



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 10:01 PM JST

PDB ID : 9L3J / pdb_00009l3j
Title : Crystal structure of endo-processive xyloglucanase Xeg5A from *Aspergillus oryzae* with GXG
Authors : Nakamichi, Y.; Shimada, N.; Watanabe, M.; Fujii, T.; Matsuzawa, T.
Deposited on : 2024-12-18
Resolution : 2.74 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

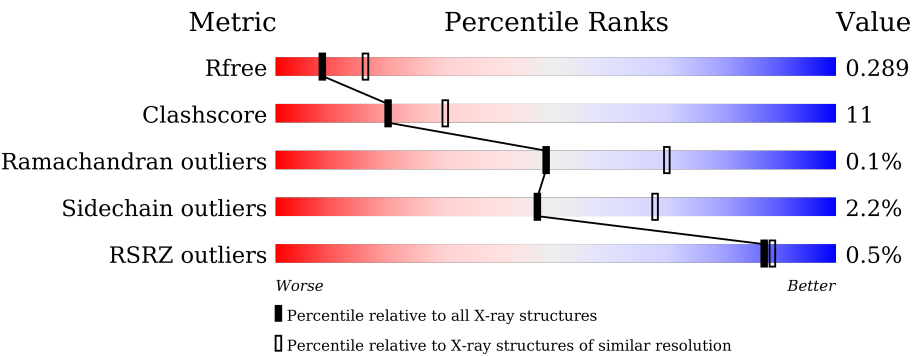
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
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 2.74 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.



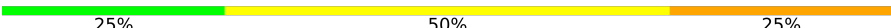


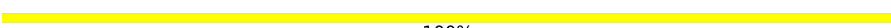
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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 $\leq 5\%$. 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	<div><div></div><div>63%21%15%</div></div>
1	B	648	<div><div></div><div>%63%21%15%</div></div>
2	C	4	<div><div></div><div>100%</div></div>
2	E	4	<div><div></div><div>25%75%</div></div>
3	D	3	<div><div></div><div>33%67%</div></div>
4	F	8	<div><div></div><div>12%62%25%</div></div>

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Mol	Chain	Length	Quality of chain
5	G	7	 29% 71%
6	H	4	 25% 50% 25%
7	I	6	 17% 83%
8	J	5	 40% 60%
9	K	2	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9209 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	0	0
			4309	2745	704	853	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

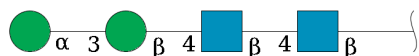
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP I8IVP5
B	-14	ASN	-	expression tag	UNP I8IVP5
B	-13	SER	-	expression tag	UNP I8IVP5
B	-12	THR	-	expression tag	UNP I8IVP5
B	-11	ASN	-	expression tag	UNP I8IVP5
B	-10	ASN	-	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

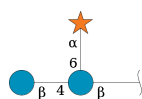
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



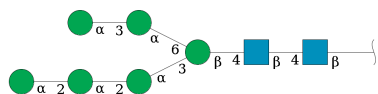
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose.



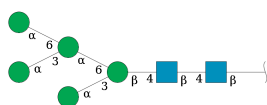
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	0	0	0
			32	17	15			

- Molecule 4 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.



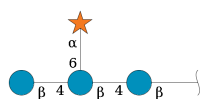
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 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.



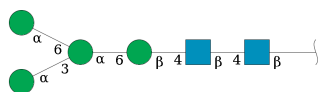
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



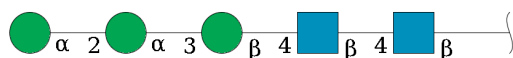
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	H	4	Total	C	O	0	0	0
			43	23	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



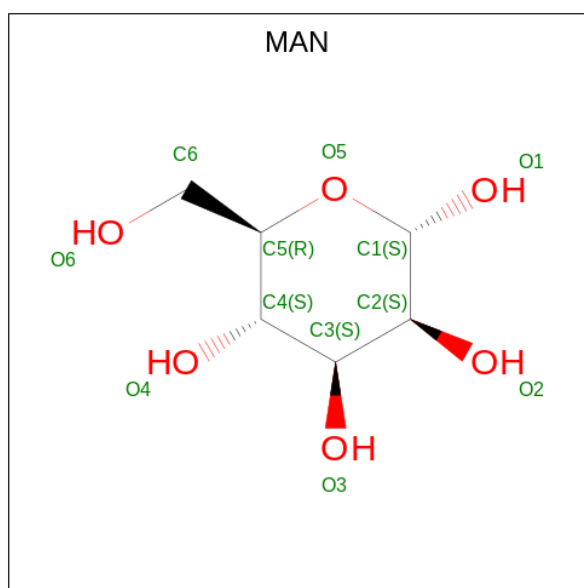
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

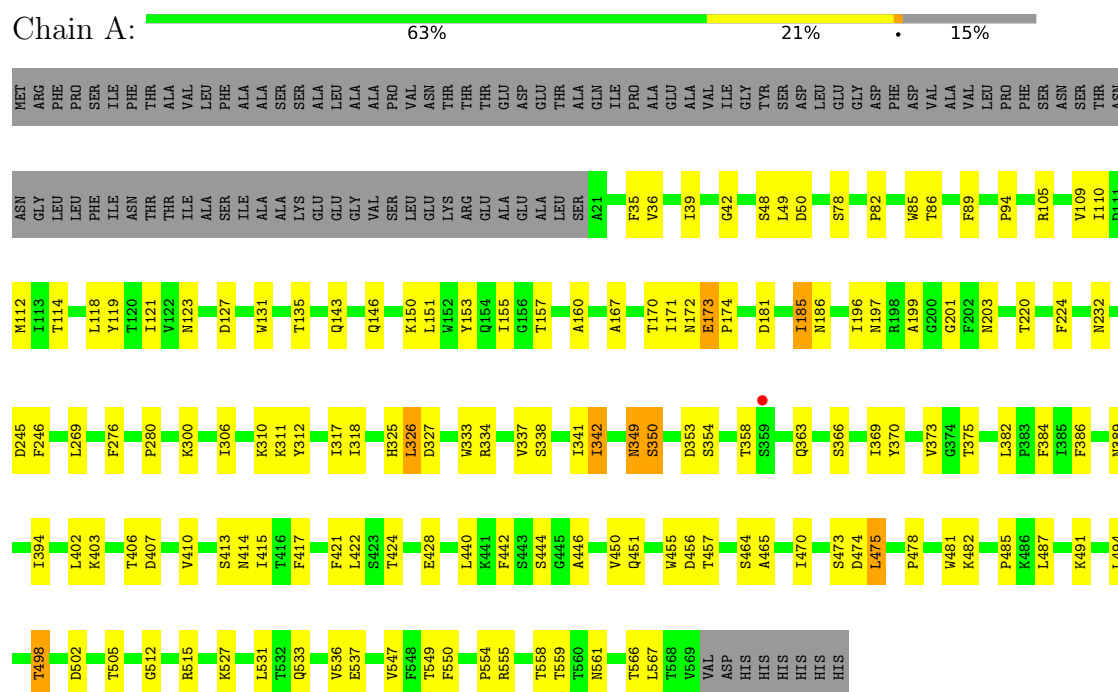


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

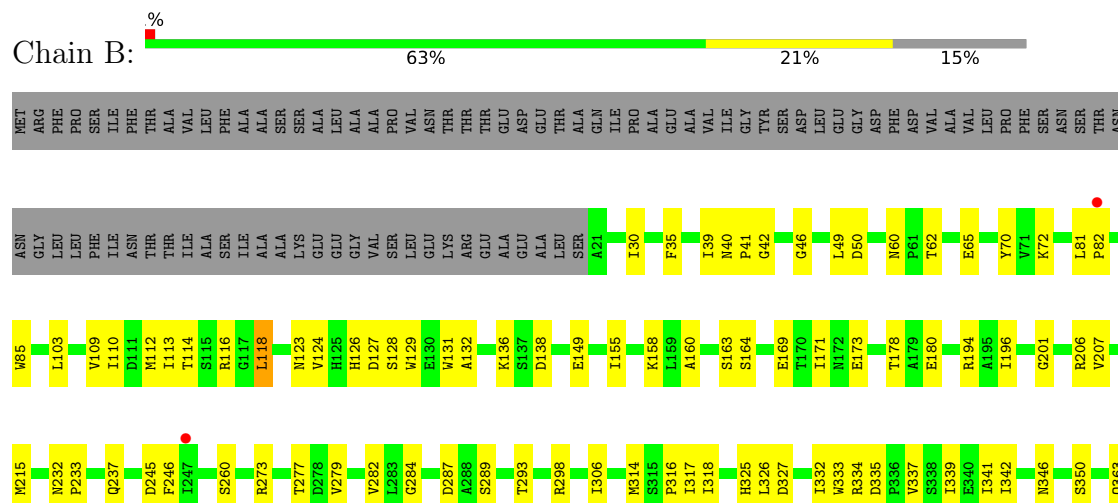
3 Residue-property plots

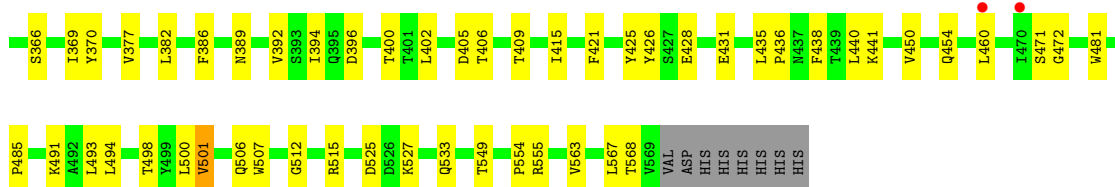
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Glycoside hydrolase superfamily





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

Chain C: 100%



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

Chain E: 25%



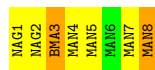
- Molecule 3: beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose

Chain D: 33%



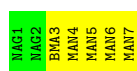
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 12%



- Molecule 5: 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 G: 29%



- Molecule 6: beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain H:  25% 50% 25%

BGC1
BGC2
BGC3
XYS4

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  17% 83%

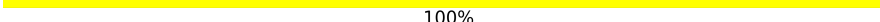
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain K:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.30Å 106.91Å 83.74Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	38.98 – 2.74 38.98 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.98-2.74) 98.3 (38.98-2.74)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.237 , 0.289 0.237 , 0.289	Depositor DCC
R_{free} test set	2257 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.119 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9209	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, YYS, BGC

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	0.20	1/4430 (0.0%)	0.38	0/6064
1	B	0.20	0/4430	0.41	0/6064
All	All	0.20	1/8860 (0.0%)	0.40	0/12128

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	CA-C	-5.81	1.49	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4309	0	4099	104	0
1	B	4309	0	4100	96	0
2	C	50	0	43	0	0
2	E	50	0	43	0	0
3	D	32	0	28	0	0
4	F	94	0	79	2	0
5	G	83	0	70	0	0
6	H	43	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	72	0	61	0	0
8	J	61	0	52	4	0
9	K	28	0	25	0	0
10	A	11	0	10	0	0
10	B	11	0	10	0	0
11	A	42	0	39	2	0
11	B	14	0	13	0	0
All	All	9209	0	8709	200	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 11.

