



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:59 PM UTC

PDB ID : 9NRU / pdb_00009nru
Title : Crystal structure of the H5 influenza virus hemagglutinin from A/duck/France/161108h/2016 (H5N8) clade 2.3.4.4b in complex with O-linked glycan 7
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2025-03-14
Resolution : 2.38 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

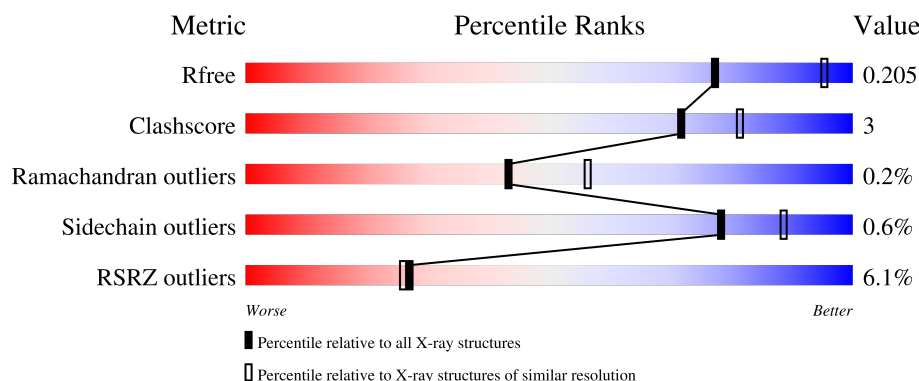
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

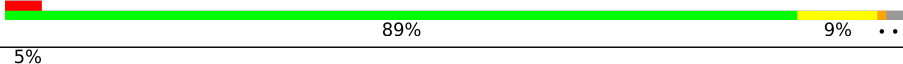
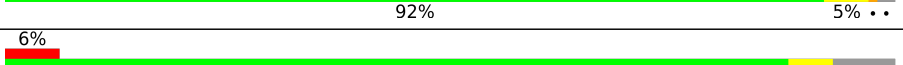
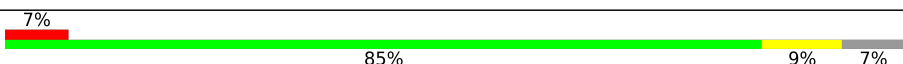
The reported resolution of this entry is 2.38 Å.

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	
1	C	329	
1	E	329	
2	B	181	
2	D	181	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	181	
3	G	5	
3	H	5	
3	I	5	
3	l	5	
4	J	5	
5	K	5	
6	L	4	
7	M	2	
7	N	2	
8	O	5	
9	P	4	
9	Q	4	
9	R	4	
9	S	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SO4	A	605	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13760 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	321	Total	C	N	O	S	0	0	0
			2537	1605	442	476	14			
1	C	324	Total	C	N	O	S	0	0	0
			2563	1623	445	481	14			
1	E	322	Total	C	N	O	S	0	0	0
			2545	1609	443	479	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	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	D	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	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 a protein called peptide linker.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			19	12	3	4			
3	G	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	H	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	I	5	Total	C	N	O	0	0	0
			37	26	5	6			

- Molecule 4 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
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

e-(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
5	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 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
6	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 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
7	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 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
8	O	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 9 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(3-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose.

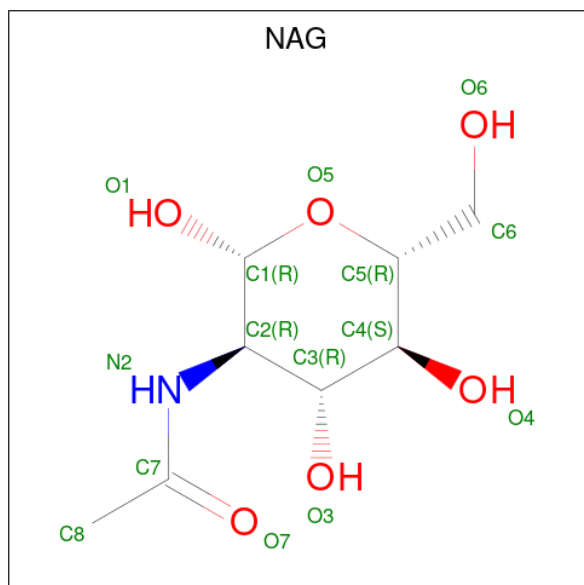
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	4	Total	C	N	O	0	0	0
			59	33	3	23			
9	Q	4	Total	C	N	O	0	0	0
			59	33	3	23			
9	R	4	Total	C	N	O	0	0	0
			59	33	3	23			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S	4	Total	C	N	O	0	0	0
			59	33	3	23			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



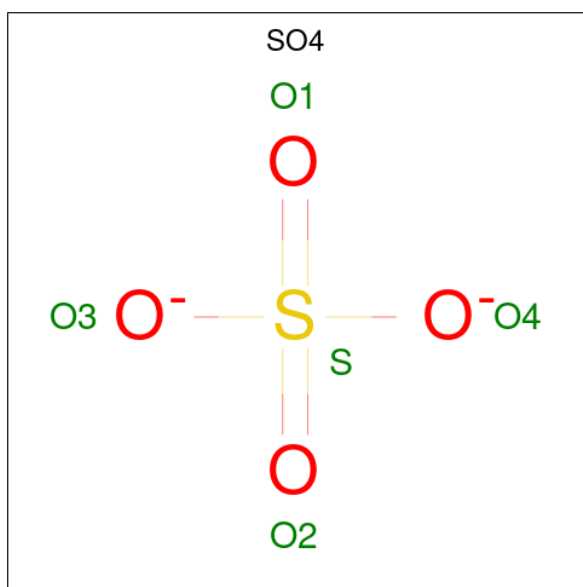
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total	O	S	0	0
			5	4	1		

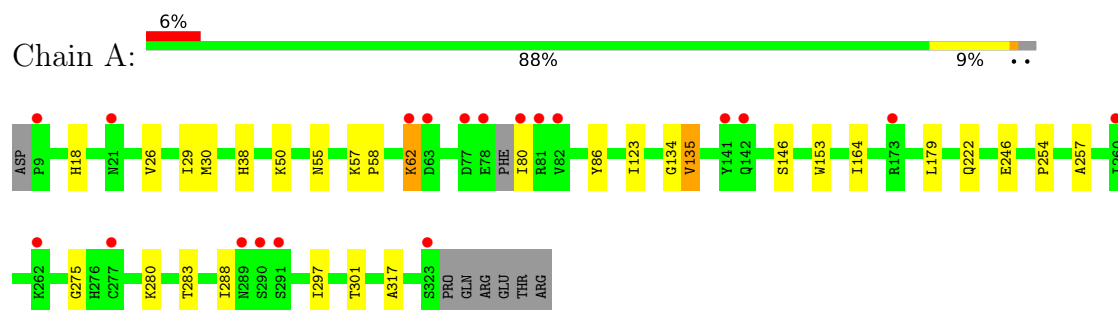
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	261	Total	O	0	0
			261	261		
13	B	112	Total	O	0	0
			112	112		
13	C	234	Total	O	0	0
			234	234		
13	D	76	Total	O	0	0
			76	76		
13	E	261	Total	O	0	0
			261	261		
13	F	142	Total	O	0	0
			142	142		
13	G	1	Total	O	0	0
			1	1		
13	H	2	Total	O	0	0
			2	2		
13	I	1	Total	O	0	0
			1	1		

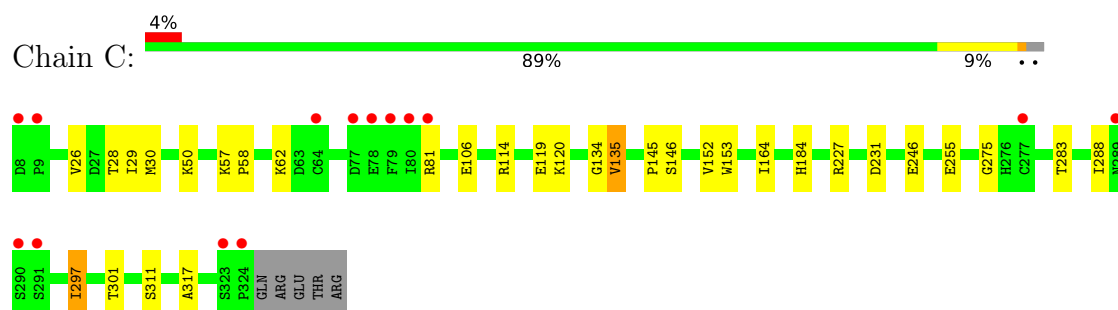
3 Residue-property plots [i](#)

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.

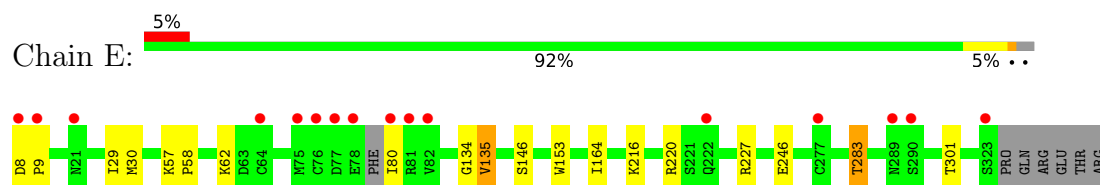
- Molecule 1: Hemagglutinin HA1 chain



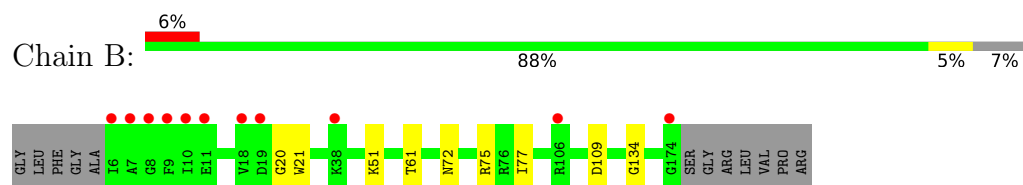
- Molecule 1: Hemagglutinin HA1 chain



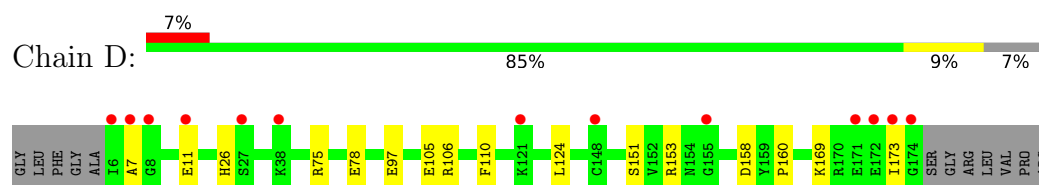
- Molecule 1: Hemagglutinin HA1 chain



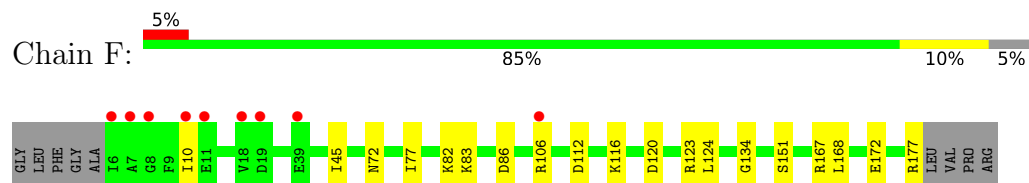
- Molecule 2: Hemagglutinin HA2 chain



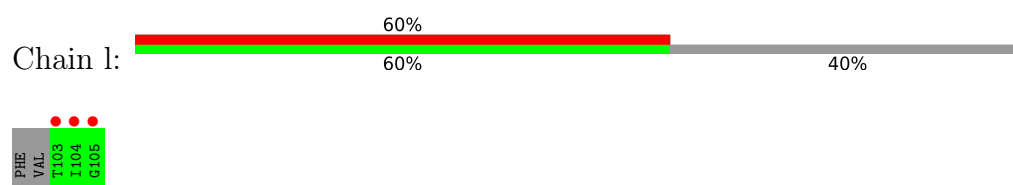
- Molecule 2: Hemagglutinin HA2 chain



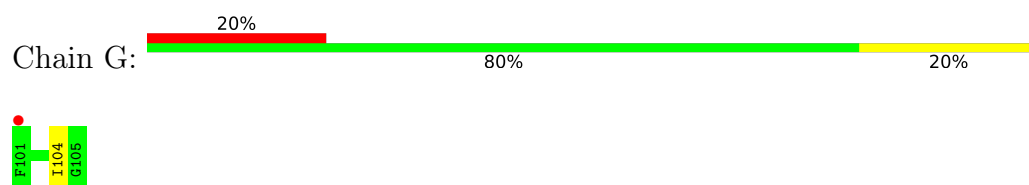
- Molecule 2: Hemagglutinin HA2 chain



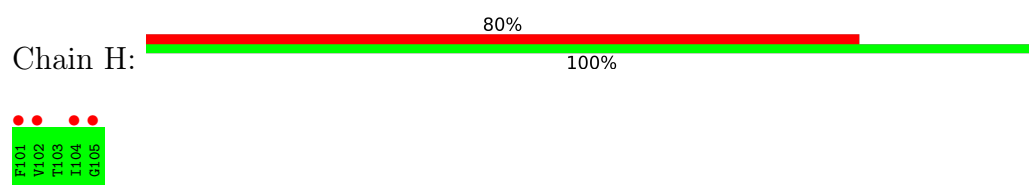
- Molecule 3: peptide linker



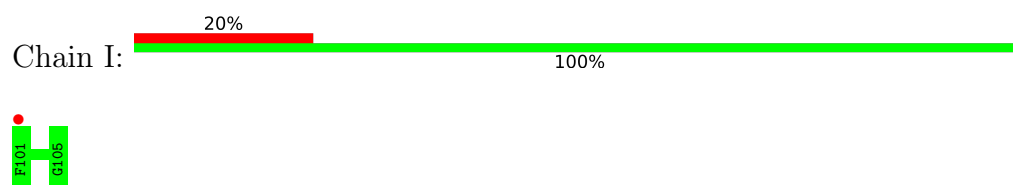
- Molecule 3: peptide linker



- Molecule 3: peptide linker



- Molecule 3: peptide linker



- Molecule 4: 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





- Molecule 5: 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



- Molecule 6: 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



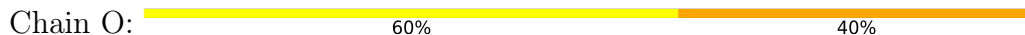
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(3-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose



- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(3-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain Q:  50% 50%



- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(3-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain R:  50% 50%



- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(3-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain S:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.75Å 171.97Å 226.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.38 46.12 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.12-2.38) 98.5 (46.12-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.182 , 0.206 0.182 , 0.205	Depositor DCC
R_{free} test set	7372 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13760	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: BMA, A2G, GOL, GAL, FUC, NAG, MAN, SIA, 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	0.13	0/2599	0.30	0/3533
1	C	0.13	0/2628	0.30	0/3576
1	E	0.13	0/2607	0.32	0/3545
2	B	0.12	0/1404	0.25	0/1887
2	D	0.12	0/1404	0.30	0/1887
2	F	0.12	0/1425	0.26	0/1914
3	G	0.08	0/37	0.19	0/49
3	H	0.22	0/37	0.26	0/49
3	I	0.12	0/37	0.21	0/49
3	I	0.15	0/18	0.27	0/23
All	All	0.13	0/12196	0.30	0/16512

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

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	2537	0	2490	18	0
1	C	2563	0	2511	22	0
1	E	2545	0	2495	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1378	0	1282	7	0
2	D	1378	0	1282	13	0
2	F	1399	0	1303	15	0
3	G	37	0	37	1	0
3	H	37	0	37	0	0
3	I	37	0	37	0	0
3	l	19	0	19	0	0
4	J	61	0	52	0	0
5	K	60	0	52	0	0
6	L	50	0	43	0	0
7	M	28	0	25	2	0
7	N	28	0	25	0	0
8	O	60	0	52	2	0
9	P	59	0	48	0	0
9	Q	59	0	48	0	0
9	R	59	0	48	0	0
9	S	59	0	48	0	0
10	A	42	0	39	0	0
10	C	28	0	26	0	0
10	E	14	0	13	0	0
11	A	6	0	8	0	0
11	C	6	0	8	0	0
11	E	6	0	8	0	0
12	A	30	0	0	3	0
12	B	10	0	0	0	0
12	C	35	0	0	3	0
12	E	35	0	0	0	0
12	F	5	0	0	1	0
13	A	261	0	0	0	0
13	B	112	0	0	0	0
13	C	234	0	0	4	0
13	D	76	0	0	1	0
13	E	261	0	0	1	0
13	F	142	0	0	4	0
13	G	1	0	0	0	0
13	H	2	0	0	0	0
13	I	1	0	0	0	0
All	All	13760	0	12036	82	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 3.

