



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:17 AM UTC

PDB ID : 6JTK / pdb_00006jtk
Title : Crystal structure of NagZ from *Neisseria gonorrhoeae* in complex with N-trifluoroacetyl-D-glucosamine
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	:	4-5-2 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

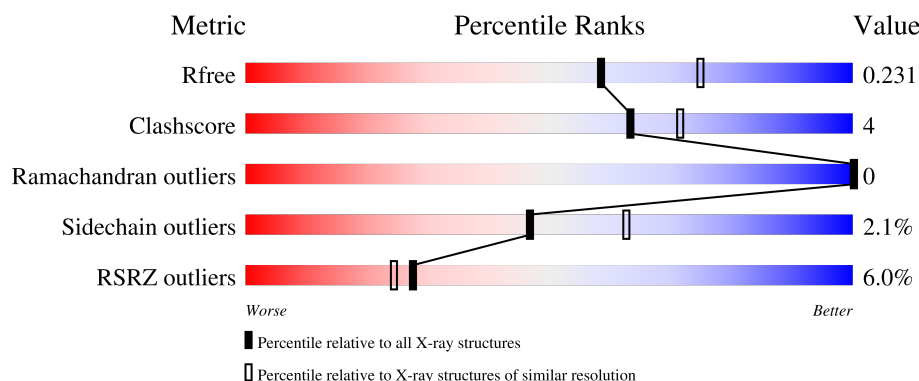
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	6% 78% 6% 16%
1	B	397	4% 80% 6% 13%
1	C	397	6% 78% 7% 15%
1	D	397	4% 81% 5% 13%
1	E	397	8% 77% 8% 15%

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Mol	Chain	Length	Quality of chain
1	F	397	4% 78% 7% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16734 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
			2636	1662	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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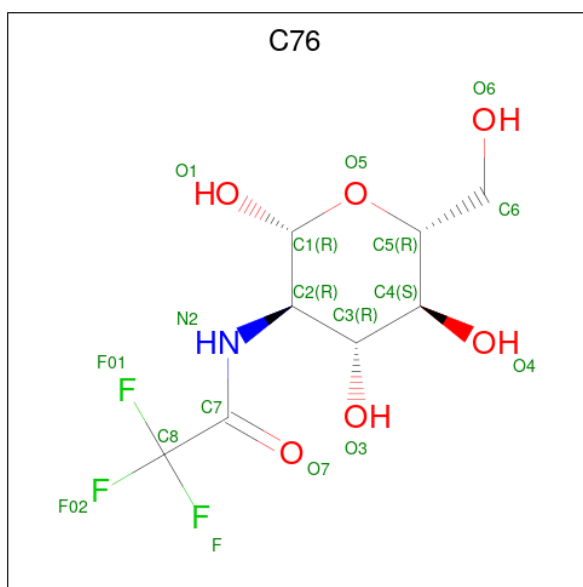
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP Q5FA94
E	-35	MET	-	expression tag	UNP Q5FA94
E	-34	GLY	-	expression tag	UNP Q5FA94
E	-33	SER	-	expression tag	UNP Q5FA94
E	-32	SER	-	expression tag	UNP Q5FA94
E	-31	HIS	-	expression tag	UNP Q5FA94
E	-30	HIS	-	expression tag	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 2,2,2-tris(fluoranyl)-N-[(2R,3R,4R,5S,6R)-6-(hydroxymethyl)-2,4,5-tris(oxidan-yl)oxan-3-yl]ethanamide (CCD ID: C76) (formula: C₈H₁₂F₃NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	
			18	8	3	1	6	0
2	B	1	Total	C	F	N	O	
			18	8	3	1	6	0
2	C	1	Total	C	F	N	O	
			18	8	3	1	6	0
2	D	1	Total	C	F	N	O	
			18	8	3	1	6	0

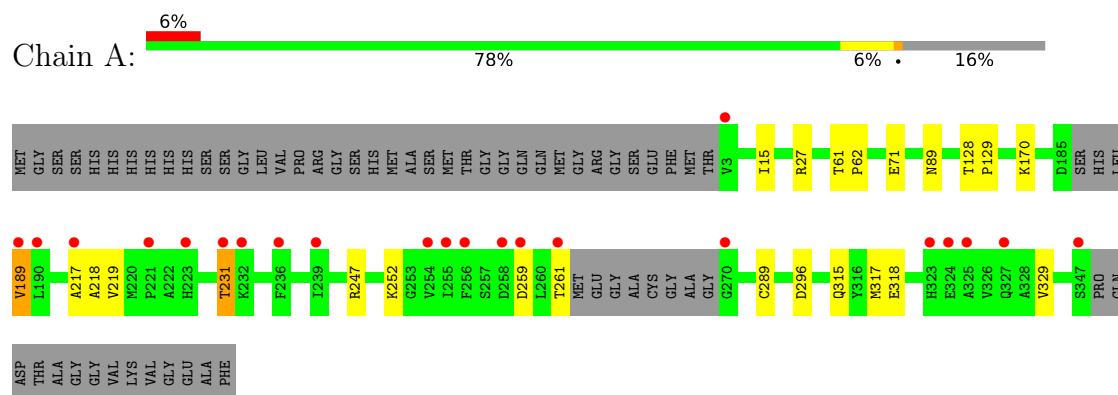
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	222	Total	O	0	0
			222	222		
3	C	140	Total	O	0	0
			140	140		
3	D	185	Total	O	0	0
			185	185		
3	E	127	Total	O	0	0
			127	127		
3	F	181	Total	O	0	0
			181	181		

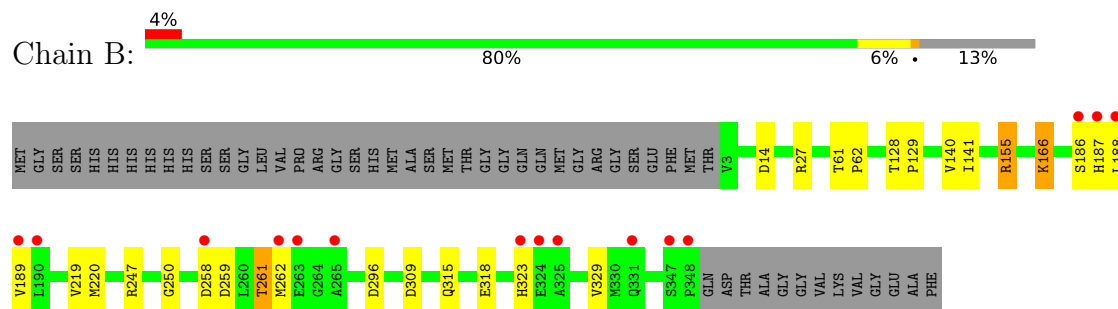
3 Residue-property plots [i](#)

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.

