Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2025 – 10:15 PM JST

PDB ID	:	9L3D / pdb_00009l3d
Title	:	Crystal structure of endo-processive xyloglucanase Xeg5A from Aspergillus oryzae
Authors	:	Nakamichi, Y.; Shimada, N.; Watanabe, M.; Fujii, T.; Matsuzawa, T.
Deposited on	:	2024-12-18
Resolution	:	1.90 Å(reported)

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

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

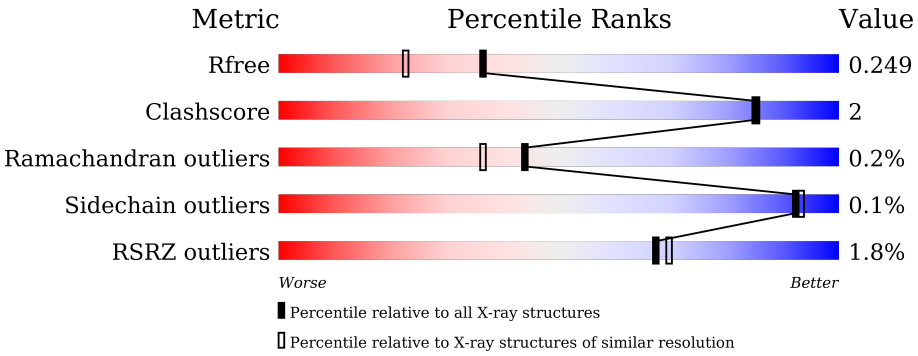
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

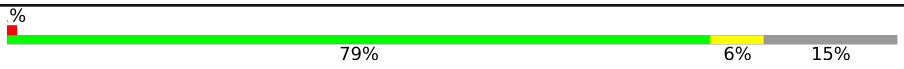
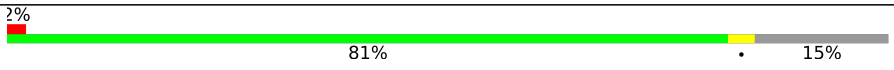
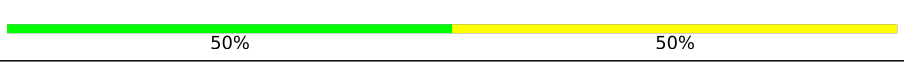
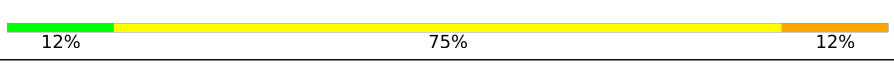
The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	648	
1	B	648	
2	C	6	
3	D	8	
3	F	8	
4	E	7	

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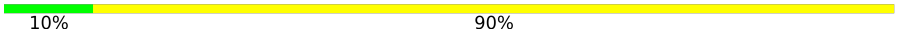
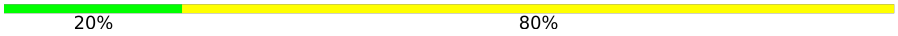
Mol	Chain	Length	Quality of chain
5	G	10	
5	H	10	
6	I	2	
6	J	2	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10332 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 Glycoside hydrolase superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	3	0
			4332	2757	707	861	7			
1	B	549	Total	C	N	O	S	0	0	0
			4309	2745	704	853	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-70	MET	-	initiating methionine	UNP I8IVP5
A	-69	ARG	-	expression tag	UNP I8IVP5
A	-68	PHE	-	expression tag	UNP I8IVP5
A	-67	PRO	-	expression tag	UNP I8IVP5
A	-66	SER	-	expression tag	UNP I8IVP5
A	-65	ILE	-	expression tag	UNP I8IVP5
A	-64	PHE	-	expression tag	UNP I8IVP5
A	-63	THR	-	expression tag	UNP I8IVP5
A	-62	ALA	-	expression tag	UNP I8IVP5
A	-61	VAL	-	expression tag	UNP I8IVP5
A	-60	LEU	-	expression tag	UNP I8IVP5
A	-59	PHE	-	expression tag	UNP I8IVP5
A	-58	ALA	-	expression tag	UNP I8IVP5
A	-57	ALA	-	expression tag	UNP I8IVP5
A	-56	SER	-	expression tag	UNP I8IVP5
A	-55	SER	-	expression tag	UNP I8IVP5
A	-54	ALA	-	expression tag	UNP I8IVP5
A	-53	LEU	-	expression tag	UNP I8IVP5
A	-52	ALA	-	expression tag	UNP I8IVP5
A	-51	ALA	-	expression tag	UNP I8IVP5
A	-50	PRO	-	expression tag	UNP I8IVP5
A	-49	VAL	-	expression tag	UNP I8IVP5
A	-48	ASN	-	expression tag	UNP I8IVP5
A	-47	THR	-	expression tag	UNP I8IVP5
A	-46	THR	-	expression tag	UNP I8IVP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-45	THR	-	expression tag	UNP I8IVP5
A	-44	GLU	-	expression tag	UNP I8IVP5
A	-43	ASP	-	expression tag	UNP I8IVP5
A	-42	GLU	-	expression tag	UNP I8IVP5
A	-41	THR	-	expression tag	UNP I8IVP5
A	-40	ALA	-	expression tag	UNP I8IVP5
A	-39	GLN	-	expression tag	UNP I8IVP5
A	-38	ILE	-	expression tag	UNP I8IVP5
A	-37	PRO	-	expression tag	UNP I8IVP5
A	-36	ALA	-	expression tag	UNP I8IVP5
A	-35	GLU	-	expression tag	UNP I8IVP5
A	-34	ALA	-	expression tag	UNP I8IVP5
A	-33	VAL	-	expression tag	UNP I8IVP5
A	-32	ILE	-	expression tag	UNP I8IVP5
A	-31	GLY	-	expression tag	UNP I8IVP5
A	-30	TYR	-	expression tag	UNP I8IVP5
A	-29	SER	-	expression tag	UNP I8IVP5
A	-28	ASP	-	expression tag	UNP I8IVP5
A	-27	LEU	-	expression tag	UNP I8IVP5
A	-26	GLU	-	expression tag	UNP I8IVP5
A	-25	GLY	-	expression tag	UNP I8IVP5
A	-24	ASP	-	expression tag	UNP I8IVP5
A	-23	PHE	-	expression tag	UNP I8IVP5
A	-22	ASP	-	expression tag	UNP I8IVP5
A	-21	VAL	-	expression tag	UNP I8IVP5
A	-20	ALA	-	expression tag	UNP I8IVP5
A	-19	VAL	-	expression tag	UNP I8IVP5
A	-18	LEU	-	expression tag	UNP I8IVP5
A	-17	PRO	-	expression tag	UNP I8IVP5
A	-16	PHE	-	expression tag	UNP I8IVP5
A	-15	SER	-	expression tag	UNP I8IVP5
A	-14	ASN	-	expression tag	UNP I8IVP5
A	-13	SER	-	expression tag	UNP I8IVP5
A	-12	THR	-	expression tag	UNP I8IVP5
A	-11	ASN	-	expression tag	UNP I8IVP5
A	-10	ASN	-	expression tag	UNP I8IVP5
A	-9	GLY	-	expression tag	UNP I8IVP5
A	-8	LEU	-	expression tag	UNP I8IVP5
A	-7	LEU	-	expression tag	UNP I8IVP5
A	-6	PHE	-	expression tag	UNP I8IVP5
A	-5	ILE	-	expression tag	UNP I8IVP5
A	-4	ASN	-	expression tag	UNP I8IVP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	THR	-	expression tag	UNP I8IVP5
A	-2	THR	-	expression tag	UNP I8IVP5
A	-1	ILE	-	expression tag	UNP I8IVP5
A	0	ALA	-	expression tag	UNP I8IVP5
A	1	SER	-	expression tag	UNP I8IVP5
A	2	ILE	-	expression tag	UNP I8IVP5
A	3	ALA	-	expression tag	UNP I8IVP5
A	4	ALA	-	expression tag	UNP I8IVP5
A	5	LYS	-	expression tag	UNP I8IVP5
A	6	GLU	-	expression tag	UNP I8IVP5
A	7	GLU	-	expression tag	UNP I8IVP5
A	8	GLY	-	expression tag	UNP I8IVP5
A	9	VAL	-	expression tag	UNP I8IVP5
A	10	SER	-	expression tag	UNP I8IVP5
A	11	LEU	-	expression tag	UNP I8IVP5
A	12	GLU	-	expression tag	UNP I8IVP5
A	13	LYS	-	expression tag	UNP I8IVP5
A	14	ARG	-	expression tag	UNP I8IVP5
A	15	GLU	-	expression tag	UNP I8IVP5
A	16	ALA	-	expression tag	UNP I8IVP5
A	17	GLU	-	expression tag	UNP I8IVP5
A	570	VAL	-	expression tag	UNP I8IVP5
A	571	ASP	-	expression tag	UNP I8IVP5
A	572	HIS	-	expression tag	UNP I8IVP5
A	573	HIS	-	expression tag	UNP I8IVP5
A	574	HIS	-	expression tag	UNP I8IVP5
A	575	HIS	-	expression tag	UNP I8IVP5
A	576	HIS	-	expression tag	UNP I8IVP5
A	577	HIS	-	expression tag	UNP I8IVP5
B	-70	MET	-	initiating methionine	UNP I8IVP5
B	-69	ARG	-	expression tag	UNP I8IVP5
B	-68	PHE	-	expression tag	UNP I8IVP5
B	-67	PRO	-	expression tag	UNP I8IVP5
B	-66	SER	-	expression tag	UNP I8IVP5
B	-65	ILE	-	expression tag	UNP I8IVP5
B	-64	PHE	-	expression tag	UNP I8IVP5
B	-63	THR	-	expression tag	UNP I8IVP5
B	-62	ALA	-	expression tag	UNP I8IVP5
B	-61	VAL	-	expression tag	UNP I8IVP5
B	-60	LEU	-	expression tag	UNP I8IVP5
B	-59	PHE	-	expression tag	UNP I8IVP5
B	-58	ALA	-	expression tag	UNP I8IVP5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-57	ALA	-	expression tag	UNP I8IVP5
B	-56	SER	-	expression tag	UNP I8IVP5
B	-55	SER	-	expression tag	UNP I8IVP5
B	-54	ALA	-	expression tag	UNP I8IVP5
B	-53	LEU	-	expression tag	UNP I8IVP5
B	-52	ALA	-	expression tag	UNP I8IVP5
B	-51	ALA	-	expression tag	UNP I8IVP5
B	-50	PRO	-	expression tag	UNP I8IVP5
B	-49	VAL	-	expression tag	UNP I8IVP5
B	-48	ASN	-	expression tag	UNP I8IVP5
B	-47	THR	-	expression tag	UNP I8IVP5
B	-46	THR	-	expression tag	UNP I8IVP5
B	-45	THR	-	expression tag	UNP I8IVP5
B	-44	GLU	-	expression tag	UNP I8IVP5
B	-43	ASP	-	expression tag	UNP I8IVP5
B	-42	GLU	-	expression tag	UNP I8IVP5
B	-41	THR	-	expression tag	UNP I8IVP5
B	-40	ALA	-	expression tag	UNP I8IVP5
B	-39	GLN	-	expression tag	UNP I8IVP5
B	-38	ILE	-	expression tag	UNP I8IVP5
B	-37	PRO	-	expression tag	UNP I8IVP5
B	-36	ALA	-	expression tag	UNP I8IVP5
B	-35	GLU	-	expression tag	UNP I8IVP5
B	-34	ALA	-	expression tag	UNP I8IVP5
B	-33	VAL	-	expression tag	UNP I8IVP5
B	-32	ILE	-	expression tag	UNP I8IVP5
B	-31	GLY	-	expression tag	UNP I8IVP5
B	-30	TYR	-	expression tag	UNP I8IVP5
B	-29	SER	-	expression tag	UNP I8IVP5
B	-28	ASP	-	expression tag	UNP I8IVP5
B	-27	LEU	-	expression tag	UNP I8IVP5
B	-26	GLU	-	expression tag	UNP I8IVP5
B	-25	GLY	-	expression tag	UNP I8IVP5
B	-24	ASP	-	expression tag	UNP I8IVP5
B	-23	PHE	-	expression tag	UNP I8IVP5
B	-22	ASP	-	expression tag	UNP I8IVP5
B	-21	VAL	-	expression tag	UNP I8IVP5
B	-20	ALA	-	expression tag	UNP I8IVP5
B	-19	VAL	-	expression tag	UNP I8IVP5
B	-18	LEU	-	expression tag	UNP I8IVP5
B	-17	PRO	-	expression tag	UNP I8IVP5
B	-16	PHE	-	expression tag	UNP I8IVP5

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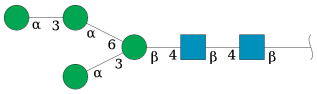
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP I8IVP5
B	-14	ASN	-	expression tag	UNP I8IVP5
B	-13	SER	-	expression tag	UNP I8IVP5
B	-12	THR	-	expression tag	UNP I8IVP5
B	-11	ASN	-	expression tag	UNP I8IVP5
B	-10	ASN	-	expression tag	UNP I8IVP5
B	-9	GLY	-	expression tag	UNP I8IVP5
B	-8	LEU	-	expression tag	UNP I8IVP5
B	-7	LEU	-	expression tag	UNP I8IVP5
B	-6	PHE	-	expression tag	UNP I8IVP5
B	-5	ILE	-	expression tag	UNP I8IVP5
B	-4	ASN	-	expression tag	UNP I8IVP5
B	-3	THR	-	expression tag	UNP I8IVP5
B	-2	THR	-	expression tag	UNP I8IVP5
B	-1	ILE	-	expression tag	UNP I8IVP5
B	0	ALA	-	expression tag	UNP I8IVP5
B	1	SER	-	expression tag	UNP I8IVP5
B	2	ILE	-	expression tag	UNP I8IVP5
B	3	ALA	-	expression tag	UNP I8IVP5
B	4	ALA	-	expression tag	UNP I8IVP5
B	5	LYS	-	expression tag	UNP I8IVP5
B	6	GLU	-	expression tag	UNP I8IVP5
B	7	GLU	-	expression tag	UNP I8IVP5
B	8	GLY	-	expression tag	UNP I8IVP5
B	9	VAL	-	expression tag	UNP I8IVP5
B	10	SER	-	expression tag	UNP I8IVP5
B	11	LEU	-	expression tag	UNP I8IVP5
B	12	GLU	-	expression tag	UNP I8IVP5
B	13	LYS	-	expression tag	UNP I8IVP5
B	14	ARG	-	expression tag	UNP I8IVP5
B	15	GLU	-	expression tag	UNP I8IVP5
B	16	ALA	-	expression tag	UNP I8IVP5
B	17	GLU	-	expression tag	UNP I8IVP5
B	570	VAL	-	expression tag	UNP I8IVP5
B	571	ASP	-	expression tag	UNP I8IVP5
B	572	HIS	-	expression tag	UNP I8IVP5
B	573	HIS	-	expression tag	UNP I8IVP5
B	574	HIS	-	expression tag	UNP I8IVP5
B	575	HIS	-	expression tag	UNP I8IVP5
B	576	HIS	-	expression tag	UNP I8IVP5
B	577	HIS	-	expression tag	UNP I8IVP5

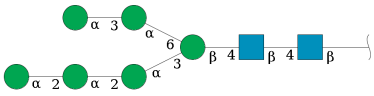
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran

ose-(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.



