



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8BBL / pdb_00008bbl
Title : SGL a GH20 family sulfoglycosidase
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Deposited on : 2022-10-13
Resolution : 2.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : **FAILED**
Xtrriage (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 2.71 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 31772 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-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	4061	2584	691	764	22	0	0	0
1	B	501	3959	2521	671	745	22	0	0	0
1	C	500	3955	2519	670	744	22	0	0	0
1	D	500	3955	2519	670	744	22	0	0	0
1	E	500	3955	2519	670	744	22	0	0	0
1	F	500	3955	2519	670	744	22	0	0	0
1	H	501	3959	2521	671	745	22	0	0	0
1	G	500	3955	2519	670	744	22	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	4	Total	O	0	0
			4	4		
2	C	4	Total	O	0	0
			4	4		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics i

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	132.95Å 133.42Å 225.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.18 – 2.71	Depositor
% Data completeness (in resolution range)	96.6 (94.18-2.71)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.283 , 0.319	Depositor
Wilson B-factor (Å ²)	47.0	Xtrriage
Anisotropy	0.089	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.055 for h,-k,-l 0.054 for -h,k,-l 0.040 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.182 for H, K, L 0.177 for h,-k,-l 0.179 for -H, K, -L 0.177 for -h,-k,l 0.071 for K, H, -L 0.071 for k,-h,l 0.070 for -K, H, L 0.072 for -K, -H, -L	Depositor
Outliers	0 of 416904 reflections	Xtrriage
Total number of atoms	31772	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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