Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 06:12 PM BST

PDB ID	:	4G1E
Title	:	Crystal structure of integrin alpha V beta 3 with coil-coiled tag.
Authors	:	Dong, X.; Mi, L.; Zhu, J.; Wang, W.; Luo, B.; Springer, T.A.
Deposited on	:	2012-07-10
Resolution	:	3.00 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 following versions of software and data (see references (1)) were used in the production of this report:

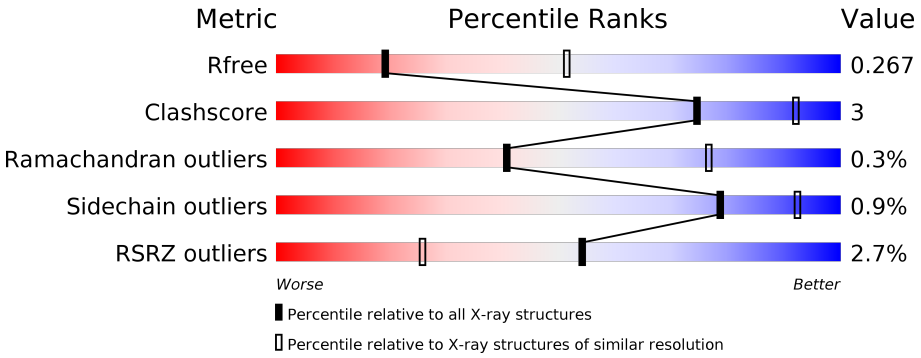
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	998	2% 88% 8%
2	B	738	4% 88% 8%
3	C	4	50% 50%
3	M	4	75% 25%
3	O	4	75% 25%
4	D	3	67% 33%

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Mol	Chain	Length	Quality of chain
4	H	3	67% 33%
4	N	3	100%
5	E	8	25% 50% 25%
6	F	4	50% 50%
7	G	2	100%
7	J	2	100%
7	K	2	100%
7	L	2	100%
8	I	6	33% 50% 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
3	MAN	C	4	-	-	-	X
3	MAN	M	4	-	-	-	X
4	BMA	D	3	-	-	-	X
4	BMA	H	3	-	-	-	X
5	MAN	E	8	-	-	-	X
7	NAG	G	2	-	-	-	X
7	NAG	K	2	-	-	-	X
8	MAN	I	5	-	-	-	X
8	MAN	I	6	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 13732 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	964	Total	C	N	O	S	0	0	0
			7512	4752	1271	1453	36			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	960	MET	-	expression tag	UNP P06756
A	961	GLY	-	expression tag	UNP P06756
A	962	SER	-	expression tag	UNP P06756
A	963	GLY	-	expression tag	UNP P06756
A	964	GLY	-	expression tag	UNP P06756
A	965	GLU	-	expression tag	UNP P06756
A	966	ASN	-	expression tag	UNP P06756
A	967	ALA	-	expression tag	UNP P06756
A	968	GLN	-	expression tag	UNP P06756
A	969	CYS	-	expression tag	UNP P06756
A	970	GLU	-	expression tag	UNP P06756
A	971	LYS	-	expression tag	UNP P06756
A	972	GLU	-	expression tag	UNP P06756
A	973	LEU	-	expression tag	UNP P06756
A	974	GLN	-	expression tag	UNP P06756
A	975	ALA	-	expression tag	UNP P06756
A	976	LEU	-	expression tag	UNP P06756
A	977	GLU	-	expression tag	UNP P06756
A	978	LYS	-	expression tag	UNP P06756
A	979	GLU	-	expression tag	UNP P06756
A	980	ASN	-	expression tag	UNP P06756
A	981	ALA	-	expression tag	UNP P06756
A	982	GLN	-	expression tag	UNP P06756
A	983	LEU	-	expression tag	UNP P06756
A	984	GLU	-	expression tag	UNP P06756
A	985	TRP	-	expression tag	UNP P06756
A	986	GLU	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	987	LEU	-	expression tag	UNP P06756
A	988	GLN	-	expression tag	UNP P06756
A	989	ALA	-	expression tag	UNP P06756
A	990	LEU	-	expression tag	UNP P06756
A	991	GLU	-	expression tag	UNP P06756
A	992	LYS	-	expression tag	UNP P06756
A	993	GLU	-	expression tag	UNP P06756
A	994	LEU	-	expression tag	UNP P06756
A	995	GLN	-	expression tag	UNP P06756
A	996	ALA	-	expression tag	UNP P06756
A	997	LEU	-	expression tag	UNP P06756
A	998	CYS	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	709	Total	C	N	O	S	0	0	0
			5454	3359	933	1091	71			

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	692	GLU	-	expression tag	UNP P05106
B	693	SER	-	expression tag	UNP P05106
B	694	MET	-	expression tag	UNP P05106
B	695	GLU	-	expression tag	UNP P05106
B	696	ASN	-	expression tag	UNP P05106
B	697	LEU	-	expression tag	UNP P05106
B	698	TYR	-	expression tag	UNP P05106
B	699	PHE	-	expression tag	UNP P05106
B	700	GLN	-	expression tag	UNP P05106
B	701	SER	-	expression tag	UNP P05106
B	702	GLY	-	expression tag	UNP P05106
B	703	GLY	-	expression tag	UNP P05106
B	704	LYS	-	expression tag	UNP P05106
B	705	ASN	-	expression tag	UNP P05106
B	706	ALA	-	expression tag	UNP P05106
B	707	GLN	-	expression tag	UNP P05106
B	708	CYS	-	expression tag	UNP P05106
B	709	LYS	-	expression tag	UNP P05106
B	710	LYS	-	expression tag	UNP P05106
B	711	LYS	-	expression tag	UNP P05106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	712	LEU	-	expression tag	UNP P05106
B	713	GLN	-	expression tag	UNP P05106
B	714	ALA	-	expression tag	UNP P05106
B	715	LEU	-	expression tag	UNP P05106
B	716	LYS	-	expression tag	UNP P05106
B	717	LYS	-	expression tag	UNP P05106
B	718	LYS	-	expression tag	UNP P05106
B	719	ASN	-	expression tag	UNP P05106
B	720	ALA	-	expression tag	UNP P05106
B	721	GLN	-	expression tag	UNP P05106
B	722	LEU	-	expression tag	UNP P05106
B	723	LYS	-	expression tag	UNP P05106
B	724	TRP	-	expression tag	UNP P05106
B	725	LYS	-	expression tag	UNP P05106
B	726	LEU	-	expression tag	UNP P05106
B	727	GLN	-	expression tag	UNP P05106
B	728	ALA	-	expression tag	UNP P05106
B	729	LEU	-	expression tag	UNP P05106
B	730	CYS	-	expression tag	UNP P05106
B	731	THR	-	expression tag	UNP P05106
B	732	GLY	-	expression tag	UNP P05106
B	733	HIS	-	expression tag	UNP P05106
B	734	HIS	-	expression tag	UNP P05106
B	735	HIS	-	expression tag	UNP P05106
B	736	HIS	-	expression tag	UNP P05106
B	737	HIS	-	expression tag	UNP P05106
B	738	HIS	-	expression tag	UNP P05106

- Molecule 3 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
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

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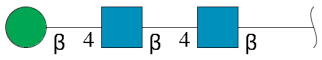
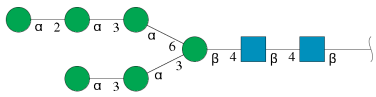
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	O	4	Total C N O 50 28 2 20	0	0	0

- Molecule 4 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
4	D	3	Total C N O 39 22 2 15	0	0	0
4	H	3	Total C N O 39 22 2 15	0	0	0
4	N	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)-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
5	E	8	Total C N O 94 52 2 40	0	0	0

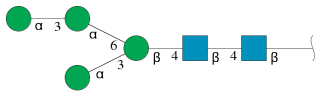
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

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

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.

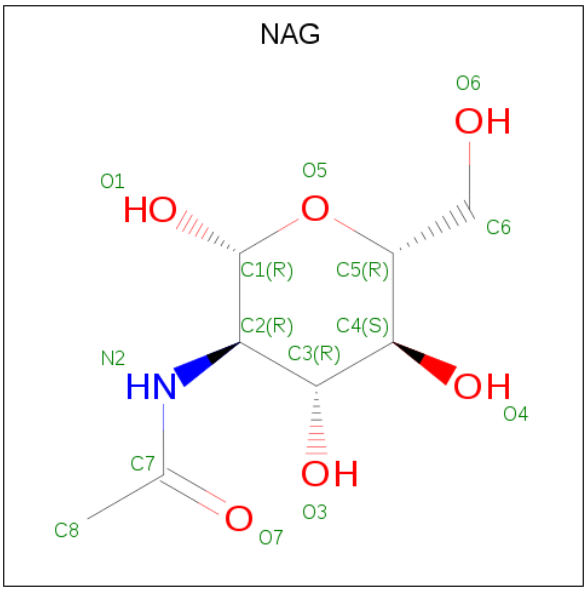


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	I	6	Total C N O 72 40 2 30	0	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

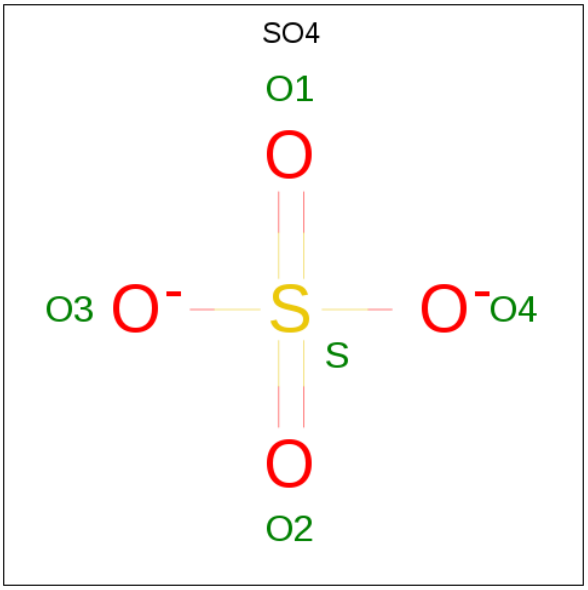
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Ca 1 1	0	0
9	A	5	Total Ca 5 5	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	3	Total Cl 3 3	0	0
12	A	4	Total Cl 4 4	0	0

- Molecule 13 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Ni 1 1	0	0

- Molecule 14 is water.

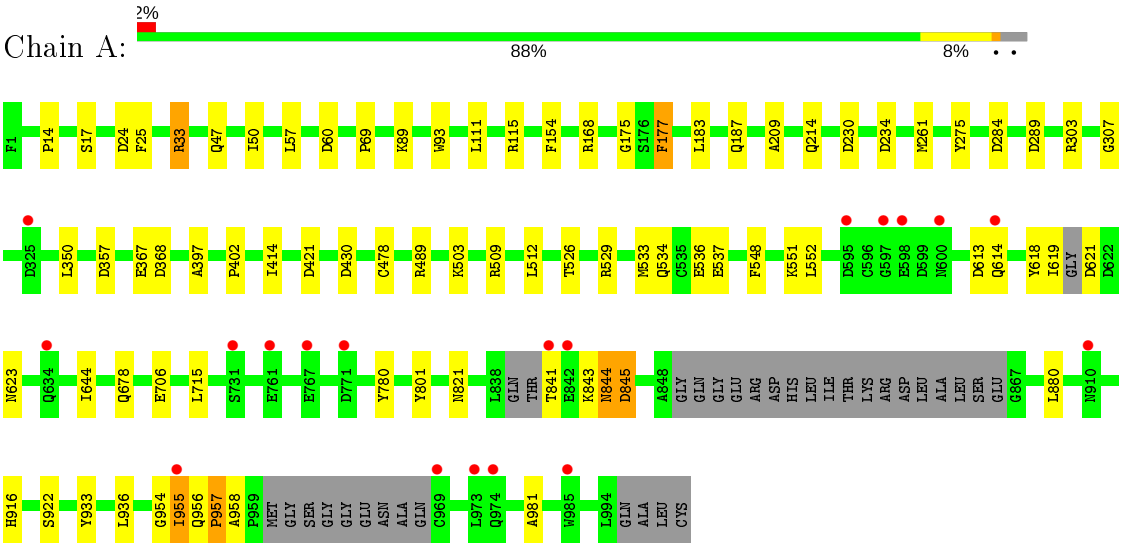
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	60	Total O 60 60	0	0
14	B	39	Total O 39 39	0	0

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.

