



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:53 AM UTC

PDB ID : 9NRV / pdb_00009nrv
Title : Crystal structure of the H5 influenza virus hemagglutinin from A/duck/France/161108h/2016 (H5N8) clade 2.3.4.4b in complex with avian receptor analog LSTa
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2025-03-14
Resolution : 2.89 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

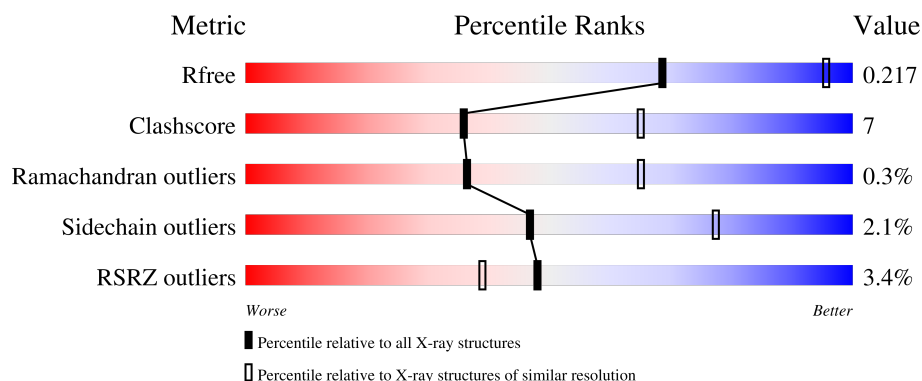
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

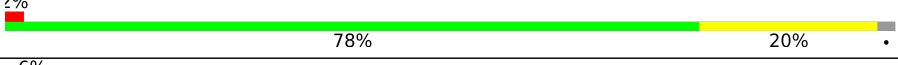
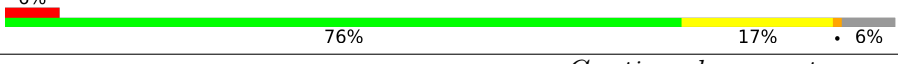
The reported resolution of this entry is 2.89 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	329	 4% 78% 19% ..
1	C	329	 3% 83% 14% ..
1	E	329	 2% 78% 20% .
2	B	181	 6% 76% 17% • 6%

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Mol	Chain	Length	Quality of chain
2	D	181	4% 75% 19% • 6%
2	F	181	% 77% 18% • 5%
3	G	5	100%
4	H	5	20% 80%
5	I	4	50% 50%
6	J	2	50% 50%
7	K	5	40% 60%
8	l	3	33% 33% 33%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 12458 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2548	1614	443	477	14			
1	C	323	Total	C	N	O	S	0	0	0
			2556	1618	444	480	14			
1	E	323	Total	C	N	O	S	0	0	0
			2556	1618	444	480	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A6M2RJB8
A	9	PRO	-	expression tag	UNP A0A6M2RJB8
A	10	GLY	-	expression tag	UNP A0A6M2RJB8
C	8	ASP	-	expression tag	UNP A0A6M2RJB8
C	9	PRO	-	expression tag	UNP A0A6M2RJB8
C	10	GLY	-	expression tag	UNP A0A6M2RJB8
E	8	ASP	-	expression tag	UNP A0A6M2RJB8
E	9	PRO	-	expression tag	UNP A0A6M2RJB8
E	10	GLY	-	expression tag	UNP A0A6M2RJB8

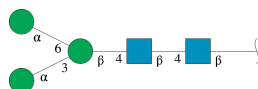
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1384	858	241	277	8			
2	D	171	Total	C	N	O	S	0	0	0
			1388	860	242	278	8			
2	F	172	Total	C	N	O	S	0	0	0
			1399	866	246	279	8			

There are 21 discrepancies between the modelled and reference sequences:

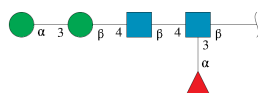
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6M2RJB8
B	176	GLY	-	expression tag	UNP A0A6M2RJB8
B	177	ARG	-	expression tag	UNP A0A6M2RJB8
B	178	LEU	-	expression tag	UNP A0A6M2RJB8
B	179	VAL	-	expression tag	UNP A0A6M2RJB8
B	180	PRO	-	expression tag	UNP A0A6M2RJB8
B	181	ARG	-	expression tag	UNP A0A6M2RJB8
D	175	SER	-	expression tag	UNP A0A6M2RJB8
D	176	GLY	-	expression tag	UNP A0A6M2RJB8
D	177	ARG	-	expression tag	UNP A0A6M2RJB8
D	178	LEU	-	expression tag	UNP A0A6M2RJB8
D	179	VAL	-	expression tag	UNP A0A6M2RJB8
D	180	PRO	-	expression tag	UNP A0A6M2RJB8
D	181	ARG	-	expression tag	UNP A0A6M2RJB8
F	175	SER	-	expression tag	UNP A0A6M2RJB8
F	176	GLY	-	expression tag	UNP A0A6M2RJB8
F	177	ARG	-	expression tag	UNP A0A6M2RJB8
F	178	LEU	-	expression tag	UNP A0A6M2RJB8
F	179	VAL	-	expression tag	UNP A0A6M2RJB8
F	180	PRO	-	expression tag	UNP A0A6M2RJB8
F	181	ARG	-	expression tag	UNP A0A6M2RJB8

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



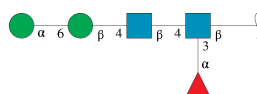
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



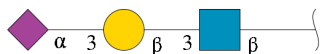
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	1	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



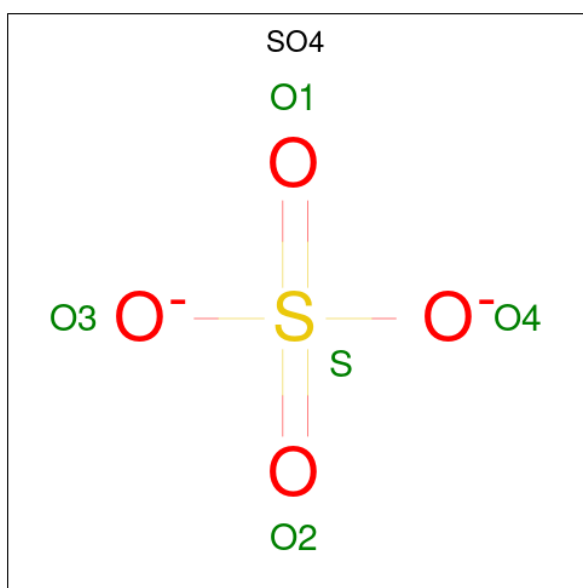
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



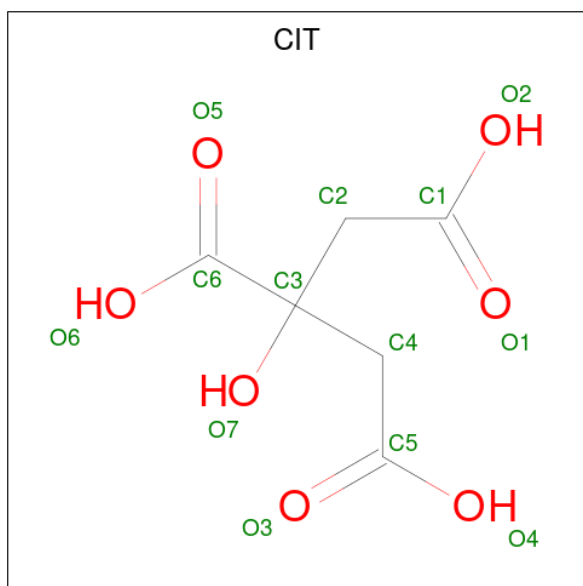
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	O	S	0	0
			5	4	1		
11	D	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		
11	F	1	Total	O	S	0	0
			5	4	1		
11	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	45	Total	O	0	0
			45	45		

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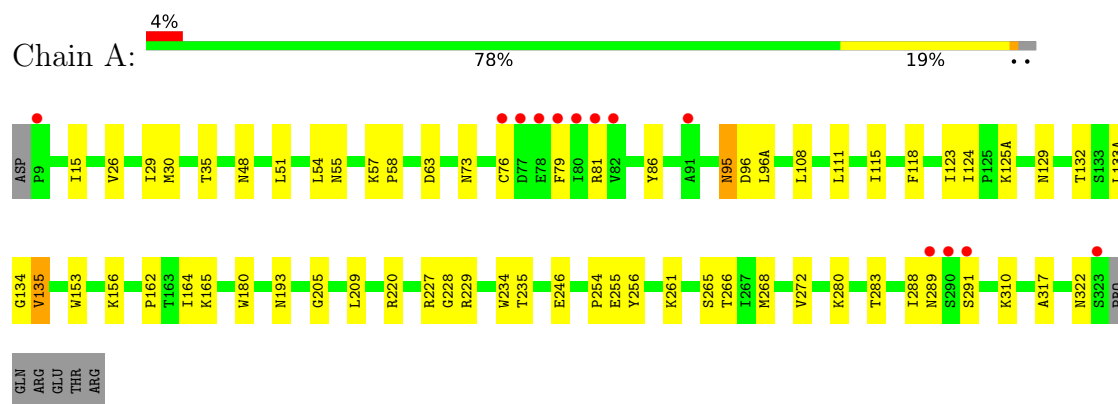
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	19	Total 19	O 19	0	0
13	C	42	Total 42	O 42	0	0
13	D	11	Total 11	O 11	0	0
13	E	44	Total 44	O 44	0	0
13	F	22	Total 22	O 22	0	0

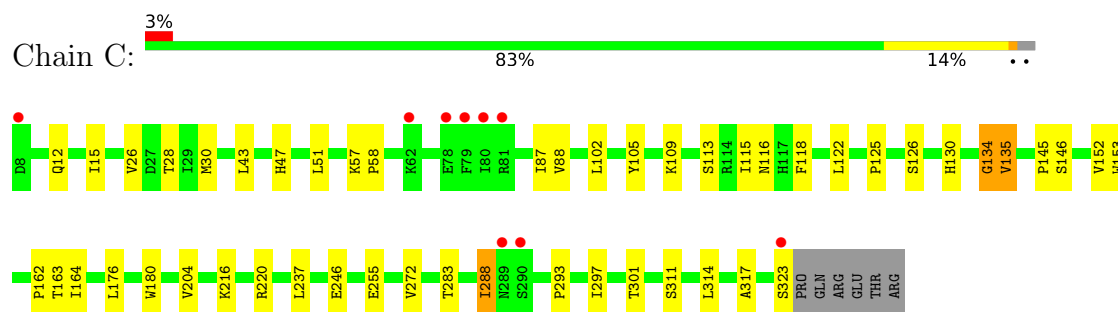
3 Residue-property plots [i](#)

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.

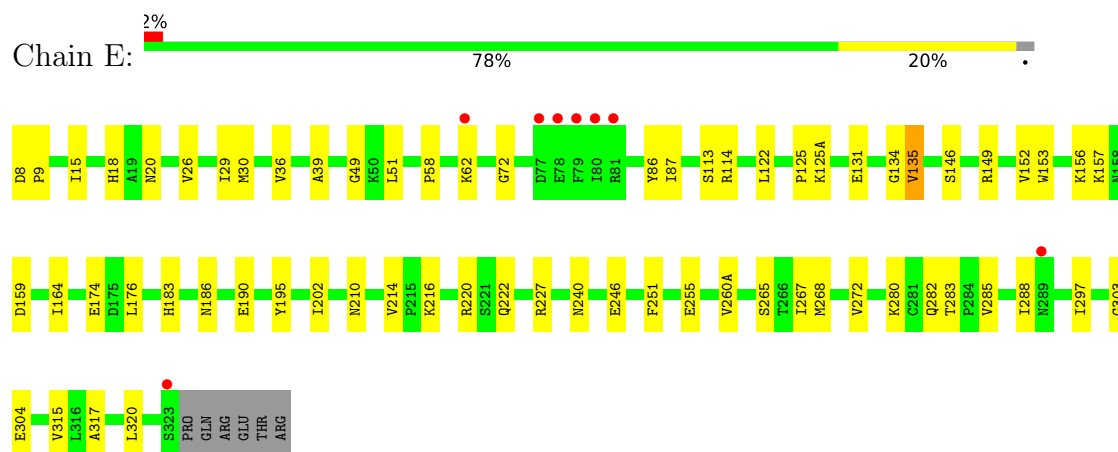
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

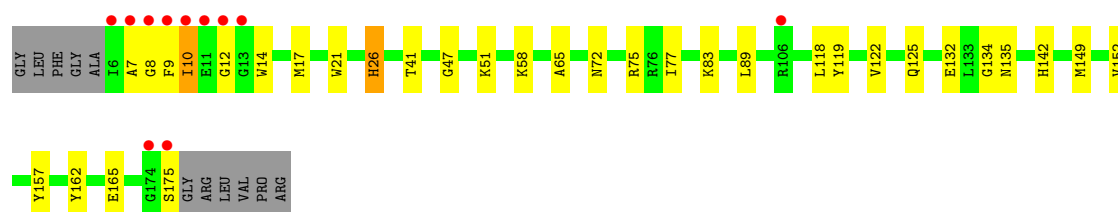


- Molecule 1: Hemagglutinin HA1 chain



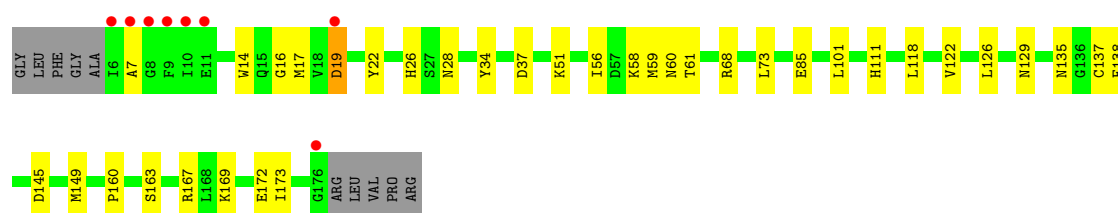
- Molecule 2: Hemagglutinin HA2 chain

Chain B: 