All (200) 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:440:LEU:HB3	1:A:442:PHE:HE1	1.40	0.86
1:A:349:ASN:HD22	1:A:446:ALA:H	1.25	0.84
1:A:366:SER:HA	1:A:382:LEU:HD12	1.63	0.81
1:A:470:ILE:HD13	1:A:475:LEU:HG	1.70	0.74
1:B:332:ILE:HD11	4:F:8:MAN:H62	1.69	0.74
1:A:109:VAL:HA	1:A:112:MET:HE3	1.71	0.71
1:B:293:THR:HG23	1:B:298:ARG:HE	1.57	0.70
1:A:410:VAL:HG22	1:A:415:ILE:HG12	1.75	0.69
1:B:160:ALA:HB1	1:B:201:GLY:HA3	1.74	0.69
1:A:417:PHE:HB3	1:A:422:LEU:HD11	1.76	0.68
1:B:49:LEU:HD12	1:B:81:LEU:HD11	1.76	0.68
1:A:494:LEU:HD12	1:A:498:THR:HB	1.76	0.68
1:B:85:TRP:CE2	1:B:155:ILE:HD11	2.28	0.68
1:B:366:SER:HA	1:B:382:LEU:HD23	1.75	0.68
1:A:558:THR:HG23	1:A:559:THR:HG23	1.75	0.67
1:A:334:ARG:NE	8:J:4:MAN:O6	2.24	0.67
1:B:306:ILE:HD11	1:B:342:ILE:HG12	1.79	0.63
1:B:369:ILE:HD11	1:B:382:LEU:HD11	1.80	0.63
1:B:525:ASP:OD1	1:B:527:LYS:N	2.27	0.62
1:A:415:ILE:HG22	1:A:417:PHE:HE2	1.62	0.62
1:B:428:GLU:OE1	1:B:428:GLU:N	2.32	0.61
1:A:110:ILE:O	1:A:114:THR:HG22	2.02	0.60
1:A:326:LEU:HB2	1:A:333:TRP:CZ3	2.37	0.60
1:A:160:ALA:HB1	1:A:201:GLY:HA3	1.83	0.60
1:A:369:ILE:HD13	1:A:450:VAL:HG11	1.84	0.59
1:A:457:THR:HG22	1:A:561:ASN:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LYS:HB3	1:B:549:THR:HB	1.83	0.59
1:B:173:GLU:OE2	6:H:1:BGC:O1	2.21	0.59
1:B:65:GLU:HB2	1:B:116:ARG:NH2	2.19	0.58
1:A:415:ILE:HG22	1:A:417:PHE:CE2	2.38	0.58
1:B:110:ILE:O	1:B:114:THR:HG23	2.04	0.58
1:B:405:ASP:HA	1:B:409:THR:HG22	1.85	0.58
1:B:326:LEU:HB2	1:B:333:TRP:CZ3	2.40	0.57
1:A:547:VAL:HG22	1:A:566:THR:HG22	1.85	0.57
1:A:421:PHE:HD2	1:A:422:LEU:HD12	1.69	0.57
1:A:35:PHE:O	1:A:39:ILE:HG23	2.05	0.57
1:A:245:ASP:OD1	1:A:246:PHE:N	2.37	0.56
1:B:491:LYS:HE3	1:B:493:LEU:HD22	1.87	0.56
1:A:349:ASN:HD22	1:A:446:ALA:N	1.99	0.56
1:B:394:ILE:HG12	1:B:440:LEU:HG	1.87	0.56
1:A:36:VAL:HG21	1:A:280:PRO:HB3	1.87	0.56
1:B:85:TRP:CZ2	1:B:155:ILE:HD11	2.40	0.56
1:A:350:SER:HB2	1:A:442:PHE:CE2	2.42	0.55
1:A:369:ILE:HD11	1:A:382:LEU:HD21	1.88	0.55
1:B:325:HIS:O	1:B:334:ARG:HD2	2.06	0.55
1:B:289:SER:O	1:B:293:THR:HG22	2.06	0.55
1:B:326:LEU:HD12	1:B:333:TRP:CE2	2.41	0.55
1:A:327:ASP:OD2	8:J:3:BMA:O4	2.25	0.55
1:B:50:ASP:HB3	1:B:82:PRO:HB2	1.87	0.55
1:A:86:THR:HG23	1:A:131:TRP:HD1	1.71	0.55
1:B:30:ILE:HG22	1:B:164:SER:HB2	1.90	0.53
1:B:245:ASP:OD1	1:B:246:PHE:N	2.41	0.53
1:B:196:ILE:HD11	1:B:232:ASN:HD21	1.73	0.53
1:A:153:TYR:O	1:A:157:THR:HG23	2.08	0.53
1:A:306:ILE:HD11	1:A:342:ILE:HG23	1.91	0.52
1:A:487:LEU:HD11	1:A:550:PHE:HD1	1.75	0.52
1:A:318:ILE:HD11	1:A:325:HIS:NE2	2.25	0.52
1:B:207:VAL:HA	1:B:233:PRO:O	2.09	0.52
1:B:472:GLY:N	1:B:533:GLN:HE22	2.07	0.52
1:B:494:LEU:HD13	1:B:498:THR:HB	1.93	0.51
1:A:78:SER:HB3	1:A:119:TYR:HB2	1.92	0.51
1:B:326:LEU:HD12	1:B:333:TRP:CZ2	2.46	0.51
1:A:269:LEU:HB3	1:A:312:TYR:HD2	1.76	0.50
1:B:435:LEU:HB3	1:B:436:PRO:HD2	1.94	0.50
1:A:487:LEU:HD11	1:A:550:PHE:CD1	2.47	0.50
1:B:65:GLU:HB2	1:B:116:ARG:HH22	1.77	0.50
1:B:392:VAL:HG22	1:B:441:LYS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:HB3	1:A:549:THR:HB	1.94	0.49
1:A:478:PRO:HA	1:A:527:LYS:O	2.12	0.49
1:A:373:VAL:HG23	1:A:455:TRP:O	2.11	0.49
1:A:337:VAL:O	1:A:341:ILE:HG13	2.12	0.49
1:B:481:TRP:CE3	1:B:485:PRO:HA	2.47	0.49
1:B:173:GLU:HG2	1:B:215:MET:HB2	1.95	0.49
1:B:293:THR:CG2	1:B:298:ARG:HE	2.23	0.48
1:A:306:ILE:HG12	1:A:342:ILE:HA	1.96	0.48
1:A:349:ASN:ND2	1:A:446:ALA:H	2.04	0.48
1:B:46:GLY:O	1:B:60:ASN:ND2	2.47	0.48
1:B:425:TYR:HE2	1:B:438:PHE:CE1	2.31	0.48
1:A:310:LYS:HE2	1:A:310:LYS:HB2	1.67	0.48
1:B:460:LEU:HG	1:B:563:VAL:HG11	1.96	0.48
1:A:153:TYR:HE1	1:A:199:ALA:HA	1.79	0.48
1:A:338:SER:O	1:A:341:ILE:N	2.45	0.47
1:B:109:VAL:O	1:B:113:ILE:HG13	2.14	0.47
1:A:350:SER:HB2	1:A:442:PHE:CD2	2.50	0.47
1:B:386:PHE:HZ	1:B:415:ILE:HD11	1.80	0.47
1:A:338:SER:HA	1:A:341:ILE:HD12	1.97	0.47
1:A:533:GLN:NE2	1:A:537:GLU:OE2	2.48	0.47
1:A:421:PHE:O	1:A:424:THR:OG1	2.19	0.47
1:A:394:ILE:HG23	1:A:440:LEU:HD12	1.97	0.47
1:A:414:ASN:HD22	11:A:602:NAG:H83	1.80	0.47
1:A:86:THR:HG23	1:A:131:TRP:CD1	2.49	0.46
1:A:384:PHE:O	1:A:413:SER:HB2	2.15	0.46
1:A:350:SER:HB3	1:A:386:PHE:HA	1.96	0.46
1:B:35:PHE:O	1:B:39:ILE:HG23	2.15	0.46
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.83	0.46
1:B:494:LEU:HD11	1:B:500:LEU:HA	1.96	0.46
1:A:470:ILE:HD13	1:A:475:LEU:CG	2.43	0.46
1:A:203:ASN:O	1:A:232:ASN:ND2	2.45	0.46
1:B:402:LEU:HD22	1:B:421:PHE:HZ	1.81	0.46
1:B:103:LEU:HB3	1:B:158:LYS:HG2	1.97	0.45
1:B:196:ILE:HD11	1:B:232:ASN:ND2	2.31	0.45
1:A:311:LYS:HE2	1:A:312:TYR:CE1	2.52	0.45
1:B:178:THR:OG1	1:B:180:GLU:HG2	2.17	0.45
1:B:284:GLY:O	1:B:317:ILE:HB	2.16	0.45
1:B:500:LEU:HG	1:B:501:VAL:HG13	1.99	0.45
1:A:82:PRO:HA	1:A:123:ASN:OD1	2.17	0.45
1:A:456:ASP:HB3	1:A:482:LYS:HD2	1.97	0.45
1:A:174:PRO:HB2	1:A:185:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HD12	1:B:498:THR:O	2.17	0.45
1:A:49:LEU:HD11	1:A:109:VAL:HG21	1.99	0.45
1:A:170:THR:HG22	1:A:171:ILE:HG22	1.99	0.45
1:A:318:ILE:HD11	1:A:325:HIS:CD2	2.51	0.45
1:B:126:HIS:CD2	1:B:129:TRP:HE1	2.35	0.45
1:B:396:ASP:OD1	1:B:400:THR:N	2.42	0.45
1:A:502:ASP:O	1:A:505:THR:HG23	2.16	0.45
1:B:366:SER:O	1:B:450:VAL:HG12	2.16	0.45
1:A:300:LYS:NZ	1:A:354:SER:OG	2.50	0.44
1:A:402:LEU:HD22	1:A:421:PHE:HZ	1.81	0.44
1:A:94:PRO:O	1:A:150:LYS:NZ	2.41	0.44
1:A:470:ILE:HD11	1:A:536:VAL:HG11	1.99	0.44
1:B:318:ILE:HD11	1:B:325:HIS:CE1	2.52	0.44
1:A:407:ASP:HB3	1:A:421:PHE:CE1	2.52	0.44
1:B:128:SER:HA	1:B:171:ILE:HD11	1.99	0.44
1:B:273:ARG:HB2	1:B:314:MET:HE3	1.99	0.44
1:A:220:THR:HG22	1:A:276:PHE:HE2	1.83	0.44
1:A:334:ARG:HE	8:J:4:MAN:HO6	1.60	0.44
1:B:35:PHE:CG	1:B:207:VAL:HG21	2.52	0.44
1:B:82:PRO:HA	1:B:123:ASN:HD21	1.81	0.44
1:B:506:GLN:HE21	1:B:507:TRP:NE1	2.16	0.44
1:B:237:GLN:HA	1:B:282:VAL:O	2.18	0.44
1:A:85:TRP:CE2	1:A:155:ILE:HD11	2.52	0.44
1:A:481:TRP:CE3	1:A:485:PRO:HA	2.53	0.44
1:B:40:ASN:OD1	1:B:316:PRO:HD2	2.17	0.44
1:A:474:ASP:OD1	1:A:533:GLN:N	2.37	0.44
1:A:442:PHE:N	1:A:442:PHE:CD1	2.86	0.43
1:A:465:ALA:HB1	1:A:470:ILE:HG21	2.00	0.43
1:B:438:PHE:HB2	1:B:450:VAL:HG22	1.99	0.43
1:A:451:GLN:OE1	8:J:1:NAG:H83	2.18	0.43
1:B:123:ASN:HB3	1:B:169:GLU:HB3	2.01	0.43
1:B:136:LYS:HD3	1:B:136:LYS:HA	1.68	0.43
1:B:85:TRP:CD1	1:B:124:VAL:HG22	2.53	0.43
1:B:363:GLN:OE1	1:B:555:ARG:HD3	2.19	0.43
1:B:402:LEU:HD22	1:B:421:PHE:CZ	2.53	0.43
1:A:269:LEU:HB3	1:A:312:TYR:CD2	2.54	0.43
1:B:337:VAL:O	1:B:341:ILE:HG13	2.19	0.43
1:B:512:GLY:O	1:B:515:ARG:HB2	2.18	0.43
1:A:146:GLN:O	1:A:150:LYS:HG2	2.19	0.43
1:A:375:THR:O	1:A:428:GLU:HG2	2.19	0.43
1:B:70:TYR:HB3	1:B:326:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HD13	1:A:185:ILE:HA	1.71	0.42
1:A:442:PHE:N	1:A:442:PHE:HD1	2.17	0.42
1:B:335:ASP:O	1:B:339:ILE:HD13	2.19	0.42
1:B:493:LEU:HA	1:B:493:LEU:HD12	1.77	0.42
1:A:512:GLY:C	1:A:515:ARG:HG2	2.44	0.42
1:B:109:VAL:HA	1:B:112:MET:SD	2.59	0.42
1:B:163:SER:O	1:B:206:ARG:NH1	2.52	0.42
1:B:438:PHE:HB2	1:B:450:VAL:CG2	2.49	0.42
1:A:353:ASP:OD2	1:A:354:SER:N	2.51	0.42
1:A:42:GLY:C	1:A:317:ILE:HG23	2.44	0.42
1:A:417:PHE:HB3	1:A:422:LEU:CD1	2.47	0.42
1:A:473:SER:C	1:A:533:GLN:HB2	2.45	0.42
1:B:42:GLY:HA3	1:B:317:ILE:HG23	2.02	0.42
1:A:89:PHE:HZ	1:A:151:LEU:HD22	1.85	0.42
1:B:128:SER:HA	1:B:132:ALA:HB3	2.02	0.42
1:A:389:ASN:ND2	1:A:444:SER:O	2.53	0.42
1:B:128:SER:HB3	1:B:171:ILE:HG12	2.00	0.42
1:B:287:ASP:OD1	1:B:325:HIS:HE1	2.03	0.42
1:A:186:ASN:HD21	1:A:224:PHE:HA	1.84	0.42
1:B:377:VAL:HG22	1:B:426:TYR:CE2	2.55	0.42
1:B:284:GLY:HA2	1:B:317:ILE:HD12	2.01	0.42
1:A:363:GLN:OE1	1:A:555:ARG:HD3	2.20	0.41
1:A:403:LYS:O	1:A:407:ASP:HB2	2.20	0.41
1:A:440:LEU:HB3	1:A:442:PHE:CE1	2.33	0.41
1:B:350:SER:OG	1:B:389:ASN:HB2	2.21	0.41
1:B:472:GLY:N	1:B:533:GLN:NE2	2.68	0.41
1:B:369:ILE:HD13	1:B:382:LEU:HD21	2.02	0.41
1:B:273:ARG:NH1	1:B:279:VAL:O	2.50	0.41
1:B:72:LYS:HB2	1:B:118:LEU:HD21	2.01	0.41
1:B:472:GLY:H	1:B:533:GLN:NE2	2.18	0.41
1:A:121:ILE:HG12	1:A:167:ALA:HB3	2.03	0.41
1:A:105:ARG:O	1:A:109:VAL:HG23	2.21	0.41
1:A:403:LYS:HG2	1:A:406:THR:HB	2.02	0.41
1:A:440:LEU:CB	1:A:442:PHE:HE1	2.23	0.41
1:B:149:GLU:OE2	1:B:194:ARG:NH2	2.54	0.41
1:B:425:TYR:HE2	1:B:438:PHE:CZ	2.39	0.41
1:A:143:GLN:HB2	11:A:604:NAG:O5	2.21	0.41
1:A:370:TYR:CE2	1:A:554:PRO:HB3	2.55	0.41
1:A:464:SER:HA	1:A:566:THR:O	2.21	0.41
1:B:40:ASN:HA	1:B:41:PRO:HA	1.94	0.41
1:B:327:ASP:OD2	4:F:3:BMA:O4	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASP:OD1	1:B:138:ASP:N	2.53	0.40
1:A:50:ASP:HB3	1:A:82:PRO:HB2	2.03	0.40
1:A:127:ASP:OD2	1:A:131:TRP:NE1	2.46	0.40
1:A:172:ASN:O	1:A:173:GLU:C	2.64	0.40
1:A:196:ILE:HG13	1:A:197:ASN:N	2.36	0.40
1:B:370:TYR:CD2	1:B:554:PRO:HB3	2.56	0.40
1:A:135:THR:HG22	1:A:181:ASP:OD2	2.21	0.40
1:B:127:ASP:HB3	1:B:131:TRP:NE1	2.37	0.40
1:B:533:GLN:OE1	1:B:533:GLN:HA	2.21	0.40
1:B:567:LEU:HD23	1:B:567:LEU:HA	1.83	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	547/648 (84%)	516 (94%)	30 (6%)	1 (0%)	44	63
1	B	547/648 (84%)	519 (95%)	28 (5%)	0	100	100
All	All	1094/1296 (84%)	1035 (95%)	58 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLU

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	481/561 (86%)	471 (98%)	10 (2%)	48	69
1	B	481/561 (86%)	470 (98%)	11 (2%)	45	66
All	All	962/1122 (86%)	941 (98%)	21 (2%)	47	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	185	ILE
1	A	326	LEU
1	A	342	ILE
1	A	349	ASN
1	A	350	SER
1	A	358	THR
1	A	475	LEU
1	A	498	THR
1	A	531	LEU
1	B	62	THR
1	B	118	LEU
1	B	260	SER
1	B	277	THR
1	B	346	ASN
1	B	406	THR
1	B	431	GLU
1	B	454	GLN
1	B	471	SER
1	B	501	VAL
1	B	568	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	47	ASN
1	A	186	ASN
1	A	209	ASN
1	A	237	GLN
1	A	349	ASN

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Mol	Chain	Res	Type
1	A	520	ASN
1	A	528	ASN
1	B	47	ASN
1	B	54	ASN
1	B	125	HIS
1	B	146	GLN
1	B	325	HIS
1	B	506	GLN

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](#)

43 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	2,1	14,14,15	0.82	0	17,19,21	1.04	1 (5%)
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	1.12	1 (5%)
2	BMA	C	3	2	11,11,12	0.94	0	15,15,17	2.54	6 (40%)
2	MAN	C	4	2	11,11,12	1.03	1 (9%)	15,15,17	1.65	3 (20%)
3	BGC	D	1	3	12,12,12	0.64	0	17,17,17	1.04	2 (11%)
3	BGC	D	2	3	11,11,12	0.73	0	15,15,17	1.07	0
3	XYS	D	3	3	9,9,10	0.92	0	10,12,14	1.37	1 (10%)
2	NAG	E	1	2,1	14,14,15	0.84	0	17,19,21	1.14	1 (5%)
2	NAG	E	2	2	14,14,15	0.80	0	17,19,21	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	E	3	2	11,11,12	1.04	1 (9%)	15,15,17	2.57	5 (33%)
2	MAN	E	4	2	11,11,12	0.75	0	15,15,17	1.49	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.71	0	17,19,21	1.10	2 (11%)
4	NAG	F	2	4	14,14,15	0.72	0	17,19,21	1.29	2 (11%)
4	BMA	F	3	4	11,11,12	0.99	1 (9%)	15,15,17	2.31	4 (26%)
4	MAN	F	4	4	11,11,12	0.71	0	15,15,17	1.31	1 (6%)
4	MAN	F	5	4	11,11,12	0.70	0	15,15,17	1.10	1 (6%)
4	MAN	F	6	4	11,11,12	0.82	0	15,15,17	1.05	0
4	MAN	F	7	4	11,11,12	0.76	0	15,15,17	2.33	4 (26%)
4	MAN	F	8	4	11,11,12	0.94	1 (9%)	15,15,17	1.29	2 (13%)
5	NAG	G	1	1,5	14,14,15	0.85	0	17,19,21	0.80	0
5	NAG	G	2	5	14,14,15	0.82	0	17,19,21	0.75	0
5	BMA	G	3	5	11,11,12	0.92	0	15,15,17	2.40	4 (26%)
5	MAN	G	4	5	11,11,12	0.90	1 (9%)	15,15,17	1.07	1 (6%)
5	MAN	G	5	5	11,11,12	0.87	1 (9%)	15,15,17	1.82	4 (26%)
5	MAN	G	6	5	11,11,12	0.79	0	15,15,17	1.03	1 (6%)
5	MAN	G	7	5	11,11,12	0.71	0	15,15,17	1.67	4 (26%)
6	BGC	H	1	6	12,12,12	0.67	0	17,17,17	1.19	2 (11%)
6	BGC	H	2	6	11,11,12	0.75	0	15,15,17	1.03	1 (6%)
6	BGC	H	3	6	11,11,12	0.77	0	15,15,17	0.91	0
6	XYS	H	4	6	9,9,10	1.01	1 (11%)	10,12,14	3.09	6 (60%)
7	NAG	I	1	1,7	14,14,15	0.79	0	17,19,21	0.93	0
7	NAG	I	2	7	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
7	BMA	I	3	7	11,11,12	0.89	0	15,15,17	2.37	3 (20%)
7	MAN	I	4	7	11,11,12	1.02	1 (9%)	15,15,17	1.38	1 (6%)
7	MAN	I	5	7	11,11,12	0.96	1 (9%)	15,15,17	1.14	1 (6%)
7	MAN	I	6	7	11,11,12	0.78	0	15,15,17	1.05	1 (6%)
8	NAG	J	1	8,1	14,14,15	0.73	0	17,19,21	1.26	1 (5%)
8	NAG	J	2	8	14,14,15	0.71	0	17,19,21	1.25	2 (11%)
8	BMA	J	3	8	11,11,12	0.80	0	15,15,17	2.58	5 (33%)
8	MAN	J	4	8	11,11,12	0.80	0	15,15,17	1.64	4 (26%)
8	MAN	J	5	8	11,11,12	0.91	1 (9%)	15,15,17	1.10	1 (6%)
9	NAG	K	1	1,9	14,14,15	0.75	0	17,19,21	1.13	2 (11%)
9	NAG	K	2	9	14,14,15	0.78	1 (7%)	17,19,21	0.88	1 (5%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	BGC	D	1	3	-	2/2/22/22	0/1/1/1
3	BGC	D	2	3	-	2/2/19/22	0/1/1/1
3	XYS	D	3	3	-	-	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	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	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
5	MAN	G	7	5	-	2/2/19/22	0/1/1/1
6	BGC	H	1	6	-	0/2/22/22	0/1/1/1
6	BGC	H	2	6	-	2/2/19/22	0/1/1/1
6	BGC	H	3	6	-	2/2/19/22	0/1/1/1
6	XYS	H	4	6	-	-	0/1/1/1
7	NAG	I	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	1/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	J	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	2/2/19/22	0/1/1/1
8	MAN	J	4	8	-	2/2/19/22	0/1/1/1
8	MAN	J	5	8	-	1/2/19/22	0/1/1/1
9	NAG	K	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	O5-C1	-2.76	1.39	1.43
2	E	3	BMA	C2-C3	2.63	1.56	1.52
7	I	5	MAN	O5-C1	-2.50	1.39	1.43
8	J	5	MAN	O5-C1	-2.42	1.39	1.43
4	F	8	MAN	O5-C1	-2.30	1.40	1.43
7	I	4	MAN	O5-C1	-2.12	1.40	1.43
4	F	3	BMA	C2-C3	2.12	1.55	1.52
9	K	2	NAG	O5-C1	-2.11	1.40	1.43
5	G	5	MAN	O5-C1	-2.10	1.40	1.43
5	G	4	MAN	O5-C1	-2.07	1.40	1.43
6	H	4	XYS	C1-C2	2.01	1.56	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	8.13	123.21	112.19
8	J	3	BMA	C1-O5-C5	7.86	122.84	112.19
7	I	3	BMA	C1-O5-C5	7.82	122.79	112.19
5	G	3	BMA	C1-O5-C5	7.37	122.18	112.19
2	C	3	BMA	C1-O5-C5	6.91	121.55	112.19
6	H	4	XYS	C1-C2-C3	6.57	117.75	109.67
4	F	3	BMA	C1-O5-C5	6.56	121.08	112.19
4	F	7	MAN	C1-C2-C3	5.33	116.22	109.67
4	F	7	MAN	C1-O5-C5	5.31	119.38	112.19
6	H	4	XYS	C4-C3-C2	4.82	116.64	110.92
7	I	4	MAN	C1-C2-C3	4.28	114.92	109.67
8	J	2	NAG	C1-O5-C5	3.78	117.31	112.19
5	G	7	MAN	C1-O5-C5	3.77	117.30	112.19
5	G	5	MAN	C1-C2-C3	3.75	114.27	109.67
4	F	4	MAN	C1-O5-C5	3.68	117.18	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C3-C4-C5	3.68	116.80	110.24
2	C	4	MAN	C2-C3-C4	3.64	117.19	110.89
4	F	3	BMA	C3-C4-C5	3.50	116.49	110.24
2	C	3	BMA	C2-C3-C4	3.49	116.94	110.89
4	F	5	MAN	C1-O5-C5	3.44	116.85	112.19
8	J	1	NAG	C1-O5-C5	3.38	116.77	112.19
2	E	4	MAN	C1-O5-C5	3.33	116.71	112.19
4	F	8	MAN	C1-C2-C3	3.33	113.76	109.67
4	F	2	NAG	C1-O5-C5	3.31	116.68	112.19
8	J	4	MAN	C3-C4-C5	-3.24	104.46	110.24
2	C	1	NAG	O5-C1-C2	-3.17	106.28	111.29
6	H	4	XYS	C5-O5-C1	3.15	116.37	111.52
5	G	5	MAN	C2-C3-C4	3.05	116.17	110.89
8	J	3	BMA	O5-C5-C4	3.03	118.19	110.83
5	G	7	MAN	O4-C4-C3	-2.99	103.44	110.35
8	J	3	BMA	C3-C4-C5	2.97	115.53	110.24
2	E	3	BMA	C3-C4-C5	2.94	115.48	110.24
8	J	4	MAN	C1-O5-C5	2.87	116.08	112.19
5	G	5	MAN	C3-C4-C5	2.84	115.30	110.24
4	F	2	NAG	O5-C1-C2	-2.83	106.83	111.29
5	G	3	BMA	O3-C3-C4	2.81	116.85	110.35
5	G	4	MAN	C1-C2-C3	2.80	113.11	109.67
8	J	4	MAN	C1-C2-C3	2.80	113.11	109.67
2	E	4	MAN	C1-C2-C3	2.79	113.09	109.67
2	E	1	NAG	O5-C1-C2	-2.78	106.89	111.29
7	I	5	MAN	C1-C2-C3	2.77	113.07	109.67
8	J	3	BMA	O3-C3-C4	2.76	116.72	110.35
8	J	4	MAN	O5-C5-C6	2.76	111.53	107.20
6	H	1	BGC	C1-C2-C3	-2.66	104.78	110.31
4	F	3	BMA	O4-C4-C3	-2.58	104.39	110.35
9	K	1	NAG	C1-O5-C5	2.53	115.62	112.19
5	G	3	BMA	C6-C5-C4	2.52	118.92	113.00
3	D	1	BGC	C1-C2-C3	-2.50	105.12	110.31
4	F	1	NAG	O4-C4-C3	-2.50	104.58	110.35
6	H	1	BGC	O5-C1-C2	-2.47	105.87	110.28
2	E	3	BMA	O5-C5-C4	2.46	116.81	110.83
6	H	4	XYS	O4-C4-C3	-2.45	105.23	110.14
7	I	6	MAN	C1-O5-C5	2.44	115.49	112.19
4	F	7	MAN	C3-C4-C5	2.43	114.57	110.24
2	C	4	MAN	C3-C4-C5	2.42	114.56	110.24
2	C	3	BMA	O4-C4-C3	-2.41	104.79	110.35
2	C	4	MAN	O4-C4-C3	-2.39	104.82	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	4	XYS	O3-C3-C2	-2.36	105.47	109.99
8	J	2	NAG	O4-C4-C3	-2.34	104.93	110.35
2	C	2	NAG	O5-C1-C2	-2.33	107.61	111.29
4	F	1	NAG	O5-C1-C2	-2.32	107.63	111.29
2	C	3	BMA	O3-C3-C2	-2.29	105.61	109.99
7	I	3	BMA	O6-C6-C5	-2.24	103.62	111.29
2	E	3	BMA	O4-C4-C3	-2.23	105.20	110.35
8	J	5	MAN	O4-C4-C3	-2.22	105.21	110.35
6	H	2	BGC	C1-C2-C3	-2.22	106.94	109.67
8	J	3	BMA	O4-C4-C3	-2.22	105.22	110.35
9	K	1	NAG	O5-C1-C2	-2.21	107.80	111.29
2	C	3	BMA	O5-C5-C4	2.20	116.19	110.83
3	D	3	XYS	O4-C4-C5	2.20	113.65	109.15
5	G	5	MAN	O4-C4-C3	-2.16	105.34	110.35
3	D	1	BGC	O5-C1-C2	-2.16	106.43	110.28
6	H	4	XYS	C5-C4-C3	2.15	112.31	109.67
4	F	7	MAN	C6-C5-C4	-2.14	107.98	113.00
5	G	3	BMA	O6-C6-C5	-2.12	104.03	111.29
7	I	3	BMA	O4-C4-C3	-2.11	105.47	110.35
2	E	3	BMA	C1-C2-C3	2.10	112.25	109.67
4	F	3	BMA	O5-C5-C4	2.08	115.89	110.83
5	G	6	MAN	C1-O5-C5	2.07	115.00	112.19
5	G	7	MAN	O5-C1-C2	-2.06	107.58	110.77
5	G	7	MAN	C2-C3-C4	2.06	114.46	110.89
9	K	2	NAG	C1-O5-C5	2.03	114.94	112.19
7	I	2	NAG	C2-N2-C7	2.02	125.78	122.90
4	F	8	MAN	C2-C3-C4	2.00	114.36	110.89

