



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2022 – 01:19 pm BST

PDB ID : 6ZU2
Title : CML1 crystal structure in complex with H-type 1 trisaccharide
Authors : Varrot, A.; Bleuler-Martinez, S.
Deposited on : 2020-07-21
Resolution : 1.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

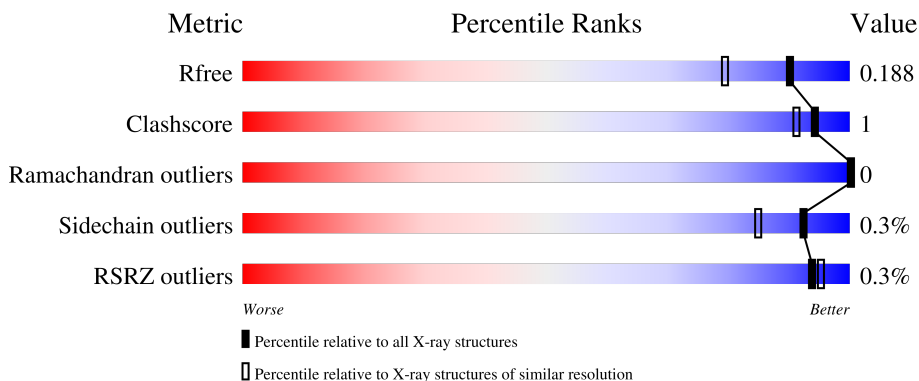
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	 97% .
1	BBB	126	 95% 5%
1	CCC	126	 94% 5% .
1	DDD	126	 98% .
1	EEE	126	 96% .

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Mol	Chain	Length	Quality of chain
1	FFF	126	 94% 5%
2	AaA	3	 100%
2	BaB	3	 100%
2	CaC	3	 100%
2	DaD	3	 33% 67%
2	EaE	3	 33% 67%
2	FaF	3	 100%

2 Entry composition [i](#)

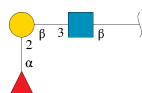
There are 4 unique types of molecules in this entry. The entry contains 7101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

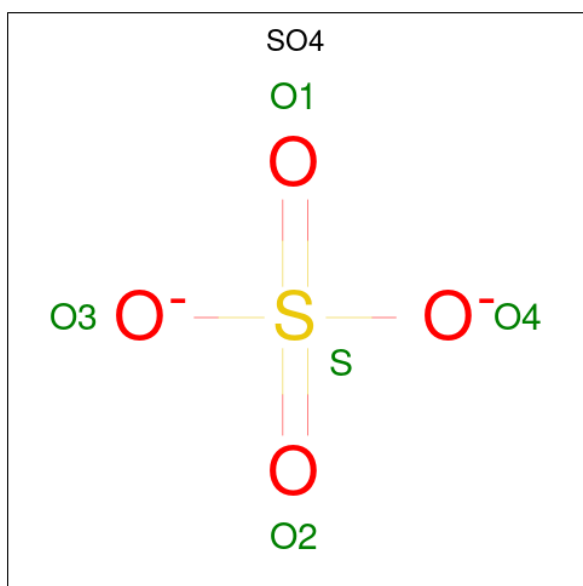
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	126	Total 984	C 622	N 171	O 190	S 1	0	3	0
1	BBB	126	Total 978	C 621	N 169	O 187	S 1	0	2	0
1	CCC	126	Total 978	C 620	N 170	O 187	S 1	0	2	0
1	DDD	126	Total 969	C 614	N 168	O 186	S 1	0	1	0
1	EEE	126	Total 978	C 622	N 169	O 186	S 1	0	2	0
1	FFF	126	Total 991	C 629	N 171	O 190	S 1	0	4	0

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	1
			10	8	2		
3	EEE	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	153	Total	O	0	5
			158	158		
4	BBB	154	Total	O	0	2
			156	156		
4	CCC	137	Total	O	0	3
			140	140		
4	DDD	158	Total	O	0	6
			164	164		
4	EEE	148	Total	O	0	3
			151	151		
4	FFF	144	Total	O	0	4
			148	148		

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



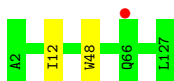
- Molecule 1: Mucin-binding lectin 1



- Molecule 1: Mucin-binding lectin 1



- Molecule 1: Mucin-binding lectin 1



- Molecule 1: Mucin-binding lectin 1



- Molecule 1: Mucin-binding lectin 1

Chain FFF:  94% 5%



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

Chain AaA:  100%



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

Chain BaB:  100%



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

Chain CaC:  100%



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

Chain DaD:  33% 67%



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

Chain EaE:  33% 67%



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

Chain FaF:  100%

MAG1
GAL2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	74.04Å 74.04Å 119.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.02 – 1.55 37.02 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.02-1.55) 100.0 (37.02-1.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.150 , 0.181 0.161 , 0.188	Depositor DCC
R_{free} test set	5401 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.006 for -h,-k,l 0.029 for h,-h-k,-l 0.019 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: SO4, GAL, NAG, FUC

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	0.87	1/1009 (0.1%)	1.05	0/1377
1	BBB	0.84	1/1003 (0.1%)	0.94	0/1370
1	CCC	0.83	2/1003 (0.2%)	0.95	2/1371 (0.1%)
1	DDD	0.82	0/994	0.98	0/1357
1	EEE	0.74	0/1003	0.92	0/1370
1	FFF	0.82	0/1016	0.93	2/1389 (0.1%)
All	All	0.82	4/6028 (0.1%)	0.96	4/8234 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	68	GLU	CD-OE1	-5.97	1.19	1.25
1	CCC	33	SER	CA-CB	-5.83	1.44	1.52
1	BBB	80	SER	CA-CB	-5.33	1.45	1.52
1	CCC	90	SER	CA-CB	-5.01	1.45	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	84	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	FFF	84	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	FFF	84	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	CCC	84	ARG	NE-CZ-NH1	-5.63	117.49	120.30