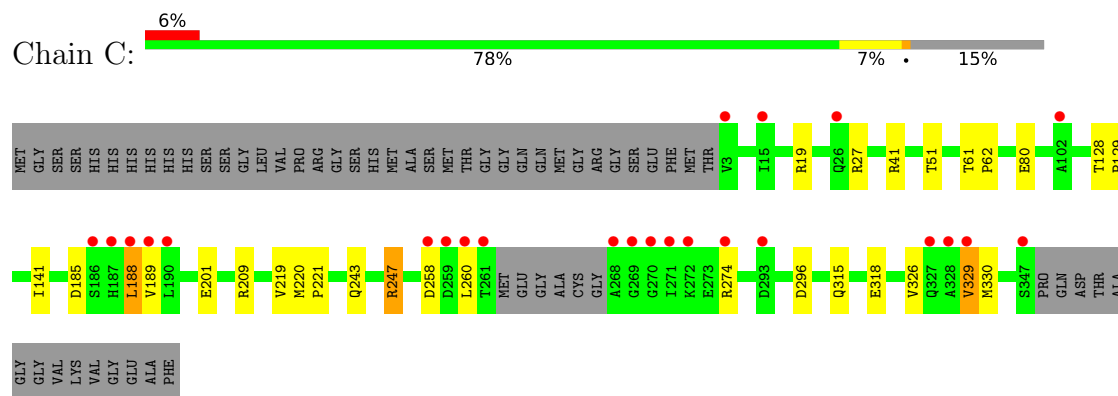
- Molecule 1: Beta-hexosaminidase



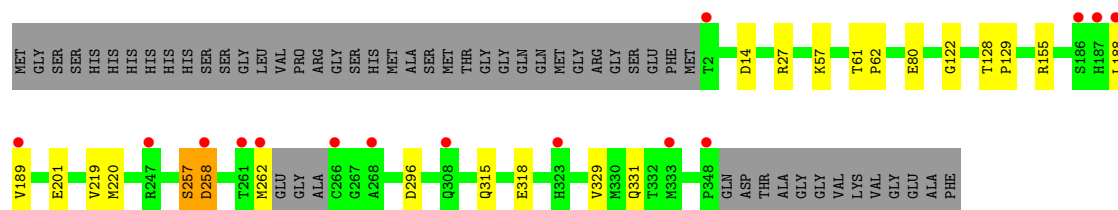
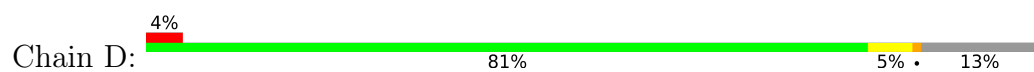
- Molecule 1: Beta-hexosaminidase



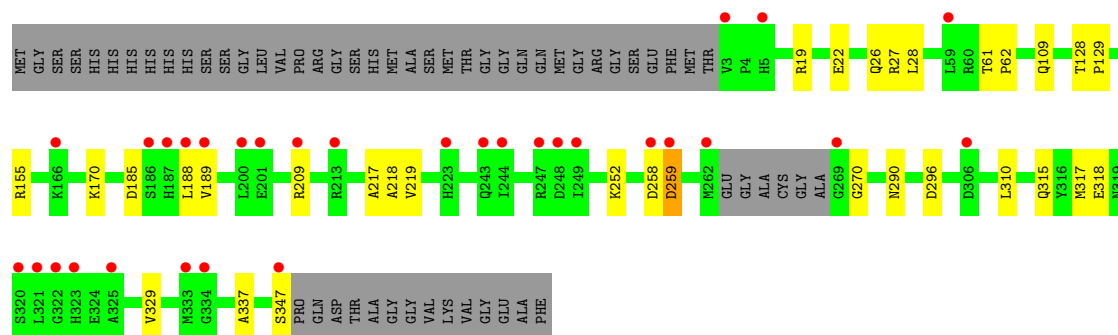
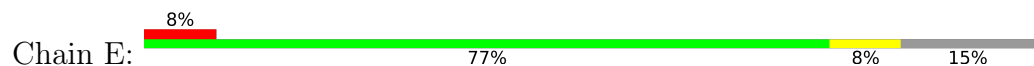
- Molecule 1: Beta-hexosaminidase



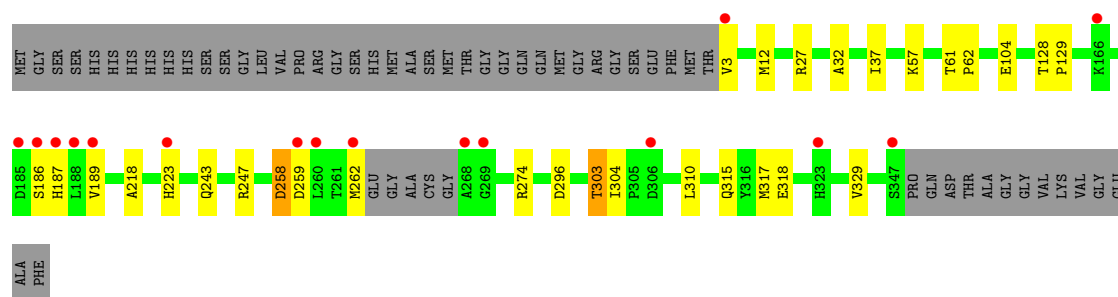
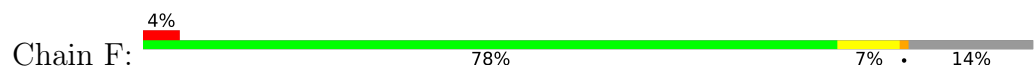
- Molecule 1: Beta-hexosaminidase



• Molecule 1: Beta-hexosaminidase



• Molecule 1: Beta-hexosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.05Å 124.75Å 190.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.5 (50.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.227 0.204 , 0.231	Depositor DCC
R_{free} test set	6227 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.2	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	0.95	EDS
Total number of atoms	16734	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 2.31% 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: C76

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	0.67	0/2607	0.78	1/3523 (0.0%)
1	B	0.67	0/2687	0.82	3/3634 (0.1%)
1	C	0.63	0/2642	0.79	2/3572 (0.1%)
1	D	0.61	0/2675	0.80	2/3617 (0.1%)
1	E	0.59	0/2645	0.76	1/3575 (0.0%)
1	F	0.63	0/2650	0.80	1/3582 (0.0%)
All	All	0.63	0/15906	0.79	10/21503 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	SER	N-CA-C	9.16	124.26	113.18
1	F	259	ASP	N-CA-C	-6.32	99.58	109.25
1	B	187	HIS	CB-CA-C	5.93	122.23	110.42
1	E	259	ASP	N-CA-C	-5.90	100.22	109.25
1	C	141	ILE	N-CA-C	-5.82	105.45	110.74
1	B	141	ILE	N-CA-C	-5.69	105.56	110.74
1	A	259	ASP	N-CA-C	5.55	122.62	110.80
1	C	330	MET	CG-SD-CE	5.29	112.53	100.90
1	B	166	LYS	CB-CG-CD	5.21	123.27	111.30
1	D	188	LEU	N-CA-C	5.05	117.38	108.24

There are no chirality outliers.

