



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 11:49 AM BST

PDB ID : 5JSD
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 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

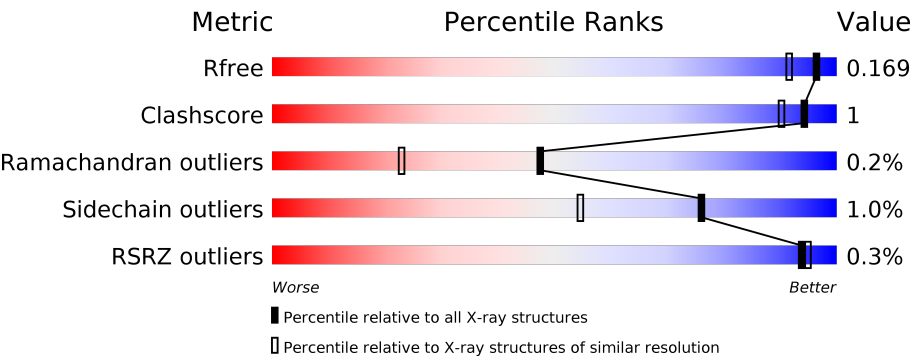
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%•24%</div></div>
1	B	719	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%•24%</div></div>
1	C	719	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%•24%</div></div>
2	D	8	<div><div></div><div><div></div><div></div></div><div>25%75%</div></div>
2	G	8	<div><div></div><div><div></div><div></div><div></div></div><div>38%50%13%</div></div>
2	H	8	<div><div></div><div><div></div><div></div></div><div>50%50%</div></div>

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Mol	Chain	Length	Quality of chain
3	E	6	
3	F	6	
3	I	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

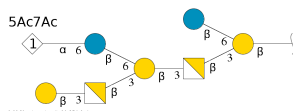
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	D	8	-	-	-	X
2	BGC	G	8	-	-	-	X
2	BGC	H	8	-	-	-	X

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.

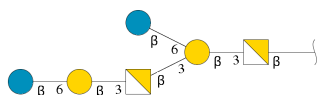
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0
1	B	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0
1	C	548	Total 4193	C 2640	N 713	O 820	S 20	0	1	0

- 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-tetradeoxy-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.



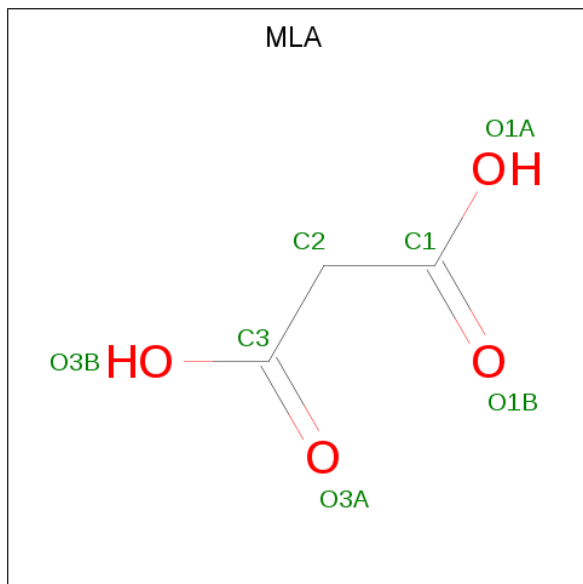
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	8	Total 100	C 55	N 4	O 41	0	0	0
2	G	8	Total 100	C 55	N 4	O 41	0	0	0
2	H	8	Total 100	C 55	N 4	O 41	0	0	0

- 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.



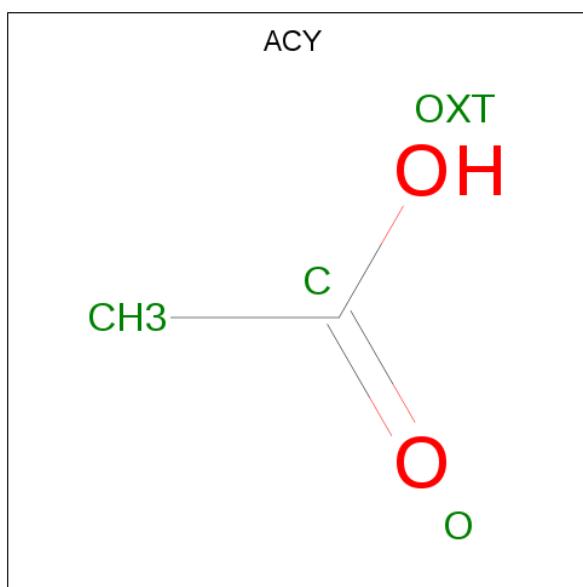
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			67	36	2	29			
3	F	6	Total	C	N	O	0	0	0
			67	36	2	29			
3	I	6	Total	C	N	O	0	0	0
			67	36	2	29			

- Molecule 4 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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 (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- 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

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.

- [illegible]

- [illegible]

- [illegible]

VAL GLU ASP LEU GLY TYR THR VAL SER GLN VAL ASN ALA VAL THR LEU LYS TLE GLU PRO ALA TLE PRO ASP GLY THR VAL ARG ARG GLU ARG GLU THR ASP TLE ASP LYS MET LYS TYR TLE PHE ASP ALA GLY ALA LEU PHE TLE ASP GLN ASN VAL ASP ALA ASP PHE ARG TLE

VAL HIS GLN GLN VAL ARG ASP GLY PHE TLE LYS LEU ARG GLY VAL LEU PRO ALA VAL HIS GLY LEU GLN VAL ALA TLE GLN ARG GLN ALA SER ASP GLU ALA ALA GLN GLU TLE ASP SER GLU MET ALA ALA GLN GLU TLE PHE ASP ASN ALA ALA ALA LEU PHE VAL ALA ALA SER Q18 T19 V70 D75 Y112

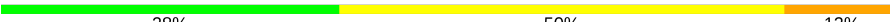
L122 T174 E202 D211 V229 T234 V255 S256 T257 Y265 H281 N314 G345 K392 V412 Y432 S504 M523 W531 S565

- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-b isacetamido-3,5,7,9-tetradeoxy-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:  25% 75%

GML1
IGN2
GML3
IGN4
GAL5
BGC6
6PZ7
BGC8

- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-b isacetamido-3,5,7,9-tetradeoxy-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:  38% 50% 13%

GML1
IGN2
GML3
IGN4
GAL5
BGC6
6PZ7
BGC8

- Molecule 2: beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[5,7-b isacetamido-3,5,7,9-tetradeoxy-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%

GML1
IGN2
GML3
IGN4
GAL5
BGC6
6PZ7
BGC8

- 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%

IGN1
GAL2
IGN3
GAL4
BGC5
BGC6

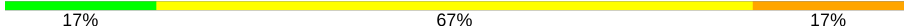
- Molecule 3: beta-D-glucopyranose-(1-6)-beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose-(1-3)-[beta-D-glucopyranose-(1-6)]beta-D-galactopyranose-(1-3)-2-amino-2-deoxy-beta-D-galactopyranose

-beta-D-galactopyranose

Chain F:  17% 67% 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

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) 87.8 (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)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.142 , 0.169 0.142 , 0.169	Depositor DCC
R_{free} test set	18826 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.469 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.470 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16020	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, 6PZ, 1GN, GAL, ACY, MLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/4289	0.63	0/5825
1	B	0.35	0/4289	0.63	0/5825
1	C	0.35	0/4289	0.63	0/5825
All	All	0.35	0/12867	0.63	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

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	11	0
1	B	4193	0	4040	11	0
1	C	4193	0	4040	10	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	33	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.