All (82) 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:D:26:HIS:HD2	2:D:153:ARG:HH12	1.33	0.73
1:E:216:LYS:O	1:E:220:ARG:NH2	2.23	0.72
1:E:227:ARG:NH2	13:E:704:HOH:O	2.26	0.69
1:A:55:ASN:HD21	1:A:280:LYS:HE3	1.59	0.68
1:E:8:ASP:HB3	1:E:9:PRO:HD3	1.76	0.67
2:F:83:LYS:NZ	13:F:302:HOH:O	2.28	0.65
1:C:288:ILE:HG21	1:C:297:ILE:HD13	1.79	0.65
1:C:81:ARG:HH22	1:C:119:GLU:HG3	1.64	0.62
1:C:135:VAL:HG22	1:C:146:SER:HA	1.82	0.61
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.84	0.60
1:A:288:ILE:HG21	1:A:297:ILE:HD13	1.84	0.59
2:D:124:LEU:HD13	2:F:134:GLY:HA2	1.83	0.59
1:A:38:HIS:ND1	12:A:605:SO4:O4	2.33	0.59
1:C:81:ARG:HH12	1:C:120:LYS:H	1.51	0.58
1:C:283:THR:HG22	1:C:301:THR:HG22	1.86	0.58
1:A:55:ASN:ND2	1:A:280:LYS:HE3	2.19	0.57
1:C:50:LYS:HD2	1:C:275:GLY:HA3	1.87	0.57
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.88	0.55
1:A:222:GLN:NE2	12:A:608:SO4:O1	2.40	0.54
1:C:106:GLU:H	1:C:106:GLU:CD	2.15	0.54
1:A:283:THR:HG22	1:A:301:THR:HG22	1.88	0.54
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.88	0.54
12:A:605:SO4:O3	2:B:21:TRP:NE1	2.41	0.54
1:A:50:LYS:HD2	1:A:275:GLY:HA3	1.89	0.53
1:E:57:LYS:HG2	1:E:58:PRO:HD2	1.89	0.53
2:F:172:GLU:HG2	2:F:177:ARG:HG3	1.90	0.52
2:F:151:SER:HB3	8:O:1:NAG:H62	1.90	0.52
1:C:114:ARG:NH1	13:C:707:HOH:O	2.43	0.52
2:F:120:ASP:OD1	2:F:123:ARG:NH1	2.42	0.52
1:C:227:ARG:NH2	12:C:606:SO4:O2	2.32	0.51
7:M:1:NAG:H4	7:M:2:NAG:N2	2.25	0.51
2:D:26:HIS:HD2	2:D:153:ARG:NH1	2.07	0.50
8:O:2:NAG:H61	8:O:5:FUC:H3	1.94	0.50
2:B:51:LYS:HE3	1:C:30:MET:HE3	1.93	0.50
1:C:81:ARG:NH2	1:C:119:GLU:HG3	2.27	0.50
2:F:72:ASN:N	12:F:201:SO4:O2	2.44	0.48
1:C:29:ILE:HG23	1:C:30:MET:HG3	1.96	0.48
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.95	0.47
2:D:75:ARG:NH1	2:D:78:GLU:OE2	2.47	0.47
2:D:151:SER:HB3	7:M:1:NAG:H62	1.96	0.47
1:C:28:THR:HB	2:D:105:GLU:HB2	1.97	0.47
2:B:134:GLY:HA2	2:F:124:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:ILE:HG23	3:G:104:ILE:HD11	1.96	0.46
1:C:57:LYS:HG2	1:C:58:PRO:HD2	1.97	0.46
1:A:164:ILE:O	1:A:246:GLU:HA	2.17	0.45
1:A:135:VAL:HG22	1:A:146:SER:HA	1.97	0.45
12:C:605:SO4:O1	13:C:702:HOH:O	2.21	0.45
1:A:62:LYS:HD3	1:A:62:LYS:HA	1.76	0.45
1:C:184:HIS:NE2	1:C:231:ASP:OD2	2.50	0.45
2:D:110:PHE:CE1	1:E:30:MET:HE1	2.52	0.45
2:F:112:ASP:O	2:F:116:LYS:HG2	2.17	0.45
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.50	0.45
1:C:164:ILE:O	1:C:246:GLU:HA	2.17	0.44
1:C:135:VAL:HG13	1:C:145:PRO:HB2	1.99	0.44
1:C:311:SER:OG	2:D:97:GLU:OE2	2.28	0.44
2:F:168:LEU:HG	13:F:301:HOH:O	2.17	0.44
1:A:179:LEU:O	1:A:254:PRO:HB3	2.18	0.43
1:E:283:THR:HG22	1:E:301:THR:HG22	1.99	0.43
1:C:152:VAL:HG23	1:C:255:GLU:HB2	2.00	0.43
2:B:109:ASP:OD2	2:F:106:ARG:NH1	2.50	0.43
12:C:608:SO4:O4	13:C:701:HOH:O	2.20	0.43
1:E:29:ILE:HG23	1:E:30:MET:HG3	2.01	0.43
2:D:169:LYS:O	2:D:173:ILE:HG13	2.18	0.42
2:B:77:ILE:HD11	2:F:77:ILE:HD13	2.01	0.42
1:E:135:VAL:HG22	1:E:146:SER:HA	2.01	0.42
2:F:167:ARG:HB3	13:F:301:HOH:O	2.19	0.42
2:F:82:LYS:NZ	2:F:86:ASP:OD2	2.52	0.42
1:E:164:ILE:O	1:E:246:GLU:HA	2.19	0.42
1:A:29:ILE:HG23	1:A:30:MET:HG3	2.02	0.41
2:D:7:ALA:HB1	2:D:11:GLU:HG3	2.01	0.41
2:F:106:ARG:HD3	13:F:376:HOH:O	2.19	0.41
2:D:158:ASP:OD1	2:D:160:PRO:HD2	2.21	0.41
1:A:18:HIS:HB2	2:B:20:GLY:O	2.21	0.41
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.02	0.41
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.56	0.41
1:E:80:ILE:HD13	1:E:80:ILE:HA	1.90	0.41
1:A:57:LYS:HG2	1:A:58:PRO:HD2	2.02	0.41
1:C:106:GLU:OE2	13:C:703:HOH:O	2.22	0.41
1:E:220:ARG:O	1:E:227:ARG:HG2	2.21	0.41
2:D:106:ARG:NH2	13:D:206:HOH:O	2.53	0.40
1:A:123:ILE:HD13	1:A:257:ALA:HB2	2.04	0.40
2:D:26:HIS:CD2	2:D:153:ARG:HH12	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	307 (97%)	9 (3%)	1 (0%)	36	48
1	C	322/329 (98%)	308 (96%)	13 (4%)	1 (0%)	36	48
1	E	318/329 (97%)	307 (96%)	10 (3%)	1 (0%)	36	48
2	B	167/181 (92%)	163 (98%)	4 (2%)	0	100	100
2	D	167/181 (92%)	165 (99%)	2 (1%)	0	100	100
2	F	170/181 (94%)	169 (99%)	1 (1%)	0	100	100
3	G	3/5 (60%)	3 (100%)	0	0	100	100
3	H	3/5 (60%)	3 (100%)	0	0	100	100
3	I	3/5 (60%)	3 (100%)	0	0	100	100
3	l	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1471/1550 (95%)	1429 (97%)	39 (3%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	E	62	LYS
1	C	62	LYS

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	286/294 (97%)	284 (99%)	2 (1%)	76	87
1	C	289/294 (98%)	287 (99%)	2 (1%)	76	87
1	E	287/294 (98%)	285 (99%)	2 (1%)	76	87
2	B	146/154 (95%)	145 (99%)	1 (1%)	76	87
2	D	146/154 (95%)	146 (100%)	0	100	100
2	F	148/154 (96%)	147 (99%)	1 (1%)	76	87
3	G	4/4 (100%)	4 (100%)	0	100	100
3	H	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
3	l	2/4 (50%)	2 (100%)	0	100	100
All	All	1316/1360 (97%)	1308 (99%)	8 (1%)	78	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	135	VAL
2	B	61	THR
1	C	135	VAL
1	C	297	ILE
1	E	135	VAL
1	E	283	THR
2	F	10	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	25	GLN
1	A	55	ASN
1	A	158	ASN
1	A	172	ASN
1	A	276	HIS
2	B	26	HIS
1	C	222	GLN
1	C	240	ASN
2	D	26	HIS
2	D	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	62	GLN
2	D	72	ASN
1	E	21	ASN
1	E	25	GLN
1	E	186	ASN
2	F	50	ASN
2	F	62	GLN
2	F	117	ASN

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](#)

39 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	$\# Z > 2$
4	NAG	J	1	4,1	14,14,15	0.71	0	17,19,21	0.97	1 (5%)
4	NAG	J	2	4	14,14,15	0.71	0	17,19,21	1.07	1 (5%)
4	BMA	J	3	4	11,11,12	0.75	0	15,15,17	1.59	1 (6%)
4	MAN	J	4	4	11,11,12	0.64	0	15,15,17	1.32	1 (6%)
4	MAN	J	5	4	11,11,12	0.70	0	15,15,17	1.09	1 (6%)
5	NAG	K	1	2,5	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
5	NAG	K	2	5	14,14,15	0.71	0	17,19,21	0.81	0
5	BMA	K	3	5	11,11,12	0.83	0	15,15,17	1.73	2 (13%)
5	MAN	K	4	5	11,11,12	0.67	0	15,15,17	1.31	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	K	5	5	10,10,11	0.75	0	14,14,16	1.01	0
6	NAG	L	1	6,1	14,14,15	0.78	0	17,19,21	1.20	1 (5%)
6	NAG	L	2	6	14,14,15	0.72	0	17,19,21	0.77	0
6	BMA	L	3	6	11,11,12	0.84	0	15,15,17	1.60	2 (13%)
6	MAN	L	4	6	11,11,12	0.66	0	15,15,17	1.33	1 (6%)
7	NAG	M	1	2,7	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
7	NAG	M	2	7	14,14,15	0.78	1 (7%)	17,19,21	1.38	2 (11%)
7	NAG	N	1	7,1	14,14,15	0.77	0	17,19,21	1.04	0
7	NAG	N	2	7	14,14,15	0.71	0	17,19,21	0.79	0
8	NAG	O	1	2,8	14,14,15	0.72	0	17,19,21	0.83	0
8	NAG	O	2	8	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
8	BMA	O	3	8	11,11,12	0.82	0	15,15,17	1.79	1 (6%)
8	MAN	O	4	8	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
8	FUC	O	5	8	10,10,11	0.73	0	14,14,16	1.07	1 (7%)
9	A2G	P	1	9,3	13,13,15	0.81	0	16,18,21	0.87	0
9	GAL	P	2	9	11,11,12	0.74	0	15,15,17	1.06	1 (6%)
9	SIA	P	3	9	20,20,21	1.60	2 (10%)	21,28,31	1.58	3 (14%)
9	NAG	P	4	9	15,15,15	0.55	0	21,21,21	0.64	0
9	A2G	Q	1	9,3	13,13,15	0.82	0	16,18,21	0.73	0
9	GAL	Q	2	9	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
9	SIA	Q	3	9	20,20,21	1.70	2 (10%)	21,28,31	1.67	3 (14%)
9	NAG	Q	4	9	15,15,15	0.56	0	21,21,21	0.60	0
9	A2G	R	1	9,3	13,13,15	0.82	0	16,18,21	0.70	0
9	GAL	R	2	9	11,11,12	0.67	0	15,15,17	1.09	1 (6%)
9	SIA	R	3	9	20,20,21	1.69	3 (15%)	21,28,31	1.65	3 (14%)
9	NAG	R	4	9	15,15,15	0.57	0	21,21,21	0.62	0
9	A2G	S	1	9,3	13,13,15	0.81	0	16,18,21	0.81	0
9	GAL	S	2	9	11,11,12	0.66	0	15,15,17	1.07	0
9	SIA	S	3	9	20,20,21	1.71	1 (5%)	21,28,31	1.66	4 (19%)
9	NAG	S	4	9	15,15,15	0.56	0	21,21,21	0.67	0

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
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	FUC	K	5	5	-	-	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
7	NAG	M	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	4/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
8	NAG	O	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	BMA	O	3	8	-	1/2/19/22	0/1/1/1
8	MAN	O	4	8	-	0/2/19/22	0/1/1/1
8	FUC	O	5	8	-	-	0/1/1/1
9	A2G	P	1	9,3	-	0/4/21/26	0/1/1/1
9	GAL	P	2	9	-	0/2/19/22	0/1/1/1
9	SIA	P	3	9	-	1/18/34/38	0/1/1/1
9	NAG	P	4	9	-	0/6/26/26	0/1/1/1
9	A2G	Q	1	9,3	-	0/4/21/26	0/1/1/1
9	GAL	Q	2	9	-	0/2/19/22	0/1/1/1
9	SIA	Q	3	9	-	3/18/34/38	0/1/1/1
9	NAG	Q	4	9	-	0/6/26/26	0/1/1/1
9	A2G	R	1	9,3	-	0/4/21/26	0/1/1/1
9	GAL	R	2	9	-	0/2/19/22	0/1/1/1
9	SIA	R	3	9	-	5/18/34/38	0/1/1/1
9	NAG	R	4	9	-	0/6/26/26	0/1/1/1
9	A2G	S	1	9,3	-	0/4/21/26	0/1/1/1
9	GAL	S	2	9	-	0/2/19/22	0/1/1/1
9	SIA	S	3	9	-	5/18/34/38	0/1/1/1
9	NAG	S	4	9	-	0/6/26/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	S	3	SIA	C2-C1	6.19	1.59	1.52
9	Q	3	SIA	C2-C1	6.01	1.59	1.52
9	R	3	SIA	C2-C1	5.95	1.59	1.52
9	P	3	SIA	C2-C1	5.72	1.59	1.52
7	M	2	NAG	C1-C2	2.10	1.55	1.52
9	P	3	SIA	O6-C2	2.10	1.47	1.43
9	R	3	SIA	C7-C6	2.08	1.55	1.52
9	Q	3	SIA	C6-C5	2.03	1.56	1.53
9	R	3	SIA	C6-C5	2.00	1.56	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	3	BMA	C1-O5-C5	5.71	119.84	112.19
5	K	3	BMA	C1-O5-C5	5.17	119.12	112.19
9	S	3	SIA	O1A-C1-C2	-4.64	112.83	122.85
9	R	3	SIA	O1A-C1-C2	-4.62	112.87	122.85
6	L	3	BMA	C1-O5-C5	4.52	118.24	112.19
9	Q	3	SIA	O1A-C1-C2	-4.43	113.27	122.85
4	J	3	BMA	C1-O5-C5	4.43	118.12	112.19
4	J	4	MAN	C1-O5-C5	4.22	117.84	112.19
5	K	4	MAN	C1-O5-C5	4.17	117.78	112.19
6	L	4	MAN	C1-O5-C5	4.10	117.68	112.19
9	P	3	SIA	O1A-C1-C2	-4.09	114.01	122.85
7	M	2	NAG	C1-O5-C5	3.80	117.27	112.19
9	Q	3	SIA	O6-C2-C3	-3.29	106.13	110.56
9	P	3	SIA	O6-C2-C3	-3.27	106.16	110.56
4	J	5	MAN	C1-O5-C5	3.19	116.46	112.19
9	R	3	SIA	O6-C2-C3	-3.11	106.38	110.56
9	S	3	SIA	O6-C2-C3	-3.08	106.42	110.56
8	O	4	MAN	C1-O5-C5	3.05	116.27	112.19
9	P	2	GAL	O3-C3-C2	-3.03	103.88	110.05
4	J	2	NAG	O4-C4-C3	-2.79	103.79	110.38
7	M	1	NAG	O5-C1-C2	-2.75	107.03	111.29
8	O	2	NAG	O5-C1-C2	-2.69	107.13	111.29
7	M	2	NAG	C2-N2-C7	2.49	126.24	122.90
6	L	1	NAG	O4-C4-C3	-2.34	104.85	110.38
9	R	3	SIA	O1B-C1-O1A	2.30	129.29	124.08
9	Q	3	SIA	O1B-C1-O1A	2.24	129.16	124.08
8	O	5	FUC	C1-O5-C5	2.22	118.20	112.97
9	S	3	SIA	O1B-C1-O1A	2.21	129.10	124.08
9	Q	2	GAL	C1-O5-C5	2.20	115.14	112.19
4	J	1	NAG	C1-O5-C5	2.18	115.11	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	2	GAL	C1-O5-C5	2.17	115.10	112.19
9	P	3	SIA	O1B-C1-O1A	2.17	129.00	124.08
5	K	1	NAG	C1-O5-C5	2.13	115.04	112.19
6	L	3	BMA	O3-C3-C2	-2.07	105.83	110.05
9	S	3	SIA	O1B-C1-C2	2.06	118.06	112.71
5	K	3	BMA	O3-C3-C2	-2.00	105.97	110.05

