Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 11:16 AM EDT

PDB ID	:	7KMD
Title	:	Crystal structure of a HIV-1 clade C isolate Du172.17 HR1.R4.664 Env trimer in complex with human Fabs PGT124 and 35O22
Authors	:	Kumar, S.; Wilson, I.A.
Deposited on	:	2020-11-02
Resolution	:	3.39 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:

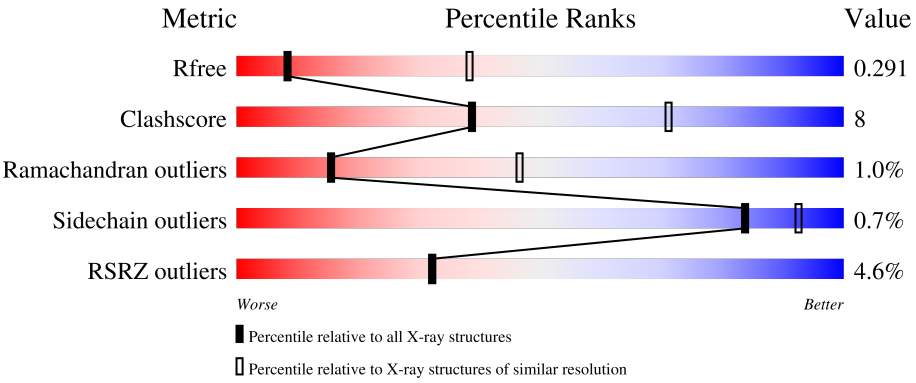
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	243	7% 84% 14%
2	E	216	% 86% 12%
3	G	480	3% 71% 22% 7%
4	T	140	% 76% 18%
5	L	214	5% 87% 11%

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Mol	Chain	Length	Quality of chain
6	H	236	9% 73% 21% 5%
7	B	9	11% 78% 11%
8	C	2	50% 50%
8	F	2	100%
8	N	2	50% 50%
9	D	3	100%
9	M	3	67% 33%
9	O	3	67% 33%
9	P	3	100%
10	I	9	22% 67% 11%
11	J	5	60% 40%
12	K	6	83% 17%

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	MAN	I	4	X	-	-	-
10	MAN	I	7	X	-	-	-
7	BMA	B	3	X	-	-	-
9	BMA	P	3	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 12033 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 35O22 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 2 is a protein called 35O22 Light chain.

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

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	447	Total	C	N	O	S	0	0	0
			3515	2213	613	662	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q202J8
G	509	ARG	-	expression tag	UNP Q202J8
G	510	ARG	-	expression tag	UNP Q202J8
G	511	ARG	-	expression tag	UNP Q202J8
G	512	ARG	-	expression tag	UNP Q202J8
G	513	ARG	-	expression tag	UNP Q202J8

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	134	Total	C	N	O	S	0	0	0
			1064	677	179	201	7			

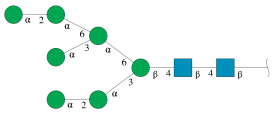
- Molecule 5 is a protein called 124 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	210	1595	1005	270	315	5	0	0	0

- Molecule 6 is a protein called 124 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	225	1716	1091	286	334	5	2	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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.

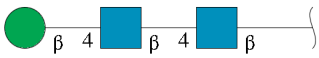


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	B	9	105	58	2	45	0	0	0

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

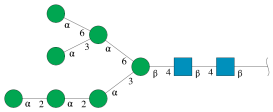
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	2	28	16	2	10	0	0	0
8	F	2	28	16	2	10	0	0	0
8	N	2	28	16	2	10	0	0	0

- Molecule 9 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.



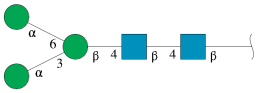
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	D	3	Total C N O 39 22 2 15	0	0	0
9	M	3	Total C N O 39 22 2 15	0	0	0
9	O	3	Total C N O 39 22 2 15	0	0	0
9	P	3	Total C N O 39 22 2 15	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[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
10	I	9	Total C N O 105 58 2 45	0	0	0

- Molecule 11 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.

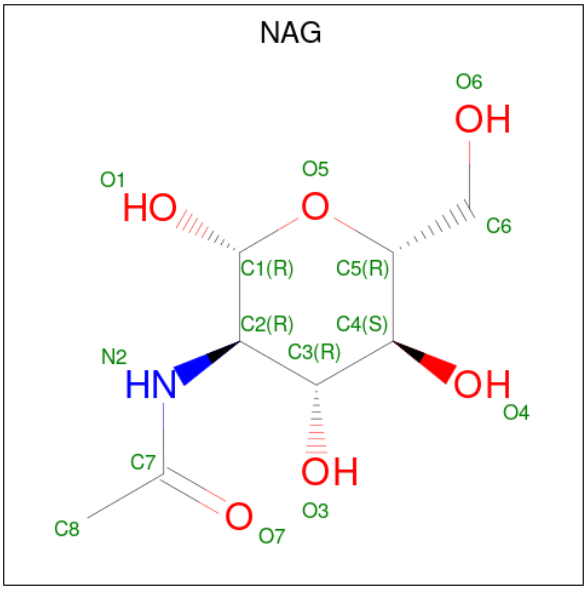


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	J	5	Total C N O 61 34 2 25	0	0	0

- Molecule 12 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-(6-8)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	K	6	Total C N O 78 44 4 30	0	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

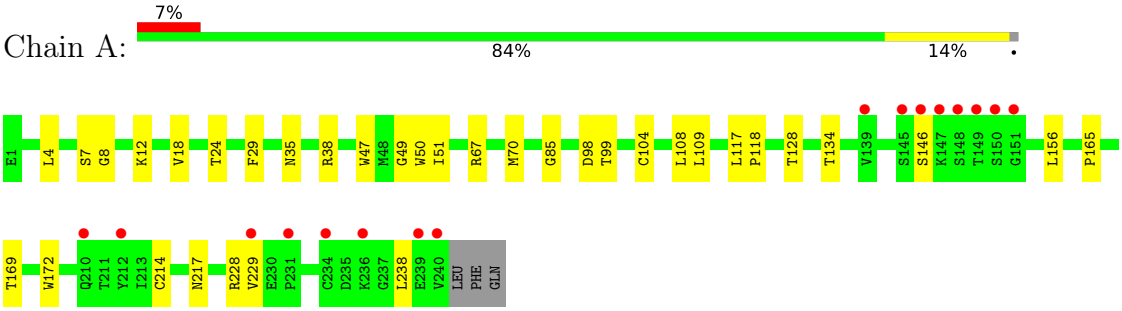


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	T	1	Total C N O 14 8 1 5	0	0
13	T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

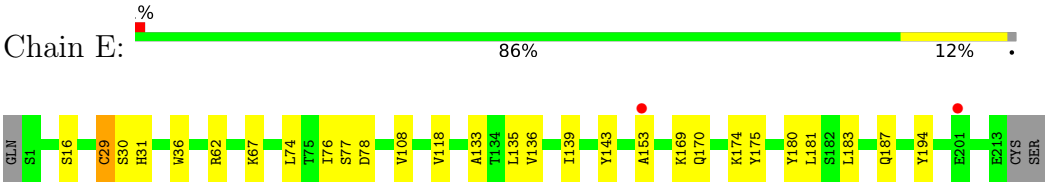
3 Residue-property plots (i)

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.

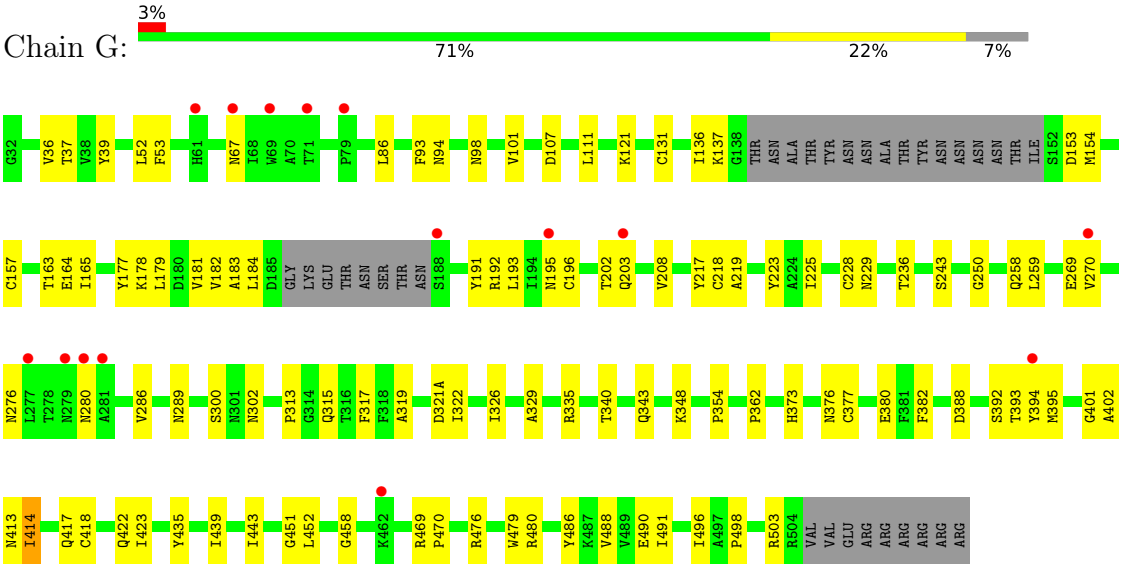
• Molecule 1: 35O22 Heavy chain



• Molecule 2: 35O22 Light chain

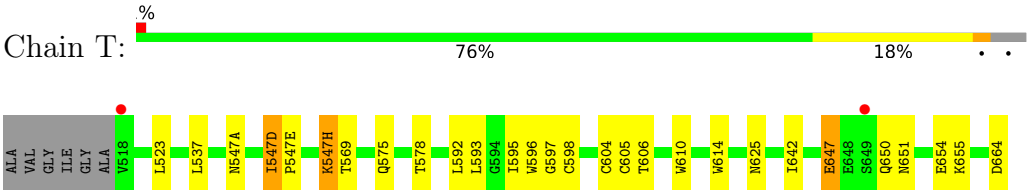


• Molecule 3: Envelope glycoprotein gp120



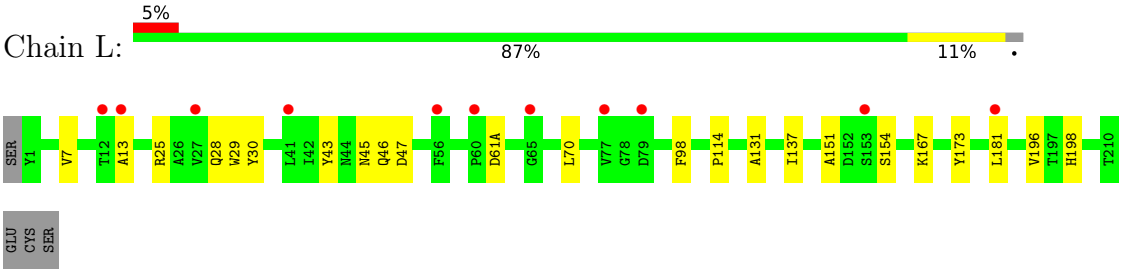
• Molecule 4: Envelope glycoprotein gp41

Chain T:



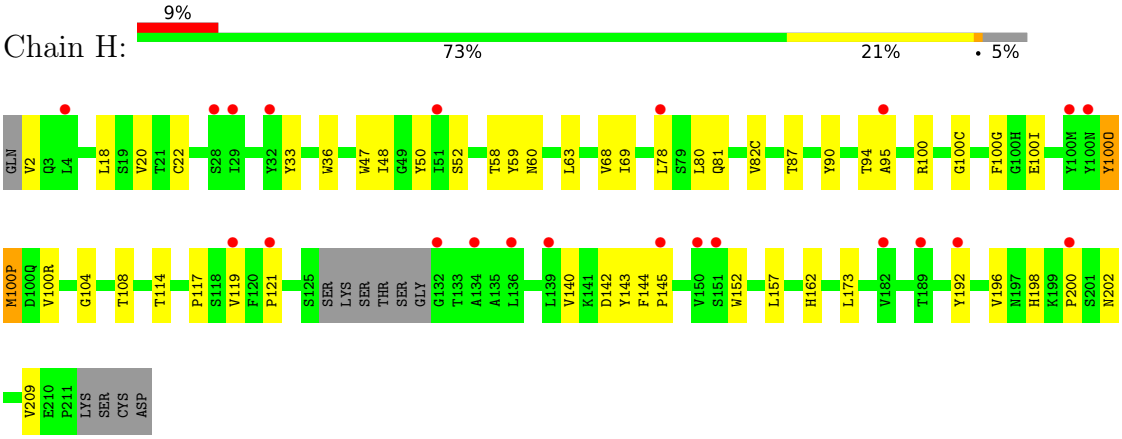
• Molecule 5: 124 Light chain

Chain L:



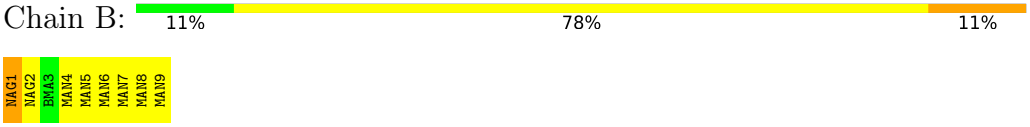
• Molecule 6: 124 Heavy chain

Chain H:



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 B:



• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

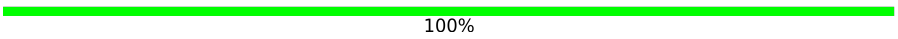
Chain F:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

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

Chain D:



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

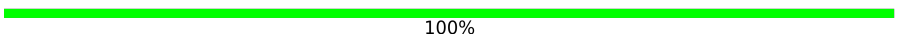
Chain M:

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

Chain O:

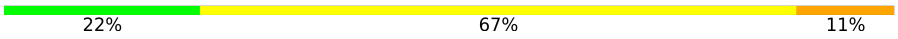
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 11: 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 12: 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-(6-8)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	127.02Å 127.02Å 316.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.53 – 3.39 49.53 – 3.39	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.53-3.39) 95.8 (49.53-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.242 , 0.292 0.242 , 0.291	Depositor DCC
R_{free} test set	1917 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	93.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12033	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: NAG, MAN, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/1860	0.46	0/2533
2	E	0.25	0/1659	0.44	0/2269
3	G	0.24	0/3587	0.44	0/4859
4	T	0.23	0/1087	0.43	0/1475
5	L	0.24	0/1638	0.43	0/2238
6	H	0.27	0/1759	0.75	3/2402 (0.1%)
All	All	0.25	0/11590	0.50	3/15776 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	100(O)	TYR	O-C-N	-20.98	89.13	122.70
6	H	100(O)	TYR	CA-C-N	14.73	149.61	117.20
6	H	100(O)	TYR	C-N-CA	13.36	155.11	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	1784	21	0
2	E	1615	0	1545	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3515	0	3468	69	0
4	T	1064	0	1038	22	0
5	L	1595	0	1544	18	0
6	H	1716	0	1683	49	0
7	B	105	0	88	2	0
8	C	28	0	25	1	0
8	F	28	0	25	0	0
8	N	28	0	25	1	0
9	D	39	0	34	0	0
9	M	39	0	34	2	0
9	O	39	0	34	2	0
9	P	39	0	34	0	0
10	I	105	0	88	2	0
11	J	61	0	52	0	0
12	K	78	0	66	0	0
13	G	98	0	91	1	0
13	T	28	0	26	0	0
All	All	12033	0	11684	178	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 8.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:30:TYR:OH	6:H:100(P):MET:CE	2.02	1.07
6:H:94:THR:HB	6:H:100(R):VAL:HG22	1.36	1.03
6:H:94:THR:HB	6:H:100(R):VAL:CG2	1.87	1.02
6:H:100(P):MET:N	6:H:100(P):MET:HE2	1.78	0.97
6:H:94:THR:CB	6:H:100(R):VAL:CG2	2.46	0.92
5:L:30:TYR:OH	6:H:100(P):MET:HE1	1.74	0.87
4:T:547(D):ILE:HB	4:T:547(E):PRO:HD3	1.55	0.87
6:H:94:THR:O	6:H:100(P):MET:HA	1.81	0.81
6:H:94:THR:OG1	6:H:100(R):VAL:CG2	2.34	0.76
2:E:135:LEU:HD12	2:E:181:LEU:HD23	1.76	0.65
3:G:154:MET:HG3	3:G:177:TYR:HA	1.79	0.65
1:A:146:SER:HB2	1:A:238:LEU:HB2	1.79	0.64
3:G:329:ALA:HB3	3:G:418:CYS:O	1.97	0.64
6:H:100(O):TYR:C	6:H:100(P):MET:HE2	2.18	0.64
6:H:2:VAL:HG22	6:H:100(R):VAL:HG11	1.80	0.64
6:H:94:THR:OG1	6:H:100(R):VAL:HG21	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:36:VAL:HG12	4:T:610:TRP:HE3	1.64	0.63
6:H:94:THR:O	6:H:100(P):MET:CA	2.47	0.63
6:H:119:VAL:HG11	6:H:196:VAL:HG21	1.79	0.63
3:G:313:PRO:HD2	3:G:315:GLN:HE22	1.64	0.61
2:E:16:SER:HA	2:E:76:ILE:O	2.01	0.61
2:E:108:VAL:O	2:E:143:TYR:OH	2.19	0.61
6:H:87:THR:HG23	6:H:108:THR:HA	1.83	0.61
3:G:300:SER:O	3:G:302:ASN:ND2	2.32	0.60
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.36	0.60
5:L:114:PRO:HG3	5:L:198:HIS:HB3	1.84	0.59
1:A:67:ARG:NH2	1:A:98:ASP:OD2	2.34	0.59
3:G:219:ALA:HB2	3:G:225:ILE:HG13	1.85	0.59
2:E:133:ALA:HB3	2:E:183:LEU:O	2.03	0.59
4:T:547(H):LYS:HG3	4:T:569:THR:HG23	1.86	0.58
5:L:30:TYR:OH	6:H:100(P):MET:HE3	2.01	0.58
5:L:131:ALA:HB3	5:L:181:LEU:O	2.03	0.58
3:G:439:ILE:HB	3:G:443:ILE:HD11	1.86	0.58
3:G:322:ILE:HG21	3:G:326:ILE:HG22	1.85	0.58
1:A:99:THR:HG23	1:A:128:THR:HA	1.85	0.57
3:G:131:CYS:HA	3:G:157:CYS:HA	1.86	0.57
6:H:100(P):MET:HE2	6:H:100(P):MET:H	1.69	0.57
3:G:335:ARG:HH11	3:G:414:ILE:HD11	1.69	0.56
3:G:362:PRO:O	3:G:469:ARG:NH1	2.37	0.56
5:L:61(A):ASP:OD2	6:H:100:ARG:NH2	2.38	0.56
6:H:18:LEU:HB2	6:H:82(C):VAL:HG11	1.88	0.56
6:H:94:THR:OG1	6:H:100(R):VAL:HG23	2.05	0.56
6:H:94:THR:CB	6:H:100(R):VAL:HG23	2.33	0.55
2:E:136:VAL:HG13	2:E:180:TYR:HE1	1.72	0.55
4:T:547(D):ILE:HB	4:T:547(E):PRO:CD	2.34	0.55
1:A:228:ARG:NH1	1:A:229:VAL:O	2.41	0.54
3:G:37:THR:HG22	4:T:605:CYS:HA	1.89	0.54
6:H:117:PRO:HB3	6:H:143:TYR:HB3	1.89	0.54
2:E:29:CYS:O	2:E:31:HIS:N	2.41	0.54
5:L:28:GLN:HG3	5:L:43:TYR:HA	1.89	0.54
3:G:392:SER:O	3:G:394:TYR:N	2.40	0.54
3:G:195:ASN:ND2	3:G:423:ILE:HD13	2.22	0.53
1:A:38:ARG:NH1	1:A:98:ASP:OD1	2.38	0.53
2:E:169:LYS:HA	2:E:175:TYR:HD1	1.74	0.53
3:G:382:PHE:HB3	3:G:418:CYS:SG	2.49	0.53
7:B:1:NAG:H3	7:B:1:NAG:H83	1.89	0.53
3:G:321(A):ASP:HB2	8:C:1:NAG:H83	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:121:LYS:HA	3:G:202:THR:HA	1.92	0.52
1:A:156:LEU:HB2	1:A:229:VAL:HG11	1.92	0.52
9:O:1:NAG:H83	9:O:1:NAG:H3	1.91	0.52
3:G:163:THR:OG1	3:G:164:GLU:N	2.41	0.52
3:G:259:LEU:HB2	3:G:373:HIS:CE1	2.45	0.52
6:H:22:CYS:HB3	6:H:78:LEU:HB3	1.92	0.51
5:L:98:PHE:HE2	6:H:47:TRP:HB2	1.74	0.51
2:E:118:VAL:HG22	2:E:139:ILE:HG23	1.91	0.51
6:H:95:ALA:HA	6:H:100(P):MET:HA	1.92	0.51
3:G:280:ASN:HD22	3:G:458:GLY:HA3	1.76	0.51
1:A:7:SER:OG	1:A:8:GLY:N	2.45	0.50
1:A:4:LEU:HD21	1:A:104:CYS:SG	2.51	0.50
5:L:46:GLN:NE2	5:L:47:ASP:OD1	2.42	0.50
4:T:650:GLN:NE2	4:T:654:GLU:OE1	2.41	0.50
3:G:380:GLU:HB2	3:G:382:PHE:HE1	1.77	0.49
6:H:68:VAL:HG13	6:H:81:GLN:HB2	1.95	0.49
2:E:36:TRP:CE2	2:E:74:LEU:HB2	2.47	0.49
1:A:109:LEU:HD22	4:T:625:ASN:HB2	1.94	0.49
3:G:203:GLN:HG3	3:G:435:TYR:HD2	1.78	0.49
3:G:94:ASN:HA	3:G:236:THR:HG22	1.94	0.48
2:E:170:GLN:N	2:E:174:LYS:O	2.44	0.48
3:G:36:VAL:HG12	4:T:610:TRP:CE3	2.48	0.48
3:G:317:PHE:CE2	3:G:319:ALA:HB2	2.49	0.48
3:G:498:PRO:HB3	4:T:610:TRP:CD2	2.49	0.48
6:H:121:PRO:HB2	6:H:209:VAL:HG13	1.96	0.48
1:A:134:THR:HG23	1:A:165:PRO:HG2	1.96	0.48
2:E:29:CYS:HA	2:E:67:LYS:HD2	1.96	0.48
5:L:167:LYS:HA	5:L:173:TYR:HA	1.96	0.47
6:H:121:PRO:HB3	6:H:209:VAL:HG22	1.95	0.47
3:G:153:ASP:HB2	3:G:178:LYS:HE3	1.96	0.47
3:G:182:VAL:O	3:G:184:LEU:N	2.48	0.47
6:H:36:TRP:HB3	6:H:48:ILE:HD12	1.95	0.47
5:L:7:VAL:HG11	5:L:13:ALA:HB2	1.97	0.47
3:G:335:ARG:NH1	3:G:414:ILE:HD11	2.28	0.47
4:T:651:ASN:HD22	4:T:655:LYS:HE3	1.78	0.47
1:A:29:PHE:CG	1:A:85:GLY:HA3	2.49	0.47
3:G:93:PHE:CE2	3:G:228:CYS:HB2	2.50	0.47
3:G:193:LEU:HB3	3:G:196:CYS:SG	2.55	0.47
3:G:86:LEU:HD22	4:T:523:LEU:O	2.15	0.47
3:G:503:ARG:HE	4:T:606:THR:HA	1.78	0.47
6:H:94:THR:CB	6:H:100(R):VAL:HG21	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:HG3	1:A:18:VAL:HB	1.98	0.46
6:H:20:VAL:HG23	6:H:80:LEU:HB3	1.96	0.46
3:G:503:ARG:NH1	4:T:597:GLY:HA3	2.31	0.46
3:G:107:ASP:O	3:G:111:LEU:HB2	2.15	0.46
3:G:53:PHE:HB2	3:G:218:CYS:HB2	1.98	0.46
3:G:101:VAL:HG21	3:G:480:ARG:HG2	1.98	0.46
3:G:340:THR:O	3:G:343:GLN:HG2	2.15	0.46
6:H:119:VAL:HG12	6:H:140:VAL:HG22	1.96	0.46
2:E:62:ARG:HD2	2:E:78:ASP:HB3	1.98	0.46
6:H:117:PRO:HA	6:H:142:ASP:O	2.14	0.46
5:L:30:TYR:OH	6:H:100(P):MET:HE2	2.04	0.46
4:T:596:TRP:CD1	4:T:647:GLU:HB2	2.51	0.46
3:G:52:LEU:HD21	3:G:488:VAL:HG21	1.98	0.45
5:L:29:TRP:CE2	5:L:70:LEU:HB2	2.51	0.45
6:H:60:ASN:HB3	6:H:63:LEU:HD23	1.98	0.45
3:G:376:ASN:OD1	3:G:377:CYS:N	2.50	0.45
3:G:491:ILE:HD11	4:T:523:LEU:HD11	1.99	0.45
1:A:51:ILE:HB	1:A:70:MET:HE3	1.99	0.45
2:E:187:GLN:O	2:E:194:TYR:OH	2.34	0.45
3:G:181:VAL:HG13	3:G:192:ARG:HB3	1.99	0.44
3:G:476:ARG:HA	3:G:479:TRP:CD1	2.52	0.44
3:G:165:ILE:HD12	3:G:165:ILE:HA	1.83	0.44
3:G:223:TYR:CE1	3:G:490:GLU:HB3	2.53	0.44
1:A:169:THR:HG23	1:A:217:ASN:HB3	2.00	0.44
4:T:664:ASP:OD1	4:T:664:ASP:N	2.51	0.44
3:G:52:LEU:HB2	3:G:217:TYR:HD2	1.83	0.44
3:G:401:GLY:O	3:G:413:ASN:N	2.51	0.44
6:H:50:TYR:CZ	6:H:58:THR:HB	2.52	0.44
3:G:335:ARG:HH22	3:G:395:MET:HG3	1.83	0.43
3:G:496:ILE:HD12	4:T:642:ILE:HG21	2.00	0.43
5:L:61(A):ASP:HB3	10:I:5:MAN:H3	2.00	0.43
4:T:593:LEU:HB3	4:T:598:CYS:O	2.18	0.43
3:G:422:GLN:O	3:G:435:TYR:HA	2.19	0.43
6:H:157:LEU:HD11	6:H:192:TYR:HD2	1.83	0.43
6:H:198:HIS:CD2	6:H:200:PRO:HD2	2.54	0.43
1:A:35:ASN:O	1:A:104:CYS:HA	2.19	0.43
3:G:276:ASN:HD22	13:G:606:NAG:H83	1.83	0.43
3:G:286:VAL:O	3:G:451:GLY:HA2	2.19	0.43
1:A:117:LEU:HD12	1:A:118:PRO:HD2	2.01	0.43
3:G:98:ASN:ND2	3:G:486:TYR:O	2.52	0.43
5:L:25:ARG:HG3	5:L:45:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:152:TRP:HB3	6:H:157:LEU:HD12	2.01	0.43
3:G:313:PRO:HD2	3:G:315:GLN:NE2	2.32	0.42
3:G:270:VAL:HG12	3:G:289:ASN:N	2.34	0.42
3:G:286:VAL:HB	3:G:452:LEU:HB2	2.01	0.42
1:A:35:ASN:OD1	1:A:50:TRP:HB3	2.18	0.42
3:G:229:ASN:ND2	8:N:1:NAG:HN2	2.18	0.42
3:G:258:GLN:HG2	3:G:470:PRO:HB2	2.01	0.42
7:B:1:NAG:H61	7:B:2:NAG:C7	2.49	0.42
3:G:269:GLU:HA	9:M:1:NAG:O5	2.19	0.42
6:H:100(C):GLY:HA3	6:H:100(I):GLU:OE1	2.19	0.42
3:G:348:LYS:HD2	3:G:348:LYS:HA	1.93	0.42
3:G:392:SER:HA	3:G:395:MET:HB3	2.02	0.42
5:L:28:GLN:HG2	6:H:100(O):TYR:HB2	2.02	0.42
5:L:151:ALA:O	5:L:154:SER:OG	2.23	0.42
3:G:67:ASN:HB3	3:G:208:VAL:HG22	2.02	0.41
6:H:59:TYR:HE2	6:H:69:ILE:HG13	1.85	0.41
3:G:498:PRO:HB3	4:T:610:TRP:CG	2.55	0.41
2:E:36:TRP:CD2	2:E:74:LEU:HB2	2.55	0.41
2:E:62:ARG:HB3	2:E:77:SER:O	2.20	0.41
6:H:144:PHE:HA	6:H:145:PRO:HA	1.86	0.41
1:A:4:LEU:HD12	1:A:24:THR:HG22	2.01	0.41
4:T:614:TRP:CH2	4:T:642:ILE:HG12	2.55	0.41
3:G:270:VAL:HG12	3:G:289:ASN:H	1.85	0.41
5:L:137:ILE:HG12	5:L:196:VAL:HG11	2.02	0.41
6:H:33:TYR:CD2	6:H:52:SER:HA	2.55	0.41
6:H:90:TYR:O	6:H:104:GLY:HA2	2.20	0.41
1:A:108:LEU:HG	1:A:109:LEU:HG	2.03	0.41
2:E:153:ALA:HA	2:E:194:TYR:HD1	1.85	0.41
3:G:39:TYR:HD1	4:T:537:LEU:HD11	1.86	0.41
3:G:269:GLU:HG2	9:M:1:NAG:H62	2.01	0.41
4:T:592:LEU:HD23	4:T:595:ILE:HD11	2.02	0.41
6:H:94:THR:O	6:H:100(P):MET:HB3	2.21	0.41
6:H:114:THR:HG22	6:H:145:PRO:HD3	2.03	0.41
3:G:192:ARG:NH2	9:O:1:NAG:O7	2.54	0.40
1:A:172:TRP:CZ3	1:A:214:CYS:HB3	2.56	0.40
3:G:131:CYS:SG	3:G:191:TYR:HB2	2.62	0.40
3:G:417:GLN:HG2	6:H:100(G):PHE:CE1	2.56	0.40
6:H:100(C):GLY:C	10:I:2:NAG:H2	2.42	0.40
6:H:142:ASP:HB3	6:H:173:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/243 (98%)	227 (95%)	11 (5%)	0	100	100
2	E	211/216 (98%)	195 (92%)	14 (7%)	2 (1%)	17	49
3	G	441/480 (92%)	382 (87%)	51 (12%)	8 (2%)	8	32
4	T	132/140 (94%)	116 (88%)	13 (10%)	3 (2%)	6	28
5	L	208/214 (97%)	196 (94%)	12 (6%)	0	100	100
6	H	221/236 (94%)	210 (95%)	10 (4%)	1 (0%)	29	61
All	All	1451/1529 (95%)	1326 (91%)	111 (8%)	14 (1%)	15	46

