wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2026 – 05:44 PM EDT

PDB ID	:	9YOB / pdb_00009yob
Title	:	Crystal structure of integrin a4b1 headpiece in complex with Bio-1211 (Mg)
Authors	:	Monroy, M.F.; Lin, F.Y.; Qiao, Q.
Deposited on	:	2025-10-13
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

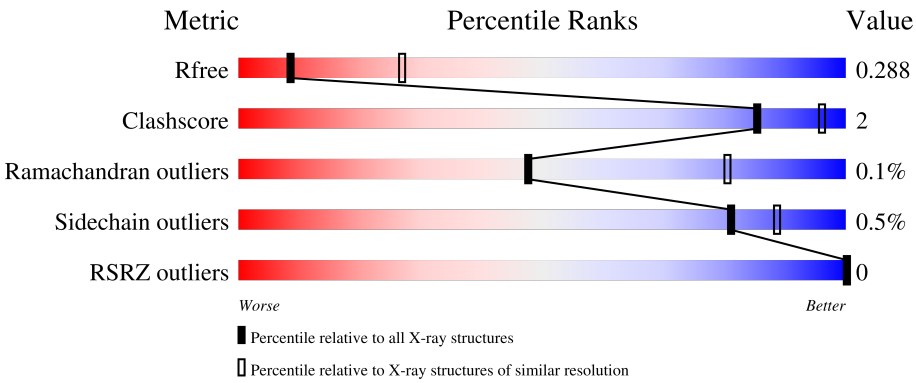
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	597	96%
2	B	490	88% 8%
3	I	5	20% 40% 20% 20%
4	C	3	100%
5	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	G	2	100%
6	E	4	25% 75%
7	F	3	33% 67%
8	H	4	50% 50%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 16264 atoms, of which 7922 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Integrin alpha-4,Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	586	8956	2857	4425	788	864	22	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	TYR	conflict	UNP P13612
A	589	GLY	-	expression tag	UNP P06756
A	590	GLY	-	expression tag	UNP P06756
A	591	SER	-	expression tag	UNP P06756
A	592	GLU	-	expression tag	UNP P06756
A	593	ASN	-	expression tag	UNP P06756
A	594	LEU	-	expression tag	UNP P06756
A	595	TYR	-	expression tag	UNP P06756
A	596	PHE	-	expression tag	UNP P06756
A	597	GLN	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	449	6798	2159	3337	582	689	31	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	conflict	UNP P05556
B	195	THR	SER	conflict	UNP P05556
B	482	GLY	-	expression tag	UNP P05556
B	483	GLY	-	expression tag	UNP P05556
B	484	SER	-	expression tag	UNP P05556
B	485	GLU	-	expression tag	UNP P05556

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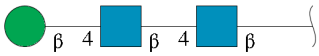
Chain	Residue	Modelled	Actual	Comment	Reference
B	486	ASN	-	expression tag	UNP P05556
B	487	LEU	-	expression tag	UNP P05556
B	488	TYR	-	expression tag	UNP P05556
B	489	PHE	-	expression tag	UNP P05556
B	490	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called Bio-1211.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	I	5	97	36	46	6	9	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	C	3	63	22	24	2	15	0	0	0

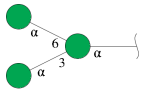
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O				
5	D	2	28	16	2	10		0	0	0
			Total	C	H	N	O			
5	G	2	47	16	19	2	10	0	0	0

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

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

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

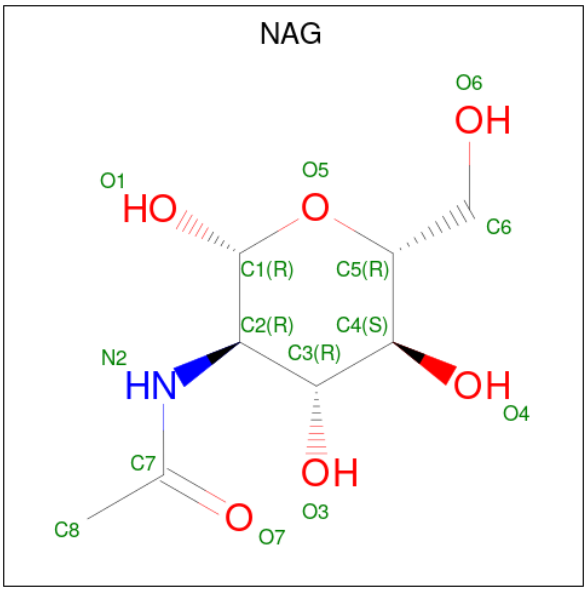


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O				
7	F	3	33	18	15		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
8	H	4	81	28	31	2	20	0	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	A	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
9	B	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
9	B	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
9	B	1	24	8	10	1	5	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
10	A	3	3	3	0	0
			Total	Ca		
10	B	2	2	2	0	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
11	B	1	1	1	0	0

- Molecule 12 is water.

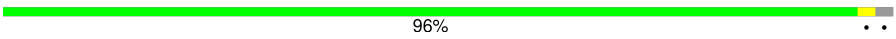
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	4	4	4	0	0
			Total	O		
12	B	4	4	4	0	0
			Total	O		
12	I	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

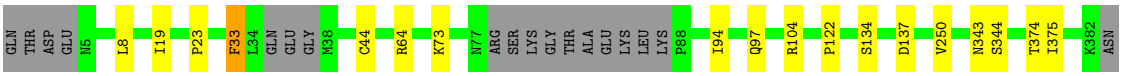
• Molecule 1: Integrin alpha-4,Integrin alpha-V heavy chain

Chain A:



• Molecule 2: Integrin beta-1

Chain B:

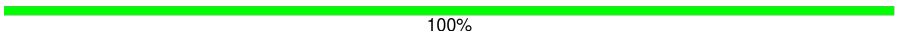


• Molecule 3: Bio-1211

Chain I:

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

Chain C:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

NAG1
NAG2

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

Chain E: 25% 75%

NAG1
NAG2
BMA3
MAN4

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

Chain F: 33% 67%

MAN1
MAN2
MAN3

• Molecule 8: 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: 50% 50%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.17Å 109.80Å 131.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.56 – 3.00 33.56 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.56-3.00) 99.5 (33.56-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.248 , 0.293 0.246 , 0.288	Depositor DCC
R_{free} test set	1530 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	82.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16264	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, A1CYX, NAG, CA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.18	0/4624	0.36	0/6256
2	B	0.15	0/3521	0.31	0/4756
3	I	4.82	6/31 (19.4%)	1.29	0/41
All	All	0.34	6/8176 (0.1%)	0.35	0/11053

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	ASP	C-N	13.71	1.48	1.33
3	I	2	LEU	C-N	10.87	1.49	1.33
3	I	3	ASP	N-CA	-10.48	1.32	1.46
3	I	4	VAL	N-CA	-10.46	1.33	1.46
3	I	4	VAL	C-N	8.55	1.48	1.34

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	4531	4425	4444	9	0
2	B	3461	3337	3336	14	0
3	I	51	46	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	39	24	34	0	0
5	D	28	0	25	5	0
5	G	28	19	25	0	0
6	E	50	0	43	2	0
7	F	33	0	28	4	0
8	H	50	31	43	0	0
9	A	14	10	13	0	0
9	B	42	30	39	2	0
10	A	3	0	0	0	0
10	B	2	0	0	0	0
11	B	1	0	0	0	0
12	A	4	0	0	0	0
12	B	4	0	0	1	0
12	I	1	0	0	0	0
All	All	8342	7922	8060	36	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.

The worst 5 of 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1:NAG:H83	5:D:1:NAG:H3	1.47	0.95
2:B:134:SER:OG	12:B:601:HOH:O	1.98	0.81
1:A:244:GLN:NE2	3:I:1:A1CYX:C04	2.50	0.75
2:B:343:ASN:O	2:B:344:SER:OG	2.09	0.70
3:I:2:LEU:HD23	3:I:2:LEU:N	2.12	0.64

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	585/597 (98%)	569 (97%)	15 (3%)	1 (0%)	43	76
2	B	439/490 (90%)	422 (96%)	17 (4%)	0	100	100
3	I	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	1026/1092 (94%)	992 (97%)	33 (3%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLN

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	488/496 (98%)	486 (100%)	2 (0%)	84	90
2	B	394/431 (91%)	393 (100%)	1 (0%)	86	91
3	I	4/4 (100%)	3 (75%)	1 (25%)	0	3
All	All	886/931 (95%)	882 (100%)	4 (0%)	81	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	SER
1	A	272	TYR
2	B	33	PHE
3	I	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	343	ASN
2	B	322	GLN
2	B	192	ASN

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Mol	Chain	Res	Type
2	B	98	GLN
2	B	201	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)

18 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	$\#\|Z\| > 2$
4	NAG	C	1	4,1	14,14,15	0.52	0	17,19,21	0.44	0
4	NAG	C	2	4	14,14,15	0.24	0	17,19,21	0.46	0
4	BMA	C	3	4	11,11,12	0.78	0	15,15,17	0.77	0
5	NAG	D	1	1,5	14,14,15	0.23	0	17,19,21	0.79	0
5	NAG	D	2	5	14,14,15	0.26	0	17,19,21	0.57	0
6	NAG	E	1	6,1	14,14,15	1.06	1 (7%)	17,19,21	2.04	4 (23%)
6	NAG	E	2	6	14,14,15	0.52	0	17,19,21	0.52	0
6	BMA	E	3	6	11,11,12	0.82	0	15,15,17	0.75	0
6	MAN	E	4	6	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
7	MAN	F	1	7	11,11,12	1.05	1 (9%)	15,15,17	0.94	0
7	MAN	F	2	7	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
7	MAN	F	3	7	11,11,12	0.92	0	15,15,17	0.79	0
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	0.38	0
5	NAG	G	2	5	14,14,15	0.39	0	17,19,21	0.45	0
8	NAG	H	1	8,1	14,14,15	0.64	1 (7%)	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	H	2	8	14,14,15	0.23	0	17,19,21	0.43	0
8	BMA	H	3	8	11,11,12	0.88	0	15,15,17	1.46	2 (13%)
8	MAN	H	4	8	11,11,12	0.77	0	15,15,17	0.79	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
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
5	NAG	D	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	2/2/19/22	0/1/1/1
6	MAN	E	4	6	-	0/2/19/22	0/1/1/1
7	MAN	F	1	7	-	1/2/19/22	0/1/1/1
7	MAN	F	2	7	-	2/2/19/22	0/1/1/1
7	MAN	F	3	7	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
8	NAG	H	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	H	2	8	-	3/6/23/26	0/1/1/1
8	BMA	H	3	8	-	1/2/19/22	0/1/1/1
8	MAN	H	4	8	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1	NAG	O5-C1	2.78	1.48	1.43
7	F	1	MAN	O5-C1	-2.49	1.39	1.43
8	H	1	NAG	O5-C1	-2.31	1.39	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1	NAG	C1-O5-C5	6.22	120.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	3	BMA	C1-O5-C5	4.49	118.20	112.19
6	E	1	NAG	O5-C5-C6	-2.92	101.99	107.66
6	E	1	NAG	C4-C3-C2	-2.71	107.05	111.02
7	F	2	MAN	C1-O5-C5	2.53	115.58	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6
7	F	3	MAN	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6

