



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:15 PM UTC

PDB ID : 6JTJ / pdb_00006jtj
Title : Crystal structure of NagZ from Neisseria gonorrhoeae in complex with N-acetylglucosamine
Authors : Chen, Y.
Deposited on : 2019-04-11
Resolution : 2.18 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

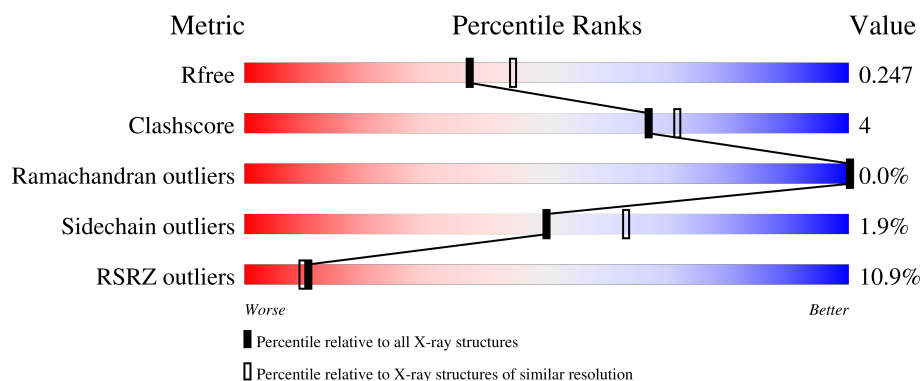
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	11% 77% 7% 16%
1	B	397	4% 79% 8% 13%
1	C	397	14% 79% 6% 15%
1	D	397	6% 81% 5% 13%
1	E	397	16% 80% 6% 15%

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Mol	Chain	Length	Quality of chain
1	F	397	 7% 79% 6% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16730 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	334	Total	C	N	O	S	0	0	0
			2560	1617	457	472	14			
1	B	346	Total	C	N	O	S	0	0	0
			2633	1659	471	487	16			
1	C	339	Total	C	N	O	S	0	0	0
			2593	1637	464	478	14			
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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

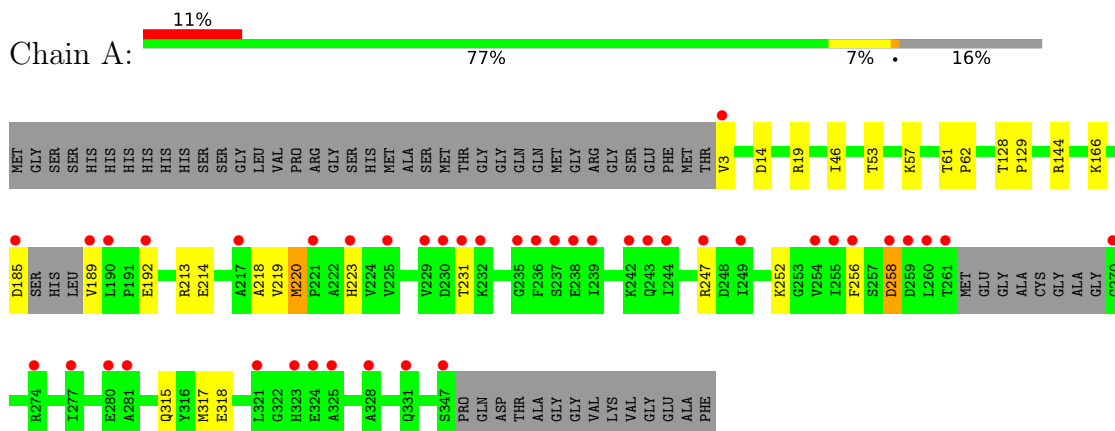
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	267	Total	O	0	0
			267	267		
3	C	153	Total	O	0	0
			153	153		
3	D	172	Total	O	0	0
			172	172		
3	E	98	Total	O	0	0
			98	98		
3	F	189	Total	O	0	0
			189	189		

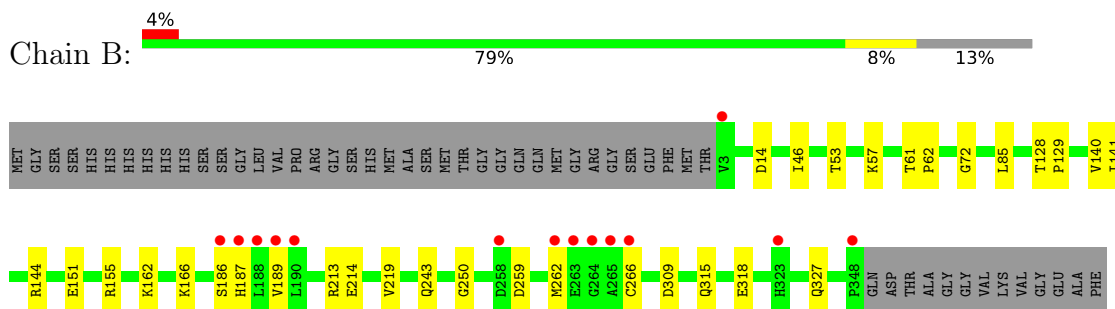
3 Residue-property plots

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.