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	8	MAN	C4-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
4	F	8	MAN	O5-C5-C6-O6
3	D	1	BGC	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
8	J	4	MAN	O5-C5-C6-O6

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

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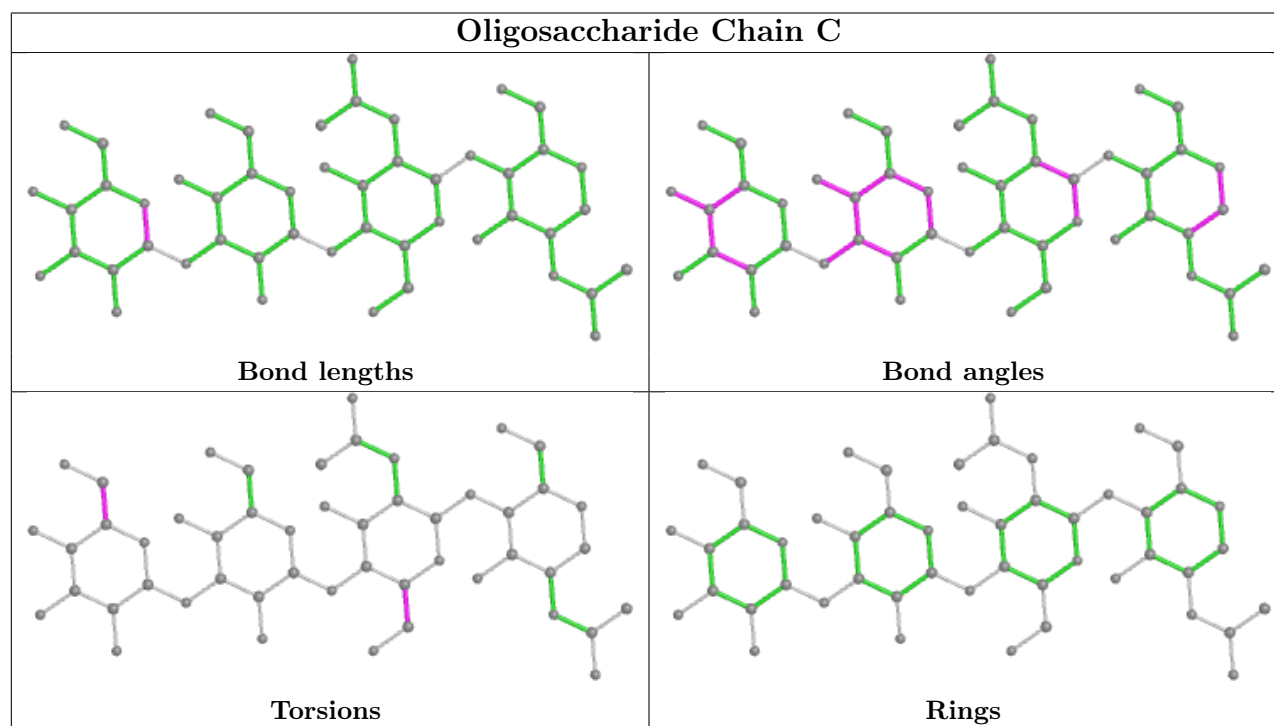
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

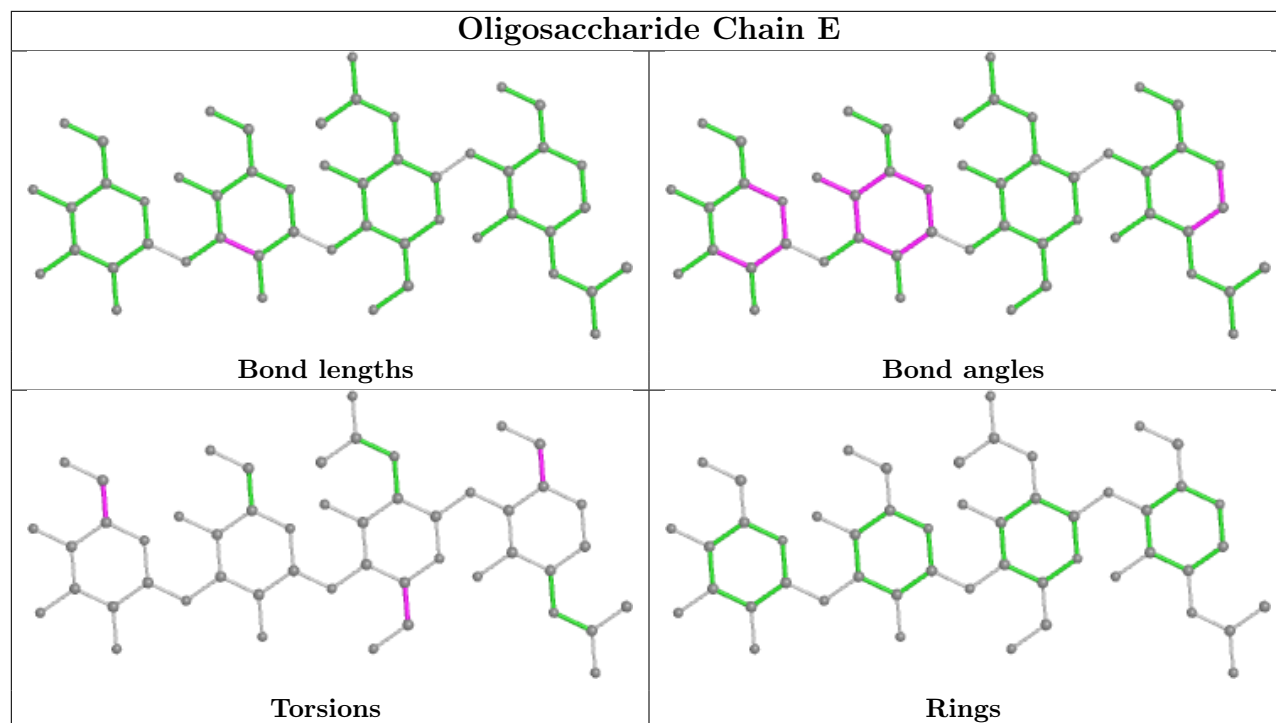
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1	NAG	1	0
8	J	3	BMA	1	0
4	F	8	MAN	1	0
6	H	1	BGC	1	0
4	F	3	BMA	1	0
8	J	4	MAN	2	0

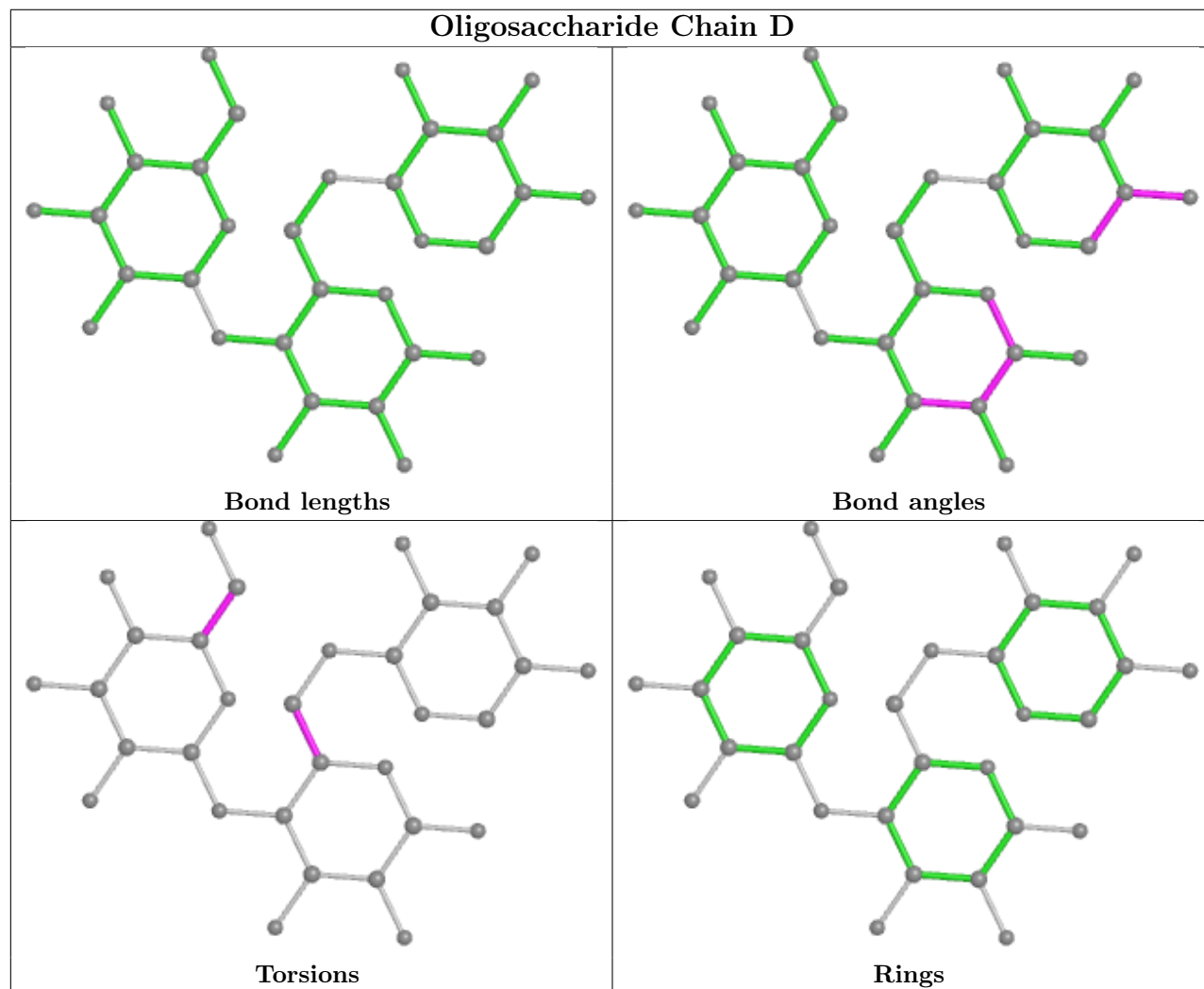
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



