Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 08:52 PM EDT

PDB ID	:	6CH9
Title	:	Crystal structure of a natively-glycosylated B41 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2018-02-22
Resolution	:	4.85 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:

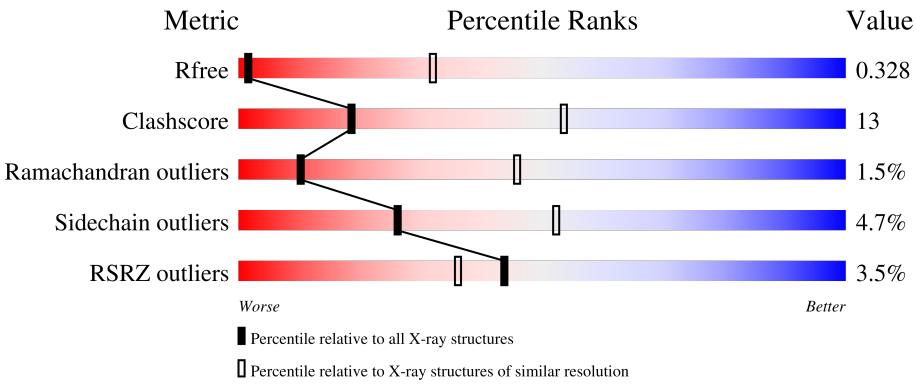
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.85 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	1098 (5.82-3.80)
Clashscore	141614	1172 (5.82-3.80)
Ramachandran outliers	138981	1107 (5.82-3.80)
Sidechain outliers	138945	1087 (5.82-3.80)
RSRZ outliers	127900	1128 (5.98-3.70)

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	B	153	4%, 67%, 21%, •, 11%
2	D	243	4%, 87%, 9%, •, •
3	E	216	4%, 88%, 10%, •
4	G	518	%, 61%, 20%, 5%, •, 14%
5	Q	240	5%, 72%, 21%, •, •

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Mol	Chain	Length	Quality of chain
6	R	215	4% 79% 16% 5%
7	A	3	100%
7	C	3	67% 33%
7	H	3	67% 33%
7	J	3	100%
7	O	3	33% 67%
7	P	3	67% 33%
7	T	3	100%
8	F	4	25% 75%
9	I	2	100%
9	K	2	50% 50%
9	N	2	50% 50%
10	L	6	50% 50%
11	M	4	75% 25%
12	S	5	60% 40%
13	U	6	33% 67%

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
10	NAG	L	1	-	-	X	-
13	NAG	U	1	-	-	X	-
13	MAN	U	5	-	-	-	X
7	NAG	A	1	-	-	-	X
7	NAG	A	2	-	-	-	X
7	BMA	A	3	-	-	-	X
7	BMA	H	3	-	-	-	X
8	MAN	F	4	-	-	X	-
9	NAG	K	1	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 11974 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	136	1094	692	188	206	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	236	1777	1129	296	344	8	0	0	0

- Molecule 3 is a protein called 35O22 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	213	1615	1012	267	328	8	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	448	3499	2198	617	658	26	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	MET	-	initiating methionine	UNP B3UES2
G	-3	ASP	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	ALA	-	expression tag	UNP B3UES2
G	-1	MET	-	expression tag	UNP B3UES2
G	0	LYS	-	expression tag	UNP B3UES2
G	1	ARG	-	expression tag	UNP B3UES2
G	2	GLY	-	expression tag	UNP B3UES2
G	3	LEU	-	expression tag	UNP B3UES2
G	4	CYS	-	expression tag	UNP B3UES2
G	5	CYS	-	expression tag	UNP B3UES2
G	6	VAL	-	expression tag	UNP B3UES2
G	7	LEU	-	expression tag	UNP B3UES2
G	8	LEU	-	expression tag	UNP B3UES2
G	9	LEU	-	expression tag	UNP B3UES2
G	10	CYS	-	expression tag	UNP B3UES2
G	11	GLY	-	expression tag	UNP B3UES2
G	12	ALA	-	expression tag	UNP B3UES2
G	13	VAL	-	expression tag	UNP B3UES2
G	14	PHE	-	expression tag	UNP B3UES2
G	15	VAL	-	expression tag	UNP B3UES2
G	16	SER	-	expression tag	UNP B3UES2
G	17	PRO	-	expression tag	UNP B3UES2
G	18	SER	-	expression tag	UNP B3UES2
G	19	GLN	-	expression tag	UNP B3UES2
G	20	GLU	-	expression tag	UNP B3UES2
G	21	ILE	-	expression tag	UNP B3UES2
G	22	HIS	-	expression tag	UNP B3UES2
G	23	ALA	-	expression tag	UNP B3UES2
G	24	ARG	-	expression tag	UNP B3UES2
G	25	PHE	-	expression tag	UNP B3UES2
G	26	ARG	-	expression tag	UNP B3UES2
G	27	ARG	-	expression tag	UNP B3UES2
G	28	GLY	-	expression tag	UNP B3UES2
G	29	ALA	-	expression tag	UNP B3UES2
G	30	ARG	-	expression tag	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2

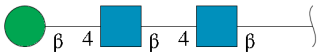
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	Q	231	1731	1089	298	336	8	0	0	0

- Molecule 6 is a protein called BG18 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	R	205	1540	963	257	314	6	0	0	0

- Molecule 7 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			
7	A	3	39	22	2	15	0	0	0
7	C	3	39	22	2	15	0	0	0
7	H	3	39	22	2	15	0	0	0
7	J	3	39	22	2	15	0	0	0
7	O	3	39	22	2	15	0	0	0
7	P	3	39	22	2	15	0	0	0
7	T	3	39	22	2	15	0	0	0

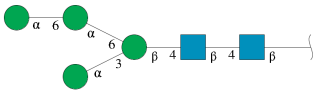
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 9 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			
9	I	2	28	16	2	10	0	0	0
9	K	2	28	16	2	10	0	0	0
9	N	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called 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.

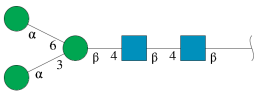


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	L	6	72	40	2	30	0	0	0

- Molecule 11 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.

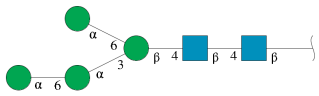
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	M	4	50	28	2	20	0	0	0

- Molecule 12 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.



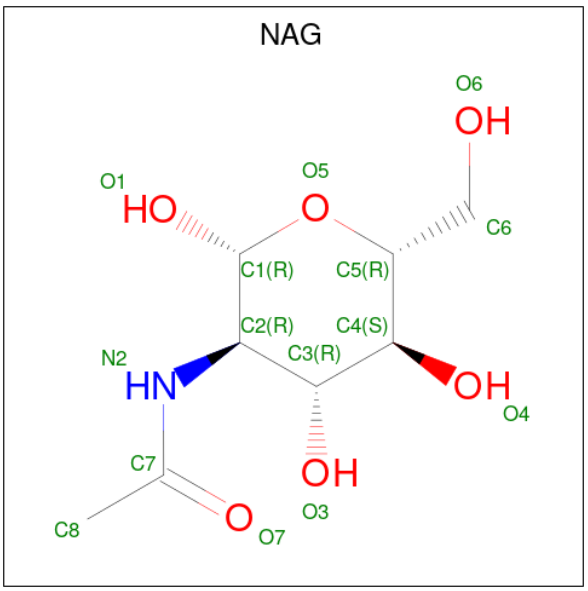
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	S	5	61	34	2	25	0	0	0

- Molecule 13 is an oligosaccharide called 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			
13	U	6	72	40	2	30	0	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



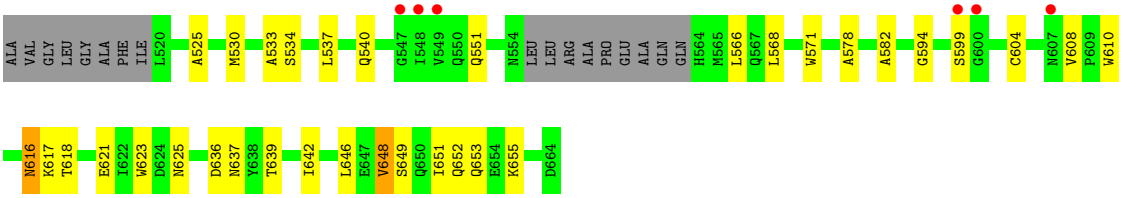
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	B	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0

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.

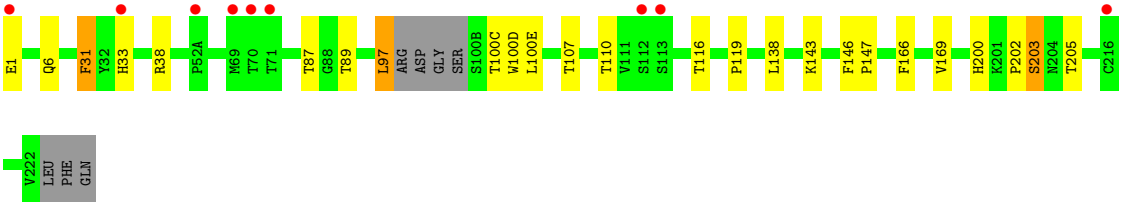
• Molecule 1: Envelope glycoprotein gp41

Chain B:



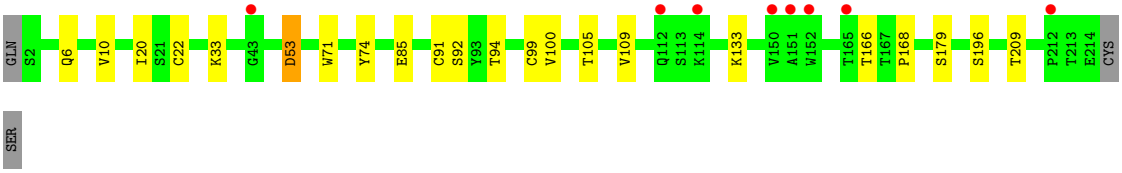
• Molecule 2: 35O22 Heavy Chain

Chain D:



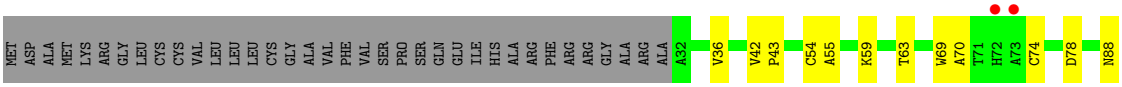
• Molecule 3: 35O22 Light Chain

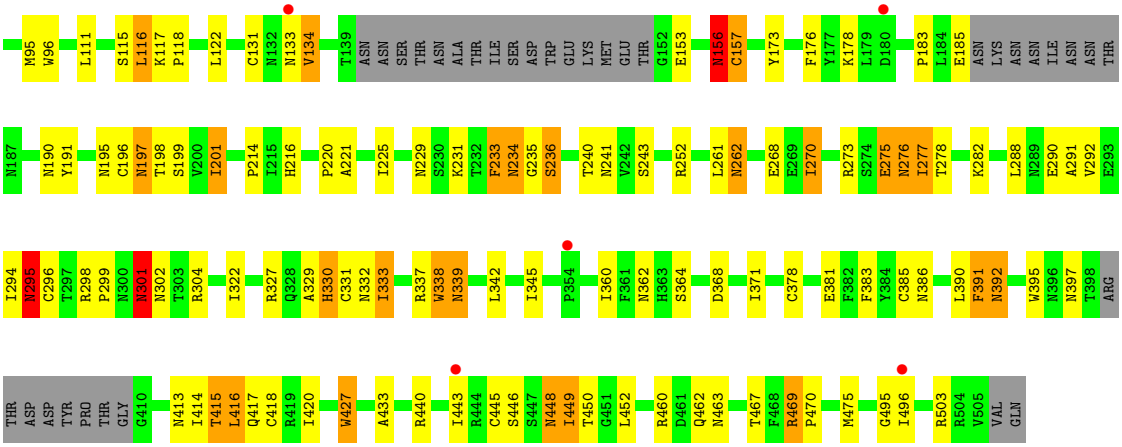
Chain E:



• Molecule 4: Envelope glycoprotein gp120

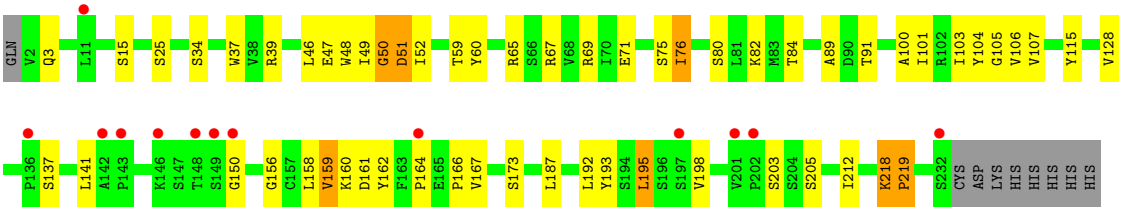
Chain G:





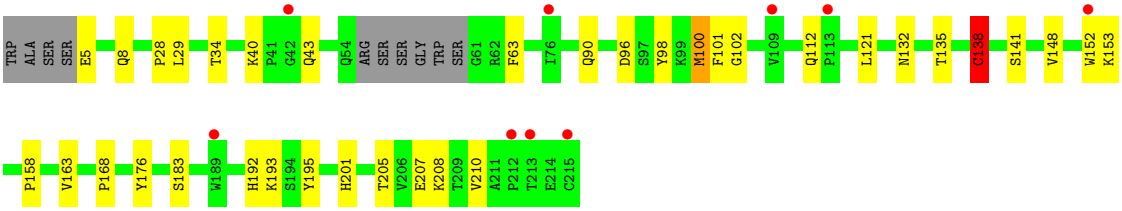
• Molecule 5: BG18 Heavy Chain

Chain Q:



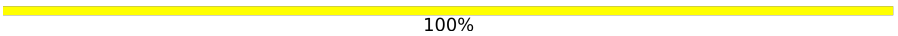
• Molecule 6: BG18 Light Chain

Chain R:



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

Chain A:



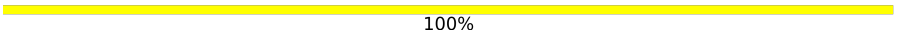
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain H:

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

Chain J: 

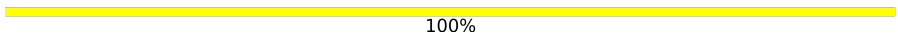
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:

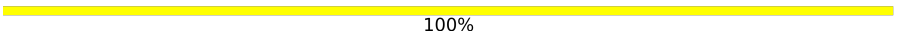
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

• Molecule 8: 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 F:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

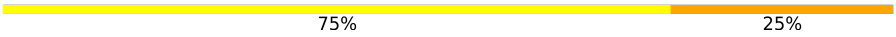
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 10: 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 L:

• Molecule 11: 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 M: 

• Molecule 12: 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 S:

• Molecule 13: 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 U:
NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	241.08Å 241.08Å 345.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.90 – 4.85 39.90 – 4.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.90-4.85) 95.3 (39.90-4.85)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 4.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.285 , 0.292 0.298 , 0.328	Depositor DCC
R_{free} test set	838 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	275.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 291.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å^2)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: MAN, BMA, 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	B	0.41	0/1113	0.61	1/1509 (0.1%)
2	D	0.41	0/1822	0.63	2/2481 (0.1%)
3	E	0.38	0/1659	0.58	0/2269
4	G	0.45	1/3572 (0.0%)	0.91	18/4857 (0.4%)
5	Q	0.38	0/1776	0.65	1/2423 (0.0%)
6	R	0.44	0/1577	0.65	0/2153
All	All	0.42	1/11519 (0.0%)	0.72	22/15692 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	392	ASN	C-N	6.72	1.49	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	234	ASN	O-C-N	-16.57	95.02	123.20
4	G	233	PHE	O-C-N	13.15	143.75	122.70
4	G	275	GLU	O-C-N	11.18	140.59	122.70
4	G	295	ASN	O-C-N	-10.77	105.46	122.70
4	G	234	ASN	CA-C-N	10.41	137.02	116.20
4	G	295	ASN	C-N-CA	10.23	147.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	233	PHE	CA-C-N	-9.94	95.33	117.20
4	G	391	PHE	C-N-CA	9.92	146.51	121.70
4	G	275	GLU	CA-C-N	-8.61	98.25	117.20
4	G	233	PHE	C-N-CA	-8.60	100.21	121.70
4	G	301	ASN	O-C-N	-8.10	109.74	122.70
4	G	295	ASN	CA-C-N	7.43	133.56	117.20
4	G	234	ASN	C-N-CA	7.28	137.59	122.30
2	D	146	PHE	C-N-CD	-6.33	106.68	120.60
5	Q	50	GLY	N-CA-C	6.27	128.78	113.10
4	G	301	ASN	C-N-CA	6.04	136.79	121.70
4	G	198	THR	N-CA-C	5.90	126.94	111.00
2	D	203	SER	N-CA-C	-5.45	96.28	111.00
4	G	275	GLU	C-N-CA	-5.45	108.08	121.70
4	G	301	ASN	CA-C-N	5.41	129.09	117.20
4	G	391	PHE	O-C-N	-5.36	114.12	122.70
1	B	648	VAL	N-CA-C	5.06	124.67	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	234	ASN	Mainchain

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	B	1094	0	1075	34	0
2	D	1777	0	1755	20	0
3	E	1615	0	1550	10	0
4	G	3499	0	3440	197	0
5	Q	1731	0	1685	45	0
6	R	1540	0	1496	15	0
7	A	39	0	34	1	0
7	C	39	0	34	1	0
7	H	39	0	34	5	0
7	J	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	39	0	34	1	0
7	P	39	0	34	1	0
7	T	39	0	34	0	0
8	F	50	0	43	11	0
9	I	28	0	25	0	0
9	K	28	0	25	10	0
9	N	28	0	25	1	0
10	L	72	0	61	11	0
11	M	50	0	43	5	0
12	S	61	0	52	4	0
13	U	72	0	61	18	0
14	B	14	0	13	4	0
14	G	42	0	39	0	0
All	All	11974	0	11626	311	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 13.