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	T	547(D)	ILE
2	E	30	SER
2	E	29	CYS
3	G	183	ALA
3	G	402	ALA
4	T	547(H)	LYS
3	G	393	THR
3	G	414	ILE
4	T	547(A)	ASN
3	G	137	LYS
6	H	202	ASN
3	G	250	GLY
3	G	136	ILE
3	G	354	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/206 (98%)	203 (100%)	0	100	100
2	E	186/189 (98%)	186 (100%)	0	100	100
3	G	397/427 (93%)	394 (99%)	3 (1%)	81	91
4	T	114/116 (98%)	110 (96%)	4 (4%)	36	65
5	L	176/180 (98%)	176 (100%)	0	100	100
6	H	194/204 (95%)	192 (99%)	2 (1%)	76	88
All	All	1270/1322 (96%)	1261 (99%)	9 (1%)	84	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	179	LEU
3	G	243	SER
3	G	388	ASP
4	T	575	GLN
4	T	578	THR
4	T	604	CYS
4	T	647	GLU
6	H	100(P)	MET
6	H	162	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	195	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

47 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	B	1	3,7	14,14,15	0.23	0	17,19,21	1.41	3 (17%)
7	NAG	B	2	7	14,14,15	0.24	0	17,19,21	0.41	0
7	BMA	B	3	7	11,11,12	0.65	0	15,15,17	0.73	0
7	MAN	B	4	7	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
7	MAN	B	5	7	11,11,12	0.73	0	15,15,17	1.04	2 (13%)
7	MAN	B	6	7	11,11,12	0.73	0	15,15,17	1.06	2 (13%)
7	MAN	B	7	7	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
7	MAN	B	8	7	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
7	MAN	B	9	7	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
8	NAG	C	1	3,8	14,14,15	0.25	0	17,19,21	0.40	0
8	NAG	C	2	8	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	D	1	3,9	14,14,15	0.29	0	17,19,21	0.39	0
9	NAG	D	2	9	14,14,15	0.21	0	17,19,21	0.40	0
9	BMA	D	3	9	11,11,12	0.60	0	15,15,17	0.80	0
8	NAG	F	1	3,8	14,14,15	0.33	0	17,19,21	0.61	0
8	NAG	F	2	8	14,14,15	0.22	0	17,19,21	0.46	0
10	NAG	I	1	3,10	14,14,15	0.21	0	17,19,21	0.44	0
10	NAG	I	2	10	14,14,15	0.19	0	17,19,21	0.45	0
10	BMA	I	3	10	11,11,12	0.65	0	15,15,17	0.92	0
10	MAN	I	4	10	11,11,12	0.76	0	15,15,17	1.16	3 (20%)
10	MAN	I	5	10	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
10	MAN	I	6	10	11,11,12	0.78	0	15,15,17	1.12	2 (13%)
10	MAN	I	7	10	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
10	MAN	I	8	10	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
10	MAN	I	9	10	11,11,12	0.71	0	15,15,17	1.09	2 (13%)
11	NAG	J	1	3,11	14,14,15	0.29	0	17,19,21	0.43	0
11	NAG	J	2	11	14,14,15	0.21	0	17,19,21	0.41	0
11	BMA	J	3	11	11,11,12	0.62	0	15,15,17	0.81	0
11	MAN	J	4	11	11,11,12	0.71	0	15,15,17	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	J	5	11	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
12	NAG	K	1	3,12	14,14,15	0.25	0	17,19,21	0.49	0
12	NAG	K	2	3,12	14,14,15	0.28	0	17,19,21	0.45	0
12	NAG	K	3	12	14,14,15	0.21	0	17,19,21	0.47	0
12	BMA	K	4	12	11,11,12	0.55	0	15,15,17	0.82	0
12	MAN	K	5	12	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
12	NAG	K	6	12	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	M	1	3,9	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
9	NAG	M	2	9	14,14,15	0.25	0	17,19,21	0.55	0
9	BMA	M	3	9	11,11,12	0.63	0	15,15,17	0.80	0
8	NAG	N	1	3,8	14,14,15	0.33	0	17,19,21	0.62	0
8	NAG	N	2	8	14,14,15	0.26	0	17,19,21	0.43	0
9	NAG	O	1	3,9	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
9	NAG	O	2	9	14,14,15	0.22	0	17,19,21	0.40	0
9	BMA	O	3	9	11,11,12	0.79	0	15,15,17	0.81	0
9	NAG	P	1	9,4	14,14,15	0.31	0	17,19,21	0.50	0
9	NAG	P	2	9	14,14,15	0.20	0	17,19,21	0.42	0
9	BMA	P	3	9	11,11,12	0.63	0	15,15,17	0.77	0

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

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

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

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1	NAG	C2-N2-C7	4.33	129.06	122.90
9	O	1	NAG	C2-N2-C7	4.08	128.72	122.90
7	B	4	MAN	C1-O5-C5	2.52	115.60	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	4	MAN	C1-O5-C5	2.49	115.57	112.19
10	I	7	MAN	C1-O5-C5	2.48	115.56	112.19
7	B	7	MAN	C1-O5-C5	2.47	115.53	112.19
7	B	1	NAG	C1-O5-C5	2.46	115.52	112.19
12	K	5	MAN	C1-O5-C5	2.40	115.44	112.19
10	I	8	MAN	C1-O5-C5	2.38	115.41	112.19
10	I	9	MAN	C1-O5-C5	2.37	115.40	112.19
10	I	5	MAN	C1-O5-C5	2.35	115.38	112.19
7	B	8	MAN	C1-O5-C5	2.34	115.36	112.19
11	J	5	MAN	C1-O5-C5	2.30	115.30	112.19
11	J	4	MAN	C1-O5-C5	2.28	115.29	112.19
7	B	6	MAN	C1-O5-C5	2.28	115.28	112.19
10	I	9	MAN	O2-C2-C3	-2.26	105.62	110.14
10	I	6	MAN	C1-O5-C5	2.25	115.24	112.19
7	B	8	MAN	O2-C2-C3	-2.24	105.66	110.14
10	I	8	MAN	O2-C2-C3	-2.23	105.67	110.14
7	B	9	MAN	O2-C2-C3	-2.21	105.72	110.14
11	J	5	MAN	O2-C2-C3	-2.19	105.75	110.14
7	B	9	MAN	C1-O5-C5	2.18	115.15	112.19
10	I	7	MAN	O2-C2-C3	-2.18	105.77	110.14
10	I	5	MAN	O2-C2-C3	-2.17	105.79	110.14
12	K	5	MAN	O2-C2-C3	-2.16	105.81	110.14
7	B	5	MAN	O2-C2-C3	-2.15	105.84	110.14
7	B	4	MAN	O2-C2-C3	-2.14	105.85	110.14
11	J	4	MAN	O2-C2-C3	-2.11	105.91	110.14
9	O	1	NAG	C1-C2-N2	2.09	114.06	110.49
7	B	1	NAG	C1-C2-N2	2.08	114.05	110.49
7	B	7	MAN	O2-C2-C3	-2.08	105.97	110.14
10	I	6	MAN	O2-C2-C3	-2.07	106.00	110.14
10	I	4	MAN	O2-C2-C3	-2.07	106.00	110.14
7	B	6	MAN	O2-C2-C3	-2.05	106.03	110.14
7	B	5	MAN	C1-O5-C5	2.04	114.95	112.19
9	M	1	NAG	C1-O5-C5	2.03	114.94	112.19
10	I	4	MAN	O5-C1-C2	2.01	113.88	110.77

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	3	BMA	C1
10	I	4	MAN	C1
10	I	7	MAN	C1

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	O	1	NAG	C4-C5-C6-O6
9	D	2	NAG	O5-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
9	D	1	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
9	D	2	NAG	C4-C5-C6-O6
7	B	1	NAG	C8-C7-N2-C2
7	B	1	NAG	O7-C7-N2-C2
9	O	1	NAG	C8-C7-N2-C2
9	O	1	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	D	1	NAG	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
9	O	2	NAG	C4-C5-C6-O6
7	B	3	BMA	O5-C5-C6-O6
11	J	1	NAG	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
11	J	1	NAG	C4-C5-C6-O6
12	K	4	BMA	O5-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
10	I	3	BMA	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
11	J	5	MAN	O5-C5-C6-O6
7	B	2	NAG	O5-C5-C6-O6
7	B	2	NAG	C4-C5-C6-O6
9	P	3	BMA	O5-C5-C6-O6
10	I	3	BMA	C4-C5-C6-O6
7	B	3	BMA	C4-C5-C6-O6
9	M	2	NAG	C3-C2-N2-C7
9	O	1	NAG	C3-C2-N2-C7
12	K	3	NAG	O5-C5-C6-O6
10	I	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	I	7	MAN	C4-C5-C6-O6
7	B	1	NAG	C3-C2-N2-C7

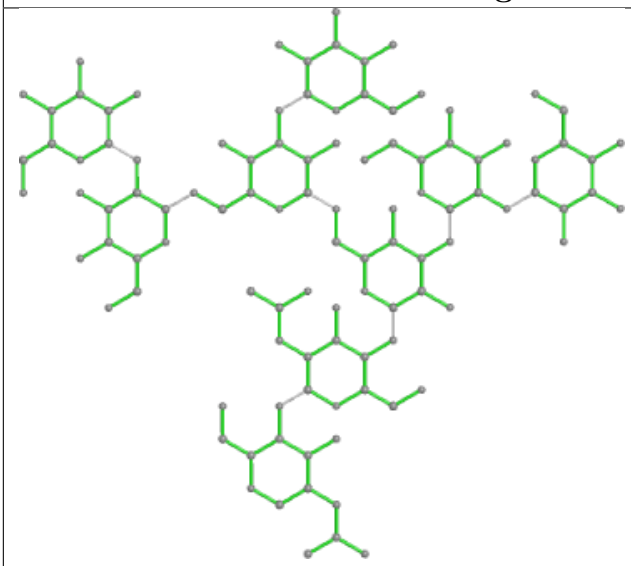
There are no ring outliers.