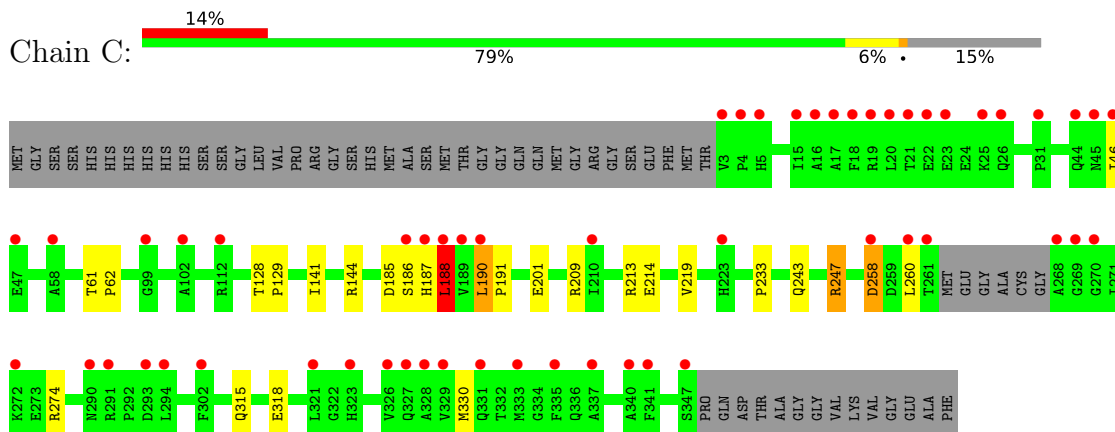
- Molecule 1: Beta-hexosaminidase



- Molecule 1: Beta-hexosaminidase

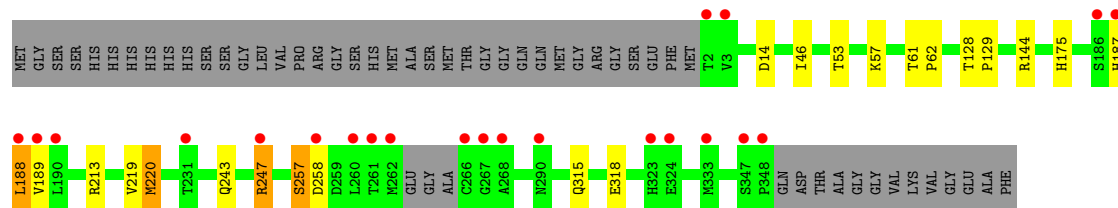


- Molecule 1: Beta-hexosaminidase



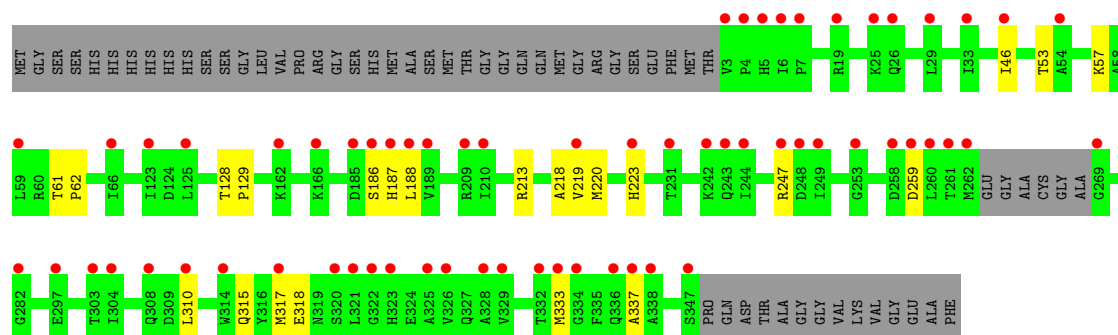
- Molecule 1: Beta-hexosaminidase

Chain D: 



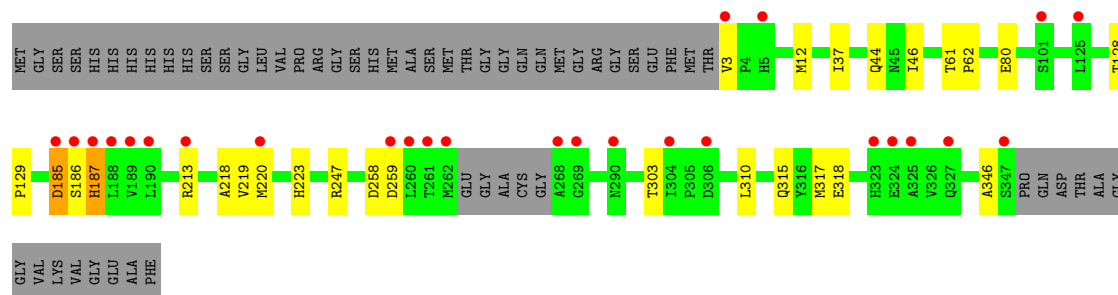
- Molecule 1: Beta-hexosaminidase

Chain E: 



- Molecule 1: Beta-hexosaminidase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.18Å 125.31Å 190.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.71 – 2.18 104.71 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (104.71-2.18) 99.7 (104.71-2.18)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.214 , 0.244 0.219 , 0.247	Depositor DCC
R_{free} test set	6401 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16730	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/2607	0.79	1/3523 (0.0%)
1	B	0.70	0/2684	0.81	1/3630 (0.0%)
1	C	0.67	0/2642	0.84	5/3572 (0.1%)
1	D	0.64	0/2675	0.78	1/3617 (0.0%)
1	E	0.62	0/2645	0.78	2/3575 (0.1%)
1	F	0.68	0/2650	0.81	5/3582 (0.1%)
All	All	0.67	0/15903	0.80	15/21499 (0.1%)

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	D	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	SER	N-CA-C	8.32	122.71	112.23
1	C	190	LEU	CA-C-N	7.59	127.54	120.03
1	C	190	LEU	C-N-CA	7.59	127.54	120.03
1	B	141	ILE	N-CA-C	-5.74	105.52	110.74
1	A	258	ASP	CA-C-O	-5.65	115.65	121.87
1	C	141	ILE	N-CA-C	-5.59	105.66	110.74
1	F	259	ASP	CA-C-N	-5.40	111.06	121.58
1	F	259	ASP	C-N-CA	-5.40	111.06	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	HIS	N-CA-C	5.39	119.80	112.04
1	C	330	MET	CG-SD-CE	5.38	112.73	100.90
1	C	188	LEU	CB-CA-C	-5.32	99.83	110.42
1	E	259	ASP	CA-C-N	-5.18	111.48	121.58
1	E	259	ASP	C-N-CA	-5.18	111.48	121.58
1	F	346	ALA	CA-C-N	5.14	130.94	121.70
1	F	346	ALA	C-N-CA	5.14	130.94	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	188	LEU	Peptide
1	F	185	ASP	Peptide

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	2560	0	2555	28	0
1	B	2633	0	2617	25	0
1	C	2593	0	2587	24	0
1	D	2625	0	2618	17	0
1	E	2596	0	2591	16	0
1	F	2601	0	2596	18	0
2	A	15	0	15	7	0
2	B	15	0	15	5	0
2	C	15	0	15	6	0
2	D	15	0	15	3	0
3	A	183	0	0	6	0
3	B	267	0	0	5	0
3	C	153	0	0	0	0
3	D	172	0	0	4	0
3	E	98	0	0	2	0
3	F	189	0	0	4	0
All	All	16730	0	15624	117	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 4.

