Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 01:54 AM EDT

PDB ID	:	5C7K
Title	:	Crystal structure BG505 SOSIP gp140 HIV-1 Env trimer bound to broadly neutralizing antibodies PGT128 and 8ANC195
Authors	:	Kong, L.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2015-06-24
Resolution	:	4.60 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 (i) 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 (i)) were used in the production of this report:

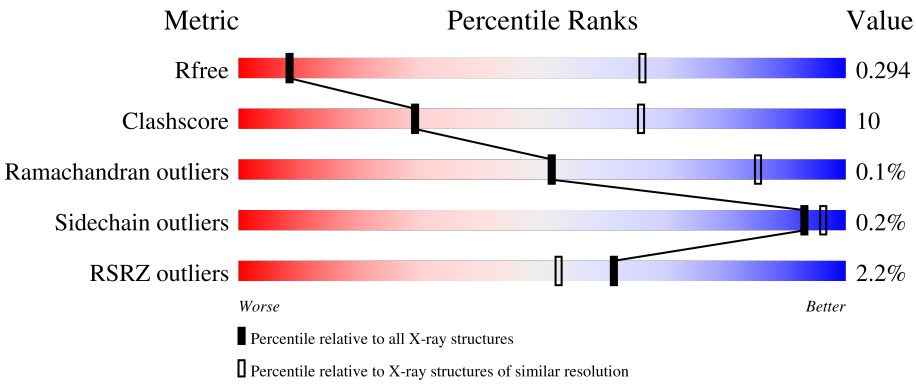
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	5% 72% 25% •
2	B	211	6% 73% 23% •
3	C	487	% 69% 23% 8%
4	D	153	61% 19% 20%
5	E	238	% 73% 21% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	215	79% 20%
7	G	2	50% 50%
7	H	2	100%
7	I	2	100%
7	J	2	100%
8	K	9	22% 67% 11%
8	M	9	11% 78% 11%
9	L	10	30% 60% 10%
10	N	7	57% 43%
11	O	5	60% 40%
12	P	3	67% 33%
12	Q	3	100%
12	R	3	33% 67%
13	S	8	12% 75% 12%
14	T	11	27% 64% 9%

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
11	MAN	O	5	-	-	-	X
12	BMA	P	3	-	-	-	X
12	NAG	Q	2	-	-	-	X
12	BMA	Q	3	-	-	-	X
12	NAG	R	1	-	-	-	X
12	BMA	R	3	-	-	-	X
13	MAN	S	5	-	-	-	X
13	MAN	S	6	-	-	-	X
13	MAN	S	7	-	-	-	X
15	NAG	C	601	-	-	-	X
15	NAG	C	621	-	-	-	X
7	NAG	G	2	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	H	1	-	-	-	X
7	NAG	H	2	-	-	-	X
7	NAG	J	2	-	-	-	X
8	MAN	K	6	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 12092 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 Antibody Fab PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1735	1105	292	332	6	0	0	0

- Molecule 2 is a protein called Antibody Fab PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	204	1514	950	254	306	4	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	450	3544	2224	628	664	28	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	508	SER	ARG	engineered mutation	UNP Q2N0S6
C	511	SER	-	expression tag	UNP Q2N0S6
C	512	GLY	-	expression tag	UNP Q2N0S6
C	513	HIS	-	expression tag	UNP Q2N0S6
C	514	HIS	-	expression tag	UNP Q2N0S6
C	515	HIS	-	expression tag	UNP Q2N0S6
C	516	HIS	-	expression tag	UNP Q2N0S6
C	517	HIS	-	expression tag	UNP Q2N0S6
C	518	HIS	-	expression tag	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	122	978	618	169	185	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6
D	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 5 is a protein called Antibody Fab 8ANC195 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	224	1686	1072	284	325	5	0	0	0

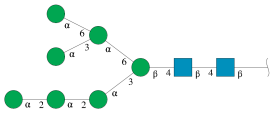
- Molecule 6 is a protein called Antibody Fab 8ANC195 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	212	1626	1018	279	324	5	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

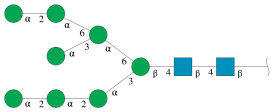
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	G	2	28	16	2	10	0	0	0
7	H	2	28	16	2	10	0	0	0
7	I	2	28	16	2	10	0	0	0
7	J	2	28	16	2	10	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



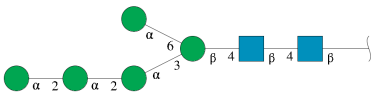
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	K	9	105	58	2	45	0	0	0
8	M	9	105	58	2	45	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



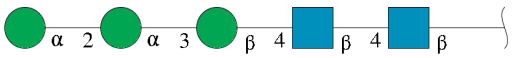
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	L	10	116	64	2	50	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.



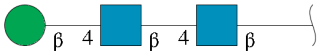
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	N	7	83	46	2	35	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



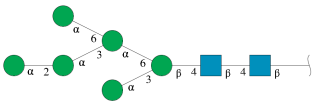
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	O	5	61	34	2	25	0	0	0

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



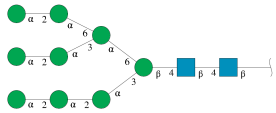
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	P	3	39	22	2	15	0	0	0
12	Q	3	39	22	2	15	0	0	0
12	R	3	39	22	2	15	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



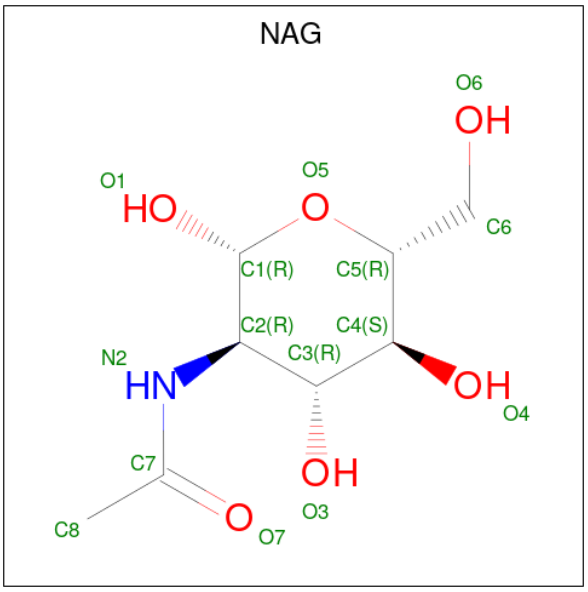
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	S	8	94	52	2	40	0	0	0

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



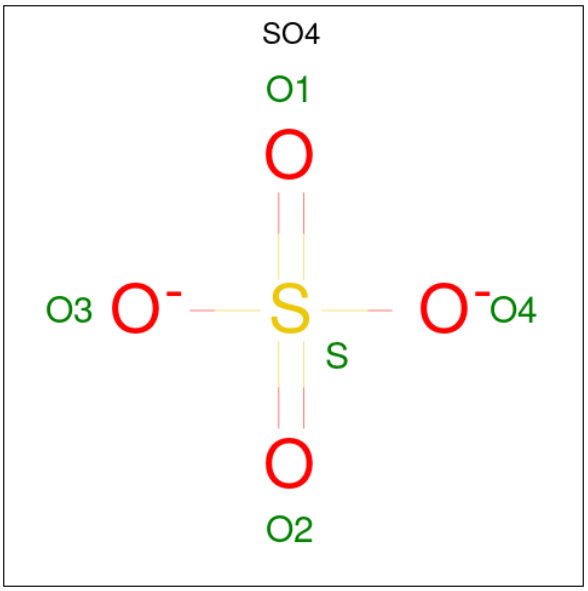
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	T	11	127	70	2	55	0	0	0

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
15	C	1	14	8	1	5	0	0
			Total	C	N	O		
15	C	1	14	8	1	5	0	0
			Total	C	N	O		
15	C	1	14	8	1	5	0	0
			Total	C	N	O		
15	C	1	14	8	1	5	0	0
			Total	C	N	O		
15	D	1	14	8	1	5	0	0
			Total	C	N	O		
15	D	1	14	8	1	5	0	0

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



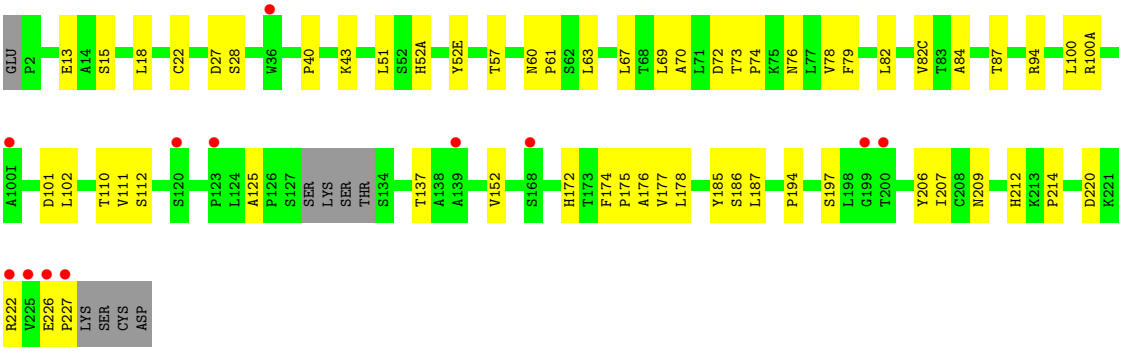
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
16	C	1	5	4	1	0	0

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.

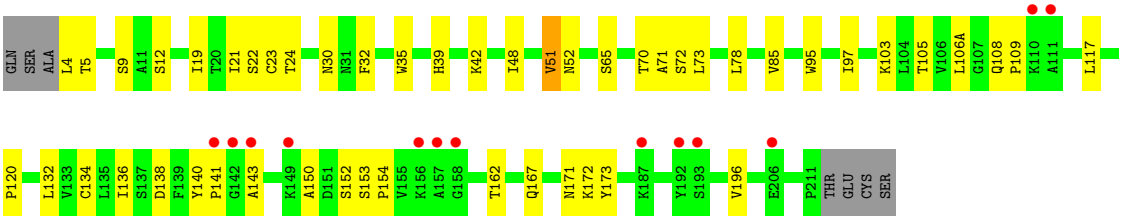
• Molecule 1: Antibody Fab PGT128 heavy chain

Chain A:



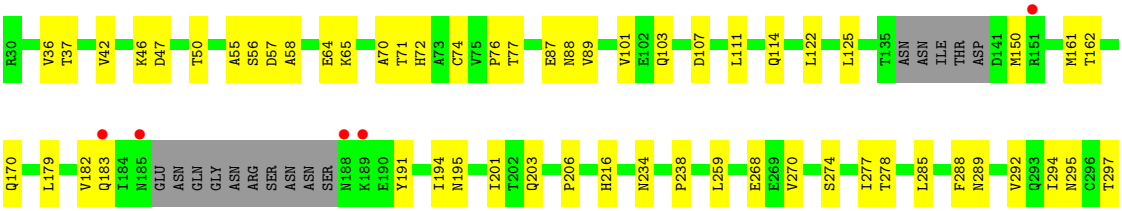
• Molecule 2: Antibody Fab PGT128 light chain

Chain B:



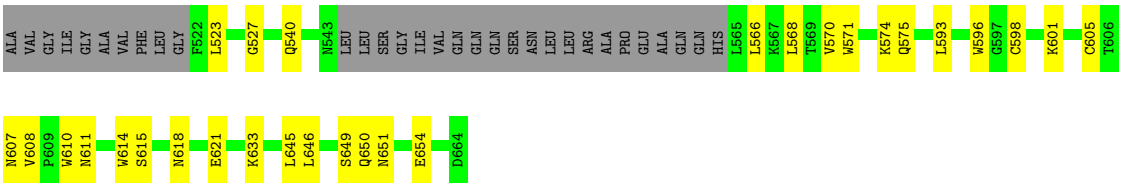
• Molecule 3: Envelope glycoprotein gp120

Chain C:



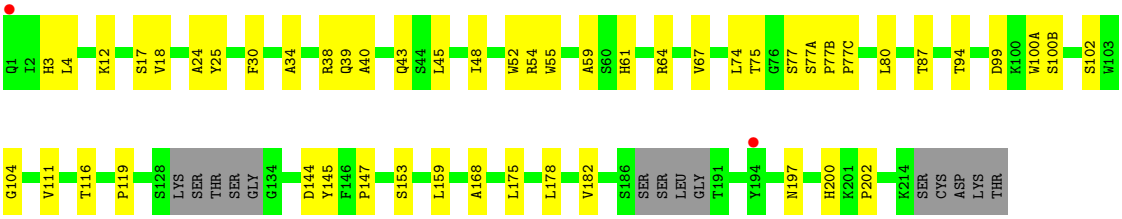
• Molecule 4: Envelope glycoprotein gp41

Chain D:



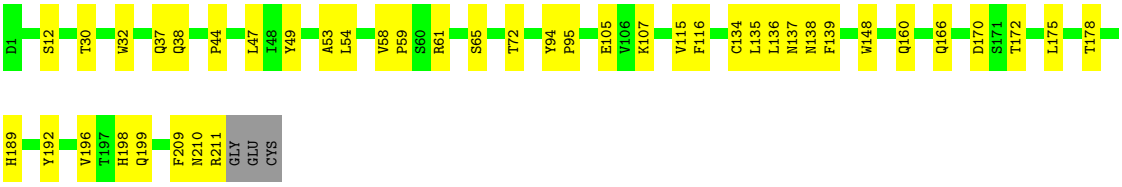
• Molecule 5: Antibody Fab 8ANC195 heavy chain

Chain E:



• Molecule 6: Antibody Fab 8ANC195 light chain

Chain F:



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

Chain G:

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

Chain H: 100%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J: 100%

NAG1 NAG2

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 K: 22% 67% 11%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8 MAN9

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 M: 11% 78% 11%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8 MAN9

• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 L: 30% 60% 10%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8 MAN9 MAN10

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 N: 57% 43%

• Molecule 11: alpha-D-mannopyranose-(1-2)-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

Chain O: 60% 40%

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 67% 33%

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 33% 67%

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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

Chain S: 12% 75% 12%

• Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	261.13Å 261.13Å 261.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 4.60 47.68 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.68-4.60) 99.8 (47.68-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.289 , 0.295 0.289 , 0.294	Depositor DCC
R_{free} test set	1637 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	157.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 113.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.23	0/1786	0.44	0/2449
2	B	0.23	0/1552	0.53	1/2121 (0.0%)
3	C	0.25	0/3617	0.48	0/4908
4	D	0.26	0/995	0.51	0/1349
5	E	0.24	0/1730	0.45	0/2361
6	F	0.24	0/1661	0.45	0/2256
All	All	0.24	0/11341	0.48	1/15444 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	108	GLN	C-N-CD	-11.29	95.77	120.60

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	1735	0	1690	38	0
2	B	1514	0	1473	31	0
3	C	3544	0	3480	84	0
4	D	978	0	959	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1686	0	1658	36	0
6	F	1626	0	1581	27	0
7	G	28	0	25	4	0
7	H	28	0	25	0	0
7	I	28	0	25	1	0
7	J	28	0	25	2	0
8	K	105	0	88	2	0
8	M	105	0	88	3	0
9	L	116	0	97	1	0
10	N	83	0	70	5	0
11	O	61	0	52	0	0
12	P	39	0	34	1	0
12	Q	39	0	34	0	0
12	R	39	0	34	3	0
13	S	94	0	79	4	0
14	T	127	0	104	1	0
15	C	56	0	52	1	0
15	D	28	0	26	0	0
16	C	5	0	0	0	0
All	All	12092	0	11699	229	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 10.

