Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:35 AM BST

PDB ID	:	4IIC
Title	:	Crystal structure of beta-glucosidase 1 from Aspergillus aculeatus in complex with isofagomine
Authors	:	Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on	:	2012-12-20
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

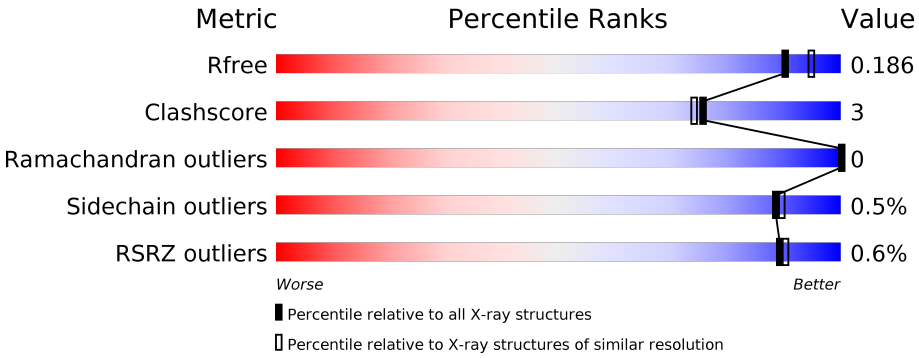
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	841	93% 5%
1	B	841	% 91% 7%
2	C	5	80% 20%
3	D	3	67% 33%
3	G	3	100%
3	L	3	100%

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Mol	Chain	Length	Quality of chain
3	N	3	100%
4	E	2	100%
5	F	10	100%
5	M	10	100%
6	H	7	86% 14%
6	O	7	86% 14%
7	I	7	86% 14%
8	J	7	86% 14%
9	K	4	75% 25%
10	P	8	75% 25%

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	BMA	P	3	-	-	X	-
12	MRD	A	941	-	-	X	-
13	MPD	A	942	-	-	X	-

2 Entry composition

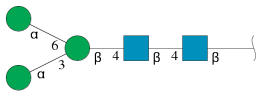
There are 16 unique types of molecules in this entry. The entry contains 15282 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-glucosidase 1.

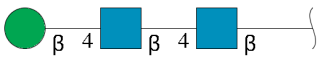
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6382	4028	1096	1240	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

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

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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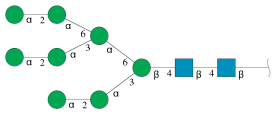
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	N	3	39	22	2	15	0	0	0

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

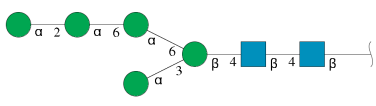
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called 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)-[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.



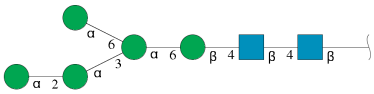
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	10	116	64	2	50	0	0	0
5	M	10	116	64	2	50	0	0	0

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



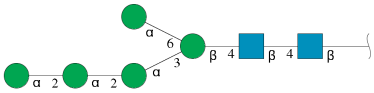
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	H	7	Total C N O 83 46 2 35	0	0	0
6	O	7	Total C N O 83 46 2 35	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



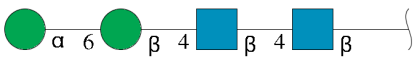
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	I	7	Total C N O 83 46 2 35	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



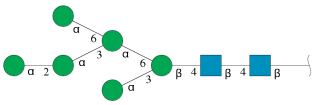
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	J	7	Total C N O 83 46 2 35	0	0	0

- Molecule 9 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.



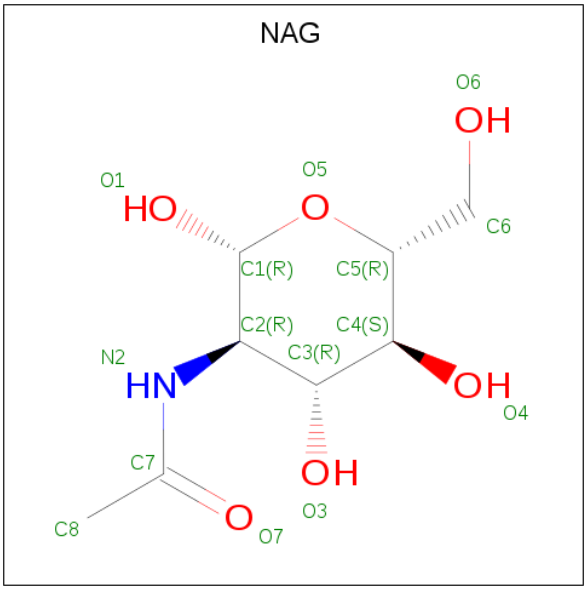
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	K	4	Total C N O 50 28 2 20	0	0	0

- Molecule 10 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
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

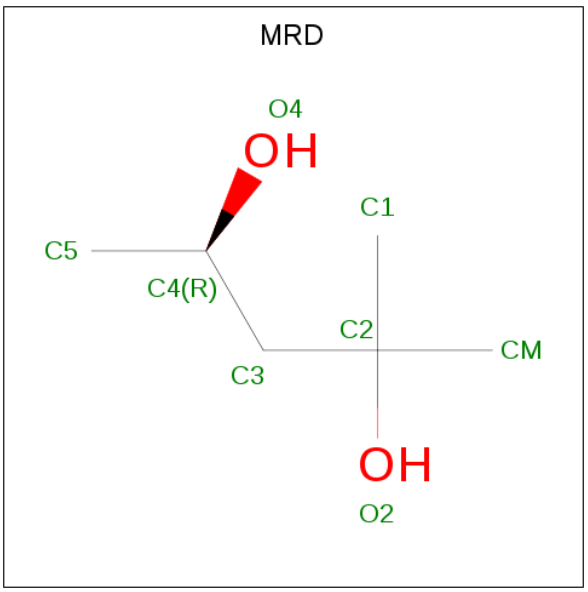
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

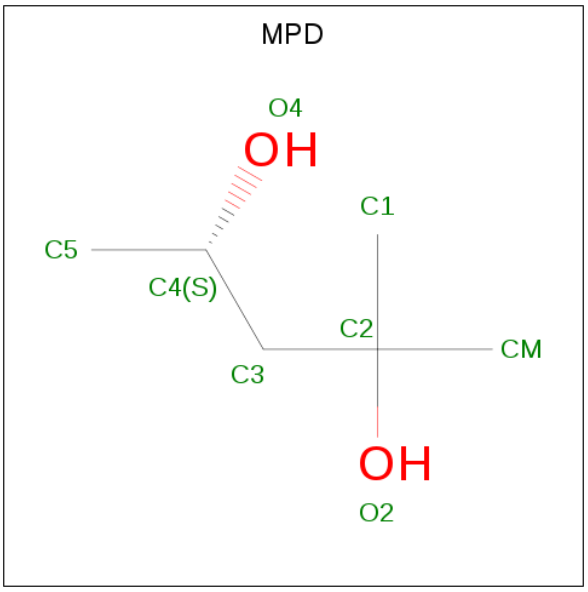
- Molecule 12 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:

$C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0

- Molecule 13 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

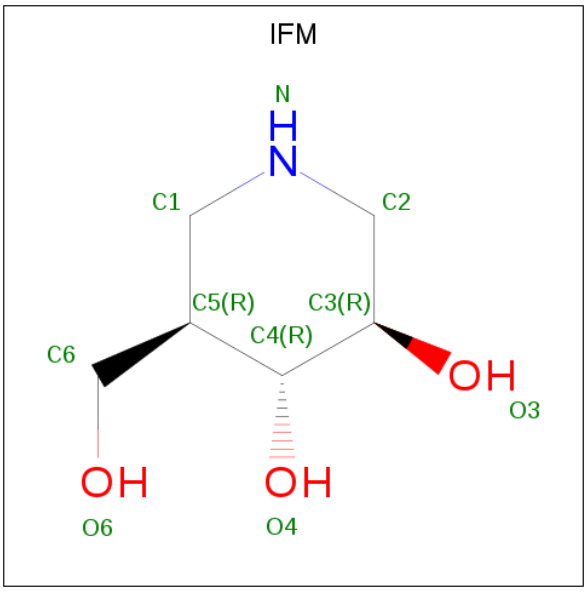


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 8 6 2	0	0

- Molecule 14 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Na 1 1	0	0
14	A	1	Total Na 1 1	0	0

- Molecule 15 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: $C_6H_{13}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C N O 10 6 1 3	0	0
15	B	1	Total C N O 10 6 1 3	0	0

- Molecule 16 is water.

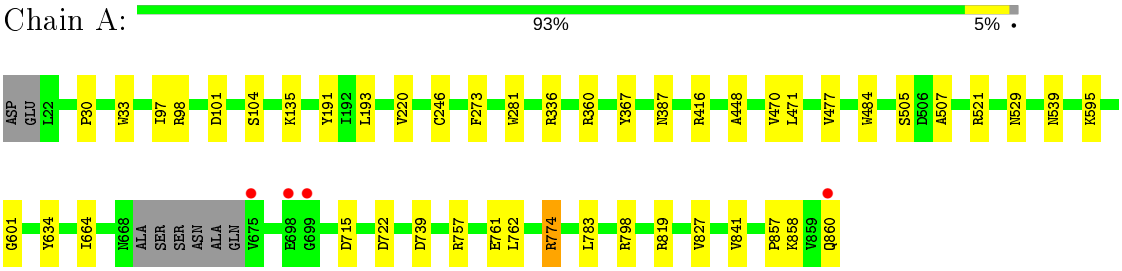
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	671	Total O 671 671	0	0
16	B	761	Total O 761 761	0	0

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.

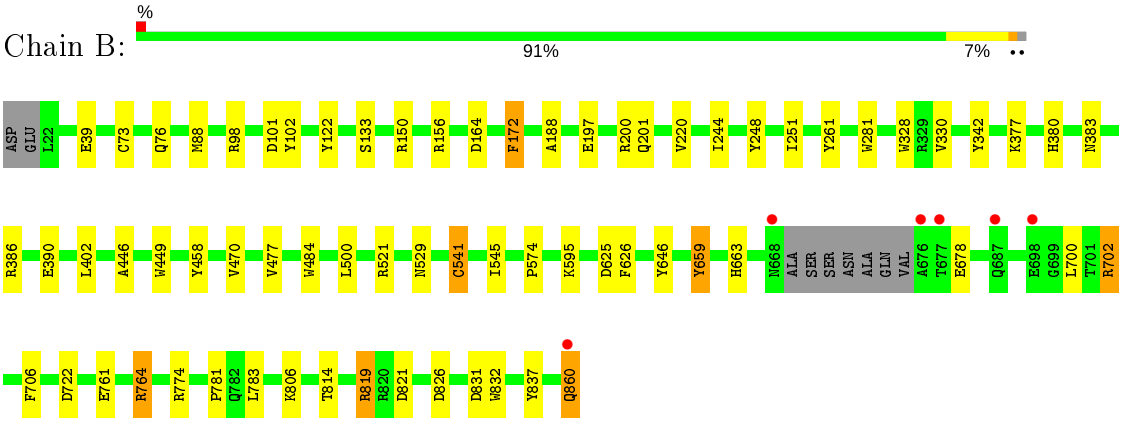
• Molecule 1: Beta-glucosidase 1

Chain A:



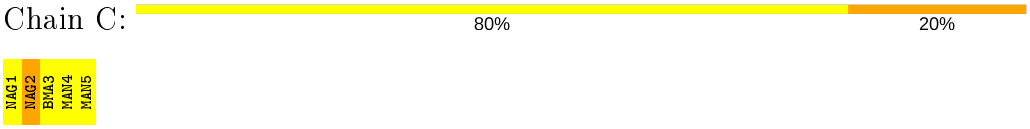
• Molecule 1: Beta-glucosidase 1

Chain B:



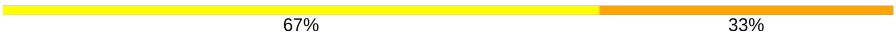
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

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

Chain E: 100%

• Molecule 5: 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)-[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 F: 100%

• Molecule 5: 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)-[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 M: 100%

• Molecule 6: alpha-D-mannopyranose-(1-2)-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

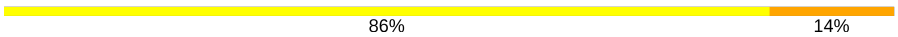
Chain H:

• Molecule 6: alpha-D-mannopyranose-(1-2)-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 O:

• Molecule 7: alpha-D-mannopyranose-(1-2)-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 I:



• Molecule 8: 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

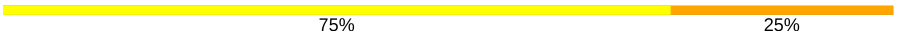
Chain J:

• Molecule 9: 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:

• Molecule 10: 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 P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.14Å 122.48Å 222.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.23 – 1.90 37.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.23-1.90) 99.7 (37.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.145 , 0.184 0.147 , 0.186	Depositor DCC
R_{free} test set	8816 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15282	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

5.1 Standard geometry

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

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	1.27	8/6545 (0.1%)	1.07	13/8923 (0.1%)
1	B	1.36	13/6538 (0.2%)	1.13	25/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.10	38/17836 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	CYS	CA-CB	9.60	1.75	1.53
1	B	122	TYR	CE1-CZ	7.42	1.48	1.38
1	B	646	TYR	CG-CD1	6.77	1.48	1.39
1	A	33	TRP	CE3-CZ3	6.75	1.50	1.38
1	B	761	GLU	CD-OE2	-5.68	1.19	1.25
1	A	761	GLU	CD-OE2	-5.65	1.19	1.25
1	B	122	TYR	CG-CD2	5.58	1.46	1.39
1	B	832	TRP	CE3-CZ3	5.51	1.47	1.38
1	B	342	TYR	CD1-CE1	5.50	1.47	1.39
1	B	197	GLU	CD-OE1	5.48	1.31	1.25
1	B	133	SER	CB-OG	5.45	1.49	1.42
1	B	328	TRP	CG-CD1	5.43	1.44	1.36
1	A	104	SER	CA-CB	5.43	1.61	1.52
1	A	601	GLY	N-CA	5.36	1.54	1.46
1	B	248	TYR	CE1-CZ	5.23	1.45	1.38
1	A	505	SER	CB-OG	5.23	1.49	1.42
1	B	458	TYR	CG-CD1	5.21	1.46	1.39
1	B	261	TYR	CE1-CZ	5.18	1.45	1.38
1	A	273	PHE	CG-CD2	5.10	1.46	1.38
1	A	471	LEU	N-CA	5.07	1.56	1.46
1	A	634	TYR	CE1-CZ	5.03	1.45	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	B	702	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	541	CYS	N-CA-CB	9.41	127.53	110.60
1	A	757	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	722	ASP	CB-CG-OD1	8.13	125.61	118.30
1	B	819	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	A	416	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	521	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	101	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	826	ASP	CB-CG-OD1	6.92	124.52	118.30
1	A	336	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	764	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	821	ASP	CB-CG-OD2	6.56	124.21	118.30
1	B	150	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	336	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	101	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	722	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	798	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	200	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	156	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	757	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	73	CYS	CA-CB-SG	-5.72	103.70	114.00
1	B	402	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	B	150	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	762	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	B	774	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	715	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	831	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	164	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	625	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	722	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	521	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	330	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	B	172	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	659	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	806	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	A	101	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	702	ARG	CB-CG-CD	-5.06	98.44	111.60

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	6382	0	6092	24	0
1	B	6375	0	6082	34	0
2	C	61	0	52	1	0
3	D	39	0	34	1	0
3	G	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	25	0	0
5	F	116	0	96	0	0
5	M	116	0	96	0	0
6	H	83	0	70	1	0
6	O	83	0	70	1	0
7	I	83	0	69	1	0
8	J	83	0	70	1	0
9	K	50	0	43	1	0
10	P	94	0	77	6	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	16	0	28	7	0
12	B	24	0	42	8	0
13	A	8	0	14	9	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
15	A	10	0	13	0	0
15	B	10	0	13	0	0
16	A	671	0	0	6	0
16	B	761	0	0	14	0
All	All	15282	0	13153	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:CYS:CA	1:B:541:CYS:CB	1.75	1.64
13:A:942:MPD:C1	13:A:942:MPD:H52	1.66	1.23
13:A:942:MPD:H52	13:A:942:MPD:H11	1.08	1.05
1:B:678:GLU:HG2	16:B:1593:HOH:O	1.59	1.02
13:A:942:MPD:C1	13:A:942:MPD:C5	2.33	1.01
13:A:942:MPD:C5	13:A:942:MPD:H11	1.91	0.90
1:B:837:TYR:HE2	16:B:1541:HOH:O	1.56	0.87
12:B:947:MRD:H1C2	12:B:947:MRD:C5	2.02	0.83
1:A:819:ARG:HH12	1:A:860:GLN:C	1.81	0.83
1:A:360:ARG:HH11	12:A:941:MRD:HMC3	1.43	0.83
13:A:942:MPD:H13	13:A:942:MPD:C5	2.09	0.80
12:B:947:MRD:H1C2	12:B:947:MRD:H5C3	1.65	0.78
13:A:942:MPD:H52	13:A:942:MPD:H13	1.63	0.78
1:B:541:CYS:CB	1:B:541:CYS:C	2.55	0.74
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.70	0.72
12:A:941:MRD:HMC1	12:A:941:MRD:H5C3	1.71	0.72
12:A:941:MRD:HMC2	16:B:1147:HOH:O	1.89	0.72
1:A:98:ARG:HH22	13:A:942:MPD:H31	1.53	0.72
1:B:819:ARG:HH12	1:B:860:GLN:C	1.93	0.71
1:B:541:CYS:CB	1:B:541:CYS:HA	2.13	0.70
1:A:819:ARG:NH1	1:A:860:GLN:C	2.44	0.70
16:A:1390:HOH:O	7:I:6:MAN:H3	1.92	0.68
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.78	0.66
1:B:201:GLN:HG3	16:B:1657:HOH:O	1.97	0.65
12:B:946:MRD:HMC2	16:B:1440:HOH:O	1.97	0.65
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.32	0.64
12:B:948:MRD:H5C3	12:B:948:MRD:O2	2.00	0.61
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.31	0.61
1:A:857:PRO:HD3	16:A:1230:HOH:O	2.01	0.60
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.37	0.59
10:P:3:BMA:H62	10:P:4:MAN:H5	1.83	0.59
12:A:941:MRD:C5	12:A:941:MRD:HMC1	2.32	0.59
1:B:595:LYS:HE2	16:B:1396:HOH:O	2.02	0.59
12:B:948:MRD:O2	12:B:948:MRD:C5	2.50	0.58
1:B:98:ARG:HH12	12:B:946:MRD:HMC3	1.68	0.57
1:A:360:ARG:HH11	12:A:941:MRD:CM	2.18	0.56
10:P:3:BMA:H62	10:P:4:MAN:H3	1.89	0.54
1:B:783:LEU:HD23	1:B:783:LEU:C	2.29	0.53
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.91	0.52
12:B:947:MRD:C1	12:B:947:MRD:H5C3	2.38	0.52
1:B:390:GLU:CG	16:B:1514:HOH:O	2.57	0.52
1:B:386:ARG:NH2	16:B:1738:HOH:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:HIS:HB3	16:B:1652:HOH:O	2.11	0.51
12:A:940:MRD:H5C3	12:A:940:MRD:O2	2.11	0.50
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.95	0.49
1:B:172:PHE:CZ	1:B:188:ALA:HB1	2.48	0.49
1:A:827:VAL:HG11	3:D:2:NAG:O3	2.13	0.48
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.49	0.47
10:P:3:BMA:C6	10:P:4:MAN:H3	2.43	0.47
1:B:390:GLU:HG3	16:B:1514:HOH:O	2.15	0.47
1:A:191:TYR:O	1:A:246:CYS:HA	2.15	0.46
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.97	0.45
1:B:76:GLN:HA	1:B:88:MET:O	2.17	0.45
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.51	0.45
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.98	0.45
1:B:251:ILE:HG21	9:K:1:NAG:H82	1.99	0.45
1:A:360:ARG:HG2	12:A:941:MRD:HMC1	1.98	0.45
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.47	0.44
12:B:946:MRD:O2	12:B:946:MRD:O4	2.30	0.44
1:B:702:ARG:HD3	16:B:1082:HOH:O	2.18	0.43
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.81	0.43
16:B:1509:HOH:O	10:P:3:BMA:H61	2.18	0.43
10:P:3:BMA:H62	10:P:4:MAN:C3	2.49	0.43
13:A:942:MPD:H12	16:A:1406:HOH:O	2.19	0.43
13:A:942:MPD:H13	13:A:942:MPD:H53	1.99	0.43
1:B:172:PHE:HZ	1:B:188:ALA:HB1	1.82	0.43
1:A:387:ASN:HB2	16:A:1200:HOH:O	2.19	0.42
1:A:774:ARG:HB3	1:A:774:ARG:HE	1.45	0.42
1:A:539:ASN:HB2	16:A:1367:HOH:O	2.19	0.42
1:B:102:TYR:HB3	1:B:383:ASN:HA	2.02	0.42
10:P:3:BMA:C6	10:P:4:MAN:C3	2.98	0.42
1:A:448:ALA:HB1	1:A:507:ALA:O	2.20	0.42
1:B:595:LYS:HE3	16:B:1204:HOH:O	2.20	0.42
1:A:97:ILE:HD13	1:A:135:LYS:HG3	2.01	0.41
1:A:595:LYS:HE3	16:A:1155:HOH:O	2.19	0.41
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.56	0.41
1:A:783:LEU:C	1:A:783:LEU:HD23	2.41	0.41
1:B:39:GLU:HG2	16:B:1324:HOH:O	2.21	0.41
1:B:706:PHE:CZ	8:J:2:NAG:H82	2.56	0.41
1:B:377:LYS:HD2	1:B:380:HIS:CE1	2.56	0.40
1:A:30:PRO:HG3	1:A:739:ASP:O	2.21	0.40
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.04	0.40
1:B:446:ALA:HA	1:B:574:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:TYR:CZ	2:C:2:NAG:H83	2.57	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	829/841 (99%)	801 (97%)	28 (3%)	0	100	100
1	B	828/841 (98%)	806 (97%)	22 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	671/677 (99%)	668 (100%)	3 (0%)	91	91
1	B	670/677 (99%)	666 (99%)	4 (1%)	86	87
All	All	1341/1354 (99%)	1334 (100%)	7 (0%)	88	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	TRP
1	A	774	ARG
1	A	858	LYS
1	B	281	TRP
1	B	449	TRP
1	B	700	LEU
1	B	860	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

