



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 03:14 PM UTC

PDB ID : 5JSD / pdb_00005jsd
Title : Crystal structure of phiAB6 tailspike in complex with five-repeated oligosaccharides of Acinetobacter baumannii surface polysaccharide
Authors : Lee, I.M.; Tu, I.F.; Huang, K.F.; Wu, S.H.
Deposited on : 2016-05-08
Resolution : 1.48 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

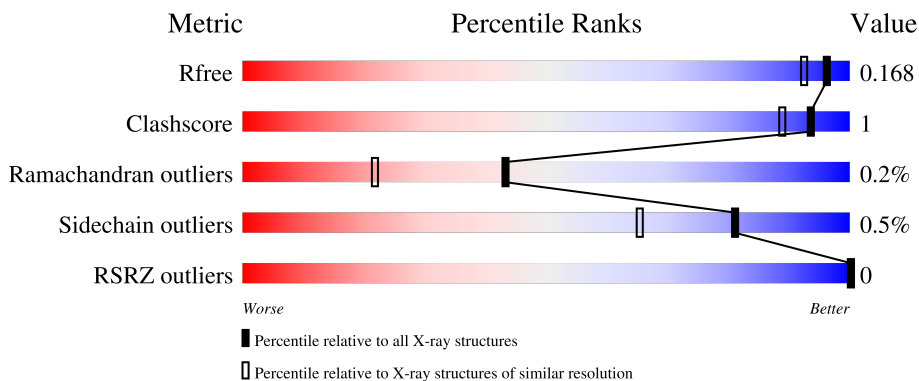
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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.






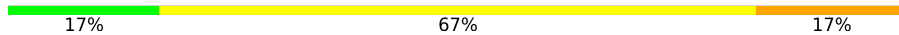
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	719	
1	B	719	
1	C	719	
2	D	8	
2	G	8	

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Mol	Chain	Length	Quality of chain
2	H	8	 50% 50%
3	E	6	 33% 50% 17%
3	F	6	 33% 50% 17%
3	I	6	 17% 67% 17%

2 Entry composition i

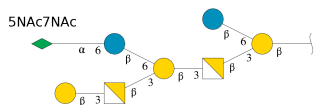
There are 6 unique types of molecules in this entry. The entry contains 16020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 phiAB6 tailspike.

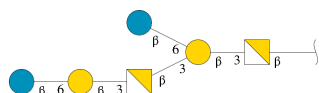
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0
1	B	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0
1	C	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-bisacetamido-3,5,7,9-tetra-deoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid-(2-6)-beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose.



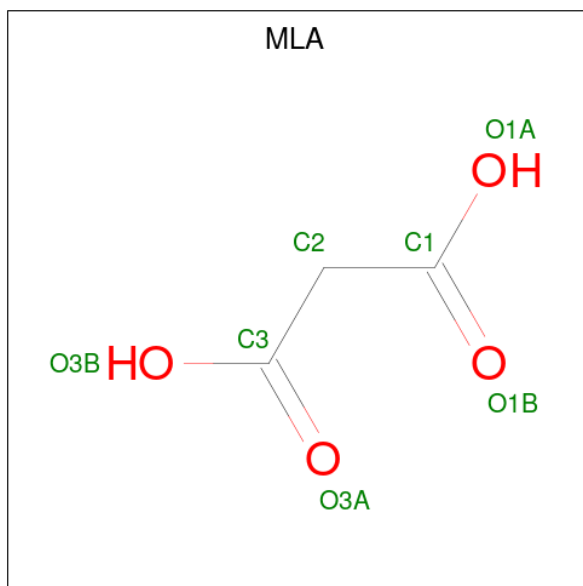
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	8	Total 100	C 55	N 4	O 41	0	0	0
2	G	8	Total 100	C 55	N 4	O 41	0	0	0
2	H	8	Total 100	C 55	N 4	O 41	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-6)-beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose.



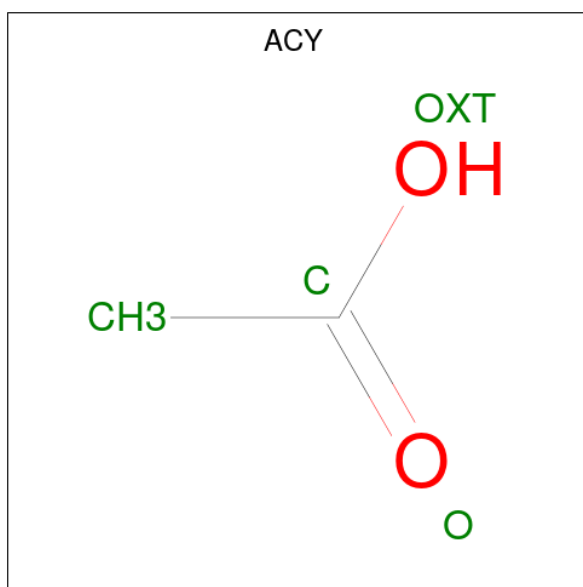
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			67	36	2	29			
3	F	6	Total	C	N	O	0	0	0
			67	36	2	29			
3	I	6	Total	C	N	O	0	0	0
			67	36	2	29			

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		

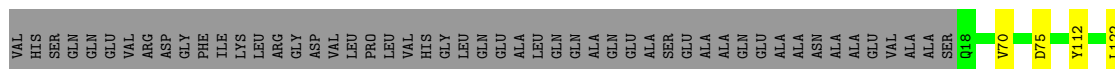
- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	A	1	Total C O 3 2 1	0	0
5	B	1	Total C O 3 2 1	0	0
5	B	1	Total C O 3 2 1	0	0
5	B	1	Total C O 3 2 1	0	0
5	B	1	Total C O 3 2 1	0	0
5	C	1	Total C O 3 2 1	0	0
5	C	1	Total C O 3 2 1	0	0
5	C	1	Total C O 3 2 1	0	0
5	C	1	Total C O 3 2 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	974	Total 974	O 974	0	0
6	B	958	Total 958	O 958	0	0
6	C	951	Total 951	O 951	0	0



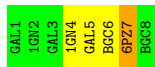
- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-bisacetamido-3,5,7,9-tetraoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid-(2-6)-beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose

Chain D: 38% 62%



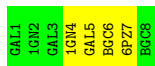
- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-bisacetamido-3,5,7,9-tetraoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid-(2-6)-beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose

Chain G: 50% 38% 12%



- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-bisacetamido-3,5,7,9-tetraoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid-(2-6)-beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose

Chain H: 50% 50%



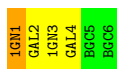
- Molecule 3: beta-D-glucopyranose-(1-6)-beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose

Chain E: 33% 50% 17%



- Molecule 3: beta-D-glucopyranose-(1-6)-beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose

Chain F: 33% 50% 17%



- Molecule 3: beta-D-glucopyranose-(1-6)-beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose

Chain I: 17% 67% 17%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.81Å 78.39Å 247.74Å 90.00° 100.53° 90.00°	Depositor
Resolution (Å)	19.77 – 1.48 19.77 – 1.48	Depositor EDS
% Data completeness (in resolution range)	87.8 (19.77-1.48) 87.9 (19.77-1.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 1.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.142 , 0.169 0.141 , 0.168	Depositor DCC
R_{free} test set	18826 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.469 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-1 0.470 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-1	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16020	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: GAL, BGC, 1GN, ACY, MLA, 6PZ

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	0.45	0/4289	0.66	0/5825
1	B	0.45	0/4289	0.66	0/5825
1	C	0.45	0/4289	0.66	0/5825
All	All	0.45	0/12867	0.66	0/17475

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4193	0	4040	12	0
1	B	4193	0	4040	12	0
1	C	4193	0	4040	11	0
2	D	100	0	63	0	0
2	G	100	0	63	4	0
2	H	100	0	63	0	0
3	E	67	0	55	1	0
3	F	67	0	55	1	0
3	I	67	0	55	1	0
4	A	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	2	0	0
4	C	7	0	2	0	0
5	A	12	0	12	0	0
5	B	12	0	12	1	0
5	C	12	0	12	1	0
6	A	974	0	0	1	0
6	B	958	0	0	1	0
6	C	951	0	0	0	0
All	All	16020	0	12516	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 1.

