



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:01 PM UTC

PDB ID : 7B6U / pdb_00007b6u
Title : Sheep Polyomavirus VP1 in complex with 5 mM Forssman antigen pentose and 20 mM 6'-sialyllactosamine
Authors : Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-12-08
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

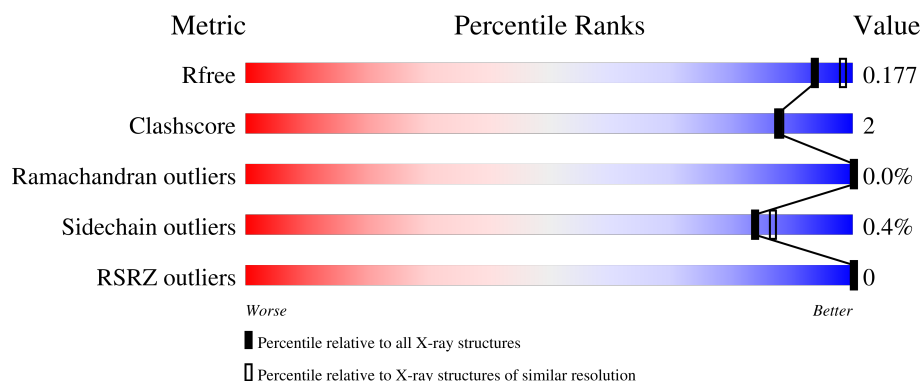
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

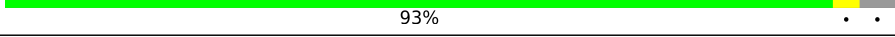
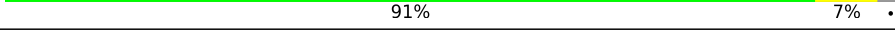
The reported resolution of this entry is 1.90 Å.

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



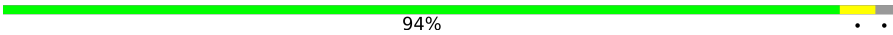
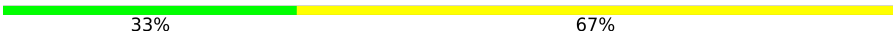
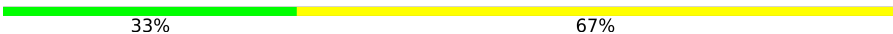
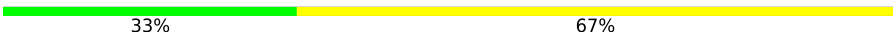
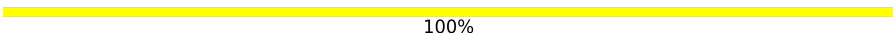
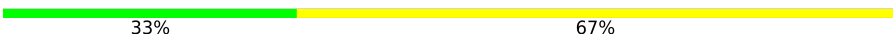
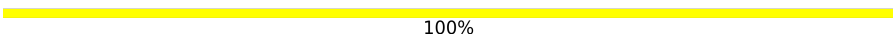
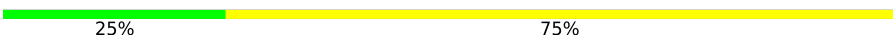
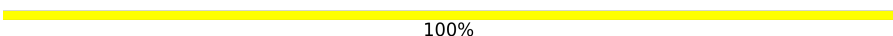
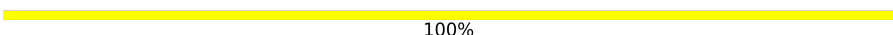
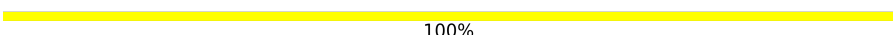
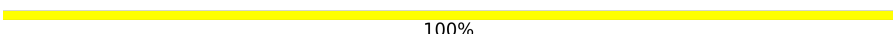
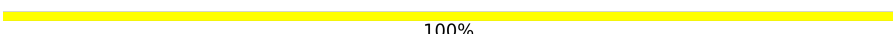
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AAA	276	 91% 6% .
1	BBB	276	 90% 5% 5%
1	CCC	276	 93% . .
1	DDD	276	 91% 7% .
1	EEE	276	 89% 6% 5%

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Mol	Chain	Length	Quality of chain
1	FFF	276	 90% 5% 5%
1	GGG	276	 88% 7% 5%
1	HHH	276	 94% . .
1	III	276	 90% . . 5%
1	JJJ	276	 89% 8% .
2	AaA	3	 33% 67%
2	DaD	3	 33% 67%
2	FaF	3	 33% 67%
2	HaH	3	 100%
2	JaJ	3	 33% 67%
3	AdA	4	 100%
3	BbB	4	 25% 75%
3	CaC	4	 100%
3	DdD	4	 100%
3	EaE	4	 100%
3	FdF	4	 100%
3	GaG	4	 100%
3	HdH	4	 50% 50%
3	IaI	4	 25% 75%
3	JdJ	4	 25% 75%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23317 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	269	Total	C	N	O	S	0	0	0
			2065	1316	347	389	13			
1	BBB	263	Total	C	N	O	S	0	0	0
			2021	1288	341	380	12			
1	CCC	264	Total	C	N	O	S	0	0	0
			2020	1288	343	377	12			
1	DDD	269	Total	C	N	O	S	0	1	0
			2077	1323	348	393	13			
1	EEE	263	Total	C	N	O	S	0	0	0
			2024	1290	342	380	12			
1	FFF	262	Total	C	N	O	S	0	1	0
			2015	1284	340	379	12			
1	GGG	263	Total	C	N	O	S	0	0	0
			2017	1287	340	378	12			
1	HHH	270	Total	C	N	O	S	0	0	0
			2073	1320	349	390	14			
1	III	261	Total	C	N	O	S	0	0	0
			2007	1282	337	376	12			
1	JJJ	270	Total	C	N	O	S	0	0	0
			2074	1319	350	391	14			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	16	GLY	-	expression tag	UNP A0A0E3ZCF3
AAA	17	SER	-	expression tag	UNP A0A0E3ZCF3
AAA	18	HIS	-	expression tag	UNP A0A0E3ZCF3
AAA	19	MET	-	expression tag	UNP A0A0E3ZCF3
AAA	95	SER	CYS	conflict	UNP A0A0E3ZCF3
BBB	16	GLY	-	expression tag	UNP A0A0E3ZCF3
BBB	17	SER	-	expression tag	UNP A0A0E3ZCF3
BBB	18	HIS	-	expression tag	UNP A0A0E3ZCF3
BBB	19	MET	-	expression tag	UNP A0A0E3ZCF3

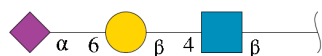
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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	95	SER	CYS	conflict	UNP A0A0E3ZCF3
CCC	16	GLY	-	expression tag	UNP A0A0E3ZCF3
CCC	17	SER	-	expression tag	UNP A0A0E3ZCF3
CCC	18	HIS	-	expression tag	UNP A0A0E3ZCF3
CCC	19	MET	-	expression tag	UNP A0A0E3ZCF3
CCC	95	SER	CYS	conflict	UNP A0A0E3ZCF3
DDD	16	GLY	-	expression tag	UNP A0A0E3ZCF3
DDD	17	SER	-	expression tag	UNP A0A0E3ZCF3
DDD	18	HIS	-	expression tag	UNP A0A0E3ZCF3
DDD	19	MET	-	expression tag	UNP A0A0E3ZCF3
DDD	95	SER	CYS	conflict	UNP A0A0E3ZCF3
EEE	16	GLY	-	expression tag	UNP A0A0E3ZCF3
EEE	17	SER	-	expression tag	UNP A0A0E3ZCF3
EEE	18	HIS	-	expression tag	UNP A0A0E3ZCF3
EEE	19	MET	-	expression tag	UNP A0A0E3ZCF3
EEE	95	SER	CYS	conflict	UNP A0A0E3ZCF3
FFF	16	GLY	-	expression tag	UNP A0A0E3ZCF3
FFF	17	SER	-	expression tag	UNP A0A0E3ZCF3
FFF	18	HIS	-	expression tag	UNP A0A0E3ZCF3
FFF	19	MET	-	expression tag	UNP A0A0E3ZCF3
FFF	95	SER	CYS	conflict	UNP A0A0E3ZCF3
GGG	16	GLY	-	expression tag	UNP A0A0E3ZCF3
GGG	17	SER	-	expression tag	UNP A0A0E3ZCF3
GGG	18	HIS	-	expression tag	UNP A0A0E3ZCF3
GGG	19	MET	-	expression tag	UNP A0A0E3ZCF3
GGG	95	SER	CYS	conflict	UNP A0A0E3ZCF3
HHH	16	GLY	-	expression tag	UNP A0A0E3ZCF3
HHH	17	SER	-	expression tag	UNP A0A0E3ZCF3
HHH	18	HIS	-	expression tag	UNP A0A0E3ZCF3
HHH	19	MET	-	expression tag	UNP A0A0E3ZCF3
HHH	95	SER	CYS	conflict	UNP A0A0E3ZCF3
III	16	GLY	-	expression tag	UNP A0A0E3ZCF3
III	17	SER	-	expression tag	UNP A0A0E3ZCF3
III	18	HIS	-	expression tag	UNP A0A0E3ZCF3
III	19	MET	-	expression tag	UNP A0A0E3ZCF3
III	95	SER	CYS	conflict	UNP A0A0E3ZCF3
JJJ	16	GLY	-	expression tag	UNP A0A0E3ZCF3
JJJ	17	SER	-	expression tag	UNP A0A0E3ZCF3
JJJ	18	HIS	-	expression tag	UNP A0A0E3ZCF3
JJJ	19	MET	-	expression tag	UNP A0A0E3ZCF3
JJJ	95	SER	CYS	conflict	UNP A0A0E3ZCF3

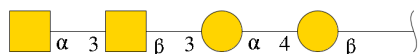
- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	DaD	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	FaF	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	HaH	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	JaJ	3	Total	C	N	O	0	0	0
			46	25	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AdA	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	BbB	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	CaC	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	DdD	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	EaE	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	FdF	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	GaG	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	HdH	4	Total	C	N	O	0	0	0
			51	28	2	21			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	IaI	4	Total	C	N	O	0	0	0
			51	28	2	21			
3	JdJ	4	Total	C	N	O	0	0	0
			51	28	2	21			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



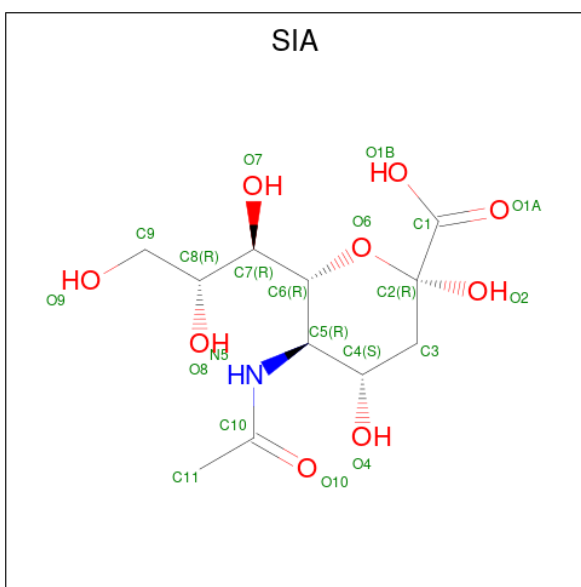
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	BBB	1	Total	C	O	0	0
			4	2	2		
4	EEE	1	Total	C	O	0	0
			4	2	2		
4	FFF	1	Total	C	O	0	0
			4	2	2		
4	GGG	1	Total	C	O	0	0
			4	2	2		
4	III	1	Total	C	O	0	0
			4	2	2		
4	III	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



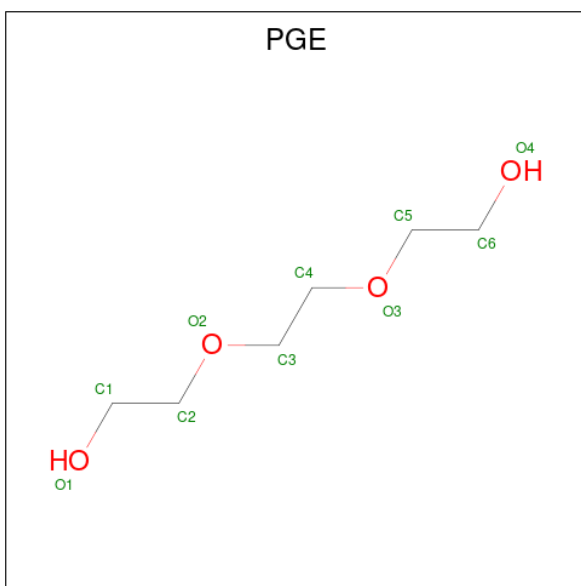
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			7	4	3		
5	BBB	1	Total	C	O	0	0
			7	4	3		
5	BBB	1	Total	C	O	0	0
			7	4	3		
5	CCC	1	Total	C	O	0	0
			7	4	3		
5	DDD	1	Total	C	O	0	0
			7	4	3		
5	EEE	1	Total	C	O	0	0
			7	4	3		
5	FFF	1	Total	C	O	0	0
			7	4	3		
5	GGG	1	Total	C	O	0	0
			7	4	3		
5	HHH	1	Total	C	O	0	0
			7	4	3		
5	HHH	1	Total	C	O	0	0
			7	4	3		
5	III	1	Total	C	O	0	0
			7	4	3		
5	JJJ	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	BBB	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	GGG	1	Total	C	O	0	0
			10	6	4		
7	HHH	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	214	Total 215	O 215	0	1
8	BBB	190	Total 190	O 190	0	0
8	CCC	204	Total 205	O 205	0	1
8	DDD	233	Total 234	O 234	0	1
8	EEE	201	Total 202	O 202	0	1
8	FFF	179	Total 179	O 179	0	0
8	GGG	186	Total 188	O 188	0	2
8	HHH	208	Total 209	O 209	0	1
8	III	202	Total 203	O 203	0	1
8	JJJ	206	Total 206	O 206	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.

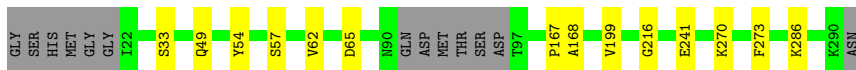
- Molecule 1: Capsid protein VP1

Chain AAA:  91% 6%



- Molecule 1: Capsid protein VP1

Chain BBB:  90% 5% 5%

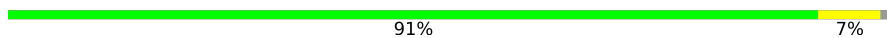


- Molecule 1: Capsid protein VP1

Chain CCC:  93% 2% 5%



- Molecule 1: Capsid protein VP1

Chain DDD:  91% 7% 2%



- Molecule 1: Capsid protein VP1

Chain EEE:  89% 6% 5%



- Molecule 1: Capsid protein VP1

Chain FFF:  90% 5% 5%



- Molecule 1: Capsid protein VP1

Chain GGG: 88% 7% 5%



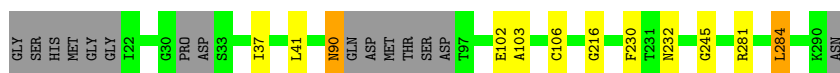
- Molecule 1: Capsid protein VP1

Chain HHH: 94% 4% 2%



- Molecule 1: Capsid protein VP1

Chain III: 90% 8% 2%



- Molecule 1: Capsid protein VP1

Chain JJJ: 89% 8% 3%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AaA: 33% 67%

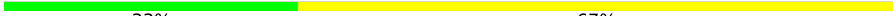


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DaD: 33% 67%

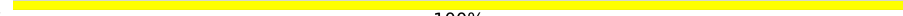


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FaF:  33% 67%

HA01
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HaH:  100%

HA01
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JaJ:  33% 67%

HA01
GAL2
SIA3

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

Chain AdA:  100%

GAL1
GLA2
NGA3
A2G4

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

Chain BbB:  25% 75%

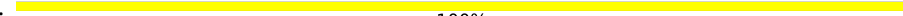
GAL1
GLA2
NGA3
A2G4

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

Chain CaC:  100%

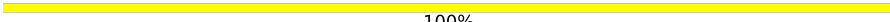
GAL1
GLA2
NGA3
A2G4

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

Chain DdD:  100%

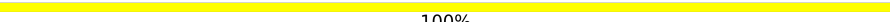
GAL1
GLA2
NGA3
A2G4

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

Chain EaE:  100%

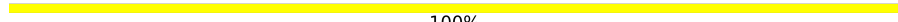
GAL1
GLA2
NGA3
A2G4

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

Chain FdF:  100%

GAL1
GLA2
NGA3
A2G4

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

Chain GaG:  100%

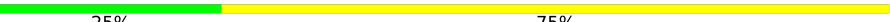
GAL1
GLA2
NGA3
A2G4

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

Chain HdH:  50% 50%

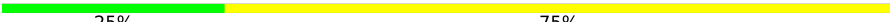
GAL1
GLA2
NGA3
A2G4

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

Chain IaI:  25% 75%

GAL1
GLA2
NGA3
A2G4

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

Chain JdJ:  25% 75%

GAL1
GLA2
NGA3
A2G4

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	129.65Å 129.65Å 220.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.47 – 1.90 49.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-1.90) 99.8 (49.47-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.146 , 0.173 0.151 , 0.177	Depositor DCC
R_{free} test set	3252 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.288 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
Reported twinning fraction	0.726 for H, K, L 0.274 for K, H, -L	Depositor
Outliers	0 of 325151 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23317	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, NGA, SIA, PEG, NAG, PGE, GLA, EDO, A2G

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	AAA	1.07	0/2118	1.24	2/2883 (0.1%)
1	BBB	1.02	0/2072	1.24	5/2818 (0.2%)
1	CCC	1.04	0/2071	1.22	0/2817
1	DDD	1.07	0/2133	1.26	1/2903 (0.0%)
1	EEE	1.03	0/2076	1.25	2/2824 (0.1%)
1	FFF	1.05	0/2069	1.26	2/2814 (0.1%)
1	GGG	1.07	3/2068 (0.1%)	1.26	1/2812 (0.0%)
1	HHH	1.05	0/2126	1.24	1/2893 (0.0%)
1	III	1.03	0/2057	1.24	0/2795
1	JJJ	1.04	1/2127 (0.0%)	1.25	1/2895 (0.0%)
All	All	1.05	4/20917 (0.0%)	1.25	15/28454 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	GGG	271	MET	C-O	6.06	1.30	1.24
1	JJJ	221	GLY	C-O	5.21	1.29	1.23
1	GGG	124	LYS	C-O	5.17	1.30	1.23
1	GGG	120	HIS	CE1-NE2	5.12	1.37	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	221	GLY	CA-C-O	-6.31	117.88	122.23
1	FFF	141	MET	CA-C-N	5.65	127.31	122.29
1	FFF	141	MET	C-N-CA	5.65	127.31	122.29
1	EEE	166	TYR	CB-CA-C	5.58	117.48	109.11
1	DDD	280	PHE	CA-CB-CG	5.48	119.28	113.80
1	EEE	177	GLY	CA-C-O	-5.48	118.45	122.23
1	BBB	65	ASP	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	128	GLU	CB-CG-CD	5.22	121.47	112.60
1	HHH	65	ASP	CA-CB-CG	5.21	117.81	112.60
1	JJJ	133	GLY	CA-C-O	-5.18	118.42	122.52
1	BBB	168	ALA	CA-C-N	5.11	127.64	120.28
1	BBB	168	ALA	C-N-CA	5.11	127.64	120.28
1	GGG	184	ASP	CA-CB-CG	5.04	117.64	112.60
1	BBB	167	PRO	CA-C-N	5.00	126.99	120.28
1	BBB	167	PRO	C-N-CA	5.00	126.99	120.28