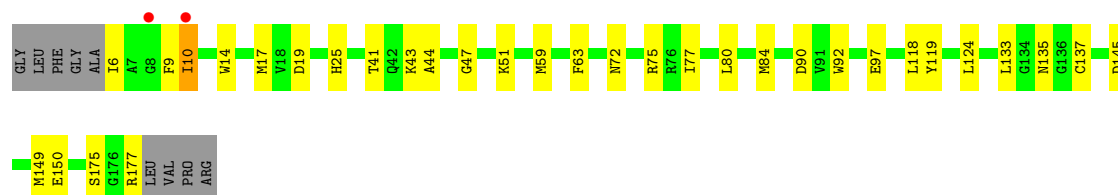
- Molecule 2: Hemagglutinin HA2 chain

Chain D: 

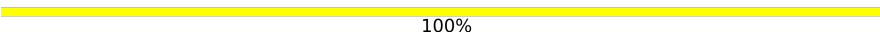


- Molecule 2: Hemagglutinin HA2 chain

Chain F: 

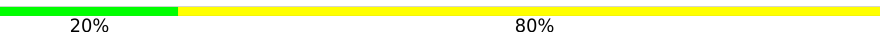


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 



- Molecule 5: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2
BMA3
MAN4

- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  50% 50%

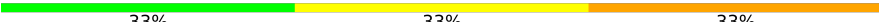
MAG1
MAG2

- Molecule 7: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-3)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  40% 60%

MAG1
MAG2
BMA3
MAN4
FUC5

- Molecule 8: N-acetyl- α -neuraminic acid-(2-3)- β -D-galactopyranose-(1-3)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain l:  33% 33% 33%

MAG1
GAL2
STA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.96Å 176.98Å 224.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.89 48.97 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.97-2.89) 99.4 (48.97-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.178 , 0.218 0.177 , 0.217	Depositor DCC
R_{free} test set	4228 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12458	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, FUC, BMA, GOL, SIA, CIT, NAG, MAN, SO4

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	0.37	0/2612	0.57	0/3552
1	C	0.37	0/2620	0.55	0/3564
1	E	0.40	0/2620	0.58	0/3564
2	B	0.39	0/1410	0.56	0/1895
2	D	0.32	0/1414	0.49	0/1900
2	F	0.36	0/1425	0.51	0/1914
All	All	0.37	0/12101	0.55	0/16389

There are no bond length outliers.

There are no bond angle outliers.

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	2548	0	2501	46	0
1	C	2556	0	2505	33	0
1	E	2556	0	2505	39	0
2	B	1384	0	1287	27	0
2	D	1388	0	1292	26	0
2	F	1399	0	1303	25	0
3	G	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	60	0	52	0	0
5	I	50	0	43	1	0
6	J	28	0	25	2	0
7	K	60	0	52	2	0
8	I	45	0	38	2	0
9	A	28	0	26	1	0
9	C	28	0	26	0	0
9	E	14	0	13	0	0
10	A	6	0	8	2	0
10	E	6	0	8	0	0
11	A	5	0	0	0	0
11	C	10	0	0	0	0
11	D	5	0	0	0	0
11	E	15	0	0	0	0
11	F	10	0	0	0	0
12	B	13	0	5	0	0
13	A	45	0	0	0	0
13	B	19	0	0	0	0
13	C	42	0	0	1	0
13	D	11	0	0	0	0
13	E	44	0	0	0	0
13	F	22	0	0	0	0
All	All	12458	0	11741	176	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 7.

All (176) 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:B:77:ILE:HD11	2:F:77:ILE:HD13	1.48	0.95
2:B:125:GLN:NE2	2:B:157:TYR:H	1.78	0.81
2:D:51:LYS:HE3	1:E:30:MET:HE3	1.64	0.79
2:B:9:PHE:CE2	2:B:10:ILE:HD13	2.23	0.73
1:E:26:VAL:HG21	1:E:317:ALA:HB2	1.71	0.73
2:D:135:ASN:ND2	2:D:137:CYS:SG	2.62	0.72
2:D:51:LYS:HG3	1:E:29:ILE:HG13	1.76	0.68
1:A:123:ILE:HG13	1:A:124:ILE:HG13	1.75	0.67
7:K:2:NAG:H61	7:K:5:FUC:H3	1.78	0.65
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.78	0.65
1:A:227:ARG:HH22	10:A:603:GOL:H12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ALA:HB3	2:D:14:TRP:HE1	1.62	0.65
1:E:216:LYS:O	1:E:220:ARG:NH2	2.30	0.64
2:B:125:GLN:HE21	2:B:157:TYR:H	1.46	0.63
1:E:8:ASP:HB3	1:E:9:PRO:HD3	1.82	0.61
1:A:125(A):LYS:HD3	1:A:132:THR:HB	1.83	0.60
1:E:288:ILE:HG21	1:E:297:ILE:HD13	1.83	0.60
2:F:19:ASP:OD1	2:F:19:ASP:N	2.34	0.60
1:C:51:LEU:HD13	1:C:272:VAL:HB	1.82	0.60
1:A:79:PHE:HE1	1:A:81:ARG:HG2	1.67	0.60
1:A:111:LEU:HD12	1:A:261:LYS:HD2	1.83	0.60
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.84	0.60
1:A:26:VAL:HG21	1:A:317:ALA:HB2	1.84	0.59
1:C:216:LYS:O	1:C:220:ARG:NH2	2.35	0.59
1:C:135:VAL:HG13	1:C:145:PRO:HB2	1.85	0.58
1:A:57:LYS:HG2	1:A:58:PRO:HD2	1.86	0.58
1:C:57:LYS:HG2	1:C:58:PRO:HD2	1.86	0.58
1:E:15:ILE:HG13	2:F:119:TYR:HA	1.85	0.58
2:D:19:ASP:OD1	2:D:19:ASP:N	2.37	0.57
2:D:58:LYS:HD2	2:F:97:GLU:HB3	1.85	0.57
1:C:283:THR:HG22	1:C:301:THR:HG22	1.87	0.57
2:B:9:PHE:CD2	2:B:10:ILE:HD13	2.39	0.57
2:B:21:TRP:HB2	2:B:41:THR:HG23	1.88	0.56
1:E:222:GLN:HG3	1:E:227:ARG:HG3	1.88	0.56
2:F:72:ASN:OD1	2:F:75:ARG:NH2	2.38	0.56
1:E:122:LEU:HD21	1:E:125:PRO:HB3	1.87	0.56
1:C:293:PRO:HD3	2:D:56:ILE:HG23	1.89	0.55
2:F:6:ILE:HG21	2:F:25:HIS:CD2	2.42	0.55
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.88	0.55
1:E:51:LEU:HD13	1:E:272:VAL:HB	1.87	0.55
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.72	0.55
1:A:29:ILE:HG23	1:A:30:MET:HG2	1.89	0.55
2:F:10:ILE:HG12	2:F:135:ASN:HA	1.89	0.55
1:A:51:LEU:HD13	1:A:272:VAL:HB	1.89	0.54
1:A:180:TRP:CZ3	1:A:235:THR:HG22	2.42	0.54
2:B:58:LYS:HE3	2:D:101:LEU:HD11	1.89	0.54
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.89	0.54
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.72	0.54
1:E:240:ASN:OD1	6:J:1:NAG:H5	2.07	0.54
1:E:268:MET:HE1	1:E:282:GLN:HG3	1.89	0.54
1:A:310:LYS:HB2	2:B:89:LEU:HD21	1.90	0.54
2:B:83:LYS:HB3	2:F:84:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:603:GOL:H11	6:J:1:NAG:H81	1.90	0.53
2:B:152:VAL:HG22	2:B:157:TYR:HB2	1.90	0.53
1:C:288:ILE:HG21	1:C:297:ILE:HD12	1.90	0.53
1:A:266:THR:HG22	2:B:65:ALA:HB1	1.90	0.53
2:D:68:ARG:NH1	2:D:85:GLU:OE2	2.40	0.53
1:A:96:ASP:CG	1:A:96(A):LEU:H	2.17	0.53
1:A:79:PHE:CE1	1:A:81:ARG:HG2	2.44	0.52
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.91	0.52
1:E:135:VAL:HG22	1:E:146:SER:HA	1.91	0.52
2:F:43:LYS:HG3	2:F:44:ALA:N	2.25	0.52
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.45	0.52
2:D:37:ASP:OD2	2:D:118:LEU:HD11	2.10	0.52
2:B:47:GLY:C	1:C:30:MET:HE2	2.34	0.52
2:B:119:TYR:OH	2:B:132:GLU:HG2	2.09	0.51
2:F:175:SER:HB2	2:F:177:ARG:HG2	1.91	0.51
2:B:7:ALA:HB1	2:B:135:ASN:O	2.09	0.51
1:E:303:GLY:HA2	2:F:63:PHE:CD2	2.44	0.51
1:A:55:ASN:HD21	1:A:280:LYS:HG2	1.76	0.51
1:C:135:VAL:HG22	1:C:146:SER:HA	1.93	0.51
1:E:114:ARG:HB2	1:E:265:SER:HB2	1.93	0.51
1:E:164:ILE:O	1:E:246:GLU:HA	2.10	0.51
1:C:164:ILE:O	1:C:246:GLU:HA	2.11	0.51
2:B:14:TRP:HE3	2:B:17:MET:HE2	1.76	0.50
1:C:43:LEU:HB2	1:C:314:LEU:HB2	1.94	0.49
1:A:265:SER:OG	1:A:266:THR:N	2.45	0.49
2:F:14:TRP:CE3	2:F:17:MET:HE2	2.47	0.49
2:F:145:ASP:O	2:F:149:MET:HG2	2.12	0.49
1:E:186:ASN:HB2	1:E:190:GLU:OE2	2.13	0.48
1:E:131:GLU:HG2	1:E:157:LYS:HB2	1.95	0.48
1:C:130:HIS:CE1	1:C:162:PRO:HD2	2.48	0.48
1:C:323:SER:HB3	13:C:719:HOH:O	2.12	0.48
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.94	0.48
2:F:133:LEU:HD12	2:F:137:CYS:HB2	1.95	0.48
2:B:26:HIS:HB2	2:B:149:MET:HE3	1.94	0.48
1:E:72:GLY:O	1:E:149:ARG:HG3	2.14	0.48
1:E:49:GLY:HA2	1:E:285:VAL:O	2.14	0.48
2:F:14:TRP:HE3	2:F:17:MET:HE2	1.78	0.48
1:C:15:ILE:HG23	2:D:118:LEU:HD23	1.96	0.48
1:E:125(A):LYS:HE2	1:E:152:VAL:HG22	1.94	0.48
2:D:160:PRO:HA	2:D:163:SER:HB2	1.96	0.47
1:A:220:ARG:HD3	1:E:210:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HE2	1:A:280:LYS:HB3	1.53	0.47
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.39	0.47
1:A:153:TRP:CH2	8:l:3:SIA:H112	2.50	0.46
2:D:22:TYR:OH	2:D:111:HIS:ND1	2.33	0.46
2:D:145:ASP:O	2:D:149:MET:HG2	2.15	0.46
1:A:30:MET:HE2	2:F:47:GLY:C	2.40	0.46
1:E:156:LYS:HE3	1:E:159:ASP:HA	1.97	0.46
1:E:174:GLU:HG2	1:E:260(A):VAL:CG2	2.45	0.46
2:F:6:ILE:HG21	2:F:25:HIS:NE2	2.30	0.46
1:E:135:VAL:HG22	1:E:146:SER:C	2.41	0.46
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.78	0.45
1:A:35:THR:HG22	1:A:322:ASN:HB3	1.99	0.45
2:B:125:GLN:NE2	2:B:157:TYR:HB3	2.31	0.45
2:D:60:ASN:ND2	2:F:90:ASP:OD1	2.50	0.45
1:E:39:ALA:HB1	1:E:315:VAL:HG12	1.98	0.45
2:D:14:TRP:HE3	2:D:17:MET:HE2	1.80	0.45
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.66	0.45
1:A:164:ILE:O	1:A:246:GLU:HA	2.17	0.45
2:B:26:HIS:ND1	2:B:26:HIS:C	2.75	0.45
1:C:135:VAL:HG22	1:C:146:SER:CA	2.47	0.45
1:E:18:HIS:CE1	1:E:20:ASN:HB3	2.51	0.45
2:B:72:ASN:HB3	2:B:75:ARG:NH2	2.31	0.45
1:E:152:VAL:HG23	1:E:255:GLU:HB2	1.98	0.45
1:C:176:LEU:HA	1:C:176:LEU:HD23	1.66	0.44
1:A:30:MET:HE3	2:F:51:LYS:HE3	1.98	0.44
2:B:9:PHE:CE2	2:B:10:ILE:CD1	2.99	0.44
2:B:142:HIS:CD2	2:B:162:TYR:HB3	2.52	0.44
1:C:87:ILE:HD12	1:C:113:SER:HA	1.98	0.44
2:B:10:ILE:HD12	2:B:10:ILE:HA	1.65	0.44
2:B:134:GLY:HA2	2:F:124:LEU:HD11	2.00	0.44
1:A:108:LEU:HD13	1:A:234:TRP:CD2	2.53	0.44
1:A:73:ASN:O	1:A:76:CYS:HB2	2.18	0.44
1:A:228:GLY:O	1:A:229:ARG:HD3	2.18	0.44
2:D:26:HIS:CD2	2:D:26:HIS:C	2.96	0.44
2:F:59:MET:HE1	2:F:92:TRP:CZ3	2.53	0.43
2:B:77:ILE:HD12	2:B:77:ILE:HG23	1.61	0.43
1:C:51:LEU:HD23	1:C:88:VAL:HG21	2.00	0.43
5:I:1:NAG:H61	5:I:2:NAG:H82	2.00	0.43
1:E:202:ILE:HD11	1:E:251:PHE:HA	2.00	0.43
1:A:129:ASN:HB3	1:A:162:PRO:HG2	2.01	0.43
2:F:9:PHE:CE1	2:F:10:ILE:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:GLY:HA3	2:D:34:TYR:CE2	2.54	0.43
1:C:122:LEU:HD21	1:C:125:PRO:HB3	2.01	0.43
2:D:59:MET:HE3	2:D:59:MET:HA	2.00	0.42
1:E:87:ILE:HB	1:E:267:ILE:HD13	2.00	0.42
2:F:150:GLU:HG3	7:K:1:NAG:O5	2.19	0.42
1:A:268:MET:HE3	1:A:268:MET:HB2	1.89	0.42
2:D:126:LEU:O	2:D:129:ASN:HB2	2.19	0.42
1:C:115:ILE:HD13	1:C:115:ILE:HA	1.81	0.42
1:A:180:TRP:HB3	1:A:254:PRO:HD3	2.01	0.42
1:A:153:TRP:CZ3	8:l:3:SIA:H112	2.54	0.42
1:C:102:LEU:O	1:C:105:TYR:HB2	2.19	0.42
1:C:105:TYR:CE2	1:C:109:LYS:HE2	2.55	0.42
1:C:115:ILE:HG21	1:C:118:PHE:HB2	2.01	0.42
1:A:156:LYS:HE2	1:A:193:ASN:O	2.19	0.42
1:E:288:ILE:HG21	1:E:288:ILE:HD13	1.74	0.42
1:C:152:VAL:HG23	1:C:255:GLU:HB2	2.02	0.42
1:A:220:ARG:HD3	1:E:210:ASN:CG	2.45	0.41
1:C:47:HIS:HB3	1:C:288:ILE:HG22	2.01	0.41
1:C:180:TRP:NE1	1:C:204:VAL:HG21	2.35	0.41
1:E:86:TYR:HA	1:E:113:SER:O	2.20	0.41
1:A:115:ILE:HG21	1:A:118:PHE:HB2	2.02	0.41
1:A:255:GLU:HG2	1:A:256:TYR:CD1	2.56	0.41
2:D:167:ARG:HE	2:D:167:ARG:HB2	1.69	0.41
2:D:169:LYS:HA	2:D:172:GLU:HG2	2.02	0.41
1:A:48:ASN:HB3	9:A:602:NAG:H81	2.02	0.41
1:A:63:ASP:O	1:A:95:ASN:ND2	2.53	0.41
1:A:133(A):LEU:O	1:A:135:VAL:N	2.54	0.41
1:A:124:ILE:HD12	1:A:254:PRO:HG2	2.03	0.41
2:F:17:MET:HB3	2:F:17:MET:HE3	1.80	0.41
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.90	0.41
1:A:205:GLY:HA2	1:A:209:LEU:O	2.21	0.41
1:A:289:ASN:C	1:A:291:SER:H	2.29	0.41
2:D:73:LEU:HD23	2:D:73:LEU:HA	1.77	0.41
1:E:135:VAL:HG22	1:E:146:SER:CA	2.50	0.41
2:F:118:LEU:HD23	2:F:118:LEU:HA	1.82	0.41
1:E:36:VAL:HA	1:E:320:LEU:O	2.21	0.41
1:C:12:GLN:HG2	2:D:138:PHE:O	2.20	0.40
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.56	0.40
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.97	0.40
1:E:29:ILE:HD12	1:E:29:ILE:HA	1.87	0.40
1:A:115:ILE:HD13	1:A:115:ILE:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LYS:HE3	1:C:30:MET:HE3	2.03	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	320/329 (97%)	298 (93%)	22 (7%)	0	100	100
1	C	321/329 (98%)	303 (94%)	17 (5%)	1 (0%)	36	65
1	E	321/329 (98%)	301 (94%)	19 (6%)	1 (0%)	36	65
2	B	168/181 (93%)	160 (95%)	6 (4%)	2 (1%)	10	34
2	D	169/181 (93%)	157 (93%)	12 (7%)	0	100	100
2	F	170/181 (94%)	163 (96%)	7 (4%)	0	100	100
All	All	1469/1530 (96%)	1382 (94%)	83 (6%)	4 (0%)	36	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLY
1	C	134	GLY
2	B	8	GLY
1	E	62	LYS

