wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2026 – 10:25 PM JST

PDB ID	:	9XEH / pdb_00009xeh
Title	:	PET hydrolase mutants V53A, C208K, C257S
Authors	:	Ma, X.
Deposited on	:	2025-10-28
Resolution	:	2.87 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

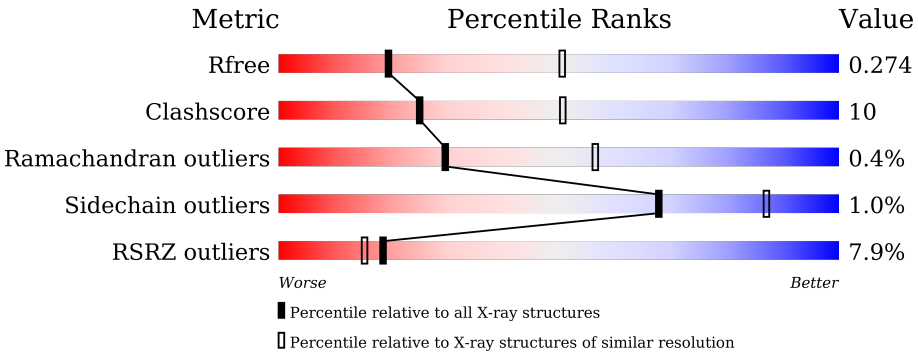
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	273	5% 83% 13% ·
1	B	273	10% 79% 17% · ·
1	C	273	8% 76% 19% · ·
1	D	273	7% 80% 15% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8173 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 PET hydrolase Z1PETase mutants V196L, C233K, C282S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1938	1199	340	386	13			
1	B	264	Total	C	N	O	S	0	0	0
			1946	1205	341	387	13			
1	C	264	Total	C	N	O	S	0	1	0
			1955	1210	342	390	13			
1	D	263	Total	C	N	O	S	0	0	0
			1938	1199	340	386	13			

- Molecule 2 is water.

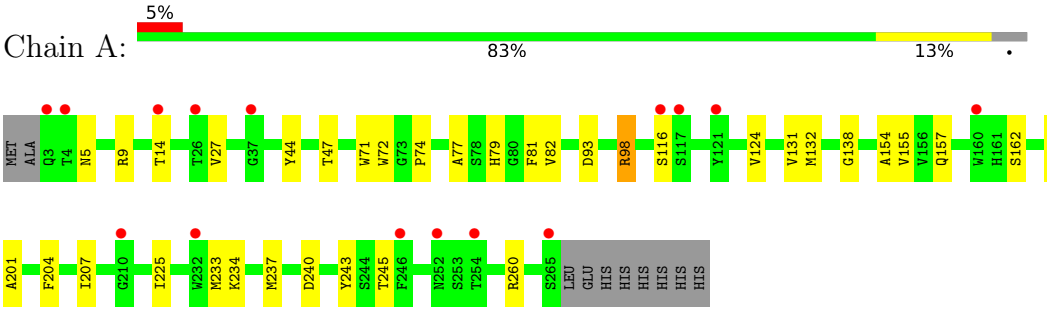
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	94	Total	O	0	0
			94	94		
2	C	100	Total	O	0	0
			100	100		
2	D	89	Total	O	0	0
			89	89		

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.

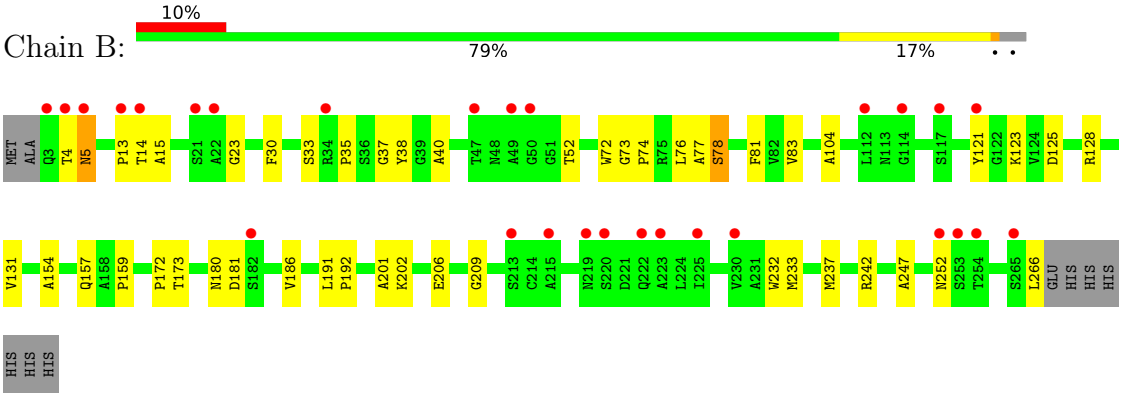
• Molecule 1: PET hydrolase Z1PETase mutants V196L, C233K, C282S

