Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:47 AM EDT

PDB ID	:	6VE1
Title	:	Crystal structure of endo-beta-N-acetylglucosaminidase H at high pH
Authors	:	Stachowski, T.R.; Snell, M.E.; Snell, E.S.
Deposited on	:	2019-12-28
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17020 atoms, of which 7767 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 Endo-beta-N-acetylglucosaminidase H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	H	N	O	S	0	0	0
			3969	1274	1942	349	402	2			
1	B	267	Total	C	H	N	O	S	0	0	0
			3969	1274	1942	349	402	2			
1	C	268	Total	C	H	N	O	S	0	0	0
			3971	1276	1940	349	403	3			
1	D	267	Total	C	H	N	O	S	0	0	0
			3969	1274	1943	348	401	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P04067
A	2	LEU	-	expression tag	UNP P04067
A	3	SER	-	expression tag	UNP P04067
A	4	THR	-	expression tag	UNP P04067
A	5	GLY	-	expression tag	UNP P04067
A	6	CYS	-	expression tag	UNP P04067
A	7	TYR	-	expression tag	UNP P04067
A	8	MET	-	expression tag	UNP P04067
A	276	HIS	-	expression tag	UNP P04067
A	277	HIS	-	expression tag	UNP P04067
A	278	HIS	-	expression tag	UNP P04067
A	279	HIS	-	expression tag	UNP P04067
A	280	HIS	-	expression tag	UNP P04067
A	281	HIS	-	expression tag	UNP P04067
B	1	SER	-	expression tag	UNP P04067
B	2	LEU	-	expression tag	UNP P04067
B	3	SER	-	expression tag	UNP P04067
B	4	THR	-	expression tag	UNP P04067
B	5	GLY	-	expression tag	UNP P04067
B	6	CYS	-	expression tag	UNP P04067
B	7	TYR	-	expression tag	UNP P04067

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	expression tag	UNP P04067
B	276	HIS	-	expression tag	UNP P04067
B	277	HIS	-	expression tag	UNP P04067
B	278	HIS	-	expression tag	UNP P04067
B	279	HIS	-	expression tag	UNP P04067
B	280	HIS	-	expression tag	UNP P04067
B	281	HIS	-	expression tag	UNP P04067
C	1	SER	-	expression tag	UNP P04067
C	2	LEU	-	expression tag	UNP P04067
C	3	SER	-	expression tag	UNP P04067
C	4	THR	-	expression tag	UNP P04067
C	5	GLY	-	expression tag	UNP P04067
C	6	CYS	-	expression tag	UNP P04067
C	7	TYR	-	expression tag	UNP P04067
C	8	MET	-	expression tag	UNP P04067
C	276	HIS	-	expression tag	UNP P04067
C	277	HIS	-	expression tag	UNP P04067
C	278	HIS	-	expression tag	UNP P04067
C	279	HIS	-	expression tag	UNP P04067
C	280	HIS	-	expression tag	UNP P04067
C	281	HIS	-	expression tag	UNP P04067
D	1	SER	-	expression tag	UNP P04067
D	2	LEU	-	expression tag	UNP P04067
D	3	SER	-	expression tag	UNP P04067
D	4	THR	-	expression tag	UNP P04067
D	5	GLY	-	expression tag	UNP P04067
D	6	CYS	-	expression tag	UNP P04067
D	7	TYR	-	expression tag	UNP P04067
D	8	MET	-	expression tag	UNP P04067
D	276	HIS	-	expression tag	UNP P04067
D	277	HIS	-	expression tag	UNP P04067
D	278	HIS	-	expression tag	UNP P04067
D	279	HIS	-	expression tag	UNP P04067
D	280	HIS	-	expression tag	UNP P04067
D	281	HIS	-	expression tag	UNP P04067

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	288	Total O 288 288	0	0
3	B	300	Total O 300 300	0	0
3	C	285	Total O 285 285	0	0
3	D	263	Total O 263 263	0	0

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

3 Data and refinement statistics (i)

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	93.48Å 99.48Å 135.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.03 – 2.10	Depositor
% Data completeness (in resolution range)	99.7 (41.03-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.221 , 0.258	Depositor
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	1.160	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17020	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1666e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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 monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

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.