All (117) 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)
2:A:401:NAG:H83	1:C:185:ASP:O	1.27	1.27
1:F:218:ALA:HB2	1:F:317:MET:HE3	1.40	1.04
1:A:185:ASP:C	2:C:401:NAG:H83	1.83	1.03
2:A:401:NAG:C8	1:C:185:ASP:O	2.07	1.02
1:E:218:ALA:HB2	1:E:317:MET:HE3	1.41	1.02
1:A:218:ALA:HB2	1:A:317:MET:HE3	1.42	1.01
1:F:218:ALA:HB2	1:F:317:MET:CE	2.02	0.90
1:C:144:ARG:HH12	2:C:401:NAG:H81	1.36	0.89
1:A:144:ARG:HH12	2:A:401:NAG:H81	1.36	0.89
1:E:218:ALA:HB2	1:E:317:MET:CE	2.03	0.88
1:A:218:ALA:HB2	1:A:317:MET:CE	2.05	0.85
1:C:243:GLN:HG3	1:C:247:ARG:NH2	1.95	0.81
1:F:303:THR:HB	3:F:553:HOH:O	1.79	0.80
1:E:315:GLN:OE1	1:E:318:GLU:OE1	2.06	0.71
1:D:144:ARG:NH2	2:D:401:NAG:O1	2.24	0.69
1:A:144:ARG:HH22	2:A:401:NAG:H82	1.58	0.68
1:B:144:ARG:HH12	2:B:401:NAG:H81	1.59	0.68
1:F:223:HIS:CD2	1:F:258:ASP:OD2	2.48	0.67
3:A:666:HOH:O	1:C:188:LEU:HD13	1.95	0.67
1:B:259:ASP:O	1:B:262:MET:HG2	1.96	0.65
1:B:144:ARG:HH22	2:B:401:NAG:H82	1.62	0.65
1:F:218:ALA:CB	1:F:317:MET:CE	2.75	0.63
1:F:44:GLN:HG2	3:F:525:HOH:O	2.00	0.62
1:A:218:ALA:CB	1:A:317:MET:CE	2.78	0.62
1:D:57:LYS:CE	3:D:530:HOH:O	2.48	0.61
3:A:666:HOH:O	1:C:188:LEU:CD1	2.48	0.61
1:E:218:ALA:CB	1:E:317:MET:CE	2.76	0.61
1:D:243:GLN:HG3	1:D:247:ARG:HH21	1.65	0.61
1:B:187:HIS:HB3	1:B:189:VAL:CG2	2.33	0.58
1:C:144:ARG:HH12	2:C:401:NAG:C8	2.11	0.58
1:A:247:ARG:HD3	1:B:250:GLY:HA2	1.86	0.57
1:B:155:ARG:HD3	3:B:707:HOH:O	2.04	0.57
1:B:140:VAL:HG21	1:F:186:SER:HB2	1.86	0.57
1:D:220:MET:SD	2:D:401:NAG:H61	2.45	0.56
1:C:144:ARG:HH22	2:C:401:NAG:H82	1.70	0.56
1:E:188:LEU:HB2	3:E:482:HOH:O	2.04	0.56
1:F:12:MET:SD	1:F:37:ILE:CG1	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ARG:NH1	2:C:401:NAG:H81	2.13	0.56
1:C:190:LEU:HD21	1:C:233:PRO:HG3	1.87	0.56
1:C:258:ASP:OD1	1:C:258:ASP:N	2.34	0.56
1:F:12:MET:SD	1:F:37:ILE:HG13	2.45	0.56
1:A:19:ARG:HD3	3:A:639:HOH:O	2.05	0.55
1:A:3:VAL:N	3:A:502:HOH:O	2.39	0.55
1:A:192:GLU:OE2	1:E:333:MET:HB3	2.07	0.55
1:B:187:HIS:CE1	3:F:401:HOH:O	2.59	0.55
1:F:80:GLU:HA	1:F:80:GLU:OE2	2.07	0.54
1:D:187:HIS:C	1:D:189:VAL:HG23	2.33	0.54
1:D:57:LYS:HE2	3:D:530:HOH:O	2.06	0.54
1:D:257:SER:O	1:D:258:ASP:CB	2.56	0.54
1:B:187:HIS:CB	1:B:189:VAL:HG23	2.37	0.53
1:C:187:HIS:C	1:C:188:LEU:HG	2.34	0.53
1:D:243:GLN:HG3	1:D:247:ARG:NH2	2.23	0.52
1:B:187:HIS:CB	1:B:189:VAL:CG2	2.87	0.52
1:D:14:ASP:HB2	3:D:555:HOH:O	2.10	0.52
2:B:401:NAG:H83	1:F:185:ASP:O	2.10	0.51
1:A:144:ARG:HH12	2:A:401:NAG:C8	2.16	0.51
1:D:61:THR:HA	1:D:62:PRO:C	2.36	0.50
1:C:260:LEU:O	1:C:274:ARG:NH2	2.44	0.50
1:E:186:SER:O	1:E:187:HIS:ND1	2.45	0.50
1:E:61:THR:HA	1:E:62:PRO:C	2.37	0.50
1:A:189:VAL:N	1:C:188:LEU:HD21	2.27	0.49
1:F:315:GLN:NE2	1:F:318:GLU:OE2	2.39	0.49
1:C:61:THR:HA	1:C:62:PRO:C	2.38	0.49
1:A:192:GLU:CD	1:E:333:MET:SD	2.96	0.49
1:B:186:SER:HB3	3:F:522:HOH:O	2.11	0.49
1:A:315:GLN:HG3	1:A:318:GLU:OE1	2.14	0.48
1:F:61:THR:HA	1:F:62:PRO:C	2.38	0.48
1:C:201:GLU:OE1	1:C:209:ARG:NH1	2.46	0.48
1:E:187:HIS:HA	3:E:473:HOH:O	2.12	0.48
1:F:223:HIS:HD2	1:F:258:ASP:OD2	1.93	0.48
1:A:231:THR:HG21	1:E:337:ALA:HA	1.96	0.48
2:B:401:NAG:H83	1:F:185:ASP:C	2.39	0.47
1:B:315:GLN:NE2	1:B:318:GLU:OE2	2.37	0.47
1:D:315:GLN:HG3	1:D:318:GLU:OE1	2.14	0.47
1:B:61:THR:HA	1:B:62:PRO:C	2.39	0.47
1:C:187:HIS:O	1:C:188:LEU:HG	2.14	0.47
1:A:61:THR:HA	1:A:62:PRO:C	2.39	0.46
1:D:175:HIS:CD2	2:D:401:NAG:H83	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:CG2	1:E:337:ALA:HA	2.45	0.46
1:A:192:GLU:HG2	1:E:333:MET:SD	2.55	0.46
1:B:144:ARG:HH12	2:B:401:NAG:C8	2.27	0.45
1:B:187:HIS:HB3	1:B:189:VAL:HG23	1.96	0.45
1:B:14:ASP:HB2	3:B:574:HOH:O	2.17	0.45
1:E:128:THR:OG1	1:E:129:PRO:HA	2.17	0.45
1:B:259:ASP:HB3	1:B:262:MET:HE3	1.99	0.44
1:A:223:HIS:CD2	1:A:258:ASP:OD2	2.70	0.44
1:B:243:GLN:HG3	3:B:718:HOH:O	2.17	0.44
1:B:128:THR:OG1	1:B:129:PRO:HA	2.18	0.44
1:C:128:THR:OG1	1:C:129:PRO:HA	2.18	0.43
1:A:185:ASP:HB2	2:C:401:NAG:C8	2.48	0.43
1:B:213:ARG:NH1	1:B:214:GLU:OE2	2.52	0.43
1:F:186:SER:OG	1:F:187:HIS:N	2.49	0.43
1:C:315:GLN:NE2	1:C:318:GLU:OE2	2.40	0.43
1:A:252:LYS:HE2	1:B:309:ASP:OD1	2.19	0.43
1:A:220:MET:HE2	1:A:256:PHE:CB	2.49	0.43
1:A:189:VAL:N	1:C:188:LEU:CD2	2.81	0.42
1:B:327:GLN:NE2	3:B:501:HOH:O	2.51	0.42
1:D:247:ARG:CZ	1:D:247:ARG:HB3	2.48	0.42
1:F:128:THR:OG1	1:F:129:PRO:HA	2.19	0.42
1:D:128:THR:OG1	1:D:129:PRO:HA	2.20	0.42
1:D:188:LEU:HD11	1:E:223:HIS:CD2	2.55	0.42
1:E:53:THR:O	1:E:57:LYS:HG3	2.20	0.41
1:A:128:THR:OG1	1:A:129:PRO:HA	2.20	0.41
2:A:401:NAG:O1	1:C:186:SER:CB	2.68	0.41
1:A:213:ARG:NH1	1:A:214:GLU:OE2	2.54	0.41
1:F:12:MET:SD	1:F:37:ILE:HD11	2.60	0.41
1:C:213:ARG:NH1	1:C:214:GLU:OE2	2.53	0.41
1:D:57:LYS:HE3	3:D:530:HOH:O	2.14	0.41
2:A:401:NAG:O1	1:C:186:SER:HB3	2.20	0.41
1:B:72:GLY:HA2	1:B:85:LEU:HB2	2.03	0.41
1:D:53:THR:O	1:D:57:LYS:HG3	2.20	0.41
1:A:14:ASP:HB2	3:A:531:HOH:O	2.21	0.40
1:B:53:THR:O	1:B:57:LYS:HG3	2.21	0.40
1:A:252:LYS:NZ	3:A:508:HOH:O	2.51	0.40
1:A:53:THR:O	1:A:57:LYS:HG3	2.22	0.40
1:B:266:CYS:SG	3:B:736:HOH:O	2.63	0.40
1:C:190:LEU:HA	1:C:191:PRO:HD3	1.68	0.40

There are no symmetry-related clashes.