The worst 5 of 33 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:N5	2:G:7:6PZ:C10	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

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%)	47	23
1	B	547/719 (76%)	528 (96%)	18 (3%)	1 (0%)	47	23
1	C	547/719 (76%)	528 (96%)	18 (3%)	1 (0%)	47	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1641/2157 (76%)	1584 (96%)	54 (3%)	3 (0%)	47 23

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 ⓘ

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%)	448 (99%)	6 (1%)	69 42
1	B	454/597 (76%)	450 (99%)	4 (1%)	78 59
1	C	454/597 (76%)	450 (99%)	4 (1%)	78 59
All	All	1362/1791 (76%)	1348 (99%)	14 (1%)	76 54

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	229	VAL
1	B	265	TYR
1	C	265	TYR
1	A	504	SER
1	C	229	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	ASN
1	B	314	ASN
1	C	267	GLN

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Mol	Chain	Res	Type
1	B	184	GLN
1	C	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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
2	1GN	D	2	2,5	11,11,12	0.43	0	12,15,17	0.87	1 (8%)
2	GAL	D	3	2	11,11,12	0.27	0	15,15,17	0.56	0
2	1GN	D	4	2,5	11,11,12	0.48	0	12,15,17	1.12	2 (16%)
2	GAL	D	5	2	11,11,12	0.38	0	15,15,17	1.08	1 (6%)
2	BGC	D	6	2	11,11,12	0.40	0	15,15,17	1.05	1 (6%)
2	6PZ	D	7	2	18,22,23	1.07	3 (16%)	22,31,34	1.52	4 (18%)
2	BGC	D	8	2	11,11,12	0.36	0	15,15,17	1.09	2 (13%)
3	1GN	E	1	3,5	12,12,12	0.95	1 (8%)	16,17,17	2.38	5 (31%)
3	GAL	E	2	3	11,11,12	0.42	0	15,15,17	1.40	1 (6%)
3	1GN	E	3	3,5	11,11,12	0.38	0	12,15,17	1.52	2 (16%)
3	GAL	E	4	3	11,11,12	0.45	0	15,15,17	1.12	2 (13%)
3	BGC	E	5	3	11,11,12	0.39	0	15,15,17	0.83	0
3	BGC	E	6	3	11,11,12	0.23	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1GN	F	1	3,5	12,12,12	0.93	1 (8%)	16,17,17	1.54	2 (12%)
3	GAL	F	2	3	11,11,12	0.42	0	15,15,17	1.48	1 (6%)
3	1GN	F	3	3,5	11,11,12	0.38	0	12,15,17	1.51	3 (25%)
3	GAL	F	4	3	11,11,12	0.27	0	15,15,17	0.94	2 (13%)
3	BGC	F	5	3	11,11,12	0.27	0	15,15,17	1.01	0
3	BGC	F	6	3	11,11,12	0.26	0	15,15,17	0.96	1 (6%)
2	GAL	G	1	2	12,12,12	0.48	0	17,17,17	0.74	0
2	1GN	G	2	2,5	11,11,12	0.41	0	12,15,17	0.81	0
2	GAL	G	3	2	11,11,12	0.24	0	15,15,17	0.50	0
2	1GN	G	4	2,5	11,11,12	0.46	0	12,15,17	1.14	2 (16%)
2	GAL	G	5	2	11,11,12	0.36	0	15,15,17	1.19	1 (6%)
2	BGC	G	6	2	11,11,12	0.40	0	15,15,17	1.13	1 (6%)
2	6PZ	G	7	2	18,22,23	7.40	2 (11%)	22,31,34	5.30	5 (22%)
2	BGC	G	8	2	11,11,12	0.39	0	15,15,17	0.97	1 (6%)
2	GAL	H	1	2	12,12,12	0.48	0	17,17,17	0.70	0
2	1GN	H	2	2,5	11,11,12	0.45	0	12,15,17	0.69	0
2	GAL	H	3	2	11,11,12	0.24	0	15,15,17	0.57	0
2	1GN	H	4	2,5	11,11,12	0.44	0	12,15,17	1.39	3 (25%)
2	GAL	H	5	2	11,11,12	0.35	0	15,15,17	1.04	1 (6%)
2	BGC	H	6	2	11,11,12	0.45	0	15,15,17	1.20	1 (6%)
2	6PZ	H	7	2	18,22,23	1.06	1 (5%)	22,31,34	1.56	6 (27%)
2	BGC	H	8	2	11,11,12	0.37	0	15,15,17	0.63	0
3	1GN	I	1	3,5	12,12,12	0.91	1 (8%)	16,17,17	1.60	2 (12%)
3	GAL	I	2	3	11,11,12	0.41	0	15,15,17	1.57	2 (13%)
3	1GN	I	3	3,5	11,11,12	0.40	0	12,15,17	1.70	2 (16%)
3	GAL	I	4	3	11,11,12	0.65	0	15,15,17	1.41	4 (26%)
3	BGC	I	5	3	11,11,12	1.71	2 (18%)	15,15,17	1.40	2 (13%)
3	BGC	I	6	3	11,11,12	0.25	0	15,15,17	0.84	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	2,5	-	0/2/19/22	0/1/1/1
2	GAL	D	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1GN	D	4	2,5	-	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	-	0/16/36/40	0/1/1/1
2	BGC	D	8	2	-	2/2/19/22	0/1/1/1
3	1GN	E	1	3,5	-	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	3,5	-	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	3,5	-	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	3,5	-	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	2,5	-	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	2,5	-	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	-	2/16/36/40	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
2	1GN	H	2	2,5	-	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	2,5	-	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	-	0/16/36/40	0/1/1/1
2	BGC	H	8	2	-	1/2/19/22	0/1/1/1
3	1GN	I	1	3,5	-	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	3,5	-	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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	6PZ	C10A-N1	22.86	2.12	1.34
2	G	7	6PZ	C10-N5	21.35	2.07	1.34
3	I	5	BGC	C1-C2	-4.56	1.41	1.52
3	I	5	BGC	C2-C3	3.08	1.57	1.52
3	E	1	1GN	C1-C2	2.57	1.55	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7	6PZ	O10A-C10A-N1	-17.80	89.23	121.95
2	G	7	6PZ	O10-C10-N5	-11.43	100.94	121.95
2	G	7	6PZ	C11A-C10A-N1	-9.48	100.05	116.10
2	G	7	6PZ	C11-C10-N5	-7.43	103.52	116.10
3	E	1	1GN	O5-C1-C2	6.13	116.67	109.51

