



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:40 PM UTC

PDB ID : 6ZV5 / pdb_00006zv5
Title : CML1 crystal structure in complex with Lewis a tetrasaccharide
Authors : Varrot, A.; Bleuler-Martinez, S.
Deposited on : 2020-07-24
Resolution : 1.95 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

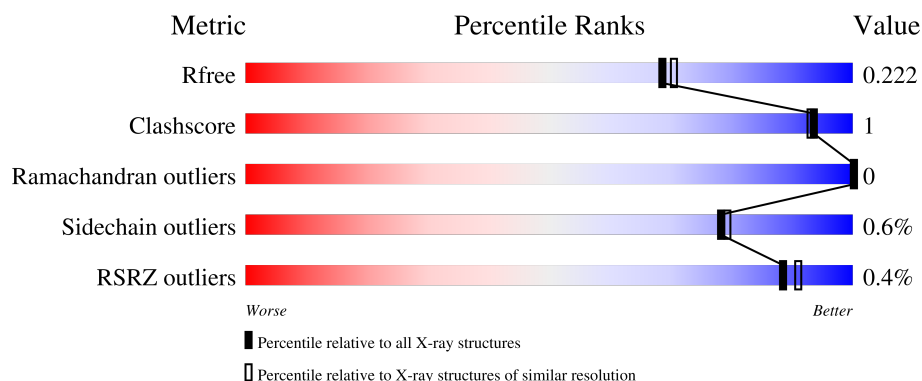
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

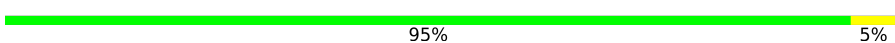
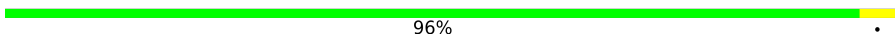
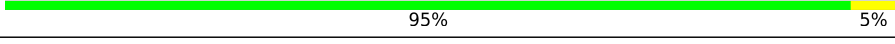
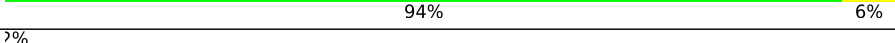
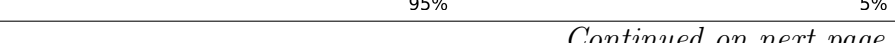
The reported resolution of this entry is 1.95 Å.

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.



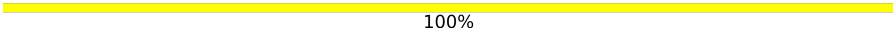
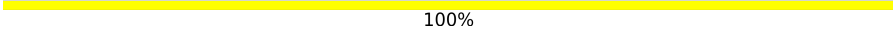
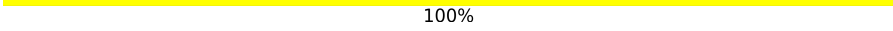
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	126	
1	BBB	126	
1	CCC	126	
1	DDD	126	
1	EEE	126	

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Mol	Chain	Length	Quality of chain
1	FFF	126	 90% 9%
2	AaA	3	 33% 67%
2	BaB	3	 100%
2	EaE	3	 100%
2	FaF	3	 33% 67%
3	CaC	4	 25% 75%
3	DaD	4	 100%

2 Entry composition [i](#)

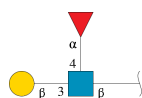
There are 5 unique types of molecules in this entry. The entry contains 6773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mucin-binding lectin 1.

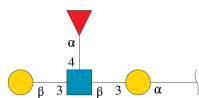
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	126	Total	C	N	O	S	0	0	0
			960	610	167	182	1			
1	BBB	126	Total	C	N	O	S	0	0	0
			961	611	165	184	1			
1	CCC	126	Total	C	N	O	S	0	0	0
			963	611	167	184	1			
1	DDD	126	Total	C	N	O	S	0	0	0
			963	611	167	184	1			
1	EEE	126	Total	C	N	O	S	0	0	0
			962	611	166	184	1			
1	FFF	126	Total	C	N	O	S	0	0	0
			963	611	167	184	1			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



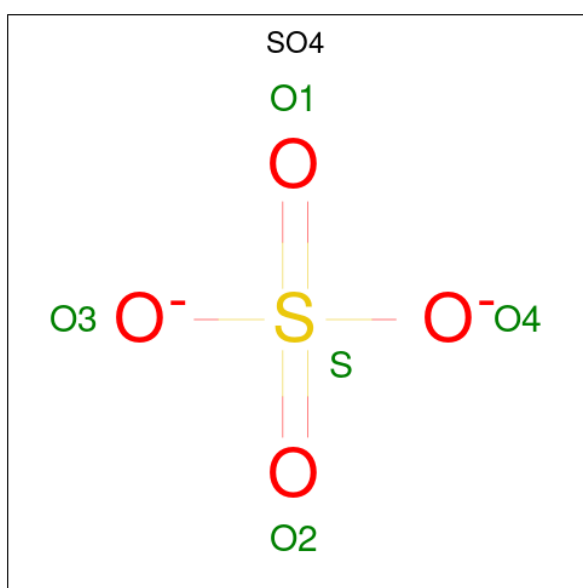
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	BaB	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	EaE	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	FaF	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CaC	4	Total	C	N	O	0	0	0
			47	26	1	20			
3	DaD	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	S	0	0
			5	4	1		
4	CCC	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		
4	EEE	1	Total	O	S	0	0
			5	4	1		
4	FFF	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	FFF	1	Total	O	S	0	0
			5	4	1		
4	FFF	1	Total	O	S	0	0
			5	4	1		
4	FFF	1	Total	O	S	0	0
			5	4	1		
4	FFF	1	Total	O	S	0	0
			5	4	1		

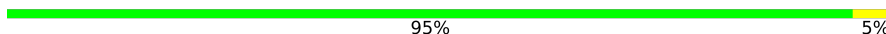
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	117	Total	O	0	9
			126	126		
5	BBB	133	Total	O	0	10
			143	143		
5	CCC	96	Total	O	0	3
			99	99		
5	DDD	135	Total	O	0	4
			139	139		
5	EEE	85	Total	O	0	6
			91	91		
5	FFF	107	Total	O	0	3
			110	110		

3 Residue-property plots [i](#)

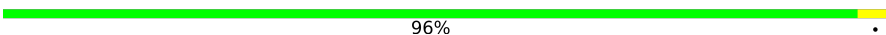
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mucin-binding lectin 1

Chain AAA:  95% 5%

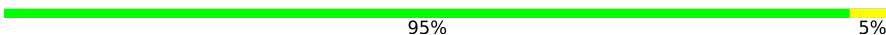


- Molecule 1: Mucin-binding lectin 1

Chain BBB:  96% .