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	287/294 (98%)	282 (98%)	5 (2%)	53	82
1	C	288/294 (98%)	281 (98%)	7 (2%)	43	75
1	E	288/294 (98%)	282 (98%)	6 (2%)	47	77
2	B	147/154 (96%)	143 (97%)	4 (3%)	39	73
2	D	147/154 (96%)	144 (98%)	3 (2%)	48	78
2	F	148/154 (96%)	145 (98%)	3 (2%)	48	78
All	All	1305/1344 (97%)	1277 (98%)	28 (2%)	47	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	135	VAL
1	A	165	LYS
1	A	283	THR
1	A	288	ILE
2	B	10	ILE
2	B	26	HIS
2	B	165	GLU
2	B	175	SER
1	C	28	THR
1	C	116	ASN
1	C	126	SER
1	C	135	VAL
1	C	163	THR
1	C	288	ILE
1	C	311	SER
2	D	19	ASP
2	D	61	THR
2	D	173	ILE
1	E	135	VAL
1	E	176	LEU
1	E	214	VAL
1	E	280	LYS
1	E	283	THR
1	E	304	GLU
2	F	10	ILE
2	F	41	THR
2	F	80	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	25	GLN
1	A	55	ASN
1	A	172	ASN
2	B	15	GLN
2	B	42	GLN
2	B	50	ASN
2	B	72	ASN
2	B	95	ASN
2	B	125	GLN
1	C	25	GLN
1	C	116	ASN
1	C	117	HIS
1	C	240	ASN
2	D	26	HIS
2	D	62	GLN
2	D	79	ASN
1	E	12	GLN
1	E	129	ASN
1	E	172	ASN
2	F	25	HIS

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 ⓘ

24 monosaccharides 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
3	NAG	G	1	3,1	14,14,15	0.85	1 (7%)	17,19,21	1.38	3 (17%)
3	NAG	G	2	3	14,14,15	0.80	0	17,19,21	1.45	2 (11%)
3	BMA	G	3	3	11,11,12	0.86	1 (9%)	15,15,17	1.87	5 (33%)
3	MAN	G	4	3	11,11,12	0.67	0	15,15,17	1.46	1 (6%)
3	MAN	G	5	3	11,11,12	0.66	0	15,15,17	1.87	1 (6%)
4	NAG	H	1	4,2	14,14,15	0.80	0	17,19,21	1.37	1 (5%)
4	NAG	H	2	4	14,14,15	0.79	0	17,19,21	0.89	0
4	BMA	H	3	4	11,11,12	0.89	0	15,15,17	1.83	2 (13%)
4	MAN	H	4	4	11,11,12	0.62	0	15,15,17	1.57	1 (6%)
4	FUC	H	5	4	10,10,11	0.74	0	14,14,16	1.07	1 (7%)
5	NAG	I	1	5,1	14,14,15	0.81	1 (7%)	17,19,21	1.15	2 (11%)
5	NAG	I	2	5	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
5	BMA	I	3	5	11,11,12	1.01	0	15,15,17	1.87	4 (26%)
5	MAN	I	4	5	11,11,12	0.62	0	15,15,17	1.51	2 (13%)
6	NAG	J	1	6,1	14,14,15	0.81	0	17,19,21	1.69	3 (17%)
6	NAG	J	2	6	14,14,15	0.72	0	17,19,21	1.49	3 (17%)
7	NAG	K	1	2,7	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
7	NAG	K	2	7	14,14,15	0.80	0	17,19,21	1.14	2 (11%)
7	BMA	K	3	7	11,11,12	0.88	0	15,15,17	2.09	2 (13%)
7	MAN	K	4	7	11,11,12	0.74	0	15,15,17	1.00	1 (6%)
7	FUC	K	5	7	10,10,11	0.63	0	14,14,16	1.31	2 (14%)
8	NAG	l	1	8	14,14,15	0.75	0	17,19,21	1.77	5 (29%)
8	GAL	l	2	8	11,11,12	0.74	0	15,15,17	1.08	0
8	SIA	l	3	8	20,20,21	1.93	3 (15%)	21,28,31	1.97	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
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	4,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	FUC	H	5	4	-	-	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	FUC	K	5	7	-	-	0/1/1/1
8	NAG	l	1	8	-	0/6/23/26	0/1/1/1
8	GAL	l	2	8	-	2/2/19/22	0/1/1/1
8	SIA	l	3	8	-	0/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	3	SIA	C2-C1	7.04	1.60	1.52
8	l	3	SIA	C7-C6	3.11	1.56	1.52
8	l	3	SIA	O6-C2	2.49	1.48	1.43
5	I	1	NAG	O5-C1	-2.11	1.40	1.43
3	G	3	BMA	C2-C3	2.08	1.55	1.52
3	G	1	NAG	O5-C1	-2.00	1.40	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	MAN	C1-O5-C5	6.24	120.55	112.19
7	K	3	BMA	C1-O5-C5	6.23	120.53	112.19
4	H	3	BMA	C1-O5-C5	5.22	119.18	112.19
4	H	4	MAN	C1-O5-C5	5.16	119.11	112.19
5	I	3	BMA	C1-O5-C5	5.11	119.03	112.19
6	J	1	NAG	C1-O5-C5	4.94	118.81	112.19
3	G	4	MAN	C1-O5-C5	4.52	118.24	112.19
8	l	3	SIA	C6-C5-N5	-4.48	103.75	110.91
8	l	3	SIA	O6-C2-C3	-4.27	104.81	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	4	MAN	C1-O5-C5	4.21	117.83	112.19
8	I	3	SIA	O1A-C1-C2	-4.08	114.03	122.85
4	H	1	NAG	C2-N2-C7	3.98	128.23	122.90
5	I	2	NAG	C1-O5-C5	3.70	117.14	112.19
3	G	2	NAG	C1-O5-C5	3.66	117.08	112.19
6	J	2	NAG	C2-N2-C7	3.65	127.79	122.90
8	I	1	NAG	C4-C3-C2	-3.43	105.99	111.02
8	I	1	NAG	O5-C1-C2	-3.35	106.10	111.29
3	G	3	BMA	C1-O5-C5	3.34	116.66	112.19
7	K	5	FUC	C1-O5-C5	3.17	120.44	112.97
3	G	1	NAG	C1-O5-C5	2.98	116.17	112.19
3	G	3	BMA	O3-C3-C2	-2.97	103.99	110.05
6	J	2	NAG	O5-C1-C2	-2.97	106.70	111.29
5	I	1	NAG	C1-C2-N2	-2.97	105.75	110.43
8	I	1	NAG	C1-C2-N2	2.94	115.06	110.43
3	G	3	BMA	O5-C5-C6	2.93	113.36	107.66
3	G	3	BMA	C2-C3-C4	2.90	115.96	110.86
8	I	1	NAG	O4-C4-C3	-2.69	104.04	110.38
3	G	1	NAG	O4-C4-C3	-2.60	104.25	110.38
5	I	3	BMA	C3-C4-C5	2.59	114.94	110.23
3	G	2	NAG	O4-C4-C3	-2.55	104.36	110.38
7	K	5	FUC	O3-C3-C4	2.54	116.36	110.38
8	I	3	SIA	O1B-C1-C2	2.43	119.03	112.71
8	I	1	NAG	O4-C4-C5	2.41	115.25	109.32
7	K	2	NAG	C3-C4-C5	2.38	114.56	110.23
5	I	4	MAN	C3-C4-C5	-2.31	106.05	110.23
7	K	3	BMA	O3-C3-C2	-2.26	105.45	110.05
3	G	1	NAG	C8-C7-N2	-2.25	112.39	116.12
3	G	3	BMA	C3-C4-C5	2.23	114.28	110.23
5	I	3	BMA	O4-C4-C3	-2.19	105.22	110.38
7	K	4	MAN	C1-O5-C5	2.17	115.10	112.19
7	K	2	NAG	O4-C4-C3	-2.16	105.28	110.38
6	J	2	NAG	O4-C4-C5	2.15	114.61	109.32
5	I	3	BMA	C2-C3-C4	2.09	114.54	110.86
6	J	1	NAG	O4-C4-C3	-2.09	105.46	110.38
7	K	1	NAG	C1-C2-N2	-2.08	107.15	110.43
4	H	3	BMA	O3-C3-C2	-2.07	105.84	110.05
4	H	5	FUC	O2-C2-C3	2.06	114.43	110.15
6	J	1	NAG	C8-C7-N2	-2.03	112.75	116.12
5	I	1	NAG	O4-C4-C3	-2.03	105.60	110.38
5	I	2	NAG	O4-C4-C3	-2.02	105.61	110.38

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
8	l	2	GAL	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
8	l	2	GAL	O5-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C3-C2-N2-C7
4	H	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