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Q	3	SIA	O8-C8-C9-O9
6	L	2	NAG	O5-C5-C6-O6
8	O	2	NAG	O5-C5-C6-O6
8	O	2	NAG	C4-C5-C6-O6
9	R	3	SIA	C6-C7-C8-O8
9	S	3	SIA	C6-C7-C8-O8
6	L	2	NAG	C4-C5-C6-O6
9	Q	3	SIA	C7-C8-C9-O9
6	L	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
9	R	3	SIA	O7-C7-C8-O8
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2
6	L	3	BMA	O5-C5-C6-O6
9	R	3	SIA	O7-C7-C8-C9
9	S	3	SIA	O7-C7-C8-C9
9	R	3	SIA	C6-C7-C8-C9
9	S	3	SIA	C6-C7-C8-C9
9	S	3	SIA	O7-C7-C8-O8
7	M	2	NAG	C4-C5-C6-O6
8	O	3	BMA	O5-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
9	R	3	SIA	O1A-C1-C2-O6
9	S	3	SIA	O1A-C1-C2-O6
4	J	5	MAN	C4-C5-C6-O6
5	K	2	NAG	C1-C2-N2-C7
4	J	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

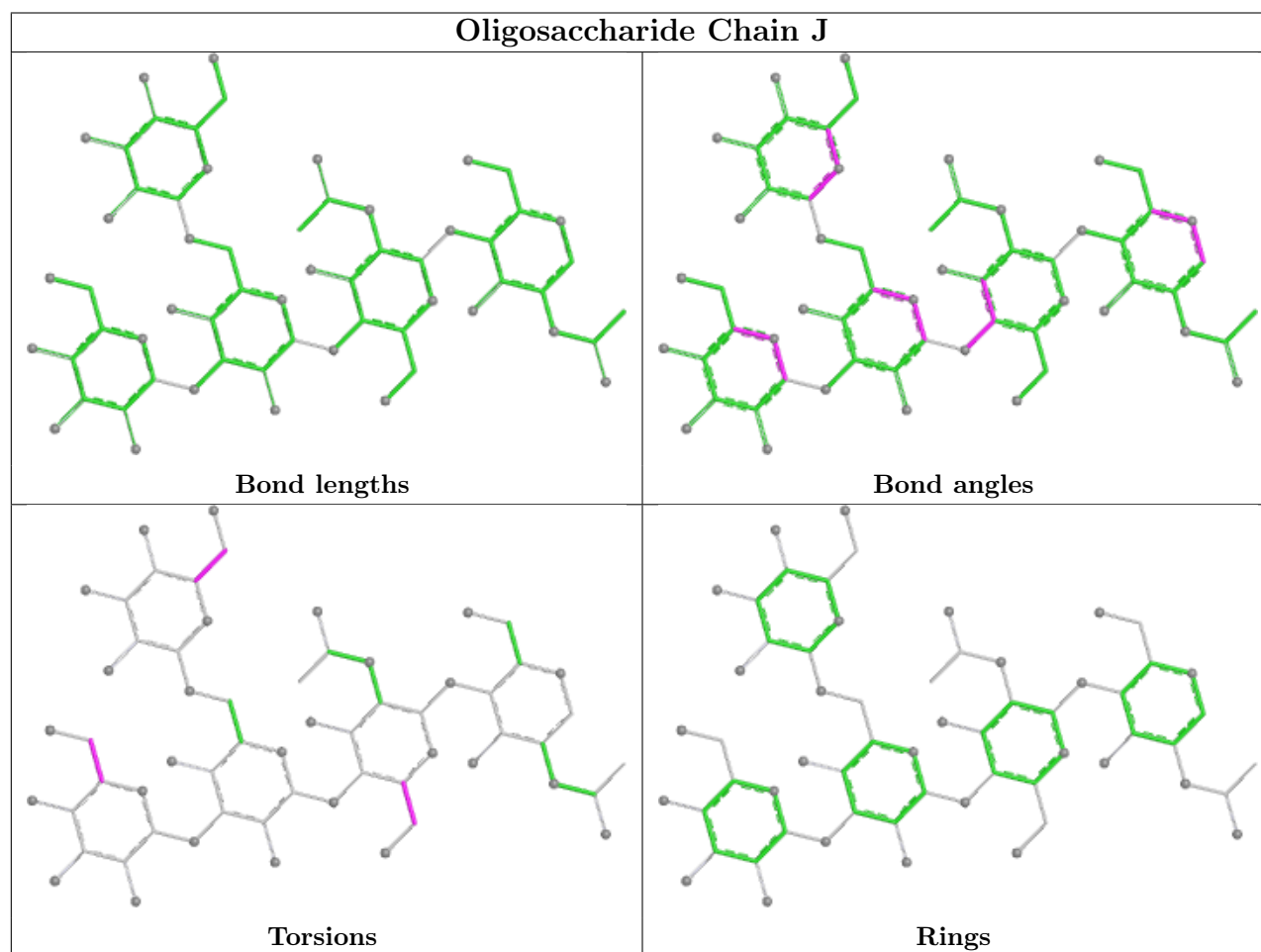
Mol	Chain	Res	Type	Atoms
9	P	3	SIA	C6-C7-C8-O8
9	Q	3	SIA	C6-C7-C8-O8

There are no ring outliers.

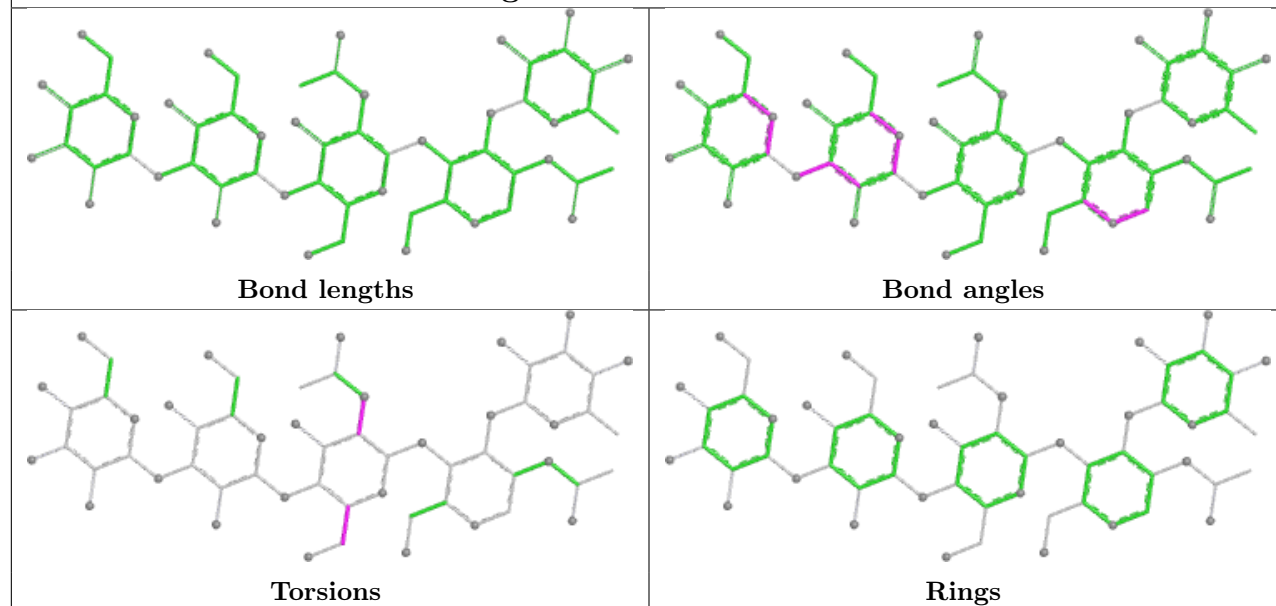
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1	NAG	2	0
8	O	2	NAG	1	0
8	O	5	FUC	1	0
7	M	2	NAG	1	0
8	O	1	NAG	1	0

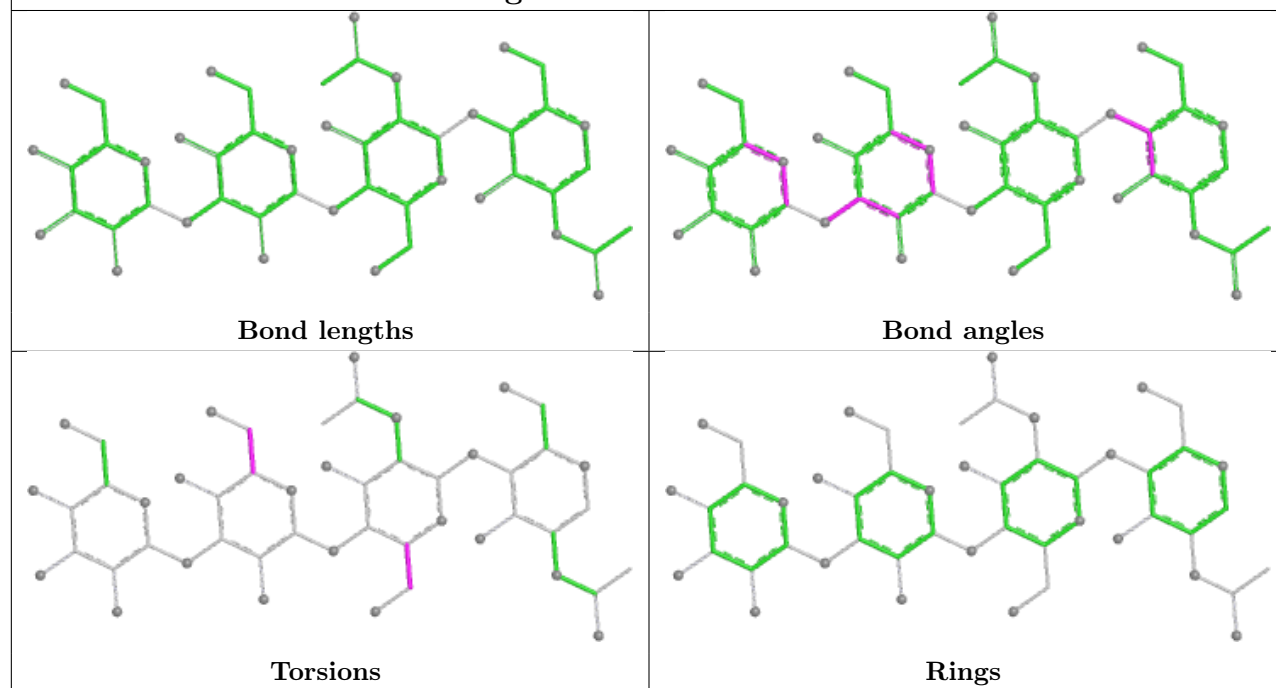
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

