wwPDB X-ray Structure Validation Summary Report (i)

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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

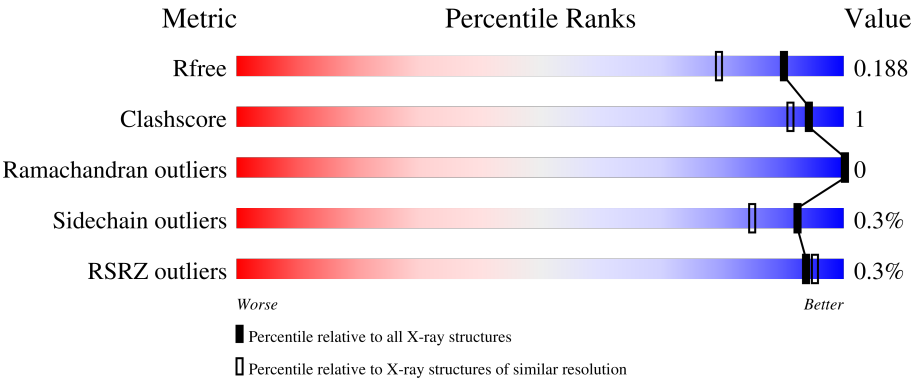
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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.



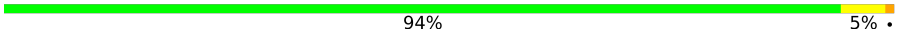
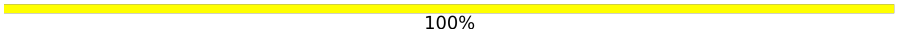
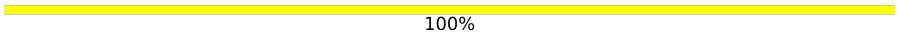
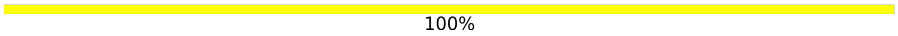
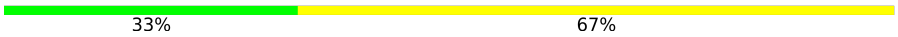
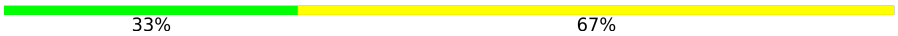
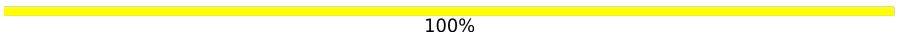
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	126	
2	AaA	3	
2	BaB	3	
2	CaC	3	
2	DaD	3	
2	EaE	3	
2	FaF	3	

2 Entry composition (i)

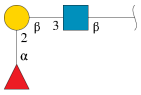
There are 4 unique types of molecules in this entry. The entry contains 7101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

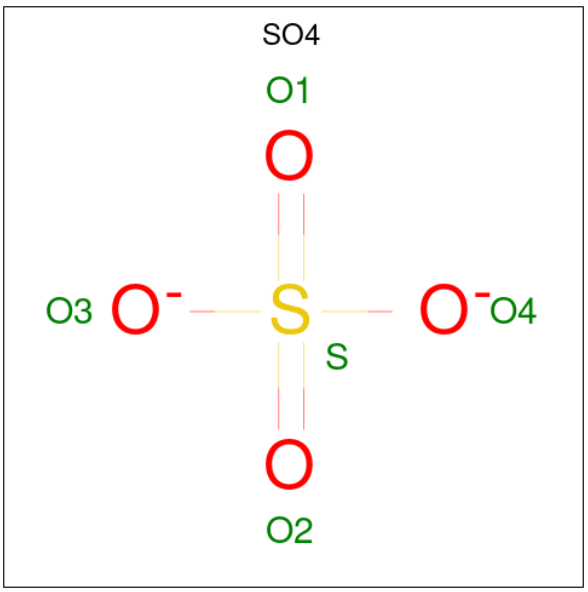
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	126	Total	C	N	O	S	0	3	0
			984	622	171	190	1			
1	BBB	126	Total	C	N	O	S	0	2	0
			978	621	169	187	1			
1	CCC	126	Total	C	N	O	S	0	2	0
			978	620	170	187	1			
1	DDD	126	Total	C	N	O	S	0	1	0
			969	614	168	186	1			
1	EEE	126	Total	C	N	O	S	0	2	0
			978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

- 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
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	CaC	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	DaD	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

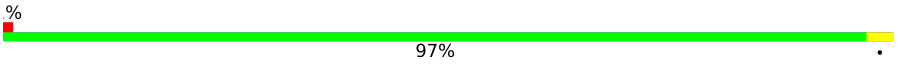
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	153	Total O 158 158	0	5
4	BBB	154	Total O 156 156	0	2
4	CCC	137	Total O 140 140	0	3
4	DDD	158	Total O 164 164	0	6
4	EEE	148	Total O 151 151	0	3
4	FFF	144	Total O 148 148	0	4

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.

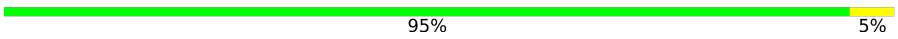
- Molecule 1: Mucin-binding lectin 1

Chain AAA:



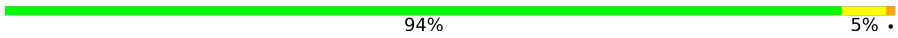
- Molecule 1: Mucin-binding lectin 1

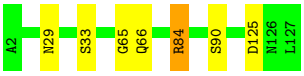
Chain BBB:



- Molecule 1: Mucin-binding lectin 1

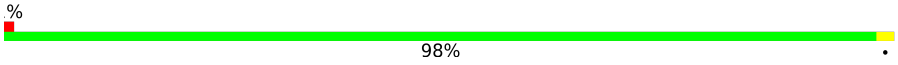
Chain CCC:

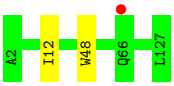




- Molecule 1: Mucin-binding lectin 1

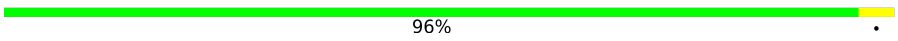
Chain DDD:

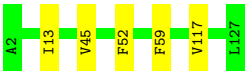




- Molecule 1: Mucin-binding lectin 1

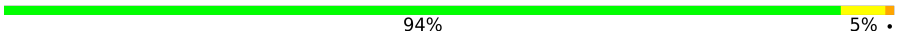
Chain EEE:

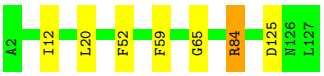




- Molecule 1: Mucin-binding lectin 1

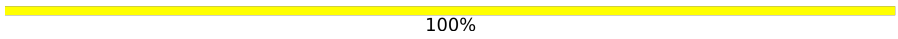
Chain FFF:





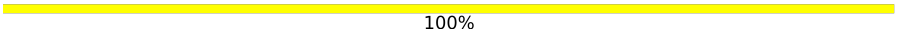
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AaA:



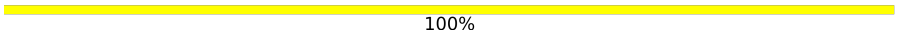
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BaB:



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

Chain CaC:

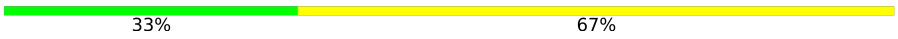


• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DaD:

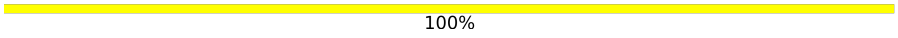
• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EaE:



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

Chain FaF:




NAG1
GAL2
FUC3

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.32 (at 1.55Å)	Xtriage
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	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.029 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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.

The worst 5 of 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

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

All (2) torsion outliers are listed below:

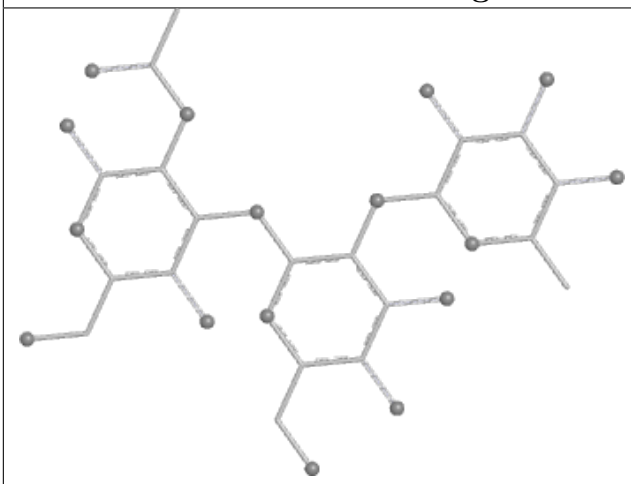
Mol	Chain	Res	Type	Atoms
2	AaA	1	NAG	O5-C5-C6-O6
2	AaA	1	NAG	C4-C5-C6-O6

There are no ring outliers.

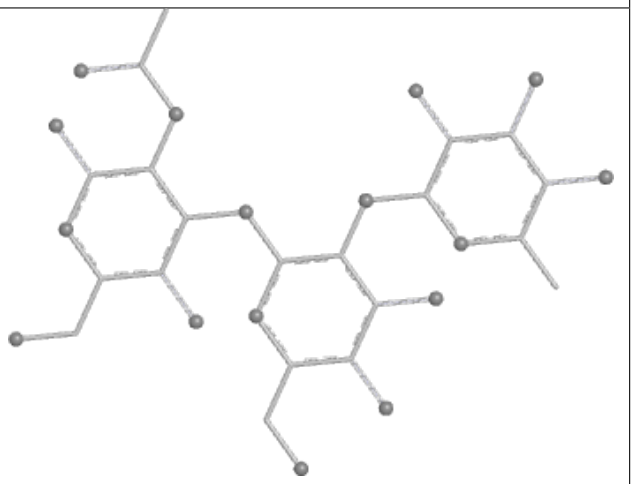
No monomer is involved in short contacts.