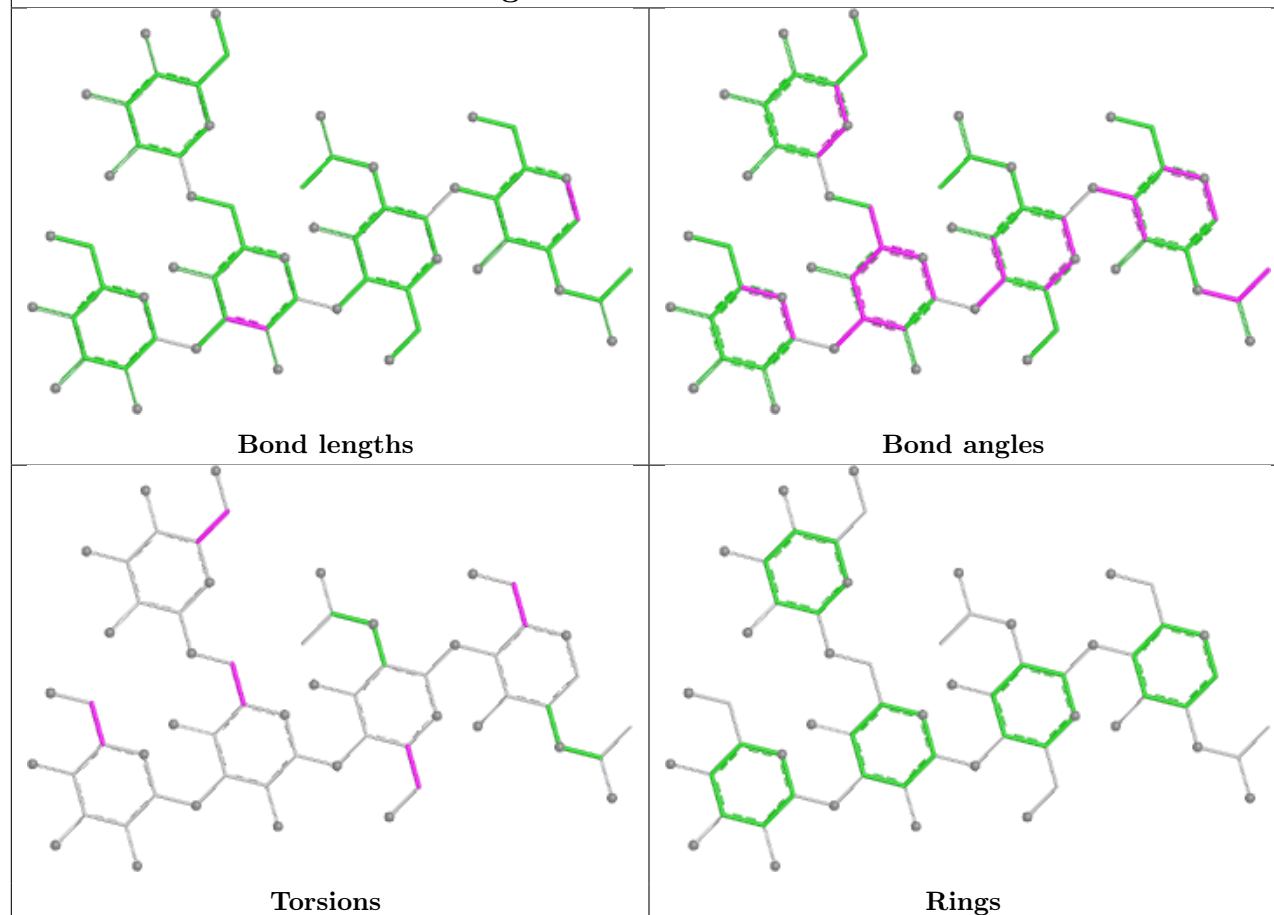
There are no ring outliers.

7 monomers are involved in 7 short contacts:

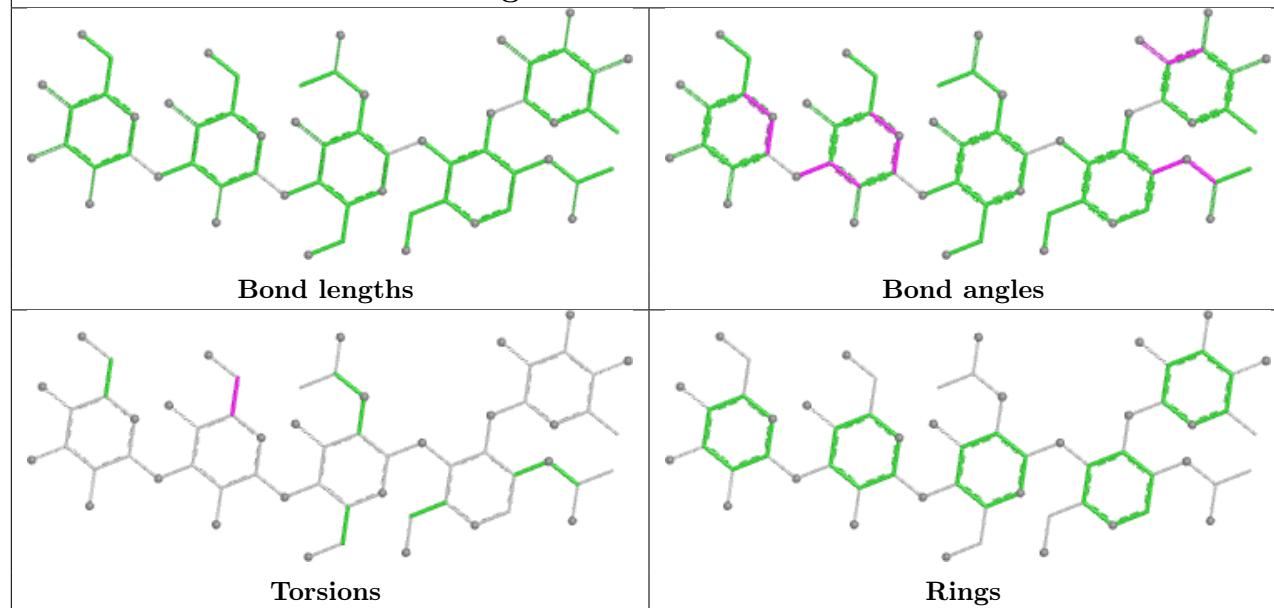
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	1	0
7	K	2	NAG	1	0
6	J	1	NAG	2	0
8	l	3	SIA	2	0
7	K	5	FUC	1	0
5	I	1	NAG	1	0
7	K	1	NAG	1	0

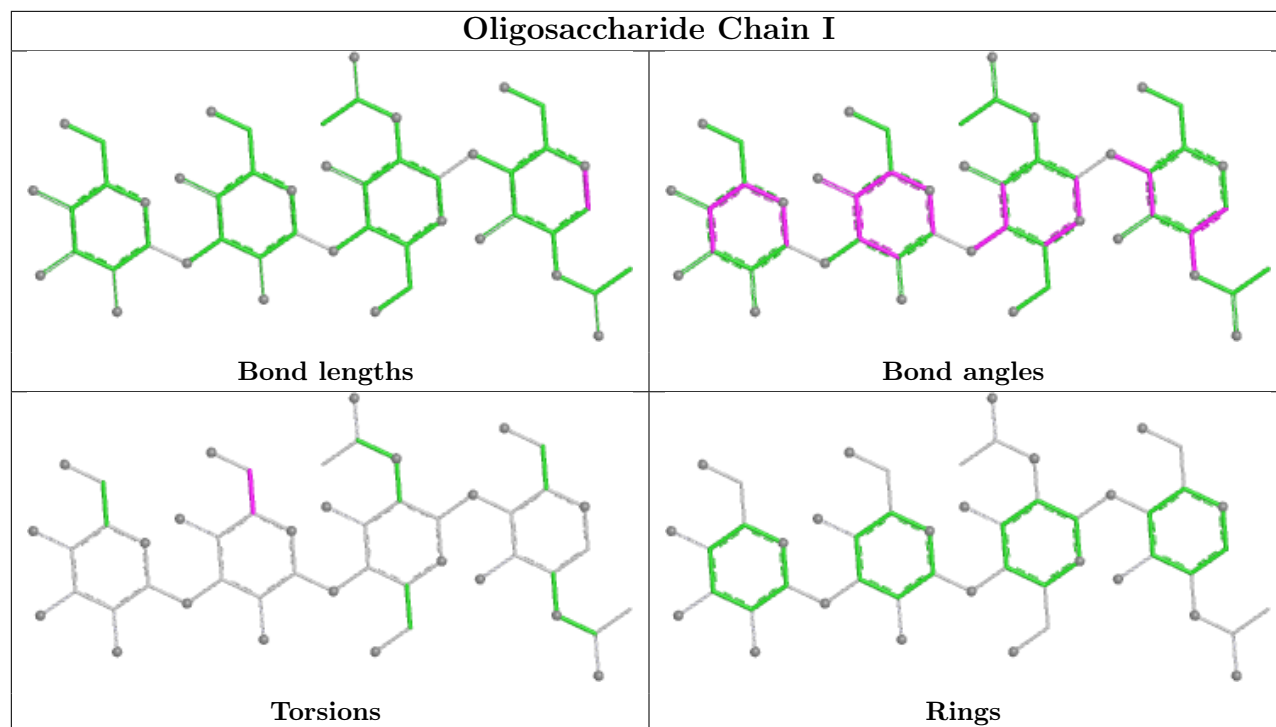
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