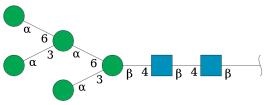
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	6	Total C N O 72 40 2 30	0	0	0

- Molecule 3 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)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



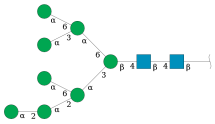
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	8	Total C N O 94 52 2 40	0	0	0
3	F	8	Total C N O 94 52 2 40	0	0	0

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



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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]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.

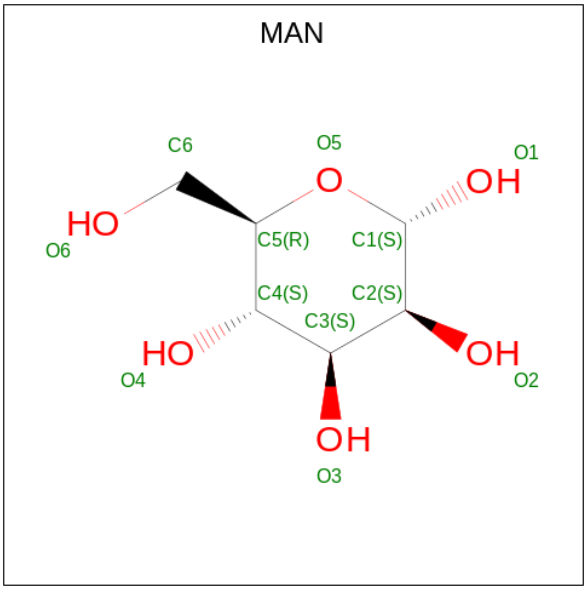


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	10	Total C N O 116 64 2 50	0	0	0
5	H	10	Total C N O 116 64 2 50	0	0	0

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

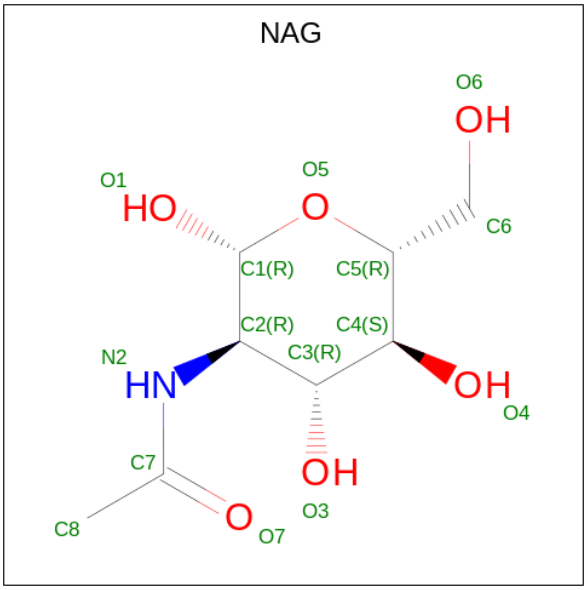
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	I	2	Total C N O 28 16 2 10	0	0	0
6	J	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



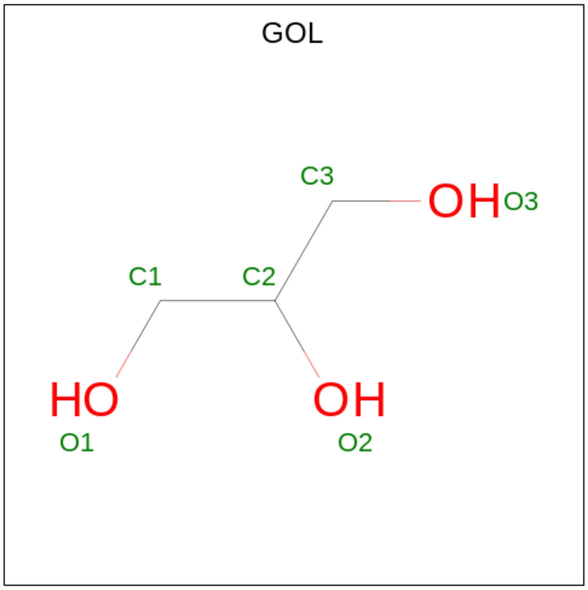
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 6 5	0	0
7	B	1	Total C O 11 6 5	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0
9	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

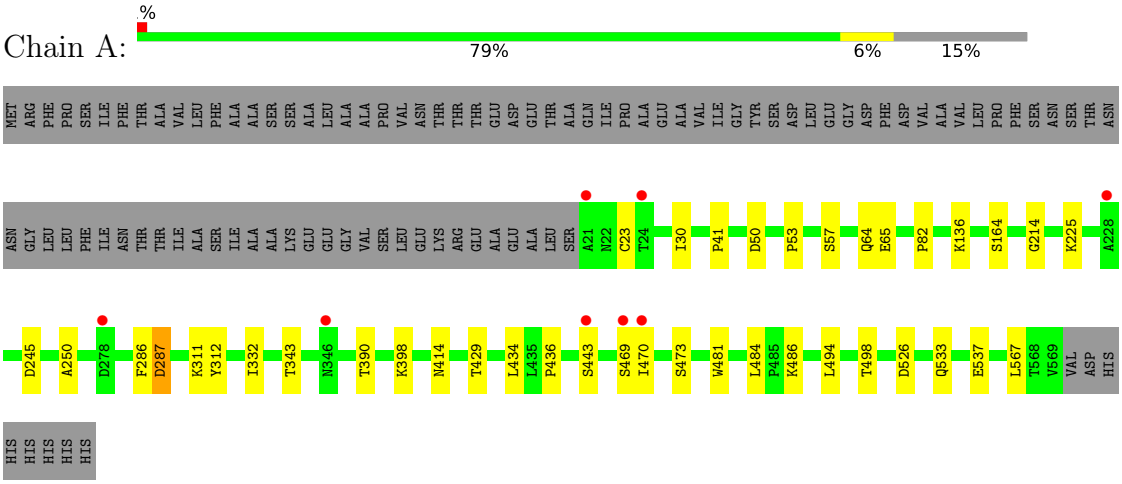
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	441	Total	O	0	0
			441	441		
10	B	451	Total	O	0	0
			451	451		

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.

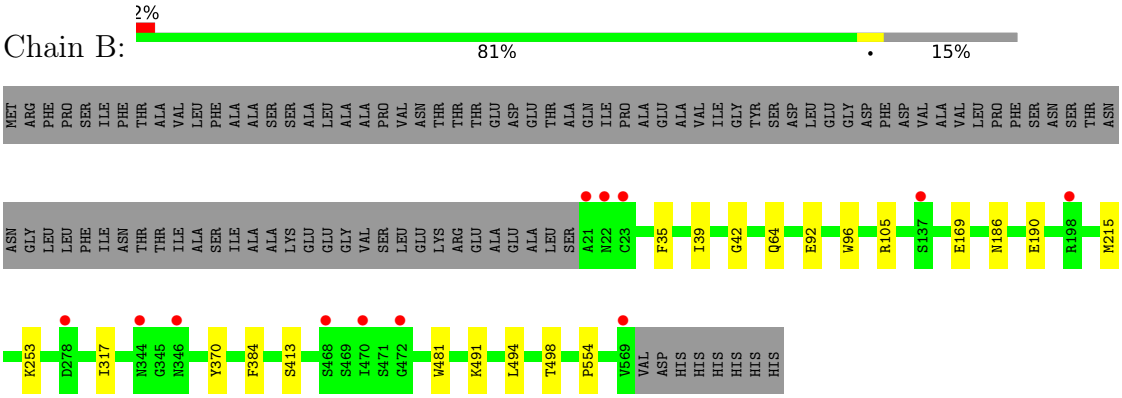
• Molecule 1: Glycoside hydrolase superfamily

Chain A:



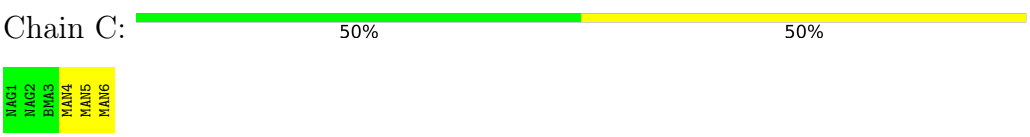
• Molecule 1: Glycoside hydrolase superfamily

Chain B:



• Molecule 2: 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 C:

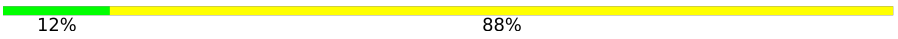


• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

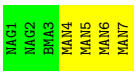
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain E:

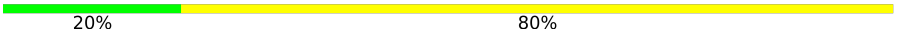


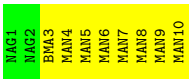
• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]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 H:





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

Chain I:

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

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.04Å 119.84Å 106.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.64 – 1.90 48.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.64-1.90) 99.3 (48.64-1.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.249 0.216 , 0.249	Depositor DCC
R_{free} test set	6329 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10332	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1231e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, 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	0.35	0/4453	0.54	0/6095
1	B	0.33	0/4430	0.52	0/6064
All	All	0.34	0/8883	0.53	0/12159

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	4332	0	4111	27	0
1	B	4309	0	4099	13	0
2	C	72	0	61	0	0
3	D	94	0	79	1	0
3	F	94	0	79	0	0
4	E	83	0	70	0	0
5	G	116	0	97	0	0
5	H	116	0	97	0	0
6	I	28	0	25	0	0
6	J	28	0	25	1	0
7	A	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	11	0	10	0	0
8	A	28	0	26	0	0
8	B	28	0	26	0	0
9	A	60	0	79	3	0
9	B	30	0	40	1	0
10	A	441	0	0	0	0
10	B	451	0	0	1	0
All	All	10332	0	8934	38	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 2.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:O	9:A:610:GOL:H32	1.94	0.67
1:A:533:GLN:O	1:A:537:GLU:HG3	1.96	0.65
1:A:23:CYS:H	9:A:612:GOL:H11	1.63	0.64
1:A:65:GLU:OE1	1:B:64:GLN:NE2	2.31	0.57
1:B:494:LEU:HD12	1:B:498:THR:HB	1.88	0.54
1:A:469:SER:OG	1:A:470:ILE:HG23	2.08	0.53
1:A:390:THR:OG1	1:A:443:SER:OG	2.22	0.51
1:A:481:TRP:HD1	9:A:605:GOL:H12	1.77	0.48
1:A:53:PRO:HD2	1:A:57:SER:OG	2.13	0.48
1:A:414:ASN:HD22	6:J:1:NAG:H83	1.78	0.48
1:A:311:LYS:HE2	1:A:312:TYR:CZ	2.50	0.46
1:A:434:LEU:HD21	1:A:484:LEU:CD1	2.46	0.45
1:B:35:PHE:O	1:B:39:ILE:HG23	2.15	0.45
1:A:332:ILE:HD11	3:D:8:MAN:O5	2.17	0.45
1:A:64:GLN:NE2	1:B:105:ARG:HH12	2.16	0.44
1:B:42:GLY:C	1:B:317:ILE:HG23	2.42	0.44
1:A:41:PRO:HG3	1:A:343:THR:HA	1.98	0.44
1:A:484:LEU:HG	1:A:486:LYS:HD3	2.00	0.43
1:B:384:PHE:O	1:B:413:SER:HB2	2.18	0.43
1:A:50:ASP:HB3	1:A:82:PRO:HB2	2.00	0.42
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.91	0.42
1:A:245:ASP:HA	1:A:250:ALA:HB3	2.01	0.42
1:B:92:GLU:HA	1:B:96:TRP:CE3	2.54	0.42
1:A:434:LEU:HD21	1:A:484:LEU:HD12	2.02	0.42
1:B:186:ASN:O	1:B:190:GLU:HG3	2.21	0.41
1:B:481:TRP:H	9:B:602:GOL:H31	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:HD12	1:A:498:THR:HB	2.01	0.41
1:B:491:LYS:NZ	10:B:705:HOH:O	2.42	0.41
1:A:225:LYS:HA	1:A:225:LYS:HD2	1.78	0.41
1:B:169:GLU:OE2	1:B:215:MET:HE1	2.21	0.41
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.80	0.41
1:A:286:PHE:O	1:A:287:ASP:HB2	2.21	0.41
1:A:470:ILE:HD11	1:A:567:LEU:HD21	2.03	0.41
1:B:253:LYS:HA	1:B:253:LYS:HD3	1.85	0.41
1:A:30:ILE:HG22	1:A:164:SER:HB2	2.03	0.41
1:A:398:LYS:NZ	1:A:436:PRO:HG3	2.36	0.40
1:B:370:TYR:CD2	1:B:554:PRO:HB3	2.56	0.40
1:A:473:SER:C	1:A:533:GLN:HB2	2.46	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	550/648 (85%)	523 (95%)	25 (4%)	2 (0%)	30 22
1	B	547/648 (84%)	524 (96%)	23 (4%)	0	100 100
All	All	1097/1296 (85%)	1047 (95%)	48 (4%)	2 (0%)	44 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLY
1	A	287	ASP