All (311) 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)
4:G:333:ILE:CD1	4:G:414:ILE:HB	1.30	1.60
4:G:338:TRP:CZ3	4:G:390:LEU:HD22	1.37	1.57
4:G:292:VAL:HB	4:G:449:ILE:CD1	1.30	1.55
4:G:292:VAL:CB	4:G:449:ILE:HD12	1.46	1.44
4:G:292:VAL:O	4:G:449:ILE:CD1	1.68	1.41
4:G:332:ASN:HD21	13:U:1:NAG:C1	1.31	1.41
4:G:292:VAL:CB	4:G:449:ILE:CD1	1.97	1.39
5:Q:158:LEU:O	5:Q:159:VAL:HG12	1.21	1.29
4:G:338:TRP:CZ3	4:G:390:LEU:CD2	2.15	1.28
4:G:333:ILE:CD1	4:G:414:ILE:CB	2.09	1.27
4:G:115:SER:O	4:G:116:LEU:HG	1.17	1.25
5:Q:75:SER:O	5:Q:76:ILE:HG12	1.07	1.24
4:G:292:VAL:O	4:G:449:ILE:CG1	1.88	1.20
4:G:115:SER:O	4:G:116:LEU:CG	1.91	1.18
4:G:292:VAL:CA	4:G:449:ILE:HD12	1.73	1.18
4:G:332:ASN:ND2	13:U:1:NAG:C1	2.08	1.15
4:G:292:VAL:HB	4:G:449:ILE:HD13	1.27	1.15
4:G:292:VAL:O	4:G:449:ILE:HD11	1.38	1.13
4:G:338:TRP:HH2	4:G:390:LEU:HB3	1.09	1.13
4:G:229:ASN:H	9:K:1:NAG:H83	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:338:TRP:CH2	4:G:390:LEU:HB3	1.86	1.10
5:Q:75:SER:O	5:Q:76:ILE:CG1	2.00	1.10
4:G:133:ASN:OD1	4:G:134:VAL:HG23	1.48	1.09
5:Q:106:VAL:H	13:U:2:NAG:H3	1.15	1.09
4:G:333:ILE:HD13	4:G:414:ILE:CB	1.78	1.07
5:Q:141:LEU:HD21	5:Q:158:LEU:HD13	1.15	1.07
4:G:333:ILE:CD1	4:G:414:ILE:O	2.03	1.06
4:G:292:VAL:O	4:G:449:ILE:HG13	1.52	1.05
4:G:333:ILE:HD11	4:G:414:ILE:CB	1.80	1.04
4:G:292:VAL:C	4:G:449:ILE:CD1	2.25	1.03
4:G:333:ILE:HD11	4:G:414:ILE:C	1.78	1.03
5:Q:106:VAL:CB	13:U:2:NAG:H5	1.90	1.01
4:G:292:VAL:C	4:G:449:ILE:HD11	1.81	1.00
4:G:338:TRP:CH2	4:G:390:LEU:HD22	1.97	0.97
4:G:333:ILE:HD12	4:G:414:ILE:O	1.63	0.97
4:G:199:SER:OG	4:G:433:ALA:HB2	1.63	0.97
2:D:200:HIS:HB3	2:D:203:SER:O	1.66	0.95
4:G:338:TRP:CH2	4:G:390:LEU:CD2	2.48	0.94
5:Q:158:LEU:O	5:Q:159:VAL:CG1	2.12	0.94
4:G:292:VAL:HG22	4:G:337:ARG:NE	1.83	0.92
4:G:338:TRP:HZ3	4:G:390:LEU:HD22	1.14	0.92
4:G:133:ASN:OD1	4:G:134:VAL:N	2.02	0.91
4:G:292:VAL:HB	4:G:449:ILE:HD12	0.91	0.90
2:D:100(D):TRP:HZ2	8:F:4:MAN:H2	1.36	0.89
4:G:252:ARG:CD	4:G:262:ASN:ND2	2.35	0.89
5:Q:106:VAL:N	13:U:2:NAG:H3	1.88	0.89
4:G:292:VAL:CG1	4:G:449:ILE:CD1	2.51	0.89
4:G:332:ASN:ND2	13:U:1:NAG:HN2	1.72	0.88
2:D:100(D):TRP:CZ2	8:F:4:MAN:H2	2.09	0.87
4:G:333:ILE:CD1	4:G:414:ILE:C	2.42	0.86
4:G:332:ASN:ND2	13:U:1:NAG:N2	2.24	0.86
4:G:133:ASN:OD1	4:G:134:VAL:CG2	2.22	0.86
4:G:252:ARG:HD2	4:G:262:ASN:CG	1.96	0.84
4:G:252:ARG:HD3	4:G:262:ASN:ND2	1.93	0.83
4:G:333:ILE:HD13	4:G:414:ILE:HB	0.83	0.83
4:G:173:TYR:HB3	7:H:1:NAG:HN2	1.43	0.82
4:G:333:ILE:HD11	4:G:414:ILE:CA	2.09	0.81
4:G:448:ASN:HB2	10:L:1:NAG:H81	1.63	0.80
4:G:338:TRP:CH2	4:G:390:LEU:CB	2.62	0.80
4:G:333:ILE:CD1	4:G:414:ILE:CA	2.60	0.80
5:Q:3:GLN:HB2	5:Q:25:SER:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:292:VAL:CA	4:G:449:ILE:CD1	2.44	0.78
4:G:229:ASN:N	9:K:1:NAG:H83	1.98	0.78
1:B:617:LYS:HD2	1:B:617:LYS:N	1.97	0.77
4:G:292:VAL:HG22	4:G:337:ARG:CZ	2.13	0.77
4:G:292:VAL:HG22	4:G:337:ARG:HE	1.50	0.77
4:G:333:ILE:HD11	4:G:414:ILE:CG2	2.14	0.77
4:G:252:ARG:HD2	4:G:262:ASN:ND2	1.99	0.77
4:G:252:ARG:NE	10:L:1:NAG:O5	2.20	0.75
4:G:115:SER:O	4:G:116:LEU:CD1	2.34	0.75
5:Q:69:ARG:HB2	5:Q:82:LYS:HB3	1.68	0.74
1:B:621:GLU:HG3	14:B:704:NAG:O7	1.87	0.74
5:Q:75:SER:C	5:Q:76:ILE:HG12	2.04	0.74
4:G:292:VAL:HG12	4:G:449:ILE:HD11	1.68	0.74
1:B:618:THR:OG1	1:B:621:GLU:HB3	1.88	0.73
4:G:278:THR:HG23	11:M:1:NAG:HN2	1.52	0.73
6:R:96:ASP:HB2	12:S:4:MAN:O4	1.87	0.73
4:G:332:ASN:HD22	13:U:1:NAG:HN2	1.37	0.73
4:G:386:ASN:ND2	4:G:417:GLN:OE1	2.22	0.72
4:G:338:TRP:CZ3	4:G:390:LEU:HD23	2.23	0.72
4:G:173:TYR:HB3	7:H:1:NAG:N2	2.05	0.72
4:G:115:SER:C	4:G:116:LEU:HG	2.06	0.72
5:Q:158:LEU:C	5:Q:159:VAL:HG12	2.10	0.71
4:G:395:TRP:NE1	4:G:397:ASN:O	2.23	0.71
2:D:100(D):TRP:HZ2	8:F:4:MAN:C2	2.03	0.71
4:G:252:ARG:HD3	10:L:1:NAG:C1	2.21	0.71
2:D:33:HIS:NE2	8:F:2:NAG:O7	2.23	0.71
4:G:332:ASN:ND2	13:U:1:NAG:C2	2.53	0.70
4:G:292:VAL:CB	4:G:449:ILE:HD11	2.19	0.69
4:G:291:ALA:HB1	4:G:448:ASN:OD1	1.92	0.69
1:B:530:MET:HB3	1:B:623:TRP:HA	1.75	0.69
4:G:88:ASN:ND2	8:F:1:NAG:H83	2.08	0.69
5:Q:141:LEU:CD2	5:Q:158:LEU:HD13	2.10	0.69
4:G:252:ARG:CD	10:L:1:NAG:C1	2.71	0.68
4:G:333:ILE:HD12	4:G:333:ILE:H	1.56	0.68
4:G:333:ILE:HD12	4:G:333:ILE:N	2.09	0.68
4:G:333:ILE:HD11	4:G:414:ILE:HG22	1.76	0.68
2:D:200:HIS:ND1	2:D:203:SER:OG	2.27	0.67
4:G:122:LEU:HB2	4:G:201:ILE:HG23	1.77	0.67
5:Q:150:GLY:HA2	5:Q:203:SER:O	1.95	0.67
1:B:604:CYS:SG	4:G:503:ARG:NH2	2.67	0.66
6:R:168:PRO:HB3	6:R:176:TYR:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:THR:OG1	1:B:621:GLU:CB	2.43	0.66
2:D:119:PRO:HD2	2:D:205:THR:HG21	1.78	0.65
4:G:117:LYS:O	4:G:117:LYS:NZ	2.24	0.65
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.79	0.65
4:G:292:VAL:HG12	4:G:449:ILE:CD1	2.25	0.65
1:B:621:GLU:OE2	14:B:704:NAG:H81	1.97	0.64
2:D:100(D):TRP:CZ2	8:F:4:MAN:C2	2.80	0.63
4:G:229:ASN:HB3	9:K:1:NAG:C7	2.28	0.63
4:G:261:LEU:N	4:G:261:LEU:HD12	2.13	0.63
4:G:333:ILE:CD1	4:G:414:ILE:CG2	2.74	0.63
4:G:332:ASN:H	4:G:415:THR:HG22	1.64	0.63
4:G:133:ASN:CG	4:G:134:VAL:H	1.97	0.62
4:G:329:ALA:HB3	4:G:418:CYS:HB3	1.81	0.62
1:B:621:GLU:OE2	14:B:704:NAG:C8	2.48	0.61
4:G:290:GLU:O	4:G:337:ARG:NH2	2.33	0.61
5:Q:141:LEU:HD21	5:Q:158:LEU:CD1	2.10	0.60
4:G:243:SER:HB3	9:K:1:NAG:H81	1.83	0.60
4:G:229:ASN:HB3	9:K:1:NAG:N2	2.16	0.60
5:Q:160:LYS:O	5:Q:160:LYS:HG2	2.02	0.60
4:G:291:ALA:C	4:G:337:ARG:HH21	2.04	0.60
4:G:252:ARG:CD	10:L:1:NAG:O5	2.50	0.59
4:G:292:VAL:HG22	4:G:337:ARG:NH2	2.17	0.59
4:G:243:SER:CB	9:K:1:NAG:H81	2.33	0.58
4:G:278:THR:OG1	11:M:1:NAG:H3	2.02	0.58
4:G:262:ASN:C	4:G:450:THR:HG21	2.22	0.58
1:B:604:CYS:HA	4:G:503:ARG:HH21	1.68	0.58
2:D:100(D):TRP:HZ2	8:F:4:MAN:C3	2.17	0.58
5:Q:103:ILE:O	13:U:3:BMA:H3	2.03	0.58
4:G:252:ARG:HD3	10:L:1:NAG:O5	2.04	0.58
4:G:462:GLN:HA	4:G:462:GLN:OE1	2.03	0.58
4:G:291:ALA:O	4:G:337:ARG:NH2	2.37	0.58
2:D:1:GLU:OE2	7:A:3:BMA:O4	2.23	0.57
4:G:338:TRP:CD1	4:G:339:ASN:N	2.72	0.57
4:G:338:TRP:CH2	4:G:390:LEU:HD23	2.34	0.57
4:G:330:HIS:NE2	13:U:1:NAG:H5	2.20	0.56
10:L:6:MAN:O4	10:L:6:MAN:O6	2.22	0.56
5:Q:48:TRP:CH2	5:Q:50:GLY:O	2.58	0.56
5:Q:106:VAL:H	13:U:2:NAG:C3	2.05	0.56
4:G:292:VAL:CG1	4:G:449:ILE:HD13	2.31	0.56
4:G:116:LEU:HD12	4:G:116:LEU:C	2.26	0.56
4:G:296:CYS:H	4:G:445:CYS:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.89	0.55
4:G:268:GLU:OE1	4:G:268:GLU:HA	2.06	0.55
7:O:1:NAG:H62	7:O:2:NAG:O7	2.07	0.55
2:D:97:LEU:HD12	2:D:100(C):THR:HG22	1.88	0.55
4:G:386:ASN:HD22	4:G:417:GLN:CD	2.10	0.54
4:G:69:TRP:HA	4:G:111:LEU:HD21	1.89	0.54
4:G:292:VAL:C	4:G:449:ILE:HD12	2.03	0.54
4:G:261:LEU:O	10:L:1:NAG:O7	2.25	0.54
4:G:292:VAL:O	4:G:449:ILE:HD12	1.87	0.54
2:D:31:PHE:HA	8:F:1:NAG:H62	1.90	0.53
4:G:360:ILE:HA	4:G:467:THR:HA	1.90	0.53
4:G:278:THR:OG1	11:M:1:NAG:H5	2.08	0.53
4:G:261:LEU:HB3	10:L:1:NAG:O7	2.08	0.53
5:Q:218:LYS:HB3	5:Q:219:PRO:HD3	1.91	0.53
1:B:636:ASP:O	1:B:639:THR:HG22	2.09	0.53
1:B:621:GLU:CG	14:B:704:NAG:O7	2.55	0.53
1:B:621:GLU:O	1:B:625:ASN:HB3	2.07	0.53
4:G:241:ASN:O	9:K:1:NAG:H82	2.08	0.53
5:Q:67:ARG:HG3	5:Q:84:THR:O	2.09	0.53
3:E:20:ILE:HG21	3:E:105:THR:HG21	1.91	0.53
4:G:117:LYS:N	4:G:118:PRO:CD	2.72	0.53
6:R:135:THR:HA	6:R:183:SER:HA	1.91	0.53
5:Q:107:VAL:HG22	13:U:1:NAG:H62	1.91	0.52
4:G:440:ARG:HG2	9:N:1:NAG:H81	1.90	0.52
4:G:196:CYS:SG	4:G:197:ASN:N	2.82	0.52
5:Q:37:TRP:HB2	5:Q:49:ILE:HB	1.91	0.52
6:R:40:LYS:HB3	6:R:43:GLN:HB2	1.91	0.52
2:D:6:GLN:HE21	2:D:107:THR:HG23	1.75	0.52
3:E:91:CYS:SG	3:E:99:CYS:HB3	2.50	0.52
4:G:298:ARG:HB3	4:G:443:ILE:HG13	1.92	0.52
4:G:278:THR:CG2	11:M:1:NAG:HN2	2.20	0.51
4:G:295:ASN:O	4:G:331:CYS:O	2.28	0.51
4:G:292:VAL:CB	4:G:449:ILE:HD13	2.03	0.51
4:G:292:VAL:CG2	4:G:337:ARG:NH2	2.73	0.51
6:R:8:GLN:HB2	6:R:102:GLY:HA3	1.93	0.51
1:B:566:LEU:HD21	1:B:568:LEU:HD12	1.93	0.51
4:G:229:ASN:CB	9:K:1:NAG:C7	2.88	0.51
4:G:117:LYS:O	4:G:117:LYS:HD2	2.11	0.51
4:G:368:ASP:HB2	4:G:371:ILE:HD12	1.92	0.51
5:Q:91:THR:HG21	5:Q:128:VAL:HB	1.93	0.51
4:G:153:GLU:HB3	4:G:178:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:299:PRO:HD3	4:G:329:ALA:O	2.10	0.50
3:E:6:GLN:HB3	3:E:105:THR:HB	1.93	0.50
4:G:338:TRP:CD1	4:G:338:TRP:C	2.85	0.50
2:D:100(D):TRP:CZ2	8:F:4:MAN:C3	2.95	0.50
1:B:617:LYS:N	1:B:617:LYS:CD	2.73	0.50
4:G:195:ASN:OD1	4:G:199:SER:O	2.29	0.50
2:D:87:THR:HG23	2:D:110:THR:HA	1.93	0.50
4:G:261:LEU:N	4:G:261:LEU:CD1	2.73	0.50
4:G:292:VAL:N	4:G:449:ILE:HD12	2.25	0.50
4:G:95:MET:H	4:G:236:SER:HB2	1.77	0.50
4:G:460:ARG:NE	4:G:463:ASN:HD22	2.09	0.50
1:B:594:GLY:HA2	1:B:599:SER:HB3	1.94	0.49
4:G:173:TYR:HB3	7:H:1:NAG:C7	2.41	0.49
4:G:332:ASN:HA	4:G:415:THR:HG23	1.94	0.49
5:Q:50:GLY:O	5:Q:51:ASP:CB	2.60	0.49
3:E:33:LYS:HG2	3:E:94:THR:HG23	1.93	0.49
1:B:608:VAL:HG21	1:B:646:LEU:HA	1.94	0.49
1:B:551:GLN:HE22	4:G:78:ASP:HB2	1.76	0.49
4:G:42:VAL:HG21	4:G:495:GLY:HA3	1.95	0.49
5:Q:34:SER:HB2	5:Q:101:ILE:HD11	1.94	0.48
5:Q:104:TYR:O	13:U:3:BMA:H2	2.13	0.48
4:G:462:GLN:O	4:G:463:ASN:HB2	2.13	0.48
2:D:100(D):TRP:CZ2	8:F:4:MAN:O3	2.65	0.48
6:R:163:VAL:HG21	6:R:183:SER:H	1.77	0.48
4:G:299:PRO:HB2	4:G:327:ARG:HD3	1.95	0.48
2:D:100(C):THR:HG21	8:F:2:NAG:O6	2.14	0.48
1:B:616:ASN:C	1:B:617:LYS:HD2	2.34	0.48
4:G:195:ASN:ND2	4:G:199:SER:O	2.46	0.48
4:G:292:VAL:CG2	4:G:337:ARG:HH21	2.27	0.48
4:G:392:ASN:OD1	12:S:1:NAG:N2	2.43	0.48
6:R:163:VAL:HG11	6:R:183:SER:HB2	1.95	0.48
4:G:117:LYS:N	4:G:118:PRO:HD2	2.29	0.47
1:B:648:VAL:HA	1:B:652:GLN:HB3	1.95	0.47
13:U:6:MAN:O6	13:U:6:MAN:O4	2.16	0.47
1:B:642:ILE:HG21	4:G:496:ILE:HG21	1.95	0.47
1:B:651:ILE:HD13	1:B:655:LYS:HG3	1.96	0.47
4:G:185:GLU:HB3	4:G:190:ASN:HB3	1.96	0.47
1:B:578:ALA:HB1	4:G:220:PRO:HB3	1.96	0.47
5:Q:173:SER:HB2	5:Q:212:ILE:HD11	1.96	0.47
4:G:337:ARG:HD2	4:G:337:ARG:O	2.14	0.47
4:G:115:SER:O	4:G:116:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:243:SER:HB2	9:K:1:NAG:C8	2.45	0.47
1:B:571:TRP:CD2	4:G:54:CYS:HB2	2.50	0.47
2:D:116:THR:HG21	2:D:202:PRO:HB2	1.97	0.47
1:B:540:GLN:HG2	4:G:43:PRO:HB3	1.97	0.46
4:G:183:PRO:HA	4:G:191:TYR:HB3	1.96	0.46
5:Q:100:ALA:HB3	5:Q:115:TYR:HB3	1.95	0.46
6:R:121:LEU:HG	6:R:208:LYS:HB2	1.96	0.46
4:G:385:CYS:HB2	4:G:416:LEU:HB2	1.97	0.46
4:G:276:ASN:HB3	4:G:282:LYS:HB2	1.97	0.46
5:Q:60:TYR:HE1	5:Q:65:ARG:HA	1.82	0.45
1:B:648:VAL:O	1:B:653:GLN:N	2.49	0.45
4:G:329:ALA:HB2	4:G:420:ILE:HD11	1.99	0.45
1:B:604:CYS:HA	4:G:503:ARG:NH2	2.32	0.45
4:G:157:CYS:HB2	4:G:176:PHE:HE2	1.82	0.45
5:Q:48:TRP:CZ2	5:Q:50:GLY:O	2.70	0.45
5:Q:160:LYS:O	5:Q:161:ASP:HB3	2.17	0.45
5:Q:161:ASP:HB2	5:Q:192:LEU:HD22	1.98	0.45
5:Q:162:TYR:CZ	5:Q:193:TYR:HB2	2.52	0.45
3:E:196:SER:HA	3:E:209:THR:HG23	1.99	0.45
4:G:116:LEU:CD1	4:G:116:LEU:C	2.86	0.45
4:G:262:ASN:CA	4:G:450:THR:HG21	2.47	0.44
4:G:278:THR:HG23	11:M:1:NAG:N2	2.27	0.44
5:Q:39:ARG:HB3	5:Q:47:GLU:HB2	1.99	0.44
1:B:637:ASN:HB2	7:C:1:NAG:C2	2.47	0.44
1:B:616:ASN:OD1	1:B:616:ASN:N	2.50	0.44
4:G:291:ALA:C	4:G:337:ARG:NH2	2.70	0.44
4:G:329:ALA:O	4:G:330:HIS:HB3	2.18	0.44
4:G:333:ILE:HD11	4:G:414:ILE:O	1.83	0.44
4:G:446:SER:HB3	10:L:2:NAG:H5	1.99	0.44
4:G:262:ASN:CG	10:L:1:NAG:H82	2.38	0.44
4:G:270:ILE:HG22	4:G:288:LEU:HA	1.99	0.44
5:Q:71:GLU:HB3	5:Q:80:SER:HB3	2.00	0.44
4:G:96:TRP:HB2	4:G:275:GLU:HG3	2.00	0.44
4:G:332:ASN:HA	4:G:414:ILE:O	2.17	0.43
4:G:59:LYS:HE3	4:G:214:PRO:HD2	2.00	0.43
4:G:338:TRP:CE3	4:G:390:LEU:CD2	2.92	0.43
4:G:469:ARG:HH21	7:P:1:NAG:C7	2.31	0.43
4:G:292:VAL:HG13	4:G:337:ARG:HG3	2.00	0.43
4:G:299:PRO:HB2	4:G:327:ARG:CD	2.49	0.43
6:R:138:CYS:O	6:R:138:CYS:SG	2.76	0.43
4:G:296:CYS:N	4:G:445:CYS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:48:TRP:HB2	6:R:101:PHE:HE1	1.83	0.43
6:R:98:TYR:CE1	6:R:100:MET:HB3	2.54	0.43
6:R:153:LYS:HA	6:R:158:PRO:HA	2.01	0.43
4:G:173:TYR:CB	7:H:1:NAG:HN2	2.22	0.42
4:G:70:ALA:O	4:G:74:CYS:HB3	2.19	0.42
5:Q:105:GLY:HA2	13:U:2:NAG:C3	2.49	0.42
4:G:241:ASN:OD1	4:G:241:ASN:N	2.53	0.42
4:G:304:ARG:HG3	4:G:440:ARG:HD2	2.02	0.42
1:B:608:VAL:HG22	1:B:649:SER:HB3	2.01	0.42
1:B:610:TRP:HE3	4:G:36:VAL:HG22	1.85	0.42
4:G:240:THR:OG1	4:G:241:ASN:OD1	2.37	0.42
5:Q:39:ARG:HB2	5:Q:49:ILE:HD11	1.99	0.42
4:G:301:ASN:O	4:G:322:ILE:HA	2.19	0.42
4:G:392:ASN:CG	12:S:1:NAG:N2	2.73	0.42
3:E:10:VAL:HG21	3:E:20:ILE:HG12	2.01	0.42
4:G:294:ILE:HG23	4:G:294:ILE:O	2.19	0.42
4:G:330:HIS:CE1	13:U:1:NAG:H3	2.55	0.42
5:Q:59:THR:HB	12:S:4:MAN:H4	2.02	0.42
1:B:534:SER:HA	1:B:537:LEU:HD23	2.01	0.42
1:B:604:CYS:CA	4:G:503:ARG:HH21	2.31	0.42
4:G:333:ILE:HD12	4:G:333:ILE:O	2.20	0.42
4:G:427:TRP:CD1	4:G:475:MET:HG3	2.54	0.42
5:Q:137:SER:O	5:Q:159:VAL:HA	2.19	0.42
1:B:525:ALA:HB1	1:B:533:ALA:HA	2.02	0.41
5:Q:156:GLY:HA2	5:Q:198:VAL:HG12	2.02	0.41
6:R:5:GLU:HB3	6:R:100:MET:HB2	2.02	0.41
4:G:386:ASN:HB2	4:G:417:GLN:HB2	2.02	0.41
2:D:143:LYS:HE3	3:E:133:LYS:HD2	2.02	0.41
3:E:85:GLU:HB3	3:E:109:VAL:H	1.85	0.41
3:E:92:SER:HB2	3:E:100:VAL:HB	2.03	0.41
5:Q:167:VAL:HG11	5:Q:195:LEU:HD22	2.02	0.41
6:R:148:VAL:HG22	6:R:201:HIS:HB2	2.02	0.41
2:D:169:VAL:HG21	3:E:166:THR:HB	2.01	0.41
4:G:156:ASN:ND2	7:H:1:NAG:C7	2.83	0.41
4:G:196:CYS:O	4:G:197:ASN:C	2.56	0.41
6:R:192:HIS:CD2	6:R:193:LYS:HG2	2.56	0.41
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.56	0.41
13:U:1:NAG:H83	13:U:1:NAG:H2	1.84	0.40
4:G:195:ASN:CG	4:G:199:SER:O	2.60	0.40
4:G:243:SER:HB2	9:K:1:NAG:H81	2.02	0.40
4:G:342:LEU:HA	4:G:345:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:164:PRO:HB2	5:Q:166:PRO:HD2	2.02	0.40
4:G:391:PHE:CE1	4:G:470:PRO:HG3	2.56	0.40
4:G:277:ILE:O	4:G:277:ILE:HG12	2.19	0.40
5:Q:51:ASP:HB3	5:Q:59:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	132/153 (86%)	119 (90%)	13 (10%)	0	100	100
2	D	232/243 (96%)	205 (88%)	26 (11%)	1 (0%)	34	72
3	E	211/216 (98%)	192 (91%)	17 (8%)	2 (1%)	17	56
4	G	440/518 (85%)	366 (83%)	69 (16%)	5 (1%)	14	51
5	Q	229/240 (95%)	178 (78%)	44 (19%)	7 (3%)	4	30
6	R	201/215 (94%)	140 (70%)	54 (27%)	7 (4%)	3	28
All	All	1445/1585 (91%)	1200 (83%)	223 (15%)	22 (2%)	10	46