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

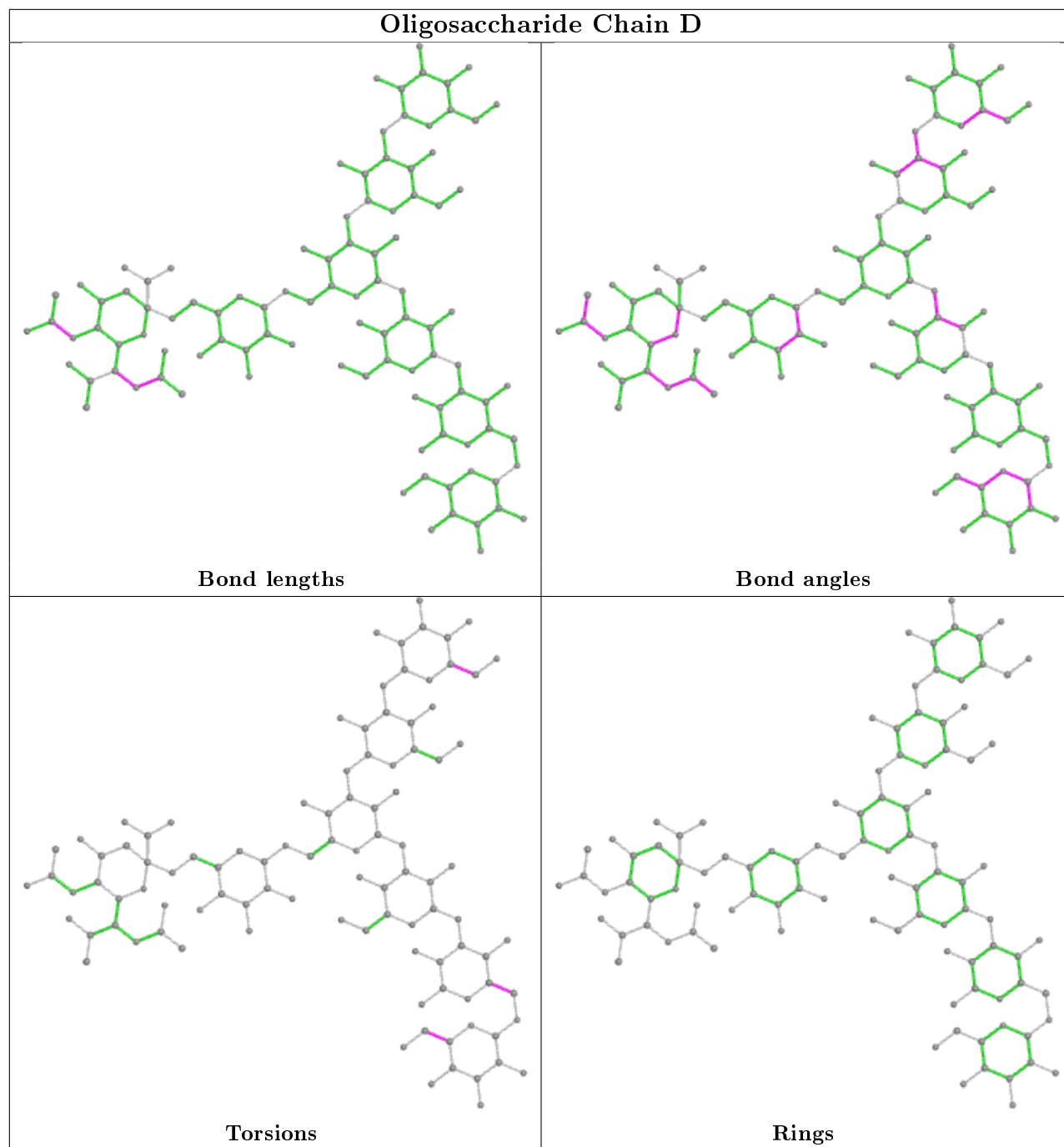
Mol	Chain	Res	Type	Atoms
2	G	7	6PZ	O10A-C10A-N1-C7
2	D	1	GAL	O5-C5-C6-O6
3	F	3	1GN	O5-C5-C6-O6
3	I	4	GAL	O5-C5-C6-O6
2	D	8	BGC	O5-C5-C6-O6

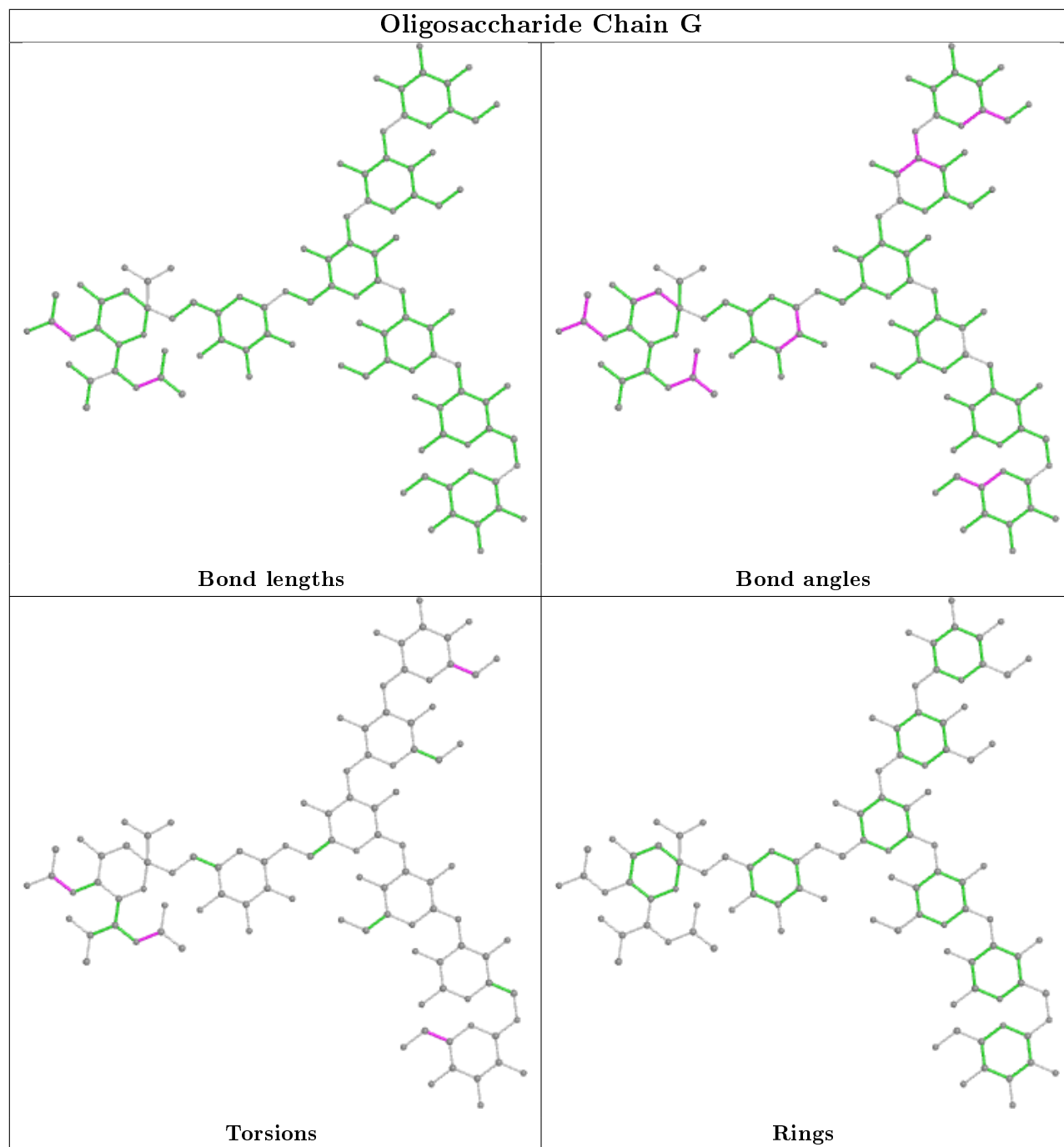
There are no ring outliers.