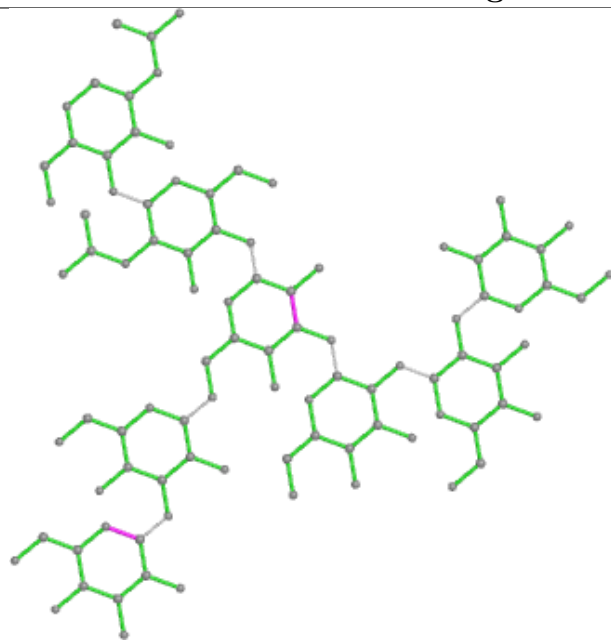
Oligosaccharide Chain E



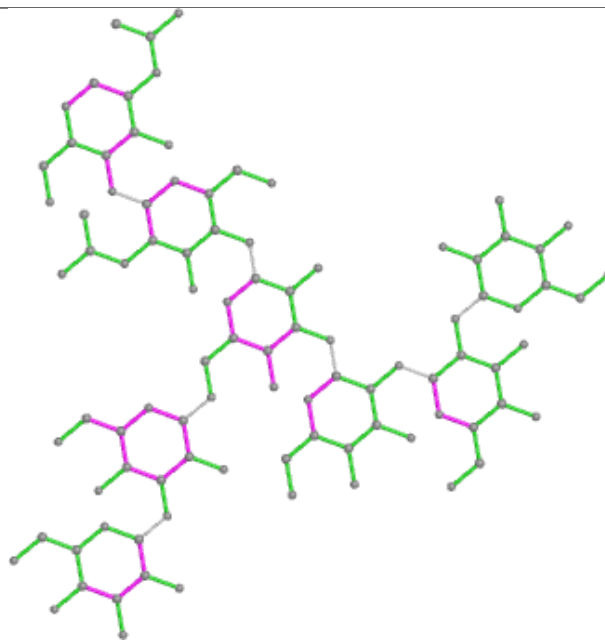
Oligosaccharide Chain D



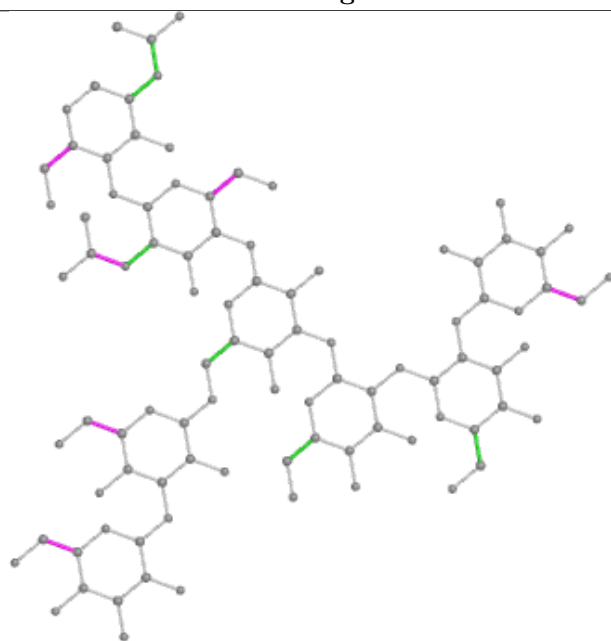
Oligosaccharide Chain F



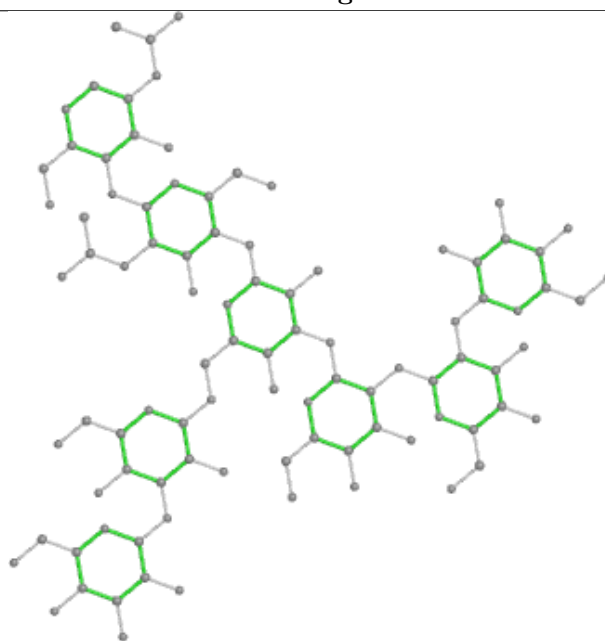
Bond lengths



Bond angles

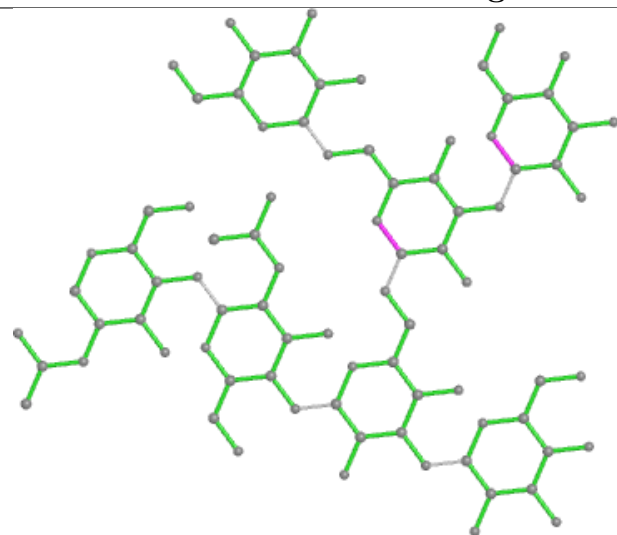


Torsions

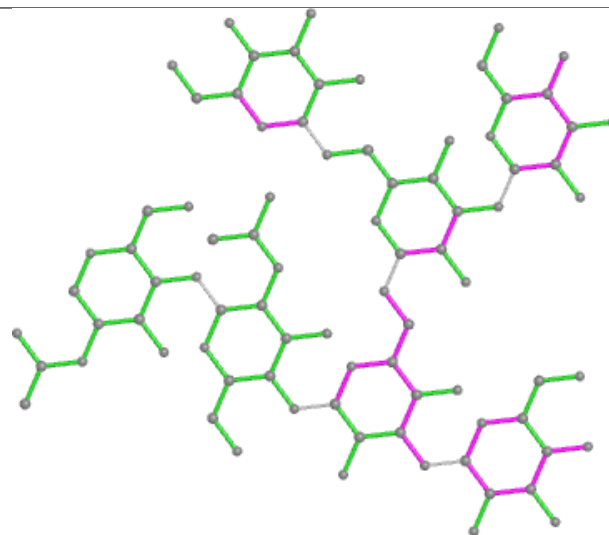


Rings

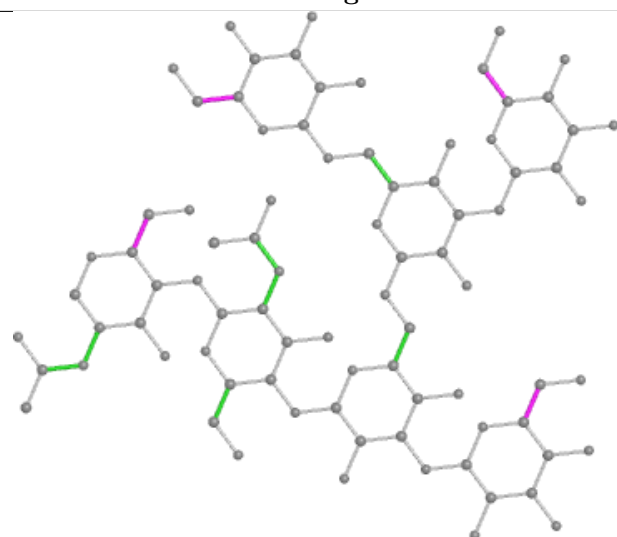
Oligosaccharide Chain G



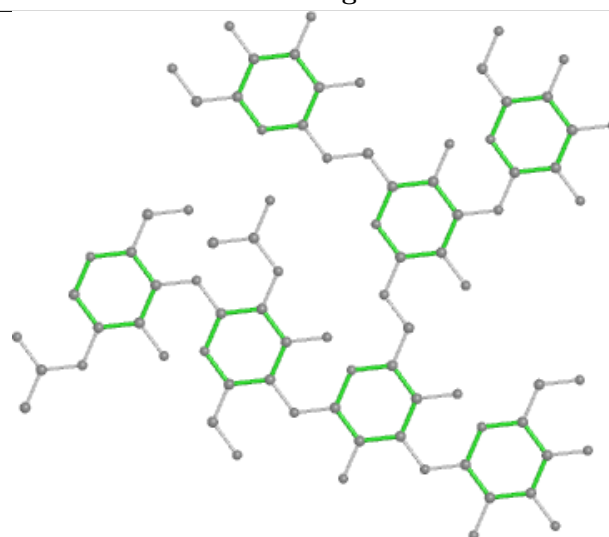
Bond lengths



Bond angles

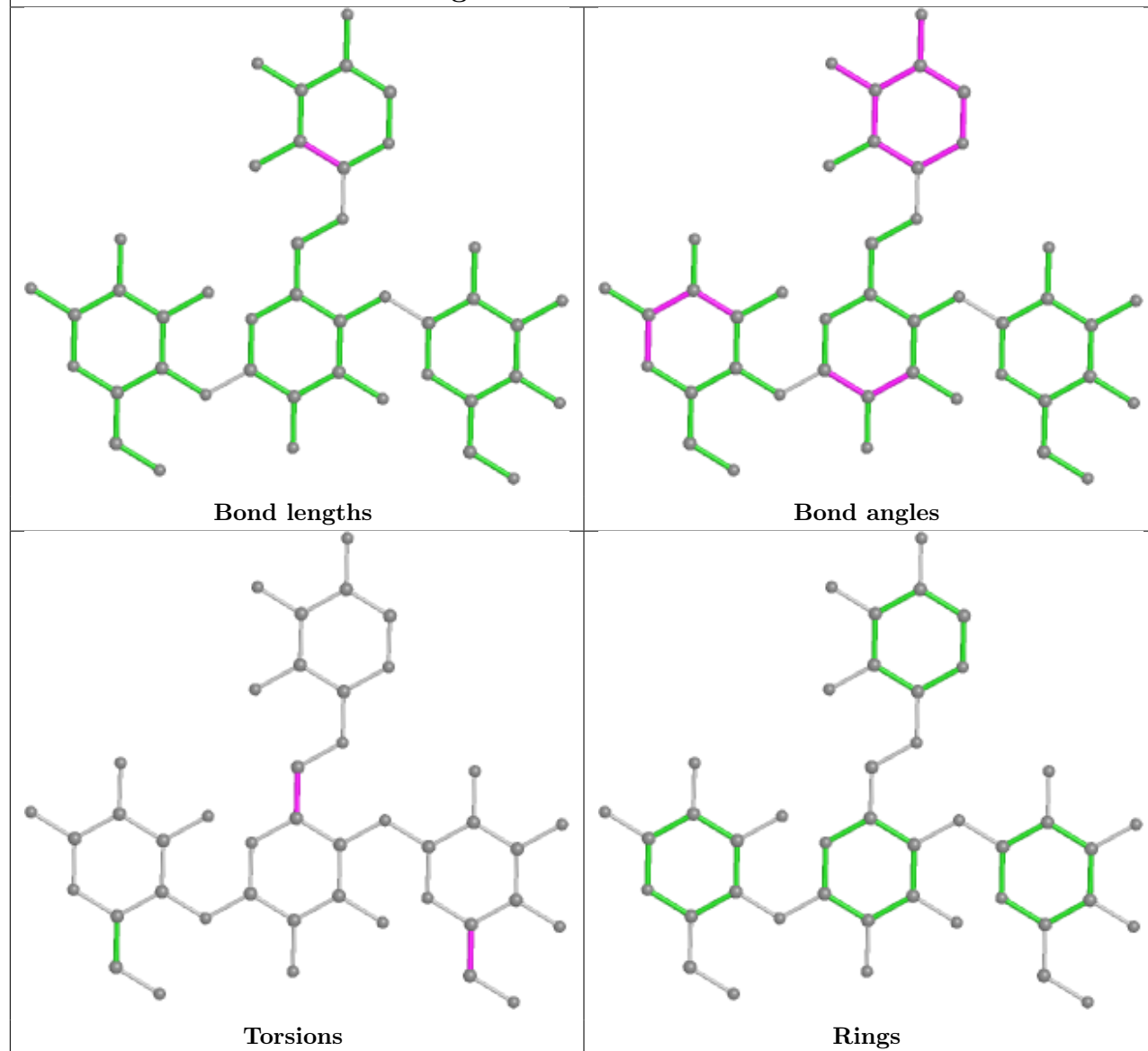


Torsions

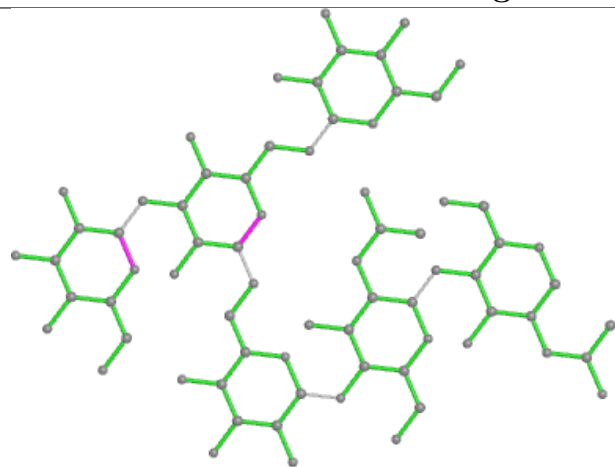


Rings

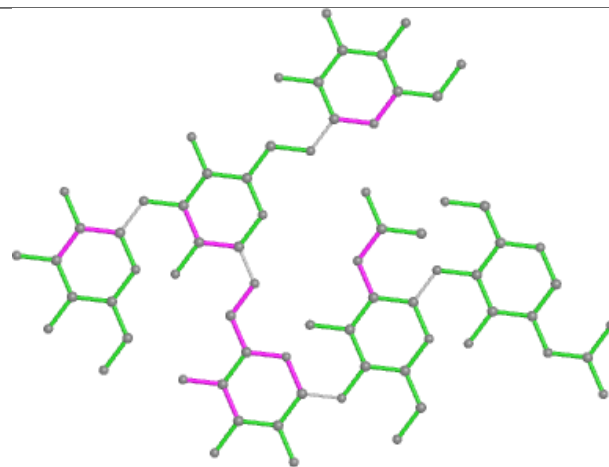
Oligosaccharide Chain H



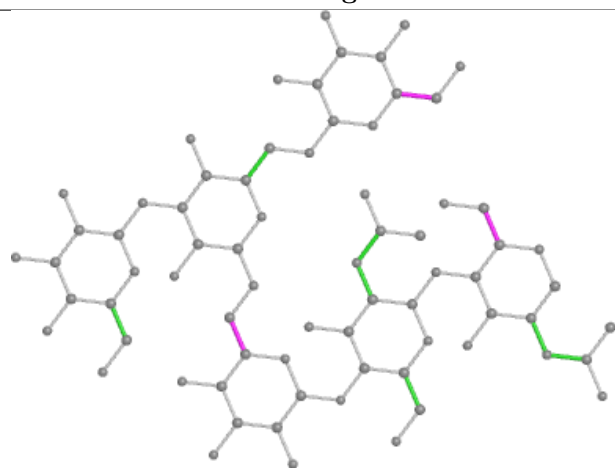
Oligosaccharide Chain I



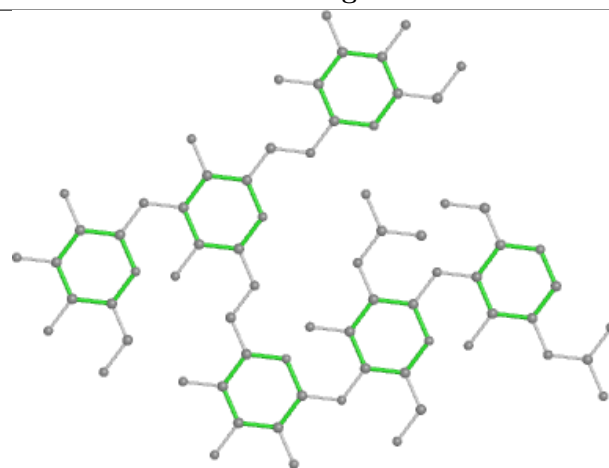
Bond lengths



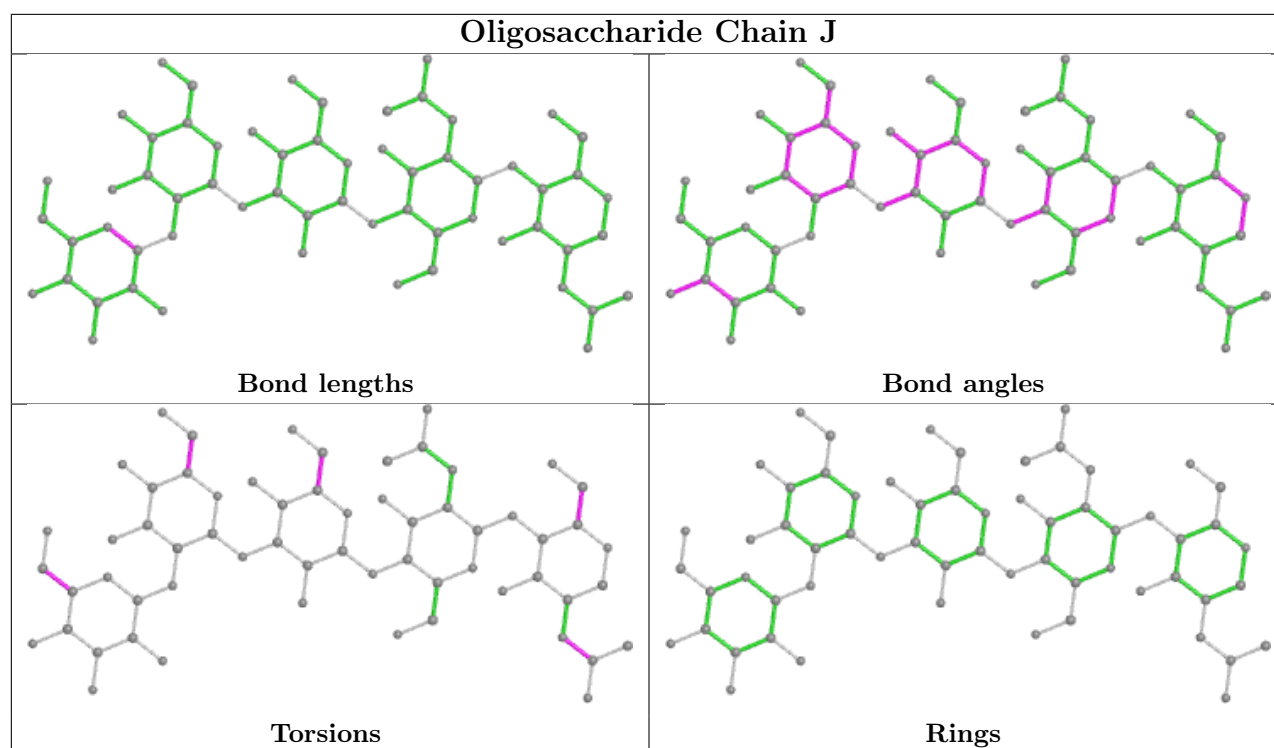
Bond angles

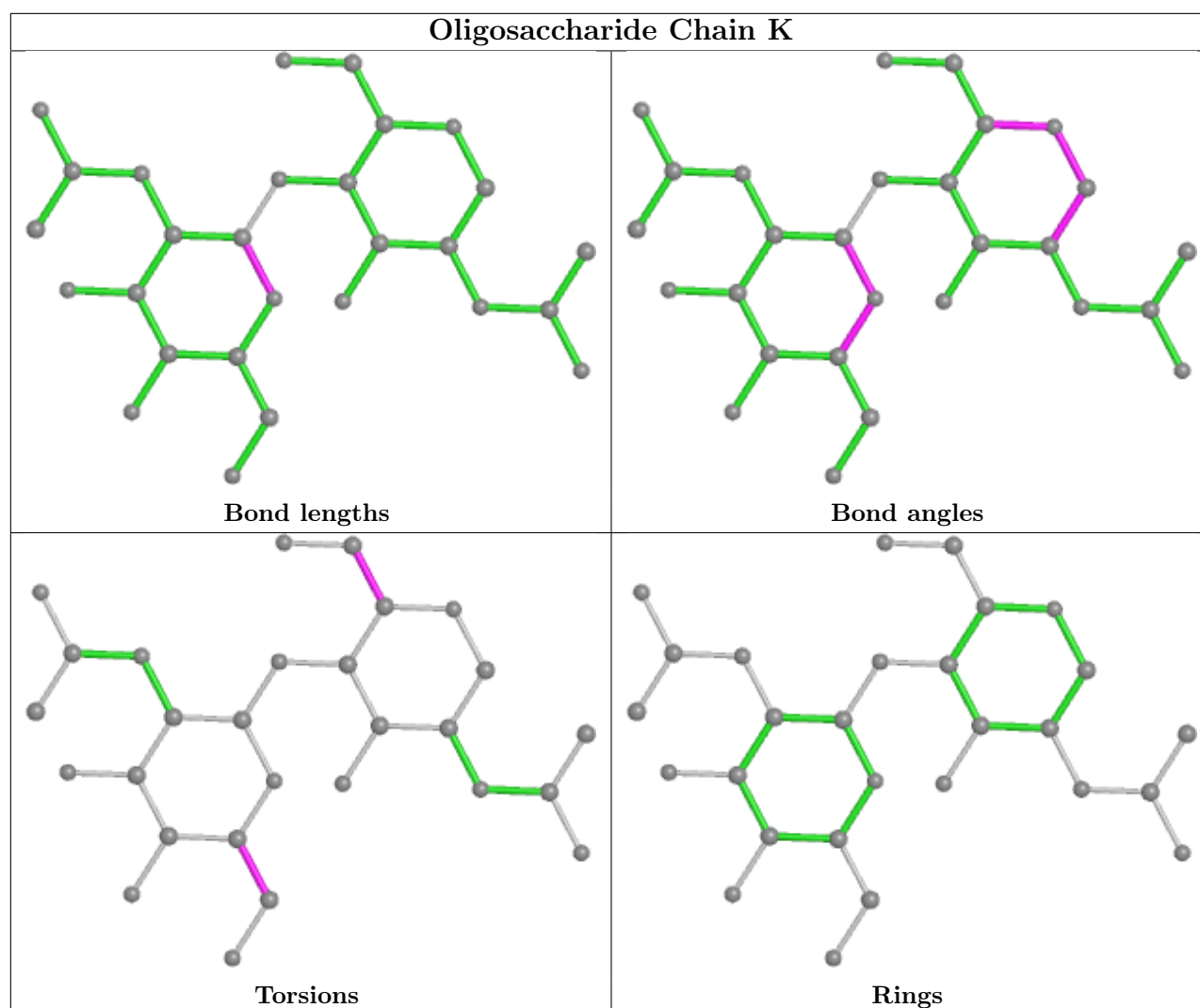


Torsions



Rings





5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
11	NAG	B	602	1	14,14,15	0.69	0	17,19,21	1.02	0
11	NAG	A	603	1	14,14,15	0.76	0	17,19,21	1.19	1 (5%)
10	MAN	A	601	1	11,11,12	0.90	1 (9%)	15,15,17	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	B	601	1	11,11,12	1.02	1 (9%)	15,15,17	1.20	1 (6%)
11	NAG	A	602	1	14,14,15	0.68	0	17,19,21	1.19	2 (11%)
11	NAG	A	604	1	14,14,15	0.76	0	17,19,21	1.12	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	602	1	-	2/6/23/26	0/1/1/1
11	NAG	A	603	1	-	2/6/23/26	0/1/1/1
10	MAN	A	601	1	-	0/2/19/22	0/1/1/1
10	MAN	B	601	1	-	2/2/19/22	0/1/1/1
11	NAG	A	602	1	-	4/6/23/26	0/1/1/1
11	NAG	A	604	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	601	MAN	O5-C1	-2.80	1.39	1.43