There are no planarity outliers.

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	22	0
1	B	2636	0	2626	27	0
1	C	2593	0	2587	17	0
1	D	2625	0	2618	18	0
1	E	2596	0	2591	26	0
1	F	2601	0	2596	29	0
2	A	18	0	0	1	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
2	D	18	0	0	2	0
3	A	196	0	0	8	0
3	B	222	0	0	7	0
3	C	140	0	0	6	0
3	D	185	0	0	11	0
3	E	127	0	0	13	0
3	F	181	0	0	11	0
All	All	16734	0	15573	124	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 (124) 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:A:189:VAL:HB	3:A:650:HOH:O	1.58	1.02
1:B:188:LEU:HD22	1:F:187:HIS:O	1.59	1.01
1:B:220:MET:SD	3:B:650:HOH:O	2.30	0.89
1:C:51:THR:HB	3:C:547:HOH:O	1.74	0.86
2:D:401:C76:O7	1:E:185:ASP:O	2.01	0.79
1:B:186:SER:HB3	3:F:518:HOH:O	1.83	0.78
1:F:61:THR:HB	3:F:551:HOH:O	1.83	0.78
1:D:257:SER:O	1:D:258:ASP:CB	2.29	0.78
1:F:57:LYS:HD2	3:F:528:HOH:O	1.85	0.76
1:F:218:ALA:HB2	1:F:317:MET:HE3	1.68	0.76
1:A:247:ARG:HD3	1:B:250:GLY:HA2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:HE3	3:D:507:HOH:O	1.86	0.76
1:A:218:ALA:HB2	1:A:317:MET:HE3	1.67	0.75
3:A:630:HOH:O	1:B:247:ARG:HB3	1.87	0.75
1:D:257:SER:O	1:D:258:ASP:HB2	1.87	0.74
1:E:218:ALA:HB2	1:E:317:MET:HE3	1.68	0.74
1:A:252:LYS:HE3	1:B:309:ASP:OD1	1.89	0.73
1:D:57:LYS:NZ	1:D:122:GLY:O	2.22	0.73
1:E:155:ARG:HG2	3:E:505:HOH:O	1.89	0.72
1:F:303:THR:HB	3:F:570:HOH:O	1.90	0.69
1:A:289:CYS:SG	3:A:673:HOH:O	2.49	0.69
1:D:57:LYS:CE	3:D:507:HOH:O	2.40	0.69
1:B:259:ASP:HB3	1:B:262:MET:HE3	1.74	0.68
1:B:220:MET:CG	3:B:650:HOH:O	2.41	0.68
2:A:401:C76:O7	1:C:185:ASP:O	2.12	0.68
1:D:80:GLU:HG2	3:D:503:HOH:O	1.94	0.68
1:C:19:ARG:CD	3:C:547:HOH:O	2.43	0.67
1:F:262:MET:HB2	3:F:563:HOH:O	1.96	0.65
1:E:259:ASP:HB2	3:E:501:HOH:O	1.95	0.65
1:A:89:ASN:HB2	3:A:577:HOH:O	1.95	0.65
1:F:218:ALA:HB2	1:F:317:MET:CE	2.27	0.64
1:E:252:LYS:NZ	3:E:403:HOH:O	2.31	0.63
1:C:260:LEU:O	1:C:274:ARG:NH2	2.31	0.63
1:E:315:GLN:OE1	1:E:318:GLU:OE1	2.16	0.63
1:E:218:ALA:HB2	1:E:317:MET:CE	2.28	0.63
1:B:188:LEU:HD23	1:F:187:HIS:HB3	1.80	0.63
1:E:290:ASN:HB3	3:E:500:HOH:O	1.99	0.62
1:A:218:ALA:HB2	1:A:317:MET:CE	2.28	0.62
1:B:140:VAL:HG21	1:F:186:SER:CB	2.31	0.61
1:B:140:VAL:HG21	1:F:186:SER:HB2	1.83	0.60
1:E:109:GLN:HG3	3:E:479:HOH:O	2.02	0.59
1:B:315:GLN:NE2	1:B:318:GLU:OE2	2.34	0.57
1:B:188:LEU:CD2	1:F:187:HIS:O	2.45	0.57
1:C:19:ARG:HD3	3:C:547:HOH:O	2.04	0.57
1:B:186:SER:CB	3:F:518:HOH:O	2.48	0.56
1:B:188:LEU:CD2	1:F:187:HIS:HB3	2.34	0.56
1:E:347:SER:HA	3:E:509:HOH:O	2.05	0.56
1:F:315:GLN:NE2	1:F:318:GLU:OE2	2.35	0.56
1:C:315:GLN:NE2	1:C:318:GLU:OE2	2.36	0.56
1:C:243:GLN:HG3	1:C:247:ARG:HH21	1.71	0.55
1:E:188:LEU:HB2	3:E:507:HOH:O	2.07	0.55
1:C:201:GLU:OE1	1:C:209:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLN:HG2	3:E:517:HOH:O	2.07	0.54
1:C:220:MET:HE3	1:C:221:PRO:HD2	1.91	0.53
1:E:19:ARG:HD2	3:E:402:HOH:O	2.08	0.53
1:F:104:GLU:CD	3:F:482:HOH:O	2.51	0.53
1:D:262:MET:HG2	3:D:504:HOH:O	2.08	0.51
1:B:188:LEU:HD11	1:F:223:HIS:ND1	2.24	0.51
1:F:274:ARG:HD2	3:F:563:HOH:O	2.10	0.51
1:B:155:ARG:HD2	3:B:607:HOH:O	2.11	0.50
1:D:315:GLN:HG3	1:D:318:GLU:OE1	2.11	0.50
1:F:223:HIS:CD2	1:F:258:ASP:OD2	2.65	0.50
1:F:27:ARG:HD3	1:F:296:ASP:OD1	2.12	0.50
1:A:315:GLN:HG3	1:A:318:GLU:OE1	2.11	0.49