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	328/397 (83%)	318 (97%)	10 (3%)	0	100	100
1	B	344/397 (87%)	329 (96%)	15 (4%)	0	100	100
1	C	335/397 (84%)	322 (96%)	12 (4%)	1 (0%)	36	39
1	D	340/397 (86%)	327 (96%)	13 (4%)	0	100	100
1	E	335/397 (84%)	325 (97%)	10 (3%)	0	100	100
1	F	336/397 (85%)	326 (97%)	10 (3%)	0	100	100
All	All	2018/2382 (85%)	1947 (96%)	70 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	LEU

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	264/309 (85%)	260 (98%)	4 (2%)	57	70
1	B	270/309 (87%)	265 (98%)	5 (2%)	50	63
1	C	267/309 (86%)	263 (98%)	4 (2%)	57	70
1	D	271/309 (88%)	266 (98%)	5 (2%)	51	65
1	E	268/309 (87%)	262 (98%)	6 (2%)	45	58
1	F	268/309 (87%)	261 (97%)	7 (3%)	40	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1608/1854 (87%)	1577 (98%)	31 (2%)	50 63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	166	LYS
1	A	219	VAL
1	A	220	MET
1	B	46	ILE
1	B	151	GLU
1	B	162	LYS
1	B	166	LYS
1	B	219	VAL
1	C	46	ILE
1	C	219	VAL
1	C	247	ARG
1	C	258	ASP
1	D	46	ILE
1	D	213	ARG
1	D	219	VAL
1	D	220	MET
1	D	247	ARG
1	E	46	ILE
1	E	213	ARG
1	E	219	VAL
1	E	220	MET
1	E	247	ARG
1	E	310	LEU
1	F	3	VAL
1	F	46	ILE
1	F	213	ARG
1	F	219	VAL
1	F	220	MET
1	F	247	ARG
1	F	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS

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Mol	Chain	Res	Type
1	A	228	GLN
1	B	161	GLN
1	B	323	HIS
1	B	327	GLN
1	B	336	GLN
1	C	26	GLN
1	C	223	HIS
1	D	161	GLN
1	D	228	GLN
1	D	336	GLN
1	E	26	GLN
1	E	228	GLN
1	E	315	GLN
1	E	327	GLN
1	E	336	GLN
1	F	161	GLN
1	F	223	HIS
1	F	228	GLN
1	F	336	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	401	-	15,15,15	1.10	1 (6%)	21,21,21	3.14	12 (57%)
2	NAG	A	401	-	15,15,15	0.90	0	21,21,21	1.53	2 (9%)
2	NAG	B	401	-	15,15,15	0.74	0	21,21,21	1.78	5 (23%)
2	NAG	C	401	-	15,15,15	0.74	0	21,21,21	1.67	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	401	-	-	4/6/26/26	0/1/1/1
2	NAG	A	401	-	-	2/6/26/26	0/1/1/1
2	NAG	B	401	-	-	2/6/26/26	0/1/1/1
2	NAG	C	401	-	-	2/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAG	O7-C7	-2.02	1.18	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAG	C1-C2-N2	-6.13	103.63	110.73
2	D	401	NAG	C8-C7-N2	5.21	124.75	116.12
2	D	401	NAG	O3-C3-C4	-4.73	99.22	110.38
2	B	401	NAG	O5-C1-C2	4.69	114.23	109.52
2	A	401	NAG	C3-C2-N2	4.55	119.00	110.62
2	C	401	NAG	O5-C1-C2	4.32	113.86	109.52
2	D	401	NAG	C3-C2-N2	4.08	118.14	110.62
2	D	401	NAG	C1-C2-C3	-4.08	104.98	110.54
2	D	401	NAG	C2-N2-C7	3.90	132.24	123.11
2	C	401	NAG	C1-O5-C5	3.84	121.07	113.65
2	D	401	NAG	O1-C1-C2	3.74	116.98	109.22
2	D	401	NAG	O3-C3-C2	3.58	116.71	109.58
2	D	401	NAG	O7-C7-C8	-3.55	115.74	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAG	O6-C6-C5	-3.30	100.09	111.33
2	B	401	NAG	C2-N2-C7	3.13	130.43	123.11
2	B	401	NAG	O1-C1-O5	-2.96	101.62	110.41
2	C	401	NAG	O1-C1-O5	-2.68	102.44	110.41
2	D	401	NAG	C1-O5-C5	-2.44	108.93	113.65
2	B	401	NAG	C3-C2-N2	2.27	114.80	110.62
2	A	401	NAG	C1-C2-N2	-2.23	108.14	110.73
2	C	401	NAG	C2-N2-C7	2.21	128.28	123.11
2	D	401	NAG	O5-C5-C6	-2.16	101.08	106.44
2	B	401	NAG	O5-C5-C6	2.06	111.56	106.44

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NAG	C8-C7-N2-C2
2	D	401	NAG	O7-C7-N2-C2
2	D	401	NAG	O5-C5-C6-O6
2	D	401	NAG	C4-C5-C6-O6
2	A	401	NAG	C8-C7-N2-C2
2	A	401	NAG	O7-C7-N2-C2
2	B	401	NAG	C8-C7-N2-C2
2	B	401	NAG	O7-C7-N2-C2
2	C	401	NAG	C8-C7-N2-C2
2	C	401	NAG	O7-C7-N2-C2

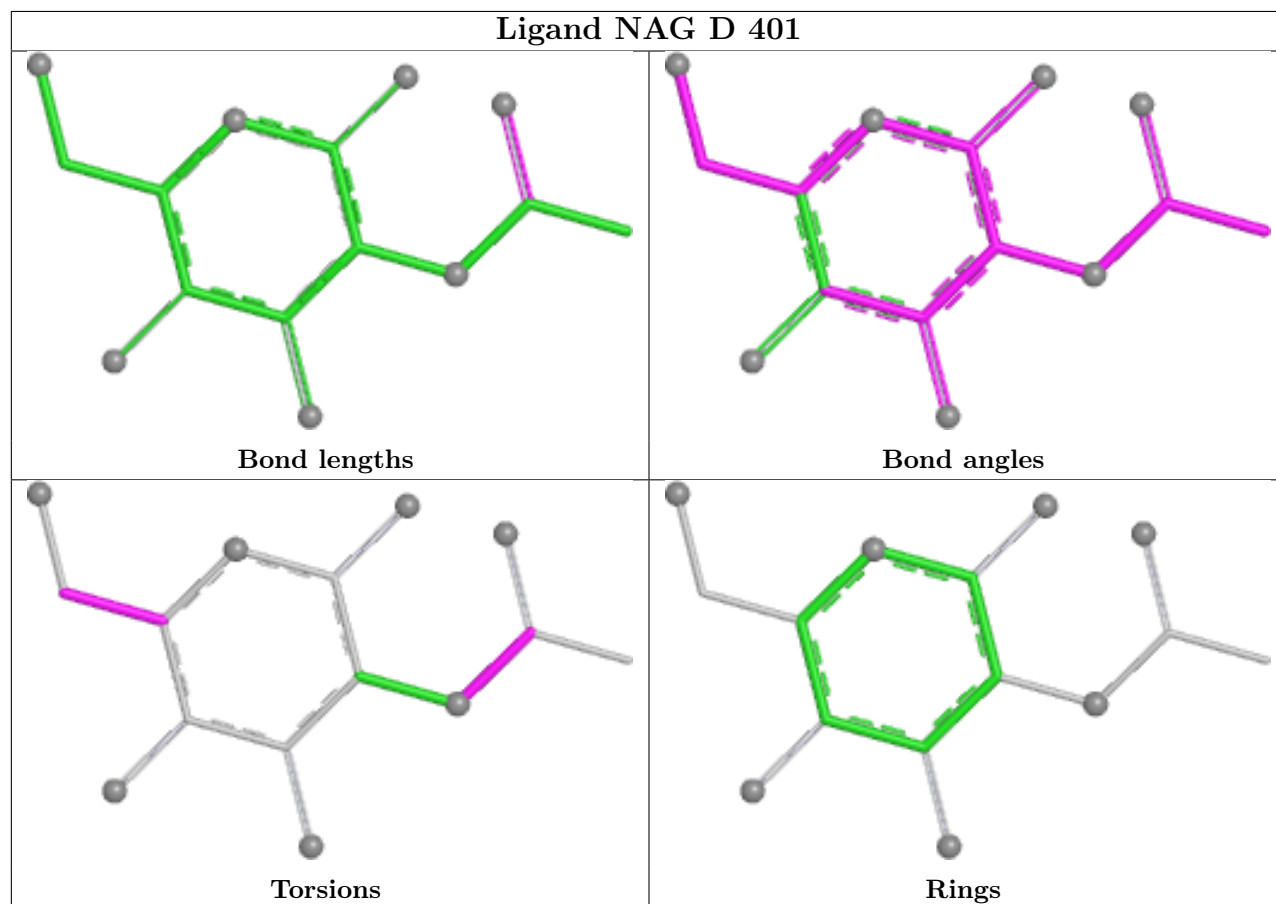
There are no ring outliers.