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	484/561 (86%)	482 (100%)	2 (0%)	89 90
1	B	481/561 (86%)	481 (100%)	0	100 100
All	All	965/1122 (86%)	963 (100%)	2 (0%)	92 93

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

Mol	Chain	Res	Type
1	A	526[A]	ASP
1	A	526[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	B	146	GLN
1	B	209	ASN
1	B	237	GLN
1	B	344	ASN
1	B	506	GLN
1	B	520	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)

53 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.44	0	17,19,21	0.74	0
2	NAG	C	2	2	14,14,15	0.40	0	17,19,21	0.47	0
2	BMA	C	3	2	11,11,12	1.05	0	15,15,17	0.94	0
2	MAN	C	4	2	11,11,12	1.22	1 (9%)	15,15,17	1.37	3 (20%)
2	MAN	C	5	2	11,11,12	1.19	1 (9%)	15,15,17	1.14	2 (13%)
2	MAN	C	6	2	11,11,12	0.88	0	15,15,17	1.09	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.68	1 (7%)	17,19,21	0.66	0
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	0.62	0
3	BMA	D	3	3	11,11,12	1.12	1 (9%)	15,15,17	1.08	1 (6%)
3	MAN	D	4	3	11,11,12	0.89	0	15,15,17	1.18	2 (13%)
3	MAN	D	5	3	11,11,12	1.20	1 (9%)	15,15,17	1.22	2 (13%)
3	MAN	D	6	3	11,11,12	1.24	2 (18%)	15,15,17	1.37	2 (13%)
3	MAN	D	7	3	11,11,12	1.24	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	D	8	3	11,11,12	1.05	1 (9%)	15,15,17	1.46	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.39	0	17,19,21	0.63	0
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.35	0
4	BMA	E	3	4	11,11,12	0.87	0	15,15,17	0.96	0
4	MAN	E	4	4	11,11,12	1.27	1 (9%)	15,15,17	1.88	3 (20%)
4	MAN	E	5	4	11,11,12	1.21	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	E	6	4	11,11,12	1.21	3 (27%)	15,15,17	1.23	2 (13%)
4	MAN	E	7	4	11,11,12	1.16	1 (9%)	15,15,17	1.09	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
3	BMA	F	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
3	MAN	F	4	3	11,11,12	1.02	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	F	5	3	11,11,12	1.12	2 (18%)	15,15,17	1.31	2 (13%)
3	MAN	F	6	3	11,11,12	1.22	2 (18%)	15,15,17	1.35	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	F	7	3	11,11,12	0.94	0	15,15,17	1.19	2 (13%)
3	MAN	F	8	3	11,11,12	0.92	0	15,15,17	1.15	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.66	1 (7%)	17,19,21	0.72	0
5	MAN	G	10	5	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
5	NAG	G	2	5	14,14,15	0.48	0	17,19,21	0.50	0
5	BMA	G	3	5	11,11,12	0.90	1 (9%)	15,15,17	0.93	1 (6%)
5	MAN	G	4	5	11,11,12	1.02	1 (9%)	15,15,17	1.37	2 (13%)
5	MAN	G	5	5	11,11,12	1.17	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	G	6	5	11,11,12	1.03	0	15,15,17	1.13	1 (6%)
5	MAN	G	7	5	11,11,12	1.21	2 (18%)	15,15,17	1.21	1 (6%)
5	MAN	G	8	5	11,11,12	1.23	1 (9%)	15,15,17	0.89	0
5	MAN	G	9	5	11,11,12	1.04	1 (9%)	15,15,17	1.44	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.32	0	17,19,21	0.71	0
5	MAN	H	10	5	11,11,12	0.90	0	15,15,17	1.17	1 (6%)
5	NAG	H	2	5	14,14,15	0.59	0	17,19,21	0.40	0
5	BMA	H	3	5	11,11,12	0.89	1 (9%)	15,15,17	0.80	0
5	MAN	H	4	5	11,11,12	1.08	0	15,15,17	1.20	2 (13%)
5	MAN	H	5	5	11,11,12	1.10	1 (9%)	15,15,17	1.01	1 (6%)
5	MAN	H	6	5	11,11,12	0.82	0	15,15,17	1.14	1 (6%)
5	MAN	H	7	5	11,11,12	1.14	1 (9%)	15,15,17	1.04	1 (6%)
5	MAN	H	8	5	11,11,12	1.04	1 (9%)	15,15,17	1.10	1 (6%)
5	MAN	H	9	5	11,11,12	1.48	2 (18%)	15,15,17	1.00	2 (13%)
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.49	0
6	NAG	J	1	6,1	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
6	NAG	J	2	6	14,14,15	0.23	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
5	MAN	H	9	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	4/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	9	MAN	C1-C2	3.33	1.59	1.52
4	E	4	MAN	C1-C2	3.27	1.59	1.52
3	D	5	MAN	C2-C3	3.23	1.57	1.52
3	D	3	BMA	C2-C3	3.01	1.56	1.52
4	E	7	MAN	C1-C2	2.96	1.59	1.52
5	H	9	MAN	O5-C1	-2.66	1.39	1.43
3	F	4	MAN	O5-C5	2.66	1.48	1.43
4	E	5	MAN	C1-C2	2.57	1.58	1.52
3	D	7	MAN	C4-C3	2.54	1.58	1.52
2	C	4	MAN	C1-C2	2.50	1.57	1.52
5	G	8	MAN	O5-C1	-2.46	1.39	1.43
3	F	3	BMA	C2-C3	2.44	1.56	1.52
2	C	5	MAN	C1-C2	2.42	1.57	1.52
5	H	7	MAN	O5-C5	2.42	1.48	1.43
5	H	5	MAN	C4-C3	2.40	1.58	1.52
5	H	8	MAN	O5-C1	-2.38	1.39	1.43
3	D	8	MAN	O5-C5	2.37	1.48	1.43
3	D	6	MAN	O5-C5	2.35	1.48	1.43
3	F	5	MAN	C2-C3	2.32	1.55	1.52
5	G	1	NAG	O5-C1	-2.31	1.40	1.43
3	D	6	MAN	C4-C3	2.30	1.58	1.52
4	E	6	MAN	C2-C3	2.27	1.55	1.52
3	D	1	NAG	C1-C2	2.27	1.55	1.52
3	F	6	MAN	O4-C4	2.24	1.48	1.43
5	G	3	BMA	O5-C1	-2.23	1.40	1.43
3	F	6	MAN	O5-C5	2.21	1.47	1.43
5	G	7	MAN	O5-C5	2.17	1.47	1.43
3	F	5	MAN	C4-C3	2.16	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	O5-C1	-2.10	1.40	1.43
4	E	6	MAN	C4-C3	2.10	1.57	1.52
5	G	4	MAN	C1-C2	2.10	1.57	1.52
5	G	7	MAN	C4-C5	2.08	1.57	1.53
4	E	6	MAN	C1-C2	2.08	1.56	1.52
5	G	9	MAN	C1-C2	2.04	1.56	1.52
5	H	3	BMA	O5-C1	-2.01	1.40	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	8	MAN	C1-O5-C5	4.77	118.65	112.19
4	E	4	MAN	C1-O5-C5	4.62	118.46	112.19
3	F	6	MAN	C1-O5-C5	4.18	117.85	112.19
5	G	9	MAN	C1-O5-C5	4.09	117.74	112.19
5	H	10	MAN	C1-O5-C5	3.69	117.19	112.19
2	C	4	MAN	C1-O5-C5	3.63	117.11	112.19
4	E	4	MAN	O2-C2-C3	-3.56	103.01	110.14
3	D	6	MAN	C1-O5-C5	3.49	116.92	112.19
5	G	4	MAN	O2-C2-C3	-3.43	103.27	110.14
3	F	5	MAN	C1-O5-C5	3.40	116.80	112.19
3	D	4	MAN	C1-O5-C5	3.40	116.79	112.19
5	H	4	MAN	O2-C2-C3	-3.38	103.36	110.14
5	G	4	MAN	C1-O5-C5	3.38	116.77	112.19
4	E	5	MAN	C1-O5-C5	3.36	116.75	112.19
2	C	6	MAN	C1-O5-C5	3.22	116.56	112.19
4	E	4	MAN	C1-C2-C3	3.18	113.58	109.67
5	G	5	MAN	O2-C2-C3	-3.16	103.81	110.14
5	G	6	MAN	C1-O5-C5	3.12	116.42	112.19
5	H	6	MAN	C1-O5-C5	3.09	116.38	112.19
3	F	4	MAN	C1-O5-C5	3.06	116.34	112.19
3	F	8	MAN	C1-O5-C5	2.98	116.23	112.19
5	H	5	MAN	O2-C2-C3	-2.89	104.36	110.14
3	F	5	MAN	O2-C2-C3	-2.88	104.36	110.14
5	H	8	MAN	O2-C2-C3	-2.80	104.53	110.14
2	C	5	MAN	C1-O5-C5	2.72	115.87	112.19
3	F	7	MAN	C1-O5-C5	2.70	115.85	112.19
5	G	10	MAN	C1-O5-C5	2.66	115.80	112.19
5	G	7	MAN	C1-O5-C5	2.64	115.76	112.19
5	H	4	MAN	C1-O5-C5	2.64	115.76	112.19
3	F	3	BMA	C1-O5-C5	2.61	115.73	112.19
3	D	6	MAN	O2-C2-C3	-2.61	104.91	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	5	MAN	O2-C2-C3	-2.55	105.03	110.14
3	D	3	BMA	C1-O5-C5	2.54	115.64	112.19
4	E	5	MAN	O2-C2-C3	-2.54	105.05	110.14
3	D	7	MAN	O2-C2-C3	-2.40	105.33	110.14
6	J	1	NAG	C1-O5-C5	2.37	115.41	112.19
5	H	7	MAN	C1-O5-C5	2.32	115.34	112.19
3	F	7	MAN	O2-C2-C3	-2.32	105.50	110.14
2	C	4	MAN	O2-C2-C3	-2.31	105.51	110.14
4	E	6	MAN	C1-O5-C5	2.31	115.32	112.19
2	C	5	MAN	O2-C2-C3	-2.30	105.52	110.14
3	D	5	MAN	C1-O5-C5	2.29	115.29	112.19
3	F	4	MAN	O2-C2-C3	-2.22	105.68	110.14
3	D	4	MAN	O2-C2-C3	-2.22	105.69	110.14
5	G	9	MAN	O3-C3-C2	2.21	114.23	109.99
4	E	6	MAN	C2-C3-C4	2.16	114.62	110.89
3	F	2	NAG	C1-O5-C5	2.13	115.08	112.19
5	G	3	BMA	O2-C2-C3	-2.11	105.91	110.14
6	I	1	NAG	C1-O5-C5	2.10	115.04	112.19
5	H	9	MAN	O2-C2-C3	-2.10	105.94	110.14
5	H	9	MAN	O3-C3-C2	2.09	113.99	109.99
4	E	7	MAN	O2-C2-C1	2.05	113.35	109.15
4	E	7	MAN	O2-C2-C3	-2.02	106.10	110.14
2	C	4	MAN	C1-C2-C3	2.01	112.14	109.67
3	D	7	MAN	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	10	MAN	O5-C5-C6-O6
4	E	7	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
5	H	9	MAN	C4-C5-C6-O6
5	H	10	MAN	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
4	E	5	MAN	C4-C5-C6-O6
4	E	7	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
5	H	9	MAN	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
5	G	10	MAN	C4-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
5	G	6	MAN	C4-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
5	G	10	MAN	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

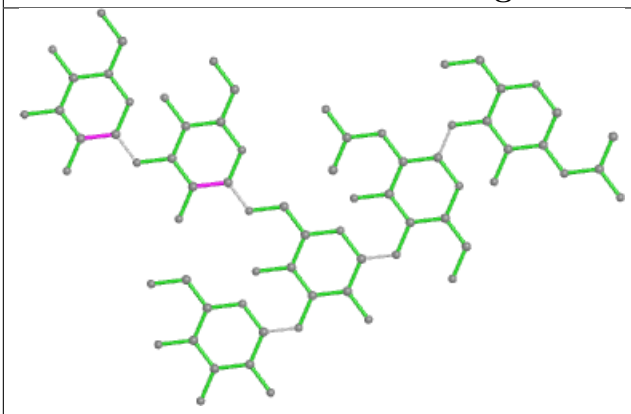
There are no ring outliers.