All (229) 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)
5:E:61:HIS:HA	5:E:64:ARG:HG3	1.59	0.84
3:C:502:LYS:HG2	3:C:503:ARG:H	1.45	0.81
7:J:1:NAG:H61	7:J:2:NAG:HN2	1.45	0.81
3:C:396:ILE:HG22	3:C:397:SER:H	1.50	0.76
3:C:58:ALA:HB2	3:C:76:PRO:HB3	1.70	0.74
2:B:95:TRP:HE1	9:L:6:MAN:HO4	1.37	0.72
2:B:12:SER:HB3	2:B:141:PRO:HG3	1.71	0.72
3:C:352:HIS:O	5:E:75:THR:OG1	2.06	0.72
1:A:100(A):ARG:NH2	7:G:1:NAG:O7	2.23	0.71
3:C:274:SER:HB3	3:C:277:ILE:HG12	1.73	0.69
2:B:138:ASP:HA	2:B:172:LYS:HB3	1.75	0.69
4:D:615:SER:H	6:F:30:THR:HG21	1.57	0.69
3:C:36:VAL:HG12	4:D:610:TRP:HE3	1.59	0.68
3:C:297:THR:HG22	3:C:444:ARG:HA	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB1	1:A:227:PRO:HA	1.77	0.66
3:C:292:VAL:HB	3:C:449:ILE:HB	1.77	0.66
5:E:159:LEU:HD21	5:E:182:VAL:HG11	1.77	0.65
4:D:650:GLN:O	4:D:654:GLU:N	2.26	0.65
3:C:238:PRO:HB3	5:E:54:ARG:HH11	1.60	0.65
3:C:72:HIS:CD2	4:D:568:LEU:HD21	2.31	0.64
2:B:24:THR:HG22	2:B:70:THR:HG22	1.80	0.64
3:C:421:LYS:HE3	3:C:424:ILE:HG22	1.80	0.64
3:C:268:GLU:O	3:C:289:ASN:ND2	2.31	0.63
2:B:106(A):LEU:HB3	2:B:140:TYR:HE1	1.63	0.63
1:A:209:ASN:ND2	1:A:220:ASP:OD2	2.31	0.63
3:C:301:ASN:HB3	3:C:323:ILE:O	1.98	0.63
3:C:55:ALA:HB3	3:C:216:HIS:HB2	1.80	0.62
5:E:25:TYR:HD1	8:K:2:NAG:H2	1.64	0.62
5:E:153:SER:HB3	5:E:197:ASN:HB2	1.82	0.62
12:R:1:NAG:O7	12:R:1:NAG:O3	2.13	0.62
2:B:85:VAL:HG22	2:B:103:LYS:HG2	1.80	0.61
4:D:615:SER:N	6:F:30:THR:HG21	2.15	0.61
4:D:523:LEU:N	4:D:540:GLN:OE1	2.34	0.61
3:C:47:ASP:HA	3:C:489:VAL:HG12	1.83	0.61
4:D:566:LEU:HD22	4:D:575:GLN:HE22	1.66	0.61
3:C:325:ASP:HB3	3:C:327:ARG:HD2	1.81	0.60
1:A:18:LEU:HD23	1:A:82:LEU:HD12	1.82	0.60
1:A:63:LEU:HB3	1:A:67:LEU:HD23	1.83	0.60
3:C:183:GLN:HA	3:C:191:TYR:HA	1.84	0.60
3:C:305:LYS:HB2	3:C:319:ALA:HB3	1.84	0.60
3:C:150:MET:SD	3:C:150:MET:N	2.75	0.60
3:C:288:PHE:HE2	3:C:449:ILE:HG22	1.67	0.59
3:C:270:VAL:HG23	3:C:348:GLN:HG3	1.83	0.59
5:E:39:GLN:HB2	5:E:45:LEU:HD23	1.84	0.59
2:B:120:PRO:HD3	2:B:132:LEU:HG	1.84	0.59
3:C:71:THR:HA	3:C:74:CYS:HB2	1.85	0.59
6:F:37:GLN:HB2	6:F:47:LEU:HD11	1.85	0.58
1:A:84:ALA:HA	1:A:111:VAL:HB	1.85	0.57
2:B:106(A):LEU:HB3	2:B:140:TYR:CE1	2.39	0.57
5:E:12:LYS:NZ	5:E:17:SER:O	2.24	0.57
3:C:161:MET:O	3:C:170:GLN:N	2.38	0.57
3:C:350:ARG:HD3	3:C:355:ASN:O	2.05	0.57
5:E:40:ALA:HB3	5:E:43:GLN:HB2	1.85	0.57
5:E:38:ARG:HB3	5:E:48:ILE:HD11	1.85	0.57
3:C:101:VAL:HG21	3:C:480:ARG:HG2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:THR:OG1	5:E:75:THR:O	2.23	0.56
5:E:119:PRO:HB3	5:E:145:TYR:HB3	1.87	0.56
3:C:503:ARG:HB2	4:D:607:ASN:OD1	2.06	0.56
1:A:137:THR:HG22	1:A:194:PRO:HA	1.87	0.56
2:B:106(A):LEU:HD22	2:B:173:TYR:HE1	1.71	0.56
4:D:618:ASN:HB3	4:D:621:GLU:HB2	1.86	0.56
5:E:200:HIS:CD2	5:E:202:PRO:HD2	2.41	0.56
7:G:1:NAG:O3	7:G:1:NAG:H83	2.05	0.56
13:S:2:NAG:H83	13:S:2:NAG:H3	1.88	0.56
6:F:53:ALA:HB1	13:S:2:NAG:H2	1.86	0.56
2:B:21:ILE:HD11	2:B:73:LEU:HD23	1.88	0.55
10:N:4:MAN:O3	10:N:6:MAN:O6	2.19	0.55
3:C:335:LYS:HG2	12:R:1:NAG:H83	1.89	0.55
5:E:4:LEU:HB2	5:E:104:GLY:HA2	1.89	0.55
1:A:172:HIS:NE2	2:B:167:GLN:OE1	2.40	0.55
10:N:1:NAG:H61	10:N:2:NAG:N2	2.20	0.55
3:C:70:ALA:HB2	3:C:111:LEU:HD11	1.89	0.55
4:D:596:TRP:O	4:D:651:ASN:ND2	2.41	0.55
5:E:144:ASP:HA	5:E:175:LEU:HB3	1.89	0.54
1:A:87:THR:HG23	1:A:110:THR:HA	1.89	0.54
1:A:72:ASP:HB2	1:A:79:PHE:HE1	1.71	0.54
2:B:106(A):LEU:HD21	2:B:171:ASN:O	2.08	0.54
2:B:51:VAL:HG12	2:B:52:ASN:H	1.71	0.54
1:A:176:ALA:HA	1:A:187:LEU:HB3	1.91	0.53
3:C:36:VAL:HG22	4:D:608:VAL:HB	1.90	0.53
3:C:502:LYS:HG2	3:C:503:ARG:N	2.21	0.53
6:F:65:SER:HB3	6:F:72:THR:HG23	1.90	0.53
7:J:1:NAG:H83	10:N:1:NAG:H62	1.90	0.53
5:E:116:THR:HG22	5:E:147:PRO:HD3	1.91	0.53
5:E:25:TYR:CE1	5:E:77(B):PRO:HG3	2.44	0.53
6:F:115:VAL:HG21	6:F:196:VAL:HG21	1.91	0.53
7:G:1:NAG:H83	7:G:1:NAG:C3	2.37	0.53
3:C:37:THR:OG1	3:C:497:ALA:O	2.26	0.52
3:C:390:LEU:HD11	3:C:416:LEU:HD11	1.91	0.52
4:D:646:LEU:O	4:D:650:GLN:HB2	2.09	0.52
2:B:106(A):LEU:HD22	2:B:173:TYR:CE1	2.44	0.52
3:C:331:CYS:HB2	3:C:416:LEU:HB2	1.92	0.52
4:D:593:LEU:HD21	4:D:601:LYS:HA	1.91	0.52
4:D:633:LYS:HG3	6:F:32:TRP:HH2	1.75	0.52
13:S:2:NAG:O3	13:S:3:BMA:O5	2.20	0.52
2:B:51:VAL:HG12	2:B:52:ASN:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:SER:O	3:C:57:ASP:HB2	2.09	0.52
3:C:278:THR:O	3:C:456:ARG:NH2	2.42	0.51
3:C:161:MET:SD	3:C:162:THR:N	2.83	0.51
2:B:5:THR:OG1	2:B:24:THR:OG1	2.28	0.51
5:E:74:LEU:HD13	5:E:77(C):PRO:HD3	1.93	0.51
2:B:136:ILE:HG12	2:B:196:VAL:HG11	1.91	0.51
1:A:52(E):TYR:HB3	3:C:442:VAL:HG11	1.92	0.51
5:E:3:HIS:CD2	8:K:5:MAN:H62	2.45	0.50
6:F:105:GLU:OE2	6:F:166:GLN:NE2	2.44	0.50
5:E:87:THR:HG22	5:E:111:VAL:H	1.76	0.50
1:A:27:ASP:OD1	1:A:28:SER:N	2.43	0.50
3:C:294:ILE:HD12	3:C:449:ILE:HD11	1.95	0.49
1:A:100:LEU:HD12	3:C:323:ILE:HG23	1.94	0.49
3:C:107:ASP:OD2	4:D:574:LYS:HE2	2.12	0.49
1:A:27:ASP:OD2	1:A:94:ARG:NH2	2.46	0.49
1:A:207:ILE:HG13	1:A:222:ARG:HA	1.95	0.49
3:C:46:LYS:HG2	5:E:100(A):TRP:NE1	2.27	0.49
1:A:22:CYS:HB3	1:A:78:VAL:HB	1.94	0.49
2:B:19:ILE:HG13	2:B:78:LEU:HD11	1.95	0.49
5:E:24:ALA:O	5:E:77(B):PRO:HB2	2.12	0.49
3:C:36:VAL:HG12	4:D:610:TRP:CE3	2.44	0.48
1:A:18:LEU:HB3	1:A:82:LEU:HB2	1.95	0.48
3:C:321(A):ASP:HB3	7:G:1:NAG:H82	1.95	0.48
5:E:75:THR:HG23	5:E:77:SER:H	1.78	0.48
3:C:179:LEU:HD11	3:C:419:ARG:HB3	1.95	0.48
6:F:160:GLN:O	6:F:178:THR:N	2.37	0.48
3:C:88:ASN:ND2	4:D:527:GLY:O	2.47	0.47
3:C:390:LEU:HG	3:C:416:LEU:HD21	1.95	0.47
5:E:99:ASP:HB3	5:E:100(B):SER:HB3	1.96	0.47
5:E:59:ALA:HB3	14:T:11:MAN:H61	1.97	0.47
6:F:49:TYR:O	6:F:53:ALA:HB3	2.13	0.47
6:F:136:LEU:HB2	6:F:175:LEU:HB3	1.96	0.46
3:C:107:ASP:O	3:C:111:LEU:HB2	2.16	0.46
3:C:378:CYS:HB3	3:C:383:PHE:CE1	2.50	0.46
1:A:101:ASP:OD1	1:A:102:LEU:N	2.49	0.46
1:A:177:VAL:HG22	2:B:162:THR:HG21	1.97	0.46
1:A:51:LEU:HD23	1:A:69:LEU:HB3	1.97	0.46
3:C:298:ARG:HD2	3:C:300:ASN:HB2	1.97	0.46
6:F:12:SER:HB3	6:F:107:LYS:HD3	1.98	0.46
7:I:2:NAG:H61	12:P:2:NAG:H5	1.97	0.46
2:B:9:SER:HB3	2:B:143:ALA:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:CYS:HA	4:D:571:TRP:CZ2	2.50	0.46
3:C:182:VAL:HG12	3:C:194:ILE:HA	1.97	0.46
5:E:144:ASP:HB3	5:E:175:LEU:HD13	1.98	0.46
3:C:206:PRO:HG3	3:C:318:TYR:CE2	2.51	0.46
5:E:30:PHE:HB2	5:E:55:TRP:CH2	2.51	0.46
1:A:197:SER:HG	1:A:206:TYR:HH	1.63	0.45
2:B:30:ASN:HB2	2:B:32:PHE:HD1	1.80	0.45
2:B:39:HIS:HB2	2:B:42:LYS:HD2	1.98	0.45
4:D:645:LEU:O	4:D:649:SER:HB3	2.16	0.45
2:B:23:CYS:N	2:B:71:ALA:O	2.48	0.45
3:C:70:ALA:HA	3:C:111:LEU:HD21	1.97	0.45
1:A:13:GLU:HA	1:A:112:SER:O	2.16	0.45
1:A:40:PRO:HB2	1:A:43:LYS:HD2	1.98	0.45
1:A:226:GLU:HA	1:A:227:PRO:HD3	1.83	0.45
2:B:105:THR:HG22	2:B:106(A):LEU:H	1.81	0.45
1:A:177:VAL:N	1:A:186:SER:O	2.49	0.45
2:B:35:TRP:HB2	2:B:48:ILE:HG22	1.99	0.45
1:A:28:SER:HA	1:A:76:ASN:HD21	1.81	0.45
3:C:71:THR:HG23	3:C:74:CYS:HB3	1.98	0.45
3:C:285:LEU:HD21	3:C:477:ASP:HB3	1.99	0.44
1:A:70:ALA:HB3	1:A:79:PHE:HB2	1.99	0.44
4:D:611:ASN:HB3	4:D:614:TRP:CD2	2.52	0.44
5:E:168:ALA:HB2	5:E:178:LEU:HD23	1.99	0.44
5:E:34:ALA:HB2	5:E:52:TRP:CD1	2.52	0.44
6:F:94:TYR:HA	6:F:95:PRO:HA	1.79	0.44
1:A:15:SER:N	1:A:82(C):VAL:O	2.39	0.44
5:E:25:TYR:CD1	5:E:77(B):PRO:HG3	2.53	0.44
5:E:61:HIS:HA	5:E:64:ARG:CG	2.39	0.44
8:M:1:NAG:O7	10:N:5:MAN:O3	2.33	0.44
3:C:464:THR:OG1	3:C:465:THR:N	2.51	0.44
3:C:358:ILE:O	3:C:465:THR:OG1	2.30	0.44
3:C:363:ASN:HB3	3:C:388:SER:HA	1.99	0.44
3:C:238:PRO:HB3	5:E:54:ARG:NH1	2.31	0.43
3:C:437:PRO:HA	3:C:438:PRO:HD3	1.80	0.43
10:N:1:NAG:H61	10:N:2:NAG:HN2	1.83	0.43
3:C:50:THR:O	3:C:103:GLN:NE2	2.32	0.43
1:A:174:PHE:HA	1:A:175:PRO:HD3	1.88	0.43
6:F:137:ASN:O	6:F:139:PHE:HD1	2.01	0.43
5:E:94:THR:HG22	5:E:102:SER:HB2	1.99	0.43
1:A:51:LEU:HB3	1:A:57:THR:HG23	2.01	0.43
6:F:116:PHE:HB2	6:F:135:LEU:HD23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:HA	1:A:61:PRO:HD3	1.93	0.43
3:C:74:CYS:HA	4:D:571:TRP:CH2	2.54	0.43
3:C:259:LEU:HD12	3:C:374:HIS:CD2	2.54	0.43
6:F:59:PRO:HB2	6:F:61:ARG:HG2	2.00	0.43
1:A:178:LEU:HD21	1:A:185:TYR:CZ	2.53	0.42
2:B:4:LEU:HG	2:B:97:ILE:HD13	2.01	0.42
3:C:42:VAL:HG22	3:C:493:PRO:O	2.19	0.42
6:F:170:ASP:HB2	6:F:172:THR:HG22	2.00	0.42
3:C:37:THR:HG22	4:D:605:CYS:HA	2.01	0.42
3:C:299:PRO:HD2	3:C:329:ALA:HA	2.01	0.42
2:B:65:SER:O	2:B:72:SER:N	2.35	0.42
1:A:212:HIS:CE1	1:A:214:PRO:HD2	2.54	0.42
3:C:460:SER:HA	3:C:461:THR:OG1	2.19	0.42
2:B:153:SER:HA	2:B:154:PRO:HD3	1.79	0.42
5:E:75:THR:HG23	5:E:77(A):SER:H	1.84	0.42
3:C:114:GLN:CD	4:D:570:VAL:HG21	2.40	0.42
3:C:295:ASN:HB2	3:C:332:ASN:HB2	2.01	0.42
3:C:195:ASN:OD1	3:C:201:ILE:HB	2.19	0.42
6:F:198:HIS:CD2	6:F:199:GLN:H	2.38	0.42
4:D:593:LEU:O	4:D:598:CYS:HB2	2.20	0.42
6:F:38:GLN:HE21	6:F:44:PRO:HD3	1.84	0.42
4:D:633:LYS:HG3	6:F:32:TRP:CH2	2.54	0.42
5:E:12:LYS:HD3	5:E:18:VAL:HB	2.01	0.42
1:A:52(A):HIS:HB3	8:M:2:NAG:C6	2.50	0.41
1:A:152:VAL:HG22	1:A:212:HIS:HD2	1.85	0.41
2:B:22:SER:OG	2:B:23:CYS:N	2.51	0.41
3:C:87:GLU:O	3:C:89:VAL:HG23	2.20	0.41
3:C:203:GLN:HG3	3:C:435:TYR:HD2	1.85	0.41
3:C:298:ARG:O	3:C:442:VAL:HG13	2.20	0.41
3:C:395:TRP:CD2	3:C:400:SER:HB3	2.55	0.41
6:F:54:LEU:O	13:S:3:BMA:H5	2.20	0.41
6:F:192:TYR:HB2	6:F:209:PHE:CE1	2.56	0.41
3:C:295:ASN:OD1	3:C:446:VAL:HG22	2.20	0.41
6:F:210:ASN:O	6:F:211:ARG:HG2	2.21	0.41
2:B:150:ALA:O	2:B:152:SER:N	2.51	0.41
3:C:64:GLU:HG3	3:C:65:LYS:H	1.86	0.41
3:C:460:SER:HB2	3:C:462:ASN:HB2	2.02	0.41
1:A:73:THR:HB	1:A:74:PRO:HD3	2.03	0.41
3:C:57:ASP:HA	3:C:77:THR:HB	2.01	0.41
3:C:122:LEU:HD13	3:C:125:LEU:HD12	2.03	0.41
3:C:335:LYS:HG2	12:R:1:NAG:C8	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:ILE:HG22	3:C:397:SER:N	2.26	0.41
5:E:67:VAL:HG13	5:E:80:LEU:HD11	2.03	0.41
6:F:134:CYS:HB2	6:F:148:TRP:CH2	2.56	0.41
2:B:117:LEU:HD13	2:B:134:CYS:SG	2.61	0.41
6:F:54:LEU:HD21	6:F:58:VAL:O	2.21	0.41
6:F:189:HIS:O	6:F:211:ARG:NH2	2.54	0.40
3:C:355:ASN:HD22	15:C:607:NAG:H83	1.87	0.40
3:C:47:ASP:OD2	3:C:487:LYS:NZ	2.33	0.40
1:A:28:SER:HB3	8:M:9:MAN:O6	2.21	0.40
6:F:138:ASN:HB3	6:F:172:THR:HG21	2.04	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	226/239 (95%)	212 (94%)	14 (6%)	0	100	100
2	B	202/211 (96%)	193 (96%)	7 (4%)	2 (1%)	15	54
3	C	442/487 (91%)	418 (95%)	24 (5%)	0	100	100
4	D	118/153 (77%)	110 (93%)	8 (7%)	0	100	100
5	E	218/238 (92%)	210 (96%)	8 (4%)	0	100	100
6	F	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
All	All	1416/1543 (92%)	1348 (95%)	66 (5%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	109	PRO

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	194/203 (96%)	194 (100%)	0	100	100
2	B	171/177 (97%)	171 (100%)	0	100	100
3	C	401/433 (93%)	399 (100%)	2 (0%)	88	93
4	D	106/129 (82%)	106 (100%)	0	100	100
5	E	192/204 (94%)	192 (100%)	0	100	100
6	F	180/182 (99%)	180 (100%)	0	100	100
All	All	1244/1328 (94%)	1242 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	234	ASN
3	C	339	ASN

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

Mol	Chain	Res	Type
3	C	195	ASN
4	D	575	GLN
5	E	39	GLN
6	F	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