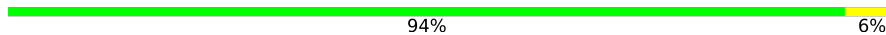


- Molecule 1: Mucin-binding lectin 1

Chain CCC:  95% 5%

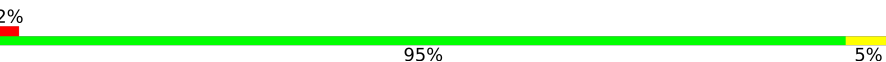


- Molecule 1: Mucin-binding lectin 1

Chain DDD:  94% 6%



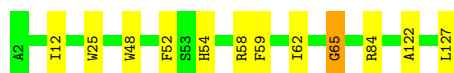
- Molecule 1: Mucin-binding lectin 1

Chain EEE:  95% 5% 2%

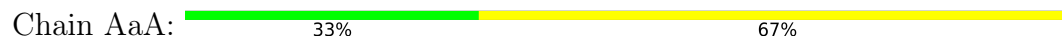


- Molecule 1: Mucin-binding lectin 1

Chain FFF:  90% 9% .



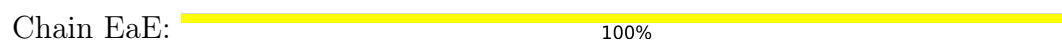
- Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



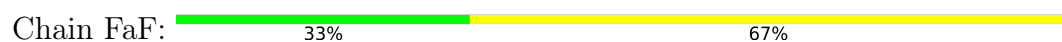
- Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-galactopyranose



- Molecule 3: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	73.92Å 73.92Å 119.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.70 – 1.95 43.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.70-1.95) 98.3 (43.70-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.239 0.171 , 0.222	Depositor DCC
R_{free} test set	2590 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.037 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6773	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: FUC, NAG, GAL, GLA, SO4

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	1.19	0/985	1.19	0/1345
1	BBB	1.23	1/986 (0.1%)	1.24	2/1346 (0.1%)
1	CCC	1.14	0/988	1.20	0/1349
1	DDD	1.15	1/988 (0.1%)	1.20	1/1349 (0.1%)
1	EEE	1.19	1/987 (0.1%)	1.20	0/1348
1	FFF	1.17	3/988 (0.3%)	1.19	1/1349 (0.1%)
All	All	1.18	6/5922 (0.1%)	1.20	4/8086 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	122	ALA	C-O	6.01	1.31	1.24
1	FFF	62	ILE	C-O	5.93	1.30	1.23
1	FFF	122	ALA	C-O	5.82	1.30	1.23
1	EEE	93	HIS	CE1-NE2	5.53	1.38	1.32
1	DDD	66	GLN	C-O	-5.24	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	65	GLY	CA-C-O	-6.83	114.93	121.49
1	BBB	26	GLY	CA-C-N	6.14	125.82	119.92
1	BBB	26	GLY	C-N-CA	6.14	125.82	119.92
1	DDD	98	THR	CA-CB-OG1	-5.23	101.76	109.60

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	960	0	937	4	0
1	BBB	961	0	932	3	0
1	CCC	963	0	939	3	0
1	DDD	963	0	939	2	0
1	EEE	962	0	934	3	0
1	FFF	963	0	939	5	0
2	AaA	36	0	33	0	0
2	BaB	36	0	33	0	0
2	EaE	36	0	33	0	0
2	FaF	36	0	33	0	0
3	CaC	47	0	42	0	0
3	DaD	47	0	42	0	0
4	BBB	5	0	0	0	0
4	CCC	5	0	0	1	0
4	DDD	15	0	0	0	0
4	EEE	5	0	0	0	0
4	FFF	25	0	0	0	0
5	AAA	126	0	0	0	0
5	BBB	143	0	0	0	0
5	CCC	99	0	0	0	0
5	DDD	139	0	0	0	0
5	EEE	91	0	0	0	0
5	FFF	110	0	0	0	0
All	All	6773	0	5836	17	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 17 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:CCC:32:ARG:NH2	4:CCC:201:SO4:O3	2.28	0.66
1:DDD:52:PHE:HB2	1:DDD:59:PHE:CZ	2.45	0.52
1:AAA:52:PHE:HB2	1:AAA:59:PHE:CZ	2.45	0.52
1:EEE:52:PHE:HB2	1:EEE:59:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:25:TRP:CE2	1:AAA:58:ARG:HB3	2.47	0.49

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	AAA	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
1	BBB	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
1	CCC	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
1	DDD	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
1	EEE	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
1	FFF	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
All	All	744/756 (98%)	723 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	104/105 (99%)	103 (99%)	1 (1%)	68	67
1	BBB	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	105/105 (100%)	104 (99%)	1 (1%)	68	67
1	DDD	105/105 (100%)	103 (98%)	2 (2%)	50	45
1	EEE	104/105 (99%)	104 (100%)	0	100	100
1	FFF	105/105 (100%)	105 (100%)	0	100	100
All	All	627/630 (100%)	623 (99%)	4 (1%)	78	79

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

Mol	Chain	Res	Type
1	AAA	19	LYS
1	CCC	19	LYS
1	DDD	29	ASN
1	DDD	47	LYS

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 ⓘ

20 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	0.49	0	21,21,21	0.94	1 (4%)
2	GAL	AaA	2	2	11,11,12	1.10	1 (9%)	15,15,17	1.05	0
2	FUC	AaA	3	2	10,10,11	0.80	0	14,14,16	0.81	0
2	NAG	BaB	1	2	15,15,15	0.55	0	21,21,21	1.73	6 (28%)
2	GAL	BaB	2	2	11,11,12	1.24	2 (18%)	15,15,17	1.56	4 (26%)
2	FUC	BaB	3	2	10,10,11	1.03	1 (10%)	14,14,16	0.77	0
3	GLA	CaC	1	3	12,12,12	1.18	1 (8%)	17,17,17	1.32	3 (17%)
3	NAG	CaC	2	3	14,14,15	0.61	0	17,19,21	1.36	2 (11%)
3	GAL	CaC	3	3	11,11,12	0.85	0	15,15,17	0.91	1 (6%)
3	FUC	CaC	4	3	10,10,11	0.84	0	14,14,16	0.71	0
3	GLA	DaD	1	3	12,12,12	1.15	1 (8%)	17,17,17	1.37	1 (5%)
3	NAG	DaD	2	3	14,14,15	0.74	0	17,19,21	1.91	4 (23%)
3	GAL	DaD	3	3	11,11,12	1.13	1 (9%)	15,15,17	1.41	2 (13%)
3	FUC	DaD	4	3	10,10,11	0.91	0	14,14,16	1.15	2 (14%)
2	NAG	EaE	1	2	15,15,15	0.70	1 (6%)	21,21,21	2.04	4 (19%)
2	GAL	EaE	2	2	11,11,12	1.12	1 (9%)	15,15,17	0.93	1 (6%)
2	FUC	EaE	3	2	10,10,11	0.55	0	14,14,16	1.29	2 (14%)
2	NAG	FaF	1	2	15,15,15	0.35	0	21,21,21	1.36	3 (14%)
2	GAL	FaF	2	2	11,11,12	0.65	0	15,15,17	0.97	0
2	FUC	FaF	3	2	10,10,11	0.93	1 (10%)	14,14,16	1.03	1 (7%)