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	984	0	952	3	0
1	BBB	978	0	955	3	0
1	CCC	978	0	949	3	0
1	DDD	969	0	943	1	0
1	EEE	978	0	957	3	0
1	FFF	991	0	964	4	0
2	AaA	36	0	33	0	0
2	BaB	36	0	33	0	0
2	CaC	36	0	33	0	0
2	DaD	36	0	33	0	0
2	EaE	36	0	33	0	0
2	FaF	36	0	33	0	0
3	AAA	10	0	0	0	0
3	BBB	15	0	0	0	0
3	CCC	15	0	0	1	0
3	DDD	25	0	0	0	0
3	EEE	20	0	0	0	0
3	FFF	5	0	0	0	0
4	AAA	158	0	0	1	0
4	BBB	156	0	0	0	0
4	CCC	140	0	0	3	0
4	DDD	164	0	0	0	0
4	EEE	151	0	0	0	0
4	FFF	148	0	0	1	0
All	All	7101	0	5918	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (16) 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)
3:CCC:203:SO4:O4	4:CCC:301:HOH:O	1.85	0.94
1:FFF:125[B]:ASP:OD2	4:FFF:301:HOH:O	1.91	0.88
1:CCC:125[B]:ASP:OD2	4:CCC:302:HOH:O	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:64[A]:GLU:O	4:AAA:301:HOH:O	2.11	0.69
1:CCC:66[B]:GLN:NE2	4:CCC:303:HOH:O	2.19	0.50
1:CCC:65:GLY:O	1:CCC:84:ARG:NH1	2.47	0.47
1:BBB:13[B]:ILE:HD11	1:BBB:45:VAL:HG11	1.98	0.46
1:EEE:117[A]:VAL:O	1:EEE:117[A]:VAL:HG13	2.16	0.45
1:DDD:12:ILE:HB	1:DDD:48:TRP:HB2	1.99	0.45
1:FFF:65:GLY:O	1:FFF:84:ARG:NH1	2.51	0.43
1:FFF:12:ILE:HD12	1:FFF:20:LEU:HD21	2.00	0.42
1:EEE:52:PHE:HB2	1:EEE:59:PHE:CZ	2.54	0.42
1:AAA:124:PRO:HD3	1:BBB:11:PHE:CE2	2.55	0.41
1:AAA:11:PHE:CE2	1:BBB:124:PRO:HD3	2.56	0.41
1:EEE:13[A]:ILE:HD11	1:EEE:45:VAL:HG11	2.03	0.40
1:FFF:52:PHE:HB2	1:FFF:59:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	127/126 (101%)	123 (97%)	4 (3%)	0	100	100
1	BBB	126/126 (100%)	121 (96%)	5 (4%)	0	100	100
1	CCC	126/126 (100%)	121 (96%)	5 (4%)	0	100	100
1	DDD	125/126 (99%)	122 (98%)	3 (2%)	0	100	100
1	EEE	126/126 (100%)	121 (96%)	5 (4%)	0	100	100
1	FFF	128/126 (102%)	124 (97%)	4 (3%)	0	100	100
All	All	758/756 (100%)	732 (97%)	26 (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	107/105 (102%)	107 (100%)	0	100	100
1	BBB	107/105 (102%)	106 (99%)	1 (1%)	78	61
1	CCC	107/105 (102%)	106 (99%)	1 (1%)	78	61
1	DDD	106/105 (101%)	106 (100%)	0	100	100
1	EEE	107/105 (102%)	107 (100%)	0	100	100
1	FFF	109/105 (104%)	109 (100%)	0	100	100
All	All	643/630 (102%)	641 (100%)	2 (0%)	92	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	32	ARG
1	CCC	29	ASN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

18 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AaA	1	2	15,15,15	1.13	2 (13%)	21,21,21	1.64	5 (23%)
2	GAL	AaA	2	2	11,11,12	0.94	0	15,15,17	1.49	5 (33%)
2	FUC	AaA	3	2	10,10,11	1.22	1 (10%)	14,14,16	2.12	5 (35%)
2	NAG	BaB	1	2	15,15,15	0.71	0	21,21,21	1.93	6 (28%)
2	GAL	BaB	2	2	11,11,12	1.15	0	15,15,17	1.28	1 (6%)
2	FUC	BaB	3	2	10,10,11	0.71	0	14,14,16	1.19	2 (14%)
2	NAG	CaC	1	2	15,15,15	0.96	0	21,21,21	0.97	1 (4%)
2	GAL	CaC	2	2	11,11,12	1.47	3 (27%)	15,15,17	1.40	3 (20%)
2	FUC	CaC	3	2	10,10,11	0.73	0	14,14,16	0.93	1 (7%)
2	NAG	DaD	1	2	15,15,15	1.02	0	21,21,21	1.17	2 (9%)
2	GAL	DaD	2	2	11,11,12	1.12	0	15,15,17	0.88	0
2	FUC	DaD	3	2	10,10,11	0.90	0	14,14,16	1.35	4 (28%)
2	NAG	EaE	1	2	15,15,15	0.71	0	21,21,21	1.33	2 (9%)
2	GAL	EaE	2	2	11,11,12	0.83	0	15,15,17	1.04	0
2	FUC	EaE	3	2	10,10,11	0.50	0	14,14,16	1.23	2 (14%)
2	NAG	FaF	1	2	15,15,15	0.80	0	21,21,21	1.48	5 (23%)
2	GAL	FaF	2	2	11,11,12	0.91	0	15,15,17	1.62	4 (26%)
2	FUC	FaF	3	2	10,10,11	1.02	0	14,14,16	1.04	2 (14%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CaC	2	GAL	O5-C1	2.90	1.48	1.43
2	AaA	3	FUC	O4-C4	2.64	1.49	1.43
2	CaC	2	GAL	O2-C2	2.55	1.48	1.43
2	AaA	1	NAG	C2-N2	-2.44	1.42	1.45
2	CaC	2	GAL	C4-C5	-2.38	1.48	1.53
2	AaA	1	NAG	C1-C2	2.11	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AaA	3	FUC	C1-C2-C3	4.40	115.08	109.67
2	BaB	1	NAG	C1-O5-C5	-4.40	105.36	113.66
2	BaB	1	NAG	O5-C5-C4	-4.07	102.30	109.69
2	AaA	3	FUC	O5-C5-C4	3.93	116.56	109.52
2	BaB	2	GAL	C1-O5-C5	-3.68	107.20	112.19
2	AaA	1	NAG	C3-C4-C5	3.62	116.69	110.24
2	FaF	1	NAG	O3-C3-C4	-3.51	102.25	110.35
2	FaF	2	GAL	C1-O5-C5	-3.34	107.66	112.19
2	EaE	1	NAG	C1-O5-C5	-3.14	107.74	113.66
2	AaA	2	GAL	O5-C5-C6	-3.13	102.30	107.20
2	AaA	3	FUC	O2-C2-C3	-2.94	104.25	110.14
2	EaE	3	FUC	O2-C2-C3	-2.83	104.47	110.14
2	EaE	1	NAG	C1-C2-C3	-2.72	106.84	110.54
2	BaB	1	NAG	O5-C5-C6	2.66	113.06	106.44
2	FaF	2	GAL	C1-C2-C3	2.61	112.88	109.67
2	FaF	2	GAL	O5-C5-C6	2.58	111.25	107.20
2	DaD	3	FUC	O4-C4-C5	2.58	115.38	109.67
2	AaA	2	GAL	O5-C1-C2	-2.56	106.81	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AaA	1	NAG	O3-C3-C4	-2.56	104.44	110.35
2	FaF	1	NAG	C1-C2-N2	2.56	113.69	110.73
2	AaA	1	NAG	C4-C3-C2	-2.54	106.62	110.34
2	FaF	3	FUC	C6-C5-C4	-2.52	108.41	113.07
2	CaC	1	NAG	C1-O5-C5	-2.51	108.92	113.66
2	AaA	1	NAG	O1-C1-O5	-2.48	102.93	110.38
2	BaB	3	FUC	C1-C2-C3	2.47	112.70	109.67
2	DaD	3	FUC	O4-C4-C3	-2.46	104.65	110.35
2	CaC	2	GAL	C6-C5-C4	-2.44	107.30	113.00
2	FaF	1	NAG	O6-C6-C5	-2.43	102.96	111.29
2	CaC	3	FUC	C1-C2-C3	2.39	112.61	109.67
2	BaB	3	FUC	O5-C1-C2	-2.36	107.12	110.77
2	AaA	3	FUC	O4-C4-C3	-2.28	105.08	110.35
2	AaA	3	FUC	O5-C5-C6	-2.25	102.48	107.33
2	FaF	3	FUC	C3-C4-C5	-2.24	106.28	109.77
2	DaD	1	NAG	O7-C7-N2	2.23	126.05	121.95
2	CaC	2	GAL	O6-C6-C5	-2.22	103.67	111.29
2	FaF	1	NAG	O1-C1-O5	-2.18	103.84	110.38
2	AaA	2	GAL	O2-C2-C3	-2.17	105.78	110.14
2	FaF	1	NAG	C3-C4-C5	2.17	114.11	110.24
2	BaB	1	NAG	C1-C2-C3	-2.15	107.61	110.54
2	FaF	2	GAL	C6-C5-C4	-2.10	108.08	113.00
2	BaB	1	NAG	C4-C3-C2	-2.10	107.27	110.34
2	DaD	3	FUC	C1-O5-C5	2.07	117.48	112.78
2	BaB	1	NAG	O3-C3-C2	2.07	113.84	109.66
2	AaA	2	GAL	O6-C6-C5	-2.07	104.20	111.29
2	CaC	2	GAL	O2-C2-C1	-2.05	104.96	109.15
2	DaD	3	FUC	O5-C5-C4	-2.05	105.85	109.52
2	EaE	3	FUC	C6-C5-C4	2.02	116.81	113.07
2	AaA	1	NAG	C1-C2-N2	2.02	113.07	110.73
2	AaA	2	GAL	O4-C4-C5	-2.01	104.31	109.30
2	DaD	1	NAG	O1-C1-C2	2.01	113.39	109.22