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

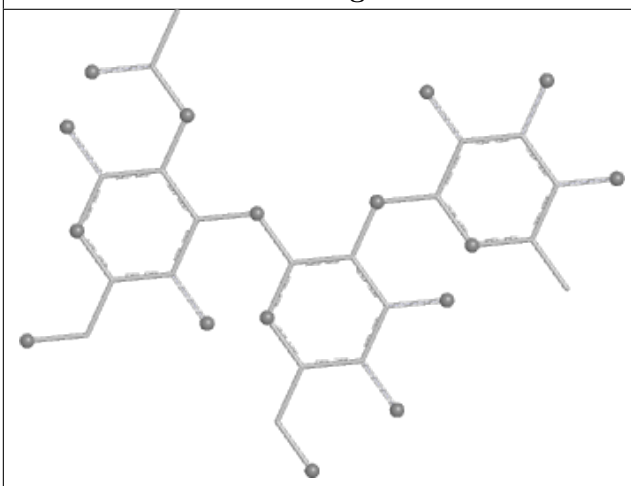
Oligosaccharide Chain AaA



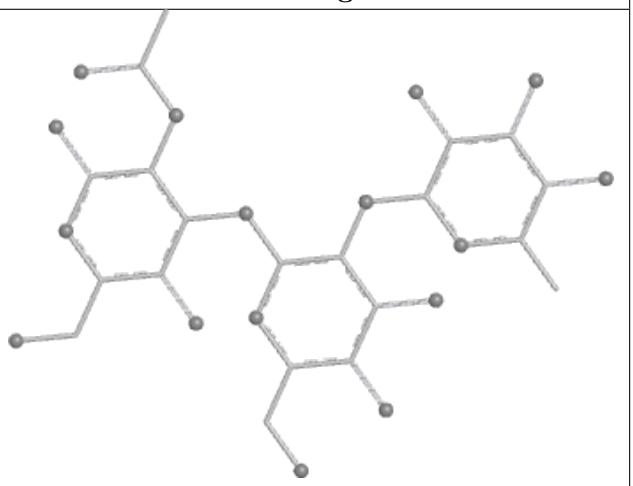
Bond lengths



Bond angles

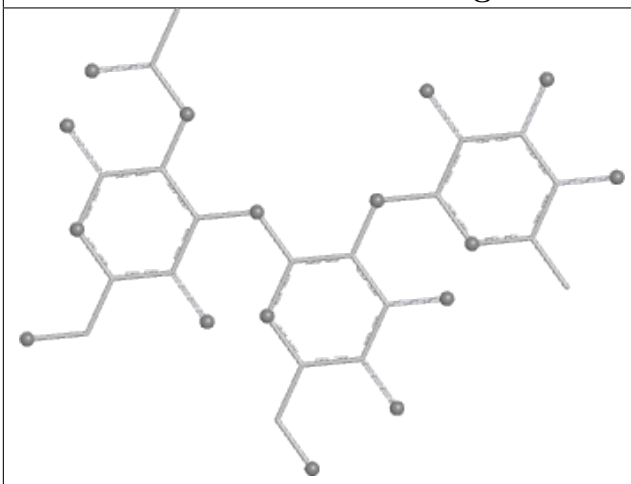


Torsions

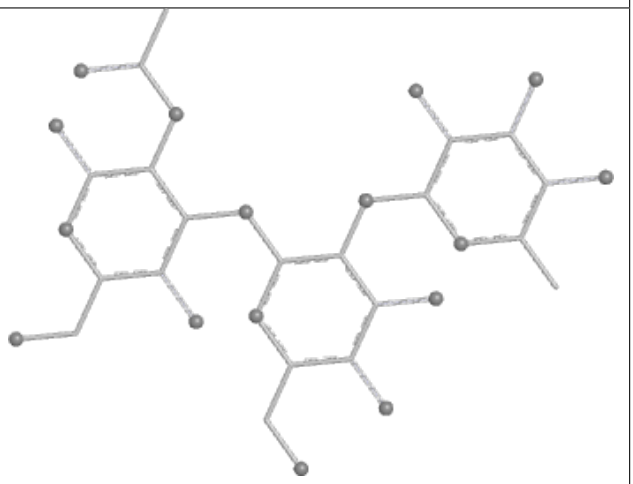


Rings

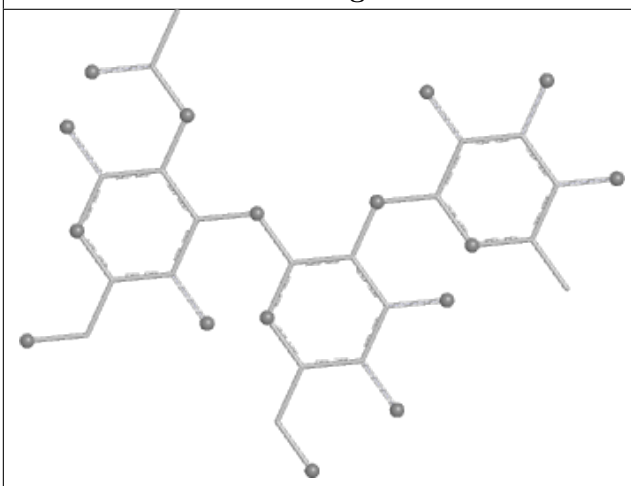
Oligosaccharide Chain BaB



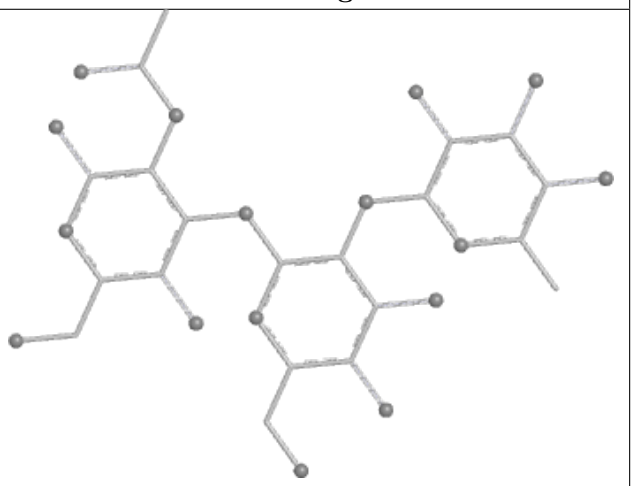
Bond lengths



Bond angles

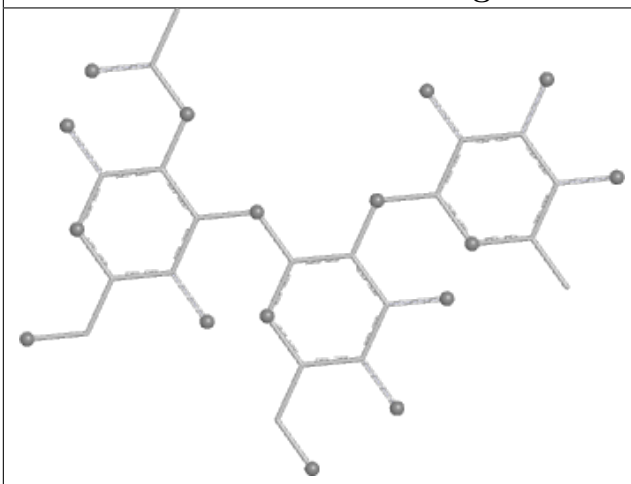


Torsions

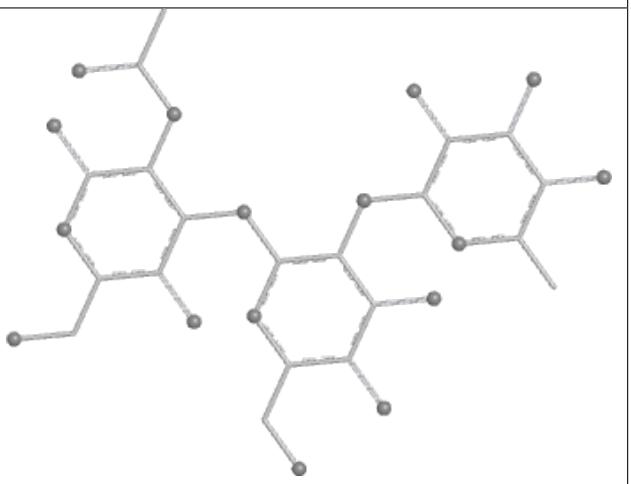


Rings

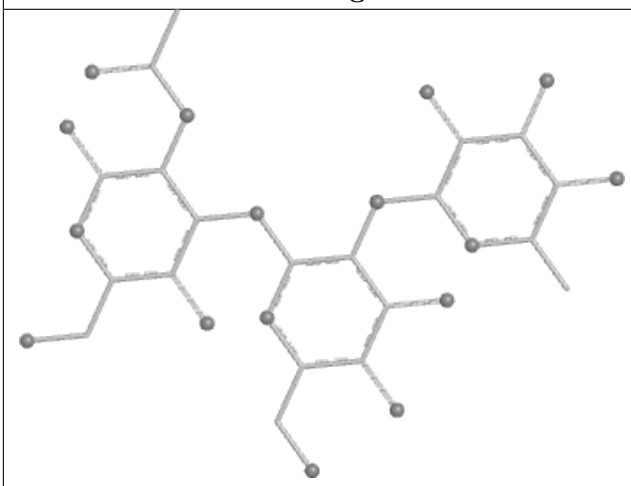