8 monomers are involved in 10 short contacts:

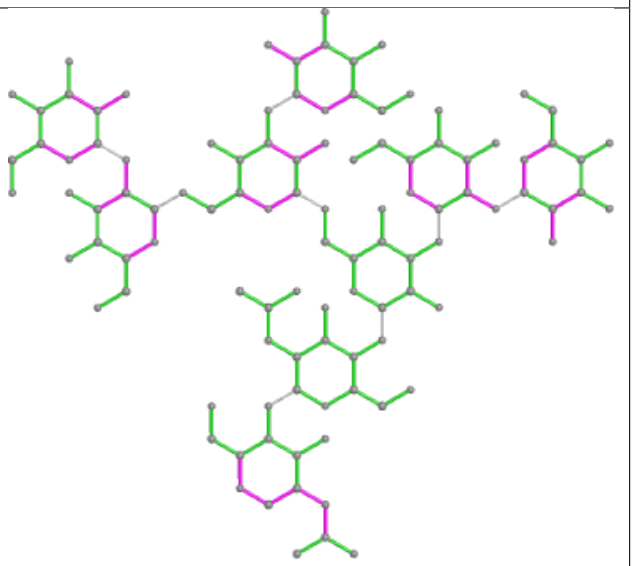
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	2	NAG	1	0
7	B	2	NAG	1	0
8	N	1	NAG	1	0
9	M	1	NAG	2	0
10	I	5	MAN	1	0
9	O	1	NAG	2	0
8	C	1	NAG	1	0
7	B	1	NAG	2	0