1:C:27:ARG:HD3	1:C:296:ASP:OD1	2.12	0.49
1:F:304:ILE:HD11	3:F:418:HOH:O	2.12	0.49
1:B:27:ARG:HD3	1:B:296:ASP:OD1	2.12	0.49
1:E:27:ARG:HD3	1:E:296:ASP:OD1	2.12	0.49
1:F:3:VAL:HG21	3:F:521:HOH:O	2.11	0.49
1:C:61:THR:HA	1:C:62:PRO:C	2.37	0.49
1:A:27:ARG:HD3	1:A:296:ASP:OD1	2.13	0.49
1:E:61:THR:HA	1:E:62:PRO:C	2.38	0.49
1:F:61:THR:HA	1:F:62:PRO:C	2.38	0.48
1:B:188:LEU:HD22	1:F:187:HIS:C	2.36	0.48
1:A:15:ILE:HD12	3:A:550:HOH:O	2.13	0.48
1:B:61:THR:HA	1:B:62:PRO:C	2.38	0.48
1:B:323:HIS:CE1	3:B:501:HOH:O	2.67	0.48
1:D:27:ARG:HD3	1:D:296:ASP:OD1	2.13	0.48
1:C:80:GLU:HB2	3:C:623:HOH:O	2.13	0.47
1:D:155:ARG:NE	3:D:501:HOH:O	2.33	0.47
1:D:14:ASP:HB2	3:D:545:HOH:O	2.13	0.47
2:D:401:C76:C7	1:E:185:ASP:O	2.61	0.47
1:E:218:ALA:CB	1:E:317:MET:CE	2.93	0.46
1:A:61:THR:HA	1:A:62:PRO:C	2.39	0.46
1:E:209:ARG:HD3	3:E:521:HOH:O	2.14	0.46
1:F:12:MET:SD	1:F:37:ILE:CG1	3.03	0.46
1:B:14:ASP:HB2	3:B:559:HOH:O	2.16	0.46
1:A:231:THR:HG21	1:E:337:ALA:HA	1.96	0.45
1:F:218:ALA:CB	1:F:317:MET:CE	2.94	0.45
1:A:231:THR:CG2	1:E:337:ALA:HA	2.47	0.45
1:E:128:THR:OG1	1:E:129:PRO:HA	2.17	0.45
1:D:61:THR:HA	1:D:62:PRO:C	2.42	0.44
1:A:218:ALA:CB	1:A:317:MET:CE	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLY:HA3	3:E:410:HOH:O	2.17	0.44
1:B:140:VAL:HG21	1:F:186:SER:HB3	1.99	0.44
1:F:243:GLN:HB3	1:F:247:ARG:NH1	2.32	0.44
1:B:128:THR:OG1	1:B:129:PRO:HA	2.18	0.43
1:A:218:ALA:CB	1:A:317:MET:HE3	2.43	0.43
1:C:128:THR:OG1	1:C:129:PRO:HA	2.19	0.43
1:E:218:ALA:CB	1:E:317:MET:HE3	2.43	0.43
1:A:189:VAL:N	3:A:510:HOH:O	2.51	0.43
1:E:22:GLU:HG3	3:E:497:HOH:O	2.19	0.43
1:D:258:ASP:HA	3:D:617:HOH:O	2.18	0.42
1:C:61:THR:HB	3:C:582:HOH:O	2.20	0.42
1:B:155:ARG:CD	3:B:607:HOH:O	2.66	0.42
1:D:220:MET:HG3	3:D:617:HOH:O	2.19	0.42
1:D:128:THR:OG1	1:D:129:PRO:HA	2.20	0.42
1:A:128:THR:OG1	1:A:129:PRO:HA	2.20	0.42
1:D:155:ARG:NH1	3:D:501:HOH:O	2.34	0.42
1:A:170:LYS:HB3	1:A:217:ALA:HB2	2.00	0.41
1:A:189:VAL:N	1:C:188:LEU:HD11	2.35	0.41
1:B:261:THR:HG21	3:B:579:HOH:O	2.20	0.41
1:F:128:THR:OG1	1:F:129:PRO:HA	2.20	0.41
1:E:19:ARG:CD	3:E:402:HOH:O	2.65	0.41
1:A:71:GLU:HB3	3:A:565:HOH:O	2.20	0.41
1:C:41:ARG:HD3	3:C:531:HOH:O	2.20	0.41
1:D:201:GLU:HG3	3:D:607:HOH:O	2.19	0.41
1:E:170:LYS:HB3	1:E:217:ALA:HB2	2.03	0.41
1:F:12:MET:SD	1:F:37:ILE:HG13	2.60	0.41
1:A:27:ARG:NH2	3:A:502:HOH:O	2.38	0.41
1:C:326:VAL:O	1:C:329:VAL:HG12	2.22	0.40
1:A:247:ARG:CD	1:B:250:GLY:HA2	2.45	0.40
1:F:32:ALA:HA	3:F:418:HOH:O	2.22	0.40
1:D:262:MET:HA	3:D:597:HOH:O	2.22	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	328/397 (83%)	317 (97%)	11 (3%)	0	100	100
1	B	344/397 (87%)	328 (95%)	16 (5%)	0	100	100
1	C	335/397 (84%)	322 (96%)	13 (4%)	0	100	100
1	D	340/397 (86%)	328 (96%)	12 (4%)	0	100	100
1	E	335/397 (84%)	323 (96%)	12 (4%)	0	100	100
1	F	336/397 (85%)	324 (96%)	12 (4%)	0	100	100
All	All	2018/2382 (85%)	1942 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	259 (98%)	5 (2%)	50	66
1	B	271/309 (88%)	264 (97%)	7 (3%)	40	55
1	C	267/309 (86%)	261 (98%)	6 (2%)	45	61
1	D	271/309 (88%)	266 (98%)	5 (2%)	51	68
1	E	268/309 (87%)	262 (98%)	6 (2%)	45	61
1	F	268/309 (87%)	263 (98%)	5 (2%)	50	66
All	All	1609/1854 (87%)	1575 (98%)	34 (2%)	47	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	VAL
1	A	219	VAL
1	A	231	THR
1	A	261	THR