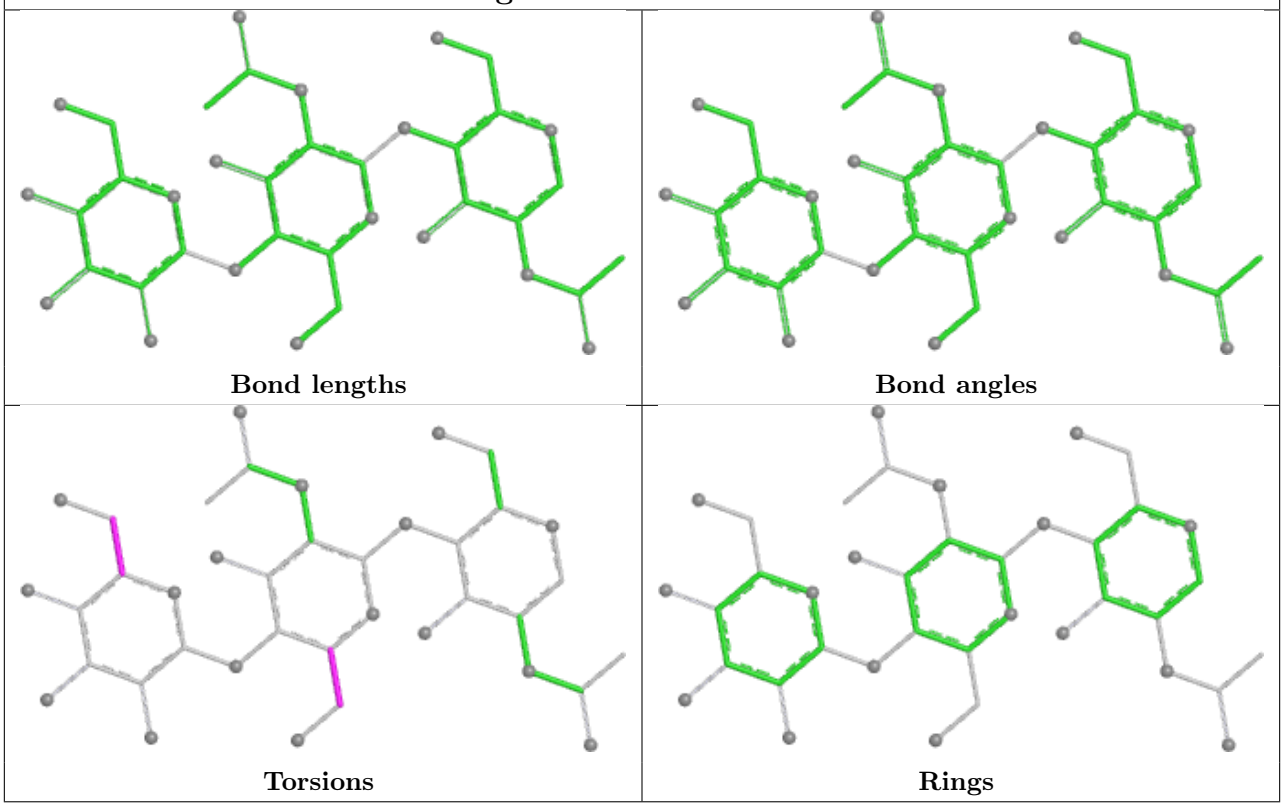
There are no ring outliers.

4 monomers are involved in 9 short contacts:

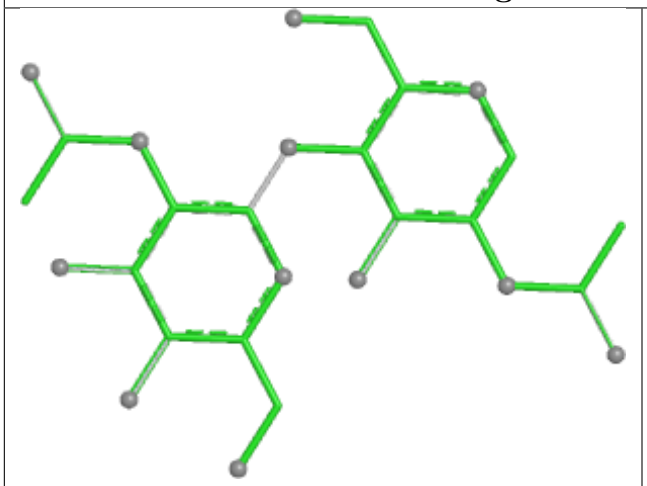
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	2	MAN	2	0
5	D	1	NAG	5	0
7	F	1	MAN	4	0
6	E	3	BMA	2	0

