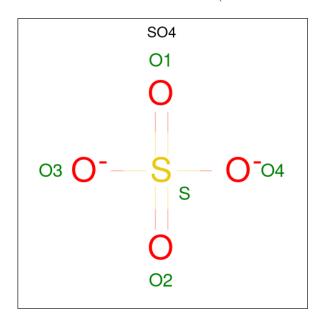




 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled	Actual	Comment	Reference
С	292	GLU	-	linker	UNP A0A0K8P6T7
С	293	HIS	-	expression tag	UNP A0A0K8P6T7
С	294	HIS	-	expression tag	UNP A0A0K8P6T7
С	295	HIS	-	expression tag	UNP A0A0K8P6T7
С	296	HIS	-	expression tag	UNP A0A0K8P6T7
С	297	HIS	-	expression tag	UNP A0A0K8P6T7
С	298	HIS	-	expression tag	UNP A0A0K8P6T7

 $\bullet$  Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



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

Continued on next page...



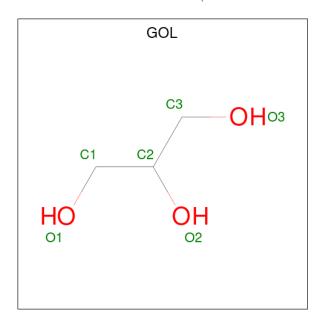
 $Continued\ from\ previous\ page...$ 

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

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C O 6 3 3	0	0
4	С	1	Total C O 6 3 3	0	0

• Molecule 5 is water.



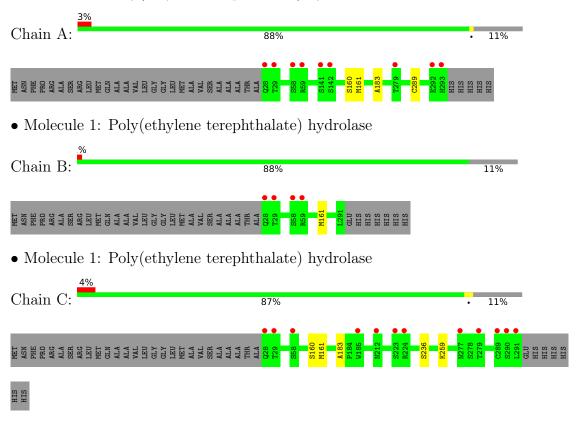
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	372	Total O 372 372	0	0
5	В	352	Total O 352 352	0	0
5	С	358	Total O 358 358	0	0



## 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	C 2 2 21	Depositor
Cell constants	52.38Å 233.96Å 164.81Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.02 - 1.45	Depositor
resolution (A)	21.02 - 1.45	EDS
% Data completeness	99.9 (21.02-1.45)	Depositor
(in resolution range)	99.9 (21.02-1.45)	EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.62  (at  1.45Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
P.P.	0.191 , $0.207$	Depositor
$R, R_{free}$	0.187 , $0.202$	DCC
$R_{free}$ test set	8759 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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: SO4, CL, 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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.46	0/2025	0.58	0/2756
1	В	0.40	0/2036	0.57	0/2770
1	С	0.41	0/2005	0.56	0/2730
All	All	0.42	0/6066	0.57	0/8256

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1973	0	1903	3	0
1	В	1973	0	1919	1	0
1	С	1954	0	1890	4	0
2	A	15	0	0	0	0
2	В	25	0	0	0	0
2	С	10	0	0	0	0
3	A	1	0	0	1	0
3	В	1	0	0	1	0
3	С	1	0	0	1	0
4	В	6	0	8	0	0

Continued on next page...



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	С	6	0	8	1	0
5	A	372	0	0	1	1
5	В	352	0	0	0	0
5	С	358	0	0	1	0
All	All	7047	0	5728	8	1

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 1.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance} (\mathrm{\AA})$	overlap (Å)
1:C:236:SER:OG	4:C:302:GOL:H12	1.92	0.69
1:B:161:MET:HG3	3:B:304:CL:CL	2.47	0.51
1:C:259:LYS:NZ	5:C:401:HOH:O	2.43	0.50
1:A:161:MET:HG3	3:A:302:CL:CL	2.51	0.48
1:C:161:MET:HG3	3:C:303:CL:CL	2.55	0.43
1:C:160:SER:HA	1:C:183:ALA:O	2.20	0.42
1:A:289:CYS:O	5:A:401:HOH:O	2.21	0.42
1:A:160:SER:HA	1:A:183:ALA:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
5:A:401:HOH:O	5:A:586:HOH:O[8_445]	1.92	0.28