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Mol	Chain	Res	Type
1	A	329	VAL
1	B	155	ARG
1	B	166	LYS
1	B	189	VAL
1	B	219	VAL
1	B	258	ASP
1	B	261	THR
1	B	329	VAL
1	C	188	LEU
1	C	189	VAL
1	C	219	VAL
1	C	247	ARG
1	C	258	ASP
1	C	329	VAL
1	D	189	VAL
1	D	219	VAL
1	D	258	ASP
1	D	329	VAL
1	D	331	GLN
1	E	28	LEU
1	E	189	VAL
1	E	219	VAL
1	E	258	ASP
1	E	310	LEU
1	E	329	VAL
1	F	189	VAL
1	F	258	ASP
1	F	303	THR
1	F	310	LEU
1	F	329	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	109	GLN
1	A	161	GLN
1	B	109	GLN
1	B	161	GLN
1	B	223	HIS
1	B	336	GLN
1	C	109	GLN

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Mol	Chain	Res	Type
1	D	5	HIS
1	D	109	GLN
1	D	161	GLN
1	D	336	GLN
1	E	109	GLN
1	E	161	GLN
1	E	223	HIS
1	E	315	GLN
1	E	336	GLN
1	F	89	ASN
1	F	109	GLN
1	F	161	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	C76	A	401	-	18,18,18	2.00	5 (27%)	27,27,27	1.90	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C76	C	401	-	18,18,18	1.95	4 (22%)	27,27,27	1.81	6 (22%)
2	C76	B	401	-	18,18,18	2.02	5 (27%)	27,27,27	1.53	3 (11%)
2	C76	D	401	-	18,18,18	2.12	5 (27%)	27,27,27	1.86	6 (22%)

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	C76	A	401	-	-	0/12/32/32	0/1/1/1
2	C76	C	401	-	-	1/12/32/32	0/1/1/1
2	C76	B	401	-	-	1/12/32/32	0/1/1/1
2	C76	D	401	-	-	1/12/32/32	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	C76	C7-N2	6.06	1.45	1.34
2	D	401	C76	C7-N2	5.41	1.44	1.34
2	C	401	C76	C7-N2	5.24	1.44	1.34
2	A	401	C76	C7-N2	4.82	1.43	1.34
2	A	401	C76	C1-C2	-3.98	1.48	1.52
2	B	401	C76	O5-C1	3.93	1.52	1.42
2	C	401	C76	O5-C1	3.93	1.52	1.42
2	D	401	C76	O5-C1	3.70	1.51	1.42
2	A	401	C76	O5-C1	3.69	1.51	1.42
2	D	401	C76	C1-C2	-3.61	1.48	1.52
2	C	401	C76	C3-C2	-2.90	1.47	1.53
2	D	401	C76	C3-C2	-2.90	1.47	1.53
2	C	401	C76	C1-C2	-2.85	1.49	1.52
2	D	401	C76	C2-N2	2.81	1.50	1.45
2	A	401	C76	C3-C2	-2.64	1.48	1.53
2	B	401	C76	C3-C2	-2.48	1.48	1.53
2	B	401	C76	C1-C2	-2.46	1.50	1.52
2	A	401	C76	C2-N2	2.10	1.49	1.45
2	B	401	C76	C2-N2	2.10	1.49	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	C76	C1-C2-N2	-7.66	101.85	110.73
2	C	401	C76	O5-C1-C2	5.62	115.16	109.52
2	D	401	C76	C1-C2-N2	-4.51	105.51	110.73
2	B	401	C76	O5-C1-C2	4.37	113.91	109.52
2	D	401	C76	O5-C1-C2	4.22	113.76	109.52
2	C	401	C76	C1-C2-N2	-4.17	105.90	110.73
2	D	401	C76	C8-C7-N2	3.74	120.56	115.24
2	B	401	C76	C1-C2-N2	-3.32	106.89	110.73
2	A	401	C76	O5-C1-C2	3.17	112.70	109.52
2	B	401	C76	C8-C7-N2	3.04	119.57	115.24
2	D	401	C76	O5-C5-C4	2.98	115.06	109.70
2	C	401	C76	C1-O5-C5	2.64	118.76	113.65
2	D	401	C76	O6-C6-C5	2.54	119.98	111.33
2	C	401	C76	C2-N2-C7	2.48	126.73	121.52
2	D	401	C76	C3-C4-C5	2.38	114.55	110.23
2	A	401	C76	C3-C2-N2	2.37	114.98	110.62
2	C	401	C76	O5-C5-C4	2.33	113.90	109.70
2	C	401	C76	O6-C6-C5	2.16	118.67	111.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	C76	C1-C2-N2-C7
2	C	401	C76	C4-C5-C6-O6
2	B	401	C76	C4-C5-C6-O6