76 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	$\#\|Z\| > 2$
7	NAG	G	1	7,3	14,14,15	0.30	0	17,19,21	0.63	0
7	NAG	G	2	7	14,14,15	0.20	0	17,19,21	0.39	0
7	NAG	H	1	7,3	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	H	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	NAG	I	1	7,3	14,14,15	0.23	0	17,19,21	1.02	1 (5%)
7	NAG	I	2	7	14,14,15	0.24	0	17,19,21	0.37	0
7	NAG	J	1	7,3	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	J	2	7	14,14,15	0.28	0	17,19,21	0.35	0
8	NAG	K	1	8,3	14,14,15	0.60	0	17,19,21	0.53	0
8	NAG	K	2	8	14,14,15	0.57	0	17,19,21	0.48	0
8	BMA	K	3	8	11,11,12	0.55	0	15,15,17	0.69	0
8	MAN	K	4	8	11,11,12	0.67	0	15,15,17	1.07	1 (6%)
8	MAN	K	5	8	11,11,12	0.57	0	15,15,17	1.04	1 (6%)
8	MAN	K	6	8	11,11,12	0.55	0	15,15,17	1.11	2 (13%)
8	MAN	K	7	8	11,11,12	0.89	0	15,15,17	0.92	2 (13%)
8	MAN	K	8	8	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
8	MAN	K	9	8	11,11,12	0.81	1 (9%)	15,15,17	1.47	2 (13%)
9	NAG	L	1	3,9	14,14,15	0.26	0	17,19,21	0.45	0
9	MAN	L	10	9	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
9	NAG	L	2	9	14,14,15	0.25	0	17,19,21	0.39	0
9	BMA	L	3	9	11,11,12	0.81	0	15,15,17	0.87	0
9	MAN	L	4	9	11,11,12	0.75	1 (9%)	15,15,17	1.14	2 (13%)
9	MAN	L	5	9	11,11,12	0.69	0	15,15,17	1.14	2 (13%)
9	MAN	L	6	9	11,11,12	0.80	0	15,15,17	0.95	1 (6%)
9	MAN	L	7	9	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
9	MAN	L	8	9	11,11,12	0.68	0	15,15,17	1.25	2 (13%)
9	MAN	L	9	9	11,11,12	0.69	0	15,15,17	0.91	1 (6%)
8	NAG	M	1	8,3	14,14,15	0.51	0	17,19,21	0.63	0
8	NAG	M	2	8	14,14,15	0.20	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BMA	M	3	8	11,11,12	0.84	0	15,15,17	1.03	0
8	MAN	M	4	8	11,11,12	0.80	0	15,15,17	1.34	2 (13%)
8	MAN	M	5	8	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
8	MAN	M	6	8	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
8	MAN	M	7	8	11,11,12	0.72	0	15,15,17	0.97	2 (13%)
8	MAN	M	8	8	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
8	MAN	M	9	8	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
10	NAG	N	1	3,10	14,14,15	0.30	0	17,19,21	0.46	0
10	NAG	N	2	10	14,14,15	0.40	0	17,19,21	0.53	0
10	BMA	N	3	10	11,11,12	0.66	0	15,15,17	1.03	1 (6%)
10	MAN	N	4	10	11,11,12	0.70	0	15,15,17	1.34	1 (6%)
10	MAN	N	5	10	11,11,12	0.54	0	15,15,17	1.16	1 (6%)
10	MAN	N	6	10	11,11,12	0.66	0	15,15,17	1.29	2 (13%)
10	MAN	N	7	10	11,11,12	0.76	1 (9%)	15,15,17	1.17	2 (13%)
11	NAG	O	1	3,11	14,14,15	0.48	0	17,19,21	0.45	0
11	NAG	O	2	11	14,14,15	0.24	0	17,19,21	0.60	0
11	BMA	O	3	11	11,11,12	0.67	0	15,15,17	1.23	1 (6%)
11	MAN	O	4	11	11,11,12	0.62	0	15,15,17	1.32	2 (13%)
11	MAN	O	5	11	11,11,12	0.22	0	15,15,17	0.58	0
12	NAG	P	1	3,12	14,14,15	0.40	0	17,19,21	0.40	0
12	NAG	P	2	12	14,14,15	0.27	0	17,19,21	0.62	0
12	BMA	P	3	12	11,11,12	0.65	0	15,15,17	0.79	0
12	NAG	Q	1	3,12	14,14,15	0.32	0	17,19,21	0.49	0
12	NAG	Q	2	12	14,14,15	0.38	0	17,19,21	0.62	0
12	BMA	Q	3	12	11,11,12	0.67	0	15,15,17	0.80	0
12	NAG	R	1	3,12	14,14,15	0.30	0	17,19,21	0.73	0
12	NAG	R	2	12	14,14,15	0.23	0	17,19,21	0.67	1 (5%)
12	BMA	R	3	12	11,11,12	0.64	0	15,15,17	0.75	0
13	NAG	S	1	13,4	14,14,15	0.24	0	17,19,21	0.41	0
13	NAG	S	2	13	14,14,15	0.42	0	17,19,21	1.52	3 (17%)
13	BMA	S	3	13	11,11,12	0.73	0	15,15,17	0.99	0
13	MAN	S	4	13	11,11,12	1.56	3 (27%)	15,15,17	1.38	2 (13%)
13	MAN	S	5	13	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
13	MAN	S	6	13	11,11,12	0.67	0	15,15,17	1.19	2 (13%)
13	MAN	S	7	13	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
13	MAN	S	8	13	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
14	NAG	T	1	14,3	14,14,15	0.19	0	17,19,21	0.39	0
14	MAN	T	10	14	11,11,12	0.64	0	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	MAN	T	11	5,14	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
14	NAG	T	2	14	14,14,15	0.38	0	17,19,21	0.45	0
14	BMA	T	3	14	11,11,12	0.52	0	15,15,17	0.70	0
14	MAN	T	4	14	11,11,12	0.52	0	15,15,17	1.11	2 (13%)
14	MAN	T	5	14	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
14	MAN	T	6	14	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
14	MAN	T	7	14	11,11,12	0.59	0	15,15,17	1.17	2 (13%)
14	MAN	T	8	14	11,11,12	0.83	0	15,15,17	1.43	3 (20%)
14	MAN	T	9	14	11,11,12	0.60	0	15,15,17	1.04	2 (13%)

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
7	NAG	G	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	NAG	H	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	NAG	I	1	7,3	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	NAG	J	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
8	NAG	K	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
8	MAN	K	4	8	-	0/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
8	MAN	K	6	8	-	1/2/19/22	0/1/1/1
8	MAN	K	7	8	-	2/2/19/22	0/1/1/1
8	MAN	K	8	8	-	0/2/19/22	0/1/1/1
8	MAN	K	9	8	-	0/2/19/22	0/1/1/1
9	NAG	L	1	3,9	-	0/6/23/26	0/1/1/1
9	MAN	L	10	9	-	1/2/19/22	0/1/1/1
9	NAG	L	2	9	-	2/6/23/26	0/1/1/1
9	BMA	L	3	9	-	0/2/19/22	0/1/1/1
9	MAN	L	4	9	-	1/2/19/22	0/1/1/1
9	MAN	L	5	9	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	L	6	9	-	0/2/19/22	0/1/1/1
9	MAN	L	7	9	-	0/2/19/22	0/1/1/1
9	MAN	L	8	9	-	0/2/19/22	0/1/1/1
9	MAN	L	9	9	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8,3	-	1/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
8	MAN	M	4	8	-	0/2/19/22	0/1/1/1
8	MAN	M	5	8	-	0/2/19/22	0/1/1/1
8	MAN	M	6	8	-	0/2/19/22	0/1/1/1
8	MAN	M	7	8	-	0/2/19/22	0/1/1/1
8	MAN	M	8	8	-	0/2/19/22	0/1/1/1
8	MAN	M	9	8	-	0/2/19/22	0/1/1/1
10	NAG	N	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	BMA	N	3	10	-	0/2/19/22	0/1/1/1
10	MAN	N	4	10	-	1/2/19/22	0/1/1/1
10	MAN	N	5	10	-	0/2/19/22	0/1/1/1
10	MAN	N	6	10	-	1/2/19/22	0/1/1/1
10	MAN	N	7	10	-	0/2/19/22	0/1/1/1
11	NAG	O	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
11	MAN	O	4	11	-	2/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	P	2	12	-	1/6/23/26	0/1/1/1
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	NAG	Q	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	2/6/23/26	0/1/1/1
12	BMA	Q	3	12	-	0/2/19/22	0/1/1/1
12	NAG	R	1	3,12	-	4/6/23/26	0/1/1/1
12	NAG	R	2	12	-	0/6/23/26	0/1/1/1
12	BMA	R	3	12	-	0/2/19/22	0/1/1/1
13	NAG	S	1	13,4	-	1/6/23/26	0/1/1/1
13	NAG	S	2	13	-	5/6/23/26	0/1/1/1
13	BMA	S	3	13	-	2/2/19/22	0/1/1/1
13	MAN	S	4	13	-	2/2/19/22	0/1/1/1
13	MAN	S	5	13	-	0/2/19/22	0/1/1/1
13	MAN	S	6	13	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	S	7	13	-	0/2/19/22	0/1/1/1
13	MAN	S	8	13	-	0/2/19/22	0/1/1/1
14	NAG	T	1	14,3	-	2/6/23/26	0/1/1/1
14	MAN	T	10	14	-	2/2/19/22	0/1/1/1
14	MAN	T	11	5,14	-	2/2/19/22	0/1/1/1
14	NAG	T	2	14	-	2/6/23/26	0/1/1/1
14	BMA	T	3	14	-	0/2/19/22	0/1/1/1
14	MAN	T	4	14	-	0/2/19/22	0/1/1/1
14	MAN	T	5	14	-	2/2/19/22	0/1/1/1
14	MAN	T	6	14	-	0/2/19/22	0/1/1/1
14	MAN	T	7	14	-	0/2/19/22	0/1/1/1
14	MAN	T	8	14	-	0/2/19/22	0/1/1/1
14	MAN	T	9	14	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	4	MAN	C2-C3	3.00	1.56	1.52
13	S	4	MAN	O2-C2	2.74	1.49	1.43
13	S	4	MAN	C1-C2	2.66	1.58	1.52
10	N	7	MAN	C1-C2	2.28	1.57	1.52
8	K	9	MAN	C1-C2	2.21	1.57	1.52
9	L	4	MAN	C1-C2	2.13	1.57	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	9	MAN	C1-O5-C5	4.62	118.46	112.19
13	S	2	NAG	C2-N2-C7	4.52	129.34	122.90
10	N	4	MAN	C1-O5-C5	4.48	118.26	112.19
8	M	4	MAN	C1-O5-C5	4.33	118.05	112.19
10	N	6	MAN	C1-O5-C5	4.04	117.67	112.19
10	N	5	MAN	C1-O5-C5	3.60	117.07	112.19
8	M	5	MAN	C1-O5-C5	3.47	116.89	112.19
13	S	6	MAN	C1-O5-C5	3.37	116.76	112.19
8	M	6	MAN	C1-O5-C5	3.35	116.73	112.19
11	O	4	MAN	O2-C2-C1	3.32	115.94	109.15
7	I	1	NAG	C2-N2-C7	3.30	127.60	122.90
14	T	8	MAN	O2-C2-C3	-3.29	103.54	110.14
14	T	4	MAN	C1-O5-C5	3.15	116.46	112.19
14	T	7	MAN	C1-O5-C5	3.15	116.46	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	5	MAN	O2-C2-C3	-3.12	103.88	110.14
8	K	6	MAN	C1-O5-C5	3.12	116.42	112.19
13	S	8	MAN	C1-O5-C5	3.09	116.38	112.19
9	L	8	MAN	C1-O5-C5	3.08	116.37	112.19
9	L	4	MAN	C1-O5-C5	3.02	116.29	112.19
9	L	8	MAN	O2-C2-C3	-3.00	104.13	110.14
11	O	3	BMA	C1-C2-C3	3.00	113.35	109.67
14	T	8	MAN	C1-O5-C5	3.00	116.25	112.19
13	S	2	NAG	C1-C2-N2	2.96	115.55	110.49
13	S	4	MAN	O2-C2-C1	2.90	115.09	109.15
8	K	5	MAN	C1-O5-C5	2.89	116.11	112.19
11	O	4	MAN	C1-O5-C5	2.89	116.10	112.19
10	N	3	BMA	C1-C2-C3	-2.88	106.13	109.67
14	T	10	MAN	C1-O5-C5	2.85	116.06	112.19
10	N	7	MAN	C1-O5-C5	2.78	115.96	112.19
14	T	6	MAN	C1-O5-C5	2.66	115.80	112.19
8	K	8	MAN	C1-O5-C5	2.66	115.79	112.19
13	S	5	MAN	C1-O5-C5	2.65	115.78	112.19
14	T	9	MAN	C1-O5-C5	2.62	115.74	112.19
9	L	7	MAN	C1-O5-C5	2.61	115.73	112.19
14	T	8	MAN	C1-C2-C3	-2.57	106.50	109.67
13	S	2	NAG	C1-O5-C5	2.51	115.59	112.19
13	S	7	MAN	C1-O5-C5	2.47	115.54	112.19
14	T	9	MAN	O2-C2-C3	-2.46	105.21	110.14
13	S	4	MAN	C1-O5-C5	2.46	115.52	112.19
9	L	4	MAN	O2-C2-C3	-2.44	105.25	110.14
8	M	9	MAN	C1-O5-C5	2.42	115.47	112.19
9	L	5	MAN	C1-O5-C5	2.42	115.47	112.19
9	L	7	MAN	O2-C2-C3	-2.29	105.55	110.14
13	S	7	MAN	O2-C2-C3	-2.27	105.59	110.14
9	L	10	MAN	C1-O5-C5	2.27	115.27	112.19
8	K	4	MAN	C1-O5-C5	2.26	115.26	112.19
14	T	6	MAN	O2-C2-C3	-2.26	105.62	110.14
14	T	7	MAN	O2-C2-C3	-2.25	105.62	110.14
8	M	7	MAN	C1-O5-C5	2.25	115.25	112.19
10	N	6	MAN	O2-C2-C3	-2.25	105.64	110.14
14	T	11	MAN	C1-O5-C5	2.24	115.23	112.19
13	S	6	MAN	O2-C2-C3	-2.24	105.65	110.14
8	M	5	MAN	O2-C2-C3	-2.23	105.66	110.14
13	S	8	MAN	O2-C2-C3	-2.23	105.67	110.14
8	M	6	MAN	O2-C2-C3	-2.23	105.67	110.14
8	M	8	MAN	O2-C2-C3	-2.23	105.68	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	7	MAN	O2-C2-C3	-2.20	105.72	110.14
9	L	9	MAN	O2-C2-C3	-2.20	105.73	110.14
8	K	8	MAN	O2-C2-C3	-2.19	105.75	110.14
9	L	10	MAN	O2-C2-C3	-2.19	105.76	110.14
8	M	9	MAN	O2-C2-C3	-2.18	105.76	110.14
8	K	7	MAN	O2-C2-C3	-2.18	105.77	110.14
14	T	4	MAN	O2-C2-C3	-2.17	105.79	110.14
14	T	11	MAN	O2-C2-C3	-2.17	105.79	110.14
8	K	6	MAN	O2-C2-C3	-2.16	105.81	110.14
10	N	7	MAN	O2-C2-C3	-2.13	105.86	110.14
12	R	2	NAG	C1-O5-C5	2.13	115.08	112.19
9	L	6	MAN	O2-C2-C3	-2.13	105.87	110.14
8	M	8	MAN	C1-O5-C5	2.11	115.06	112.19
8	K	9	MAN	O2-C2-C3	-2.10	105.93	110.14
8	M	4	MAN	O2-C2-C3	-2.10	105.94	110.14
14	T	10	MAN	O2-C2-C3	-2.08	105.97	110.14
8	K	7	MAN	C1-O5-C5	2.04	114.95	112.19
14	T	5	MAN	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1	NAG	C3-C2-N2-C7
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
7	I	1	NAG	C3-C2-N2-C7
12	R	1	NAG	C8-C7-N2-C2
12	R	1	NAG	O7-C7-N2-C2
8	K	1	NAG	O5-C5-C6-O6
13	S	2	NAG	C4-C5-C6-O6
14	T	1	NAG	O5-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
11	O	2	NAG	O5-C5-C6-O6
13	S	2	NAG	O5-C5-C6-O6
8	K	2	NAG	C4-C5-C6-O6
14	T	10	MAN	O5-C5-C6-O6
12	R	1	NAG	C1-C2-N2-C7
7	H	2	NAG	O5-C5-C6-O6
8	K	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	O	2	NAG	C4-C5-C6-O6
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
13	S	2	NAG	C8-C7-N2-C2
13	S	2	NAG	O7-C7-N2-C2
9	L	2	NAG	O5-C5-C6-O6
14	T	1	NAG	C4-C5-C6-O6
14	T	10	MAN	C4-C5-C6-O6
8	K	7	MAN	O5-C5-C6-O6
14	T	5	MAN	O5-C5-C6-O6
8	K	7	MAN	C4-C5-C6-O6
13	S	3	BMA	O5-C5-C6-O6
14	T	11	MAN	O5-C5-C6-O6
14	T	5	MAN	C4-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
13	S	3	BMA	C4-C5-C6-O6
11	O	4	MAN	C4-C5-C6-O6
9	L	2	NAG	C4-C5-C6-O6
14	T	9	MAN	O5-C5-C6-O6
9	L	4	MAN	O5-C5-C6-O6
8	K	6	MAN	O5-C5-C6-O6
9	L	10	MAN	O5-C5-C6-O6
13	S	1	NAG	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
14	T	2	NAG	C4-C5-C6-O6
7	G	1	NAG	C1-C2-N2-C7
7	J	2	NAG	O5-C5-C6-O6
12	R	1	NAG	C3-C2-N2-C7
7	J	1	NAG	C1-C2-N2-C7
14	T	11	MAN	C4-C5-C6-O6
12	Q	2	NAG	C4-C5-C6-O6
13	S	4	MAN	C4-C5-C6-O6
10	N	4	MAN	O5-C5-C6-O6
14	T	2	NAG	O5-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
8	M	1	NAG	C3-C2-N2-C7
13	S	2	NAG	C3-C2-N2-C7
13	S	4	MAN	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
12	Q	2	NAG	O5-C5-C6-O6
10	N	6	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	J	1	NAG	C3-C2-N2-C7
8	M	2	NAG	C3-C2-N2-C7
8	M	2	NAG	C1-C2-N2-C7

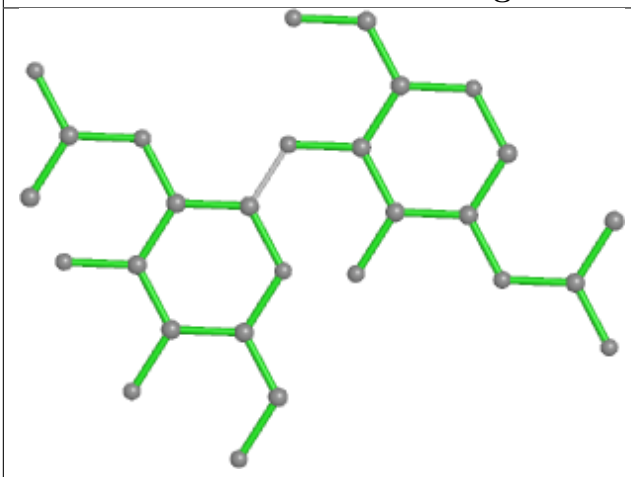
There are no ring outliers.