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	53	ASP
4	G	197	ASN
5	Q	51	ASP
5	Q	159	VAL
6	R	29	LEU
6	R	100	MET
4	G	156	ASN
6	R	28	PRO

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Mol	Chain	Res	Type
3	E	71	TRP
5	Q	218	LYS
6	R	195	TYR
2	D	147	PRO
4	G	235	GLY
4	G	236	SER
5	Q	219	PRO
6	R	132	ASN
4	G	330	HIS
5	Q	15	SER
5	Q	89	ALA
6	R	138	CYS
5	Q	76	ILE
6	R	112	GLN

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	B	119/130 (92%)	118 (99%)	1 (1%)	81	89
2	D	199/206 (97%)	192 (96%)	7 (4%)	36	60
3	E	186/189 (98%)	181 (97%)	5 (3%)	44	66
4	G	393/455 (86%)	361 (92%)	32 (8%)	11	37
5	Q	193/207 (93%)	188 (97%)	5 (3%)	46	67
6	R	174/182 (96%)	165 (95%)	9 (5%)	23	49
All	All	1264/1369 (92%)	1205 (95%)	59 (5%)	26	52

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	616	ASN
2	D	31	PHE
2	D	38	ARG
2	D	89	THR

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Mol	Chain	Res	Type
2	D	97	LEU
2	D	100(E)	LEU
2	D	138	LEU
2	D	166	PHE
3	E	22	CYS
3	E	53	ASP
3	E	74	TYR
3	E	168	PRO
3	E	179	SER
4	G	63	THR
4	G	116	LEU
4	G	131	CYS
4	G	134	VAL
4	G	156	ASN
4	G	157	CYS
4	G	201	ILE
4	G	225	ILE
4	G	231	LYS
4	G	233	PHE
4	G	262	ASN
4	G	270	ILE
4	G	273	ARG
4	G	276	ASN
4	G	277	ILE
4	G	295	ASN
4	G	301	ASN
4	G	302	ASN
4	G	333	ILE
4	G	338	TRP
4	G	339	ASN
4	G	362	ASN
4	G	364	SER
4	G	381	GLU
4	G	413	ASN
4	G	415	THR
4	G	416	LEU
4	G	427	TRP
4	G	448	ASN
4	G	449	ILE
4	G	452	LEU
4	G	469	ARG
5	Q	46	LEU

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Mol	Chain	Res	Type
5	Q	52	ILE
5	Q	187	LEU
5	Q	195	LEU
5	Q	205	SER
6	R	34	THR
6	R	63	PHE
6	R	90	GLN
6	R	138	CYS
6	R	141	SER
6	R	152	TRP
6	R	205	THR
6	R	207	GLU
6	R	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	551	GLN
2	D	6	GLN
2	D	197	ASN
4	G	130	ASN
4	G	132	ASN
4	G	302	ASN
4	G	332	ASN
4	G	363	HIS
4	G	463	ASN
4	G	478	ASN
6	R	188	GLN
6	R	192	HIS

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)

52 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	A	1	1,7	14,14,15	0.92	0	17,19,21	2.23	5 (29%)
7	NAG	A	2	7	14,14,15	0.81	1 (7%)	17,19,21	1.21	2 (11%)
7	BMA	A	3	7	11,11,12	0.40	0	15,15,17	0.90	0
7	NAG	C	1	1,7	14,14,15	0.79	0	17,19,21	1.88	3 (17%)
7	NAG	C	2	7	14,14,15	0.67	0	17,19,21	2.17	4 (23%)
7	BMA	C	3	7	11,11,12	0.44	0	15,15,17	0.98	1 (6%)
8	NAG	F	1	8	14,14,15	0.95	0	17,19,21	2.21	6 (35%)
8	NAG	F	2	8	14,14,15	1.12	2 (14%)	17,19,21	2.75	7 (41%)
8	BMA	F	3	8	11,11,12	1.53	2 (18%)	15,15,17	2.28	6 (40%)
8	MAN	F	4	8	11,11,12	2.18	2 (18%)	15,15,17	2.22	8 (53%)
7	NAG	H	1	4,7	14,14,15	0.95	1 (7%)	17,19,21	1.89	7 (41%)
7	NAG	H	2	7	14,14,15	1.21	2 (14%)	17,19,21	2.30	5 (29%)
7	BMA	H	3	7	11,11,12	0.84	0	15,15,17	1.72	3 (20%)
9	NAG	I	1	9,4	14,14,15	1.02	0	17,19,21	1.23	1 (5%)
9	NAG	I	2	9	14,14,15	1.14	1 (7%)	17,19,21	1.64	4 (23%)
7	NAG	J	1	4,7	14,14,15	0.81	0	17,19,21	1.71	4 (23%)
7	NAG	J	2	7	14,14,15	1.35	1 (7%)	17,19,21	1.47	3 (17%)
7	BMA	J	3	7	11,11,12	0.76	0	15,15,17	1.27	2 (13%)
9	NAG	K	1	9,4	14,14,15	0.89	1 (7%)	17,19,21	2.26	6 (35%)
9	NAG	K	2	9	14,14,15	0.65	1 (7%)	17,19,21	0.98	0
10	NAG	L	1	10,4	14,14,15	1.13	1 (7%)	17,19,21	2.94	8 (47%)
10	NAG	L	2	10	14,14,15	0.73	0	17,19,21	2.42	7 (41%)
10	BMA	L	3	10	11,11,12	0.74	0	15,15,17	2.73	7 (46%)
10	MAN	L	4	10	11,11,12	0.42	0	15,15,17	2.10	3 (20%)
10	MAN	L	5	10	11,11,12	0.77	0	15,15,17	1.57	1 (6%)
10	MAN	L	6	10	11,11,12	1.02	1 (9%)	15,15,17	1.58	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	M	1	4,11	14,14,15	1.36	2 (14%)	17,19,21	2.47	5 (29%)
11	NAG	M	2	11	14,14,15	0.58	0	17,19,21	1.49	2 (11%)
11	BMA	M	3	11	11,11,12	0.91	1 (9%)	15,15,17	1.89	5 (33%)
11	MAN	M	4	11	11,11,12	0.67	0	15,15,17	1.68	3 (20%)
9	NAG	N	1	9,4	14,14,15	0.81	1 (7%)	17,19,21	2.23	3 (17%)
9	NAG	N	2	9	14,14,15	0.47	0	17,19,21	1.28	3 (17%)
7	NAG	O	1	4,7	14,14,15	0.37	0	17,19,21	1.28	3 (17%)
7	NAG	O	2	7	14,14,15	0.72	0	17,19,21	1.64	3 (17%)
7	BMA	O	3	7	11,11,12	0.39	0	15,15,17	1.19	1 (6%)
7	NAG	P	1	4,7	14,14,15	0.64	0	17,19,21	1.49	2 (11%)
7	NAG	P	2	7	14,14,15	0.81	1 (7%)	17,19,21	1.24	2 (11%)
7	BMA	P	3	7	11,11,12	0.46	0	15,15,17	1.01	1 (6%)
12	NAG	S	1	4,12	14,14,15	1.28	1 (7%)	17,19,21	1.66	4 (23%)
12	NAG	S	2	12	14,14,15	1.36	2 (14%)	17,19,21	2.61	6 (35%)
12	BMA	S	3	12	11,11,12	1.34	1 (9%)	15,15,17	2.64	5 (33%)
12	MAN	S	4	12	11,11,12	0.86	1 (9%)	15,15,17	2.75	8 (53%)
12	MAN	S	5	12	11,11,12	0.73	0	15,15,17	1.28	2 (13%)
7	NAG	T	1	4,7	14,14,15	0.68	0	17,19,21	1.64	4 (23%)
7	NAG	T	2	7	14,14,15	0.82	0	17,19,21	1.45	4 (23%)
7	BMA	T	3	7	11,11,12	0.66	0	15,15,17	1.72	3 (20%)
13	NAG	U	1	13	14,14,15	1.48	4 (28%)	17,19,21	2.16	5 (29%)
13	NAG	U	2	13	14,14,15	0.86	0	17,19,21	2.91	7 (41%)
13	BMA	U	3	13	11,11,12	0.78	0	15,15,17	2.42	5 (33%)
13	MAN	U	4	13	11,11,12	0.65	0	15,15,17	1.94	5 (33%)
13	MAN	U	5	13	11,11,12	0.53	0	15,15,17	1.35	1 (6%)
13	MAN	U	6	13	11,11,12	0.87	1 (9%)	15,15,17	3.02	9 (60%)

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	A	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	S	2	12	-	2/6/23/26	0/1/1/1
12	BMA	S	3	12	-	2/2/19/22	0/1/1/1
12	MAN	S	4	12	-	2/2/19/22	0/1/1/1
12	MAN	S	5	12	-	1/2/19/22	0/1/1/1
7	NAG	T	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	1/2/19/22	0/1/1/1
13	NAG	U	1	13	-	4/6/23/26	0/1/1/1
13	NAG	U	2	13	-	2/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	1/2/19/22	0/1/1/1
13	MAN	U	5	13	-	0/2/19/22	0/1/1/1
13	MAN	U	6	13	-	2/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4	MAN	O5-C1	5.83	1.53	1.43
8	F	4	MAN	C1-C2	3.43	1.60	1.52
11	M	1	NAG	C1-C2	3.42	1.57	1.52
12	S	3	BMA	C2-C3	3.39	1.57	1.52
7	J	2	NAG	C1-C2	3.33	1.57	1.52
13	U	1	NAG	O4-C4	3.29	1.50	1.43
9	I	2	NAG	C1-C2	3.03	1.56	1.52
12	S	2	NAG	O4-C4	2.97	1.50	1.43
8	F	3	BMA	C1-C2	2.77	1.58	1.52
7	H	1	NAG	O4-C4	2.76	1.49	1.43
12	S	2	NAG	C1-C2	2.64	1.56	1.52
7	H	2	NAG	O4-C4	2.62	1.49	1.43
7	H	2	NAG	C1-C2	2.54	1.56	1.52
12	S	1	NAG	C4-C5	2.43	1.58	1.53
13	U	1	NAG	O5-C1	-2.40	1.39	1.43
8	F	2	NAG	C4-C5	2.37	1.58	1.53
9	K	1	NAG	C1-C2	2.28	1.55	1.52
8	F	2	NAG	O4-C4	2.27	1.48	1.43
7	A	2	NAG	C1-C2	2.26	1.55	1.52
10	L	6	MAN	C2-C3	2.23	1.55	1.52
7	P	2	NAG	C1-C2	2.21	1.55	1.52
11	M	1	NAG	O5-C1	2.17	1.47	1.43
13	U	6	MAN	C1-C2	2.14	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	S	4	MAN	C1-C2	2.14	1.57	1.52
13	U	1	NAG	C1-C2	-2.10	1.49	1.52
11	M	3	BMA	O3-C3	2.06	1.47	1.43
9	K	2	NAG	C1-C2	2.05	1.55	1.52
9	N	1	NAG	C1-C2	2.05	1.55	1.52
13	U	1	NAG	C4-C3	2.04	1.57	1.52
10	L	1	NAG	C1-C2	2.01	1.55	1.52
8	F	3	BMA	O6-C6	2.01	1.50	1.42

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	1	NAG	C2-N2-C7	7.59	133.71	122.90
9	N	1	NAG	C2-N2-C7	7.43	133.49	122.90
13	U	6	MAN	C1-C2-C3	7.37	118.73	109.67
12	S	2	NAG	C2-N2-C7	6.73	132.49	122.90
13	U	2	NAG	O4-C4-C5	-6.68	92.71	109.30
11	M	1	NAG	C2-N2-C7	6.48	132.14	122.90
12	S	3	BMA	O5-C5-C6	6.40	117.24	107.20
8	F	2	NAG	C1-O5-C5	6.01	120.34	112.19
10	L	3	BMA	O5-C5-C6	5.83	116.34	107.20
8	F	2	NAG	O4-C4-C5	5.70	123.46	109.30
7	A	1	NAG	C1-O5-C5	-5.70	104.47	112.19
8	F	3	BMA	O5-C5-C6	5.29	115.50	107.20
10	L	4	MAN	O5-C5-C6	5.29	115.50	107.20
7	H	2	NAG	O5-C1-C2	-5.28	102.95	111.29
8	F	1	NAG	O5-C1-C2	-5.23	103.03	111.29
10	L	2	NAG	C2-N2-C7	5.15	130.24	122.90
12	S	2	NAG	O5-C1-C2	-5.13	103.19	111.29
13	U	2	NAG	O5-C5-C6	5.08	115.17	107.20
9	K	1	NAG	C2-N2-C7	5.06	130.11	122.90
7	C	2	NAG	C1-O5-C5	5.04	119.02	112.19
13	U	2	NAG	O5-C1-C2	-5.03	103.35	111.29
13	U	1	NAG	C1-C2-N2	-5.00	101.95	110.49
7	H	2	NAG	C3-C4-C5	-4.98	101.35	110.24
7	C	2	NAG	C2-N2-C7	4.93	129.93	122.90
12	S	4	MAN	O4-C4-C3	-4.91	99.00	110.35
11	M	1	NAG	C4-C3-C2	4.82	118.08	111.02
7	O	2	NAG	C2-N2-C7	4.80	129.74	122.90
12	S	4	MAN	C1-O5-C5	-4.69	105.83	112.19
11	M	4	MAN	O5-C1-C2	-4.69	103.53	110.77
12	S	3	BMA	O3-C3-C2	4.67	118.94	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	3	BMA	O6-C6-C5	4.66	127.30	111.29
10	L	2	NAG	C1-O5-C5	4.65	118.50	112.19
13	U	3	BMA	O3-C3-C2	-4.54	101.30	109.99
8	F	1	NAG	C2-N2-C7	-4.52	116.46	122.90
13	U	6	MAN	O5-C1-C2	-4.50	103.83	110.77
9	K	1	NAG	C1-O5-C5	-4.47	106.13	112.19
7	P	1	NAG	O5-C5-C6	-4.39	100.32	107.20
10	L	3	BMA	O3-C3-C4	-4.35	100.28	110.35
10	L	5	MAN	O5-C1-C2	-4.35	104.06	110.77
10	L	1	NAG	C1-C2-N2	4.34	117.90	110.49
10	L	1	NAG	O5-C1-C2	-4.32	104.47	111.29
13	U	1	NAG	O4-C4-C3	4.31	120.31	110.35
13	U	2	NAG	C4-C3-C2	4.22	117.20	111.02
7	A	1	NAG	C2-N2-C7	4.15	128.82	122.90
7	T	1	NAG	C2-N2-C7	4.11	128.76	122.90
7	C	1	NAG	C1-C2-N2	4.06	117.42	110.49
12	S	4	MAN	O2-C2-C1	4.05	117.43	109.15
12	S	3	BMA	O5-C1-C2	-4.03	104.54	110.77
13	U	3	BMA	O5-C5-C6	4.01	113.50	107.20
7	H	2	NAG	C1-O5-C5	4.01	117.62	112.19
10	L	1	NAG	C8-C7-N2	3.99	122.85	116.10
10	L	3	BMA	C6-C5-C4	-3.99	103.67	113.00
7	H	3	BMA	O5-C5-C6	3.98	113.44	107.20
7	T	3	BMA	O5-C5-C6	3.94	113.37	107.20
7	C	1	NAG	O3-C3-C2	-3.89	101.41	109.47
8	F	4	MAN	C2-C3-C4	3.89	117.62	110.89
7	H	3	BMA	O5-C1-C2	-3.89	104.77	110.77
10	L	2	NAG	C1-C2-N2	3.85	117.06	110.49
9	I	2	NAG	O5-C1-C2	-3.84	105.23	111.29
12	S	1	NAG	O5-C5-C6	3.83	113.20	107.20
11	M	2	NAG	O5-C1-C2	-3.80	105.29	111.29
10	L	4	MAN	C3-C4-C5	-3.78	103.49	110.24
12	S	4	MAN	C3-C4-C5	3.77	116.97	110.24
13	U	6	MAN	O4-C4-C3	3.76	119.05	110.35
7	C	1	NAG	C2-N2-C7	3.70	128.17	122.90
7	J	1	NAG	C4-C3-C2	-3.70	105.60	111.02
9	K	1	NAG	O4-C4-C3	-3.68	101.83	110.35
13	U	4	MAN	C2-C3-C4	-3.60	104.67	110.89
7	J	2	NAG	C2-N2-C7	3.53	127.93	122.90
13	U	1	NAG	C3-C4-C5	-3.48	104.04	110.24
11	M	1	NAG	O4-C4-C3	-3.47	102.33	110.35
11	M	3	BMA	O5-C1-C2	-3.38	105.55	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	6	MAN	C1-O5-C5	3.37	116.76	112.19
10	L	4	MAN	O5-C1-C2	-3.37	105.57	110.77
12	S	2	NAG	C1-C2-N2	3.36	116.23	110.49
7	J	1	NAG	C1-O5-C5	3.35	116.73	112.19
13	U	3	BMA	O5-C1-C2	-3.35	105.60	110.77
10	L	3	BMA	O4-C4-C3	-3.35	102.60	110.35
8	F	4	MAN	C3-C4-C5	-3.35	104.27	110.24
8	F	2	NAG	O5-C5-C6	-3.35	101.96	107.20
7	H	1	NAG	O5-C1-C2	-3.34	106.01	111.29
11	M	2	NAG	C1-O5-C5	3.28	116.63	112.19
7	T	3	BMA	O2-C2-C1	3.26	115.82	109.15
8	F	2	NAG	C6-C5-C4	3.23	120.57	113.00
7	O	1	NAG	O4-C4-C5	-3.22	101.29	109.30
10	L	6	MAN	O5-C5-C6	3.22	112.25	107.20
10	L	1	NAG	C1-O5-C5	3.21	116.54	112.19
8	F	3	BMA	O2-C2-C1	3.19	115.68	109.15
7	P	2	NAG	O5-C1-C2	-3.19	106.25	111.29
8	F	2	NAG	O3-C3-C2	3.18	116.05	109.47
7	P	1	NAG	O4-C4-C3	-3.18	103.00	110.35
11	M	3	BMA	O3-C3-C4	3.17	117.69	110.35
10	L	2	NAG	O5-C5-C6	3.16	112.16	107.20
8	F	3	BMA	O6-C6-C5	3.16	122.13	111.29
9	I	2	NAG	C1-O5-C5	3.12	116.43	112.19
7	H	1	NAG	O4-C4-C5	3.12	117.05	109.30
9	N	2	NAG	C1-O5-C5	3.12	116.41	112.19
13	U	6	MAN	O3-C3-C2	-3.10	104.06	109.99
9	I	1	NAG	O4-C4-C5	3.07	116.93	109.30
8	F	3	BMA	O4-C4-C5	3.07	116.92	109.30
7	J	3	BMA	O5-C5-C6	3.04	111.96	107.20
8	F	3	BMA	O5-C1-C2	-3.02	106.11	110.77
8	F	2	NAG	O6-C6-C5	3.00	121.57	111.29
7	T	2	NAG	C1-O5-C5	2.99	116.25	112.19
12	S	4	MAN	O2-C2-C3	-2.99	104.15	110.14
10	L	3	BMA	O5-C1-C2	-2.98	106.17	110.77
7	A	1	NAG	O4-C4-C3	-2.98	103.46	110.35
13	U	4	MAN	C1-C2-C3	2.98	113.33	109.67
7	J	3	BMA	O5-C1-C2	-2.97	106.19	110.77
7	C	2	NAG	O4-C4-C3	2.93	117.12	110.35
7	H	2	NAG	O4-C4-C5	2.92	116.55	109.30
13	U	4	MAN	O4-C4-C3	2.90	117.06	110.35
13	U	3	BMA	O3-C3-C4	2.88	117.01	110.35
12	S	4	MAN	O5-C5-C6	2.88	111.71	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1	NAG	O5-C5-C6	-2.85	102.74	107.20
13	U	6	MAN	O5-C5-C4	-2.81	103.98	110.83
12	S	2	NAG	C4-C3-C2	2.81	115.13	111.02
10	L	3	BMA	O3-C3-C2	-2.80	104.63	109.99
9	I	2	NAG	O5-C5-C6	2.80	111.59	107.20
9	N	1	NAG	O7-C7-N2	2.79	127.09	121.95
11	M	3	BMA	C1-C2-C3	2.79	113.09	109.67
7	O	2	NAG	C8-C7-N2	2.78	120.81	116.10
10	L	6	MAN	O2-C2-C3	2.78	115.70	110.14
12	S	2	NAG	O3-C3-C2	-2.77	103.73	109.47
13	U	4	MAN	O5-C5-C4	-2.77	104.09	110.83
11	M	3	BMA	C2-C3-C4	-2.76	106.11	110.89
7	O	3	BMA	O5-C1-C2	-2.76	106.51	110.77
8	F	4	MAN	O2-C2-C3	2.76	115.66	110.14
12	S	3	BMA	C1-C2-C3	2.73	113.03	109.67
12	S	1	NAG	O4-C4-C3	-2.73	104.04	110.35
10	L	1	NAG	O7-C7-C8	-2.71	117.02	122.06
8	F	4	MAN	O4-C4-C5	2.71	116.02	109.30
8	F	2	NAG	C3-C4-C5	-2.70	105.42	110.24
8	F	1	NAG	C3-C4-C5	-2.70	105.42	110.24
13	U	4	MAN	O4-C4-C5	2.69	115.97	109.30
9	I	2	NAG	C1-C2-N2	2.68	115.06	110.49
7	A	2	NAG	C2-N2-C7	2.67	126.70	122.90
7	A	1	NAG	O5-C1-C2	2.66	115.50	111.29
8	F	4	MAN	O3-C3-C4	-2.64	104.24	110.35
7	C	3	BMA	O5-C1-C2	-2.64	106.70	110.77
12	S	4	MAN	O4-C4-C5	-2.64	102.75	109.30
12	S	5	MAN	O5-C5-C6	2.62	111.31	107.20
8	F	1	NAG	O3-C3-C4	2.61	116.39	110.35
7	H	1	NAG	C1-C2-N2	2.60	114.93	110.49
7	H	1	NAG	O4-C4-C3	-2.58	104.37	110.35
13	U	5	MAN	C6-C5-C4	2.58	119.04	113.00
7	J	2	NAG	C1-O5-C5	2.57	115.68	112.19
13	U	6	MAN	O2-C2-C1	2.55	114.38	109.15
7	T	1	NAG	C8-C7-N2	2.55	120.41	116.10
8	F	1	NAG	C1-O5-C5	2.53	115.62	112.19
9	K	1	NAG	O3-C3-C2	2.53	114.70	109.47
12	S	2	NAG	O5-C5-C6	-2.51	103.27	107.20
10	L	2	NAG	C6-C5-C4	2.50	118.87	113.00
8	F	4	MAN	C6-C5-C4	-2.49	107.17	113.00
8	F	1	NAG	C4-C3-C2	-2.49	107.37	111.02
8	F	3	BMA	C1-C2-C3	2.48	112.72	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	4	MAN	O5-C1-C2	-2.48	106.94	110.77
11	M	4	MAN	C1-O5-C5	2.47	115.54	112.19
7	O	1	NAG	O4-C4-C3	-2.45	104.68	110.35
13	U	2	NAG	C1-O5-C5	2.43	115.49	112.19
7	J	1	NAG	O3-C3-C4	2.42	115.94	110.35
7	H	2	NAG	C4-C3-C2	2.40	114.54	111.02
11	M	1	NAG	C1-C2-N2	2.40	114.59	110.49
7	P	3	BMA	O5-C1-C2	-2.39	107.09	110.77
11	M	3	BMA	O5-C5-C6	2.38	110.93	107.20
7	T	2	NAG	O5-C1-C2	-2.38	107.53	111.29
12	S	1	NAG	O6-C6-C5	2.35	119.34	111.29
10	L	2	NAG	O4-C4-C5	2.34	115.11	109.30
13	U	1	NAG	C1-O5-C5	2.34	115.36	112.19
9	N	2	NAG	O5-C1-C2	-2.34	107.59	111.29
12	S	1	NAG	O4-C4-C5	2.34	115.10	109.30
7	H	3	BMA	C1-C2-C3	2.33	112.54	109.67
12	S	3	BMA	O4-C4-C3	2.33	115.73	110.35
7	O	2	NAG	O5-C5-C6	2.32	110.84	107.20
10	L	2	NAG	C3-C4-C5	-2.31	106.12	110.24
7	J	1	NAG	O4-C4-C3	2.31	115.69	110.35
12	S	5	MAN	O2-C2-C1	2.31	113.87	109.15
7	P	2	NAG	O5-C5-C6	2.27	110.77	107.20
11	M	1	NAG	O7-C7-C8	-2.27	117.84	122.06
7	T	1	NAG	O5-C1-C2	-2.26	107.72	111.29
7	T	2	NAG	C3-C4-C5	-2.26	106.21	110.24
11	M	4	MAN	C1-C2-C3	2.24	112.42	109.67
9	N	1	NAG	O4-C4-C5	-2.22	103.77	109.30
7	O	1	NAG	C6-C5-C4	-2.22	107.81	113.00
7	C	2	NAG	C1-C2-N2	2.22	114.27	110.49
10	L	1	NAG	O4-C4-C5	2.21	114.78	109.30
7	T	2	NAG	C1-C2-N2	2.21	114.26	110.49
9	K	1	NAG	C8-C7-N2	-2.21	112.36	116.10
7	A	1	NAG	O5-C5-C6	2.20	110.66	107.20
12	S	4	MAN	C1-C2-C3	2.20	112.37	109.67
7	J	2	NAG	C1-C2-N2	2.20	114.24	110.49
13	U	1	NAG	O4-C4-C5	2.19	114.75	109.30
7	H	1	NAG	C4-C3-C2	2.18	114.21	111.02
13	U	2	NAG	O3-C3-C2	-2.14	105.03	109.47
9	K	1	NAG	O7-C7-N2	2.14	125.89	121.95
13	U	6	MAN	O2-C2-C3	-2.11	105.92	110.14
9	N	2	NAG	O5-C5-C6	2.10	110.50	107.20
13	U	6	MAN	C6-C5-C4	-2.10	108.10	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	3	BMA	O5-C1-C2	-2.08	107.56	110.77
13	U	2	NAG	O4-C4-C3	2.06	115.11	110.35
7	T	1	NAG	O5-C5-C6	2.04	110.40	107.20
7	A	2	NAG	C1-O5-C5	2.03	114.94	112.19
10	L	1	NAG	C3-C4-C5	-2.01	106.65	110.24
7	H	1	NAG	C2-N2-C7	2.01	125.76	122.90
8	F	4	MAN	O4-C4-C3	2.01	114.99	110.35
10	L	3	BMA	C1-C2-C3	2.01	112.13	109.67