2 monomers are involved in 2 short contacts:

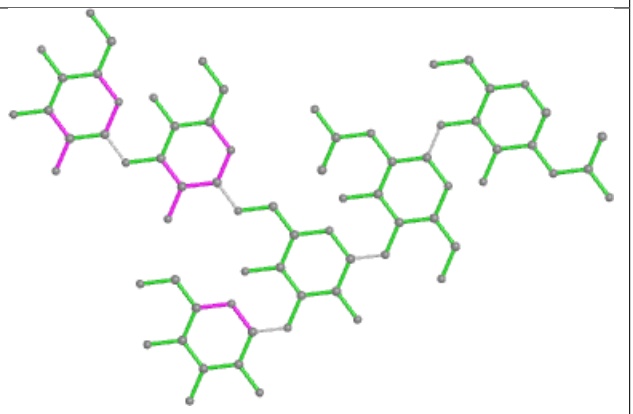
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
3	D	8	MAN	1	0

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

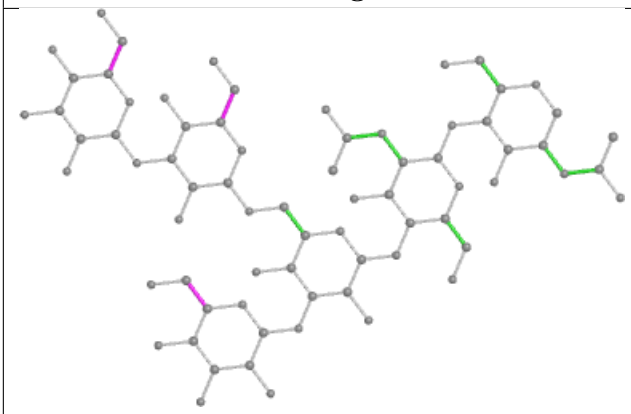
Oligosaccharide Chain C



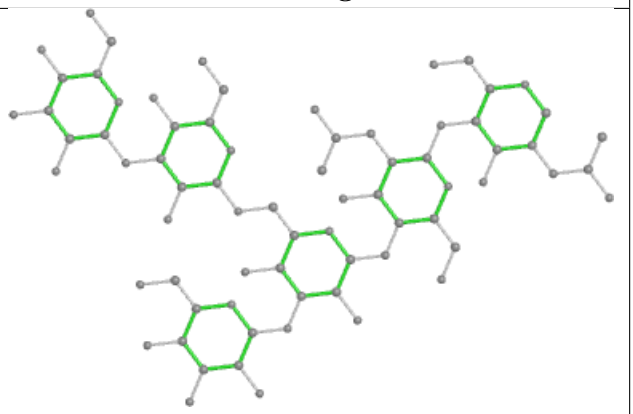
Bond lengths



Bond angles

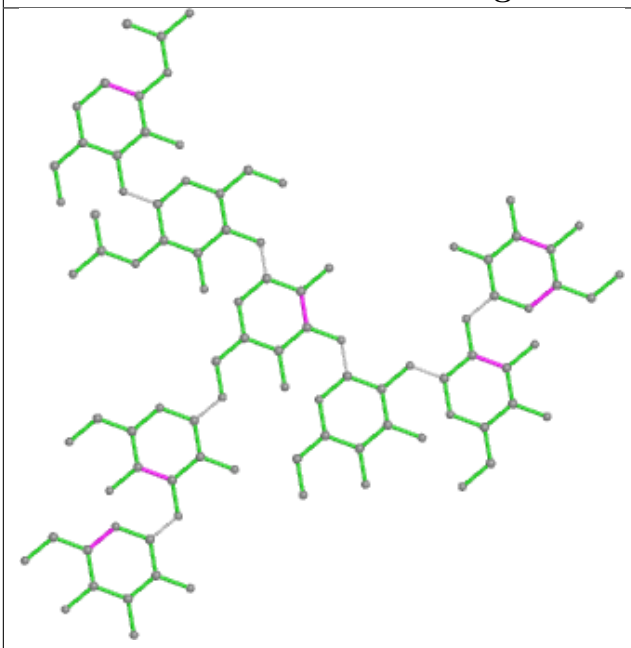


Torsions

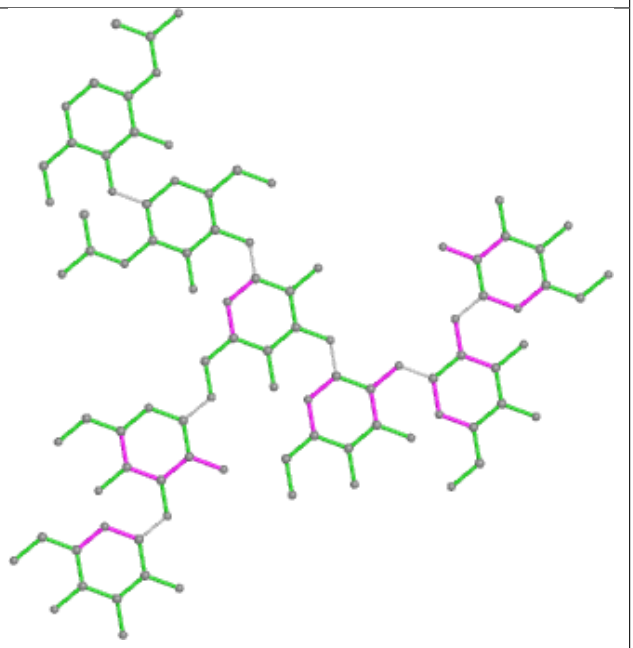


Rings

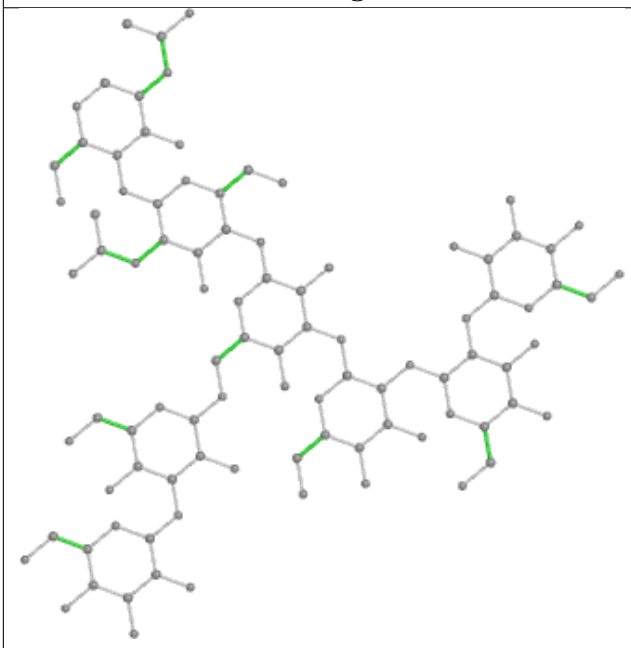
Oligosaccharide Chain D



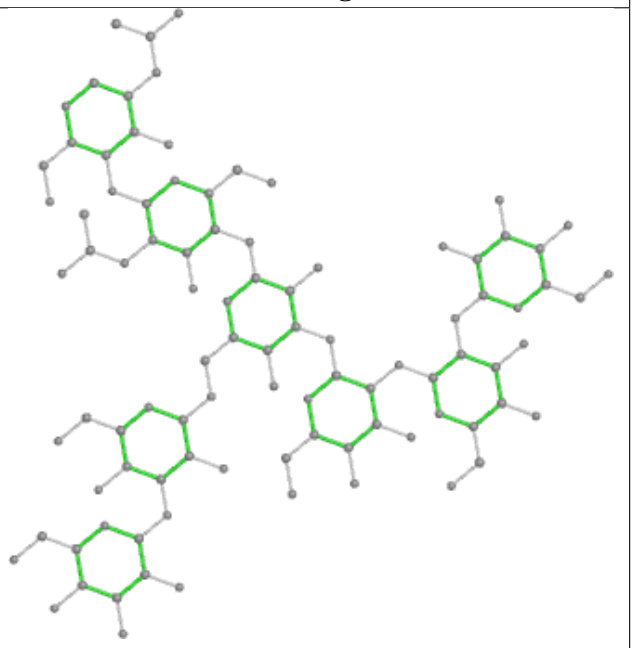
Bond lengths



Bond angles

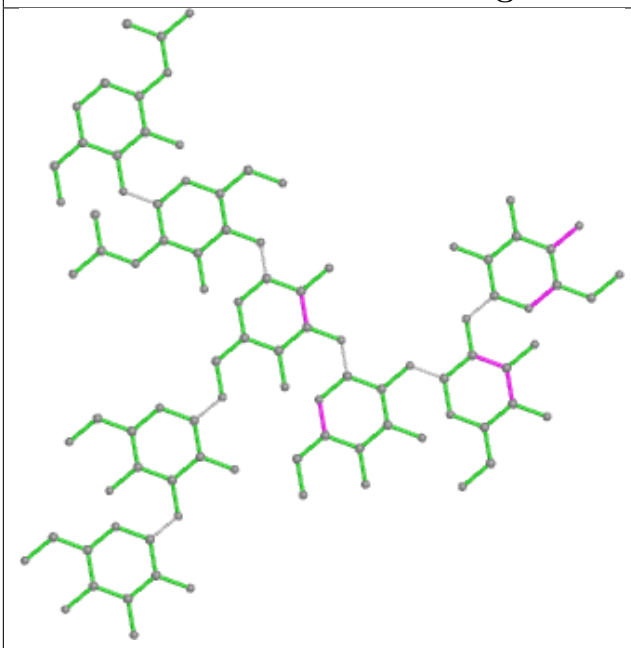


Torsions

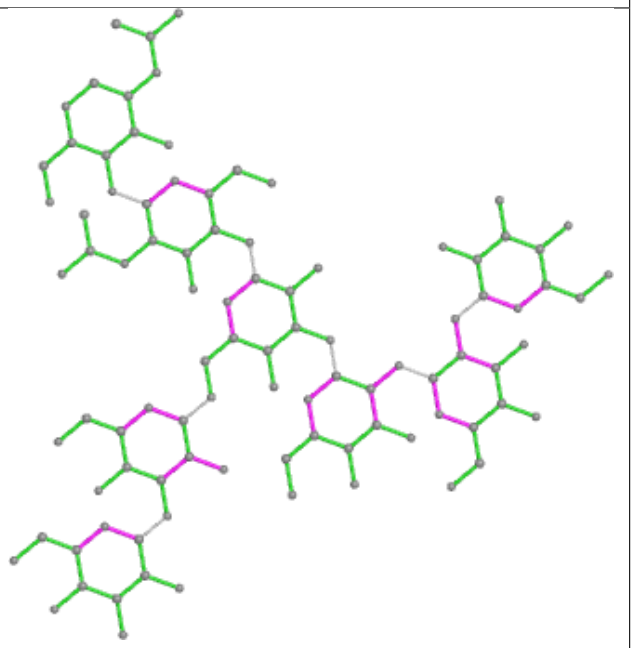


Rings

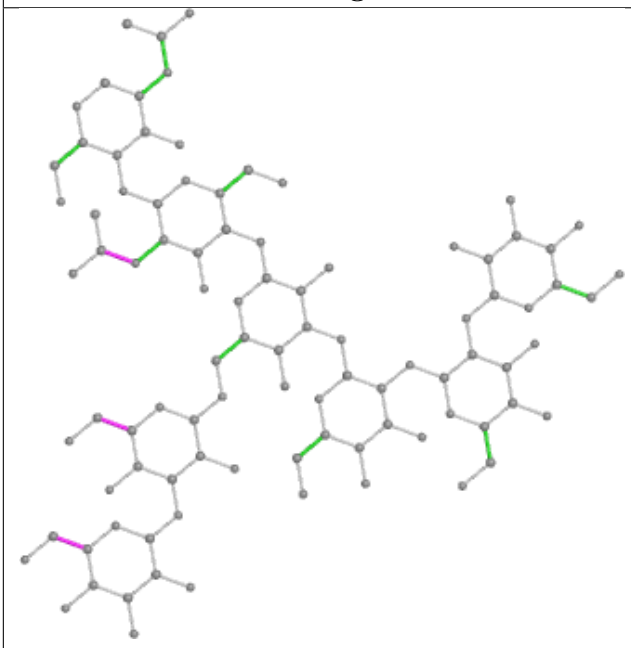
Oligosaccharide Chain F



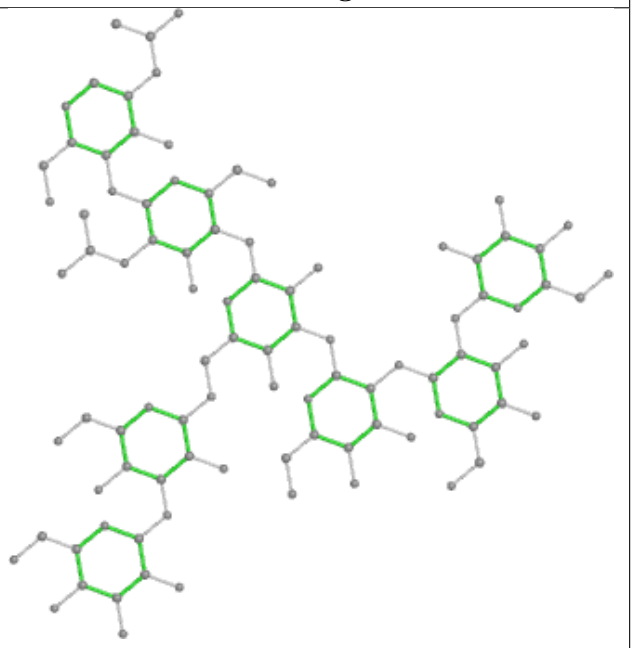
Bond lengths



Bond angles

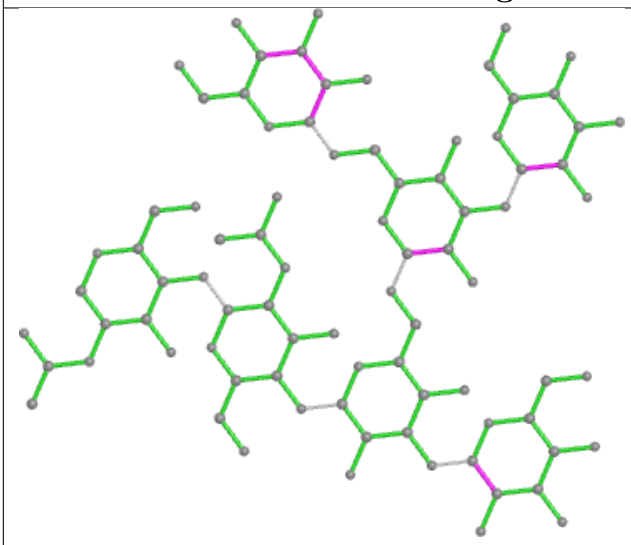


Torsions

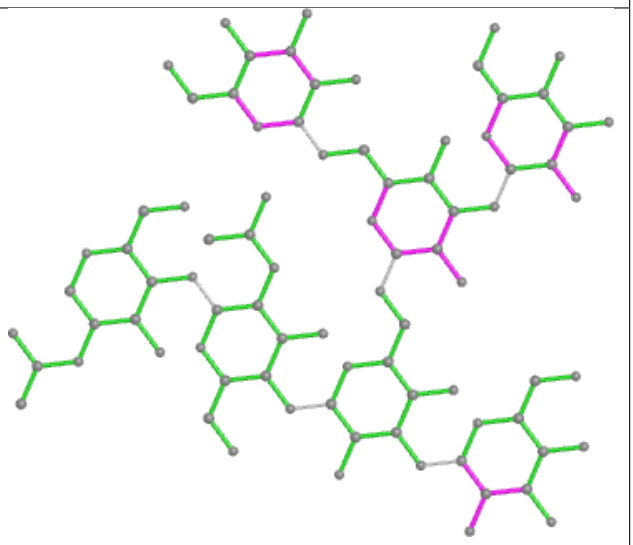


Rings

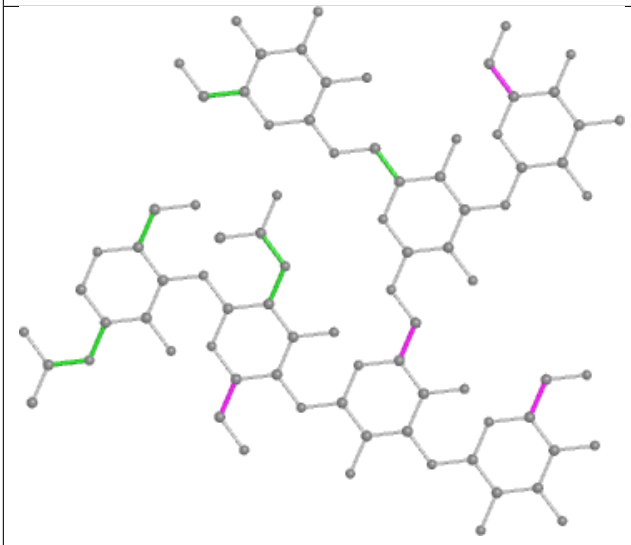
Oligosaccharide Chain E



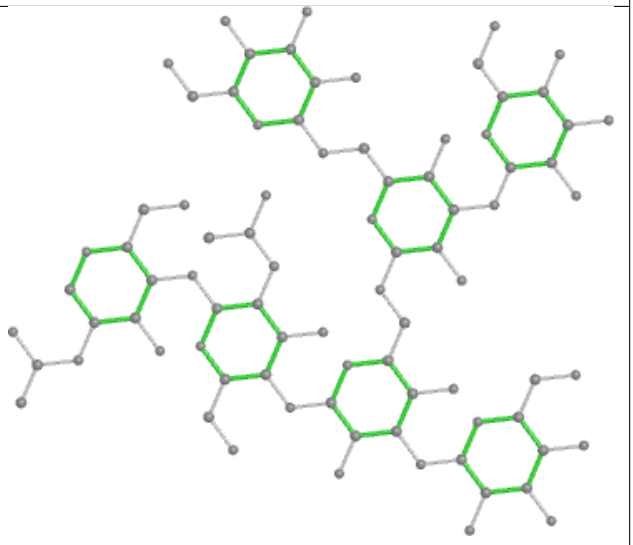
Bond lengths



Bond angles

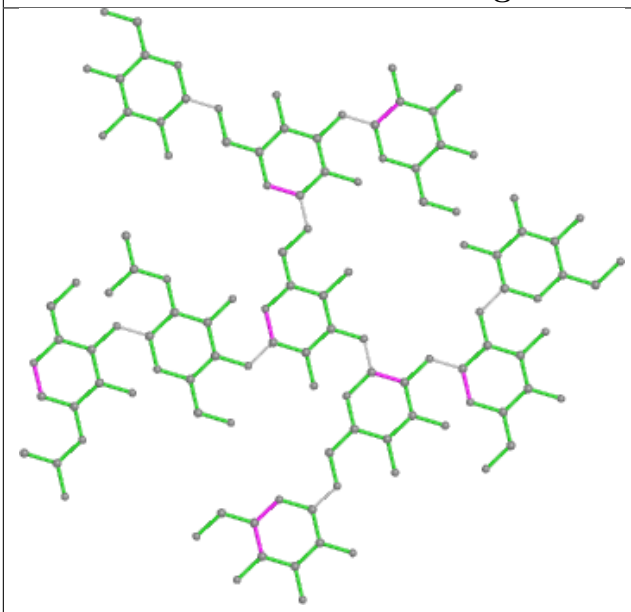


Torsions

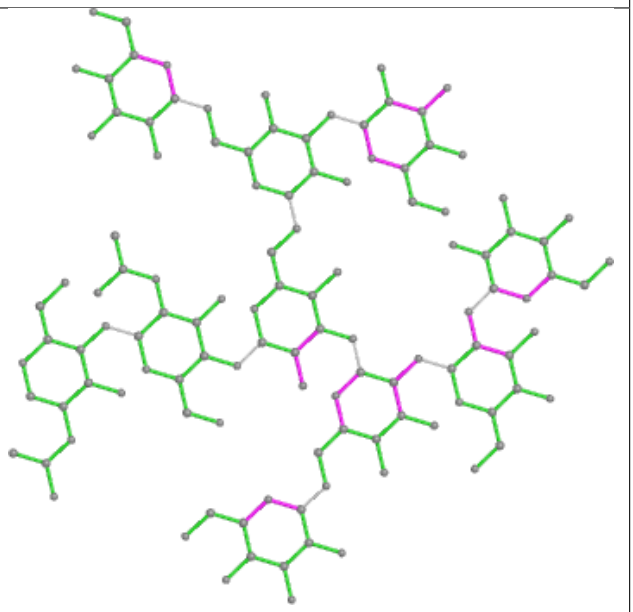


Rings

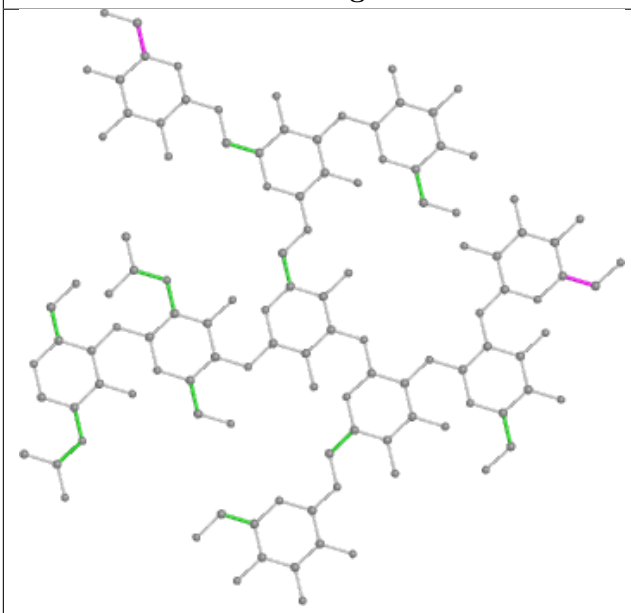
Oligosaccharide Chain G



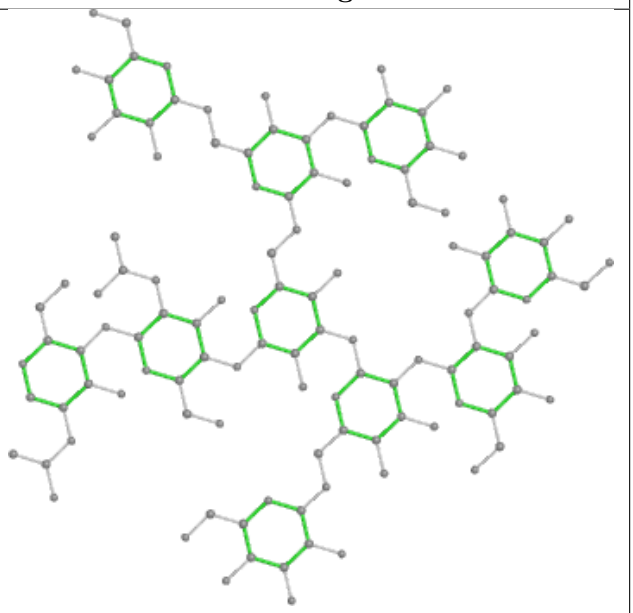
Bond lengths



Bond angles

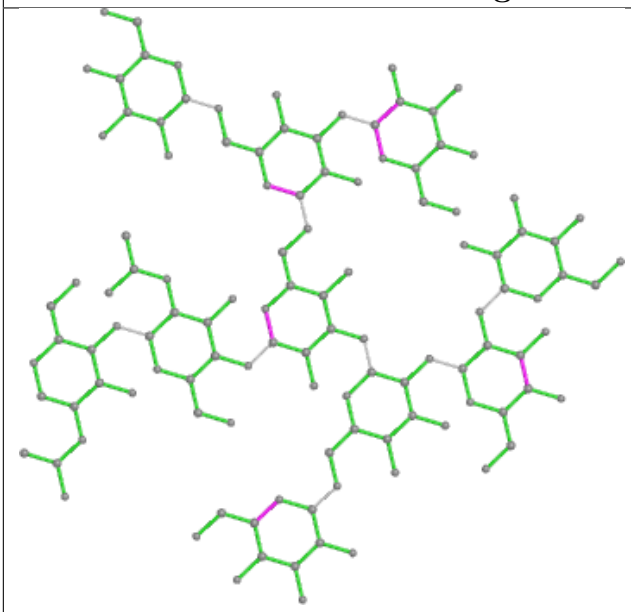


Torsions

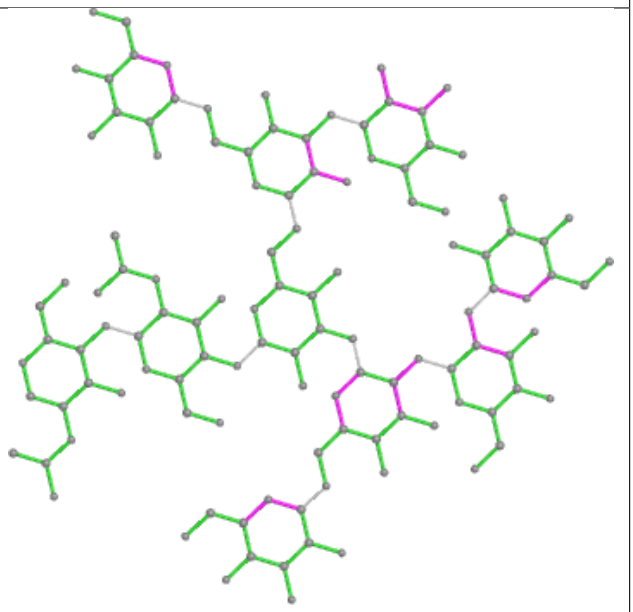


Rings

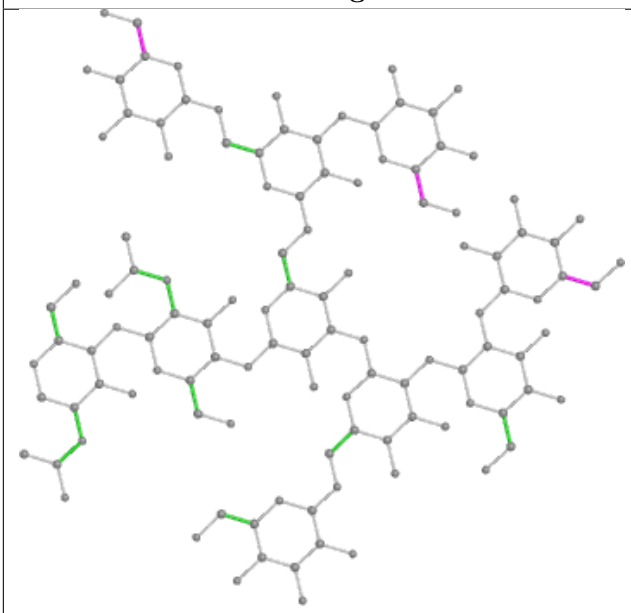
Oligosaccharide Chain H



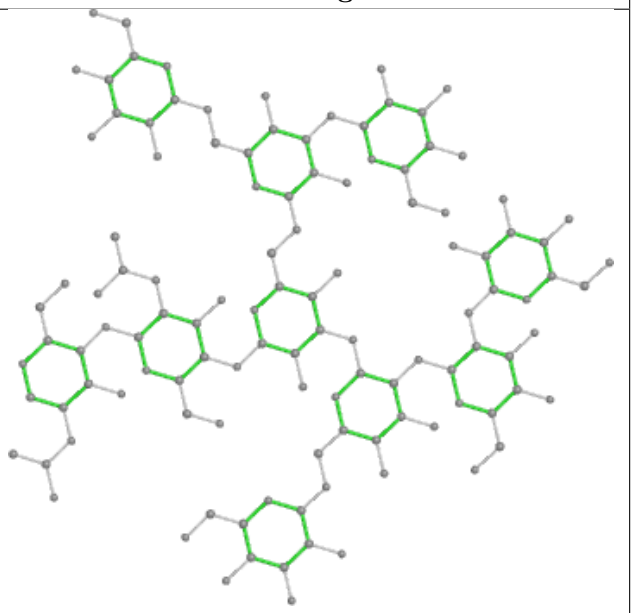
Bond lengths



Bond angles

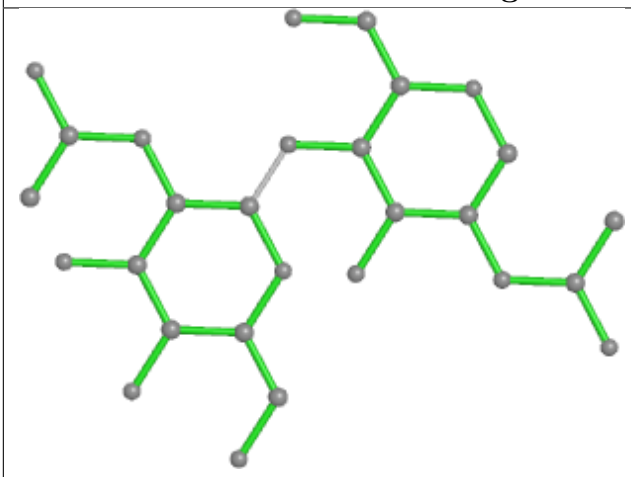


Torsions

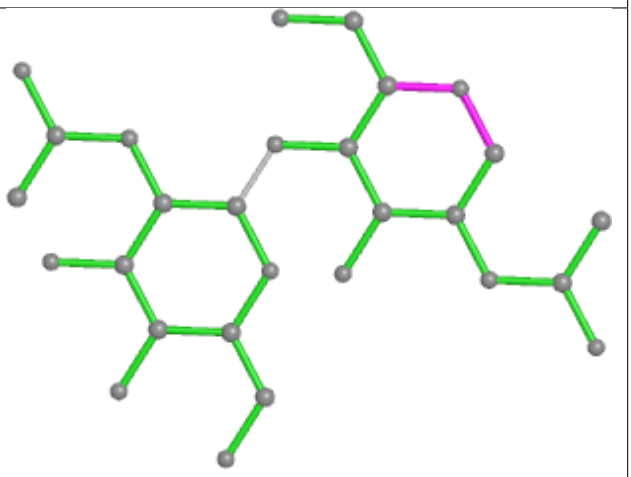


Rings

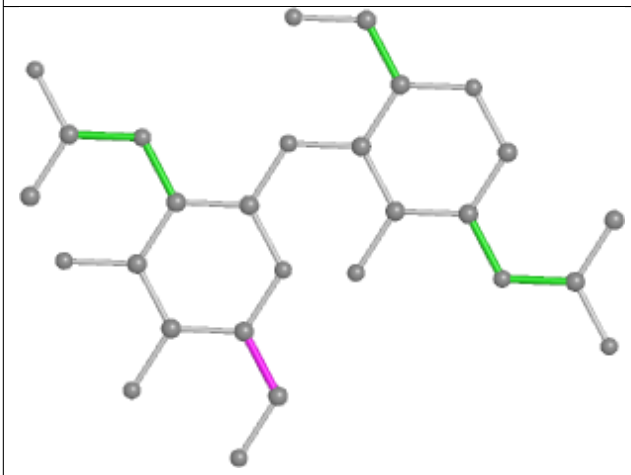
Oligosaccharide Chain I



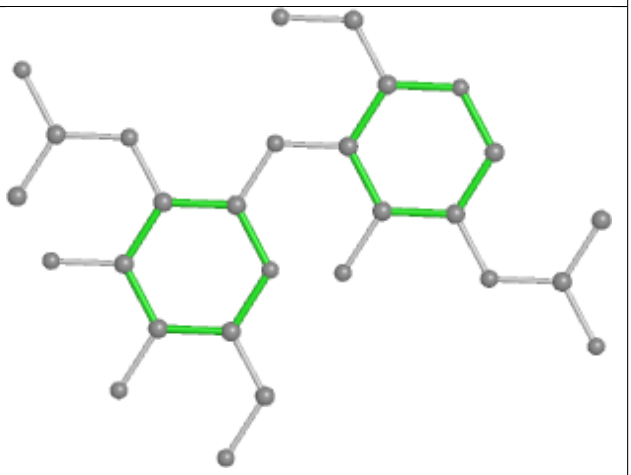
Bond lengths



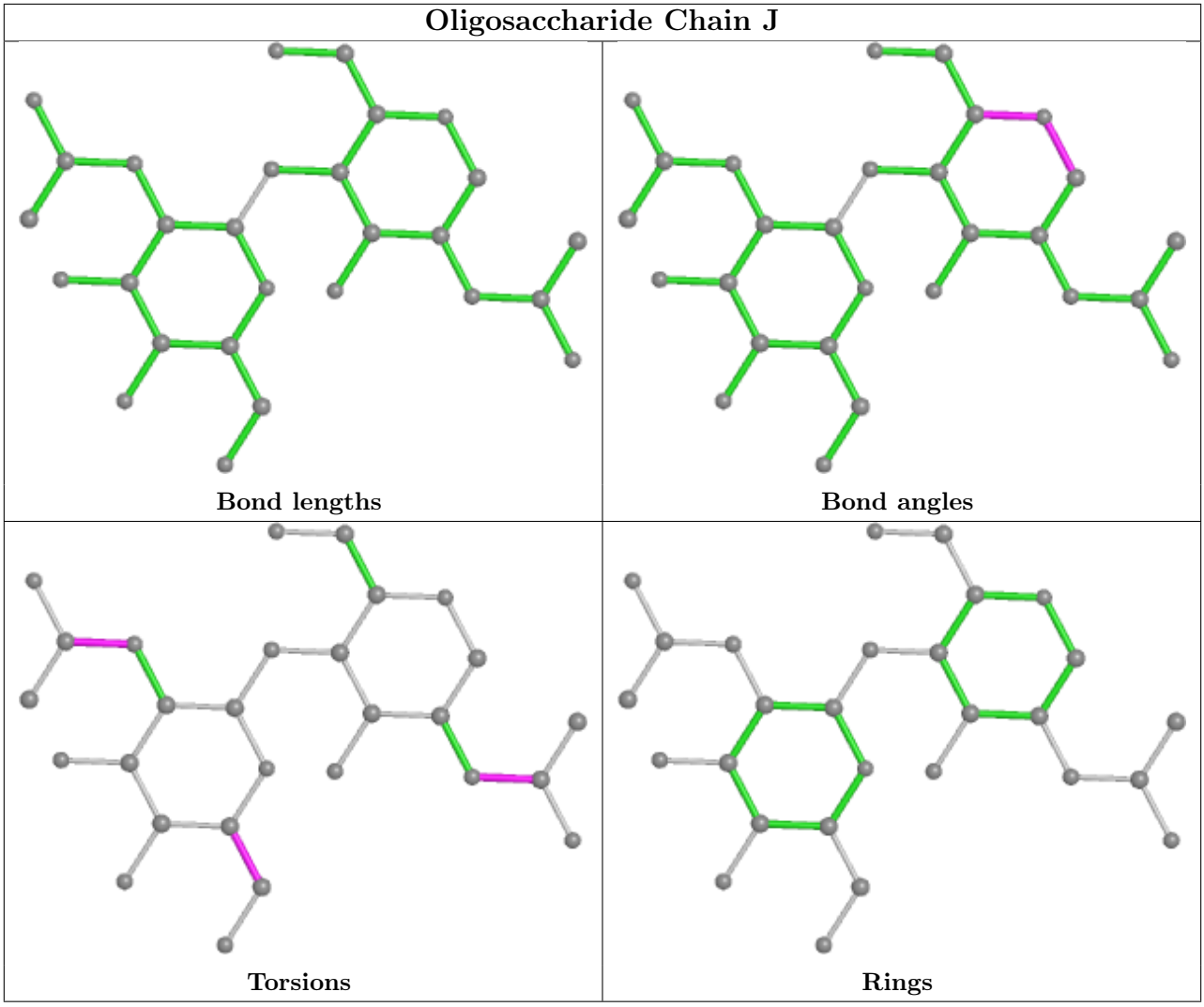
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
9	GOL	A	606	-	5,5,5	0.74	0	5,5,5	1.27	0
8	NAG	A	602	1	14,14,15	0.49	0	17,19,21	0.64	0
9	GOL	B	606	-	5,5,5	1.09	0	5,5,5	0.87	0
9	GOL	B	608	-	5,5,5	1.08	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GOL	A	607	-	5,5,5	1.15	0	5,5,5	0.91	0
9	GOL	A	610	-	5,5,5	0.89	0	5,5,5	1.11	0
9	GOL	B	602	-	5,5,5	0.82	0	5,5,5	1.15	1 (20%)
9	GOL	A	612	-	5,5,5	0.95	0	5,5,5	0.97	0