There are no chirality outliers.

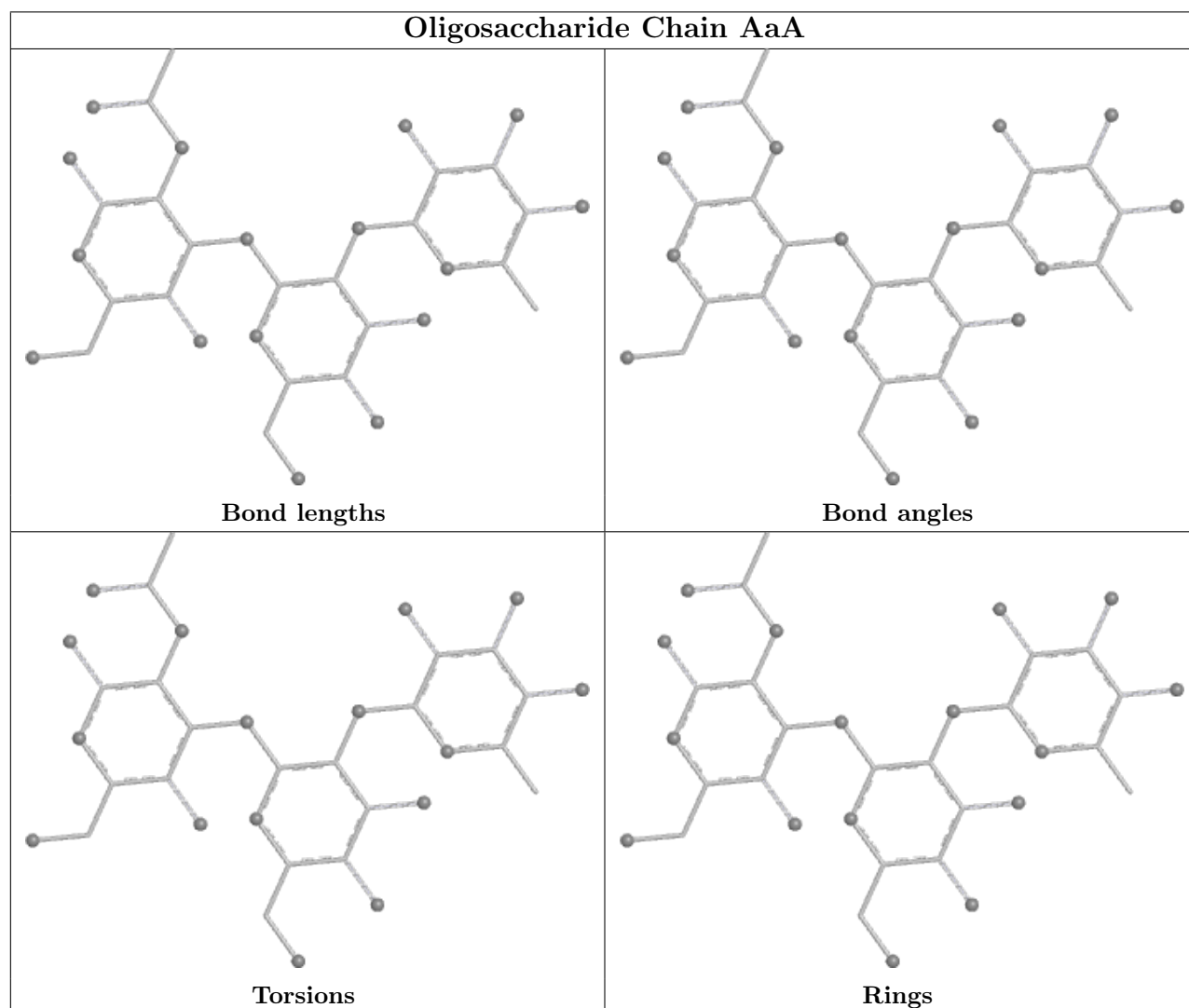
All (2) torsion outliers are listed below:

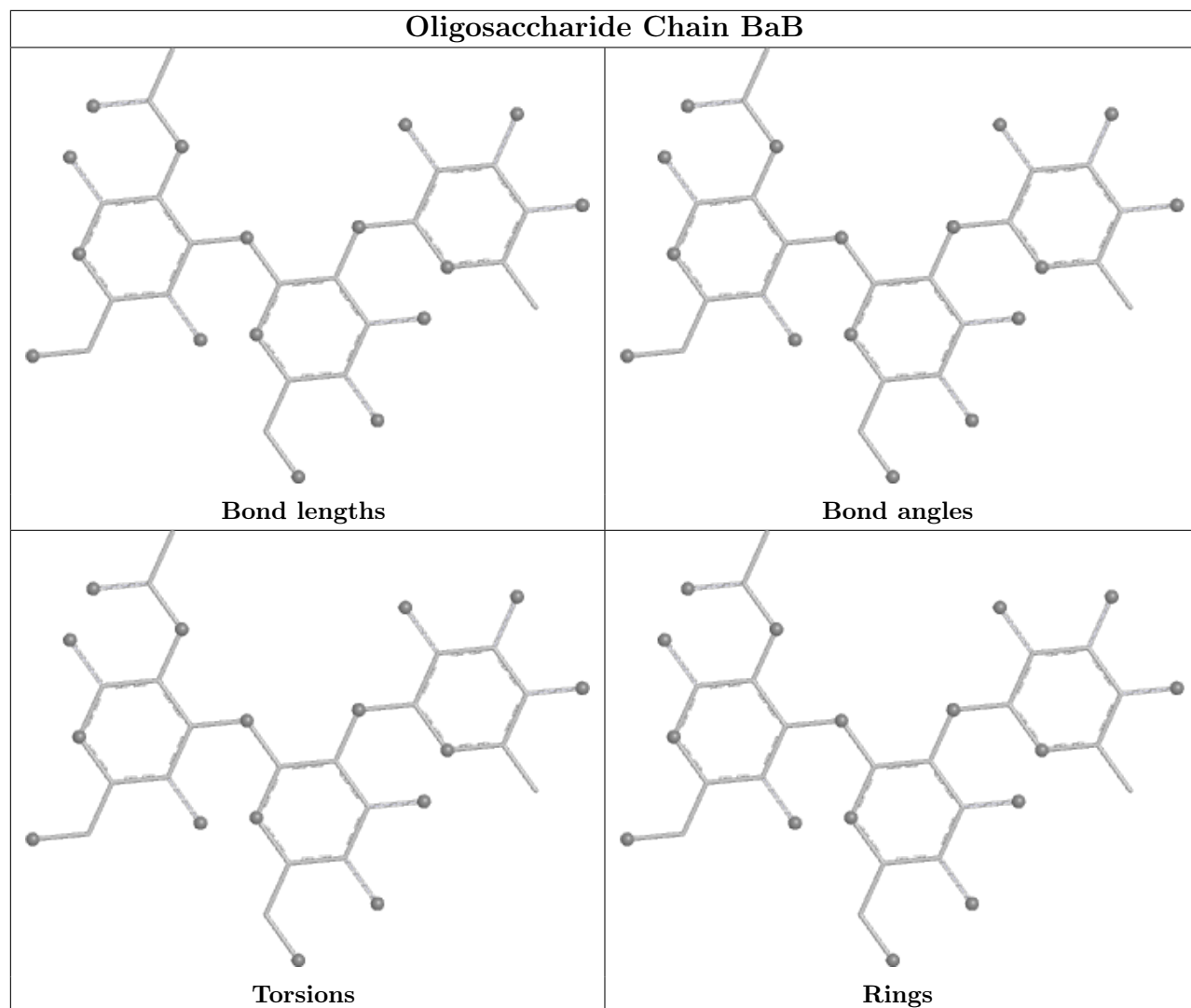
Mol	Chain	Res	Type	Atoms
2	AaA	1	NAG	O5-C5-C6-O6
2	AaA	1	NAG	C4-C5-C6-O6