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	AAA	2065	0	1972	10	0
1	BBB	2021	0	1922	8	0
1	CCC	2020	0	1929	5	0
1	DDD	2077	0	1992	11	0
1	EEE	2024	0	1933	11	0
1	FFF	2015	0	1915	7	0
1	GGG	2017	0	1928	10	0
1	HHH	2073	0	1978	6	0
1	III	2007	0	1924	10	0
1	JJJ	2074	0	1978	14	0
2	AaA	46	0	40	0	0
2	DaD	46	0	40	0	0
2	FaF	46	0	40	0	0
2	HaH	46	0	40	0	0
2	JaJ	46	0	40	0	0
3	AdA	51	0	44	0	0
3	BbB	51	0	44	1	0
3	CaC	51	0	44	0	0
3	DdD	51	0	44	0	0
3	EaE	51	0	44	0	0
3	FdF	51	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GaG	51	0	44	0	0
3	HdH	51	0	44	0	0
3	IaI	51	0	44	0	0
3	JdJ	51	0	44	0	0
4	AAA	4	0	6	0	0
4	BBB	4	0	6	0	0
4	EEE	4	0	6	0	0
4	FFF	4	0	6	0	0
4	GGG	4	0	6	0	0
4	III	8	0	12	0	0
5	AAA	7	0	10	0	0
5	BBB	14	0	20	0	0
5	CCC	7	0	10	0	0
5	DDD	7	0	10	0	0
5	EEE	7	0	10	0	0
5	FFF	7	0	10	0	0
5	GGG	7	0	10	0	0
5	HHH	14	0	20	0	0
5	III	7	0	10	0	0
5	JJJ	7	0	10	0	0
6	BBB	21	0	18	1	0
7	GGG	10	0	14	0	0
7	HHH	10	0	14	0	0
8	AAA	215	0	0	1	0
8	BBB	190	0	0	0	0
8	CCC	205	0	0	2	0
8	DDD	234	0	0	1	0
8	EEE	202	0	0	1	0
8	FFF	179	0	0	1	0
8	GGG	188	0	0	0	0
8	HHH	209	0	0	1	0
8	III	203	0	0	1	0
8	JJJ	206	0	0	1	0
All	All	23317	0	20319	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:27:VAL:HG11	1:JJJ:285:ARG:HD2	1.83	0.61
1:GGG:229:THR:HG22	1:HHH:217:GLN:HG3	1.83	0.61
1:EEE:281:ARG:NH1	8:EEE:601:HOH:O	2.35	0.60
1:BBB:62:VAL:O	6:BBB:301:SIA:H91	2.01	0.60
1:FFF:217:GLN:CB	8:FFF:771:HOH:O	2.52	0.58
1:III:281:ARG:NH1	8:III:604:HOH:O	2.37	0.56
1:CCC:281:ARG:NH1	8:CCC:605:HOH:O	2.42	0.52
1:HHH:27:VAL:HG12	1:HHH:28:ARG:O	2.09	0.52
1:III:90:ASN:C	1:III:90:ASN:HD22	2.18	0.51
1:HHH:230:PHE:CZ	1:III:216:GLY:HA3	2.46	0.50
1:JJJ:27:VAL:CG1	1:JJJ:285:ARG:HD2	2.40	0.50
1:JJJ:152:PRO:HB2	1:JJJ:190:THR:CG2	2.41	0.50
1:AAA:92:ASP:CB	8:AAA:780:HOH:O	2.61	0.49
1:III:37:ILE:C	1:III:37:ILE:HD12	2.38	0.49
1:JJJ:141:MET:O	1:JJJ:141:MET:HG3	2.14	0.47
1:BBB:57:SER:HB3	1:BBB:273:PHE:HB2	1.96	0.47
1:AAA:216:GLY:HA3	1:EEE:230:PHE:CZ	2.50	0.47
1:EEE:106:CYS:HA	1:EEE:281:ARG:O	2.16	0.46
1:DDD:37:ILE:C	1:DDD:37:ILE:HD12	2.40	0.46
1:DDD:281:ARG:NH1	8:DDD:608:HOH:O	2.49	0.46
1:AAA:89:LEU:HD23	1:AAA:286:LYS:HE2	1.98	0.46
1:GGG:33:SER:HA	1:GGG:286:LYS:HD2	1.97	0.45
8:CCC:702:HOH:O	1:DDD:124:LYS:HE3	2.16	0.45
1:JJJ:143:TYR:HB3	1:JJJ:260:ILE:HD12	1.97	0.45
1:FFF:232:ASN:HB3	1:GGG:214:TYR:CZ	2.52	0.45
1:GGG:261:VAL:HG22	1:GGG:274:ARG:O	2.16	0.45
1:DDD:34:ILE:HD13	1:DDD:285:ARG:HB3	1.99	0.45
1:DDD:145:MET:HA	1:DDD:215:PHE:O	2.17	0.45
1:III:102:GLU:O	1:III:284:LEU:HA	2.16	0.45
1:BBB:49:GLN:HG3	1:BBB:54:TYR:CZ	2.52	0.44
1:BBB:270:LYS:HE3	3:BbB:2:GLA:O2	2.17	0.44
1:CCC:230:PHE:CZ	1:DDD:216:GLY:HA3	2.53	0.44
1:AAA:114:ASN:HB2	1:BBB:199:VAL:O	2.17	0.44
1:GGG:89:LEU:HD21	1:GGG:101:TRP:CE2	2.53	0.44
1:DDD:107:ARG:HH21	1:DDD:107:ARG:HB3	1.83	0.44
1:III:106:CYS:HA	1:III:281:ARG:O	2.18	0.43
1:III:232:ASN:HB3	1:JJJ:214:TYR:CZ	2.53	0.43
1:BBB:33:SER:HA	1:BBB:286:LYS:CD	2.49	0.43
1:CCC:151:GLU:HB2	1:CCC:152:PRO:HD2	2.00	0.43
1:GGG:159:VAL:O	1:GGG:181:GLN:HA	2.19	0.43
1:GGG:230:PHE:CZ	1:HHH:216:GLY:HA3	2.54	0.43
1:AAA:106:CYS:HA	1:AAA:281:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:145:MET:HE2	1:CCC:145:MET:HB2	1.95	0.43
1:CCC:264:PHE:O	1:CCC:271:MET:HA	2.19	0.43
1:EEE:37:ILE:C	1:EEE:37:ILE:HD12	2.44	0.43
1:AAA:162:HIS:CD2	1:AAA:178:ALA:HA	2.54	0.43
1:EEE:107:ARG:HH11	1:EEE:107:ARG:HB3	1.84	0.43
1:HHH:159:VAL:HG12	1:HHH:201:ALA:HA	2.00	0.42
1:FFF:188:LYS:NZ	1:FFF:205:ASP:OD2	2.51	0.42
1:BBB:33:SER:HA	1:BBB:286:LYS:HD3	2.02	0.42
1:HHH:31:PRO:HD2	8:HHH:780:HOH:O	2.18	0.42
1:III:103:ALA:O	1:III:245:GLY:HA3	2.20	0.42
1:JJJ:103:ALA:O	1:JJJ:245:GLY:HA3	2.20	0.42
1:EEE:107:ARG:HB3	1:EEE:107:ARG:NH1	2.35	0.42
1:JJJ:166:TYR:HB2	1:JJJ:172:VAL:HG21	2.02	0.42
1:JJJ:281:ARG:NH2	8:JJJ:615:HOH:O	2.53	0.42
1:DDD:128:GLU:HG3	1:DDD:129:ASN:N	2.34	0.42
1:GGG:106:CYS:HA	1:GGG:281:ARG:O	2.20	0.41
1:AAA:230:PHE:CZ	1:BBB:216:GLY:HA3	2.55	0.41
1:EEE:162:HIS:CD2	1:EEE:178:ALA:HA	2.55	0.41
1:GGG:57:SER:HB3	1:GGG:273:PHE:HB2	2.03	0.41
1:DDD:79:TYR:CE2	1:DDD:199:VAL:HA	2.55	0.41
1:FFF:112:GLY:O	1:FFF:115:MET:HG2	2.21	0.41
1:JJJ:70:ALA:O	1:JJJ:72:PRO:HD3	2.20	0.41
1:AAA:141:MET:SD	1:EEE:117:THR:HA	2.61	0.41
1:GGG:264:PHE:O	1:GGG:271:MET:HA	2.20	0.41
1:FFF:264:PHE:O	1:FFF:271:MET:HA	2.20	0.41
1:DDD:99:LEU:HD13	1:DDD:286:LYS:HD3	2.03	0.41
1:EEE:108:THR:HA	1:EEE:279:TYR:O	2.20	0.41
1:FFF:79:TYR:CE2	1:FFF:199:VAL:HA	2.56	0.41
1:III:230:PHE:CZ	1:JJJ:216:GLY:HA3	2.56	0.41
1:AAA:102:GLU:O	1:AAA:284:LEU:HA	2.20	0.41
1:EEE:80:SER:HA	1:EEE:194:ASP:OD1	2.20	0.40
1:JJJ:37:ILE:HD12	1:JJJ:37:ILE:C	2.46	0.40
1:JJJ:40:TYR:HA	1:JJJ:278:ARG:O	2.22	0.40
1:EEE:35:THR:HG22	1:EEE:101:TRP:CZ3	2.56	0.40
1:DDD:254:PHE:CD1	1:DDD:254:PHE:N	2.89	0.40
1:FFF:145:MET:HA	1:FFF:215:PHE:O	2.20	0.40
1:JJJ:106:CYS:HA	1:JJJ:281:ARG:O	2.22	0.40
1:AAA:145:MET:HA	1:AAA:215:PHE:O	2.22	0.40
1:III:41:LEU:HD23	1:III:41:LEU:HA	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	AAA	267/276 (97%)	254 (95%)	13 (5%)	0	100	100
1	BBB	259/276 (94%)	247 (95%)	12 (5%)	0	100	100
1	CCC	260/276 (94%)	248 (95%)	12 (5%)	0	100	100
1	DDD	268/276 (97%)	256 (96%)	11 (4%)	1 (0%)	30	22
1	EEE	259/276 (94%)	246 (95%)	13 (5%)	0	100	100
1	FFF	259/276 (94%)	248 (96%)	11 (4%)	0	100	100
1	GGG	259/276 (94%)	248 (96%)	11 (4%)	0	100	100
1	HHH	268/276 (97%)	255 (95%)	13 (5%)	0	100	100
1	III	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	JJJ	268/276 (97%)	258 (96%)	10 (4%)	0	100	100
All	All	2622/2760 (95%)	2503 (96%)	118 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	74	LYS

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	AAA	218/234 (93%)	218 (100%)	0	100	100
1	BBB	212/234 (91%)	211 (100%)	1 (0%)	81	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	212/234 (91%)	211 (100%)	1 (0%)	81	84
1	DDD	222/234 (95%)	221 (100%)	1 (0%)	81	84
1	EEE	214/234 (92%)	213 (100%)	1 (0%)	81	84
1	FFF	211/234 (90%)	211 (100%)	0	100	100
1	GGG	212/234 (91%)	212 (100%)	0	100	100
1	HHH	219/234 (94%)	218 (100%)	1 (0%)	81	84
1	III	212/234 (91%)	210 (99%)	2 (1%)	70	73
1	JJJ	220/234 (94%)	219 (100%)	1 (0%)	81	84
All	All	2152/2340 (92%)	2144 (100%)	8 (0%)	84	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	241	GLU
1	CCC	90	ASN
1	DDD	95	SER
1	EEE	139	GLU
1	HHH	139	GLU
1	III	90	ASN
1	III	284	LEU
1	JJJ	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