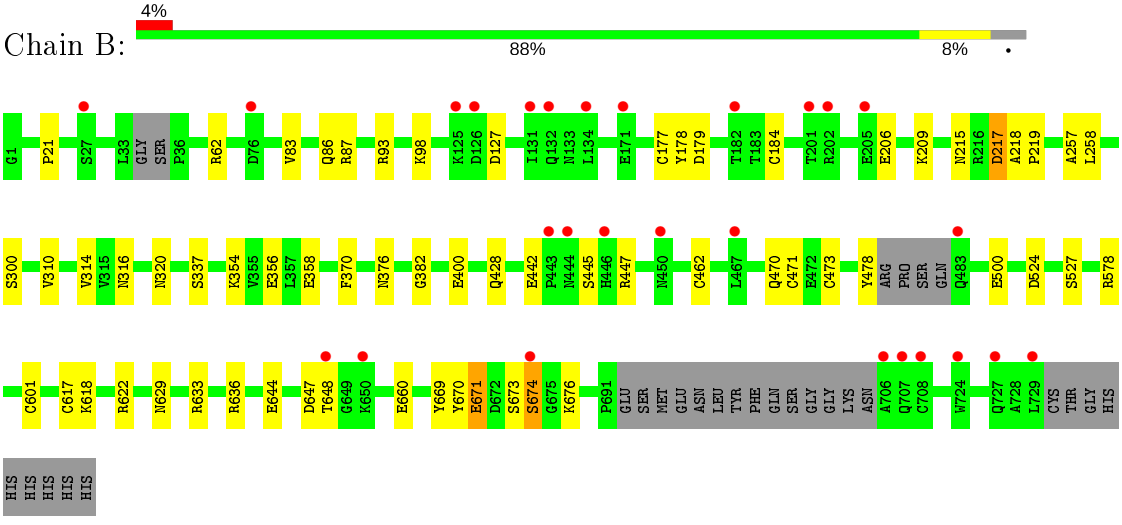
• Molecule 1: Integrin alpha-V

Chain A:



• Molecule 2: Integrin beta-3

Chain B:



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

Chain M:

• Molecule 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 O:

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

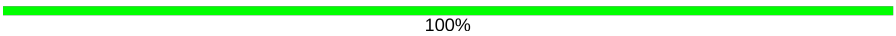
Chain D:

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

Chain H:

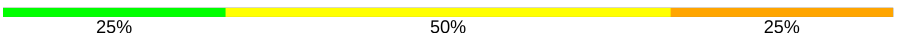
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

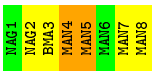
Chain N:



• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)-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 E:



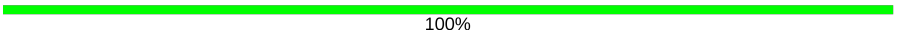


• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

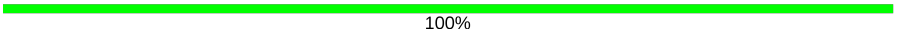
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



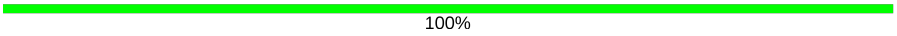
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



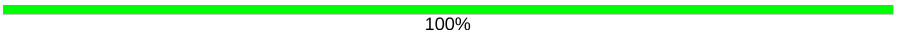
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



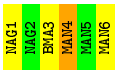
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• Molecule 8: alpha-D-mannopyranose-(1-3)-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 I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.56Å 128.56Å 352.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 3.00 47.52 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.52-3.00) 100.0 (47.52-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.241 , 0.261 0.245 , 0.267	Depositor DCC
R_{free} test set	1168 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 98.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: NI, BMA, NAG, CL, CA, SO4, 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	0.21	0/7669	0.37	0/10392
2	B	0.22	0/5549	0.36	0/7493
All	All	0.21	0/13218	0.37	0/17885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7512	0	7319	44	1
2	B	5454	0	5220	35	1
3	C	50	0	43	1	0
3	M	50	0	43	1	0
3	O	50	0	43	2	0
4	D	39	0	34	0	0
4	H	39	0	34	0	0
4	N	39	0	34	0	0
5	E	94	0	79	2	0
6	F	50	0	43	4	0
7	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	28	0	25	0	0
7	K	28	0	25	0	0
7	L	28	0	25	0	0
8	I	72	0	61	4	0
9	A	5	0	0	0	0
9	B	1	0	0	0	0
10	A	28	0	26	0	0
11	A	15	0	0	0	0
11	B	15	0	0	0	0
12	A	4	0	0	0	0
12	B	3	0	0	0	0
13	A	1	0	0	0	0
14	A	60	0	0	1	0
14	B	39	0	0	1	0
All	All	13732	0	13079	86	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:CYS:N	2:B:184:CYS:SG	2.62	0.73
1:A:503:LYS:O	1:A:509:ARG:NH1	2.21	0.73
6:F:3:BMA:H4	6:F:4:MAN:H2	1.71	0.71
1:A:618:TYR:O	1:A:623:ASN:ND2	2.25	0.70
2:B:87:ARG:NH1	2:B:428:GLN:OE1	2.25	0.69
1:A:619:ILE:O	1:A:621:ASP:N	2.26	0.68
2:B:21:PRO:O	2:B:93:ARG:NH1	2.29	0.65
2:B:617:CYS:SG	2:B:618:LYS:N	2.73	0.61
1:A:303:ARG:NH1	1:A:307:GLY:O	2.34	0.61
2:B:447:ARG:O	2:B:470:GLN:NE2	2.34	0.60
6:F:3:BMA:C4	6:F:4:MAN:H2	2.31	0.60
8:I:3:BMA:H61	8:I:4:MAN:H3	1.83	0.60
1:A:24:ASP:OD1	1:A:25:PHE:N	2.39	0.56
2:B:300:SER:OG	2:B:358:GLU:OE1	2.24	0.55
2:B:462:CYS:SG	2:B:471:CYS:N	2.79	0.55
2:B:633:ARG:O	2:B:636:ARG:NH1	2.40	0.55
3:C:2:NAG:O3	3:C:3:BMA:H2	2.07	0.55
1:A:526:THR:O	1:A:534:GLN:NE2	2.40	0.54
1:A:780:TYR:OH	1:A:922:SER:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:OD2	1:A:289:ASP:N	2.37	0.53
2:B:400:GLU:HB2	3:M:1:NAG:H83	1.90	0.52
1:A:844:ASN:ND2	2:B:671:GLU:OE1	2.43	0.52
2:B:83:VAL:O	2:B:86:GLN:NE2	2.43	0.51
1:A:548:PHE:O	1:A:551:LYS:NZ	2.44	0.50
6:F:3:BMA:H4	6:F:4:MAN:C2	2.41	0.50
1:A:489:ARG:HA	1:A:529:ARG:NH1	2.27	0.50
2:B:310:VAL:HB	2:B:314:VAL:HG23	1.94	0.50
2:B:370:PHE:O	2:B:382:GLY:N	2.41	0.50
2:B:671:GLU:OE2	2:B:671:GLU:HA	2.12	0.49
1:A:214:GLN:OE1	1:A:214:GLN:N	2.44	0.49
1:A:956:GLN:N	1:A:957:PRO:CD	2.76	0.48
2:B:644:GLU:OE1	3:O:2:NAG:H81	2.12	0.48
1:A:706:GLU:N	14:A:2132:HOH:O	2.45	0.48
2:B:376:ASN:OD1	2:B:629:ASN:ND2	2.46	0.48
8:I:3:BMA:H61	8:I:4:MAN:C3	2.38	0.47
2:B:316:ASN:O	2:B:320:ASN:ND2	2.45	0.47
1:A:261:MET:HG3	1:A:261:MET:O	2.15	0.47
1:A:230:ASP:OD2	1:A:234:ASP:O	2.33	0.47
2:B:578:ARG:NH1	2:B:601:CYS:HB3	2.30	0.46
1:A:50:ILE:HD13	1:A:89:LYS:HB2	1.97	0.46
1:A:168:ARG:NH1	1:A:187:GLN:HG3	2.31	0.45
6:F:3:BMA:C4	6:F:4:MAN:C2	2.93	0.45
1:A:14:PRO:O	1:A:430:ASP:OD2	2.35	0.45
2:B:622:ARG:NH1	2:B:660:GLU:HB2	2.31	0.45
1:A:845:ASP:O	2:B:578:ARG:NH1	2.46	0.44
2:B:473:CYS:HB3	2:B:478:TYR:CE1	2.52	0.44
5:E:4:MAN:H2	5:E:5:MAN:H2	1.99	0.44
1:A:956:GLN:N	1:A:957:PRO:HD3	2.32	0.44
1:A:414:ILE:HG22	1:A:421:ASP:OD2	2.18	0.44
1:A:397:ALA:HB2	1:A:402:PRO:HD3	2.00	0.44
2:B:316:ASN:ND2	14:B:2124:HOH:O	2.51	0.44
1:A:933:TYR:HB3	1:A:936:LEU:HD23	2.00	0.44
2:B:127:ASP:OD2	2:B:337:SER:HB2	2.17	0.44
1:A:33:ARG:NH2	1:A:60:ASP:OD1	2.51	0.43
2:B:257:ALA:O	2:B:258:LEU:HB2	2.17	0.43
5:E:4:MAN:O2	5:E:5:MAN:C1	2.66	0.43
2:B:178:TYR:CG	2:B:179:ASP:N	2.87	0.43
1:A:954:GLY:C	1:A:955:ILE:HG13	2.39	0.43
2:B:669:TYR:OH	8:I:1:NAG:O6	2.33	0.42
1:A:14:PRO:O	1:A:17:SER:OG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HD11	1:A:678:GLN:HB3	2.00	0.42
1:A:154:PHE:O	1:A:175:GLY:HA3	2.19	0.42
1:A:613:ASP:O	1:A:614:GLN:HB3	2.20	0.42
1:A:916:HIS:NE2	1:A:981:ALA:HB1	2.34	0.42
1:A:478:CYS:HB3	1:A:533:MET:SD	2.60	0.42
1:A:93:TRP:CD1	1:A:111:LEU:HD22	2.55	0.42
2:B:648:THR:HG1	2:B:670:TYR:HD1	1.63	0.42
1:A:715:LEU:HD12	1:A:715:LEU:N	2.35	0.41
1:A:801:TYR:HB2	1:A:880:LEU:HB2	2.02	0.41
1:A:47:GLN:HB3	1:A:50:ILE:HD12	2.02	0.41
1:A:183:LEU:O	1:A:209:ALA:HA	2.20	0.41
2:B:218:ALA:N	2:B:219:PRO:CD	2.84	0.41
1:A:367:GLU:O	1:A:368:ASP:HB2	2.20	0.41
8:I:3:BMA:O2	8:I:6:MAN:H2	2.20	0.41
1:A:350:LEU:N	1:A:357:ASP:OD2	2.44	0.41
2:B:524:ASP:OD2	2:B:527:SER:OG	2.39	0.41
1:A:115:ARG:HG2	1:A:115:ARG:O	2.21	0.41
1:A:536:GLU:HG2	1:A:537:GLU:N	2.36	0.41
2:B:647:ASP:OD2	3:O:2:NAG:O6	2.28	0.41
1:A:552:LEU:HB3	2:B:500:GLU:HG2	2.02	0.41
2:B:206:GLU:OE2	2:B:209:LYS:HD2	2.20	0.41
2:B:354:LYS:NZ	2:B:356:GLU:HB2	2.36	0.41
2:B:673:SER:O	2:B:674:SER:CB	2.69	0.41
2:B:442:GLU:HB3	2:B:445:SER:HB3	2.02	0.40
1:A:177:PHE:N	1:A:177:PHE:CD1	2.87	0.40
1:A:57:LEU:HA	1:A:69:PRO:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:ALA:O	2:B:62:ARG:NH1[4_555]	2.17	0.03

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	954/998 (96%)	900 (94%)	50 (5%)	4 (0%)	34 72
2	B	701/738 (95%)	669 (95%)	31 (4%)	1 (0%)	51 85
All	All	1655/1736 (95%)	1569 (95%)	81 (5%)	5 (0%)	41 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	843	LYS
2	B	217	ASP
1	A	957	PRO
1	A	955	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	819/844 (97%)	812 (99%)	7 (1%)	78 92
2	B	628/653 (96%)	622 (99%)	6 (1%)	76 91
All	All	1447/1497 (97%)	1434 (99%)	13 (1%)	78 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	PHE
1	A	275	TYR
1	A	512	LEU
1	A	821	ASN
1	A	841	THR
1	A	844	ASN
1	A	845	ASP
2	B	98	LYS

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Mol	Chain	Res	Type
2	B	215	ASN
2	B	217	ASP
2	B	671	GLU
2	B	674	SER
2	B	676	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	623	ASN
2	B	376	ASN
2	B	629	ASN

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

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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	0.63	0
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	1.50	4 (23%)
3	BMA	C	3	3	11,11,12	0.49	0	15,15,17	1.14	1 (6%)
3	MAN	C	4	3	11,11,12	0.65	0	15,15,17	0.66	0
4	NAG	D	1	1,4	14,14,15	0.53	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	0.67	0
4	BMA	D	3	4	11,11,12	0.70	0	15,15,17	0.70	0
5	NAG	E	1	1,5	14,14,15	0.58	0	17,19,21	0.80	0
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	0.82	1 (5%)
5	BMA	E	3	5	11,11,12	0.83	1 (9%)	15,15,17	0.92	0
5	MAN	E	4	5	11,11,12	0.60	0	15,15,17	1.35	3 (20%)
5	MAN	E	5	5	11,11,12	0.65	0	15,15,17	1.12	1 (6%)
5	MAN	E	6	5	11,11,12	0.63	0	15,15,17	0.69	0
5	MAN	E	7	5	11,11,12	0.63	0	15,15,17	1.39	3 (20%)
5	MAN	E	8	5	11,11,12	0.67	0	15,15,17	0.81	1 (6%)
6	NAG	F	1	1,6	14,14,15	0.56	0	17,19,21	0.71	1 (5%)
6	NAG	F	2	6	14,14,15	0.63	0	17,19,21	1.01	1 (5%)
6	BMA	F	3	6	11,11,12	0.98	0	15,15,17	1.33	2 (13%)
6	MAN	F	4	6	11,11,12	0.67	0	15,15,17	1.32	1 (6%)
7	NAG	G	1	1,7	14,14,15	0.54	0	17,19,21	0.62	0
7	NAG	G	2	7	14,14,15	0.52	0	17,19,21	0.61	0
4	NAG	H	1	1,4	14,14,15	0.53	0	17,19,21	0.68	0
4	NAG	H	2	4	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
4	BMA	H	3	4	11,11,12	0.71	0	15,15,17	0.70	0
8	NAG	I	1	1,8	14,14,15	0.58	0	17,19,21	0.74	0
8	NAG	I	2	8	14,14,15	0.59	0	17,19,21	0.78	0
8	BMA	I	3	8	11,11,12	0.70	0	15,15,17	0.85	0
8	MAN	I	4	8	11,11,12	0.66	0	15,15,17	1.19	3 (20%)
8	MAN	I	5	8	11,11,12	0.63	0	15,15,17	0.70	0
8	MAN	I	6	8	11,11,12	0.66	0	15,15,17	0.77	0
7	NAG	J	1	1,7	14,14,15	0.54	0	17,19,21	0.68	0
7	NAG	J	2	7	14,14,15	0.52	0	17,19,21	0.68	0
7	NAG	K	1	2,7	14,14,15	0.56	0	17,19,21	0.61	0
7	NAG	K	2	7	14,14,15	0.52	0	17,19,21	0.72	0
7	NAG	L	1	2,7	14,14,15	0.62	0	17,19,21	0.71	0
7	NAG	L	2	7	14,14,15	0.51	0	17,19,21	0.63	0
3	NAG	M	1	3,2	14,14,15	0.52	0	17,19,21	0.76	0
3	NAG	M	2	3	14,14,15	0.56	0	17,19,21	0.71	0
3	BMA	M	3	3	11,11,12	0.59	0	15,15,17	0.77	0
3	MAN	M	4	3	11,11,12	0.67	0	15,15,17	0.80	0
4	NAG	N	1	2,4	14,14,15	0.52	0	17,19,21	0.75	0
4	NAG	N	2	4	14,14,15	0.55	0	17,19,21	0.64	0
4	BMA	N	3	4	11,11,12	0.63	0	15,15,17	0.78	0
3	NAG	O	1	3,2	14,14,15	0.60	0	17,19,21	0.68	0
3	NAG	O	2	3	14,14,15	0.60	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	O	3	3	11,11,12	0.72	0	15,15,17	0.75	0
3	MAN	O	4	3	11,11,12	0.67	0	15,15,17	0.76	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
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	1/2/19/22	0/1/1/1
5	MAN	E	8	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
8	NAG	I	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1
8	BMA	I	3	8	-	2/2/19/22	0/1/1/1
8	MAN	I	4	8	-	1/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
8	MAN	I	6	8	-	0/2/19/22	0/1/1/1
7	NAG	J	1	1,7	-	2/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3	BMA	O5-C1	-2.04	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	4	MAN	O5-C1-C2	-4.25	104.20	110.77
5	E	7	MAN	C1-C2-C3	-3.50	105.36	109.67
3	C	3	BMA	C1-O5-C5	3.49	116.92	112.19
3	C	2	NAG	O5-C1-C2	3.27	116.45	111.29
5	E	5	MAN	O5-C1-C2	-3.27	105.72	110.77
3	C	2	NAG	C1-O5-C5	3.17	116.49	112.19
5	E	4	MAN	O3-C3-C2	2.95	115.64	109.99
6	F	3	BMA	C1-C2-C3	2.67	112.95	109.67
8	I	4	MAN	C1-C2-C3	2.52	112.77	109.67
5	E	7	MAN	O5-C1-C2	-2.44	107.00	110.77
3	C	2	NAG	O4-C4-C3	2.43	115.97	110.35
6	F	3	BMA	O5-C1-C2	2.42	114.50	110.77
5	E	2	NAG	O5-C5-C6	2.41	110.98	107.20
5	E	4	MAN	C1-C2-C3	-2.36	106.76	109.67
8	I	4	MAN	O5-C1-C2	-2.34	107.15	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1	NAG	O5-C5-C6	2.25	110.73	107.20
5	E	7	MAN	O3-C3-C2	2.20	114.21	109.99
4	H	2	NAG	C4-C3-C2	2.18	114.21	111.02
6	F	2	NAG	C4-C3-C2	2.10	114.10	111.02
3	O	2	NAG	O5-C1-C2	-2.09	107.99	111.29
4	D	1	NAG	O5-C5-C6	2.06	110.43	107.20
5	E	8	MAN	O5-C1-C2	-2.05	107.61	110.77
5	E	4	MAN	C2-C3-C4	-2.04	107.36	110.89
8	I	4	MAN	O5-C5-C6	2.01	110.35	107.20
3	C	2	NAG	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
7	L	1	NAG	C3-C2-N2-C7
7	L	1	NAG	C8-C7-N2-C2
7	L	1	NAG	O7-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	3	BMA	C4-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
5	E	3	BMA	O5-C5-C6-O6
8	I	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
7	J	2	NAG	C8-C7-N2-C2
8	I	3	BMA	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
4	H	1	NAG	C1-C2-N2-C7
3	C	3	BMA	O5-C5-C6-O6
8	I	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	J	2	NAG	O7-C7-N2-C2
3	O	3	BMA	C4-C5-C6-O6
8	I	2	NAG	C8-C7-N2-C2
3	M	3	BMA	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
5	E	7	MAN	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
8	I	4	MAN	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
6	F	2	NAG	C8-C7-N2-C2
4	H	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C8-C7-N2-C2
8	I	2	NAG	O7-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2