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

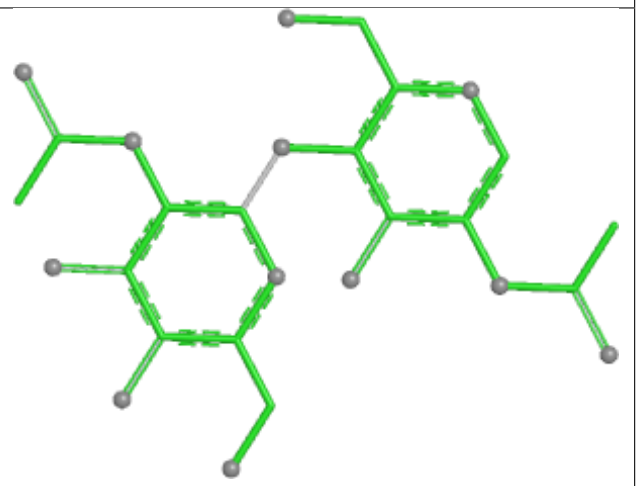
Oligosaccharide Chain C



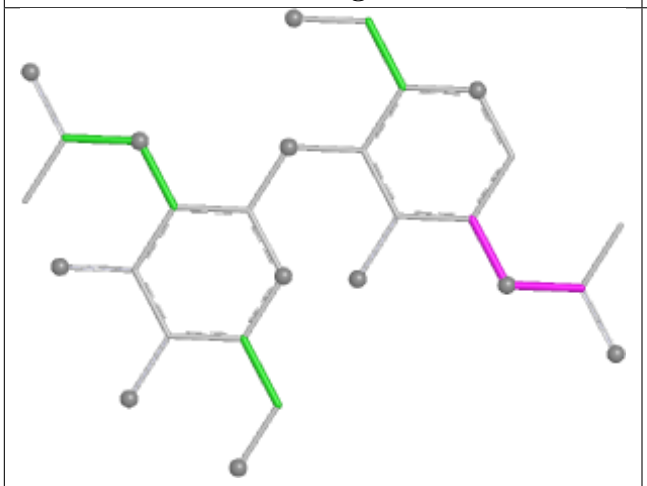
Oligosaccharide Chain D



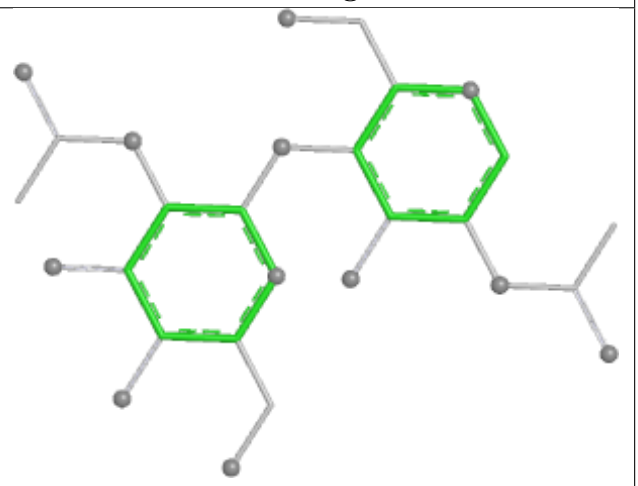
Bond lengths



Bond angles

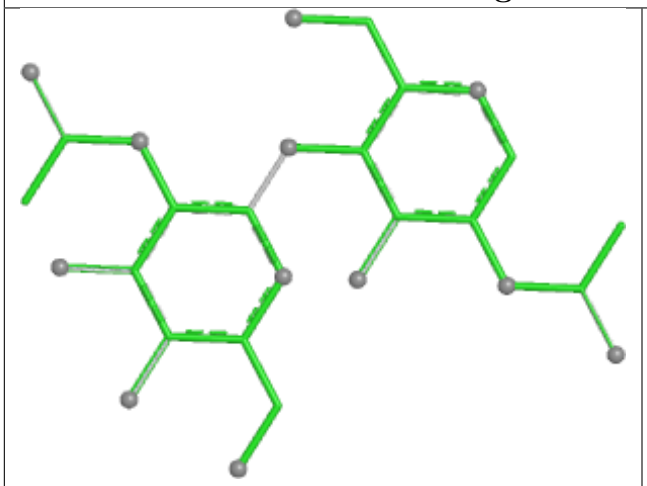


Torsions

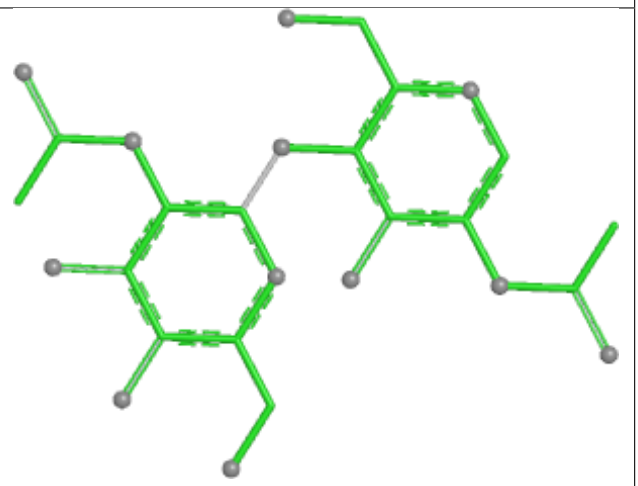


Rings

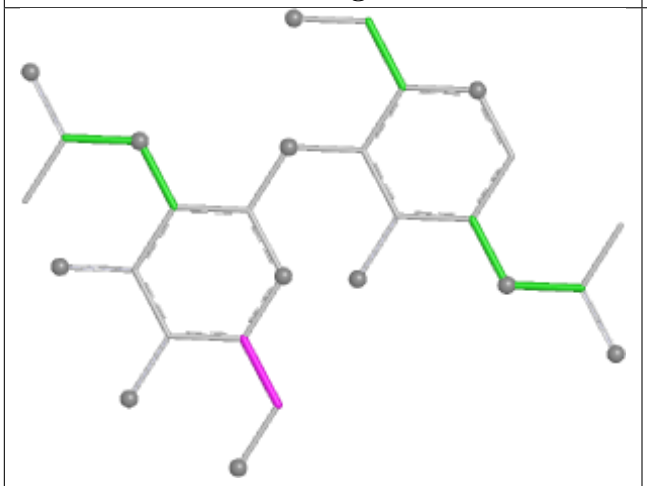
Oligosaccharide Chain G



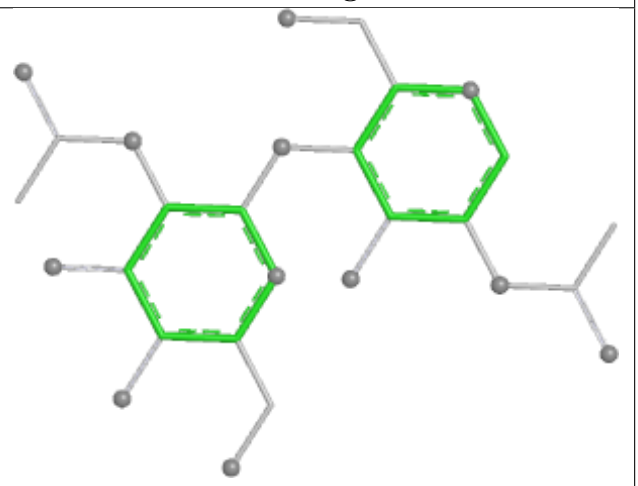
Bond lengths



Bond angles

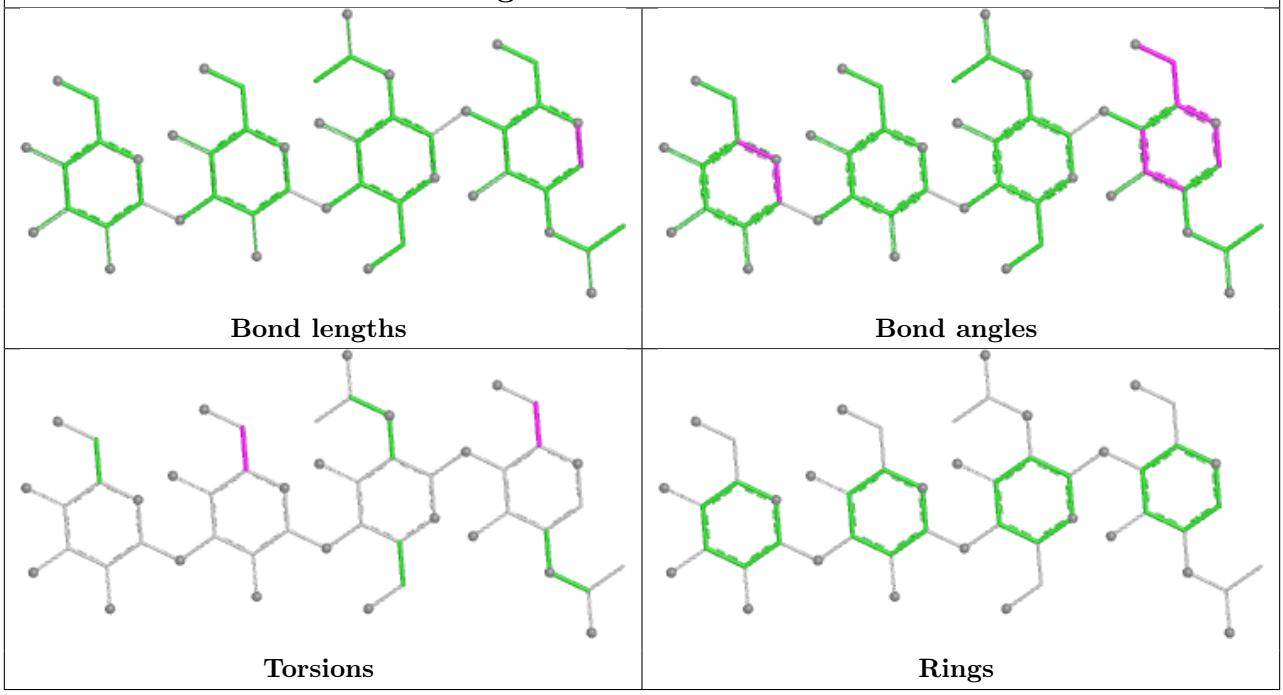


Torsions

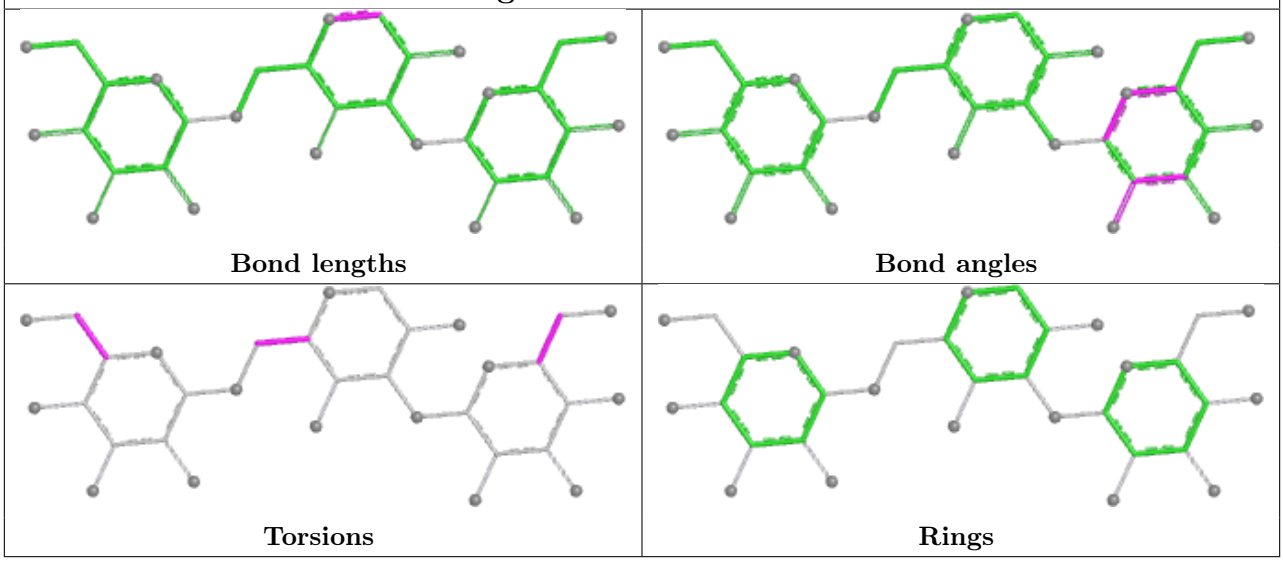


Rings

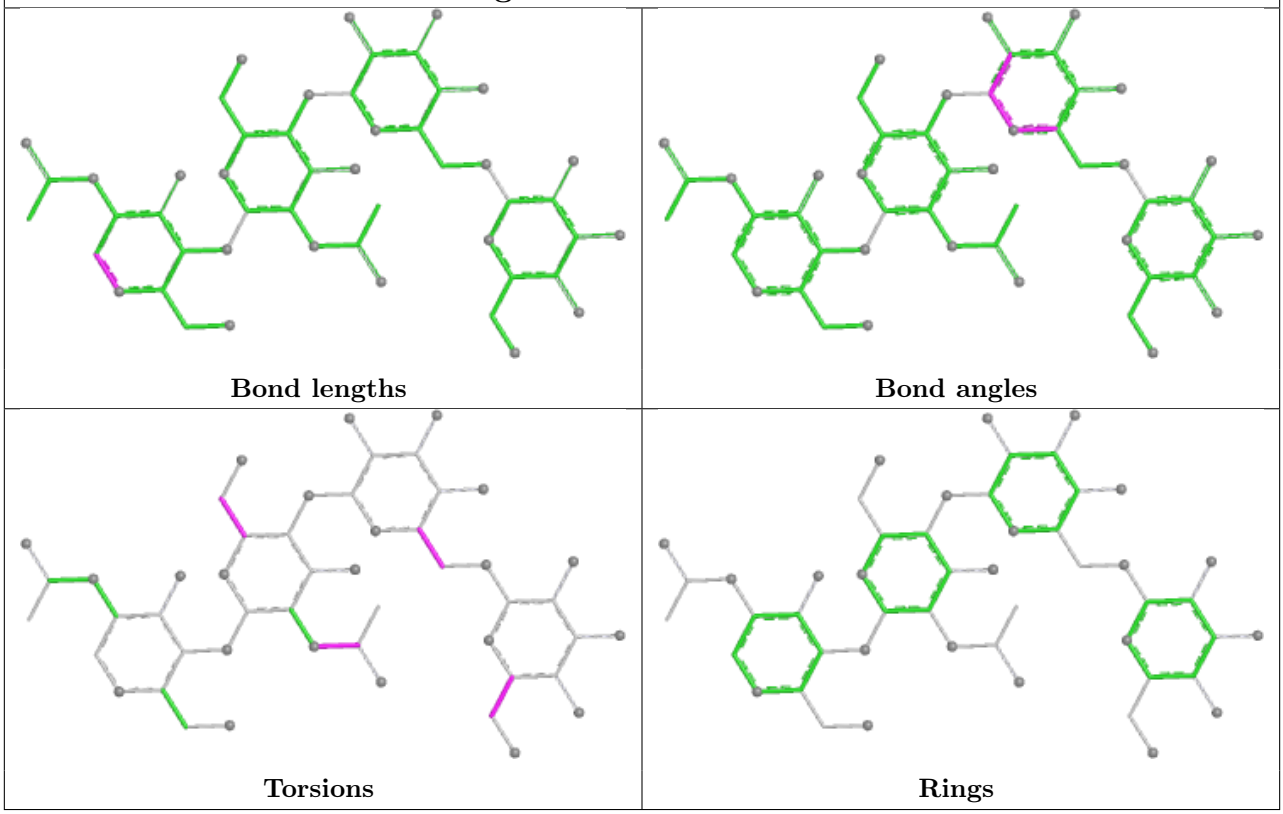
Oligosaccharide Chain E



Oligosaccharide Chain F



Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	B	505	2	14,14,15	0.42	0	17,19,21	0.37	0
9	NAG	B	506	-	14,14,15	0.68	1 (7%)	17,19,21	0.58	0
9	NAG	B	504	-	14,14,15	0.43	0	17,19,21	0.41	0
9	NAG	A	601	1	14,14,15	0.37	0	17,19,21	0.47	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	NAG	B	505	2	-	0/6/23/26	0/1/1/1
9	NAG	B	506	-	-	4/6/23/26	0/1/1/1
9	NAG	B	504	-	-	3/6/23/26	0/1/1/1
9	NAG	A	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	506	NAG	O5-C1	-2.32	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	NAG	O5-C5-C6-O6
9	B	506	NAG	O5-C5-C6-O6
9	B	506	NAG	C4-C5-C6-O6
9	A	601	NAG	C4-C5-C6-O6
9	B	504	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	505	NAG	1	0
9	B	504	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	586/597 (98%)	-0.25	0	100	100	46, 94, 133, 164	1 (0%)
2	B	449/490 (91%)	-0.06	0	100	100	69, 123, 156, 181	0
3	I	4/5 (80%)	0.43	0	100	100	67, 67, 72, 79	0
All	All	1039/1092 (95%)	-0.17	0	100	100	46, 104, 147, 181	1 (0%)

There are no RSRZ outliers to report.

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
4	NAG	C	1	14/15	-	-	94,112,129,136	0
4	NAG	C	2	14/15	-	-	114,125,152,152	0
4	BMA	C	3	11/12	-	-	129,131,168,169	0
6	NAG	E	2	14/15	0.37	0.10	97,102,112,113	0
5	NAG	D	2	14/15	0.38	0.12	123,126,131,132	0
5	NAG	G	1	14/15	-	-	103,122,148,149	0
5	NAG	G	2	14/15	-	-	125,142,180,180	0
6	NAG	E	1	14/15	0.52	0.11	105,110,118,121	0
8	NAG	H	2	14/15	0.63	0.12	123,136,164,165	0
6	BMA	E	3	11/12	-	-	91,93,97,98	0