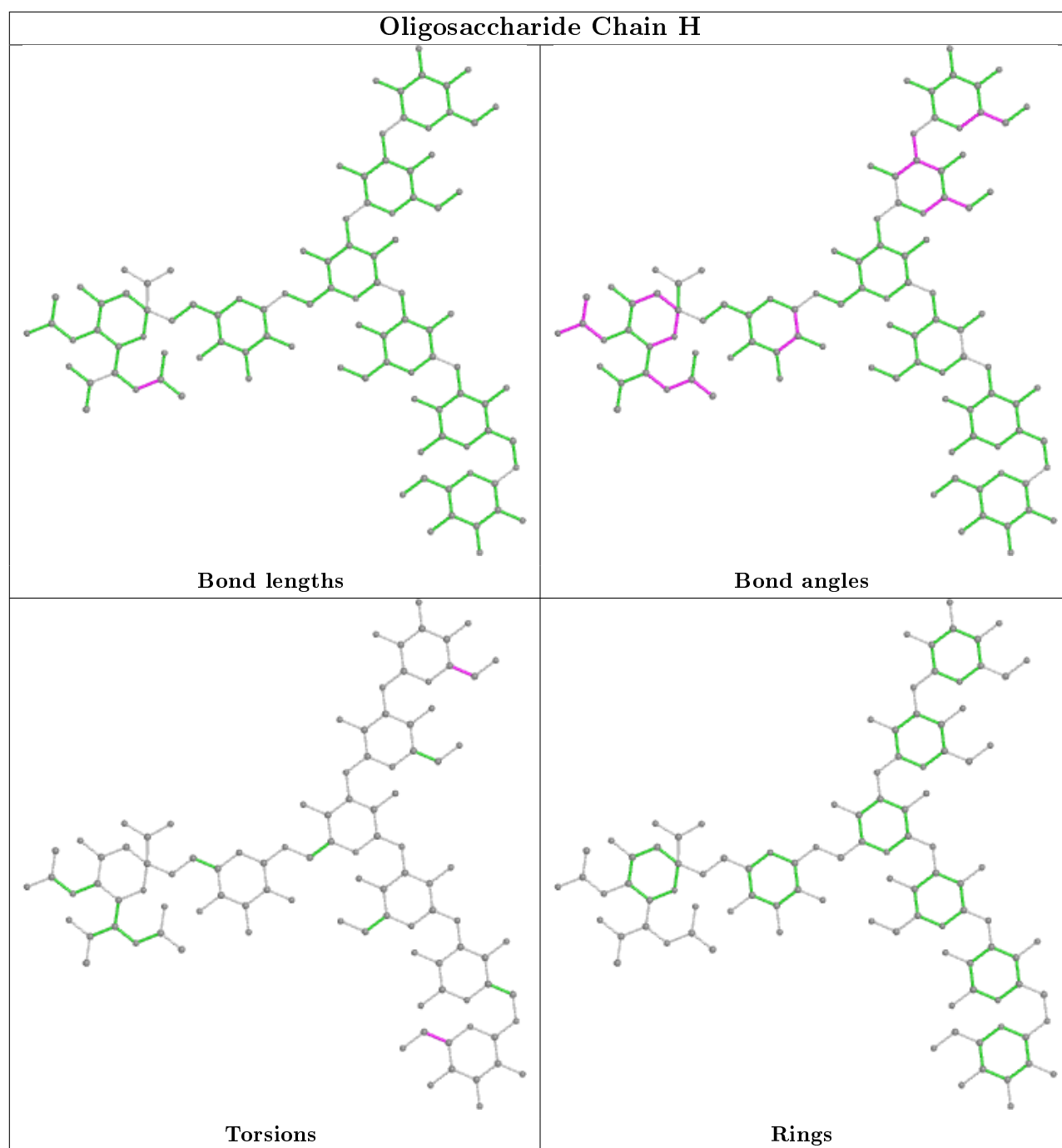
4 monomers are involved in 7 short contacts:

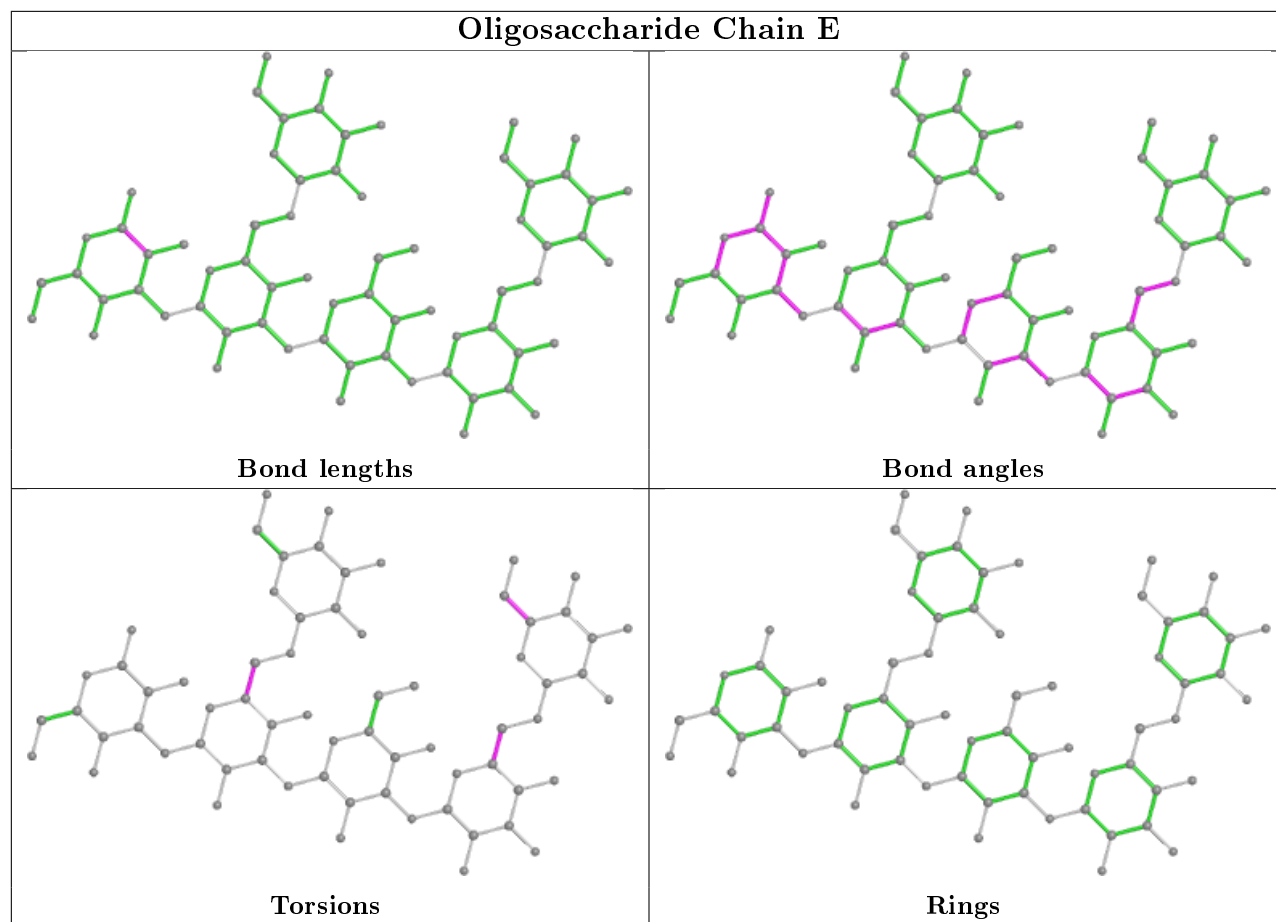
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	1GN	1	0
2	G	7	6PZ	4	0
3	I	1	1GN	1	0
3	F	1	1GN	1	0