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	-	1/2/19/22	0/1/1/1
2	FUC	AaA	3	2	-	-	0/1/1/1
2	NAG	BaB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	BaB	2	2	-	1/2/19/22	0/1/1/1
2	FUC	BaB	3	2	-	-	0/1/1/1
3	GLA	CaC	1	3	-	1/2/22/22	0/1/1/1
3	NAG	CaC	2	3	-	0/6/23/26	0/1/1/1
3	GAL	CaC	3	3	-	1/2/19/22	0/1/1/1
3	FUC	CaC	4	3	-	-	0/1/1/1
3	GLA	DaD	1	3	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	DaD	2	3	-	0/6/23/26	0/1/1/1
3	GAL	DaD	3	3	-	1/2/19/22	0/1/1/1
3	FUC	DaD	4	3	-	-	0/1/1/1
2	NAG	EaE	1	2	-	2/6/26/26	0/1/1/1
2	GAL	EaE	2	2	-	1/2/19/22	0/1/1/1
2	FUC	EaE	3	2	-	-	0/1/1/1
2	NAG	FaF	1	2	-	4/6/26/26	0/1/1/1
2	GAL	FaF	2	2	-	1/2/19/22	0/1/1/1
2	FUC	FaF	3	2	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EaE	2	GAL	C2-C3	-2.74	1.48	1.52
3	DaD	1	GLA	O1-C1	2.32	1.46	1.39
3	CaC	1	GLA	O3-C3	2.28	1.48	1.43
2	FaF	3	FUC	C1-C2	2.22	1.57	1.52
2	BaB	2	GAL	O5-C1	-2.22	1.40	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EaE	1	NAG	O5-C1-C2	-6.14	103.35	109.52
3	DaD	2	NAG	C2-N2-C7	-4.86	116.39	122.90
3	DaD	2	NAG	C1-O5-C5	4.50	118.22	112.19
2	EaE	1	NAG	C1-C2-C3	4.16	116.21	110.54
3	DaD	1	GLA	C1-O5-C5	-4.08	105.75	113.65

There are no chirality outliers.

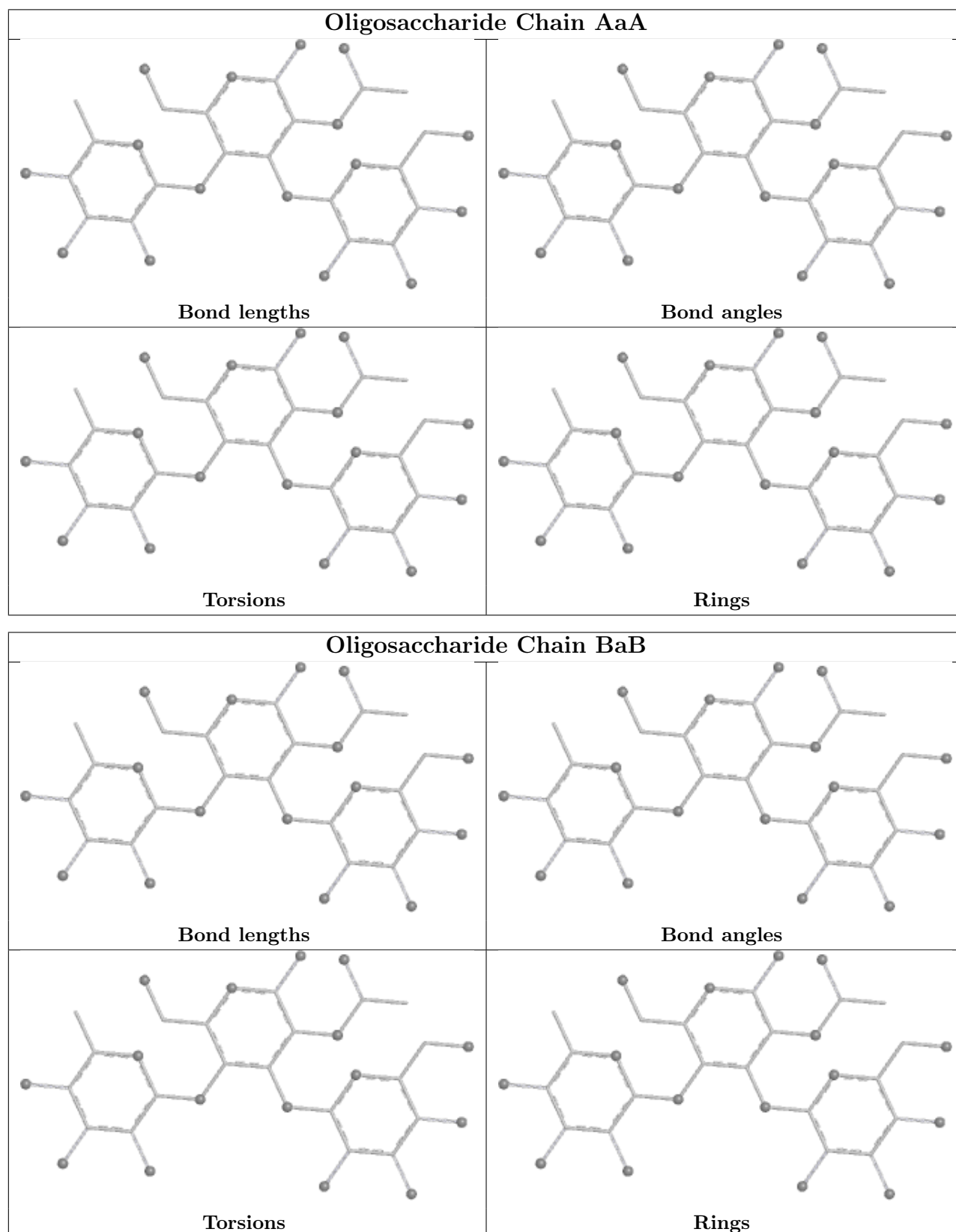
5 of 17 torsion outliers are listed below:

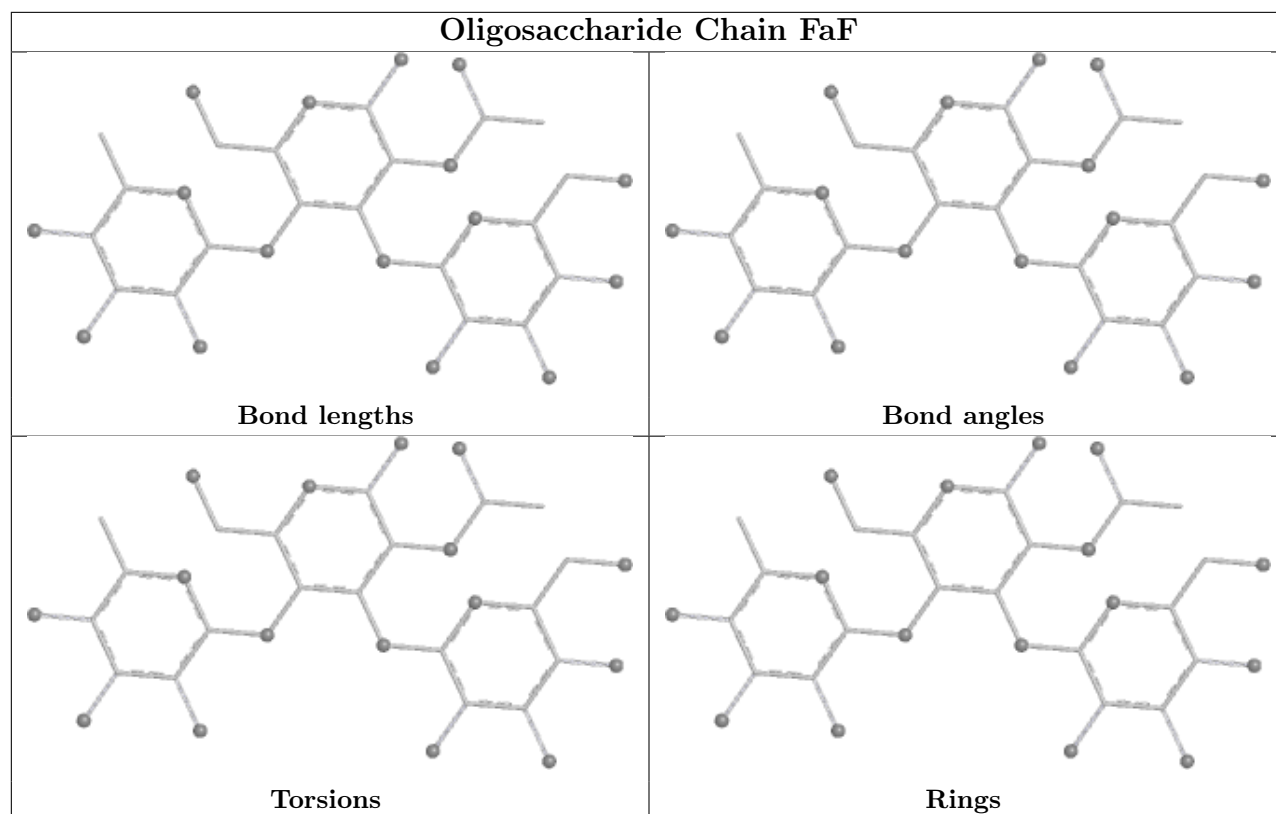
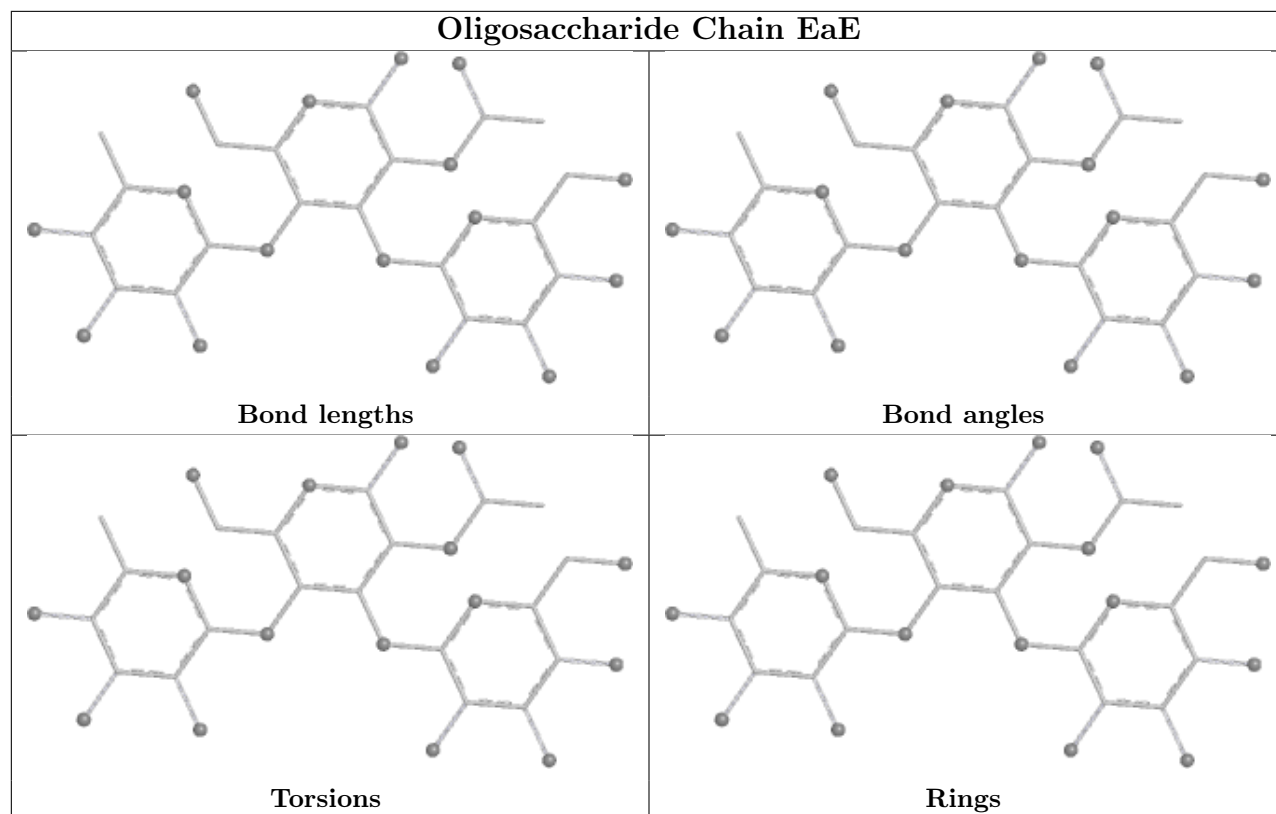
Mol	Chain	Res	Type	Atoms
2	FaF	1	NAG	O5-C5-C6-O6
2	FaF	1	NAG	C4-C5-C6-O6
3	DaD	1	GLA	O5-C5-C6-O6
3	DaD	1	GLA	C4-C5-C6-O6
2	EaE	1	NAG	C8-C7-N2-C2