20 monomers are involved in 24 short contacts:

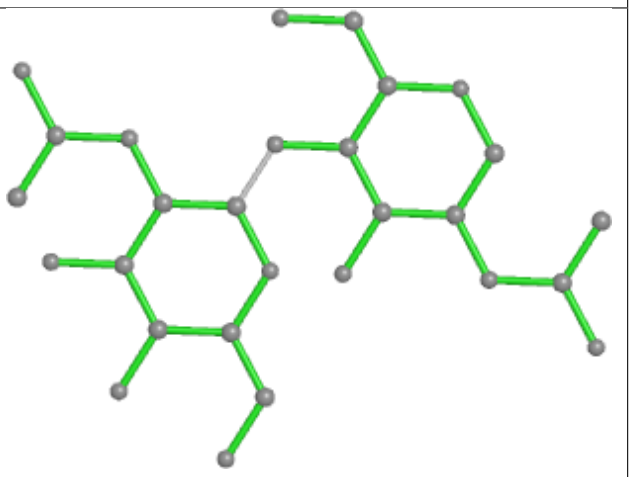
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	6	MAN	1	0
8	K	2	NAG	1	0
8	K	5	MAN	1	0
8	M	9	MAN	1	0
7	G	1	NAG	4	0
12	R	1	NAG	3	0
7	J	1	NAG	2	0
14	T	11	MAN	1	0
8	M	2	NAG	1	0
10	N	4	MAN	1	0
9	L	6	MAN	1	0
8	M	1	NAG	1	0
13	S	2	NAG	3	0
7	J	2	NAG	1	0
12	P	2	NAG	1	0
13	S	3	BMA	2	0
10	N	2	NAG	2	0
10	N	1	NAG	3	0
10	N	5	MAN	1	0
7	I	2	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.