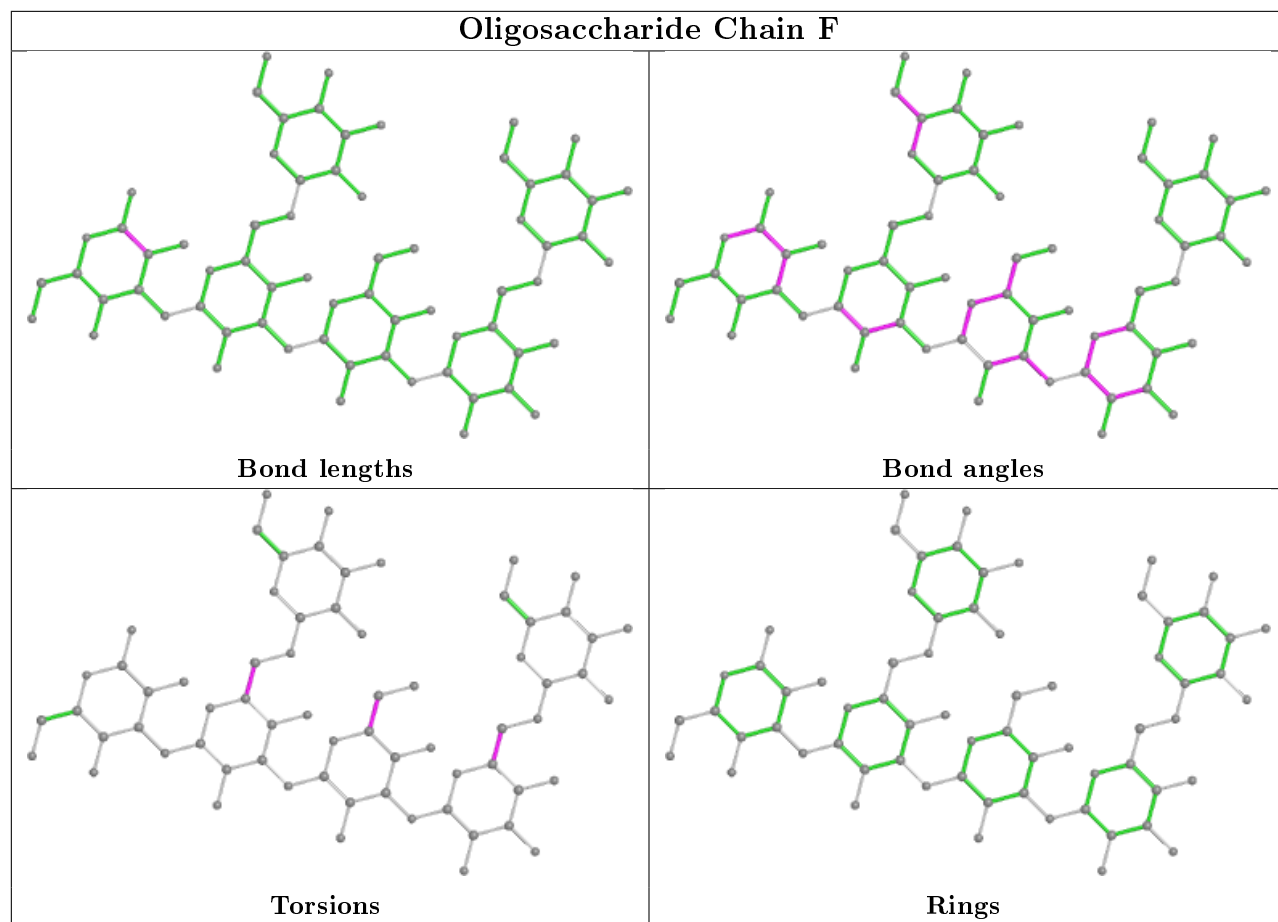
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