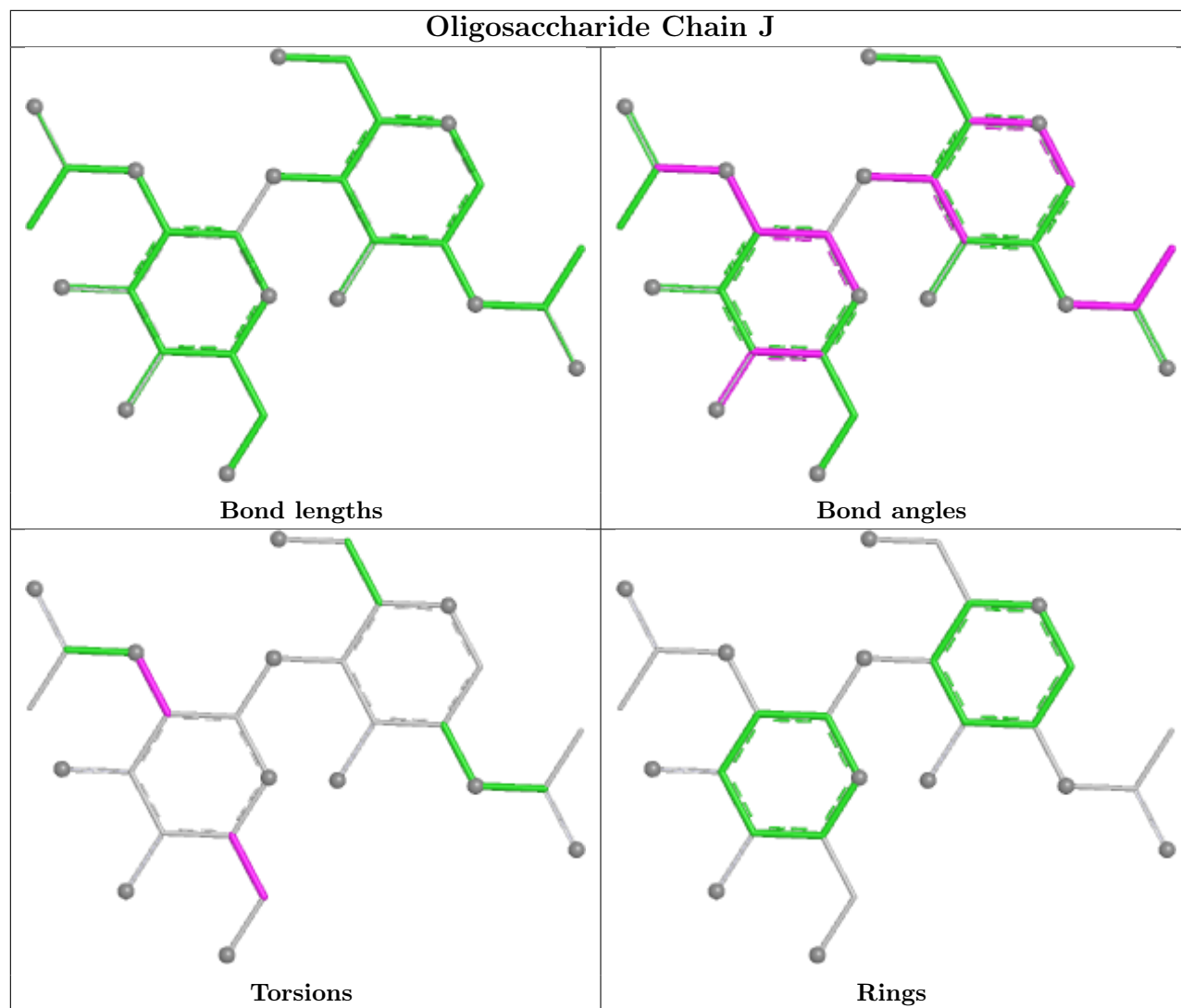
Oligosaccharide Chain G

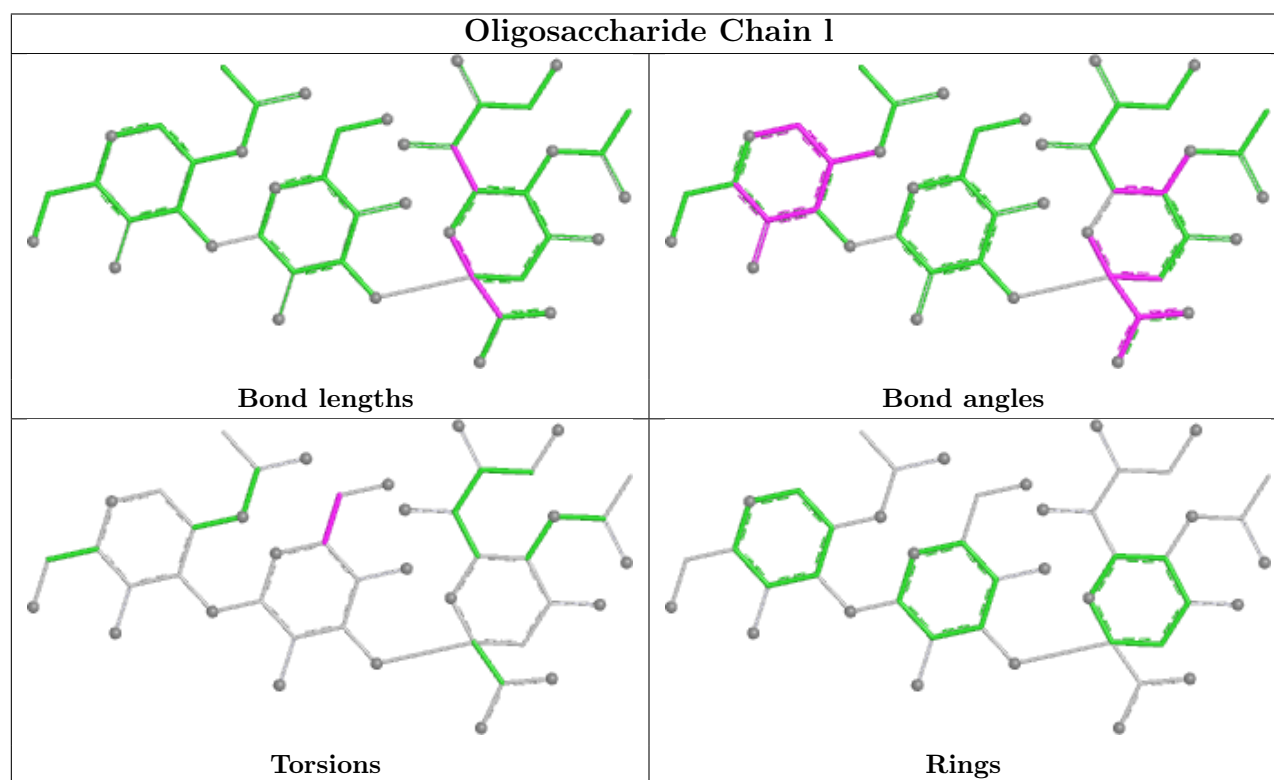
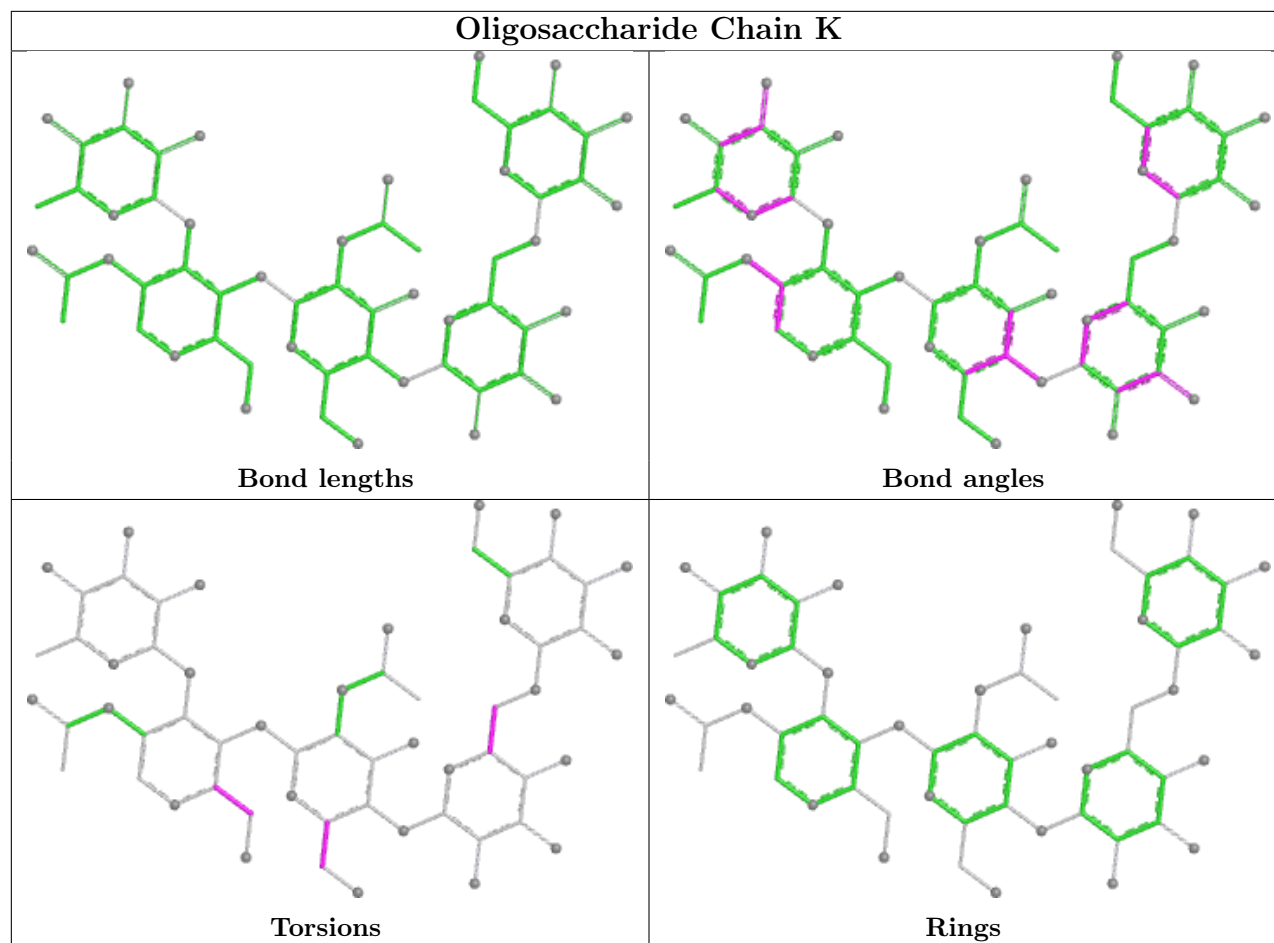


Oligosaccharide Chain H









5.6 Ligand geometry

17 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$
9	NAG	E	601	1	14,14,15	0.66	0	17,19,21	1.84	2 (11%)
9	NAG	A	601	1	14,14,15	0.82	1 (7%)	17,19,21	1.04	1 (5%)
9	NAG	C	602	1	14,14,15	0.77	1 (7%)	17,19,21	1.58	2 (11%)
11	SO4	E	604	-	4,4,4	0.74	0	6,6,6	0.32	0
11	SO4	C	603	-	4,4,4	1.00	0	6,6,6	0.62	0
11	SO4	D	201	-	4,4,4	0.75	0	6,6,6	0.54	0
9	NAG	A	602	1	14,14,15	0.78	0	17,19,21	2.44	3 (17%)
11	SO4	F	202	-	4,4,4	0.77	0	6,6,6	0.17	0
11	SO4	C	604	-	4,4,4	0.92	0	6,6,6	0.42	0
10	GOL	A	603	-	5,5,5	0.45	0	5,5,5	0.72	0
11	SO4	F	201	-	4,4,4	0.86	0	6,6,6	0.53	0
11	SO4	A	604	-	4,4,4	0.74	0	6,6,6	0.31	0
11	SO4	E	605	-	4,4,4	0.80	0	6,6,6	0.35	0
9	NAG	C	601	1	14,14,15	0.72	0	17,19,21	1.35	1 (5%)
11	SO4	E	603	-	4,4,4	0.96	0	6,6,6	0.67	0
10	GOL	E	602	-	5,5,5	0.40	0	5,5,5	0.86	0
12	CIT	B	201	-	12,12,12	1.84	1 (8%)	17,17,17	1.76	5 (29%)

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
9	NAG	E	601	1	-	0/6/23/26	0/1/1/1
9	NAG	A	601	1	-	2/6/23/26	0/1/1/1
9	NAG	C	602	1	-	0/6/23/26	0/1/1/1
9	NAG	A	602	1	-	5/6/23/26	0/1/1/1
10	GOL	A	603	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	601	1	-	0/6/23/26	0/1/1/1
10	GOL	E	602	-	-	2/4/4/4	-
12	CIT	B	201	-	-	10/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	201	CIT	C3-C6	4.74	1.58	1.53
9	A	601	NAG	C1-C2	2.30	1.55	1.52
9	C	602	NAG	C1-C2	2.14	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	602	NAG	C2-N2-C7	8.30	134.02	122.90
9	E	601	NAG	C1-O5-C5	6.32	120.66	112.19
9	C	601	NAG	C1-O5-C5	4.26	117.89	112.19
9	C	602	NAG	C1-O5-C5	3.99	117.53	112.19
12	B	201	CIT	O6-C6-C3	3.50	119.86	113.14
12	B	201	CIT	O5-C6-C3	-3.37	115.55	122.09
9	A	602	NAG	C8-C7-N2	2.88	120.89	116.12
9	A	602	NAG	C1-C2-N2	2.67	114.63	110.43
9	C	602	NAG	C2-N2-C7	2.58	126.36	122.90
9	A	601	NAG	C1-O5-C5	2.32	115.30	112.19
12	B	201	CIT	O7-C3-C6	2.27	112.17	108.96
9	E	601	NAG	C2-N2-C7	2.26	125.93	122.90
12	B	201	CIT	O1-C1-C2	-2.12	116.96	122.95
12	B	201	CIT	O3-C5-C4	-2.03	117.20	122.95

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	603	GOL	C1-C2-C3-O3
10	E	602	GOL	C1-C2-C3-O3
10	E	602	GOL	O2-C2-C3-O3
12	B	201	CIT	C1-C2-C3-O7
12	B	201	CIT	C1-C2-C3-C6
12	B	201	CIT	O7-C3-C6-O5
12	B	201	CIT	O7-C3-C6-O6
12	B	201	CIT	C4-C3-C6-O5

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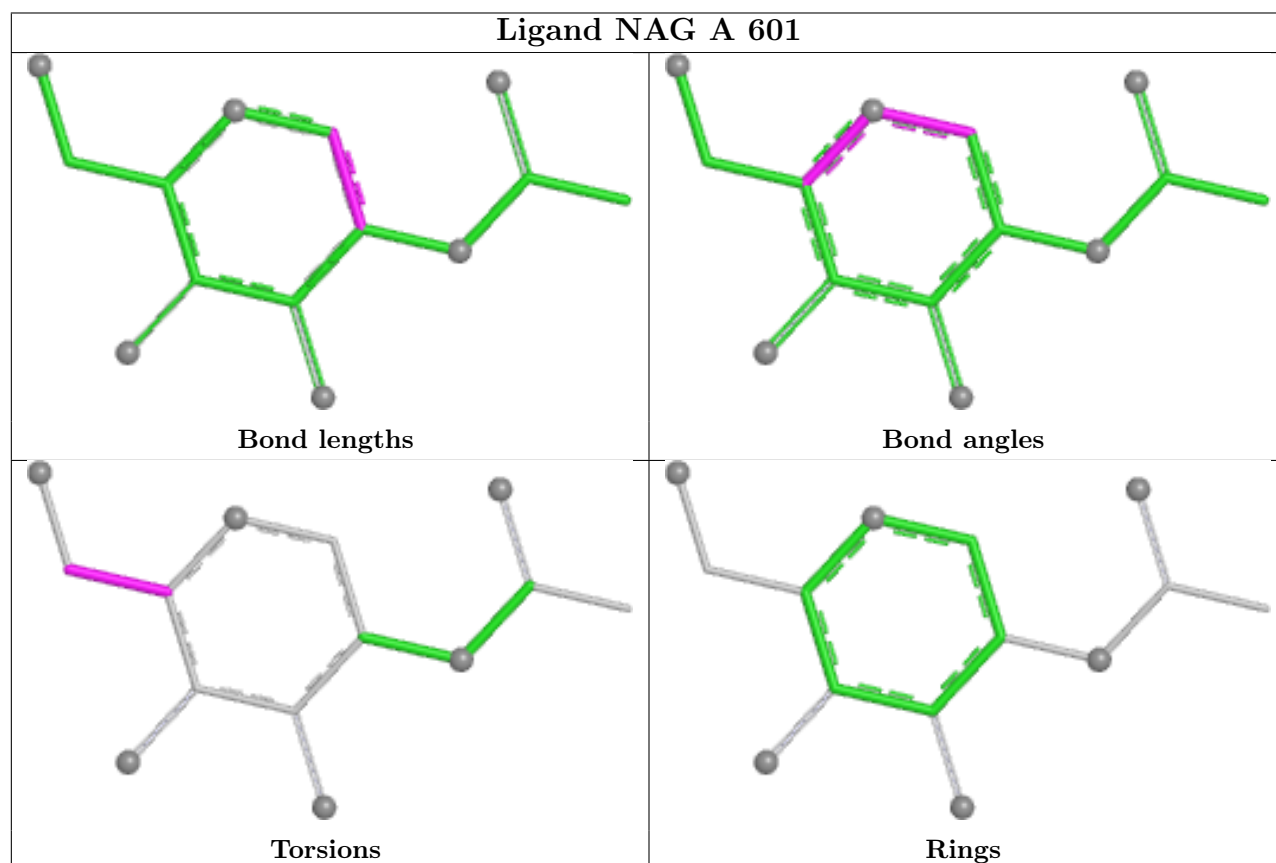
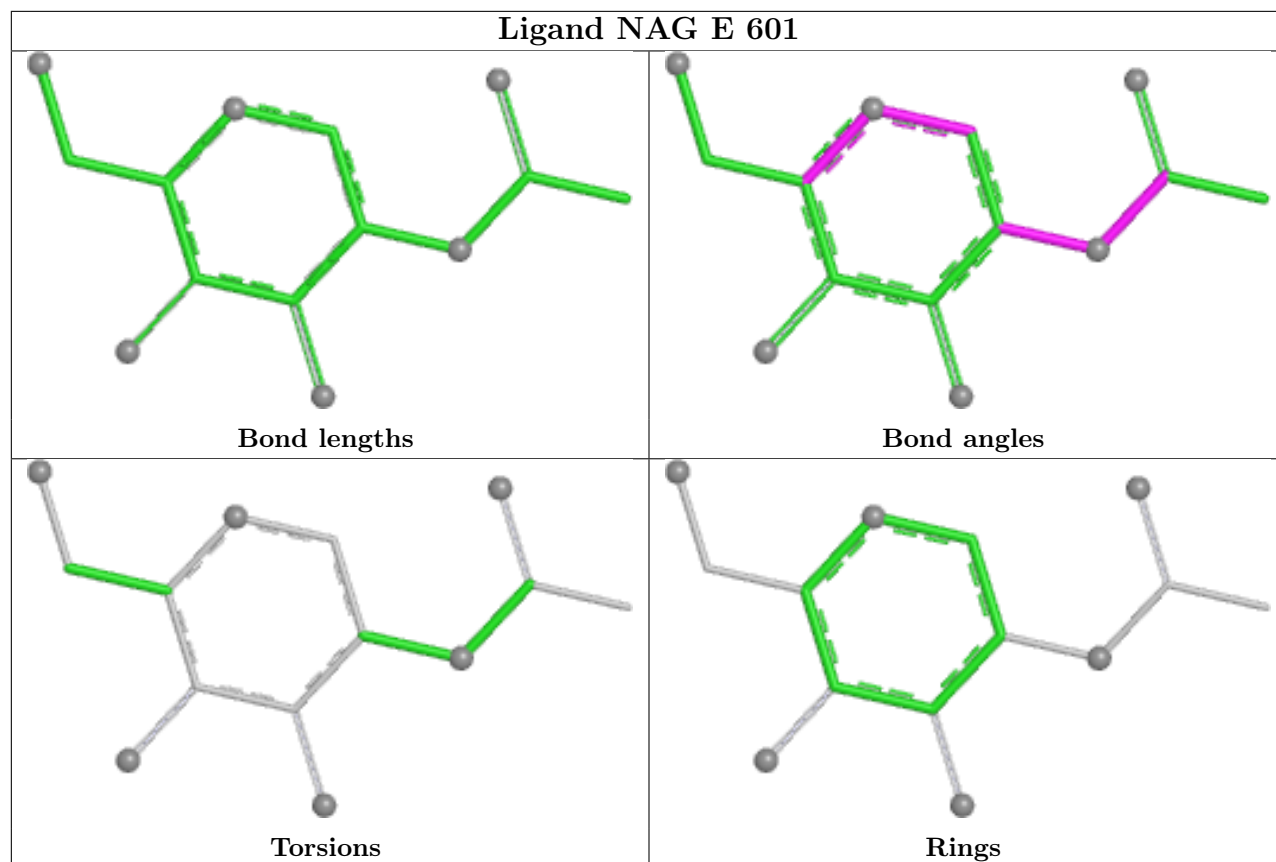
Mol	Chain	Res	Type	Atoms
12	B	201	CIT	C4-C3-C6-O6
9	A	601	NAG	O5-C5-C6-O6
9	A	601	NAG	C4-C5-C6-O6
12	B	201	CIT	C1-C2-C3-C4
9	A	602	NAG	C8-C7-N2-C2
9	A	602	NAG	O7-C7-N2-C2
10	A	603	GOL	O2-C2-C3-O3
12	B	201	CIT	C2-C3-C4-C5
12	B	201	CIT	C6-C3-C4-C5
9	A	602	NAG	C1-C2-N2-C7
10	A	603	GOL	O1-C1-C2-O2
9	A	602	NAG	C3-C2-N2-C7
12	B	201	CIT	O7-C3-C4-C5
10	A	603	GOL	O1-C1-C2-C3
9	A	602	NAG	O5-C5-C6-O6