9	GOL	B	601	-	5,5,5	0.76	0	5,5,5	1.06	0
7	MAN	B	603	1	11,11,12	1.09	1 (9%)	15,15,17	0.98	1 (6%)
8	NAG	A	603	1	14,14,15	0.64	0	17,19,21	0.53	0
7	MAN	A	601	1	11,11,12	1.02	0	15,15,17	0.86	0
9	GOL	A	609	-	5,5,5	0.78	0	5,5,5	1.04	0
9	GOL	A	608	-	5,5,5	0.99	0	5,5,5	0.83	0
9	GOL	A	605	-	5,5,5	0.73	0	5,5,5	1.10	0
9	GOL	B	607	-	5,5,5	1.14	1 (20%)	5,5,5	0.82	0
8	NAG	B	605	1	14,14,15	0.49	0	17,19,21	0.38	0
9	GOL	A	613	-	5,5,5	0.54	0	5,5,5	0.96	0
9	GOL	A	611	-	5,5,5	0.87	0	5,5,5	0.95	0
8	NAG	B	604	1	14,14,15	0.41	0	17,19,21	0.49	0
9	GOL	A	604	-	5,5,5	1.17	1 (20%)	5,5,5	0.92	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
9	GOL	A	606	-	-	4/4/4/4	-
8	NAG	A	602	1	-	2/6/23/26	0/1/1/1
9	GOL	B	606	-	-	0/4/4/4	-
9	GOL	B	608	-	-	2/4/4/4	-
9	GOL	A	607	-	-	3/4/4/4	-
9	GOL	A	610	-	-	4/4/4/4	-
9	GOL	B	602	-	-	2/4/4/4	-
9	GOL	A	612	-	-	0/4/4/4	-
9	GOL	B	601	-	-	2/4/4/4	-
7	MAN	B	603	1	-	1/2/19/22	0/1/1/1
8	NAG	A	603	1	-	2/6/23/26	0/1/1/1
7	MAN	A	601	1	-	2/2/19/22	0/1/1/1
9	GOL	A	609	-	-	2/4/4/4	-
9	GOL	A	608	-	-	2/4/4/4	-
9	GOL	A	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	B	607	-	-	2/4/4/4	-
8	NAG	B	605	1	-	0/6/23/26	0/1/1/1
9	GOL	A	613	-	-	2/4/4/4	-
9	GOL	A	611	-	-	0/4/4/4	-
8	NAG	B	604	1	-	1/6/23/26	0/1/1/1
9	GOL	A	604	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	604	GOL	O2-C2	-2.49	1.36	1.43
7	B	603	MAN	C4-C5	2.47	1.58	1.53
9	B	607	GOL	C3-C2	2.24	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	603	MAN	C1-O5-C5	2.23	115.21	112.19
9	B	602	GOL	C3-C2-C1	-2.14	103.38	111.70

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	608	GOL	C1-C2-C3-O3
9	A	609	GOL	C1-C2-C3-O3
9	A	610	GOL	O1-C1-C2-C3
9	A	610	GOL	C1-C2-C3-O3
9	A	613	GOL	O1-C1-C2-C3
9	B	601	GOL	C1-C2-C3-O3
9	B	602	GOL	C1-C2-C3-O3
9	B	608	GOL	C1-C2-C3-O3
7	A	601	MAN	O5-C5-C6-O6
7	A	601	MAN	C4-C5-C6-O6
8	A	602	NAG	O5-C5-C6-O6
9	A	610	GOL	O1-C1-C2-O2
9	A	610	GOL	O2-C2-C3-O3
8	B	604	NAG	O5-C5-C6-O6
9	A	605	GOL	C1-C2-C3-O3
9	A	606	GOL	O1-C1-C2-C3
9	A	607	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	B	607	GOL	C1-C2-C3-O3
9	A	605	GOL	O2-C2-C3-O3
9	A	608	GOL	O2-C2-C3-O3
9	A	613	GOL	O1-C1-C2-O2
9	B	601	GOL	O2-C2-C3-O3
9	B	602	GOL	O2-C2-C3-O3
9	B	607	GOL	O2-C2-C3-O3
9	B	608	GOL	O2-C2-C3-O3
9	A	607	GOL	O1-C1-C2-O2
