Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 07:56 PM JST

PDB ID	:	6JTI
Title	:	Crystal structure of native NagZ from Neisseria gonorrhoeae
Authors	:	Chen, Y.
Deposited on	:	2019-04-11
Resolution	:	2.20 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:

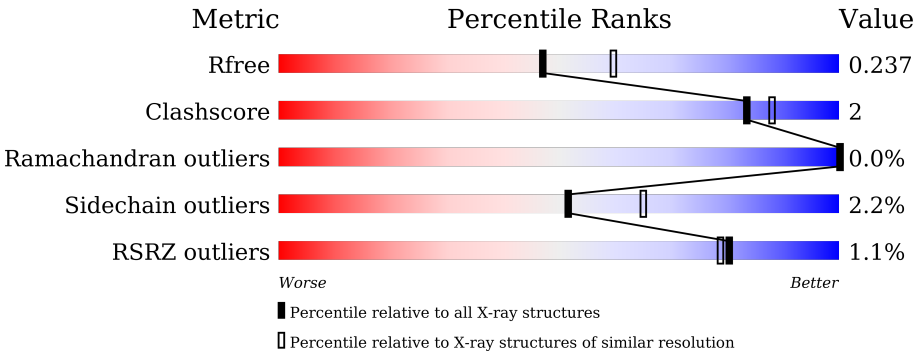
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	397	79% 6% • 15%
1	B	397	81% 5% • 13%
1	C	397	81% 5% • 14%
1	D	397	80% 6% • 13%
1	E	397	79% 6% 15%
1	F	397	80% 5% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16208 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-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2599	1642	464	478	15			
1	B	344	Total	C	N	O	S	0	0	0
			2623	1655	469	483	16			
1	C	343	Total	C	N	O	S	0	0	0
			2623	1654	468	485	16			
1	D	344	Total	C	N	O	S	0	0	0
			2625	1656	469	484	16			
1	E	339	Total	C	N	O	S	0	0	0
			2596	1639	464	478	15			
1	F	340	Total	C	N	O	S	0	0	0
			2601	1642	465	479	15			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP Q5FA94
A	-34	GLY	-	expression tag	UNP Q5FA94
A	-33	SER	-	expression tag	UNP Q5FA94
A	-32	SER	-	expression tag	UNP Q5FA94
A	-31	HIS	-	expression tag	UNP Q5FA94
A	-30	HIS	-	expression tag	UNP Q5FA94
A	-29	HIS	-	expression tag	UNP Q5FA94
A	-28	HIS	-	expression tag	UNP Q5FA94
A	-27	HIS	-	expression tag	UNP Q5FA94
A	-26	HIS	-	expression tag	UNP Q5FA94
A	-25	SER	-	expression tag	UNP Q5FA94
A	-24	SER	-	expression tag	UNP Q5FA94
A	-23	GLY	-	expression tag	UNP Q5FA94
A	-22	LEU	-	expression tag	UNP Q5FA94
A	-21	VAL	-	expression tag	UNP Q5FA94
A	-20	PRO	-	expression tag	UNP Q5FA94
A	-19	ARG	-	expression tag	UNP Q5FA94