79 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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	1.34	2 (14%)	17,19,21	1.50	2 (11%)
2	NAG	C	2	2	14,14,15	0.99	1 (7%)	17,19,21	2.06	9 (52%)
2	BMA	C	3	2	11,11,12	1.16	1 (9%)	15,15,17	2.55	7 (46%)
2	MAN	C	4	2	11,11,12	0.94	0	15,15,17	2.80	8 (53%)
2	MAN	C	5	2	11,11,12	0.89	0	15,15,17	1.68	3 (20%)
3	NAG	D	1	1,3	14,14,15	1.14	1 (7%)	17,19,21	1.57	5 (29%)
3	NAG	D	2	3	14,14,15	1.27	2 (14%)	17,19,21	1.64	5 (29%)
3	BMA	D	3	3	11,11,12	1.05	0	15,15,17	3.22	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	1	1,4	14,14,15	0.72	0	17,19,21	1.50	3 (17%)
4	NAG	E	2	4	14,14,15	1.03	1 (7%)	17,19,21	2.08	5 (29%)
5	NAG	F	1	1,5	14,14,15	1.51	4 (28%)	17,19,21	1.20	3 (17%)
5	MAN	F	10	5	11,11,12	1.17	1 (9%)	15,15,17	1.76	5 (33%)
5	NAG	F	2	5	14,14,15	1.21	2 (14%)	17,19,21	1.33	1 (5%)
5	BMA	F	3	5	11,11,12	0.87	0	15,15,17	1.48	3 (20%)
5	MAN	F	4	5	11,11,12	0.99	2 (18%)	15,15,17	1.26	2 (13%)
5	MAN	F	5	5	11,11,12	0.77	0	15,15,17	1.81	3 (20%)
5	MAN	F	6	5	11,11,12	0.73	0	15,15,17	2.13	3 (20%)
5	MAN	F	7	5	11,11,12	1.44	2 (18%)	15,15,17	1.46	2 (13%)
5	MAN	F	8	5	11,11,12	1.09	0	15,15,17	1.61	3 (20%)
5	MAN	F	9	5	11,11,12	1.20	1 (9%)	15,15,17	1.44	3 (20%)
3	NAG	G	1	1,3	14,14,15	1.16	1 (7%)	17,19,21	1.80	4 (23%)
3	NAG	G	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.56	2 (11%)
3	BMA	G	3	3	11,11,12	1.08	1 (9%)	15,15,17	3.07	7 (46%)
6	NAG	H	1	1,6	14,14,15	0.92	0	17,19,21	1.44	3 (17%)
6	NAG	H	2	6	14,14,15	0.78	0	17,19,21	1.85	5 (29%)
6	BMA	H	3	6	11,11,12	0.89	0	15,15,17	1.54	4 (26%)
6	MAN	H	4	6	11,11,12	0.84	0	15,15,17	1.79	6 (40%)
6	MAN	H	5	6	11,11,12	0.92	0	15,15,17	1.45	2 (13%)
6	MAN	H	6	6	11,11,12	1.24	1 (9%)	15,15,17	1.20	1 (6%)
6	MAN	H	7	6	11,11,12	0.71	0	15,15,17	1.80	4 (26%)
7	NAG	I	1	1,14,7	14,14,15	1.27	1 (7%)	17,19,21	1.57	6 (35%)
7	NAG	I	2	7	14,14,15	1.40	1 (7%)	17,19,21	1.26	4 (23%)
7	BMA	I	3	7	11,11,12	0.87	1 (9%)	15,15,17	2.41	5 (33%)
7	MAN	I	4	7	11,11,12	1.16	1 (9%)	15,15,17	2.17	3 (20%)
7	MAN	I	5	7	11,11,12	0.84	0	15,15,17	2.30	6 (40%)
7	MAN	I	6	7	11,11,12	0.93	0	15,15,17	2.16	7 (46%)
7	MAN	I	7	7	11,11,12	0.76	0	15,15,17	1.88	4 (26%)
8	NAG	J	1	1,8	14,14,15	1.37	1 (7%)	17,19,21	2.69	7 (41%)
8	NAG	J	2	8	14,14,15	1.08	1 (7%)	17,19,21	1.91	4 (23%)
8	BMA	J	3	8	11,11,12	1.37	1 (9%)	15,15,17	1.82	5 (33%)
8	MAN	J	4	8	11,11,12	0.58	0	15,15,17	1.95	5 (33%)
8	MAN	J	5	8	11,11,12	0.97	0	15,15,17	1.34	2 (13%)
8	MAN	J	6	8	11,11,12	0.88	0	15,15,17	1.51	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	J	7	8	11,11,12	0.70	0	15,15,17	1.88	5 (33%)
9	NAG	K	1	1,9	14,14,15	1.09	1 (7%)	17,19,21	1.80	5 (29%)
9	NAG	K	2	9	14,14,15	1.67	5 (35%)	17,19,21	1.58	4 (23%)
9	BMA	K	3	9	11,11,12	0.73	0	15,15,17	1.87	3 (20%)
9	MAN	K	4	9	11,11,12	1.21	2 (18%)	15,15,17	2.28	6 (40%)
3	NAG	L	1	1,3	14,14,15	1.02	0	17,19,21	1.72	4 (23%)
3	NAG	L	2	3	14,14,15	0.66	0	17,19,21	1.71	4 (23%)
3	BMA	L	3	3	11,11,12	0.82	0	15,15,17	2.26	6 (40%)
5	NAG	M	1	1,5	14,14,15	1.25	2 (14%)	17,19,21	1.78	6 (35%)
5	MAN	M	10	5	11,11,12	1.17	1 (9%)	15,15,17	2.07	7 (46%)
5	NAG	M	2	5	14,14,15	1.29	2 (14%)	17,19,21	1.43	3 (17%)
5	BMA	M	3	5	11,11,12	1.18	1 (9%)	15,15,17	1.72	2 (13%)
5	MAN	M	4	5	11,11,12	0.93	0	15,15,17	1.71	5 (33%)
5	MAN	M	5	5	11,11,12	0.83	0	15,15,17	2.04	5 (33%)
5	MAN	M	6	5	11,11,12	1.07	1 (9%)	15,15,17	1.61	2 (13%)
5	MAN	M	7	5	11,11,12	1.21	2 (18%)	15,15,17	2.27	6 (40%)
5	MAN	M	8	5	11,11,12	1.20	1 (9%)	15,15,17	1.89	3 (20%)
5	MAN	M	9	5	11,11,12	1.12	0	15,15,17	1.74	5 (33%)
3	NAG	N	1	1,3	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
3	NAG	N	2	3	14,14,15	1.21	1 (7%)	17,19,21	1.40	2 (11%)
3	BMA	N	3	3	11,11,12	0.88	0	15,15,17	2.33	4 (26%)
6	NAG	O	1	1,6	14,14,15	0.98	0	17,19,21	1.30	1 (5%)
6	NAG	O	2	6	14,14,15	1.11	1 (7%)	17,19,21	1.93	5 (29%)
6	BMA	O	3	6	11,11,12	1.06	1 (9%)	15,15,17	1.25	2 (13%)
6	MAN	O	4	6	11,11,12	1.00	1 (9%)	15,15,17	2.02	7 (46%)
6	MAN	O	5	6	11,11,12	0.83	0	15,15,17	1.77	5 (33%)
6	MAN	O	6	6	11,11,12	0.78	0	15,15,17	1.74	5 (33%)
6	MAN	O	7	6	11,11,12	0.76	0	15,15,17	2.58	5 (33%)
10	NAG	P	1	1,10,14	14,14,15	1.38	2 (14%)	17,19,21	1.57	4 (23%)
10	NAG	P	2	10	14,14,15	0.94	0	17,19,21	1.45	3 (17%)
10	BMA	P	3	10	11,11,12	1.09	1 (9%)	15,15,17	3.72	8 (53%)
10	MAN	P	4	10	11,11,12	0.97	0	15,15,17	1.91	4 (26%)
10	MAN	P	5	10	11,11,12	0.95	0	15,15,17	2.49	7 (46%)
10	MAN	P	6	10	11,11,12	0.87	0	15,15,17	2.41	6 (40%)
10	MAN	P	7	10	11,11,12	0.98	1 (9%)	15,15,17	1.95	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	P	8	10	11,11,12	0.92	0	15,15,17	2.15	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	2/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/19/22	0/1/1/1
6	MAN	H	6	6	-	1/2/19/22	0/1/1/1
6	MAN	H	7	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	1,14,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1
7	MAN	I	7	7	-	2/2/19/22	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	2/2/19/22	0/1/1/1
8	MAN	J	6	8	-	2/2/19/22	0/1/1/1
8	MAN	J	7	8	-	0/2/19/22	0/1/1/1
9	NAG	K	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	M	10	5	-	2/2/19/22	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	0/2/19/22	0/1/1/1
5	MAN	M	9	5	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
6	MAN	O	7	6	-	1/2/19/22	0/1/1/1
10	NAG	P	1	1,10,14	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	P	4	10	-	2/2/19/22	0/1/1/1
10	MAN	P	5	10	-	0/2/19/22	0/1/1/1
10	MAN	P	6	10	-	2/2/19/22	0/1/1/1
10	MAN	P	7	10	-	2/2/19/22	0/1/1/1
10	MAN	P	8	10	-	1/2/19/22	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	C1-C2	4.02	1.58	1.52
7	I	2	NAG	O5-C1	-3.96	1.37	1.43
3	N	2	NAG	C1-C2	3.53	1.57	1.52
2	C	1	NAG	C1-C2	3.49	1.57	1.52
8	J	3	BMA	C2-C3	3.28	1.57	1.52
9	K	2	NAG	C3-C2	3.20	1.59	1.52
10	P	1	NAG	O7-C7	2.98	1.30	1.23
10	P	1	NAG	C1-C2	-2.97	1.47	1.52
5	F	7	MAN	C4-C3	2.96	1.59	1.52
5	F	1	NAG	C1-C2	2.92	1.56	1.52
5	M	2	NAG	C4-C3	2.81	1.59	1.52
5	M	3	BMA	O4-C4	-2.79	1.36	1.43
5	M	1	NAG	C1-C2	2.78	1.56	1.52
5	F	9	MAN	O4-C4	-2.78	1.36	1.43
9	K	2	NAG	C4-C5	2.68	1.58	1.53
9	K	2	NAG	O5-C1	-2.67	1.39	1.43
6	O	4	MAN	O2-C2	-2.66	1.37	1.43
5	F	10	MAN	O5-C1	-2.63	1.39	1.43
5	M	8	MAN	O5-C5	2.58	1.48	1.43
6	O	2	NAG	C3-C2	2.54	1.57	1.52
4	E	2	NAG	O3-C3	-2.52	1.37	1.43
5	F	2	NAG	C1-C2	2.50	1.56	1.52
5	F	1	NAG	C4-C3	2.49	1.58	1.52
8	J	2	NAG	C4-C5	2.48	1.58	1.53
10	P	7	MAN	C2-C3	2.44	1.56	1.52
6	O	3	BMA	C1-C2	2.42	1.57	1.52
7	I	1	NAG	O5-C1	2.42	1.47	1.43
10	P	3	BMA	O5-C1	-2.40	1.39	1.43
3	G	1	NAG	C1-C2	2.39	1.55	1.52
5	M	10	MAN	O5-C1	-2.36	1.39	1.43
6	H	6	MAN	C4-C5	2.36	1.58	1.53
5	F	7	MAN	O5-C1	-2.36	1.40	1.43
3	G	2	NAG	O5-C1	-2.35	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.31	1.55	1.52
2	C	2	NAG	C1-C2	2.26	1.55	1.52
5	M	7	MAN	O3-C3	2.25	1.48	1.43
3	D	2	NAG	O5-C1	-2.23	1.40	1.43
9	K	4	MAN	C4-C3	2.22	1.58	1.52
9	K	2	NAG	O7-C7	2.19	1.28	1.23
3	G	3	BMA	C1-C2	2.19	1.57	1.52
5	M	7	MAN	C4-C3	2.16	1.57	1.52
9	K	2	NAG	C1-C2	2.16	1.55	1.52
7	I	3	BMA	O2-C2	-2.13	1.38	1.43
5	F	1	NAG	C2-N2	2.13	1.49	1.46
5	M	2	NAG	O5-C1	2.09	1.47	1.43
7	I	4	MAN	O5-C5	2.08	1.47	1.43
9	K	1	NAG	C1-C2	2.08	1.55	1.52
9	K	4	MAN	C2-C3	2.07	1.55	1.52
5	M	6	MAN	O5-C1	2.06	1.47	1.43
2	C	3	BMA	O3-C3	2.05	1.47	1.43
5	M	1	NAG	C2-N2	2.04	1.49	1.46
5	F	2	NAG	C6-C5	2.03	1.58	1.51
3	D	2	NAG	C4-C5	2.02	1.57	1.53
2	C	1	NAG	C8-C7	2.02	1.54	1.50
5	F	1	NAG	O3-C3	2.01	1.47	1.43
5	F	4	MAN	C2-C3	2.01	1.55	1.52
5	F	4	MAN	O5-C1	-2.01	1.40	1.43