8	A	603	NAG	C4-C5-C6-O6
8	A	603	NAG	O5-C5-C6-O6
9	A	606	GOL	O2-C2-C3-O3
9	A	609	GOL	O2-C2-C3-O3
9	A	606	GOL	O1-C1-C2-O2
7	B	603	MAN	O5-C5-C6-O6
9	A	606	GOL	C1-C2-C3-O3
8	A	602	NAG	C4-C5-C6-O6
9	A	607	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	610	GOL	1	0
9	B	602	GOL	1	0
9	A	612	GOL	1	0
9	A	605	GOL	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	549/648 (84%)	-0.02	8 (1%)	71	74	13, 24, 40, 57	3 (0%)
1	B	549/648 (84%)	-0.04	12 (2%)	62	64	20, 26, 42, 62	0
All	All	1098/1296 (84%)	-0.03	20 (1%)	67	70	13, 25, 41, 62	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	3.8
1	B	470	ILE	3.7
1	A	21	ALA	3.2
1	B	346	ASN	3.2
1	A	24	THR	2.8
1	B	22	ASN	2.7
1	A	443	SER	2.7
1	B	569	VAL	2.5
1	B	344	ASN	2.5
1	B	278	ASP	2.5
1	A	346	ASN	2.5
1	A	469	SER	2.4
1	A	470	ILE	2.4
1	A	278	ASP	2.4
1	B	472	GLY	2.3
1	B	198	ARG	2.2
1	B	137	SER	2.2
1	B	468	SER	2.1
1	A	228	ALA	2.1
1	B	23	CYS	2.1

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
2	MAN	C	6	11/12	0.48	0.16	58,63,65,71	0
4	MAN	E	7	11/12	0.51	0.16	63,66,71,73	0
6	NAG	J	2	14/15	0.62	0.16	71,76,81,81	0
6	NAG	I	2	14/15	0.69	0.14	60,69,75,75	0
4	MAN	E	6	11/12	0.70	0.17	51,58,63,64	0
2	BMA	C	3	11/12	0.72	0.14	46,50,57,61	0
6	NAG	J	1	14/15	0.74	0.15	49,57,65,70	0
3	MAN	F	8	11/12	0.76	0.14	51,56,63,65	0
3	MAN	D	8	11/12	0.76	0.14	49,53,55,55	0
5	MAN	G	10	11/12	0.78	0.12	48,49,53,54	0
4	BMA	E	3	11/12	0.78	0.12	47,51,58,64	0
3	MAN	F	7	11/12	0.80	0.13	45,49,52,58	0
5	MAN	G	9	11/12	0.80	0.13	29,31,33,37	0
3	MAN	D	7	11/12	0.80	0.12	43,48,52,53	0
2	MAN	C	5	11/12	0.81	0.18	29,37,41,41	0
4	MAN	E	4	11/12	0.81	0.13	44,45,53,56	0
5	MAN	H	10	11/12	0.81	0.11	42,45,48,50	0
2	MAN	C	4	11/12	0.83	0.11	35,42,46,50	0
6	NAG	I	1	14/15	0.84	0.11	40,46,58,62	0
4	MAN	E	5	11/12	0.84	0.17	27,36,43,44	0
5	MAN	H	6	11/12	0.85	0.12	34,38,45,46	0
5	MAN	H	5	11/12	0.86	0.12	29,34,37,47	0
5	MAN	H	7	11/12	0.87	0.11	30,38,41,41	0
5	MAN	G	6	11/12	0.87	0.11	29,35,41,46	0
5	MAN	G	5	11/12	0.88	0.11	28,33,35,40	0
3	NAG	F	2	14/15	0.88	0.11	28,32,38,42	0
5	MAN	H	9	11/12	0.88	0.11	27,29,35,39	0
5	MAN	G	7	11/12	0.88	0.10	32,36,38,38	0
2	NAG	C	2	14/15	0.89	0.11	32,38,42,44	0
5	NAG	G	2	14/15	0.90	0.09	25,27,29,31	0
5	MAN	G	8	11/12	0.90	0.10	27,32,39,44	0
5	MAN	H	4	11/12	0.90	0.09	30,32,36,37	0