All (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)
2:G:7:6PZ:C10	2:G:7:6PZ:N5	2.07	1.18
2:G:7:6PZ:N1	2:G:7:6PZ:C10A	2.12	1.12
1:B:184:GLN:NE2	6:B:701:HOH:O	2.24	0.69
1:A:184:GLN:NE2	6:A:701:HOH:O	2.30	0.64
5:B:602:ACY:O	3:F:1:1GN:H1	2.09	0.53
1:B:174:THR:HG21	1:B:202:GLU:HG3	1.91	0.52
1:B:112:TYR:CE1	1:B:122:LEU:HA	2.46	0.51
5:C:618:ACY:O	3:I:1:1GN:H1	2.11	0.50
1:A:174:THR:HG21	1:A:202:GLU:HG3	1.93	0.50
1:C:112:TYR:CE1	1:C:122:LEU:HA	2.46	0.50
1:A:112:TYR:CE1	1:A:122:LEU:HA	2.47	0.49
1:C:174:THR:HG21	1:C:202:GLU:HG3	1.95	0.49
1:B:18:GLN:HG3	1:B:21:TYR:CZ	2.47	0.49
1:B:257:THR:HA	1:B:281:HIS:O	2.14	0.48
1:A:523:MET:HG3	1:A:531:TRP:CE2	2.48	0.48
1:C:523:MET:HG3	1:C:531:TRP:CE2	2.50	0.47
1:B:523:MET:HG3	1:B:531:TRP:CE2	2.50	0.47
1:C:257:THR:HA	1:C:281:HIS:O	2.17	0.45
2:G:7:6PZ:N1	2:G:7:6PZ:O10A	2.45	0.45
1:A:70:VAL:HG22	1:C:75:ASP:HA	1.98	0.45
1:B:75:ASP:HA	1:C:70:VAL:HG22	1.99	0.45
1:A:257:THR:HA	1:A:281:HIS:O	2.17	0.45
1:A:75:ASP:HA	1:B:70:VAL:HG22	2.00	0.44
1:C:211:ASP:HA	1:C:234:THR:O	2.18	0.44
1:B:211:ASP:HA	1:B:234:THR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:6PZ:N1	2:G:7:6PZ:C11A	2.81	0.43
1:A:211:ASP:HA	1:A:234:THR:O	2.20	0.42
1:B:401:THR:O	1:C:392:LYS:HA	2.20	0.41
1:A:78:TYR:HB2	1:A:80:ILE:HG12	2.03	0.41
1:A:314:ASN:HD22	1:A:345:GLY:HA3	1.86	0.41
1:B:313:GLU:OE2	3:E:1:1GN:O1	2.37	0.41
1:A:112:TYR:CD1	1:A:112:TYR:C	2.98	0.41
1:B:112:TYR:CD1	1:B:112:TYR:C	2.99	0.41
1:C:112:TYR:CD1	1:C:112:TYR:C	3.00	0.40
1:C:314:ASN:HD22	1:C:345:GLY:HA3	1.85	0.40
1:A:397:THR:HA	1:C:412:VAL:O	2.21	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	547/719 (76%)	528 (96%)	18 (3%)	1 (0%)	43 22
1	B	547/719 (76%)	528 (96%)	18 (3%)	1 (0%)	43 22
1	C	547/719 (76%)	528 (96%)	18 (3%)	1 (0%)	43 22
All	All	1641/2157 (76%)	1584 (96%)	54 (3%)	3 (0%)	43 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	255	VAL
1	C	255	VAL

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	454/597 (76%)	451 (99%)	3 (1%)	76	56
1	B	454/597 (76%)	452 (100%)	2 (0%)	84	70
1	C	454/597 (76%)	452 (100%)	2 (0%)	84	70
All	All	1362/1791 (76%)	1355 (100%)	7 (0%)	81	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	VAL
1	A	395	ASN
1	A	504	SER
1	B	229	VAL
1	B	504	SER
1	C	229	VAL
1	C	504	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	52	ASN
1	A	184	GLN
1	A	209	ASN
1	A	235	ASN
1	A	243	ASN
1	A	263	ASN
1	A	314	ASN
1	A	377	ASN
1	A	395	ASN
1	A	447	ASN
1	A	522	GLN
1	B	18	GLN
1	B	35	ASN

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Mol	Chain	Res	Type
1	B	52	ASN
1	B	209	ASN
1	B	235	ASN
1	B	243	ASN
1	B	263	ASN
1	B	314	ASN
1	B	377	ASN
1	B	447	ASN
1	B	522	GLN
1	C	52	ASN
1	C	235	ASN
1	C	243	ASN
1	C	263	ASN
1	C	267	GLN
1	C	314	ASN
1	C	377	ASN
1	C	447	ASN
1	C	522	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](#)