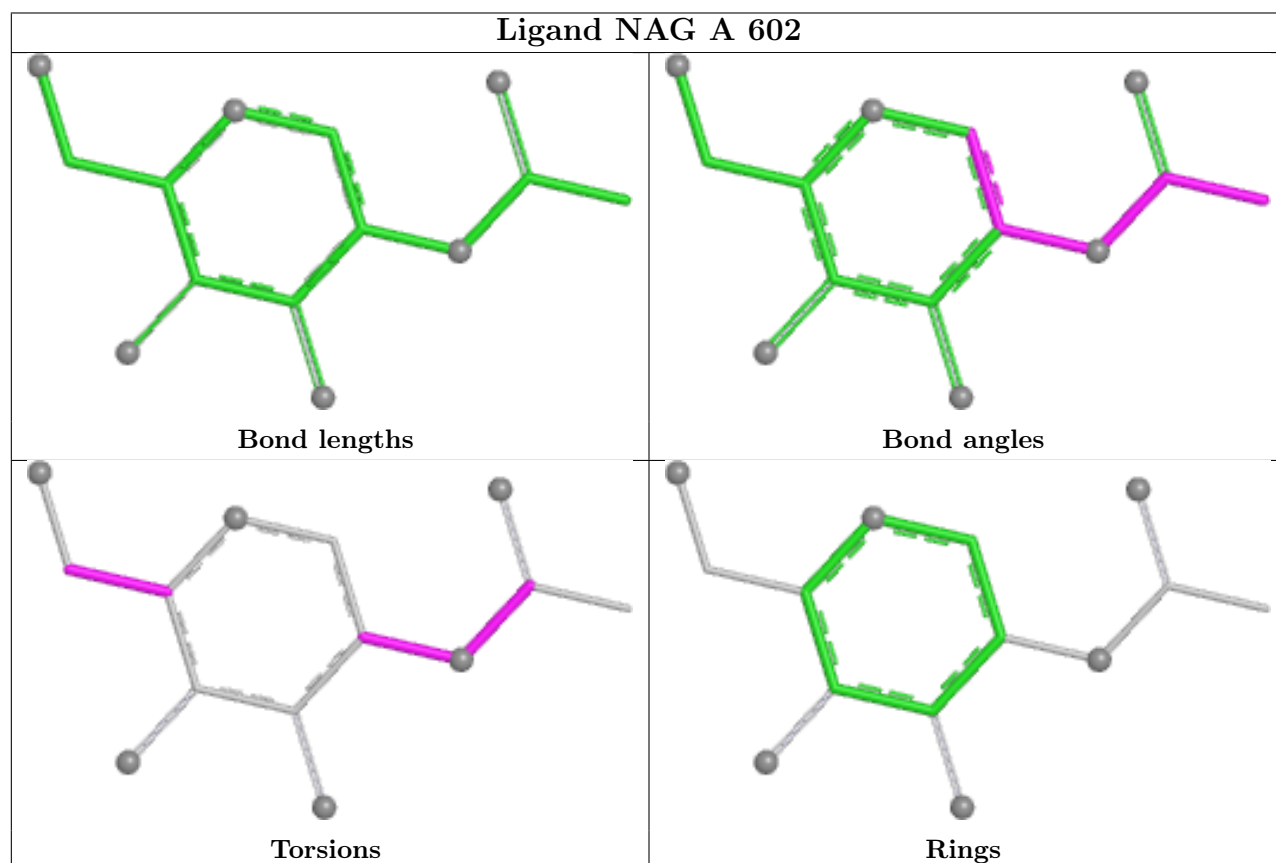
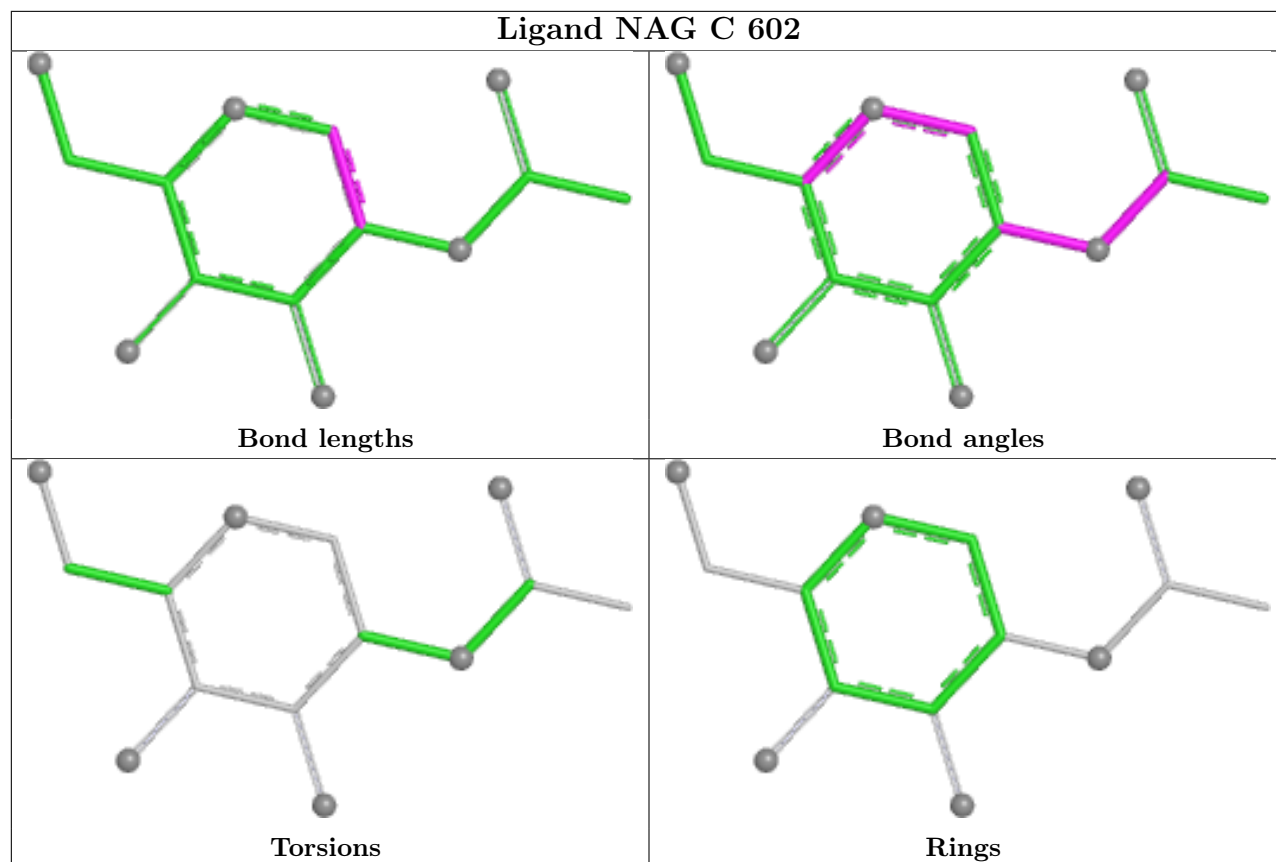
There are no ring outliers.

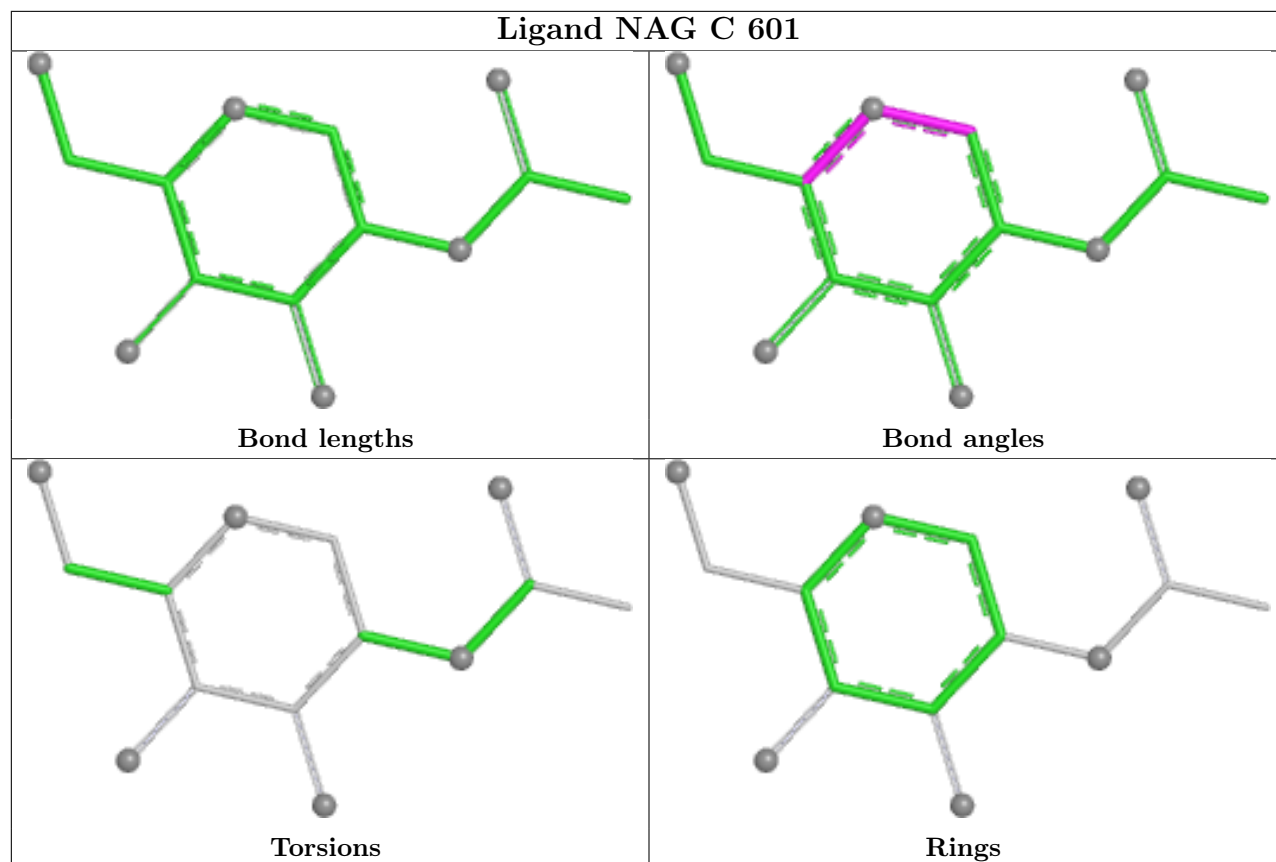
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	602	NAG	1	0
10	A	603	GOL	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 [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	322/329 (97%)	-0.31	13 (4%) 42 34	32, 51, 85, 170	0
1	C	323/329 (98%)	-0.37	9 (2%) 55 46	30, 50, 89, 152	0
1	E	323/329 (98%)	-0.45	8 (2%) 58 48	27, 47, 78, 165	0
2	B	170/181 (93%)	-0.10	11 (6%) 25 20	38, 60, 96, 169	0
2	D	171/181 (94%)	0.19	8 (4%) 36 28	41, 79, 109, 122	0
2	F	172/181 (95%)	-0.30	2 (1%) 76 69	40, 59, 81, 110	0
All	All	1481/1530 (96%)	-0.27	51 (3%) 48 39	27, 54, 96, 170	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	9	PHE	7.0
2	D	6	ILE	7.0
1	A	9	PRO	6.7
1	A	78	GLU	6.3
1	A	79	PHE	5.9
1	E	80	ILE	5.9
1	E	79	PHE	5.3
2	B	6	ILE	5.2
1	A	323	SER	5.1
1	C	79	PHE	4.8
1	C	8	ASP	4.7
1	C	78	GLU	4.6
2	D	7	ALA	4.6
1	A	81	ARG	4.2
1	A	80	ILE	4.0
2	B	175	SER	4.0
1	A	77	ASP	3.9
1	E	323	SER	3.9
2	B	106	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	81	ARG	3.8
1	E	78	GLU	3.7
1	C	80	ILE	3.6
1	C	290	SER	3.6
2	B	10	ILE	3.6
1	C	323	SER	3.5
2	D	19	ASP	3.5
2	D	10	ILE	3.5
1	A	289	ASN	3.2
2	D	176	GLY	3.1
2	B	174	GLY	3.0
1	A	91	ALA	2.8
2	B	7	ALA	2.8
2	D	8	GLY	2.8
1	A	82	VAL	2.8
1	C	81	ARG	2.7
2	B	12	GLY	2.7
1	C	289	ASN	2.7
2	D	11	GLU	2.7
2	B	11	GLU	2.5
1	E	289	ASN	2.5
1	E	77	ASP	2.4
2	D	9	PHE	2.4
2	B	8	GLY	2.4
1	A	76	CYS	2.3
1	A	291	SER	2.3
1	C	62	LYS	2.3
1	E	62	LYS	2.3
2	F	10	ILE	2.2
2	B	13	GLY	2.0
2	F	8	GLY	2.0
1	A	290	SER	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](#)