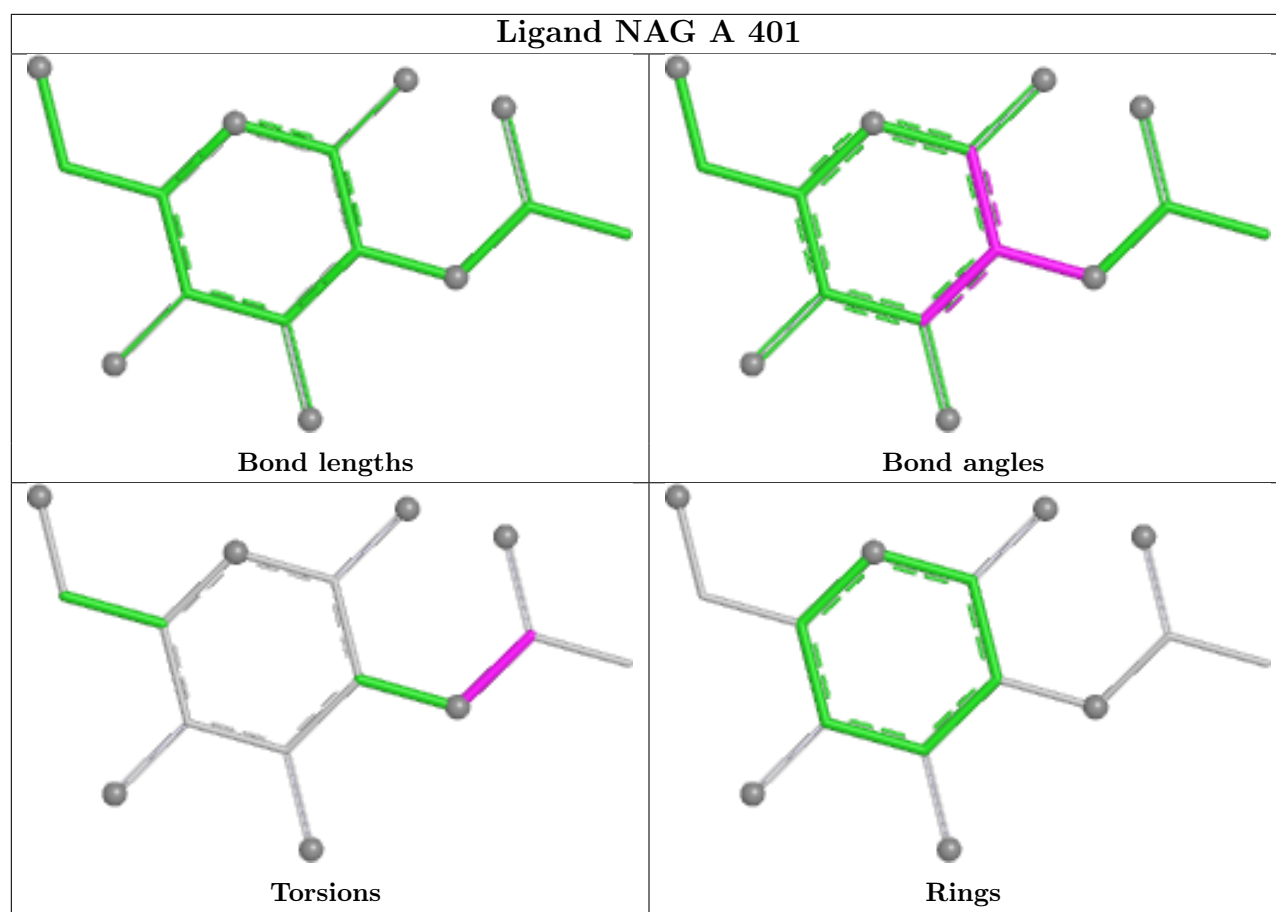
4 monomers are involved in 21 short contacts:

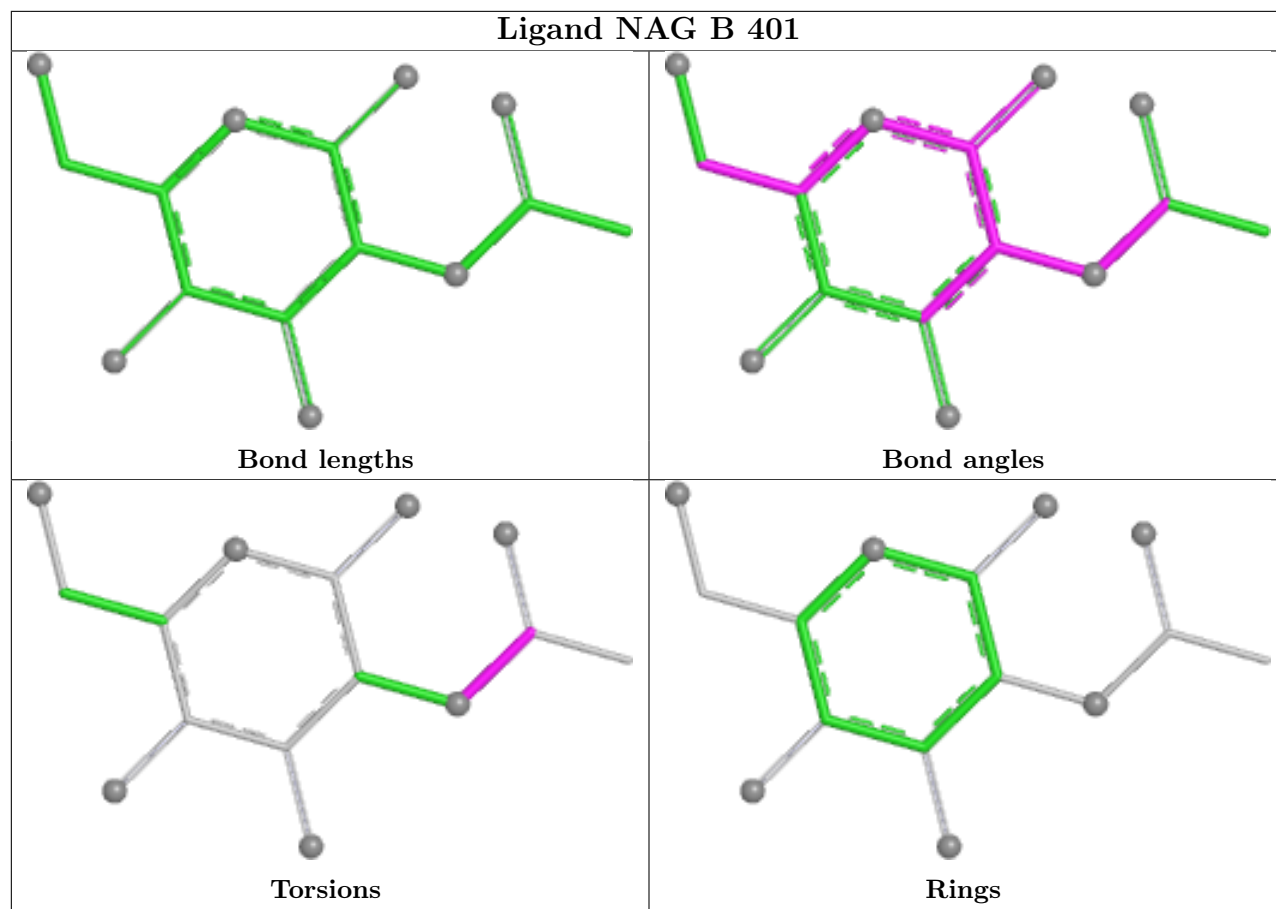
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAG	3	0
2	A	401	NAG	7	0
2	B	401	NAG	5	0
2	C	401	NAG	6	0