42 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	GAL	D	1	2	12,12,12	0.48	0	17,17,17	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1GN	D	2	5,2	11,11,12	0.41	0	13,15,17	0.84	1 (7%)
2	GAL	D	3	2	11,11,12	0.26	0	15,15,17	0.56	0
2	1GN	D	4	5,2	11,11,12	0.46	0	13,15,17	1.07	2 (15%)
2	GAL	D	5	2	11,11,12	0.38	0	15,15,17	0.88	1 (6%)
2	BGC	D	6	2	11,11,12	0.39	0	15,15,17	0.92	1 (6%)
2	6PZ	D	7	2	21,22,23	1.15	3 (14%)	22,31,34	1.89	9 (40%)
2	BGC	D	8	2	11,11,12	0.36	0	15,15,17	0.85	0
3	1GN	E	1	5,3	12,12,12	0.95	1 (8%)	16,17,17	2.39	5 (31%)
3	GAL	E	2	3	11,11,12	0.41	0	15,15,17	1.24	1 (6%)
3	1GN	E	3	5,3	11,11,12	0.37	0	13,15,17	1.50	2 (15%)
3	GAL	E	4	3	11,11,12	0.44	0	15,15,17	1.02	2 (13%)
3	BGC	E	5	3	11,11,12	0.38	0	15,15,17	0.80	0
3	BGC	E	6	3	11,11,12	0.23	0	15,15,17	0.66	0
3	1GN	F	1	5,3	12,12,12	0.93	1 (8%)	16,17,17	1.53	2 (12%)
3	GAL	F	2	3	11,11,12	0.41	0	15,15,17	1.31	1 (6%)
3	1GN	F	3	5,3	11,11,12	0.38	0	13,15,17	1.44	3 (23%)
3	GAL	F	4	3	11,11,12	0.26	0	15,15,17	0.87	1 (6%)
3	BGC	F	5	3	11,11,12	0.26	0	15,15,17	0.95	0
3	BGC	F	6	3	11,11,12	0.26	0	15,15,17	0.84	0
2	GAL	G	1	2	12,12,12	0.49	0	17,17,17	0.74	0
2	1GN	G	2	5,2	11,11,12	0.38	0	13,15,17	0.72	0
2	GAL	G	3	2	11,11,12	0.23	0	15,15,17	0.48	0
2	1GN	G	4	5,2	11,11,12	0.45	0	13,15,17	1.09	2 (15%)
2	GAL	G	5	2	11,11,12	0.35	0	15,15,17	0.98	1 (6%)
2	BGC	G	6	2	11,11,12	0.40	0	15,15,17	1.00	1 (6%)
2	6PZ	G	7	2	21,22,23	7.31	2 (9%)	22,31,34	5.57	9 (40%)
2	BGC	G	8	2	11,11,12	0.39	0	15,15,17	0.78	0
2	GAL	H	1	2	12,12,12	0.48	0	17,17,17	0.70	0
2	1GN	H	2	5,2	11,11,12	0.43	0	13,15,17	0.73	0
2	GAL	H	3	2	11,11,12	0.24	0	15,15,17	0.52	0
2	1GN	H	4	5,2	11,11,12	0.43	0	13,15,17	1.24	3 (23%)
2	GAL	H	5	2	11,11,12	0.35	0	15,15,17	0.84	1 (6%)
2	BGC	H	6	2	11,11,12	0.44	0	15,15,17	1.03	1 (6%)
2	6PZ	H	7	2	21,22,23	1.12	4 (19%)	22,31,34	1.92	8 (36%)
2	BGC	H	8	2	11,11,12	0.37	0	15,15,17	0.56	0
3	1GN	I	1	5,3	12,12,12	0.91	1 (8%)	16,17,17	1.60	2 (12%)
3	GAL	I	2	3	11,11,12	0.40	0	15,15,17	1.40	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1GN	I	3	5,3	11,11,12	0.39	0	13,15,17	1.67	2 (15%)
3	GAL	I	4	3	11,11,12	0.64	0	15,15,17	1.21	2 (13%)
3	BGC	I	5	3	11,11,12	1.64	2 (18%)	15,15,17	1.29	2 (13%)
3	BGC	I	6	3	11,11,12	0.25	0	15,15,17	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	1	2	-	2/2/22/22	0/1/1/1
2	1GN	D	2	5,2	-	0/2/19/22	0/1/1/1
2	GAL	D	3	2	-	0/2/19/22	0/1/1/1
2	1GN	D	4	5,2	-	0/2/19/22	0/1/1/1
2	GAL	D	5	2	-	2/2/19/22	0/1/1/1
2	BGC	D	6	2	-	0/2/19/22	0/1/1/1
2	6PZ	D	7	2	-	0/20/36/40	0/1/1/1
2	BGC	D	8	2	-	2/2/19/22	0/1/1/1
3	1GN	E	1	5,3	-	0/2/22/22	0/1/1/1
3	GAL	E	2	3	-	1/2/19/22	0/1/1/1
3	1GN	E	3	5,3	-	0/2/19/22	0/1/1/1
3	GAL	E	4	3	-	1/2/19/22	0/1/1/1
3	BGC	E	5	3	-	2/2/19/22	0/1/1/1
3	BGC	E	6	3	-	0/2/19/22	0/1/1/1
3	1GN	F	1	5,3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	1/2/19/22	0/1/1/1
3	1GN	F	3	5,3	-	2/2/19/22	0/1/1/1
3	GAL	F	4	3	-	1/2/19/22	0/1/1/1
3	BGC	F	5	3	-	0/2/19/22	0/1/1/1
3	BGC	F	6	3	-	0/2/19/22	0/1/1/1
2	GAL	G	1	2	-	0/2/22/22	0/1/1/1
2	1GN	G	2	5,2	-	0/2/19/22	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	1GN	G	4	5,2	-	0/2/19/22	0/1/1/1
2	GAL	G	5	2	-	1/2/19/22	0/1/1/1
2	BGC	G	6	2	-	0/2/19/22	0/1/1/1
2	6PZ	G	7	2	-	2/20/36/40	0/1/1/1
2	BGC	G	8	2	-	2/2/19/22	0/1/1/1
2	GAL	H	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1GN	H	2	5,2	-	0/2/19/22	0/1/1/1
2	GAL	H	3	2	-	0/2/19/22	0/1/1/1
2	1GN	H	4	5,2	-	0/2/19/22	0/1/1/1
2	GAL	H	5	2	-	2/2/19/22	0/1/1/1
2	BGC	H	6	2	-	0/2/19/22	0/1/1/1
2	6PZ	H	7	2	-	0/20/36/40	0/1/1/1
2	BGC	H	8	2	-	1/2/19/22	0/1/1/1
3	1GN	I	1	5,3	-	0/2/22/22	0/1/1/1
3	GAL	I	2	3	-	1/2/19/22	0/1/1/1
3	1GN	I	3	5,3	-	0/2/19/22	0/1/1/1
3	GAL	I	4	3	-	2/2/19/22	0/1/1/1
3	BGC	I	5	3	-	0/2/19/22	0/1/1/1
3	BGC	I	6	3	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	6PZ	C10A-N1	24.35	2.12	1.34
2	G	7	6PZ	C10-N5	22.74	2.07	1.34
3	I	5	BGC	C1-C2	-4.35	1.41	1.52
3	I	5	BGC	C2-C3	2.98	1.57	1.52
3	E	1	1GN	C1-C2	2.57	1.55	1.52
2	D	7	6PZ	C10A-N1	-2.45	1.26	1.34
3	I	1	1GN	C1-C2	2.37	1.55	1.52
3	F	1	1GN	C1-C2	2.33	1.55	1.52
2	H	7	6PZ	C10A-N1	-2.31	1.26	1.34
2	D	7	6PZ	C10-N5	-2.14	1.27	1.34
2	D	7	6PZ	C7-N1	2.13	1.49	1.45
2	H	7	6PZ	C7-N1	2.03	1.49	1.45
2	H	7	6PZ	C5-N5	2.03	1.49	1.45
2	H	7	6PZ	C10-N5	-2.01	1.27	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7	6PZ	O10A-C10A-N1	-18.53	89.23	121.98
2	G	7	6PZ	O10-C10-N5	-11.91	100.94	121.98
2	G	7	6PZ	C11A-C10A-N1	-9.69	100.05	116.12
2	G	7	6PZ	C11-C10-N5	-7.59	103.52	116.12
3	E	1	1GN	O5-C1-C2	6.13	116.67	109.51
3	E	1	1GN	C1-C2-C3	5.17	117.41	110.60
3	I	3	1GN	O3-C3-C2	-4.86	100.81	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	1GN	C1-C2-C3	4.00	115.87	110.60
3	I	2	GAL	C1-C2-C3	3.92	115.35	109.64
3	F	2	GAL	C1-C2-C3	3.86	115.27	109.64
3	E	3	1GN	O3-C3-C2	-3.86	102.69	109.90
3	F	1	1GN	C1-C2-C3	3.86	115.68	110.60
2	D	7	6PZ	C11A-C10A-N1	3.66	122.18	116.12
3	E	2	GAL	C1-C2-C3	3.61	114.91	109.64
2	H	7	6PZ	C11A-C10A-N1	3.38	121.73	116.12
2	H	7	6PZ	O1B-C1-C2	3.35	121.42	112.71
2	D	7	6PZ	O6-C2-C1	-3.27	101.55	107.72
2	D	7	6PZ	O1B-C1-C2	3.25	121.16	112.71
2	H	7	6PZ	C7-N1-C10A	3.25	130.71	123.11
2	G	7	6PZ	O1B-C1-C2	3.22	121.09	112.71
2	D	7	6PZ	C7-N1-C10A	3.15	130.47	123.11
2	H	7	6PZ	O6-C2-C1	-3.03	102.00	107.72
3	F	3	1GN	O3-C3-C2	-3.00	104.29	109.90
2	G	7	6PZ	O6-C2-C3	-2.92	106.64	110.56
3	E	3	1GN	C1-O5-C5	2.90	116.08	112.19
3	E	1	1GN	O3-C3-C2	-2.88	105.05	110.22
2	H	6	BGC	C1-C2-C3	2.86	113.80	109.64
2	G	7	6PZ	O6-C2-C1	-2.82	102.39	107.72
2	H	7	6PZ	O10-C10-C11	-2.80	117.07	122.05
2	H	7	6PZ	O6-C2-C3	-2.77	106.83	110.56
2	G	5	GAL	O5-C5-C6	2.77	113.06	107.66
2	G	6	BGC	C1-C2-C3	2.71	113.59	109.64
3	E	1	1GN	O1-C1-O5	-2.68	102.44	110.41
3	I	1	1GN	O5-C1-C2	2.56	112.50	109.51
2	D	5	GAL	O5-C5-C6	2.56	112.64	107.66
2	D	7	6PZ	O6-C2-C3	-2.56	107.12	110.56
3	F	3	1GN	C1-O5-C5	2.55	115.60	112.19
3	E	4	GAL	O6-C6-C5	-2.54	102.69	111.33
3	I	5	BGC	C1-O5-C5	-2.51	108.82	112.19
2	H	5	GAL	O5-C5-C6	2.46	112.46	107.66
3	I	3	1GN	C1-O5-C5	2.46	115.49	112.19
3	I	4	GAL	C1-O5-C5	2.45	115.47	112.19
2	H	7	6PZ	C11-C10-N5	2.41	120.11	116.12
2	G	4	1GN	O3-C3-C2	-2.37	105.47	109.90
2	H	4	1GN	O3-C3-C2	-2.36	105.48	109.90
3	E	4	GAL	C1-C2-C3	2.36	113.08	109.64
2	D	4	1GN	O3-C3-C2	-2.36	105.49	109.90
2	D	7	6PZ	O1A-C1-C2	-2.35	117.78	122.85
2	D	7	6PZ	C11-C10-N5	2.31	119.94	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	4	GAL	O6-C6-C5	2.29	119.13	111.33
2	D	6	BGC	C1-C2-C3	2.28	112.96	109.64
2	H	7	6PZ	O1A-C1-C2	-2.25	117.98	122.85
2	H	4	1GN	O3-C3-C4	2.25	115.68	110.38
3	I	2	GAL	C1-O5-C5	2.24	115.19	112.19
3	F	3	1GN	O5-C5-C6	2.20	111.94	107.66
2	G	4	1GN	O3-C3-C4	2.20	115.56	110.38
3	I	5	BGC	O3-C3-C2	2.19	114.53	110.05
2	G	7	6PZ	O1A-C1-C2	-2.19	118.13	122.85
2	D	4	1GN	O3-C3-C4	2.18	115.50	110.38
3	E	1	1GN	C1-O5-C5	2.09	117.70	113.65
3	F	4	GAL	C1-O5-C5	2.04	114.93	112.19
3	F	1	1GN	O5-C1-C2	2.04	111.89	109.51
2	D	7	6PZ	O10-C10-C11	-2.04	118.43	122.05
2	D	7	6PZ	O10A-C10A-N1	-2.04	118.38	121.98
2	H	4	1GN	O5-C5-C6	2.03	111.61	107.66
2	D	2	1GN	O3-C3-C2	-2.02	106.12	109.90
2	G	7	6PZ	O10-C10-C11	2.00	125.62	122.05

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	7	6PZ	O10A-C10A-N1-C7
2	D	1	GAL	O5-C5-C6-O6
3	F	3	1GN	O5-C5-C6-O6
2	D	8	BGC	O5-C5-C6-O6
3	I	4	GAL	O5-C5-C6-O6
2	G	8	BGC	O5-C5-C6-O6
3	F	3	1GN	C4-C5-C6-O6
3	E	5	BGC	C4-C5-C6-O6
2	D	1	GAL	C4-C5-C6-O6
2	G	8	BGC	C4-C5-C6-O6
2	D	8	BGC	C4-C5-C6-O6
3	E	5	BGC	O5-C5-C6-O6
2	D	5	GAL	O5-C5-C6-O6
2	G	7	6PZ	O10-C10-N5-C5
3	I	4	GAL	C4-C5-C6-O6
2	H	5	GAL	O5-C5-C6-O6
3	E	4	GAL	O5-C5-C6-O6
2	H	8	BGC	O5-C5-C6-O6
3	F	4	GAL	O5-C5-C6-O6