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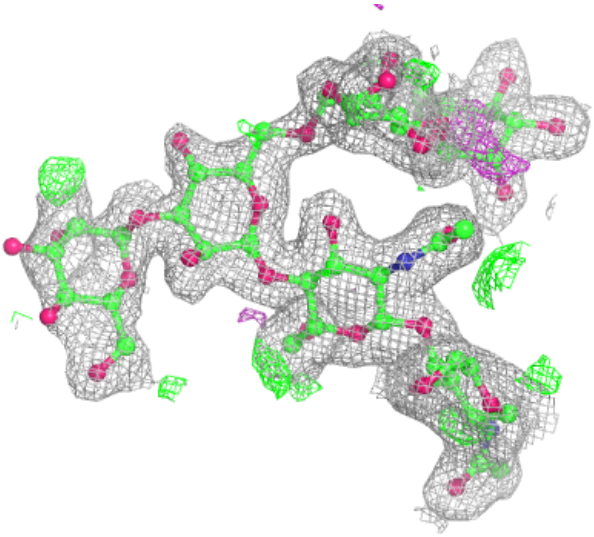
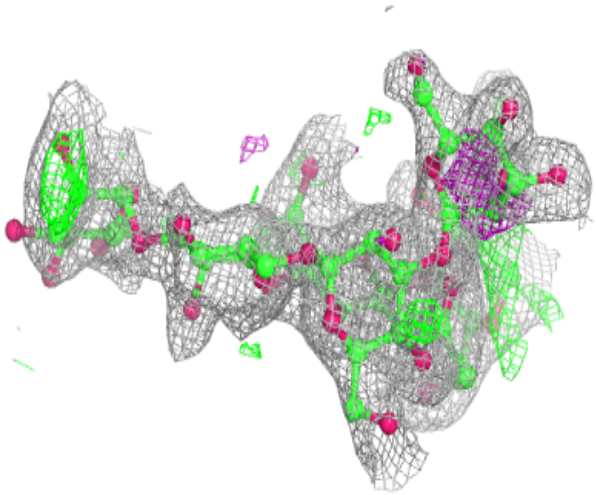
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	D	6	11/12	0.91	0.09	31,33,37,37	0
3	NAG	D	2	14/15	0.91	0.10	29,31,37,39	0
3	MAN	D	4	11/12	0.91	0.08	23,28,29,30	0
4	NAG	E	2	14/15	0.91	0.10	33,37,43,48	0
5	BMA	H	3	11/12	0.91	0.09	27,28,33,34	0
3	MAN	F	4	11/12	0.92	0.08	22,27,29,30	0
3	MAN	F	6	11/12	0.92	0.09	29,30,34,34	0
5	NAG	G	1	14/15	0.92	0.08	25,28,29,31	0
5	MAN	G	4	11/12	0.93	0.08	25,32,35,35	0
3	NAG	F	1	14/15	0.93	0.07	26,30,33,34	0
2	NAG	C	1	14/15	0.93	0.08	23,27,29,31	0
5	NAG	H	2	14/15	0.93	0.08	24,29,30,33	0
5	BMA	G	3	11/12	0.93	0.07	26,28,32,33	0
3	MAN	D	5	11/12	0.94	0.07	23,26,28,30	0
3	MAN	F	5	11/12	0.94	0.07	24,26,29,29	0
4	NAG	E	1	14/15	0.94	0.09	19,25,27,30	0
5	NAG	H	1	14/15	0.94	0.08	22,26,29,33	0
3	NAG	D	1	14/15	0.94	0.07	25,28,31,33	0
5	MAN	H	8	11/12	0.94	0.08	25,29,35,38	0
3	BMA	F	3	11/12	0.95	0.06	26,29,34,37	0
3	BMA	D	3	11/12	0.96	0.06	25,29,34,38	0

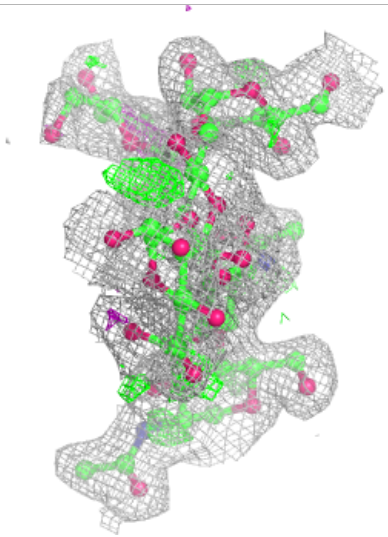
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

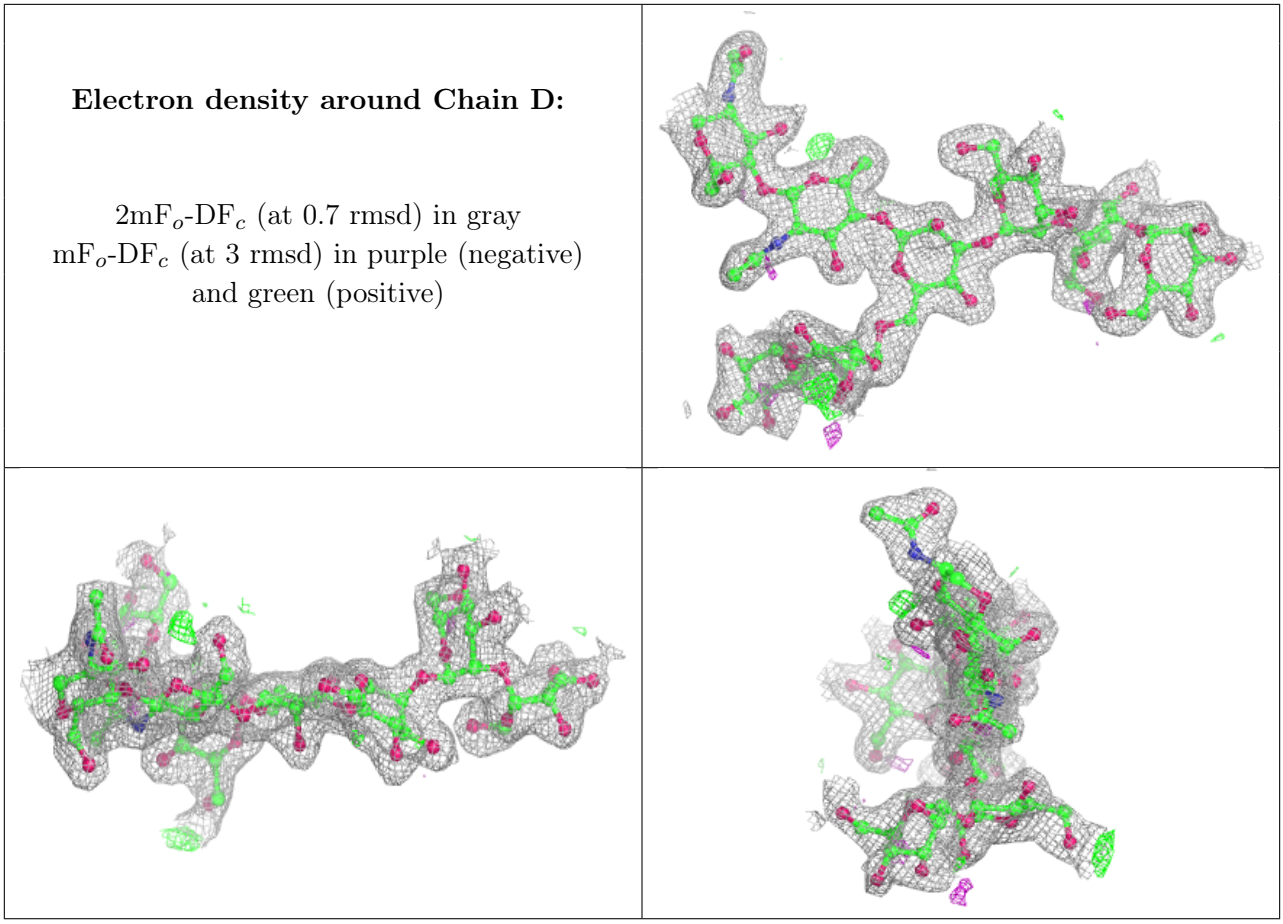






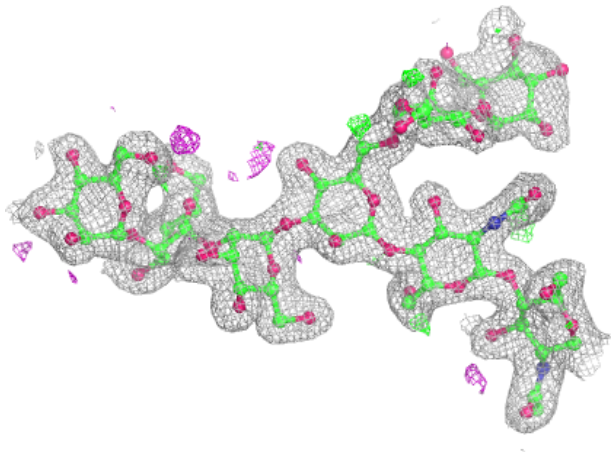
Electron density around Chain D:

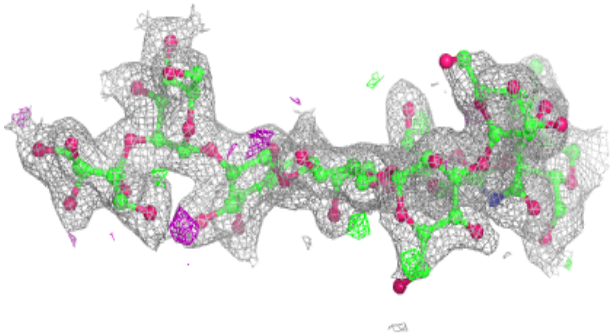
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

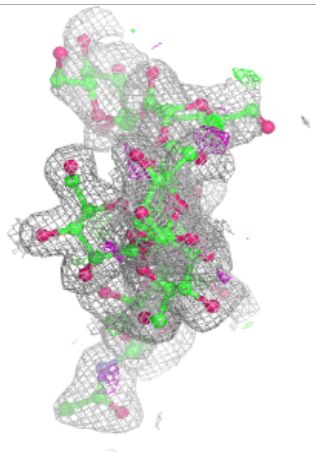


Electron density around Chain F:

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

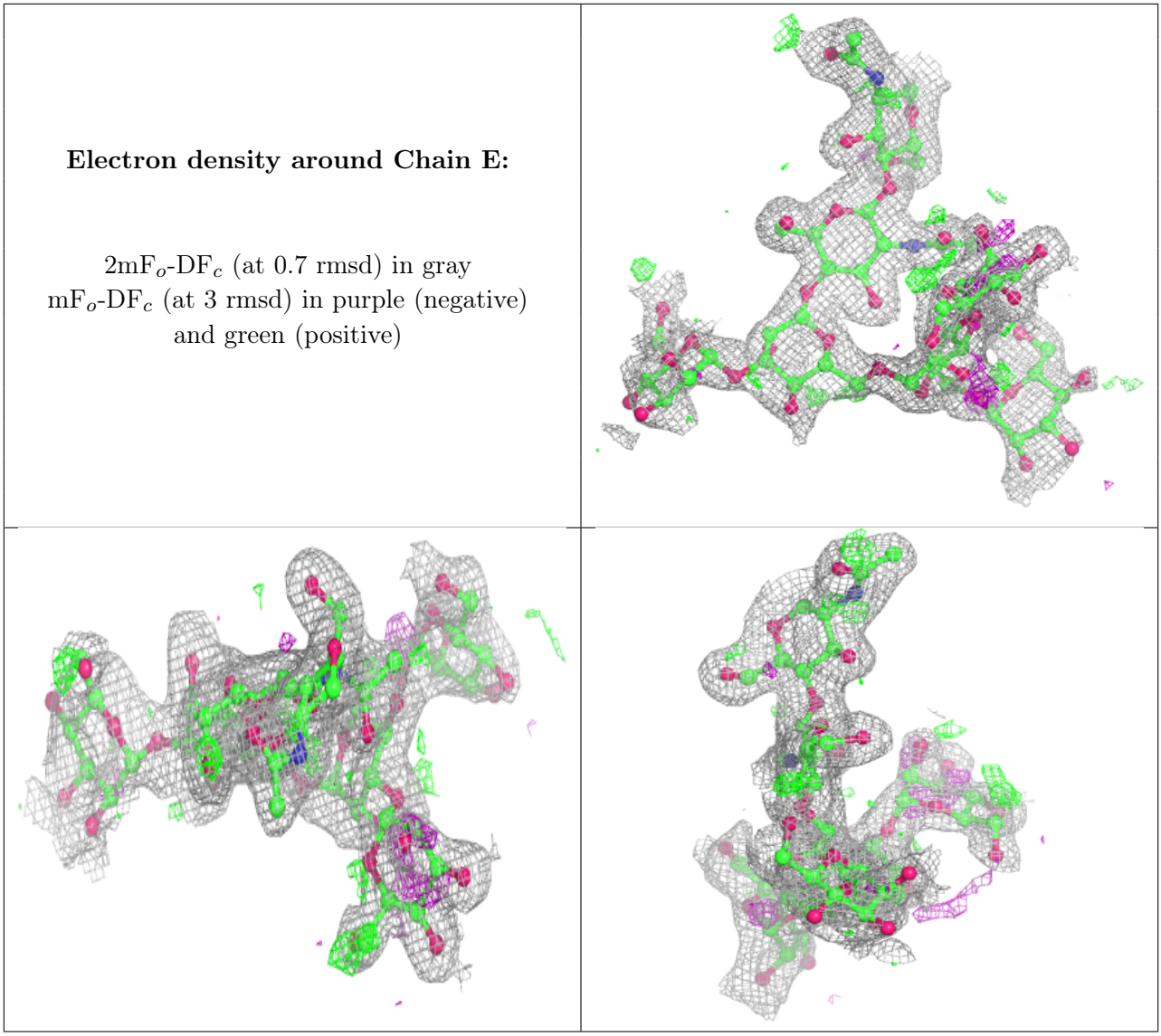






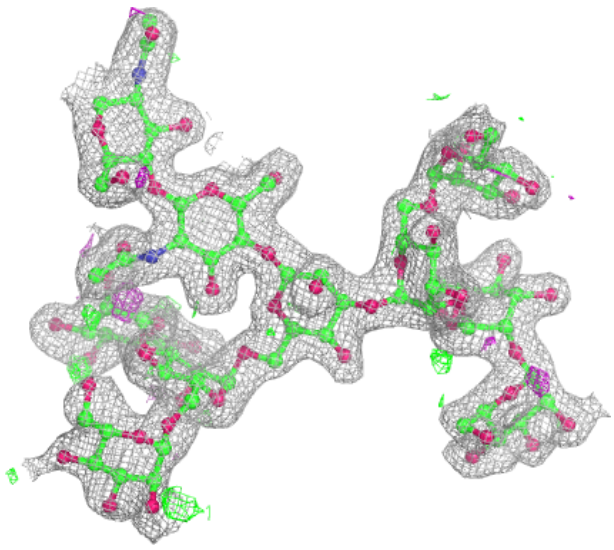
Electron density around Chain E:

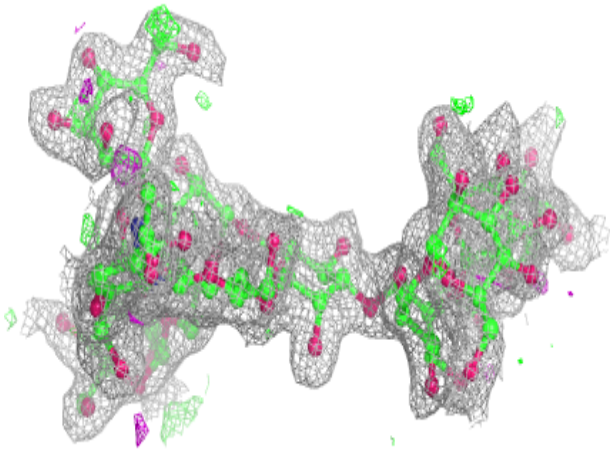
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

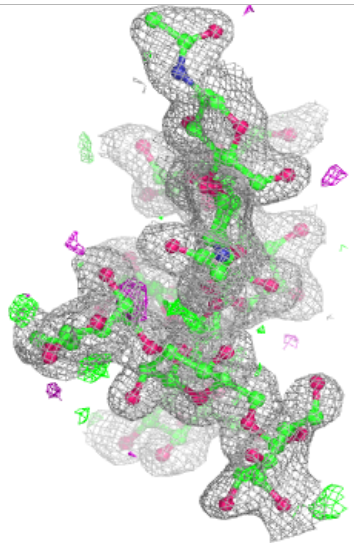


Electron density around Chain G:

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

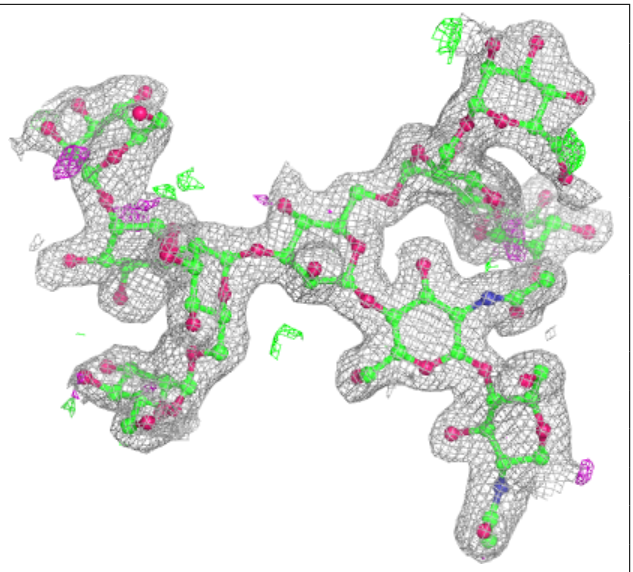


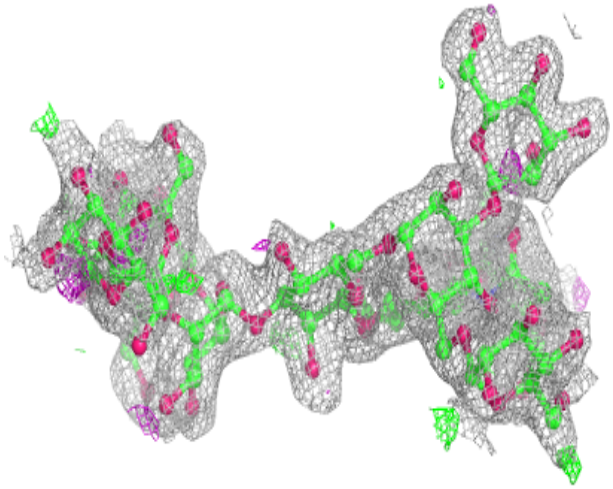


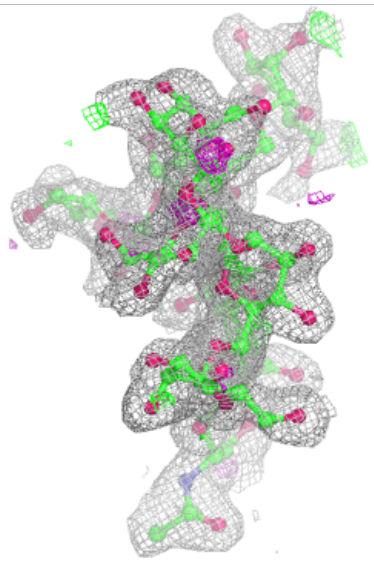


Electron density around Chain H:

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

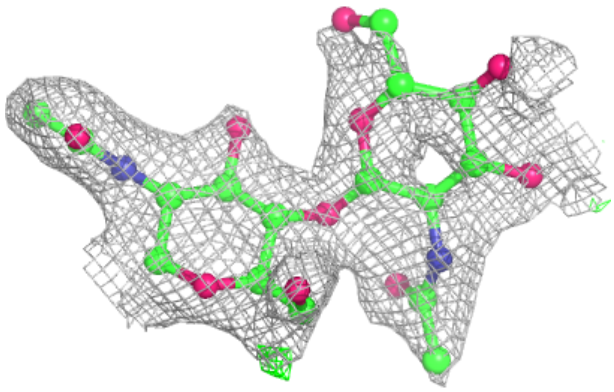


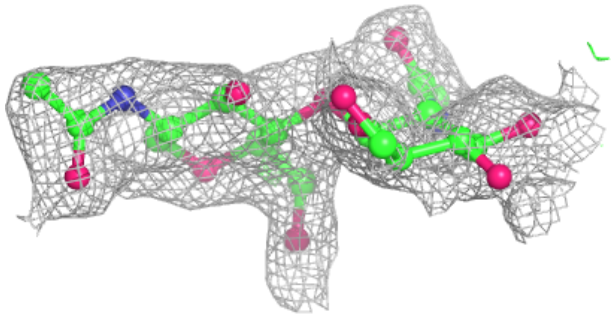


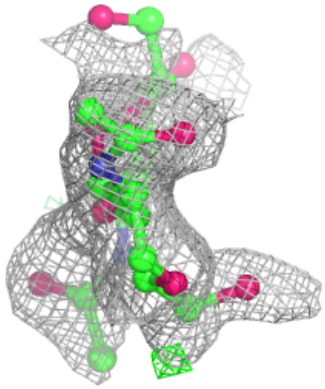


Electron density around Chain I:

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

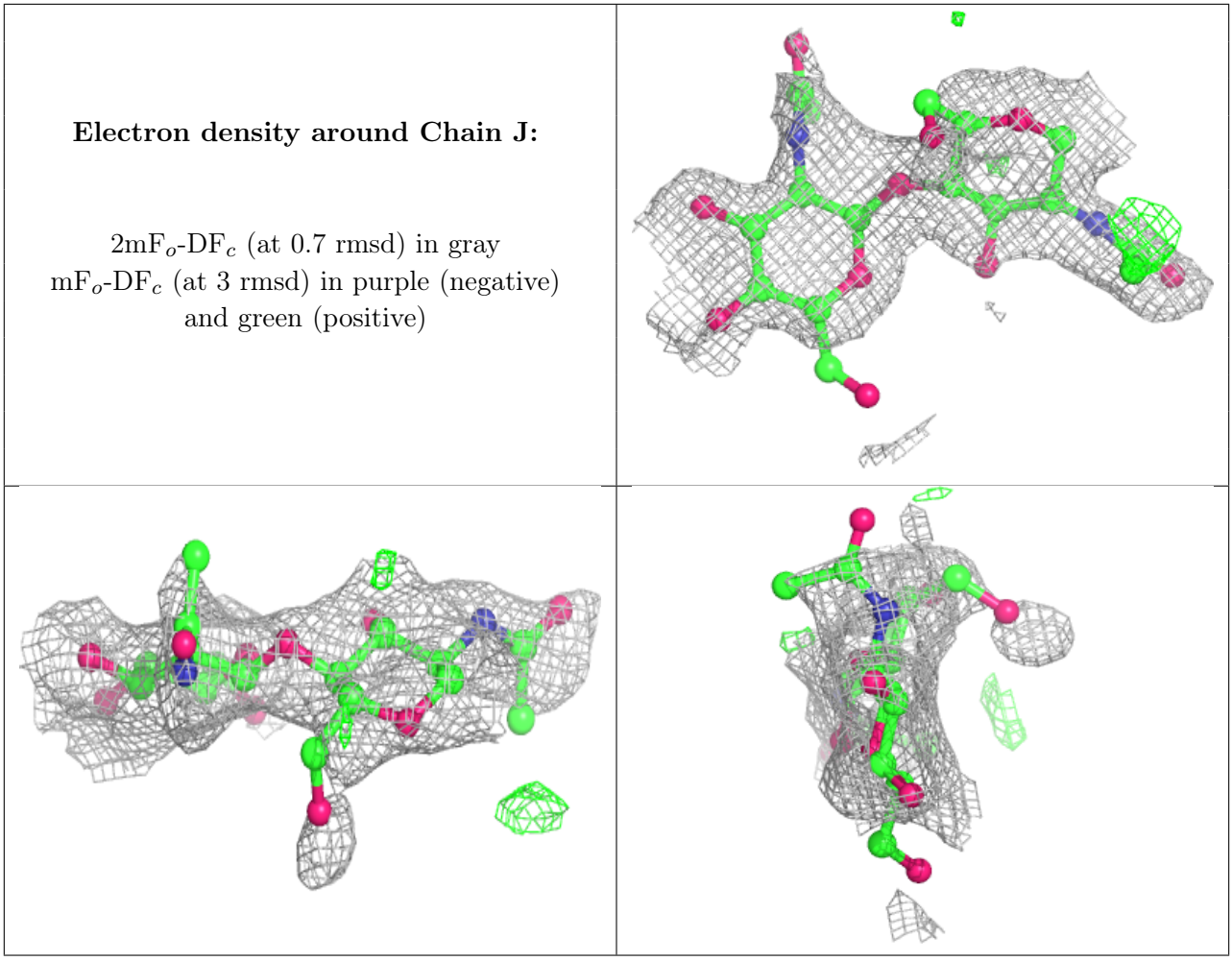






Electron density around Chain J:

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



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
8	NAG	A	603	14/15	0.67	0.15	53,60,67,67	0
7	MAN	A	601	11/12	0.68	0.15	35,39,46,53	0
8	NAG	B	605	14/15	0.71	0.14	50,59,63,66	0
8	NAG	A	602	14/15	0.73	0.15	45,47,51,51	0
9	GOL	A	610	6/6	0.73	0.17	37,39,40,43	0
8	NAG	B	604	14/15	0.76	0.14	48,51,54,59	0
9	GOL	A	609	6/6	0.78	0.15	36,37,40,46	0
7	MAN	B	603	11/12	0.81	0.12	37,41,47,48	0
9	GOL	A	613	6/6	0.81	0.16	26,33,37,40	0
9	GOL	A	612	6/6	0.82	0.14	38,40,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	A	604	6/6	0.82	0.13	34,37,40,43	0
9	GOL	B	607	6/6	0.82	0.15	32,34,38,40	0
9	GOL	B	608	6/6	0.83	0.14	30,37,40,45	0
9	GOL	A	606	6/6	0.84	0.13	32,37,40,42	0
9	GOL	A	611	6/6	0.84	0.15	28,35,36,45	0
9	GOL	A	608	6/6	0.85	0.15	25,34,38,39	0
9	GOL	A	605	6/6	0.86	0.12	31,37,40,44	0
9	GOL	B	601	6/6	0.87	0.14	27,33,37,41	0
9	GOL	B	602	6/6	0.88	0.12	31,36,40,41	0
9	GOL	A	607	6/6	0.91	0.09	31,36,38,40	0
9	GOL	B	606	6/6	0.94	0.08	30,34,35,38	0

6.5 Other polymers (i)

There are no such residues in this entry.