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C3-C2-N2-C7
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	J	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C8-C7-N2-C2
7	J	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	T	1	NAG	C8-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
7	T	2	NAG	C8-C7-N2-C2
7	T	2	NAG	O7-C7-N2-C2
8	F	2	NAG	C3-C2-N2-C7
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
9	K	2	NAG	C8-C7-N2-C2
9	K	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	N	1	NAG	C3-C2-N2-C7
11	M	1	NAG	C8-C7-N2-C2
11	M	1	NAG	O7-C7-N2-C2
13	U	1	NAG	C8-C7-N2-C2
13	U	1	NAG	O7-C7-N2-C2
8	F	4	MAN	C4-C5-C6-O6
13	U	6	MAN	C4-C5-C6-O6
8	F	1	NAG	C8-C7-N2-C2
9	I	2	NAG	C8-C7-N2-C2
9	I	2	NAG	O7-C7-N2-C2
12	S	4	MAN	O5-C5-C6-O6
7	O	2	NAG	C1-C2-N2-C7
8	F	4	MAN	O5-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
8	F	3	BMA	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
8	F	1	NAG	O7-C7-N2-C2
8	F	2	NAG	C8-C7-N2-C2
8	F	2	NAG	O7-C7-N2-C2
9	N	1	NAG	C8-C7-N2-C2
9	N	1	NAG	O7-C7-N2-C2
9	N	2	NAG	C8-C7-N2-C2
7	C	1	NAG	C4-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
13	U	2	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
10	L	4	MAN	O5-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
13	U	6	MAN	O5-C5-C6-O6
7	C	1	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
10	L	1	NAG	O5-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
13	U	2	NAG	C4-C5-C6-O6
12	S	3	BMA	O5-C5-C6-O6
12	S	4	MAN	C4-C5-C6-O6
7	H	1	NAG	C1-C2-N2-C7
9	K	1	NAG	C1-C2-N2-C7
9	N	1	NAG	O5-C5-C6-O6
12	S	1	NAG	O5-C5-C6-O6

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

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Mol	Chain	Res	Type	Atoms
7	J	3	BMA	O5-C5-C6-O6
10	L	2	NAG	C1-C2-N2-C7
7	C	1	NAG	C8-C7-N2-C2
9	K	1	NAG	O5-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
7	C	1	NAG	C1-C2-N2-C7
7	T	3	BMA	C4-C5-C6-O6
7	C	1	NAG	O7-C7-N2-C2
8	F	1	NAG	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
10	L	3	BMA	C4-C5-C6-O6
7	C	2	NAG	C3-C2-N2-C7
7	O	1	NAG	C3-C2-N2-C7
9	K	1	NAG	C3-C2-N2-C7
7	A	1	NAG	C4-C5-C6-O6
7	C	1	NAG	C3-C2-N2-C7

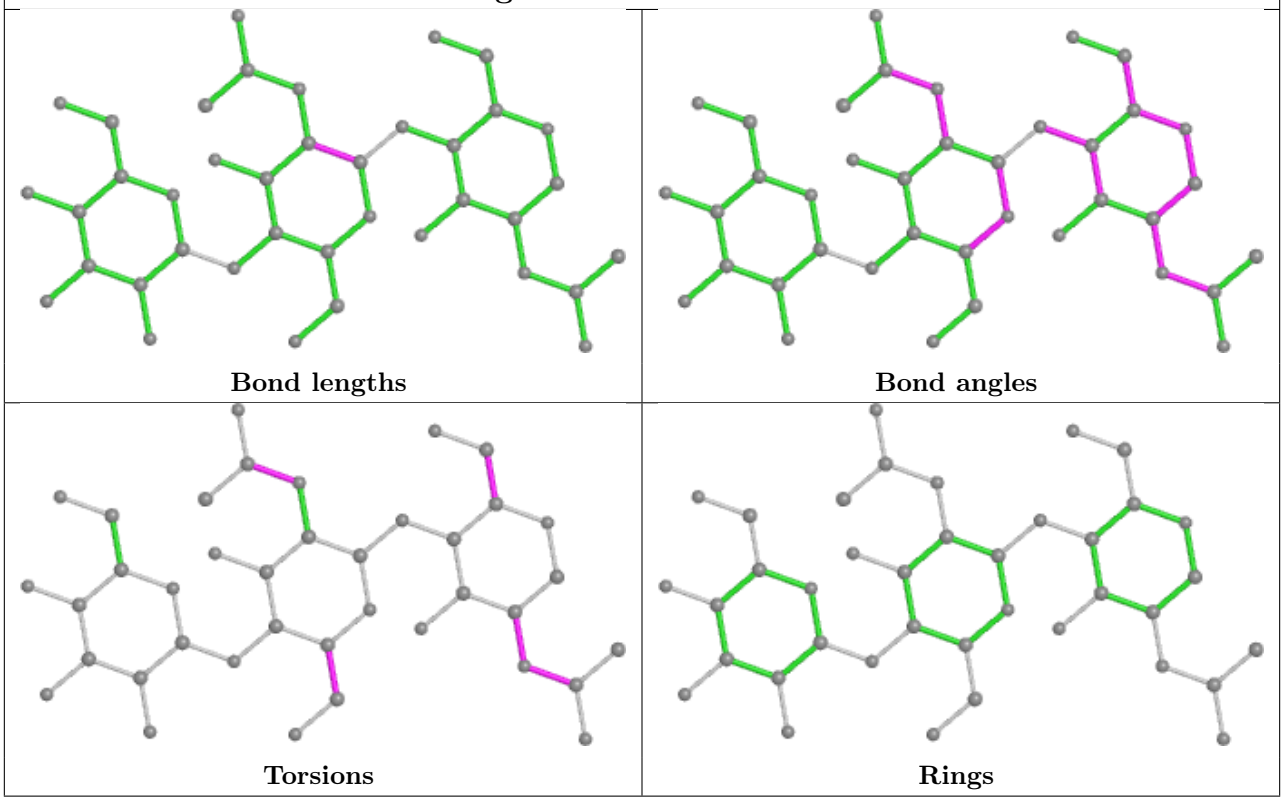
There are no ring outliers.

21 monomers are involved in 69 short contacts:

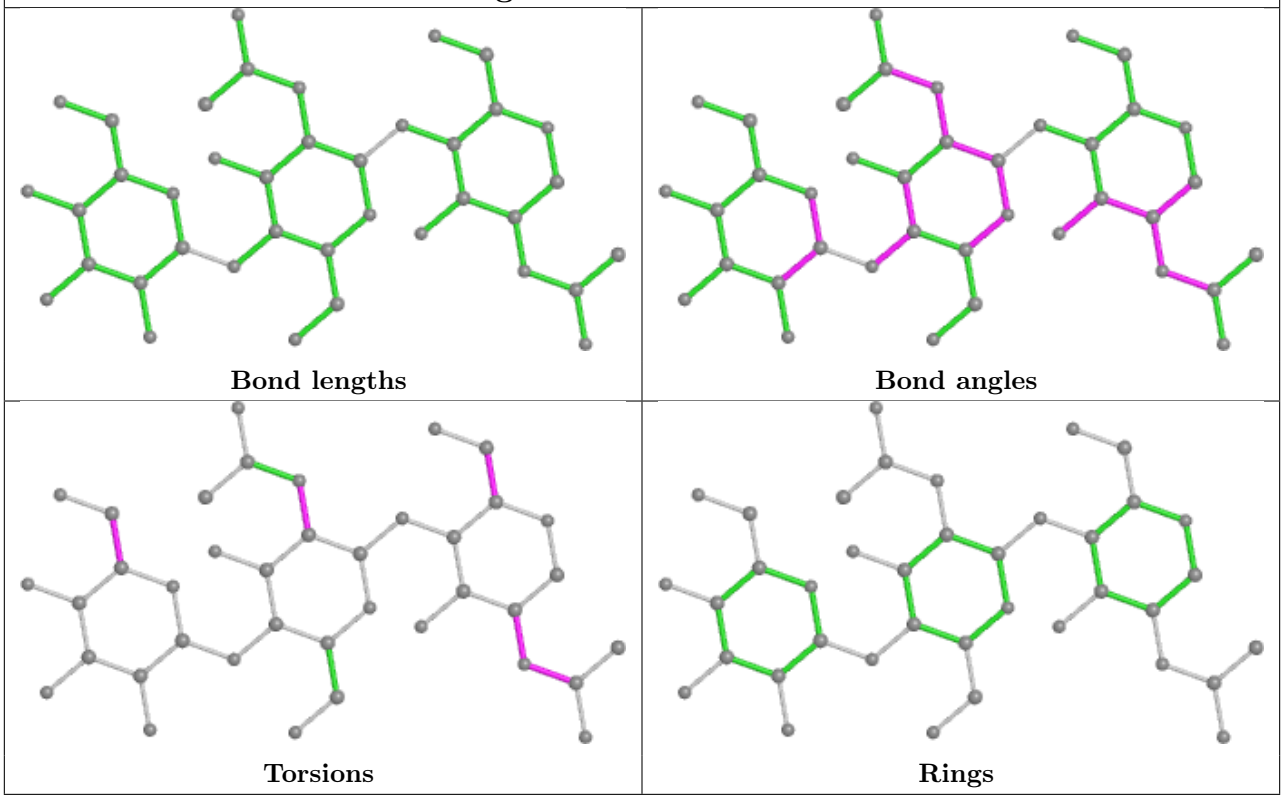
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	S	4	MAN	2	0
10	L	1	NAG	9	0
10	L	6	MAN	1	0
8	F	1	NAG	2	0
9	N	1	NAG	1	0
13	U	3	BMA	2	0
13	U	2	NAG	5	0
7	O	1	NAG	1	0
8	F	4	MAN	7	0
7	P	1	NAG	1	0
9	K	1	NAG	10	0
10	L	2	NAG	1	0
11	M	1	NAG	5	0
7	O	2	NAG	1	0
7	H	1	NAG	5	0
8	F	2	NAG	2	0
13	U	1	NAG	10	0
13	U	6	MAN	1	0
12	S	1	NAG	2	0
7	C	1	NAG	1	0
7	A	3	BMA	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.