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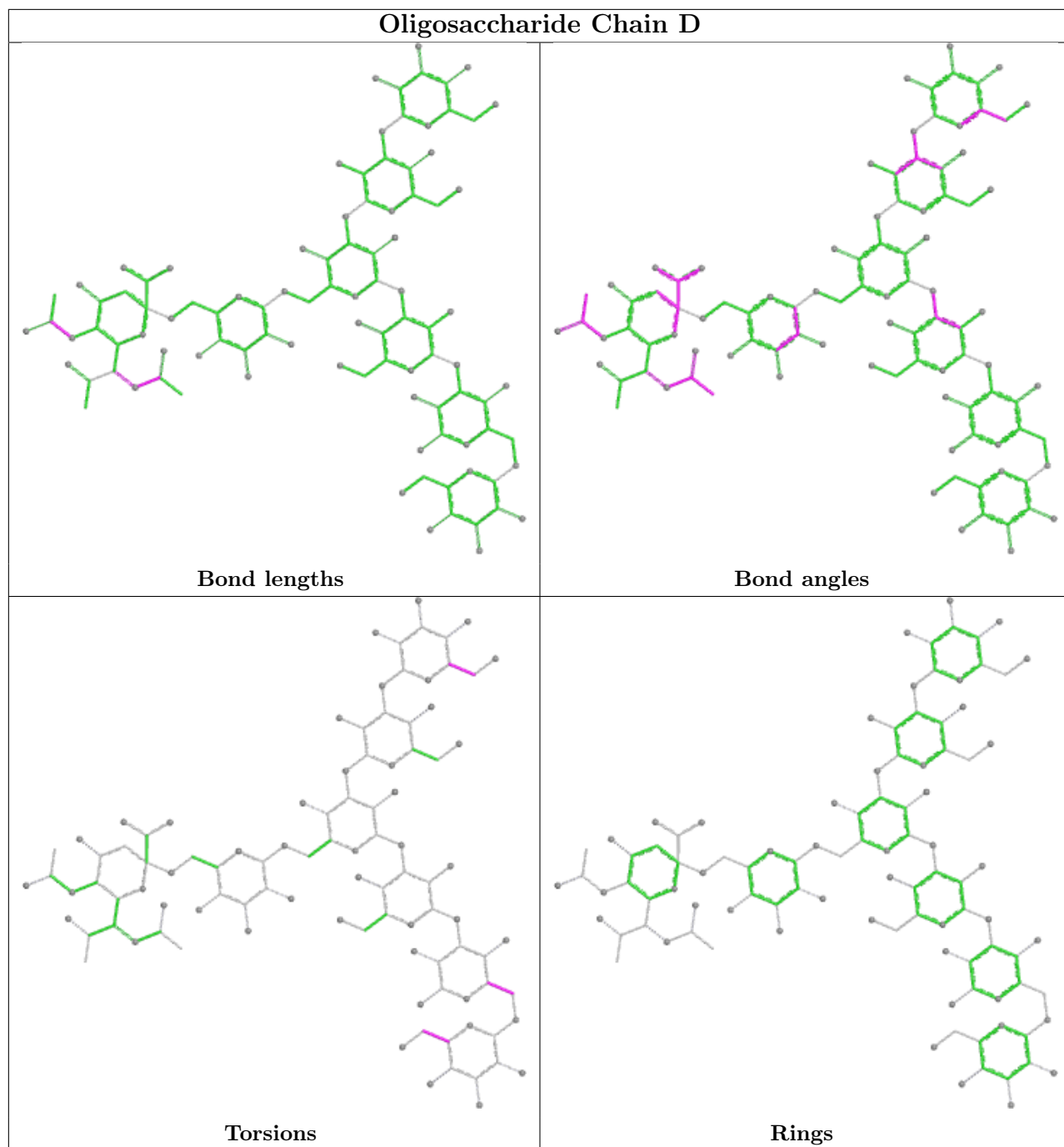
Mol	Chain	Res	Type	Atoms
3	E	2	GAL	O5-C5-C6-O6
3	F	2	GAL	O5-C5-C6-O6
3	I	2	GAL	O5-C5-C6-O6
2	G	5	GAL	O5-C5-C6-O6
2	D	5	GAL	C4-C5-C6-O6
2	H	5	GAL	C4-C5-C6-O6

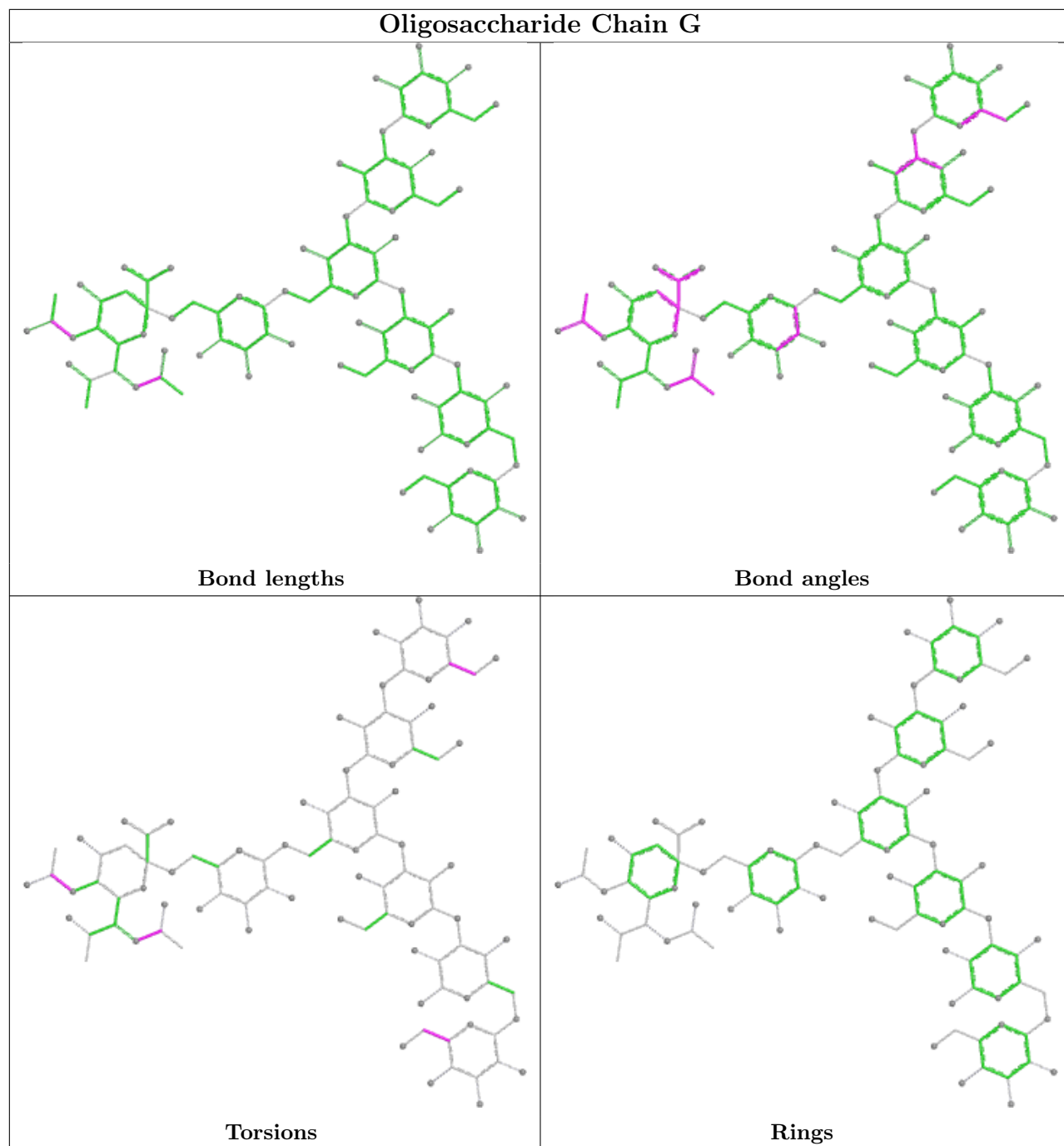
There are no ring outliers.