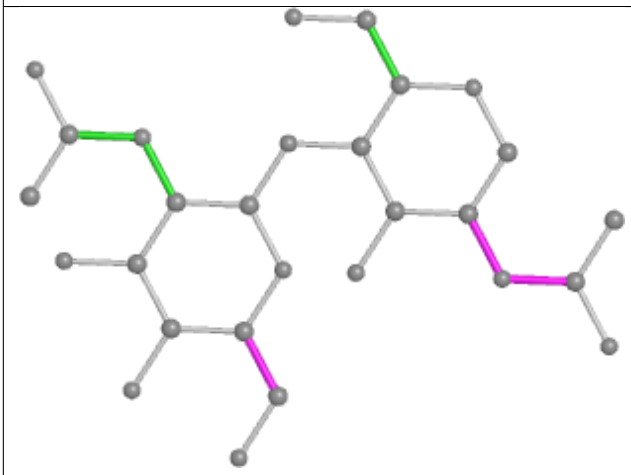
Oligosaccharide Chain G



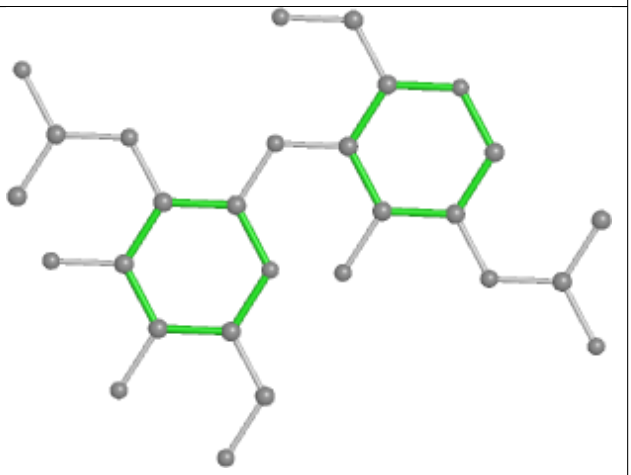
Bond lengths



Bond angles

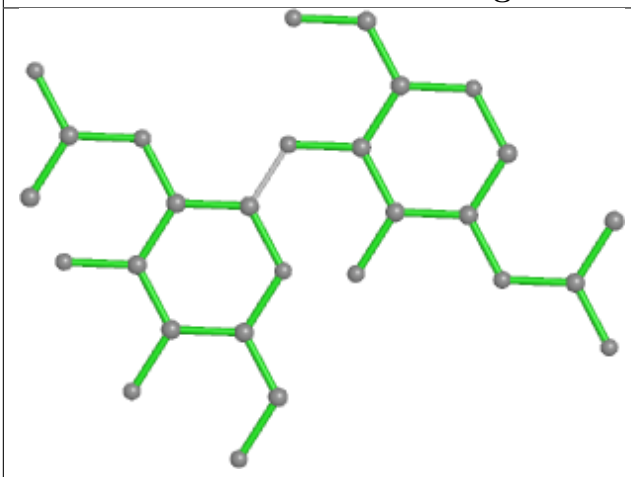


Torsions

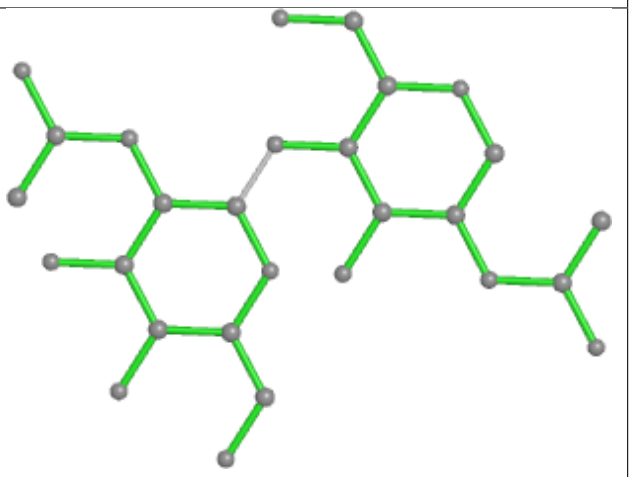


Rings

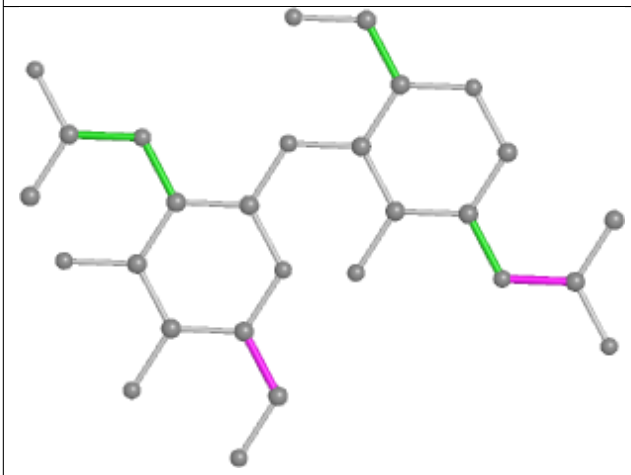
Oligosaccharide Chain H



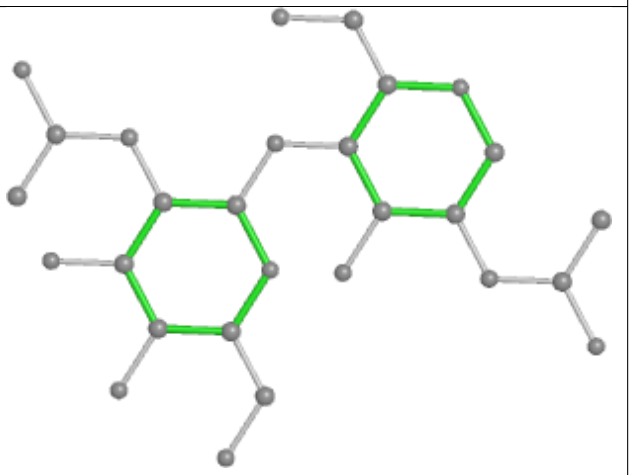
Bond lengths



Bond angles

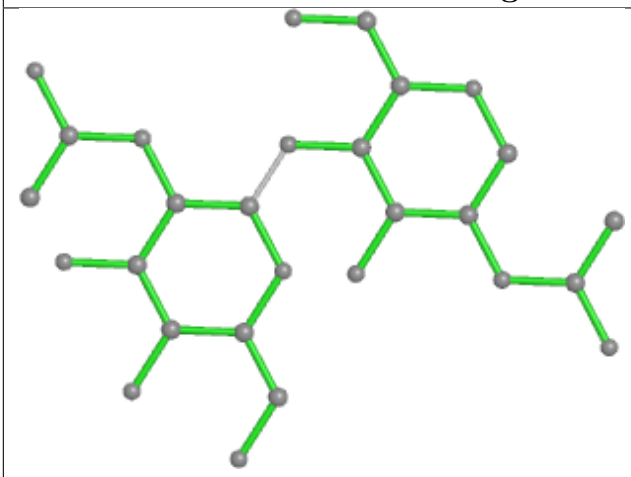


Torsions

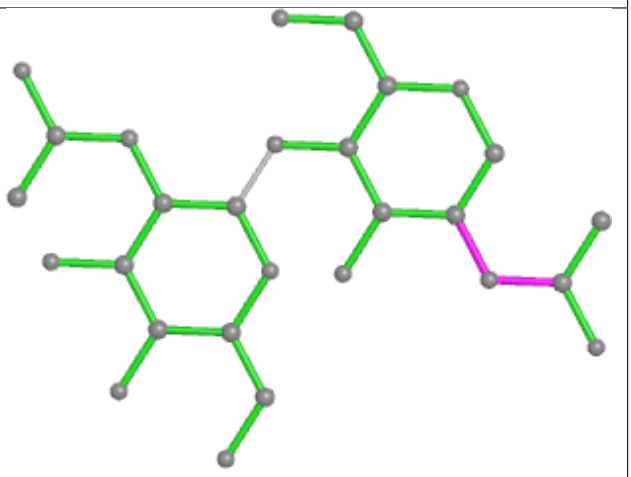


Rings

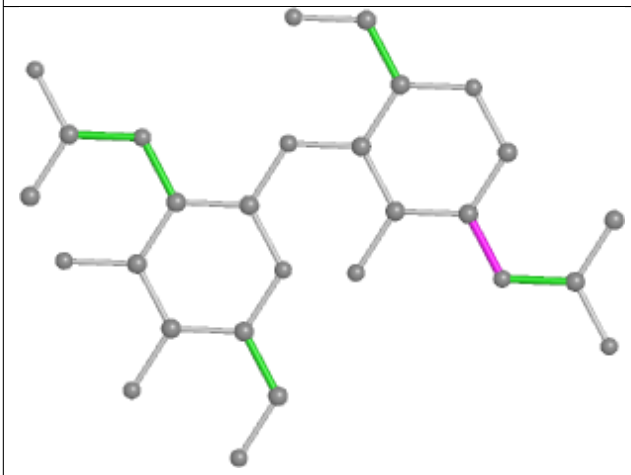
Oligosaccharide Chain I



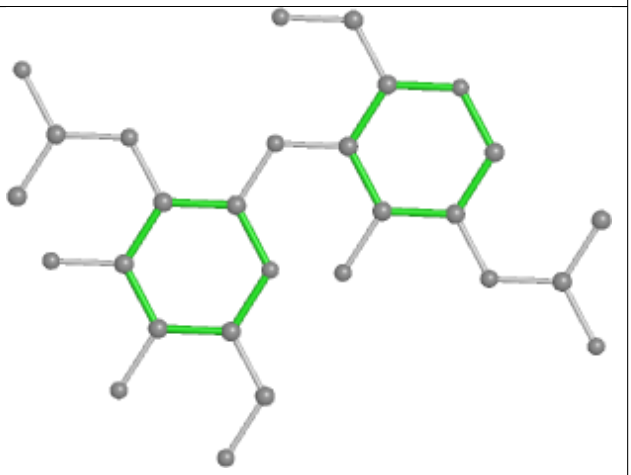
Bond lengths



Bond angles

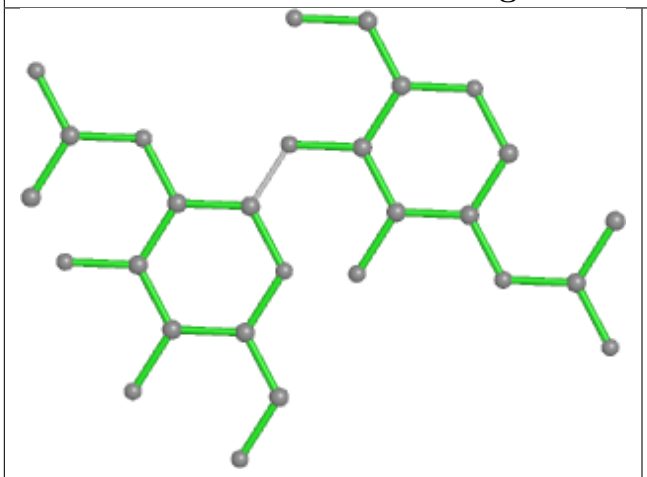


Torsions

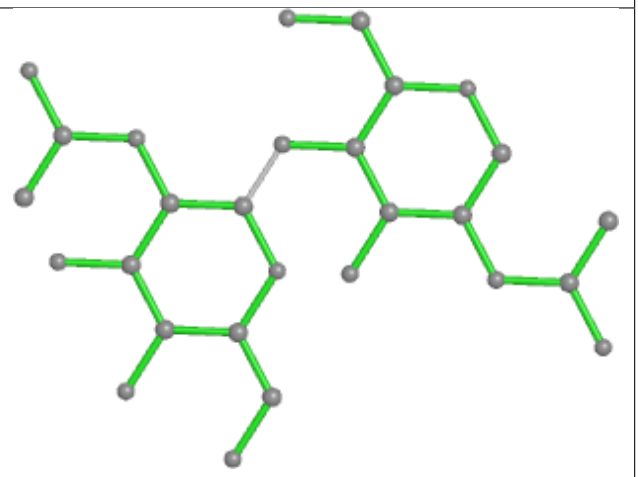


Rings

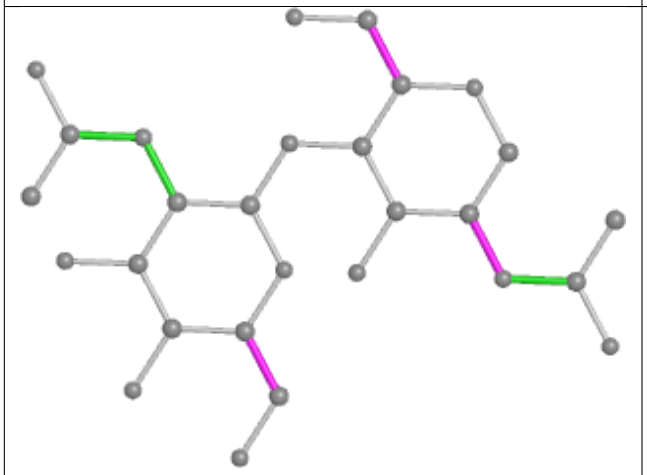
Oligosaccharide Chain J



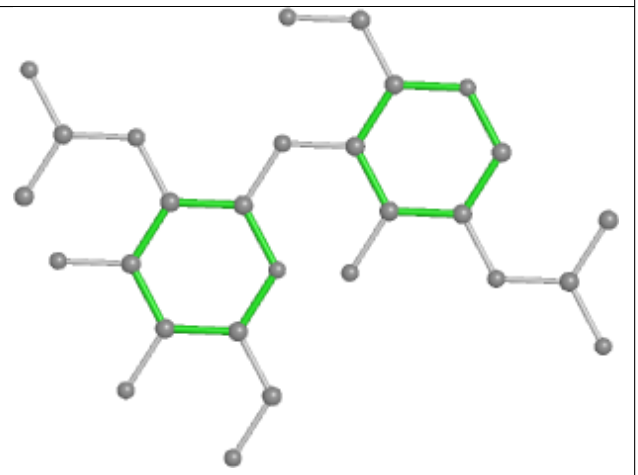
Bond lengths



Bond angles

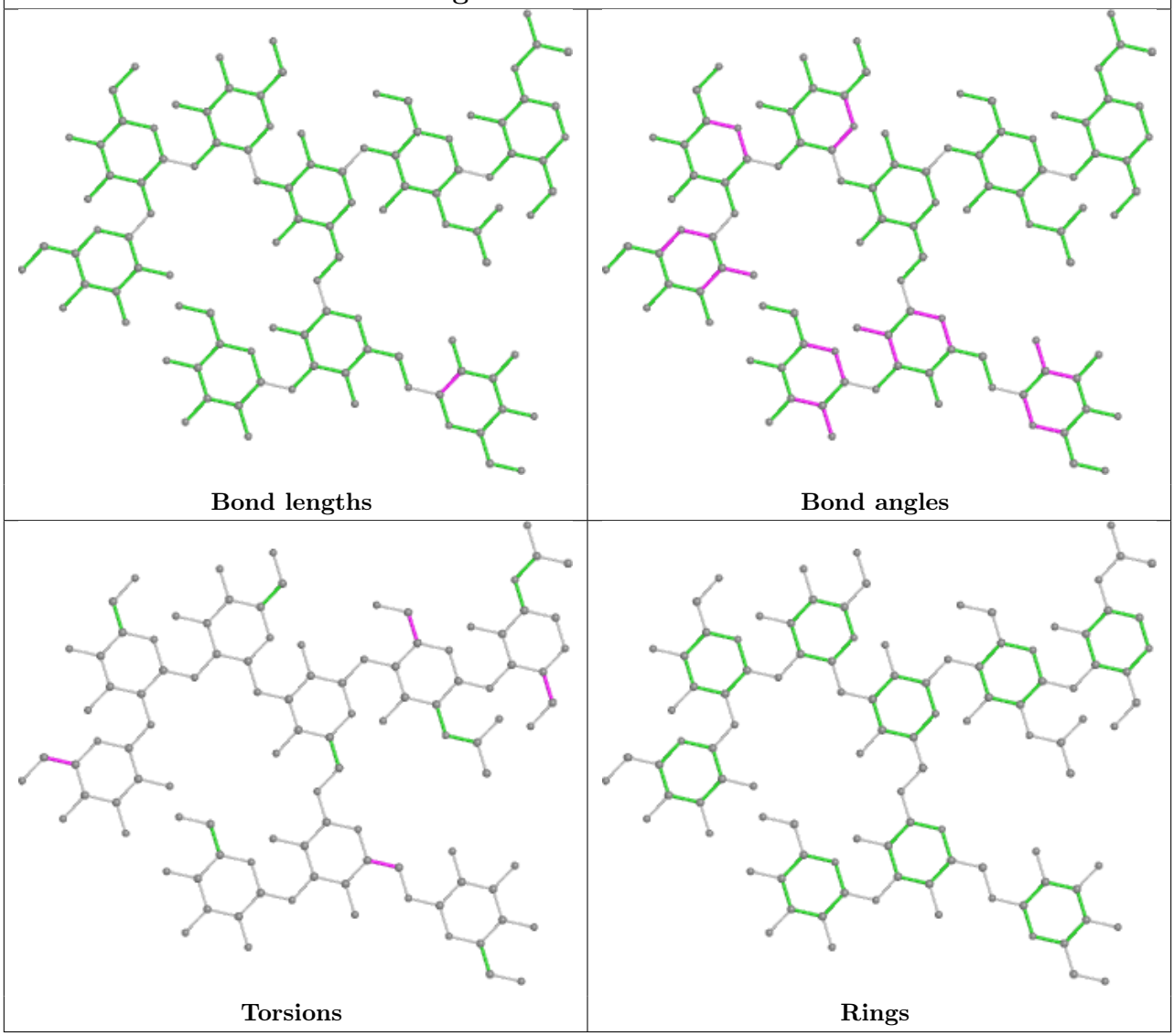


Torsions

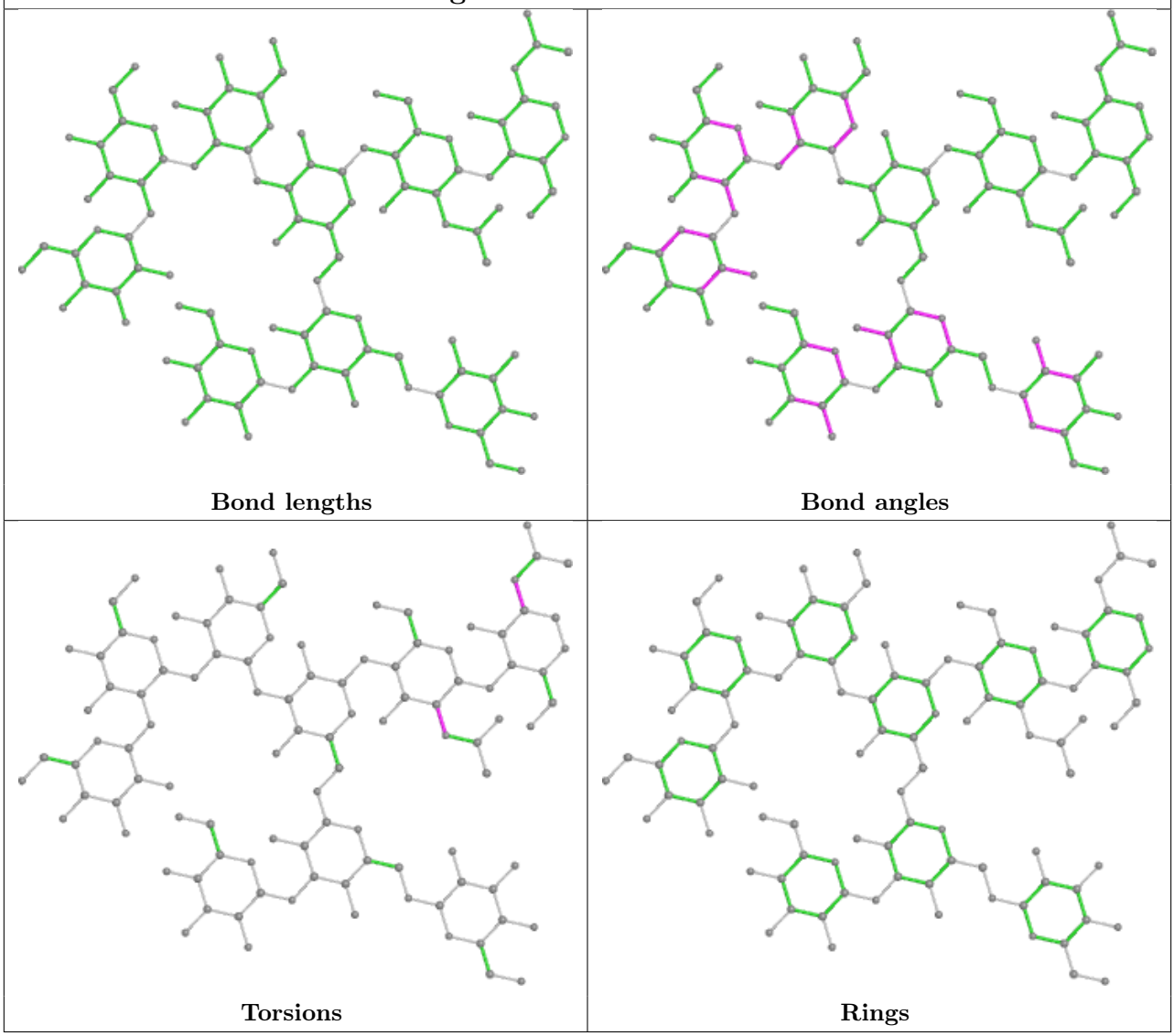


Rings

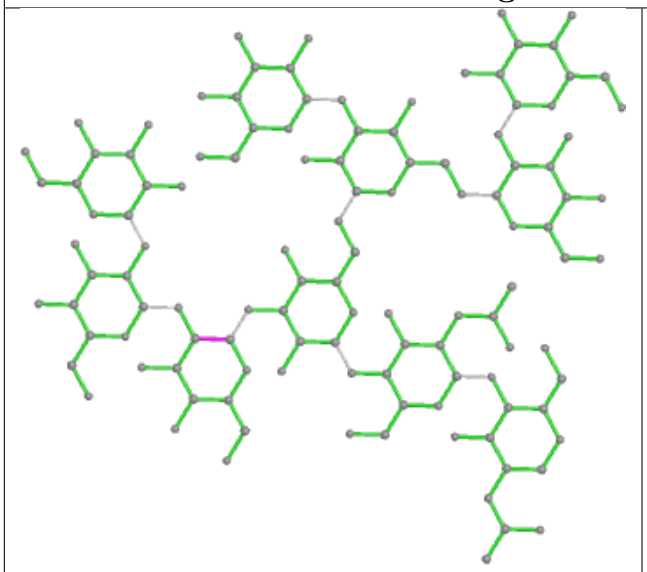
Oligosaccharide Chain K



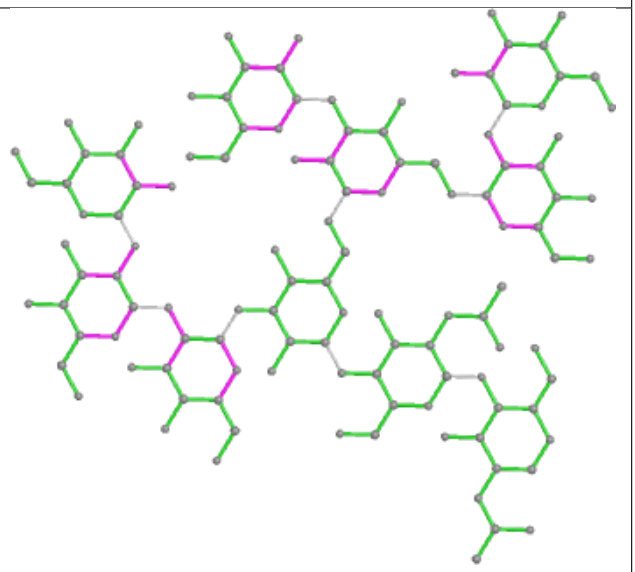
Oligosaccharide Chain M



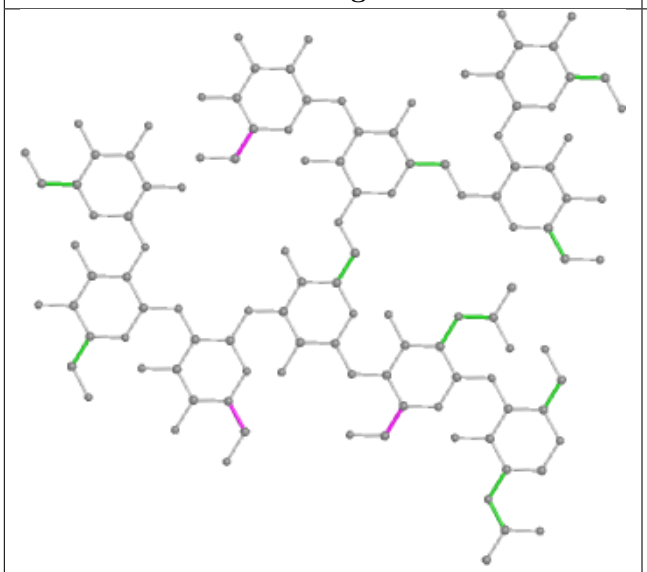
Oligosaccharide Chain L



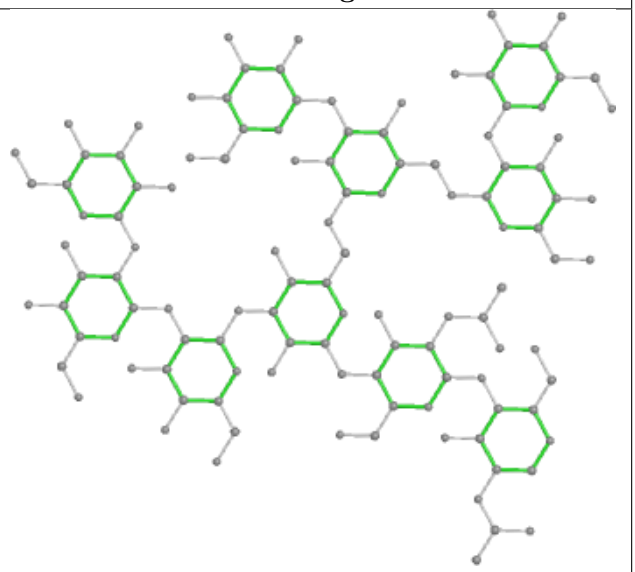
Bond lengths



Bond angles

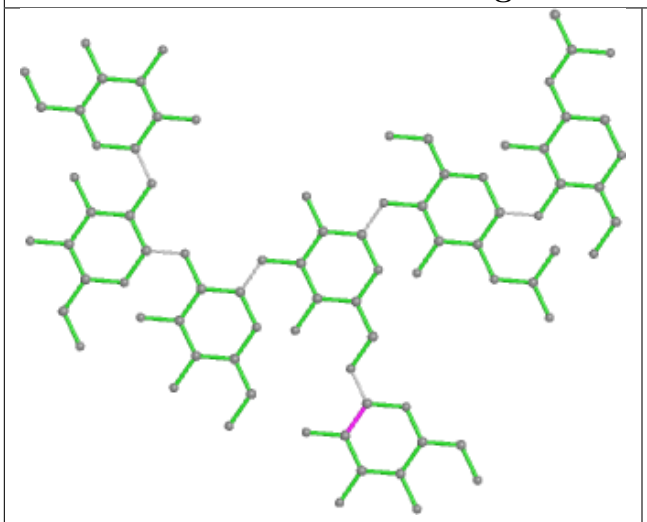


Torsions

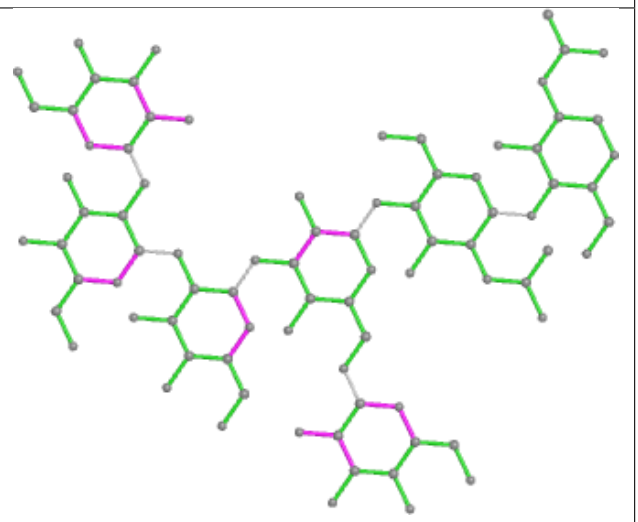


Rings

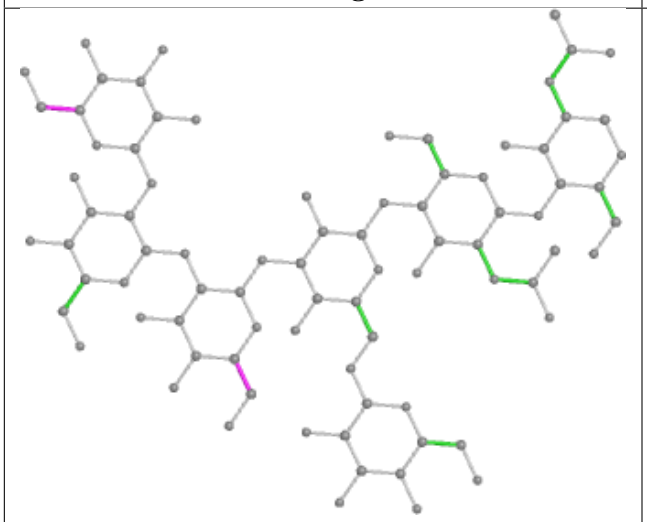
Oligosaccharide Chain N



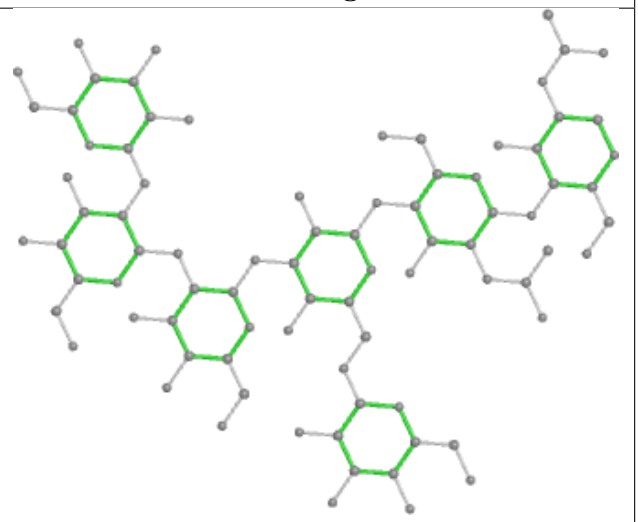
Bond lengths



Bond angles

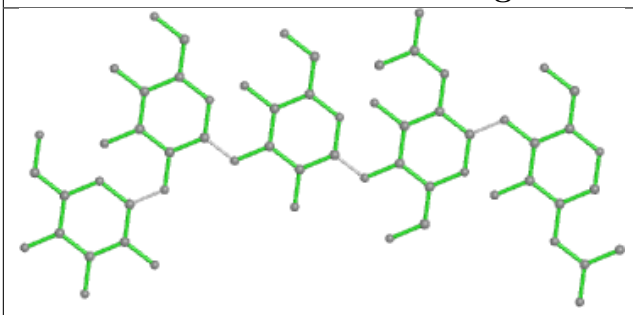


Torsions

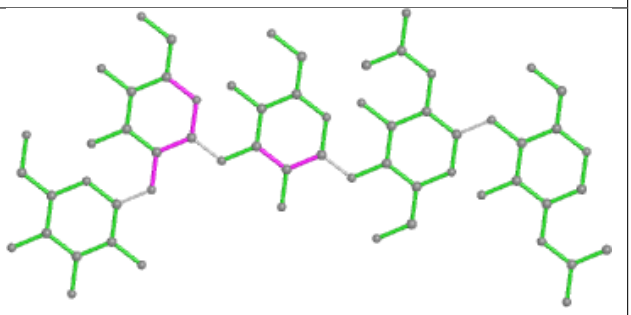


Rings

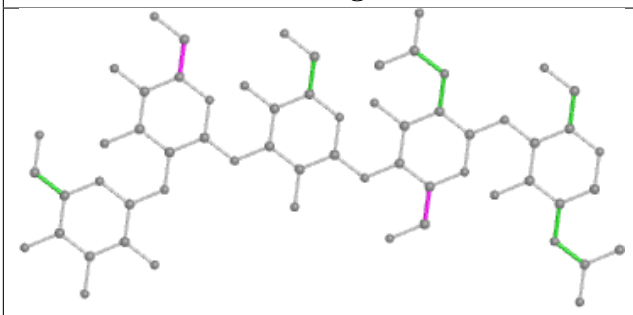
Oligosaccharide Chain O



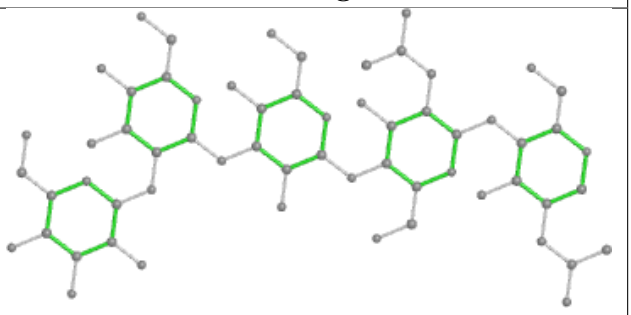
Bond lengths



Bond angles

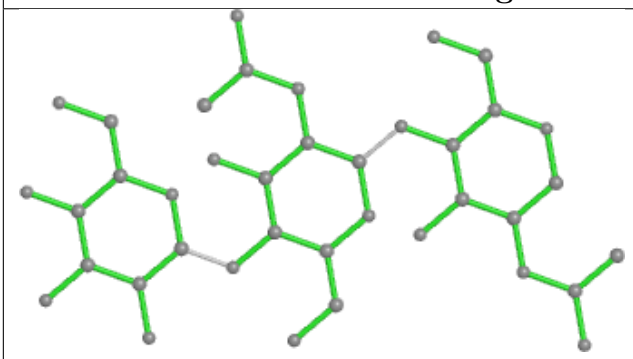


Torsions

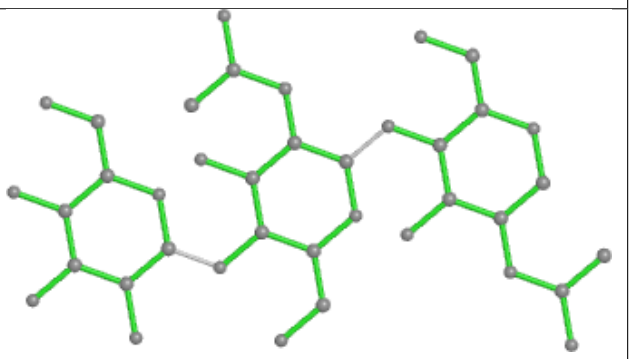


Rings

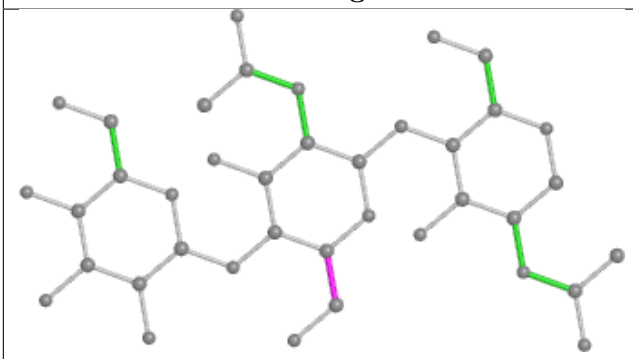
Oligosaccharide Chain P



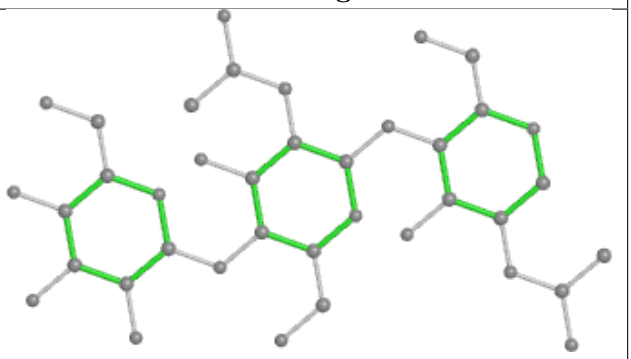
Bond lengths



Bond angles

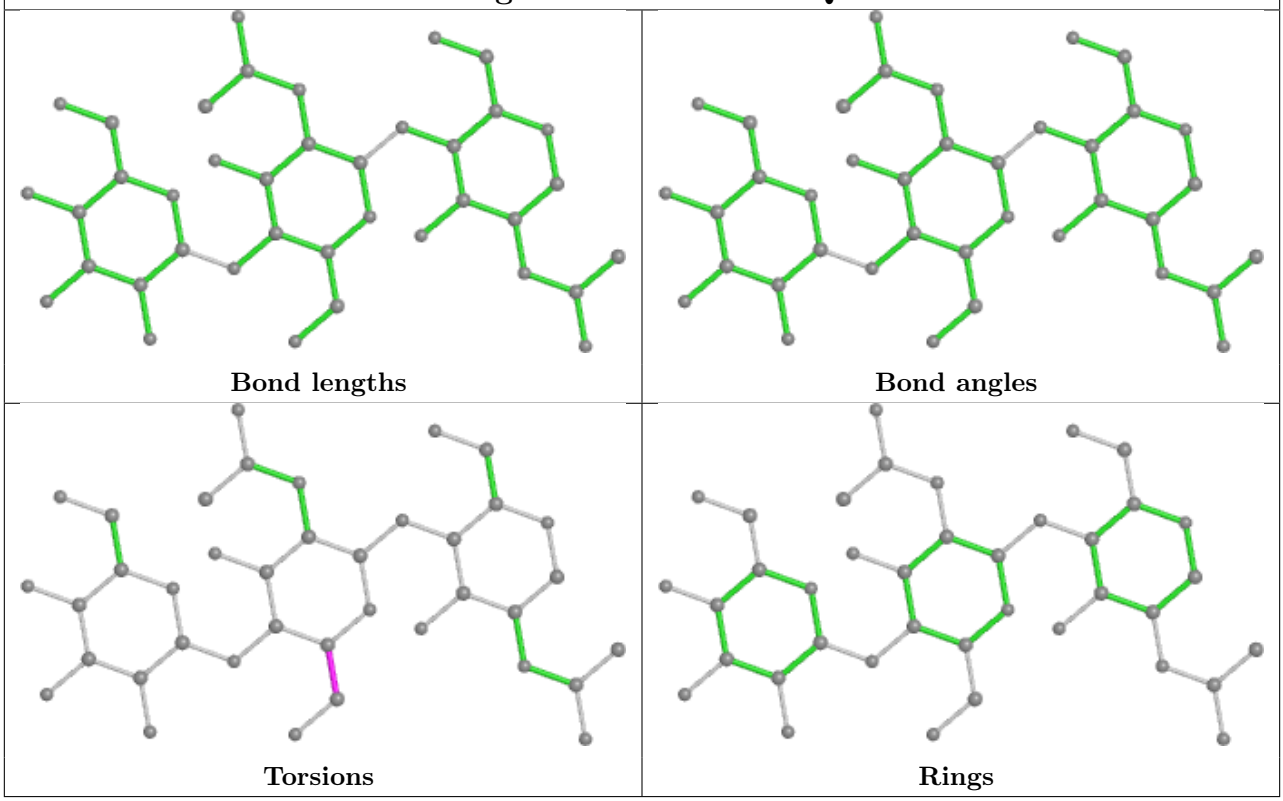


Torsions

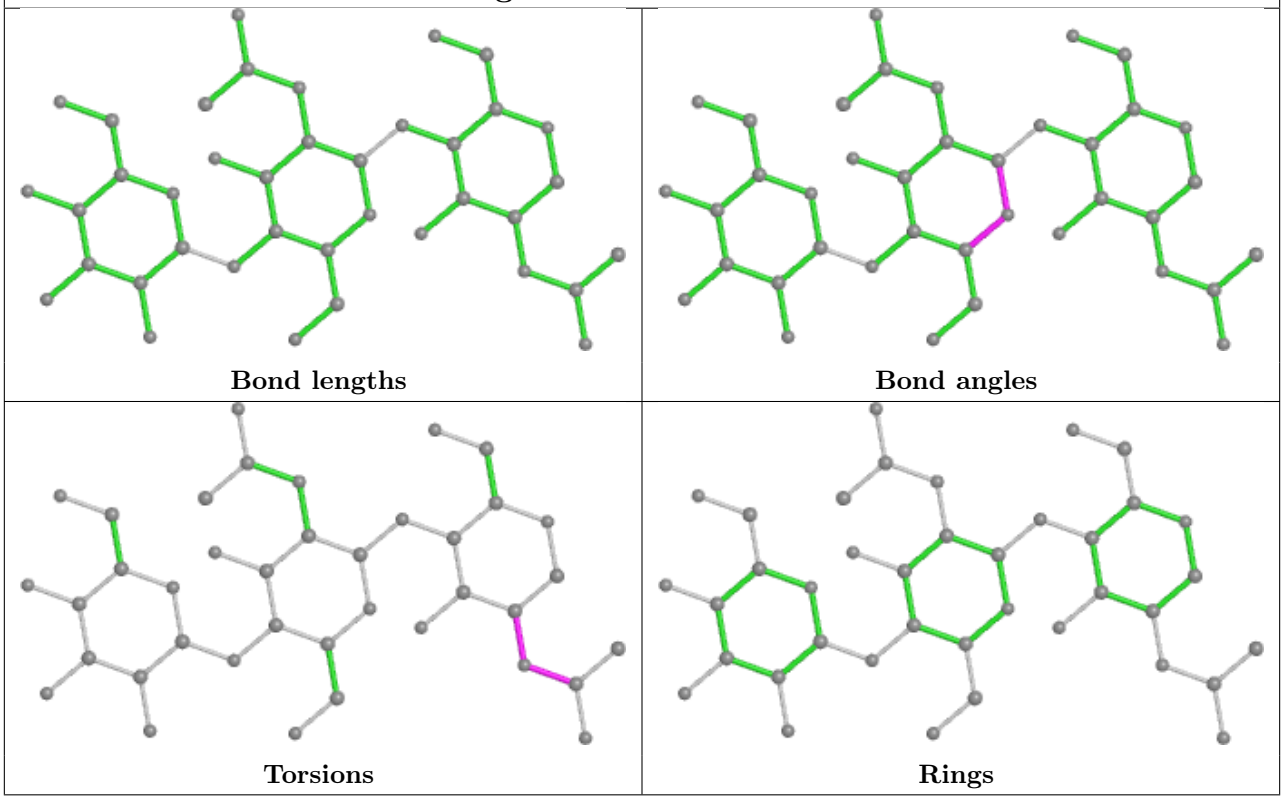


Rings

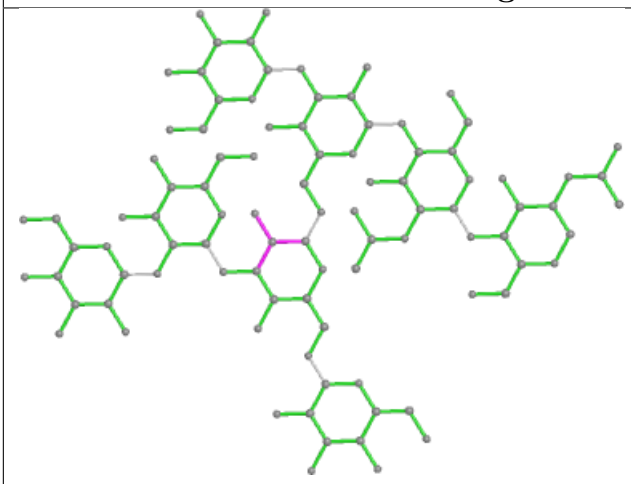
Oligosaccharide Chain Q



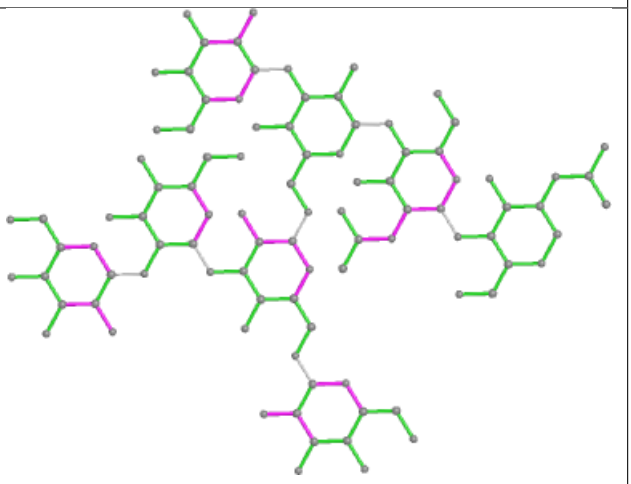
Oligosaccharide Chain R



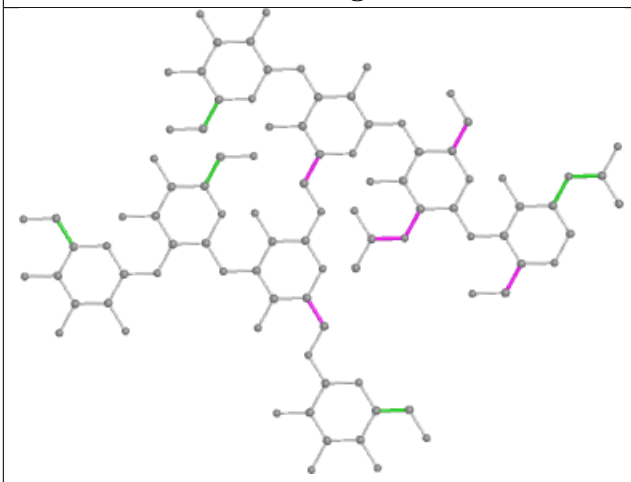
Oligosaccharide Chain S



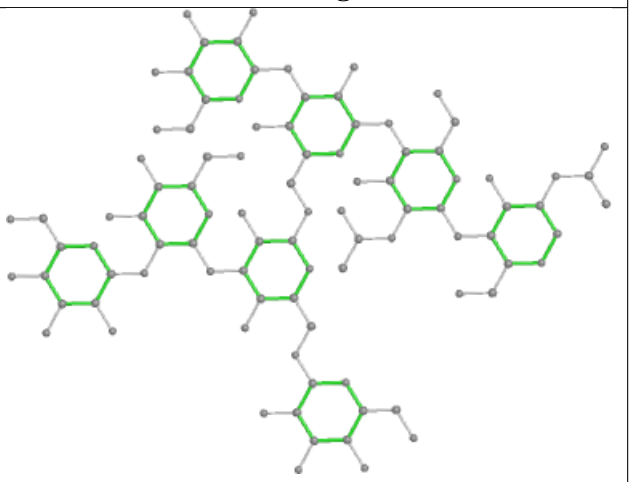
Bond lengths



Bond angles

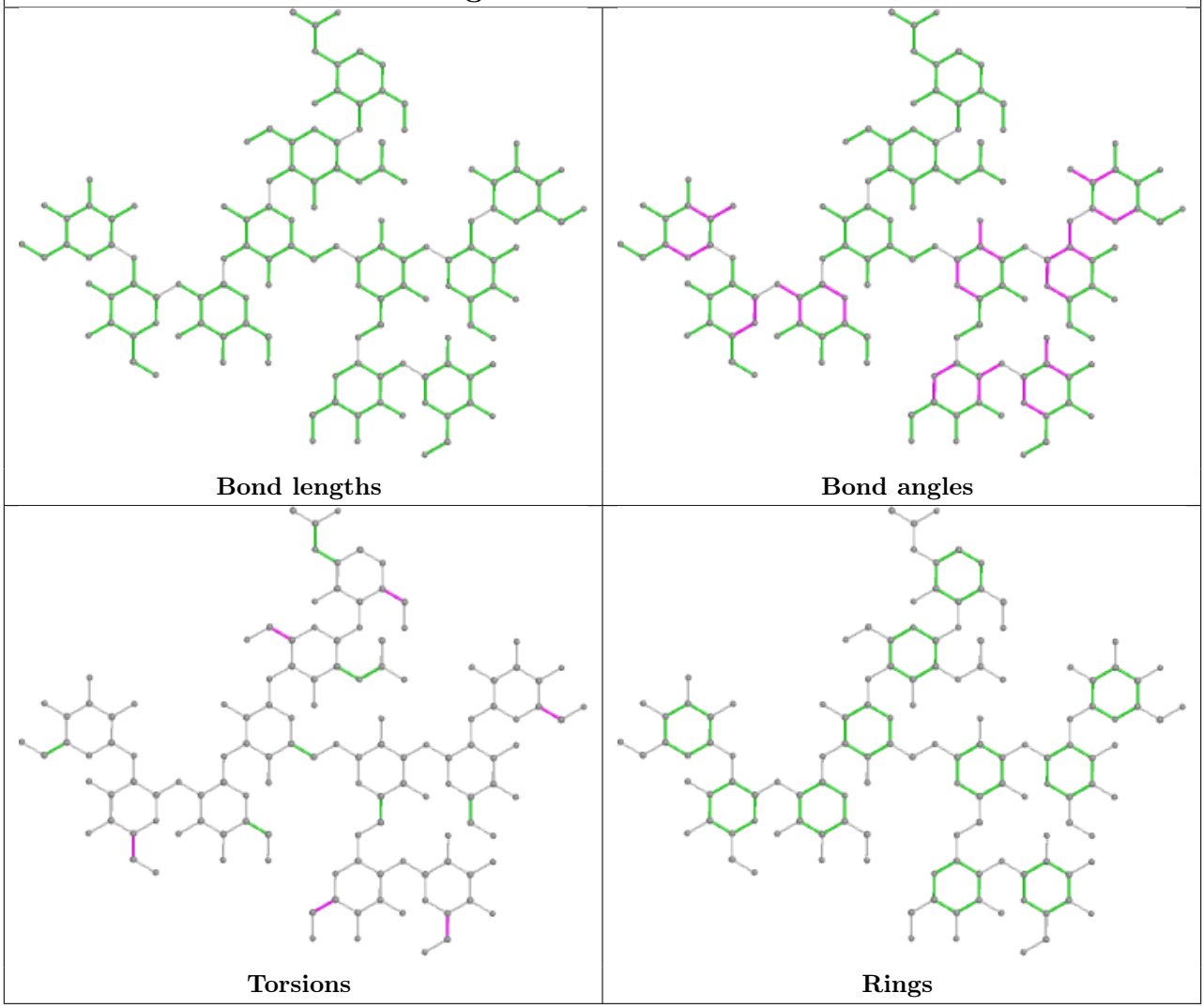


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
15	NAG	C	621	3	14,14,15	0.35	0	17,19,21	0.35	0
16	SO4	C	656	3	4,4,4	0.13	0	6,6,6	0.04	0
15	NAG	D	710	4	14,14,15	0.31	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	NAG	C	607	3	14,14,15	0.35	0	17,19,21	0.54	0
15	NAG	C	601	3	14,14,15	0.35	0	17,19,21	0.61	1 (5%)
15	NAG	C	604	3	14,14,15	0.29	0	17,19,21	0.44	0
15	NAG	D	709	4	14,14,15	0.22	0	17,19,21	0.41	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
15	NAG	C	621	3	-	2/6/23/26	0/1/1/1
15	NAG	D	710	4	-	2/6/23/26	0/1/1/1
15	NAG	C	607	3	-	4/6/23/26	0/1/1/1
15	NAG	C	601	3	-	2/6/23/26	0/1/1/1
15	NAG	C	604	3	-	4/6/23/26	0/1/1/1