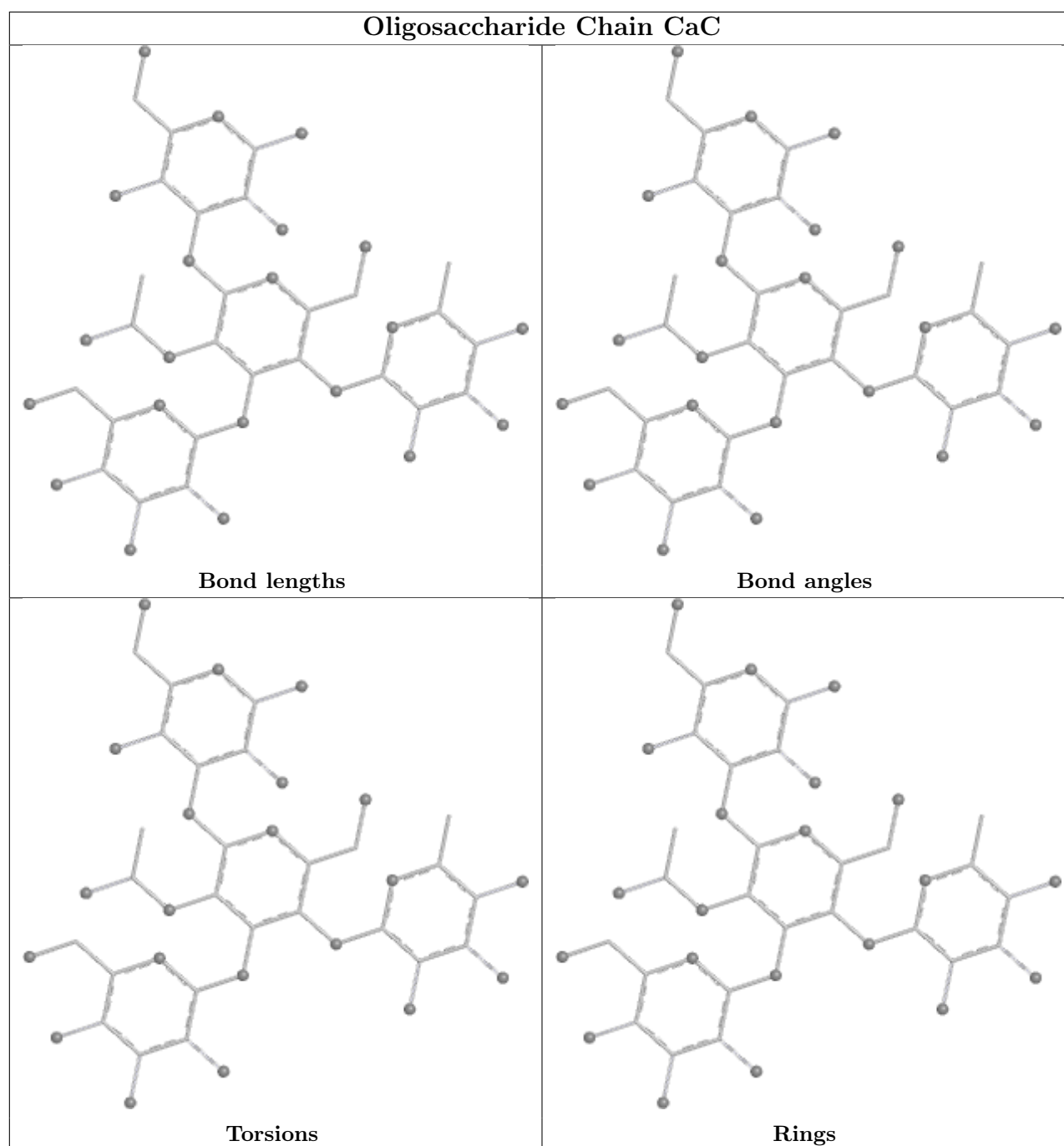
There are no ring outliers.

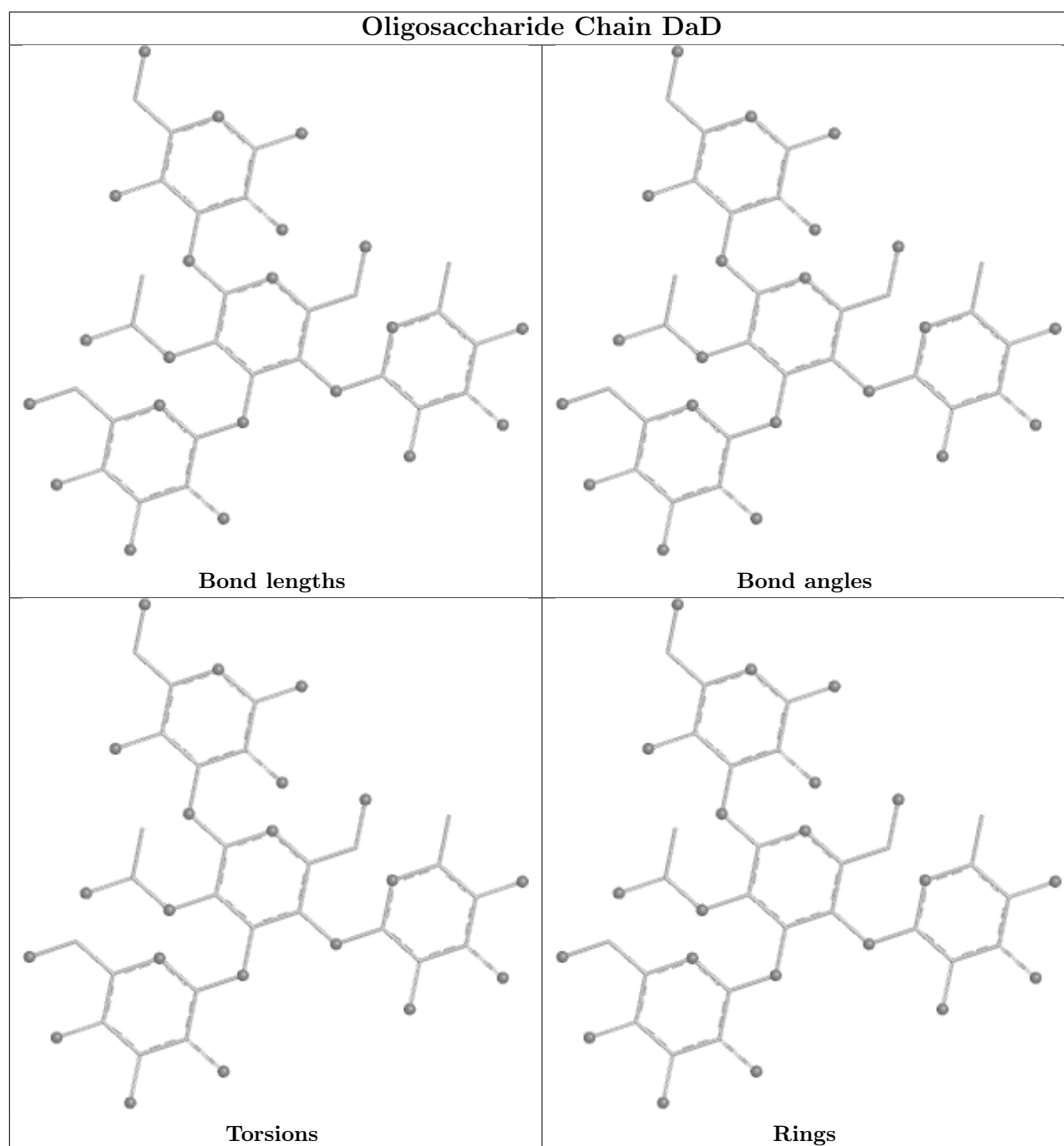
No monomer is involved in short contacts.