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q5FA94
A	-17	SER	-	expression tag	UNP Q5FA94
A	-16	HIS	-	expression tag	UNP Q5FA94
A	-15	MET	-	expression tag	UNP Q5FA94
A	-14	ALA	-	expression tag	UNP Q5FA94
A	-13	SER	-	expression tag	UNP Q5FA94
A	-12	MET	-	expression tag	UNP Q5FA94
A	-11	THR	-	expression tag	UNP Q5FA94
A	-10	GLY	-	expression tag	UNP Q5FA94
A	-9	GLY	-	expression tag	UNP Q5FA94
A	-8	GLN	-	expression tag	UNP Q5FA94
A	-7	GLN	-	expression tag	UNP Q5FA94
A	-6	MET	-	expression tag	UNP Q5FA94
A	-5	GLY	-	expression tag	UNP Q5FA94
A	-4	ARG	-	expression tag	UNP Q5FA94
A	-3	GLY	-	expression tag	UNP Q5FA94
A	-2	SER	-	expression tag	UNP Q5FA94
A	-1	GLU	-	expression tag	UNP Q5FA94
A	0	PHE	-	expression tag	UNP Q5FA94
B	-35	MET	-	expression tag	UNP Q5FA94
B	-34	GLY	-	expression tag	UNP Q5FA94
B	-33	SER	-	expression tag	UNP Q5FA94
B	-32	SER	-	expression tag	UNP Q5FA94
B	-31	HIS	-	expression tag	UNP Q5FA94
B	-30	HIS	-	expression tag	UNP Q5FA94
B	-29	HIS	-	expression tag	UNP Q5FA94
B	-28	HIS	-	expression tag	UNP Q5FA94
B	-27	HIS	-	expression tag	UNP Q5FA94
B	-26	HIS	-	expression tag	UNP Q5FA94
B	-25	SER	-	expression tag	UNP Q5FA94
B	-24	SER	-	expression tag	UNP Q5FA94
B	-23	GLY	-	expression tag	UNP Q5FA94
B	-22	LEU	-	expression tag	UNP Q5FA94
B	-21	VAL	-	expression tag	UNP Q5FA94
B	-20	PRO	-	expression tag	UNP Q5FA94
B	-19	ARG	-	expression tag	UNP Q5FA94
B	-18	GLY	-	expression tag	UNP Q5FA94
B	-17	SER	-	expression tag	UNP Q5FA94
B	-16	HIS	-	expression tag	UNP Q5FA94
B	-15	MET	-	expression tag	UNP Q5FA94
B	-14	ALA	-	expression tag	UNP Q5FA94
B	-13	SER	-	expression tag	UNP Q5FA94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	expression tag	UNP Q5FA94
B	-11	THR	-	expression tag	UNP Q5FA94
B	-10	GLY	-	expression tag	UNP Q5FA94
B	-9	GLY	-	expression tag	UNP Q5FA94
B	-8	GLN	-	expression tag	UNP Q5FA94
B	-7	GLN	-	expression tag	UNP Q5FA94
B	-6	MET	-	expression tag	UNP Q5FA94
B	-5	GLY	-	expression tag	UNP Q5FA94
B	-4	ARG	-	expression tag	UNP Q5FA94
B	-3	GLY	-	expression tag	UNP Q5FA94
B	-2	SER	-	expression tag	UNP Q5FA94
B	-1	GLU	-	expression tag	UNP Q5FA94
B	0	PHE	-	expression tag	UNP Q5FA94
C	-35	MET	-	expression tag	UNP Q5FA94
C	-34	GLY	-	expression tag	UNP Q5FA94
C	-33	SER	-	expression tag	UNP Q5FA94
C	-32	SER	-	expression tag	UNP Q5FA94
C	-31	HIS	-	expression tag	UNP Q5FA94
C	-30	HIS	-	expression tag	UNP Q5FA94
C	-29	HIS	-	expression tag	UNP Q5FA94
C	-28	HIS	-	expression tag	UNP Q5FA94
C	-27	HIS	-	expression tag	UNP Q5FA94
C	-26	HIS	-	expression tag	UNP Q5FA94
C	-25	SER	-	expression tag	UNP Q5FA94
C	-24	SER	-	expression tag	UNP Q5FA94
C	-23	GLY	-	expression tag	UNP Q5FA94
C	-22	LEU	-	expression tag	UNP Q5FA94
C	-21	VAL	-	expression tag	UNP Q5FA94
C	-20	PRO	-	expression tag	UNP Q5FA94
C	-19	ARG	-	expression tag	UNP Q5FA94
C	-18	GLY	-	expression tag	UNP Q5FA94
C	-17	SER	-	expression tag	UNP Q5FA94
C	-16	HIS	-	expression tag	UNP Q5FA94
C	-15	MET	-	expression tag	UNP Q5FA94
C	-14	ALA	-	expression tag	UNP Q5FA94
C	-13	SER	-	expression tag	UNP Q5FA94
C	-12	MET	-	expression tag	UNP Q5FA94
C	-11	THR	-	expression tag	UNP Q5FA94
C	-10	GLY	-	expression tag	UNP Q5FA94
C	-9	GLY	-	expression tag	UNP Q5FA94
C	-8	GLN	-	expression tag	UNP Q5FA94
C	-7	GLN	-	expression tag	UNP Q5FA94