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

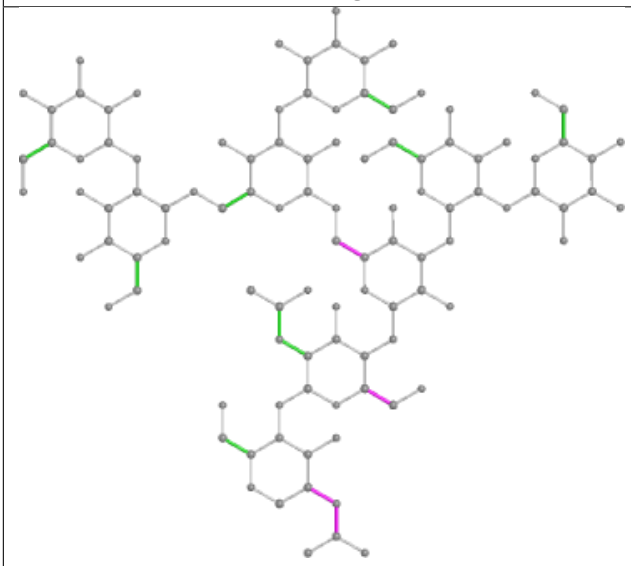
Oligosaccharide Chain B



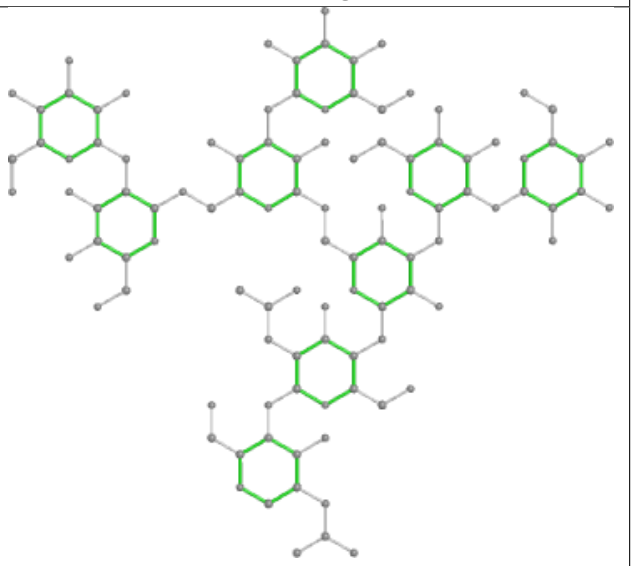
Bond lengths



Bond angles

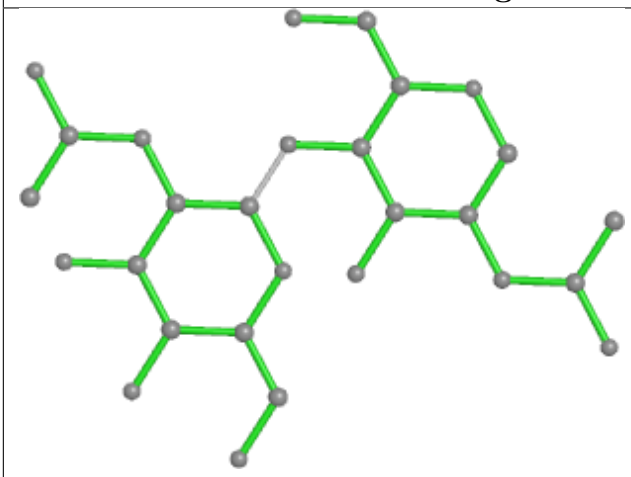


Torsions

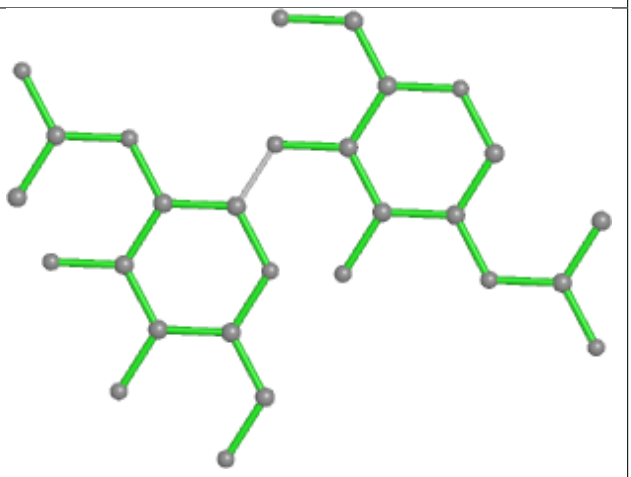


Rings

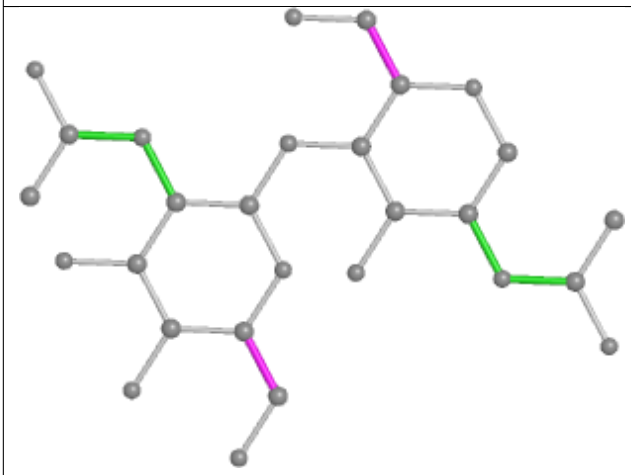
Oligosaccharide Chain C



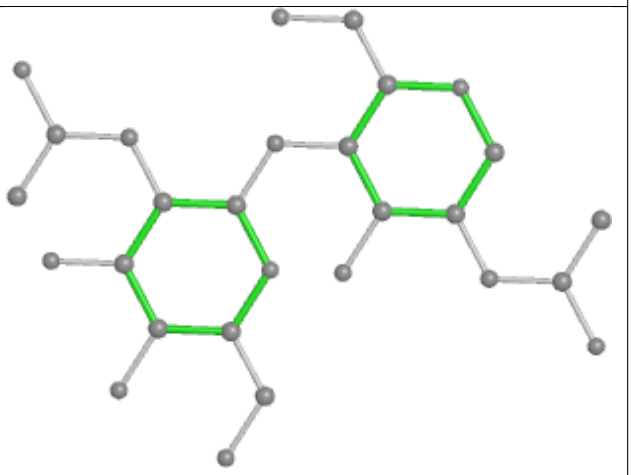
Bond lengths



Bond angles

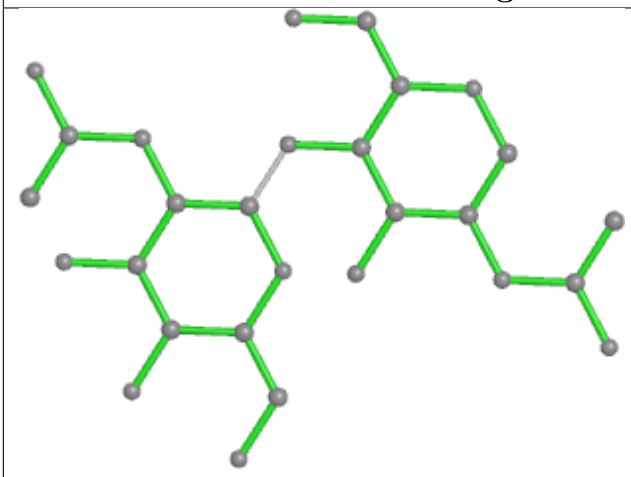


Torsions

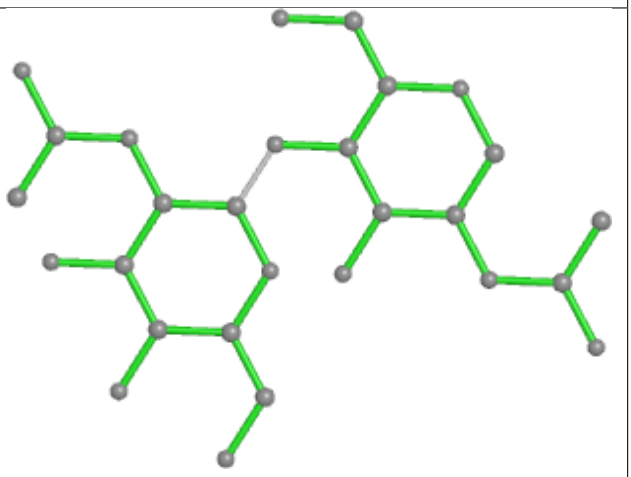


Rings

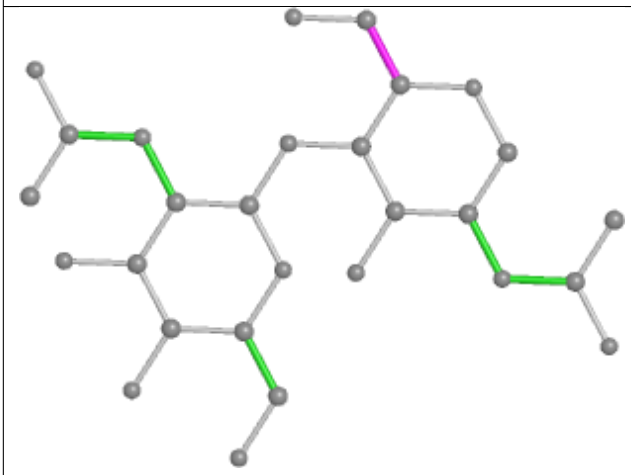
Oligosaccharide Chain F



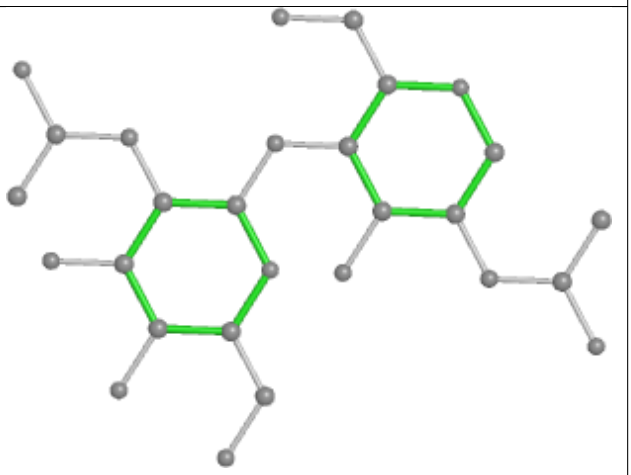
Bond lengths



Bond angles

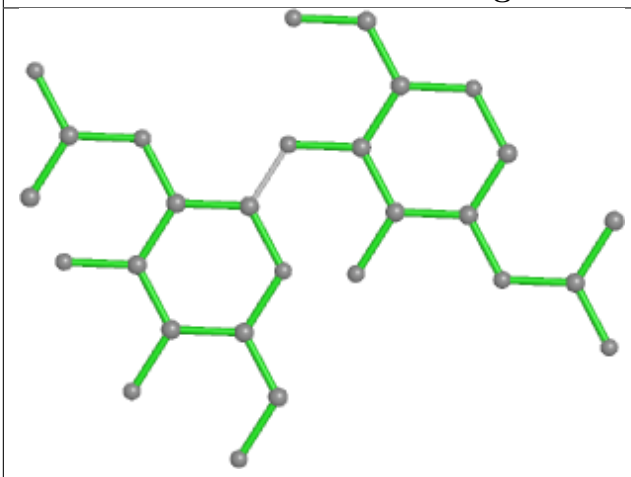


Torsions

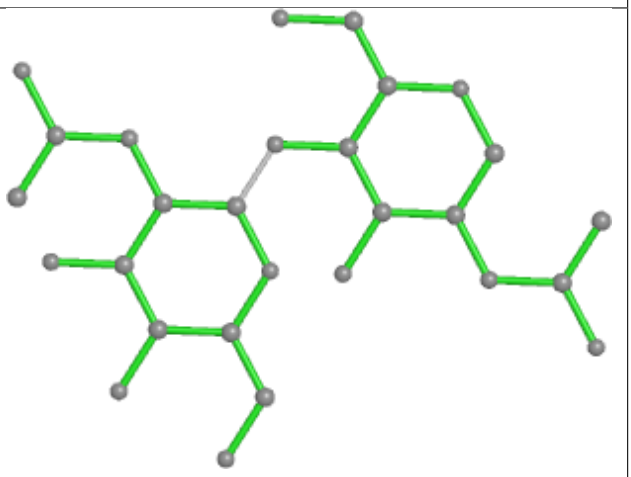


Rings

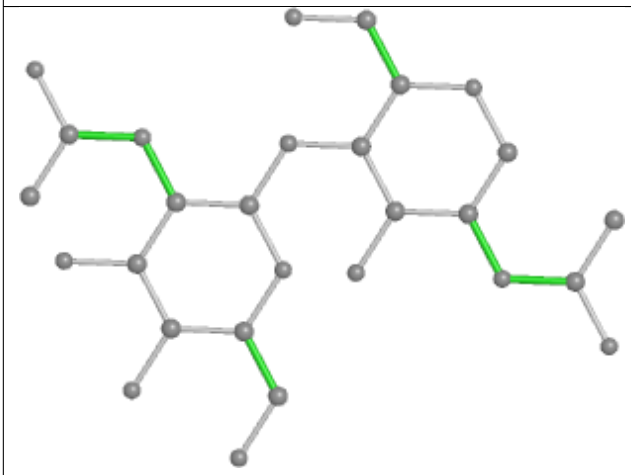
Oligosaccharide Chain N



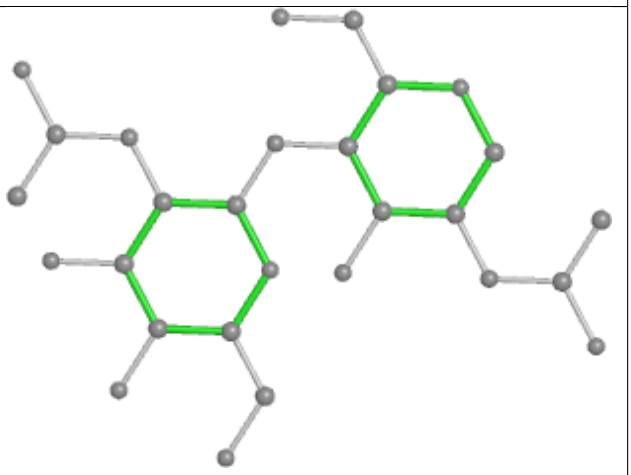
Bond lengths



Bond angles

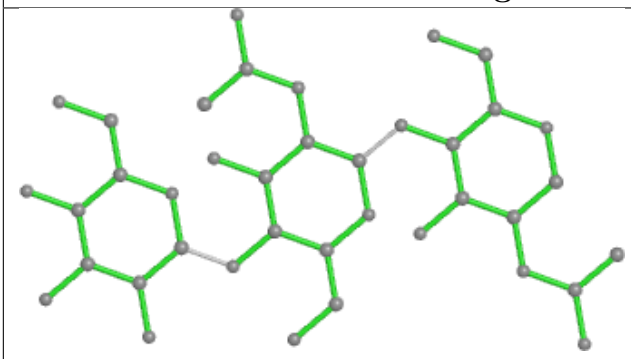


Torsions

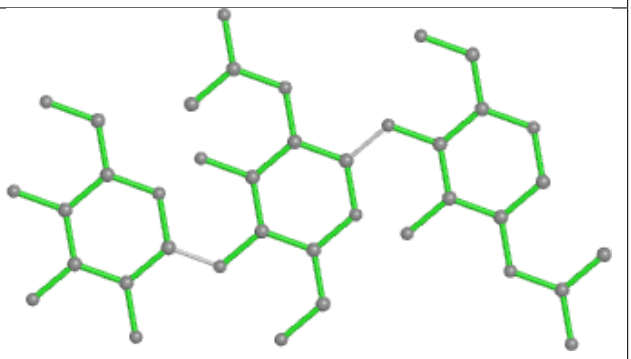


Rings

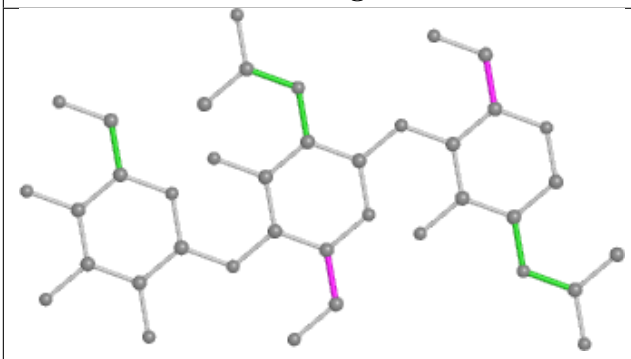
Oligosaccharide Chain D



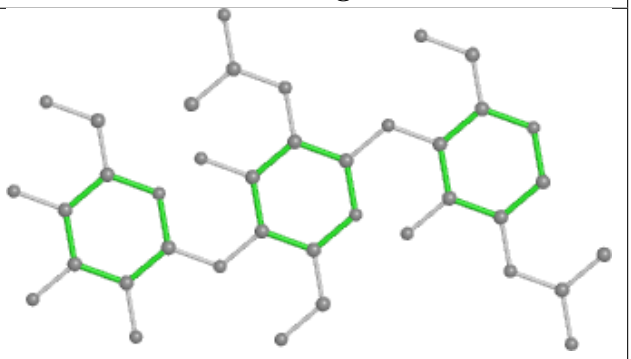
Bond lengths



Bond angles

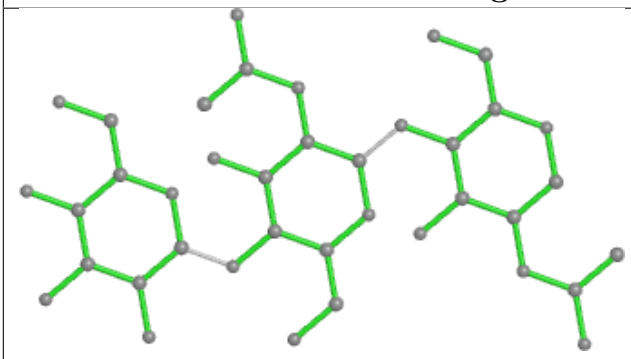


Torsions

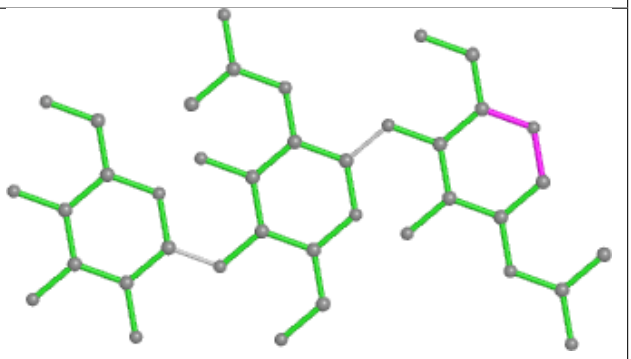


Rings

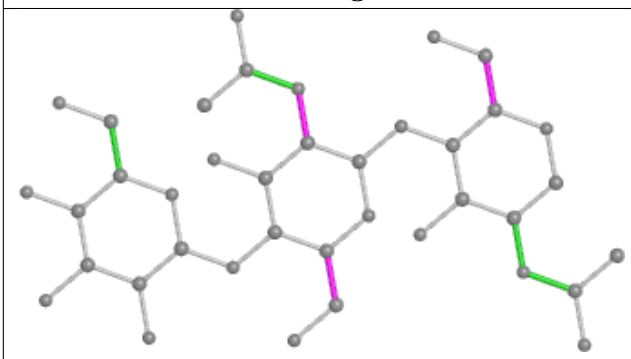
Oligosaccharide Chain M



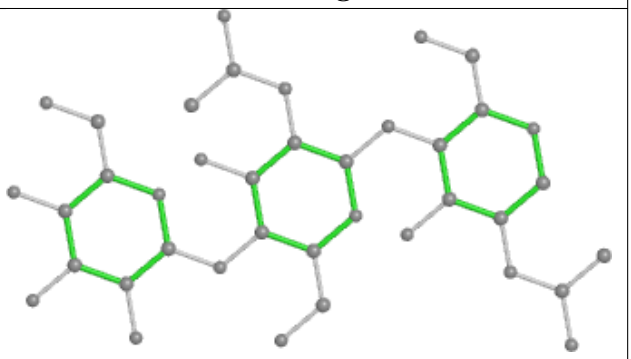
Bond lengths



Bond angles

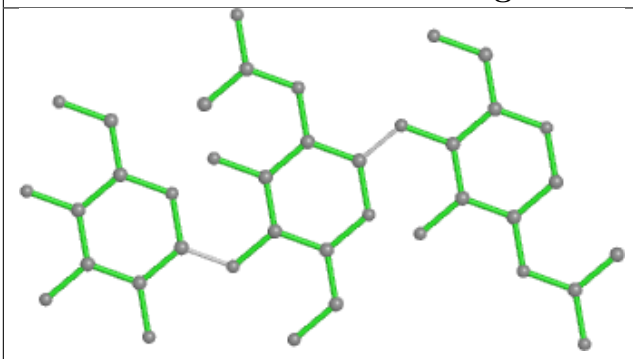


Torsions

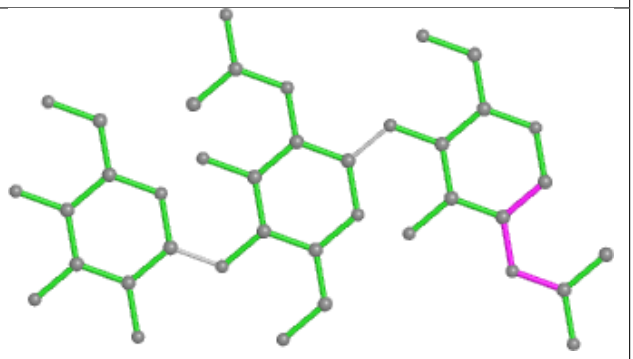


Rings

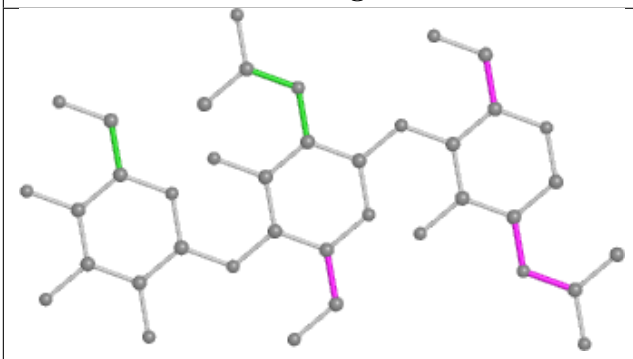
Oligosaccharide Chain O



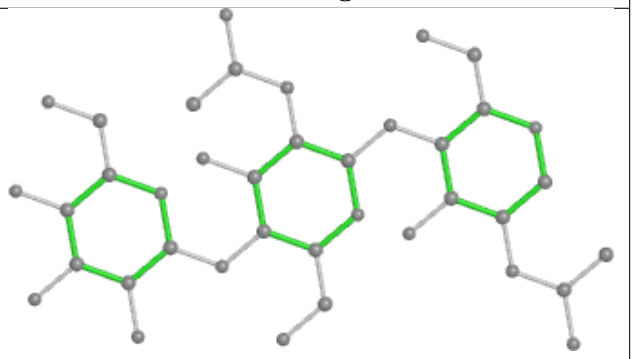
Bond lengths



Bond angles

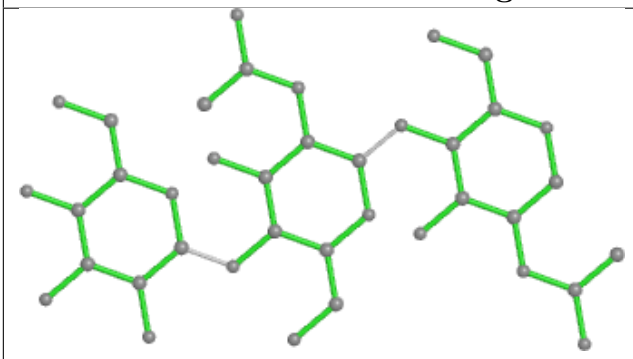


Torsions

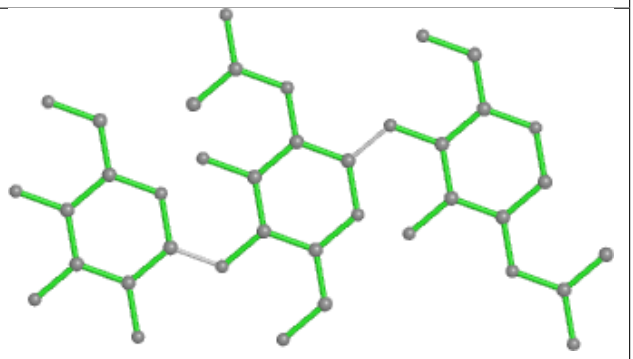


Rings

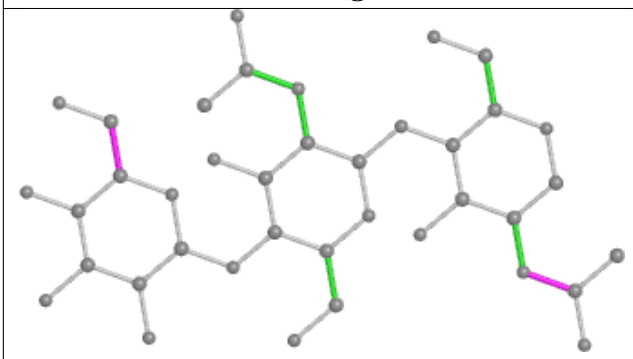
Oligosaccharide Chain P



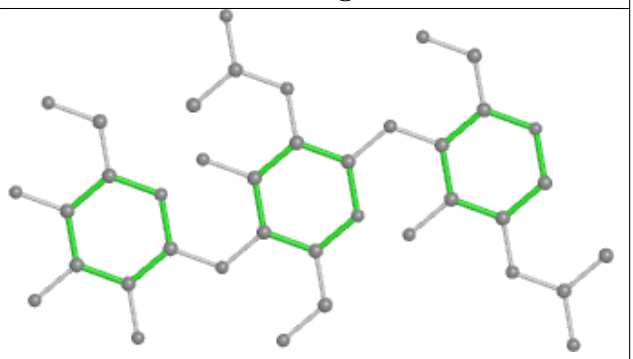
Bond lengths



Bond angles

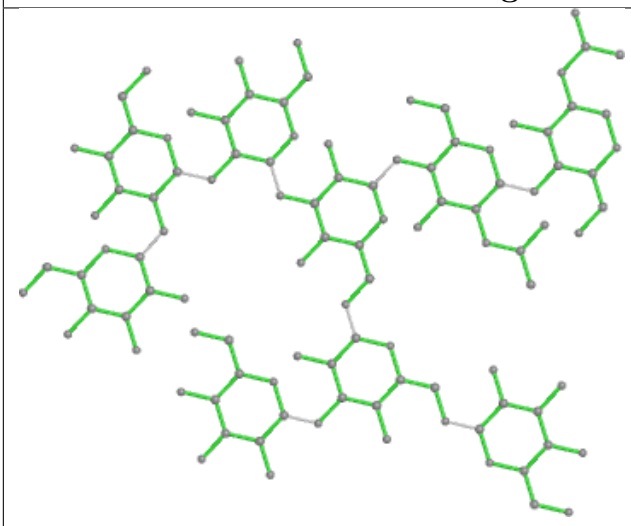


Torsions

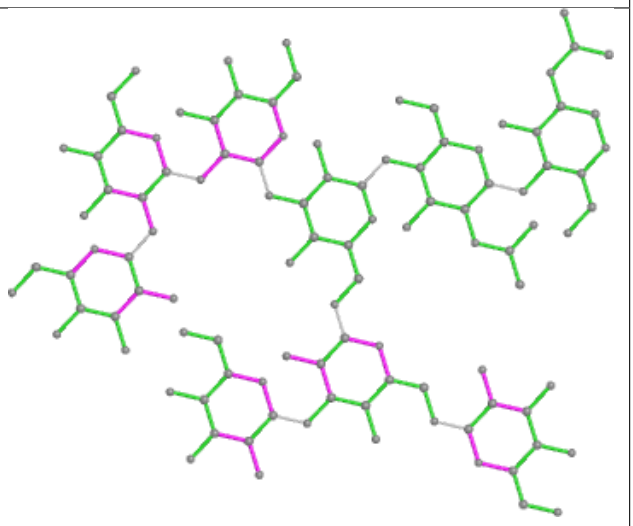


Rings

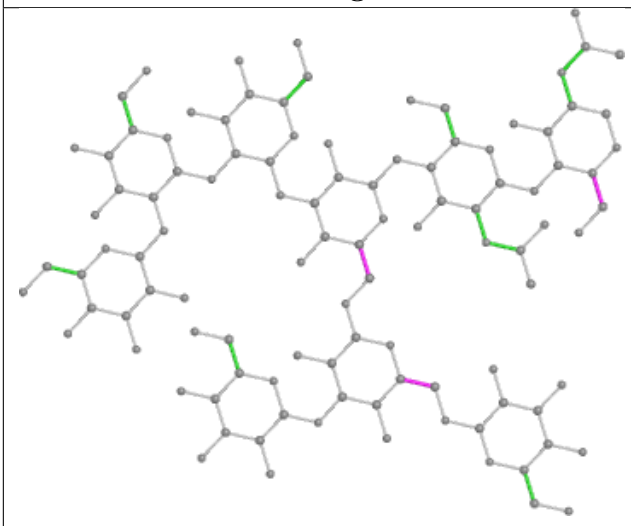
Oligosaccharide Chain I



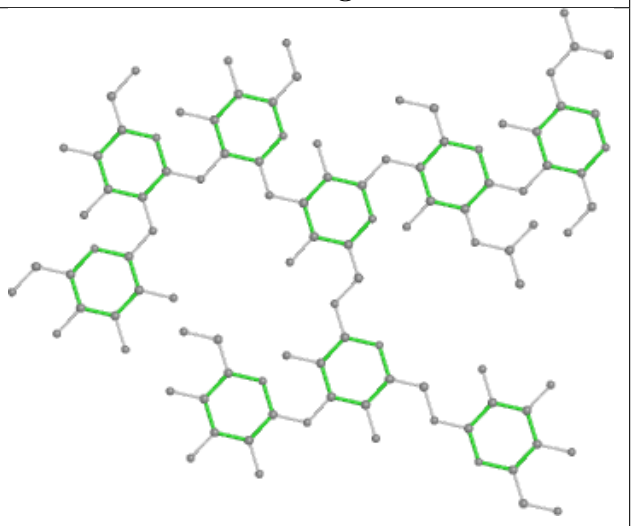
Bond lengths



Bond angles

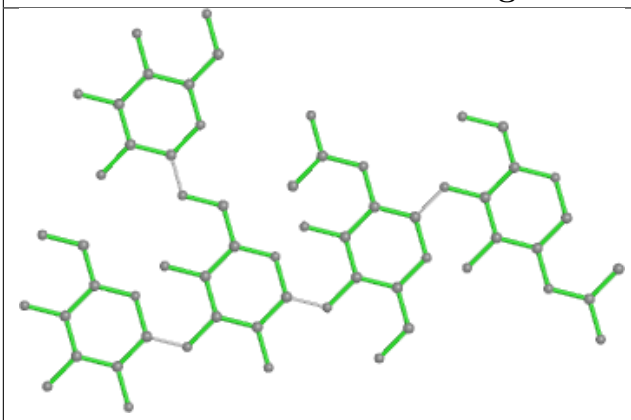


Torsions

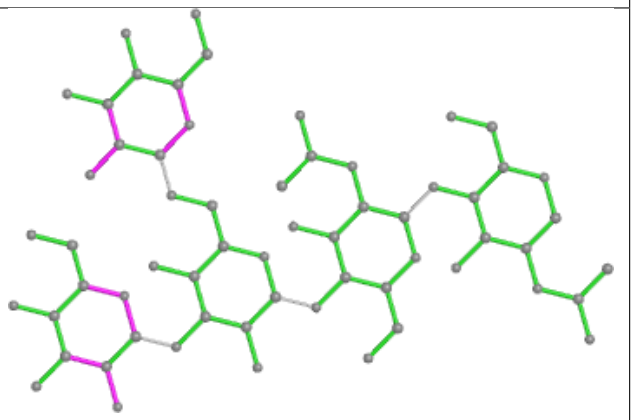


Rings

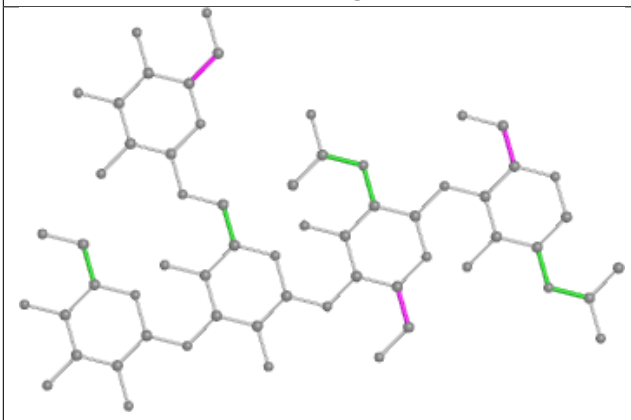
Oligosaccharide Chain J



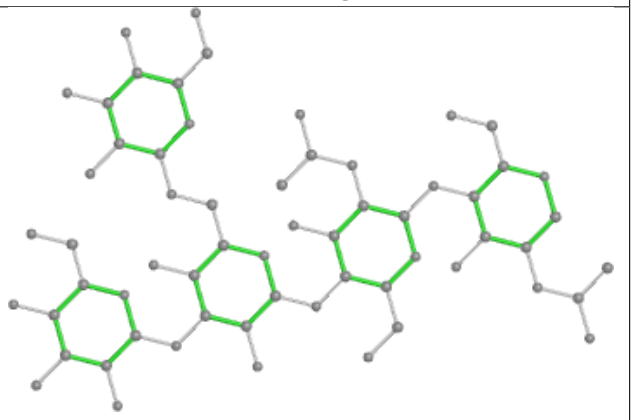
Bond lengths



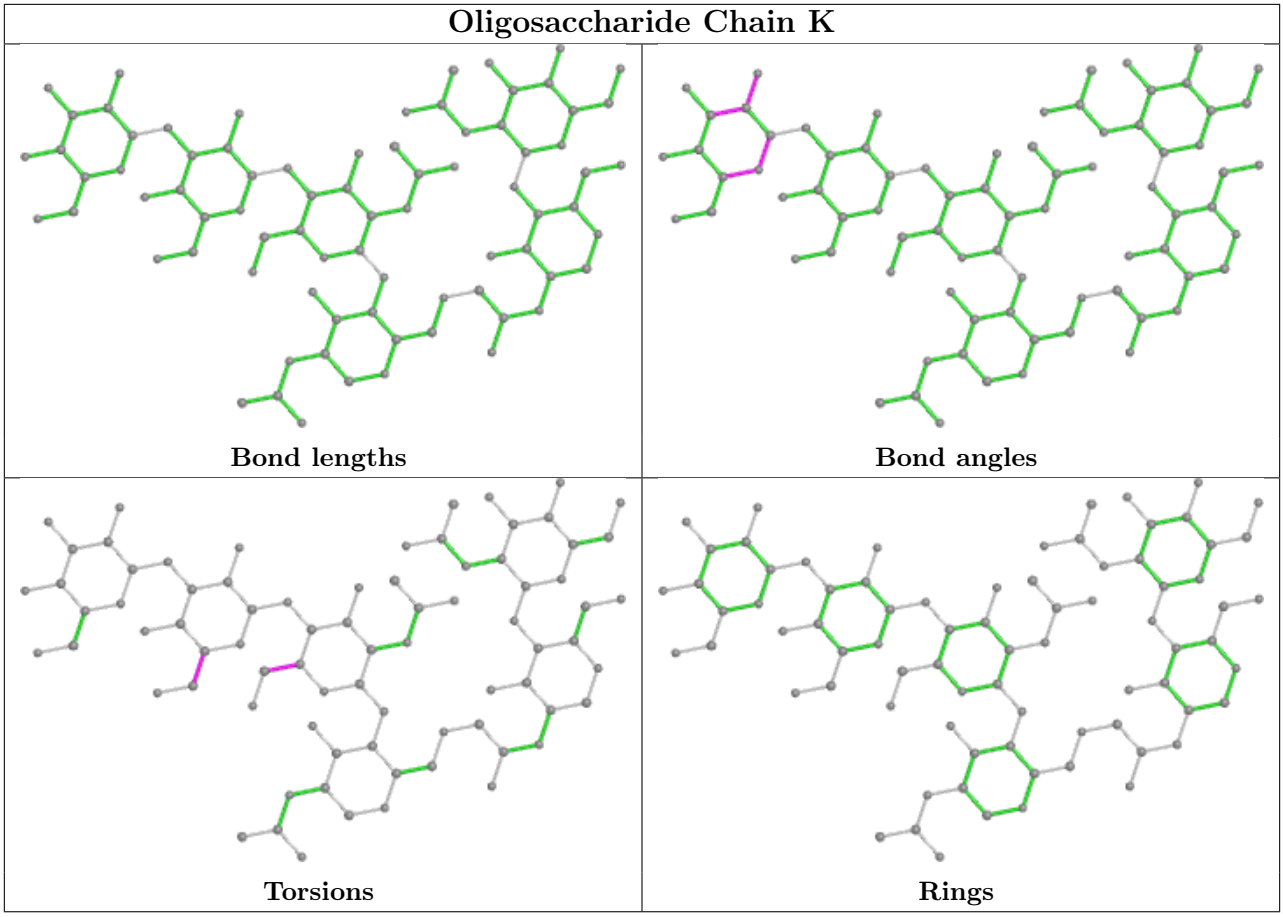
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
13	NAG	T	702	4	14,14,15	0.27	0	17,19,21	0.54	0
13	NAG	G	605	3	14,14,15	0.28	0	17,19,21	0.42	0
13	NAG	T	701	4	14,14,15	0.25	0	17,19,21	0.39	0
