



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:45 PM UTC

PDB ID : 6Z68 / pdb_00006z68
Title : A novel metagenomic alpha/beta-fold esterase
Authors : Bollinger, A.; Thies, S.; Hoepfner, A.; Kobus, S.; Jaeger, K.-E.; Smits, S.H.J.
Deposited on : 2020-05-28
Resolution : 1.35 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 ⓘ 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 ⓘ](#)) 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 : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

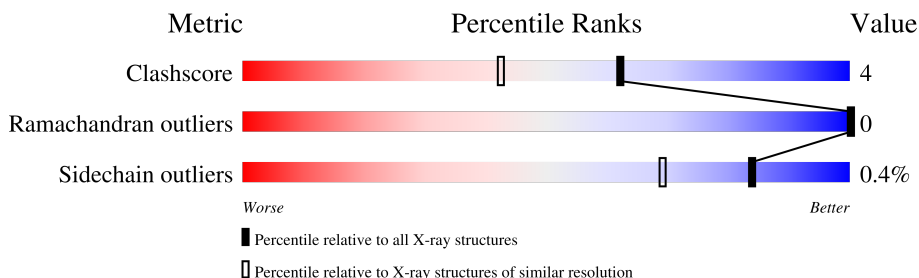
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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))
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6484 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.

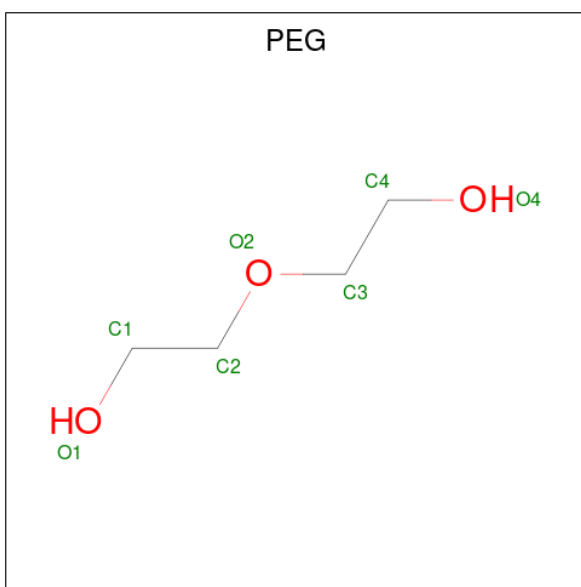
- Molecule 1 is a protein called Acetyl esterase/lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	6	0
			2773	1749	495	514	15			
1	B	357	Total	C	N	O	S	0	8	0
			2734	1726	486	506	16			

There are 18 discrepancies between the modelled and reference sequences:

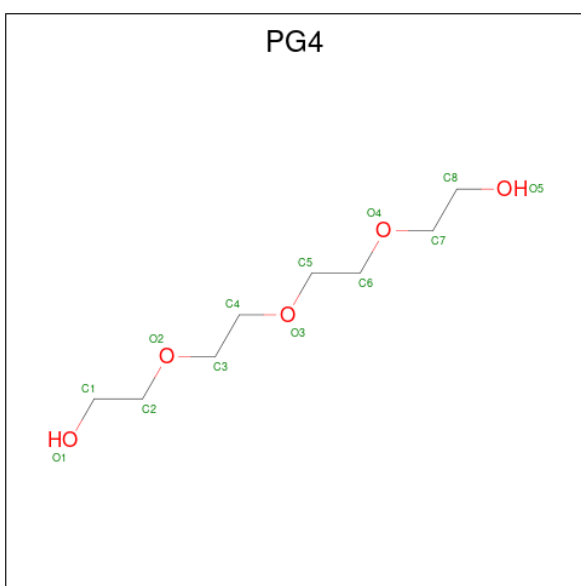
Chain	Residue	Modelled	Actual	Comment	Reference
A	271	VAL	LEU	conflict	UNP A0A1M6Y2K1
A	369	LEU	-	expression tag	UNP A0A1M6Y2K1
A	370	GLU	-	expression tag	UNP A0A1M6Y2K1
A	371	HIS	-	expression tag	UNP A0A1M6Y2K1
A	372	HIS	-	expression tag	UNP A0A1M6Y2K1
A	373	HIS	-	expression tag	UNP A0A1M6Y2K1
A	374	HIS	-	expression tag	UNP A0A1M6Y2K1
A	375	HIS	-	expression tag	UNP A0A1M6Y2K1
A	376	HIS	-	expression tag	UNP A0A1M6Y2K1
B	271	VAL	LEU	conflict	UNP A0A1M6Y2K1
B	369	LEU	-	expression tag	UNP A0A1M6Y2K1
B	370	GLU	-	expression tag	UNP A0A1M6Y2K1
B	371	HIS	-	expression tag	UNP A0A1M6Y2K1
B	372	HIS	-	expression tag	UNP A0A1M6Y2K1
B	373	HIS	-	expression tag	UNP A0A1M6Y2K1
B	374	HIS	-	expression tag	UNP A0A1M6Y2K1
B	375	HIS	-	expression tag	UNP A0A1M6Y2K1
B	376	HIS	-	expression tag	UNP A0A1M6Y2K1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	477	Total 477	O 477	0	0
5	B	459	Total 459	O 459	0	0