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3	BMA	C1-O5-C5	9.17	124.61	112.19
10	P	3	BMA	C1-O5-C5	8.46	123.65	112.19
10	P	3	BMA	C6-C5-C4	-7.27	95.98	113.00
7	I	4	MAN	O5-C5-C6	6.92	118.05	107.20
3	D	3	BMA	O5-C5-C6	6.71	117.72	107.20
2	C	4	MAN	C1-O5-C5	6.47	120.96	112.19
6	O	7	MAN	C1-C2-C3	-6.07	102.20	109.67
7	I	3	BMA	C1-O5-C5	5.79	120.04	112.19
2	C	3	BMA	C1-C2-C3	5.56	116.50	109.67
8	J	1	NAG	O5-C1-C2	-5.45	102.68	111.29
5	M	7	MAN	C1-O5-C5	5.41	119.52	112.19
10	P	6	MAN	O5-C5-C6	5.31	115.53	107.20
9	K	4	MAN	O5-C5-C6	5.27	115.46	107.20
3	D	3	BMA	C3-C4-C5	5.18	119.47	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	3	BMA	C1-O5-C5	5.17	119.20	112.19
9	K	3	BMA	C1-O5-C5	5.13	119.14	112.19
3	D	3	BMA	O6-C6-C5	5.05	128.62	111.29
10	P	7	MAN	O5-C5-C6	5.04	115.11	107.20
3	N	3	BMA	C1-O5-C5	5.03	119.01	112.19
3	N	3	BMA	O5-C5-C6	5.03	115.08	107.20
5	F	6	MAN	O5-C5-C6	4.96	114.97	107.20
8	J	4	MAN	O5-C5-C6	4.90	114.89	107.20
10	P	5	MAN	C6-C5-C4	-4.89	101.55	113.00
5	M	6	MAN	O5-C5-C6	4.86	114.83	107.20
7	I	5	MAN	C3-C4-C5	-4.84	101.61	110.24
10	P	3	BMA	O6-C6-C5	-4.71	95.14	111.29
5	M	5	MAN	O6-C6-C5	-4.69	95.19	111.29
9	K	1	NAG	C4-C3-C2	-4.68	104.15	111.02
10	P	8	MAN	C2-C3-C4	4.58	118.83	110.89
5	M	8	MAN	O3-C3-C4	-4.56	99.80	110.35
4	E	2	NAG	C3-C4-C5	-4.55	102.12	110.24
5	F	5	MAN	O6-C6-C5	-4.53	95.76	111.29
8	J	1	NAG	C1-O5-C5	-4.51	106.09	112.19
8	J	1	NAG	C4-C3-C2	-4.50	104.43	111.02
3	L	2	NAG	C3-C4-C5	-4.48	102.25	110.24
2	C	4	MAN	C1-C2-C3	4.39	115.06	109.67
10	P	3	BMA	O2-C2-C3	4.36	118.88	110.14
6	O	7	MAN	O5-C1-C2	-4.30	104.14	110.77
8	J	2	NAG	O7-C7-C8	-4.22	114.22	122.06
5	F	6	MAN	O3-C3-C2	4.13	117.91	109.99
3	D	3	BMA	O3-C3-C2	-4.11	102.12	109.99
2	C	4	MAN	C3-C4-C5	4.10	117.56	110.24
8	J	1	NAG	O7-C7-N2	4.10	129.48	121.95
6	H	7	MAN	O5-C1-C2	-4.08	104.48	110.77
8	J	1	NAG	C8-C7-N2	-4.05	109.24	116.10
3	G	3	BMA	O2-C2-C1	4.05	117.43	109.15
10	P	6	MAN	O3-C3-C4	4.04	119.68	110.35
10	P	4	MAN	O2-C2-C1	-4.03	100.92	109.15
2	C	3	BMA	O2-C2-C3	-4.02	102.09	110.14
7	I	5	MAN	O2-C2-C3	-3.96	102.21	110.14
3	G	2	NAG	C1-C2-N2	-3.95	103.75	110.49
10	P	8	MAN	C1-C2-C3	3.92	114.48	109.67
7	I	3	BMA	C6-C5-C4	-3.89	103.89	113.00
2	C	2	NAG	O6-C6-C5	-3.89	97.94	111.29
8	J	7	MAN	O3-C3-C2	3.89	117.44	109.99
3	D	3	BMA	C1-C2-C3	3.88	114.44	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	5	MAN	C1-O5-C5	3.87	117.44	112.19
8	J	5	MAN	O5-C5-C6	3.86	113.25	107.20
7	I	6	MAN	C1-O5-C5	3.85	117.41	112.19
6	O	4	MAN	C1-C2-C3	3.85	114.40	109.67
5	M	1	NAG	O4-C4-C5	-3.83	99.78	109.30
5	M	3	BMA	C2-C3-C4	-3.83	104.27	110.89
10	P	5	MAN	C1-O5-C5	3.83	117.38	112.19
2	C	1	NAG	O5-C1-C2	-3.82	105.25	111.29
5	M	8	MAN	O5-C5-C6	3.82	113.19	107.20
3	G	1	NAG	C1-C2-N2	-3.81	103.98	110.49
5	M	7	MAN	O2-C2-C3	-3.81	102.51	110.14
9	K	4	MAN	O3-C3-C4	3.78	119.09	110.35
5	F	6	MAN	O2-C2-C1	-3.77	101.45	109.15
5	M	10	MAN	O2-C2-C1	3.75	116.83	109.15
10	P	5	MAN	O5-C5-C6	3.75	113.08	107.20
3	L	3	BMA	O4-C4-C3	-3.75	101.68	110.35
4	E	2	NAG	O6-C6-C5	-3.74	98.47	111.29
2	C	3	BMA	C2-C3-C4	-3.74	104.43	110.89
9	K	4	MAN	C1-C2-C3	3.74	114.26	109.67
6	O	7	MAN	O4-C4-C3	-3.71	101.77	110.35
7	I	6	MAN	O3-C3-C4	3.68	118.86	110.35
7	I	3	BMA	O3-C3-C4	-3.65	101.91	110.35
7	I	7	MAN	C1-O5-C5	3.65	117.14	112.19
10	P	5	MAN	O2-C2-C3	-3.65	102.83	110.14
3	G	1	NAG	C2-N2-C7	3.63	128.08	122.90
8	J	3	BMA	O5-C5-C4	-3.63	102.00	110.83
8	J	2	NAG	O6-C6-C5	-3.54	99.14	111.29
10	P	4	MAN	O5-C1-C2	3.53	116.23	110.77
6	H	1	NAG	C1-C2-N2	-3.52	104.48	110.49
6	H	2	NAG	O4-C4-C3	-3.48	102.31	110.35
3	D	3	BMA	C1-O5-C5	3.47	116.90	112.19
5	F	7	MAN	O5-C1-C2	-3.46	105.43	110.77
3	L	1	NAG	O4-C4-C5	-3.44	100.74	109.30
5	M	9	MAN	C1-C2-C3	3.44	113.89	109.67
2	C	4	MAN	O5-C1-C2	3.43	116.06	110.77
3	L	1	NAG	C3-C4-C5	3.42	116.34	110.24
10	P	7	MAN	C1-C2-C3	-3.40	105.49	109.67
3	G	3	BMA	O3-C3-C4	3.40	118.21	110.35
7	I	7	MAN	O5-C5-C6	3.39	112.52	107.20
4	E	2	NAG	O5-C5-C6	3.38	112.51	107.20
7	I	6	MAN	O2-C2-C1	3.38	116.06	109.15
5	F	8	MAN	C3-C4-C5	3.35	116.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	3	BMA	C6-C5-C4	-3.35	105.15	113.00
3	N	2	NAG	O7-C7-C8	-3.34	115.85	122.06
10	P	3	BMA	O5-C5-C4	3.34	118.94	110.83
4	E	1	NAG	O4-C4-C5	-3.33	101.03	109.30
6	H	4	MAN	O5-C1-C2	3.33	115.91	110.77
5	M	3	BMA	O5-C5-C4	-3.30	102.80	110.83
6	O	5	MAN	O5-C5-C6	3.29	112.37	107.20
10	P	4	MAN	O4-C4-C3	-3.29	102.74	110.35
3	N	3	BMA	C3-C4-C5	3.29	116.11	110.24
6	O	2	NAG	O4-C4-C3	-3.29	102.75	110.35
6	O	7	MAN	O2-C2-C3	3.27	116.69	110.14
10	P	3	BMA	C3-C4-C5	3.26	116.06	110.24
6	O	6	MAN	C1-O5-C5	3.26	116.61	112.19
10	P	8	MAN	O3-C3-C4	-3.26	102.82	110.35
7	I	7	MAN	C1-C2-C3	-3.23	105.69	109.67
9	K	2	NAG	C6-C5-C4	3.22	120.54	113.00
8	J	3	BMA	O6-C6-C5	-3.22	100.26	111.29
2	C	3	BMA	O3-C3-C4	3.21	117.76	110.35
3	G	1	NAG	C4-C3-C2	-3.21	106.32	111.02
6	O	6	MAN	C1-C2-C3	-3.20	105.73	109.67
6	H	2	NAG	C2-N2-C7	-3.19	118.36	122.90
10	P	6	MAN	O4-C4-C5	-3.15	101.47	109.30
3	L	3	BMA	C3-C4-C5	3.13	115.81	110.24
5	M	2	NAG	C1-C2-N2	-3.12	105.15	110.49
8	J	7	MAN	C1-O5-C5	-3.12	107.96	112.19
8	J	7	MAN	O5-C5-C6	3.12	112.10	107.20
5	M	7	MAN	O5-C5-C6	3.11	112.08	107.20
6	O	4	MAN	O3-C3-C4	3.09	117.49	110.35
2	C	4	MAN	O5-C5-C6	-3.08	102.37	107.20
10	P	6	MAN	C3-C4-C5	-3.08	104.75	110.24
6	O	7	MAN	O3-C3-C2	3.06	115.85	109.99
2	C	1	NAG	O5-C5-C6	3.05	111.99	107.20
5	M	10	MAN	O6-C6-C5	-3.05	100.84	111.29
7	I	5	MAN	O2-C2-C1	3.04	115.37	109.15
5	F	7	MAN	C2-C3-C4	-3.04	105.64	110.89
3	L	2	NAG	O6-C6-C5	-3.03	100.88	111.29
8	J	2	NAG	O7-C7-N2	3.02	127.51	121.95
3	L	1	NAG	O5-C5-C6	3.01	111.92	107.20
3	D	1	NAG	O5-C5-C4	-3.00	103.52	110.83
2	C	5	MAN	C6-C5-C4	3.00	120.03	113.00
6	O	4	MAN	O2-C2-C3	-3.00	104.13	110.14
8	J	6	MAN	C1-O5-C5	2.97	116.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	2	NAG	O6-C6-C5	-2.96	101.13	111.29
5	F	5	MAN	C1-O5-C5	2.95	116.19	112.19
3	L	3	BMA	O3-C3-C2	2.95	115.64	109.99
7	I	4	MAN	O4-C4-C3	-2.94	103.55	110.35
3	L	3	BMA	O5-C1-C2	-2.93	106.25	110.77
5	M	1	NAG	O5-C5-C6	-2.93	102.61	107.20
5	F	10	MAN	C2-C3-C4	2.92	115.95	110.89
6	O	2	NAG	C6-C5-C4	2.92	119.85	113.00
8	J	6	MAN	C6-C5-C4	-2.92	106.17	113.00
5	F	3	BMA	C1-C2-C3	2.92	113.25	109.67
10	P	6	MAN	C1-O5-C5	2.90	116.12	112.19
5	M	9	MAN	O3-C3-C2	-2.90	104.44	109.99
5	F	5	MAN	C6-C5-C4	-2.90	106.22	113.00
5	F	4	MAN	O6-C6-C5	-2.89	101.37	111.29
8	J	3	BMA	C1-C2-C3	-2.89	106.12	109.67
3	D	2	NAG	C1-O5-C5	-2.89	108.28	112.19
6	H	7	MAN	O4-C4-C3	-2.88	103.68	110.35
2	C	5	MAN	O3-C3-C4	2.88	117.02	110.35
3	N	3	BMA	C6-C5-C4	-2.88	106.25	113.00
5	M	10	MAN	C1-C2-C3	-2.88	106.12	109.67
5	M	4	MAN	C1-O5-C5	2.87	116.08	112.19
7	I	5	MAN	C1-O5-C5	2.87	116.08	112.19
10	P	8	MAN	C3-C4-C5	2.84	115.31	110.24
5	M	4	MAN	O2-C2-C3	2.84	115.83	110.14
5	M	1	NAG	C1-C2-N2	-2.84	105.64	110.49
3	D	2	NAG	C6-C5-C4	2.83	119.64	113.00
9	K	2	NAG	O6-C6-C5	-2.81	101.65	111.29
7	I	6	MAN	O5-C5-C4	2.81	117.65	110.83
10	P	1	NAG	O5-C5-C6	2.80	111.60	107.20
6	O	2	NAG	O3-C3-C2	-2.80	103.66	109.47
7	I	5	MAN	C6-C5-C4	2.80	119.57	113.00
6	H	4	MAN	C6-C5-C4	2.77	119.48	113.00
6	H	3	BMA	C1-O5-C5	-2.76	108.45	112.19
7	I	6	MAN	C6-C5-C4	-2.76	106.54	113.00
6	H	6	MAN	O5-C5-C6	2.76	111.53	107.20
6	O	5	MAN	C6-C5-C4	-2.74	106.58	113.00
7	I	1	NAG	O5-C5-C6	2.73	111.48	107.20
8	J	1	NAG	O5-C5-C4	-2.73	104.19	110.83
3	G	3	BMA	O5-C1-C2	2.72	114.97	110.77
6	O	2	NAG	C3-C4-C5	-2.71	105.40	110.24
5	F	3	BMA	O5-C5-C6	2.70	111.44	107.20
8	J	4	MAN	C6-C5-C4	-2.69	106.69	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	C1-C2-N2	2.68	115.07	110.49
6	H	7	MAN	C1-C2-C3	-2.68	106.37	109.67
2	C	2	NAG	O4-C4-C5	-2.68	102.65	109.30
3	D	1	NAG	C1-C2-N2	2.67	115.06	110.49
3	G	1	NAG	O3-C3-C2	-2.67	103.93	109.47
5	M	4	MAN	O6-C6-C5	-2.67	102.14	111.29
3	D	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	H	2	NAG	C4-C3-C2	2.66	114.92	111.02
7	I	2	NAG	C1-O5-C5	2.66	115.80	112.19
6	H	5	MAN	O2-C2-C3	-2.65	104.82	110.14
5	F	10	MAN	O2-C2-C3	2.65	115.44	110.14
3	G	3	BMA	C3-C4-C5	2.65	114.96	110.24
2	C	2	NAG	C6-C5-C4	2.64	119.18	113.00
7	I	1	NAG	C2-N2-C7	-2.63	119.15	122.90
2	C	3	BMA	C3-C4-C5	2.62	114.91	110.24
2	C	2	NAG	O7-C7-C8	-2.62	117.19	122.06
7	I	3	BMA	C1-C2-C3	2.61	112.87	109.67
5	F	9	MAN	O4-C4-C3	-2.61	104.32	110.35
3	N	1	NAG	C1-O5-C5	-2.60	108.67	112.19
6	H	5	MAN	C3-C4-C5	-2.59	105.62	110.24
3	D	2	NAG	O3-C3-C2	-2.58	104.12	109.47
6	H	4	MAN	O6-C6-C5	-2.57	102.47	111.29
6	H	3	BMA	O2-C2-C1	-2.57	103.89	109.15
5	M	5	MAN	O3-C3-C4	-2.57	104.41	110.35
7	I	2	NAG	O5-C1-C2	-2.57	107.23	111.29
7	I	1	NAG	O6-C6-C5	-2.57	102.49	111.29
2	C	5	MAN	C1-O5-C5	2.56	115.66	112.19
5	M	9	MAN	O2-C2-C3	-2.56	105.00	110.14
3	G	3	BMA	O4-C4-C5	-2.56	102.94	109.30
5	M	4	MAN	C2-C3-C4	-2.56	106.47	110.89
10	P	1	NAG	O7-C7-C8	2.55	126.80	122.06
7	I	5	MAN	O4-C4-C3	-2.55	104.45	110.35
5	M	10	MAN	O5-C5-C6	-2.54	103.22	107.20
5	M	2	NAG	O4-C4-C3	-2.54	104.47	110.35
7	I	7	MAN	O2-C2-C3	2.54	115.23	110.14
6	H	2	NAG	O6-C6-C5	-2.54	102.58	111.29
4	E	1	NAG	O5-C5-C6	2.54	111.18	107.20
10	P	4	MAN	O3-C3-C4	-2.53	104.50	110.35
5	M	7	MAN	O5-C5-C4	-2.52	104.69	110.83
7	I	1	NAG	C6-C5-C4	-2.51	107.13	113.00
5	M	7	MAN	O6-C6-C5	-2.50	102.73	111.29
5	F	4	MAN	O5-C5-C6	2.49	111.11	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	5	MAN	O6-C6-C5	-2.49	102.75	111.29
3	L	2	NAG	C2-N2-C7	2.48	126.43	122.90
10	P	2	NAG	C8-C7-N2	2.47	120.27	116.10
6	H	3	BMA	O5-C5-C4	-2.46	104.83	110.83
10	P	8	MAN	O2-C2-C1	2.45	114.17	109.15
5	F	10	MAN	O3-C3-C4	-2.45	104.68	110.35
5	F	9	MAN	O3-C3-C2	-2.43	105.33	109.99
6	O	4	MAN	O2-C2-C1	2.43	114.12	109.15
2	C	2	NAG	O5-C5-C4	-2.43	104.92	110.83
8	J	7	MAN	O4-C4-C3	-2.43	104.74	110.35
2	C	2	NAG	O3-C3-C4	2.42	115.95	110.35
5	M	5	MAN	C6-C5-C4	-2.42	107.33	113.00
5	M	9	MAN	O5-C5-C6	-2.42	103.41	107.20
7	I	6	MAN	C2-C3-C4	-2.41	106.73	110.89
6	H	2	NAG	C3-C4-C5	-2.41	105.95	110.24
6	O	5	MAN	O4-C4-C3	-2.40	104.79	110.35
10	P	5	MAN	O3-C3-C4	-2.40	104.80	110.35
10	P	5	MAN	C1-C2-C3	2.40	112.62	109.67
10	P	1	NAG	C1-O5-C5	2.40	115.44	112.19
10	P	5	MAN	O6-C6-C5	-2.39	103.08	111.29
2	C	4	MAN	C2-C3-C4	2.39	115.03	110.89
7	I	3	BMA	O2-C2-C3	2.38	114.91	110.14
6	O	3	BMA	O4-C4-C5	-2.38	103.39	109.30
9	K	2	NAG	O4-C4-C5	-2.38	103.39	109.30
9	K	4	MAN	C6-C5-C4	2.37	118.56	113.00
10	P	7	MAN	O4-C4-C5	-2.37	103.41	109.30
2	C	3	BMA	O5-C1-C2	2.36	114.41	110.77
6	H	1	NAG	O5-C5-C4	-2.35	105.10	110.83
6	O	4	MAN	O4-C4-C5	-2.35	103.46	109.30
6	O	1	NAG	C1-O5-C5	2.35	115.38	112.19
6	O	6	MAN	O6-C6-C5	-2.35	103.23	111.29
2	C	2	NAG	O3-C3-C2	-2.35	104.61	109.47
2	C	3	BMA	O3-C3-C2	-2.34	105.51	109.99
8	J	6	MAN	O5-C5-C6	2.33	110.86	107.20
7	I	1	NAG	C1-O5-C5	2.33	115.35	112.19
5	M	10	MAN	O2-C2-C3	2.33	114.80	110.14
10	P	3	BMA	O4-C4-C5	-2.32	103.53	109.30
8	J	2	NAG	O4-C4-C5	-2.32	103.54	109.30
3	G	2	NAG	C4-C3-C2	2.30	114.39	111.02
3	L	1	NAG	C6-C5-C4	-2.29	107.64	113.00
3	D	1	NAG	C2-N2-C7	-2.29	119.65	122.90
3	N	2	NAG	C2-N2-C7	-2.28	119.65	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	F	2	NAG	O5-C1-C2	-2.28	107.69	111.29
9	K	2	NAG	C1-O5-C5	-2.27	109.12	112.19
3	D	2	NAG	O5-C1-C2	-2.26	107.73	111.29
5	F	10	MAN	C1-O5-C5	2.25	115.24	112.19
8	J	7	MAN	C2-C3-C4	-2.25	107.00	110.89
7	I	2	NAG	C6-C5-C4	-2.24	107.75	113.00
5	F	8	MAN	O2-C2-C1	-2.24	104.58	109.15
5	M	1	NAG	O5-C5-C4	-2.23	105.41	110.83
5	M	10	MAN	C1-O5-C5	2.23	115.21	112.19
9	K	1	NAG	O3-C3-C2	-2.22	104.88	109.47
2	C	2	NAG	O7-C7-N2	2.22	126.03	121.95
8	J	3	BMA	O3-C3-C4	-2.21	105.23	110.35
5	F	8	MAN	O4-C4-C5	2.21	114.79	109.30
6	O	2	NAG	O6-C6-C5	-2.21	103.72	111.29
5	F	1	NAG	O5-C5-C6	-2.21	103.75	107.20
8	J	4	MAN	O2-C2-C3	-2.20	105.72	110.14
9	K	3	BMA	O3-C3-C2	2.20	114.20	109.99
9	K	4	MAN	O4-C4-C5	-2.19	103.85	109.30
3	D	1	NAG	O6-C6-C5	-2.19	103.77	111.29
5	M	8	MAN	C1-O5-C5	2.19	115.16	112.19
5	F	1	NAG	C3-C4-C5	2.19	114.15	110.24
6	H	4	MAN	O4-C4-C3	-2.19	105.29	110.35
6	H	4	MAN	O3-C3-C2	2.18	114.17	109.99
3	D	2	NAG	O6-C6-C5	-2.17	103.84	111.29
8	J	1	NAG	O4-C4-C3	-2.16	105.35	110.35
2	C	2	NAG	C2-N2-C7	2.16	125.97	122.90
5	M	6	MAN	O2-C2-C1	-2.16	104.74	109.15
7	I	6	MAN	O6-C6-C5	-2.15	103.90	111.29
5	M	4	MAN	O5-C5-C4	-2.15	105.59	110.83
10	P	2	NAG	O6-C6-C5	-2.15	103.92	111.29
6	O	6	MAN	O4-C4-C3	-2.13	105.41	110.35
6	O	6	MAN	C6-C5-C4	-2.13	108.01	113.00
2	C	4	MAN	O3-C3-C2	2.13	114.08	109.99
8	J	3	BMA	C3-C4-C5	2.13	114.04	110.24
6	O	4	MAN	C1-O5-C5	2.13	115.08	112.19
10	P	1	NAG	O3-C3-C2	-2.12	105.07	109.47
5	M	10	MAN	O5-C1-C2	2.12	114.05	110.77
9	K	1	NAG	C1-C2-N2	2.12	114.10	110.49
6	O	3	BMA	O5-C5-C6	2.10	110.50	107.20
7	I	1	NAG	C1-C2-N2	-2.10	106.90	110.49
5	M	9	MAN	C1-O5-C5	2.10	115.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	3	BMA	C2-C3-C4	-2.09	107.27	110.89
8	J	5	MAN	O2-C2-C1	-2.09	104.87	109.15
6	H	7	MAN	O6-C6-C5	-2.09	104.12	111.29
3	L	3	BMA	O5-C5-C4	2.08	115.89	110.83
5	M	1	NAG	C4-C3-C2	2.08	114.07	111.02
9	K	1	NAG	O5-C5-C4	-2.08	105.76	110.83
4	E	2	NAG	O5-C5-C4	-2.08	105.77	110.83
5	M	1	NAG	O5-C1-C2	-2.08	108.01	111.29
6	O	5	MAN	C1-O5-C5	2.08	115.01	112.19
8	J	4	MAN	O6-C6-C5	-2.07	104.18	111.29
3	L	2	NAG	C6-C5-C4	-2.07	108.15	113.00
5	F	9	MAN	C1-O5-C5	2.07	115.00	112.19
7	I	4	MAN	O4-C4-C5	2.07	114.43	109.30
6	O	4	MAN	O6-C6-C5	-2.06	104.22	111.29
5	F	10	MAN	O4-C4-C3	-2.06	105.58	110.35
9	K	3	BMA	O2-C2-C1	-2.06	104.94	109.15
7	I	2	NAG	O3-C3-C2	-2.06	105.21	109.47
9	K	4	MAN	O4-C4-C3	2.06	115.10	110.35
4	E	1	NAG	C1-O5-C5	2.05	114.97	112.19
6	H	1	NAG	C8-C7-N2	2.05	119.56	116.10
6	H	4	MAN	C1-O5-C5	2.04	114.96	112.19
9	K	1	NAG	O6-C6-C5	-2.04	104.30	111.29
3	G	3	BMA	O5-C5-C4	2.03	115.77	110.83
8	J	4	MAN	C1-O5-C5	-2.02	109.45	112.19
10	P	6	MAN	O2-C2-C3	2.02	114.19	110.14
5	M	5	MAN	C1-C2-C3	-2.02	107.19	109.67
10	P	7	MAN	C6-C5-C4	-2.01	108.29	113.00
5	F	1	NAG	C6-C5-C4	2.01	117.70	113.00
2	C	4	MAN	O4-C4-C3	-2.01	105.71	110.35
5	M	7	MAN	O3-C3-C4	-2.00	105.71	110.35
10	P	3	BMA	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	4	MAN	O5-C5-C6-O6
8	J	5	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
10	P	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	F	10	MAN	C4-C5-C6-O6
8	J	5	MAN	C4-C5-C6-O6
5	M	10	MAN	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
10	P	3	BMA	C4-C5-C6-O6
8	J	6	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
10	P	7	MAN	C4-C5-C6-O6
5	M	10	MAN	O5-C5-C6-O6
5	F	10	MAN	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6
10	P	4	MAN	O5-C5-C6-O6
8	J	6	MAN	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
10	P	3	BMA	O5-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
7	I	7	MAN	C4-C5-C6-O6
10	P	8	MAN	O5-C5-C6-O6
7	I	7	MAN	O5-C5-C6-O6
6	O	7	MAN	C4-C5-C6-O6
7	I	6	MAN	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C3-C2-N2-C7
10	P	4	MAN	C4-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	BMA	1	0
8	J	2	NAG	1	0
9	K	1	NAG	1	0
10	P	4	MAN	5	0
6	O	3	BMA	1	0
10	P	3	BMA	6	0
3	D	2	NAG	1	0
7	I	6	MAN	1	0

