



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2025 – 12:31 AM JST

PDB ID : 9JLQ / pdb_00009jlq
Title : Crystal structure of GH57 family amylopullulanase from Aquifex aeolicus wild type apo
Authors : Zhu, Z.M.; Wang, W.W.; Yu, F.; Wang, Q.S.
Deposited on : 2024-09-19
Resolution : 2.54 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

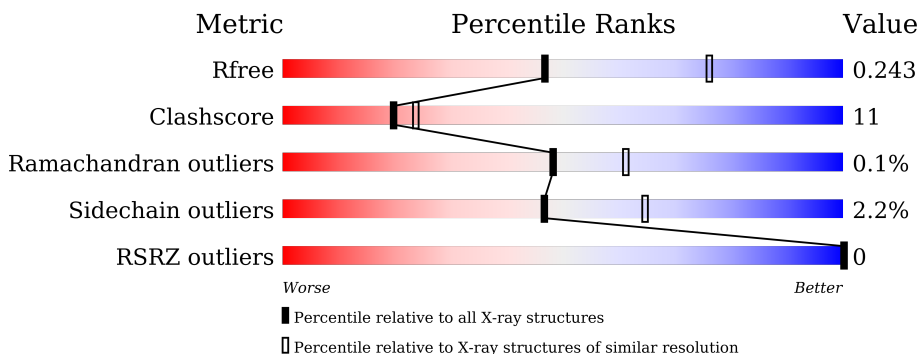
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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 $\leq 5\%$. 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	484	<div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	B	484	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	C	484	<div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	D	484	<div> <div>63%</div> <div>36%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16492 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 Glycoside hydrolase family 57 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			4052	2651	648	743	10			
1	B	477	Total	C	N	O	S	0	0	0
			4052	2651	648	743	10			
1	C	484	Total	C	N	O	S	0	0	0
			4119	2692	665	752	10			
1	D	483	Total	C	N	O	S	0	0	0
			4109	2686	662	751	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	LEU	-	expression tag	UNP O66934
A	479	GLU	-	expression tag	UNP O66934
A	480	HIS	-	expression tag	UNP O66934
A	481	HIS	-	expression tag	UNP O66934
A	482	HIS	-	expression tag	UNP O66934
A	483	HIS	-	expression tag	UNP O66934
A	484	HIS	-	expression tag	UNP O66934
B	478	LEU	-	expression tag	UNP O66934
B	479	GLU	-	expression tag	UNP O66934
B	480	HIS	-	expression tag	UNP O66934
B	481	HIS	-	expression tag	UNP O66934
B	482	HIS	-	expression tag	UNP O66934
B	483	HIS	-	expression tag	UNP O66934
B	484	HIS	-	expression tag	UNP O66934
C	478	LEU	-	expression tag	UNP O66934
C	479	GLU	-	expression tag	UNP O66934
C	480	HIS	-	expression tag	UNP O66934
C	481	HIS	-	expression tag	UNP O66934
C	482	HIS	-	expression tag	UNP O66934
C	483	HIS	-	expression tag	UNP O66934

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Chain	Residue	Modelled	Actual	Comment	Reference
C	484	HIS	-	expression tag	UNP O66934
D	478	LEU	-	expression tag	UNP O66934
D	479	GLU	-	expression tag	UNP O66934
D	480	HIS	-	expression tag	UNP O66934
D	481	HIS	-	expression tag	UNP O66934
D	482	HIS	-	expression tag	UNP O66934
D	483	HIS	-	expression tag	UNP O66934
D	484	HIS	-	expression tag	UNP O66934

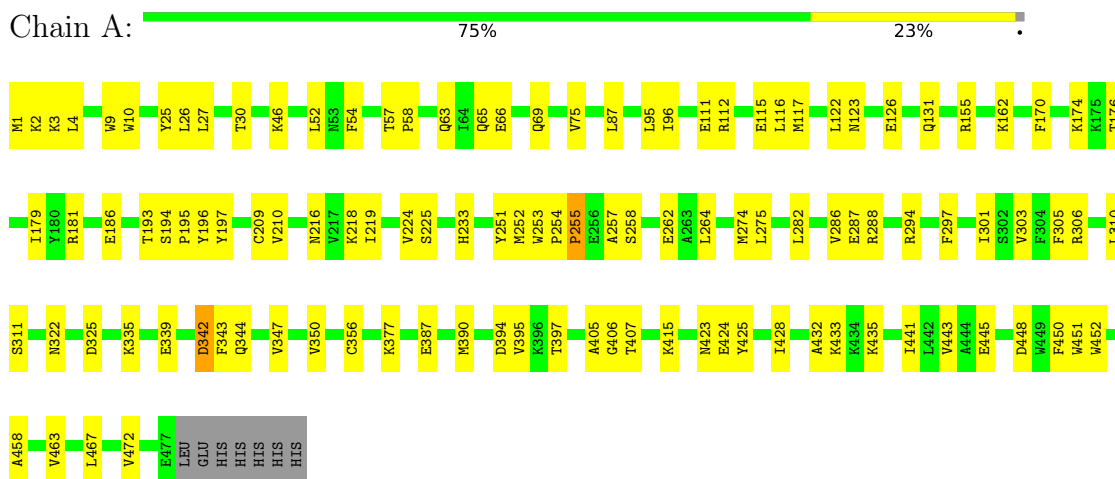
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	41	Total O 41 41	0	0
2	C	32	Total O 32 32	0	0
2	D	22	Total O 22 22	0	0