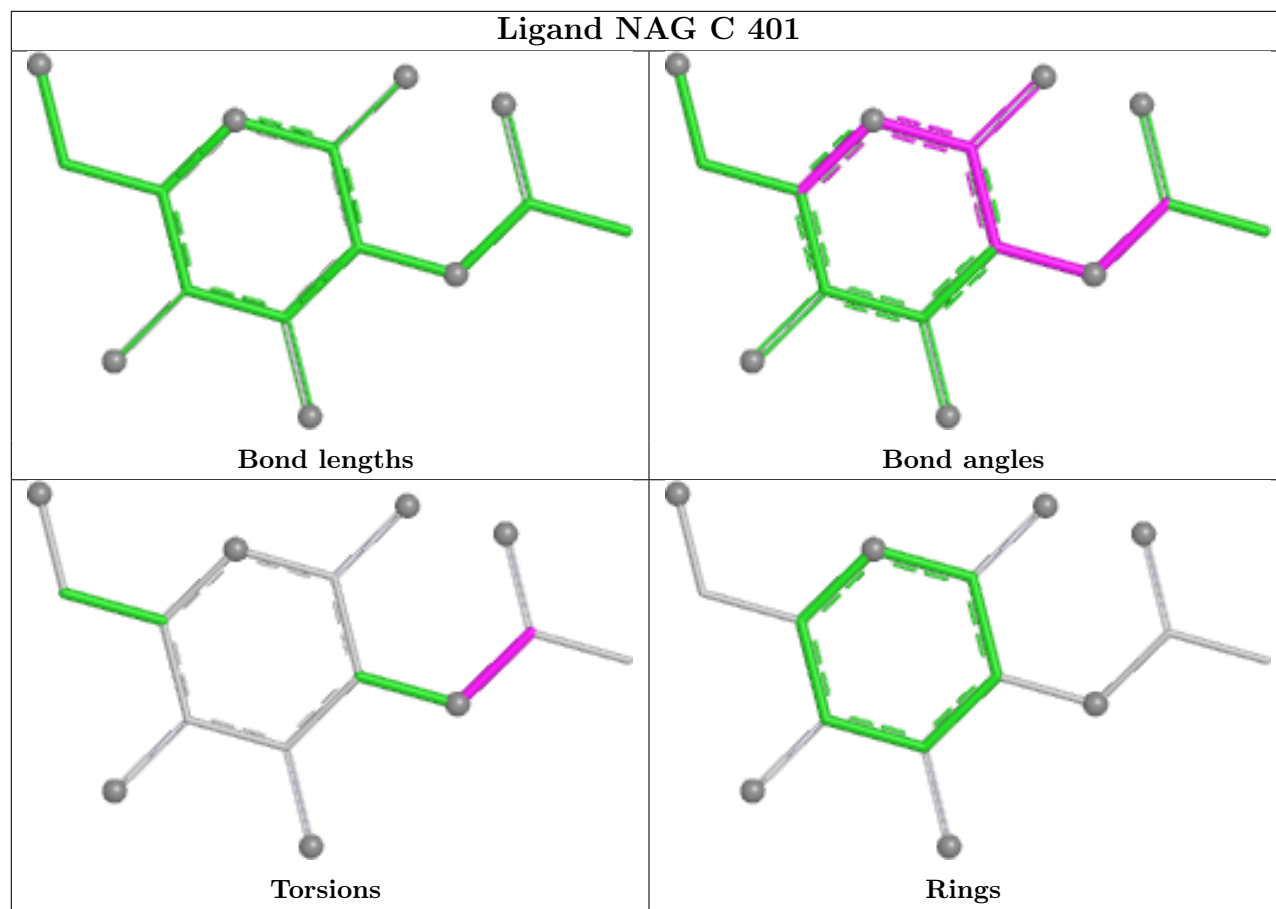
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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

