



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 12:47 AM JST

PDB ID : 8J17  
Title : Crystal structure of IsPETase variant  
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Deposited on : 2023-04-12  
Resolution : 1.97 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](mailto: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>.

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

MolProbity : 4.02b-467  
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

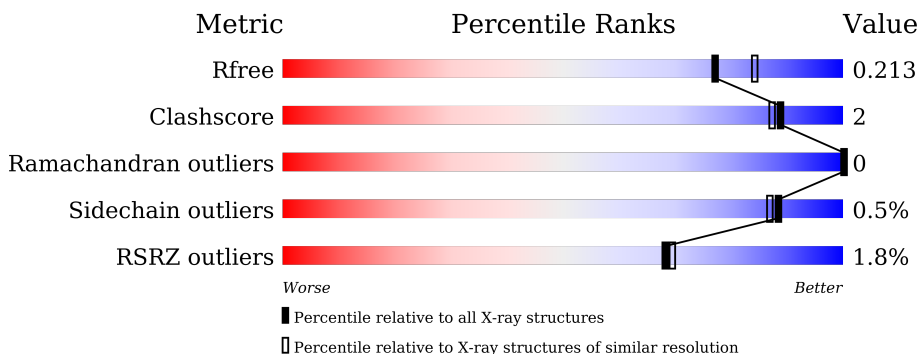
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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	272	 2% 95% 7% . .
1	B	272	 2% 90% 7% .
1	C	272	 % 91% 5% .

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6530 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
			Total	C	N	O	S			
1	A	262	1923	1190	344	378	11	0	0	0
1	B	262	1923	1190	344	378	11	0	0	0
1	C	262	1923	1190	344	378	11	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0A0K8P6T7
A	92	PRO	SER	variant	UNP A0A0K8P6T7
A	157	ALA	ASP	variant	UNP A0A0K8P6T7
A	262	LEU	-	expression tag	UNP A0A0K8P6T7
A	263	GLU	-	expression tag	UNP A0A0K8P6T7
A	264	HIS	-	expression tag	UNP A0A0K8P6T7
A	265	HIS	-	expression tag	UNP A0A0K8P6T7
A	266	HIS	-	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
B	-2	MET	-	initiating methionine	UNP A0A0K8P6T7
B	92	PRO	SER	variant	UNP A0A0K8P6T7
B	157	ALA	ASP	variant	UNP A0A0K8P6T7
B	262	LEU	-	expression tag	UNP A0A0K8P6T7
B	263	GLU	-	expression tag	UNP A0A0K8P6T7
B	264	HIS	-	expression tag	UNP A0A0K8P6T7
B	265	HIS	-	expression tag	UNP A0A0K8P6T7
B	266	HIS	-	expression tag	UNP A0A0K8P6T7
B	267	HIS	-	expression tag	UNP A0A0K8P6T7
B	268	HIS	-	expression tag	UNP A0A0K8P6T7
B	269	HIS	-	expression tag	UNP A0A0K8P6T7
C	-2	MET	-	initiating methionine	UNP A0A0K8P6T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	92	PRO	SER	variant	UNP A0A0K8P6T7
C	157	ALA	ASP	variant	UNP A0A0K8P6T7
C	262	LEU	-	expression tag	UNP A0A0K8P6T7
C	263	GLU	-	expression tag	UNP A0A0K8P6T7
C	264	HIS	-	expression tag	UNP A0A0K8P6T7
C	265	HIS	-	expression tag	UNP A0A0K8P6T7
C	266	HIS	-	expression tag	UNP A0A0K8P6T7
C	267	HIS	-	expression tag	UNP A0A0K8P6T7
C	268	HIS	-	expression tag	UNP A0A0K8P6T7
C	269	HIS	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	323	Total O 323 323	0	0
2	B	219	Total O 219 219	0	0
2	C	219	Total O 219 219	0	0

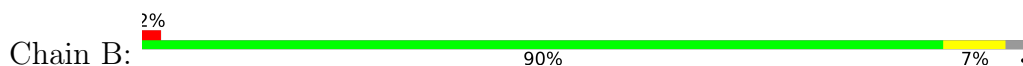
### 3 Residue-property plots [i](#)