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP Q5FA94
C	-5	GLY	-	expression tag	UNP Q5FA94
C	-4	ARG	-	expression tag	UNP Q5FA94
C	-3	GLY	-	expression tag	UNP Q5FA94
C	-2	SER	-	expression tag	UNP Q5FA94
C	-1	GLU	-	expression tag	UNP Q5FA94
C	0	PHE	-	expression tag	UNP Q5FA94
D	-35	MET	-	expression tag	UNP Q5FA94
D	-34	GLY	-	expression tag	UNP Q5FA94
D	-33	SER	-	expression tag	UNP Q5FA94
D	-32	SER	-	expression tag	UNP Q5FA94
D	-31	HIS	-	expression tag	UNP Q5FA94
D	-30	HIS	-	expression tag	UNP Q5FA94
D	-29	HIS	-	expression tag	UNP Q5FA94
D	-28	HIS	-	expression tag	UNP Q5FA94
D	-27	HIS	-	expression tag	UNP Q5FA94
D	-26	HIS	-	expression tag	UNP Q5FA94
D	-25	SER	-	expression tag	UNP Q5FA94
D	-24	SER	-	expression tag	UNP Q5FA94
D	-23	GLY	-	expression tag	UNP Q5FA94
D	-22	LEU	-	expression tag	UNP Q5FA94
D	-21	VAL	-	expression tag	UNP Q5FA94
D	-20	PRO	-	expression tag	UNP Q5FA94
D	-19	ARG	-	expression tag	UNP Q5FA94
D	-18	GLY	-	expression tag	UNP Q5FA94
D	-17	SER	-	expression tag	UNP Q5FA94
D	-16	HIS	-	expression tag	UNP Q5FA94
D	-15	MET	-	expression tag	UNP Q5FA94
D	-14	ALA	-	expression tag	UNP Q5FA94
D	-13	SER	-	expression tag	UNP Q5FA94
D	-12	MET	-	expression tag	UNP Q5FA94
D	-11	THR	-	expression tag	UNP Q5FA94
D	-10	GLY	-	expression tag	UNP Q5FA94
D	-9	GLY	-	expression tag	UNP Q5FA94
D	-8	GLN	-	expression tag	UNP Q5FA94
D	-7	GLN	-	expression tag	UNP Q5FA94
D	-6	MET	-	expression tag	UNP Q5FA94
D	-5	GLY	-	expression tag	UNP Q5FA94
D	-4	ARG	-	expression tag	UNP Q5FA94
D	-3	GLY	-	expression tag	UNP Q5FA94
D	-2	SER	-	expression tag	UNP Q5FA94
D	-1	GLU	-	expression tag	UNP Q5FA94

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP Q5FA94
E	-35	MET	-	expression tag	UNP Q5FA94
E	-34	GLY	-	expression tag	UNP Q5FA94
E	-33	SER	-	expression tag	UNP Q5FA94
E	-32	SER	-	expression tag	UNP Q5FA94
E	-31	HIS	-	expression tag	UNP Q5FA94
E	-30	HIS	-	expression tag	UNP Q5FA94
E	-29	HIS	-	expression tag	UNP Q5FA94
E	-28	HIS	-	expression tag	UNP Q5FA94
E	-27	HIS	-	expression tag	UNP Q5FA94
E	-26	HIS	-	expression tag	UNP Q5FA94
E	-25	SER	-	expression tag	UNP Q5FA94
E	-24	SER	-	expression tag	UNP Q5FA94
E	-23	GLY	-	expression tag	UNP Q5FA94
E	-22	LEU	-	expression tag	UNP Q5FA94
E	-21	VAL	-	expression tag	UNP Q5FA94
E	-20	PRO	-	expression tag	UNP Q5FA94
E	-19	ARG	-	expression tag	UNP Q5FA94
E	-18	GLY	-	expression tag	UNP Q5FA94
E	-17	SER	-	expression tag	UNP Q5FA94
E	-16	HIS	-	expression tag	UNP Q5FA94
E	-15	MET	-	expression tag	UNP Q5FA94
E	-14	ALA	-	expression tag	UNP Q5FA94
E	-13	SER	-	expression tag	UNP Q5FA94
E	-12	MET	-	expression tag	UNP Q5FA94
E	-11	THR	-	expression tag	UNP Q5FA94
E	-10	GLY	-	expression tag	UNP Q5FA94
E	-9	GLY	-	expression tag	UNP Q5FA94
E	-8	GLN	-	expression tag	UNP Q5FA94
E	-7	GLN	-	expression tag	UNP Q5FA94
E	-6	MET	-	expression tag	UNP Q5FA94
E	-5	GLY	-	expression tag	UNP Q5FA94
E	-4	ARG	-	expression tag	UNP Q5FA94
E	-3	GLY	-	expression tag	UNP Q5FA94
E	-2	SER	-	expression tag	UNP Q5FA94
E	-1	GLU	-	expression tag	UNP Q5FA94
E	0	PHE	-	expression tag	UNP Q5FA94
F	-35	MET	-	expression tag	UNP Q5FA94
F	-34	GLY	-	expression tag	UNP Q5FA94
F	-33	SER	-	expression tag	UNP Q5FA94
F	-32	SER	-	expression tag	UNP Q5FA94
F	-31	HIS	-	expression tag	UNP Q5FA94