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, 95th 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	334/397 (84%)	0.63	42 (12%) 8 7	17, 32, 56, 81	0
1	B	346/397 (87%)	0.11	14 (4%) 42 41	15, 24, 46, 106	0
1	C	339/397 (85%)	0.85	55 (16%) 4 4	16, 34, 61, 91	0
1	D	344/397 (86%)	0.42	22 (6%) 25 24	22, 33, 53, 103	0
1	E	339/397 (85%)	1.34	64 (18%) 3 3	26, 44, 70, 130	0
1	F	340/397 (85%)	0.55	26 (7%) 20 19	20, 32, 53, 108	0
All	All	2042/2382 (85%)	0.65	223 (10%) 10 9	15, 33, 60, 130	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	188	LEU	9.4
1	F	262	MET	8.3
1	B	189	VAL	8.2
1	E	187	HIS	7.7
1	A	189	VAL	7.4
1	B	264	GLY	6.8
1	B	188	LEU	6.7
1	B	265	ALA	6.6
1	D	188	LEU	6.6
1	E	262	MET	6.5
1	E	188	LEU	6.5
1	C	189	VAL	6.3
1	D	348	PRO	6.3
1	D	262	MET	6.2
1	F	188	LEU	6.2
1	C	269	GLY	6.0
1	C	190	LEU	5.9
1	F	187	HIS	5.9
1	D	189	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	268	ALA	5.6
1	C	187	HIS	5.5
1	E	186	SER	5.4
1	A	261	THR	5.2
1	E	189	VAL	5.2
1	F	189	VAL	5.1
1	F	3	VAL	5.0
1	B	263	GLU	5.0
1	C	268	ALA	4.8
1	A	236	PHE	4.8
1	D	187	HIS	4.6
1	F	347	SER	4.6
1	E	3	VAL	4.6
1	E	322	GLY	4.5
1	A	259	ASP	4.5
1	A	232	LYS	4.5
1	B	262	MET	4.4
1	C	186	SER	4.4
1	B	187	HIS	4.3
1	E	333	MET	4.2
1	D	2	THR	4.2
1	C	261	THR	4.1
1	F	186	SER	4.1
1	F	269	GLY	4.1
1	A	231	THR	4.0
1	C	3	VAL	3.9
1	A	270	GLY	3.9
1	D	333	MET	3.9
1	A	323	HIS	3.9
1	E	269	GLY	3.8
1	A	223	HIS	3.6
1	E	347	SER	3.6
1	B	348	PRO	3.6
1	E	334	GLY	3.6
1	E	325	ALA	3.6
1	A	260	LEU	3.6
1	C	18	PHE	3.6
1	B	3	VAL	3.5
1	E	249	ILE	3.5
1	E	46	ILE	3.4
1	A	256	PHE	3.4
1	A	321	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	254	VAL	3.3
1	E	259	ASP	3.3
1	A	190	LEU	3.3
1	E	321	LEU	3.3
1	E	323	HIS	3.2
1	A	238	GLU	3.2
1	F	261	THR	3.1
1	A	258	ASP	3.1
1	C	102	ALA	3.1
1	D	186	SER	3.1
1	A	192	GLU	3.1
1	A	255	ILE	3.1
1	F	259	ASP	3.1
1	C	46	ILE	3.1
1	E	320	SER	3.1
1	D	268	ALA	3.0
1	B	190	LEU	3.0
1	C	44	GLN	3.0
1	E	326	VAL	3.0
1	C	327	GLN	3.0
1	C	270	GLY	2.9
1	E	166	LYS	2.9
1	C	26	GLN	2.9
1	A	217	ALA	2.9
1	C	20	LEU	2.9
1	A	229	VAL	2.9
1	E	59	LEU	2.9
1	F	260	LEU	2.9
1	D	266	CYS	2.9
1	F	323	HIS	2.9
1	C	16	ALA	2.9
1	C	293	ASP	2.8
1	E	260	LEU	2.8
1	D	3	VAL	2.8
1	A	239	ILE	2.8
1	C	347	SER	2.8
1	B	258	ASP	2.8
1	A	3	VAL	2.8
1	C	99	GLY	2.7
1	C	335	PHE	2.7
1	A	281	ALA	2.7
1	C	328	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	325	ALA	2.7
1	E	209	ARG	2.7
1	D	258	ASP	2.7
1	C	321	LEU	2.7
1	E	329	VAL	2.7
1	C	272	LYS	2.7
1	C	340	ALA	2.6
1	F	190	LEU	2.6
1	E	162	LYS	2.6
1	A	247	ARG	2.6
1	E	243	GLN	2.6
1	C	22	GLU	2.6
1	C	21	THR	2.6
1	B	186	SER	2.6
1	A	225	VAL	2.6
1	E	338	ALA	2.6
1	B	323	HIS	2.6
1	C	25	LYS	2.6
1	C	17	ALA	2.6
1	E	261	THR	2.6
1	E	303	THR	2.6
1	E	297	GLU	2.5
1	E	123	ILE	2.5
1	E	244	ILE	2.5
1	C	45	ASN	2.5
1	E	242	LYS	2.5
1	C	112	ARG	2.5
1	E	231	THR	2.5
1	C	323	HIS	2.5
1	A	230	ASP	2.5
1	E	337	ALA	2.5
1	E	317	MET	2.5
1	E	5	HIS	2.5
1	D	267	GLY	2.5
1	A	347	SER	2.4
1	C	337	ALA	2.4
1	C	290	ASN	2.4
1	A	324	GLU	2.4
1	A	237	SER	2.4
1	D	347	SER	2.4
1	C	19	ARG	2.4
1	C	223	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	223	HIS	2.4
1	A	235	GLY	2.4
1	F	327	GLN	2.4
1	C	258	ASP	2.4
1	C	15	ILE	2.4
1	E	210	ILE	2.4
1	E	332	THR	2.4
1	E	328	ALA	2.4
1	E	247	ARG	2.4
1	E	4	PRO	2.4
1	E	66	ILE	2.3
1	A	221	PRO	2.3
1	E	6	ILE	2.3
1	C	329	VAL	2.3
1	E	26	GLN	2.3
1	E	336	GLN	2.3
1	C	260	LEU	2.3
1	E	125	LEU	2.3
1	F	213	ARG	2.3
1	F	306	ASP	2.3
1	D	324	GLU	2.3
1	C	210	ILE	2.3
1	A	185	ASP	2.3
1	E	258	ASP	2.3
1	F	290	ASN	2.2
1	E	25	LYS	2.2
1	E	248	ASP	2.2
1	F	220	MET	2.2
1	C	47	GLU	2.2
1	F	5	HIS	2.2
1	C	302	PHE	2.2
1	A	244	ILE	2.2
1	D	323	HIS	2.2
1	E	314	TRP	2.2
1	A	242	LYS	2.2
1	A	277	ILE	2.2
1	E	282	GLY	2.2
1	B	266	CYS	2.2
1	D	190	LEU	2.2
1	D	290	ASN	2.2
1	D	261	THR	2.2
1	F	185	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	ILE	2.1
1	E	219	VAL	2.1
1	A	243	GLN	2.1
1	D	247	ARG	2.1
1	E	29	LEU	2.1
1	A	280	GLU	2.1
1	F	324	GLU	2.1
1	E	7	PRO	2.1
1	A	331	GLN	2.1
1	C	331	GLN	2.1
1	C	5	HIS	2.1
1	E	253	GLY	2.1
1	A	274	ARG	2.1
1	C	291	ARG	2.1
1	D	260	LEU	2.1
1	E	185	ASP	2.1
1	A	328	ALA	2.1
1	F	101	SER	2.1
1	F	125	LEU	2.1
1	C	23	GLU	2.1
1	C	4	PRO	2.1
1	E	19	ARG	2.1
1	C	326	VAL	2.1
1	E	54	ALA	2.1
1	E	310	LEU	2.0
1	E	308	GLN	2.0
1	E	33	ILE	2.0
1	E	304	ILE	2.0
1	F	304	ILE	2.0
1	C	341	PHE	2.0
1	C	333	MET	2.0
1	A	325	ALA	2.0
1	C	58	ALA	2.0
1	C	294	LEU	2.0
1	C	31	PRO	2.0
1	D	231	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

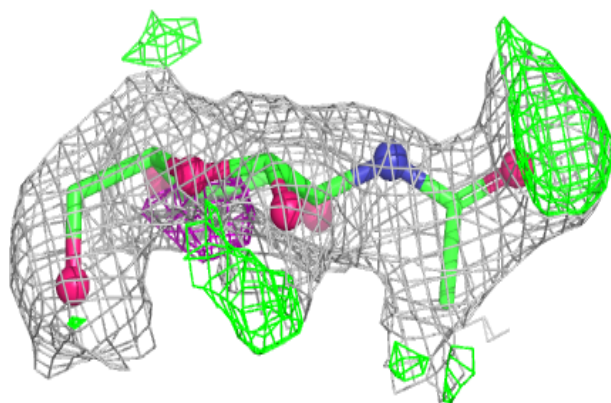
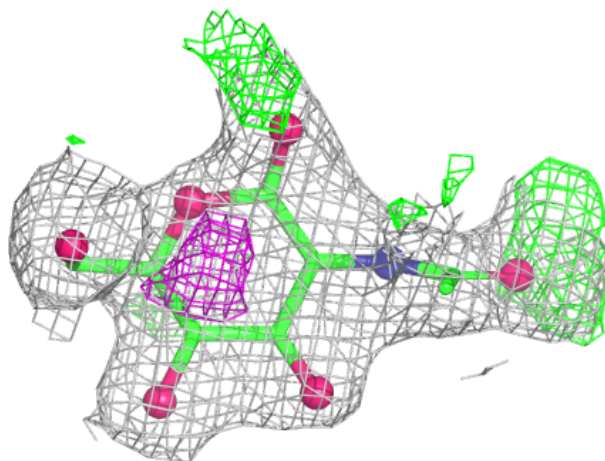
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	401	15/15	0.72	0.17	39,47,55,55	0
2	NAG	A	401	15/15	0.74	0.16	36,47,55,56	0
2	NAG	D	401	15/15	0.78	0.15	50,58,62,62	0
2	NAG	B	401	15/15	0.79	0.13	28,32,38,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