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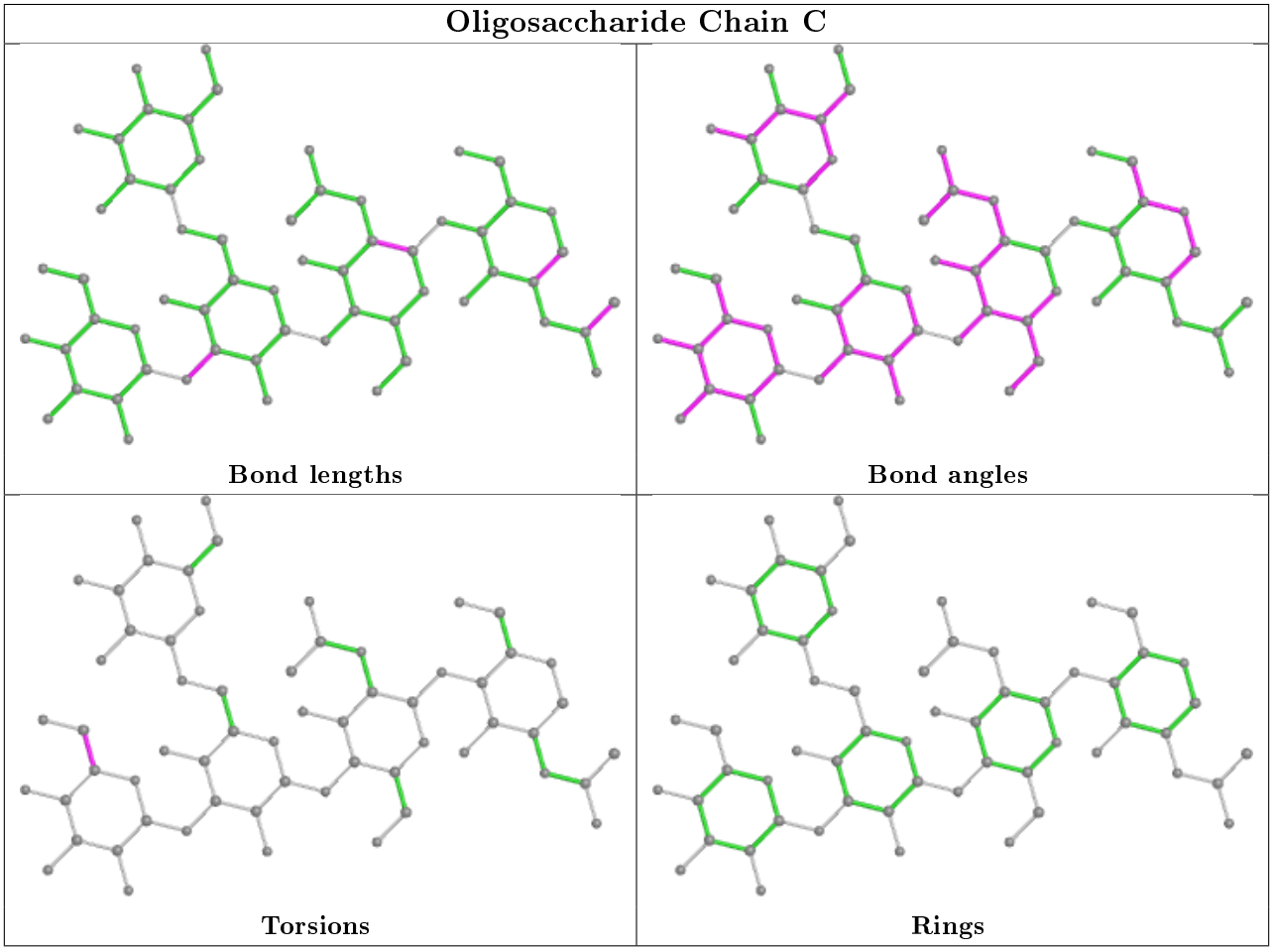
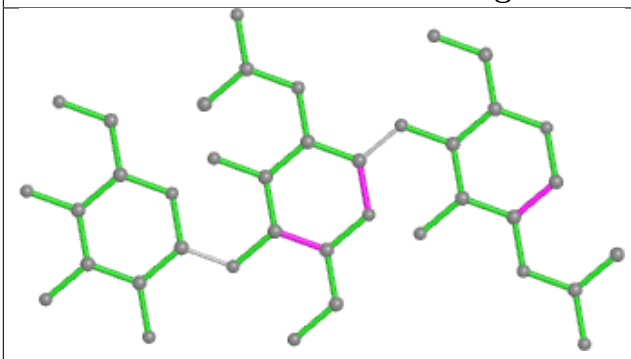
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

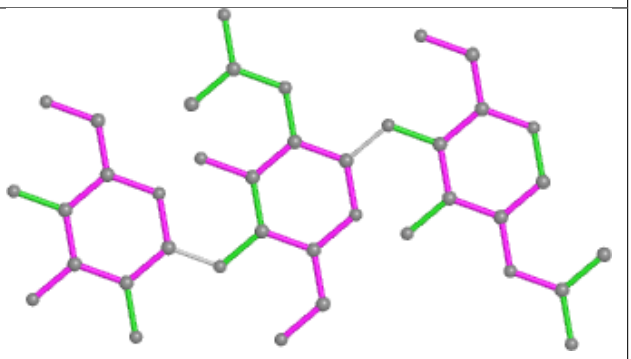
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



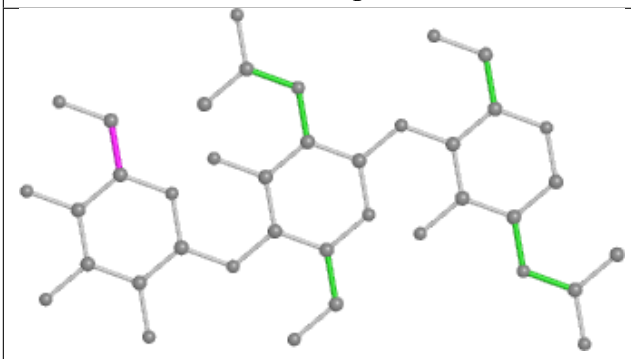
Oligosaccharide Chain D



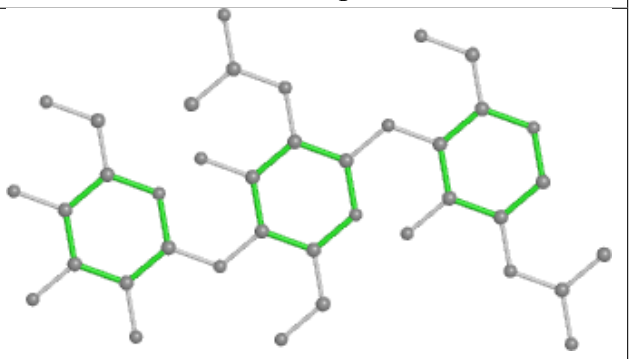
Bond lengths



Bond angles

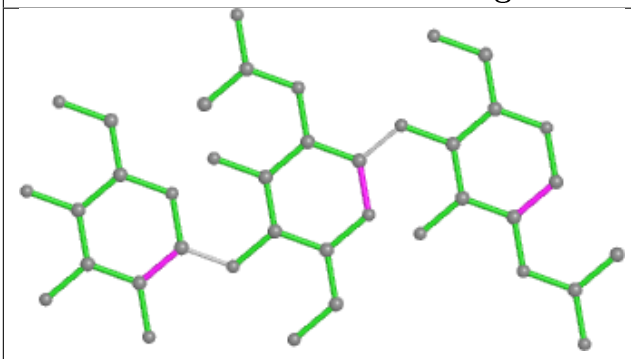


Torsions

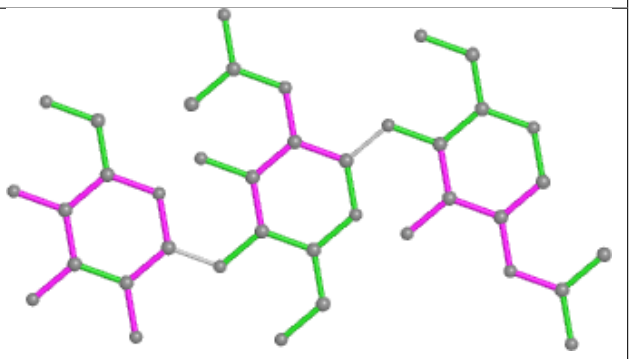


Rings

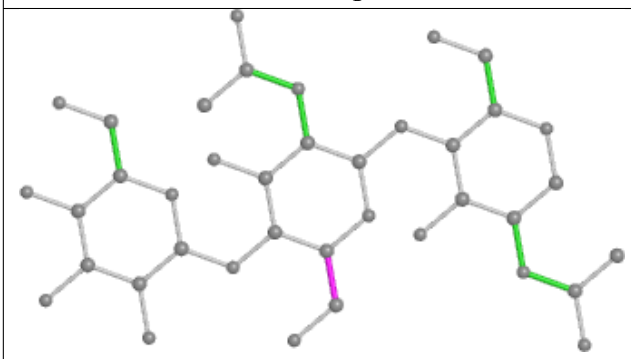
Oligosaccharide Chain G



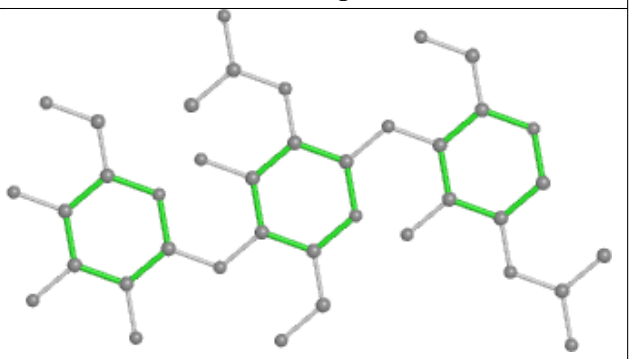
Bond lengths



Bond angles

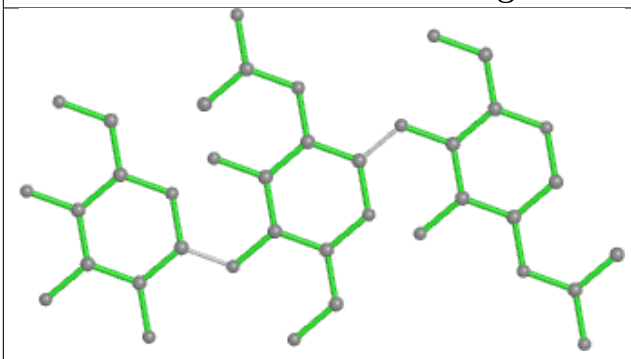


Torsions

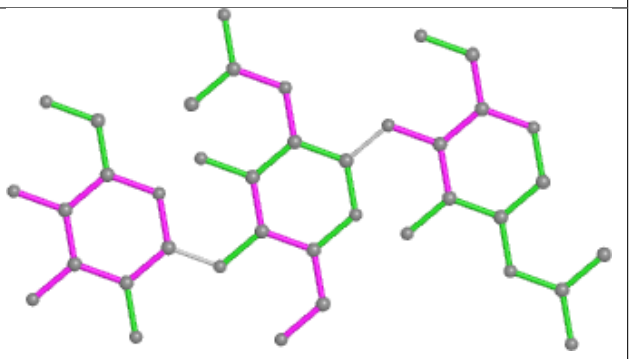


Rings

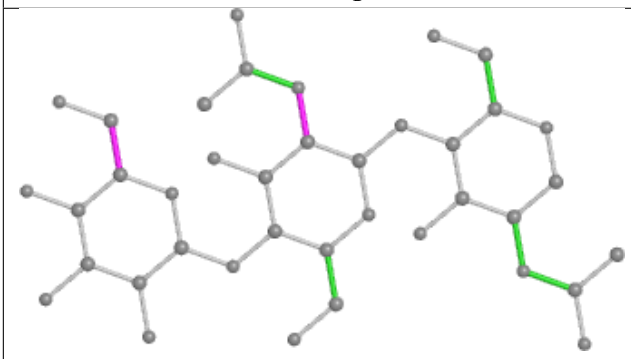
Oligosaccharide Chain L



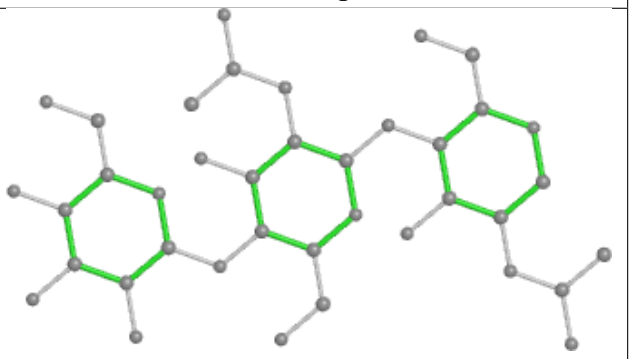
Bond lengths



Bond angles

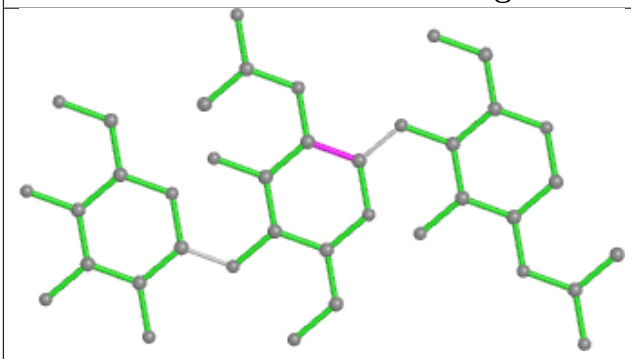


Torsions

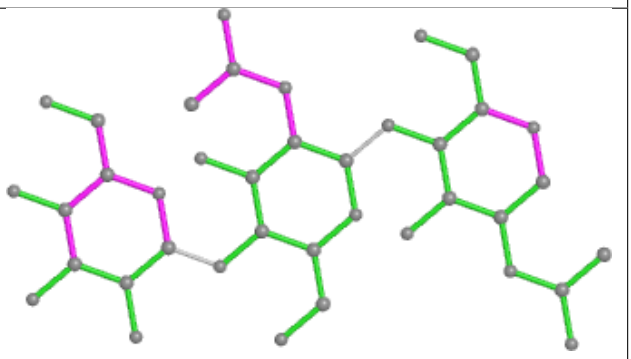


Rings

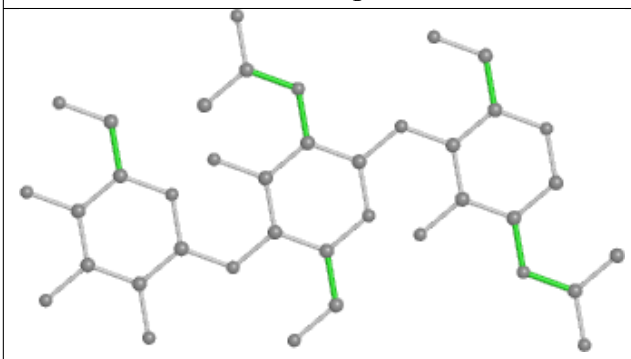
Oligosaccharide Chain N



Bond lengths



Bond angles



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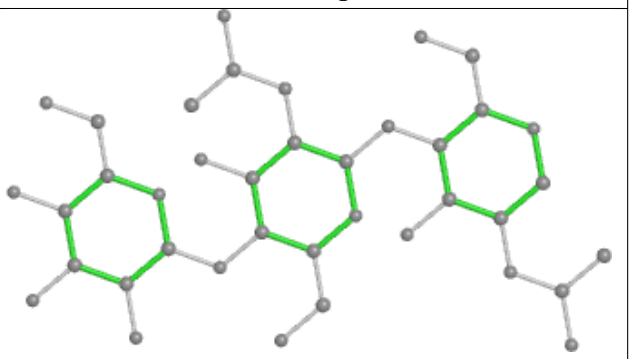
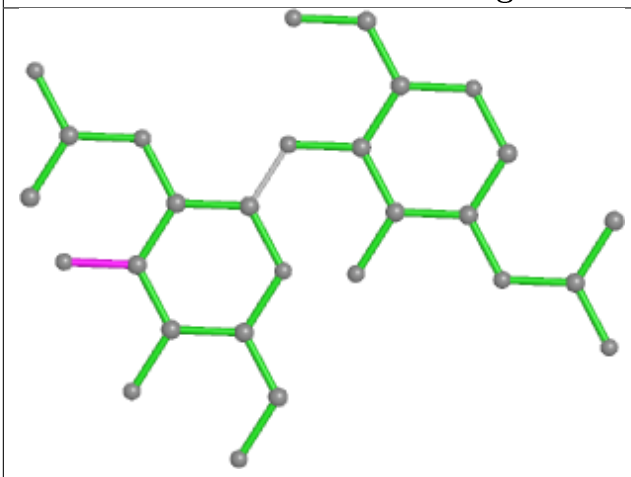
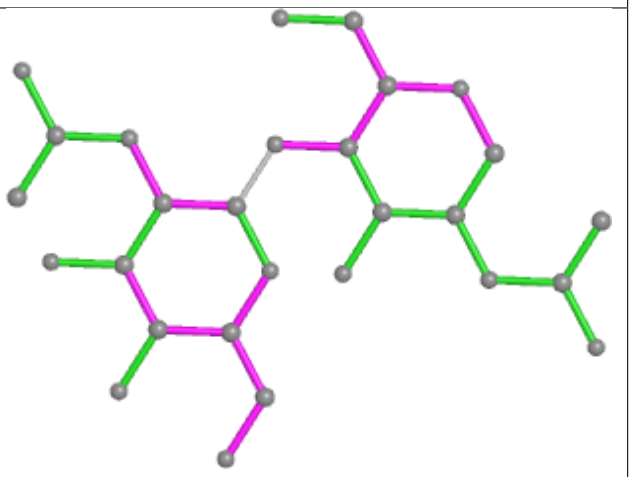


Rings

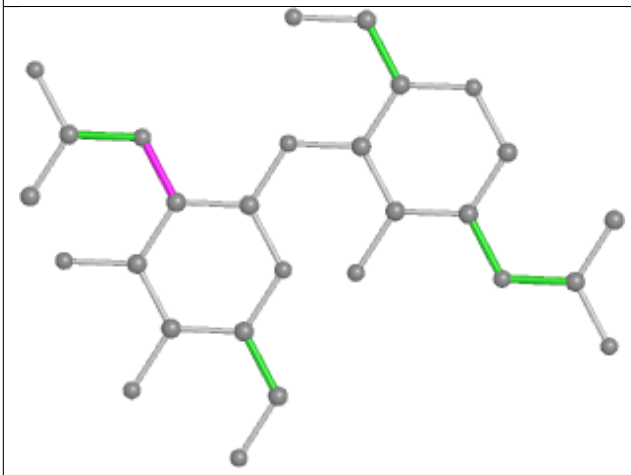
Oligosaccharide Chain E



Bond lengths



Bond angles



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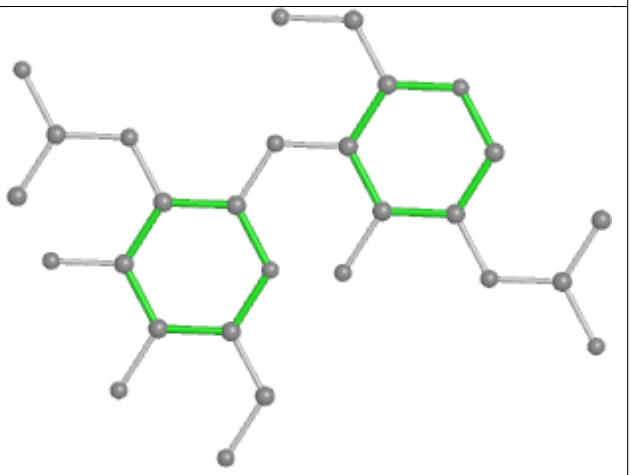
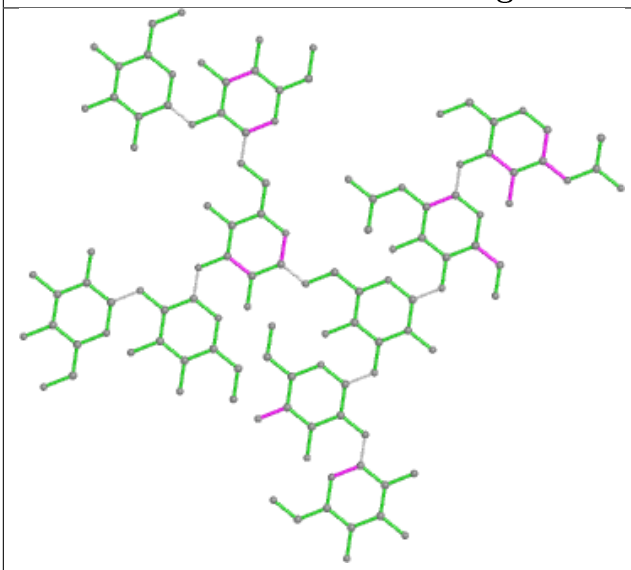
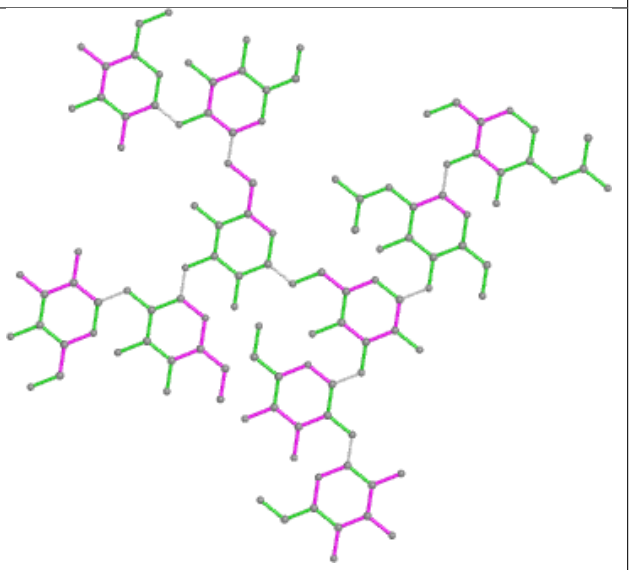