#### 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	Perce	entiles
1	A	$266/298\ (89\%)$	262 (98%)	4 (2%)	0	100	100
1	В	268/298 (90%)	263 (98%)	5 (2%)	0	100	100
1	С	264/298~(89%)	260 (98%)	4 (2%)	0	100	100
All	All	798/894 (89%)	785 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Perce	ntiles
1	A	214/234~(92%)	214 (100%)	0	100	100
1	В	216/234 (92%)	216 (100%)	0	100	100
1	С	212/234 (91%)	212 (100%)	0	100	100
All	All	642/702 (92%)	642 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

#### 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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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).

Mal	Trino	Chain	Dag	Timle	В	ond leng	gths	В	ond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	SO4	В	305	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	С	304	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	В	301	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	В	306	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	В	302	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	A	301	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	С	301	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.05	0
4	GOL	В	303	-	5,5,5	0.11	0	5,5,5	0.32	0
2	SO4	В	307	-	4,4,4	0.38	0	6,6,6	0.05	0
4	GOL	С	302	-	5,5,5	0.10	0	5,5,5	0.34	0
2	SO4	A	303	-	4,4,4	0.38	0	6,6,6	0.06	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	GOL	С	302	-	-	2/4/4/4	_
4	GOL	В	303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	302	GOL	O1-C1-C2-C3
4	С	302	GOL	O1-C1-C2-O2



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	302	GOL	1	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 (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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	266/298~(89%)	-0.22	9 (3%) 45 48	16, 22, 36, 54	0
1	В	264/298 (88%)	-0.13	4 (1%) 73 74	22, 28, 36, 56	0
1	С	264/298 (88%)	-0.02	12 (4%) 33 36	22, 29, 39, 60	0
All	All	794/894 (88%)	-0.13	25 (3%) 49 52	16, 27, 37, 60	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	28	GLN	9.3
1	В	28	GLN	8.1
1	A	28	GLN	6.6
1	С	291	LEU	6.4
1	A	293	HIS	5.2
1	С	290	SER	4.5
1	A	279	THR	3.5
1	С	29	THR	3.4
1	В	58	SER	3.4
1	В	59	ARG	3.0
1	A	292	GLU	2.9
1	С	277	ASN	2.7
1	A	29	THR	2.6
1	С	279	THR	2.6
1	В	29	THR	2.5
1	A	59	ARG	2.4
1	С	58	SER	2.3
1	С	223	SER	2.3
1	A	142	SER	2.2
1	С	185	TRP	2.2
1	С	289	CYS	2.1
1	A	58[A]	SER	2.1
1	С	224	ARG	2.1

Continued on next page...



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Res	Type	RSRZ
1	A	141	SER	2.0
1	С	212	ASN	2.0

### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	SO4	В	307	5/5	0.59	0.20	132,132,132,132	0
4	GOL	С	302	6/6	0.70	0.20	51,53,54,55	0
2	SO4	В	306	5/5	0.76	0.18	105,105,105,105	0
2	SO4	A	304	5/5	0.81	0.19	87,87,87,87	0
2	SO4	С	304	5/5	0.87	0.25	64,64,65,65	0
4	GOL	В	303	6/6	0.88	0.13	35,38,40,42	0
2	SO4	В	305	5/5	0.88	0.26	64,64,64,64	0
2	SO4	A	303	5/5	0.93	0.20	71,71,71,71	0
2	SO4	A	301	5/5	0.95	0.14	37,37,38,38	0
3	CL	В	304	1/1	0.95	0.07	37,37,37,37	0
3	CL	A	302	1/1	0.97	0.05	32,32,32,32	0
2	SO4	В	302	5/5	0.97	0.23	49,49,50,50	0
3	CL	С	303	1/1	0.98	0.05	33,33,33,33	0
2	SO4	С	301	5/5	0.98	0.16	35,36,36,36	0
2	SO4	В	301	5/5	0.98	0.16	42,42,42,43	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