Oligosaccharide Chain CaC



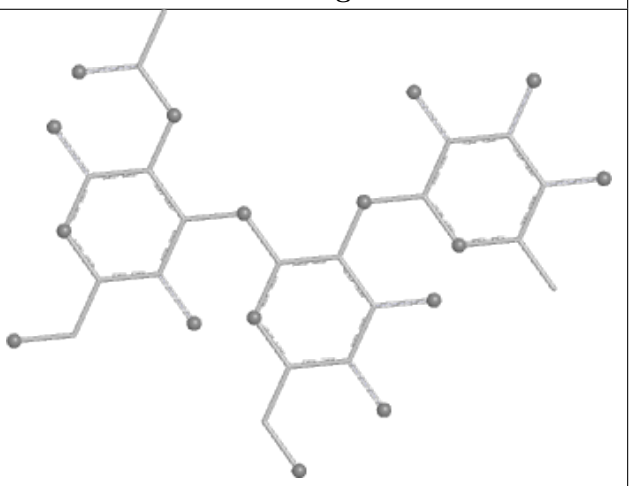
Bond lengths



Bond angles

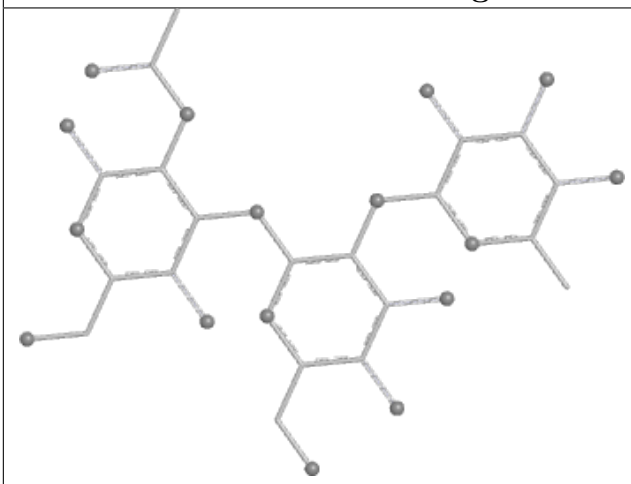


Torsions

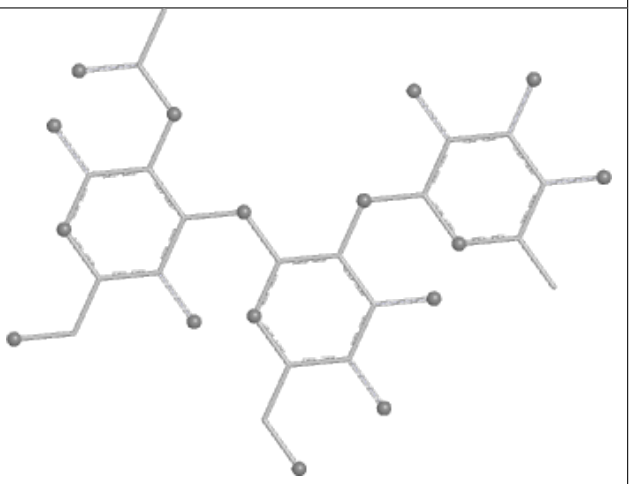


Rings

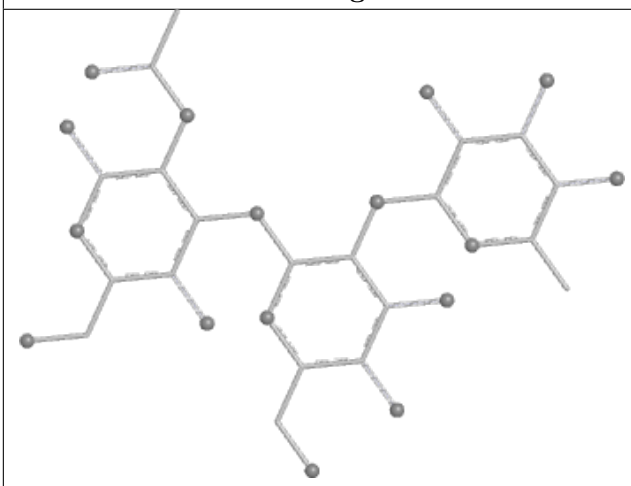
Oligosaccharide Chain DaD



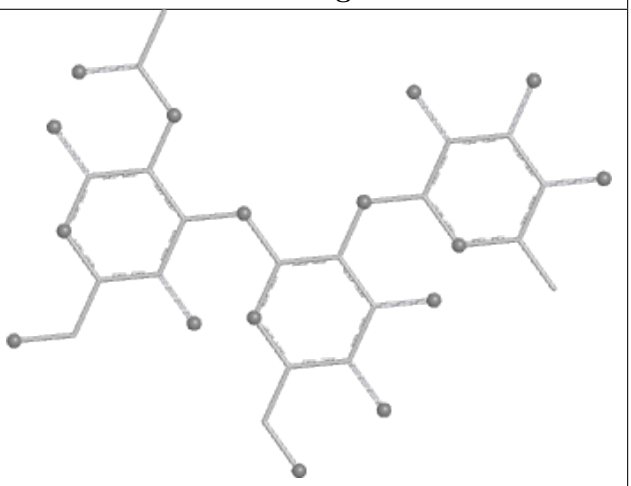
Bond lengths



Bond angles

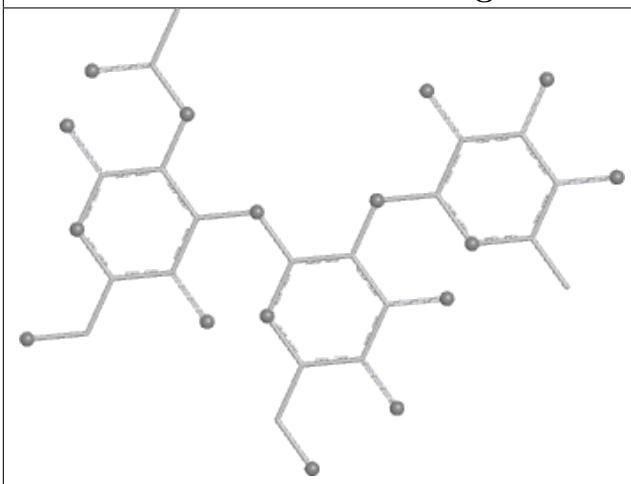


Torsions

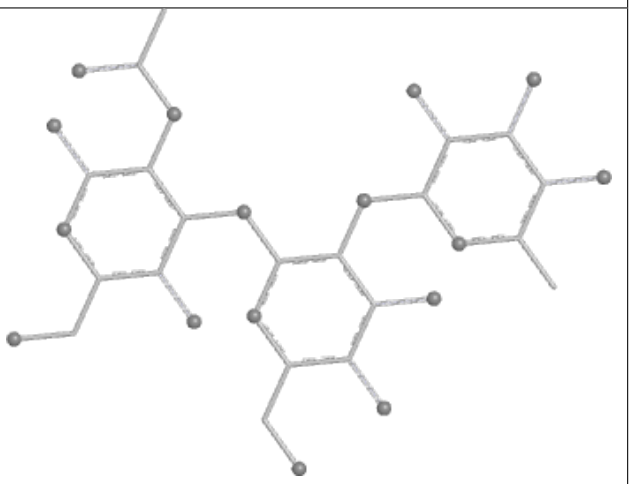


Rings

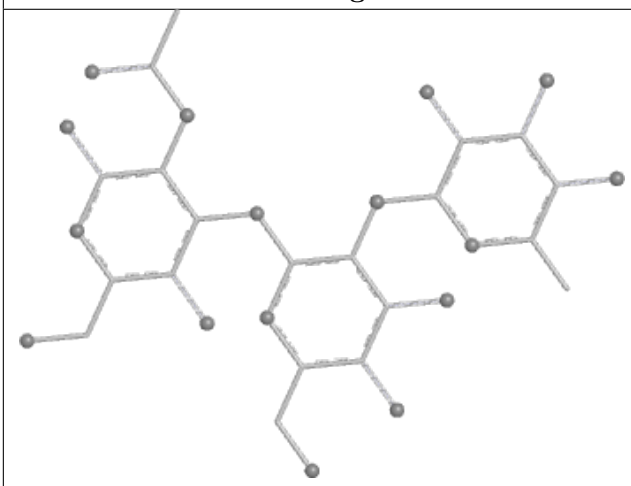
Oligosaccharide Chain EaE



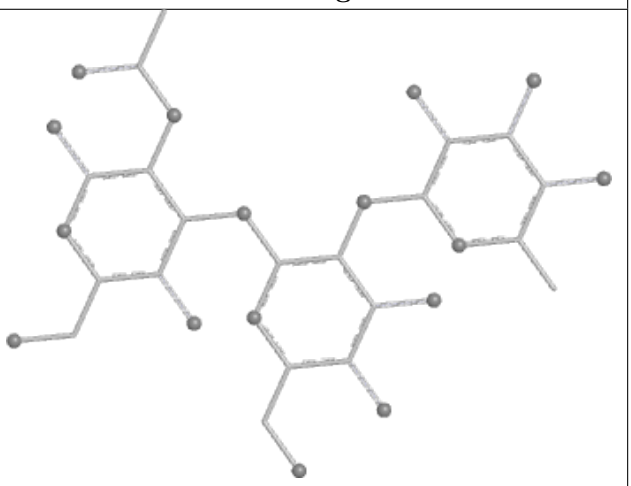