13	NAG	G	603	3	14,14,15	0.25	0	17,19,21	0.42	0
13	NAG	G	606	3	14,14,15	0.24	0	17,19,21	0.44	0
13	NAG	G	604	3	14,14,15	0.32	0	17,19,21	0.50	0
13	NAG	G	601	3	14,14,15	0.29	0	17,19,21	0.54	0
13	NAG	G	602	3	14,14,15	0.26	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	G	607	3	14,14,15	0.26	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	T	702	4	-	2/6/23/26	0/1/1/1
13	NAG	G	605	3	-	0/6/23/26	0/1/1/1
13	NAG	T	701	4	-	0/6/23/26	0/1/1/1
13	NAG	G	603	3	-	2/6/23/26	0/1/1/1
13	NAG	G	606	3	-	4/6/23/26	0/1/1/1
13	NAG	G	604	3	-	2/6/23/26	0/1/1/1
13	NAG	G	601	3	-	2/6/23/26	0/1/1/1
13	NAG	G	602	3	-	2/6/23/26	0/1/1/1
13	NAG	G	607	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	603	NAG	O5-C5-C6-O6
13	G	606	NAG	C8-C7-N2-C2
13	G	606	NAG	O7-C7-N2-C2
13	G	606	NAG	O5-C5-C6-O6
13	G	606	NAG	C4-C5-C6-O6
13	G	604	NAG	O5-C5-C6-O6
13	G	601	NAG	O5-C5-C6-O6
13	G	602	NAG	O5-C5-C6-O6
13	T	702	NAG	O5-C5-C6-O6
13	G	603	NAG	C4-C5-C6-O6
13	G	601	NAG	C3-C2-N2-C7
13	G	602	NAG	C3-C2-N2-C7
13	T	702	NAG	C3-C2-N2-C7
13	G	604	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	606	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	240/243 (98%)	0.48	16 (6%) 17 19	47, 105, 230, 252	0
2	E	213/216 (98%)	0.07	2 (0%) 84 83	58, 118, 178, 198	0
3	G	447/480 (93%)	0.24	15 (3%) 45 44	44, 98, 176, 203	0
4	T	134/140 (95%)	0.14	2 (1%) 73 72	42, 75, 166, 184	0
5	L	210/214 (98%)	0.30	11 (5%) 27 27	71, 129, 153, 183	0
6	H	225/236 (95%)	0.72	22 (9%) 7 9	79, 124, 185, 258	1 (0%)
All	All	1469/1529 (96%)	0.33	68 (4%) 32 32	42, 108, 180, 258	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	SER	9.7
1	A	240	VAL	8.4
1	A	149	THR	8.0
1	A	151	GLY	7.2
1	A	148	SER	6.7
1	A	236	LYS	6.6
1	A	147	LYS	6.5
6	H	4	LEU	5.6
1	A	231	PRO	5.3
6	H	150	VAL	4.6
3	G	67	ASN	4.6
6	H	136	LEU	4.4
3	G	462	LYS	4.3
6	H	100(N)	TYR	3.8
1	A	210	GLN	3.8
6	H	192	TYR	3.6
6	H	28	SER	3.6
6	H	145	PRO	3.5
6	H	139	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	279	ASN	3.4
5	L	77	VAL	3.4
5	L	153	SER	3.3
5	L	41	LEU	3.2
1	A	234	CYS	3.2
6	H	182	VAL	3.2
6	H	200	PRO	3.2
3	G	79	PRO	3.1
1	A	146	SER	3.1
5	L	79	ASP	3.0
5	L	56	PHE	3.0
6	H	51	ILE	2.7
2	E	153	ALA	2.7
6	H	78	LEU	2.7
6	H	134	ALA	2.7
3	G	195	ASN	2.6
3	G	277	LEU	2.6
3	G	394	TYR	2.6
1	A	239	GLU	2.5
3	G	280	ASN	2.5
6	H	119	VAL	2.5
6	H	151	SER	2.4
3	G	71	THR	2.4
1	A	229	VAL	2.4
6	H	95	ALA	2.4
3	G	281	ALA	2.4
1	A	212	TYR	2.4
2	E	201	GLU	2.4
6	H	132	GLY	2.4
5	L	181	LEU	2.3
6	H	32	TYR	2.3
4	T	518	VAL	2.3
3	G	203	GLN	2.2
6	H	29	ILE	2.2
3	G	69	TRP	2.2
5	L	65	GLY	2.2
5	L	12	THR	2.2
3	G	188	SER	2.2
4	T	649	SER	2.1
1	A	145	SER	2.1
3	G	61	HIS	2.1
6	H	189	THR	2.1