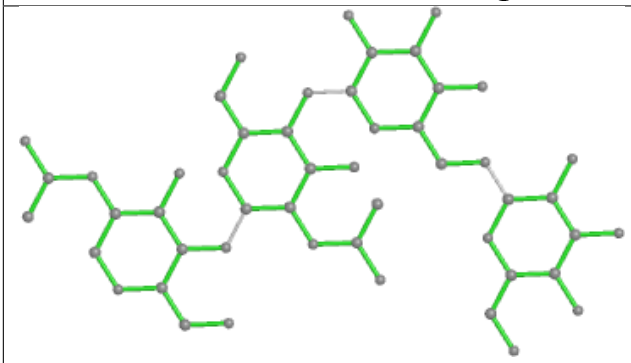
There are no ring outliers.

12 monomers are involved in 14 short contacts:

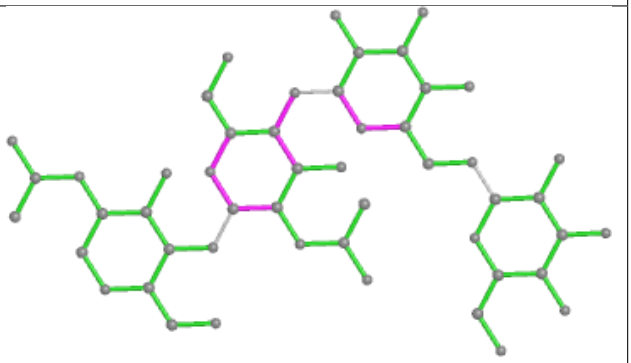
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BMA	1	0
8	I	4	MAN	2	0
5	E	4	MAN	2	0
3	O	2	NAG	2	0
8	I	3	BMA	3	0
5	E	5	MAN	2	0
8	I	6	MAN	1	0
6	F	4	MAN	4	0
8	I	1	NAG	1	0
3	C	2	NAG	1	0
3	M	1	NAG	1	0
6	F	3	BMA	4	0