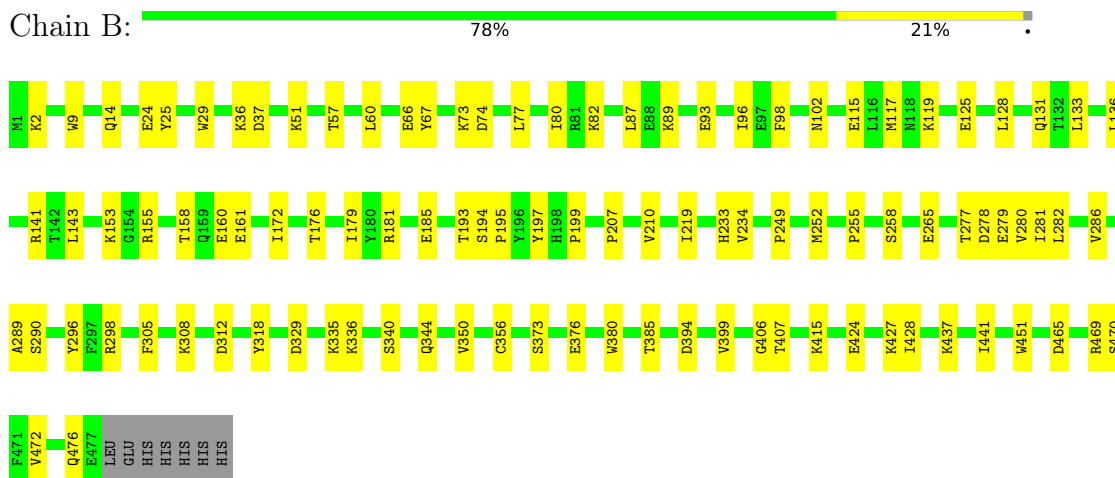
3 Residue-property plots

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: Glycoside hydrolase family 57 N-terminal domain-containing protein