Bond lengths



Bond angles

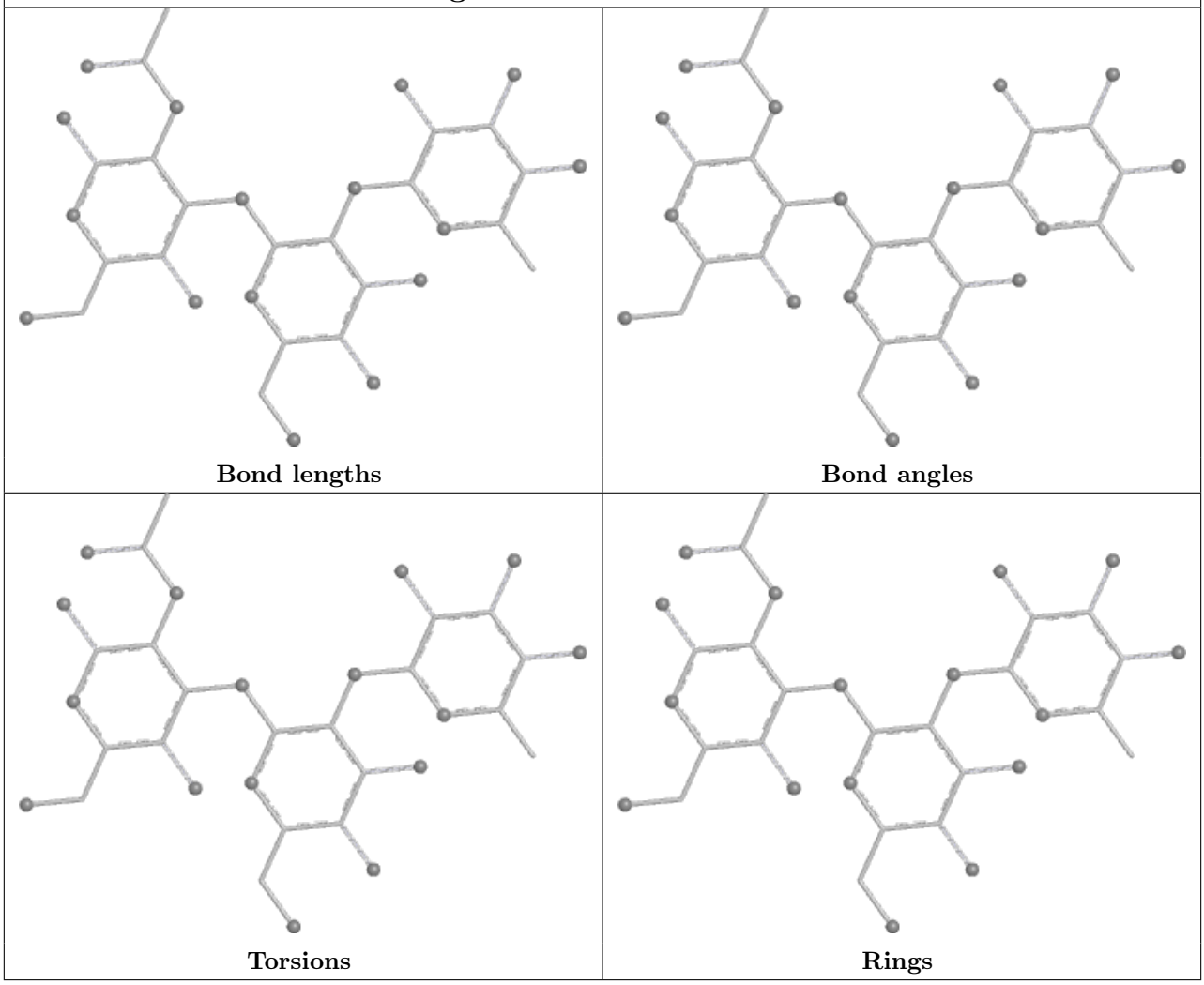


Torsions



Rings

Oligosaccharide Chain FaF



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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

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

6.3 Carbohydrates

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, 95^{th} 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

Continued on next page...

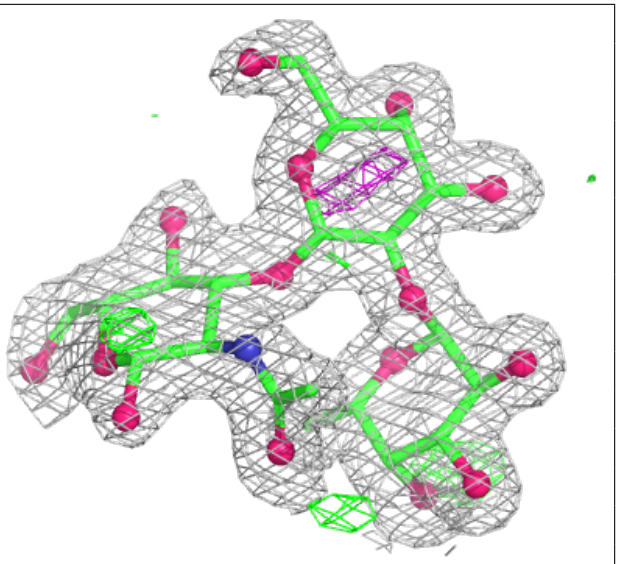
Continued from previous page...

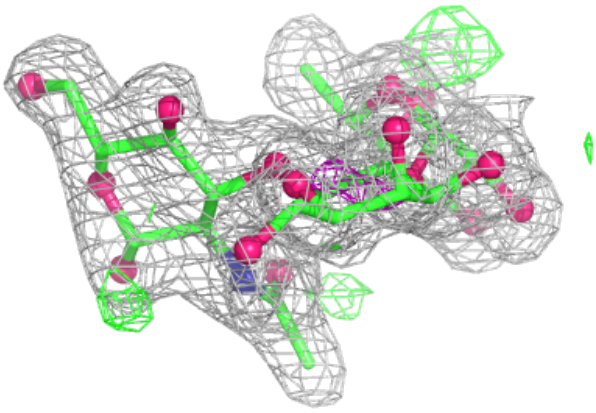
