



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:57 AM UTC

PDB ID : 8A2C / pdb\_00008a2c  
Title : The crystal structure of the S178A mutant of PET40, a PETase enzyme from an unclassified *Amycolatopsis*  
Authors : Costanzi, E.; Applegate, V.; Port, A.; Smits, S.H.J.  
Deposited on : 2022-06-03  
Resolution : 1.60 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
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) : 2.49

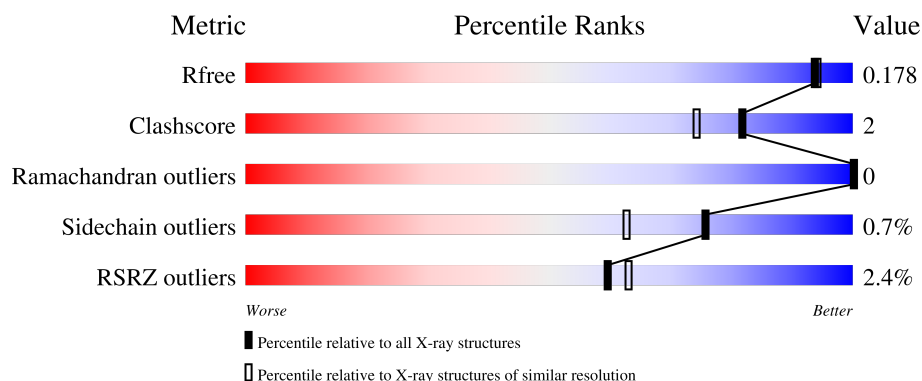
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	278	
1	B	278	

## 2 Entry composition [i](#)

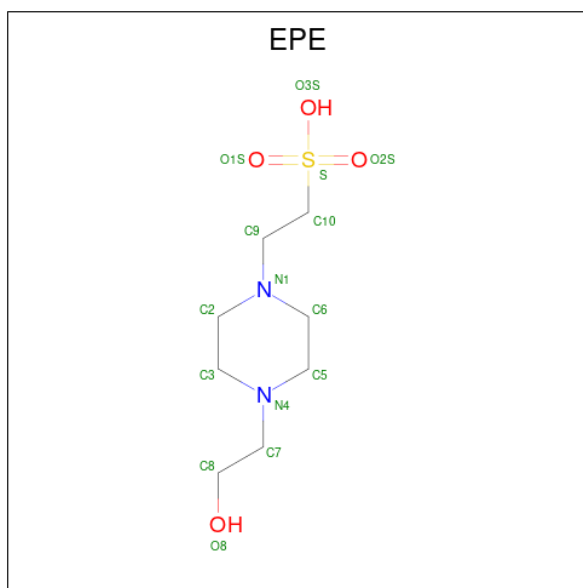
There are 6 unique types of molecules in this entry. The entry contains 8773 atoms, of which 4028 are hydrogens and 0 are deuteriums.

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 PET40 S178A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	H	N	O	S	0	7	0
			4039	1282	1994	364	396	3			
1	B	267	Total	C	H	N	O	S	0	4	0
			3992	1268	1970	360	391	3			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Cl	0	0
			7	7		
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

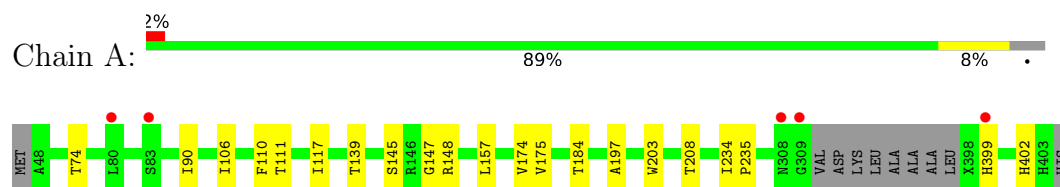
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	323	Total 323	O 323	0	0
6	B	293	Total 293	O 293	0	0

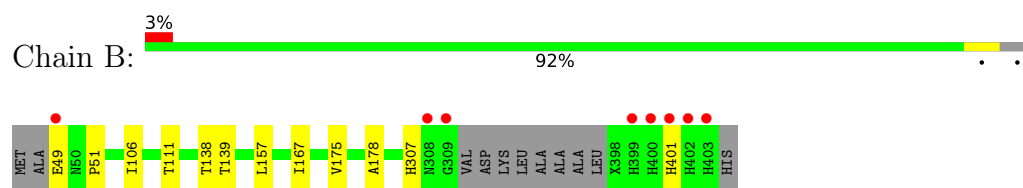
### 3 Residue-property plots [i](#)

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: PET40 S178A



#### • Molecule 1: PET40 S178A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.04Å 110.00Å 47.96Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	31.51 – 1.60 31.51 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (31.51-1.60) 97.7 (31.51-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.146 , 0.179 0.145 , 0.178	Depositor DCC
$R_{free}$ test set	3066 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, EPE, MG

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	0.58	4/2106 (0.2%)	0.66	0/2877
1	B	0.57	2/2082 (0.1%)	0.60	0/2844
All	All	0.58	6/4188 (0.1%)	0.63	0/5721

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	PRO	C-O	-6.02	1.16	1.24
1	B	307	HIS	CE1-NE2	-5.74	1.26	1.32
1	A	147	GLY	C-O	-5.63	1.17	1.23
1	A	145	SER	C-O	-5.34	1.17	1.24
1	A	402	HIS	CG-ND1	-5.22	1.32	1.38