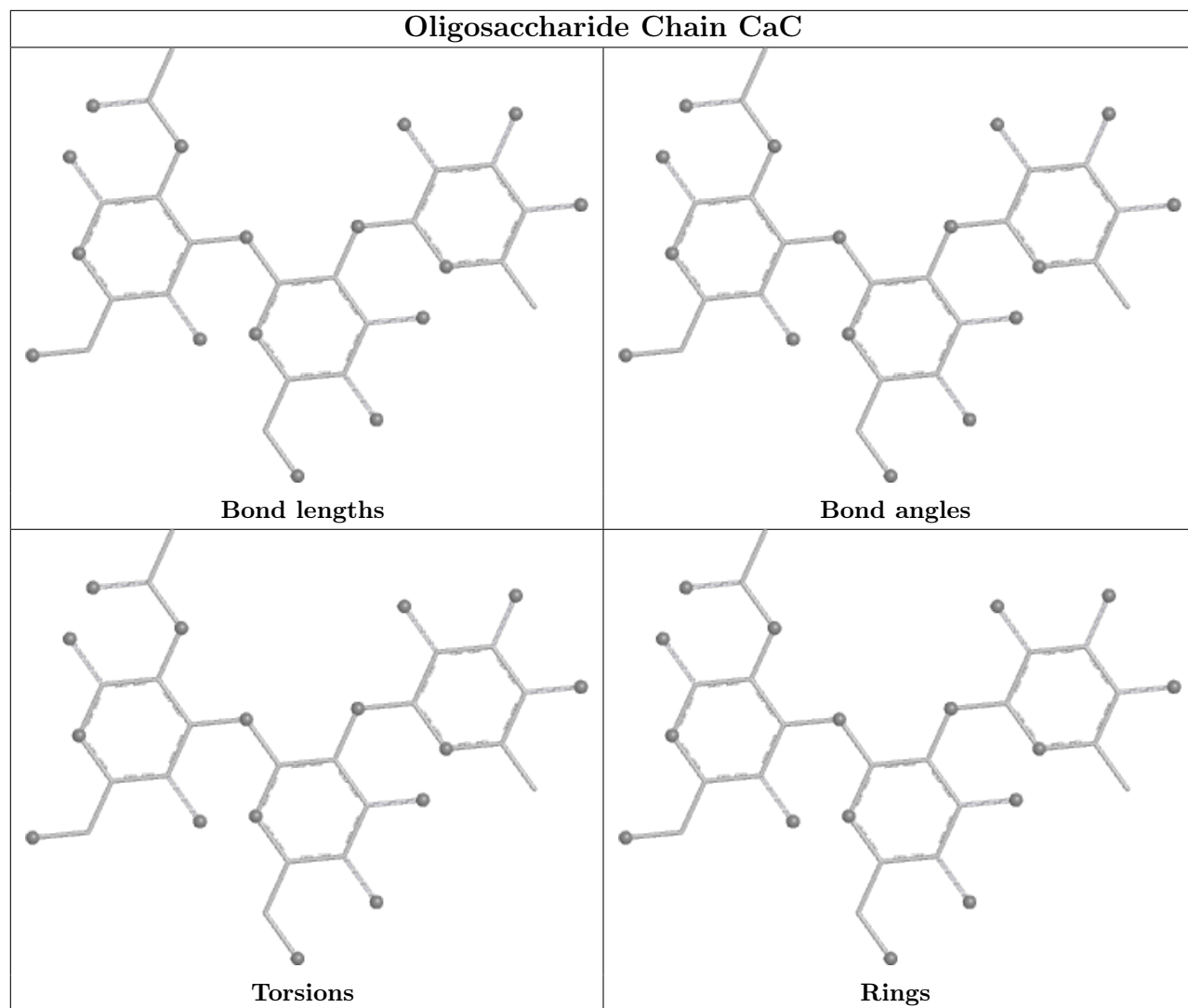
There are no ring outliers.