10	A	601	MAN	O5-C1	-2.44	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	603	NAG	C2-N2-C7	3.02	127.21	122.90
11	A	602	NAG	C4-C3-C2	-2.81	106.90	111.02
11	A	602	NAG	C1-O5-C5	2.76	115.93	112.19
10	B	601	MAN	O5-C1-C2	-2.33	107.18	110.77
11	A	604	NAG	C2-N2-C7	2.32	126.20	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	602	NAG	O5-C5-C6-O6
11	A	602	NAG	C8-C7-N2-C2
11	A	602	NAG	O7-C7-N2-C2
11	A	602	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	B	601	MAN	O5-C5-C6-O6
11	B	602	NAG	C4-C5-C6-O6
11	B	602	NAG	O5-C5-C6-O6
11	A	603	NAG	O5-C5-C6-O6
10	B	601	MAN	C4-C5-C6-O6
11	A	603	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	602	NAG	1	0
11	A	604	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/648 (84%)	0.19	1 (0%) 92 92	55, 74, 92, 101	0
1	B	549/648 (84%)	0.16	4 (0%) 84 85	53, 72, 91, 106	0
All	All	1098/1296 (84%)	0.17	5 (0%) 87 88	53, 73, 92, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	SER	3.1
1	B	470	ILE	2.4
1	B	460	LEU	2.3
1	B	247	ILE	2.1
1	B	82	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	E	4	11/12	0.54	0.12	113,120,123,128	0
4	MAN	F	7	11/12	0.55	0.10	104,109,113,115	0
5	MAN	G	7	11/12	0.57	0.14	81,85,93,94	0
2	BMA	E	3	11/12	0.58	0.10	93,96,111,115	0

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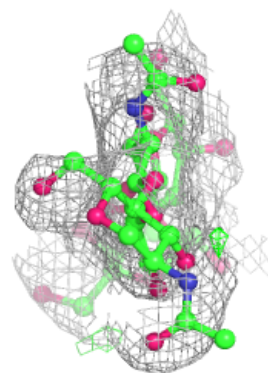
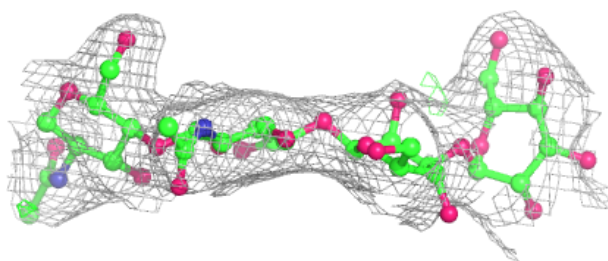
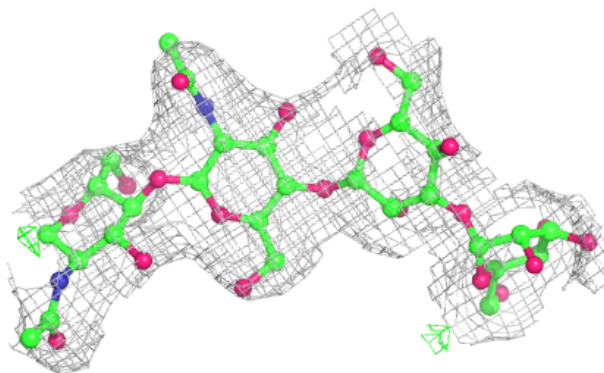
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.59	0.11	105,109,114,114	0
2	BMA	C	3	11/12	0.61	0.10	100,104,115,116	0
7	MAN	I	6	11/12	0.61	0.11	97,99,102,104	0
7	BMA	I	3	11/12	0.62	0.13	87,94,102,103	0
5	MAN	G	6	11/12	0.64	0.10	93,98,101,105	0
6	BGC	H	1	12/12	0.65	0.15	71,87,95,98	0