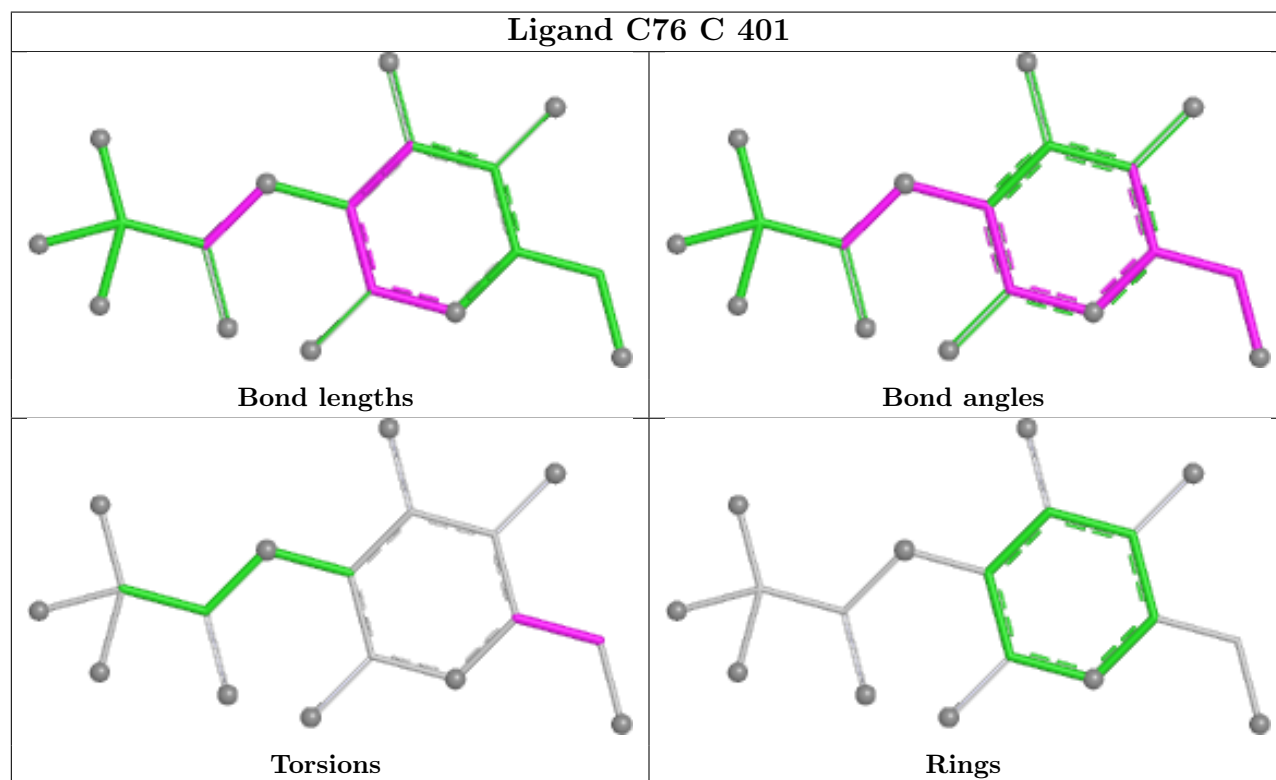
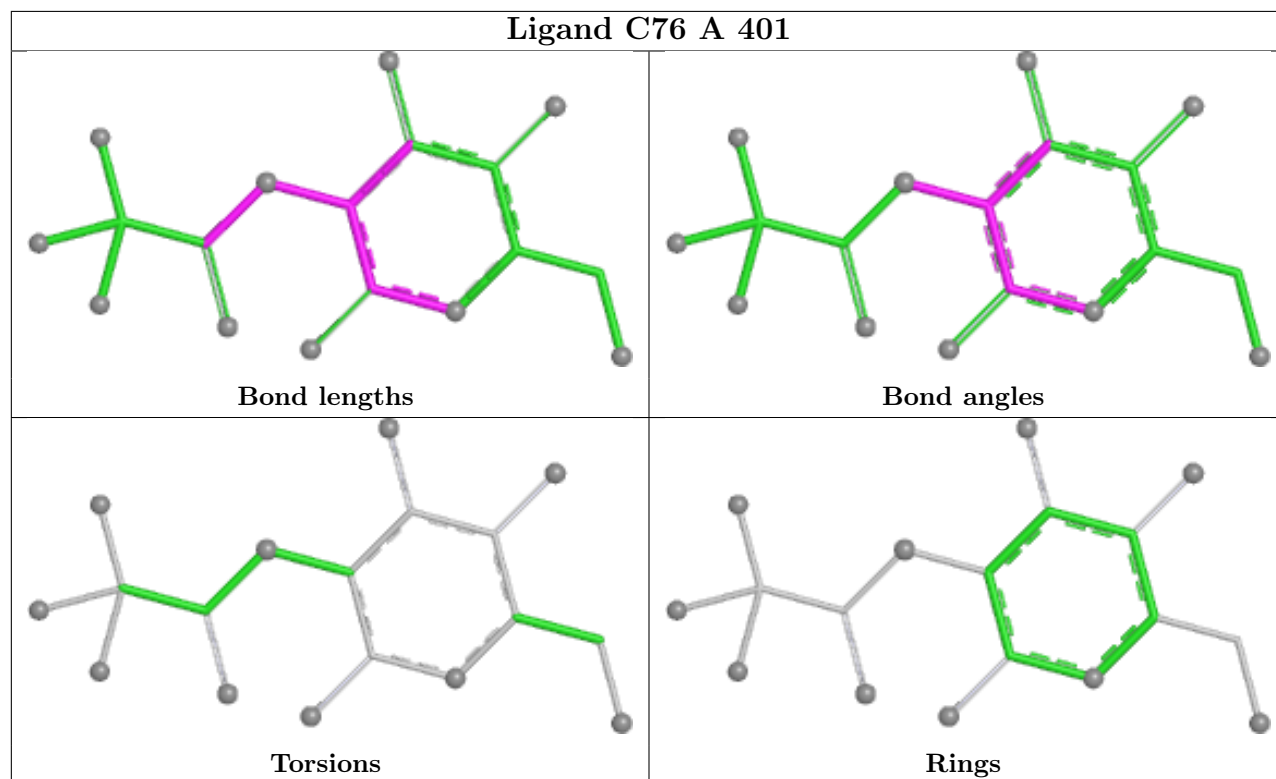
There are no ring outliers.

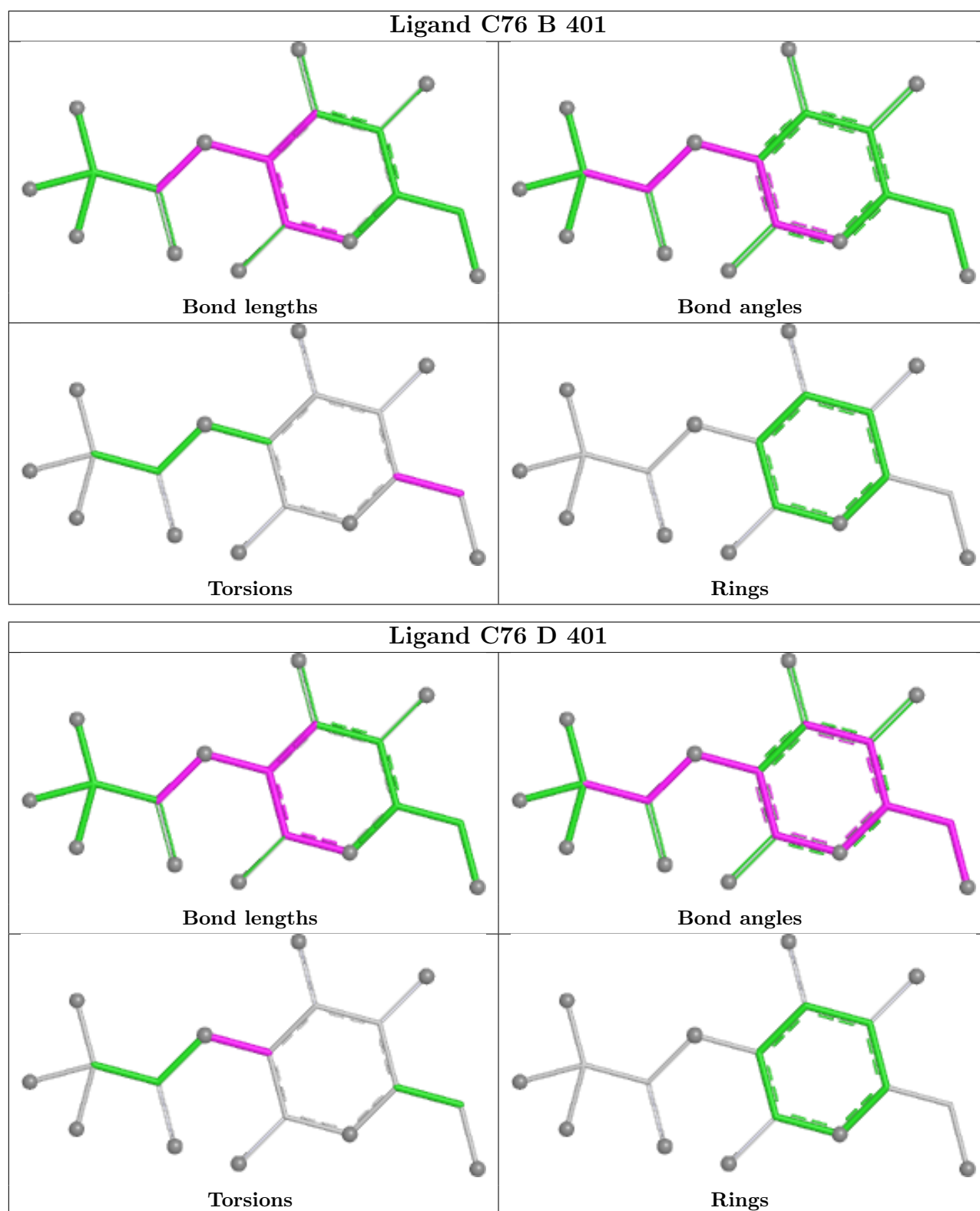
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	C76	1	0
2	D	401	C76	2	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