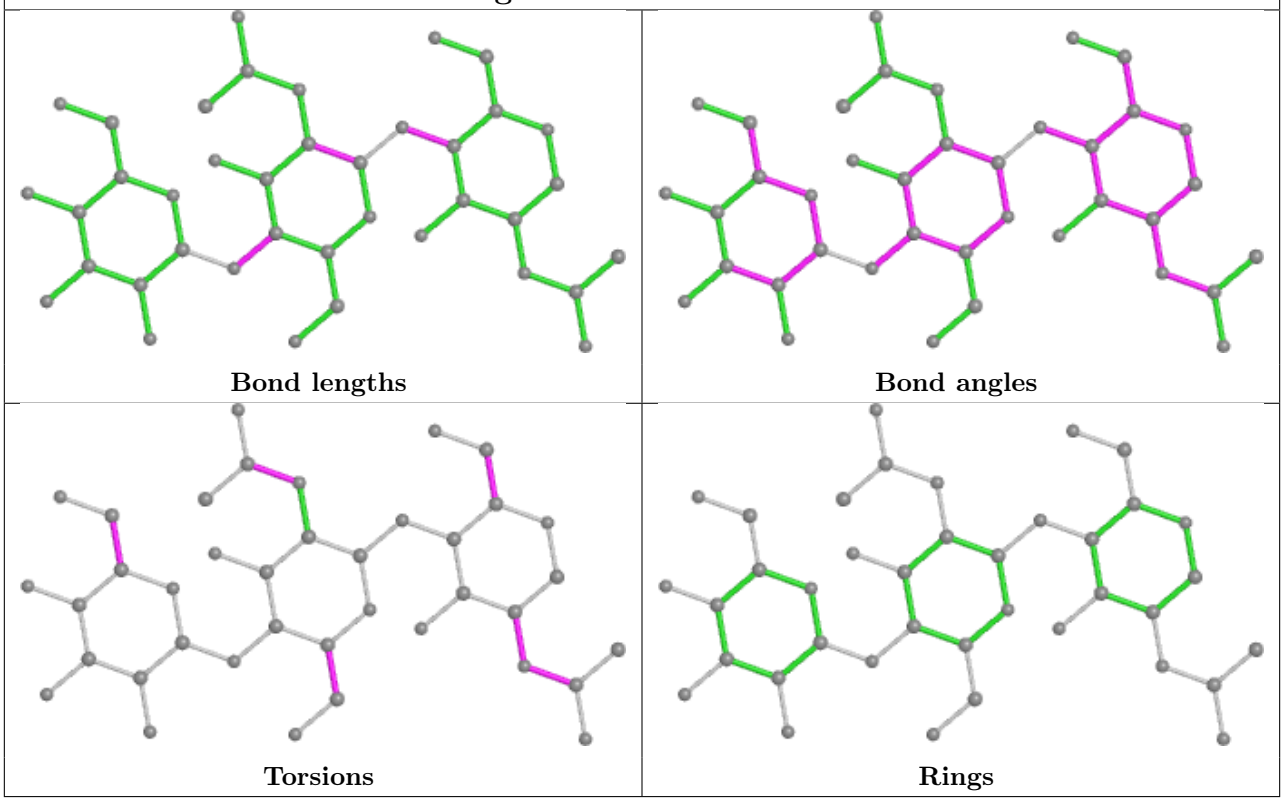
Oligosaccharide Chain A



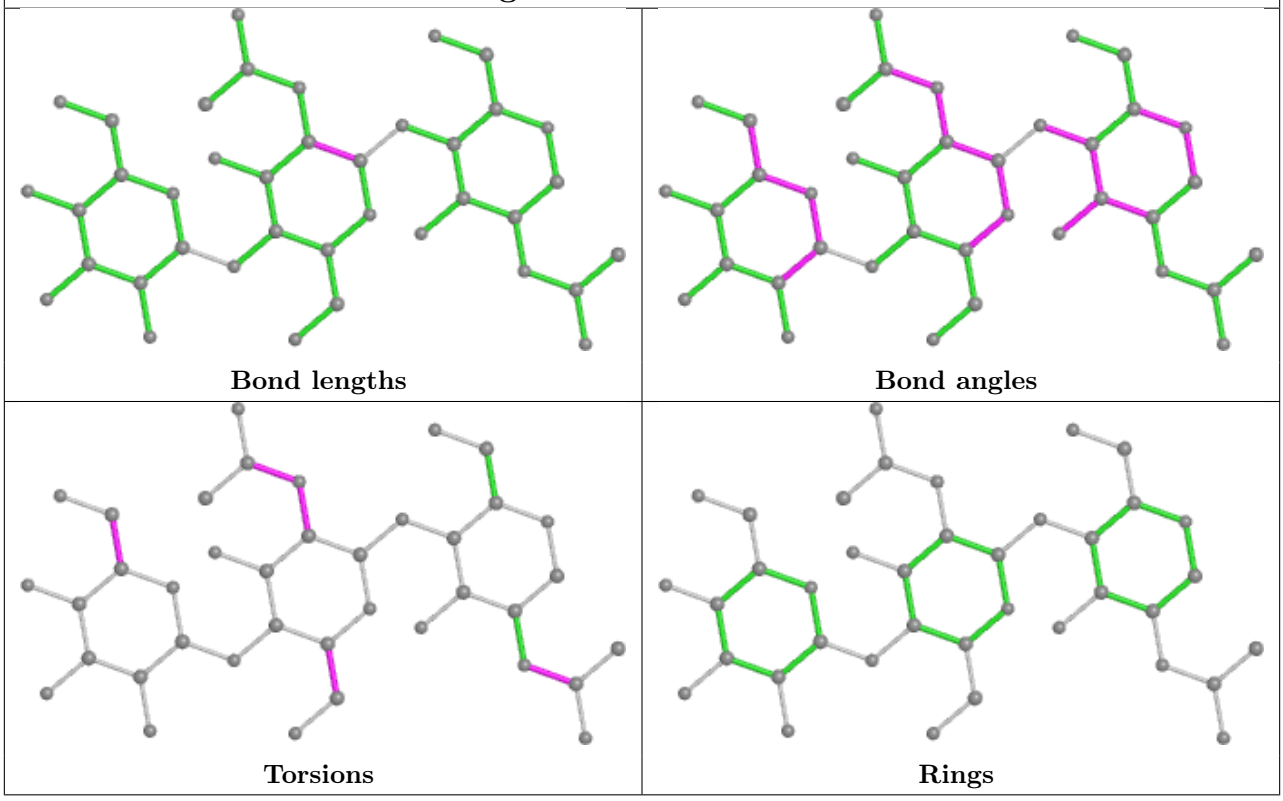
Oligosaccharide Chain C



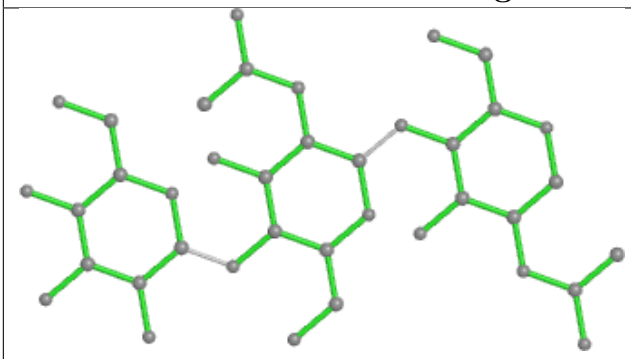
Oligosaccharide Chain H



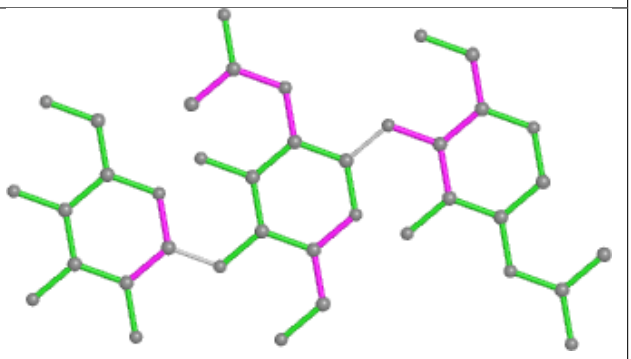
Oligosaccharide Chain J



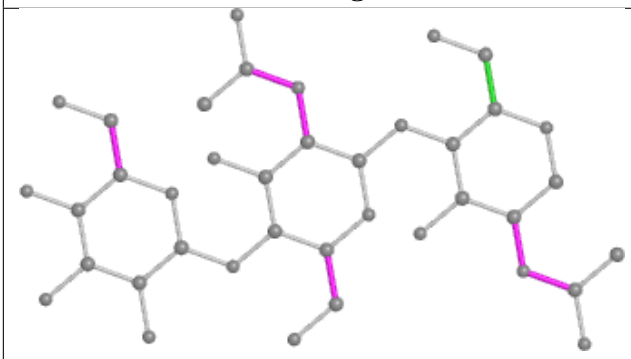
Oligosaccharide Chain O



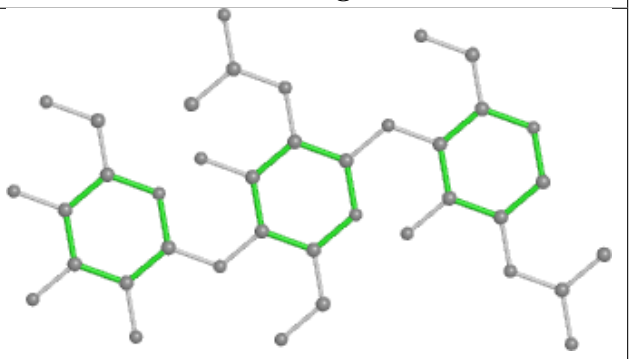
Bond lengths



Bond angles

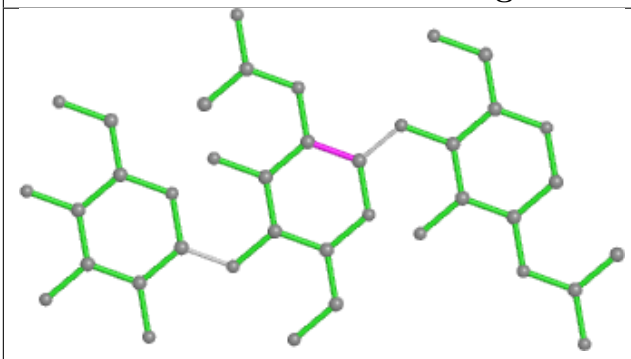


Torsions

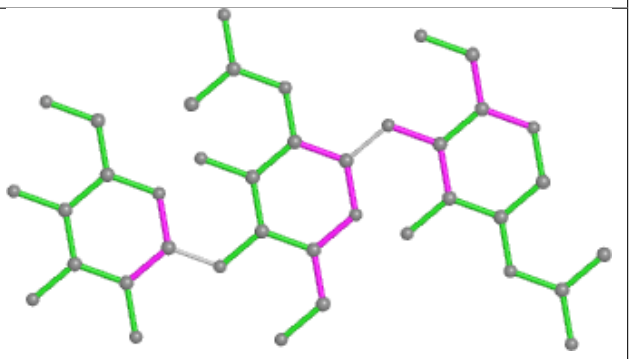


Rings

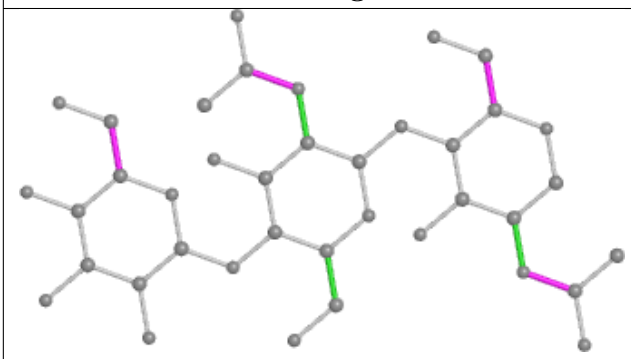
Oligosaccharide Chain P



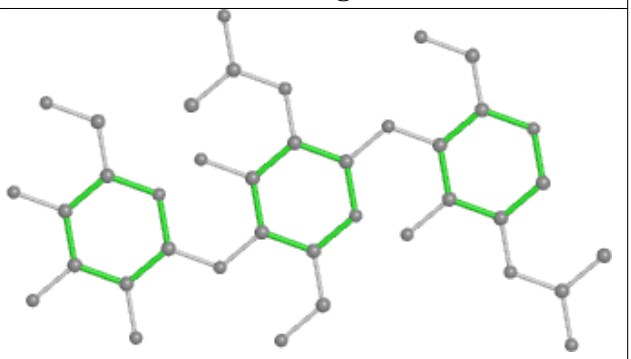
Bond lengths



Bond angles

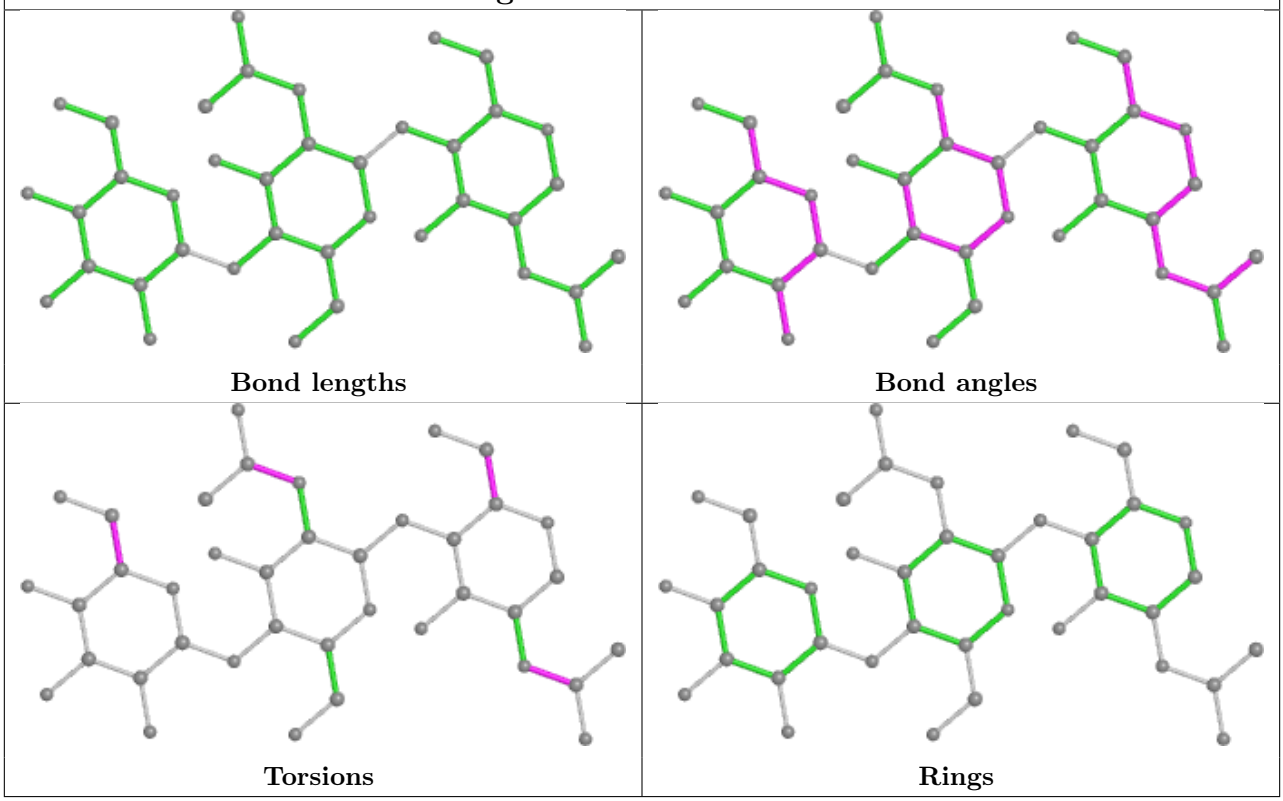


Torsions

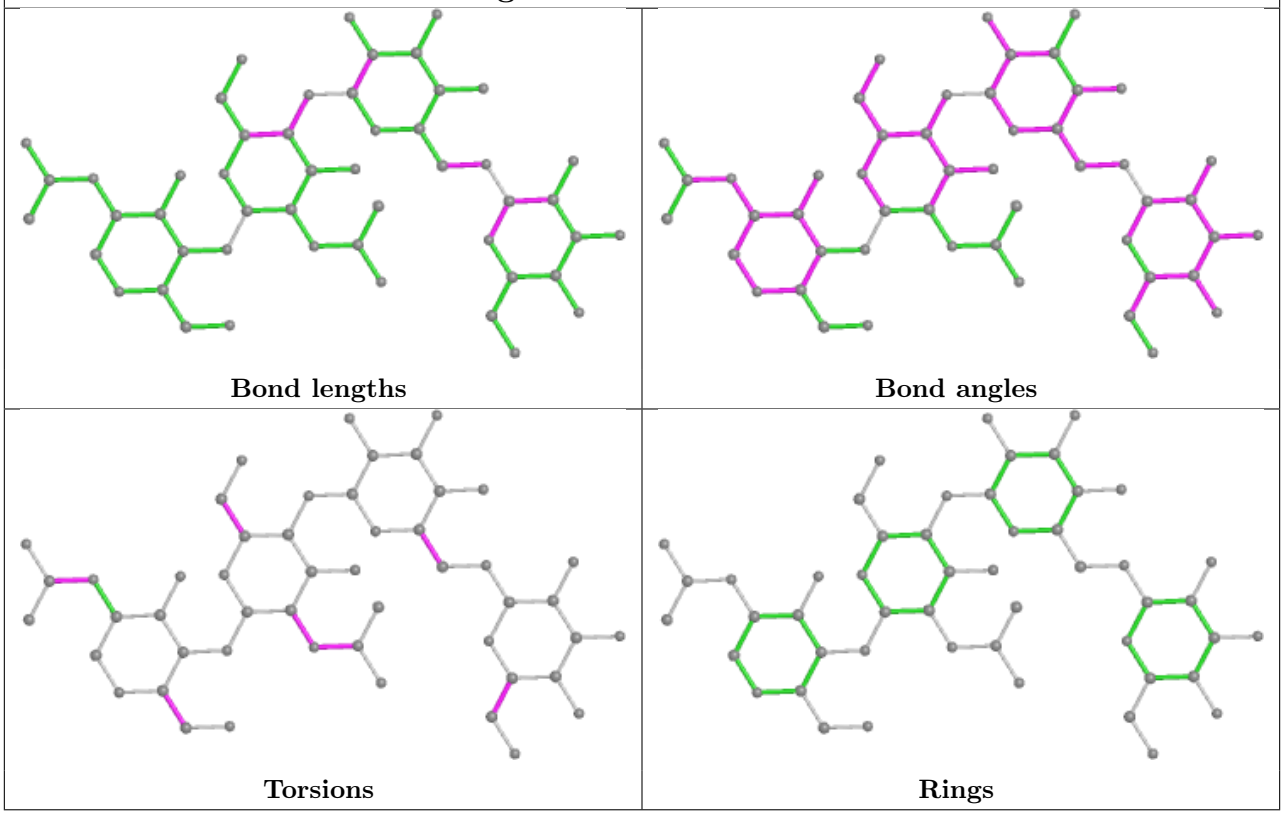


Rings

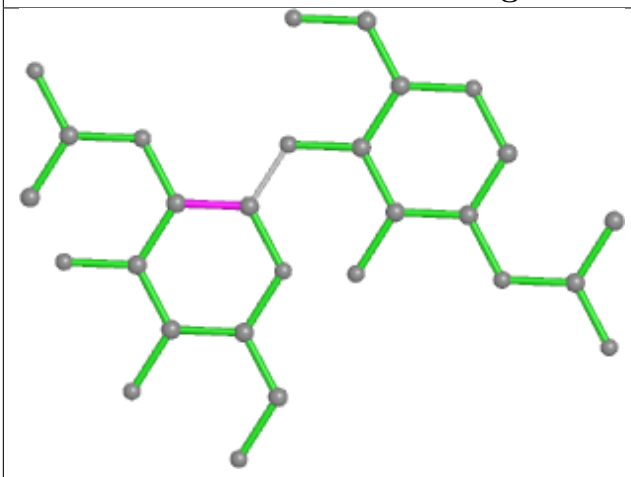
Oligosaccharide Chain T



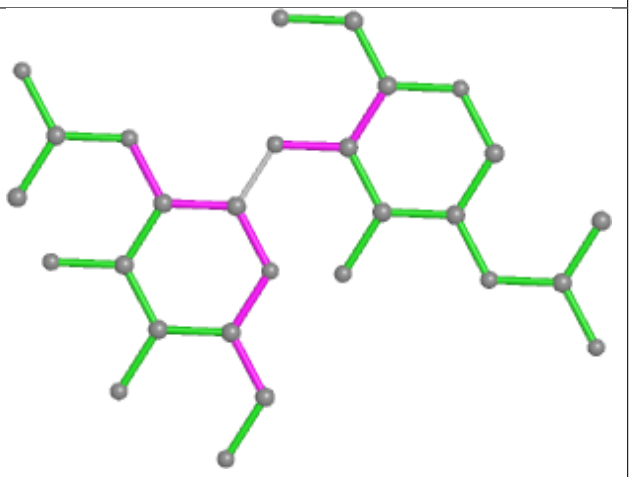
Oligosaccharide Chain F



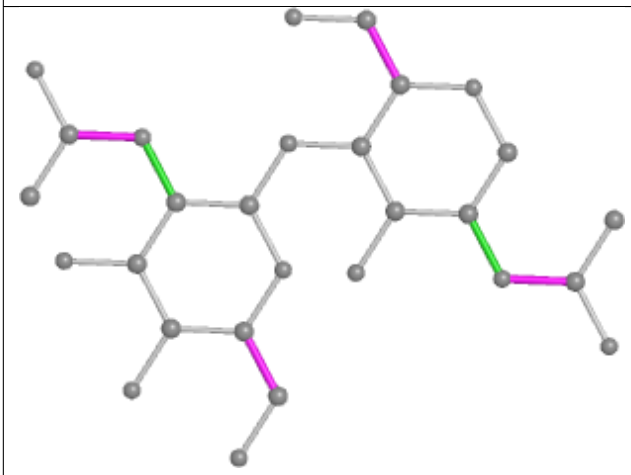
Oligosaccharide Chain I



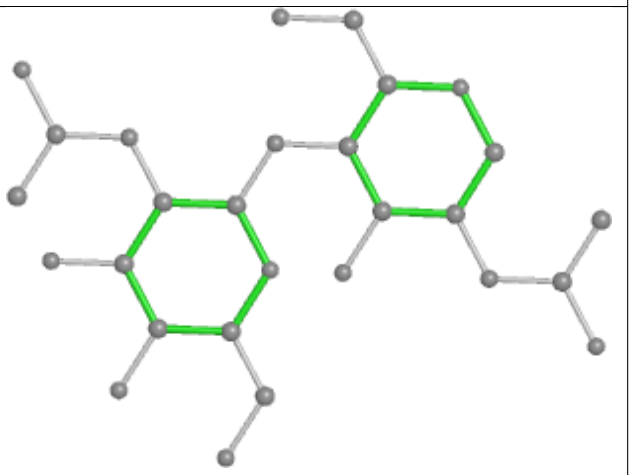
Bond lengths



Bond angles

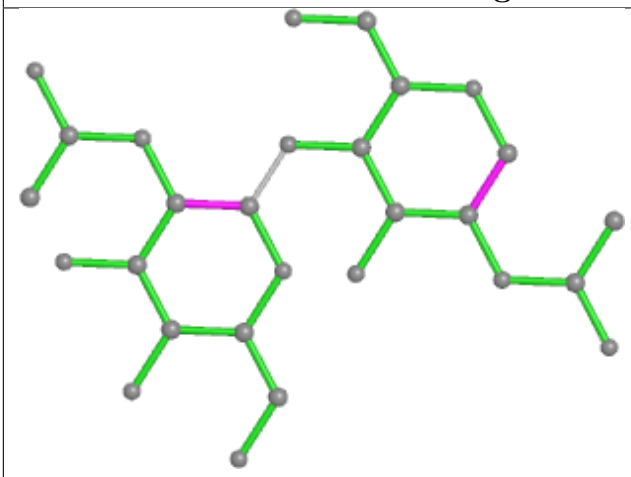


Torsions

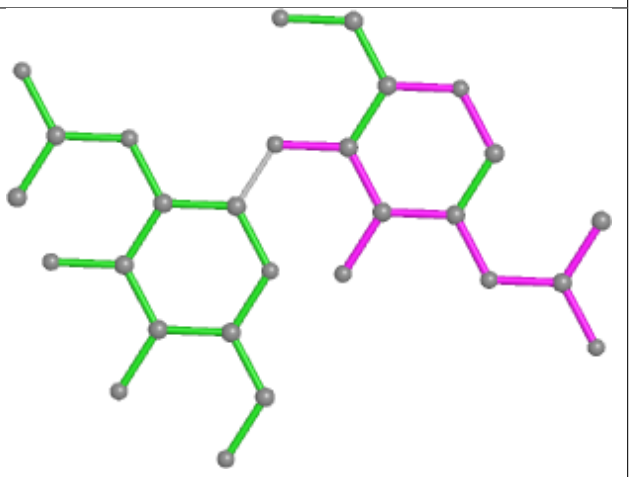


Rings

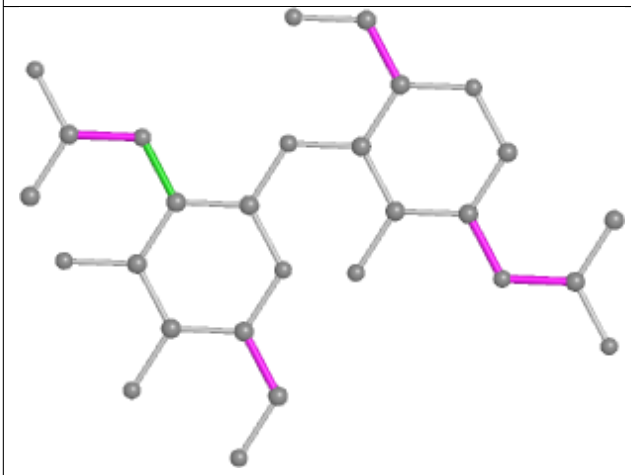
Oligosaccharide Chain K



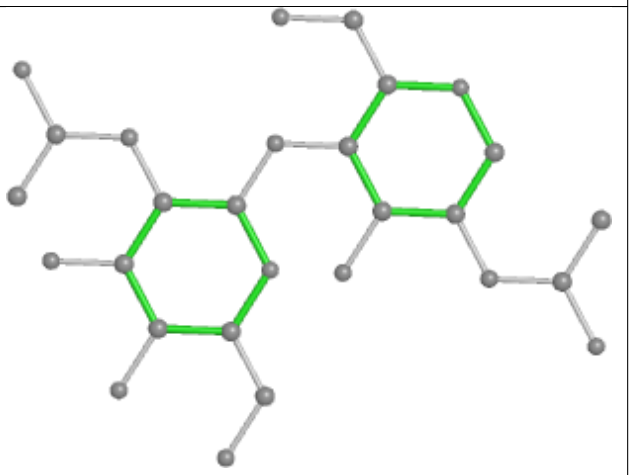
Bond lengths



Bond angles

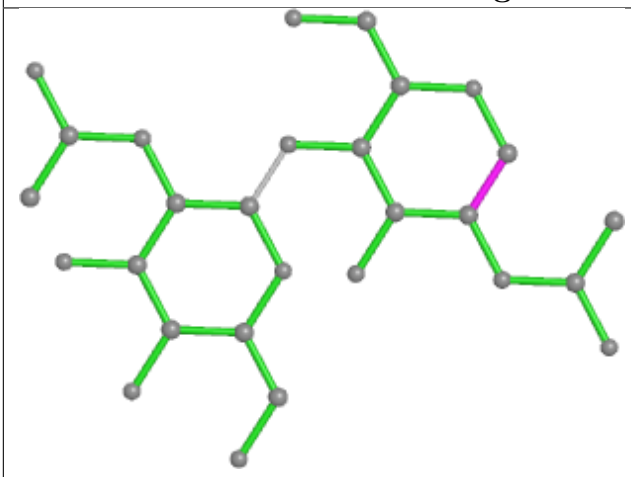


Torsions

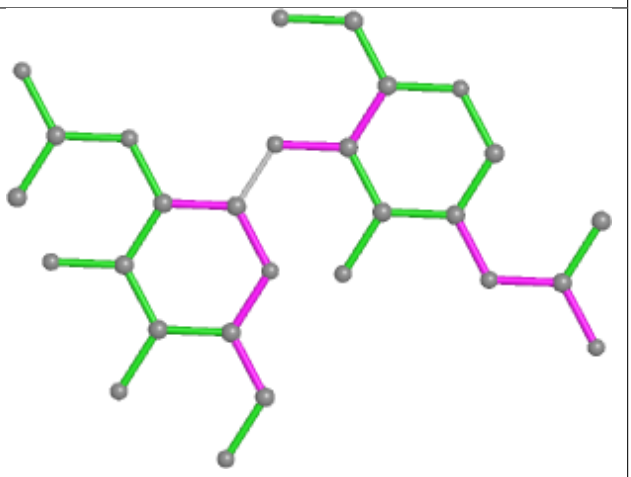


Rings

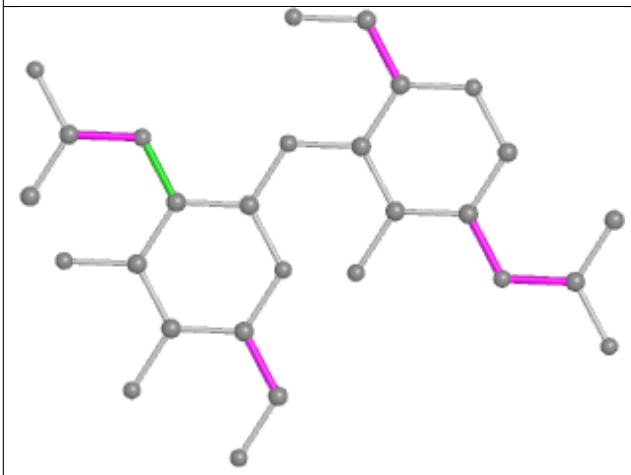
Oligosaccharide Chain N



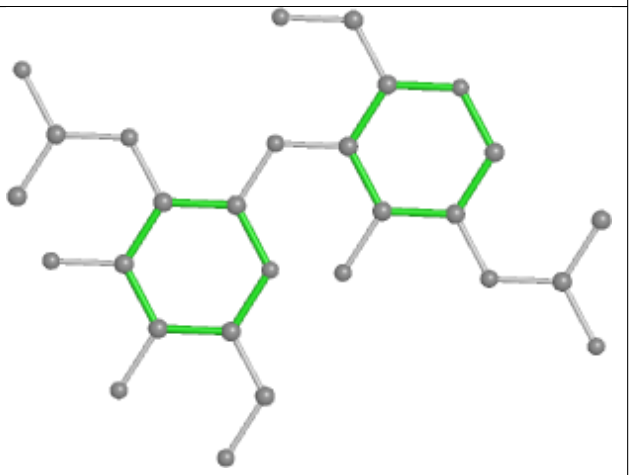
Bond lengths



Bond angles

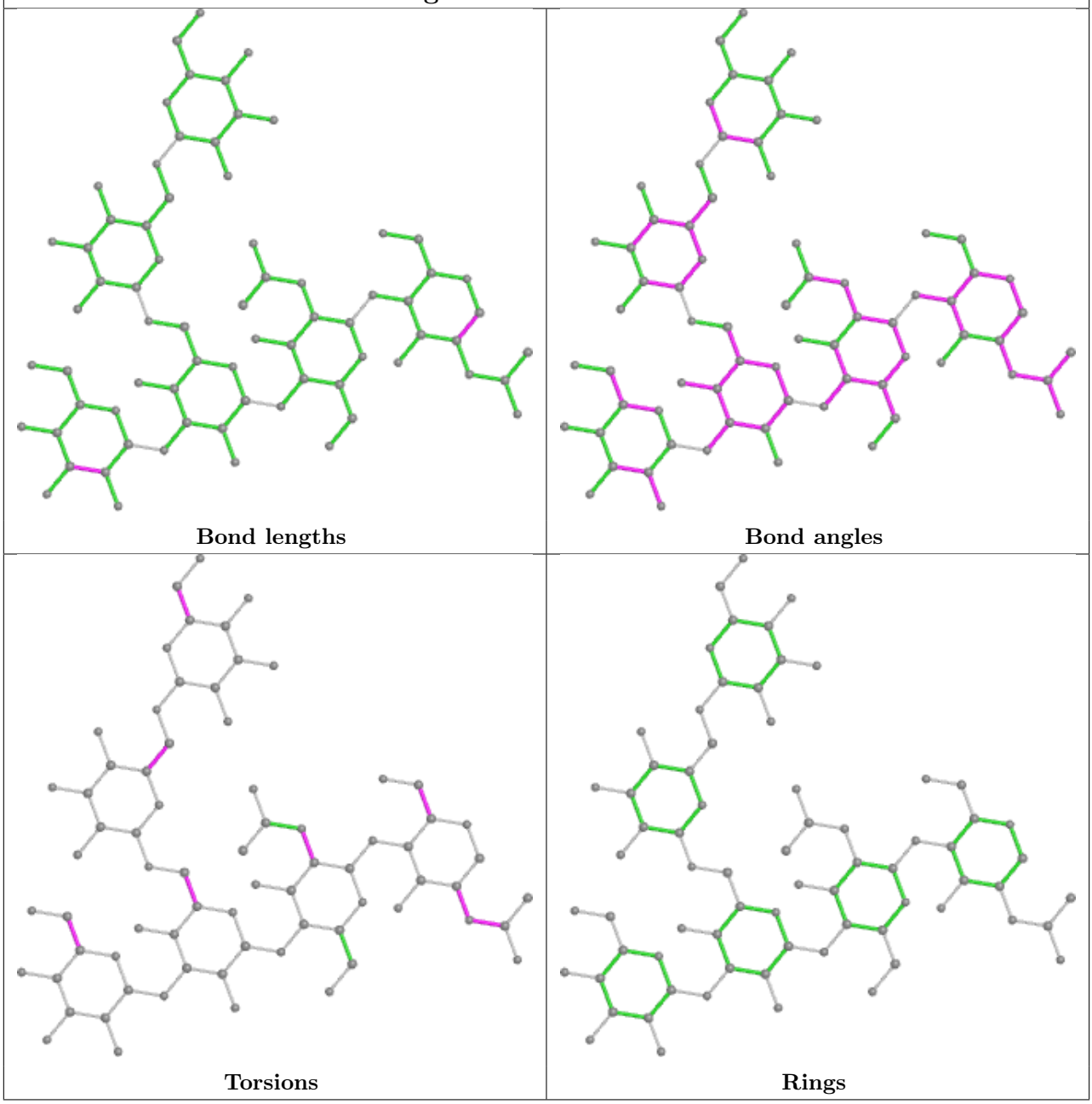


Torsions

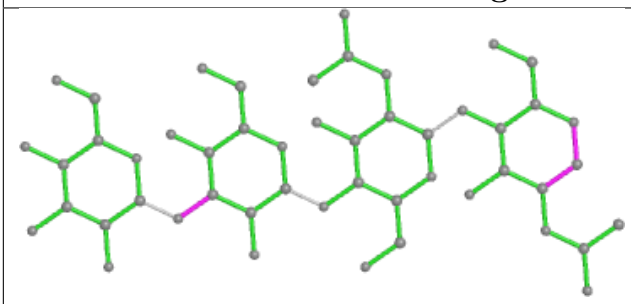


Rings

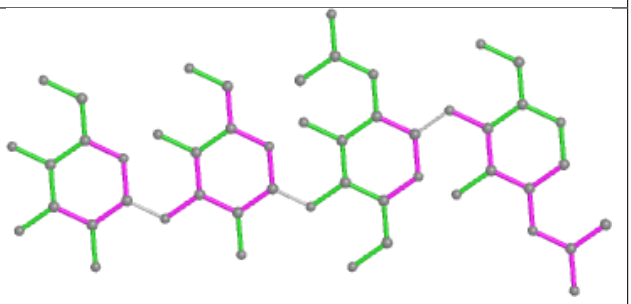
Oligosaccharide Chain L



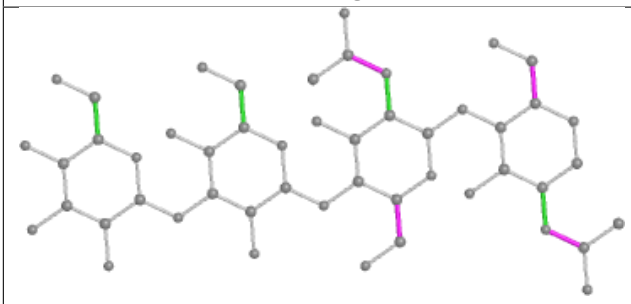
Oligosaccharide Chain M



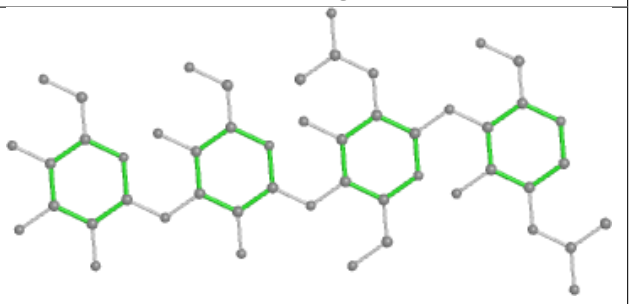
Bond lengths



Bond angles

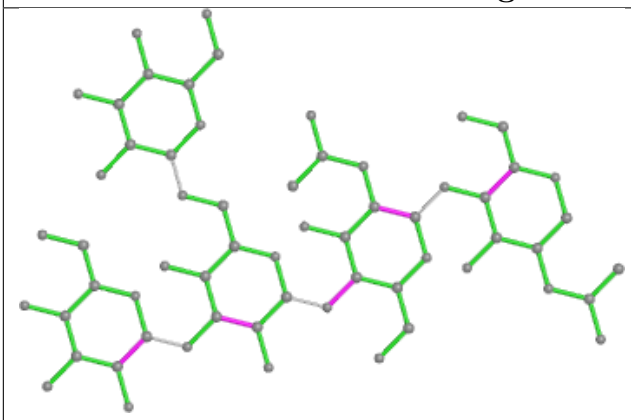


Torsions

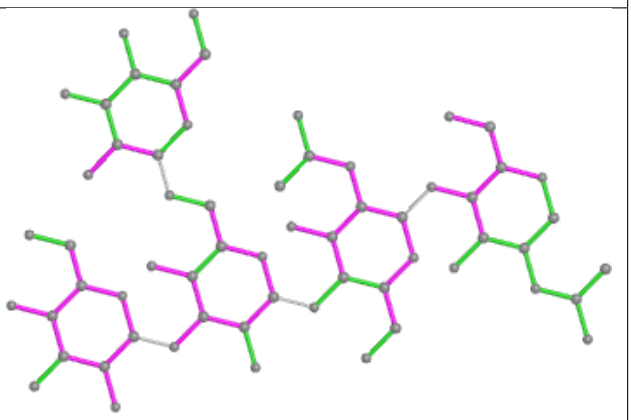


Rings

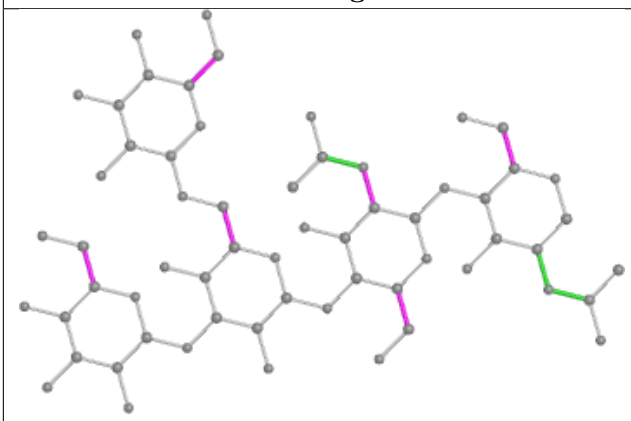
Oligosaccharide Chain S



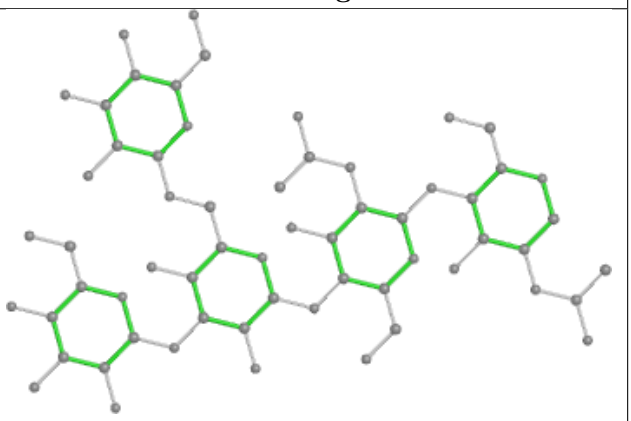
Bond lengths



Bond angles

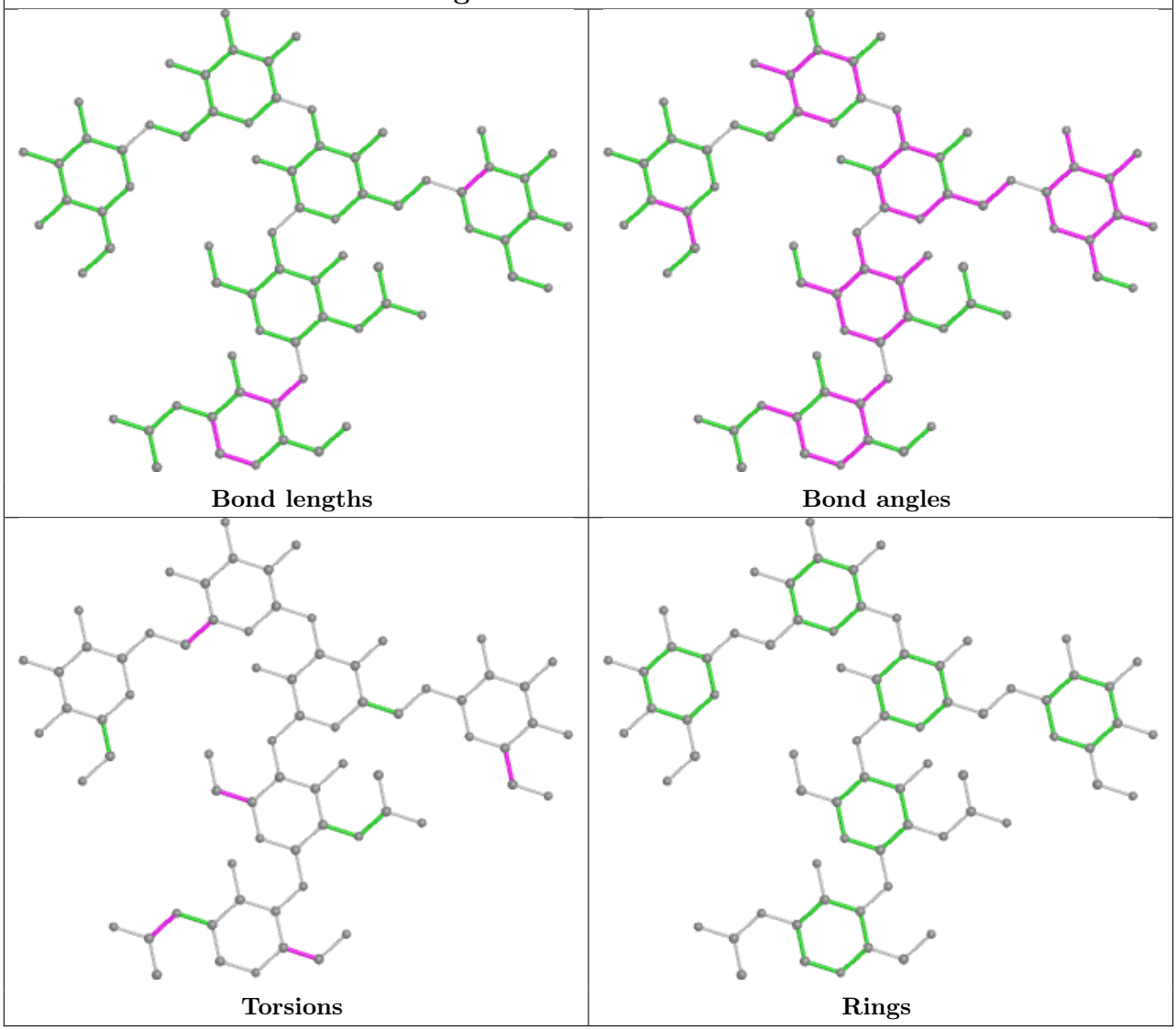


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	NAG	G	606	4	14,14,15	1.20	1 (7%)	17,19,21	1.93	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	NAG	G	622	4	14,14,15	0.90	1 (7%)	17,19,21	1.92	6 (35%)
14	NAG	G	631	4	14,14,15	0.60	0	17,19,21	1.77	4 (23%)