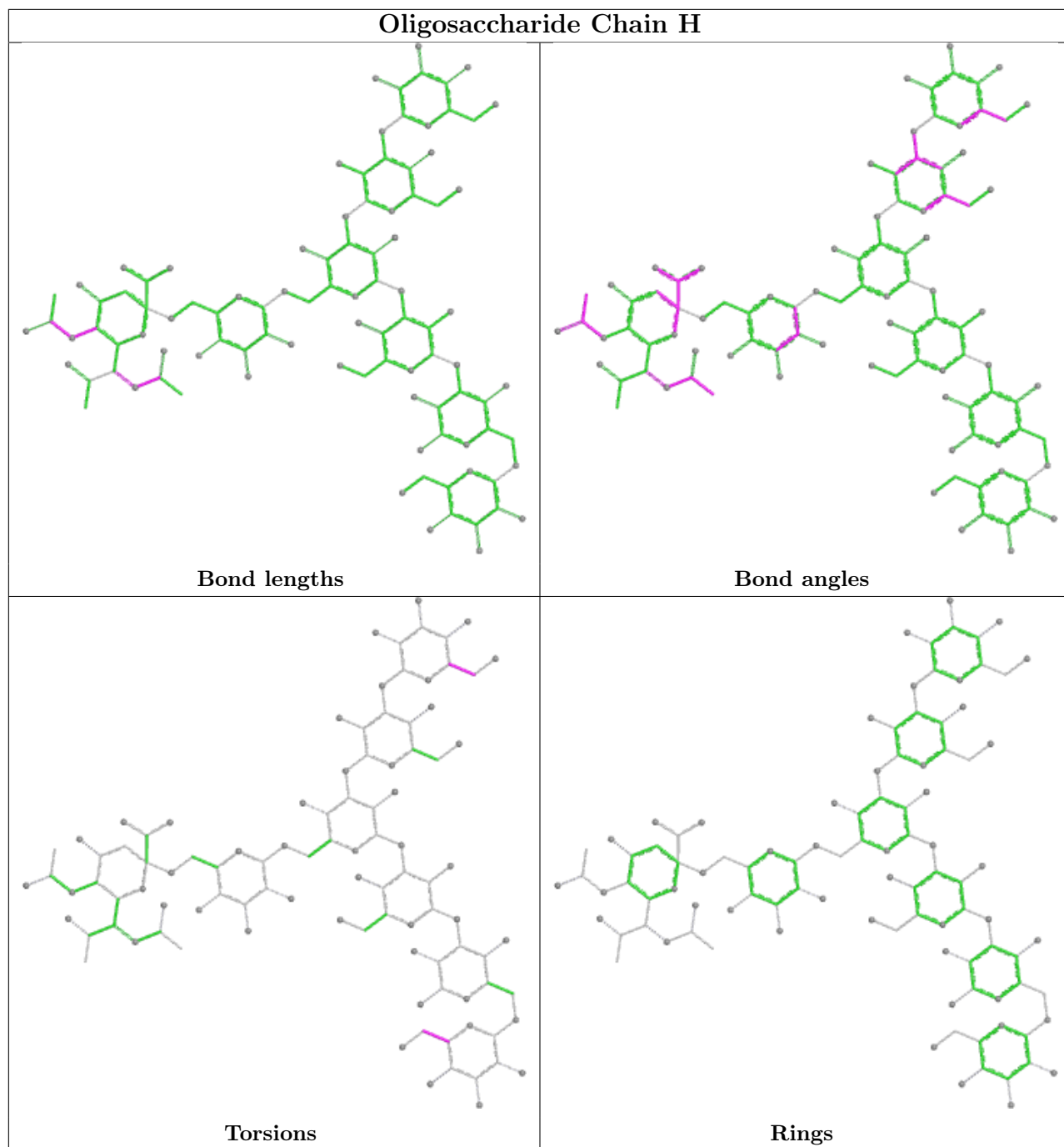
4 monomers are involved in 7 short contacts:

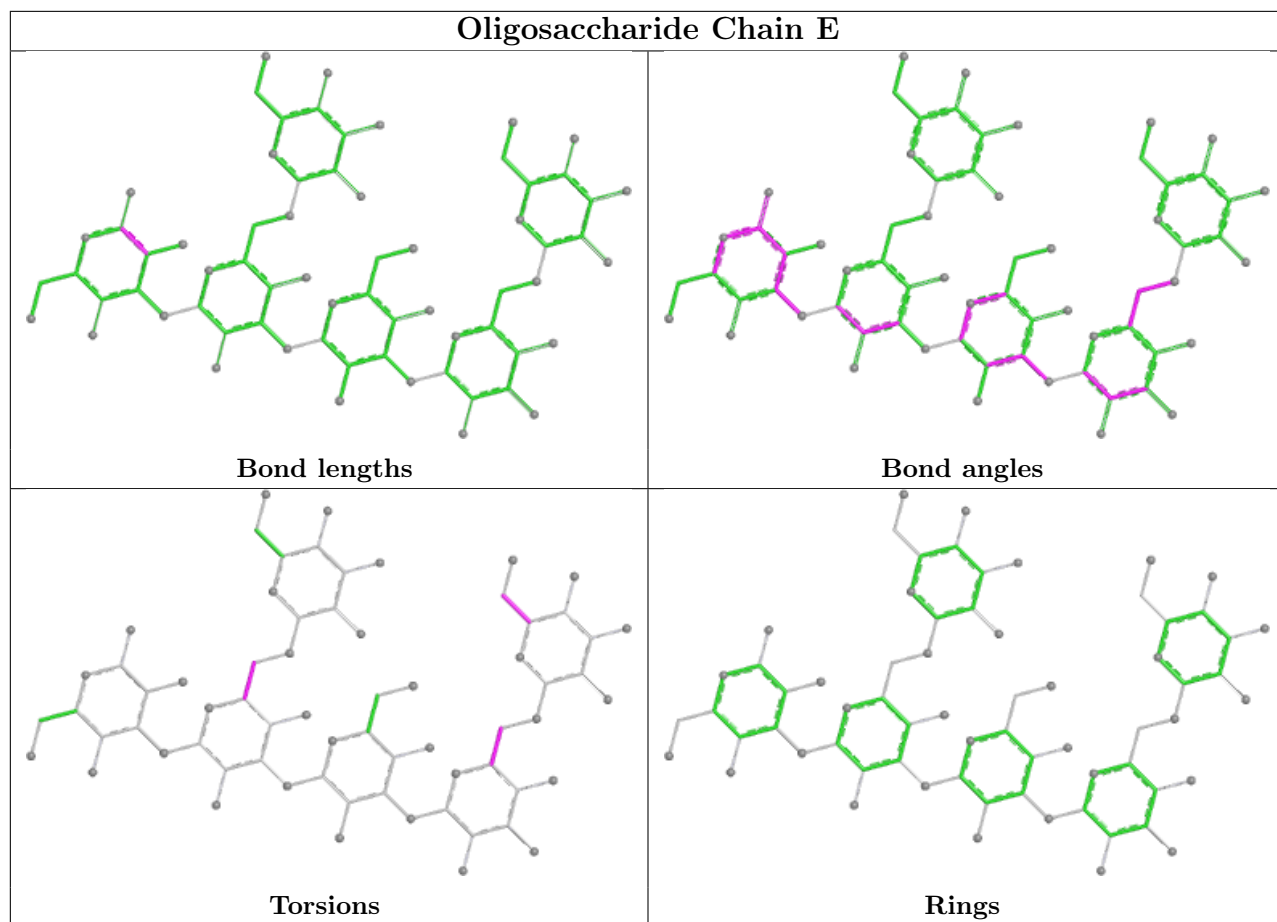
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7	6PZ	4	0
3	I	1	1GN	1	0
3	E	1	1GN	1	0
3	F	1	1GN	1	0

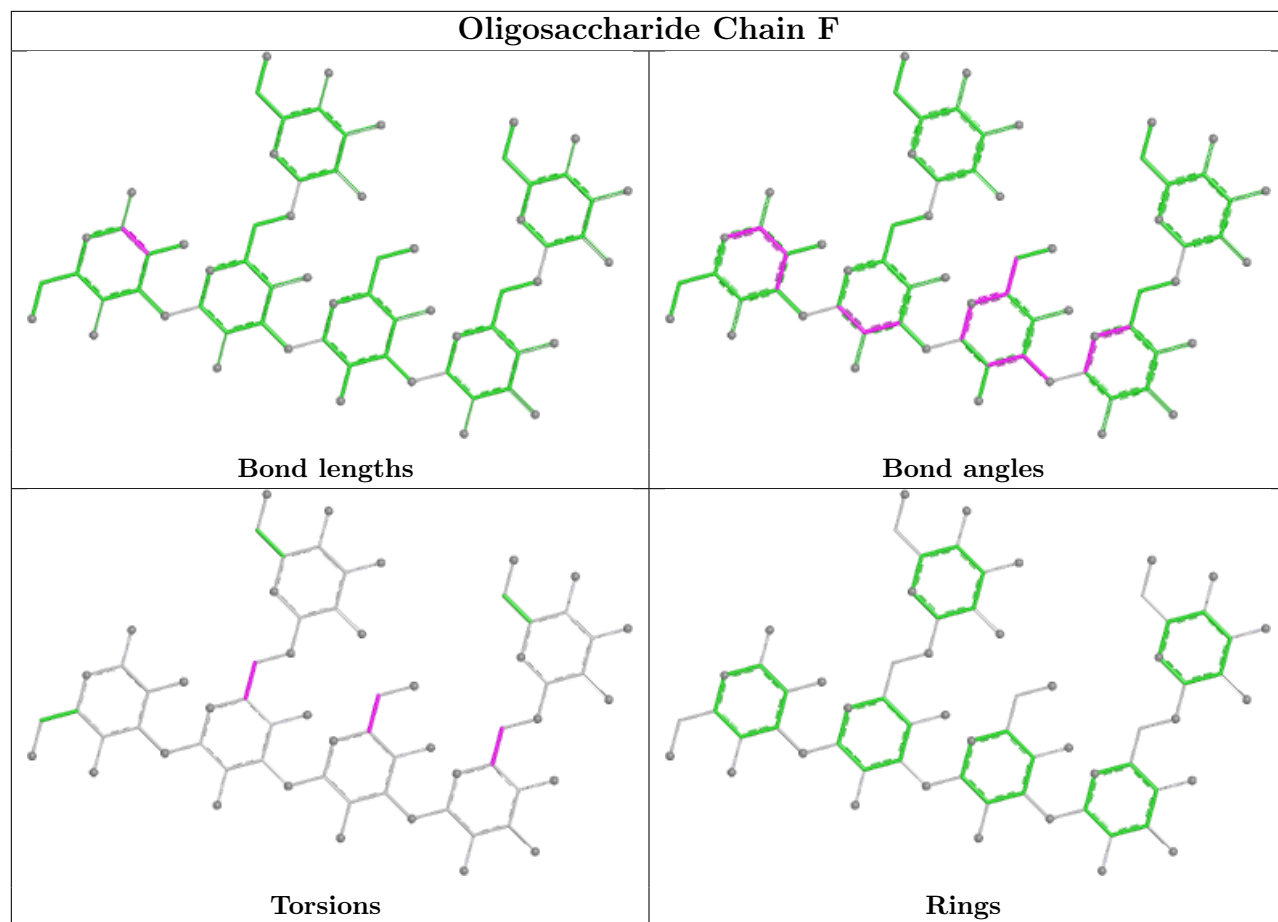
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