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%)	0.31	22 (6%) 24 21	22, 38, 63, 93	0
1	B	346/397 (87%)	-0.03	15 (4%) 40 36	22, 31, 57, 105	0
1	C	339/397 (85%)	0.55	24 (7%) 22 19	24, 41, 72, 100	0
1	D	344/397 (86%)	0.16	15 (4%) 39 36	26, 38, 67, 116	0
1	E	339/397 (85%)	0.70	31 (9%) 15 12	31, 47, 78, 139	0
1	F	340/397 (85%)	0.26	16 (4%) 36 33	26, 39, 64, 132	0
All	All	2042/2382 (85%)	0.32	123 (6%) 27 24	22, 39, 68, 139	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	LEU	6.6
1	C	189	VAL	6.5
1	B	189	VAL	5.9
1	C	188	LEU	5.8
1	B	188	LEU	5.8
1	F	188	LEU	5.3
1	B	187	HIS	4.9
1	F	262	MET	4.8
1	E	186	SER	4.7
1	E	189	VAL	4.6
1	D	258	ASP	4.6
1	F	259	ASP	4.5
1	A	323	HIS	4.5
1	F	189	VAL	4.4
1	A	189	VAL	4.4
1	A	258	ASP	4.2
1	C	269	GLY	4.2
1	E	259	ASP	4.1
1	E	188	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	3	VAL	4.1
1	C	268	ALA	4.1
1	D	186	SER	4.1
1	A	259	ASP	4.0
1	E	325	ALA	4.0
1	B	258	ASP	4.0
1	E	187	HIS	4.0
1	B	323	HIS	3.9
1	D	188	LEU	3.8
1	E	262	MET	3.7
1	D	187	HIS	3.7
1	B	262	MET	3.7
1	C	259	ASP	3.6
1	D	262	MET	3.6
1	C	327	GLN	3.5
1	A	190	LEU	3.4
1	C	261	THR	3.3
1	E	209	ARG	3.3
1	A	270	GLY	3.3
1	E	333	MET	3.3
1	B	190	LEU	3.3
1	F	347	SER	3.3
1	D	323	HIS	3.2
1	B	348	PRO	3.2
1	E	322	GLY	3.2
1	D	261	THR	3.2
1	D	189	VAL	3.2
1	B	186	SER	3.1
1	E	347	SER	3.1
1	C	260	LEU	3.1
1	C	293	ASP	3.1
1	E	269	GLY	3.1
1	F	268	ALA	3.1
1	F	187	HIS	3.0
1	E	320	SER	3.0
1	E	213	ARG	2.9
1	A	231	THR	2.9
1	E	323	HIS	2.9
1	D	266	CYS	2.9
1	C	270	GLY	2.9
1	C	328	ALA	2.9
1	E	247	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	201	GLU	2.9
1	F	323	HIS	2.8
1	D	2	THR	2.8
1	E	334	GLY	2.8
1	C	258	ASP	2.7
1	B	263	GLU	2.7
1	C	187	HIS	2.6
1	E	248	ASP	2.6
1	E	258	ASP	2.6
1	B	347	SER	2.6
1	E	59	LEU	2.6
1	F	223	HIS	2.6
1	C	329	VAL	2.6
1	D	348	PRO	2.6
1	E	243	GLN	2.6
1	C	274	ARG	2.5
1	C	347	SER	2.5
1	E	223	HIS	2.5
1	F	3	VAL	2.5
1	E	321	LEU	2.5
1	A	236	PHE	2.4
1	A	223	HIS	2.4
1	C	102	ALA	2.4
1	A	327	GLN	2.4
1	A	261	THR	2.4
1	A	3	VAL	2.4
1	C	271	ILE	2.4
1	F	186	SER	2.4
1	A	324	GLU	2.4
1	F	185	ASP	2.3
1	B	265	ALA	2.3
1	A	347	SER	2.3
1	E	5	HIS	2.3
1	D	308	GLN	2.3
1	F	260	LEU	2.3
1	C	186	SER	2.3
1	D	247	ARG	2.3
1	E	244	ILE	2.3
1	C	3	VAL	2.3
1	F	306	ASP	2.3
1	A	256	PHE	2.2
1	D	333	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	325	ALA	2.2
1	E	249	ILE	2.2
1	F	269	GLY	2.2
1	B	324	GLU	2.2
1	E	166	LYS	2.2
1	C	15	ILE	2.2
1	E	200	LEU	2.2
1	A	217	ALA	2.2
1	A	239	ILE	2.1
1	E	306	ASP	2.1
1	A	232	LYS	2.1
1	A	221	PRO	2.1
1	B	331	GLN	2.1
1	A	255	ILE	2.1
1	B	325	ALA	2.1
1	D	268	ALA	2.1
1	A	254	VAL	2.1
1	F	166	LYS	2.0
1	C	26	GLN	2.0
1	C	272	LYS	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 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(Å ²)	Q<0.9
2	C76	C	401	18/18	0.85	0.12	42,53,64,67	0
2	C76	D	401	18/18	0.86	0.11	39,56,65,69	0
2	C76	B	401	18/18	0.88	0.09	35,42,46,50	0

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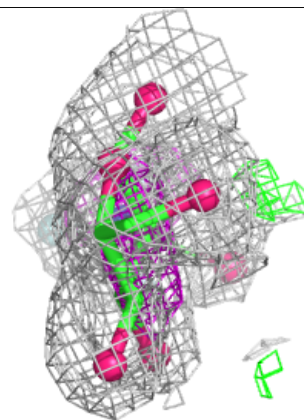
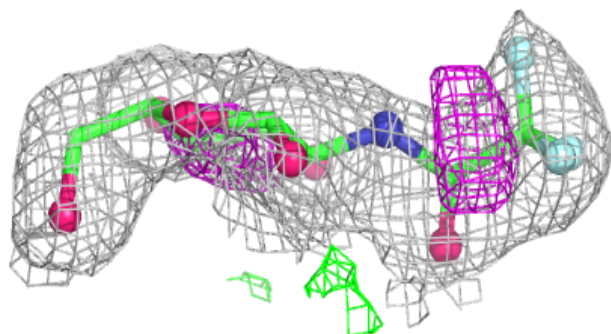
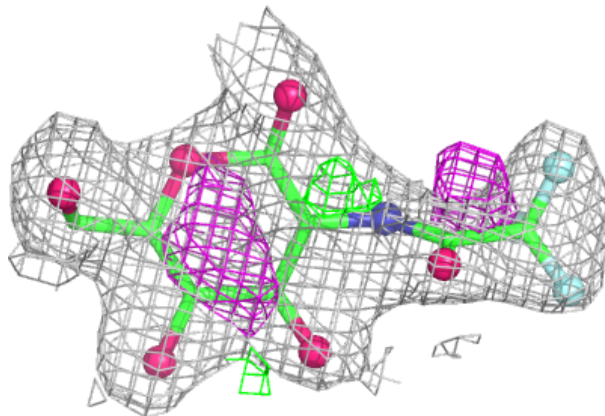
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C76	A	401	18/18	0.90	0.10	41,50,58,59	0

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.