55 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	AaA	1	2	15,15,15	0.54	0	21,21,21	1.28	1 (4%)
2	GAL	AaA	2	2	11,11,12	0.48	0	15,15,17	0.77	0
2	SIA	AaA	3	2	20,20,21	0.92	0	21,28,31	1.61	5 (23%)
3	GAL	AdA	1	3	12,12,12	0.46	0	17,17,17	0.90	1 (5%)
3	GLA	AdA	2	3	11,11,12	0.40	0	15,15,17	1.24	3 (20%)
3	NGA	AdA	3	3	14,14,15	0.87	0	17,19,21	1.07	1 (5%)
3	A2G	AdA	4	3	14,14,15	0.58	0	17,19,21	1.36	2 (11%)
3	GAL	BbB	1	3	12,12,12	0.54	0	17,17,17	1.20	1 (5%)
3	GLA	BbB	2	3	11,11,12	0.53	0	15,15,17	1.02	0
3	NGA	BbB	3	3	14,14,15	0.69	0	17,19,21	0.85	0
3	A2G	BbB	4	3	14,14,15	0.81	0	17,19,21	1.35	1 (5%)
3	GAL	CaC	1	3	12,12,12	0.51	0	17,17,17	1.17	1 (5%)
3	GLA	CaC	2	3	11,11,12	0.97	1 (9%)	15,15,17	1.27	2 (13%)
3	NGA	CaC	3	3	14,14,15	0.80	1 (7%)	17,19,21	1.16	2 (11%)
3	A2G	CaC	4	3	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
2	NAG	DaD	1	2	15,15,15	0.44	0	21,21,21	1.29	3 (14%)
2	GAL	DaD	2	2	11,11,12	0.42	0	15,15,17	0.85	0
2	SIA	DaD	3	2	20,20,21	0.87	0	21,28,31	1.78	5 (23%)
3	GAL	DdD	1	3	12,12,12	0.59	0	17,17,17	1.49	4 (23%)
3	GLA	DdD	2	3	11,11,12	0.72	0	15,15,17	1.60	5 (33%)
3	NGA	DdD	3	3	14,14,15	0.73	0	17,19,21	1.09	1 (5%)
3	A2G	DdD	4	3	14,14,15	1.03	1 (7%)	17,19,21	1.33	3 (17%)
3	GAL	EaE	1	3	12,12,12	0.60	0	17,17,17	1.02	1 (5%)
3	GLA	EaE	2	3	11,11,12	0.80	1 (9%)	15,15,17	1.17	2 (13%)
3	NGA	EaE	3	3	14,14,15	0.76	0	17,19,21	1.14	1 (5%)
3	A2G	EaE	4	3	14,14,15	0.72	1 (7%)	17,19,21	1.51	3 (17%)
2	NAG	FaF	1	2	15,15,15	0.48	0	21,21,21	1.71	4 (19%)
2	GAL	FaF	2	2	11,11,12	0.50	0	15,15,17	1.00	0
2	SIA	FaF	3	2	20,20,21	0.79	1 (5%)	21,28,31	1.15	1 (4%)
3	GAL	FdF	1	3	12,12,12	0.49	0	17,17,17	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLA	FdF	2	3	11,11,12	0.70	0	15,15,17	1.41	3 (20%)
3	NGA	FdF	3	3	14,14,15	0.69	0	17,19,21	1.00	1 (5%)
3	A2G	FdF	4	3	14,14,15	0.81	0	17,19,21	1.41	2 (11%)
3	GAL	GaG	1	3	12,12,12	0.88	0	17,17,17	1.72	2 (11%)
3	GLA	GaG	2	3	11,11,12	0.68	0	15,15,17	1.26	3 (20%)
3	NGA	GaG	3	3	14,14,15	0.84	1 (7%)	17,19,21	0.56	0
3	A2G	GaG	4	3	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
2	NAG	HaH	1	2	15,15,15	0.48	0	21,21,21	1.13	1 (4%)
2	GAL	HaH	2	2	11,11,12	0.45	0	15,15,17	1.09	1 (6%)
2	SIA	HaH	3	2	20,20,21	0.64	0	21,28,31	1.47	6 (28%)
3	GAL	HdH	1	3	12,12,12	0.53	0	17,17,17	1.02	0
3	GLA	HdH	2	3	11,11,12	0.57	0	15,15,17	1.36	4 (26%)
3	NGA	HdH	3	3	14,14,15	0.76	0	17,19,21	0.79	0
3	A2G	HdH	4	3	14,14,15	0.68	0	17,19,21	1.49	3 (17%)
3	GAL	IaI	1	3	12,12,12	0.69	0	17,17,17	1.21	2 (11%)
3	GLA	IaI	2	3	11,11,12	0.62	0	15,15,17	1.40	1 (6%)
3	NGA	IaI	3	3	14,14,15	0.91	0	17,19,21	1.25	3 (17%)
3	A2G	IaI	4	3	14,14,15	0.45	0	17,19,21	0.88	0
2	NAG	JaJ	1	2	15,15,15	0.50	0	21,21,21	1.21	2 (9%)
2	GAL	JaJ	2	2	11,11,12	0.32	0	15,15,17	0.74	0
2	SIA	JaJ	3	2	20,20,21	0.86	0	21,28,31	1.56	4 (19%)
3	GAL	JdJ	1	3	12,12,12	0.69	0	17,17,17	1.13	2 (11%)
3	GLA	JdJ	2	3	11,11,12	0.47	0	15,15,17	1.16	1 (6%)
3	NGA	JdJ	3	3	14,14,15	0.49	0	17,19,21	0.85	0
3	A2G	JdJ	4	3	14,14,15	0.62	0	17,19,21	1.46	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	AaA	1	2	-	0/6/26/26	0/1/1/1
2	GAL	AaA	2	2	-	0/2/19/22	0/1/1/1
2	SIA	AaA	3	2	-	4/18/34/38	0/1/1/1
3	GAL	AdA	1	3	-	2/2/22/22	0/1/1/1
3	GLA	AdA	2	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NGA	AdA	3	3	-	0/6/23/26	0/1/1/1
3	A2G	AdA	4	3	-	0/6/23/26	0/1/1/1
3	GAL	BbB	1	3	-	1/2/22/22	0/1/1/1
3	GLA	BbB	2	3	-	1/2/19/22	0/1/1/1
3	NGA	BbB	3	3	-	0/6/23/26	0/1/1/1
3	A2G	BbB	4	3	-	0/6/23/26	0/1/1/1
3	GAL	CaC	1	3	-	1/2/22/22	0/1/1/1
3	GLA	CaC	2	3	-	1/2/19/22	0/1/1/1
3	NGA	CaC	3	3	-	0/6/23/26	0/1/1/1
3	A2G	CaC	4	3	-	0/6/23/26	0/1/1/1
2	NAG	DaD	1	2	-	0/6/26/26	0/1/1/1
2	GAL	DaD	2	2	-	0/2/19/22	0/1/1/1
2	SIA	DaD	3	2	-	4/18/34/38	0/1/1/1
3	GAL	DdD	1	3	-	2/2/22/22	0/1/1/1
3	GLA	DdD	2	3	-	1/2/19/22	0/1/1/1
3	NGA	DdD	3	3	-	0/6/23/26	0/1/1/1
3	A2G	DdD	4	3	-	1/6/23/26	0/1/1/1
3	GAL	EaE	1	3	-	1/2/22/22	0/1/1/1
3	GLA	EaE	2	3	-	1/2/19/22	0/1/1/1
3	NGA	EaE	3	3	-	0/6/23/26	0/1/1/1
3	A2G	EaE	4	3	-	0/6/23/26	0/1/1/1
2	NAG	FaF	1	2	-	2/6/26/26	0/1/1/1
2	GAL	FaF	2	2	-	0/2/19/22	0/1/1/1
2	SIA	FaF	3	2	-	3/18/34/38	0/1/1/1
3	GAL	FdF	1	3	-	0/2/22/22	0/1/1/1
3	GLA	FdF	2	3	-	1/2/19/22	0/1/1/1
3	NGA	FdF	3	3	-	0/6/23/26	0/1/1/1
3	A2G	FdF	4	3	-	0/6/23/26	0/1/1/1
3	GAL	GaG	1	3	-	1/2/22/22	0/1/1/1
3	GLA	GaG	2	3	-	1/2/19/22	0/1/1/1
3	NGA	GaG	3	3	-	0/6/23/26	0/1/1/1
3	A2G	GaG	4	3	-	0/6/23/26	0/1/1/1
2	NAG	HaH	1	2	-	0/6/26/26	0/1/1/1
2	GAL	HaH	2	2	-	0/2/19/22	0/1/1/1
2	SIA	HaH	3	2	-	4/18/34/38	0/1/1/1
3	GAL	HdH	1	3	-	2/2/22/22	0/1/1/1
3	GLA	HdH	2	3	-	1/2/19/22	0/1/1/1
3	NGA	HdH	3	3	-	0/6/23/26	0/1/1/1
3	A2G	HdH	4	3	-	1/6/23/26	0/1/1/1
3	GAL	IaI	1	3	-	1/2/22/22	0/1/1/1
3	GLA	IaI	2	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NGA	IaI	3	3	-	0/6/23/26	0/1/1/1
3	A2G	IaI	4	3	-	1/6/23/26	0/1/1/1
2	NAG	JaJ	1	2	-	2/6/26/26	0/1/1/1
2	GAL	JaJ	2	2	-	0/2/19/22	0/1/1/1
2	SIA	JaJ	3	2	-	2/18/34/38	0/1/1/1
3	GAL	JdJ	1	3	-	1/2/22/22	0/1/1/1
3	GLA	JdJ	2	3	-	1/2/19/22	0/1/1/1
3	NGA	JdJ	3	3	-	0/6/23/26	0/1/1/1
3	A2G	JdJ	4	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CaC	3	NGA	O5-C1	-2.59	1.39	1.43
3	EaE	2	GLA	O5-C1	-2.36	1.39	1.43
3	CaC	2	GLA	O2-C2	-2.36	1.38	1.43
3	DdD	4	A2G	O5-C1	2.19	1.47	1.43
3	GaG	3	NGA	O4-C4	2.12	1.48	1.43
2	FaF	3	SIA	O1B-C1	-2.12	1.23	1.30
3	EaE	4	A2G	C4-C5	-2.03	1.48	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GaG	1	GAL	C3-C4-C5	-4.36	102.33	110.23
2	DaD	3	SIA	O6-C2-C1	4.21	115.66	107.72
2	JaJ	3	SIA	O6-C2-C1	3.89	115.05	107.72
3	JdJ	4	A2G	C1-O5-C5	3.88	117.39	112.19
2	FaF	1	NAG	C1-C2-C3	-3.70	105.50	110.54
2	AaA	1	NAG	O5-C1-C2	-3.67	105.83	109.52
3	EaE	4	A2G	O5-C1-C2	-3.47	105.92	111.29
2	DaD	3	SIA	O8-C8-C9	-3.46	101.16	109.03
2	FaF	1	NAG	O5-C1-C2	-3.29	106.21	109.52
3	HdH	4	A2G	O5-C5-C6	3.28	114.04	107.66
3	GaG	1	GAL	O3-C3-C4	3.22	117.97	110.38
3	AdA	4	A2G	C1-O5-C5	3.21	116.49	112.19
2	FaF	1	NAG	C3-C4-C5	3.16	115.96	110.23
3	IaI	2	GLA	O3-C3-C2	-3.13	103.67	110.05
3	DdD	4	A2G	O5-C5-C6	3.05	113.60	107.66
2	DaD	1	NAG	C1-C2-N2	3.04	114.25	110.73
2	AaA	3	SIA	O10-C10-N5	3.02	127.32	121.98
3	FdF	2	GLA	O3-C3-C4	2.94	117.31	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AaA	3	SIA	C11-C10-N5	-2.91	111.30	116.12
2	HaH	2	GAL	C1-O5-C5	2.86	116.02	112.19
3	JdJ	1	GAL	C3-C4-C5	-2.86	105.05	110.23
3	EaE	4	A2G	C6-C5-C4	-2.83	106.07	113.02
3	DdD	1	GAL	C3-C4-C5	-2.82	105.11	110.23
3	BbB	1	GAL	O5-C1-C2	-2.82	105.34	110.30
3	FdF	4	A2G	O4-C4-C3	-2.81	103.76	110.38
2	AaA	3	SIA	O1B-C1-C2	2.77	119.91	112.71
3	GaG	2	GLA	O3-C3-C2	-2.75	104.45	110.05
3	BbB	4	A2G	C4-C3-C2	-2.73	107.01	111.02
2	HaH	3	SIA	O1B-C1-C2	2.69	119.72	112.71
3	AdA	3	NGA	C4-C3-C2	-2.69	107.08	111.02
2	JaJ	1	NAG	O5-C1-C2	-2.65	106.86	109.52
2	FaF	3	SIA	O1B-C1-C2	2.64	119.59	112.71
3	FdF	2	GLA	O2-C2-C3	-2.64	104.69	110.15
2	HaH	3	SIA	O6-C2-C1	2.64	112.69	107.72
2	HaH	1	NAG	C3-C4-C5	2.63	115.01	110.23
3	JdJ	4	A2G	C2-N2-C7	2.63	126.42	122.90
3	DdD	1	GAL	O5-C1-C2	-2.63	105.68	110.30
3	FdF	2	GLA	C1-O5-C5	2.61	115.68	112.19
2	HaH	3	SIA	O1A-C1-C2	-2.61	117.22	122.85
3	JdJ	2	GLA	C1-O5-C5	2.60	115.67	112.19
3	DdD	1	GAL	C6-C5-C4	2.59	119.39	113.02
3	EaE	3	NGA	C2-N2-C7	-2.57	119.45	122.90
3	FdF	3	NGA	O3-C3-C2	-2.55	104.10	109.40
2	JaJ	1	NAG	C1-C2-N2	2.55	113.68	110.73
3	DdD	2	GLA	C2-C3-C4	-2.54	106.39	110.86
3	DdD	4	A2G	C1-C2-N2	2.51	114.38	110.43
3	AdA	2	GLA	O5-C5-C6	-2.49	102.83	107.66
2	JaJ	3	SIA	O6-C2-C3	-2.48	107.22	110.56
3	AdA	2	GLA	O2-C2-C3	-2.48	105.01	110.15
3	FdF	4	A2G	O5-C1-C2	-2.45	107.50	111.29
3	IaI	1	GAL	C3-C4-C5	-2.44	105.81	110.23
3	HdH	2	GLA	O3-C3-C2	-2.44	105.08	110.05
2	HaH	3	SIA	O8-C8-C9	-2.38	103.61	109.03
3	EaE	4	A2G	O6-C6-C5	-2.37	103.25	111.33
3	CaC	2	GLA	O3-C3-C2	-2.37	105.22	110.05
3	HdH	4	A2G	O3-C3-C2	2.36	114.30	109.40
3	IaI	3	NGA	O7-C7-C8	-2.36	117.86	122.05
3	HdH	2	GLA	O2-C2-C3	-2.34	105.30	110.15
3	DdD	2	GLA	O4-C4-C3	2.32	115.85	110.38
2	HaH	3	SIA	O9-C9-C8	-2.32	106.28	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AdA	4	A2G	O6-C6-C5	-2.32	103.44	111.33
2	AaA	3	SIA	O6-C2-C3	2.32	113.67	110.56
3	EaE	1	GAL	C4-C3-C2	-2.30	106.78	110.83
3	CaC	3	NGA	O5-C5-C6	2.27	112.08	107.66
3	CaC	4	A2G	C1-O5-C5	2.26	115.22	112.19
3	FdF	1	GAL	O5-C5-C6	2.25	112.01	106.44
3	IaI	3	NGA	C8-C7-N2	2.24	119.83	116.12
2	AaA	3	SIA	O6-C2-C1	2.23	111.94	107.72
2	DaD	1	NAG	O4-C4-C5	-2.23	103.84	109.32
2	DaD	1	NAG	C3-C4-C5	2.22	114.25	110.23
3	GaG	2	GLA	O3-C3-C4	2.20	115.57	110.38
2	DaD	3	SIA	C11-C10-N5	-2.20	112.48	116.12
3	JdJ	1	GAL	O5-C5-C4	2.19	113.64	109.70
2	DaD	3	SIA	O4-C4-C3	-2.18	104.44	109.86
3	DdD	2	GLA	C3-C4-C5	-2.18	106.28	110.23
3	CaC	2	GLA	O2-C2-C3	-2.17	105.66	110.15
2	JaJ	3	SIA	O1B-C1-O1A	-2.16	119.17	124.08
3	JdJ	4	A2G	O7-C7-N2	2.15	125.77	121.98
3	AdA	1	GAL	C3-C4-C5	-2.14	106.35	110.23
2	JaJ	3	SIA	O10-C10-N5	2.14	125.77	121.98
3	HdH	2	GLA	C1-O5-C5	2.14	115.06	112.19
3	EaE	2	GLA	C1-O5-C5	2.13	115.05	112.19
3	HdH	2	GLA	O4-C4-C3	-2.13	105.35	110.38
3	CaC	1	GAL	O2-C2-C1	2.10	114.10	109.25
3	DdD	4	A2G	C4-C3-C2	-2.10	107.94	111.02
3	GaG	4	A2G	O6-C6-C5	-2.09	104.21	111.33
3	DdD	2	GLA	C1-C2-C3	2.09	112.69	109.64
3	IaI	3	NGA	C1-O5-C5	2.08	114.98	112.19
3	DdD	1	GAL	O5-C5-C4	-2.08	105.94	109.70
2	FaF	1	NAG	O4-C4-C5	-2.06	104.25	109.32
2	HaH	3	SIA	C6-C5-N5	-2.06	107.62	110.91
3	IaI	1	GAL	C6-C5-C4	2.04	118.04	113.02
3	DdD	2	GLA	O5-C5-C6	-2.03	103.70	107.66
3	AdA	2	GLA	O3-C3-C4	2.02	115.15	110.38
2	DaD	3	SIA	C9-C8-C7	2.02	116.29	112.17
3	EaE	2	GLA	O2-C2-C1	2.02	113.85	109.22
3	GaG	2	GLA	C1-C2-C3	2.02	112.58	109.64
3	DdD	3	NGA	O5-C1-C2	2.01	114.41	111.29
3	HdH	4	A2G	O3-C3-C4	-2.00	105.66	110.38
3	CaC	3	NGA	O3-C3-C2	-2.00	105.25	109.40

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DdD	1	GAL	O5-C5-C6-O6
2	FaF	1	NAG	O5-C5-C6-O6
3	AdA	1	GAL	O5-C5-C6-O6
2	AaA	3	SIA	O7-C7-C8-C9
2	DaD	3	SIA	O7-C7-C8-C9
2	DaD	3	SIA	C6-C7-C8-C9
3	DdD	1	GAL	C4-C5-C6-O6
3	IaI	2	GLA	O5-C5-C6-O6
2	HaH	3	SIA	O7-C7-C8-C9
2	DaD	3	SIA	C6-C7-C8-O8
2	JaJ	1	NAG	C4-C5-C6-O6
3	FdF	2	GLA	O5-C5-C6-O6
3	DdD	2	GLA	O5-C5-C6-O6
3	BbB	1	GAL	O5-C5-C6-O6
3	HdH	1	GAL	C4-C5-C6-O6
3	EaE	1	GAL	O5-C5-C6-O6
3	JdJ	2	GLA	O5-C5-C6-O6
3	GaG	2	GLA	O5-C5-C6-O6
3	JdJ	1	GAL	O5-C5-C6-O6
3	AdA	2	GLA	O5-C5-C6-O6
3	CaC	2	GLA	O5-C5-C6-O6
3	IaI	1	GAL	O5-C5-C6-O6
3	EaE	2	GLA	O5-C5-C6-O6
3	HdH	2	GLA	O5-C5-C6-O6
3	CaC	1	GAL	O5-C5-C6-O6
3	HdH	1	GAL	O5-C5-C6-O6
3	BbB	2	GLA	O5-C5-C6-O6
3	GaG	1	GAL	O5-C5-C6-O6
2	AaA	3	SIA	C6-C7-C8-O8
2	HaH	3	SIA	C6-C7-C8-C9
2	AaA	3	SIA	O7-C7-C8-O8
2	JaJ	1	NAG	O5-C5-C6-O6
2	FaF	3	SIA	C6-C7-C8-O8
3	DdD	4	A2G	O5-C5-C6-O6
3	AdA	1	GAL	C4-C5-C6-O6
2	AaA	3	SIA	C6-C7-C8-C9
2	HaH	3	SIA	C6-C7-C8-O8
2	DaD	3	SIA	O7-C7-C8-O8
2	FaF	1	NAG	C4-C5-C6-O6
3	HdH	4	A2G	O5-C5-C6-O6
2	FaF	3	SIA	C6-C7-C8-C9
2	JaJ	3	SIA	O8-C8-C9-O9

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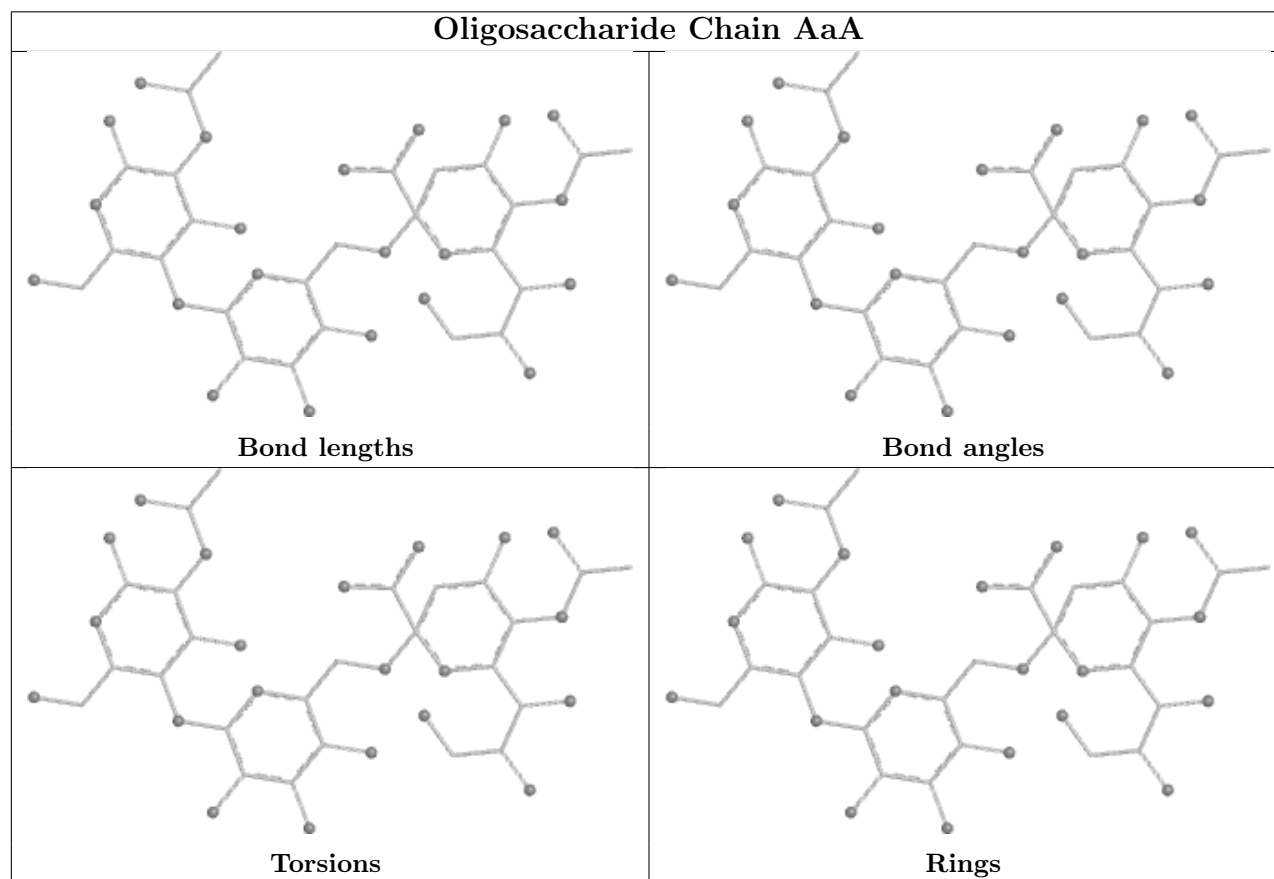
Mol	Chain	Res	Type	Atoms
2	FaF	3	SIA	O7-C7-C8-C9
2	JaJ	3	SIA	C7-C8-C9-O9
2	HaH	3	SIA	O7-C7-C8-O8
3	IaI	4	A2G	O5-C5-C6-O6

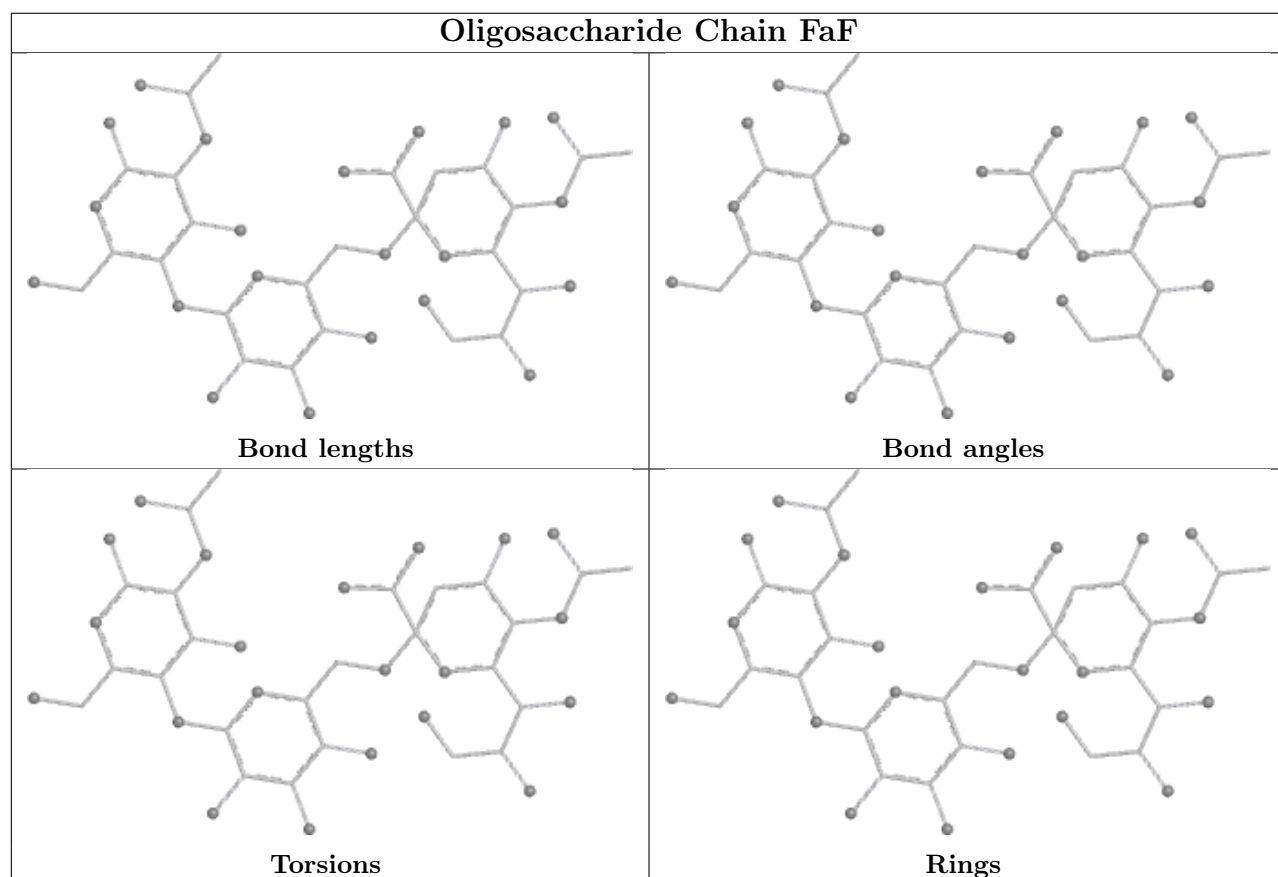
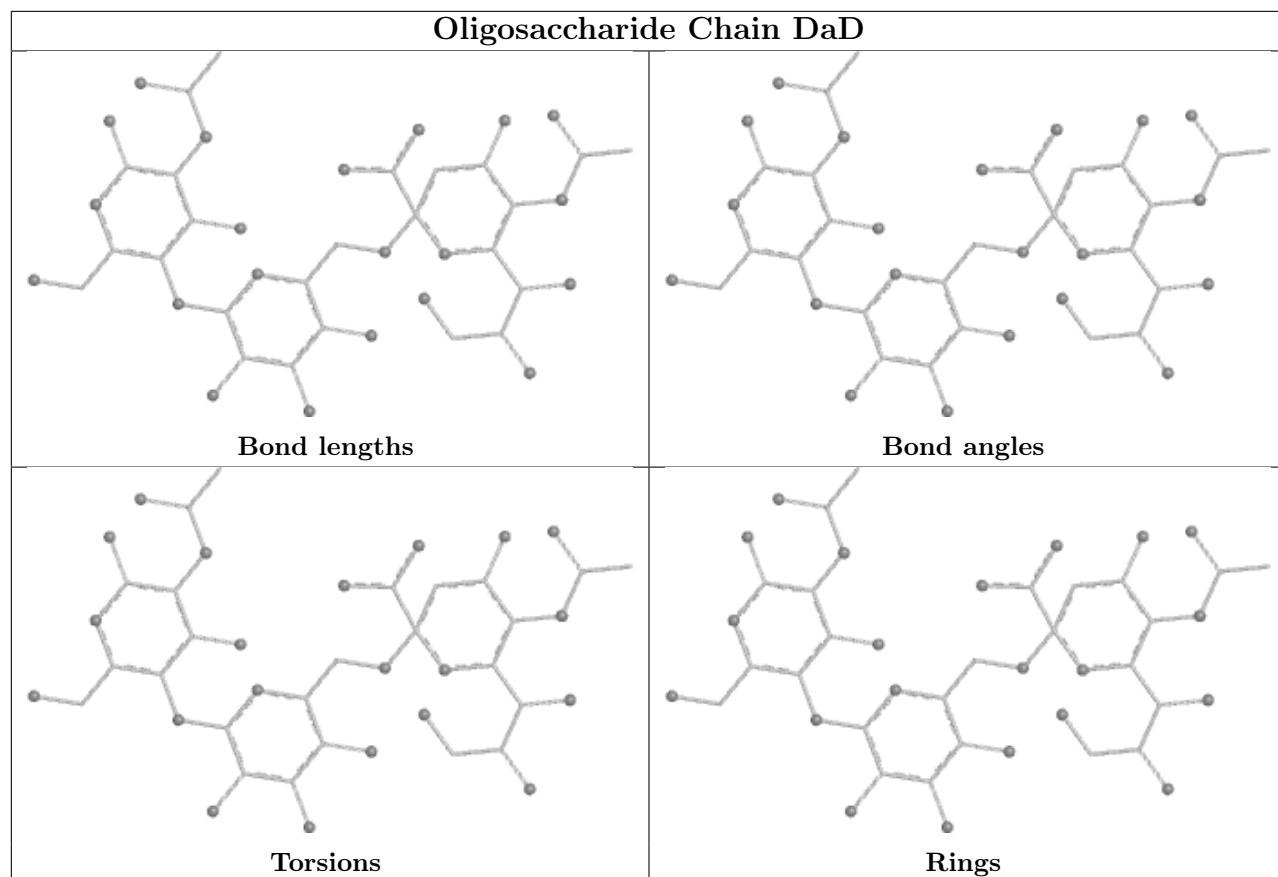
There are no ring outliers.

