



wwPDB Geometry-Only Validation Summary Report ⓘ

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PDB ID : 5ZO0 / pdb_00005zo0
Title : Neutron structure of xylanase at pD5.4
Authors : Wan, Q.; Li, Z.H.
Deposited on : 2018-04-12
Resolution : 1.65 Å(reported)

This is a wwPDB Geometry-Only 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
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

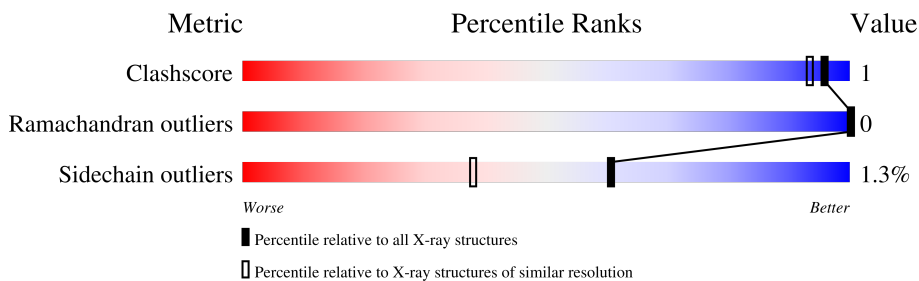
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION

The reported resolution of this entry is 1.65 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	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	189	 98% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3654 atoms, of which 1351 are hydrogens and 659 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 Endo-1,4-beta-xylanase 2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	189	Total	C	D	H	N	O	S	152	182	0
			3192	939	351	1351	256	294	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	154	Total	D	O	0	0
			462	308	154		

Note EDS was not executed.

- Molecule 1: Endo-1,4-beta-xylanase 2

98%



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOD

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	0.40	2/2998 (0.1%)	0.59	2/4087 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4[A]	GLN	C-N	6.50	1.49	1.33
1	A	4[B]	GLN	C-N	6.50	1.49	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3[A]	ILE	O-C-N	5.06	128.65	123.04
1	A	3[B]	ILE	O-C-N	5.06	128.65	123.04

There are no chirality outliers.

There are no planarity outliers.

4.2 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	1841	1351	81	1	0
2	A	462	0	0	3	0
All	All	2303	1351	81	3	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 1.

All (3) 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:4[A]:GLN:NE2	2:A:209:DOD:O	2.48	0.47

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	369/189 (195%)	364 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	305/155 (197%)	301 (99%)	4 (1%)	61	38

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

Mol	Chain	Res	Type
1	A	4[A]	GLN

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Mol	Chain	Res	Type
1	A	4[B]	GLN
1	A	75[A]	SER
1	A	75[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.