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP Q5FA94
F	-29	HIS	-	expression tag	UNP Q5FA94
F	-28	HIS	-	expression tag	UNP Q5FA94
F	-27	HIS	-	expression tag	UNP Q5FA94
F	-26	HIS	-	expression tag	UNP Q5FA94
F	-25	SER	-	expression tag	UNP Q5FA94
F	-24	SER	-	expression tag	UNP Q5FA94
F	-23	GLY	-	expression tag	UNP Q5FA94
F	-22	LEU	-	expression tag	UNP Q5FA94
F	-21	VAL	-	expression tag	UNP Q5FA94
F	-20	PRO	-	expression tag	UNP Q5FA94
F	-19	ARG	-	expression tag	UNP Q5FA94
F	-18	GLY	-	expression tag	UNP Q5FA94
F	-17	SER	-	expression tag	UNP Q5FA94
F	-16	HIS	-	expression tag	UNP Q5FA94
F	-15	MET	-	expression tag	UNP Q5FA94
F	-14	ALA	-	expression tag	UNP Q5FA94
F	-13	SER	-	expression tag	UNP Q5FA94
F	-12	MET	-	expression tag	UNP Q5FA94
F	-11	THR	-	expression tag	UNP Q5FA94
F	-10	GLY	-	expression tag	UNP Q5FA94
F	-9	GLY	-	expression tag	UNP Q5FA94
F	-8	GLN	-	expression tag	UNP Q5FA94
F	-7	GLN	-	expression tag	UNP Q5FA94
F	-6	MET	-	expression tag	UNP Q5FA94
F	-5	GLY	-	expression tag	UNP Q5FA94
F	-4	ARG	-	expression tag	UNP Q5FA94
F	-3	GLY	-	expression tag	UNP Q5FA94
F	-2	SER	-	expression tag	UNP Q5FA94
F	-1	GLU	-	expression tag	UNP Q5FA94
F	0	PHE	-	expression tag	UNP Q5FA94

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0
2	B	124	Total O 124 124	0	0
2	C	114	Total O 114 114	0	0
2	D	67	Total O 67 67	0	0

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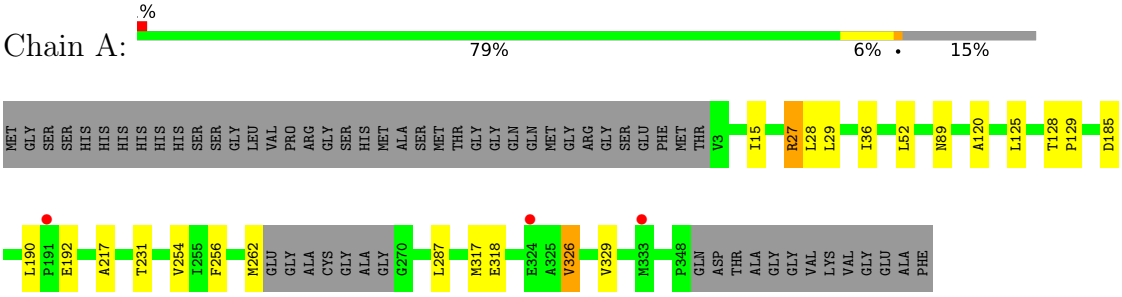
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	45	Total O 45 45	0	0
2	F	63	Total O 63 63	0	0

3 Residue-property plots (i)

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.