1 monomer is involved in 1 short contact:

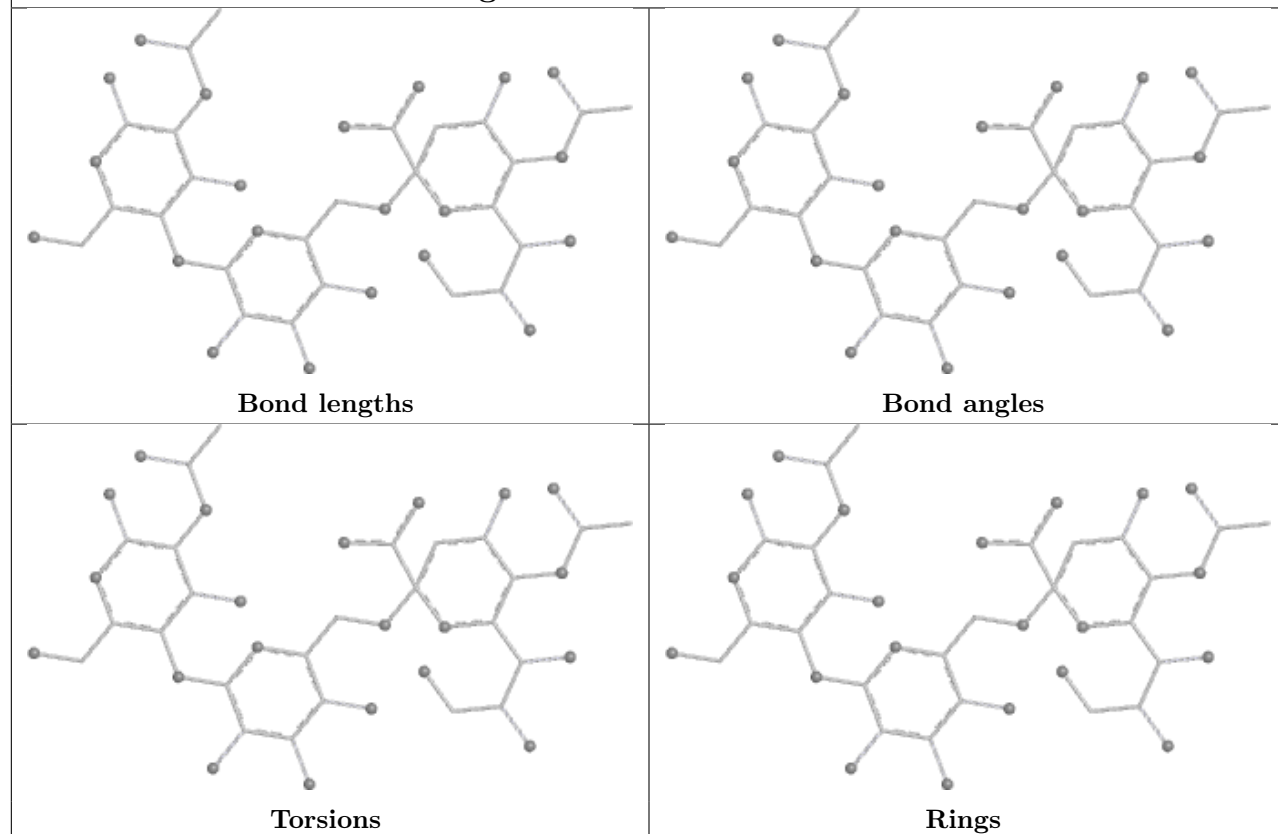
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BbB	2	GLA	1	0

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

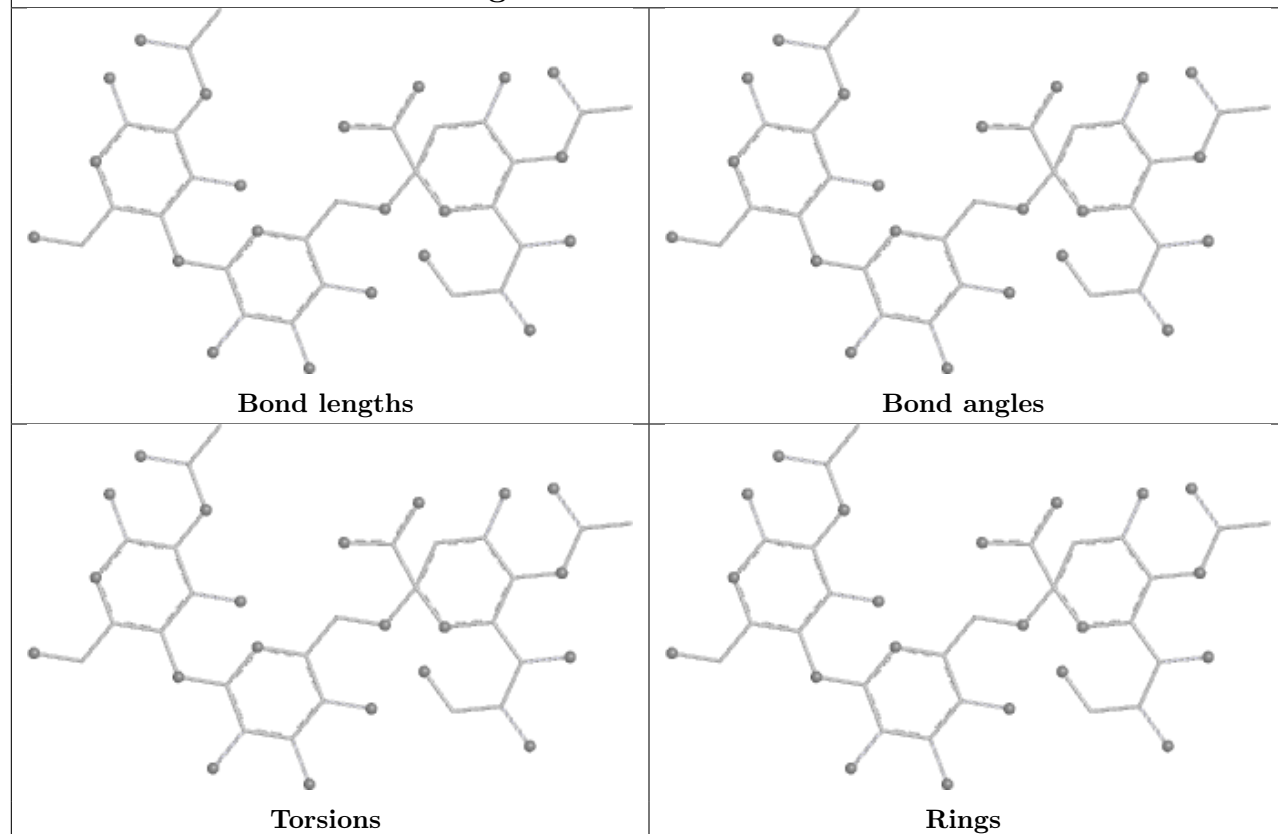


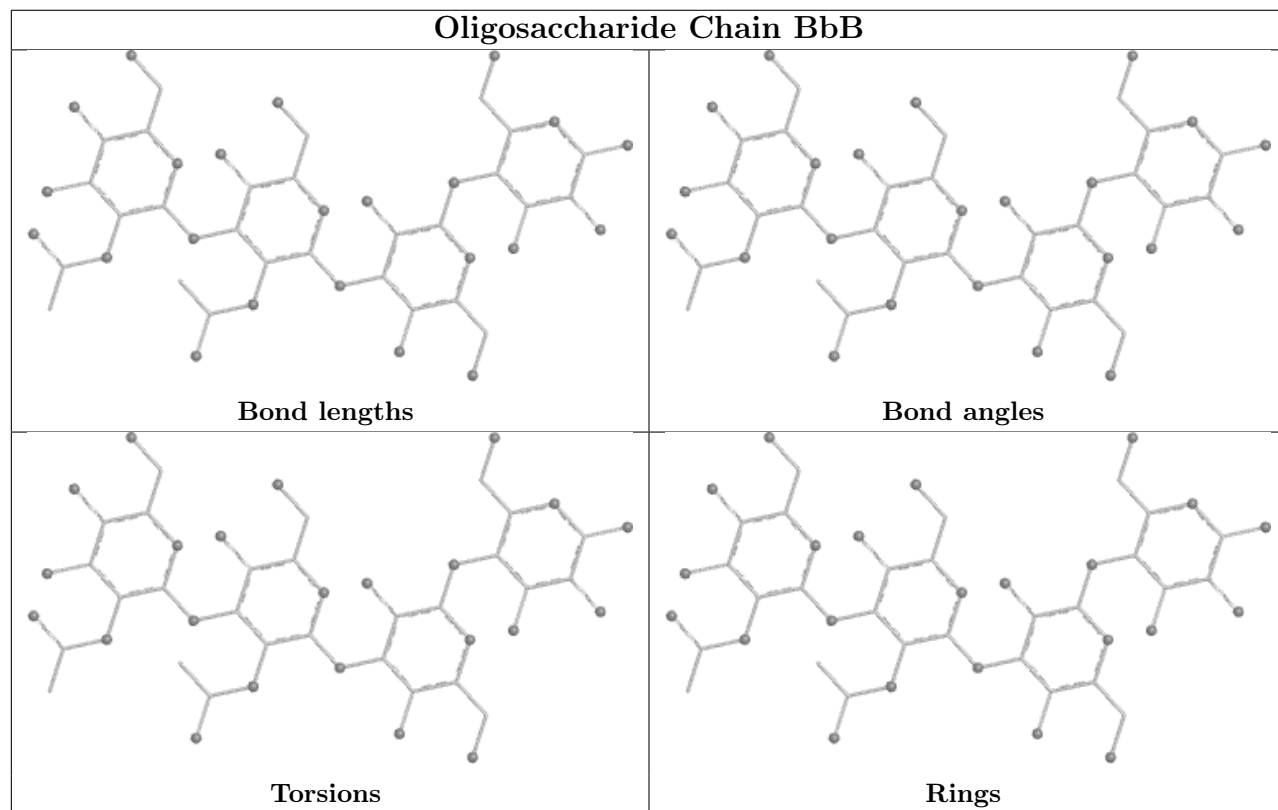
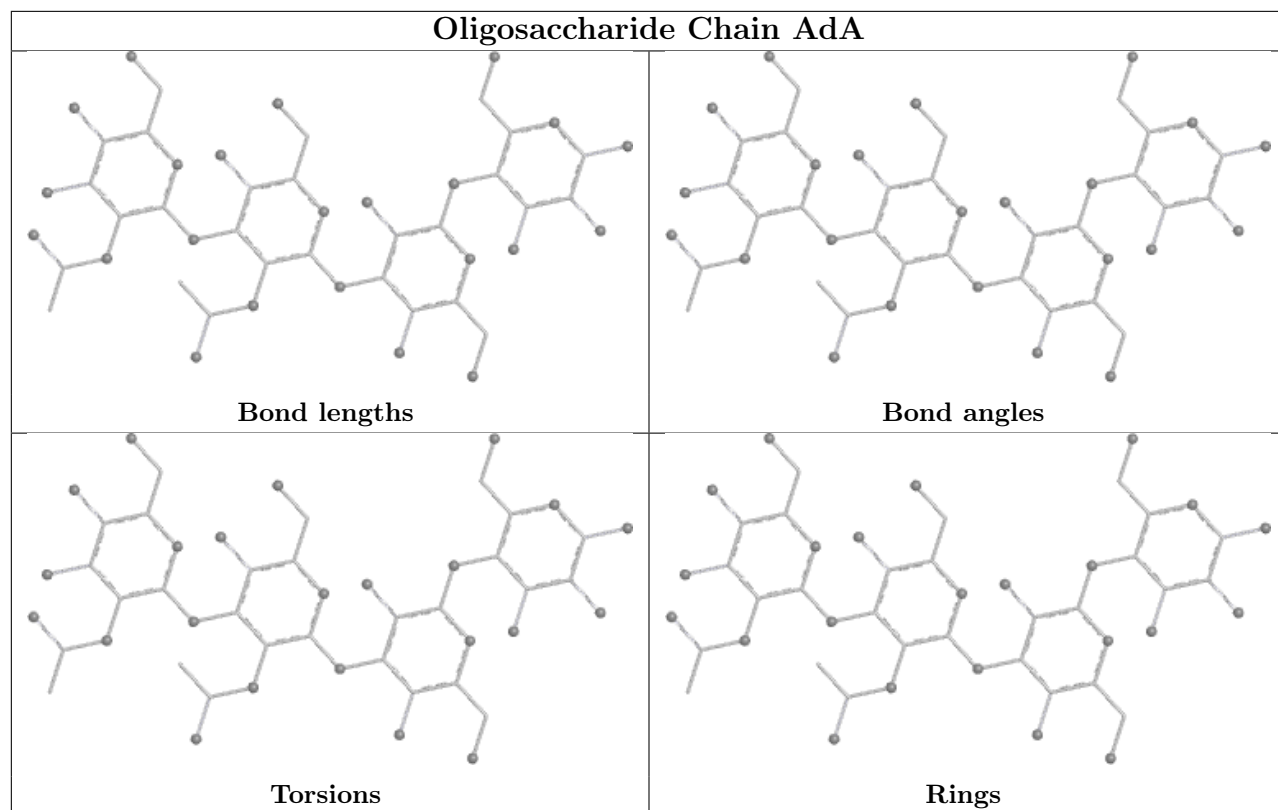


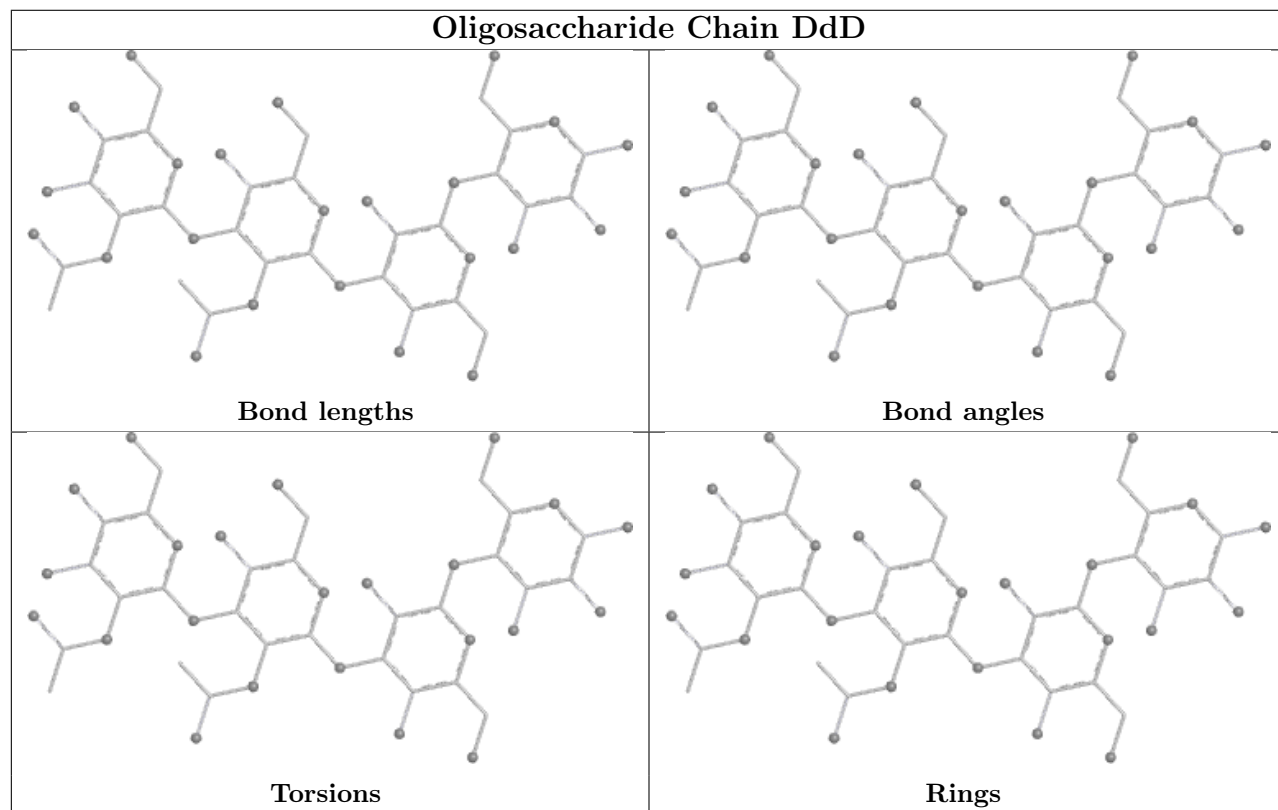
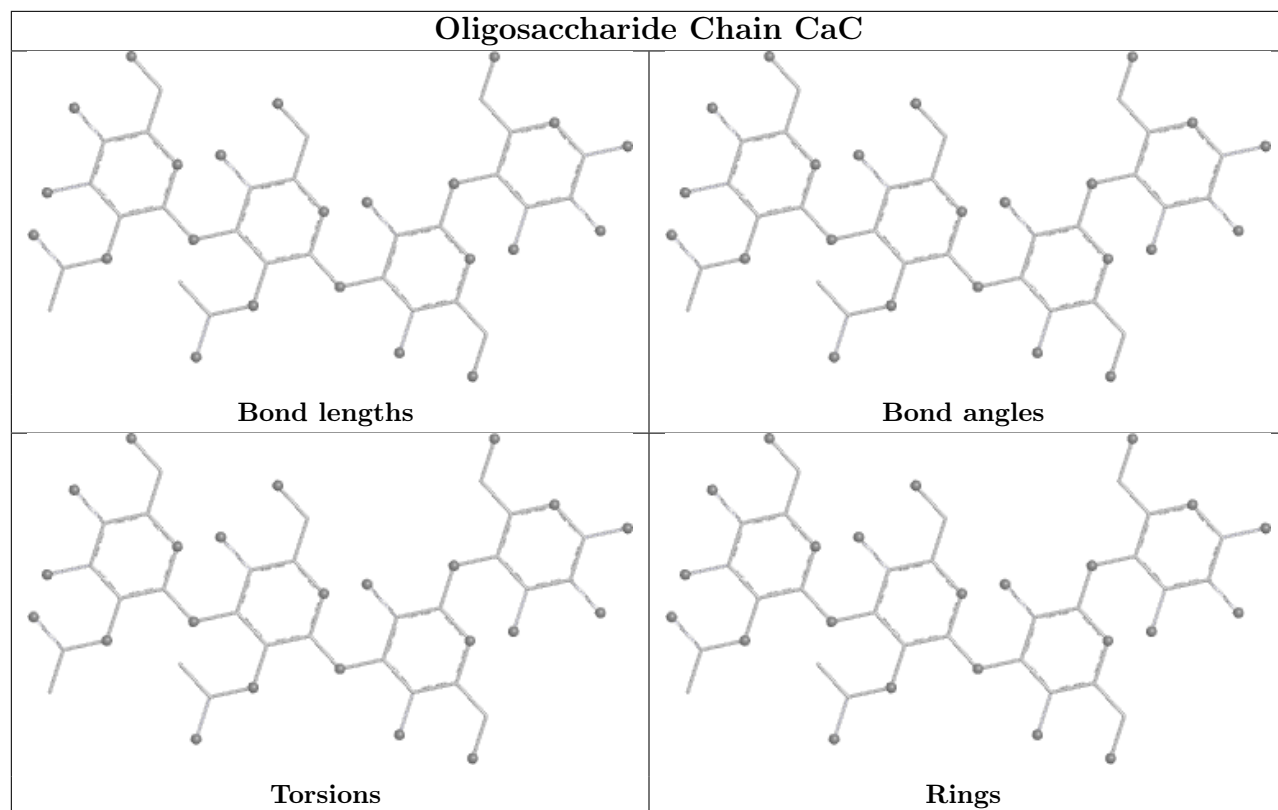
Oligosaccharide Chain HaH