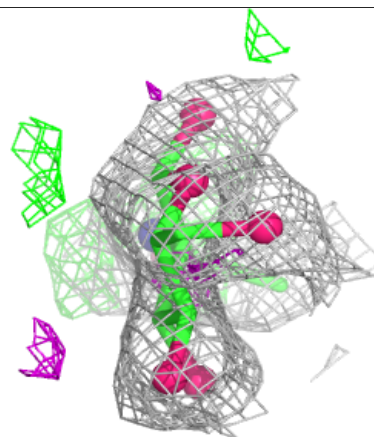
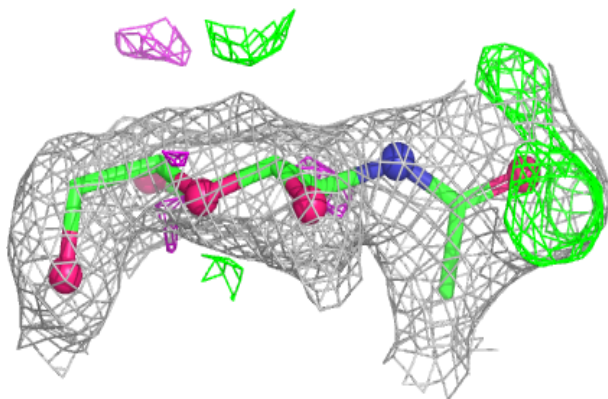
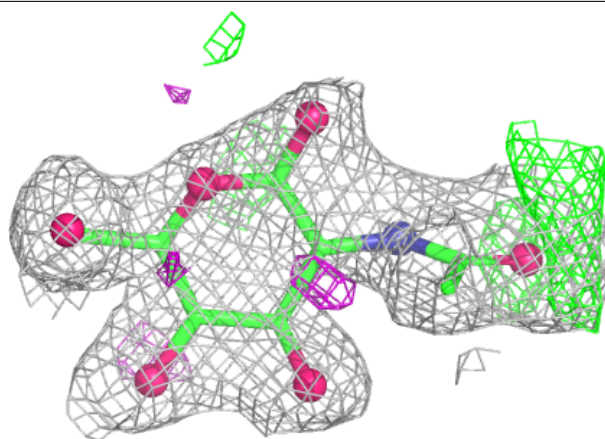
Electron density around NAG C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



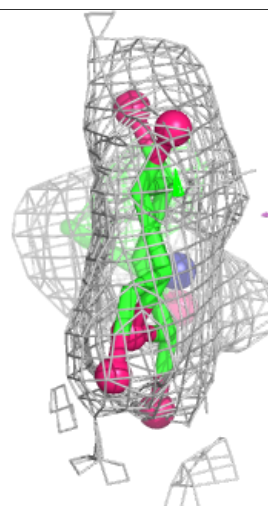
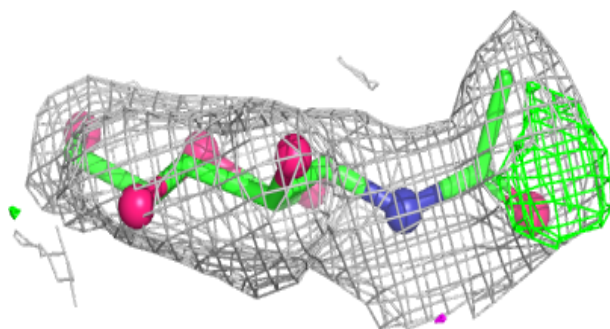
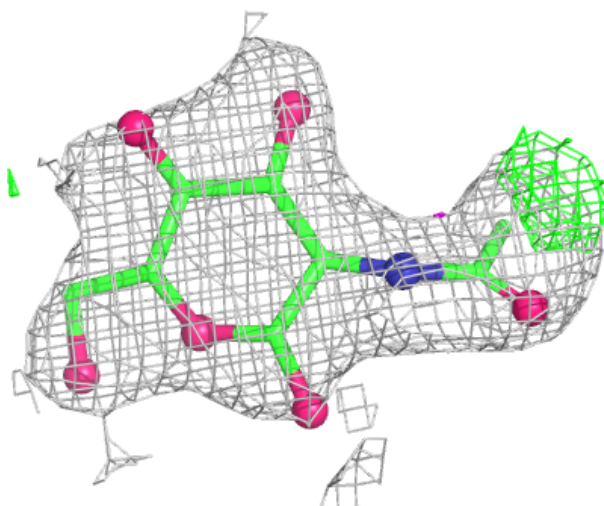
Electron density around NAG A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



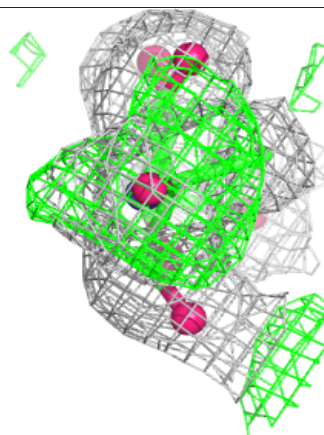
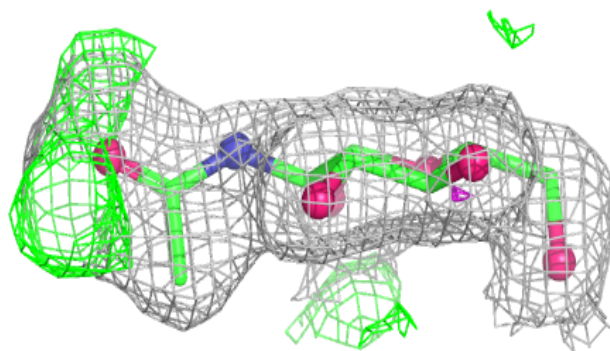
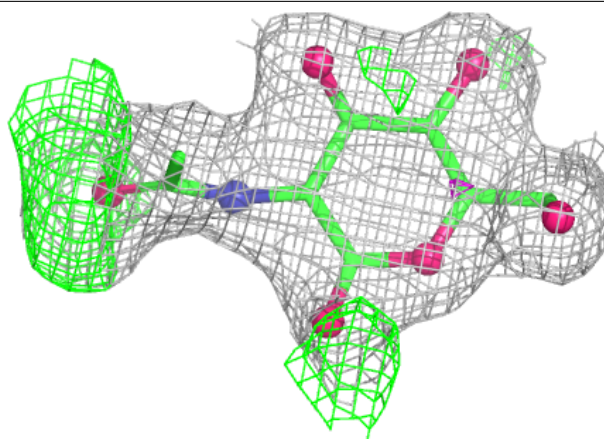
Electron density around NAG D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG B 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.