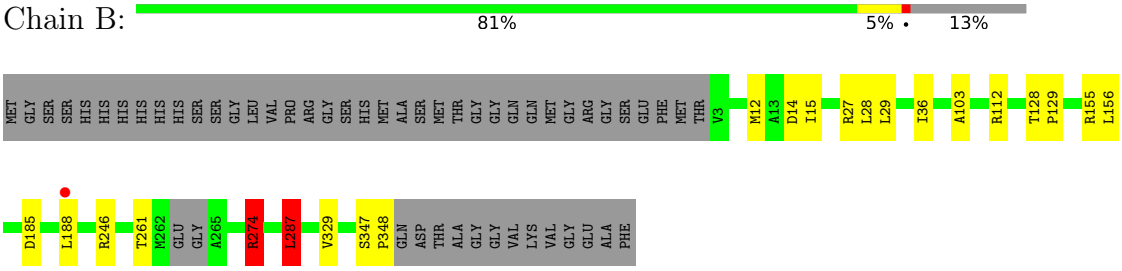
• Molecule 1: Beta-hexosaminidase

Chain A:



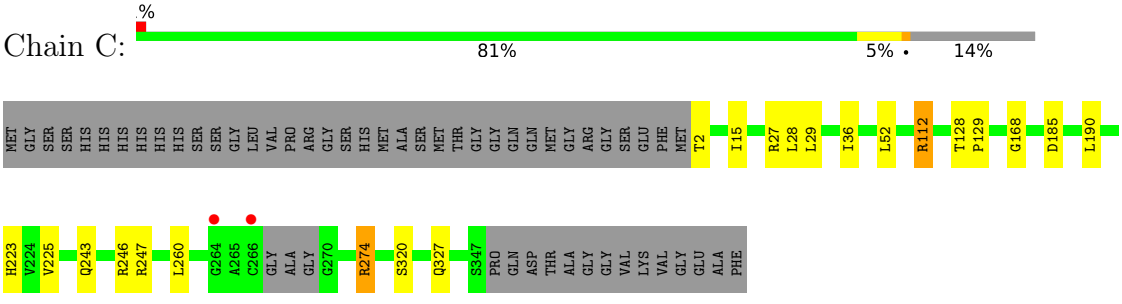
• Molecule 1: Beta-hexosaminidase

Chain B:



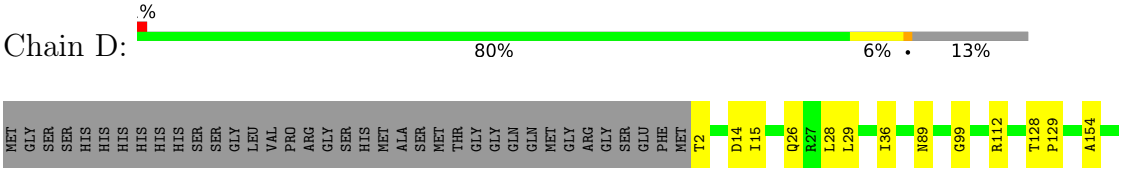
• Molecule 1: Beta-hexosaminidase

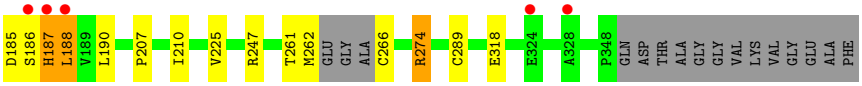
Chain C:



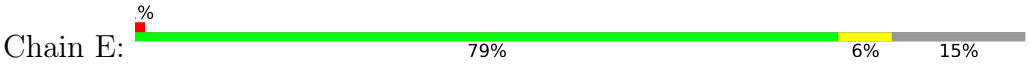
• Molecule 1: Beta-hexosaminidase

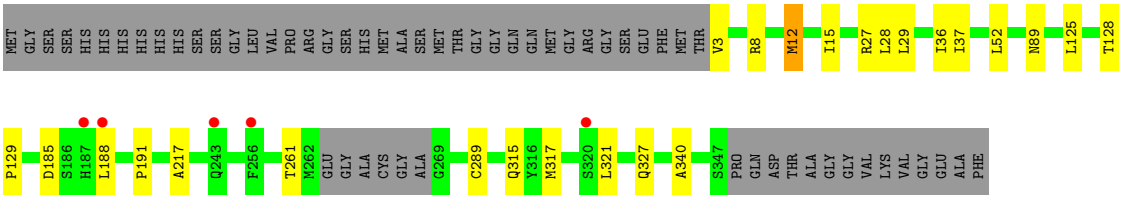
Chain D:



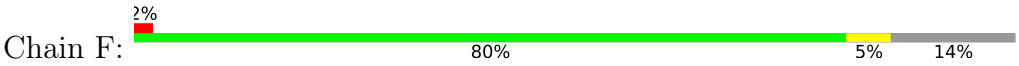


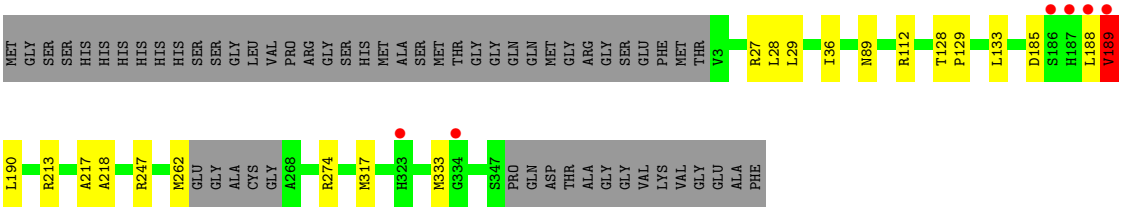
• Molecule 1: Beta-hexosaminidase





• Molecule 1: Beta-hexosaminidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.02Å 124.09Å 189.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.88 – 2.20 94.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.88-2.20) 100.0 (94.96-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.214 , 0.233 0.217 , 0.237	Depositor DCC
R_{free} test set	6172 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16208	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

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	0.57	0/2649	0.77	5/3582 (0.1%)
1	B	0.57	0/2673	0.76	6/3614 (0.2%)
1	C	0.56	0/2672	0.75	4/3612 (0.1%)
1	D	0.53	1/2675 (0.0%)	0.76	3/3617 (0.1%)
1	E	0.50	0/2645	0.73	2/3575 (0.1%)
1	F	0.54	1/2650 (0.0%)	0.77	5/3582 (0.1%)
All	All	0.55	2/15964 (0.0%)	0.76	25/21582 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	189	VAL	C-O	-5.49	1.12	1.23
1	D	318	GLU	CD-OE2	-5.01	1.20	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	112	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	E	27	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	F	333	MET	N-CA-C	-6.74	92.81	111.00
1	C	274	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	27	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	112	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	F	27	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	274	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	E	12	MET	CG-SD-CE	-5.94	90.69	100.20
1	A	192	GLU	CB-CA-C	5.90	122.20	110.40
1	D	112	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	287	LEU	CA-CB-CG	5.71	128.42	115.30
1	F	112	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	246	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	274	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	274	ARG	NE-CZ-NH1	-5.41	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	246	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	262	MET	CB-CG-SD	5.27	128.20	112.40
1	C	112	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	318	GLU	CG-CD-OE2	5.07	128.43	118.30
1	F	274	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	27	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	F	213	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	27	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	29	LEU	CB-CG-CD2	5.00	119.50	111.00

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	2599	0	2595	13	0
1	B	2623	0	2616	17	0
1	C	2623	0	2614	12	0
1	D	2625	0	2618	12	0
1	E	2596	0	2591	18	0
1	F	2601	0	2596	14	0
2	A	128	0	0	1	0
2	B	124	0	0	0	0
2	C	114	0	0	1	0
2	D	67	0	0	0	0
2	E	45	0	0	0	0
2	F	63	0	0	0	0
All	All	16208	0	15630	74	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 2.