Rings

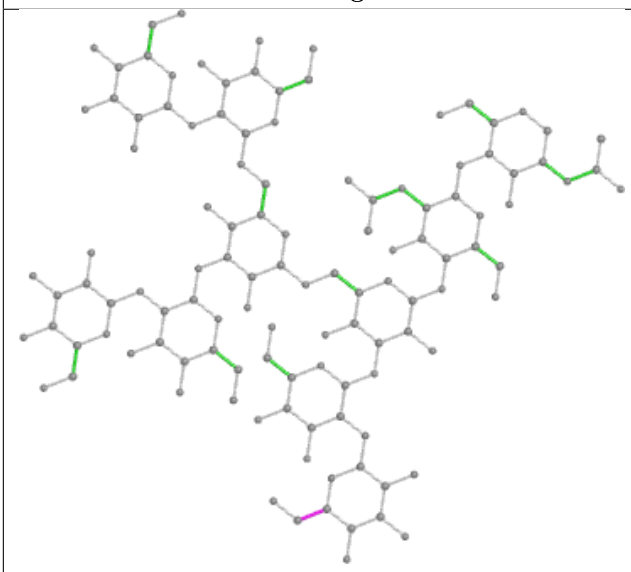
Oligosaccharide Chain F



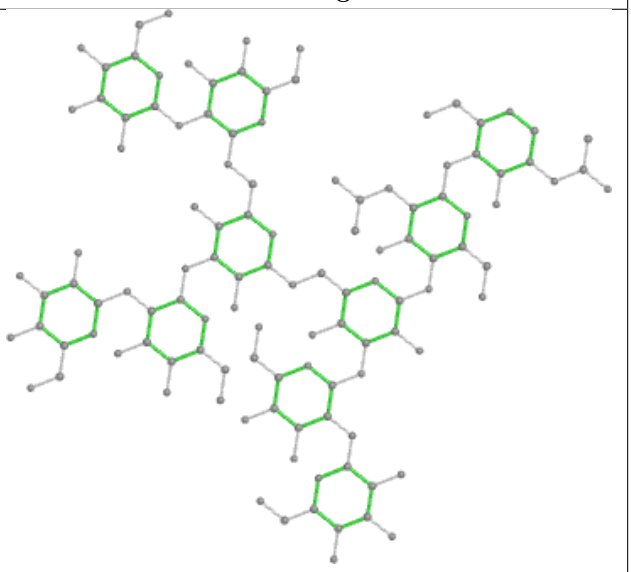
Bond lengths



Bond angles

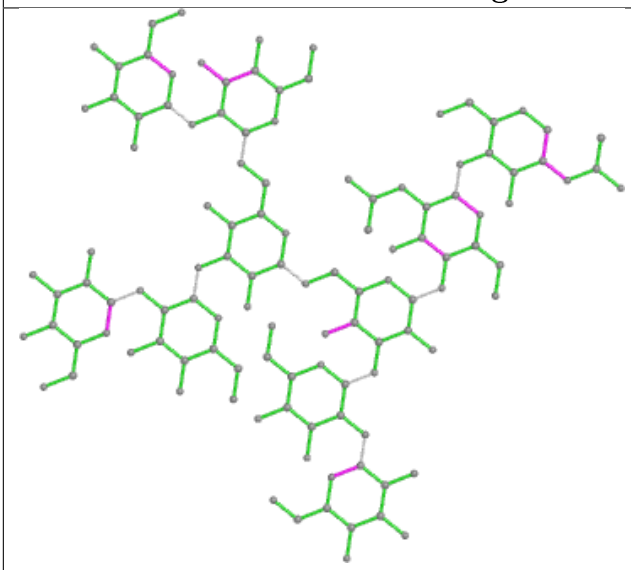


Torsions

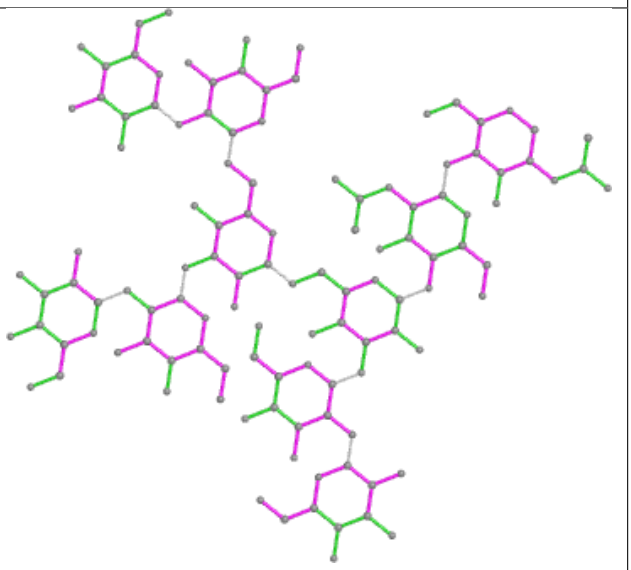


Rings

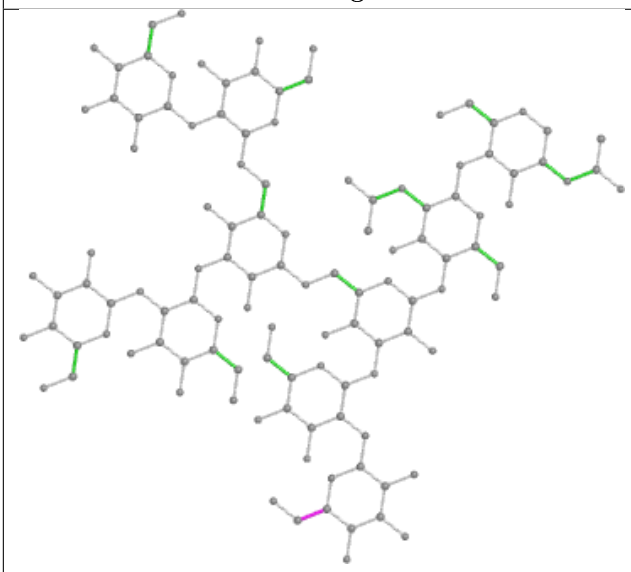
Oligosaccharide Chain M



Bond lengths



Bond angles



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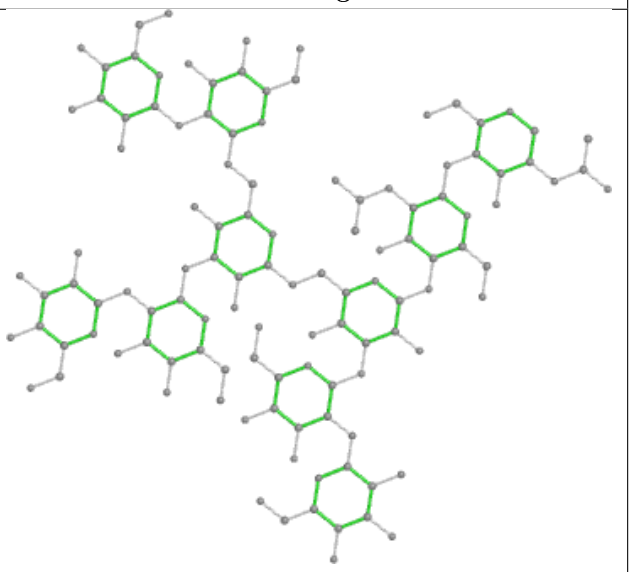
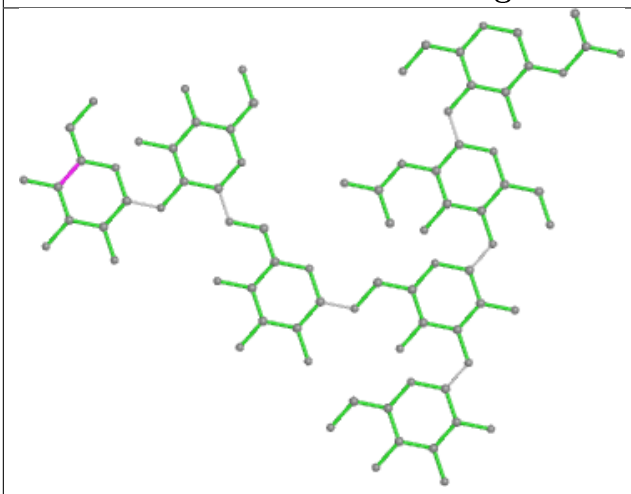
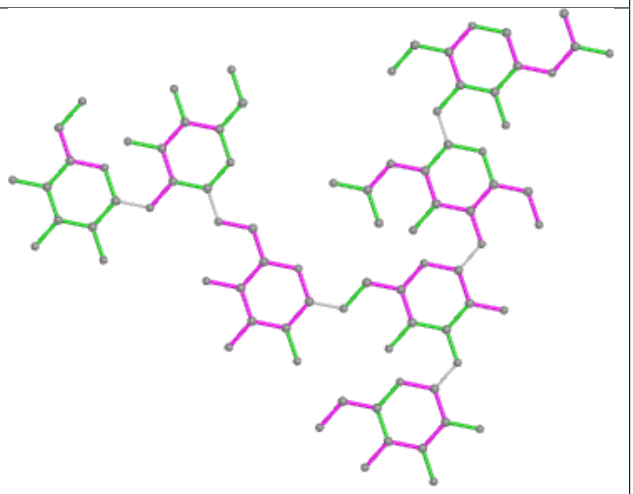


Rings

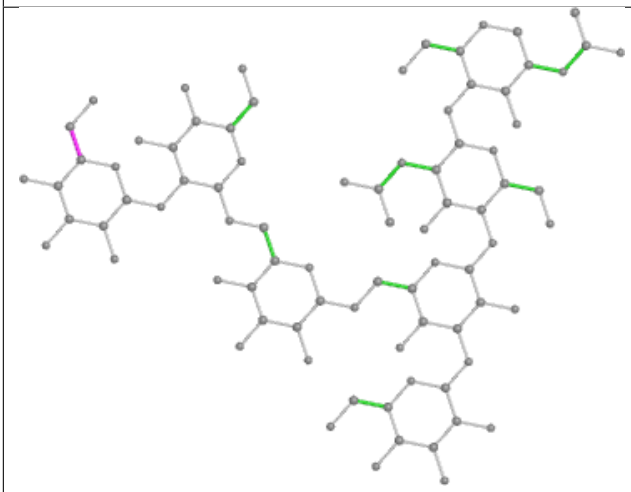
Oligosaccharide Chain H



Bond lengths



Bond angles



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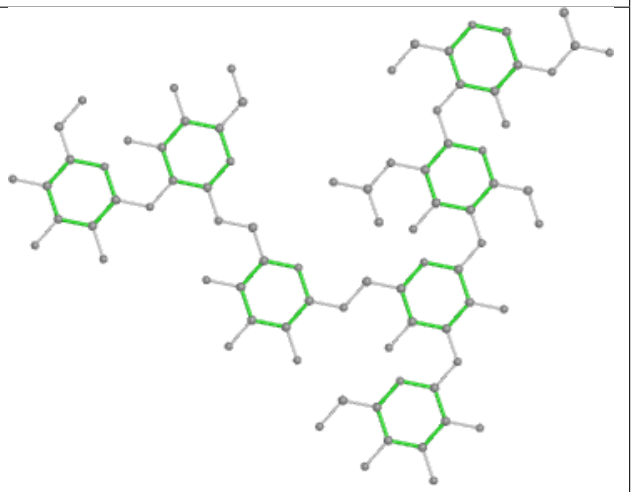
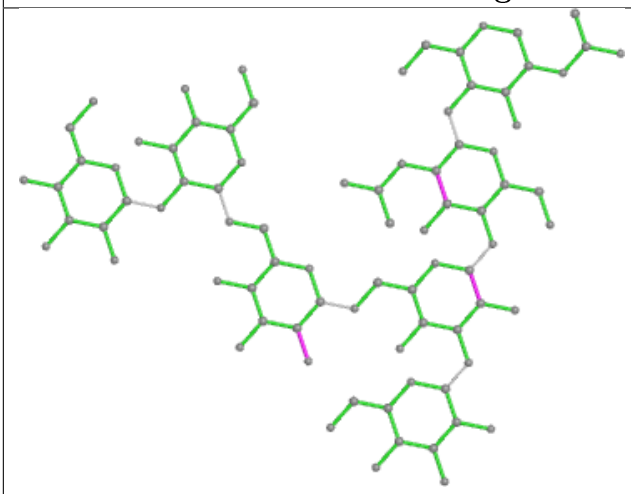
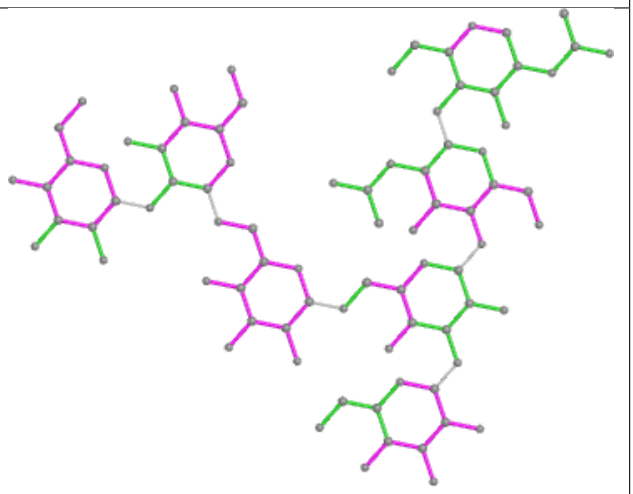