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	FaF	2	11/12	0.90	0.11	23,29,36,37	0
2	FUC	AaA	3	10/11	0.91	0.07	20,22,23,24	0
2	NAG	FaF	1	15/15	0.91	0.07	24,31,40,46	0
2	NAG	CaC	1	15/15	0.91	0.11	22,26,34,36	0
2	GAL	EaE	2	11/12	0.92	0.16	24,28,38,43	0
2	FUC	EaE	3	10/11	0.92	0.08	21,22,24,25	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

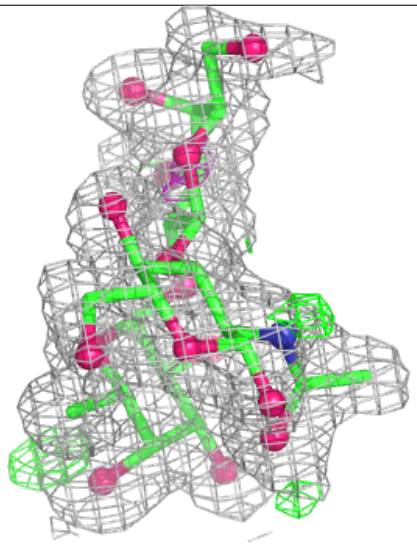
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

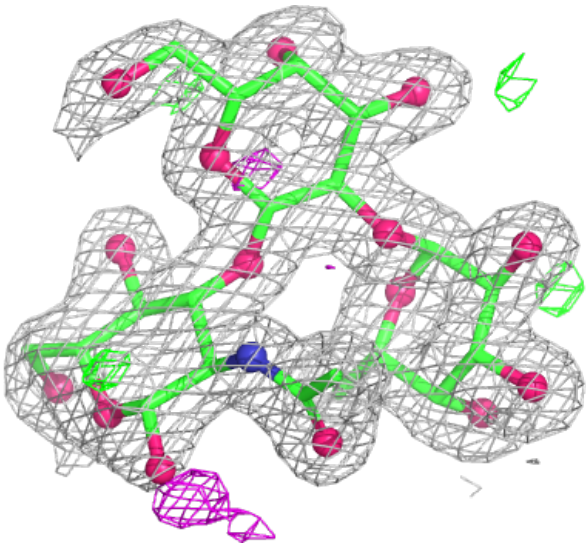


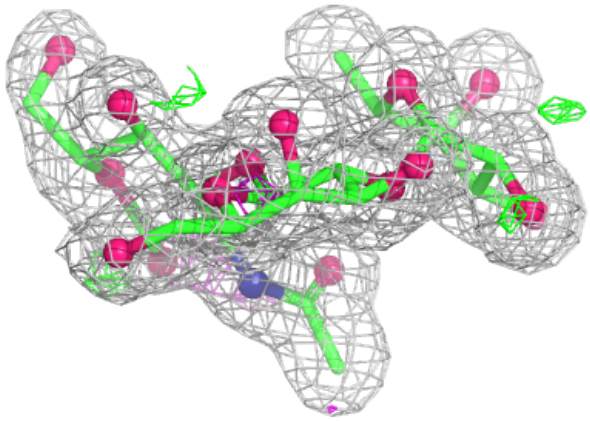




Electron density around Chain BaB:

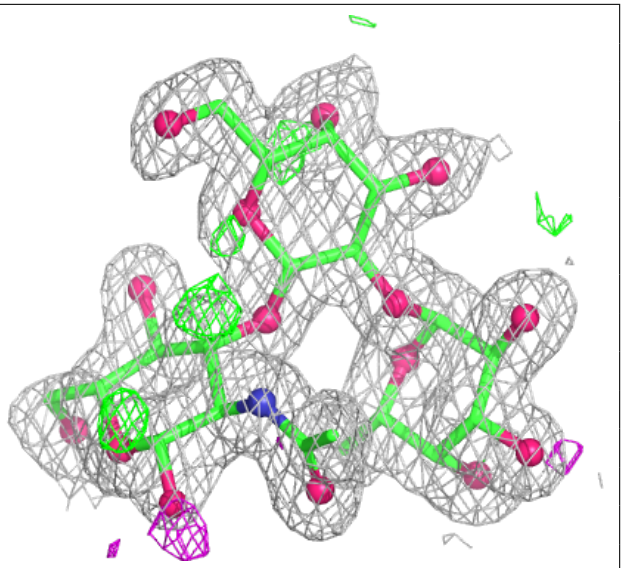
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

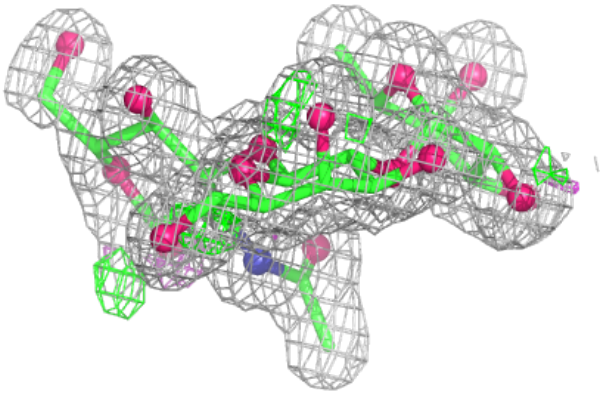


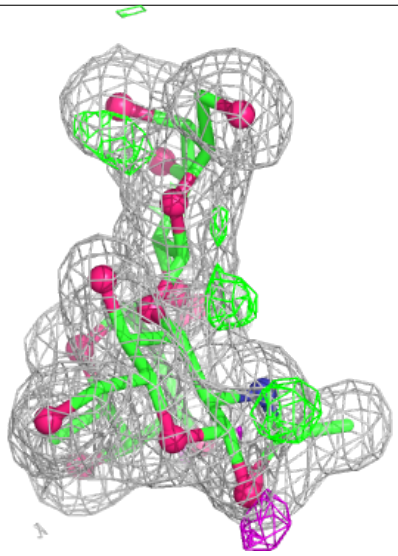


Electron density around Chain CaC:

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

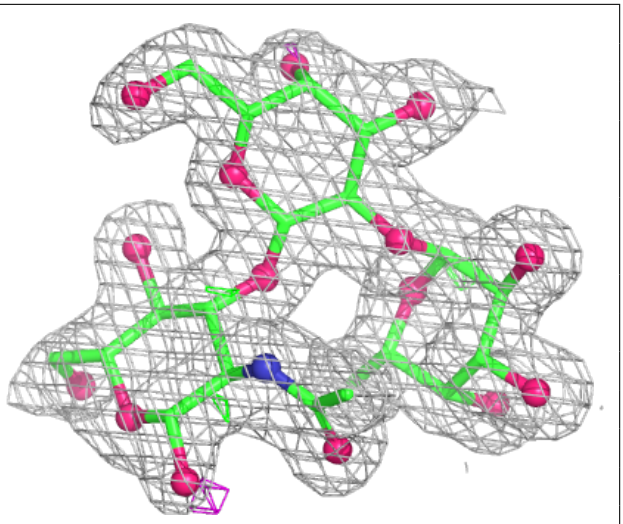


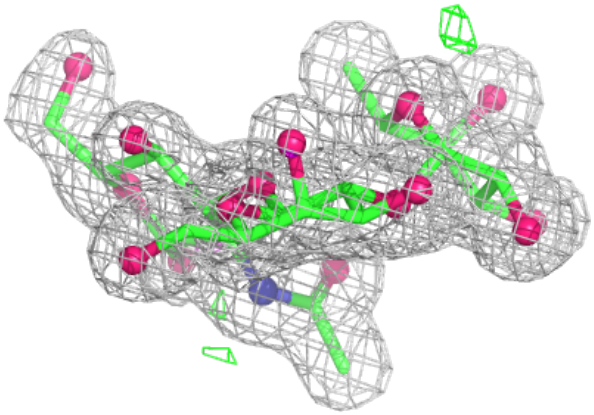


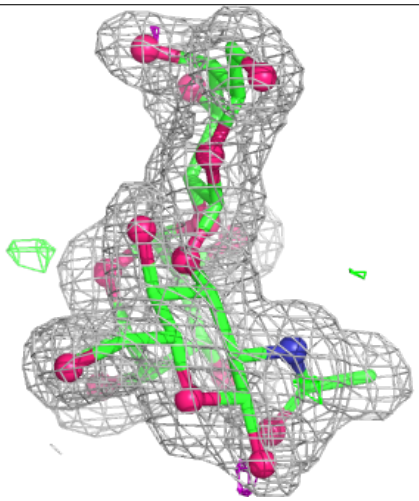


Electron density around Chain DaD:

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

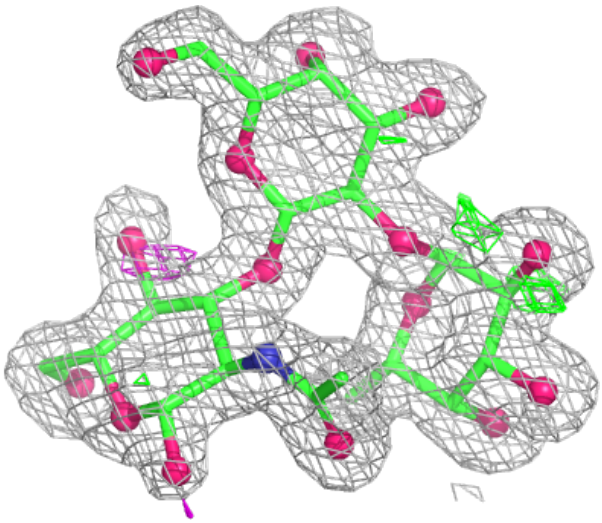


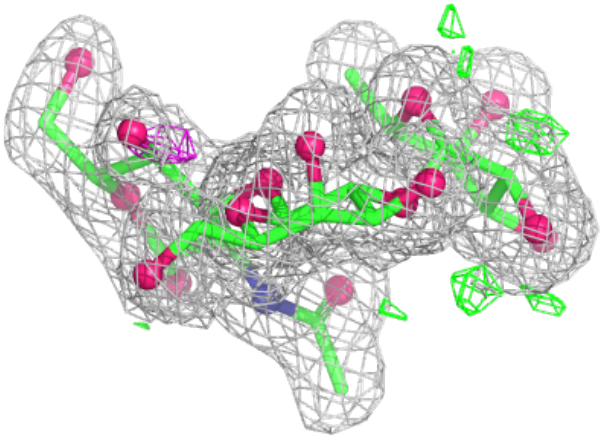


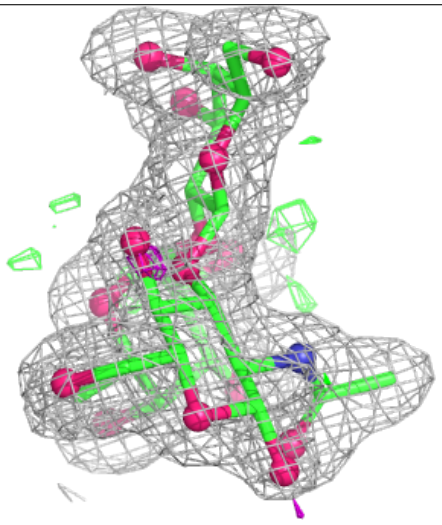


Electron density around Chain EaE:

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

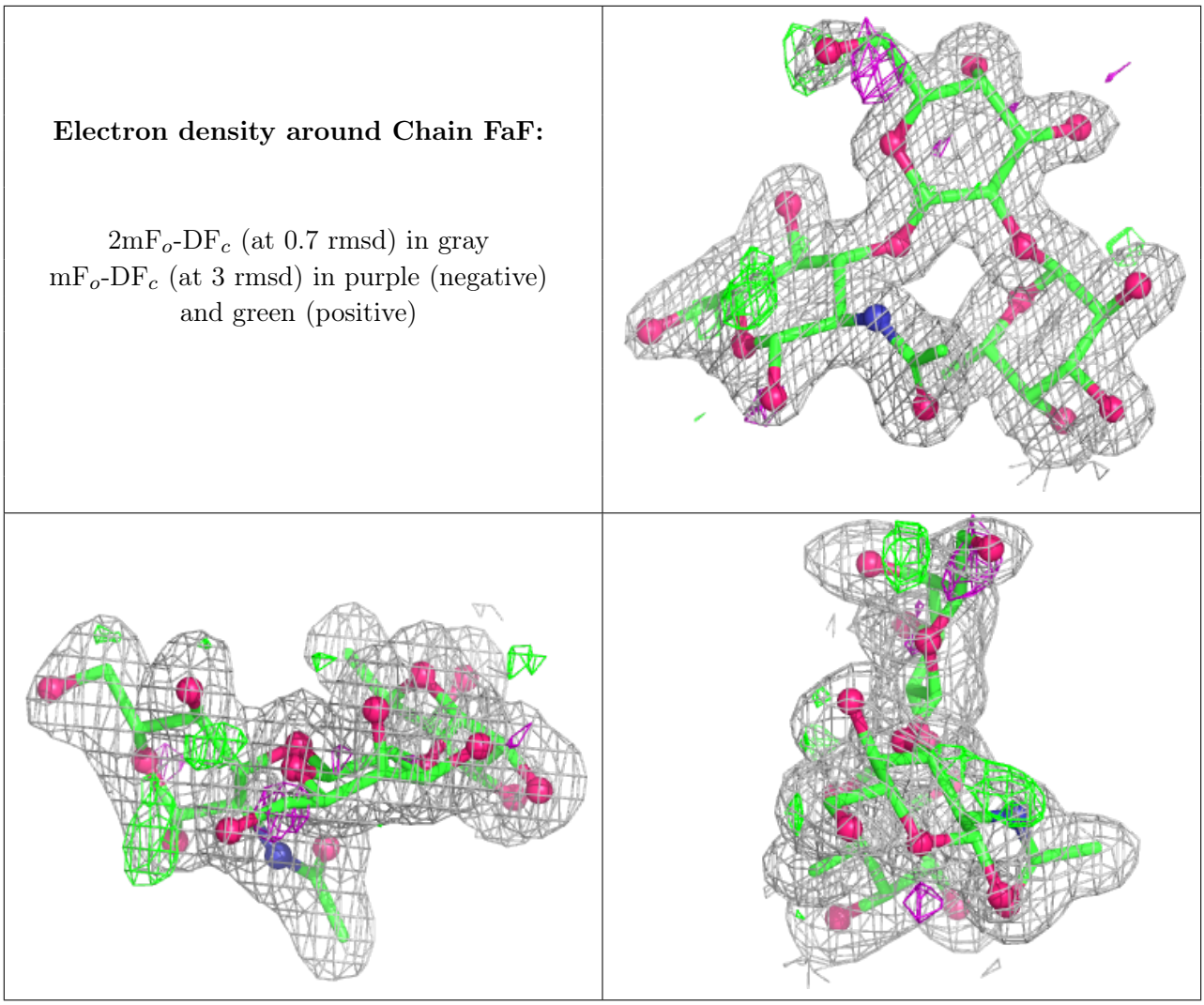






Electron density around Chain FaF:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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

Continued on next page...

Continued from previous page...

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.