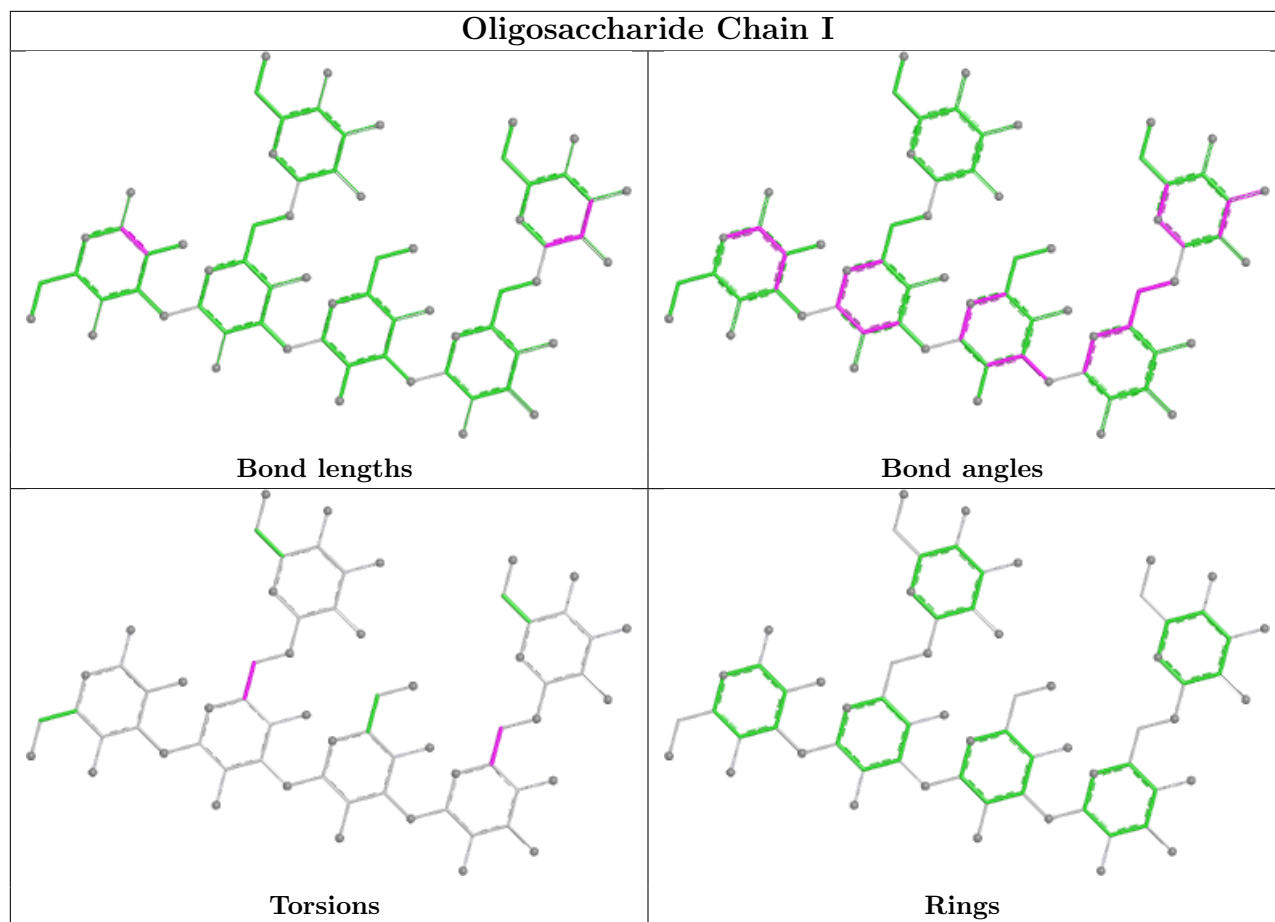












5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
5	ACY	A	619	3	1,2,3	1.48	0	0,1,3	-	-
4	MLA	B	601	-	6,6,6	1.14	0	7,7,7	1.08	0
5	ACY	B	619	2	1,2,3	1.51	0	0,1,3	-	-
5	ACY	B	602	3	1,2,3	1.48	0	0,1,3	-	-
4	MLA	A	601	-	6,6,6	1.10	0	7,7,7	1.13	0
5	ACY	A	618	2	1,2,3	1.47	0	0,1,3	-	-
4	MLA	C	601	-	6,6,6	1.12	0	7,7,7	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACY	C	617	2	1,2,3	1.51	0	0,1,3	-	-
5	ACY	C	619	2	1,2,3	1.49	0	0,1,3	-	-
5	ACY	C	618	3	1,2,3	1.55	0	0,1,3	-	-
5	ACY	A	610	2	1,2,3	1.55	0	0,1,3	-	-
5	ACY	B	609	2	1,2,3	1.45	0	0,1,3	-	-
5	ACY	B	610	3	1,2,3	1.49	0	0,1,3	-	-
5	ACY	C	602	3	1,2,3	1.47	0	0,1,3	-	-
5	ACY	A	611	3	1,2,3	1.45	0	0,1,3	-	-

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	MLA	B	601	-	-	0/4/4/4	-
4	MLA	A	601	-	-	0/4/4/4	-
4	MLA	C	601	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	ACY	1	0
5	C	618	ACY	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	548/719 (76%)	-1.18	0 100 100	9, 14, 22, 45	1 (0%)
1	B	548/719 (76%)	-1.18	0 100 100	9, 14, 22, 44	1 (0%)
1	C	548/719 (76%)	-1.16	0 100 100	9, 14, 23, 48	1 (0%)
All	All	1644/2157 (76%)	-1.18	0 100 100	9, 14, 23, 48	3 (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
2	BGC	D	8	11/12	0.95	0.10	40,50,54,57	0
2	BGC	G	8	11/12	0.95	0.12	44,56,60,64	0
2	BGC	H	8	11/12	0.96	0.09	44,50,53,56	0
3	GAL	E	4	11/12	0.97	0.06	45,50,54,57	0
3	GAL	F	4	11/12	0.97	0.06	46,49,54,58	0
3	BGC	F	5	11/12	0.97	0.07	34,39,42,47	0
3	BGC	I	5	11/12	0.97	0.06	36,40,42,45	0
3	1GN	E	3	11/12	0.98	0.05	25,29,32,38	0
2	GAL	D	5	11/12	0.98	0.06	26,28,33,38	0
3	BGC	E	5	11/12	0.98	0.06	35,37,41,47	0