3	BGC	D	1	12/12	0.67	0.12	66,83,91,92	0
8	NAG	J	2	14/15	0.67	0.12	85,97,100,102	0
3	XYS	D	3	9/10	0.68	0.11	74,81,88,89	0
8	BMA	J	3	11/12	0.68	0.11	80,91,96,97	0
4	MAN	F	8	11/12	0.69	0.11	114,121,128,128	0
6	XYS	H	4	9/10	0.69	0.13	75,82,89,91	0
6	BGC	H	3	11/12	0.71	0.13	76,83,86,88	0
6	BGC	H	2	11/12	0.72	0.09	64,84,88,93	0
3	BGC	D	2	11/12	0.73	0.12	75,82,85,85	0
4	MAN	F	6	11/12	0.73	0.12	84,93,96,96	0
7	MAN	I	4	11/12	0.74	0.10	86,93,97,97	0
4	MAN	F	5	11/12	0.75	0.12	84,90,95,95	0
8	NAG	J	1	14/15	0.75	0.12	75,85,94,96	0
9	NAG	K	2	14/15	0.75	0.10	107,116,121,126	0
9	NAG	K	1	14/15	0.79	0.08	90,96,104,111	0
5	NAG	G	2	14/15	0.80	0.10	77,87,94,98	0
2	NAG	C	2	14/15	0.80	0.11	87,93,99,103	0
4	BMA	F	3	11/12	0.80	0.07	84,94,101,103	0
5	MAN	G	5	11/12	0.81	0.10	86,90,92,92	0
4	NAG	F	2	14/15	0.82	0.10	77,95,104,107	0
8	MAN	J	4	11/12	0.82	0.10	86,93,96,96	0
8	MAN	J	5	11/12	0.83	0.12	81,92,98,98	0
7	MAN	I	5	11/12	0.83	0.11	81,92,94,99	0
5	BMA	G	3	11/12	0.83	0.10	87,93,98,99	0
2	NAG	E	2	14/15	0.84	0.09	67,78,83,95	0
2	NAG	E	1	14/15	0.84	0.11	64,67,73,74	0
2	NAG	C	1	14/15	0.86	0.11	72,82,89,92	0
4	NAG	F	1	14/15	0.86	0.10	74,89,92,93	0
7	NAG	I	2	14/15	0.87	0.08	78,89,94,95	0
5	NAG	G	1	14/15	0.87	0.09	59,67,72,75	0
4	MAN	F	4	11/12	0.87	0.09	79,90,96,98	0
5	MAN	G	4	11/12	0.89	0.08	84,88,91,91	0
7	NAG	I	1	14/15	0.90	0.07	71,80,83,88	0

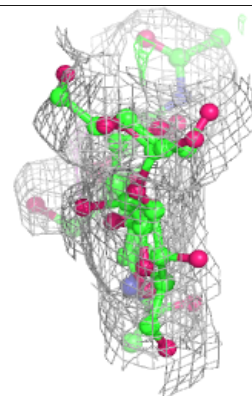
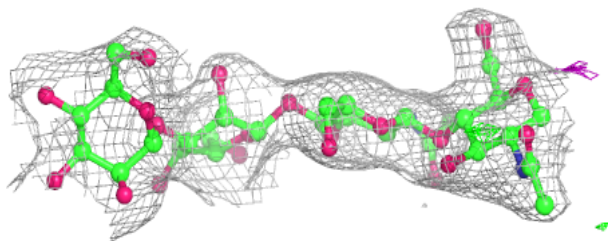
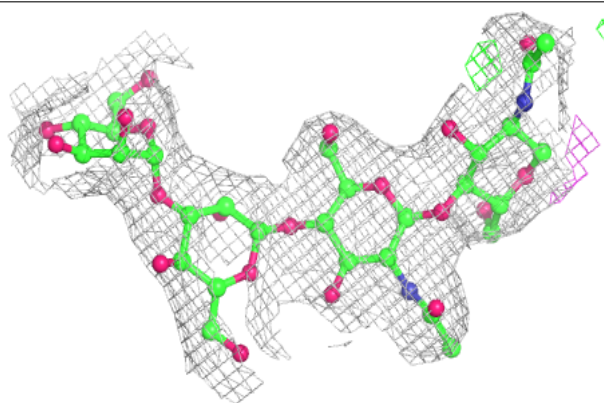
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

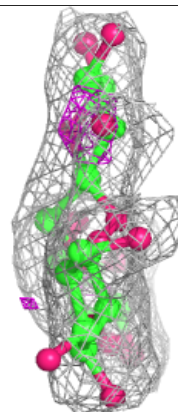
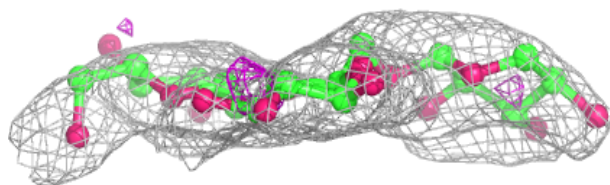
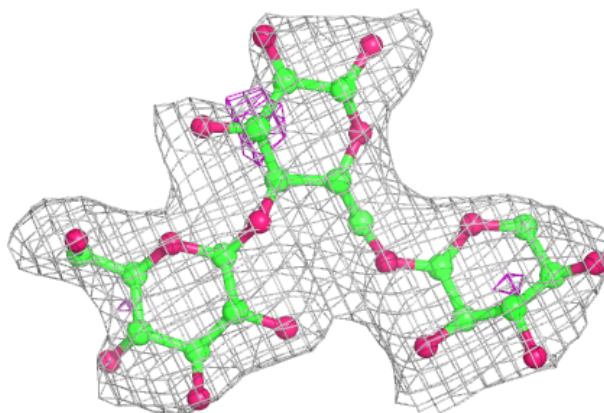
**Electron density around Chain E:**