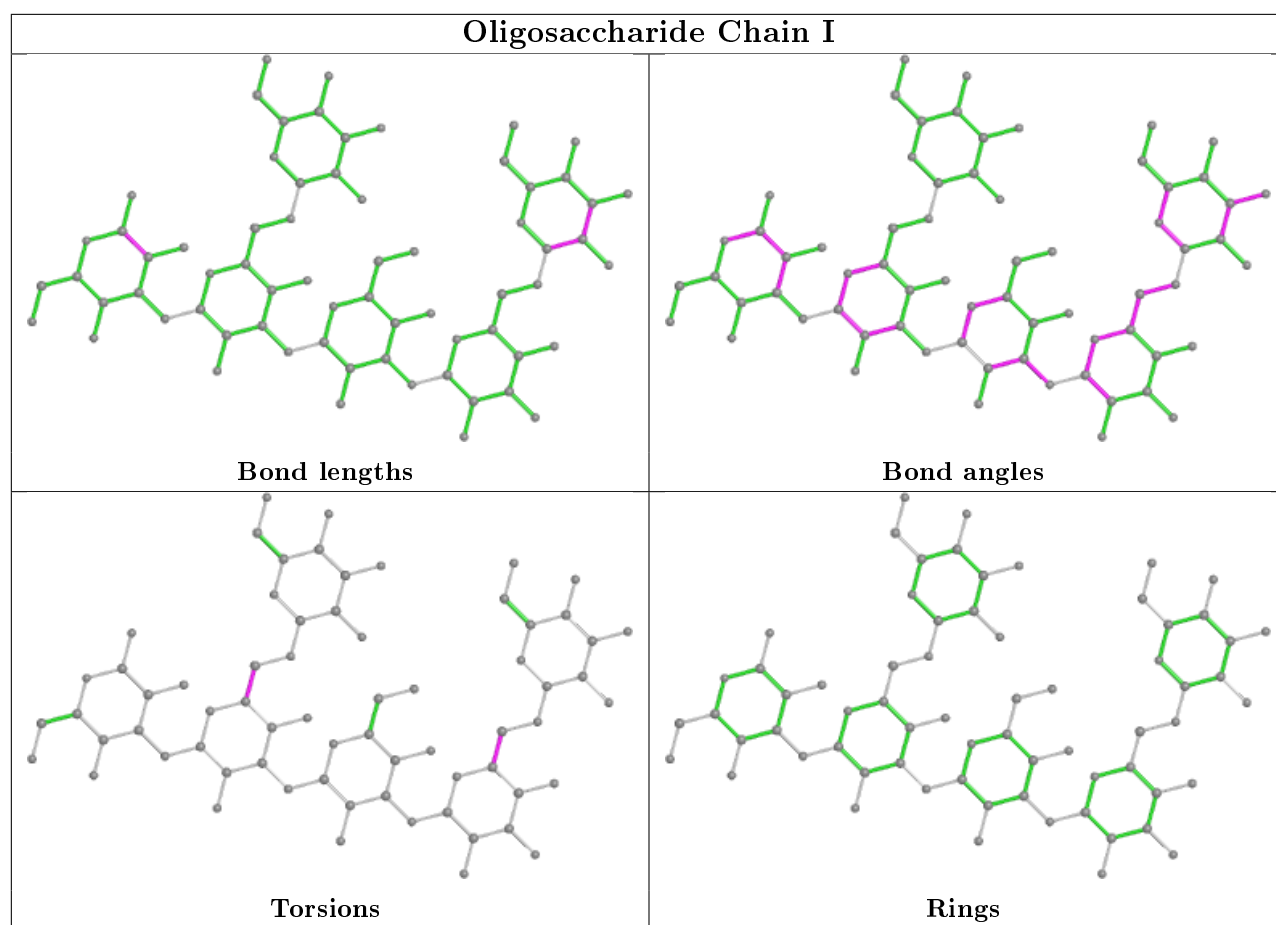












5.6 Ligand geometry [i](#)

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	611	3	1,2,3	1.38	0	1,1,3	1.02	0
4	MLA	C	601	-	0,6,6	0.00	-	0,7,7	0.00	-
5	ACY	B	602	3	1,2,3	1.42	0	1,1,3	1.15	0
5	ACY	A	618	2	1,2,3	1.40	0	1,1,3	0.99	0
5	ACY	B	619	2	1,2,3	1.45	0	1,1,3	1.23	0
5	ACY	B	610	3	1,2,3	1.42	0	1,1,3	1.16	0
5	ACY	C	617	2	1,2,3	1.45	0	1,1,3	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACY	A	610	2	1,2,3	1.48	0	1,1,3	1.06	0
5	ACY	C	618	3	1,2,3	1.48	0	1,1,3	1.20	0
5	ACY	B	609	2	1,2,3	1.39	0	1,1,3	0.99	0
5	ACY	C	602	3	1,2,3	1.41	0	1,1,3	1.19	0
5	ACY	A	619	3	1,2,3	1.41	0	1,1,3	1.24	0
5	ACY	C	619	2	1,2,3	1.42	0	1,1,3	1.10	0
4	MLA	B	601	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLA	A	601	-	0,6,6	0.00	-	0,7,7	0.00	-

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

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%)	-0.40	1 (0%) 95 95	9, 14, 22, 45	0
1	B	548/719 (76%)	-0.40	2 (0%) 92 94	9, 14, 22, 44	0
1	C	548/719 (76%)	-0.37	2 (0%) 92 94	9, 14, 23, 48	0
All	All	1644/2157 (76%)	-0.39	5 (0%) 94 95	9, 14, 23, 48	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	GLN	6.4
1	C	18	GLN	5.5
1	A	18	GLN	4.0
1	B	19	THR	3.8
1	C	19	THR	2.3

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	H	8	11/12	0.32	0.46	44,50,53,56	0
2	BGC	G	8	11/12	0.38	0.69	44,56,60,64	0
2	BGC	D	8	11/12	0.44	0.45	40,50,54,57	0

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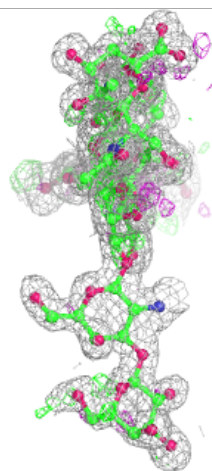
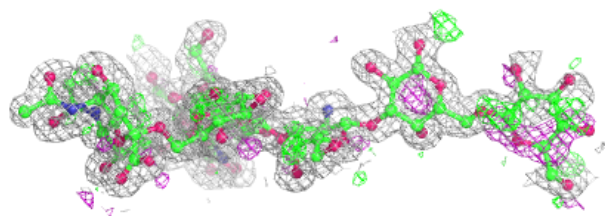
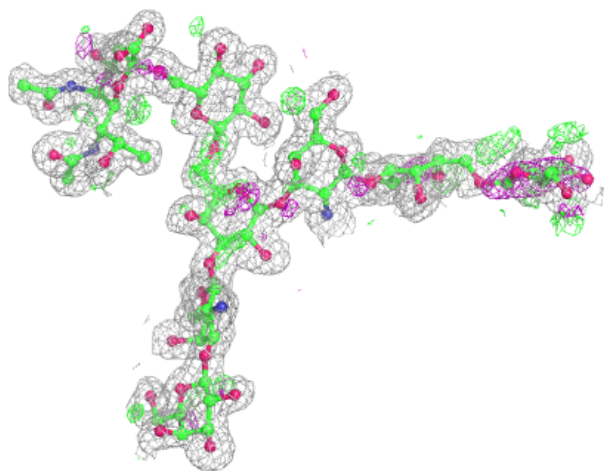
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAL	E	4	11/12	0.72	0.16	45,50,54,57	0
3	GAL	I	4	11/12	0.73	0.16	46,50,54,56	0
3	GAL	F	4	11/12	0.73	0.15	46,49,54,58	0
3	BGC	F	5	11/12	0.78	0.15	34,39,42,47	0
3	BGC	I	5	11/12	0.79	0.16	36,40,42,45	0
3	1GN	E	1	12/12	0.80	0.21	26,30,33,38	0
3	1GN	F	3	11/12	0.80	0.19	29,31,39,43	0
3	1GN	F	1	12/12	0.81	0.24	27,30,33,39	0
3	1GN	I	3	11/12	0.83	0.14	23,29,33,39	0
2	GAL	H	3	11/12	0.85	0.14	27,36,50,54	0
3	GAL	E	2	11/12	0.86	0.12	26,26,28,29	0
3	BGC	E	5	11/12	0.86	0.15	35,37,41,47	0
3	1GN	I	1	12/12	0.86	0.21	25,30,33,38	0
2	1GN	G	4	11/12	0.86	0.15	25,26,32,38	0
3	BGC	F	6	11/12	0.87	0.22	21,27,34,37	0
3	BGC	E	6	11/12	0.88	0.24	21,27,33,37	0
2	GAL	D	5	11/12	0.88	0.17	26,28,33,38	0
3	1GN	E	3	11/12	0.89	0.10	25,29,32,38	0
3	BGC	I	6	11/12	0.89	0.20	20,28,33,37	0
2	GAL	G	1	12/12	0.90	0.09	21,25,30,35	0
2	GAL	G	5	11/12	0.90	0.12	27,28,34,40	0
2	GAL	D	1	12/12	0.90	0.12	21,25,33,42	0
2	GAL	G	3	11/12	0.91	0.16	26,34,48,50	0
3	GAL	I	2	11/12	0.91	0.15	26,27,28,28	0
2	6PZ	G	7	22/23	0.91	0.11	15,17,23,23	0
2	GAL	H	1	12/12	0.91	0.08	21,26,30,35	0
2	1GN	H	4	11/12	0.92	0.14	23,26,31,34	0
2	1GN	D	4	11/12	0.92	0.11	26,27,30,32	0
2	GAL	H	5	11/12	0.93	0.12	26,27,34,40	0
2	GAL	D	3	11/12	0.93	0.14	27,33,48,51	0
2	1GN	D	2	11/12	0.93	0.08	16,19,20,23	0
2	BGC	H	6	11/12	0.93	0.08	15,16,18,18	0
3	GAL	F	2	11/12	0.93	0.10	25,27,28,29	0
2	6PZ	H	7	22/23	0.94	0.07	16,17,20,21	0
2	1GN	G	2	11/12	0.94	0.08	17,19,20,23	0
2	6PZ	D	7	22/23	0.95	0.07	16,17,21,22	0
2	BGC	D	6	11/12	0.96	0.06	14,16,17,19	0
2	1GN	H	2	11/12	0.96	0.06	17,19,20,23	0
2	BGC	G	6	11/12	0.97	0.07	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.