14	NAG	B	704	1	14,14,15	0.30	0	17,19,21	1.11	2 (11%)

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
14	NAG	G	606	4	-	5/6/23/26	0/1/1/1
14	NAG	G	622	4	-	5/6/23/26	0/1/1/1
14	NAG	G	631	4	-	1/6/23/26	0/1/1/1
14	NAG	B	704	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	606	NAG	C1-C2	3.53	1.57	1.52
14	G	622	NAG	C1-C2	2.36	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	606	NAG	C2-N2-C7	5.43	130.64	122.90
14	G	631	NAG	C2-N2-C7	4.16	128.83	122.90
14	G	631	NAG	O5-C5-C6	3.74	113.07	107.20
14	G	622	NAG	C2-N2-C7	3.10	127.31	122.90
14	G	622	NAG	C6-C5-C4	-3.07	105.82	113.00
14	B	704	NAG	C2-N2-C7	-3.04	118.57	122.90
14	G	622	NAG	C1-O5-C5	2.76	115.94	112.19
14	G	606	NAG	C1-O5-C5	-2.59	108.69	112.19
14	G	622	NAG	O3-C3-C2	2.43	114.49	109.47
14	G	622	NAG	O5-C1-C2	-2.41	107.49	111.29
14	G	606	NAG	C1-C2-N2	2.34	114.48	110.49
14	G	606	NAG	C8-C7-N2	2.31	120.02	116.10
14	G	606	NAG	O3-C3-C2	2.29	114.21	109.47
14	G	622	NAG	O7-C7-C8	-2.29	117.81	122.06
14	B	704	NAG	C4-C3-C2	-2.27	107.69	111.02
14	G	631	NAG	C4-C3-C2	2.05	114.02	111.02
14	G	631	NAG	C6-C5-C4	-2.03	108.25	113.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	704	NAG	C8-C7-N2-C2
14	B	704	NAG	O7-C7-N2-C2
14	G	606	NAG	C3-C2-N2-C7
14	G	606	NAG	C8-C7-N2-C2
14	G	606	NAG	O7-C7-N2-C2
14	G	622	NAG	C8-C7-N2-C2
14	G	622	NAG	O7-C7-N2-C2
14	G	606	NAG	C4-C5-C6-O6
14	B	704	NAG	O5-C5-C6-O6
14	G	606	NAG	O5-C5-C6-O6
14	G	622	NAG	C1-C2-N2-C7
14	B	704	NAG	C4-C5-C6-O6
14	G	622	NAG	C3-C2-N2-C7
14	G	631	NAG	C3-C2-N2-C7
14	G	622	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	704	NAG	4	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	B	136/153 (88%)	0.13	6 (4%)	34	29	183, 285, 325, 365	0
2	D	236/243 (97%)	0.22	9 (3%)	40	33	207, 303, 325, 325	0
3	E	213/216 (98%)	0.02	8 (3%)	40	33	196, 297, 325, 325	0
4	G	448/518 (86%)	-0.00	7 (1%)	72	63	186, 292, 325, 375	0
5	Q	231/240 (96%)	0.24	13 (5%)	24	21	210, 298, 325, 325	0
6	R	205/215 (95%)	0.25	9 (4%)	34	29	219, 309, 325, 325	0
All	All	1469/1585 (92%)	0.12	52 (3%)	44	36	183, 298, 325, 375	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	CYS	5.0
4	G	73	ALA	4.9
5	Q	150	GLY	4.8
5	Q	149	SER	4.7
1	B	600	GLY	4.4
5	Q	142	ALA	4.3
3	E	112	GLN	4.2
5	Q	201	VAL	4.1
1	B	549	VAL	4.1
4	G	72	HIS	4.0
5	Q	11	LEU	3.5
2	D	33	HIS	3.5
5	Q	148	THR	3.4
5	Q	202	PRO	3.3
6	R	215	CYS	3.2
6	R	42	GLY	3.1
4	G	133	ASN	3.1
2	D	69	MET	3.0
2	D	71	THR	3.0