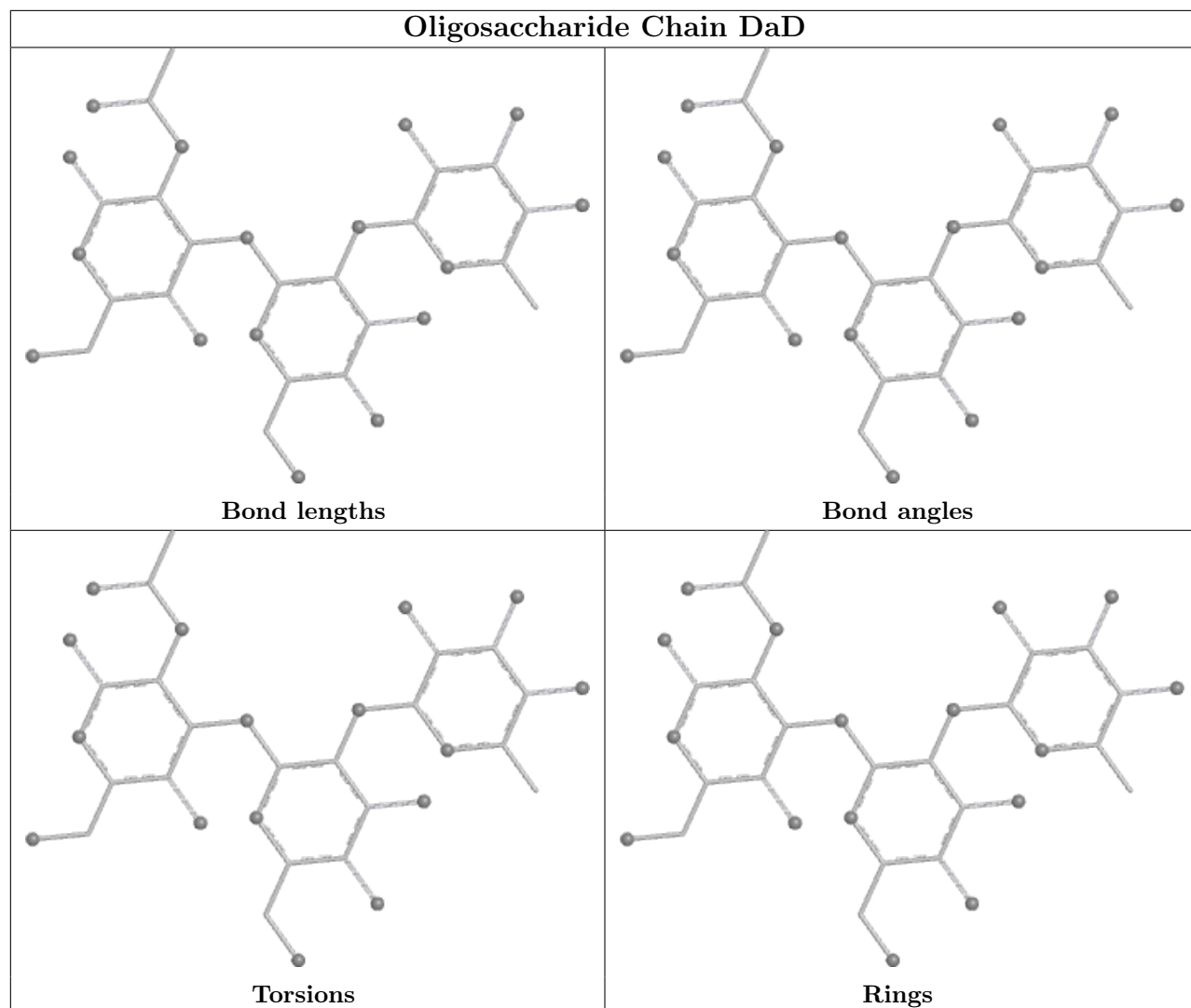
No monomer is involved in short contacts.

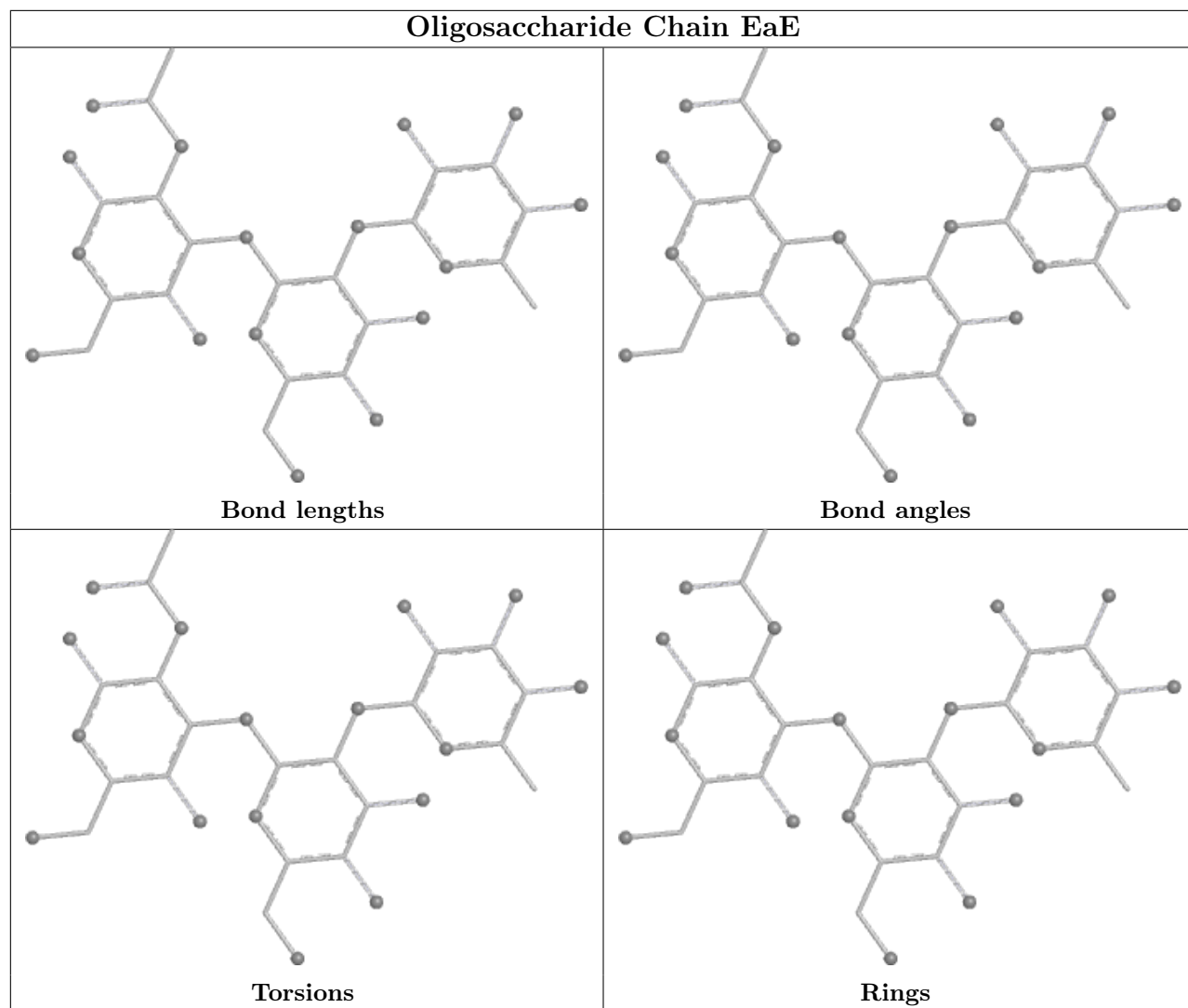
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