15	NAG	D	709	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	601	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	709	NAG	O5-C5-C6-O6
15	C	601	NAG	O5-C5-C6-O6
15	C	621	NAG	C4-C5-C6-O6
15	C	621	NAG	O5-C5-C6-O6
15	D	710	NAG	O5-C5-C6-O6
15	D	709	NAG	C4-C5-C6-O6
15	C	604	NAG	C8-C7-N2-C2
15	C	604	NAG	O7-C7-N2-C2
15	C	607	NAG	C8-C7-N2-C2
15	C	607	NAG	O7-C7-N2-C2
15	C	604	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	601	NAG	C4-C5-C6-O6
15	D	710	NAG	C4-C5-C6-O6
15	C	607	NAG	O5-C5-C6-O6
15	C	604	NAG	O5-C5-C6-O6
15	C	607	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	607	NAG	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	230/239 (96%)	0.25	12 (5%)	27	24	183, 200, 258, 262	0
2	B	204/211 (96%)	0.48	13 (6%)	19	16	186, 226, 250, 255	0
3	C	450/487 (92%)	-0.10	5 (1%)	80	73	126, 172, 188, 202	0
4	D	122/153 (79%)	-0.25	0	100	100	128, 139, 177, 187	0
5	E	224/238 (94%)	-0.08	2 (0%)	84	77	136, 154, 186, 196	0
6	F	212/215 (98%)	-0.08	0	100	100	136, 157, 189, 192	0
All	All	1442/1543 (93%)	0.03	32 (2%)	62	53	126, 177, 247, 262	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	ALA	5.7
1	A	200	THR	5.2
2	B	142	GLY	4.5
2	B	141	PRO	4.2
2	B	158	GLY	4.0
1	A	225	VAL	4.0
2	B	156	LYS	3.6
2	B	143	ALA	3.6
2	B	110	LYS	3.5
3	C	189	LYS	3.4
5	E	1	GLN	3.4
3	C	185	ASN	3.3
1	A	199	GLY	3.3
2	B	111	ALA	3.2
1	A	226	GLU	3.1
2	B	149	LYS	3.0
2	B	206	GLU	2.8
1	A	100(I)	ALA	2.7
1	A	123	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	192	TYR	2.6
3	C	183	GLN	2.4
3	C	151	ARG	2.4
3	C	188	ASN	2.4
5	E	194	TYR	2.4
1	A	120	SER	2.4
1	A	168	SER	2.2
1	A	227	PRO	2.1
2	B	187	LYS	2.1
2	B	193	SER	2.1
1	A	222	ARG	2.1
1	A	36	TRP	2.0
1	A	139	ALA	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
12	BMA	Q	3	11/12	0.53	0.59	211,211,211,211	0
11	MAN	O	5	11/12	0.61	0.50	225,225,225,225	0
13	MAN	S	6	11/12	0.61	0.73	199,199,199,199	0
7	NAG	H	1	14/15	0.66	0.52	196,196,196,196	0
12	NAG	R	1	14/15	0.67	0.61	198,198,198,198	0
12	BMA	R	3	11/12	0.68	0.47	222,222,222,222	0
7	NAG	H	2	14/15	0.69	0.49	199,199,199,199	0
11	BMA	O	3	11/12	0.70	0.37	217,217,217,217	0
10	MAN	N	7	11/12	0.72	0.35	193,193,193,193	0
7	NAG	J	2	14/15	0.73	0.56	194,194,194,194	0
13	MAN	S	5	11/12	0.74	0.42	189,189,189,189	0
11	MAN	O	4	11/12	0.74	0.37	221,221,221,221	0
9	MAN	L	5	11/12	0.75	0.27	183,183,183,183	0
7	NAG	G	2	14/15	0.75	0.40	192,192,192,192	0
13	MAN	S	7	11/12	0.75	0.46	190,190,190,190	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	BMA	P	3	11/12	0.76	0.41	198,198,198,198	0
9	NAG	L	2	14/15	0.78	0.31	183,183,183,183	0
11	NAG	O	2	14/15	0.78	0.31	204,204,204,204	0
13	MAN	S	8	11/12	0.78	0.29	178,178,178,178	0
8	MAN	K	6	11/12	0.79	0.43	196,196,196,196	0
14	MAN	T	11	11/12	0.79	0.29	151,151,151,151	0
7	NAG	J	1	14/15	0.80	0.25	182,182,182,182	0
13	MAN	S	4	11/12	0.80	0.41	180,180,180,180	0
12	NAG	Q	1	14/15	0.80	0.56	197,197,197,197	0
12	NAG	Q	2	14/15	0.80	0.51	206,206,206,206	0
8	MAN	M	4	11/12	0.80	0.25	194,194,194,194	0
7	NAG	I	2	14/15	0.80	0.48	191,191,191,191	0
12	NAG	R	2	14/15	0.80	0.49	211,211,211,211	0
11	NAG	O	1	14/15	0.81	0.29	187,187,187,187	0
8	MAN	M	9	11/12	0.81	0.44	200,200,200,200	0