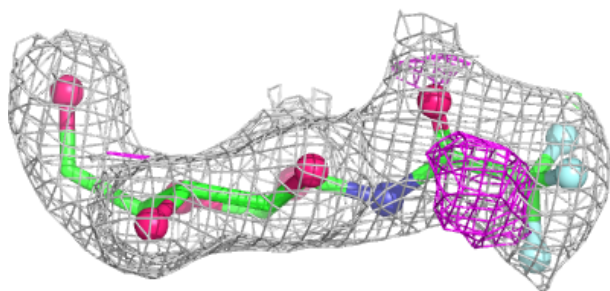
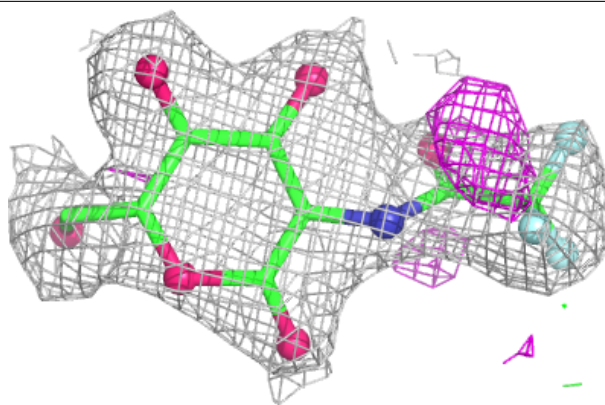
Electron density around C76 C 401:

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

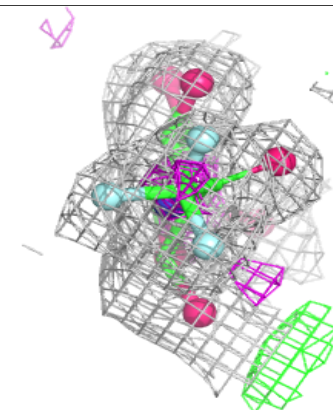
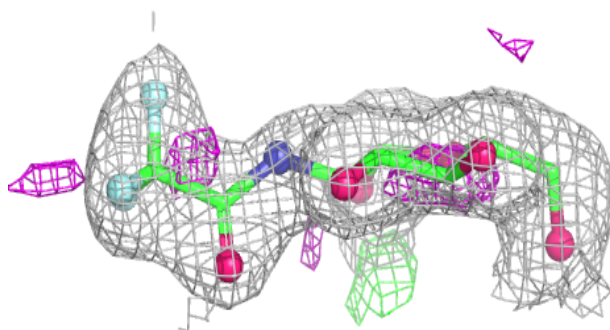
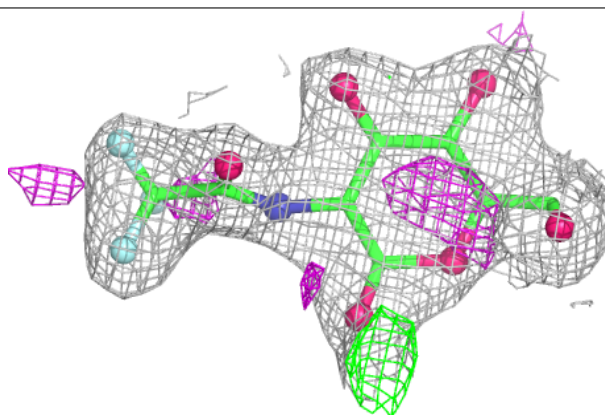


Electron density around C76 D 401:

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

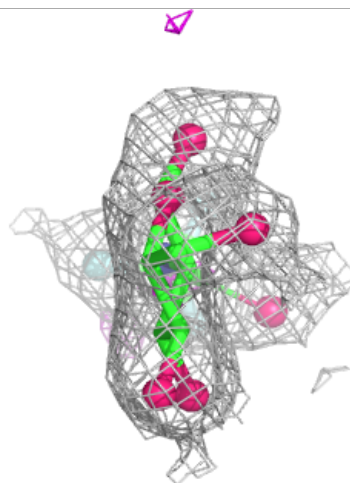
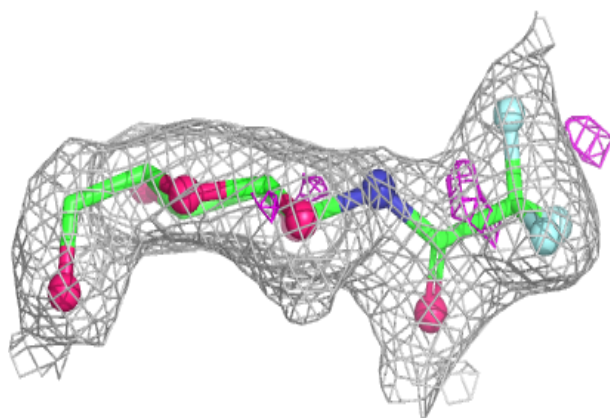
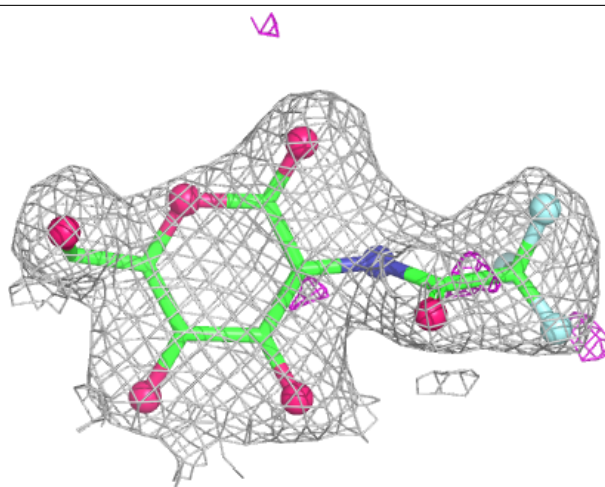
**Electron density around C76 B 401:**

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



Electron density around C76 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.