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,

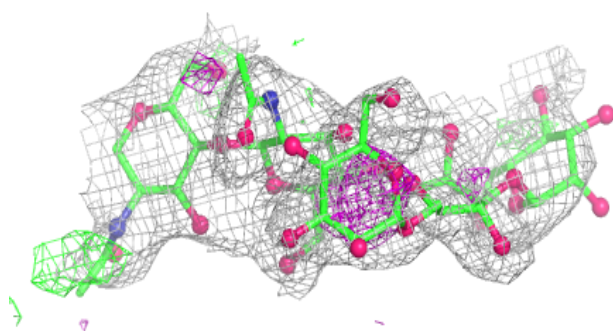
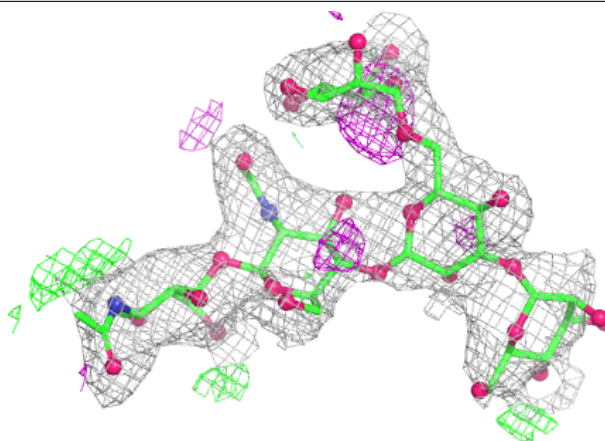
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	K	4	11/12	0.26	0.18	139,173,177,178	0
4	MAN	H	4	11/12	0.31	0.20	152,177,188,190	0
4	BMA	H	3	11/12	0.45	0.16	138,167,180,189	0
7	BMA	K	3	11/12	0.51	0.18	110,141,154,161	0
3	MAN	G	4	11/12	0.71	0.18	109,139,149,161	0
7	FUC	K	5	10/11	0.73	0.19	111,125,141,142	0
7	NAG	K	2	14/15	0.76	0.20	103,113,126,129	0
6	NAG	J	2	14/15	0.76	0.14	63,104,112,116	0
4	NAG	H	2	14/15	0.80	0.17	103,125,148,149	0
3	MAN	G	5	11/12	0.82	0.21	85,99,115,129	0
5	BMA	I	3	11/12	0.85	0.14	63,70,92,100	0
7	NAG	K	1	14/15	0.85	0.15	80,98,113,125	0
3	BMA	G	3	11/12	0.86	0.16	83,117,136,140	0
4	NAG	H	1	14/15	0.86	0.14	64,107,117,123	0
3	NAG	G	2	14/15	0.87	0.18	73,100,124,129	0
4	FUC	H	5	10/11	0.88	0.17	87,112,116,119	0
3	NAG	G	1	14/15	0.88	0.16	69,84,94,102	0
5	NAG	I	2	14/15	0.93	0.10	50,58,74,84	0
5	NAG	I	1	14/15	0.93	0.11	46,64,71,89	0
5	MAN	I	4	11/12	0.94	0.08	51,58,74,77	0
6	NAG	J	1	14/15	0.96	0.07	49,71,83,101	0
8	NAG	l	1	14/15	-	-	59,86,102,112	0
8	GAL	l	2	11/12	-	-	40,48,60,63	0
8	SIA	l	3	20/21	-	-	35,44,51,57	0

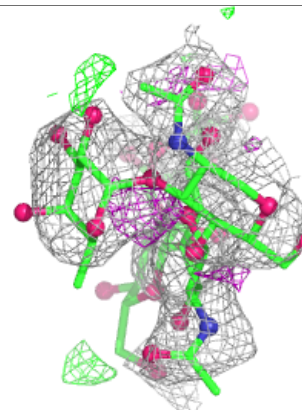
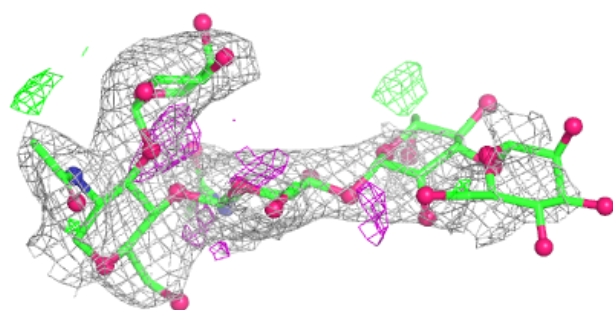
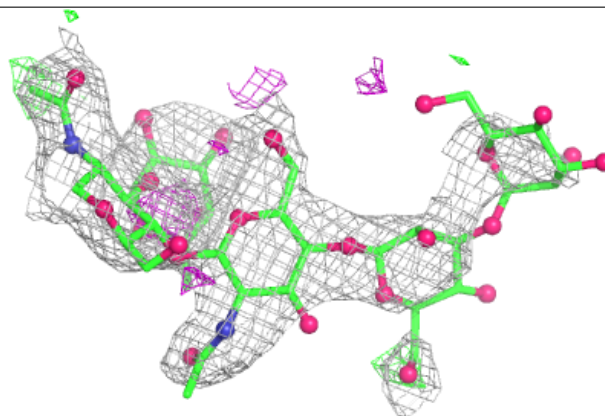
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

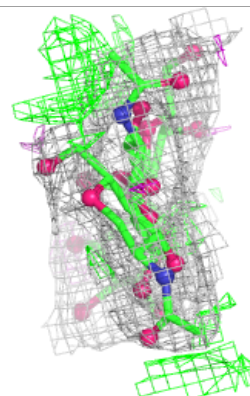
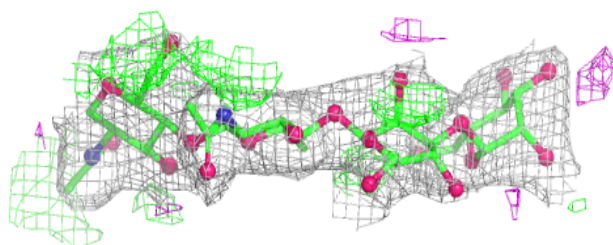
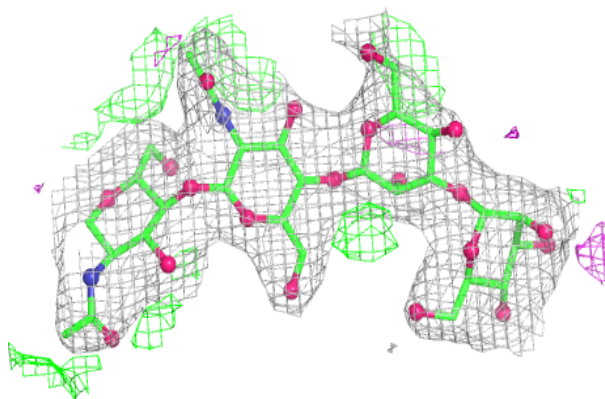
**Electron density around Chain H:**

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

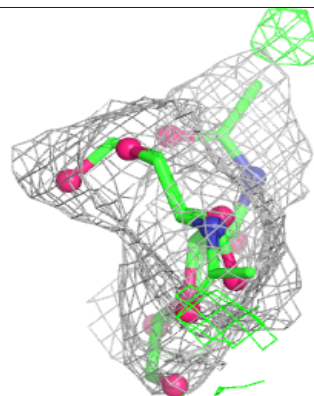
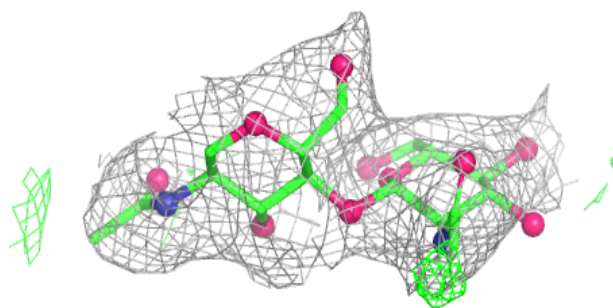
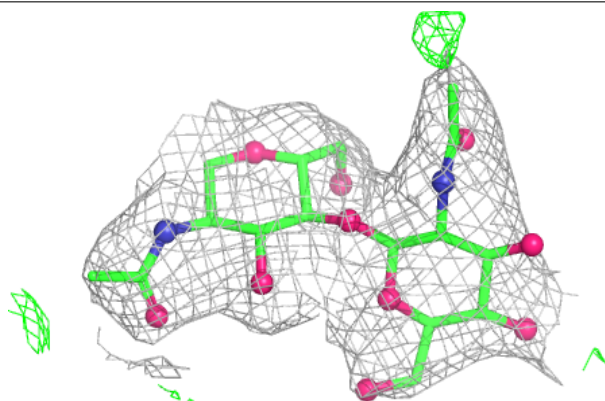


Electron density around Chain I:

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

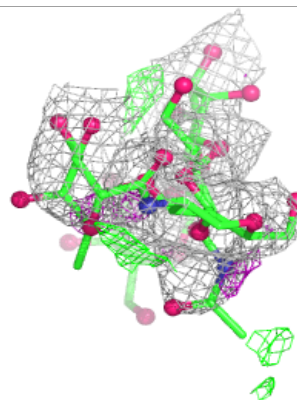
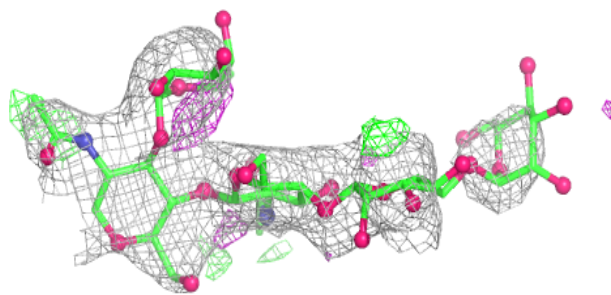
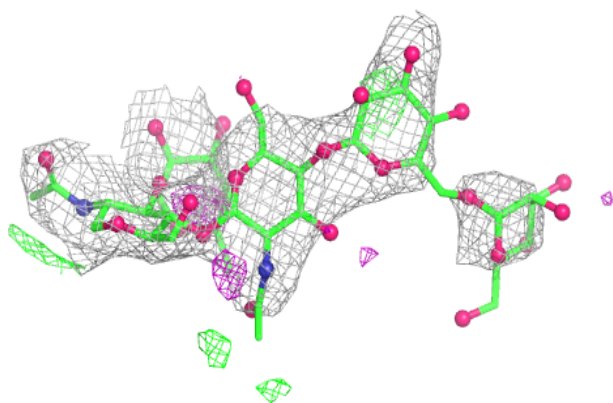
**Electron density around Chain J:**