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](#)

11 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	$\# Z > 2$
4	SO4	FFF	203	-	4,4,4	0.43	0	6,6,6	0.44	0
4	SO4	FFF	202	-	4,4,4	0.25	0	6,6,6	0.28	0
4	SO4	CCC	201	-	4,4,4	0.58	0	6,6,6	0.30	0
4	SO4	FFF	204	-	4,4,4	0.31	0	6,6,6	0.40	0
4	SO4	DDD	201	-	4,4,4	0.17	0	6,6,6	0.44	0
4	SO4	EEE	201	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	BBB	201	-	4,4,4	0.35	0	6,6,6	0.19	0
4	SO4	DDD	203	-	4,4,4	0.29	0	6,6,6	0.23	0
4	SO4	FFF	201	-	4,4,4	0.27	0	6,6,6	0.30	0
4	SO4	DDD	202	-	4,4,4	0.25	0	6,6,6	0.24	0
4	SO4	FFF	205	-	4,4,4	0.38	0	6,6,6	0.16	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	201	SO4	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	AAA	126/126 (100%)	-0.11	0 100 100	25, 31, 42, 55	0
1	BBB	126/126 (100%)	-0.31	0 100 100	24, 28, 34, 55	1 (0%)
1	CCC	126/126 (100%)	-0.03	0 100 100	26, 34, 45, 54	0
1	DDD	126/126 (100%)	-0.21	0 100 100	25, 30, 38, 48	0
1	EEE	126/126 (100%)	0.20	3 (2%) 59 66	26, 35, 50, 68	0
1	FFF	126/126 (100%)	-0.16	0 100 100	25, 31, 40, 56	0
All	All	756/756 (100%)	-0.10	3 (0%) 88 91	24, 31, 44, 68	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	109	PRO	2.6
1	EEE	110	GLY	2.6
1	EEE	108	VAL	2.6

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	-	-	34,44,49,53	0

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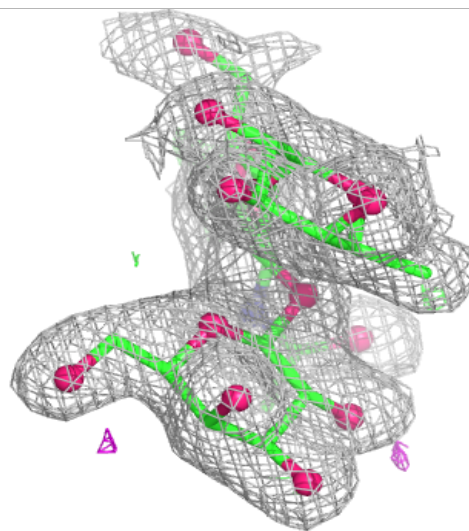
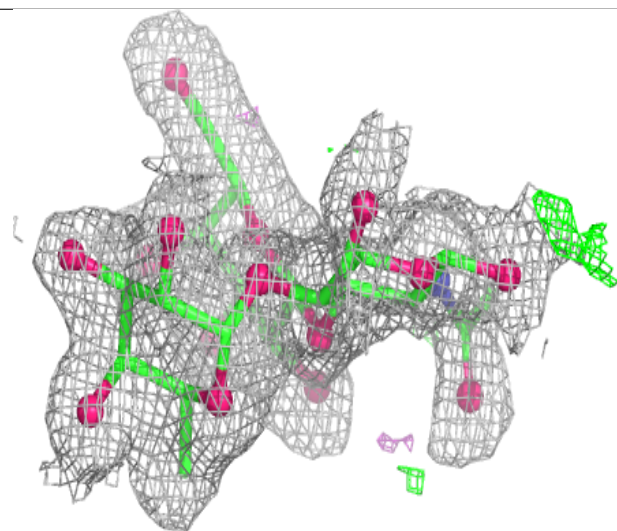
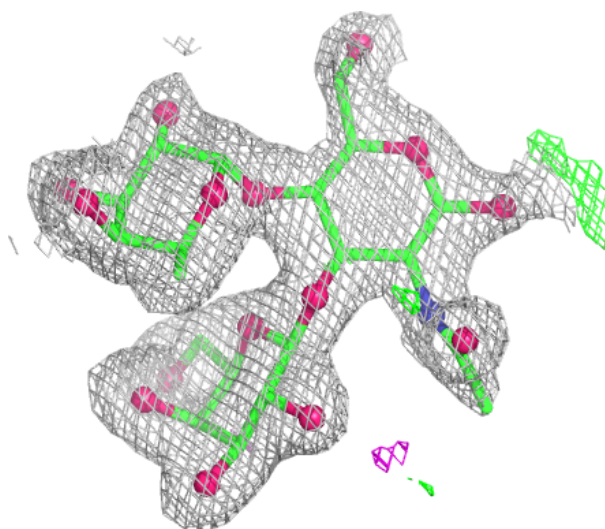
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	AaA	2	11/12	-	-	33,38,43,43	0
2	FUC	AaA	3	10/11	-	-	30,31,33,33	0
2	NAG	BaB	1	15/15	-	-	34,41,53,53	0
2	GAL	BaB	2	11/12	-	-	33,36,41,49	0
2	FUC	BaB	3	10/11	-	-	28,31,35,37	0
2	NAG	EaE	1	15/15	-	-	38,53,63,66	0
2	GAL	EaE	2	11/12	-	-	39,42,51,52	0
2	FUC	EaE	3	10/11	-	-	32,38,41,43	0
2	NAG	FaF	1	15/15	-	-	41,56,67,67	0
2	GAL	FaF	2	11/12	-	-	39,50,62,62	0
2	FUC	FaF	3	10/11	-	-	37,43,49,50	0
3	GLA	CaC	1	12/12	-	-	38,43,48,54	0
3	NAG	CaC	2	14/15	-	-	30,46,59,59	0
3	GAL	CaC	3	11/12	-	-	35,45,51,54	0
3	FUC	CaC	4	10/11	-	-	25,30,32,34	0
3	GLA	DaD	1	12/12	-	-	45,50,57,63	0
3	NAG	DaD	2	14/15	-	-	29,49,59,60	0
3	GAL	DaD	3	11/12	-	-	36,40,44,45	0
3	FUC	DaD	4	10/11	-	-	28,31,34,35	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.