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Mol	Chain	Res	Type	RSRZ
5	Q	143	PRO	2.9
3	E	152	TRP	2.9
3	E	150	VAL	2.7
1	B	548	ILE	2.7
3	E	212	PRO	2.7
5	Q	146	LYS	2.7
2	D	112	SER	2.6
2	D	1	GLU	2.6
2	D	70	THR	2.6
6	R	152	TRP	2.5
6	R	213	THR	2.5
5	Q	136	PRO	2.5
3	E	114	LYS	2.4
6	R	189	TRP	2.4
2	D	113	SER	2.3
5	Q	197	SER	2.3
3	E	43	GLY	2.3
4	G	180	ASP	2.3
5	Q	232	SER	2.3
1	B	547	GLY	2.2
4	G	354	PRO	2.2
1	B	599	SER	2.2
6	R	212	PRO	2.2
4	G	443	ILE	2.2
3	E	151	ALA	2.2
6	R	109	VAL	2.2
6	R	113	PRO	2.2
2	D	52(A)	PRO	2.2
5	Q	164	PRO	2.2
4	G	496	ILE	2.1
1	B	607	ASN	2.1
3	E	165	THR	2.0
6	R	76	ILE	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BMA	A	3	11/12	0.42	0.41	420,420,420,420	0
7	BMA	O	3	11/12	0.47	0.22	435,435,435,435	0
13	MAN	U	5	11/12	0.48	0.73	366,366,366,366	0
7	NAG	A	2	14/15	0.52	0.69	430,430,430,430	0
7	BMA	H	3	11/12	0.52	0.42	478,478,478,478	0
12	MAN	S	4	11/12	0.56	0.35	327,327,327,327	0
7	BMA	J	3	11/12	0.57	0.34	441,441,441,441	0
9	NAG	I	2	14/15	0.60	0.33	433,433,433,433	0
8	MAN	F	4	11/12	0.62	0.26	360,360,360,360	0
8	NAG	F	2	14/15	0.64	0.29	337,337,337,337	0
7	BMA	C	3	11/12	0.66	0.29	450,450,450,450	0
11	MAN	M	4	11/12	0.67	0.25	456,456,456,456	0
8	NAG	F	1	14/15	0.67	0.31	343,343,343,343	0
7	NAG	H	2	14/15	0.67	0.40	449,449,449,449	0
12	BMA	S	3	11/12	0.70	0.23	415,415,415,415	0
9	NAG	I	1	14/15	0.73	0.30	396,396,396,396	0
7	BMA	T	3	11/12	0.74	0.18	415,415,415,415	0
7	NAG	A	1	14/15	0.76	0.40	411,411,411,411	0
7	NAG	C	2	14/15	0.76	0.38	449,449,449,449	0
8	BMA	F	3	11/12	0.76	0.25	349,349,349,349	0
9	NAG	N	1	14/15	0.76	0.36	391,391,391,391	0
10	NAG	L	1	14/15	0.78	0.28	396,396,396,396	0
11	BMA	M	3	11/12	0.78	0.21	432,432,432,432	0
9	NAG	K	1	14/15	0.78	0.17	311,311,311,311	0
10	MAN	L	4	11/12	0.79	0.12	387,387,387,387	0
12	NAG	S	2	14/15	0.80	0.16	398,398,398,398	0
12	MAN	S	5	11/12	0.81	0.30	397,397,397,397	0
7	NAG	H	1	14/15	0.81	0.21	383,383,383,383	0
10	MAN	L	6	11/12	0.82	0.19	369,369,369,369	0
10	MAN	L	5	11/12	0.85	0.13	416,416,416,416	0
7	BMA	P	3	11/12	0.86	0.18	417,417,417,417	0
7	NAG	O	2	14/15	0.86	0.32	428,428,428,428	0
7	NAG	O	1	14/15	0.86	0.40	394,394,394,394	0
12	NAG	S	1	14/15	0.87	0.17	343,343,343,343	0
9	NAG	K	2	14/15	0.88	0.19	333,333,333,333	0
13	NAG	U	1	14/15	0.88	0.17	352,352,352,352	0
13	BMA	U	3	11/12	0.88	0.13	334,334,334,334	0

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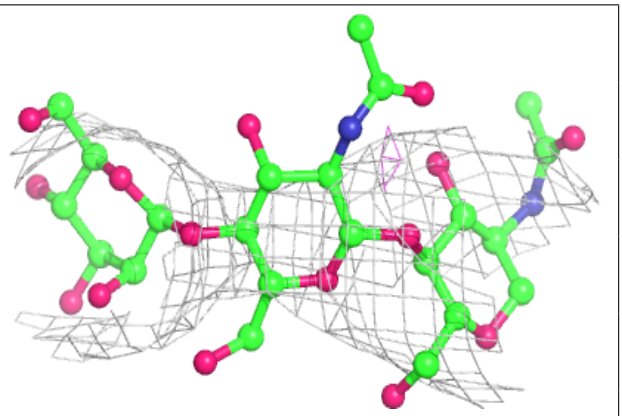
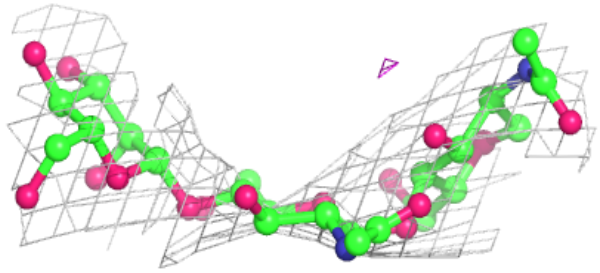
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	J	1	14/15	0.88	0.22	384,384,384,384	0
10	NAG	L	2	14/15	0.89	0.24	340,340,340,340	0
9	NAG	N	2	14/15	0.90	0.28	422,422,422,422	0
7	NAG	P	1	14/15	0.90	0.36	386,386,386,386	0
7	NAG	C	1	14/15	0.90	0.14	428,428,428,428	0
13	MAN	U	4	11/12	0.90	0.17	373,373,373,373	0
7	NAG	J	2	14/15	0.90	0.29	418,418,418,418	0
13	MAN	U	6	11/12	0.90	0.12	331,331,331,331	0
7	NAG	T	2	14/15	0.91	0.24	425,425,425,425	0
7	NAG	T	1	14/15	0.93	0.16	380,380,380,380	0
13	NAG	U	2	14/15	0.93	0.26	359,359,359,359	0
11	NAG	M	2	14/15	0.94	0.12	405,405,405,405	0
11	NAG	M	1	14/15	0.94	0.21	390,390,390,390	0
7	NAG	P	2	14/15	0.95	0.23	409,409,409,409	0
10	BMA	L	3	11/12	0.95	0.07	386,386,386,386	0

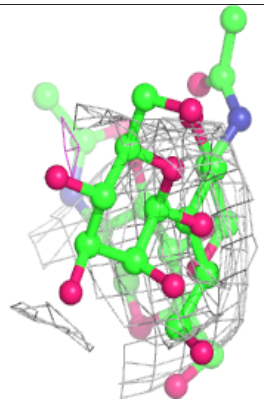
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

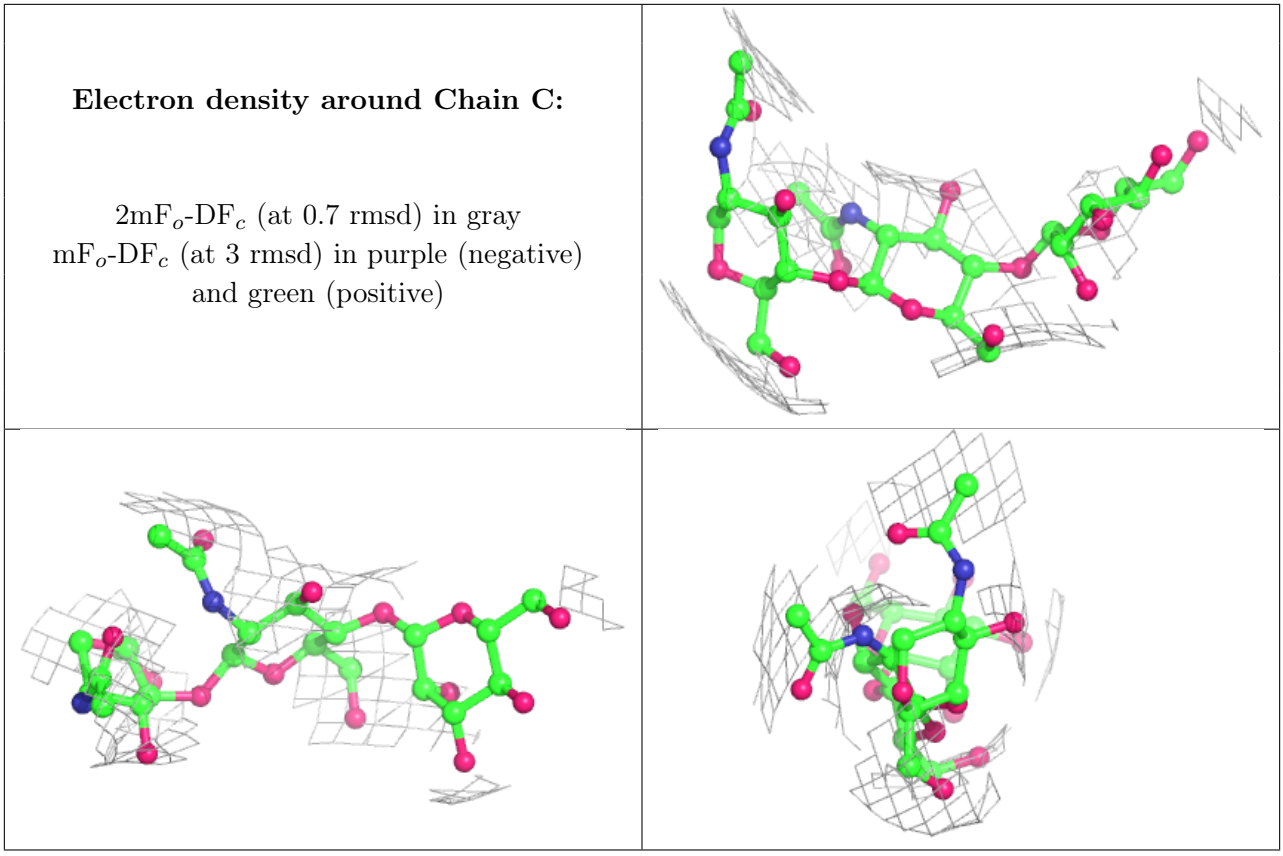






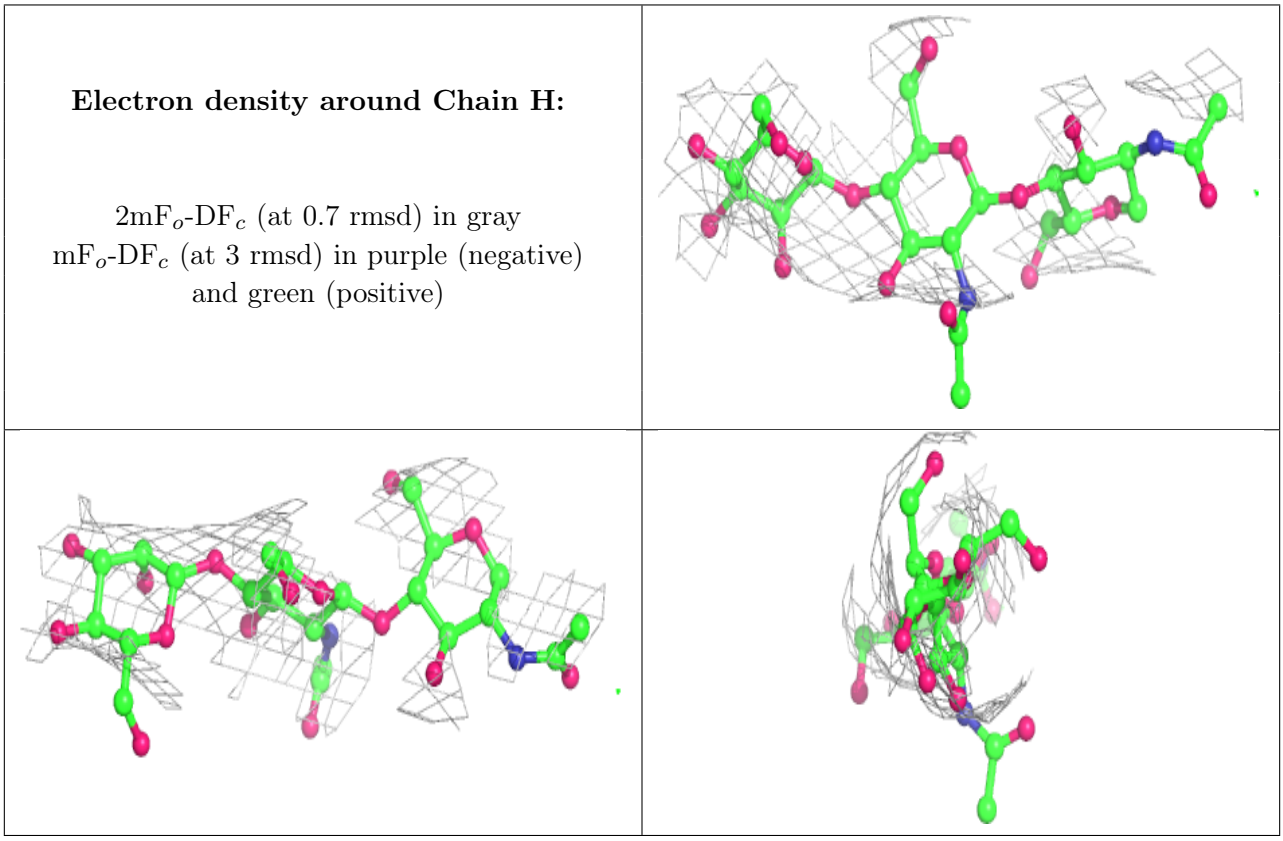
Electron density around Chain C:

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



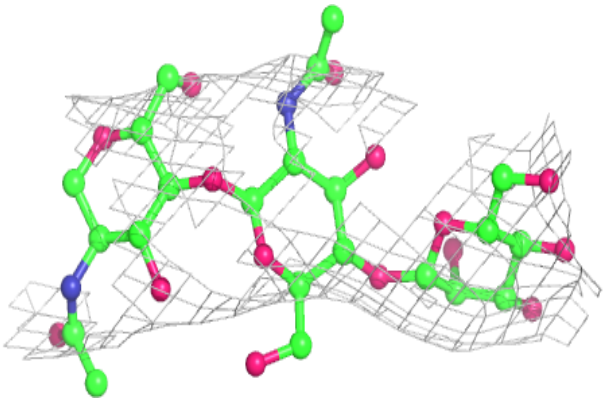
Electron density around Chain H:

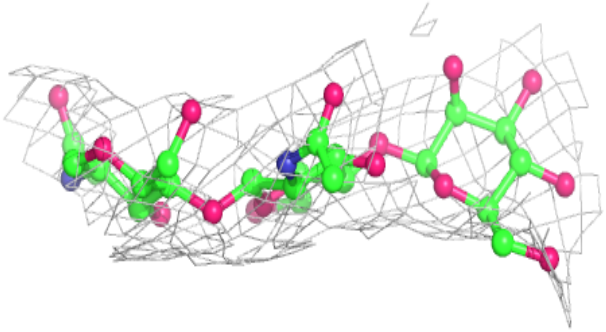
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

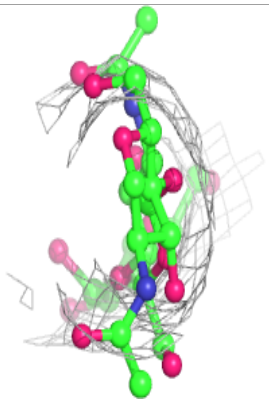


Electron density around Chain J:

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

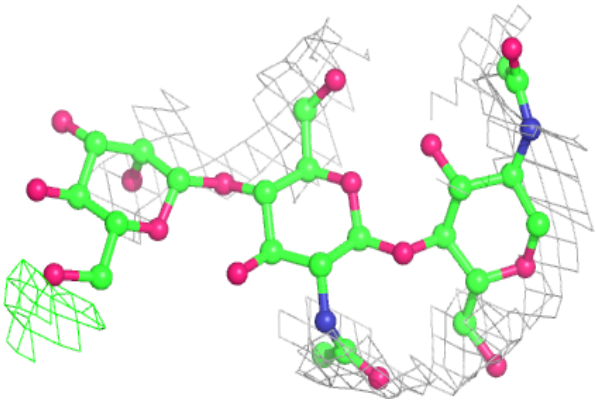


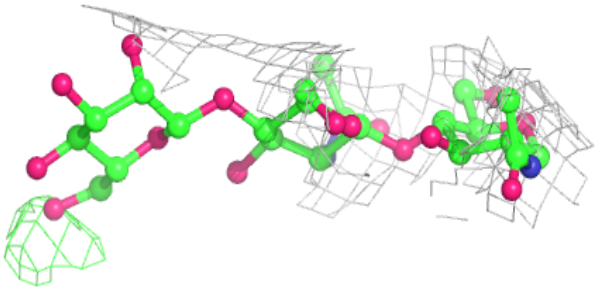


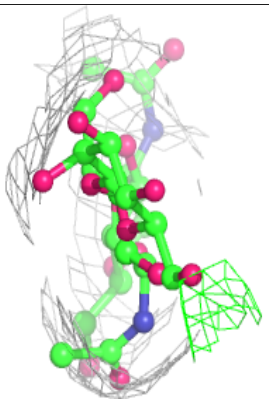


Electron density around Chain O:

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

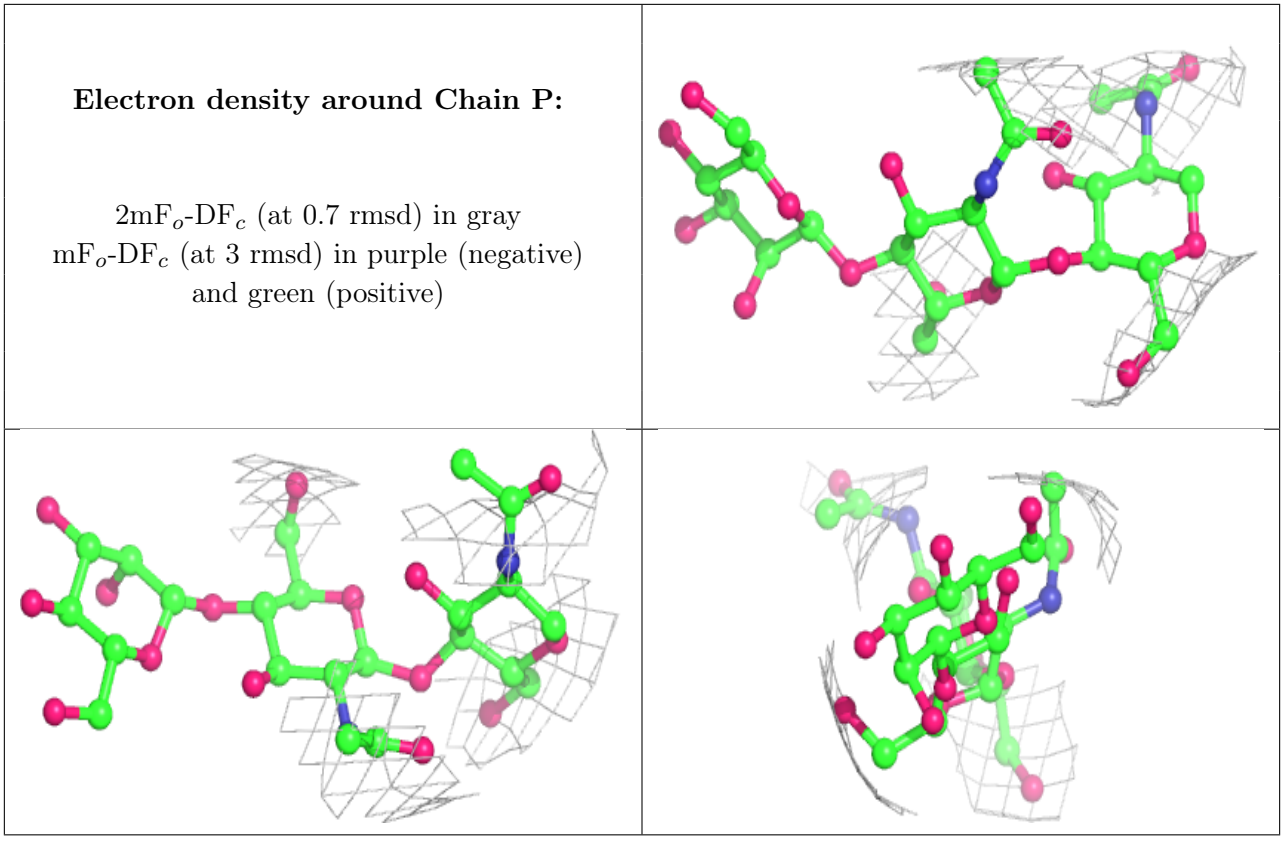






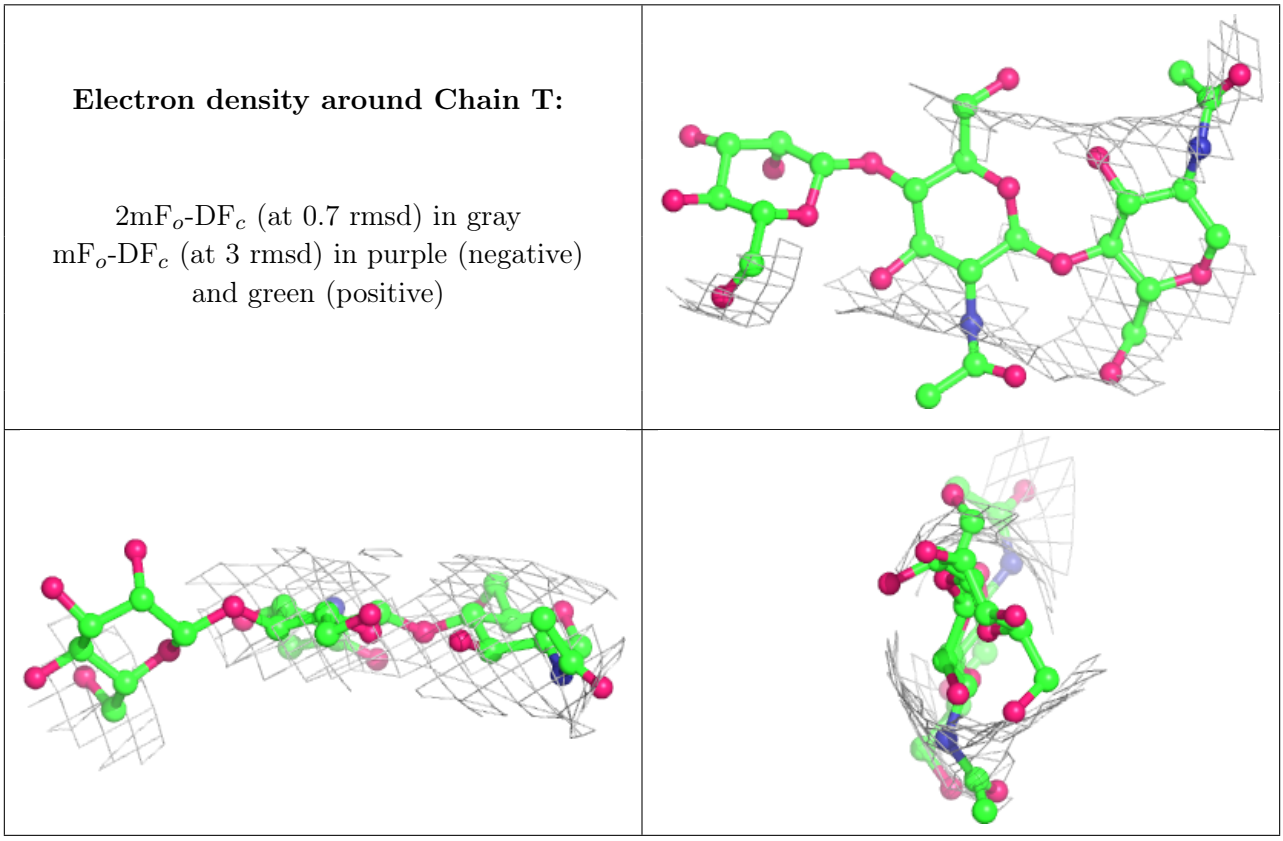
Electron density around Chain P:

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



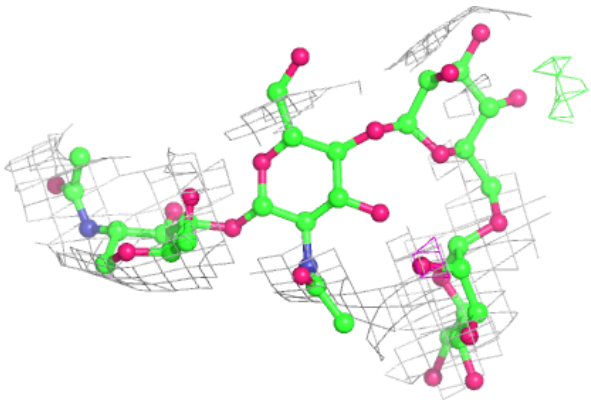
Electron density around Chain T:

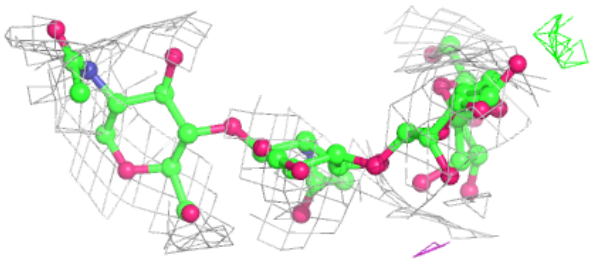
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

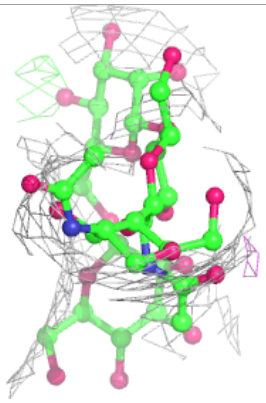


Electron density around Chain F:

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

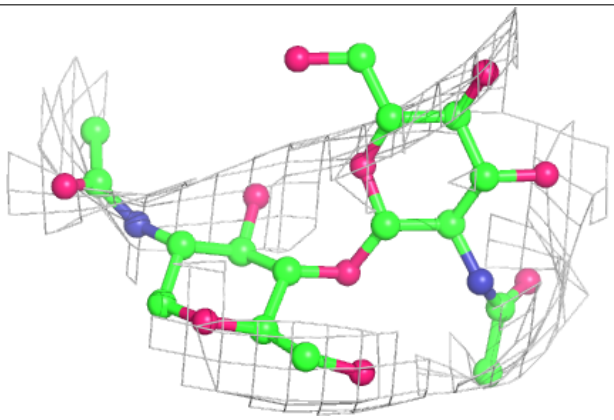


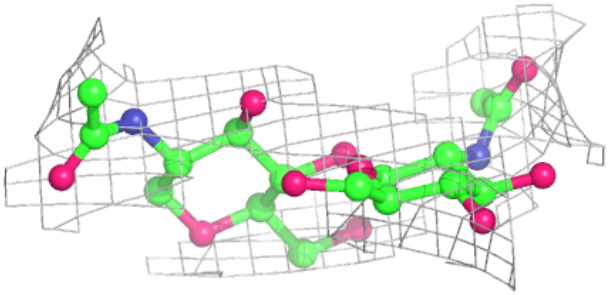


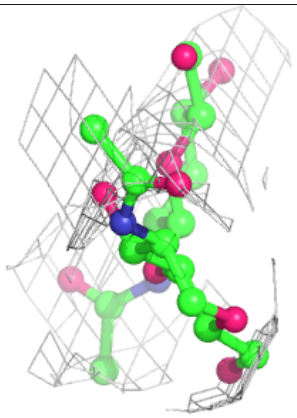


Electron density around Chain I:

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

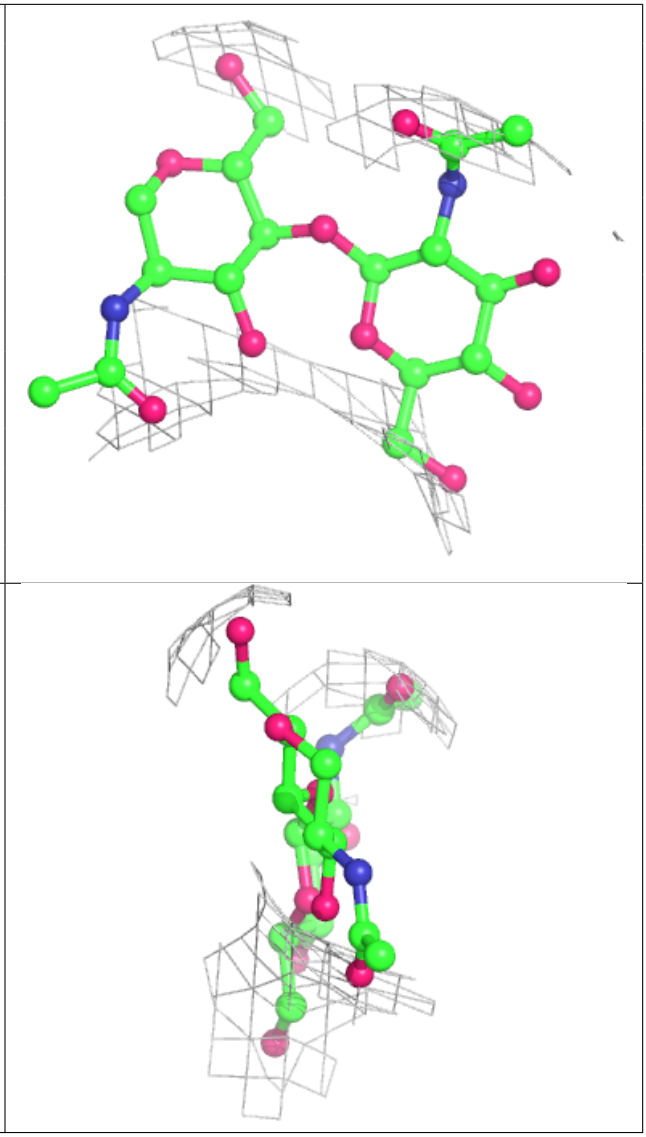


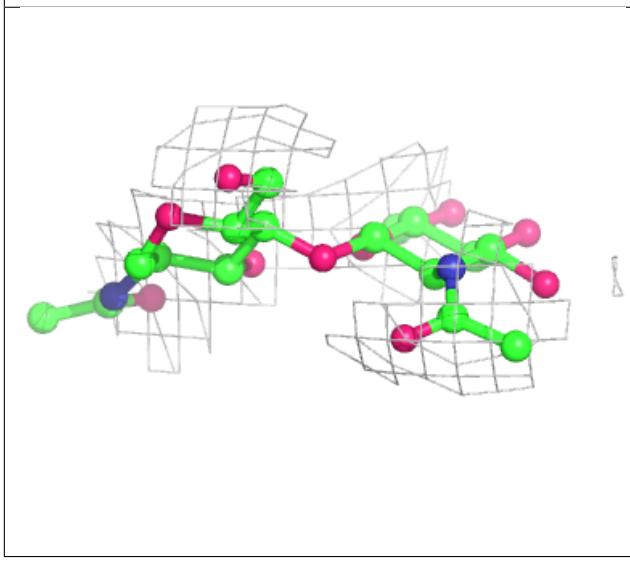




Electron density around Chain K:

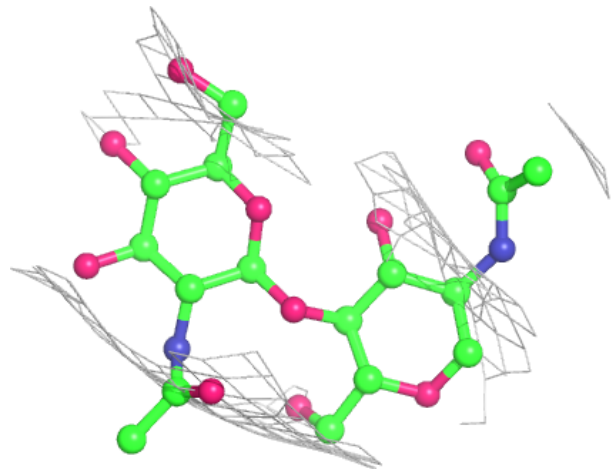
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

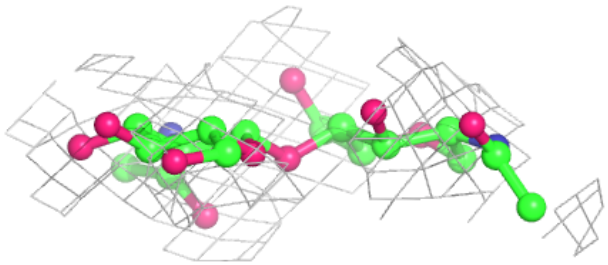


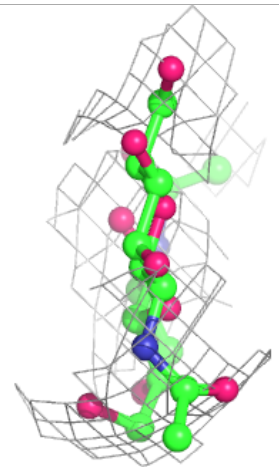


Electron density around Chain N:

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

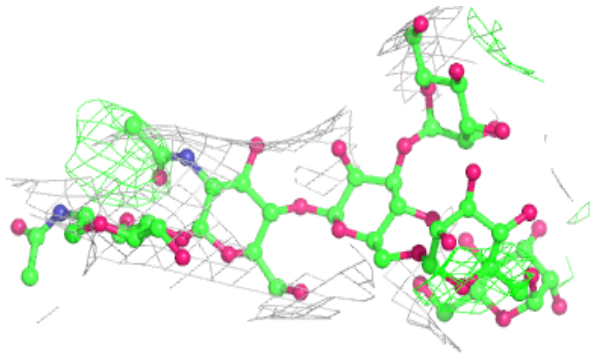


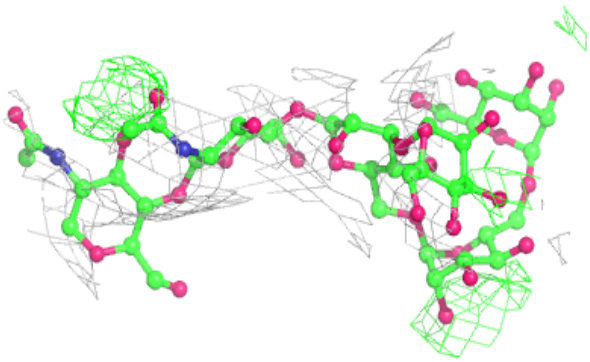


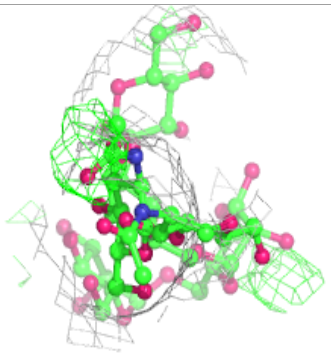


Electron density around Chain L:

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

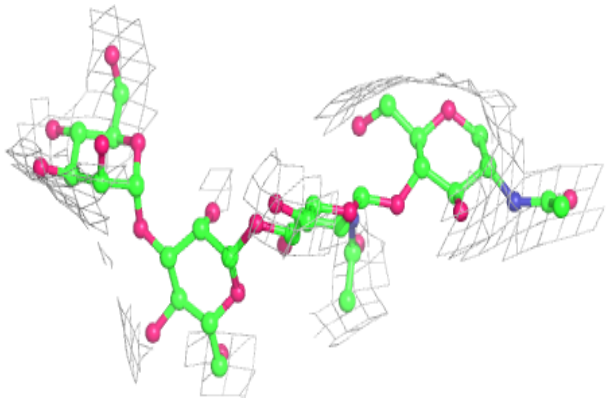


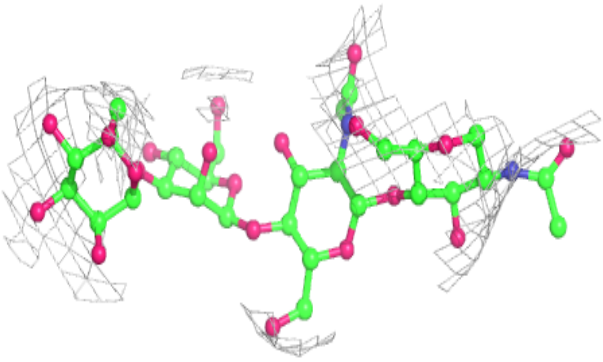


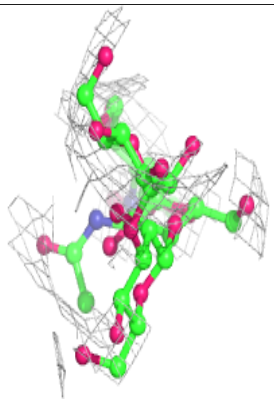


Electron density around Chain M:

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

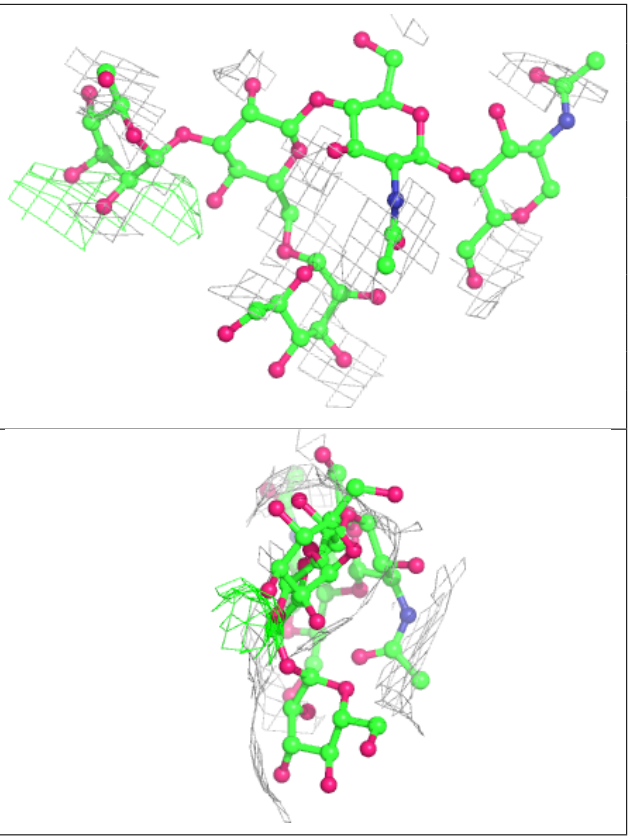


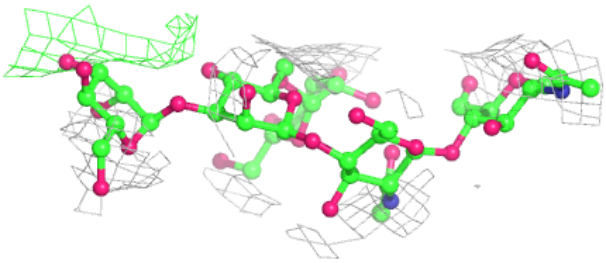




Electron density around Chain S:

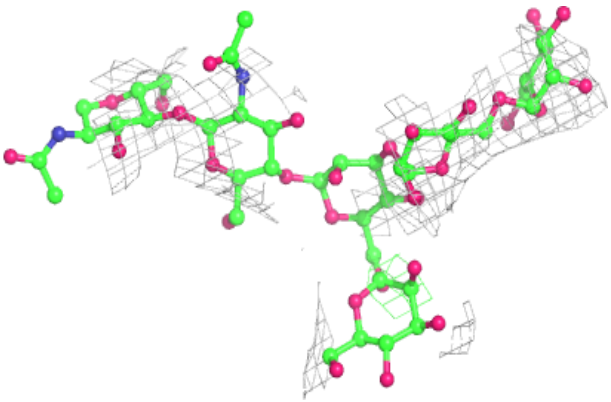
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

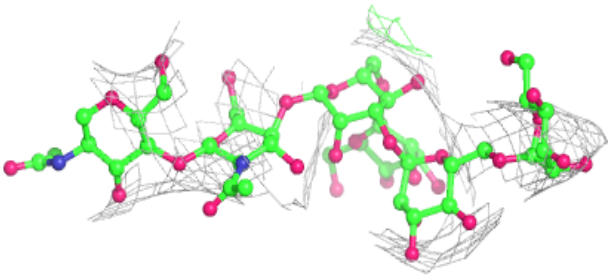


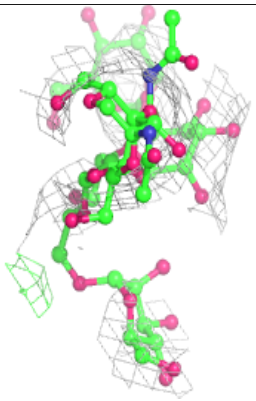


Electron density around Chain U:

$2mF_o$-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
14	NAG	B	704	14/15	0.78	0.40	326,326,326,326	0
14	NAG	G	631	14/15	0.84	0.40	365,365,365,365	0
14	NAG	G	622	14/15	0.89	0.23	367,367,367,367	0
14	NAG	G	606	14/15	0.92	0.17	368,368,368,368	0

6.5 Other polymers (i)

There are no such residues in this entry.