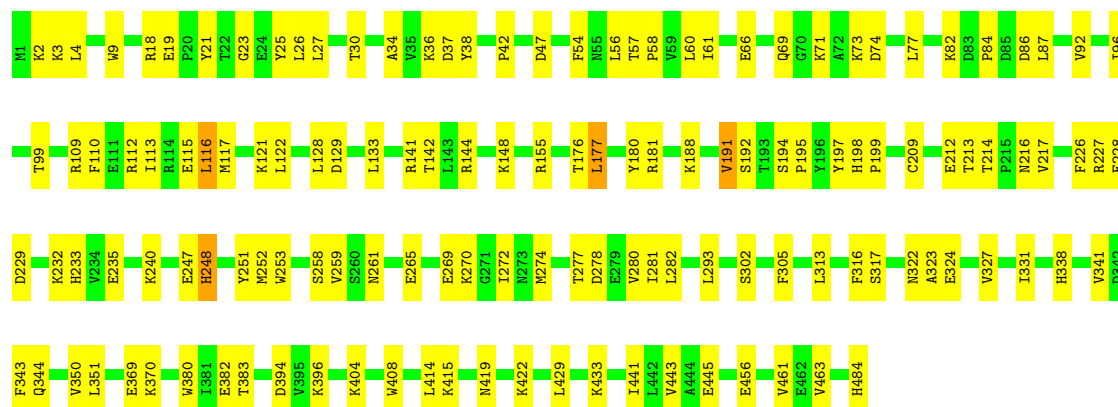


- Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein



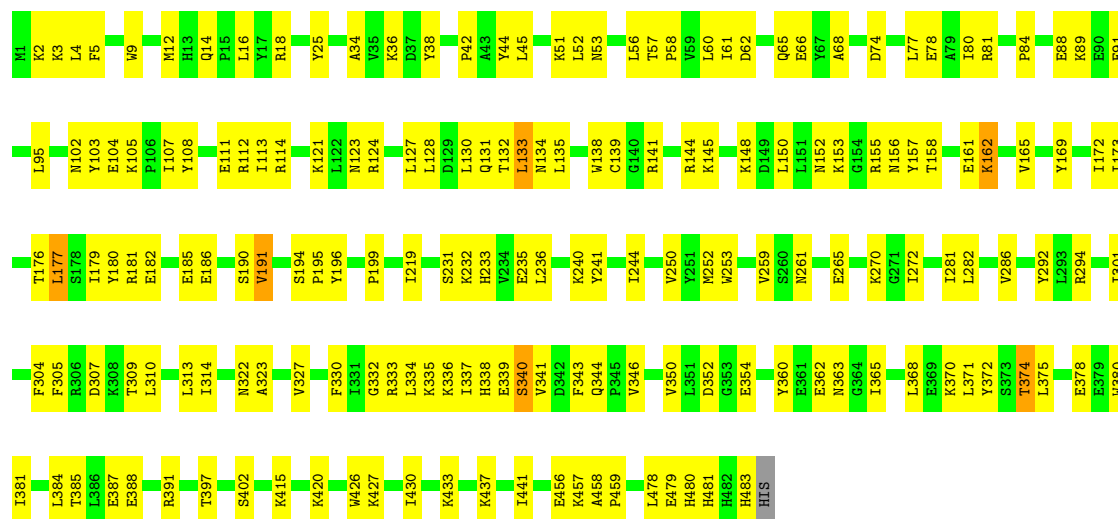
- Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein





- Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain D: 63% 36% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.66Å 166.73Å 99.51Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	93.33 – 2.54 93.33 – 2.54	Depositor EDS
% Data completeness (in resolution range)	62.3 (93.33-2.54) 62.4 (93.33-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.198 , 0.243 0.198 , 0.243	Depositor DCC
R_{free} test set	2259 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 9.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16492	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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](#)

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	0.19	1/4165 (0.0%)	0.31	0/5633
1	B	0.12	0/4165	0.31	0/5633
1	C	0.25	1/4237 (0.0%)	0.36	1/5731 (0.0%)
1	D	0.19	0/4226	0.39	0/5716
All	All	0.19	2/16793 (0.0%)	0.34	1/22713 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	PRO	C-O	-5.20	1.17	1.24
1	C	198	HIS	C-O	5.20	1.26	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	LEU	N-CA-CB	-5.54	103.14	111.56

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	4052	0	3987	75	0
1	B	4052	0	3987	63	0
1	C	4119	0	4039	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4109	0	4032	138	0
2	A	65	0	0	13	0
2	B	41	0	0	6	0
2	C	32	0	0	7	0
2	D	22	0	0	4	0
All	All	16492	0	16045	366	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 11.

The worst 5 of 366 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:113:ILE:HG12	1:D:133:LEU:HD21	1.54	0.89
1:A:186:GLU:OE1	2:A:501:HOH:O	1.96	0.82
1:D:34:ALA:HA	1:D:38:TYR:HB2	1.60	0.82
1:D:18:ARG:NH1	2:D:502:HOH:O	2.15	0.80
1:A:356:CYS:O	2:A:502:HOH:O	2.00	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	475/484 (98%)	465 (98%)	10 (2%)	0	100	100
1	B	475/484 (98%)	466 (98%)	9 (2%)	0	100	100
1	C	482/484 (100%)	462 (96%)	19 (4%)	1 (0%)	44	56
1	D	481/484 (99%)	456 (95%)	25 (5%)	0	100	100
All	All	1913/1936 (99%)	1849 (97%)	63 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	HIS

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	437/444 (98%)	433 (99%)	4 (1%)	75	87
1	B	437/444 (98%)	431 (99%)	6 (1%)	62	77
1	C	444/444 (100%)	431 (97%)	13 (3%)	37	54
1	D	443/444 (100%)	428 (97%)	15 (3%)	32	47
All	All	1761/1776 (99%)	1723 (98%)	38 (2%)	47	65

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	VAL
1	D	479	GLU
1	D	250	VAL
1	D	322	ASN
1	D	483	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	453	GLN
1	D	11	HIS
1	D	273	ASN
1	D	206	ASN
1	D	208	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, 95th 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	477/484 (98%)	-1.90	0 100 100	9, 23, 46, 80	0
1	B	477/484 (98%)	-1.90	0 100 100	11, 27, 51, 97	0
1	C	484/484 (100%)	-1.84	0 100 100	18, 39, 73, 93	0
1	D	483/484 (99%)	-1.72	0 100 100	18, 61, 96, 109	0
All	All	1921/1936 (99%)	-1.84	0 100 100	9, 34, 84, 109	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 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.