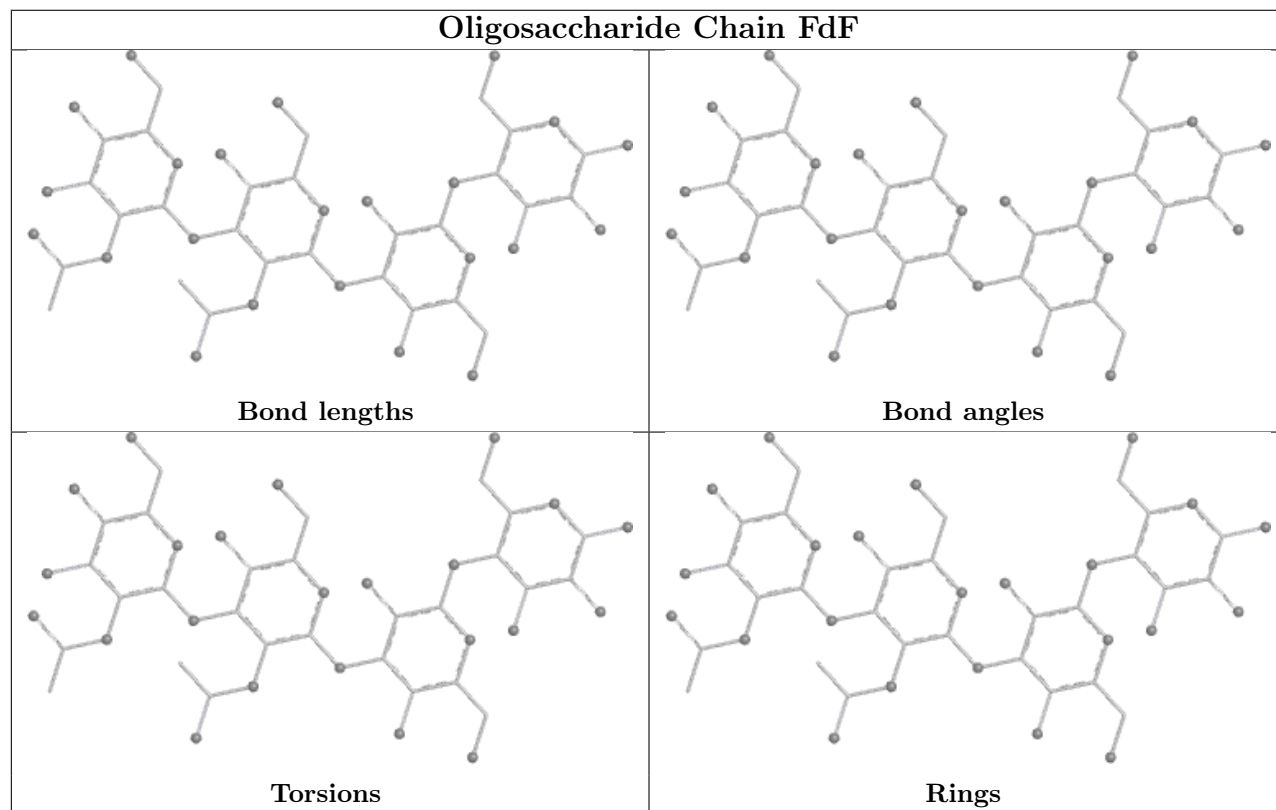
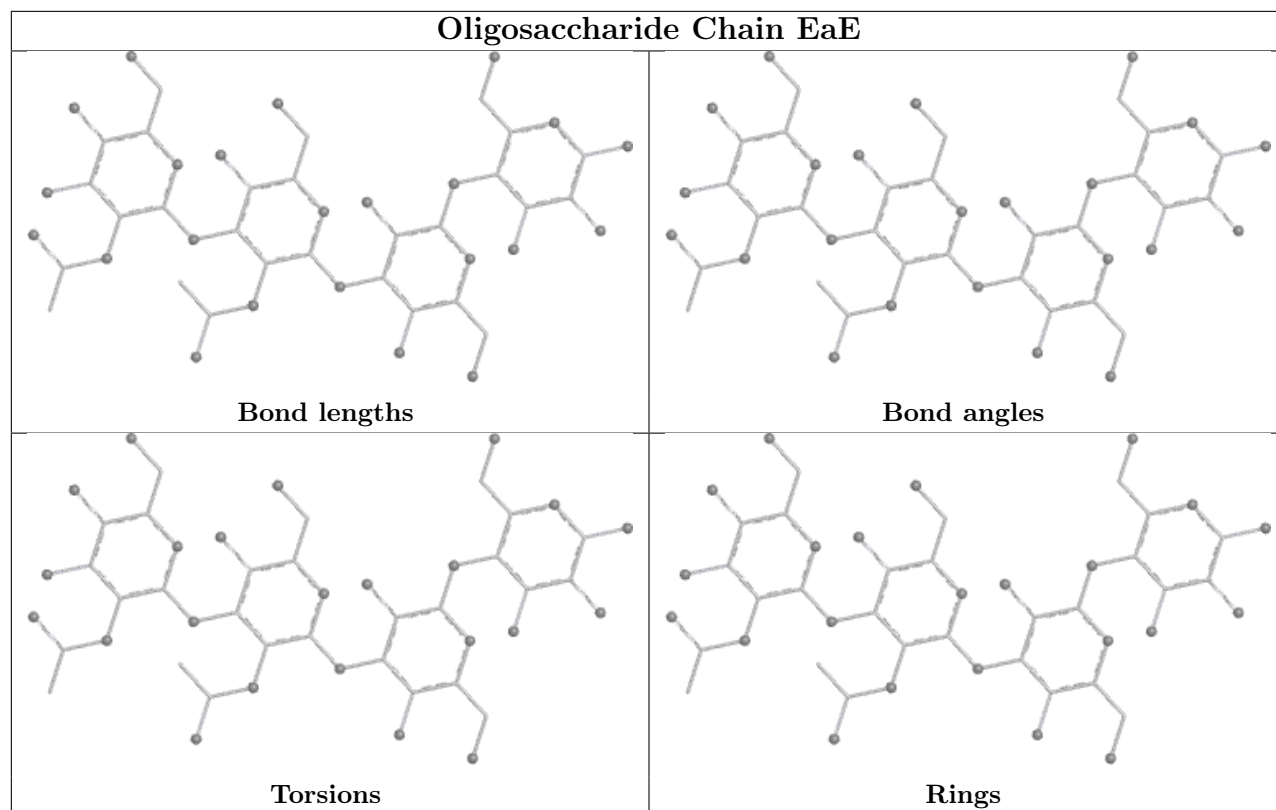


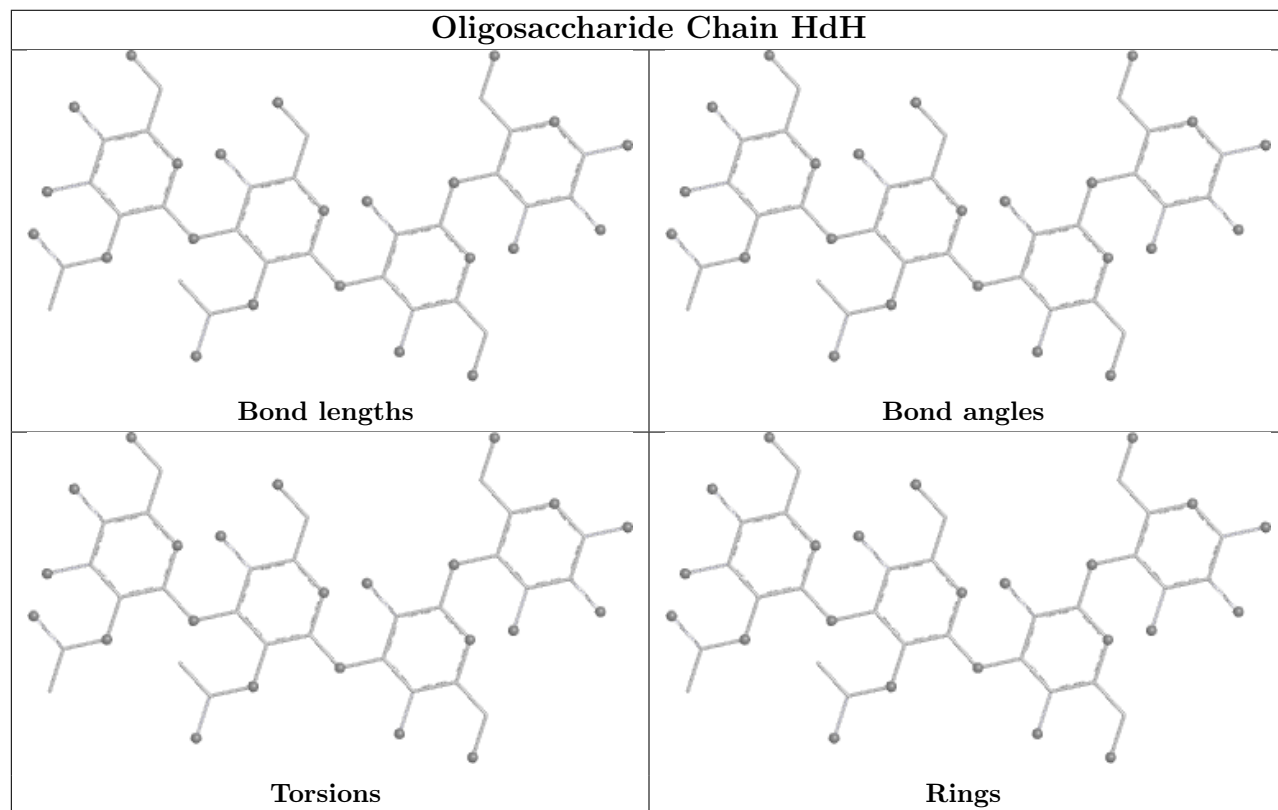
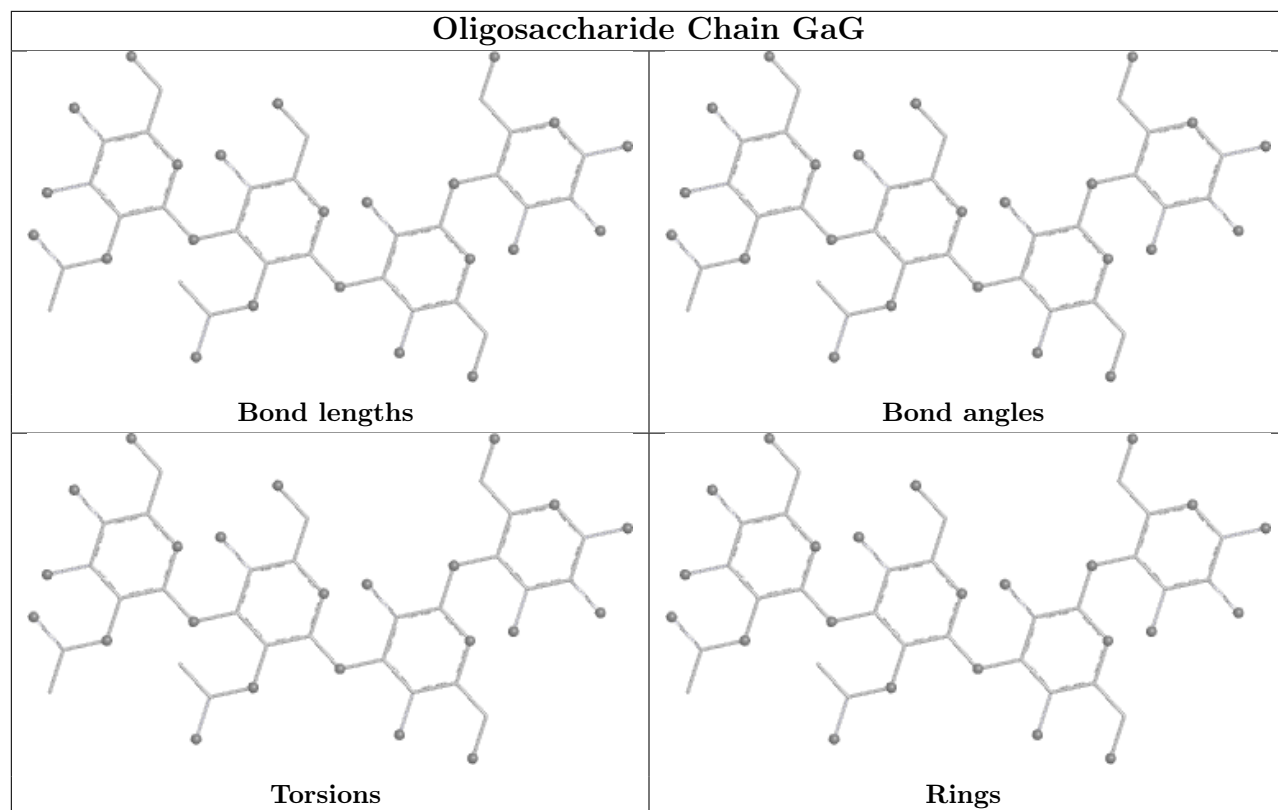
Oligosaccharide Chain JaJ

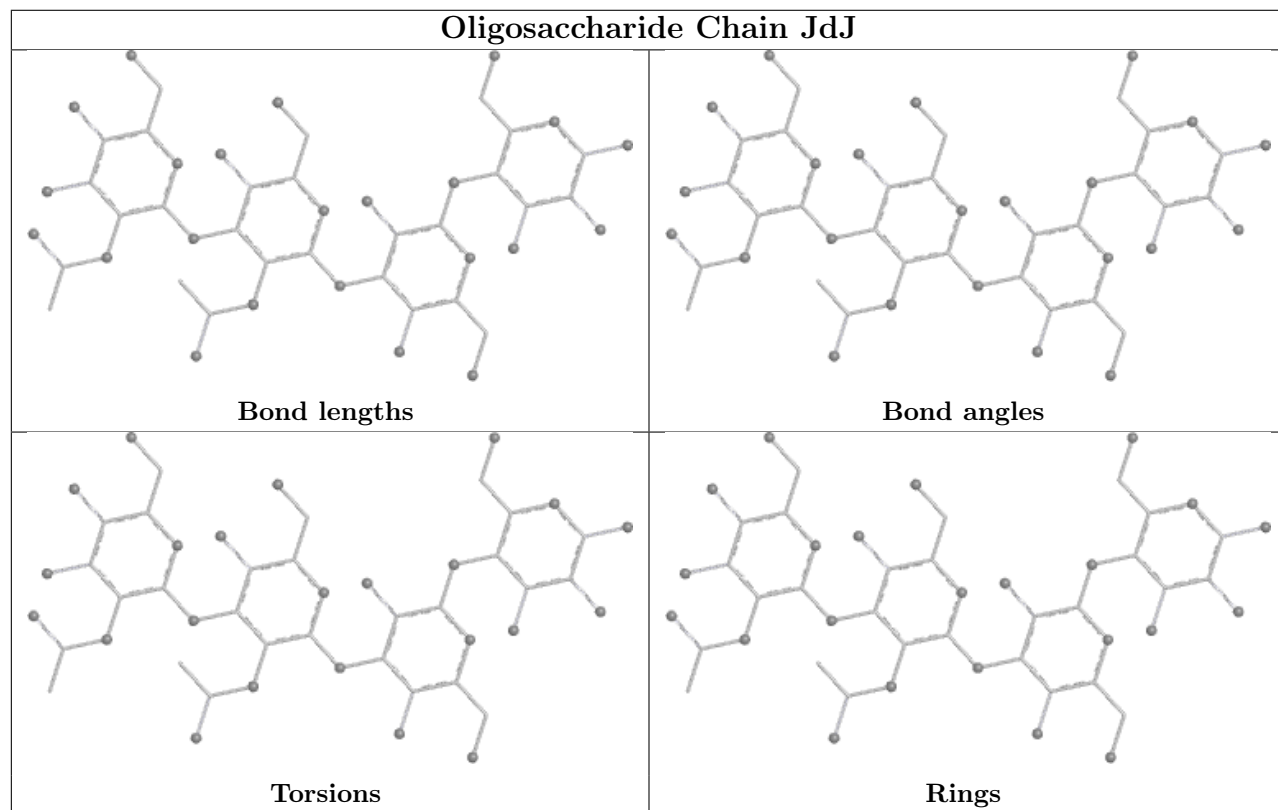
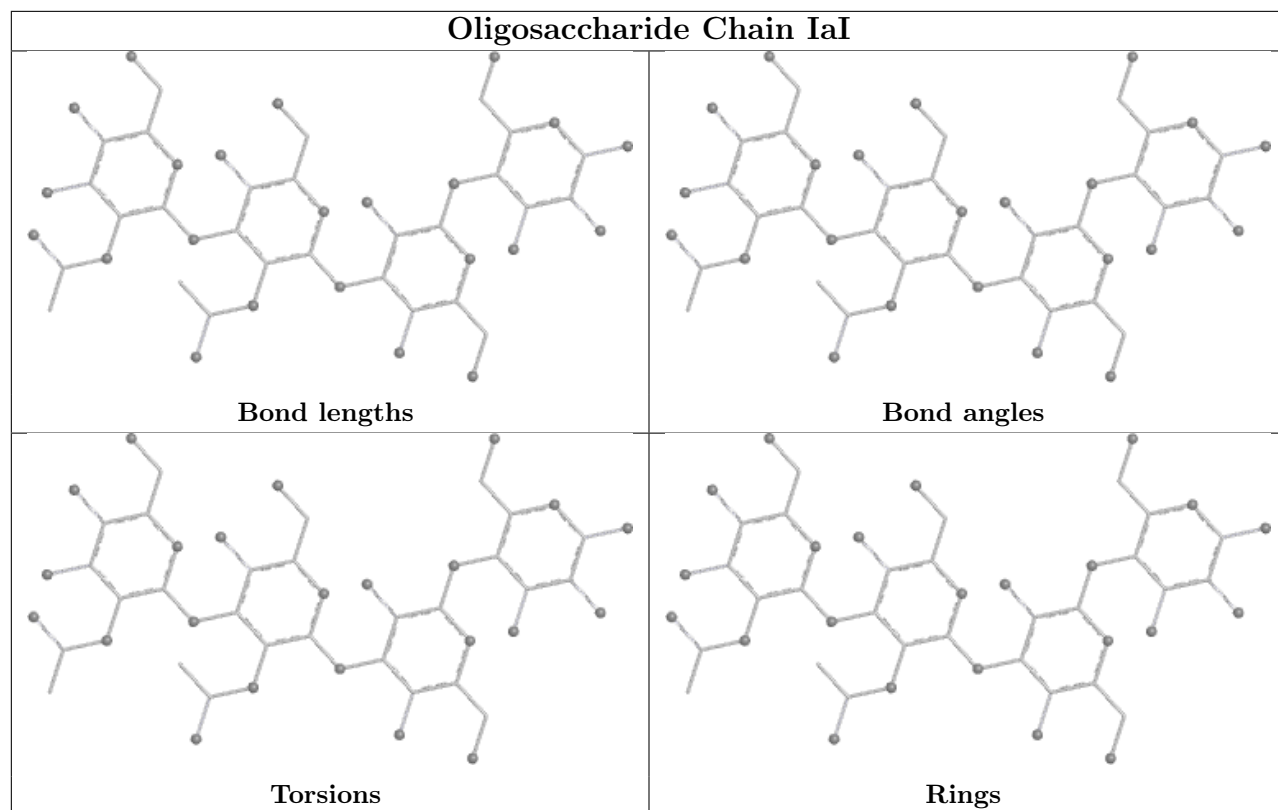