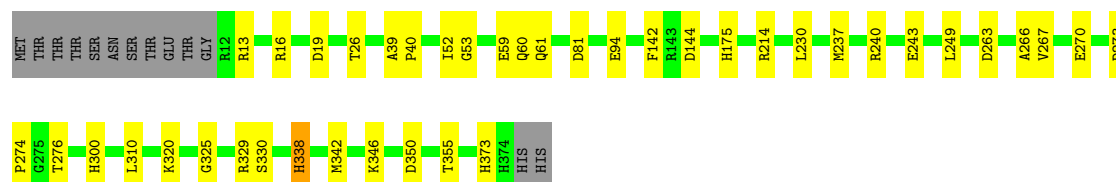
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

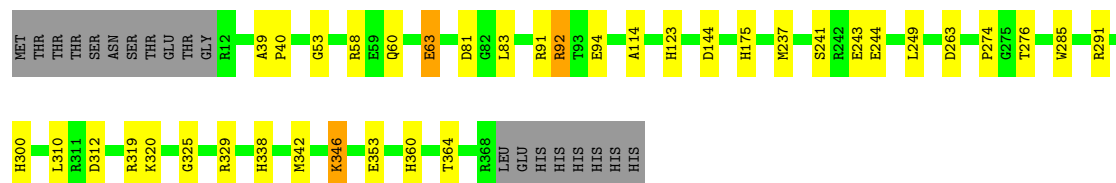
- Molecule 1: Acetyl esterase/lipase

Chain A: 



- Molecule 1: Acetyl esterase/lipase

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.71Å 77.19Å 162.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.28 – 1.35	Depositor
% Data completeness (in resolution range)	96.5 (55.28-1.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.138 , 0.184	Depositor
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	1.651	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6484	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, PG4, PEG

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	1.36	19/2861 (0.7%)	1.35	17/3899 (0.4%)
1	B	1.22	8/2827 (0.3%)	1.27	10/3852 (0.3%)
All	All	1.29	27/5688 (0.5%)	1.31	27/7751 (0.3%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	PRO	N-CA	16.51	1.66	1.47
1	A	243	GLU	CD-OE2	10.99	1.46	1.25
1	A	13	ARG	C-N	10.92	1.46	1.33
1	B	274	PRO	C-N	9.84	1.49	1.33
1	A	240	ARG	C-N	7.62	1.43	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	CA-C-N	10.03	130.66	119.93
1	A	273	ASP	C-N-CA	10.03	130.66	119.93
1	A	13	ARG	O-C-N	-8.95	111.40	121.43
1	A	13	ARG	CG-CD-NE	-8.16	94.05	112.00
1	A	266	ALA	O-C-N	8.15	130.76	122.12

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	2773	0	2707	22	0
1	B	2734	0	2691	21	0
2	A	7	0	10	0	0
2	B	7	0	10	2	0
3	A	13	0	18	0	0
3	B	13	0	18	0	0
4	B	1	0	0	0	0
5	A	477	0	0	6	0
5	B	459	0	0	15	0
All	All	6484	0	5454	45	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 4.

The worst 5 of 45 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:230:LEU:HD22	1:A:342[B]:MET:CE	1.67	1.25
1:A:230:LEU:CD2	1:A:342[B]:MET:HE1	1.82	1.10
1:A:230:LEU:HD22	1:A:342[B]:MET:HE1	1.06	1.04
1:A:320:LYS:HE2	5:A:787:HOH:O	1.57	0.99
1:A:230:LEU:HD22	1:A:342[B]:MET:HE3	1.67	0.76

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	367/376 (98%)	354 (96%)	13 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/376 (96%)	353 (97%)	10 (3%)	0	100	100
All	All	730/752 (97%)	707 (97%)	23 (3%)	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	283/291 (97%)	283 (100%)	0	100	100
1	B	280/291 (96%)	278 (99%)	2 (1%)	76	54
All	All	563/582 (97%)	561 (100%)	2 (0%)	84	69

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	ARG
1	B	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	GLN

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	PG4	A	402	-	12,12,12	0.60	0	11,11,11	0.43	0
2	PEG	A	401	-	6,6,6	0.35	0	5,5,5	0.20	0
3	PG4	B	402	-	12,12,12	0.41	0	11,11,11	0.35	0
2	PEG	B	401	-	6,6,6	0.47	0	5,5,5	0.35	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	PG4	A	402	-	-	3/10/10/10	-
2	PEG	A	401	-	-	1/4/4/4	-
3	PG4	B	402	-	-	0/10/10/10	-
2	PEG	B	401	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PEG	O1-C1-C2-O2
2	B	401	PEG	O1-C1-C2-O2
3	A	402	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	A	402	PG4	O1-C1-C2-O2
3	A	402	PG4	O4-C7-C8-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PEG	2	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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.