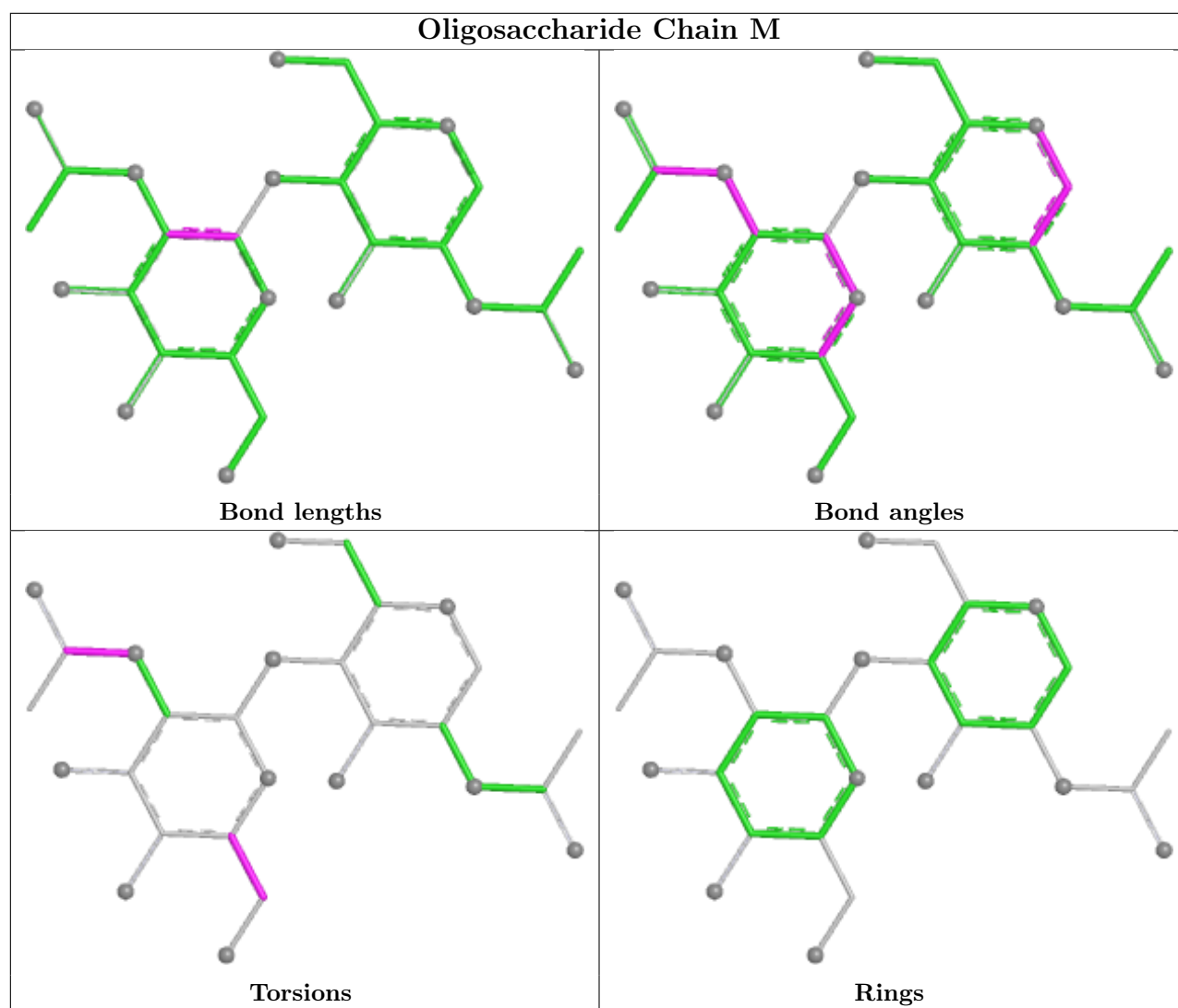


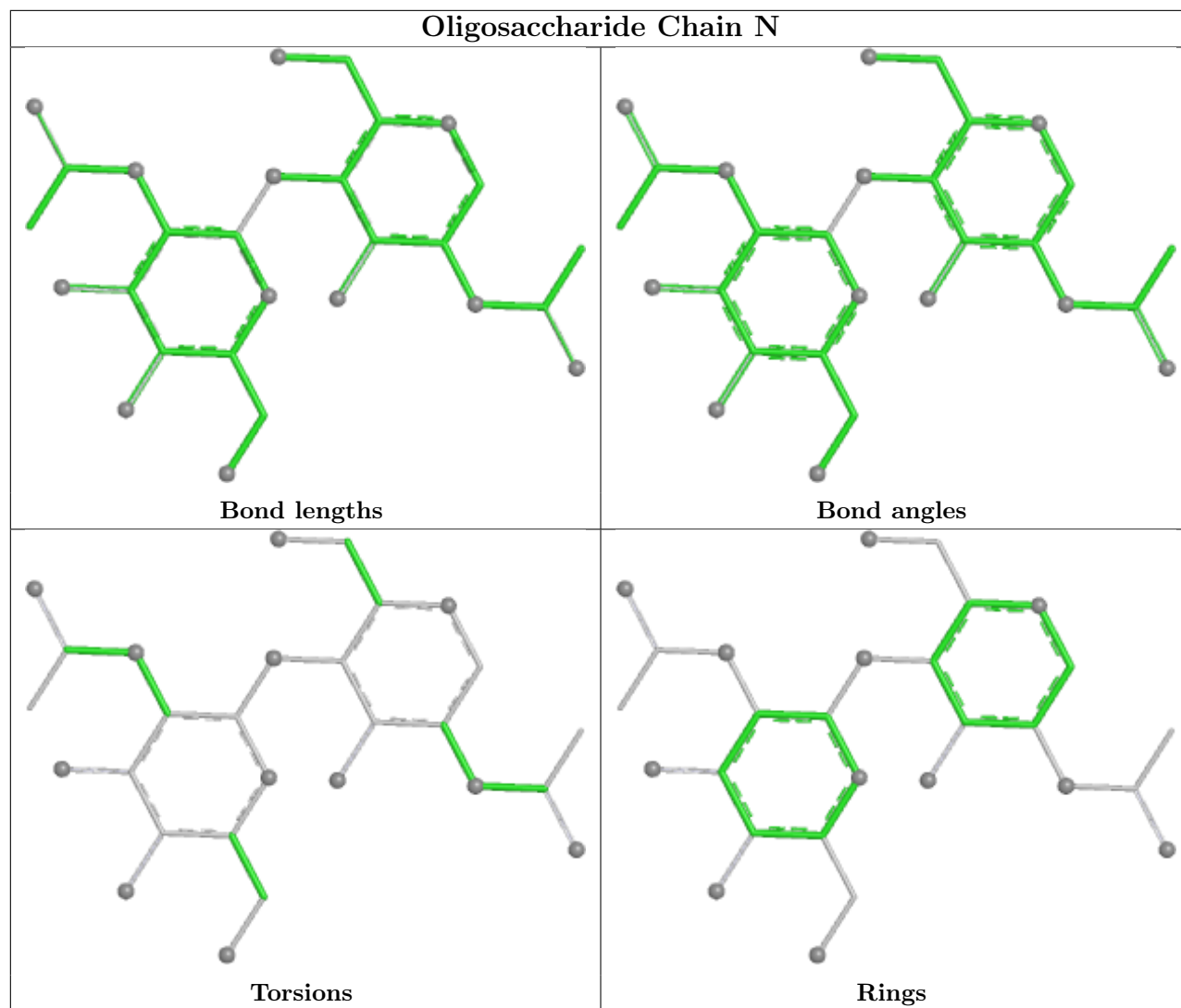
Oligosaccharide Chain K



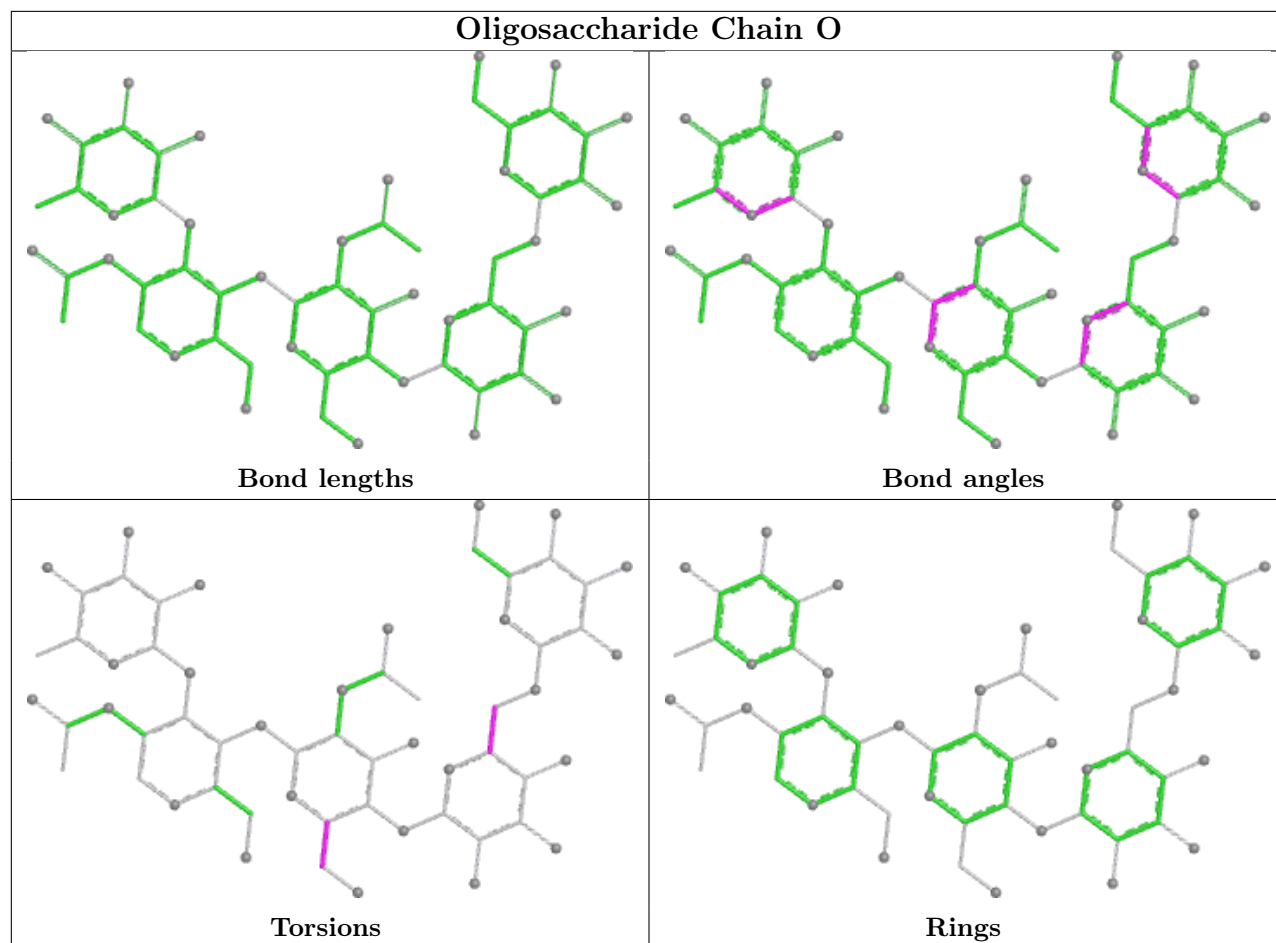
Oligosaccharide Chain L



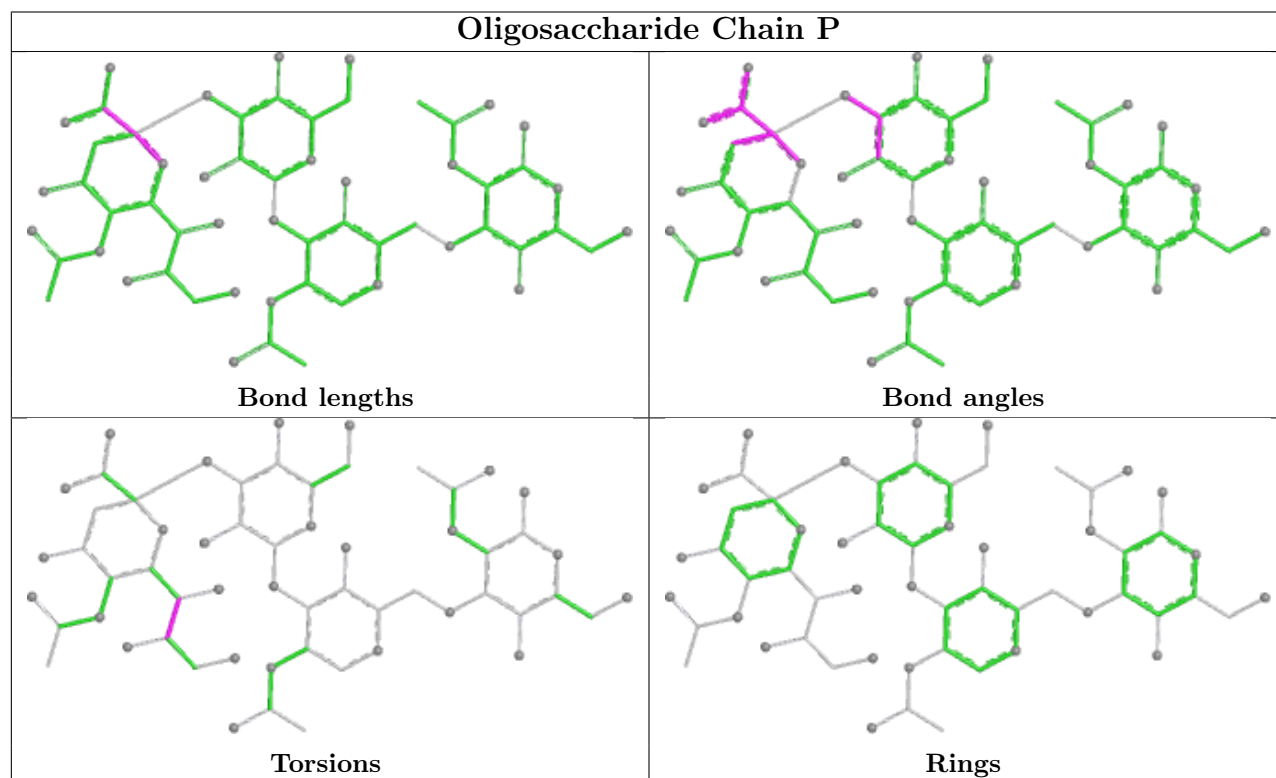




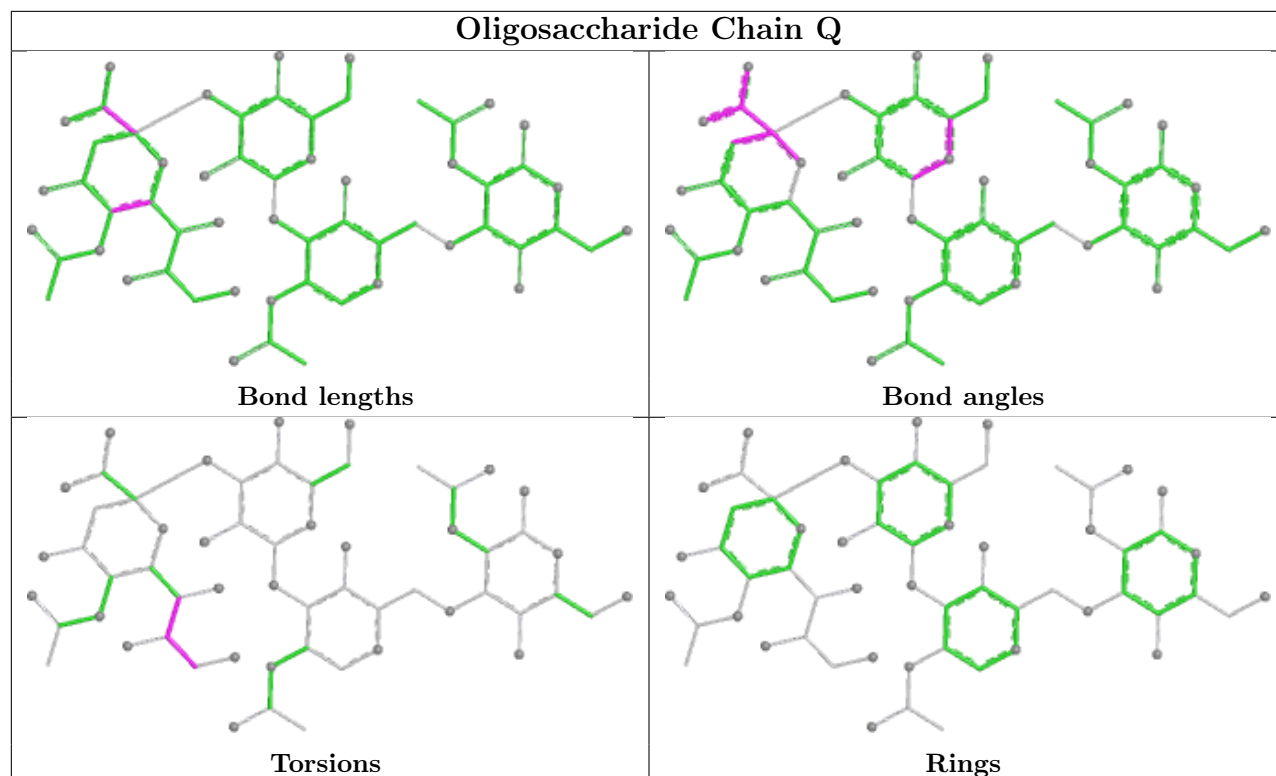
Oligosaccharide Chain O



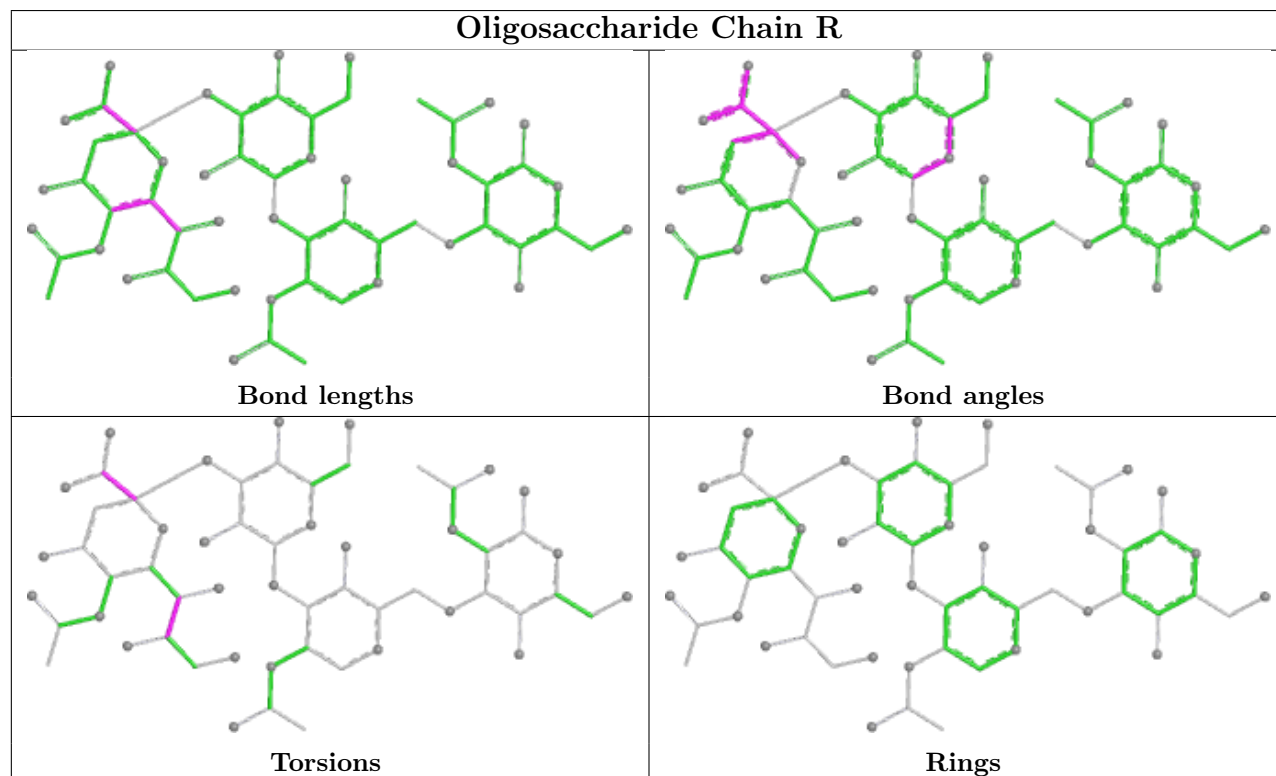
Oligosaccharide Chain P

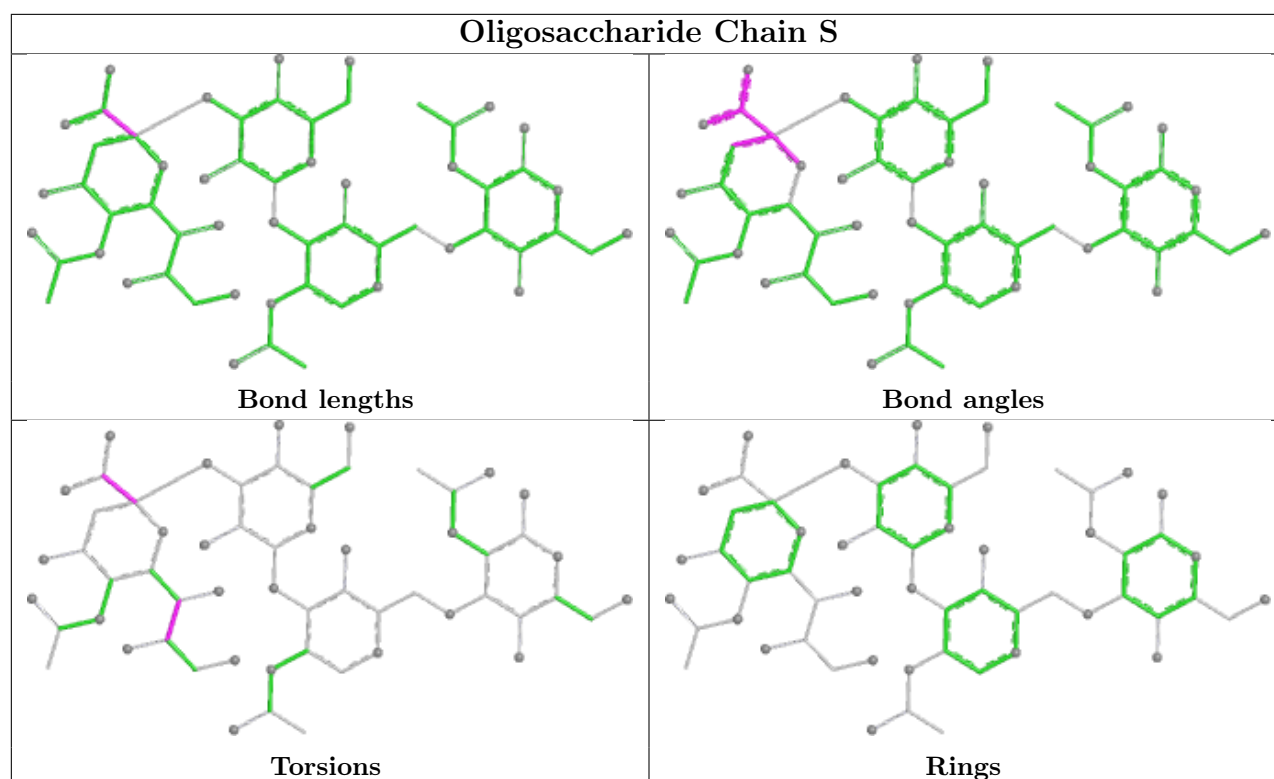


Oligosaccharide Chain Q



Oligosaccharide Chain R





5.6 Ligand geometry [i](#)

32 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	$\# Z > 2$
12	SO4	A	608	-	4,4,4	0.66	0	6,6,6	0.09	0
10	NAG	C	602	1	14,14,15	0.71	0	17,19,21	0.92	0
10	NAG	A	603	1	14,14,15	0.69	0	17,19,21	0.88	0
12	SO4	C	605	-	4,4,4	0.71	0	6,6,6	0.14	0
12	SO4	E	607	-	4,4,4	0.71	0	6,6,6	0.11	0
12	SO4	E	608	-	4,4,4	0.68	0	6,6,6	0.08	0
11	GOL	E	602	-	5,5,5	0.34	0	5,5,5	0.42	0
10	NAG	A	601	1	14,14,15	0.68	0	17,19,21	0.90	0
12	SO4	A	605	-	4,4,4	0.67	0	6,6,6	0.07	0
10	NAG	E	601	1	14,14,15	0.68	0	17,19,21	0.96	1 (5%)
12	SO4	C	608	-	4,4,4	0.73	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	SO4	E	609	-	4,4,4	0.68	0	6,6,6	0.07	0
12	SO4	A	606	-	4,4,4	0.66	0	6,6,6	0.10	0
12	SO4	C	606	-	4,4,4	0.73	0	6,6,6	0.15	0
12	SO4	B	201	-	4,4,4	0.67	0	6,6,6	0.10	0
12	SO4	F	201	-	4,4,4	0.66	0	6,6,6	0.10	0
12	SO4	C	604	-	4,4,4	0.67	0	6,6,6	0.09	0
12	SO4	E	604	-	4,4,4	0.66	0	6,6,6	0.08	0
10	NAG	A	602	1	14,14,15	0.72	0	17,19,21	2.33	3 (17%)
12	SO4	E	605	-	4,4,4	0.67	0	6,6,6	0.09	0
12	SO4	C	609	-	4,4,4	0.66	0	6,6,6	0.10	0
11	GOL	A	604	-	5,5,5	0.32	0	5,5,5	0.45	0