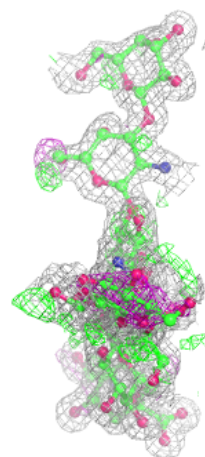
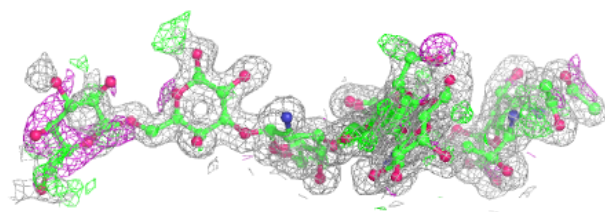
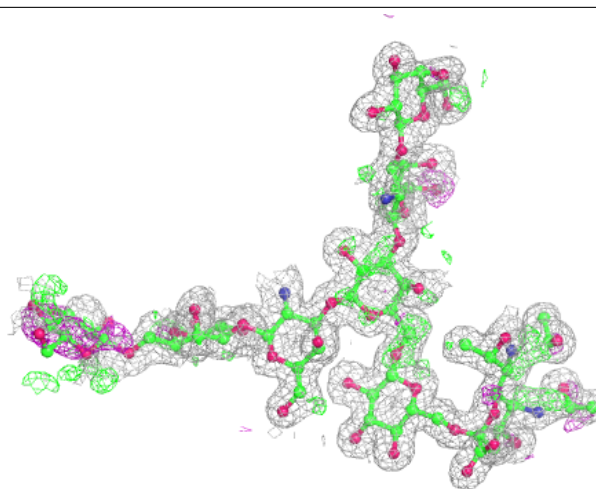
Electron density around Chain D:

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



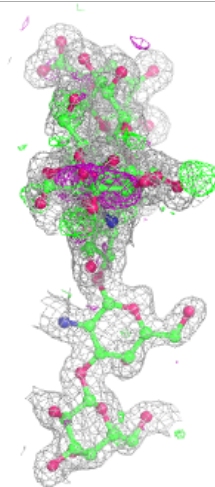
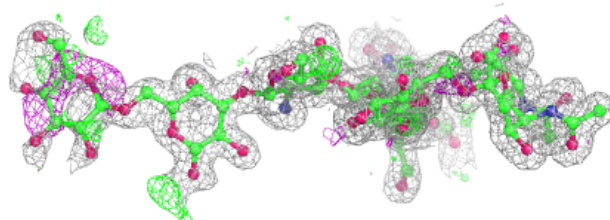
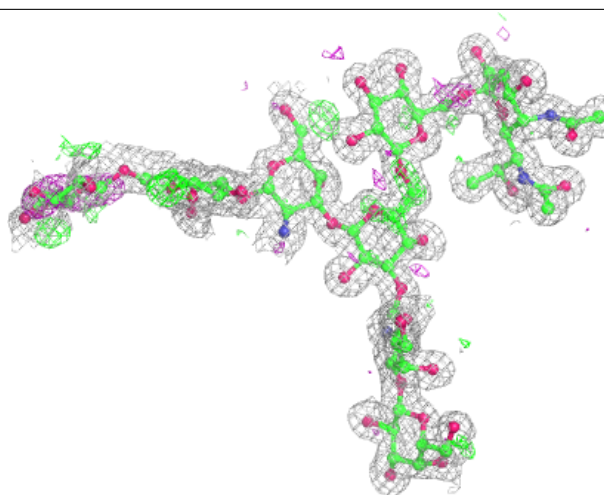
Electron density around Chain G:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



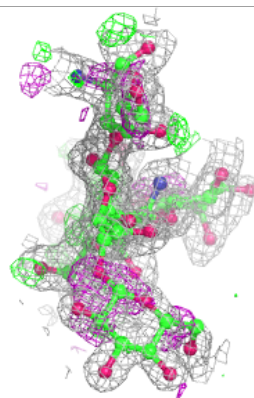
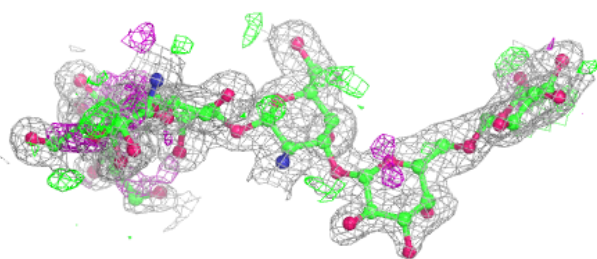
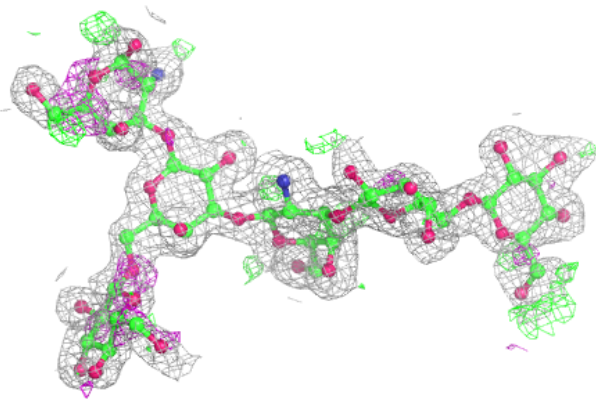
Electron density around Chain H:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