Rings

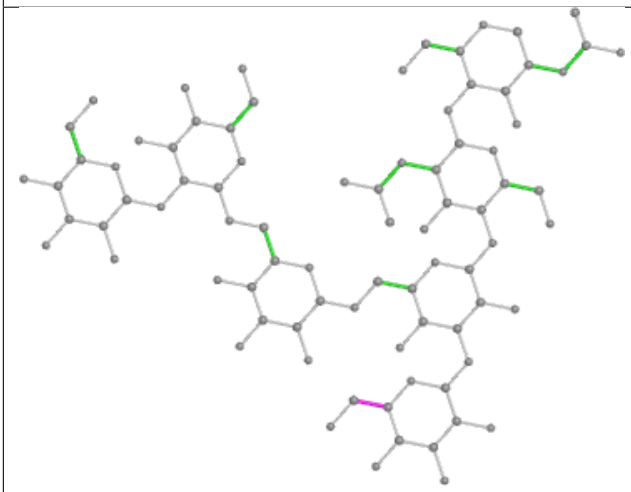
Oligosaccharide Chain O



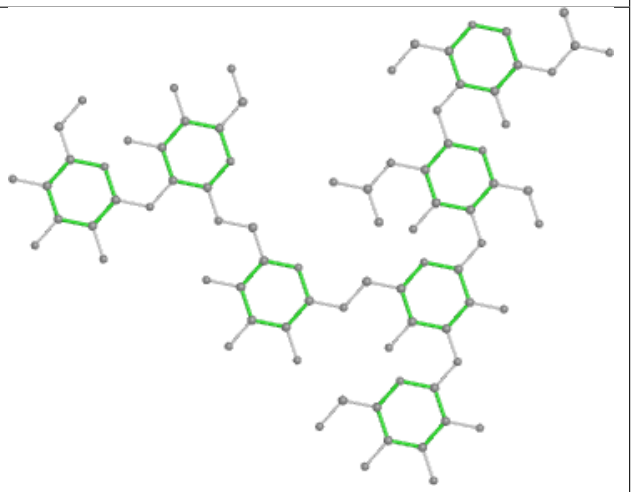
Bond lengths



Bond angles

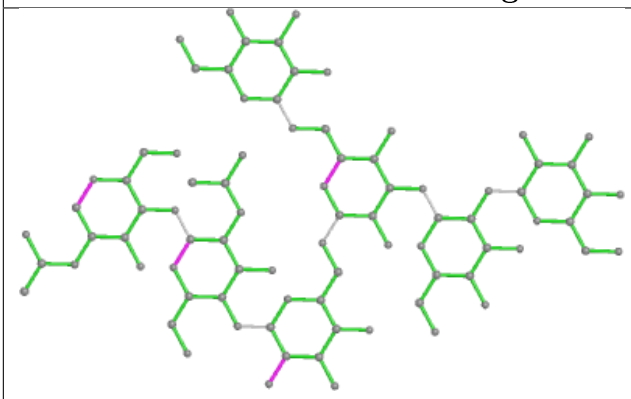


Torsions

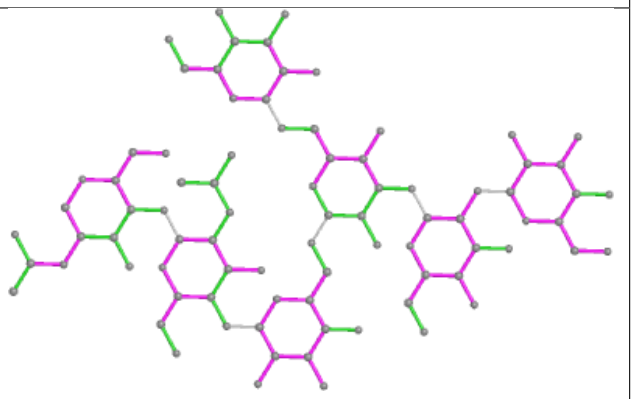


Rings

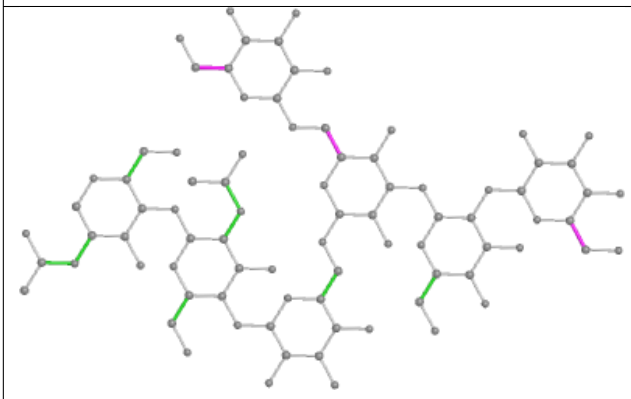
Oligosaccharide Chain I



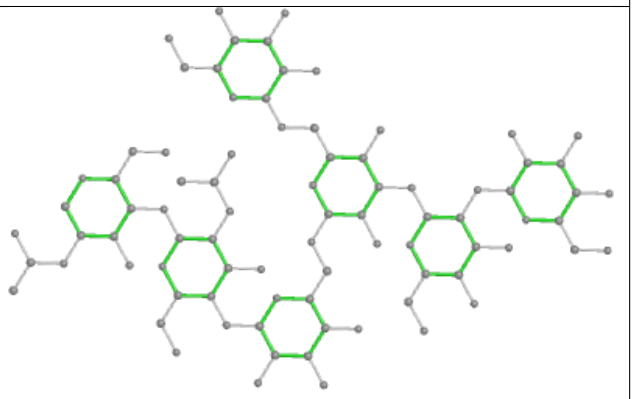
Bond lengths



Bond angles

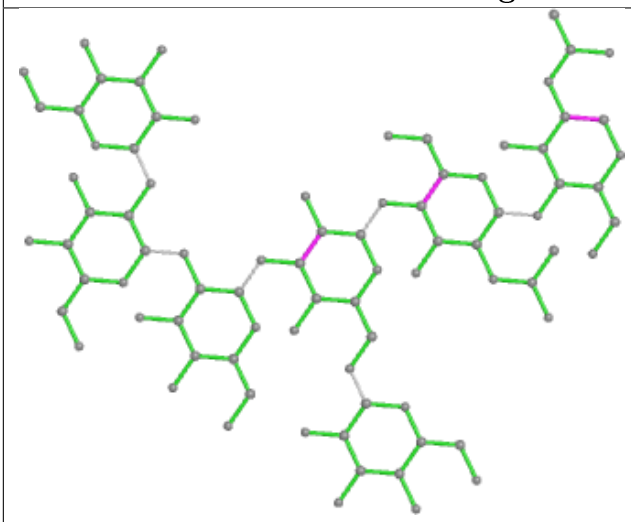


Torsions

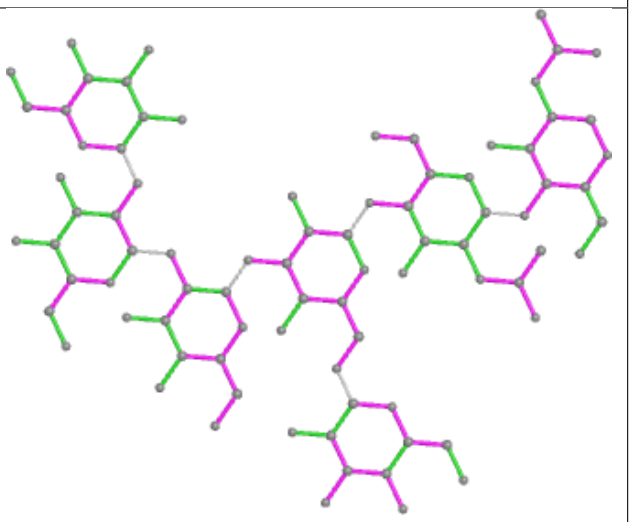


Rings

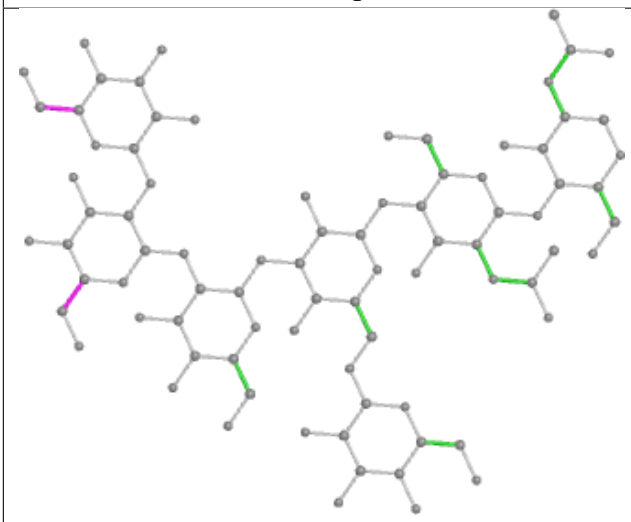
Oligosaccharide Chain J



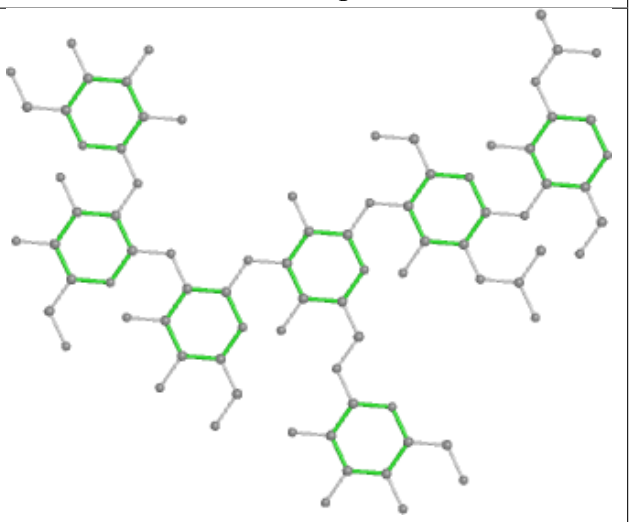
Bond lengths



Bond angles

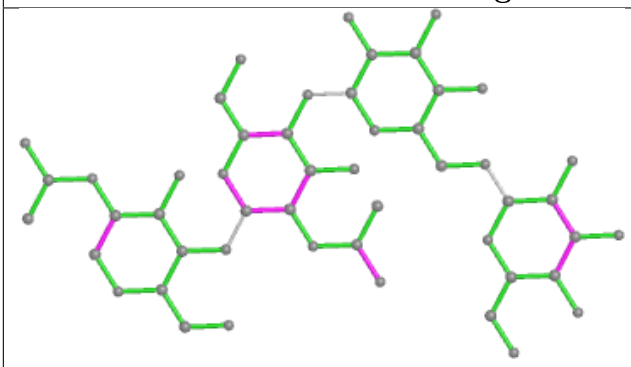


Torsions

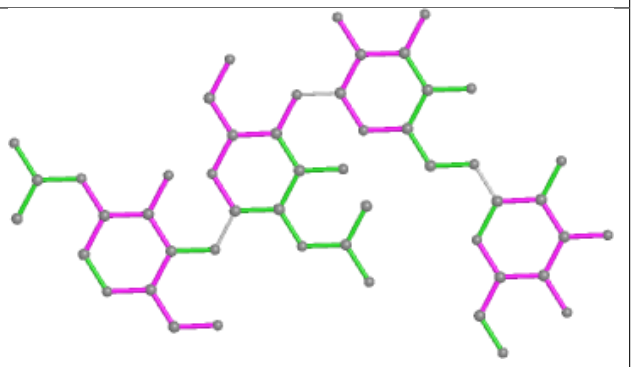


Rings

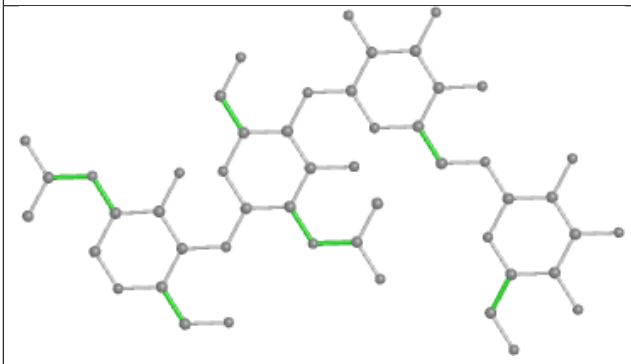
Oligosaccharide Chain K



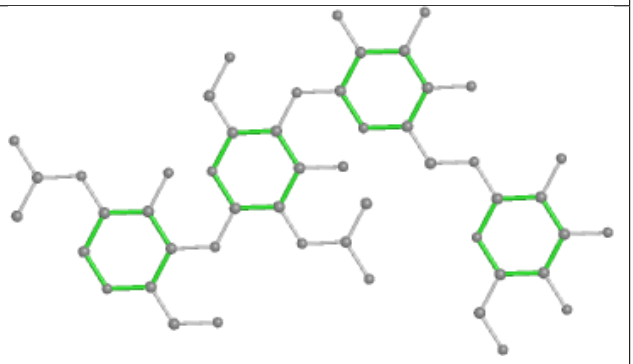
Bond lengths



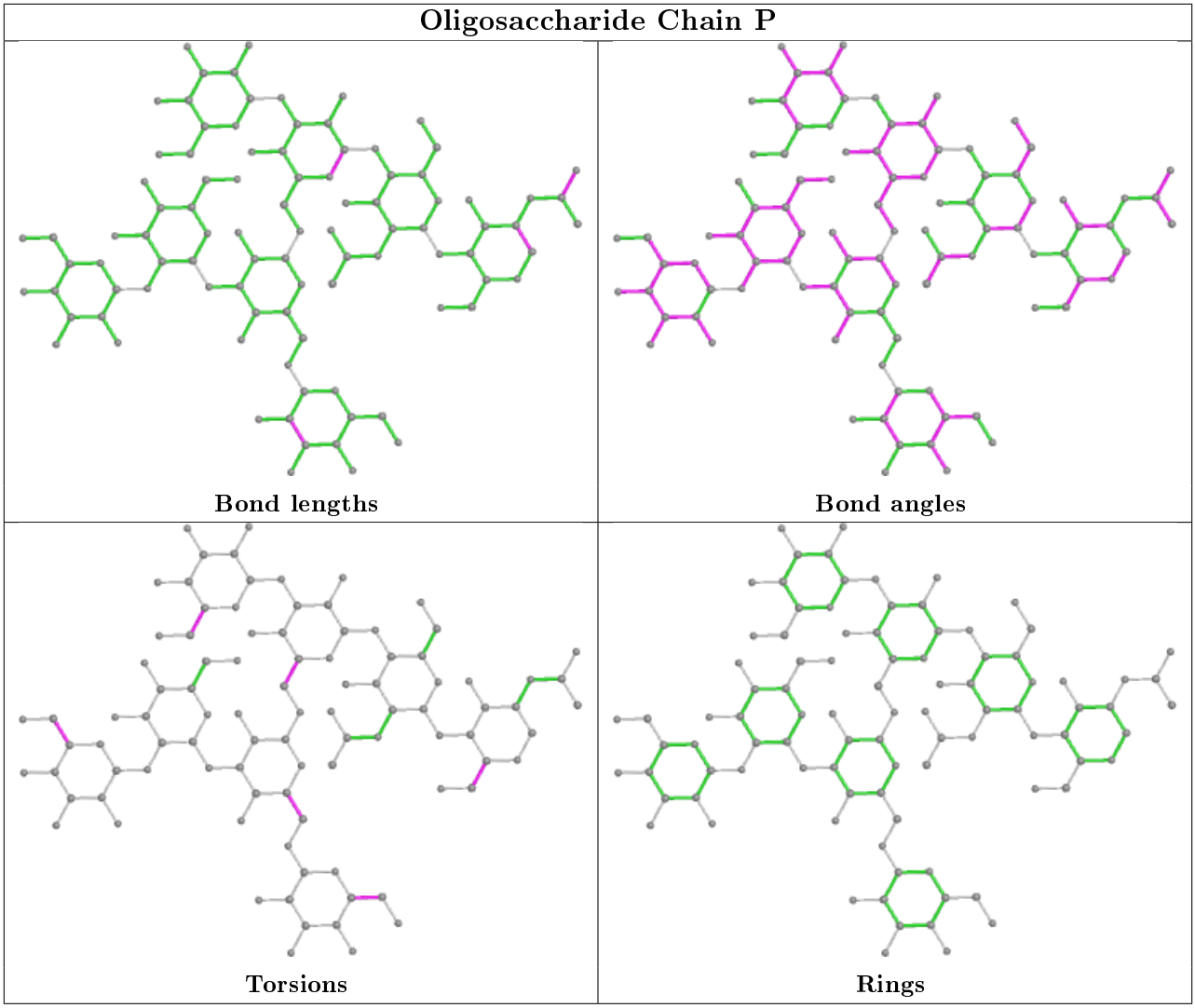
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
11	NAG	B	908	1	14,14,15	0.94	1 (7%)	17,19,21	2.89	8 (47%)
11	NAG	A	906	1	14,14,15	0.82	0	17,19,21	1.74	3 (17%)
15	IFM	A	944	-	9,10,10	3.61	5 (55%)	9,13,13	1.52	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MRD	B	948	-	7,7,7	1.13	1 (14%)	9,10,10	0.52	0
11	NAG	A	939	1	14,14,15	1.11	2 (14%)	17,19,21	2.12	9 (52%)
15	IFM	B	950	-	9,10,10	2.43	5 (55%)	9,13,13	1.37	2 (22%)
12	MRD	B	946	-	7,7,7	1.26	0	9,10,10	0.60	0
12	MRD	A	940	-	7,7,7	1.33	0	9,10,10	0.48	0
12	MRD	B	947	-	7,7,7	1.14	1 (14%)	9,10,10	1.45	3 (33%)
11	NAG	B	945	1	14,14,15	0.80	0	17,19,21	1.73	4 (23%)
13	MPD	A	942	-	7,7,7	0.73	0	9,10,10	1.06	0
12	MRD	A	941	-	7,7,7	1.38	0	9,10,10	1.31	2 (22%)
11	NAG	B	944	1	14,14,15	0.76	0	17,19,21	2.21	6 (35%)

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
11	NAG	B	908	1	-	6/6/23/26	0/1/1/1
11	NAG	A	906	1	-	0/6/23/26	0/1/1/1
15	IFM	A	944	-	-	0/2/16/16	0/1/1/1
12	MRD	B	948	-	-	2/5/5/5	-
11	NAG	A	939	1	-	0/6/23/26	0/1/1/1
15	IFM	B	950	-	-	0/2/16/16	0/1/1/1
12	MRD	B	946	-	-	4/5/5/5	-
12	MRD	A	940	-	-	1/5/5/5	-
12	MRD	B	947	-	-	2/5/5/5	-
11	NAG	B	945	1	-	1/6/23/26	0/1/1/1
13	MPD	A	942	-	-	2/5/5/5	-
12	MRD	A	941	-	-	2/5/5/5	-
11	NAG	B	944	1	-	4/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	944	IFM	C2-C3	6.95	1.59	1.52
15	A	944	IFM	C5-C4	5.60	1.60	1.53
15	B	950	IFM	C2-C3	4.90	1.57	1.52
15	A	944	IFM	C1-N	4.16	1.53	1.46
15	A	944	IFM	C6-C5	3.00	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	944	IFM	C2-N	2.85	1.51	1.46
15	B	950	IFM	C1-N	2.72	1.50	1.46
11	B	908	NAG	O5-C1	-2.64	1.39	1.43
12	B	947	MRD	C3-C2	-2.48	1.46	1.53
12	B	948	MRD	O2-C2	-2.43	1.38	1.44
11	A	939	NAG	O3-C3	-2.35	1.37	1.43
11	A	939	NAG	O4-C4	-2.10	1.38	1.43
15	B	950	IFM	C2-N	2.06	1.49	1.46
15	B	950	IFM	O4-C4	2.05	1.47	1.43
15	B	950	IFM	C6-C5	2.04	1.56	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	908	NAG	C8-C7-N2	6.00	126.26	116.10
11	B	908	NAG	C2-N2-C7	5.34	130.50	122.90
11	B	908	NAG	O5-C5-C6	4.89	114.86	107.20
11	B	944	NAG	C8-C7-N2	4.78	124.18	116.10
11	A	906	NAG	C1-C2-N2	4.69	118.50	110.49
11	B	944	NAG	O5-C1-C2	-4.25	104.58	111.29
11	B	908	NAG	O5-C1-C2	-3.65	105.53	111.29
11	A	939	NAG	C2-N2-C7	-3.64	117.72	122.90
11	B	944	NAG	O7-C7-C8	-3.47	115.61	122.06
15	A	944	IFM	C1-C5-C6	-3.16	105.20	110.66
11	B	945	NAG	C3-C4-C5	-3.12	104.67	110.24
11	A	939	NAG	C1-O5-C5	3.12	116.42	112.19
11	B	908	NAG	O3-C3-C4	-3.12	103.14	110.35
11	B	908	NAG	O7-C7-N2	-3.11	116.24	121.95
12	B	947	MRD	O4-C4-C3	-3.05	99.05	111.36
11	A	939	NAG	C8-C7-N2	2.98	121.14	116.10
15	B	950	IFM	C2-C3-C4	-2.81	107.02	110.33
11	B	945	NAG	O5-C5-C6	2.70	111.43	107.20
11	B	945	NAG	C1-O5-C5	-2.69	108.55	112.19
11	A	939	NAG	O5-C5-C4	-2.62	104.45	110.83
11	B	908	NAG	C1-C2-N2	-2.57	106.11	110.49
11	B	945	NAG	O5-C5-C4	-2.53	104.67	110.83
11	A	939	NAG	O5-C1-C2	2.53	115.28	111.29
11	A	939	NAG	O3-C3-C4	-2.50	104.58	110.35
12	A	941	MRD	O4-C4-C3	-2.49	101.33	111.36
11	B	944	NAG	O5-C5-C6	2.47	111.08	107.20
11	B	908	NAG	O7-C7-C8	-2.46	117.49	122.06
11	A	906	NAG	O5-C5-C6	2.40	110.96	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	939	NAG	O5-C5-C6	2.36	110.90	107.20
11	A	939	NAG	C4-C3-C2	-2.23	107.75	111.02
11	A	906	NAG	C2-N2-C7	-2.21	119.75	122.90
11	A	939	NAG	C3-C4-C5	-2.18	106.35	110.24
12	B	947	MRD	O2-C2-C1	2.15	114.98	108.08
15	B	950	IFM	O4-C4-C3	-2.13	105.92	109.99
12	A	941	MRD	CM-C2-C1	2.13	115.01	110.57
12	B	947	MRD	C1-C2-C3	-2.08	100.29	109.96
11	B	944	NAG	O4-C4-C3	2.03	115.05	110.35
11	B	944	NAG	O6-C6-C5	-2.03	104.32	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	948	MRD	C2-C3-C4-O4
12	B	948	MRD	C2-C3-C4-C5
11	B	908	NAG	C4-C5-C6-O6
11	B	908	NAG	O5-C5-C6-O6
11	B	908	NAG	C8-C7-N2-C2
11	B	908	NAG	O7-C7-N2-C2
11	B	944	NAG	C8-C7-N2-C2
11	B	944	NAG	O7-C7-N2-C2
11	B	944	NAG	C4-C5-C6-O6
12	B	946	MRD	O2-C2-C3-C4
13	A	942	MPD	O2-C2-C3-C4
12	B	947	MRD	C2-C3-C4-C5
12	B	946	MRD	C1-C2-C3-C4
12	B	946	MRD	CM-C2-C3-C4
12	B	947	MRD	C1-C2-C3-C4
11	B	945	NAG	O5-C5-C6-O6
11	B	908	NAG	C1-C2-N2-C7
11	B	944	NAG	O5-C5-C6-O6
11	B	908	NAG	C3-C2-N2-C7
12	A	940	MRD	C2-C3-C4-C5
13	A	942	MPD	C2-C3-C4-C5
12	A	941	MRD	C2-C3-C4-C5
12	B	946	MRD	C2-C3-C4-O4
12	A	941	MRD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	948	MRD	2	0
12	B	946	MRD	3	0
12	A	940	MRD	1	0
12	B	947	MRD	3	0
13	A	942	MPD	9	0
12	A	941	MRD	6	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	833/841 (99%)	-0.30	4 (0%) 91 92	10, 17, 30, 53	0
1	B	832/841 (98%)	-0.43	6 (0%) 87 88	9, 14, 26, 53	0
All	All	1665/1682 (98%)	-0.37	10 (0%) 89 90	9, 15, 29, 53	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	VAL	2.9
1	A	699	GLY	2.7
1	B	860	GLN	2.6
1	B	698	GLU	2.5
1	B	668	ASN	2.4
1	B	687	GLN	2.3
1	A	698	GLU	2.2
1	B	677	THR	2.1
1	A	860	GLN	2.0
1	B	676	ALA	2.0

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	4	11/12	0.49	0.30	60,74,81,87	0
9	MAN	K	4	11/12	0.61	0.29	53,60,64,65	0
3	BMA	G	3	11/12	0.74	0.32	41,51,62,72	0
6	MAN	O	7	11/12	0.75	0.32	58,63,67,71	0
10	MAN	P	8	11/12	0.76	0.25	59,67,77,86	0
10	MAN	P	7	11/12	0.81	0.27	42,50,57,62	0
6	MAN	H	7	11/12	0.81	0.33	52,62,64,67	0
3	BMA	L	3	11/12	0.81	0.36	56,73,91,97	0
7	MAN	I	7	11/12	0.82	0.24	50,55,60,72	0
2	MAN	C	5	11/12	0.84	0.18	41,50,56,62	0
10	BMA	P	3	11/12	0.84	0.17	35,38,46,58	0
7	MAN	I	6	11/12	0.86	0.25	40,51,55,66	0
3	BMA	D	3	11/12	0.86	0.22	34,42,51,57	0
3	NAG	G	2	14/15	0.86	0.23	36,43,52,56	0
2	BMA	C	3	11/12	0.87	0.18	33,46,53,57	0
10	MAN	P	6	11/12	0.90	0.28	47,52,60,63	0
7	BMA	I	3	11/12	0.90	0.19	30,37,47,51	0
10	MAN	P	4	11/12	0.91	0.17	27,31,39,42	0
3	BMA	N	3	11/12	0.91	0.21	35,42,55,67	0
6	BMA	O	3	11/12	0.91	0.17	24,28,34,45	0
5	MAN	M	6	11/12	0.92	0.13	25,28,34,35	0
7	MAN	I	4	11/12	0.93	0.10	22,29,39,50	0
6	BMA	H	3	11/12	0.93	0.18	21,25,32,43	0
9	BMA	K	3	11/12	0.93	0.18	32,38,48,49	0
5	MAN	F	6	11/12	0.93	0.16	27,29,34,40	0
5	MAN	M	10	11/12	0.93	0.12	27,36,41,43	0
10	NAG	P	2	14/15	0.94	0.11	24,29,35,36	0
7	NAG	I	2	14/15	0.94	0.13	22,27,32,37	0
8	MAN	J	7	11/12	0.94	0.13	22,29,34,34	0
6	NAG	O	2	14/15	0.94	0.12	18,23,32,33	0
5	MAN	F	10	11/12	0.94	0.16	31,37,44,57	0
6	NAG	H	2	14/15	0.95	0.12	17,23,28,34	0
3	NAG	L	2	14/15	0.95	0.10	18,23,42,43	0
3	NAG	D	2	14/15	0.95	0.15	23,27,34,37	0
3	NAG	N	2	14/15	0.95	0.15	24,29,41,41	0
6	MAN	O	4	11/12	0.95	0.15	23,28,38,43	0
7	MAN	I	5	11/12	0.95	0.11	24,31,40,43	0
2	NAG	C	2	14/15	0.95	0.09	20,28,38,42	0
9	NAG	K	1	14/15	0.95	0.09	16,18,20,21	0
6	MAN	H	6	11/12	0.95	0.15	18,22,33,38	0
6	NAG	O	1	14/15	0.95	0.10	16,20,39,43	0
6	NAG	H	1	14/15	0.96	0.09	15,18,39,42	0
8	MAN	J	6	11/12	0.96	0.13	22,26,29,37	0

