



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1GOW / pdb_00001gow
Title : BETA-GLYCOSIDASE FROM SULFOLOBUS SOLFATARICUS
Authors : Pearl, L.H.; Aguilar, C.F.; Sanderson, I.
Deposited on : 1996-09-19
Resolution : 2.60 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

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

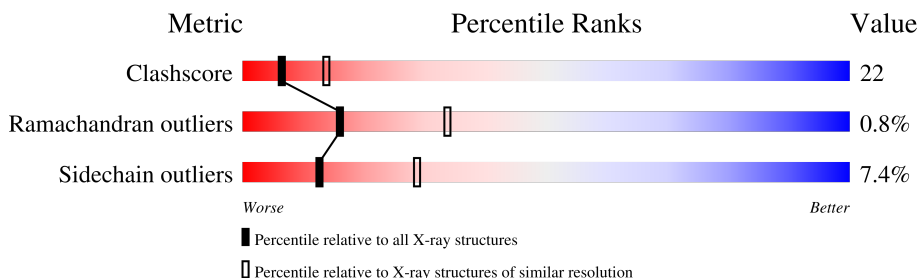
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 ≥ 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	489	 62% 30% 7%
1	B	489	 63% 30% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8304 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 BETA-GLYCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			4020	2575	692	741	12			
1	B	489	Total	C	N	O	S	0	0	0
			4020	2575	692	741	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	SER	VAL	conflict	UNP P22498
A	87	GLN	ILE	conflict	UNP P22498
A	146	GLN	LEU	conflict	UNP P22498
A	190	THR	ILE	conflict	UNP P22498
A	235	ALA	HIS	conflict	UNP P22498
B	82	SER	VAL	conflict	UNP P22498
B	87	GLN	ILE	conflict	UNP P22498
B	146	GLN	LEU	conflict	UNP P22498
B	190	THR	ILE	conflict	UNP P22498
B	235	ALA	HIS	conflict	UNP P22498

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	132	Total	O	0	0
			132	132		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.40 Å 169.40 Å 98.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.9 (10.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8304	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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	0.97	3/4149 (0.1%)	1.13	28/5636 (0.5%)
1	B	0.97	3/4149 (0.1%)	1.13	28/5636 (0.5%)
All	All	0.97	6/8298 (0.1%)	1.13	56/11272 (0.5%)

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	1
1	B	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	MET	SD-CE	12.18	2.10	1.79
1	B	275	MET	SD-CE	12.13	2.09	1.79
1	A	280	MET	SD-CE	6.36	1.95	1.79
1	B	280	MET	SD-CE	6.31	1.95	1.79
1	B	65	THR	CA-CB	-5.19	1.45	1.53

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	SER	N-CA-C	10.07	132.25	110.80
1	A	426	SER	N-CA-C	10.04	132.18	110.80
1	A	409	VAL	N-CA-C	-9.10	101.47	110.30
1	B	409	VAL	N-CA-C	-9.09	101.49	110.30
1	A	20	GLU	N-CA-C	7.97	119.59	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	TYR	Sidechain
1	B	382	TYR	Sidechain

5.2 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	4020	0	3799	170	4
1	B	4020	0	3799	173	0
2	A	132	0	0	12	0
2	B	132	0	0	13	4
All	All	8304	0	7598	343	4

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 22.

The worst 5 of 343 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:B:275:MET:SD	1:B:275:MET:CE	2.09	1.40
1:A:275:MET:CE	1:A:275:MET:SD	2.10	1.40
1:B:201:TYR:HA	2:B:541:HOH:O	1.52	1.09
1:A:201:TYR:HA	2:A:541:HOH:O	1.52	1.07
1:A:329:ARG:HD3	1:A:330:THR:H	1.21	1.06

All (4) 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:A:90:ASN:CB	2:B:616:HOH:O[4_546]	1.25	0.95
1:A:90:ASN:CA	2:B:616:HOH:O[4_546]	1.56	0.64
1:A:90:ASN:CG	2:B:616:HOH:O[4_546]	1.69	0.51
1:A:90:ASN:ND2	2:B:616:HOH:O[4_546]	1.79	0.41

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	487/489 (100%)	442 (91%)	41 (8%)	4 (1%)	16	34
1	B	487/489 (100%)	442 (91%)	41 (8%)	4 (1%)	16	34
All	All	974/978 (100%)	884 (91%)	82 (8%)	8 (1%)	16	34

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	151	TRP
1	B	96	GLN
1	B	151	TRP
1	A	306	VAL

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	421/421 (100%)	390 (93%)	31 (7%)	13	29
1	B	421/421 (100%)	390 (93%)	31 (7%)	13	29
All	All	842/842 (100%)	780 (93%)	62 (7%)	13	29

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ASN

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Mol	Chain	Res	Type
1	B	386	THR
1	B	100	GLU
1	B	359	PHE
1	B	449	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	HIS
1	B	479	ASN
1	B	87	GLN
1	B	342	HIS
1	B	71	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.