12	SO4	B	202	-	4,4,4	0.67	0	6,6,6	0.08	0
12	SO4	C	607	-	4,4,4	0.67	0	6,6,6	0.07	0
12	SO4	C	610	-	4,4,4	0.68	0	6,6,6	0.16	0
10	NAG	C	601	1	14,14,15	0.66	0	17,19,21	0.92	0
12	SO4	E	603	-	4,4,4	0.66	0	6,6,6	0.07	0
12	SO4	E	606	-	4,4,4	0.67	0	6,6,6	0.11	0
11	GOL	C	603	-	5,5,5	0.32	0	5,5,5	0.44	0
12	SO4	A	609	-	4,4,4	0.67	0	6,6,6	0.08	0
12	SO4	A	610	-	4,4,4	0.67	0	6,6,6	0.14	0
12	SO4	A	607	-	4,4,4	0.67	0	6,6,6	0.11	0

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
10	NAG	E	601	1	-	0/6/23/26	0/1/1/1
10	NAG	C	602	1	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	3/6/23/26	0/1/1/1
10	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	GOL	A	604	-	-	0/4/4/4	-
11	GOL	E	602	-	-	0/4/4/4	-
11	GOL	C	603	-	-	0/4/4/4	-
10	NAG	C	601	1	-	0/6/23/26	0/1/1/1
10	NAG	A	602	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	602	NAG	C2-N2-C7	8.21	133.90	122.90
10	A	602	NAG	C8-C7-N2	2.64	120.50	116.12
10	E	601	NAG	C1-O5-C5	2.59	115.65	112.19
10	A	602	NAG	C1-C2-N2	2.26	114.00	110.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	601	NAG	O5-C5-C6-O6
10	A	601	NAG	C4-C5-C6-O6
10	A	602	NAG	C8-C7-N2-C2
10	A	602	NAG	O7-C7-N2-C2
10	A	603	NAG	C8-C7-N2-C2
10	A	603	NAG	O7-C7-N2-C2
10	C	602	NAG	C4-C5-C6-O6
10	C	602	NAG	O5-C5-C6-O6
10	A	603	NAG	C4-C5-C6-O6
10	A	602	NAG	C1-C2-N2-C7
10	A	602	NAG	C3-C2-N2-C7

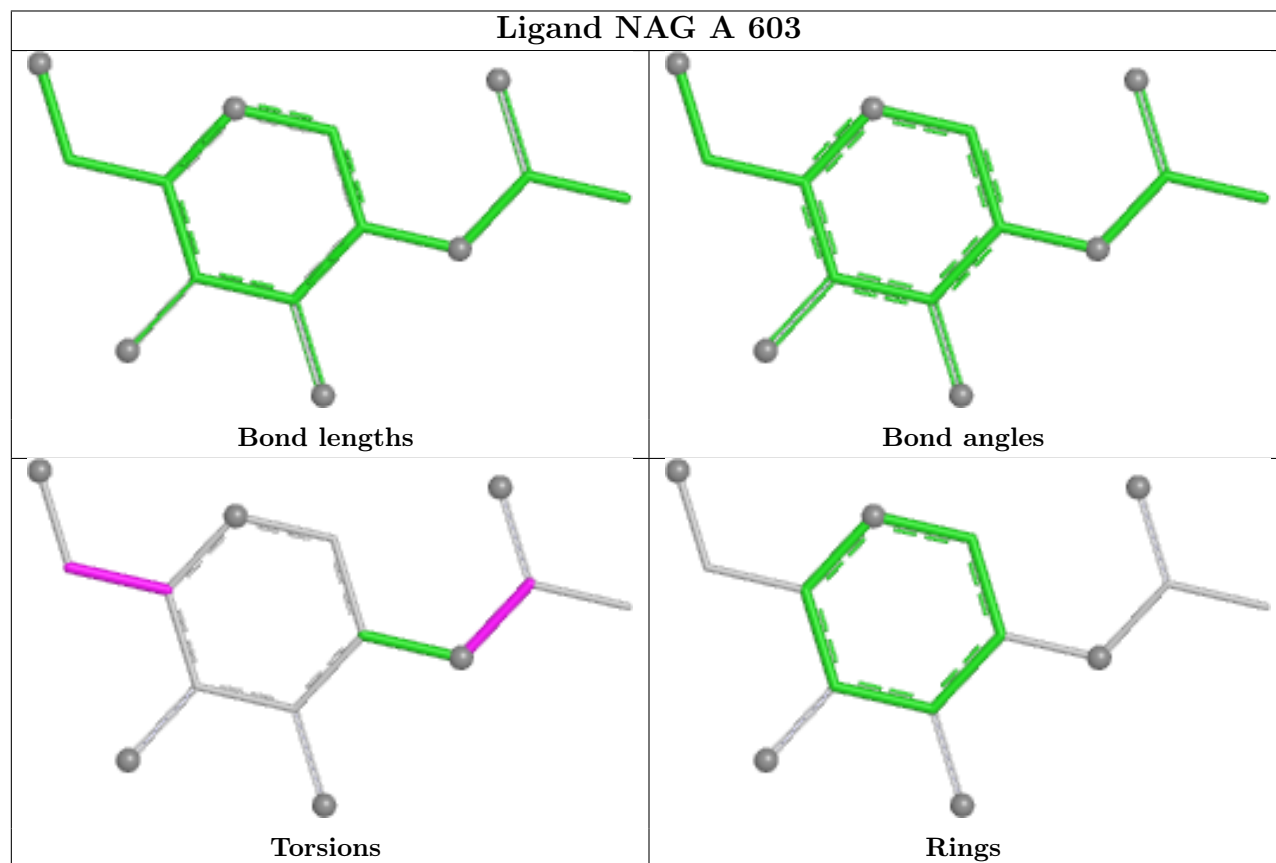
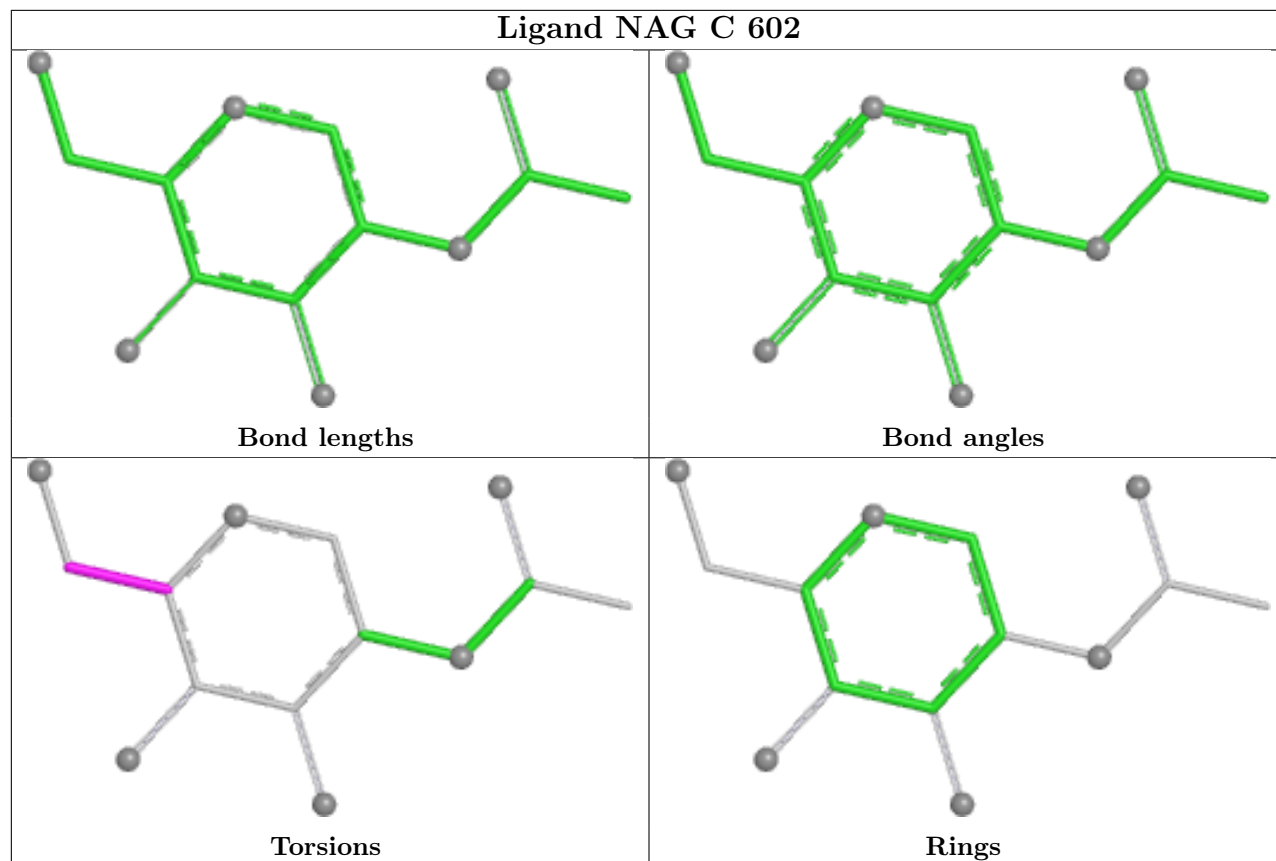
There are no ring outliers.

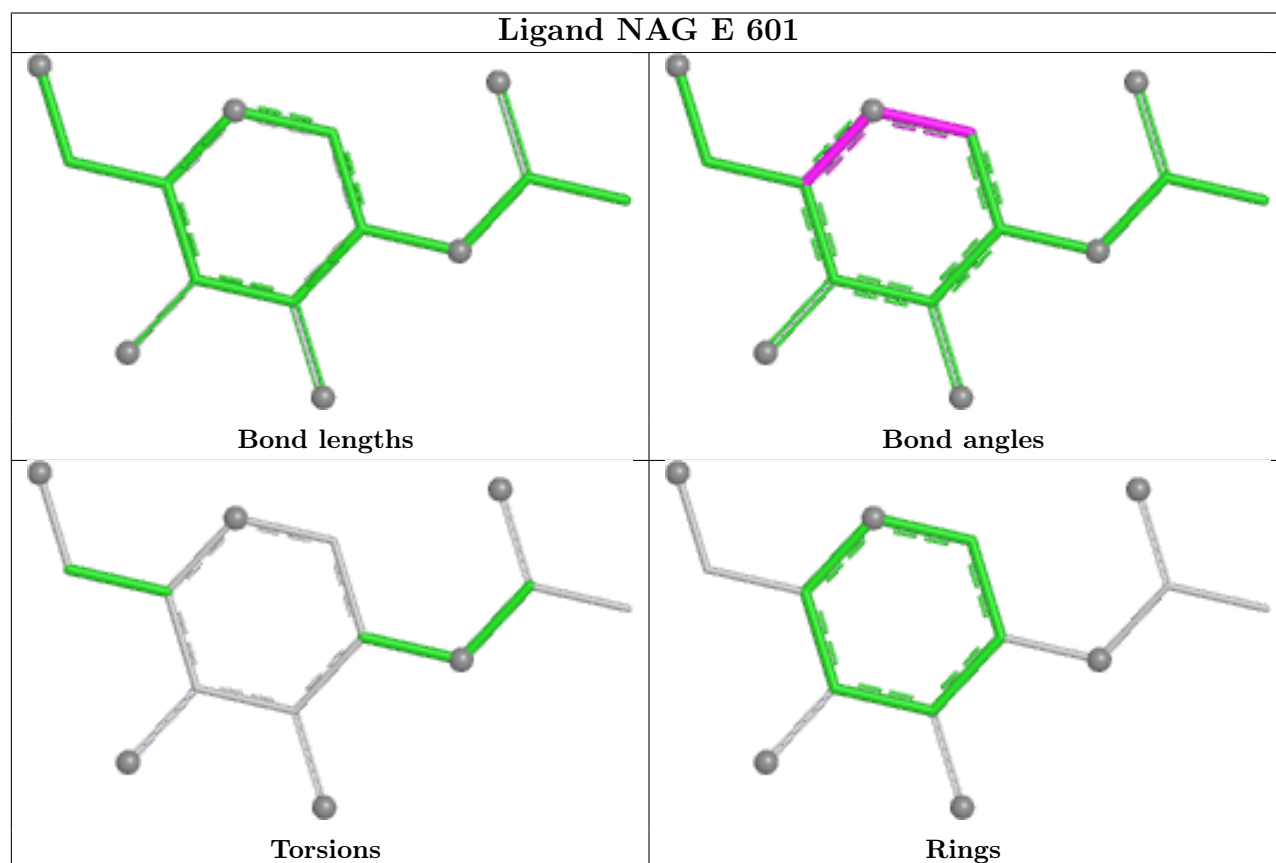
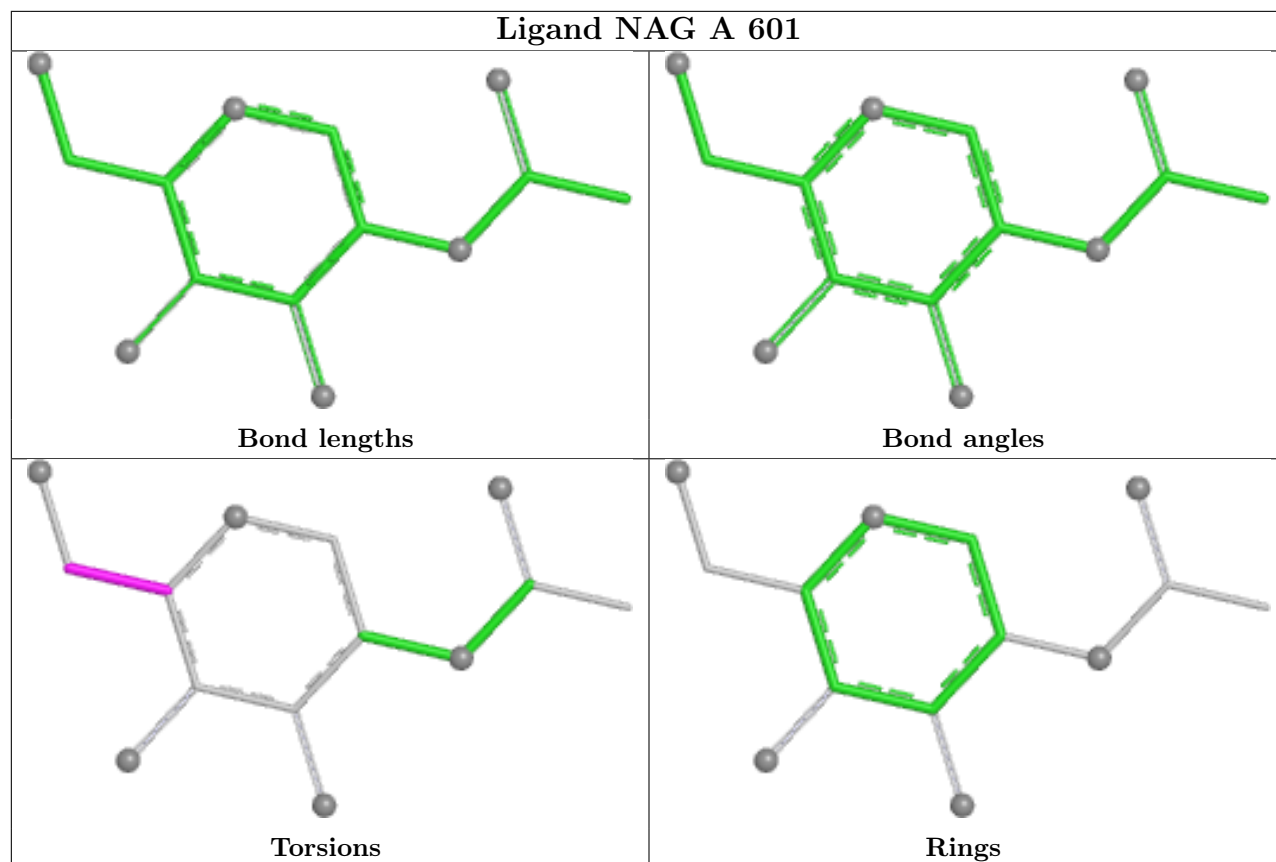
6 monomers are involved in 7 short contacts:

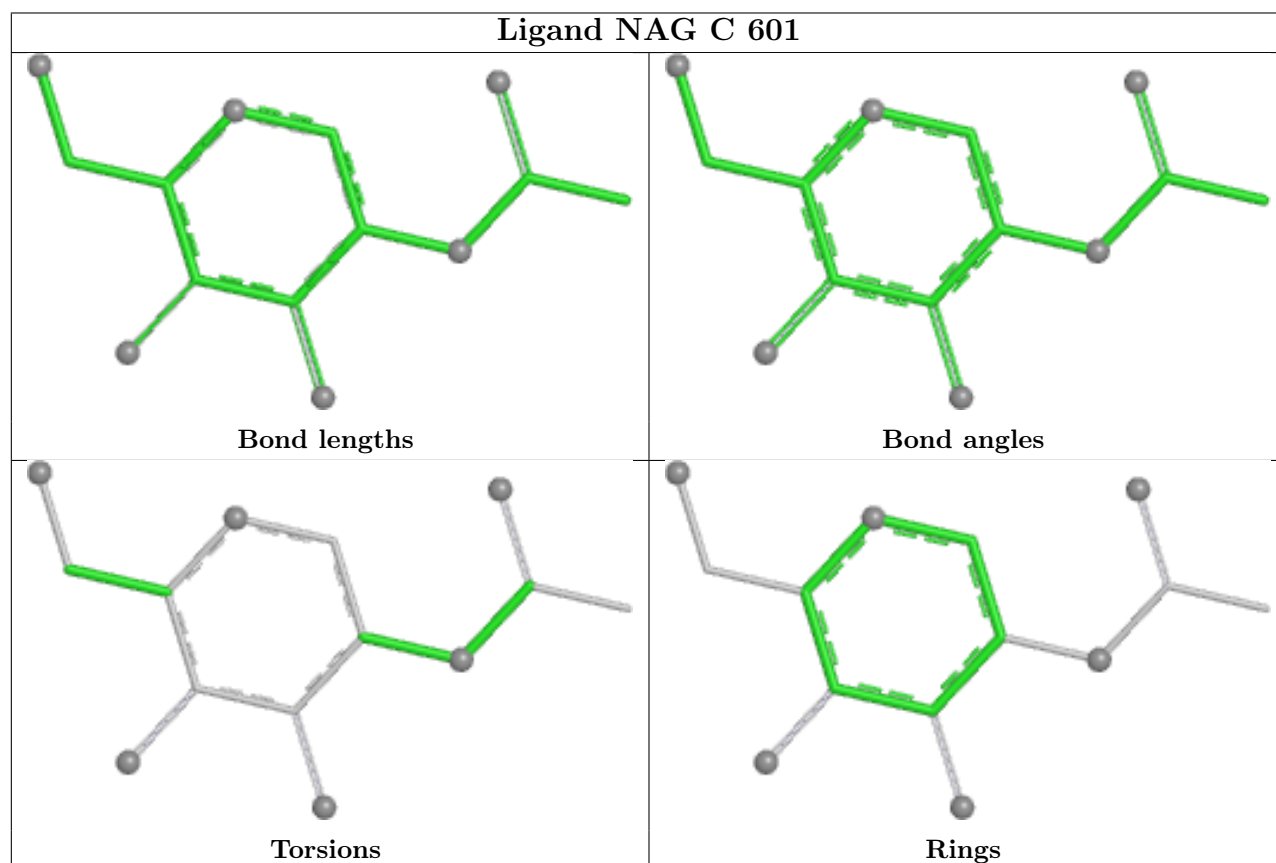
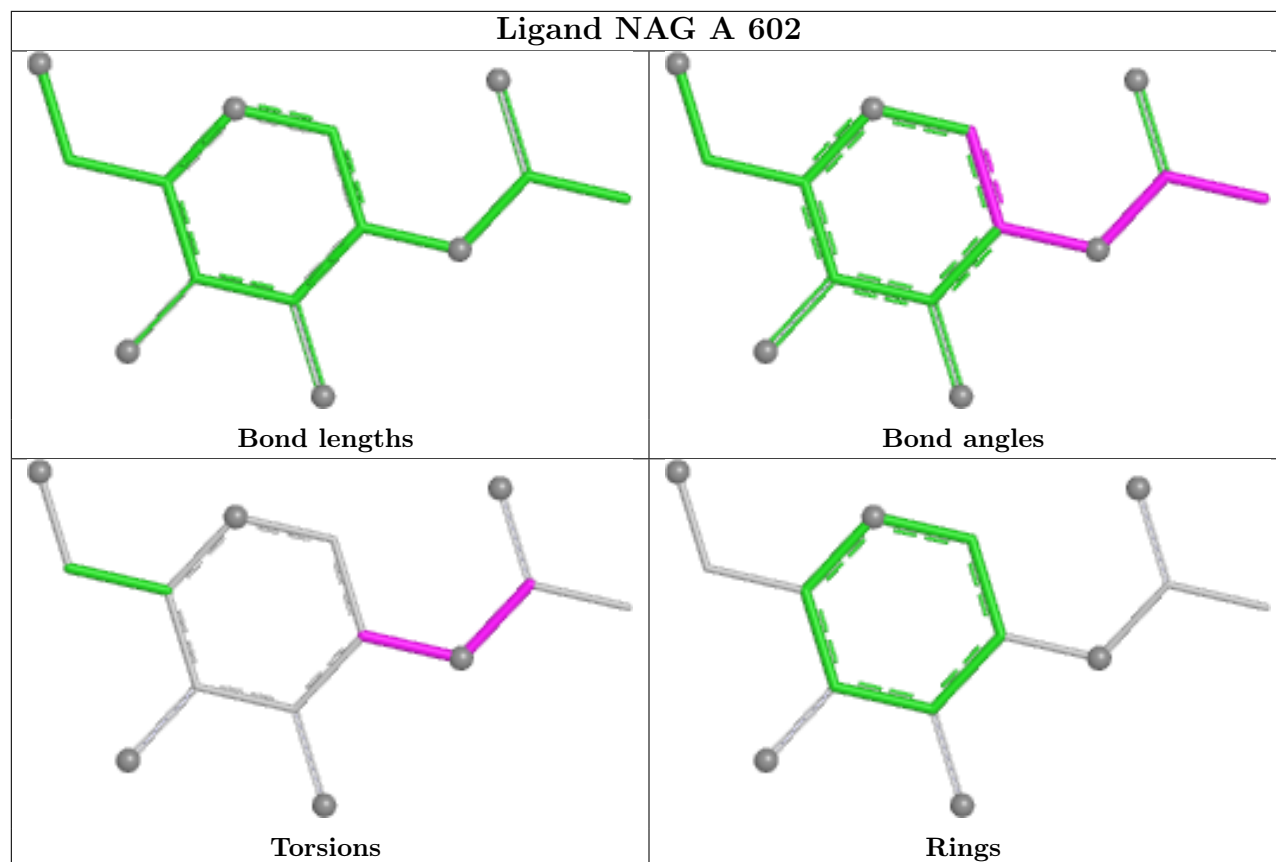
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	608	SO4	1	0
12	C	605	SO4	1	0
12	A	605	SO4	2	0
12	C	608	SO4	1	0
12	C	606	SO4	1	0
12	F	201	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	321/329 (97%)	0.10	19 (5%) 28 27	26, 41, 69, 150	0
1	C	324/329 (98%)	0.07	14 (4%) 40 39	24, 40, 68, 159	0
1	E	322/329 (97%)	-0.01	16 (4%) 34 34	26, 39, 64, 172	0
2	B	169/181 (93%)	0.32	11 (6%) 25 23	32, 48, 80, 138	0
2	D	169/181 (93%)	0.56	13 (7%) 19 18	32, 55, 84, 108	0
2	F	172/181 (95%)	0.13	9 (5%) 33 32	33, 46, 66, 97	0
3	G	5/5 (100%)	2.05	1 (20%) 3 2	51, 53, 59, 104	0
3	H	5/5 (100%)	3.40	4 (80%) 0 0	61, 64, 84, 108	0
3	I	5/5 (100%)	2.18	1 (20%) 3 2	59, 60, 70, 116	0
3	l	3/5 (60%)	6.04	3 (100%) 0 0	104, 104, 111, 115	0
All	All	1495/1550 (96%)	0.19	91 (6%) 27 26	24, 43, 74, 172	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	ALA	8.2
3	I	101	PHE	7.9
1	C	9	PRO	7.8
2	D	7	ALA	7.8
2	D	6	ILE	7.5
1	A	78	GLU	7.4
1	A	9	PRO	7.4
3	G	101	PHE	7.2
2	B	6	ILE	7.2
1	C	324	PRO	7.2
2	D	174	GLY	7.1
3	l	103	THR	6.9
3	l	104	ILE	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	174	GLY	6.6
3	H	101	PHE	6.4
1	E	323	SER	6.2
2	D	173	ILE	6.1
1	E	78	GLU	6.1
1	C	323	SER	6.0
1	A	80	ILE	5.7
1	E	80	ILE	5.6
1	E	77	ASP	5.5
1	C	79	PHE	5.4
1	C	290	SER	5.4
1	C	78	GLU	5.1
3	H	105	GLY	5.1
1	C	81	ARG	4.9
2	B	10	ILE	4.9
1	A	77	ASP	4.9
1	C	80	ILE	4.8
1	C	8	ASP	4.8
3	I	105	GLY	4.6
1	E	290	SER	4.4
1	E	8	ASP	4.4
2	D	155	GLY	4.4
1	C	289	ASN	4.2
1	A	323	SER	4.1
2	B	9	PHE	4.1
2	B	8	GLY	3.9
2	F	6	ILE	3.9
1	A	290	SER	3.8
1	E	289	ASN	3.8
1	A	289	ASN	3.7
1	E	277	CYS	3.6
1	A	173	ARG	3.5
2	D	8	GLY	3.5
2	D	171	GLU	3.4
2	B	11	GLU	3.4
2	F	8	GLY	3.3
1	C	277	CYS	3.3
2	B	106	ARG	3.3
1	E	81	ARG	3.1
1	A	277	CYS	3.1
2	F	10	ILE	3.1
2	F	19	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	11	GLU	3.0
1	A	291	SER	2.9
1	A	81	ARG	2.9
2	D	172	GLU	2.8
1	A	63	ASP	2.7
1	E	76	CYS	2.7
2	F	39	GLU	2.7
1	A	141	TYR	2.7
1	E	75	MET	2.7
1	E	222	GLN	2.6
2	B	38	LYS	2.6
1	A	82	VAL	2.5
1	C	291	SER	2.5
2	F	7	ALA	2.5
1	A	142	GLN	2.5
3	H	102	VAL	2.5
1	C	64	CYS	2.4
2	B	18	VAL	2.3
2	F	18	VAL	2.3
1	A	62	LYS	2.3
1	E	64	CYS	2.3
1	E	21	ASN	2.3
1	A	260	ILE	2.3
3	H	104	ILE	2.3
2	F	106	ARG	2.2
2	F	11	GLU	2.2
2	B	19	ASP	2.2
1	E	9	PRO	2.2
1	A	262	LYS	2.1
2	D	148	CYS	2.1
2	D	27	SER	2.1
1	A	21	ASN	2.1
1	E	82	VAL	2.1
2	D	121	LYS	2.1
1	C	77	ASP	2.0
2	D	38	LYS	2.0

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

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

6.3 Carbohydrates

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.

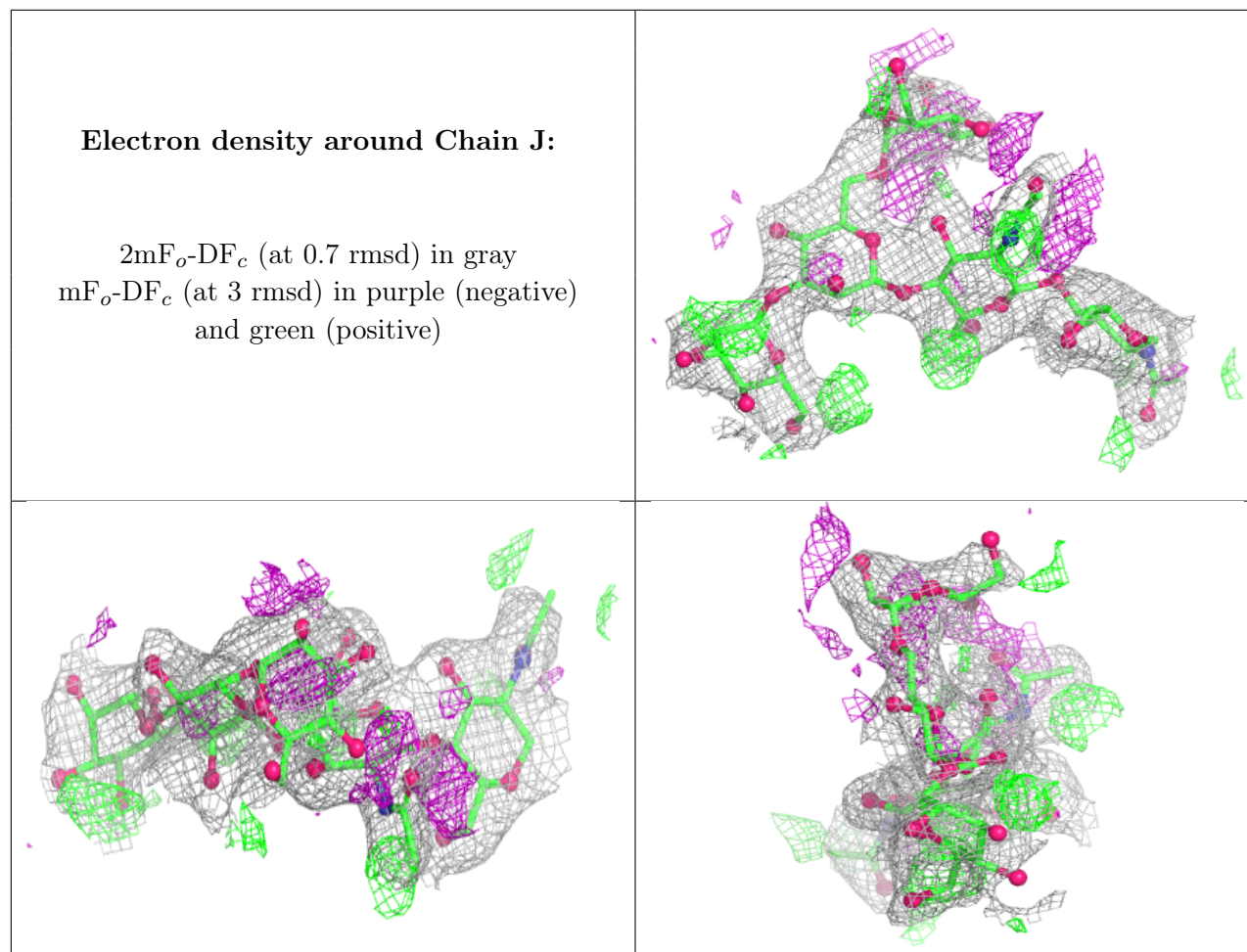
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	1	14/15	-	-	43,62,74,81	0
4	NAG	J	2	14/15	-	-	58,74,86,87	0
4	BMA	J	3	11/12	-	-	81,89,110,114	0
4	MAN	J	4	11/12	-	-	100,130,137,138	0
4	MAN	J	5	11/12	-	-	85,98,113,115	0
6	BMA	L	3	11/12	0.26	0.19	61,74,90,96	0
6	MAN	L	4	11/12	0.30	0.25	52,58,62,87	0
9	NAG	S	4	15/15	0.38	0.27	116,137,153,155	0
9	NAG	Q	4	15/15	0.41	0.27	96,137,142,145	0
5	FUC	K	5	10/11	-	-	74,104,107,107	0
9	SIA	S	3	20/21	0.48	0.26	138,154,170,172	0
9	SIA	R	3	20/21	0.55	0.27	148,170,181,184	0
5	MAN	K	4	11/12	0.57	0.25	144,178,184,184	0
7	NAG	N	2	14/15	0.61	0.22	72,99,113,122	0
9	NAG	R	4	15/15	0.62	0.24	121,142,151,156	0
8	NAG	O	2	14/15	0.73	0.16	56,76,91,100	0
9	GAL	S	2	11/12	0.74	0.16	97,130,138,139	0
7	NAG	N	1	14/15	0.75	0.22	45,70,87,95	0
9	GAL	R	2	11/12	0.77	0.18	96,106,127,143	0
6	NAG	L	2	14/15	0.77	0.19	46,59,68,70	0
8	BMA	O	3	11/12	-	-	123,135,152,157	0
8	MAN	O	4	11/12	-	-	161,164,172,175	0
8	FUC	O	5	10/11	-	-	95,101,107,114	0
9	A2G	P	1	13/15	-	-	70,81,103,114	0
9	GAL	P	2	11/12	-	-	32,43,51,53	0
9	SIA	P	3	20/21	-	-	28,36,43,49	0
9	NAG	P	4	15/15	-	-	123,154,161,163	0
5	NAG	K	2	14/15	0.78	0.18	99,113,132,145	0
5	BMA	K	3	11/12	0.80	0.17	152,159,169,174	0
6	NAG	L	1	14/15	0.82	0.16	46,55,77,83	0
9	A2G	S	1	13/15	0.86	0.16	64,82,92,92	0
9	A2G	Q	1	13/15	0.88	0.15	56,64,76,80	0
7	NAG	M	1	14/15	0.90	0.13	100,114,122,136	0
8	NAG	O	1	14/15	0.90	0.12	56,73,79,91	0
7	NAG	M	2	14/15	0.92	0.12	124,136,141,142	0
5	NAG	K	1	14/15	0.92	0.12	64,93,102,108	0
9	A2G	R	1	13/15	0.94	0.10	68,82,94,98	0