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

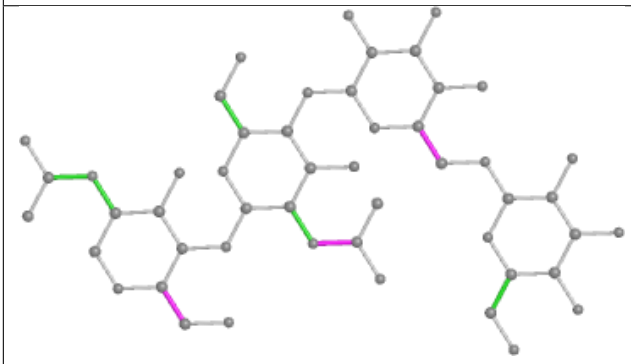
Oligosaccharide Chain C



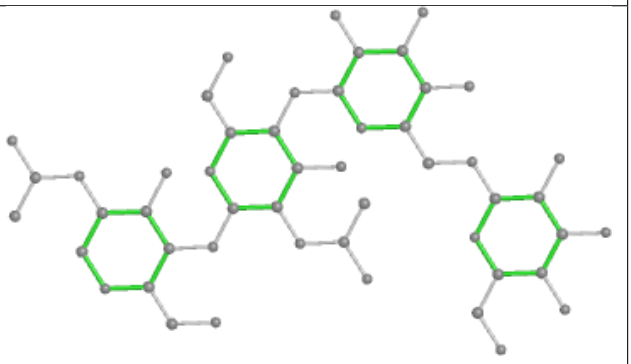
Bond lengths



Bond angles

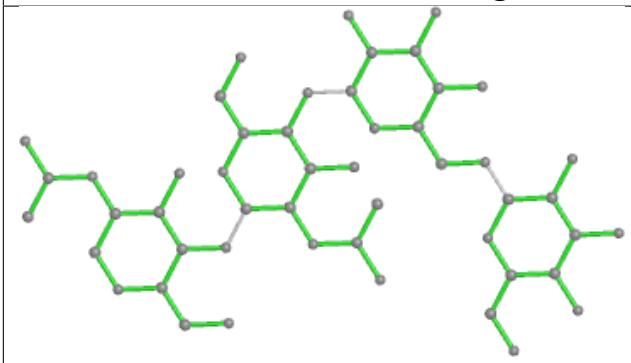


Torsions

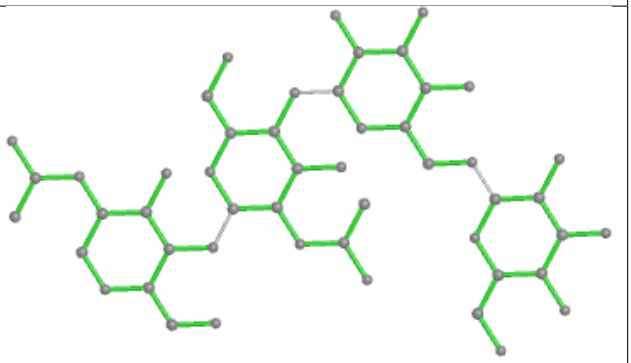


Rings

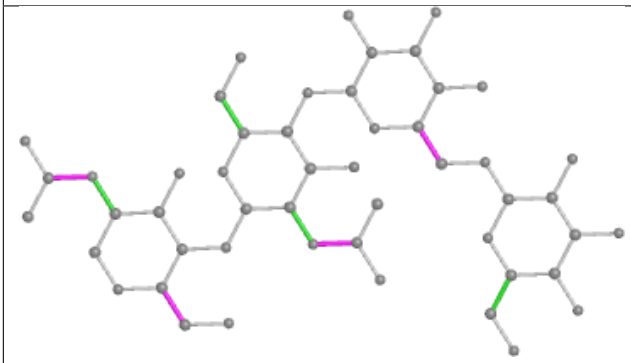
Oligosaccharide Chain M



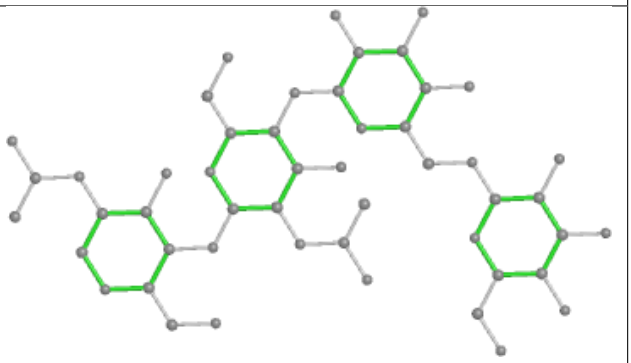
Bond lengths



Bond angles

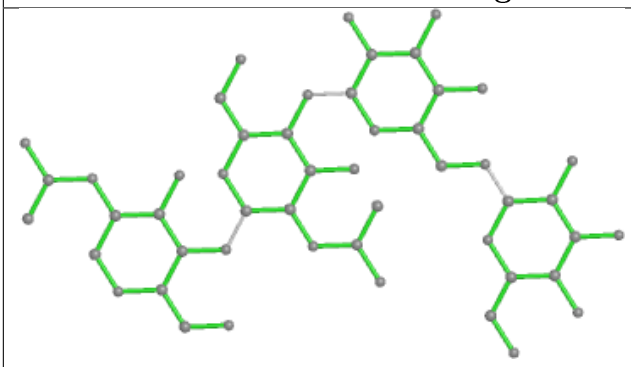


Torsions

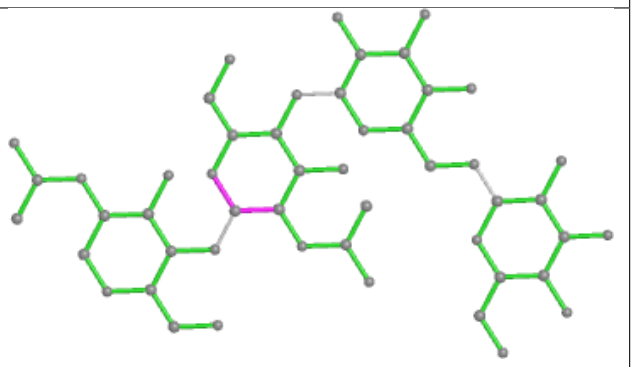


Rings

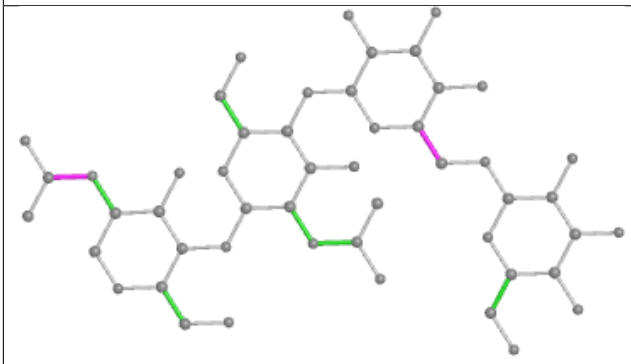
Oligosaccharide Chain O



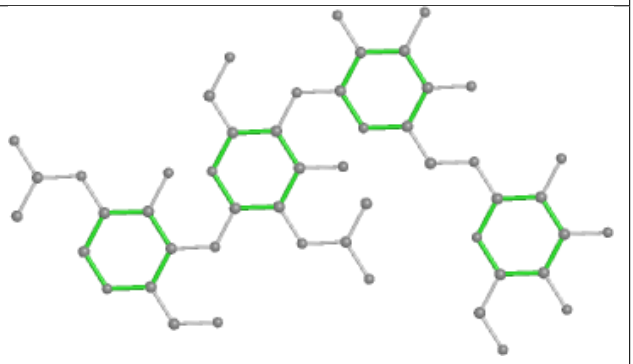
Bond lengths



Bond angles

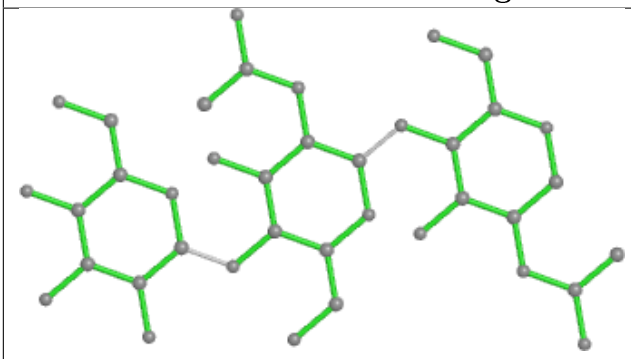


Torsions

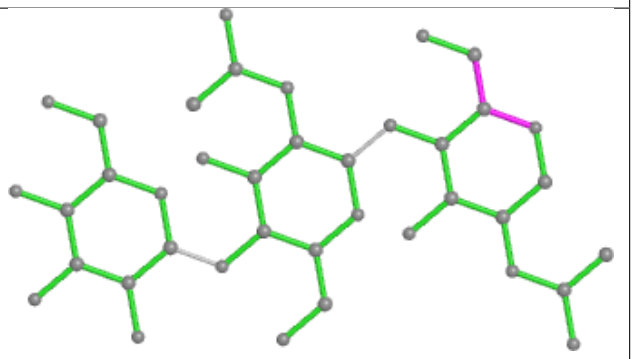


Rings

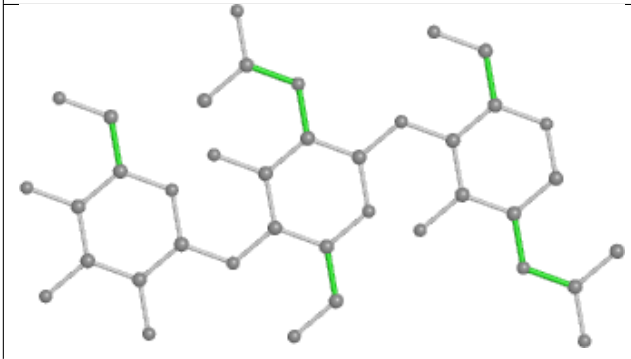
Oligosaccharide Chain D



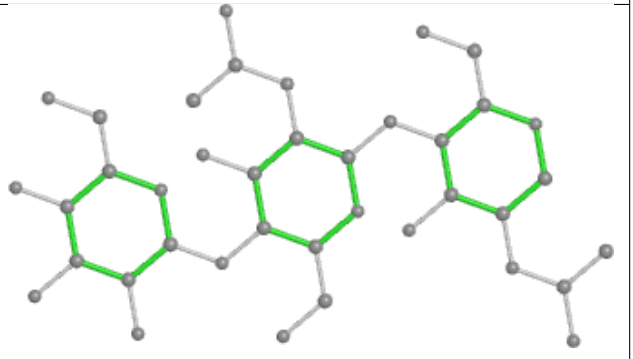
Bond lengths



Bond angles

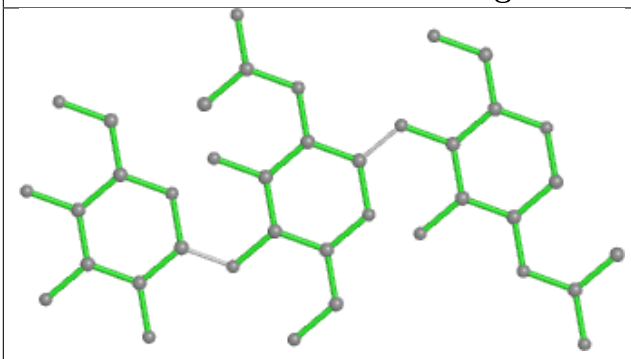


Torsions

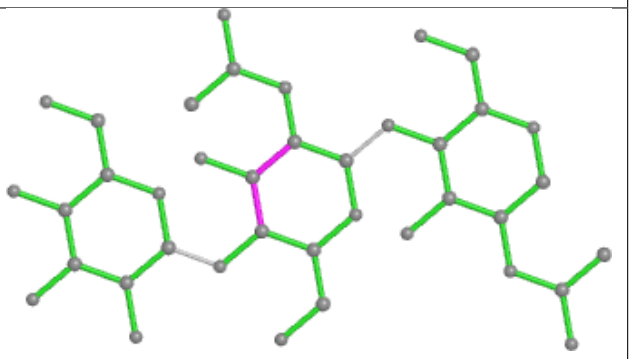


Rings

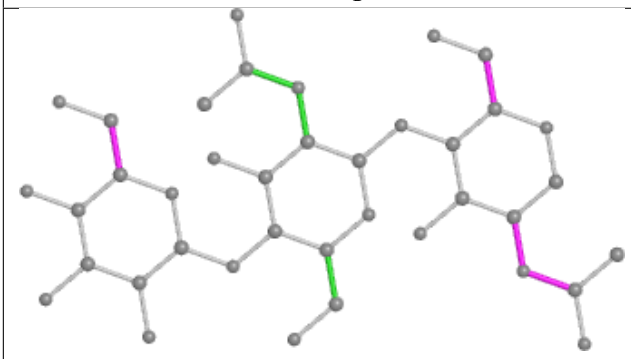
Oligosaccharide Chain H