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

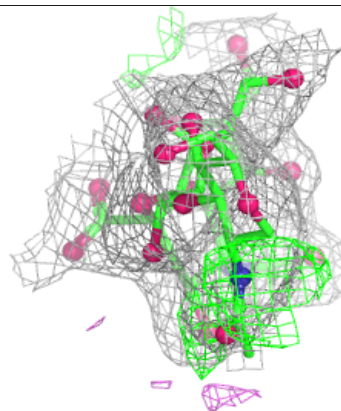
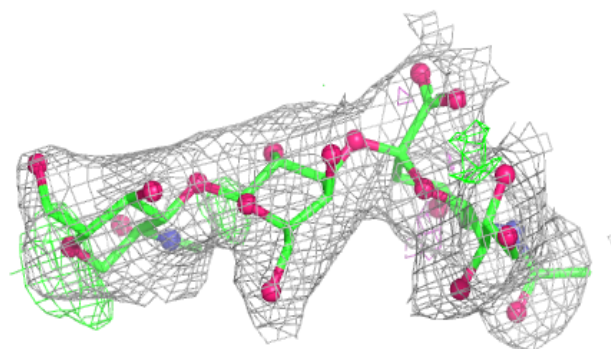
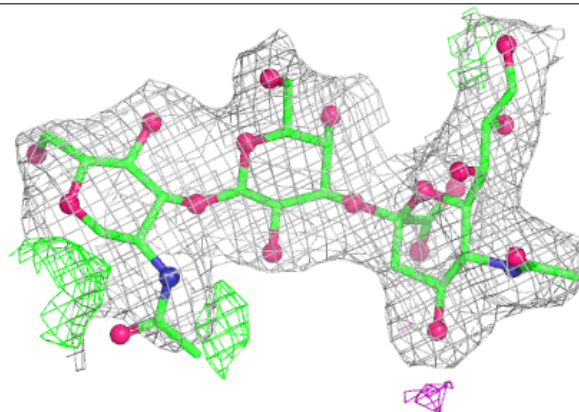


Electron density around Chain K:

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

**Electron density around Chain I:**

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



6.4 Ligands ⓘ

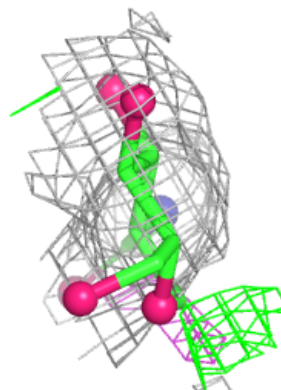
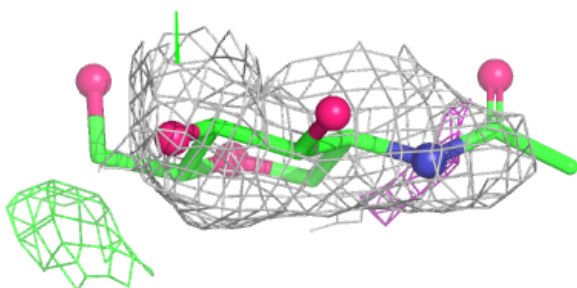
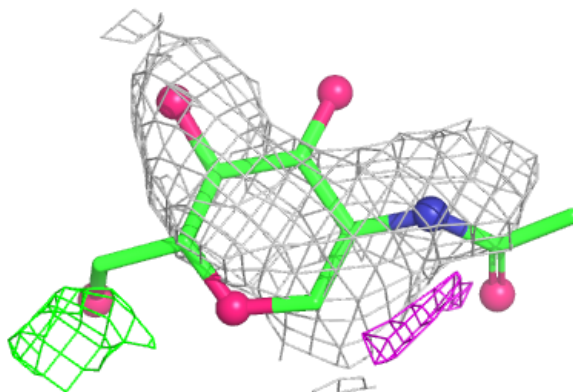
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	C	602	14/15	0.60	0.22	96,139,149,154	0
9	NAG	A	602	14/15	0.64	0.24	114,144,148,150	0
10	GOL	A	603	6/6	0.71	0.24	62,90,92,94	0
9	NAG	C	601	14/15	0.82	0.16	87,113,130,131	0
12	CIT	B	201	13/13	0.83	0.16	64,102,118,120	0
9	NAG	A	601	14/15	0.84	0.16	89,116,128,138	0
11	SO4	D	201	5/5	0.84	0.22	97,109,128,150	0
9	NAG	E	601	14/15	0.84	0.14	94,117,123,133	0
11	SO4	F	201	5/5	0.85	0.23	72,90,107,124	0
11	SO4	A	604	5/5	0.90	0.23	72,81,122,131	0
11	SO4	C	604	5/5	0.92	0.22	73,74,83,124	0
11	SO4	F	202	5/5	0.92	0.19	91,106,121,142	0
11	SO4	E	603	5/5	0.92	0.26	64,68,109,126	0
10	GOL	E	602	6/6	0.93	0.14	51,57,63,65	0
11	SO4	C	603	5/5	0.93	0.29	57,64,95,125	0
11	SO4	E	604	5/5	0.94	0.20	61,66,102,114	0
11	SO4	E	605	5/5	0.95	0.21	82,88,105,132	0

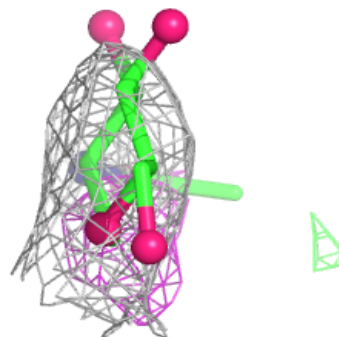
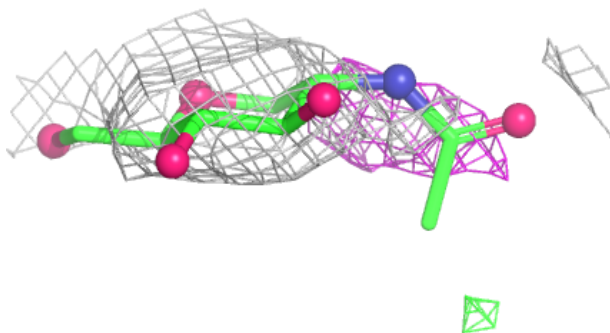
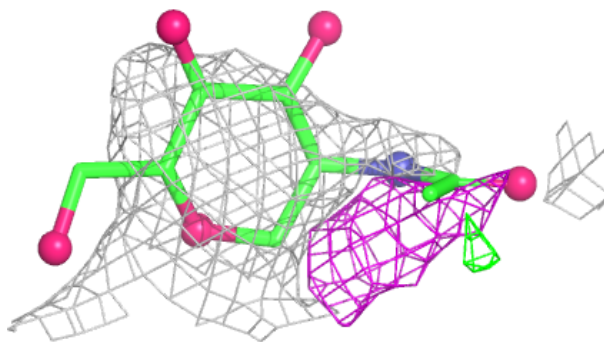
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG C 602:

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

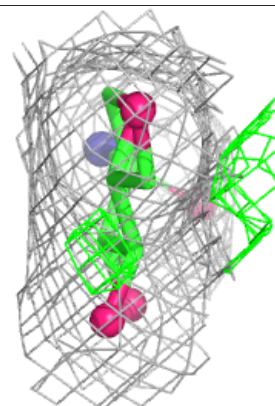
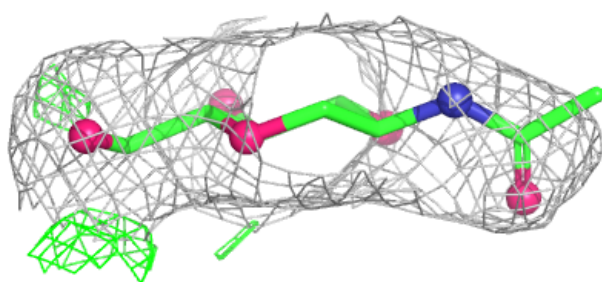
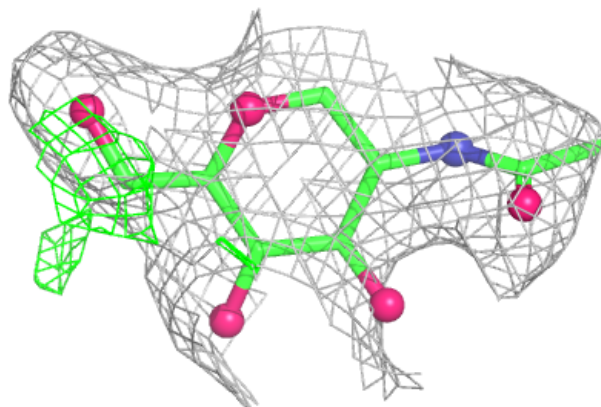
**Electron density around NAG A 602:**

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

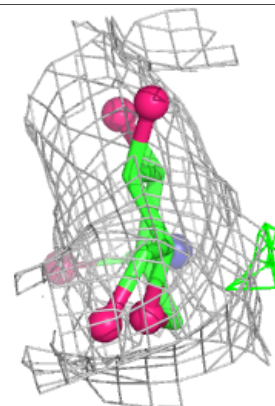
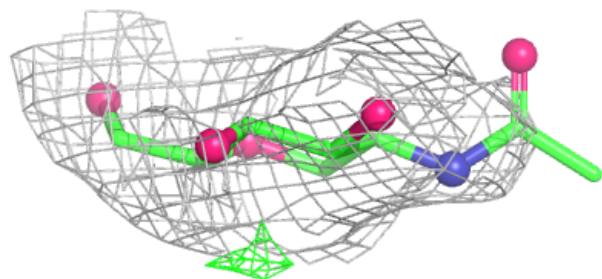
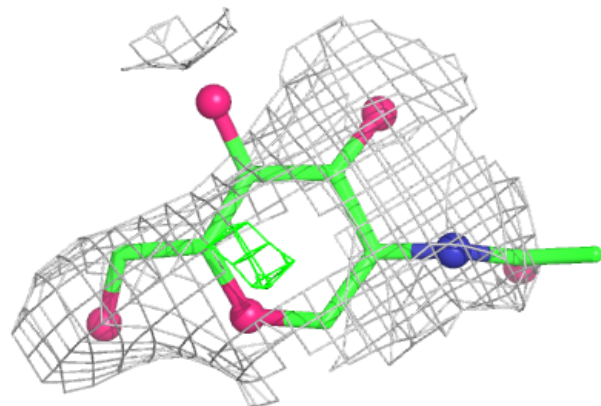


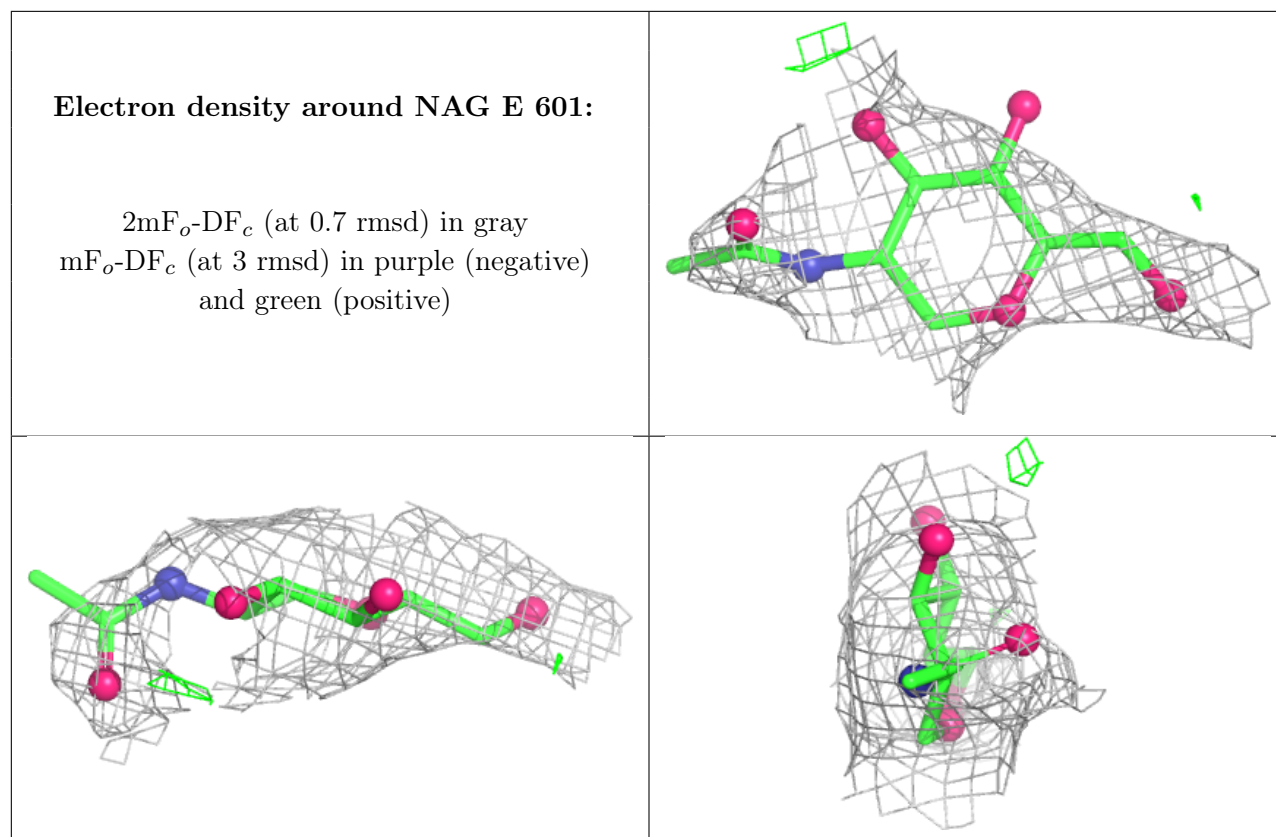
Electron density around NAG C 601:

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

**Electron density around NAG A 601:**

$2mF_o-DF_c$ (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.