5.6 Ligand geometry

22 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	PEG	DDD	501	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	EEE	502	-	6,6,6	0.19	0	5,5,5	0.17	0
4	EDO	GGG	502	-	3,3,3	0.07	0	2,2,2	0.35	0
5	PEG	CCC	501	-	6,6,6	0.14	0	5,5,5	0.12	0
5	PEG	HHH	503	-	6,6,6	0.16	0	5,5,5	0.09	0
5	PEG	HHH	502	-	6,6,6	0.10	0	5,5,5	0.20	0
4	EDO	FFF	502	-	3,3,3	0.13	0	2,2,2	0.36	0
5	PEG	FFF	501	-	6,6,6	0.33	0	5,5,5	0.20	0
7	PGE	GGG	501	-	9,9,9	0.15	0	8,8,8	0.13	0
5	PEG	AAA	502	-	6,6,6	0.20	0	5,5,5	0.19	0
6	SIA	BBB	301	-	21,21,21	1.53	4 (19%)	24,31,31	2.36	8 (33%)
4	EDO	BBB	303	-	3,3,3	0.31	0	2,2,2	0.44	0
4	EDO	III	503	-	3,3,3	0.09	0	2,2,2	0.16	0
4	EDO	AAA	501	-	3,3,3	0.26	0	2,2,2	0.15	0
5	PEG	BBB	302	-	6,6,6	0.20	0	5,5,5	0.17	0
5	PEG	III	502	-	6,6,6	0.22	0	5,5,5	0.08	0
4	EDO	EEE	501	-	3,3,3	0.14	0	2,2,2	0.21	0
7	PGE	HHH	501	-	9,9,9	0.25	0	8,8,8	0.15	0
4	EDO	III	501	-	3,3,3	0.12	0	2,2,2	0.12	0
5	PEG	BBB	304	-	6,6,6	0.19	0	5,5,5	0.10	0
5	PEG	JJJ	501	-	6,6,6	0.17	0	5,5,5	0.16	0
5	PEG	GGG	503	-	6,6,6	0.17	0	5,5,5	0.09	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
5	PEG	DDD	501	-	-	3/4/4/4	-
5	PEG	EEE	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	GGG	502	-	-	0/1/1/1	-
5	PEG	CCC	501	-	-	2/4/4/4	-
5	PEG	HHH	503	-	-	2/4/4/4	-
5	PEG	HHH	502	-	-	3/4/4/4	-
4	EDO	FFF	502	-	-	1/1/1/1	-
5	PEG	FFF	501	-	-	3/4/4/4	-
7	PGE	GGG	501	-	-	5/7/7/7	-
5	PEG	AAA	502	-	-	3/4/4/4	-
6	SIA	BBB	301	-	-	10/20/38/38	0/1/1/1
4	EDO	BBB	303	-	-	1/1/1/1	-
4	EDO	III	503	-	-	0/1/1/1	-
4	EDO	AAA	501	-	-	0/1/1/1	-
5	PEG	BBB	302	-	-	1/4/4/4	-
5	PEG	III	502	-	-	0/4/4/4	-
4	EDO	EEE	501	-	-	1/1/1/1	-
7	PGE	HHH	501	-	-	3/7/7/7	-
4	EDO	III	501	-	-	0/1/1/1	-
5	PEG	BBB	304	-	-	2/4/4/4	-
5	PEG	JJJ	501	-	-	2/4/4/4	-
5	PEG	GGG	503	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BBB	301	SIA	C2-C1	-3.16	1.49	1.53
6	BBB	301	SIA	O2-C2	3.14	1.44	1.39
6	BBB	301	SIA	C3-C2	2.42	1.55	1.51
6	BBB	301	SIA	C5-N5	2.18	1.49	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	BBB	301	SIA	O2-C2-C1	-6.61	96.76	110.73
6	BBB	301	SIA	O1A-C1-C2	-4.69	116.03	123.85
6	BBB	301	SIA	O6-C6-C5	4.27	113.75	109.84
6	BBB	301	SIA	O2-C2-C3	3.32	114.47	109.44
6	BBB	301	SIA	C4-C5-N5	2.50	115.36	110.44
6	BBB	301	SIA	O6-C6-C7	2.42	110.43	106.65
6	BBB	301	SIA	C5-N5-C10	2.32	128.53	123.11
6	BBB	301	SIA	O10-C10-C11	-2.17	118.18	122.05

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BBB	301	SIA	O1A-C1-C2-O2
6	BBB	301	SIA	O1A-C1-C2-O6
6	BBB	301	SIA	O1B-C1-C2-O6
6	BBB	301	SIA	C6-C7-C8-C9
6	BBB	301	SIA	O7-C7-C8-C9
6	BBB	301	SIA	C7-C8-C9-O9
6	BBB	301	SIA	O8-C8-C9-O9
6	BBB	301	SIA	C6-C7-C8-O8
7	GGG	501	PGE	O2-C3-C4-O3
7	HHH	501	PGE	O2-C3-C4-O3
6	BBB	301	SIA	O7-C7-C8-O8
5	AAA	502	PEG	O1-C1-C2-O2
5	FFF	501	PEG	O2-C3-C4-O4
5	HHH	503	PEG	O1-C1-C2-O2
5	BBB	304	PEG	O1-C1-C2-O2
5	FFF	501	PEG	O1-C1-C2-O2
7	HHH	501	PGE	O3-C5-C6-O4
5	HHH	503	PEG	O2-C3-C4-O4
7	GGG	501	PGE	O1-C1-C2-O2
4	FFF	502	EDO	O1-C1-C2-O2
5	HHH	502	PEG	O1-C1-C2-O2
5	DDD	501	PEG	O2-C3-C4-O4
5	HHH	502	PEG	O2-C3-C4-O4
5	DDD	501	PEG	C1-C2-O2-C3
5	HHH	502	PEG	C1-C2-O2-C3
5	GGG	503	PEG	C4-C3-O2-C2
5	EEE	502	PEG	O2-C3-C4-O4
5	JJJ	501	PEG	C4-C3-O2-C2
5	AAA	502	PEG	C1-C2-O2-C3
7	GGG	501	PGE	C4-C3-O2-C2
5	BBB	302	PEG	C1-C2-O2-C3
5	CCC	501	PEG	C4-C3-O2-C2
5	DDD	501	PEG	O1-C1-C2-O2
5	GGG	503	PEG	C1-C2-O2-C3
5	AAA	502	PEG	O2-C3-C4-O4
5	EEE	502	PEG	C1-C2-O2-C3
7	GGG	501	PGE	C6-C5-O3-C4
4	BBB	303	EDO	O1-C1-C2-O2
7	GGG	501	PGE	C3-C4-O3-C5
5	FFF	501	PEG	C1-C2-O2-C3

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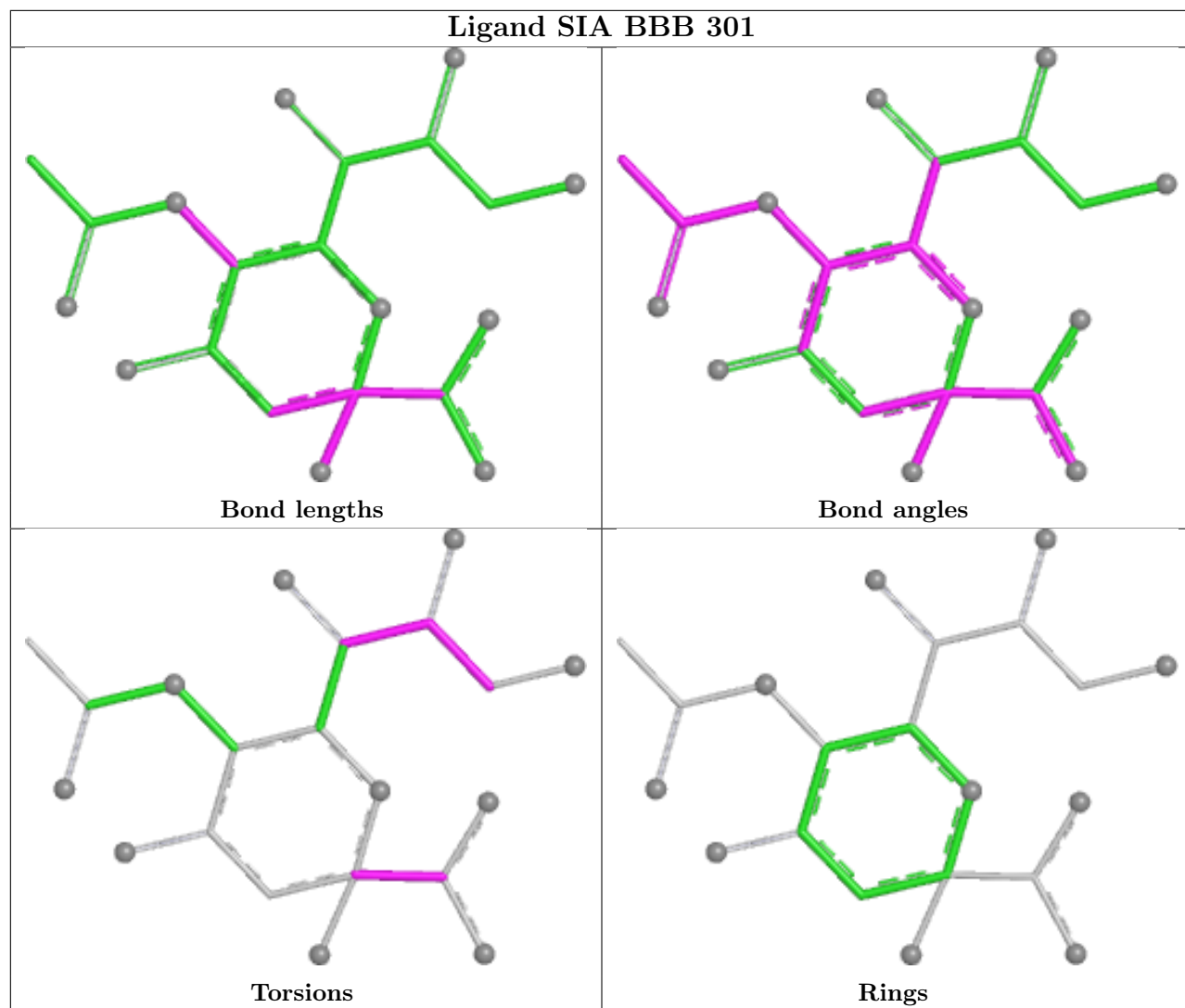
Mol	Chain	Res	Type	Atoms
5	JJJ	501	PEG	O1-C1-C2-O2
4	EEE	501	EDO	O1-C1-C2-O2
5	BBB	304	PEG	C1-C2-O2-C3
6	BBB	301	SIA	O1B-C1-C2-O2
7	HHH	501	PGE	C6-C5-O3-C4
5	GGG	503	PEG	O2-C3-C4-O4
5	CCC	501	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	301	SIA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	AAA	269/276 (97%)	-1.28	0 100 100	21, 26, 44, 61	0
1	BBB	263/276 (95%)	-1.25	0 100 100	19, 28, 51, 65	0
1	CCC	264/276 (95%)	-1.29	0 100 100	18, 25, 49, 73	0
1	DDD	269/276 (97%)	-1.31	0 100 100	13, 25, 45, 59	1 (0%)
1	EEE	263/276 (95%)	-1.29	0 100 100	20, 25, 48, 75	0
1	FFF	262/276 (94%)	-1.23	0 100 100	19, 28, 51, 68	1 (0%)
1	GGG	263/276 (95%)	-1.28	0 100 100	19, 25, 46, 64	0
1	HHH	270/276 (97%)	-1.31	0 100 100	18, 24, 45, 68	0
1	III	261/276 (94%)	-1.28	0 100 100	19, 25, 46, 69	0
1	JJJ	270/276 (97%)	-1.29	0 100 100	20, 26, 44, 60	0
All	All	2654/2760 (96%)	-1.28	0 100 100	13, 26, 47, 75	2 (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	NAG	AaA	1	15/15	-	-	48,53,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	AaA	2	11/12	-	-	38,50,54,56	0
2	SIA	AaA	3	20/21	-	-	26,29,35,36	0
2	NAG	DaD	1	15/15	-	-	49,57,61,61	0
2	GAL	DaD	2	11/12	-	-	32,40,48,48	0
2	SIA	DaD	3	20/21	-	-	20,29,34,35	0
2	NAG	FaF	1	15/15	-	-	55,63,67,72	0
2	GAL	FaF	2	11/12	-	-	49,57,62,66	0
2	SIA	FaF	3	20/21	-	-	28,34,37,38	0
2	NAG	HaH	1	15/15	-	-	50,55,61,65	0
2	GAL	HaH	2	11/12	-	-	38,45,56,60	0
2	SIA	HaH	3	20/21	-	-	21,28,35,36	0
2	NAG	JaJ	1	15/15	-	-	51,54,59,62	0
2	GAL	JaJ	2	11/12	-	-	37,53,61,64	0
2	SIA	JaJ	3	20/21	-	-	23,31,35,40	0
3	GAL	AdA	1	12/12	-	-	36,48,51,52	0
3	GLA	AdA	2	11/12	-	-	24,27,30,33	0
3	NGA	AdA	3	14/15	-	-	24,27,30,33	0
3	A2G	AdA	4	14/15	-	-	25,28,31,37	0
3	GAL	BbB	1	12/12	-	-	36,46,50,55	0
3	GLA	BbB	2	11/12	-	-	26,29,31,33	0
3	NGA	BbB	3	14/15	-	-	22,24,26,27	0
3	A2G	BbB	4	14/15	-	-	24,26,33,38	0
3	GAL	CaC	1	12/12	-	-	23,29,36,47	0
3	GLA	CaC	2	11/12	-	-	19,22,23,23	0
3	NGA	CaC	3	14/15	-	-	20,23,26,27	0
3	A2G	CaC	4	14/15	-	-	20,22,25,33	0
3	GAL	DdD	1	12/12	-	-	33,41,49,49	0
3	GLA	DdD	2	11/12	-	-	22,26,27,30	0
3	NGA	DdD	3	14/15	-	-	20,23,26,28	0
3	A2G	DdD	4	14/15	-	-	23,24,27,28	0
3	GAL	EaE	1	12/12	-	-	27,33,39,44	0
3	GLA	EaE	2	11/12	-	-	21,24,25,26	0
3	NGA	EaE	3	14/15	-	-	22,25,27,29	0
3	A2G	EaE	4	14/15	-	-	24,26,28,34	0
3	GAL	FdF	1	12/12	-	-	34,40,48,49	0
3	GLA	FdF	2	11/12	-	-	27,30,31,33	0
3	NGA	FdF	3	14/15	-	-	27,29,32,32	0
3	A2G	FdF	4	14/15	-	-	26,28,35,37	0
3	GAL	GaG	1	12/12	-	-	29,34,38,42	0
3	GLA	GaG	2	11/12	-	-	20,22,25,26	0
3	NGA	GaG	3	14/15	-	-	20,23,26,27	0
3	A2G	GaG	4	14/15	-	-	21,25,30,31	0

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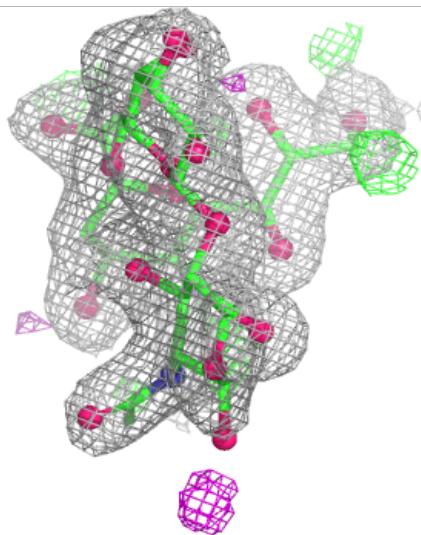
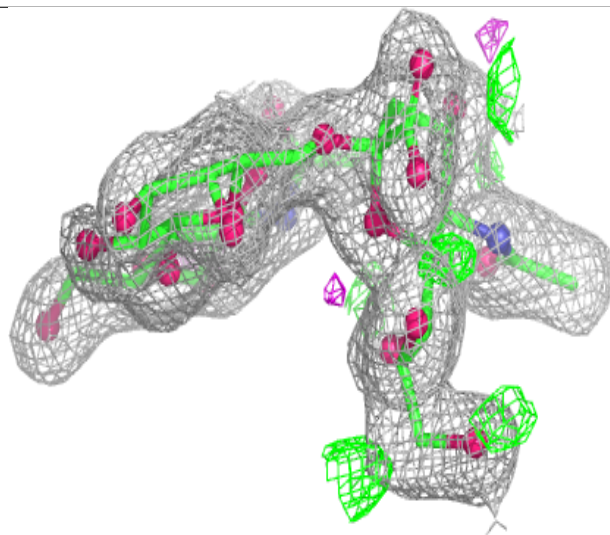
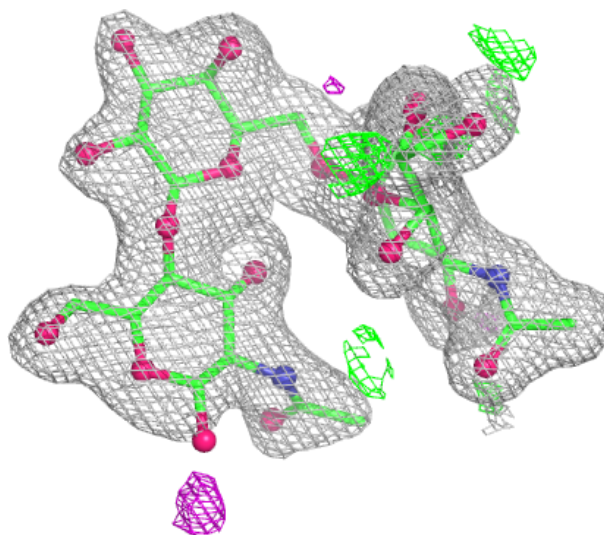
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	HdH	1	12/12	-	-	31,37,41,43	0
3	GLA	HdH	2	11/12	-	-	22,24,27,28	0
3	NGA	HdH	3	14/15	-	-	19,23,24,25	0
3	A2G	HdH	4	14/15	-	-	19,25,35,39	0
3	GAL	IaI	1	12/12	-	-	28,33,39,41	0
3	GLA	IaI	2	11/12	-	-	23,24,25,26	0
3	NGA	IaI	3	14/15	-	-	22,23,27,27	0
3	A2G	IaI	4	14/15	-	-	24,26,30,34	0
3	GAL	JdJ	1	12/12	-	-	36,42,50,50	0
3	GLA	JdJ	2	11/12	-	-	27,31,34,35	0
3	NGA	JdJ	3	14/15	-	-	26,27,28,29	0
3	A2G	JdJ	4	14/15	-	-	26,29,38,42	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.