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	2045	1994	1976	15	0
1	B	2022	1970	1960	5	0
2	A	15	17	17	1	0
2	B	15	17	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	24	24	0	0
3	B	4	6	6	0	0
4	A	7	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	323	0	0	2	0
6	B	293	0	0	1	0
All	All	4745	4028	4000	20	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 20 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:174:VAL:HG23	1:A:184[A]:THR:HG23	1.49	0.90
1:A:184[A]:THR:HG22	1:A:197:ALA:HB1	1.91	0.52
1:A:106:ILE:HG22	1:A:117:ILE:HD12	1.93	0.51
1:A:148:ARG:HH11	1:A:148:ARG:HG2	1.75	0.51
1:A:184[A]:THR:CG2	1:A:197:ALA:HB1	2.40	0.51

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	271/278 (98%)	267 (98%)	4 (2%)	0	100	100
1	B	267/278 (96%)	262 (98%)	5 (2%)	0	100	100
All	All	538/556 (97%)	529 (98%)	9 (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	224/225 (100%)	222 (99%)	2 (1%)	70	55
1	B	222/225 (99%)	220 (99%)	2 (1%)	70	55
All	All	446/450 (99%)	442 (99%)	4 (1%)	76	55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157[A]	LEU
1	A	157[B]	LEU
1	B	138	THR
1	B	401	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	286	GLN
1	A	403	HIS
1	B	260	ASN
1	B	402	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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
3	EDO	A	605	-	3,3,3	0.32	0	2,2,2	0.28	0
2	EPE	B	502	-	15,15,15	2.06	2 (13%)	19,20,20	1.89	6 (31%)
3	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	B	501	-	3,3,3	0.38	0	2,2,2	0.32	0
2	EPE	A	601	-	15,15,15	2.54	3 (20%)	19,20,20	2.01	6 (31%)
3	EDO	A	603	-	3,3,3	0.38	0	2,2,2	0.60	0
3	EDO	A	604	-	3,3,3	0.49	0	2,2,2	0.23	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	EDO	A	605	-	-	0/1/1/1	-
2	EPE	B	502	-	-	8/9/19/19	0/1/1/1
3	EDO	A	602	-	-	0/1/1/1	-
3	EDO	B	501	-	-	0/1/1/1	-
2	EPE	A	601	-	-	5/9/19/19	0/1/1/1
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	EPE	C10-S	-6.72	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	EPE	C10-S	-6.60	1.68	1.77
2	A	601	EPE	O1S-S	-4.82	1.31	1.45
2	A	601	EPE	O2S-S	-3.96	1.34	1.45
2	B	502	EPE	O3S-S	-2.53	1.37	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	EPE	O3S-S-C10	4.58	114.97	106.00
2	A	601	EPE	O1S-S-C10	4.29	113.21	106.73
2	A	601	EPE	C2-C3-N4	4.10	118.91	110.65
2	A	601	EPE	C9-N1-C2	3.62	120.87	111.24
2	A	601	EPE	C6-N1-C2	-3.51	101.27	108.84

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EPE	C10-C9-N1-C2
2	A	601	EPE	C9-C10-S-O2S
2	B	502	EPE	C10-C9-N1-C2
2	B	502	EPE	C9-C10-S-O1S
2	B	502	EPE	C9-C10-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	EPE	1	0
2	A	601	EPE	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<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	267/278 (96%)	-0.56	5 (1%) 66 70	7, 16, 31, 85	5 (1%)
1	B	266/278 (95%)	-0.53	8 (3%) 52 55	9, 17, 33, 74	2 (0%)
All	All	533/556 (95%)	-0.55	13 (2%) 59 63	7, 17, 33, 85	7 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	HIS	4.3
1	A	309	GLY	3.7
1	A	80	LEU	3.4
1	B	309	GLY	3.0
1	B	49	GLU	2.9

### 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](#)

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	602	4/4	0.82	0.15	34,43,52,57	0
3	EDO	A	604	4/4	0.85	0.15	25,31,42,50	0
3	EDO	A	603	4/4	0.86	0.12	33,40,52,53	0
5	MG	A	613	1/1	0.90	0.12	37,37,37,37	0
3	EDO	A	605	4/4	0.91	0.11	20,26,32,32	0
3	EDO	B	501	4/4	0.94	0.11	19,24,29,29	0
4	CL	B	505	1/1	0.94	0.09	34,34,34,34	0
2	EPE	B	502	15/15	0.94	0.12	15,49,73,78	0
5	MG	B	506	1/1	0.94	0.16	32,32,32,32	0
4	CL	A	610	1/1	0.96	0.06	33,33,33,33	0
2	EPE	A	601	15/15	0.97	0.09	13,37,47,50	0
4	CL	A	608	1/1	0.98	0.07	26,26,26,26	0
4	CL	A	612	1/1	0.98	0.07	22,22,22,22	0
4	CL	B	504	1/1	0.98	0.07	24,24,24,24	0
4	CL	A	607	1/1	0.99	0.07	25,25,25,25	0
4	CL	A	611	1/1	0.99	0.02	20,20,20,20	0
4	CL	A	606	1/1	0.99	0.03	19,19,19,19	0
4	CL	B	503	1/1	0.99	0.02	15,15,15,15	0
4	CL	A	609	1/1	1.00	0.04	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.