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

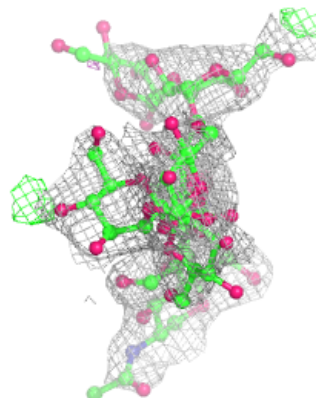
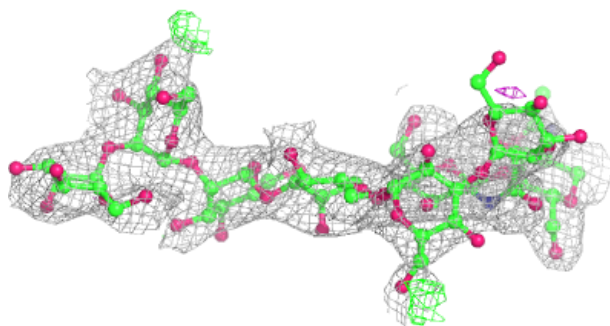
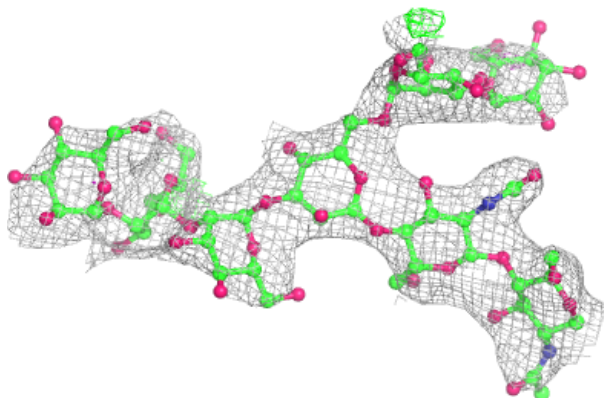


Electron density around Chain D:

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

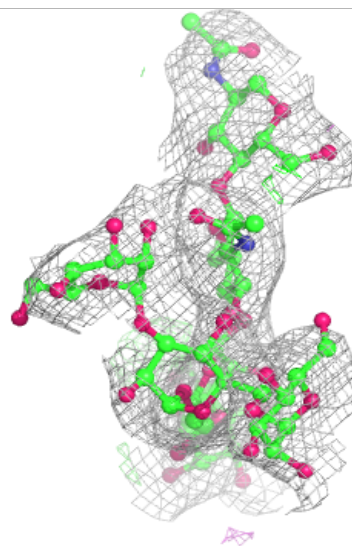
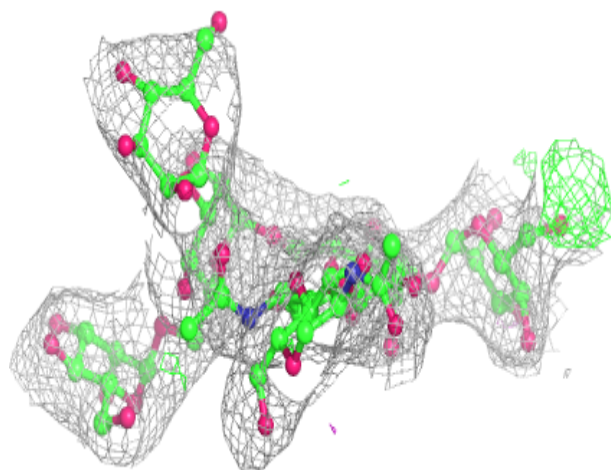
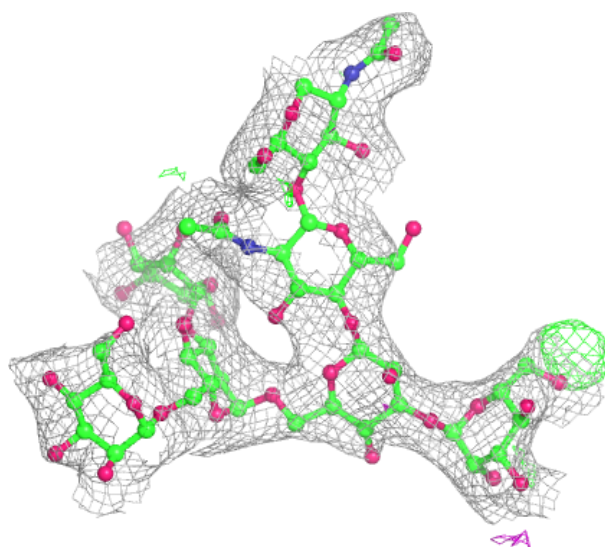
**Electron density around Chain F:**

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



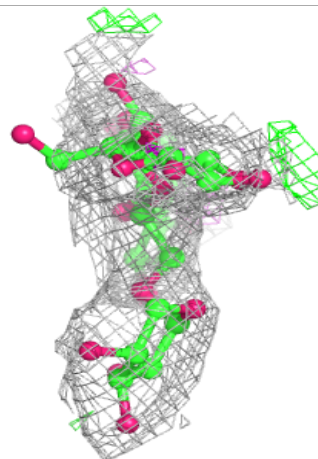
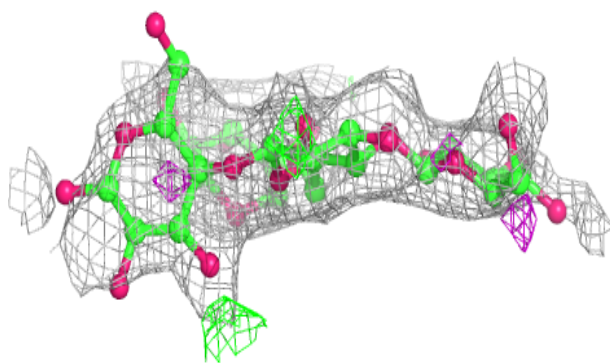
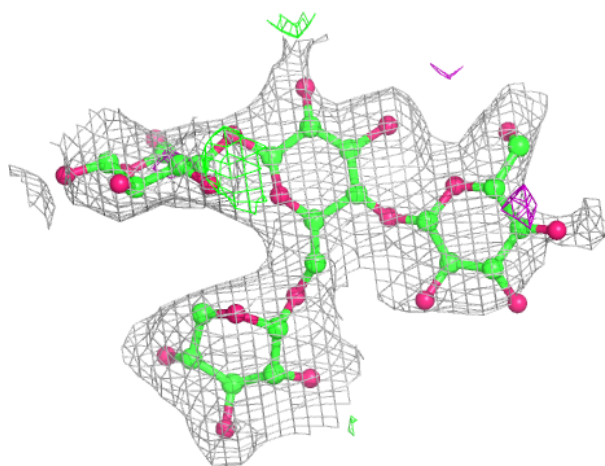
Electron density around Chain G:

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



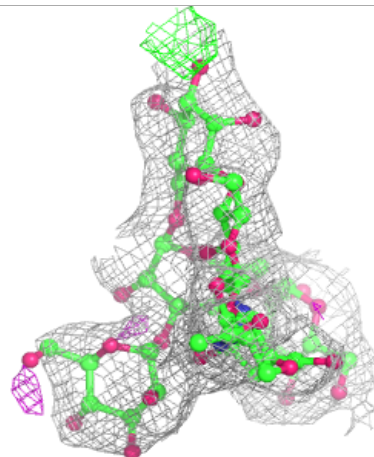
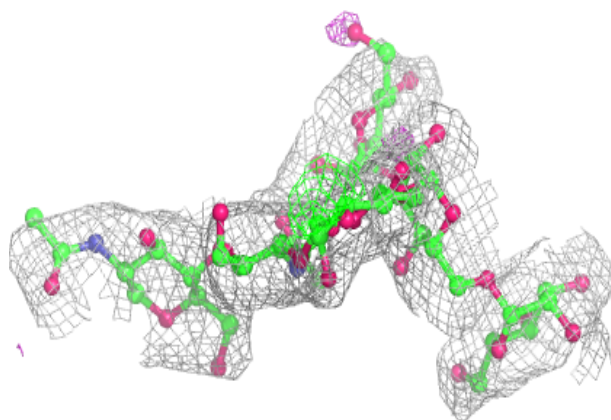
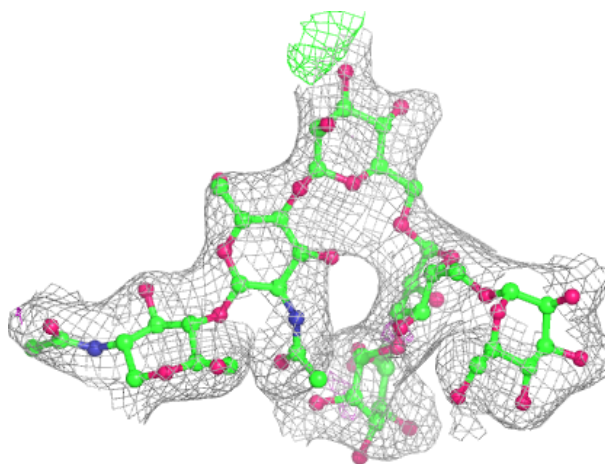
Electron density around Chain H:

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



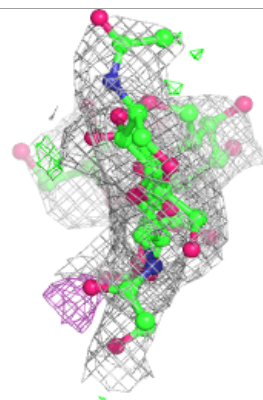
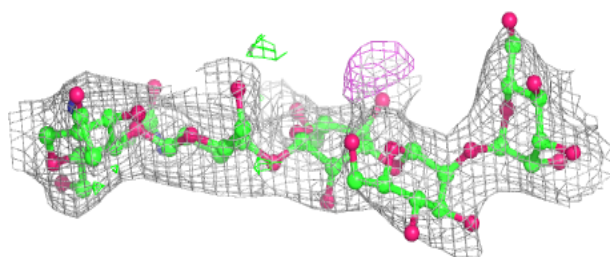
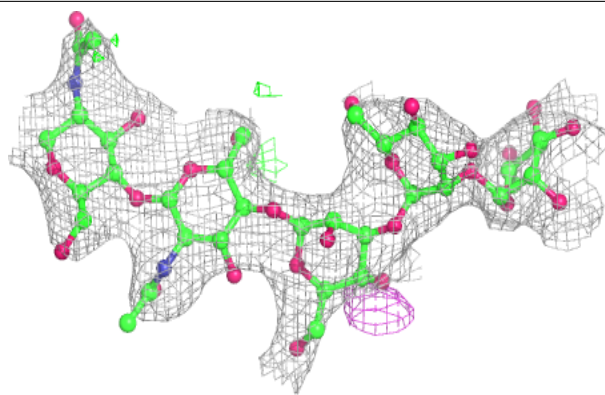
Electron density around Chain I:

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

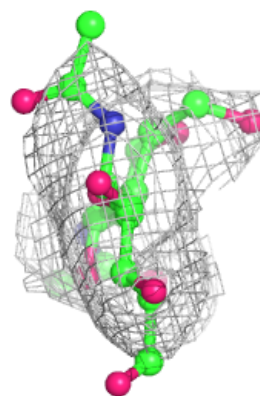
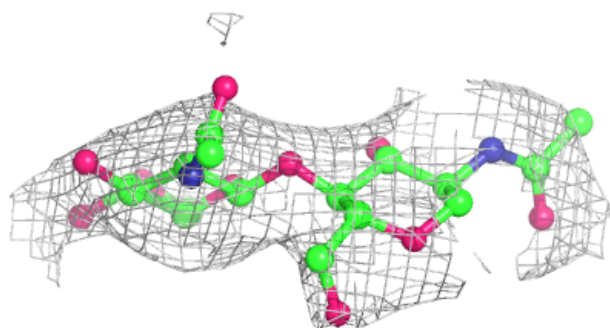
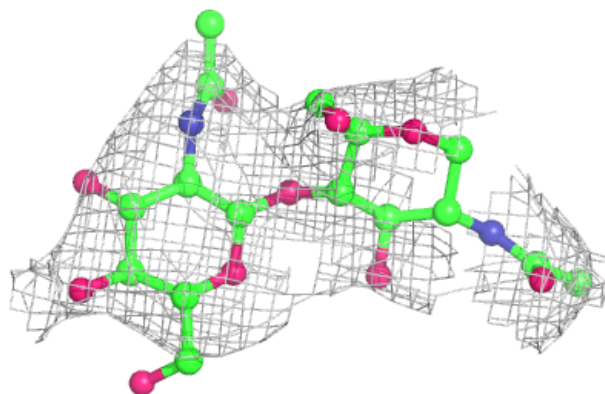


Electron density around Chain J:

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

**Electron density around Chain K:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	A	602	14/15	0.59	0.10	96,105,118,118	0
10	MAN	B	601	11/12	0.64	0.12	97,100,108,112	0
10	MAN	A	601	11/12	0.74	0.10	94,96,102,104	0
11	NAG	A	603	14/15	0.82	0.07	80,92,101,103	0
11	NAG	A	604	14/15	0.84	0.07	78,93,97,101	0
11	NAG	B	602	14/15	0.85	0.07	88,99,102,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.