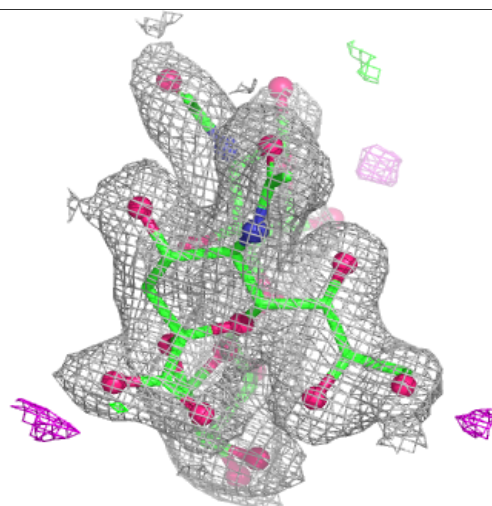
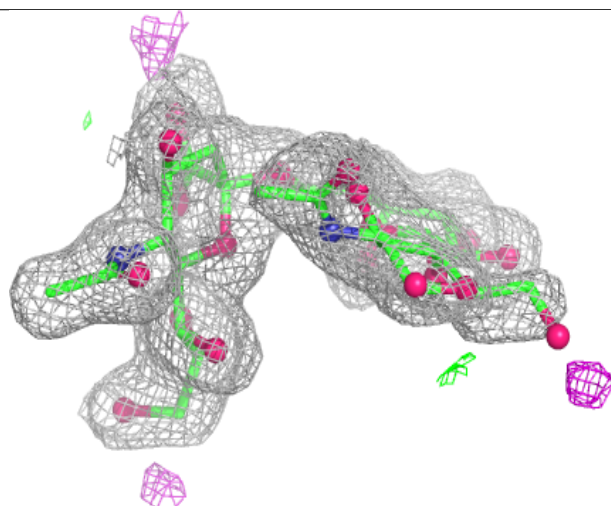
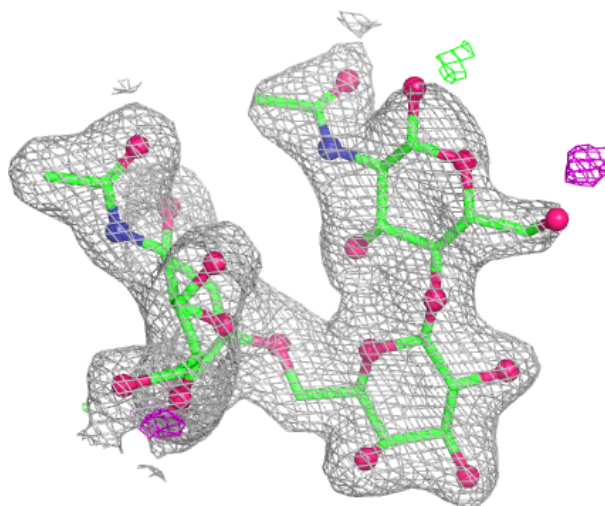
Electron density around Chain AaA:

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



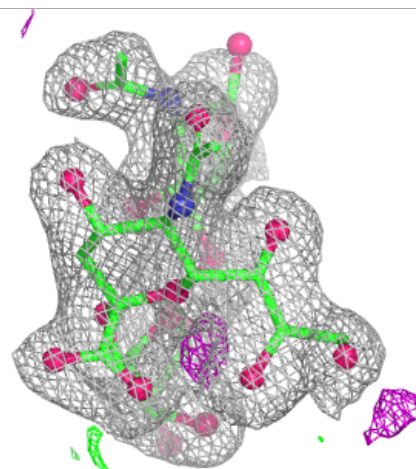
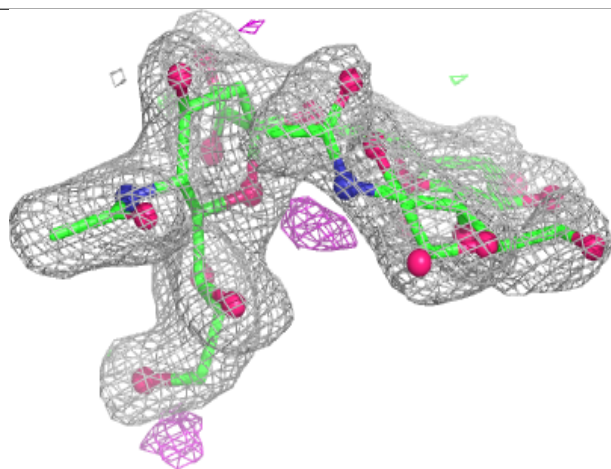
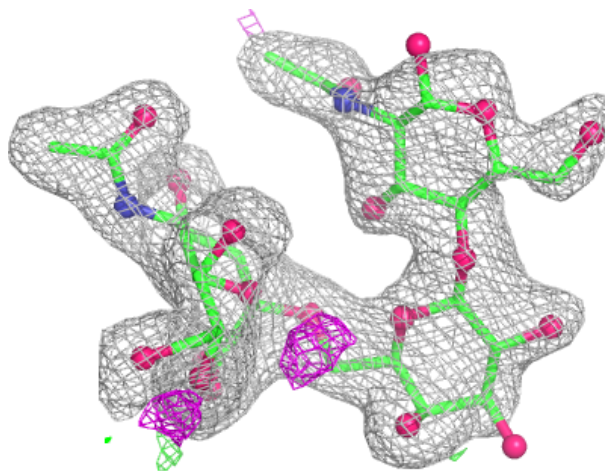
Electron density around Chain DaD:

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



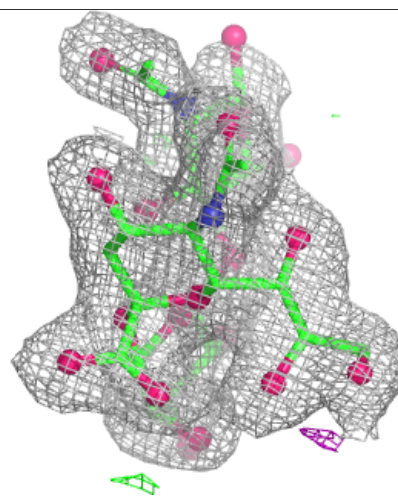
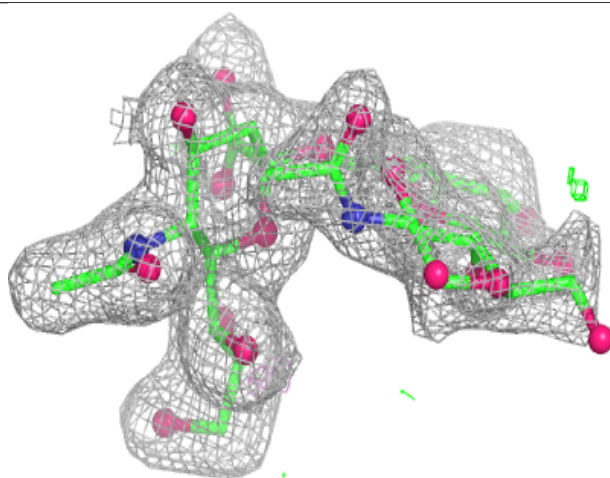
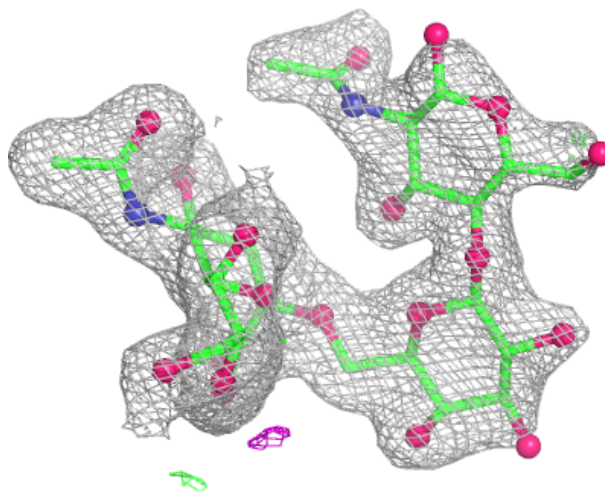
Electron density around Chain FaF:

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



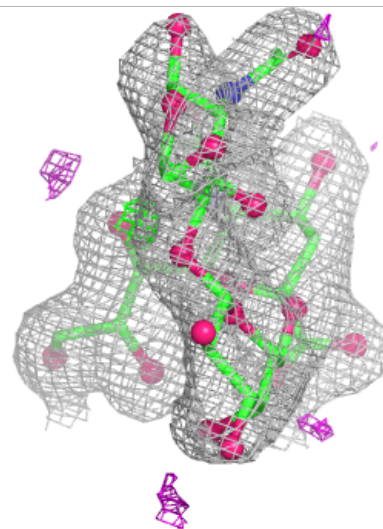
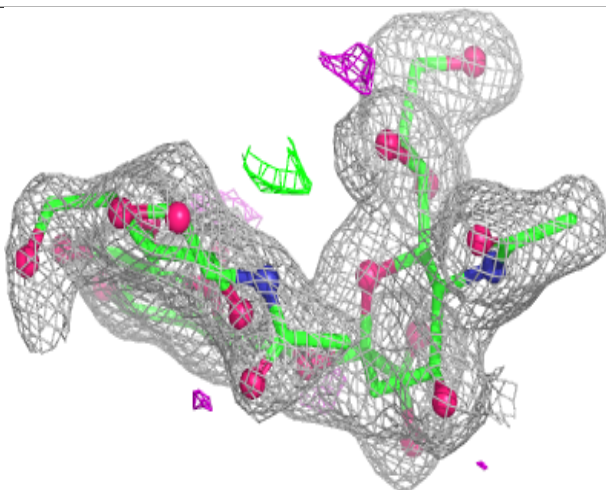
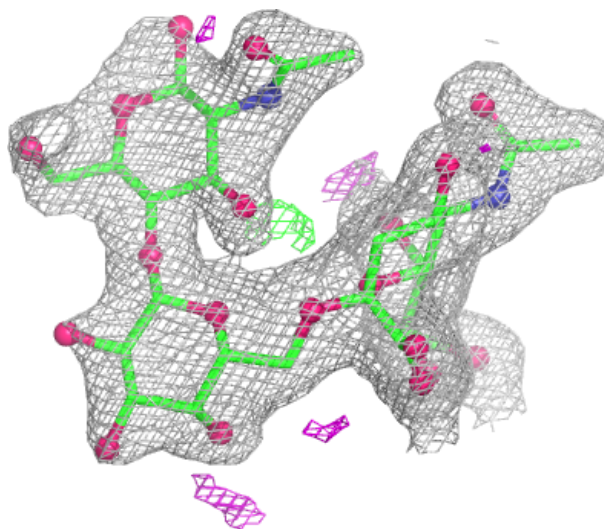
Electron density around Chain HaH:

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



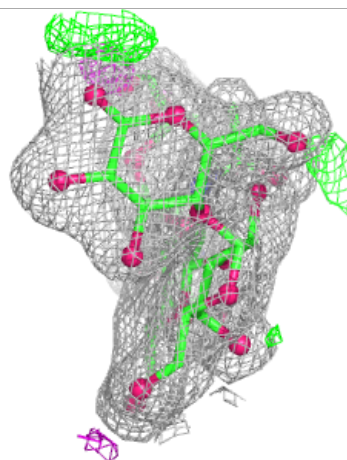
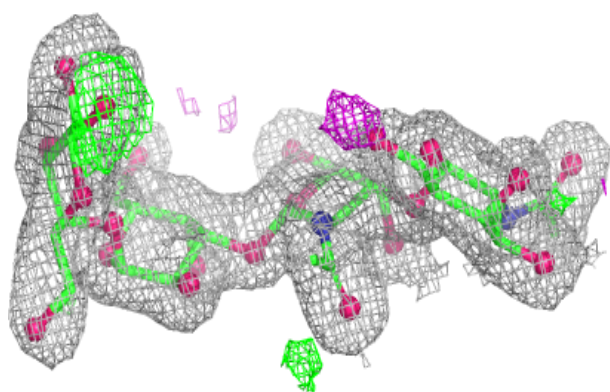
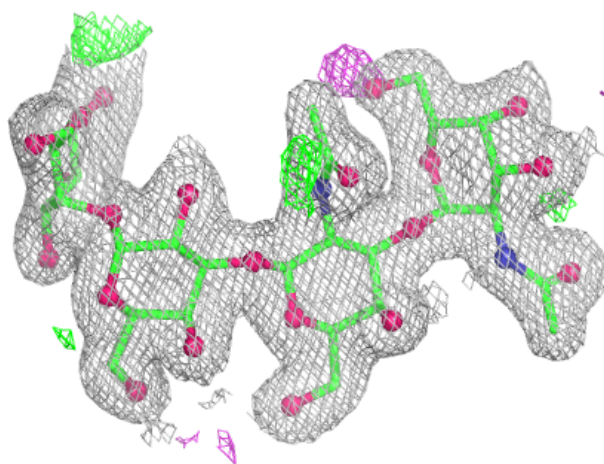
Electron density around Chain JaJ:

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



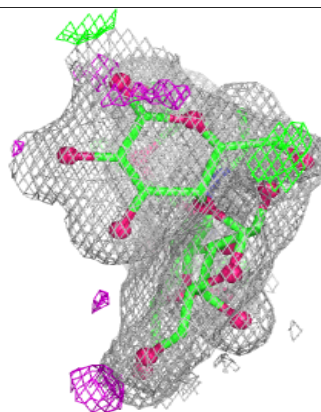
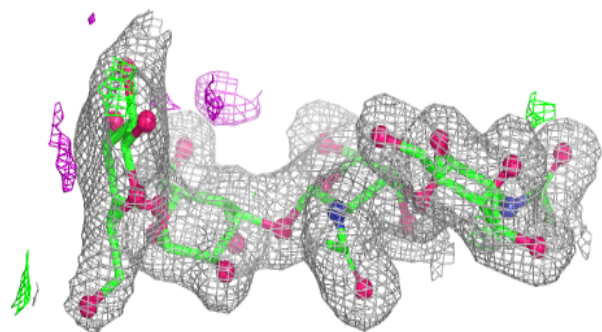
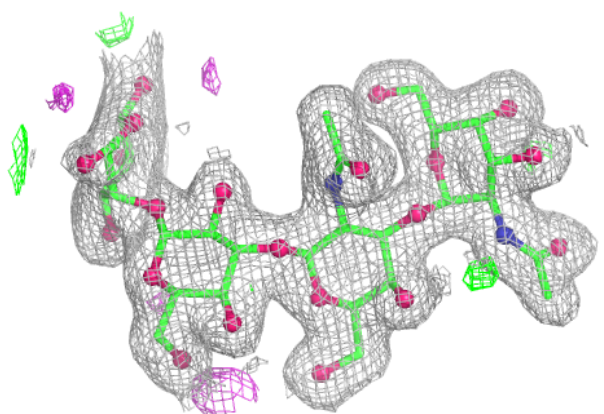
Electron density around Chain AdA:

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



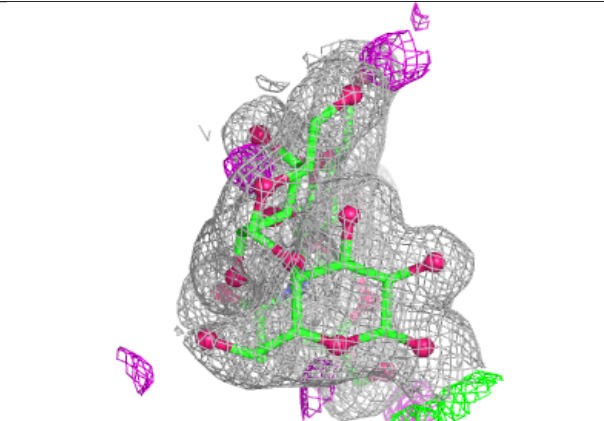
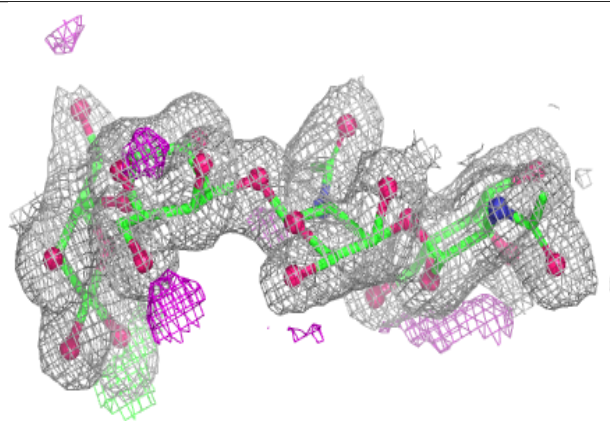
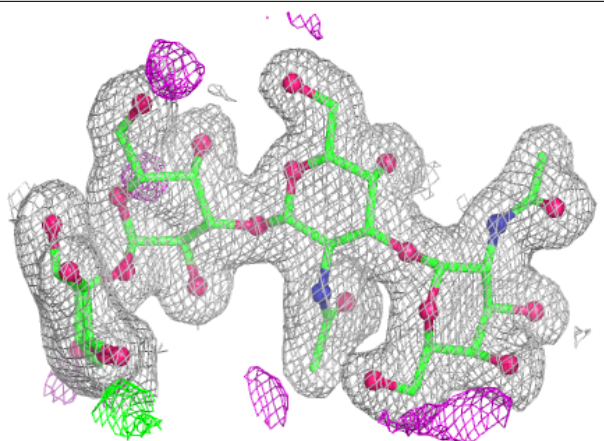
Electron density around Chain BbB:

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



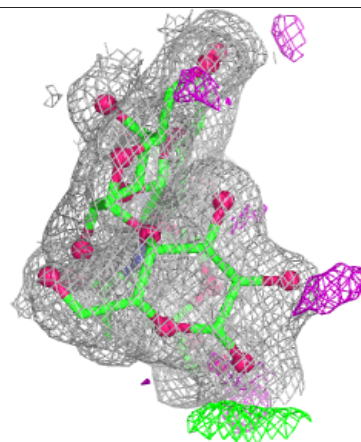
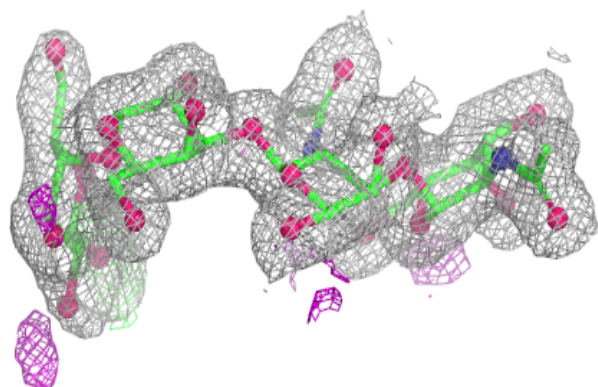
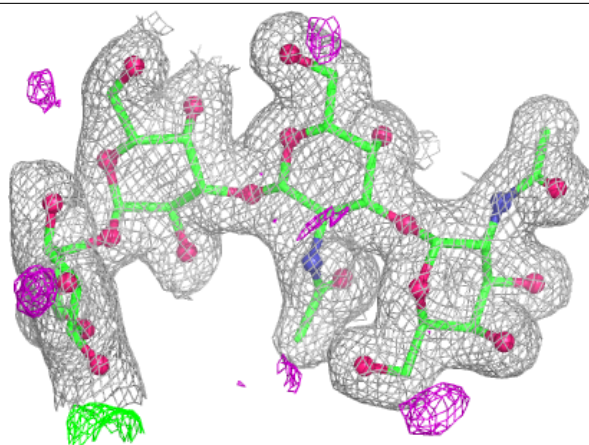
Electron density around Chain CaC:

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



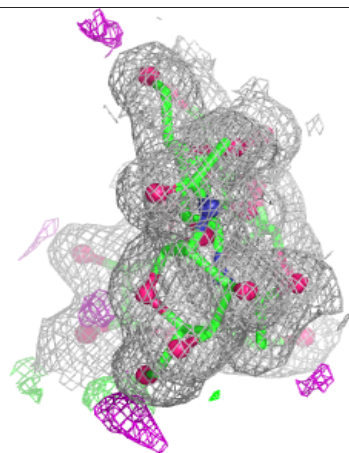
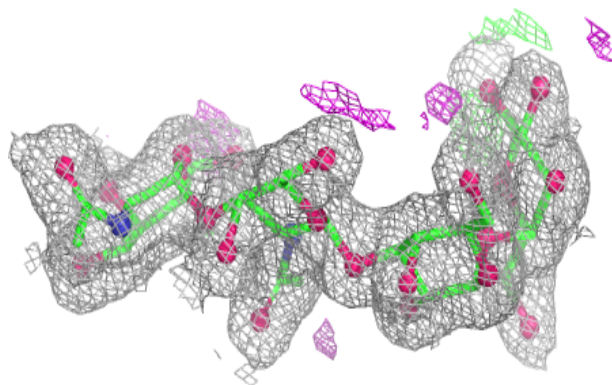
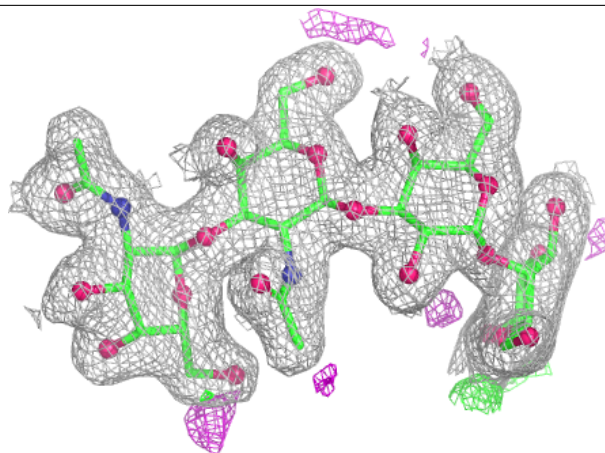
Electron density around Chain DdD:

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



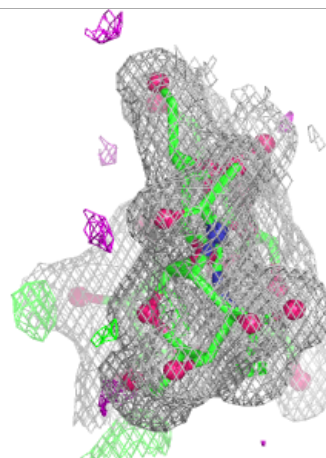
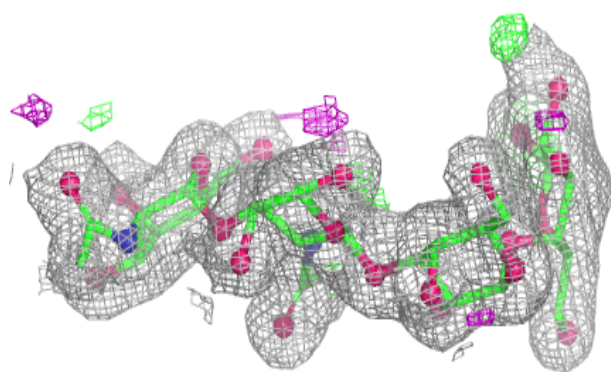
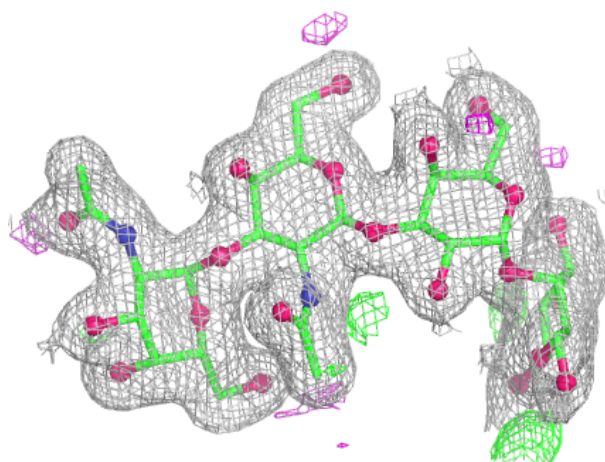
Electron density around Chain EaE:

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



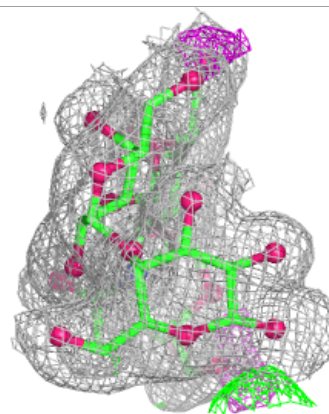
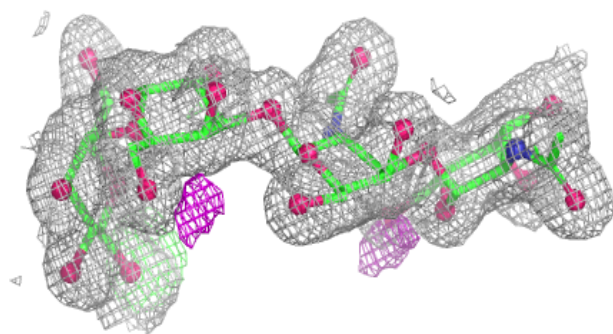
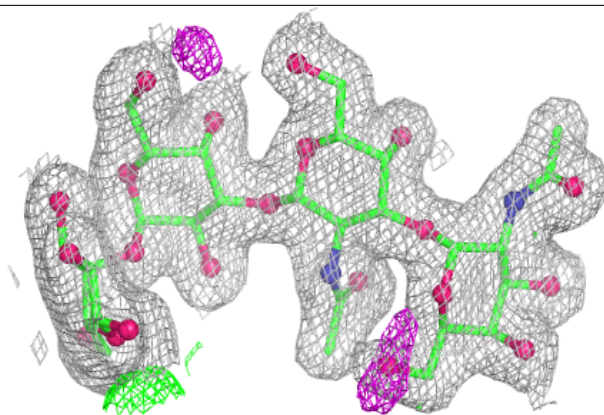
Electron density around Chain FdF:

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



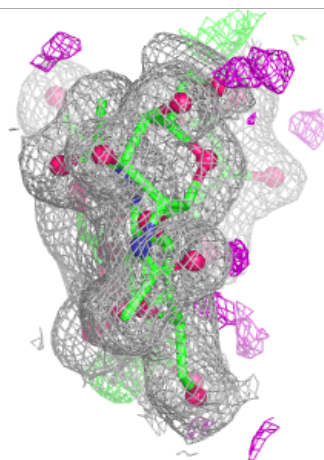
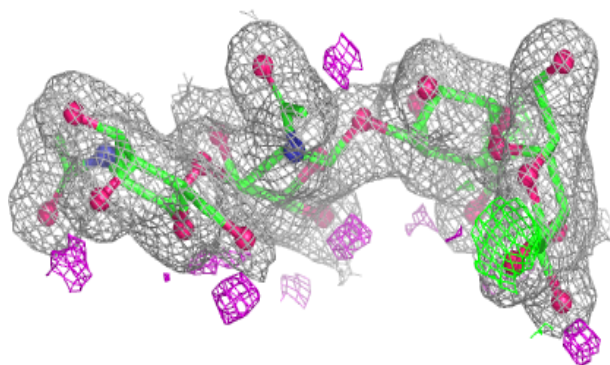
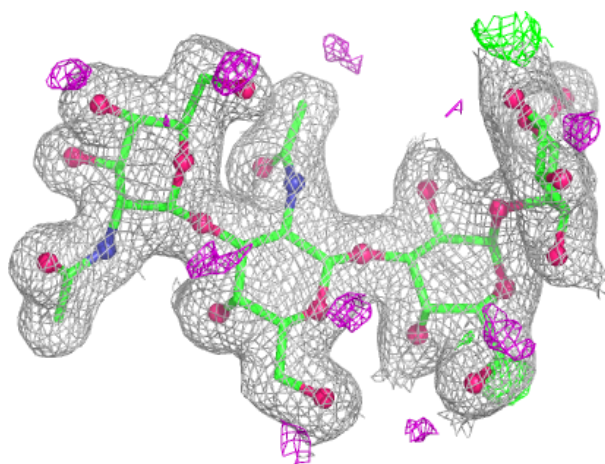
Electron density around Chain GaG:

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



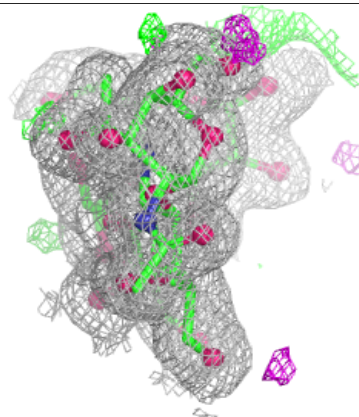
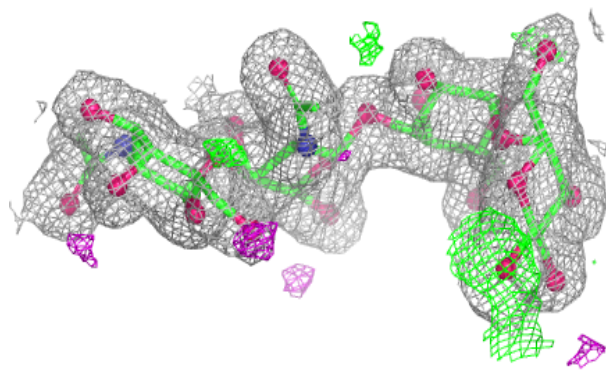
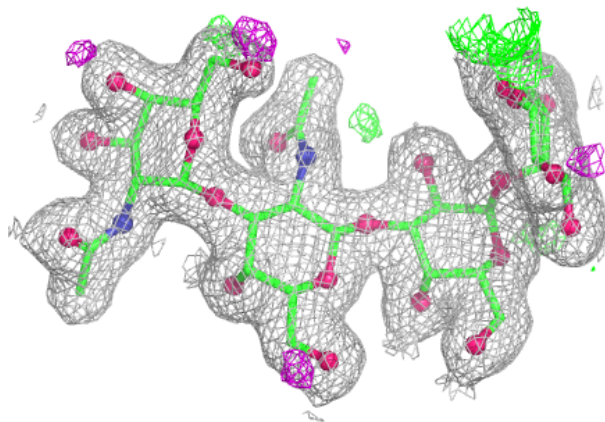
Electron density around Chain HdH:

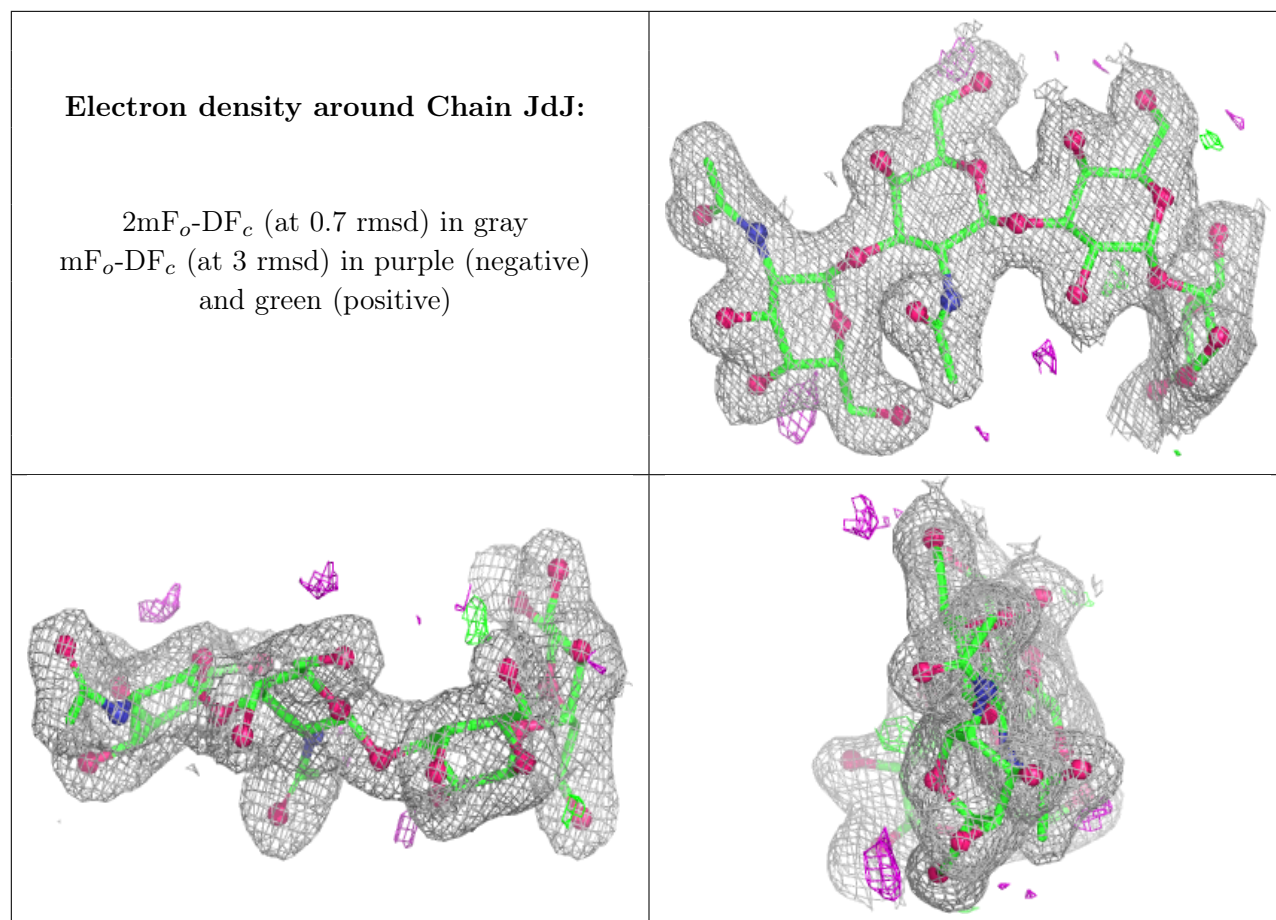
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain IaI:

$2mF_o-DF_c$ (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.

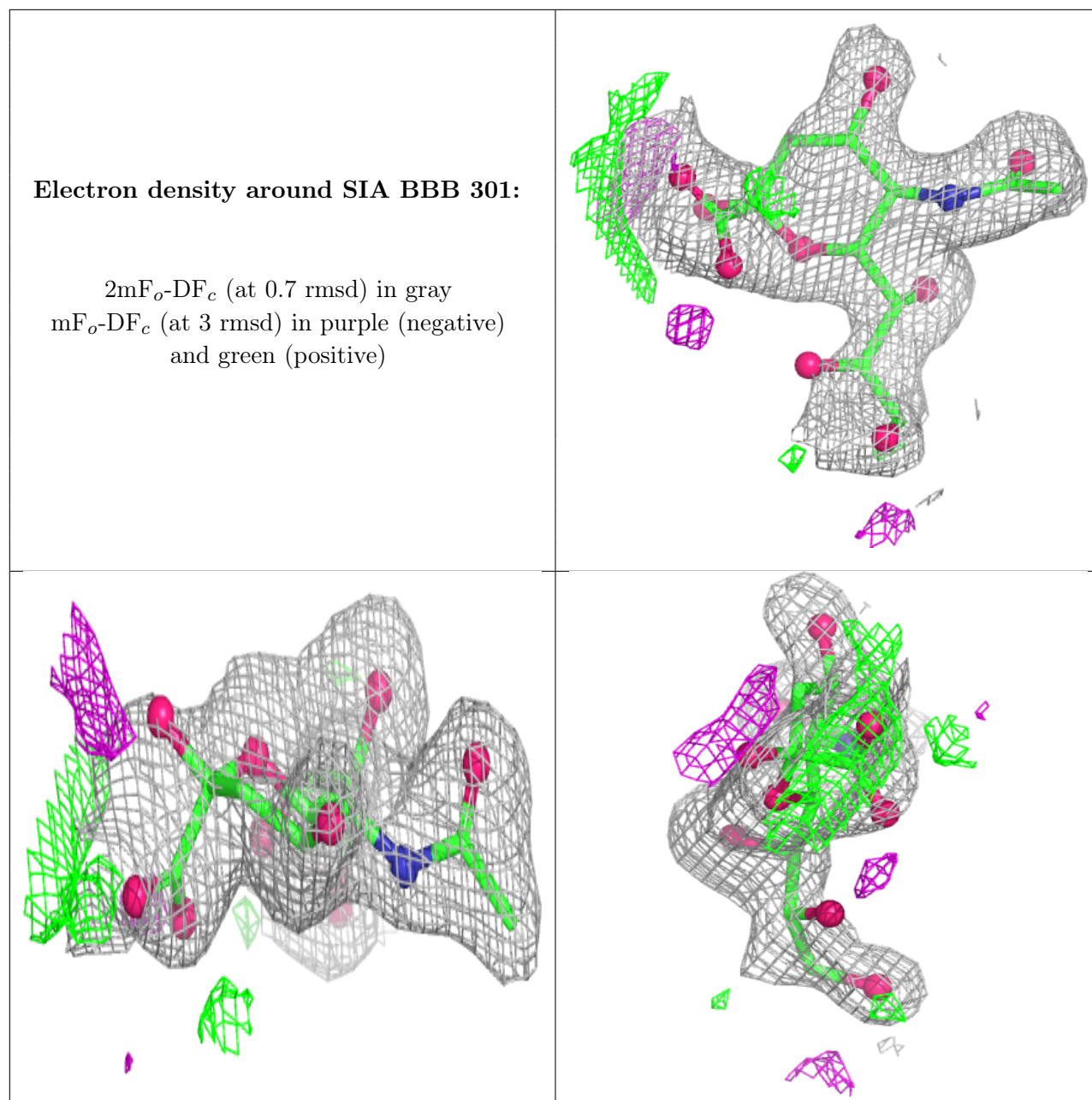
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	HHH	503	7/7	0.96	0.08	68,68,71,72	0
4	EDO	III	501	4/4	0.97	0.07	45,49,50,57	0
4	EDO	III	503	4/4	0.97	0.07	44,44,44,50	0
5	PEG	BBB	304	7/7	0.97	0.07	49,54,63,66	0
5	PEG	CCC	501	7/7	0.97	0.08	54,58,60,60	0
4	EDO	GGG	502	4/4	0.97	0.09	48,49,49,53	0
5	PEG	III	502	7/7	0.97	0.07	44,47,54,56	0
4	EDO	BBB	303	4/4	0.98	0.06	39,42,46,49	0
5	PEG	EEE	502	7/7	0.98	0.05	45,49,51,55	0
5	PEG	GGG	503	7/7	0.98	0.07	60,62,67,67	0
5	PEG	HHH	502	7/7	0.98	0.05	47,51,54,54	0
5	PEG	AAA	502	7/7	0.98	0.06	50,51,53,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	FFF	502	4/4	0.98	0.08	45,46,47,47	0
6	SIA	BBB	301	21/21	0.98	0.05	27,43,56,60	0
7	PGE	GGG	501	10/10	0.98	0.07	45,50,53,53	0
4	EDO	AAA	501	4/4	0.99	0.06	43,45,47,47	0
5	PEG	DDD	501	7/7	0.99	0.05	55,58,63,70	0
5	PEG	BBB	302	7/7	0.99	0.05	50,53,59,60	0
5	PEG	JJJ	501	7/7	0.99	0.05	54,55,58,59	0
5	PEG	FFF	501	7/7	0.99	0.06	46,48,50,50	0
4	EDO	EEE	501	4/4	0.99	0.04	50,53,54,55	0
7	PGE	HHH	501	10/10	0.99	0.05	45,53,58,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.