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



- Molecule 1: Poly(ethylene terephthalate) hydrolase



- Molecule 1: Poly(ethylene terephthalate) hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.56Å 233.80Å 163.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 1.97 58.45 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.92-1.97) 99.8 (58.45-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.97Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.175 , 0.213 0.175 , 0.213	Depositor DCC
$R_{free}$ test set	3531 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtrriage
Anisotropy	0.638	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.37	0/1969	0.55	0/2684
1	B	0.37	0/1969	0.54	0/2684
1	C	0.37	0/1969	0.53	0/2684
All	All	0.37	0/5907	0.54	0/8052

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	1923	0	1858	2	0
1	B	1923	0	1858	10	0
1	C	1923	0	1858	10	0
2	A	323	0	0	0	0
2	B	219	0	0	2	0
2	C	219	0	0	5	0
All	All	6530	0	5574	22	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 (22) 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:C:63:SER:HA	1:C:66:LYS:HD2	1.72	0.70
1:B:54:ILE:HG22	1:B:65:ILE:HD13	1.79	0.64
1:B:54:ILE:CG2	1:B:65:ILE:HD13	2.36	0.55
1:C:66:LYS:NZ	2:C:304:HOH:O	2.29	0.53
1:C:75:HIS:HD2	2:C:346:HOH:O	1.92	0.50
1:C:103:ARG:HD3	2:C:366:HOH:O	2.13	0.48
1:C:194:SER:HB2	2:C:450:HOH:O	2.13	0.47
1:B:72:LEU:HD23	1:B:226:VAL:HG22	1.97	0.46
1:C:24:ARG:HH11	1:C:43:THR:HG21	1.80	0.45
1:C:75:HIS:HE1	2:C:329:HOH:O	2.00	0.45
1:A:66:LYS:HE2	1:A:66:LYS:HB3	1.59	0.44
1:B:194:SER:HB2	2:B:406:HOH:O	2.18	0.43
1:C:168:PRO:HA	1:C:197:ALA:O	2.18	0.43
1:B:168:PRO:HA	1:B:197:ALA:O	2.17	0.43
1:B:190:TYR:CD1	1:B:200:PHE:HB2	2.54	0.42
1:B:252:VAL:O	2:B:301:HOH:O	2.21	0.42
1:B:58:TYR:CD2	1:B:59:THR:HG23	2.54	0.42
1:C:51:ALA:HA	1:C:78:VAL:O	2.20	0.42
1:B:51:ALA:HA	1:B:78:VAL:O	2.20	0.41
1:A:131:SER:HA	1:A:154:ALA:O	2.21	0.41
1:B:84:THR:HG21	1:B:94:ARG:HG2	2.02	0.41
1:C:152:PRO:HG2	1:C:171:ILE:HD13	2.03	0.40

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	260/272 (96%)	257 (99%)	3 (1%)	0	100	100
1	B	260/272 (96%)	255 (98%)	5 (2%)	0	100	100
1	C	260/272 (96%)	256 (98%)	4 (2%)	0	100	100
All	All	780/816 (96%)	768 (98%)	12 (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	Percentiles	
1	A	207/217 (95%)	207 (100%)	0	100	100
1	B	207/217 (95%)	205 (99%)	2 (1%)	76	73
1	C	207/217 (95%)	206 (100%)	1 (0%)	88	87
All	All	621/651 (95%)	618 (100%)	3 (0%)	88	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	SER
1	B	261	SER
1	C	209	SER

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](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/272 (96%)	0.59	6 (2%) 60 62	30, 39, 50, 68	0
1	B	262/272 (96%)	0.22	5 (1%) 66 68	34, 43, 55, 71	0
1	C	262/272 (96%)	0.20	3 (1%) 80 82	33, 44, 55, 80	0
All	All	786/816 (96%)	0.33	14 (1%) 68 69	30, 42, 55, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	CYS	3.2
1	B	30	ARG	3.0
1	A	100	ALA	2.7
1	A	261	SER	2.5
1	C	261	SER	2.4
1	A	251	ARG	2.4
1	B	260	CYS	2.4
1	B	58	TYR	2.3
1	A	147	LEU	2.2
1	B	201	LEU	2.2
1	A	201	LEU	2.1
1	B	156	TRP	2.1
1	A	171	ILE	2.1
1	C	220	LEU	2.1

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.