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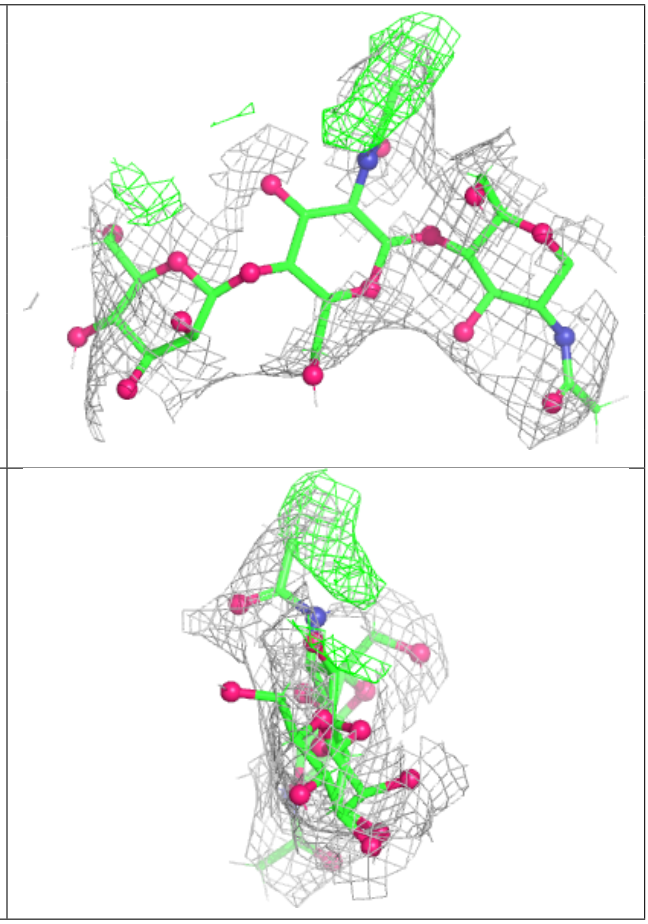
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	E	4	11/12	-	-	97,100,102,103	0
7	MAN	F	1	11/12	-	-	88,95,99,100	0
7	MAN	F	2	11/12	-	-	99,104,107,109	0
7	MAN	F	3	11/12	-	-	104,104,104,104	0
8	NAG	H	1	14/15	0.73	0.10	108,130,149,150	0
5	NAG	D	1	14/15	0.82	0.08	110,118,125,128	0
8	BMA	H	3	11/12	-	-	140,143,186,186	0
8	MAN	H	4	11/12	-	-	144,151,196,198	0

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

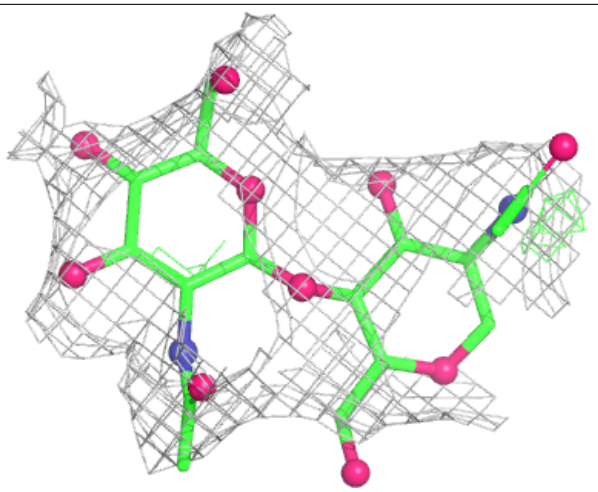
Electron density around Chain C:

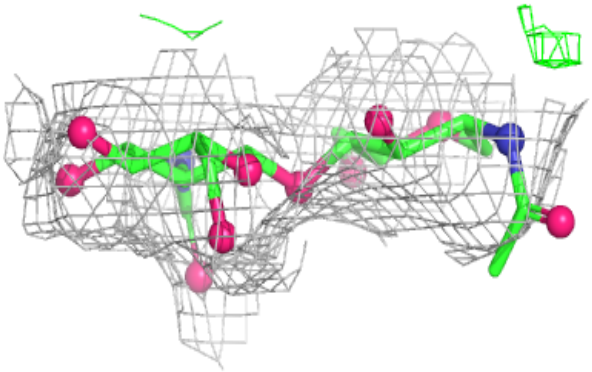
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

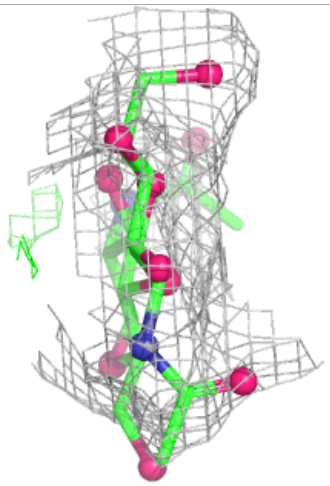


Electron density around Chain D:

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

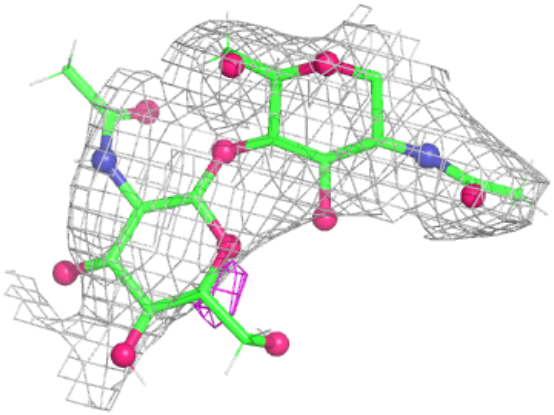


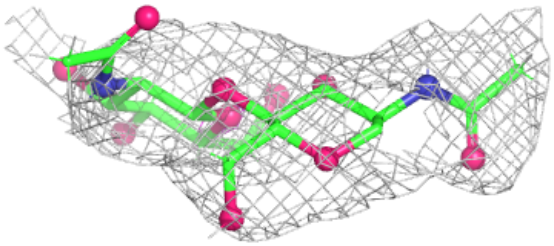


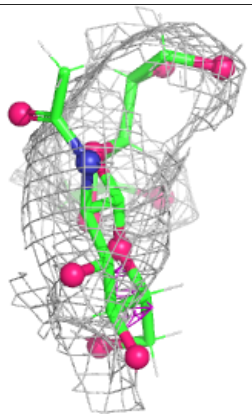


Electron density around Chain G:

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

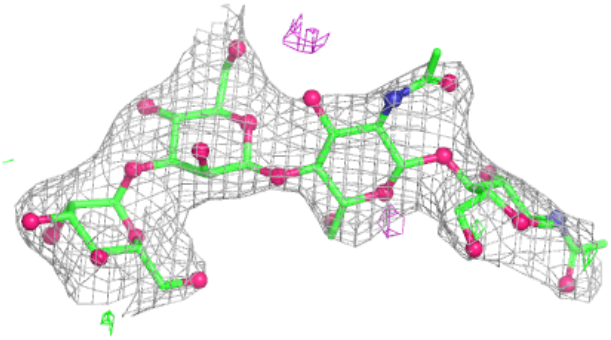


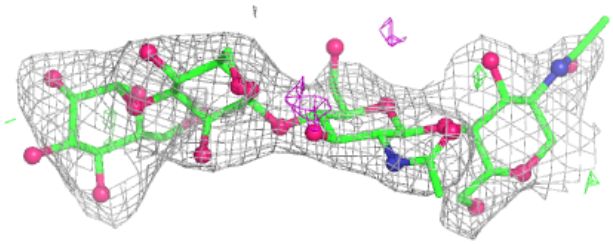


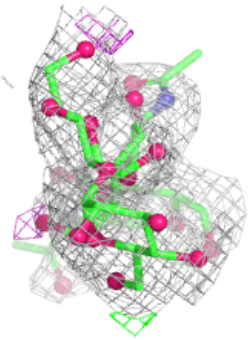


Electron density around Chain E:

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

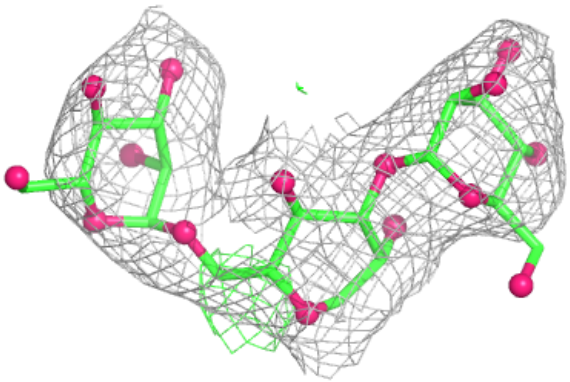


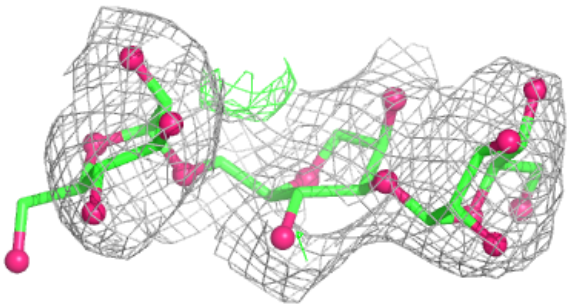


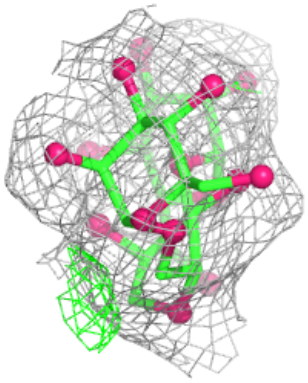


Electron density around Chain F:

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

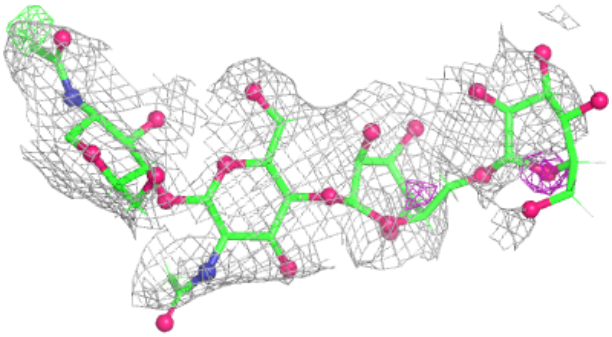


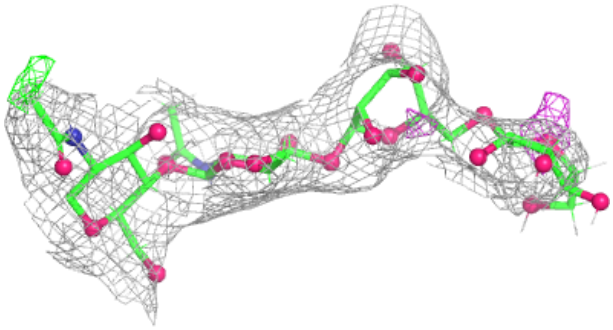


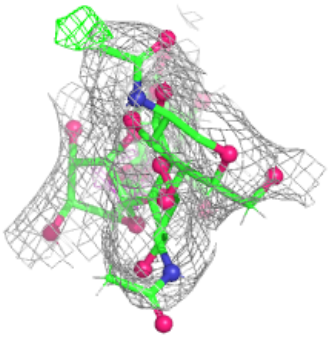


Electron density around Chain H:

$2mF_o$-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
9	NAG	B	506	14/15	0.50	0.14	115,124,155,156	0
9	NAG	B	505	14/15	0.55	0.12	134,172,232,232	0
9	NAG	A	601	14/15	0.73	0.09	108,124,156,156	0
9	NAG	B	504	14/15	0.75	0.13	125,143,170,172	0
10	CA	B	502	1/1	0.94	0.05	117,117,117,117	0
10	CA	A	603	1/1	0.98	0.05	78,78,78,78	0
11	MG	B	503	1/1	0.98	0.09	99,99,99,99	0
10	CA	B	501	1/1	0.99	0.03	78,78,78,78	0
10	CA	A	602	1/1	0.99	0.02	71,71,71,71	0
10	CA	A	604	1/1	0.99	0.04	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.