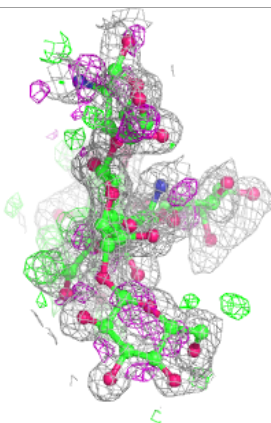
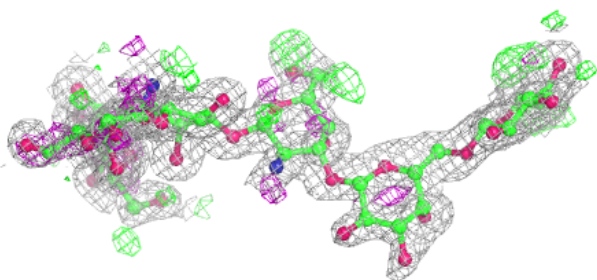
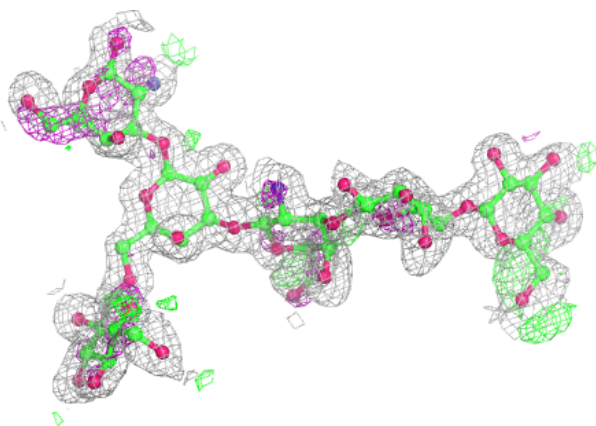


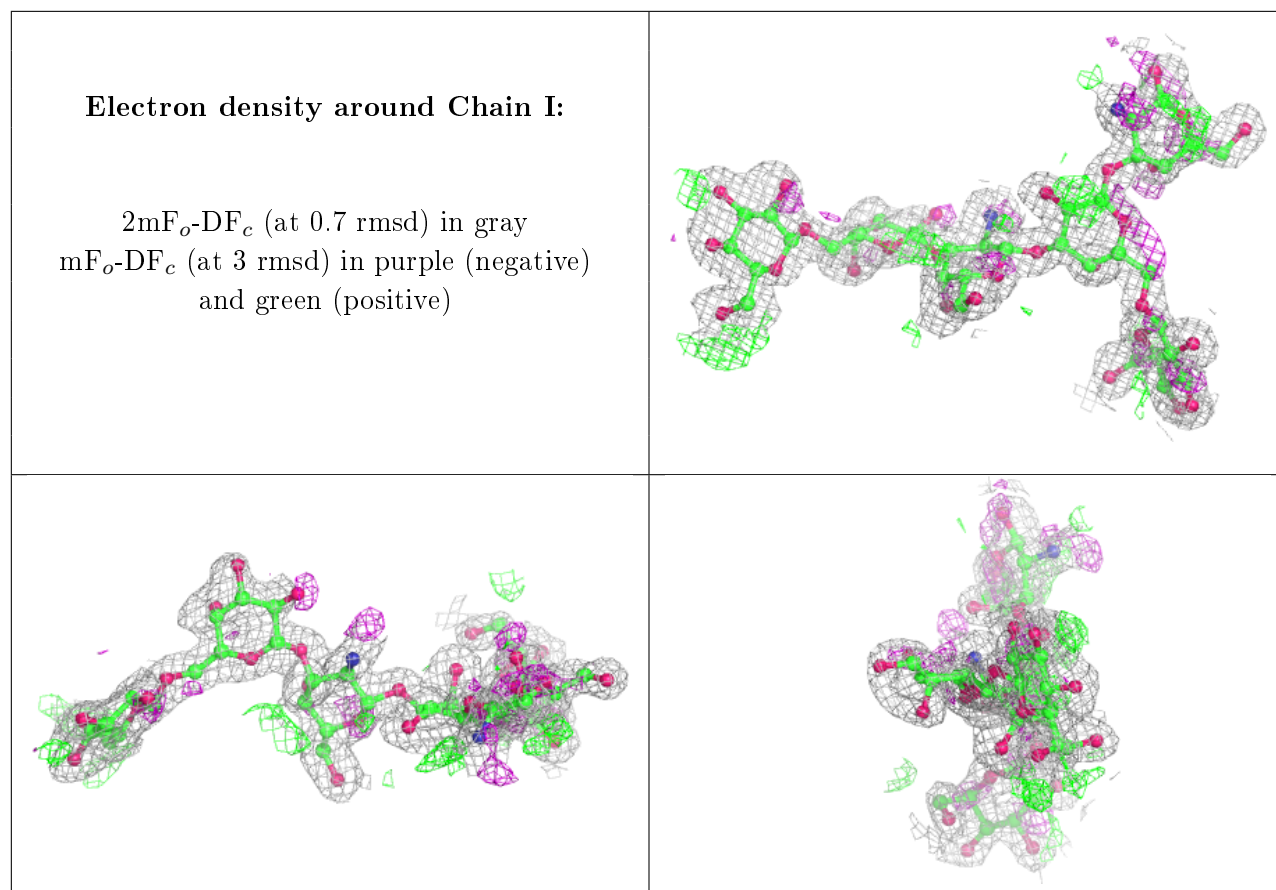
Electron density around Chain E:

$2mF_o-DF_c$ (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 ⓘ

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	C	602	3/4	0.80	0.22	35,35,35,40	0
5	ACY	A	619	3/4	0.81	0.26	32,32,35,44	0
5	ACY	C	618	3/4	0.82	0.20	27,27,28,29	0
5	ACY	B	610	3/4	0.84	0.17	34,34,35,38	0
5	ACY	B	602	3/4	0.85	0.15	27,27,29,29	0
5	ACY	A	611	3/4	0.86	0.18	27,27,27,29	0
5	ACY	C	619	3/4	0.86	0.12	25,25,25,26	0
4	MLA	A	601	7/7	0.87	0.18	22,27,33,37	0
4	MLA	B	601	7/7	0.88	0.15	20,27,33,38	0
4	MLA	C	601	7/7	0.92	0.15	22,28,34,41	0
5	ACY	A	610	3/4	0.94	0.09	21,21,21,22	0
5	ACY	B	609	3/4	0.95	0.10	25,25,25,26	0
5	ACY	A	618	3/4	0.96	0.07	24,24,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACY	B	619	3/4	0.97	0.06	21,21,22,22	0
5	ACY	C	617	3/4	0.97	0.09	21,21,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.