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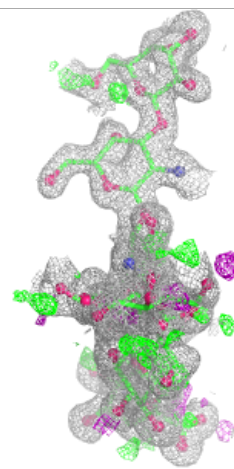
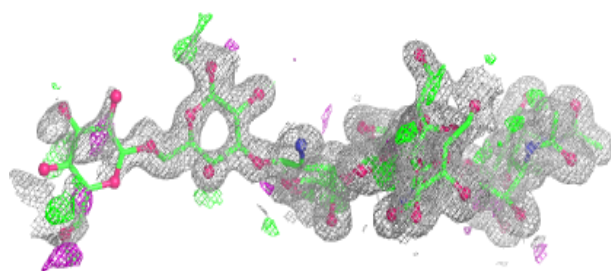
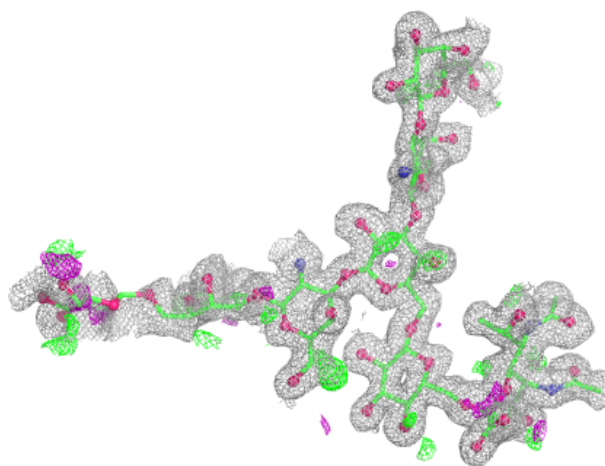
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BGC	E	6	11/12	0.98	0.06	21,27,33,37	0
3	1GN	F	1	12/12	0.98	0.07	27,30,33,39	0
3	1GN	F	3	11/12	0.98	0.05	29,31,39,43	0
2	1GN	G	4	11/12	0.98	0.06	25,26,32,38	0
3	1GN	E	1	12/12	0.98	0.06	26,30,33,38	0
3	BGC	F	6	11/12	0.98	0.06	21,27,34,37	0
3	1GN	I	1	12/12	0.98	0.05	25,30,33,38	0
3	1GN	I	3	11/12	0.98	0.04	23,29,33,39	0
3	GAL	I	4	11/12	0.98	0.06	46,50,54,56	0
3	GAL	E	2	11/12	0.98	0.04	26,26,28,29	0
3	BGC	I	6	11/12	0.98	0.05	20,28,33,37	0
2	6PZ	H	7	22/23	0.99	0.03	16,17,20,21	0
2	GAL	D	1	12/12	0.99	0.04	21,25,33,42	0
2	BGC	D	6	11/12	0.99	0.03	14,16,17,19	0
2	6PZ	D	7	22/23	0.99	0.03	16,17,21,22	0
2	1GN	D	2	11/12	0.99	0.04	16,19,20,23	0
2	GAL	G	1	12/12	0.99	0.04	21,25,30,35	0
2	1GN	G	2	11/12	0.99	0.03	17,19,20,23	0
2	GAL	G	3	11/12	0.99	0.06	26,34,48,50	0
2	GAL	D	3	11/12	0.99	0.06	27,33,48,51	0
3	GAL	F	2	11/12	0.99	0.04	25,27,28,29	0
2	GAL	G	5	11/12	0.99	0.04	27,28,34,40	0
2	6PZ	G	7	22/23	0.99	0.04	15,17,23,23	0
2	1GN	D	4	11/12	0.99	0.04	26,27,30,32	0
2	GAL	H	1	12/12	0.99	0.03	21,26,30,35	0
2	1GN	H	2	11/12	0.99	0.03	17,19,20,23	0
3	GAL	I	2	11/12	0.99	0.05	26,27,28,28	0
2	GAL	H	3	11/12	0.99	0.06	27,36,50,54	0
2	1GN	H	4	11/12	0.99	0.04	23,26,31,34	0
2	GAL	H	5	11/12	0.99	0.04	26,27,34,40	0
2	BGC	H	6	11/12	0.99	0.03	15,16,18,18	0
2	BGC	G	6	11/12	1.00	0.02	15,15,18,19	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.

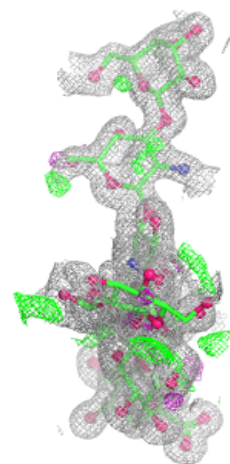
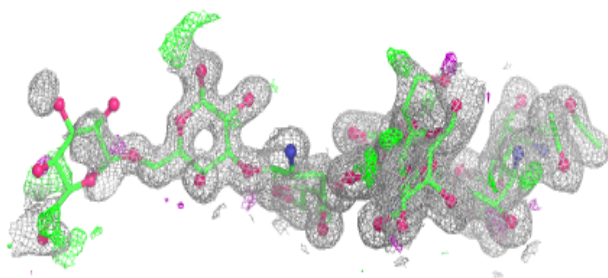
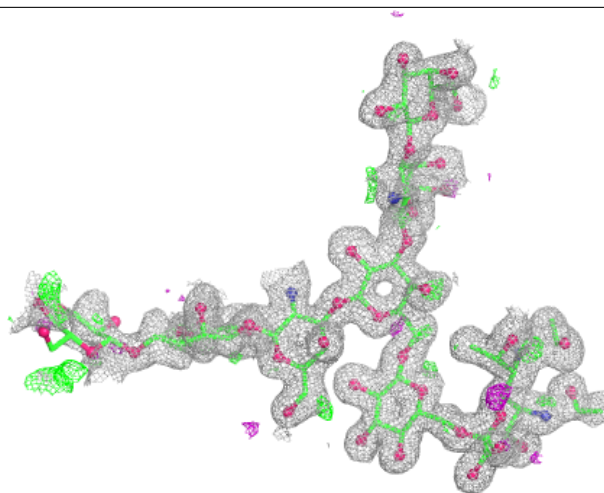
Electron density around Chain D:

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



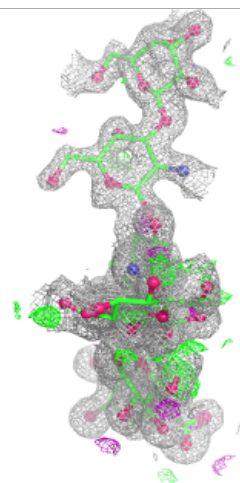
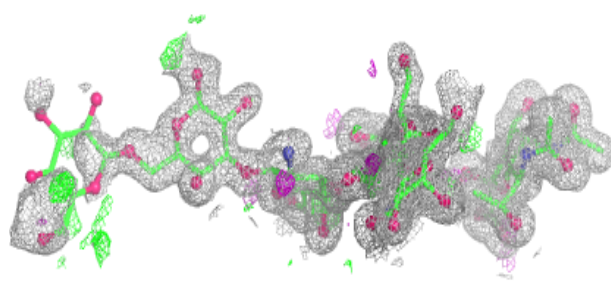
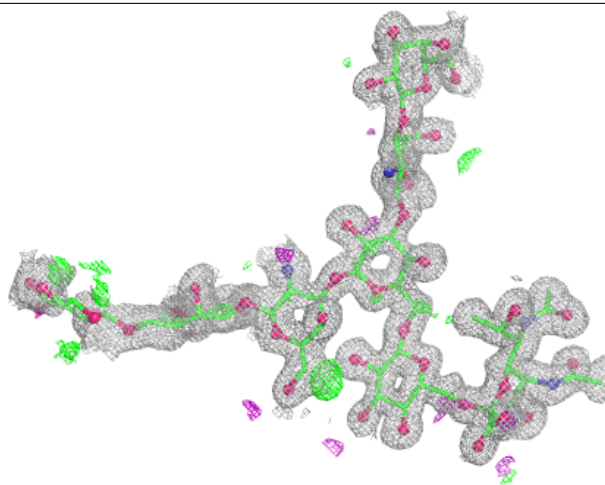
Electron density around Chain G:

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



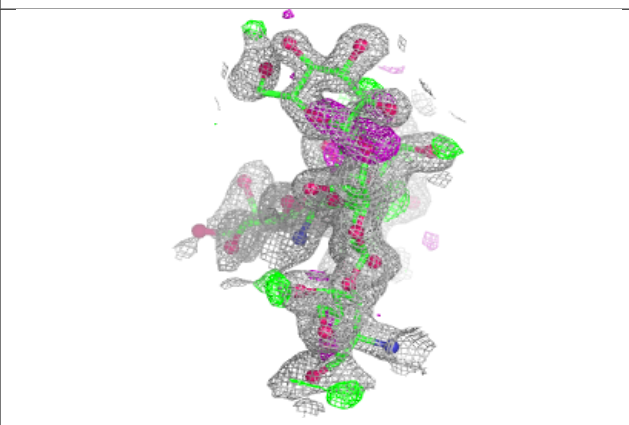
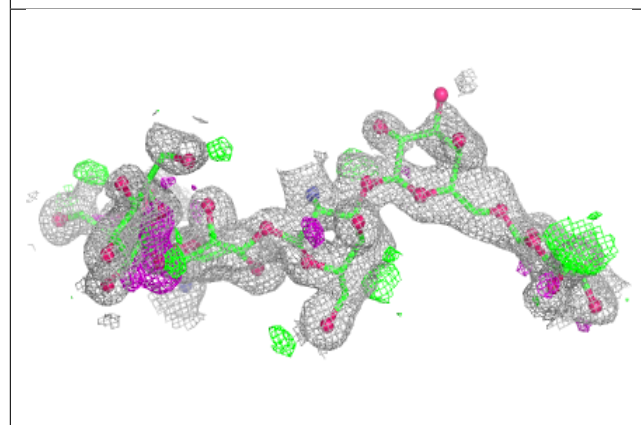
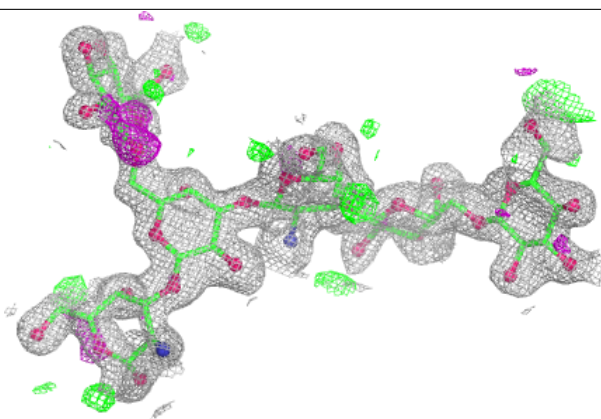
Electron density around Chain H:

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

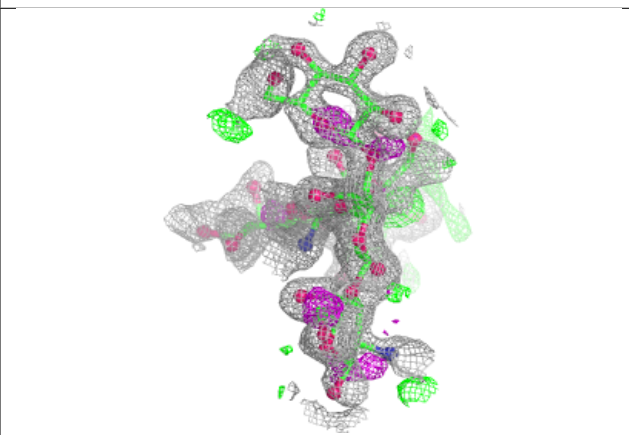
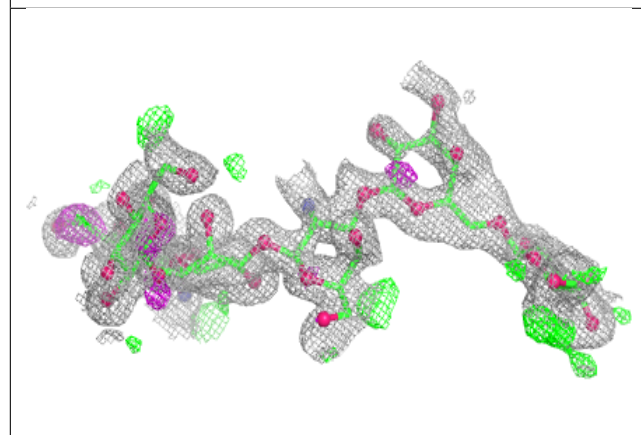
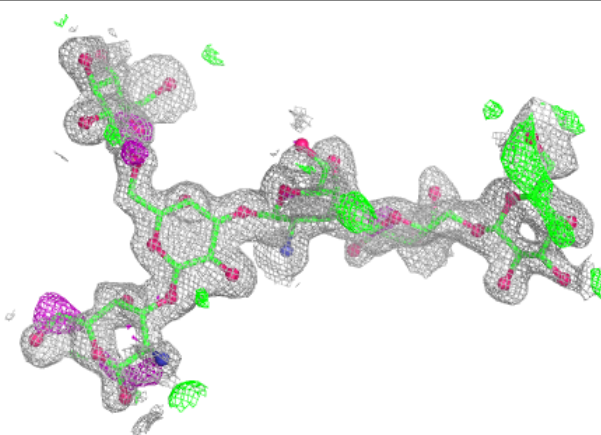


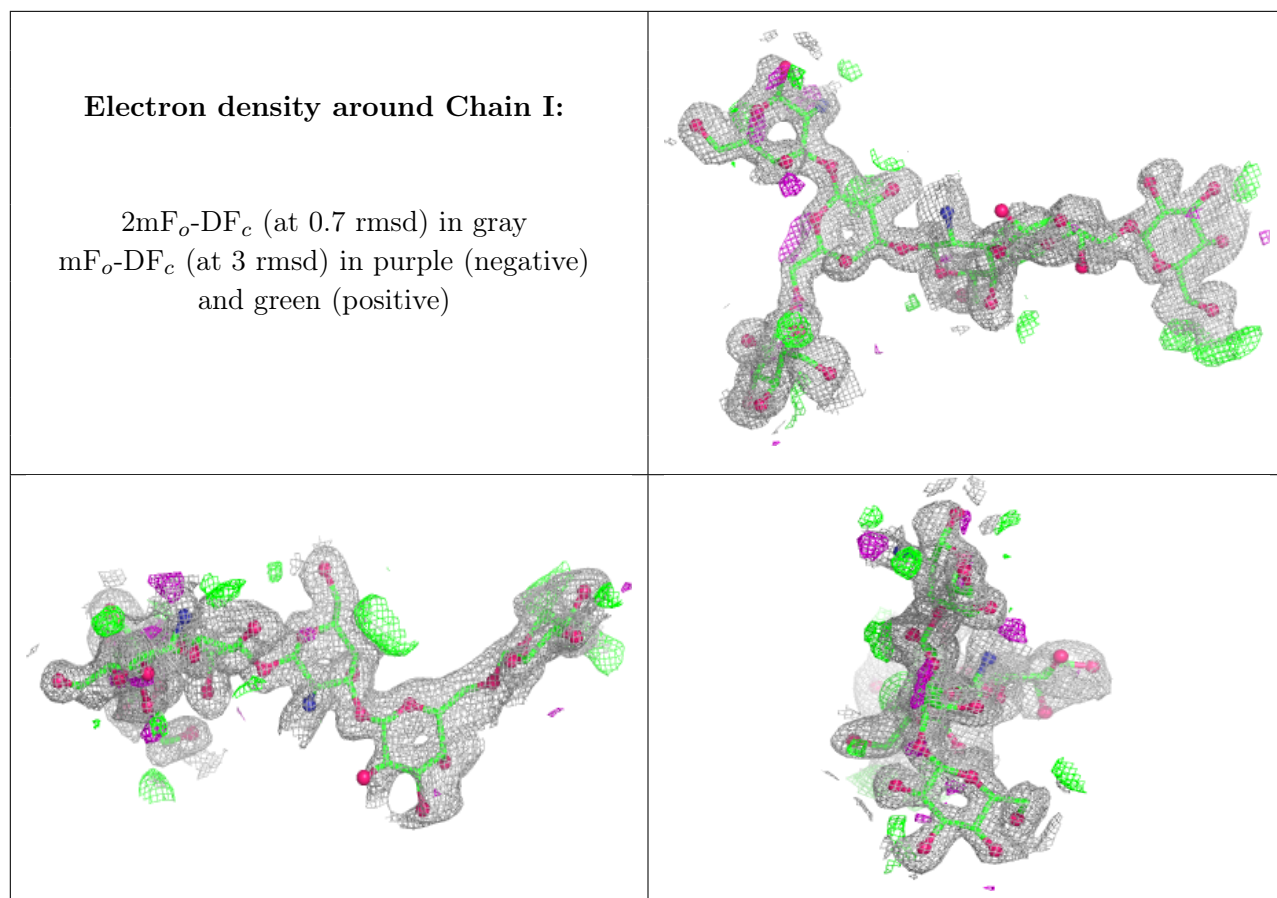
Electron density around Chain E:

$2mF_o-DF_c$ (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)





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
5	ACY	A	619	3/4	0.95	0.08	32,32,35,44	0
5	ACY	C	602	3/4	0.97	0.06	35,35,35,40	0
5	ACY	B	602	3/4	0.98	0.07	27,27,29,29	0
5	ACY	B	610	3/4	0.98	0.04	34,34,35,38	0
4	MLA	A	601	7/7	0.98	0.05	22,27,33,37	0
5	ACY	C	618	3/4	0.98	0.09	27,27,28,29	0
5	ACY	C	619	3/4	0.98	0.06	25,25,25,26	0
4	MLA	C	601	7/7	0.99	0.04	22,28,34,41	0
5	ACY	B	609	3/4	0.99	0.03	25,25,25,26	0
5	ACY	A	610	3/4	0.99	0.05	21,21,21,22	0
5	ACY	A	611	3/4	0.99	0.08	27,27,27,29	0
5	ACY	C	617	3/4	0.99	0.05	21,21,22,23	0
5	ACY	A	618	3/4	0.99	0.03	24,24,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MLA	B	601	7/7	0.99	0.05	20,27,33,38	0
5	ACY	B	619	3/4	1.00	0.03	21,21,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.