All (74) 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:347:SER:HB2	1:B:348:PRO:HD2	1.36	1.04
1:B:188:LEU:HD13	1:F:262:MET:C	1.83	0.97
1:B:347:SER:CB	1:B:348:PRO:HD2	1.97	0.94
1:E:12:MET:CE	1:E:37:ILE:HB	2.00	0.91
1:D:188:LEU:HG	1:E:188:LEU:HB3	1.52	0.90
1:C:112:ARG:NH1	2:C:401:HOH:O	1.96	0.89
1:B:347:SER:HB2	1:B:348:PRO:CD	2.03	0.87
1:B:188:LEU:CD1	1:F:262:MET:C	2.46	0.84
1:E:12:MET:HE3	1:E:37:ILE:HB	1.62	0.81
1:D:188:LEU:CG	1:E:188:LEU:HB3	2.15	0.75
1:E:8:ARG:HH12	1:E:315:GLN:HE21	1.34	0.73
1:B:347:SER:CB	1:B:348:PRO:CD	2.66	0.71
1:F:218:ALA:HB2	1:F:317:MET:HE1	1.75	0.68
1:A:231:THR:HG21	1:E:340:ALA:HB3	1.77	0.66
1:E:217:ALA:HB1	1:E:317:MET:SD	2.39	0.63
1:B:155:ARG:NH1	1:D:99:GLY:HA2	2.13	0.63
1:C:190:LEU:HD22	1:C:225:VAL:HG23	1.81	0.62
1:A:231:THR:HG21	1:E:340:ALA:CB	2.28	0.62
1:D:154:ALA:HB1	1:D:210:ILE:HG21	1.83	0.61
1:F:217:ALA:HB1	1:F:317:MET:SD	2.41	0.60
1:F:189:VAL:HG23	1:F:190:LEU:H	1.67	0.60
1:C:223:HIS:HE1	1:C:260:LEU:HD22	1.67	0.59
1:E:261:THR:HG21	1:E:289:CYS:O	2.03	0.59
1:E:8:ARG:HH12	1:E:315:GLN:NE2	2.01	0.58
1:A:217:ALA:HB1	1:A:317:MET:SD	2.44	0.57
1:C:15:ILE:HD11	1:C:52:LEU:HD21	1.87	0.56
1:D:261:THR:HG21	1:D:289:CYS:O	2.05	0.55
1:D:190:LEU:HD11	1:D:225:VAL:HG23	1.89	0.55
1:C:243:GLN:O	1:C:247:ARG:CG	2.56	0.55
1:A:15:ILE:HD11	1:A:52:LEU:HD21	1.90	0.54
1:E:15:ILE:HD11	1:E:52:LEU:HD21	1.89	0.53
1:B:188:LEU:HD12	1:F:262:MET:O	2.09	0.53
1:D:207:PRO:HA	1:D:210:ILE:HG22	1.91	0.53
1:D:188:LEU:CD2	1:E:188:LEU:HB3	2.40	0.52
1:A:190:LEU:O	1:A:190:LEU:HG	2.11	0.51
1:C:243:GLN:O	1:C:247:ARG:HG2	2.13	0.49
1:C:243:GLN:O	1:C:247:ARG:HG3	2.13	0.48
1:F:217:ALA:O	1:F:317:MET:HE1	2.13	0.48
1:B:12:MET:HB3	1:B:287:LEU:HD22	1.95	0.48
1:B:188:LEU:CD1	1:F:262:MET:O	2.61	0.48
1:F:217:ALA:C	1:F:317:MET:HE1	2.35	0.47
1:C:243:GLN:HA	1:C:247:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:HIS:CE1	1:C:260:LEU:HD22	2.48	0.47
1:B:347:SER:OG	1:B:348:PRO:HD2	2.15	0.46
1:E:12:MET:HE2	1:E:37:ILE:HB	1.92	0.46
1:B:261:THR:O	1:B:274:ARG:NH1	2.48	0.46
1:F:217:ALA:O	1:F:317:MET:CE	2.64	0.45
1:A:28:LEU:HD22	1:A:36:ILE:HD11	1.99	0.44
1:A:254:VAL:HG11	1:A:256:PHE:CE1	2.52	0.43
1:E:12:MET:HE3	1:E:37:ILE:CB	2.42	0.43
1:F:28:LEU:HD22	1:F:36:ILE:HD11	2.00	0.43
1:F:188:LEU:O	1:F:189:VAL:HG22	2.18	0.43
1:E:28:LEU:HD22	1:E:36:ILE:HD11	2.00	0.43
1:B:128:THR:OG1	1:B:129:PRO:HA	2.19	0.42
1:A:120:ALA:HA	1:A:326:VAL:HG11	2.01	0.42
1:A:125:LEU:HD13	1:A:317:MET:HE3	2.00	0.42
1:B:188:LEU:HD12	1:F:262:MET:C	2.32	0.42
1:A:128:THR:OG1	1:A:129:PRO:HA	2.19	0.42
1:C:28:LEU:HD22	1:C:36:ILE:HD11	2.02	0.42
1:D:128:THR:OG1	1:D:129:PRO:HA	2.20	0.42
1:E:128:THR:OG1	1:E:129:PRO:HA	2.19	0.42
1:C:128:THR:OG1	1:C:129:PRO:HA	2.20	0.42
1:D:28:LEU:HD22	1:D:36:ILE:HD11	2.01	0.42
1:F:128:THR:OG1	1:F:129:PRO:HA	2.20	0.42
1:B:14:ASP:O	1:B:15:ILE:HD13	2.20	0.41
1:B:28:LEU:HD22	1:B:36:ILE:HD11	2.02	0.41
1:B:103:ALA:HB1	1:B:156:LEU:HD21	2.03	0.41
1:D:14:ASP:O	1:D:15:ILE:HD13	2.21	0.41
1:A:256:PHE:HD2	1:A:287:LEU:HD11	1.86	0.41
1:E:125:LEU:HD13	1:E:317:MET:HE3	2.03	0.41
1:C:168:GLY:HA2	1:C:320:SER:OG	2.20	0.40
1:A:27:ARG:NH2	2:A:403:HOH:O	2.43	0.40
1:A:326:VAL:O	1:A:329:VAL:HG12	2.22	0.40
1:D:187:HIS:CE1	1:E:191:PRO:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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	335/397 (84%)	323 (96%)	12 (4%)	0	100	100
1	B	340/397 (86%)	329 (97%)	11 (3%)	0	100	100
1	C	339/397 (85%)	329 (97%)	10 (3%)	0	100	100
1	D	340/397 (86%)	328 (96%)	12 (4%)	0	100	100
1	E	335/397 (84%)	322 (96%)	13 (4%)	0	100	100
1	F	336/397 (85%)	322 (96%)	13 (4%)	1 (0%)	41	46
All	All	2025/2382 (85%)	1953 (96%)	71 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	189	VAL