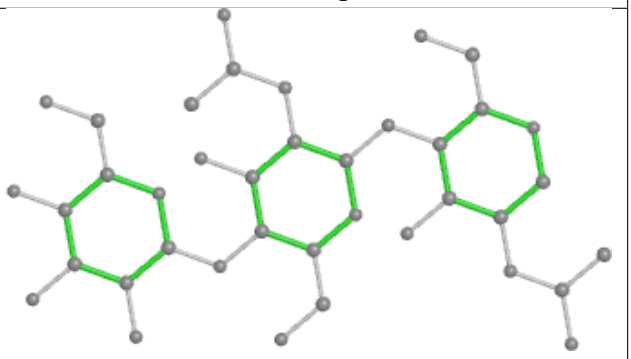
Bond lengths



Bond angles

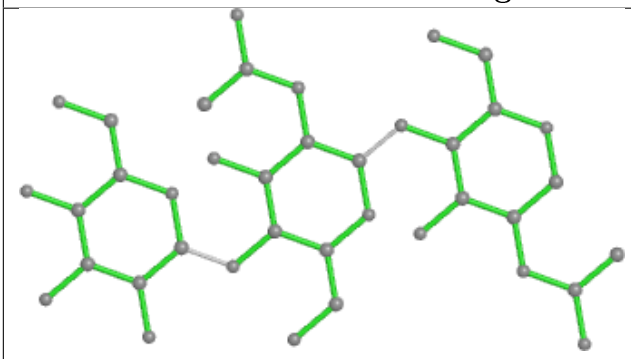


Torsions

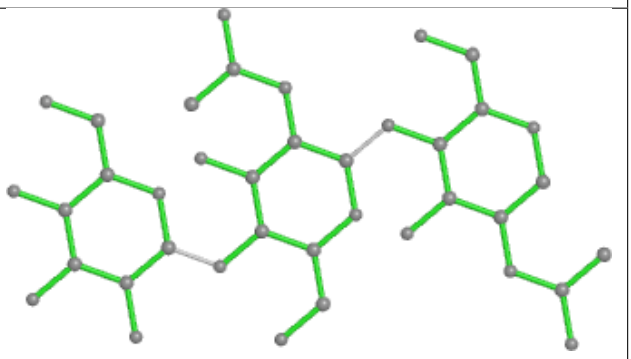


Rings

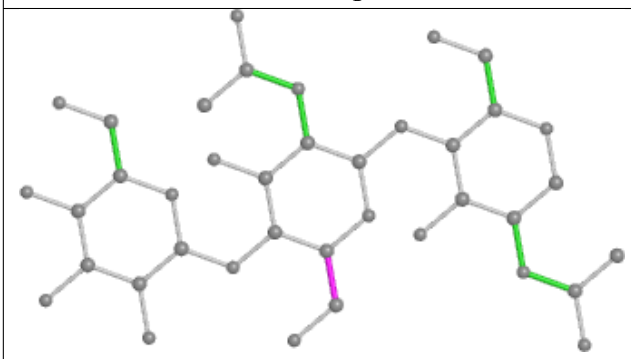
Oligosaccharide Chain N



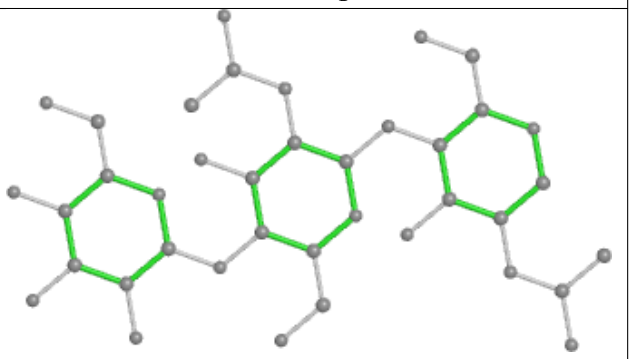
Bond lengths



Bond angles

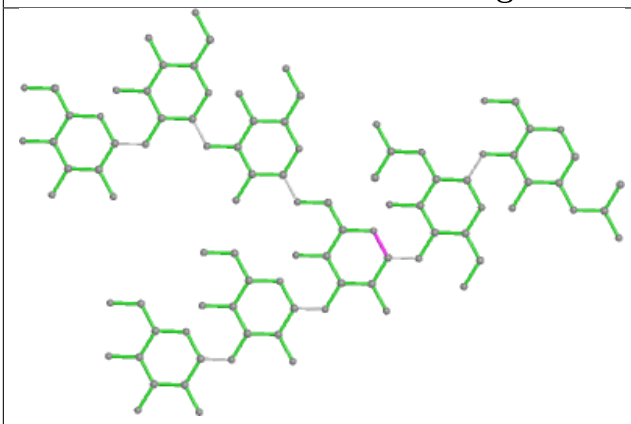


Torsions

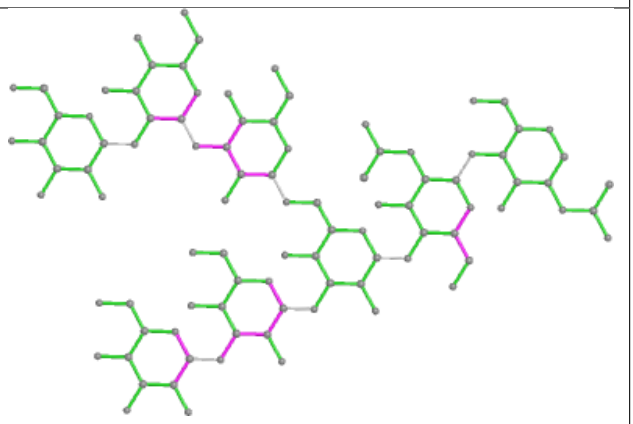


Rings

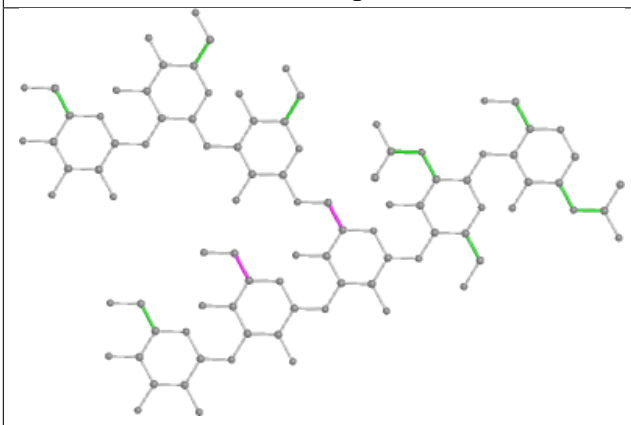
Oligosaccharide Chain E



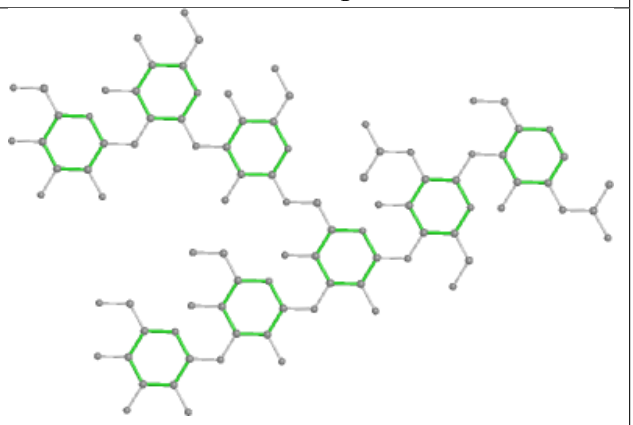
Bond lengths



Bond angles

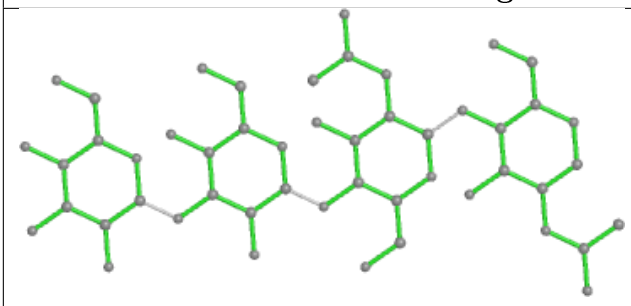


Torsions

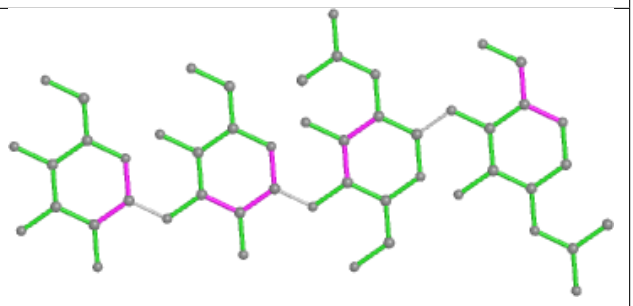


Rings

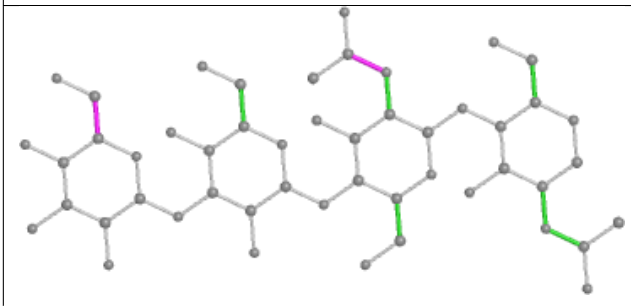
Oligosaccharide Chain F



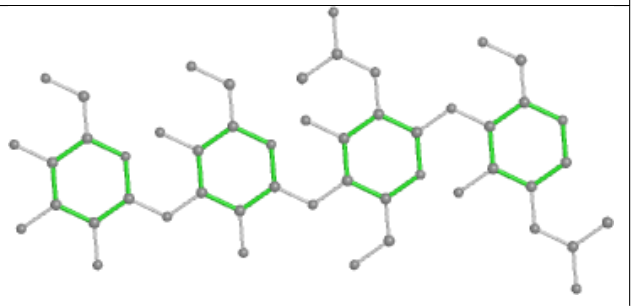
Bond lengths



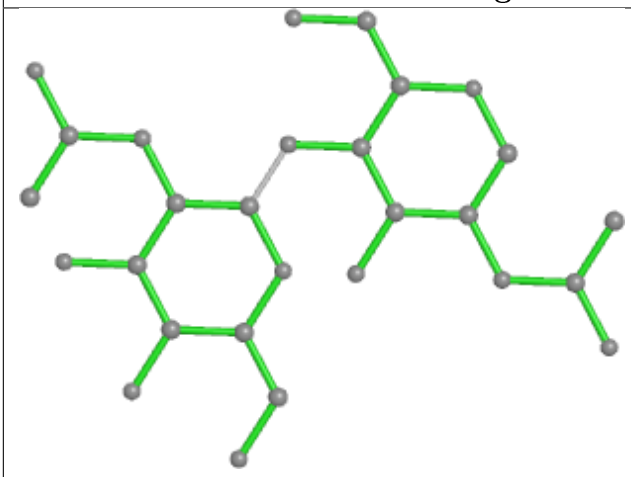
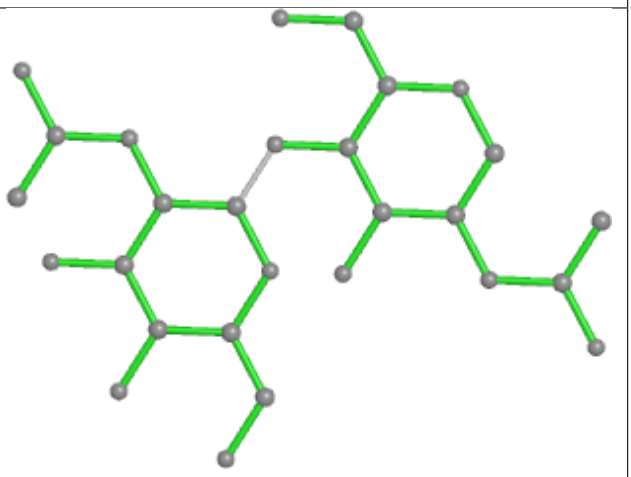
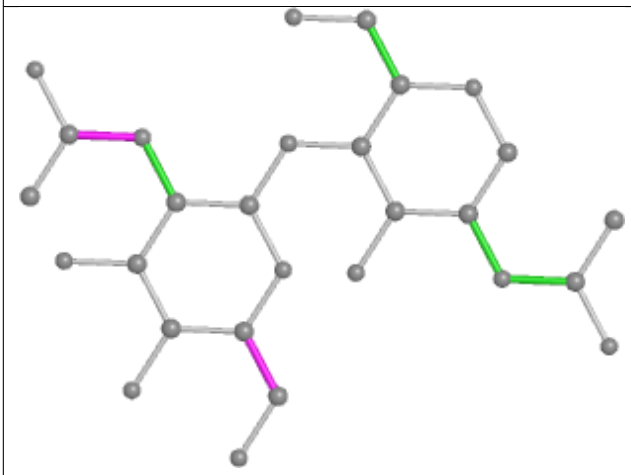
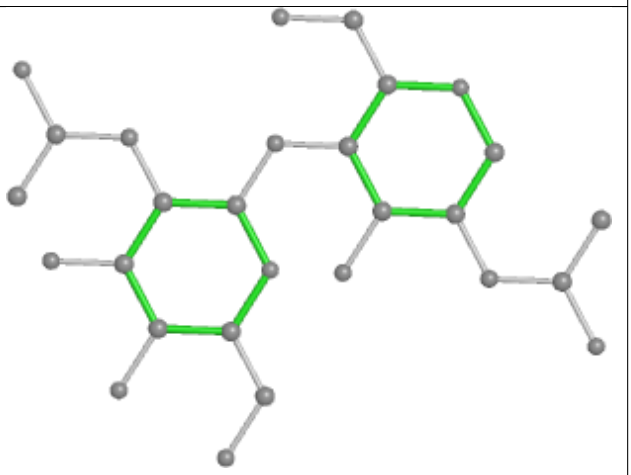
Bond angles



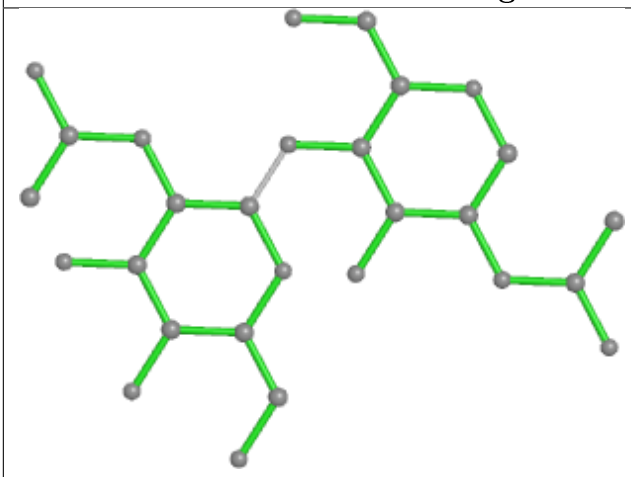
Torsions



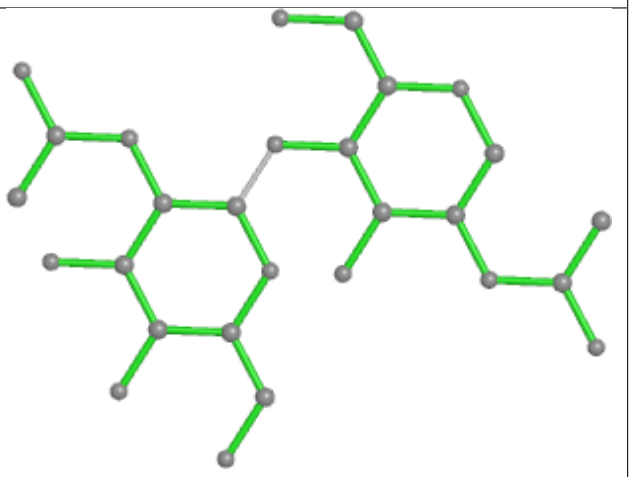
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