8	MAN	M	7	11/12	0.81	0.19	192,192,192,192	0
10	MAN	N	6	11/12	0.82	0.46	191,191,191,191	0
8	MAN	K	9	11/12	0.82	0.34	184,184,184,184	0
13	BMA	S	3	11/12	0.82	0.24	168,168,168,168	0
10	BMA	N	3	11/12	0.83	0.22	188,188,188,188	0
14	MAN	T	9	11/12	0.83	0.36	159,159,159,159	0
12	NAG	P	2	14/15	0.83	0.43	194,194,194,194	0
8	MAN	K	8	11/12	0.84	0.36	186,186,186,186	0
14	MAN	T	10	11/12	0.84	0.36	147,147,147,147	0
8	MAN	M	6	11/12	0.84	0.33	202,202,202,202	0
8	MAN	K	7	11/12	0.85	0.19	180,180,180,180	0
8	MAN	M	8	11/12	0.85	0.29	193,193,193,193	0
10	MAN	N	4	11/12	0.85	0.30	190,190,190,190	0
9	NAG	L	1	14/15	0.86	0.27	180,180,180,180	0
9	MAN	L	6	11/12	0.86	0.33	184,184,184,184	0
14	MAN	T	6	11/12	0.87	0.28	151,151,151,151	0
8	NAG	M	1	14/15	0.87	0.29	184,184,184,184	0
13	NAG	S	2	14/15	0.87	0.32	155,155,155,155	0
14	NAG	T	1	14/15	0.87	0.37	144,144,144,144	0
8	MAN	K	5	11/12	0.88	0.33	188,188,188,188	0
12	NAG	P	1	14/15	0.88	0.30	186,186,186,186	0
8	MAN	M	5	11/12	0.88	0.33	199,199,199,199	0
14	MAN	T	5	11/12	0.88	0.26	148,148,148,148	0
10	MAN	N	5	11/12	0.89	0.40	192,192,192,192	0
7	NAG	G	1	14/15	0.89	0.20	187,187,187,187	0
8	BMA	M	3	11/12	0.89	0.20	188,188,188,188	0
7	NAG	I	1	14/15	0.90	0.35	186,186,186,186	0

Continued on next page...

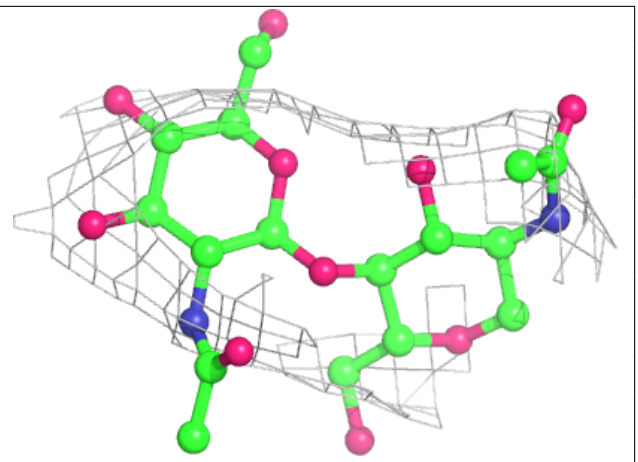
Continued from previous page...

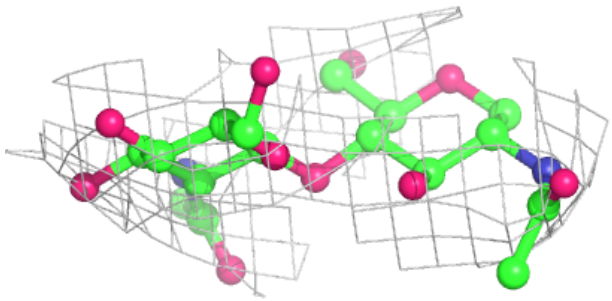
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	NAG	S	1	14/15	0.90	0.31	144,144,144,144	0
9	MAN	L	7	11/12	0.90	0.18	184,184,184,184	0
14	MAN	T	4	11/12	0.91	0.26	147,147,147,147	0
8	BMA	K	3	11/12	0.91	0.30	169,169,169,169	0
8	NAG	K	2	14/15	0.91	0.29	159,159,159,159	0
9	BMA	L	3	11/12	0.91	0.19	182,182,182,182	0
10	NAG	N	2	14/15	0.91	0.24	180,180,180,180	0
14	NAG	T	2	14/15	0.91	0.31	144,144,144,144	0
14	MAN	T	7	11/12	0.92	0.32	147,147,147,147	0
14	BMA	T	3	11/12	0.92	0.33	146,146,146,146	0
9	MAN	L	4	11/12	0.93	0.19	181,181,181,181	0
8	MAN	K	4	11/12	0.93	0.32	179,179,179,179	0
8	NAG	M	2	14/15	0.94	0.22	186,186,186,186	0
8	NAG	K	1	14/15	0.94	0.22	154,154,154,154	0
14	MAN	T	8	11/12	0.94	0.26	154,154,154,154	0
10	NAG	N	1	14/15	0.95	0.24	173,173,173,173	0
9	MAN	L	8	11/12	0.95	0.17	180,180,180,180	0
9	MAN	L	9	11/12	0.95	0.11	182,182,182,182	0
9	MAN	L	10	11/12	0.95	0.15	186,186,186,186	0

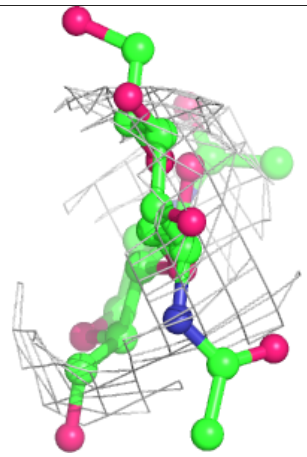
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

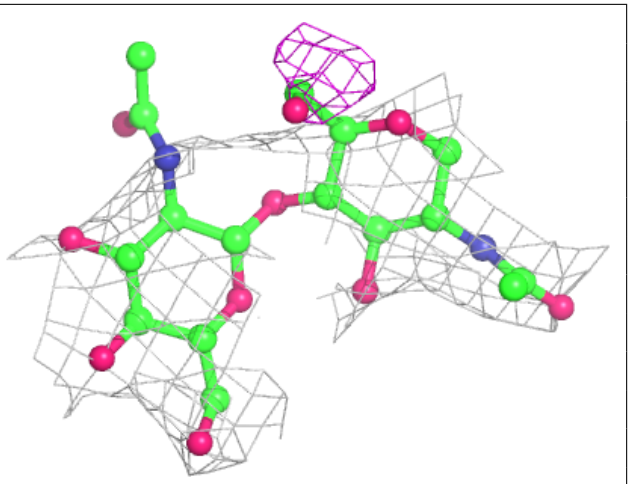


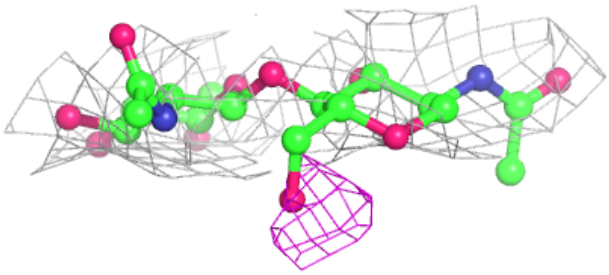


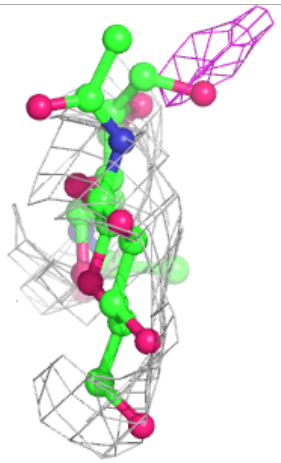


Electron density around Chain H:

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

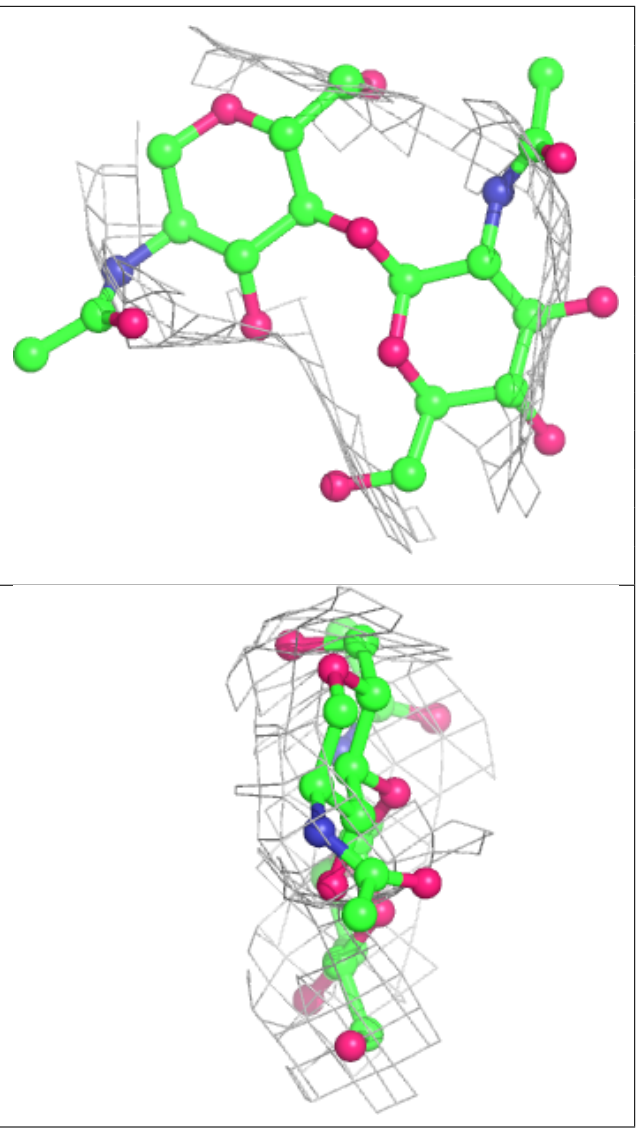






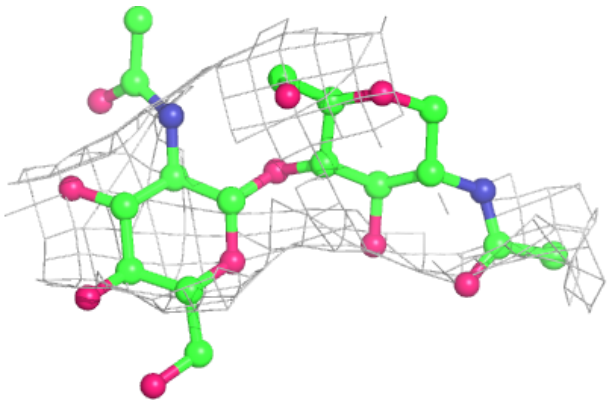
Electron density around Chain I:

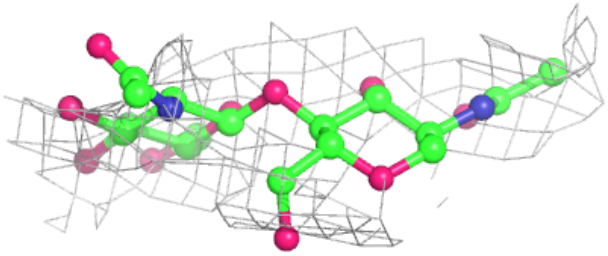
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

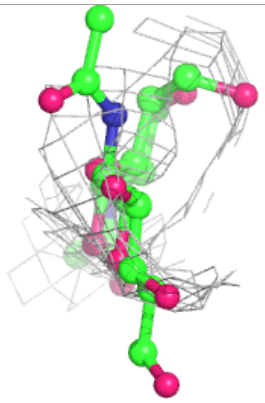


Electron density around Chain J:

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

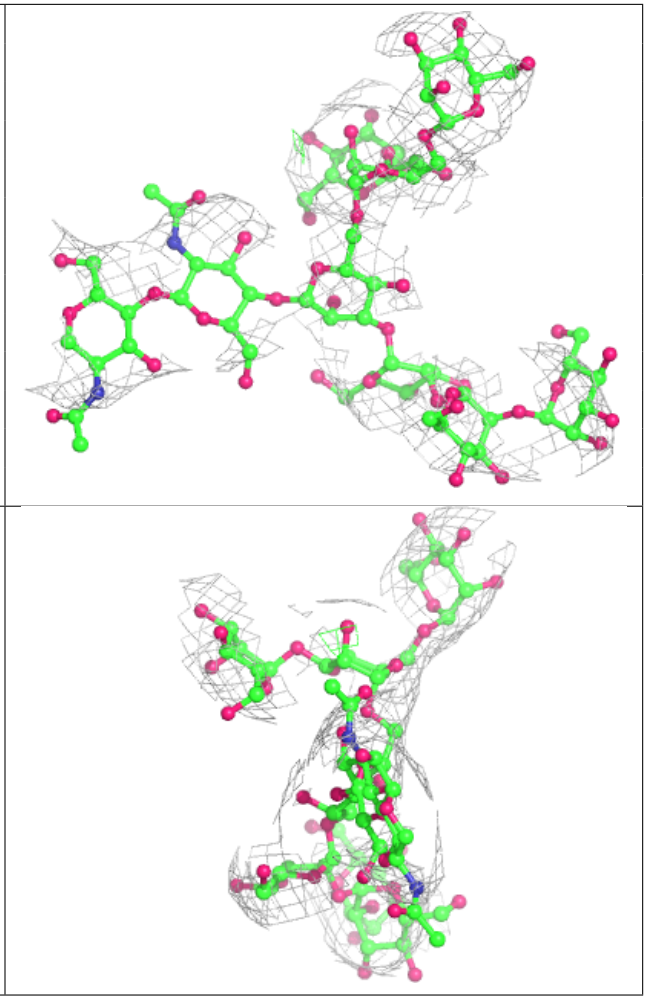






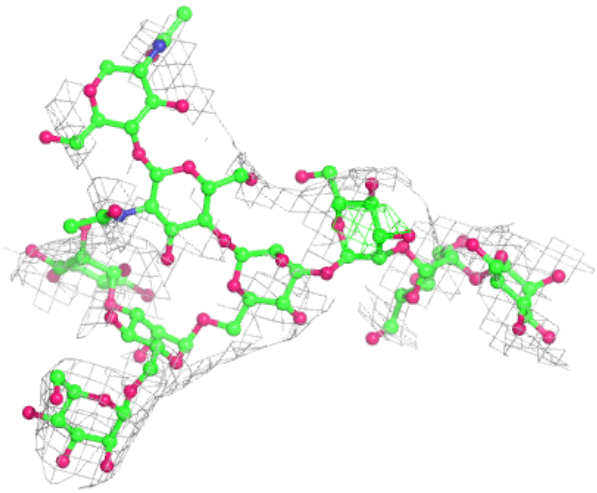
Electron density around Chain K:

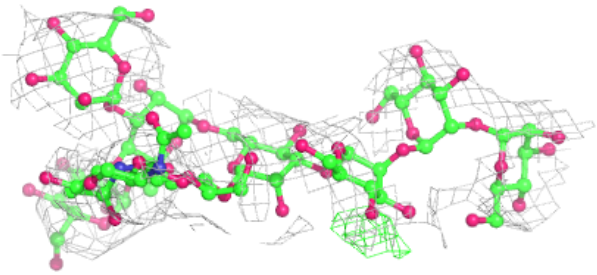
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

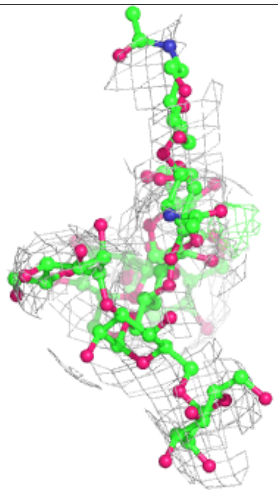


Electron density around Chain M:

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

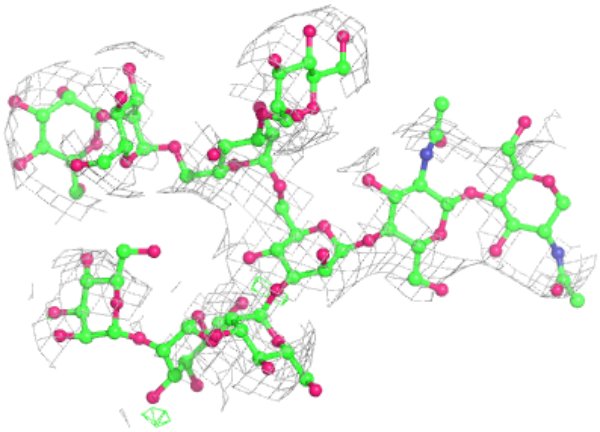


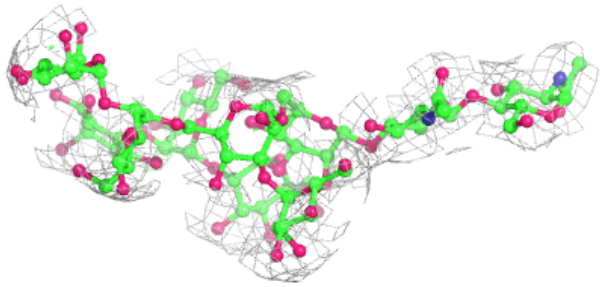


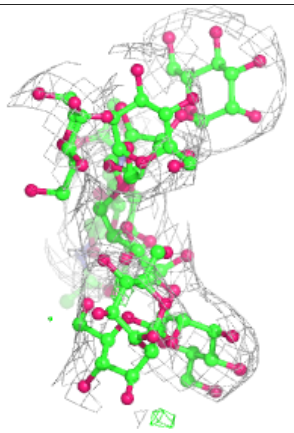


Electron density around Chain L:

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

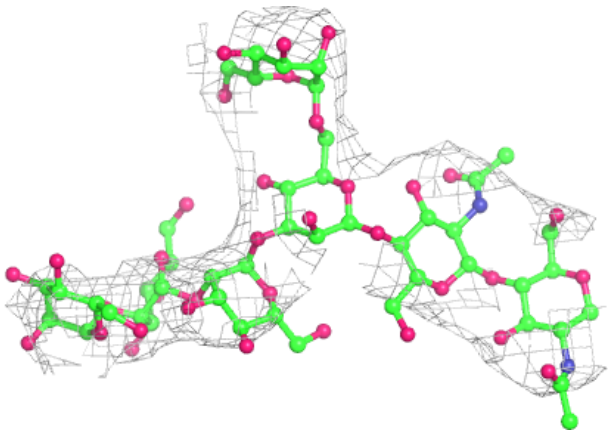


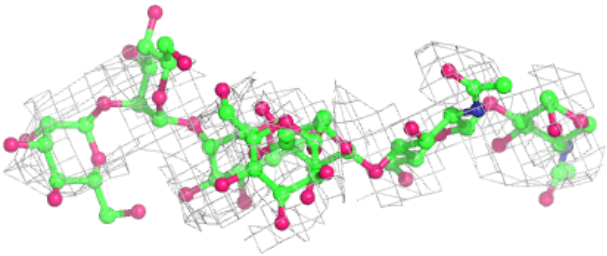


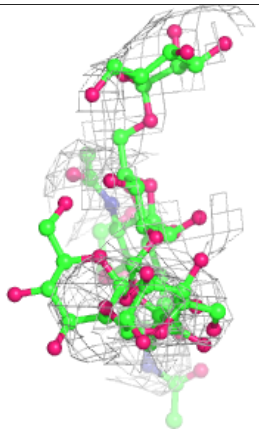


Electron density around Chain N:

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

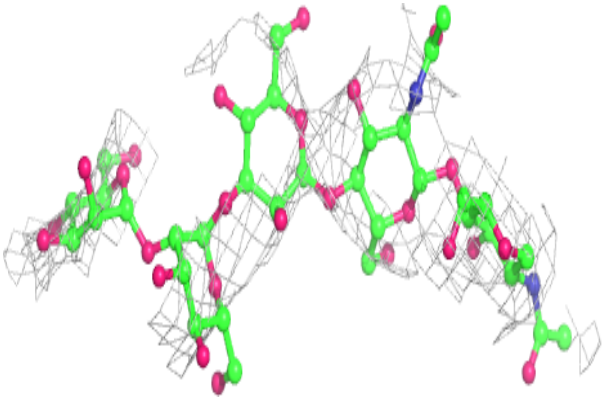


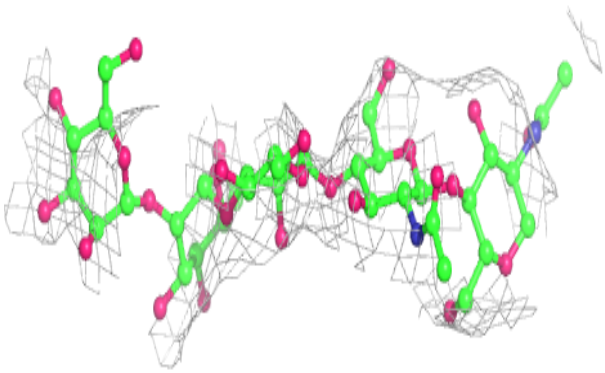


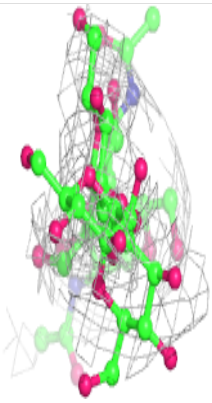


Electron density around Chain O:

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

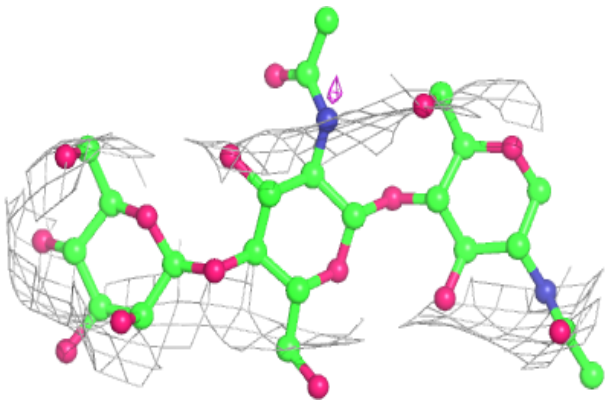


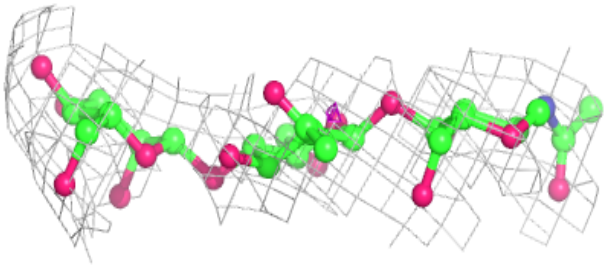


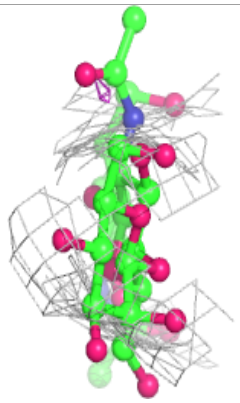


Electron density around Chain P:

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

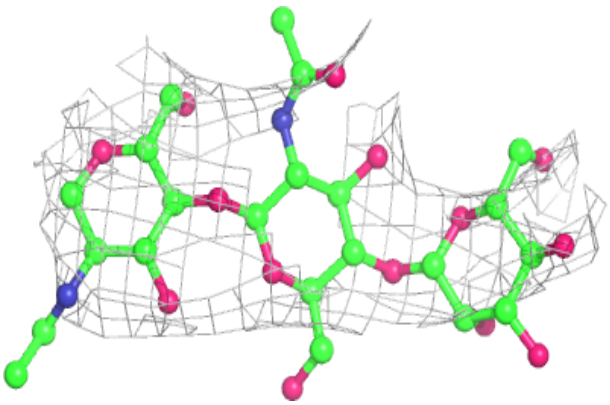


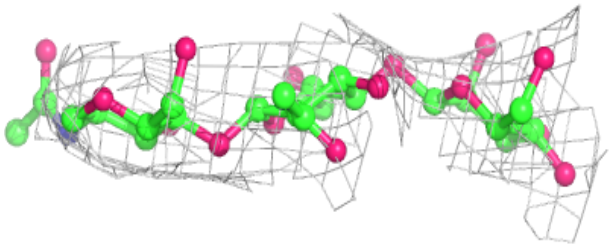


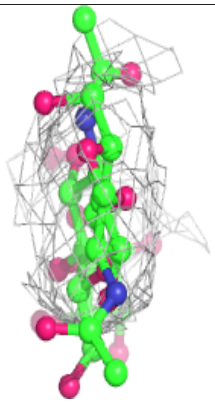


Electron density around Chain Q:

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

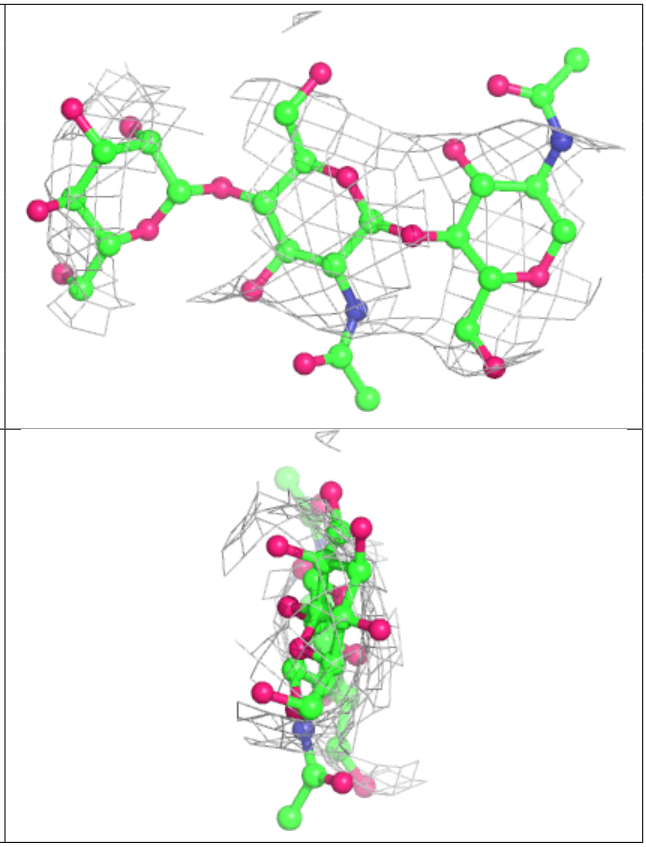






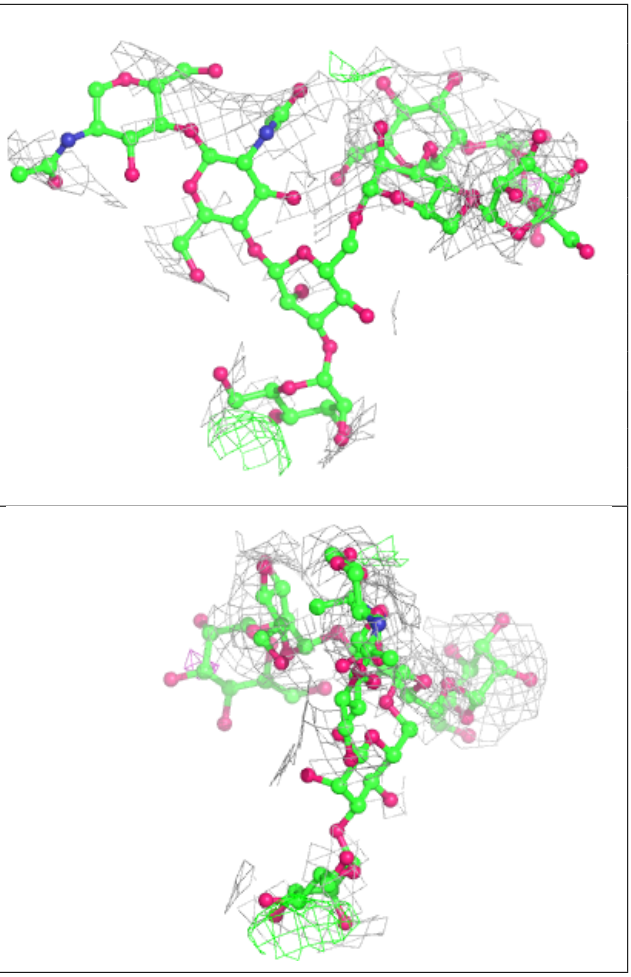
Electron density around Chain R:

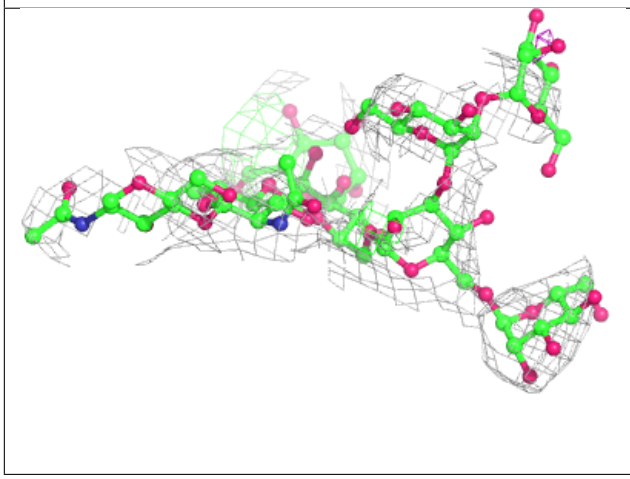
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain S:

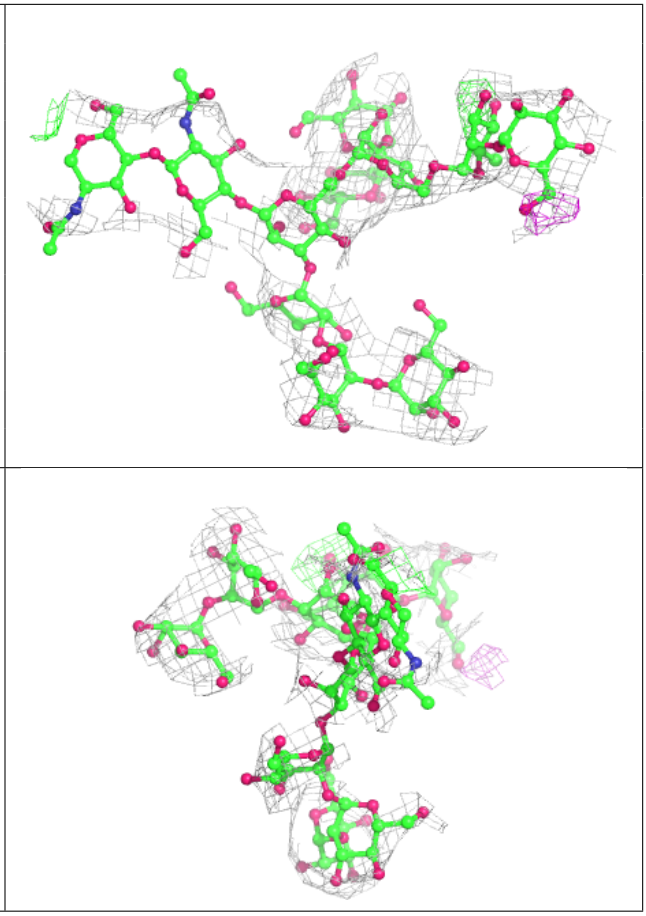
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around Chain T:

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



6.4 Ligands (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
15	NAG	C	621	14/15	0.57	0.66	198,198,198,198	0
16	SO4	C	656	5/5	0.66	0.39	171,171,171,171	0
15	NAG	C	601	14/15	0.70	0.47	144,144,144,144	0
15	NAG	C	604	14/15	0.77	0.37	184,184,184,184	0
15	NAG	D	709	14/15	0.79	0.37	143,143,143,143	0
15	NAG	C	607	14/15	0.89	0.21	177,177,177,177	0
15	NAG	D	710	14/15	0.91	0.23	145,145,145,145	0

6.5 Other polymers (i)

There are no such residues in this entry.