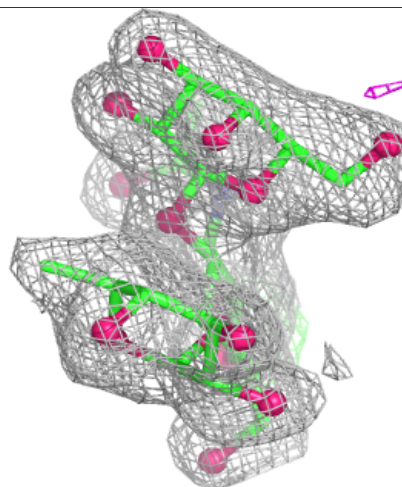
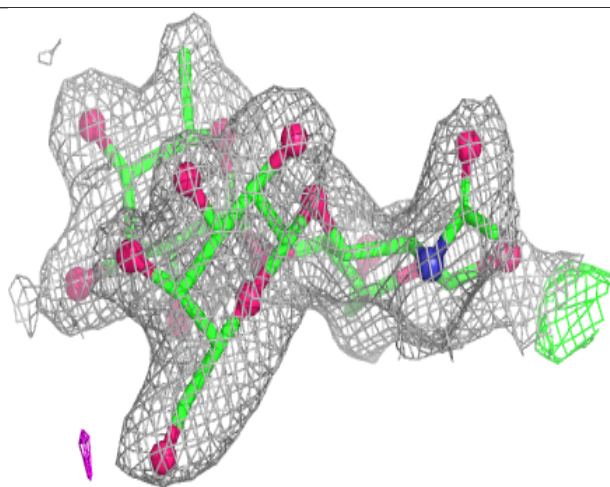
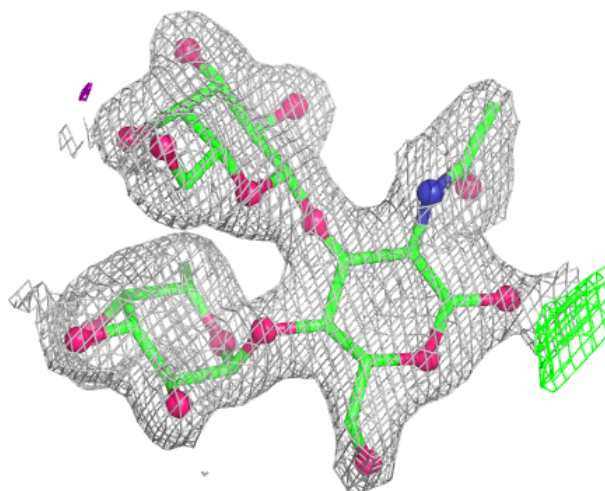
Electron density around Chain AaA:

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



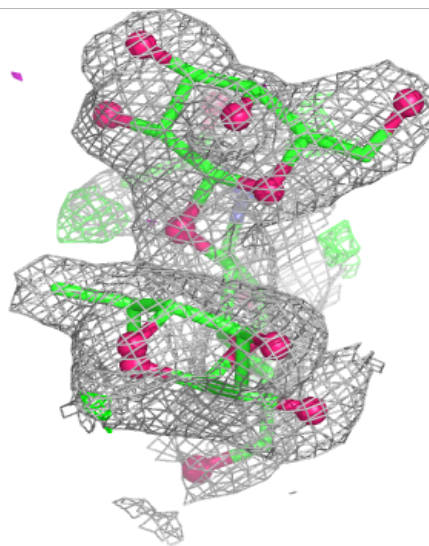
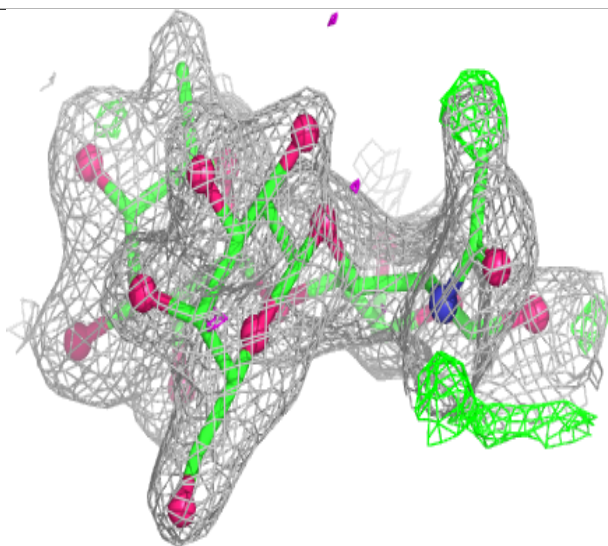
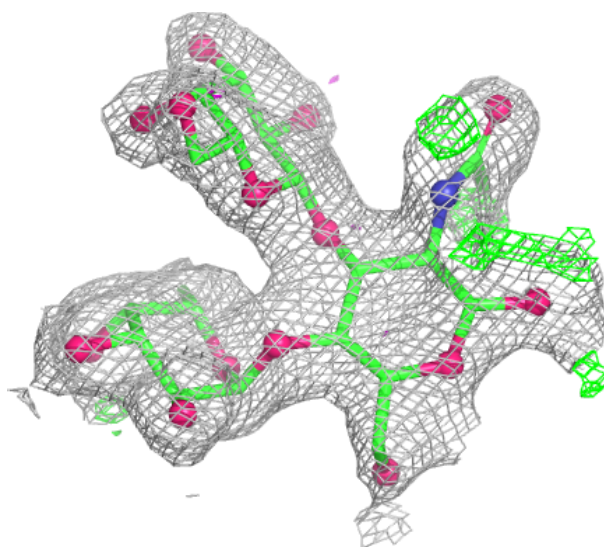
Electron density around Chain BaB:

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



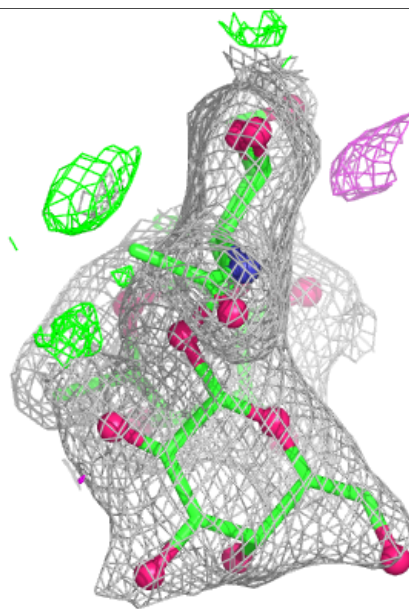
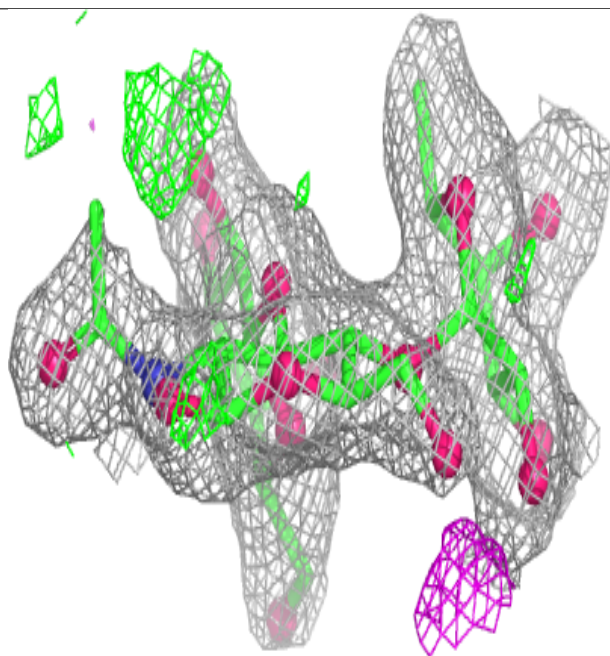
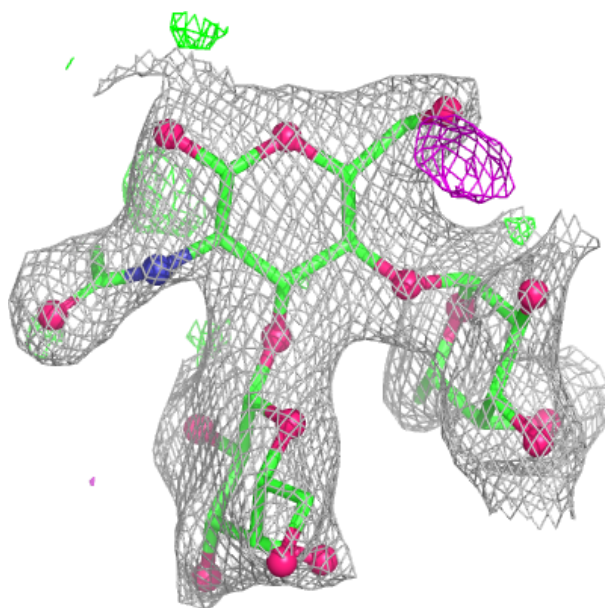
Electron density around Chain EaE:

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



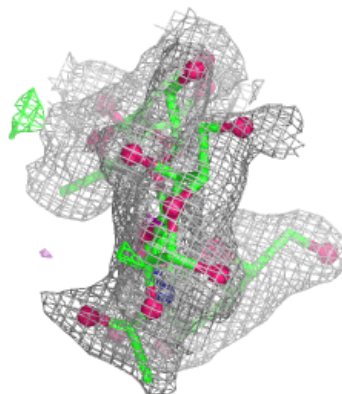
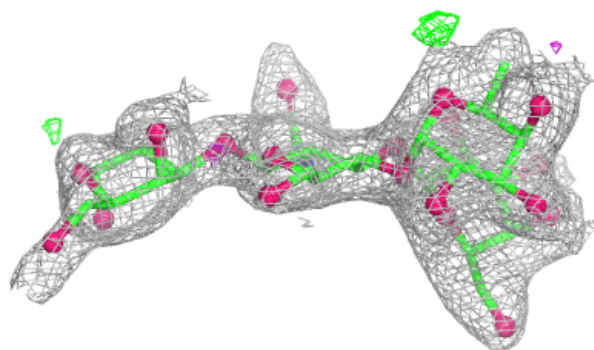
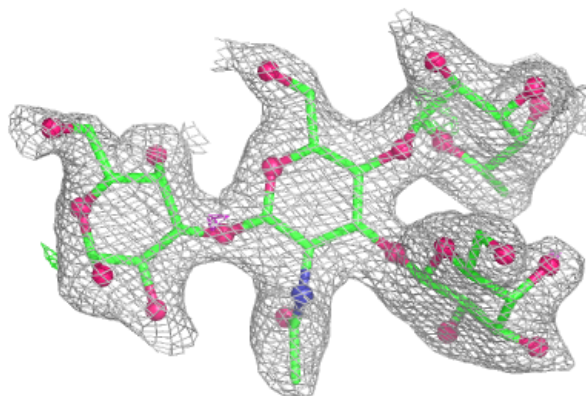
Electron density around Chain FaF:

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

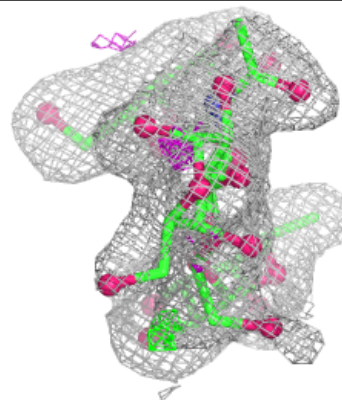
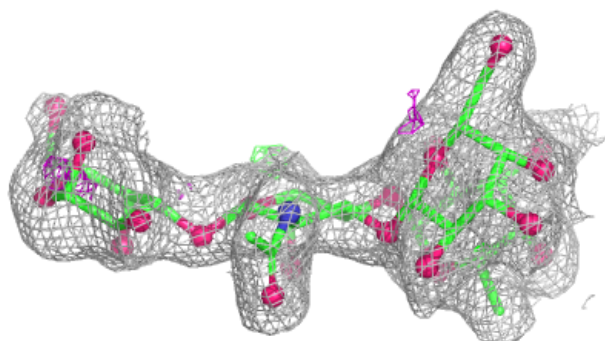
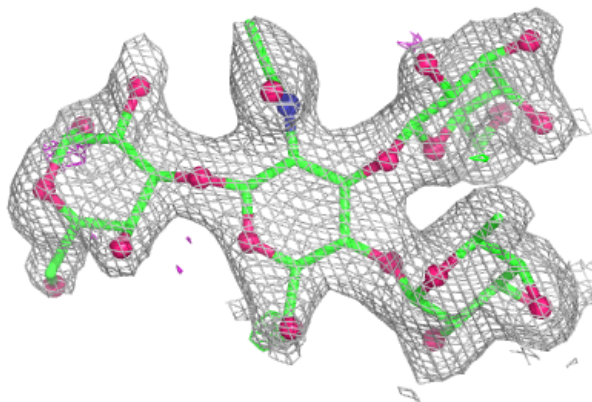


Electron density around Chain CaC:

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

**Electron density around Chain DaD:**

$2mF_o-DF_c$ (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
4	SO4	DDD	203	5/5	0.75	0.09	60,66,66,75	0
4	SO4	FFF	201	5/5	0.77	0.10	61,61,85,88	0
4	SO4	FFF	202	5/5	0.80	0.10	67,72,88,109	0
4	SO4	CCC	201	5/5	0.83	0.14	40,41,44,46	5
4	SO4	BBB	201	5/5	0.83	0.09	68,70,72,79	0
4	SO4	DDD	201	5/5	0.87	0.10	57,61,62,65	0
4	SO4	FFF	205	5/5	0.91	0.08	54,56,60,65	0
4	SO4	EEE	201	5/5	0.92	0.07	49,63,79,80	0
4	SO4	FFF	203	5/5	0.93	0.07	41,47,55,57	0
4	SO4	DDD	202	5/5	0.94	0.06	58,62,64,70	0
4	SO4	FFF	204	5/5	0.95	0.08	35,38,48,49	5

6.5 Other polymers [i](#)

There are no such residues in this entry.