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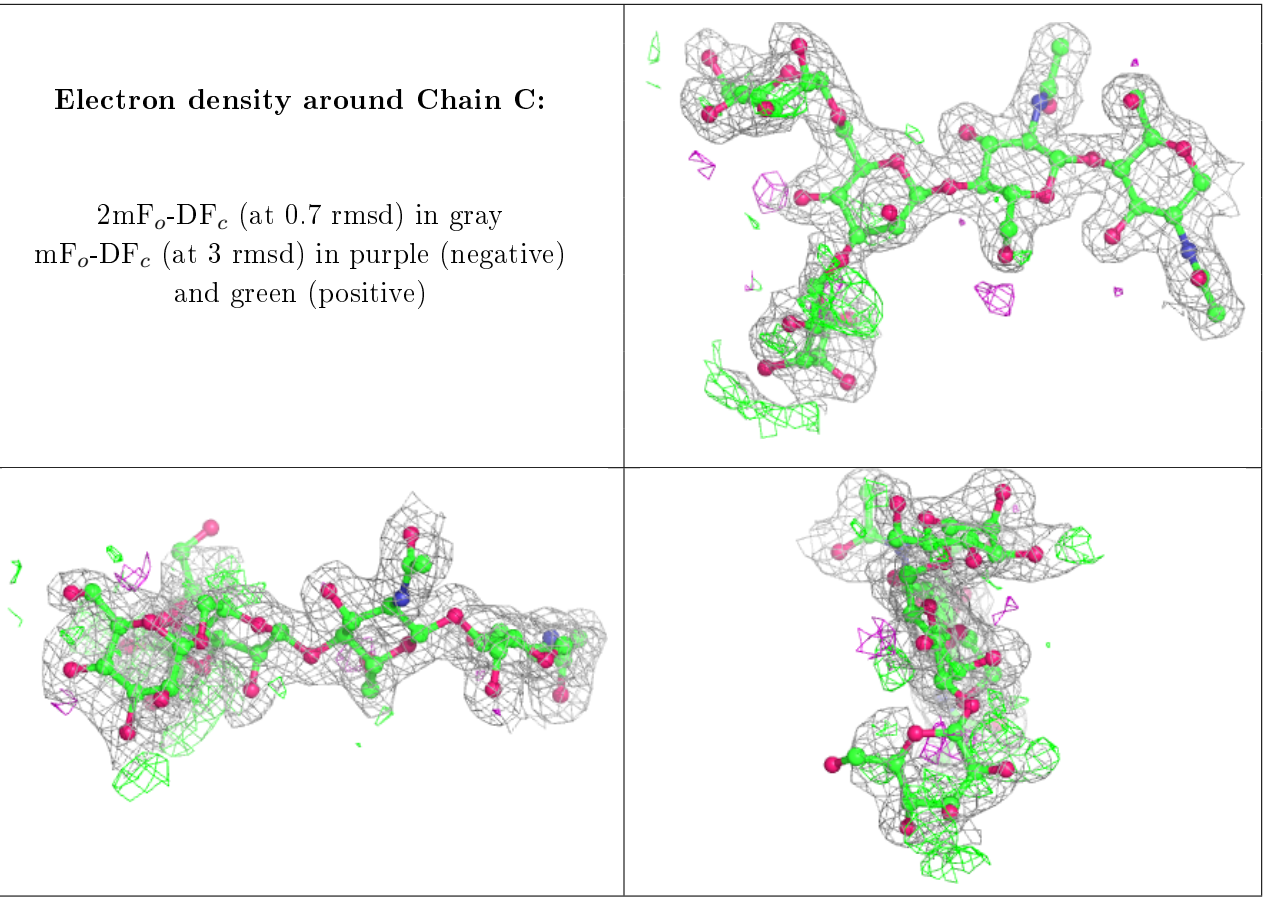
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	F	5	11/12	0.96	0.08	20,24,30,34	0
3	NAG	N	1	14/15	0.96	0.09	18,23,32,33	0
6	MAN	H	5	11/12	0.96	0.14	19,22,34,37	0
10	MAN	P	5	11/12	0.96	0.16	24,31,35,42	0
5	NAG	F	1	14/15	0.96	0.08	20,23,26,29	0
9	NAG	K	2	14/15	0.96	0.10	17,23,31,31	0
6	MAN	H	4	11/12	0.96	0.15	24,26,38,39	0
3	NAG	G	1	14/15	0.96	0.09	19,25,35,38	0
4	NAG	E	2	14/15	0.96	0.09	25,30,47,49	0
5	MAN	F	7	11/12	0.96	0.07	16,18,21,22	0
6	MAN	O	6	11/12	0.97	0.13	18,22,29,32	0
6	MAN	O	5	11/12	0.97	0.13	21,23,29,34	0
3	NAG	D	1	14/15	0.97	0.09	17,20,22,24	0
5	MAN	M	8	11/12	0.97	0.08	16,17,19,21	0
8	MAN	J	4	11/12	0.97	0.16	24,31,40,41	0
5	MAN	M	9	11/12	0.97	0.06	18,20,24,26	0
5	NAG	F	2	14/15	0.97	0.07	17,19,20,22	0
5	MAN	F	9	11/12	0.97	0.11	24,25,32,33	0
5	MAN	F	8	11/12	0.97	0.09	18,20,21,22	0
2	NAG	C	1	14/15	0.97	0.07	16,19,21,23	0
5	MAN	M	5	11/12	0.97	0.08	18,21,22,33	0
5	MAN	F	4	11/12	0.97	0.06	17,20,22,23	0
5	BMA	F	3	11/12	0.97	0.07	19,21,26,27	0
8	MAN	J	5	11/12	0.97	0.14	23,30,37,47	0
8	BMA	J	3	11/12	0.97	0.10	19,21,22,24	0
5	NAG	M	2	14/15	0.97	0.07	12,15,15,16	0
7	NAG	I	1	14/15	0.97	0.07	17,20,23,24	0
5	MAN	M	7	11/12	0.98	0.07	13,14,16,16	0
3	NAG	L	1	14/15	0.98	0.06	14,16,19,19	0
4	NAG	E	1	14/15	0.98	0.07	16,19,23,25	0
5	BMA	M	3	11/12	0.98	0.06	14,16,18,18	0
10	NAG	P	1	14/15	0.98	0.07	15,18,21,22	0
8	NAG	J	2	14/15	0.98	0.06	14,16,20,28	0
5	NAG	M	1	14/15	0.98	0.07	12,14,19,22	0
8	NAG	J	1	14/15	0.98	0.06	12,14,17,18	0
5	MAN	M	4	11/12	0.99	0.06	14,15,15,16	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.

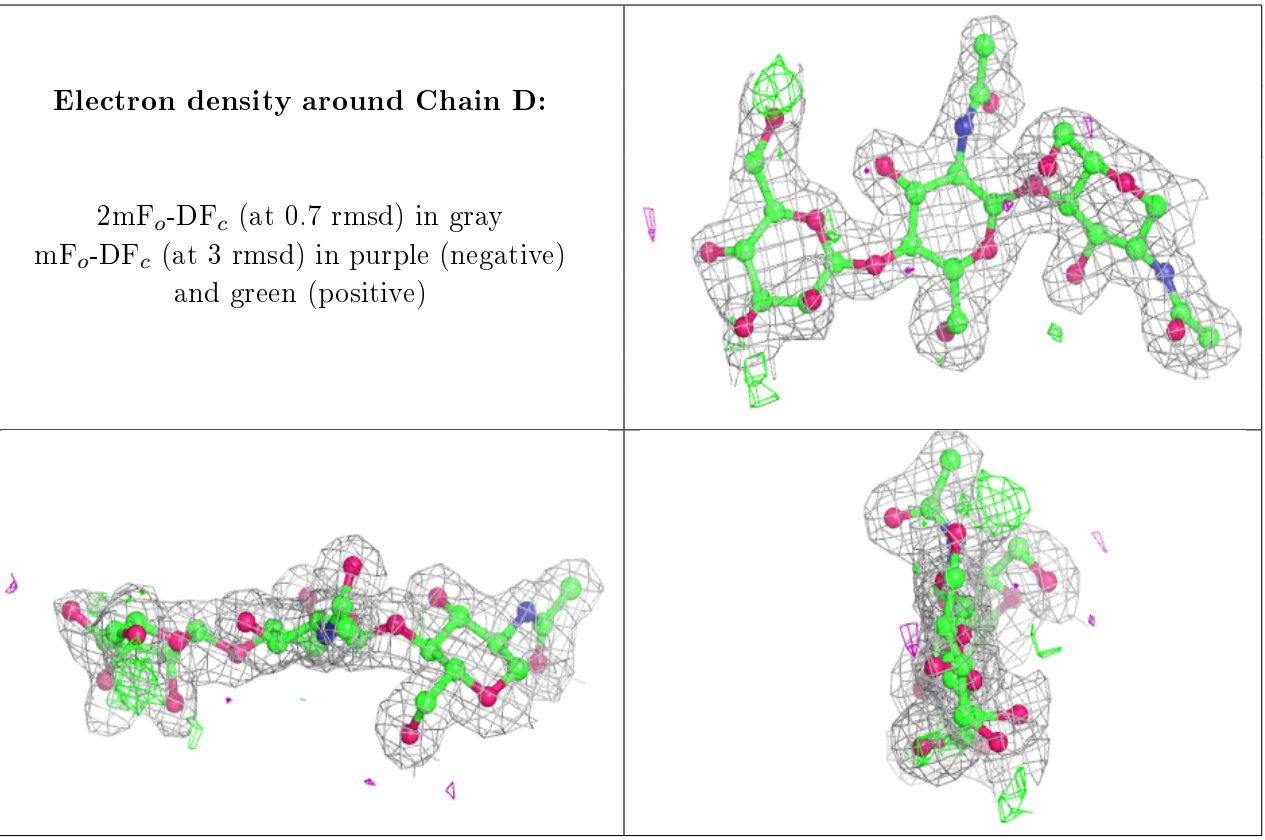
Electron density around Chain C:

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



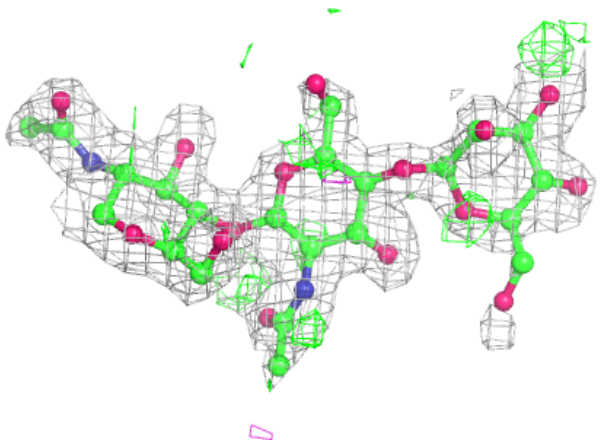
Electron density around Chain D:

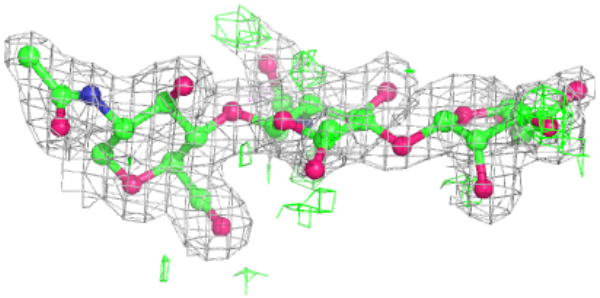
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

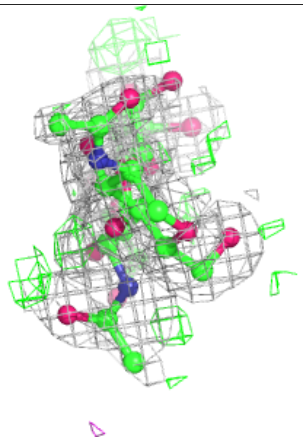


Electron density around Chain G:

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

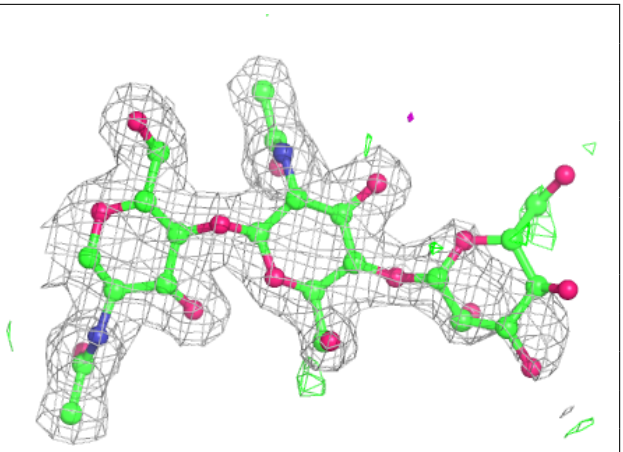


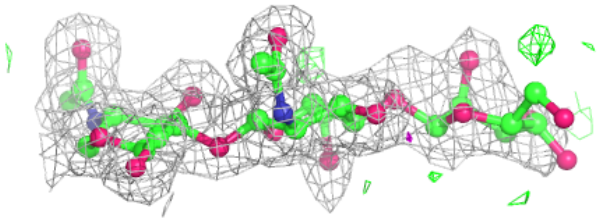


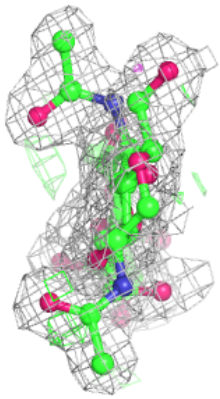


Electron density around Chain L:

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

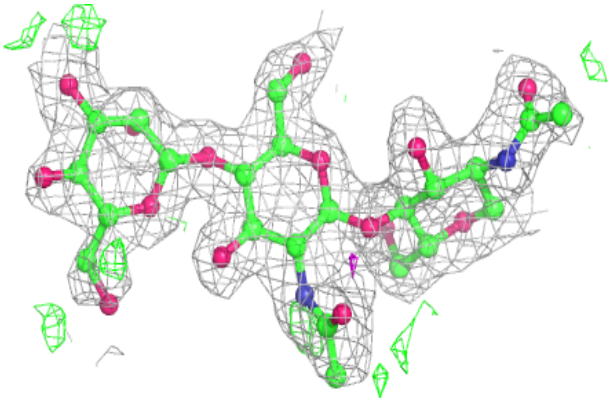


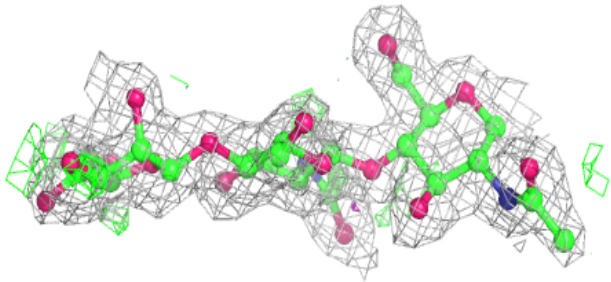


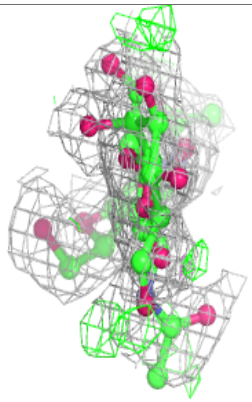


Electron density around Chain N:

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

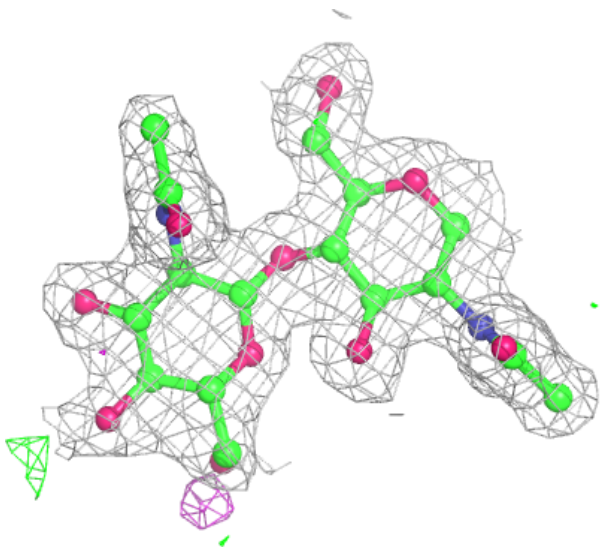


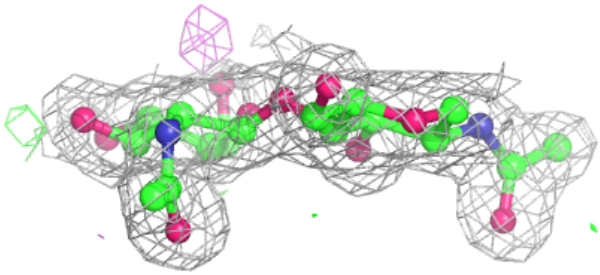


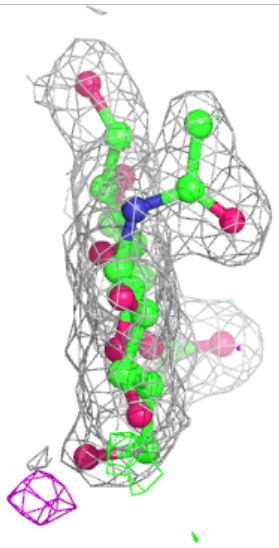


Electron density around Chain E:

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

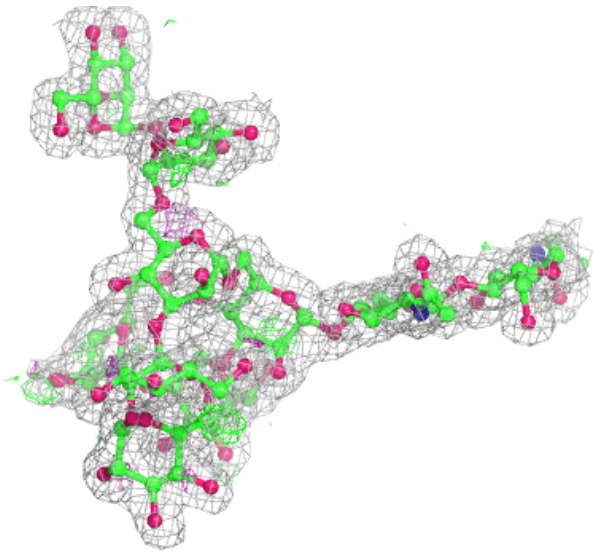


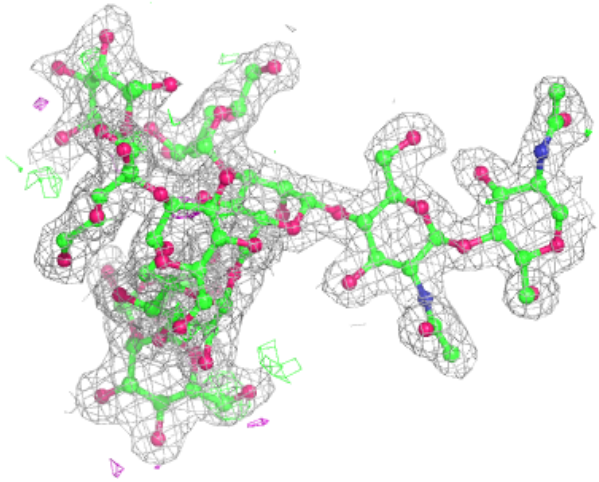


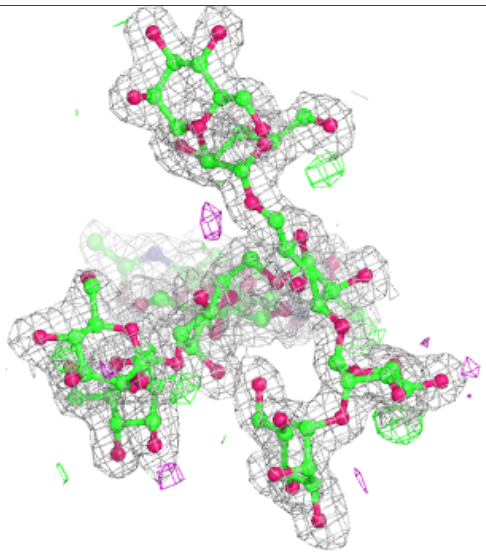


Electron density around Chain F:

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

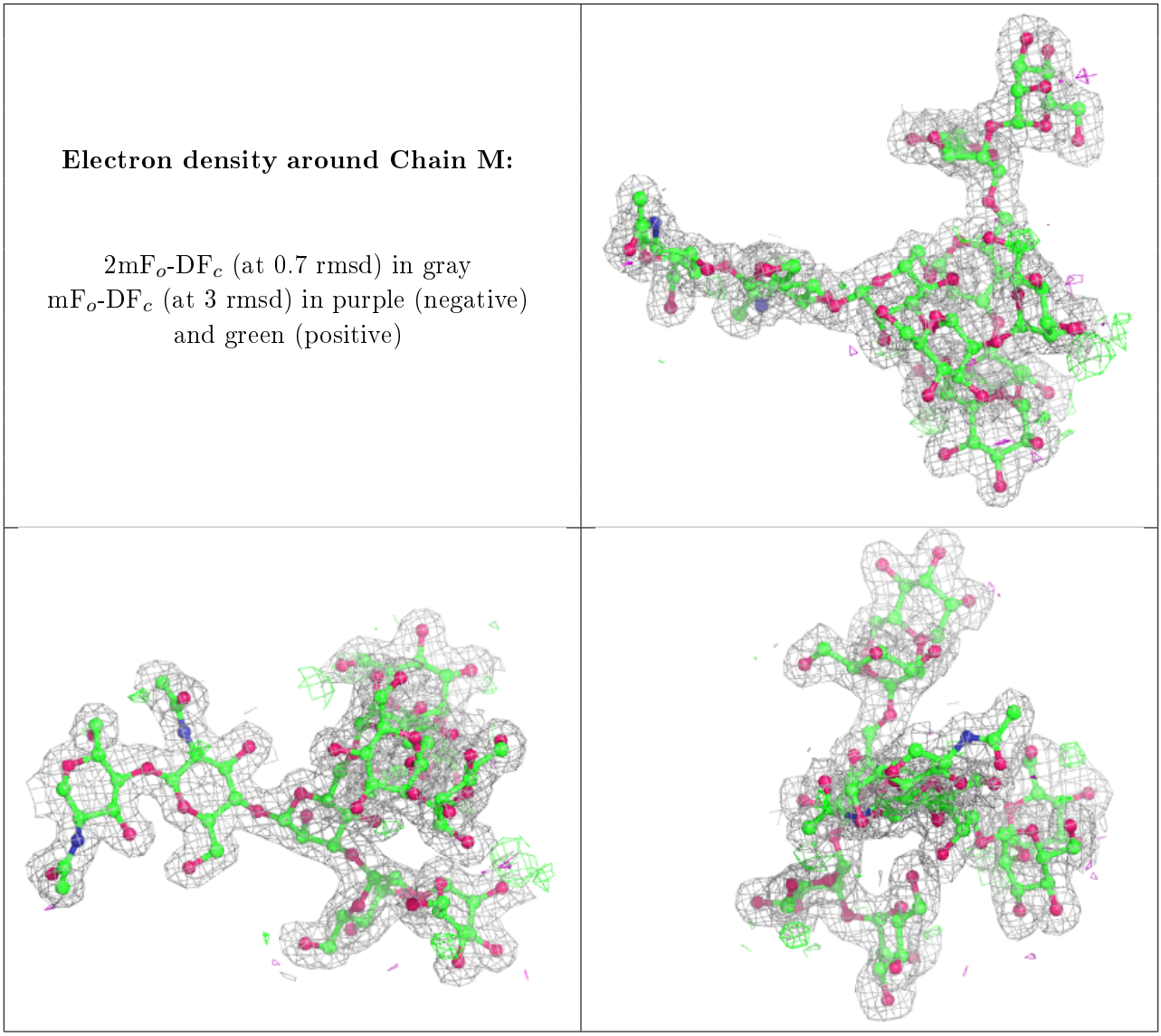






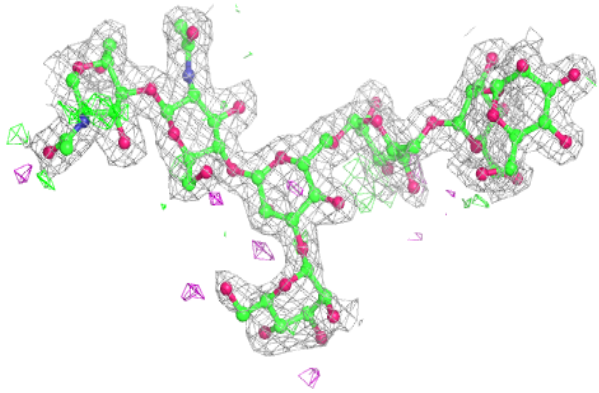
Electron density around Chain M:

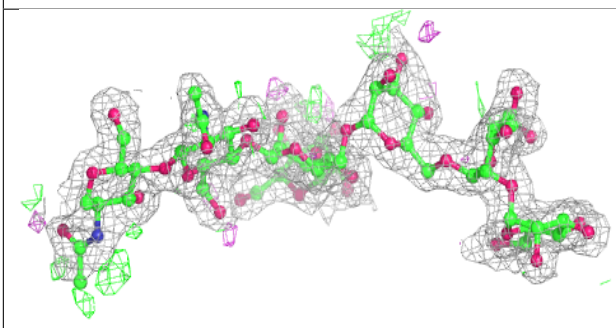
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

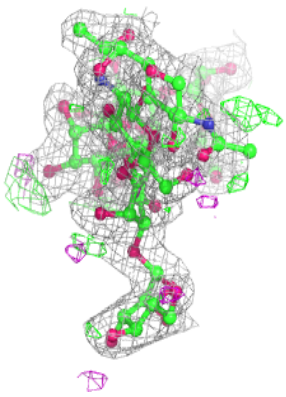


Electron density around Chain H:

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

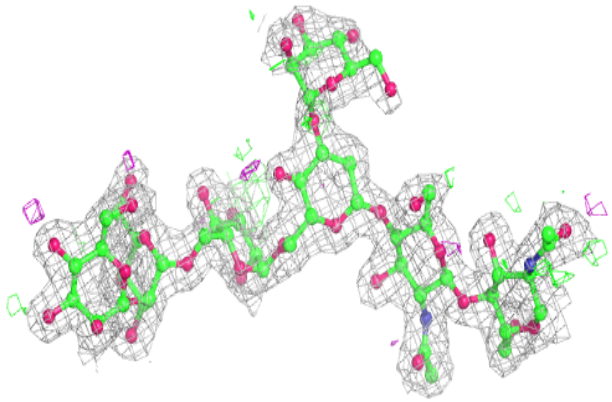


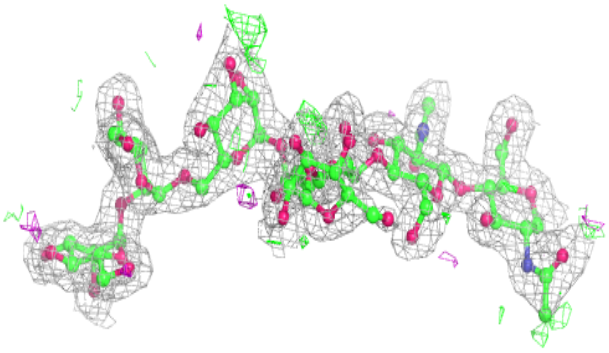


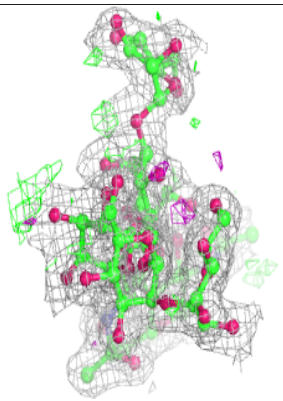


Electron density around Chain O:

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

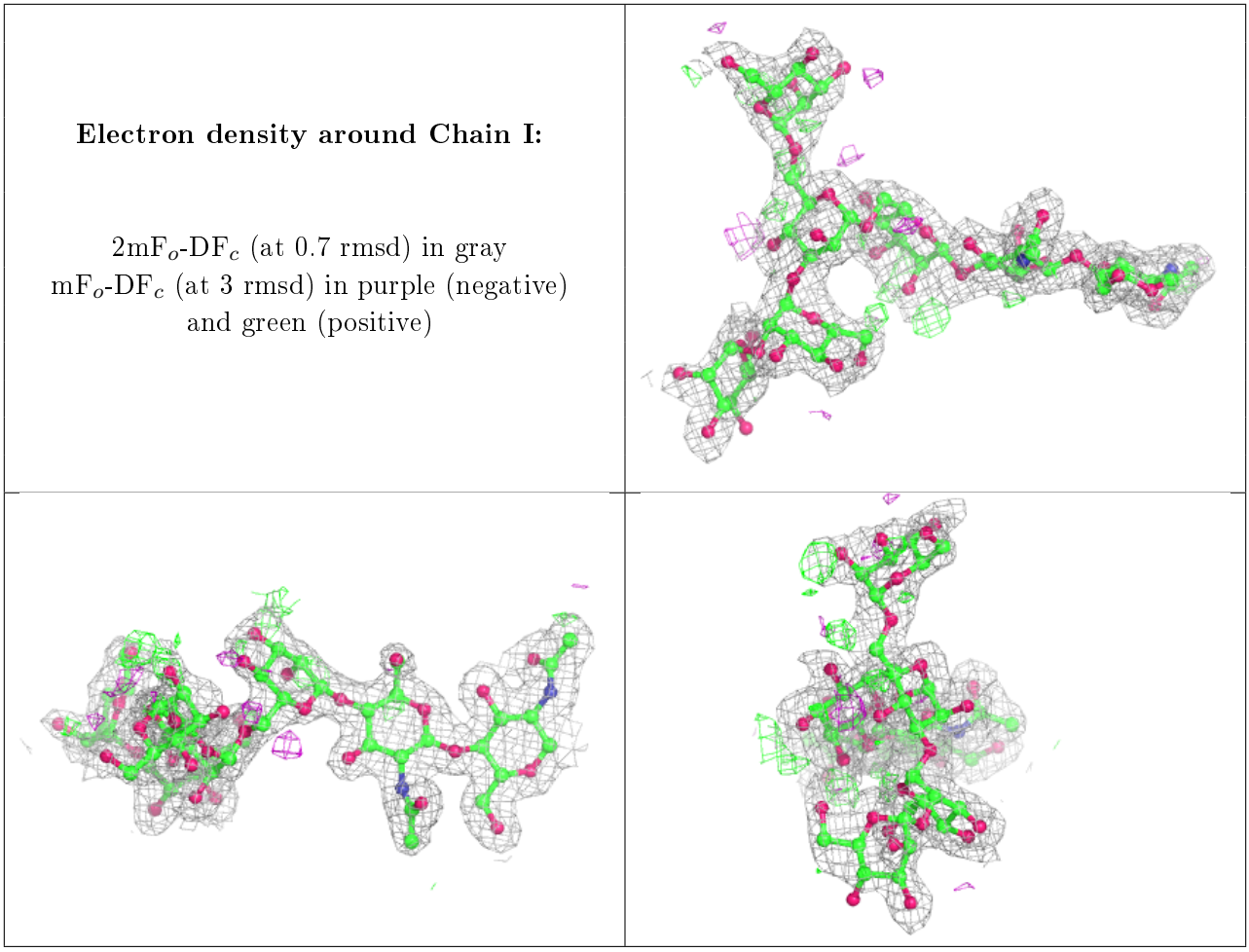






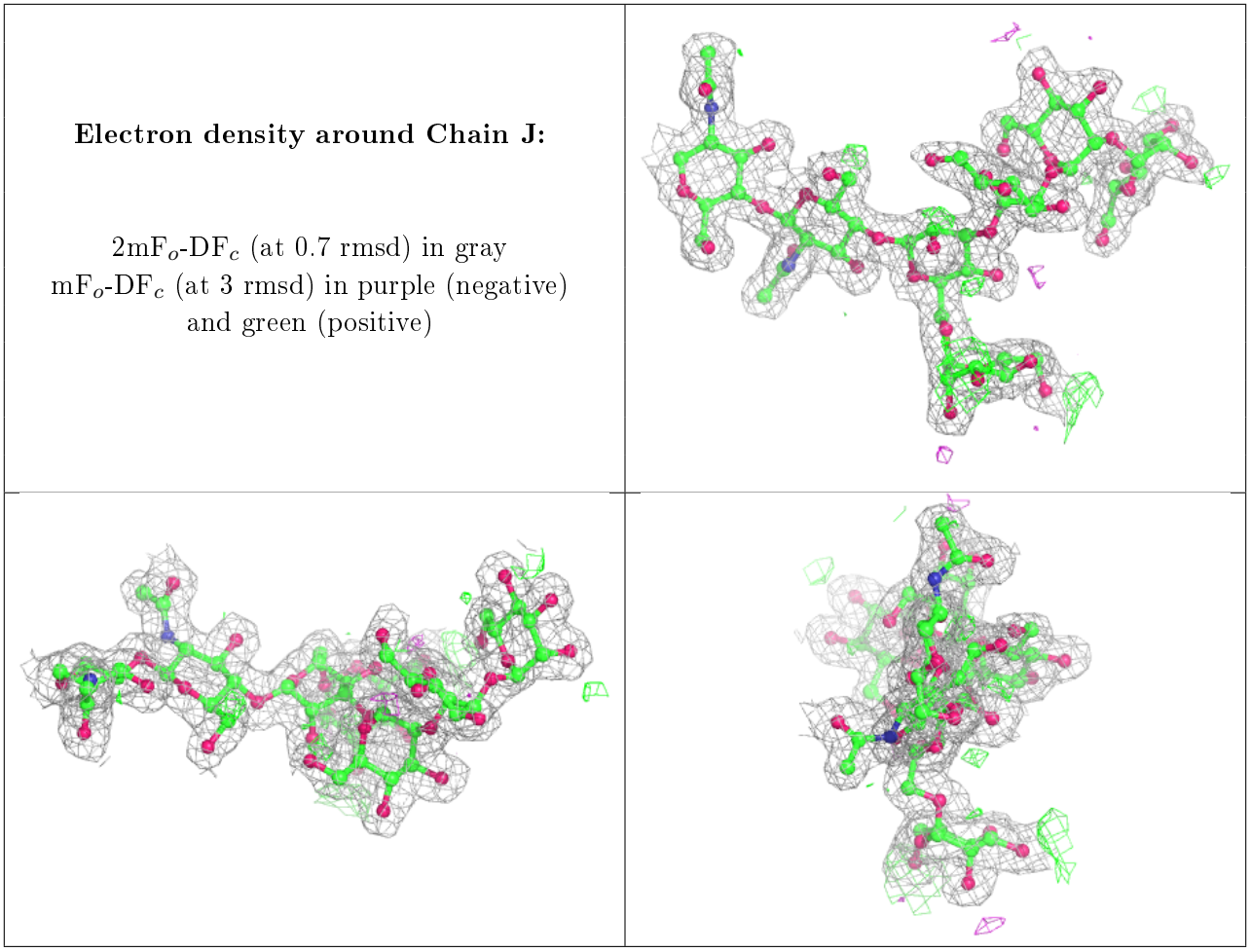
Electron density around Chain I:

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



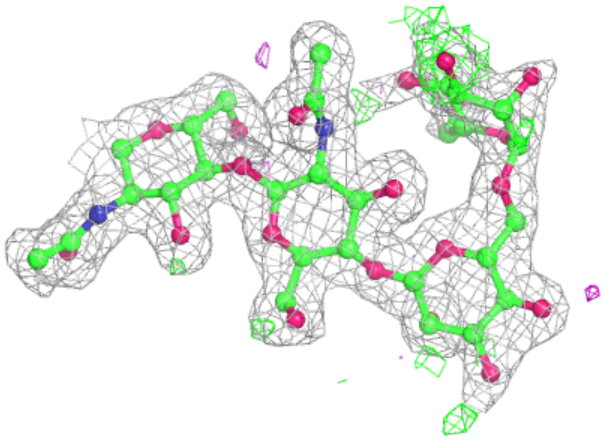
Electron density around Chain J:

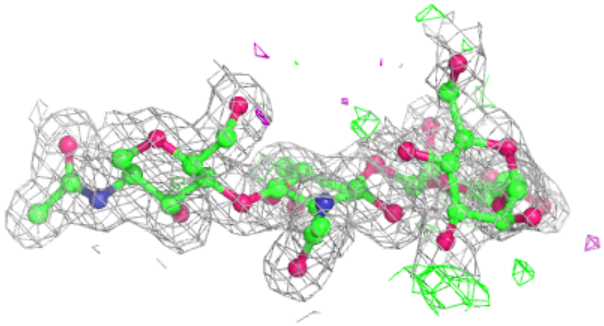
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

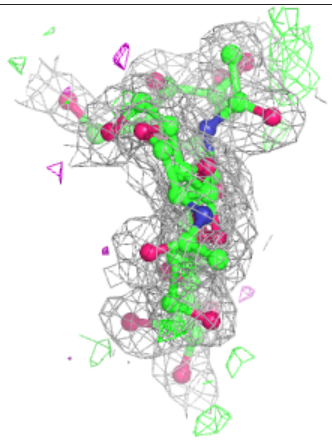


Electron density around Chain K:

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

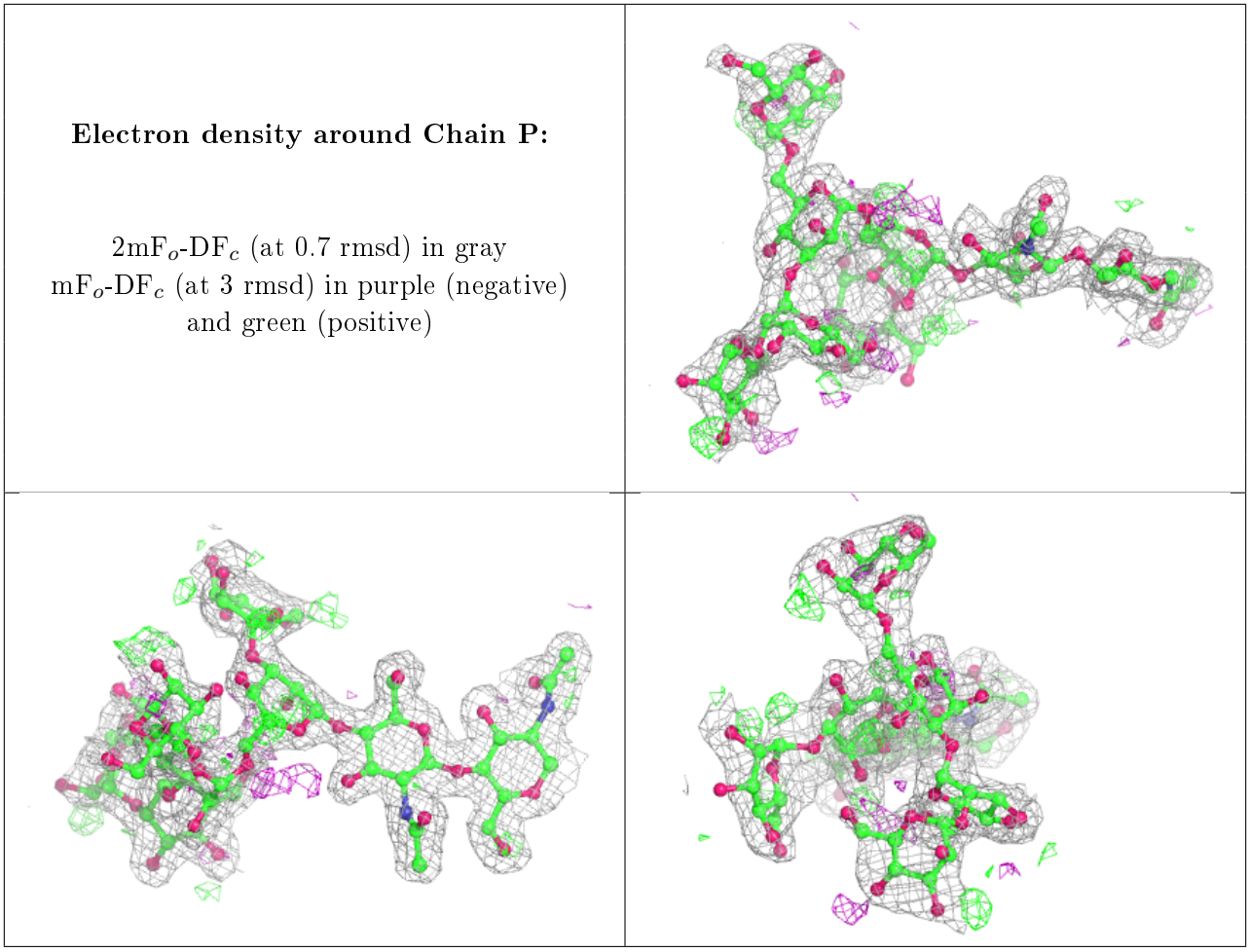






Electron density around Chain P:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
13	MPD	A	942	8/8	0.84	0.21	37,39,45,48	0
12	MRD	A	941	8/8	0.85	0.17	18,30,41,43	0
11	NAG	A	906	14/15	0.86	0.36	42,52,57,58	0
11	NAG	B	908	14/15	0.87	0.32	39,48,52,53	0
12	MRD	B	946	8/8	0.87	0.20	19,32,40,43	0
11	NAG	B	944	14/15	0.91	0.25	36,50,55,59	0
12	MRD	B	948	8/8	0.94	0.15	32,41,42,43	0
12	MRD	B	947	8/8	0.95	0.11	20,25,37,37	0
11	NAG	A	939	14/15	0.95	0.15	35,38,42,46	0
14	NA	A	943	1/1	0.96	0.17	26,26,26,26	0
14	NA	B	949	1/1	0.97	0.22	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MRD	A	940	8/8	0.97	0.06	20,22,25,26	0
11	NAG	B	945	14/15	0.98	0.18	26,29,33,34	0
15	IFM	A	944	10/10	0.98	0.15	12,13,14,15	0
15	IFM	B	950	10/10	0.99	0.12	10,11,11,11	0

6.5 Other polymers

There are no such residues in this entry.