Chain A:



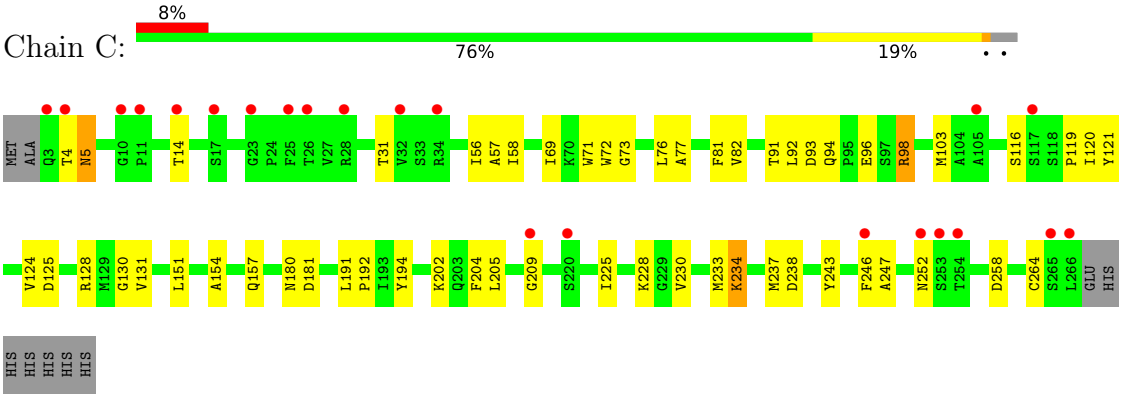
• Molecule 1: PET hydrolase Z1PETase mutants V196L, C233K, C282S

Chain B:



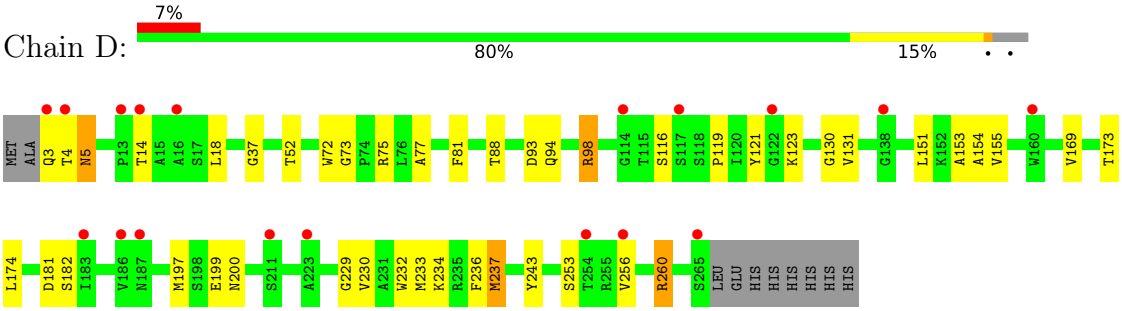
• Molecule 1: PET hydrolase Z1PETase mutants V196L, C233K, C282S

Chain C:



• Molecule 1: PET hydrolase Z1PETase mutants V196L, C233K, C282S

Chain D:


7%
80%
15%
MET ALA Q3 T4 N5 P13 T14 A15 A16 S17 L18 G37 T52 W72 G73 P74 R75 L76 A77 F81 T88 D93 Q94 R98 G114 T115 S116 S117 S118 P119 I120 Y121 G122 K123 G130 V131 G138 L151 K152 A153 A154 V155 W160 V169 T173
L174 D181 S182 I183 V186 N187 M197 S198 E199 N200 S211 A223 G229 V230 A231 W232 M233 K234 R235 F236 M237 Y243 S253 T254 R255 V256 R260 S265 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.41Å 132.89Å 79.10Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	51.41 – 2.87 51.41 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.8 (51.41-2.87) 98.8 (51.41-2.87)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.225 , 0.265 0.231 , 0.274	Depositor DCC
R_{free} test set	1231 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8173	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5300e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.55	0/1983	0.92	2/2701 (0.1%)
1	B	0.55	0/1991	0.91	1/2712 (0.0%)
1	C	0.54	0/2000	0.92	3/2724 (0.1%)
1	D	0.54	0/1983	0.93	1/2701 (0.0%)
All	All	0.54	0/7957	0.92	7/10838 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	THR	CA-CB-OG1	-7.13	98.90	109.60
1	D	181	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	258	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	238	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	181	ASP	CA-CB-CG	5.11	117.70	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	98	ARG	Sidechain
1	C	98	ARG	Sidechain
1	D	260	ARG	Sidechain
1	D	98	ARG	Sidechain

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	1938	0	1855	27	1
1	B	1946	0	1866	38	1
1	C	1955	0	1871	44	2
1	D	1938	0	1855	38	2
2	A	113	0	0	17	0
2	B	94	0	0	24	0
2	C	100	0	0	26	0
2	D	89	0	0	19	0
All	All	8173	0	7447	147	3

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 10.

The worst 5 of 147 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:D:197:MET:HE2	1:D:200:ASN:HD21	1.16	1.09
1:C:103:MET:SD	2:C:399:HOH:O	2.24	0.95
1:B:252:ASN:HA	2:B:350:HOH:O	1.75	0.87
1:B:247:ALA:HB1	2:B:384:HOH:O	1.78	0.84
1:D:197:MET:CE	1:D:200:ASN:HD21	1.91	0.83

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TYR:OH	1:D:116:SER:O[1_554]	1.37	0.83
1:C:116:SER:O	1:D:121:TYR:OH[1_554]	1.78	0.42
1:A:116:SER:O	1:B:121:TYR:OH[1_455]	1.79	0.41

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	261/273 (96%)	251 (96%)	9 (3%)	1 (0%)	30	56
1	B	262/273 (96%)	251 (96%)	10 (4%)	1 (0%)	30	56
1	C	263/273 (96%)	251 (95%)	11 (4%)	1 (0%)	30	56
1	D	261/273 (96%)	250 (96%)	10 (4%)	1 (0%)	30	56
All	All	1047/1092 (96%)	1003 (96%)	40 (4%)	4 (0%)	30	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	5	ASN
1	C	5	ASN
1	D	5	ASN

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	210/219 (96%)	208 (99%)	2 (1%)	68	87
1	B	211/219 (96%)	209 (99%)	2 (1%)	70	88
1	C	212/219 (97%)	210 (99%)	2 (1%)	70	88
1	D	210/219 (96%)	208 (99%)	2 (1%)	68	87
All	All	843/876 (96%)	835 (99%)	8 (1%)	68	88

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	237	MET
1	D	199	GLU
1	C	14	THR
1	B	78	SER
1	C	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	C	157	GLN
1	D	263	ASN
1	C	222	GLN
1	A	222	GLN

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

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, 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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	263/273 (96%)	0.70	15 (5%)	29	23	15, 28, 42, 92	0
1	B	264/273 (96%)	0.97	28 (10%)	11	10	18, 33, 53, 89	0
1	C	264/273 (96%)	0.86	22 (8%)	17	14	10, 27, 45, 96	1 (0%)
1	D	263/273 (96%)	0.92	18 (6%)	23	18	18, 31, 48, 86	0
All	All	1054/1092 (96%)	0.86	83 (7%)	18	15	10, 30, 49, 96	1 (0%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	ASN	4.8
1	D	4	THR	4.2
1	D	160	TRP	3.7
1	C	254	THR	3.7
1	C	4	THR	3.4

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.