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Mol	Chain	Res	Type	RSRZ
6	H	100(M)	TYR	2.1
5	L	13	ALA	2.1
1	A	139	VAL	2.0
5	L	60	PRO	2.0
6	H	121	PRO	2.0
3	G	270	VAL	2.0
5	L	27	VAL	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, 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
9	BMA	M	3	11/12	0.52	0.32	168,198,210,211	0
9	BMA	P	3	11/12	0.57	0.46	178,185,199,203	0
9	BMA	D	3	11/12	0.61	0.24	176,189,199,199	0
11	MAN	J	4	11/12	0.71	0.23	175,198,202,203	0
9	NAG	O	1	14/15	0.78	0.34	139,159,167,175	0
9	BMA	O	3	11/12	0.78	0.26	148,187,194,196	0
9	NAG	O	2	14/15	0.79	0.26	159,175,181,195	0
9	NAG	P	2	14/15	0.79	0.35	134,162,171,178	0
11	BMA	J	3	11/12	0.80	0.19	172,186,195,197	0
8	NAG	N	2	14/15	0.81	0.22	80,133,142,145	0
11	MAN	J	5	11/12	0.81	0.17	166,186,196,197	0
9	NAG	D	2	14/15	0.83	0.36	129,164,188,192	0
12	MAN	K	5	11/12	0.83	0.19	133,150,158,160	0
8	NAG	F	2	14/15	0.85	0.20	117,149,157,159	0
7	MAN	B	6	11/12	0.85	0.25	120,128,152,159	0
9	NAG	P	1	14/15	0.86	0.27	76,114,150,156	0
11	NAG	J	2	14/15	0.86	0.24	115,138,159,167	0
8	NAG	N	1	14/15	0.86	0.30	70,101,135,136	0
8	NAG	F	1	14/15	0.88	0.24	110,129,149,163	0
8	NAG	C	2	14/15	0.88	0.23	138,160,178,181	0
12	NAG	K	1	14/15	0.89	0.19	100,119,141,141	0

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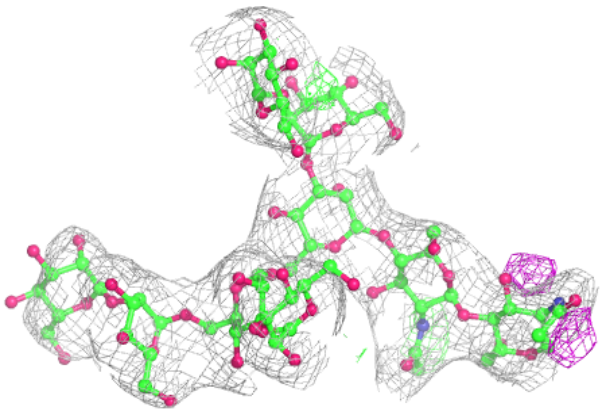
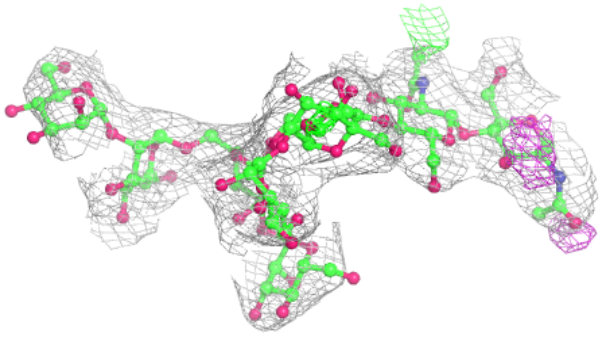
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	NAG	K	6	14/15	0.89	0.28	140,154,169,170	0
10	MAN	I	8	11/12	0.90	0.17	126,156,161,166	0
12	BMA	K	4	11/12	0.91	0.14	106,133,143,145	0
10	MAN	I	9	11/12	0.91	0.12	132,148,151,158	0
8	NAG	C	1	14/15	0.91	0.22	109,130,146,153	0
9	NAG	M	2	14/15	0.92	0.26	120,138,160,183	0
7	MAN	B	9	11/12	0.92	0.44	91,100,113,118	0
12	NAG	K	3	14/15	0.92	0.18	91,112,129,131	0
7	MAN	B	4	11/12	0.92	0.28	69,79,104,119	0
7	MAN	B	7	11/12	0.92	0.35	93,122,132,135	0
10	NAG	I	2	14/15	0.92	0.17	80,109,121,124	0
12	NAG	K	2	14/15	0.93	0.25	67,91,107,118	0
10	MAN	I	7	11/12	0.93	0.10	126,141,155,158	0
7	NAG	B	1	14/15	0.93	0.29	40,54,70,83	0
10	NAG	I	1	14/15	0.93	0.27	98,109,122,128	0
7	MAN	B	5	11/12	0.93	0.25	75,89,103,127	0
10	MAN	I	5	11/12	0.94	0.17	81,94,103,104	0
7	MAN	B	8	11/12	0.95	0.39	56,70,82,83	0
10	MAN	I	6	11/12	0.95	0.13	85,91,97,99	0
9	NAG	M	1	14/15	0.95	0.21	76,86,106,117	0
9	NAG	D	1	14/15	0.96	0.15	85,111,127,137	0
7	NAG	B	2	14/15	0.96	0.29	36,49,70,71	0
10	MAN	I	4	11/12	0.96	0.15	72,87,102,108	0
10	BMA	I	3	11/12	0.97	0.12	86,96,104,120	0
11	NAG	J	1	14/15	0.97	0.24	77,96,111,113	0
7	BMA	B	3	11/12	0.97	0.29	48,58,68,75	0

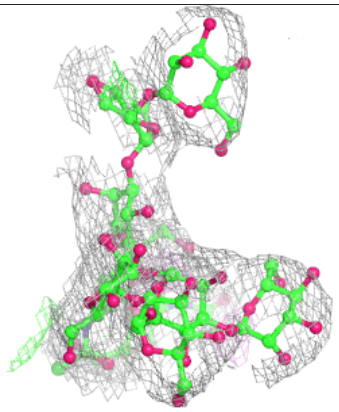
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

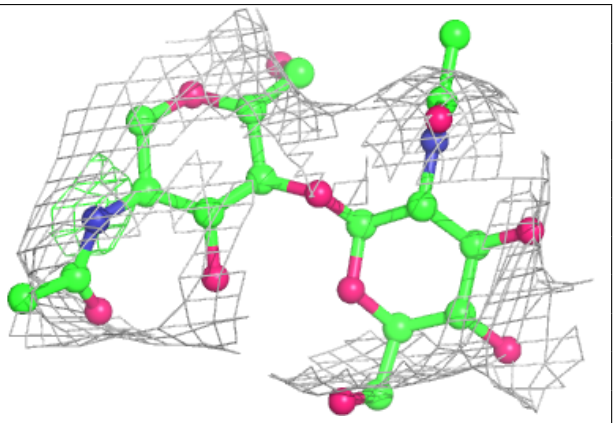


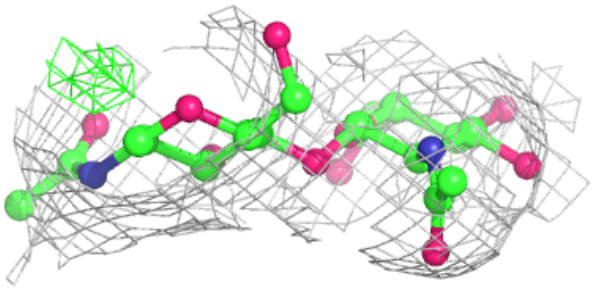


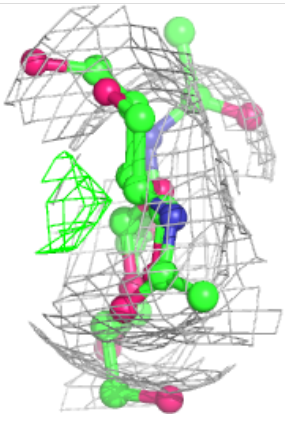


Electron density around Chain C:

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

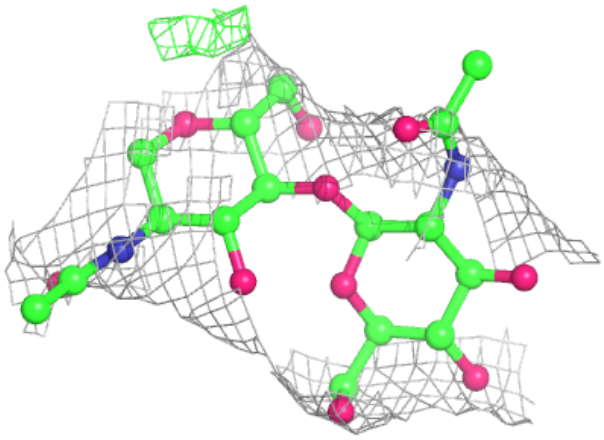


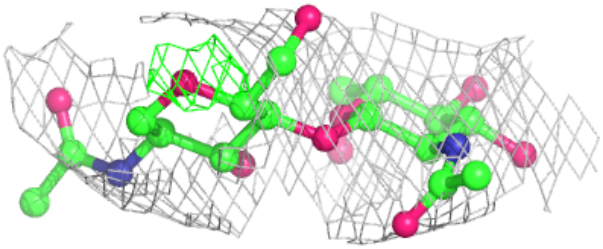


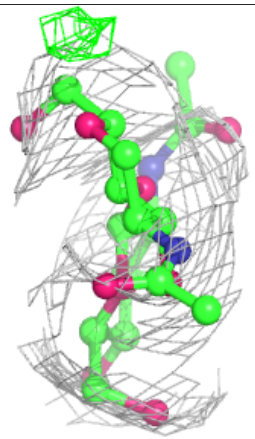


Electron density around Chain F:

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

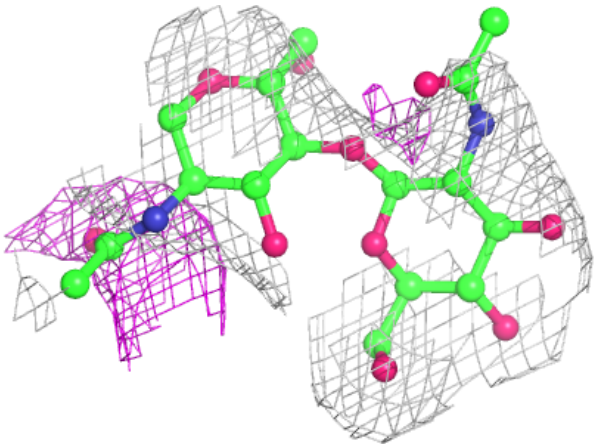


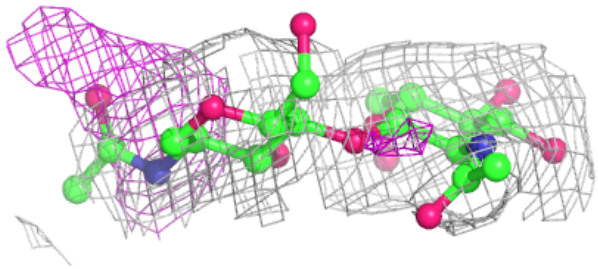


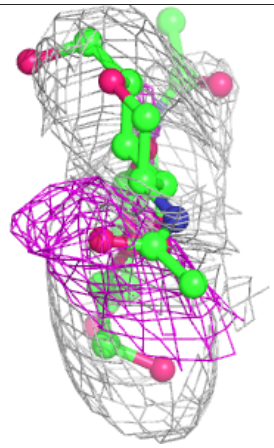


Electron density around Chain N:

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

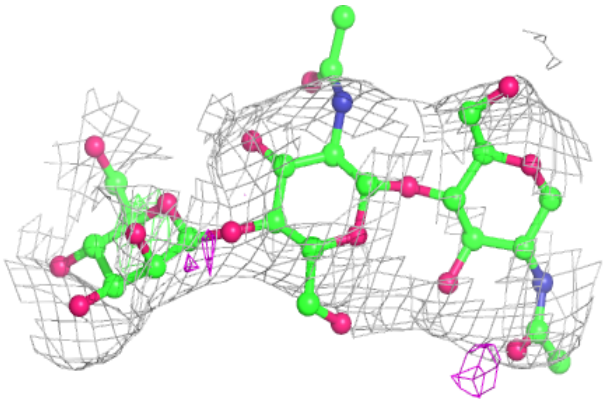


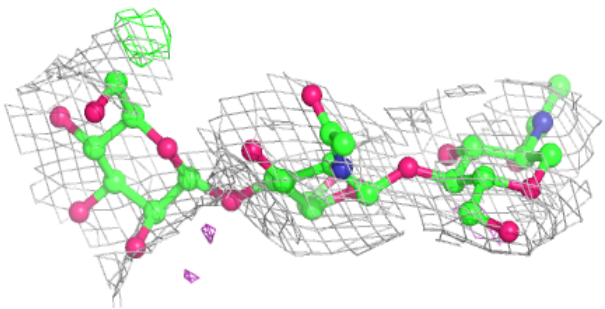


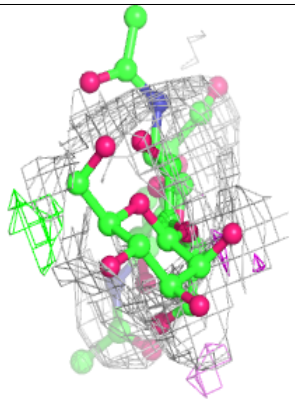


Electron density around Chain D:

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

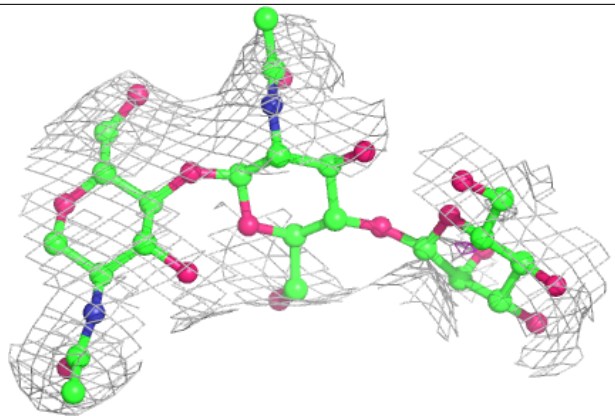


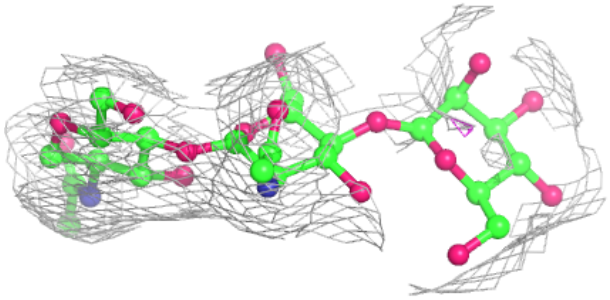


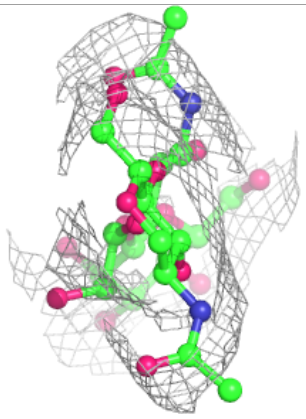


Electron density around Chain M:

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

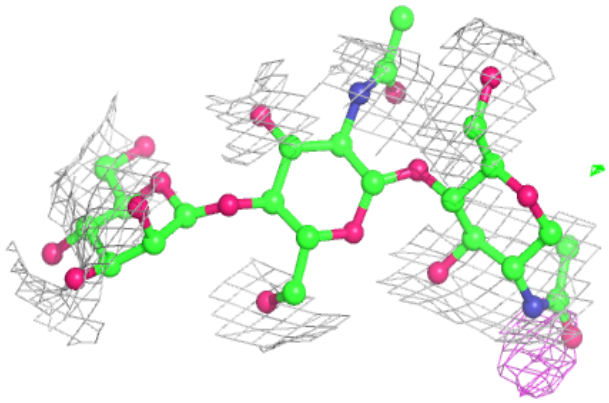


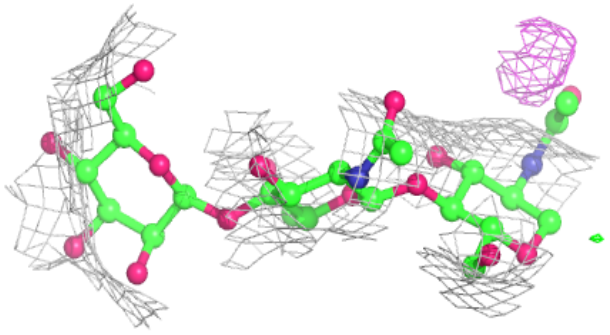


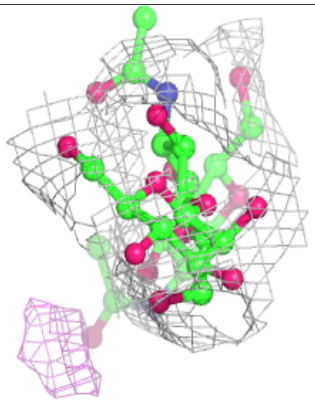


Electron density around Chain O:

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

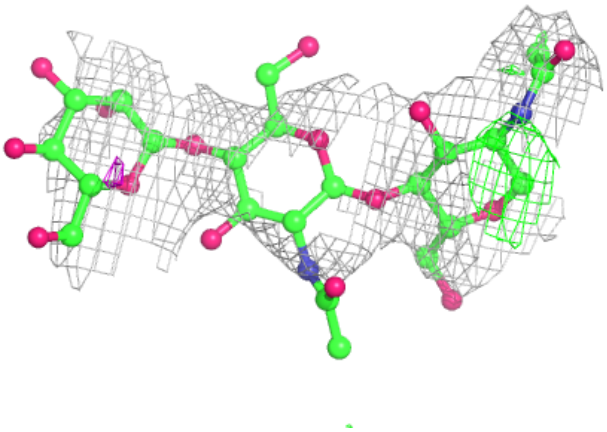


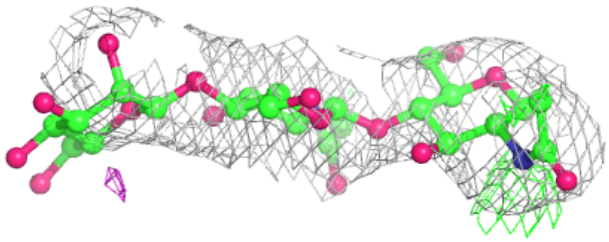


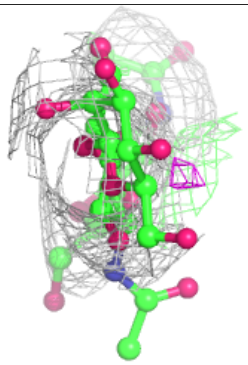


Electron density around Chain P:

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

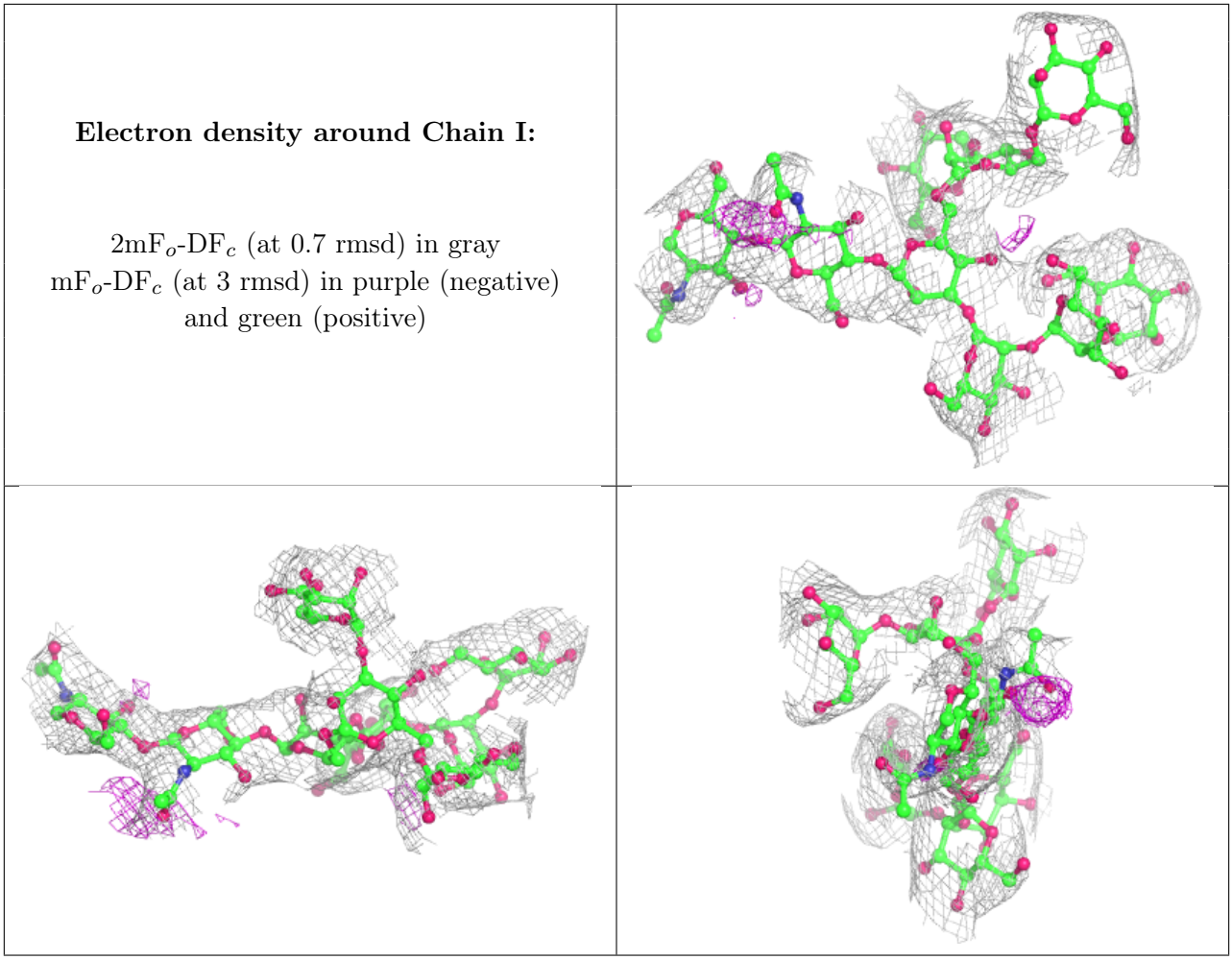






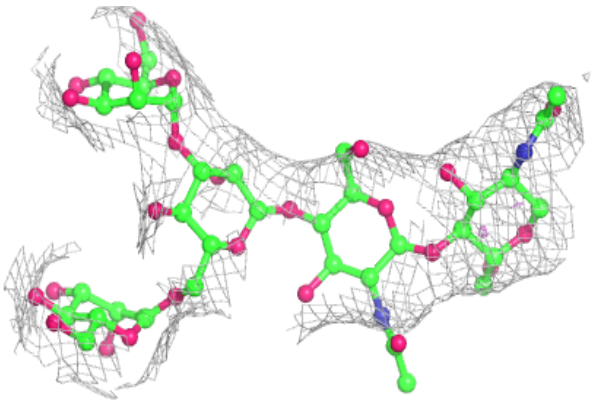
Electron density around Chain I:

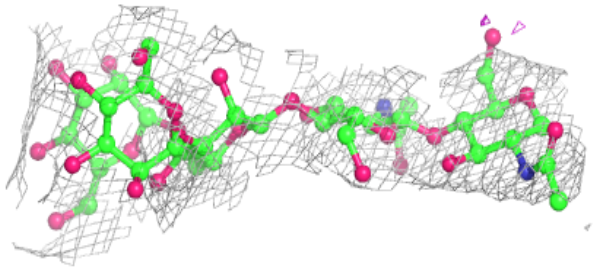
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

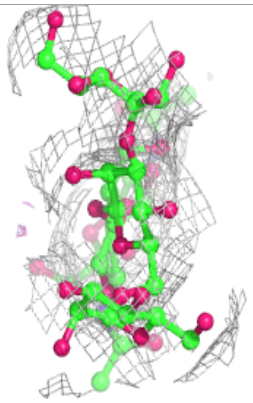


Electron density around Chain J:

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

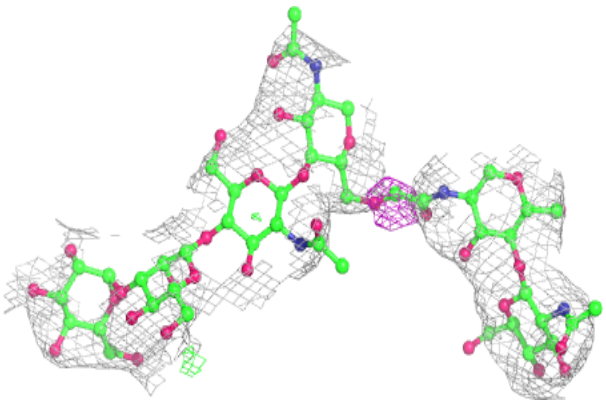


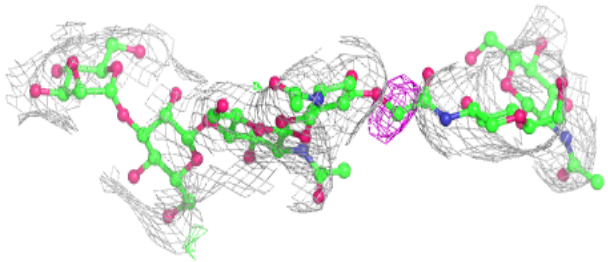




Electron density around Chain K:

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





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, 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	NAG	G	605	14/15	0.63	0.36	117,156,174,179	0
13	NAG	G	603	14/15	0.77	0.36	98,150,159,161	0
13	NAG	G	601	14/15	0.79	0.22	133,156,189,194	0
13	NAG	G	607	14/15	0.83	0.18	139,155,163,164	0
13	NAG	T	702	14/15	0.83	0.40	114,148,159,166	0
13	NAG	T	701	14/15	0.84	0.20	94,129,147,160	0
13	NAG	G	602	14/15	0.87	0.28	95,124,135,137	0
13	NAG	G	604	14/15	0.87	0.38	80,105,131,133	0
13	NAG	G	606	14/15	0.90	0.39	144,156,164,167	0

6.5 Other polymers (i)

There are no such residues in this entry.