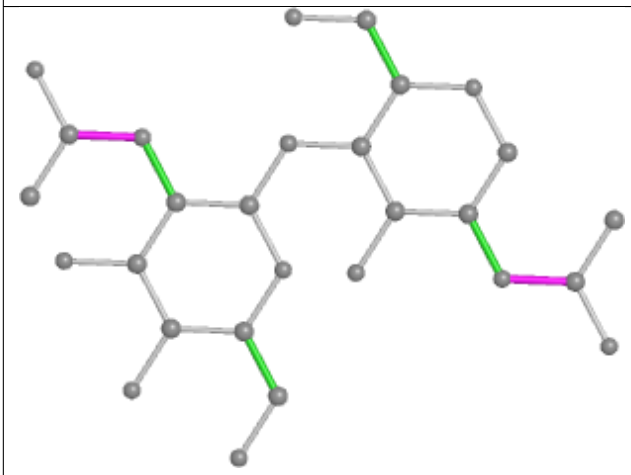
Oligosaccharide Chain J



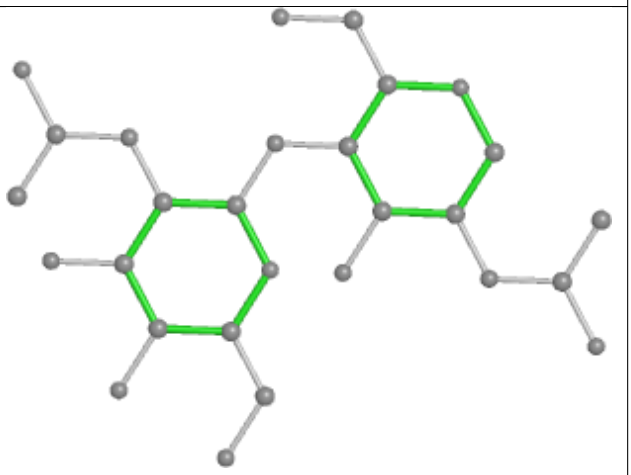
Bond lengths



Bond angles

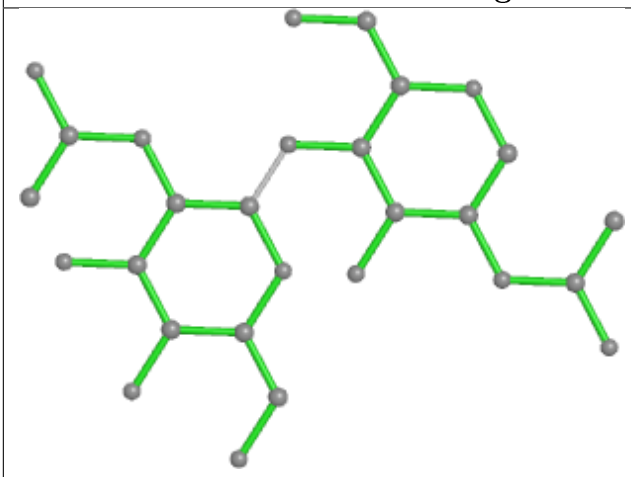


Torsions

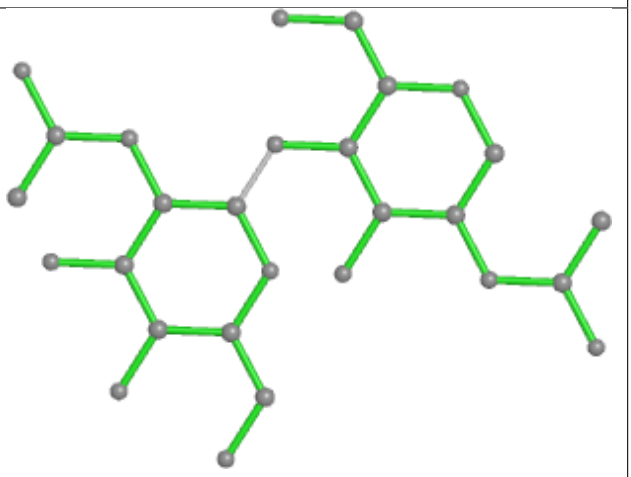


Rings

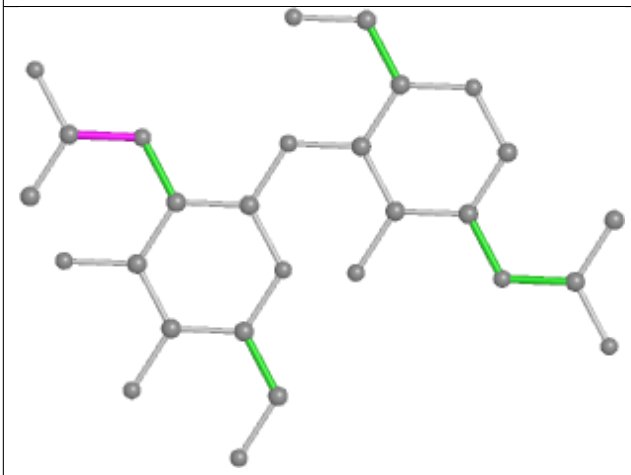
Oligosaccharide Chain K



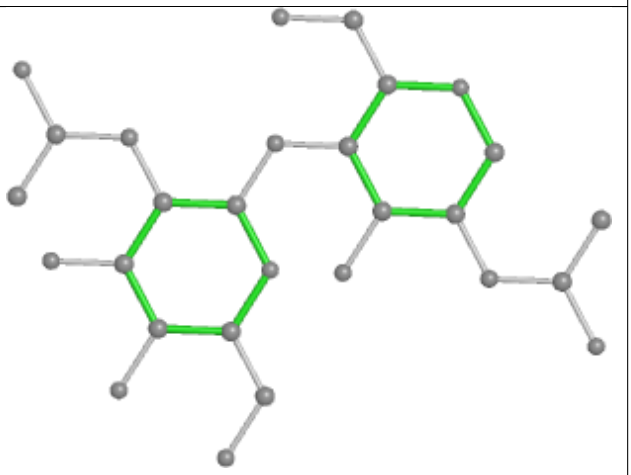
Bond lengths



Bond angles

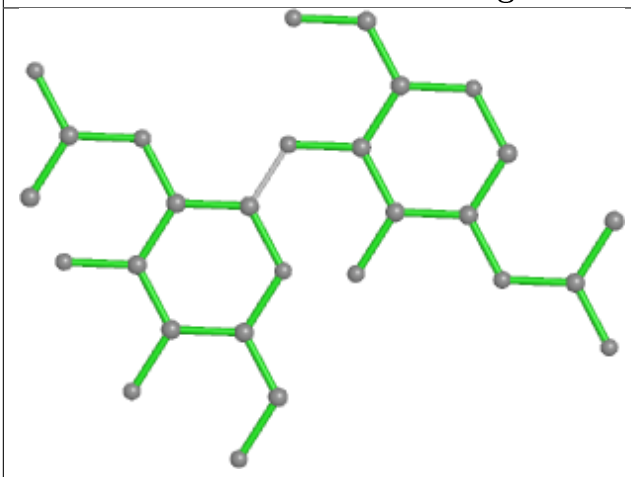


Torsions

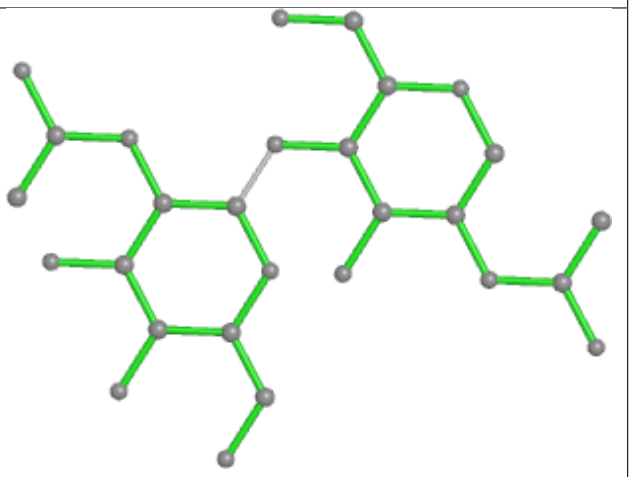


Rings

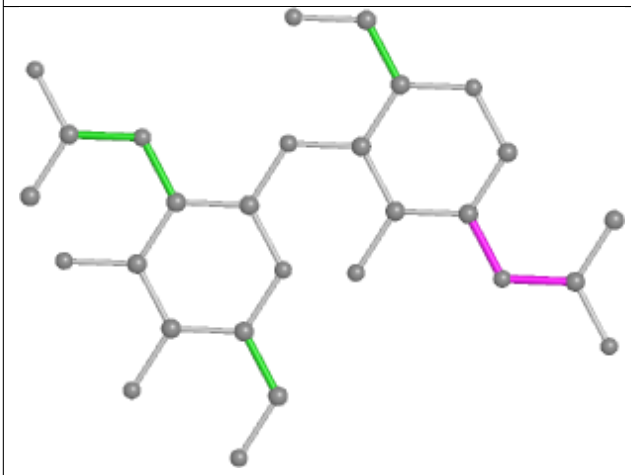
Oligosaccharide Chain L



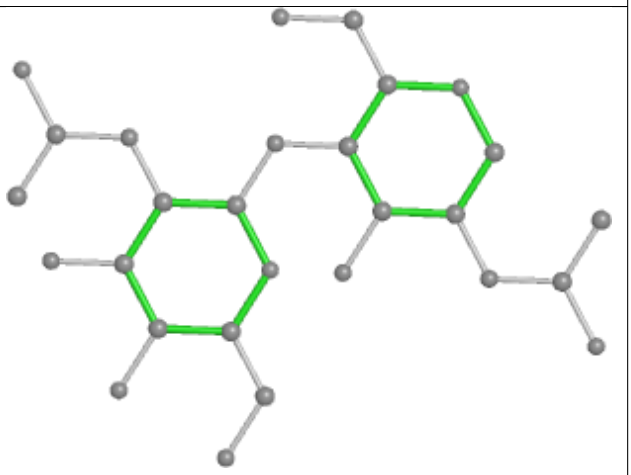
Bond lengths



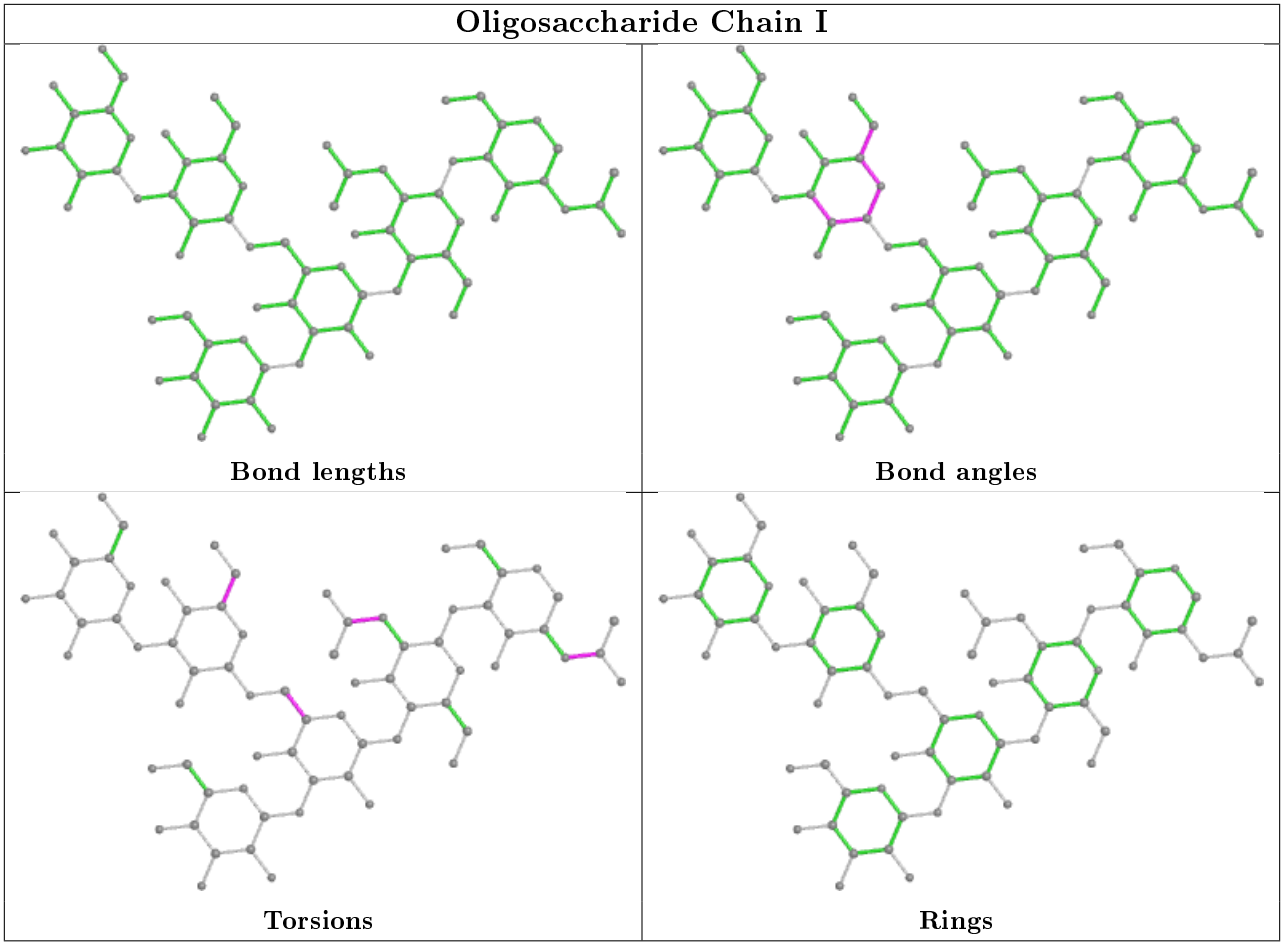
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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	SO4	A	2042	-	4,4,4	0.14	0	6,6,6	0.04	0
10	NAG	A	2025	1	14,14,15	0.57	0	17,19,21	0.71	0
11	SO4	B	2018	-	4,4,4	0.14	0	6,6,6	0.05	0
11	SO4	B	2019	-	4,4,4	0.13	0	6,6,6	0.05	0
11	SO4	A	2040	-	4,4,4	0.15	0	6,6,6	0.04	0
11	SO4	A	2041	-	4,4,4	0.14	0	6,6,6	0.05	0
11	SO4	B	2017	-	4,4,4	0.14	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	A	2039	1	14,14,15	0.52	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	2025	1	-	2/6/23/26	0/1/1/1
10	NAG	A	2039	1	-	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2025	NAG	C8-C7-N2-C2
10	A	2025	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	964/998 (96%)	0.15	19 (1%)	65	36	74, 119, 180, 268	0
2	B	709/738 (96%)	0.16	27 (3%)	40	16	81, 126, 177, 254	0
All	All	1673/1736 (96%)	0.16	46 (2%)	54	26	74, 122, 178, 268	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	598	GLU	5.4
2	B	446	HIS	5.3
1	A	974	GLN	5.3
2	B	706	ALA	5.0
2	B	648	THR	4.2
1	A	597	GLY	4.1
1	A	973	LEU	4.0
1	A	969	CYS	3.9
2	B	27	SER	3.9
2	B	729	LEU	3.8
2	B	707	GLN	3.5
2	B	708	CYS	3.5
1	A	842	GLU	3.4
1	A	910	ASN	3.4
2	B	674	SER	3.4
2	B	182	THR	3.4
1	A	985	TRP	3.3
2	B	467	LEU	3.2
2	B	76	ASP	3.2
1	A	841	THR	3.2
1	A	614	GLN	3.1
1	A	325	ASP	3.0
1	A	731	SER	2.9
1	A	955	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	132	GLN	2.6
2	B	134	LEU	2.6
2	B	727	GLN	2.6
2	B	483	GLN	2.5
1	A	595	ASP	2.5
2	B	126	ASP	2.4
2	B	205	GLU	2.4
1	A	634	GLN	2.3
2	B	125	LYS	2.3
2	B	201	THR	2.3
2	B	131	ILE	2.3
1	A	761	GLU	2.3
1	A	600	ASN	2.2
1	A	771	ASP	2.2
2	B	650	LYS	2.2
2	B	444	ASN	2.2
2	B	450	ASN	2.2
1	A	767	GLU	2.1
2	B	171	GLU	2.0
2	B	724	TRP	2.0
2	B	443	PRO	2.0
2	B	202	ARG	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
4	BMA	D	3	11/12	0.48	0.50	162,180,184,184	0
4	BMA	H	3	11/12	0.50	0.51	131,166,172,175	0
3	BMA	M	3	11/12	0.52	0.35	164,178,186,187	0
3	BMA	O	3	11/12	0.56	0.36	155,172,179,184	0
8	MAN	I	5	11/12	0.56	0.53	186,196,206,206	0
5	MAN	E	8	11/12	0.65	0.44	175,184,191,191	0

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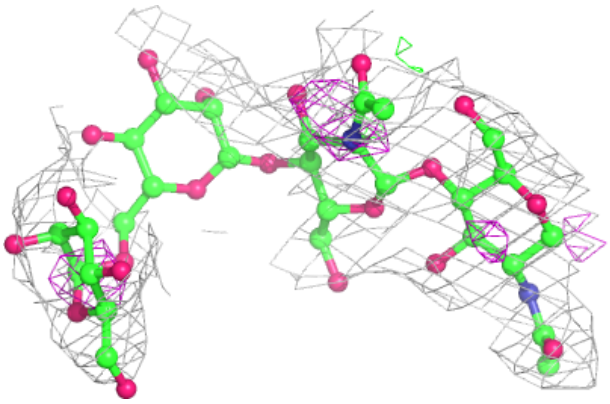
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MAN	I	6	11/12	0.66	0.42	191,208,215,217	0
3	MAN	M	4	11/12	0.66	0.43	130,156,162,163	0
8	MAN	I	4	11/12	0.68	0.34	180,192,207,210	0
3	BMA	C	3	11/12	0.68	0.28	157,163,167,172	0
8	NAG	I	1	14/15	0.72	0.25	167,179,191,198	0
8	NAG	I	2	14/15	0.72	0.31	165,190,195,196	0
7	NAG	J	1	14/15	0.73	0.21	101,150,165,181	0
7	NAG	K	2	14/15	0.73	0.42	172,182,191,192	0
4	BMA	N	3	11/12	0.73	0.27	148,170,176,178	0
4	NAG	H	2	14/15	0.73	0.34	141,166,172,175	0
3	MAN	C	4	11/12	0.73	0.41	148,158,171,173	0
6	NAG	F	2	14/15	0.74	0.18	97,164,173,174	0
7	NAG	G	2	14/15	0.75	0.41	181,197,204,205	0
7	NAG	L	2	14/15	0.75	0.29	143,198,213,218	0
7	NAG	J	2	14/15	0.75	0.37	171,179,183,184	0
4	NAG	H	1	14/15	0.76	0.24	98,150,168,170	0
3	NAG	C	2	14/15	0.76	0.23	123,144,158,160	0
8	BMA	I	3	11/12	0.76	0.27	195,200,203,207	0
5	MAN	E	6	11/12	0.77	0.35	184,194,202,207	0
3	NAG	O	2	14/15	0.78	0.35	174,183,191,193	0
4	NAG	N	2	14/15	0.79	0.18	136,145,162,176	0
7	NAG	L	1	14/15	0.80	0.24	122,155,172,186	0
6	MAN	F	4	11/12	0.80	0.23	150,162,176,179	0
5	MAN	E	5	11/12	0.81	0.24	122,159,167,186	0
5	BMA	E	3	11/12	0.82	0.15	133,145,155,165	0
3	MAN	O	4	11/12	0.84	0.42	160,174,181,183	0
4	NAG	D	2	14/15	0.87	0.39	144,176,189,189	0
7	NAG	K	1	14/15	0.90	0.25	116,140,152,166	0
3	NAG	M	2	14/15	0.90	0.26	143,151,168,173	0
5	MAN	E	7	11/12	0.90	0.23	132,167,174,179	0
6	BMA	F	3	11/12	0.90	0.22	162,173,180,180	0
6	NAG	F	1	14/15	0.91	0.28	121,147,175,176	0
7	NAG	G	1	14/15	0.91	0.23	136,163,178,192	0
5	MAN	E	4	11/12	0.92	0.17	146,156,163,166	0
3	NAG	O	1	14/15	0.92	0.20	87,119,143,159	0
4	NAG	D	1	14/15	0.92	0.25	97,120,152,152	0
4	NAG	N	1	14/15	0.93	0.16	102,123,128,136	0
5	NAG	E	2	14/15	0.94	0.15	87,102,133,135	0
5	NAG	E	1	14/15	0.94	0.20	75,85,110,117	0
3	NAG	M	1	14/15	0.94	0.20	85,121,133,133	0
3	NAG	C	1	14/15	0.95	0.18	78,98,114,119	0

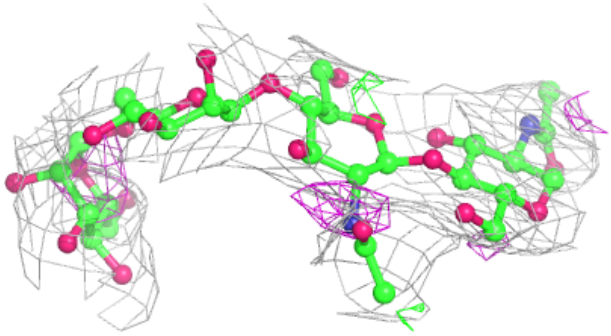
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

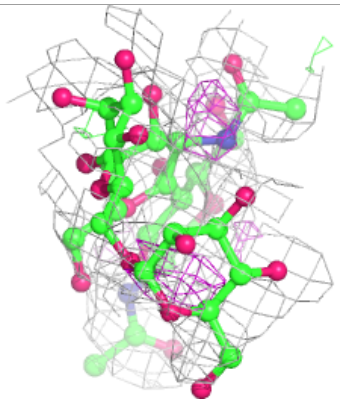
charide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

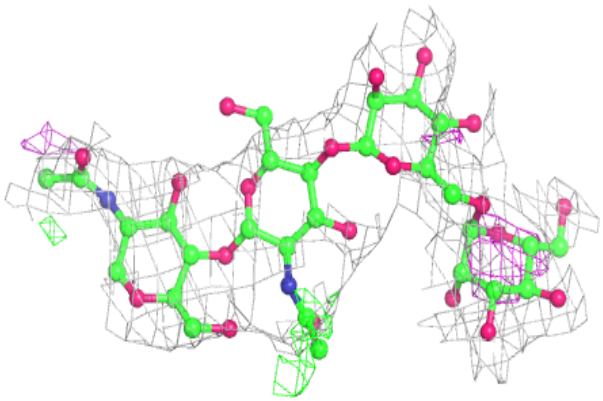


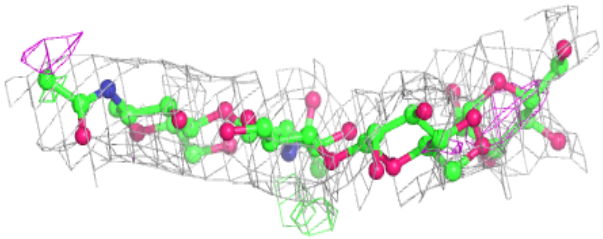


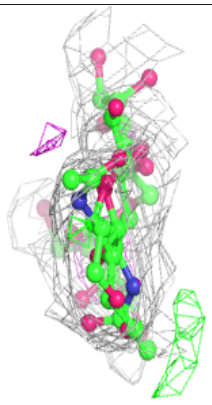


Electron density around Chain M:

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

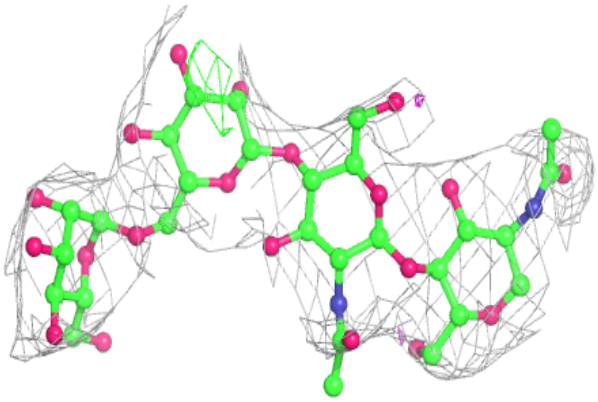


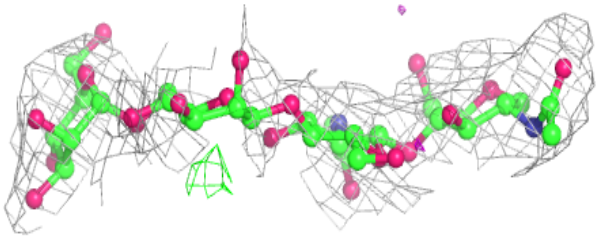


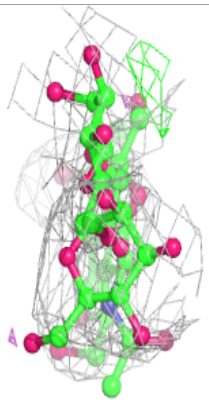


Electron density around Chain O:

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

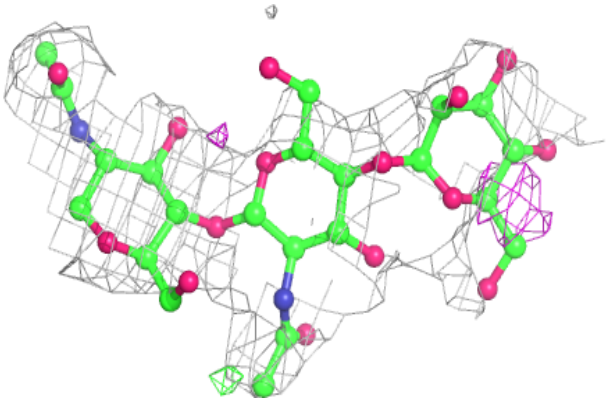


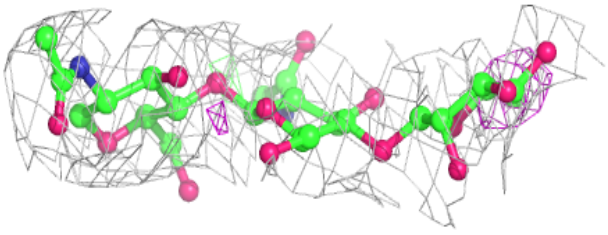


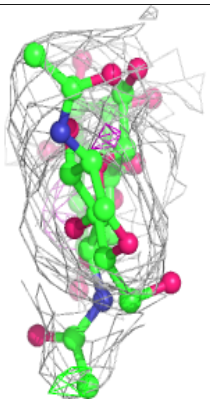


Electron density around Chain D:

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

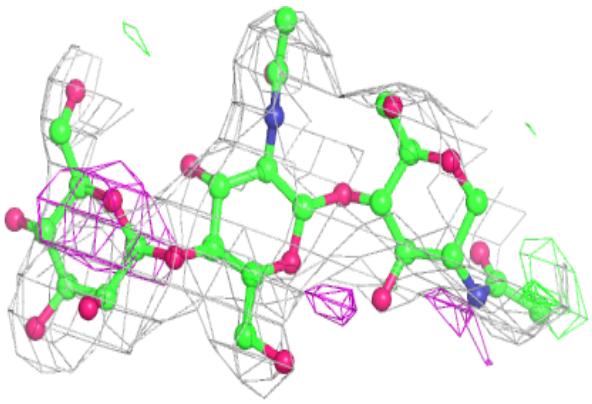


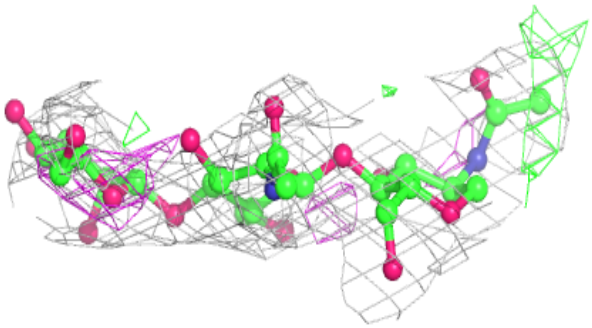




Electron density around Chain H:

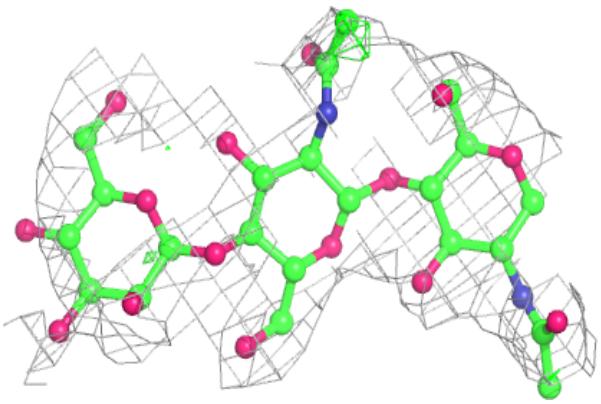
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

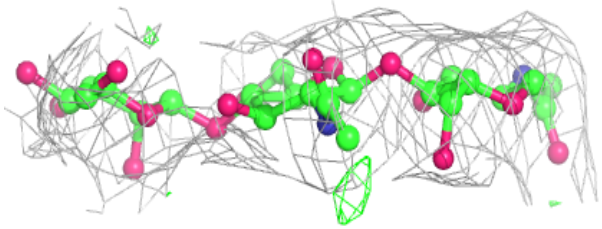


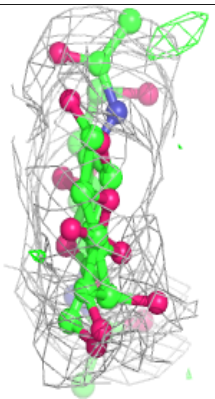


Electron density around Chain N:

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

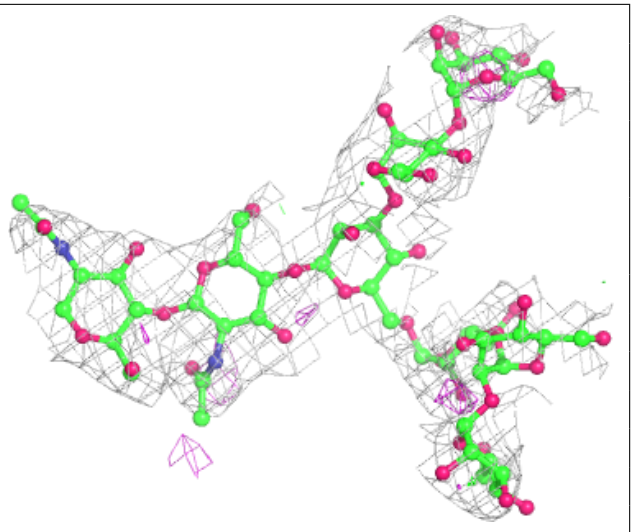


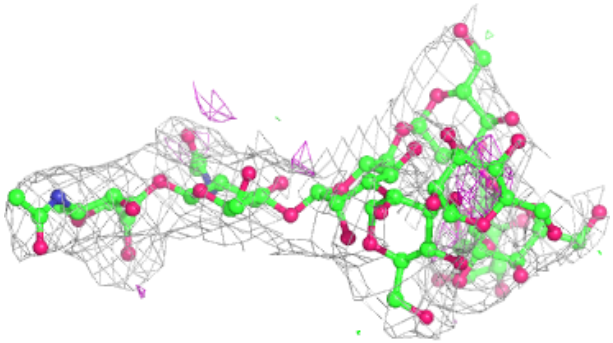


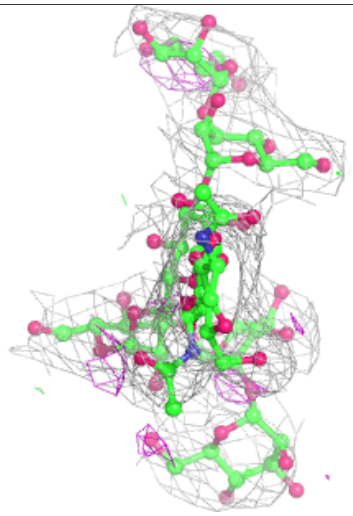


Electron density around Chain E:

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

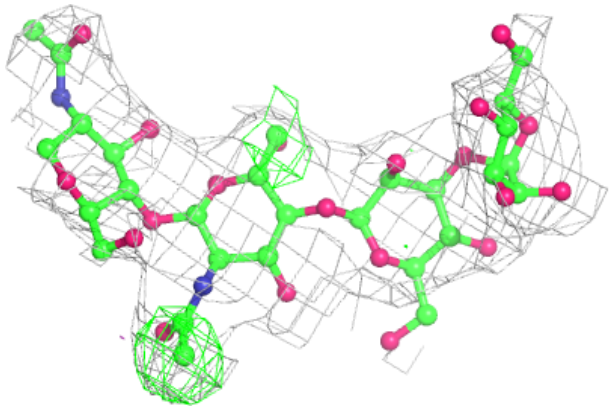


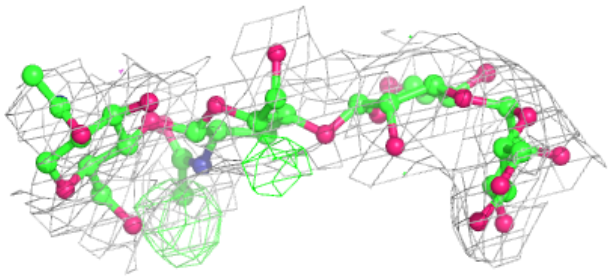


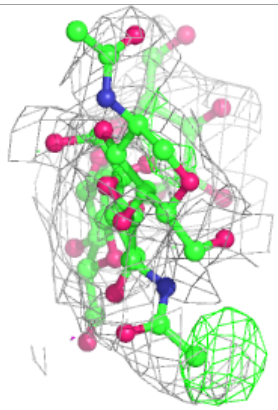


Electron density around Chain F:

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

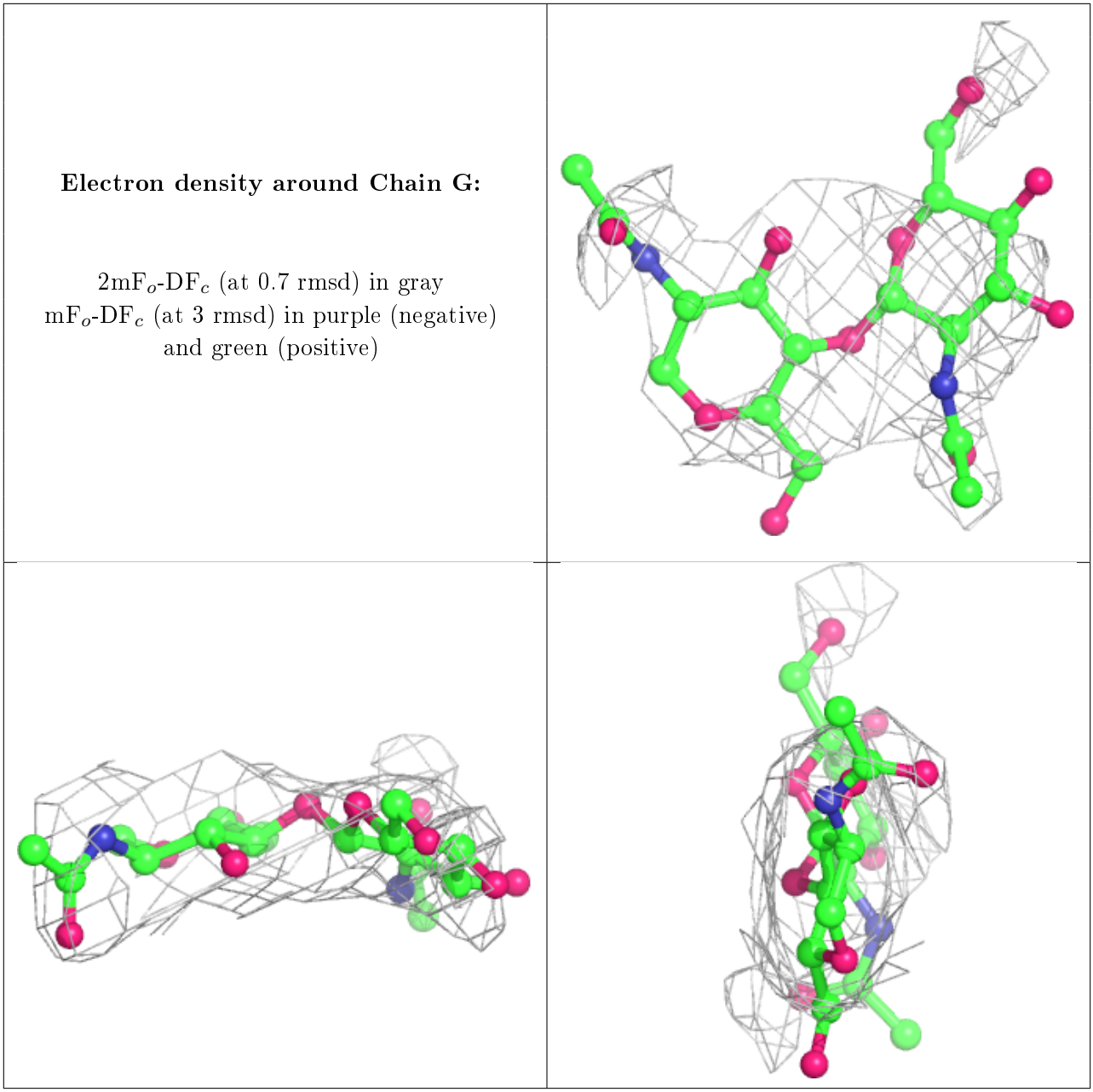






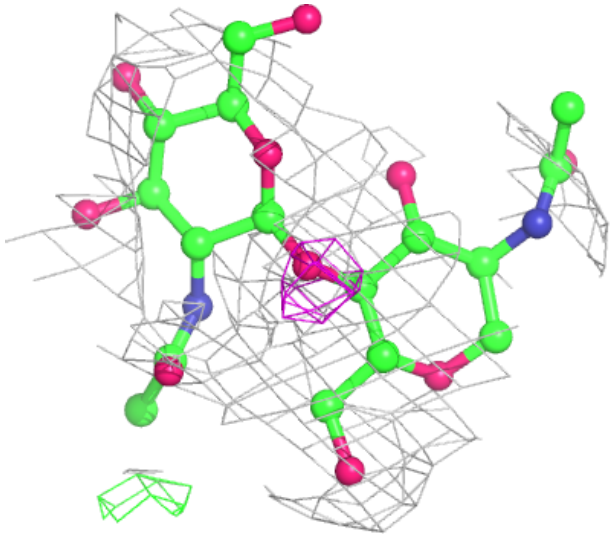
Electron density around Chain G:

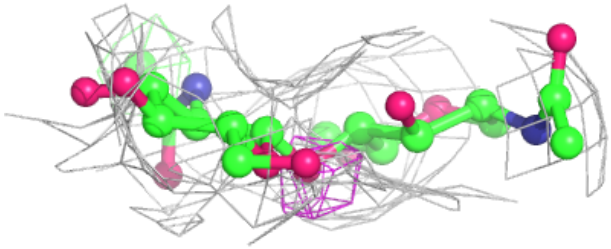
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

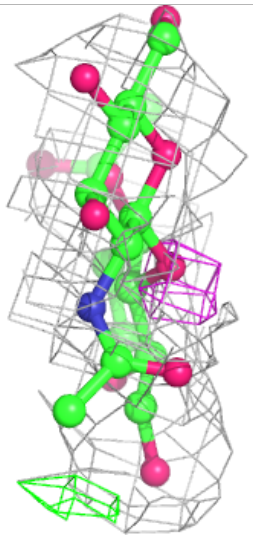


Electron density around Chain J:

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

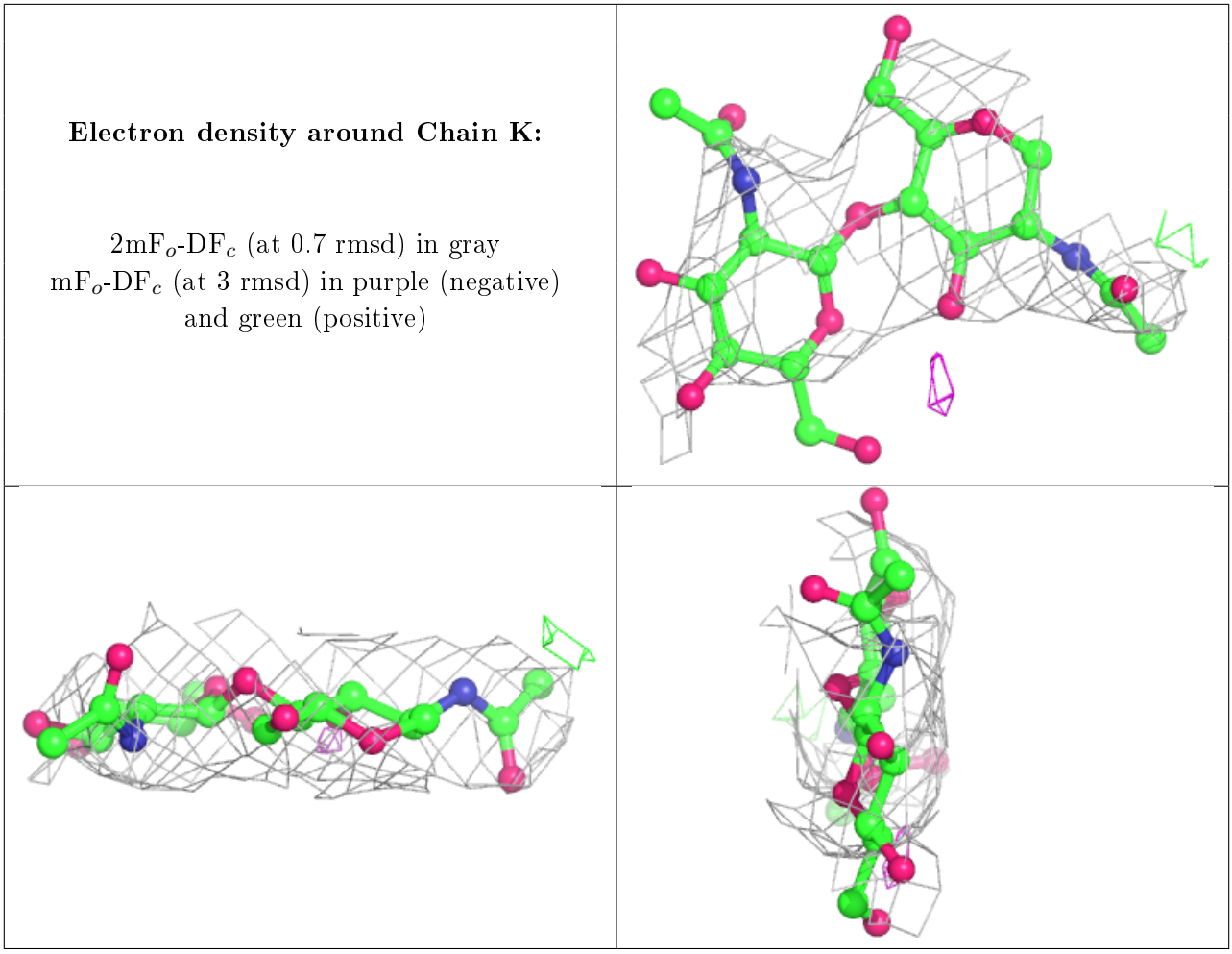






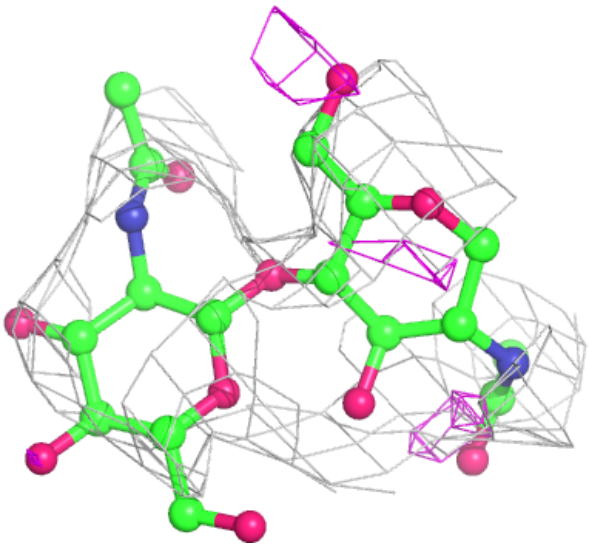
Electron density around Chain K:

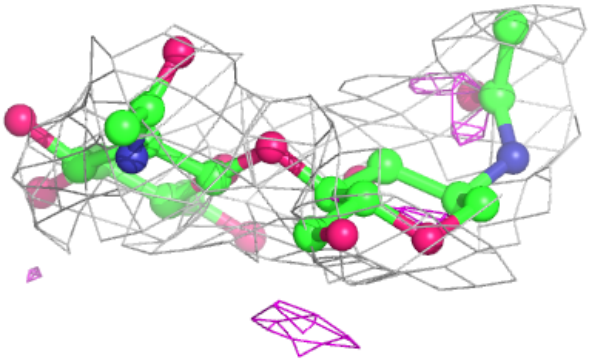
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

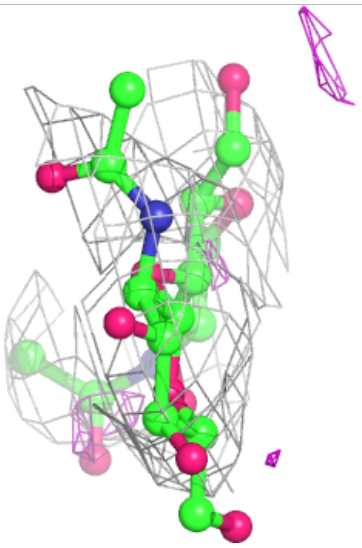


Electron density around Chain L:

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

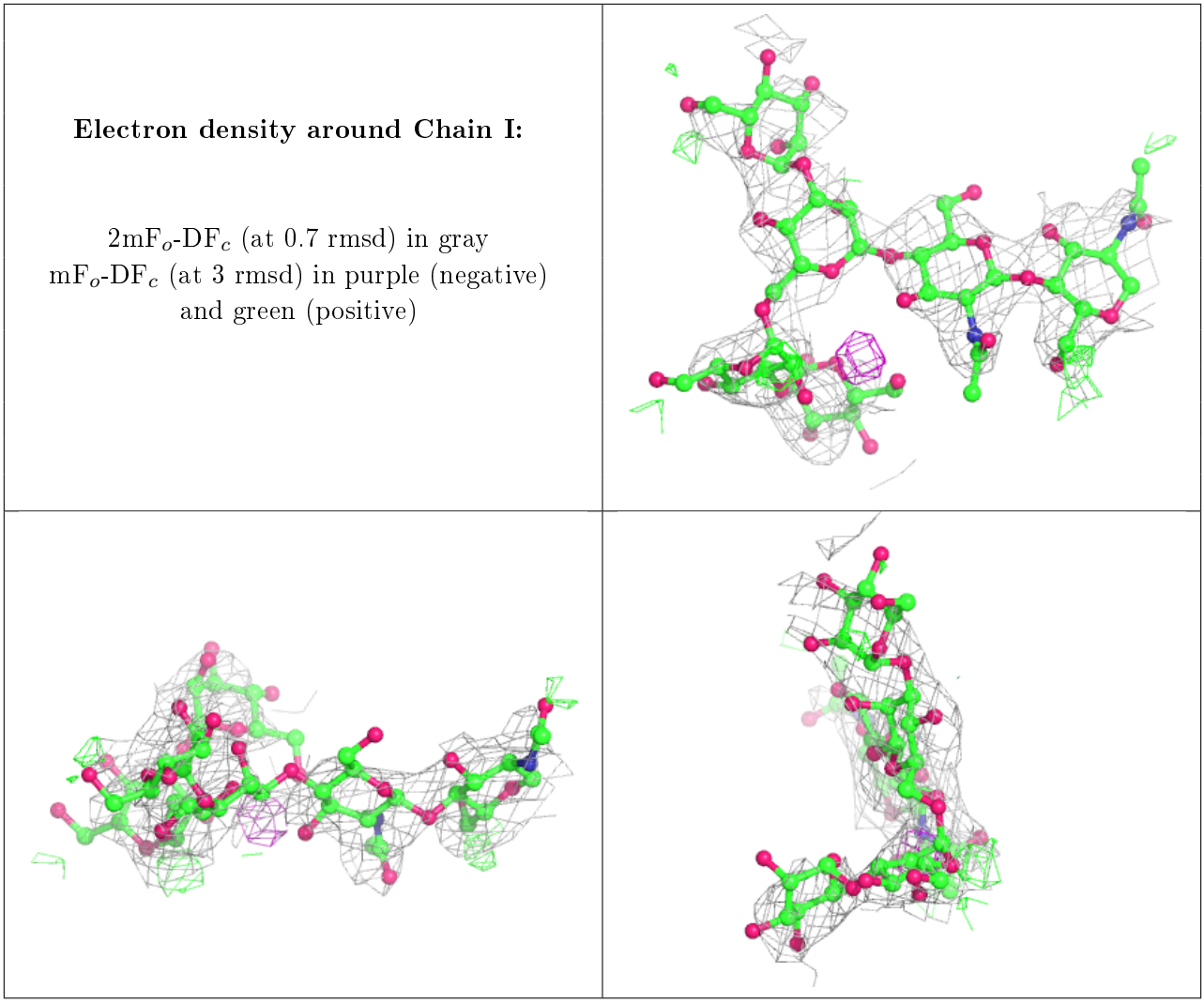






Electron density around Chain I:

$2mF_o$-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
12	CL	A	2045	1/1	0.26	0.40	141,141,141,141	0
9	CA	B	2001	1/1	0.59	0.18	302,302,302,302	0
12	CL	B	2020	1/1	0.75	0.19	106,106,106,106	0
10	NAG	A	2025	14/15	0.76	0.25	136,151,161,163	0
10	NAG	A	2039	14/15	0.78	0.29	128,152,160,163	0
9	CA	A	2005	1/1	0.80	0.45	267,267,267,267	0
11	SO4	B	2019	5/5	0.90	0.17	171,174,175,178	0
12	CL	B	2022	1/1	0.90	0.10	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CL	A	2043	1/1	0.90	0.21	100,100,100,100	0
12	CL	B	2021	1/1	0.91	0.14	89,89,89,89	0
11	SO4	B	2018	5/5	0.92	0.20	123,128,144,146	0
12	CL	A	2046	1/1	0.92	0.07	88,88,88,88	0
9	CA	A	2003	1/1	0.92	0.10	117,117,117,117	0
9	CA	A	2001	1/1	0.94	0.06	124,124,124,124	0
11	SO4	A	2042	5/5	0.94	0.16	135,139,141,142	0
11	SO4	A	2040	5/5	0.95	0.16	108,121,128,142	0
9	CA	A	2004	1/1	0.96	0.12	115,115,115,115	0
11	SO4	A	2041	5/5	0.96	0.15	126,129,132,134	0
12	CL	A	2044	1/1	0.96	0.21	107,107,107,107	0
9	CA	A	2002	1/1	0.96	0.05	121,121,121,121	0
11	SO4	B	2017	5/5	0.97	0.14	103,108,116,122	0
13	NI	A	2047	1/1	0.97	0.12	128,128,128,128	0

6.5 Other polymers (i)

There are no such residues in this entry.