



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9KL9 / pdb\_00009kl9  
Title : crystal structure of a mutant Poly(Ethylene terephthalate) hydrolase  
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Deposited on : 2024-11-14  
Resolution : 2.90 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](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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Metric

(#Entries)

 $(\# \text{Entries, resolution range}(\text{\AA}))$  $R_{free}$ 

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164625

2335 (2.90-2.90)

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Clashscore

180529

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2564 (2.90-2.90)

### Ramachandran outliers

177936

2514 (2.90-2.90)

Sidechain outliers

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177891

2516 (2.90-2.90)

RSRZ outliers

164620

2337 (2.90-2.90)

*Worse*

*Better*

Percentile relative to all X-ray structures

▮ Percentile relative to X-ray structures of similar resolution

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
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Quality of chain

1

A

270

81%

14%

•

1

B

270

85%

119

•

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3916 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	A	259	Total	C	N	O	S	0	0	0
			1962	1231	350	375	6			
1	B	258	Total	C	N	O	S	0	0	0
			1954	1225	349	374	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A2H5Z9R5
A	185	ASN	HIS	conflict	UNP A0A2H5Z9R5
A	189	MET	PHE	conflict	UNP A0A2H5Z9R5
A	210	THR	PHE	conflict	UNP A0A2H5Z9R5
A	261	LEU	-	expression tag	UNP A0A2H5Z9R5
A	262	GLU	-	expression tag	UNP A0A2H5Z9R5
A	263	LEU	-	expression tag	UNP A0A2H5Z9R5
A	264	GLU	-	expression tag	UNP A0A2H5Z9R5
A	265	HIS	-	expression tag	UNP A0A2H5Z9R5
A	266	HIS	-	expression tag	UNP A0A2H5Z9R5
A	267	HIS	-	expression tag	UNP A0A2H5Z9R5
A	268	HIS	-	expression tag	UNP A0A2H5Z9R5
A	269	HIS	-	expression tag	UNP A0A2H5Z9R5
A	270	HIS	-	expression tag	UNP A0A2H5Z9R5
B	1	MET	-	initiating methionine	UNP A0A2H5Z9R5
B	185	ASN	HIS	conflict	UNP A0A2H5Z9R5
B	189	MET	PHE	conflict	UNP A0A2H5Z9R5
B	210	THR	PHE	conflict	UNP A0A2H5Z9R5
B	261	LEU	-	expression tag	UNP A0A2H5Z9R5
B	262	GLU	-	expression tag	UNP A0A2H5Z9R5
B	263	LEU	-	expression tag	UNP A0A2H5Z9R5
B	264	GLU	-	expression tag	UNP A0A2H5Z9R5
B	265	HIS	-	expression tag	UNP A0A2H5Z9R5
B	266	HIS	-	expression tag	UNP A0A2H5Z9R5
B	267	HIS	-	expression tag	UNP A0A2H5Z9R5

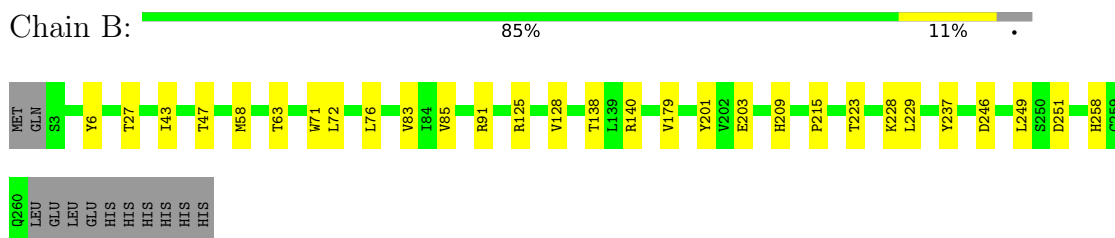
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Chain	Residue	Modelled	Actual	Comment	Reference
B	268	HIS	-	expression tag	UNP A0A2H5Z9R5
B	269	HIS	-	expression tag	UNP A0A2H5Z9R5
B	270	HIS	-	expression tag	UNP A0A2H5Z9R5



- Molecule 1: Poly(Ethylene terephthalate) hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.71Å 51.62Å 56.68Å 103.23° 103.61° 96.66°	Depositor
Resolution (Å)	32.17 – 2.90 32.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.17-2.90) 97.2 (32.17-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286, PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.195 , 0.235 0.194 , 0.236	Depositor DCC
$R_{free}$ test set	507 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% 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

### 5.1 Standard geometry

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	0.20	0/2012	0.38	2/2757 (0.1%)
1	B	0.15	0/2004	0.35	0/2746
All	All	0.18	0/4016	0.37	2/5503 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	HIS	CA-C-N	5.19	131.45	121.54
1	A	131	HIS	C-N-CA	5.19	131.45	121.54

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	1962	0	1922	24	0
1	B	1954	0	1911	17	0
All	All	3916	0	3833	40	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 5.

The worst 5 of 40 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:58:MET:HE1	1:A:72:LEU:HG	1.74	0.68
1:B:246:ASP:HB3	1:B:249:LEU:HG	1.76	0.67
1:B:63:THR:HA	1:B:91:ARG:HB3	1.82	0.59
1:A:128:VAL:HG12	1:A:138:THR:HG23	1.86	0.58
1:A:63:THR:HA	1:A:91:ARG:HB3	1.86	0.57

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	257/270 (95%)	250 (97%)	7 (3%)	0	100	100
1	B	256/270 (95%)	248 (97%)	8 (3%)	0	100	100
All	All	513/540 (95%)	498 (97%)	15 (3%)	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	215/226 (95%)	215 (100%)	0	100	100
1	B	214/226 (95%)	213 (100%)	1 (0%)	86	96
All	All	429/452 (95%)	428 (100%)	1 (0%)	92	98



All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	HIS
1	B	213	ASN
1	B	256	ASN
1	A	144	GLN
1	A	89	ASN

### 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 oligosaccharides 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	259/270 (95%)	0.13	0 100 100	11, 20, 34, 45	0
1	B	258/270 (95%)	0.09	0 100 100	12, 20, 31, 50	0
All	All	517/540 (95%)	0.11	0 100 100	11, 20, 33, 50	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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.