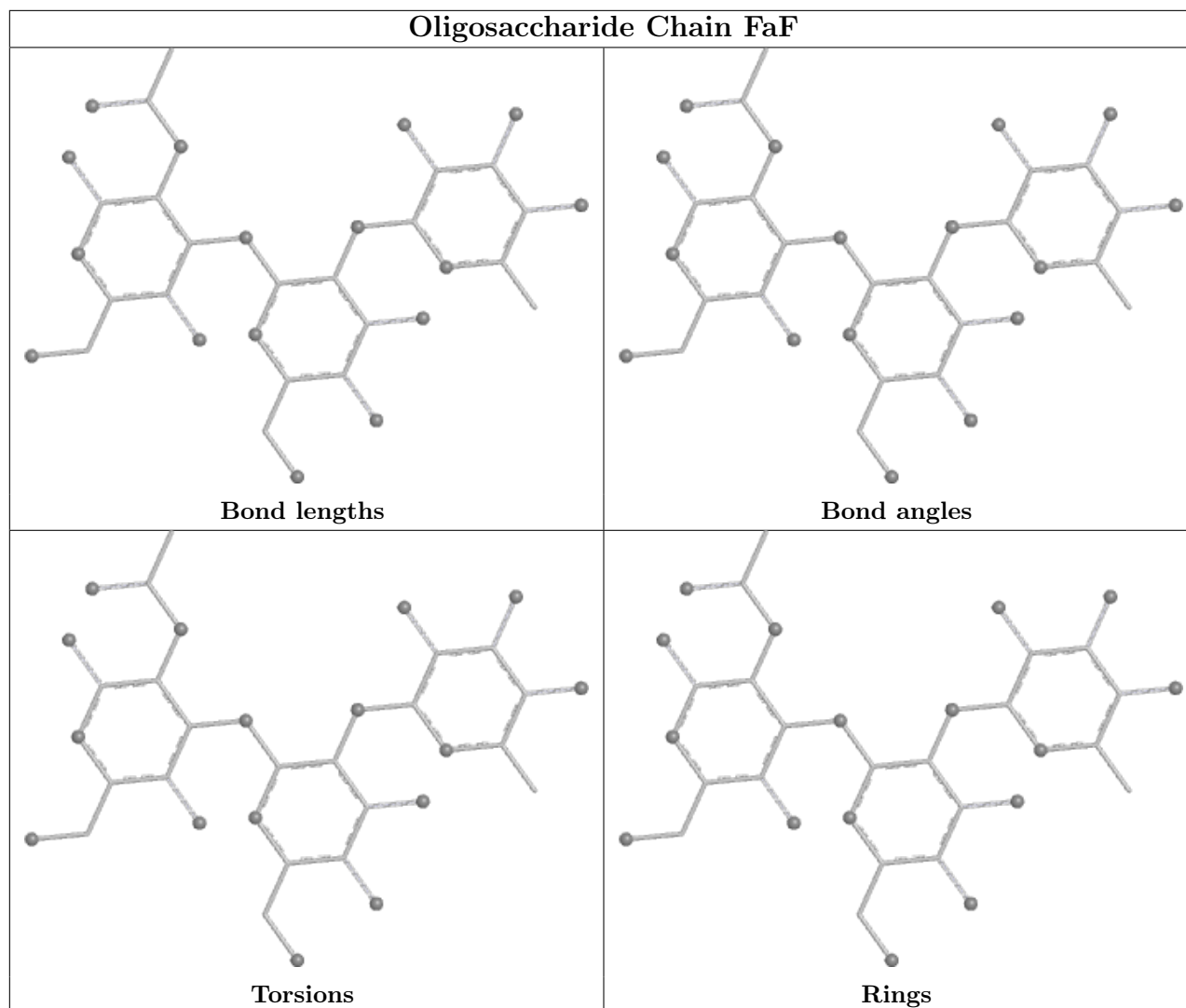












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
3	SO4	BBB	203	-	4,4,4	0.19	0	6,6,6	0.15	0
3	SO4	EEE	202	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	CCC	203	-	4,4,4	0.39	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	DDD	201	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	DDD	202	-	4,4,4	0.28	0	6,6,6	0.37	0
3	SO4	BBB	202	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	EEE	204	-	4,4,4	0.28	0	6,6,6	0.25	0
3	SO4	FFF	201	-	4,4,4	0.38	0	6,6,6	0.17	0
3	SO4	AAA	202	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	CCC	202	-	4,4,4	0.11	0	6,6,6	0.21	0
3	SO4	EEE	201	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	EEE	203	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	CCC	201	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	BBB	201	-	4,4,4	0.34	0	6,6,6	0.23	0
3	SO4	AAA	201	-	4,4,4	0.37	0	6,6,6	0.20	0
3	SO4	DDD	204[B]	-	4,4,4	0.31	0	6,6,6	0.32	0
3	SO4	DDD	204[A]	-	4,4,4	0.41	0	6,6,6	0.14	0
3	SO4	DDD	203	-	4,4,4	0.31	0	6,6,6	0.13	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
3	CCC	203	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%)	-0.27	1 (0%) 86 89	16, 21, 34, 38	1 (0%)
1	BBB	126/126 (100%)	-0.33	0 100 100	15, 18, 27, 41	1 (0%)
1	CCC	126/126 (100%)	-0.28	0 100 100	17, 23, 31, 37	0
1	DDD	126/126 (100%)	-0.23	1 (0%) 86 89	15, 20, 28, 41	0
1	EEE	126/126 (100%)	-0.29	0 100 100	17, 22, 31, 43	0
1	FFF	126/126 (100%)	-0.39	0 100 100	18, 21, 29, 38	0
All	All	756/756 (100%)	-0.30	2 (0%) 94 95	15, 21, 31, 43	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	66	GLN	2.8
1	AAA	127	LEU	2.1

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	EaE	1	15/15	0.88	0.18	26,29,38,38	0
2	GAL	AaA	2	11/12	0.89	0.13	22,32,38,43	0

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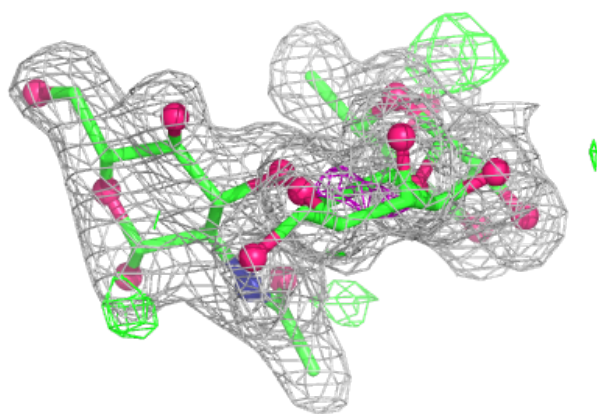
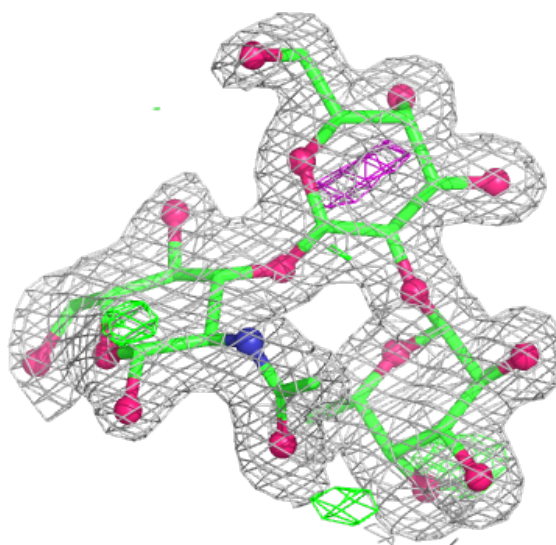
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GAL	FaF	2	11/12	0.90	0.11	23,29,36,37	0
2	FUC	AaA	3	10/11	0.91	0.07	20,22,23,24	0
2	NAG	FaF	1	15/15	0.91	0.07	24,31,40,46	0
2	NAG	CaC	1	15/15	0.91	0.11	22,26,34,36	0
2	GAL	EaE	2	11/12	0.92	0.16	24,28,38,43	0
2	FUC	EaE	3	10/11	0.92	0.08	21,22,24,25	0
2	GAL	DaD	2	11/12	0.92	0.11	19,25,30,36	0
2	GAL	BaB	2	11/12	0.92	0.13	21,26,35,41	0
2	GAL	CaC	2	11/12	0.93	0.07	19,24,28,38	0
2	NAG	DaD	1	15/15	0.93	0.13	22,27,38,41	0
2	NAG	BaB	1	15/15	0.94	0.14	24,27,39,39	0
2	NAG	AaA	1	15/15	0.94	0.08	30,35,41,55	0
2	FUC	BaB	3	10/11	0.94	0.08	17,18,20,20	0
2	FUC	DaD	3	10/11	0.95	0.06	16,18,19,19	0
2	FUC	FaF	3	10/11	0.95	0.06	20,22,23,24	0
2	FUC	CaC	3	10/11	0.96	0.08	17,18,20,20	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.