5.3.2 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	269/309 (87%)	266 (99%)	3 (1%)	73	85
1	B	270/309 (87%)	265 (98%)	5 (2%)	57	71
1	C	271/309 (88%)	266 (98%)	5 (2%)	59	72
1	D	271/309 (88%)	259 (96%)	12 (4%)	28	35
1	E	268/309 (87%)	262 (98%)	6 (2%)	52	65
1	F	268/309 (87%)	263 (98%)	5 (2%)	57	71
All	All	1617/1854 (87%)	1581 (98%)	36 (2%)	52	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	185	ASP
1	A	326	VAL
1	B	29	LEU
1	B	185	ASP
1	B	274	ARG
1	B	287	LEU
1	B	329	VAL
1	C	2	THR
1	C	29	LEU
1	C	185	ASP
1	C	274	ARG
1	C	327	GLN
1	D	2	THR
1	D	26	GLN
1	D	29	LEU
1	D	89	ASN
1	D	185	ASP
1	D	186	SER
1	D	187	HIS
1	D	188	LEU
1	D	247	ARG
1	D	262	MET
1	D	266	CYS
1	D	274	ARG
1	E	3	VAL
1	E	29	LEU
1	E	89	ASN
1	E	185	ASP
1	E	321	LEU
1	E	327	GLN
1	F	29	LEU
1	F	89	ASN
1	F	133	LEU
1	F	185	ASP
1	F	247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	327	GLN
1	D	187	HIS
1	E	315	GLN

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Mol	Chain	Res	Type
1	E	331	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	339/397 (85%)	-0.22	3 (0%)	84	83	22, 33, 57, 90	0
1	B	344/397 (86%)	-0.24	1 (0%)	94	93	22, 33, 57, 94	0
1	C	343/397 (86%)	-0.18	2 (0%)	89	88	21, 34, 60, 93	0
1	D	344/397 (86%)	-0.08	5 (1%)	73	72	26, 40, 69, 104	0
1	E	339/397 (85%)	0.13	5 (1%)	73	72	29, 50, 73, 118	0
1	F	340/397 (85%)	0.01	6 (1%)	68	66	27, 45, 72, 126	0
All	All	2049/2382 (86%)	-0.10	22 (1%)	80	79	21, 39, 68, 126	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	HIS	8.2
1	F	188	LEU	7.3
1	B	188	LEU	7.2
1	E	187	HIS	5.2
1	D	188	LEU	4.6
1	D	324	GLU	4.3
1	F	187	HIS	4.2
1	C	266	CYS	3.9
1	F	334	GLY	3.5
1	F	323	HIS	3.1
1	F	189	VAL	3.0
1	C	264	GLY	2.7
1	A	324	GLU	2.6
1	E	320	SER	2.5
1	D	186	SER	2.5
1	A	333	MET	2.4
1	E	256	PHE	2.3
1	D	328	ALA	2.1
1	A	191	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	243	GLN	2.0
1	F	186	SER	2.0
1	E	188	LEU	2.0

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.