Continued on next page...

Continued from previous page...

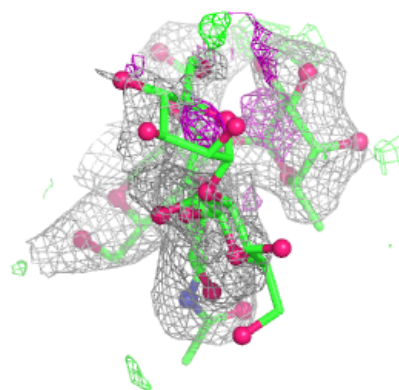
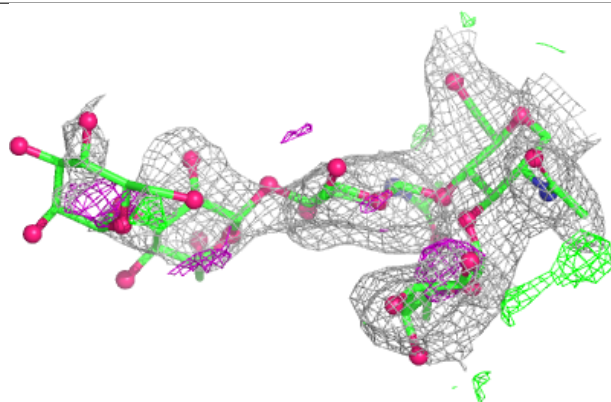
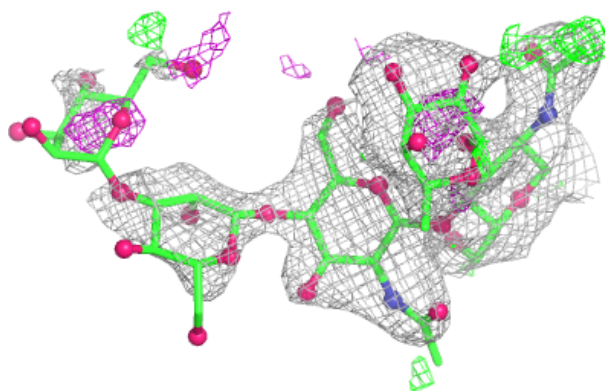
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SIA	Q	3	20/21	0.95	0.08	120,154,169,171	0
9	GAL	Q	2	11/12	0.97	0.06	78,94,115,125	0

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.

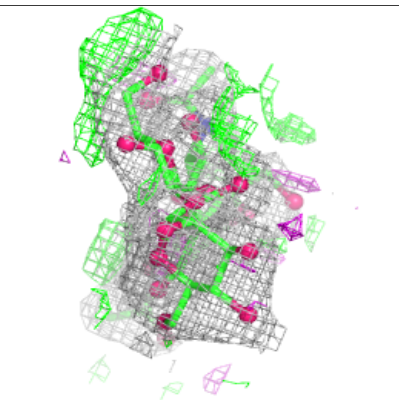
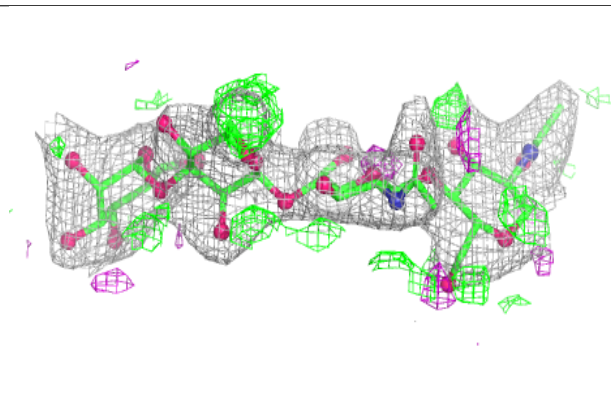
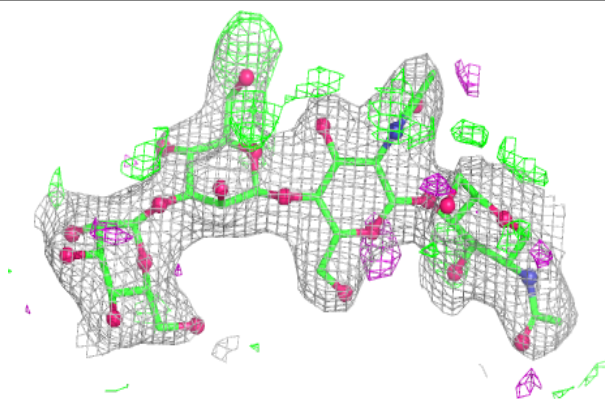


Electron density around Chain K:

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

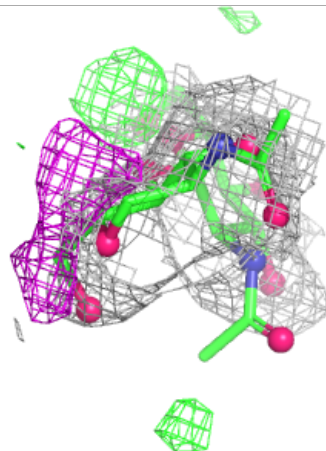
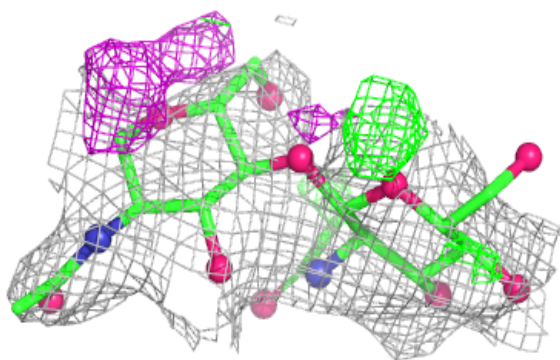
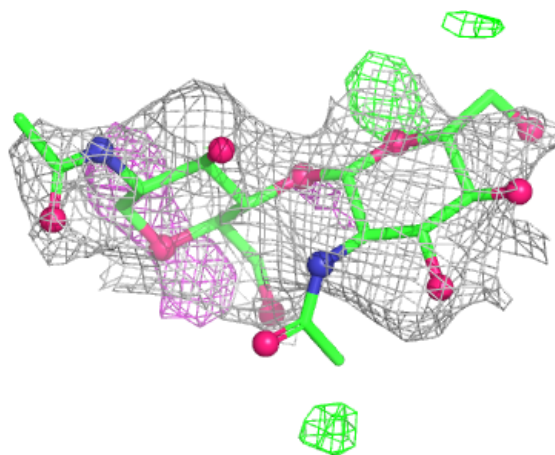
**Electron density around Chain L:**

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



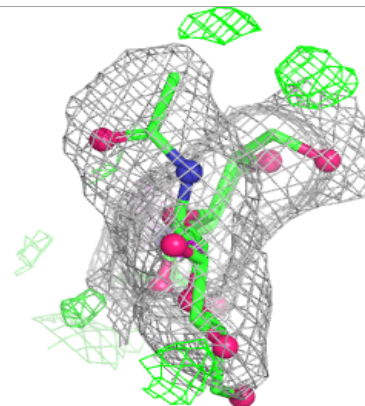
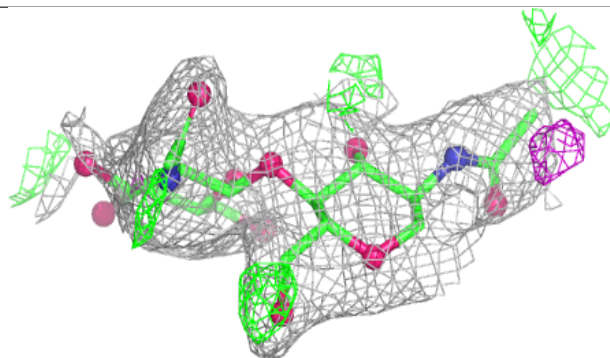
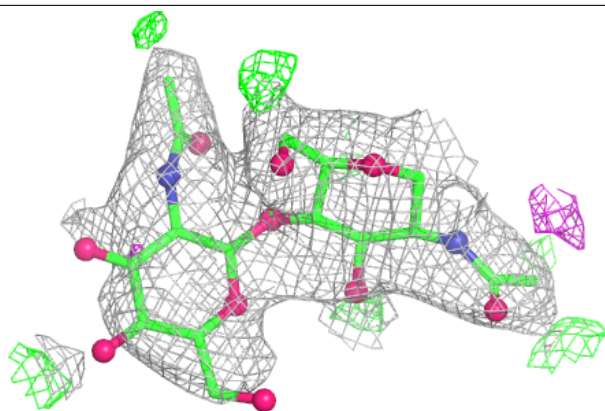
Electron density around Chain M:

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

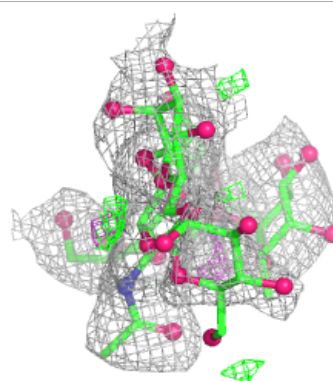
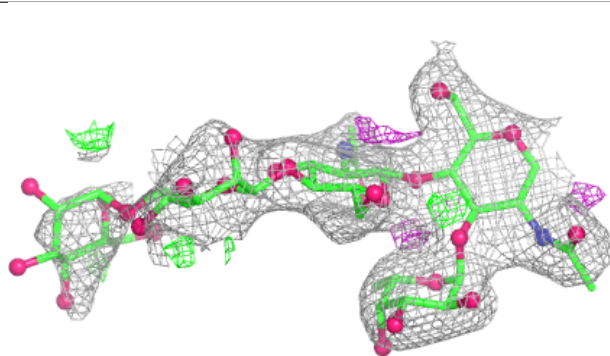
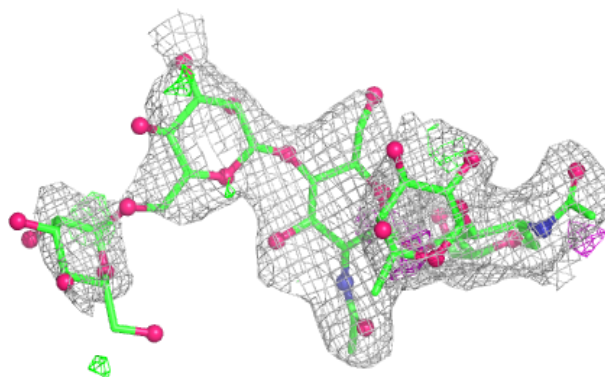


Electron density around Chain N:

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

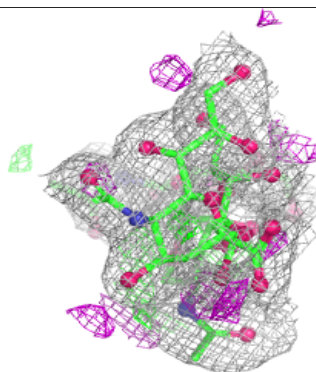
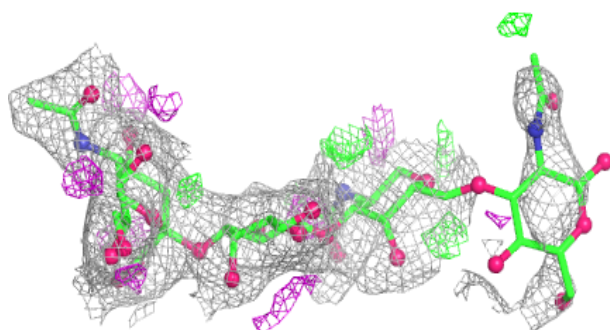
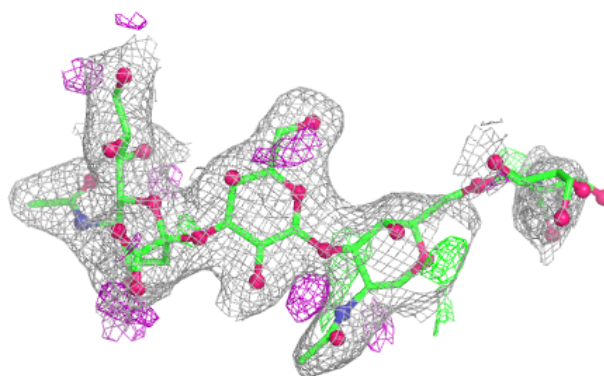
**Electron density around Chain O:**

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

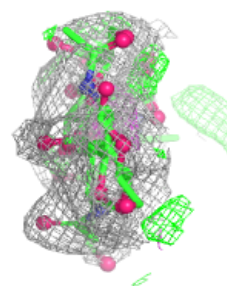
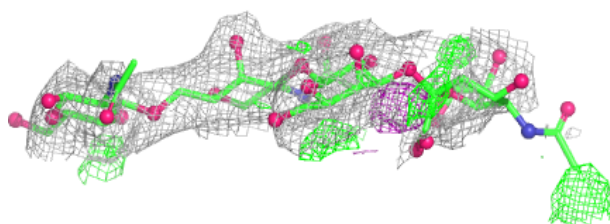
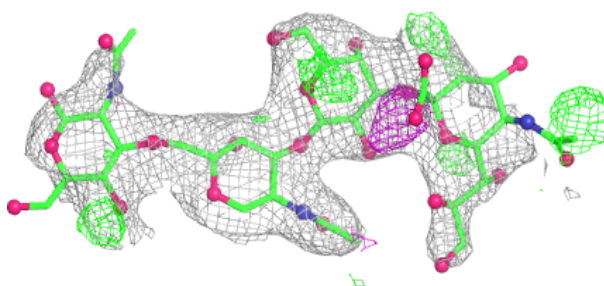


Electron density around Chain P:

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

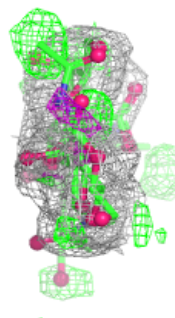
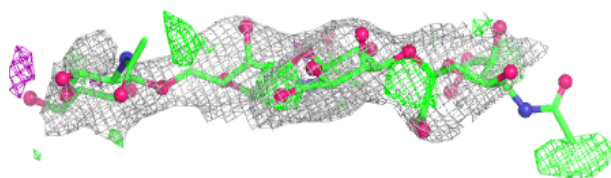
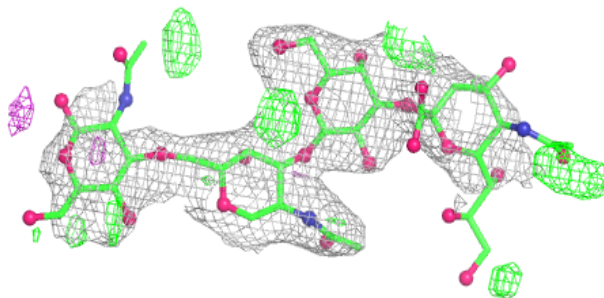
**Electron density around Chain Q:**

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

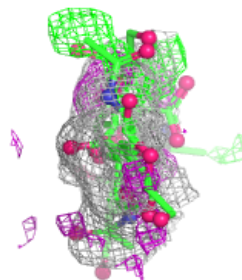
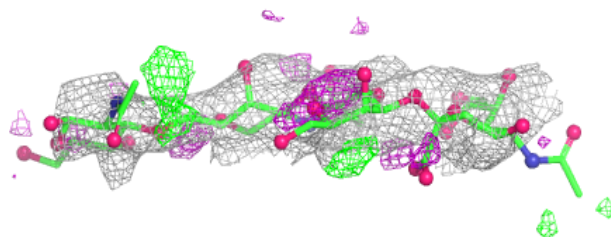
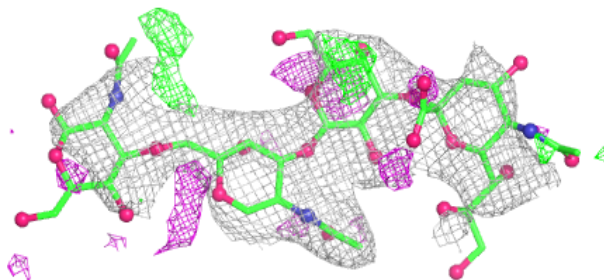


Electron density around Chain R:

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

**Electron density around Chain S:**

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



6.4 Ligands ⓘ

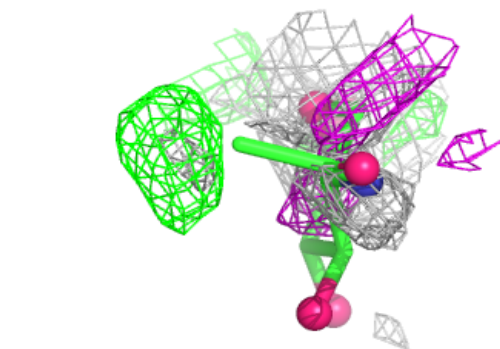
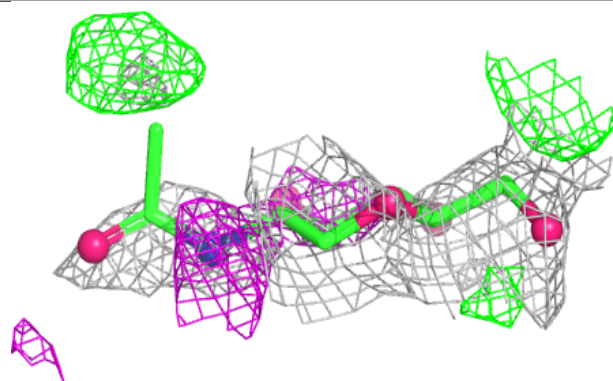
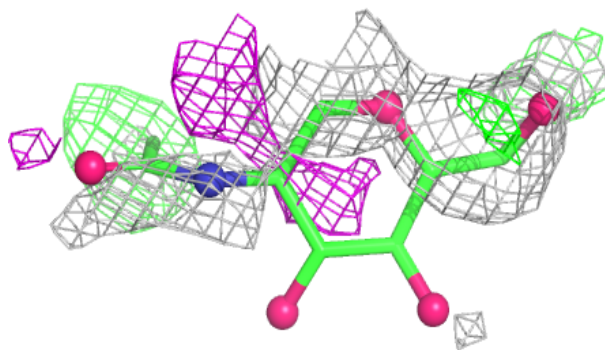
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	A	603	14/15	0.44	0.27	122,143,155,161	0
12	SO4	F	201	5/5	0.56	0.20	89,106,132,158	0
10	NAG	A	602	14/15	0.62	0.27	129,146,153,159	0
10	NAG	C	601	14/15	0.65	0.20	86,103,112,116	0
10	NAG	C	602	14/15	0.68	0.24	113,150,169,177	0
12	SO4	E	607	5/5	0.69	0.25	52,64,96,152	0
10	NAG	E	601	14/15	0.70	0.20	96,107,122,127	0
12	SO4	A	610	5/5	0.72	0.18	120,131,135,168	0
12	SO4	B	201	5/5	0.72	0.19	121,142,154,194	0
12	SO4	C	606	5/5	0.73	0.22	52,54,91,129	0
12	SO4	E	604	5/5	0.73	0.26	77,86,137,147	0
12	SO4	E	609	5/5	0.75	0.24	120,124,149,174	0
12	SO4	A	609	5/5	0.76	0.11	117,127,137,175	0
12	SO4	C	609	5/5	0.77	0.25	79,92,134,137	0
12	SO4	E	608	5/5	0.79	0.14	86,86,129,131	0
12	SO4	A	608	5/5	0.79	0.16	89,98,119,146	0
12	SO4	B	202	5/5	0.79	0.29	124,153,180,208	0
10	NAG	A	601	14/15	0.81	0.15	66,86,103,112	0
12	SO4	A	607	5/5	0.81	0.20	56,58,123,145	0
12	SO4	C	605	5/5	0.82	0.16	67,70,84,140	0
12	SO4	C	610	5/5	0.83	0.16	82,97,103,120	0
12	SO4	A	605	5/5	0.84	0.18	103,116,122,157	0
12	SO4	C	604	5/5	0.85	0.11	64,79,100,104	0
12	SO4	E	605	5/5	0.85	0.23	71,90,127,159	0
12	SO4	A	606	5/5	0.86	0.12	87,92,100,115	0
12	SO4	C	607	5/5	0.86	0.20	48,49,129,140	0
12	SO4	C	608	5/5	0.88	0.15	36,50,92,138	0
12	SO4	E	606	5/5	0.88	0.25	97,113,123,173	0
11	GOL	A	604	6/6	0.88	0.20	53,68,72,83	0
11	GOL	C	603	6/6	0.90	0.27	46,61,65,74	0
11	GOL	E	602	6/6	0.90	0.20	68,73,76,85	0
12	SO4	E	603	5/5	0.94	0.10	77,78,83,86	0

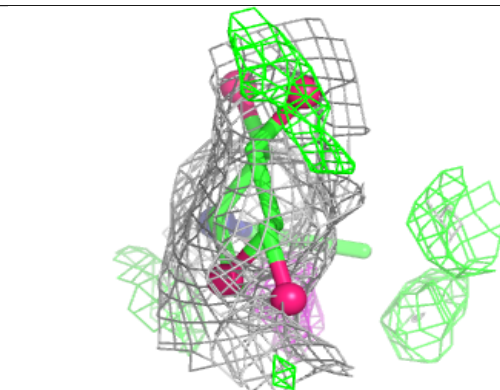
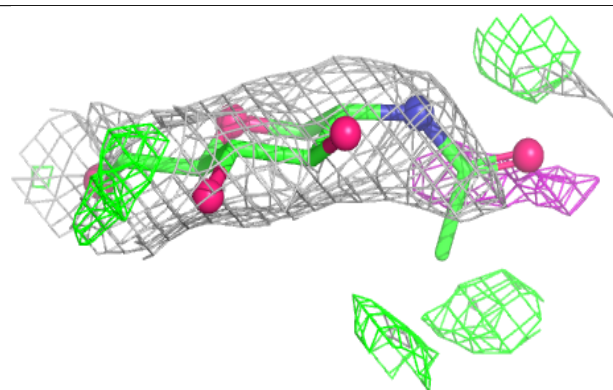
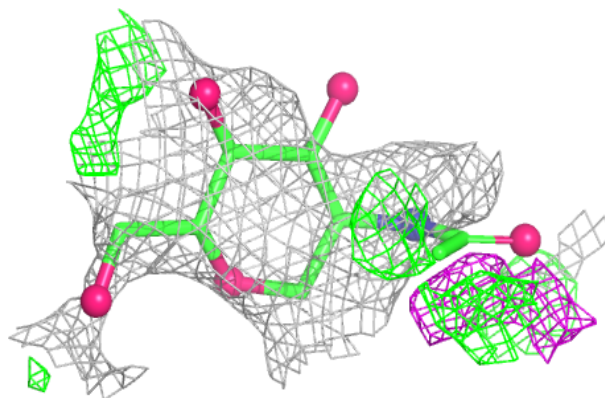
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 603:

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

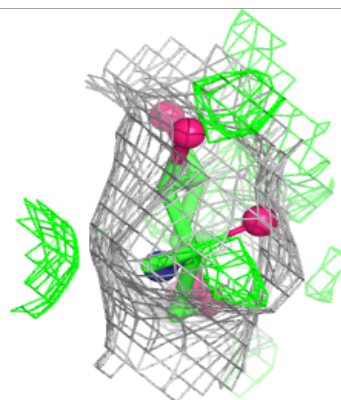
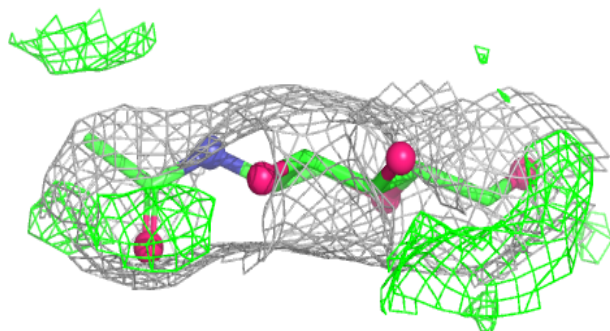
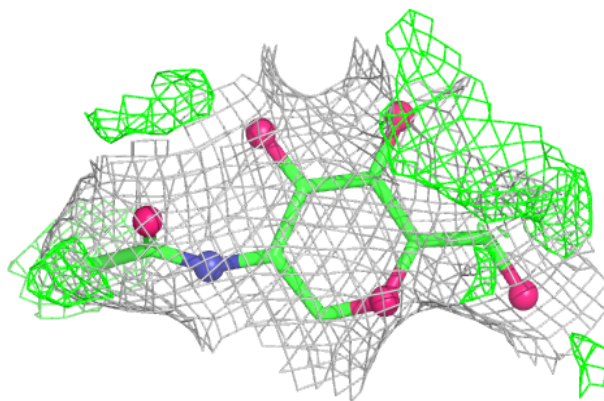
**Electron density around NAG A 602:**

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

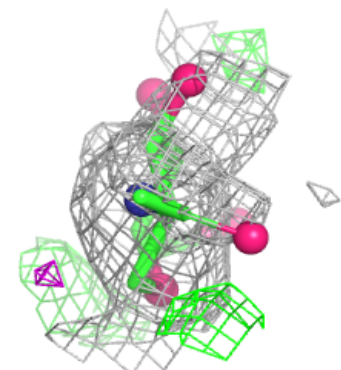
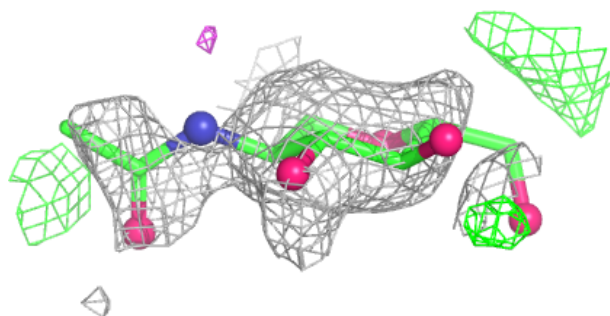
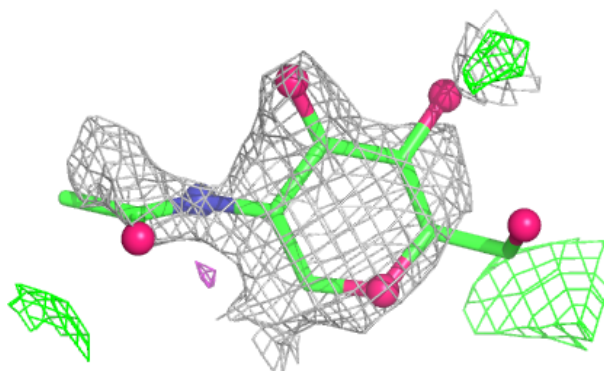


Electron density around NAG C 601:

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

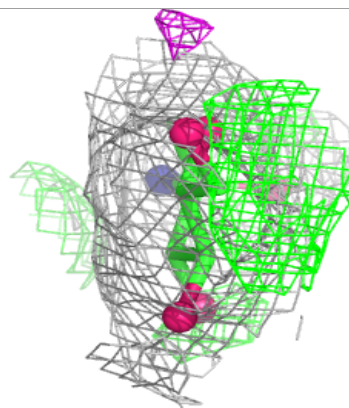
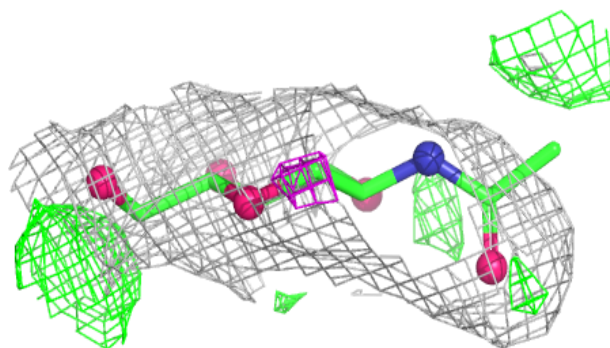
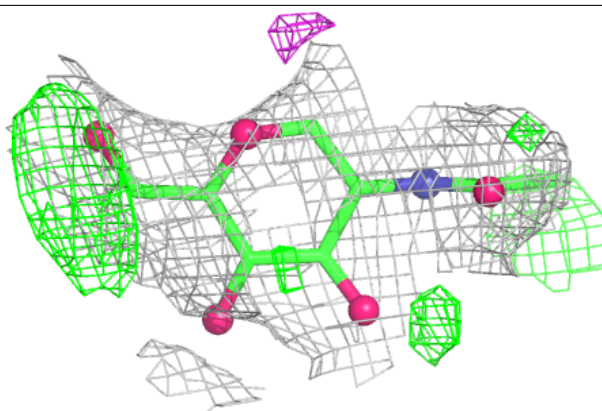
**Electron density around NAG C 602:**

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

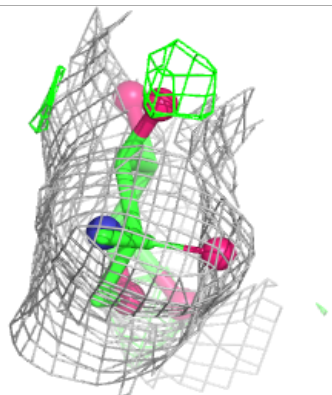
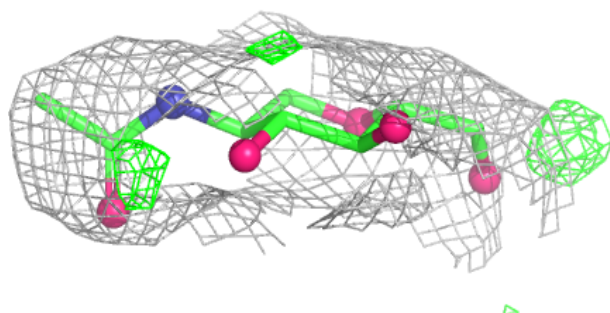
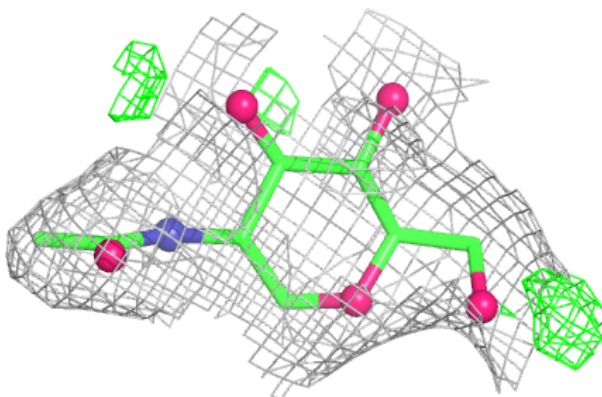


Electron density around NAG E 601:

$2mF_o-DF_c$ (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.