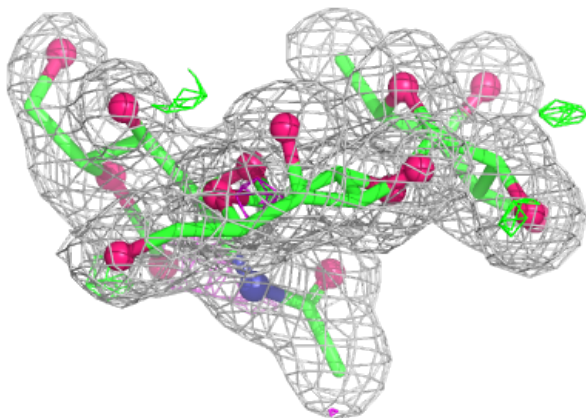
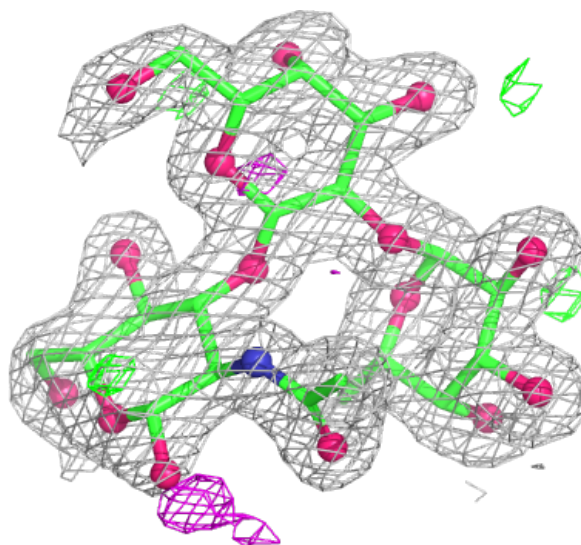
Electron density around Chain AaA:

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



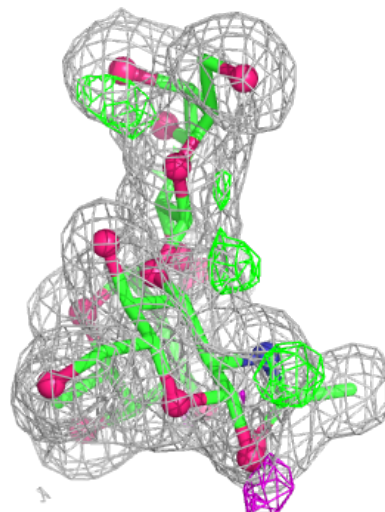
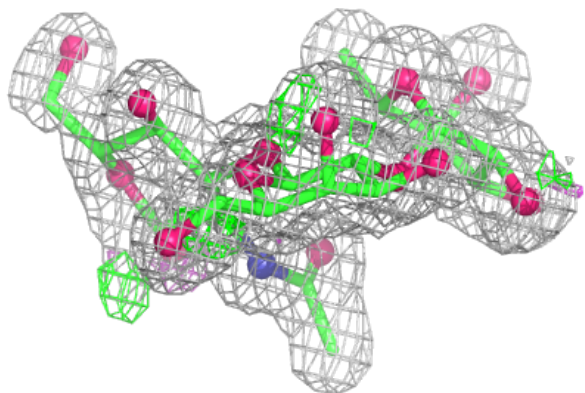
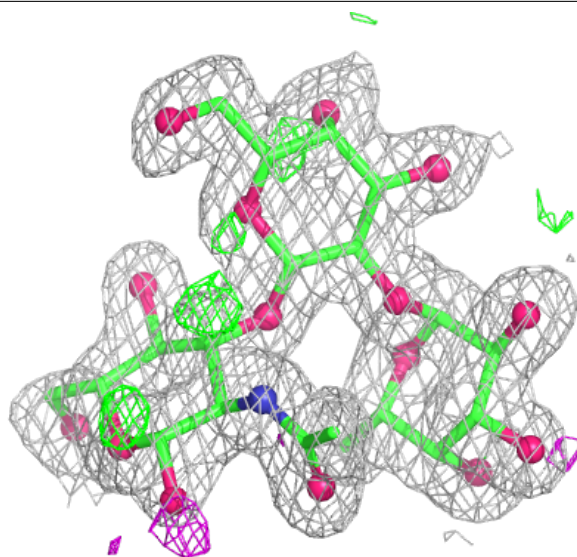
Electron density around Chain BaB:

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



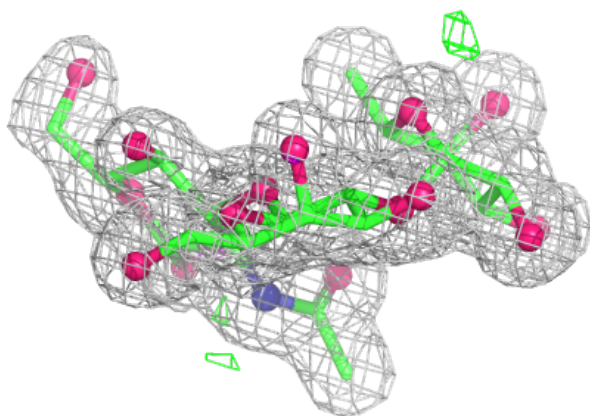
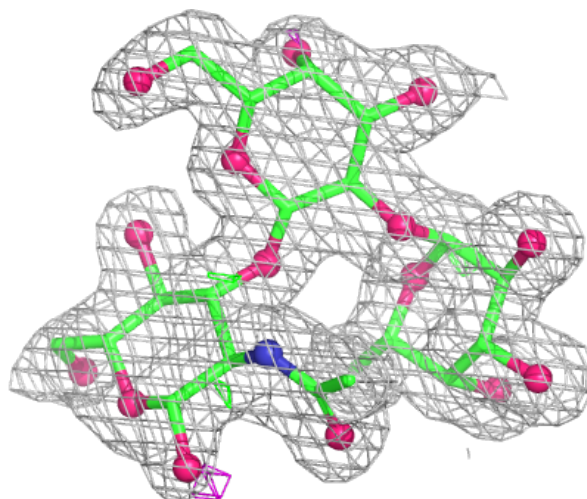
Electron density around Chain CaC:

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



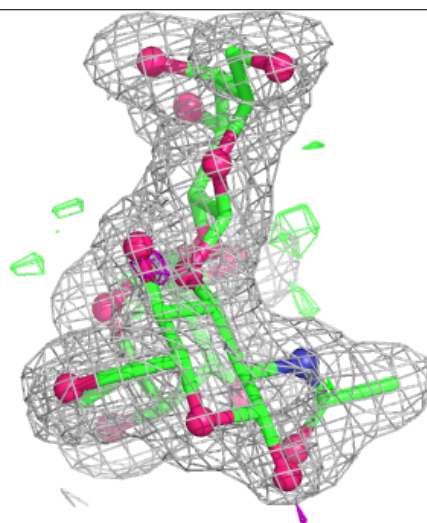
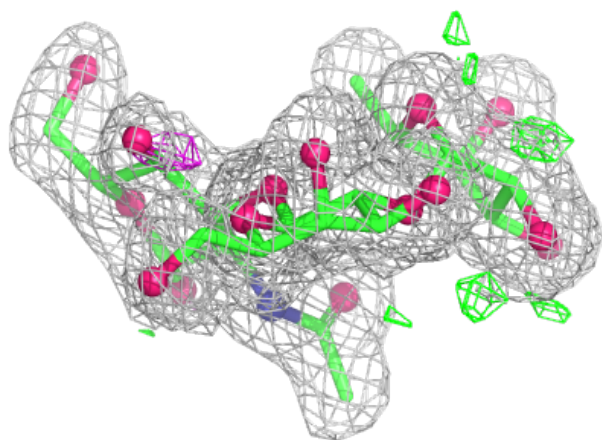
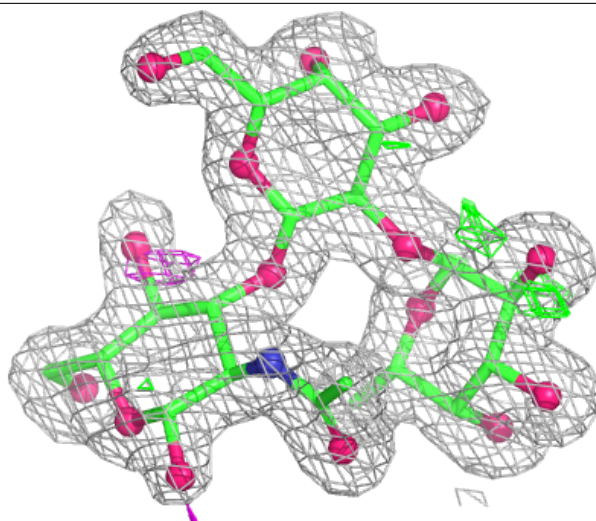
Electron density around Chain DaD:

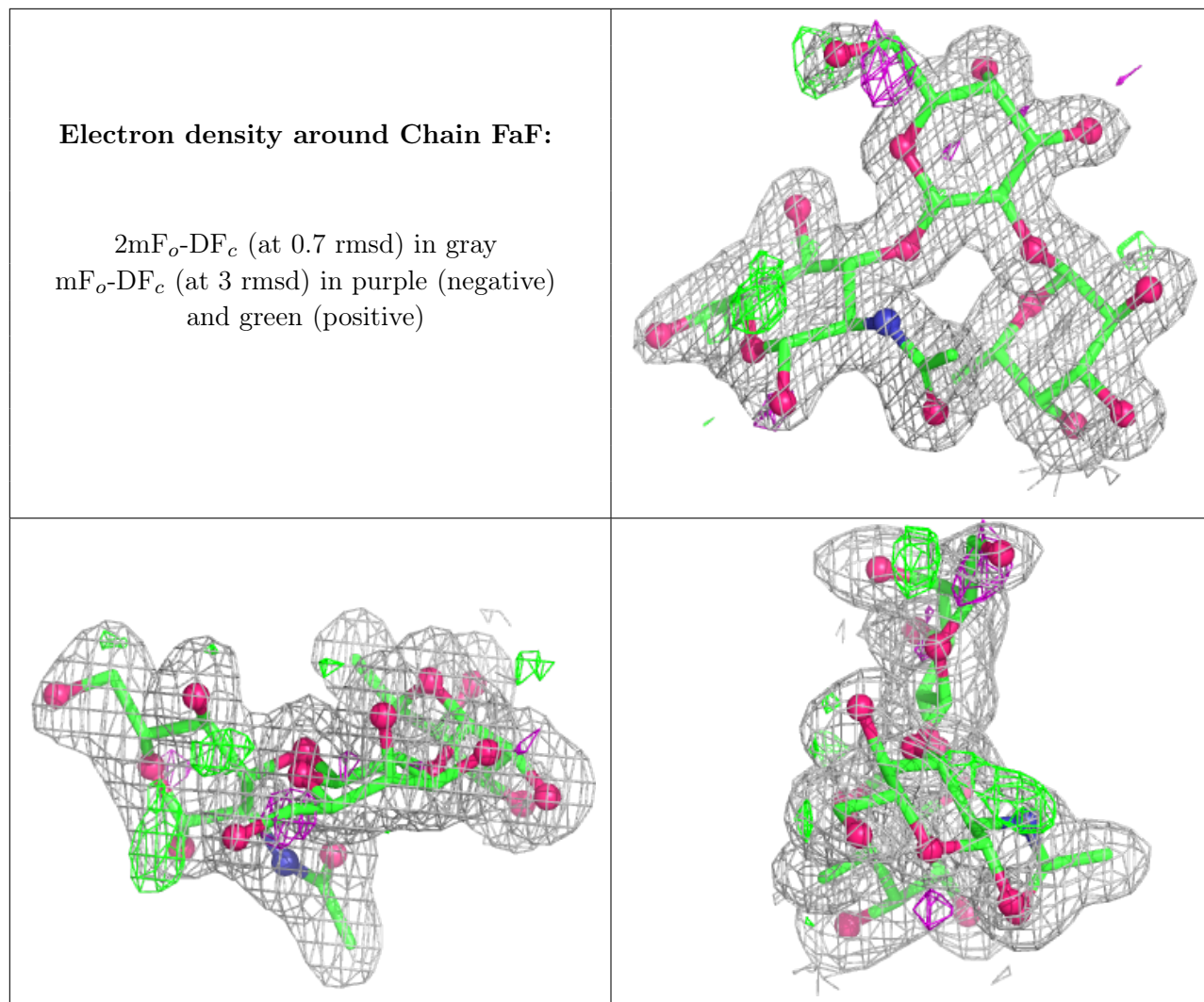
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
3	SO4	CCC	201	5/5	0.76	0.36	57,78,84,88	0
3	SO4	BBB	201	5/5	0.82	0.22	46,47,59,62	0
3	SO4	CCC	203	5/5	0.84	0.17	34,35,42,44	5
3	SO4	BBB	202	5/5	0.87	0.26	60,62,71,74	0
3	SO4	DDD	204[A]	5/5	0.88	0.15	30,30,34,38	5
3	SO4	DDD	204[B]	5/5	0.88	0.15	24,33,33,36	5
3	SO4	EEE	201	5/5	0.88	0.26	64,66,72,75	0
3	SO4	AAA	202	5/5	0.89	0.35	41,53,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	DDD	203	5/5	0.90	0.29	53,59,64,64	0
3	SO4	CCC	202	5/5	0.90	0.26	42,51,51,54	0
3	SO4	BBB	203	5/5	0.90	0.27	44,44,50,57	0
3	SO4	DDD	201	5/5	0.90	0.21	67,73,75,79	0
3	SO4	FFF	201	5/5	0.90	0.22	51,53,62,64	0
3	SO4	AAA	201	5/5	0.91	0.21	53,54,57,61	0
3	SO4	EEE	202	5/5	0.92	0.31	70,70,72,73	0
3	SO4	EEE	203	5/5	0.93	0.17	63,64,69,70	0
3	SO4	EEE	204	5/5	0.95	0.17	45,49,56,57	0
3	SO4	DDD	202	5/5	0.97	0.12	36,39,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.