Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 03:49 pm GMT

PDB ID	:	7ODK
Title	:	Plant peptide hormone receptor H1
Authors	:	Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.
Deposited on	:	2021-04-29
Resolution	:	1.83 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 (i) 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 (1)) were used in the production of this report:

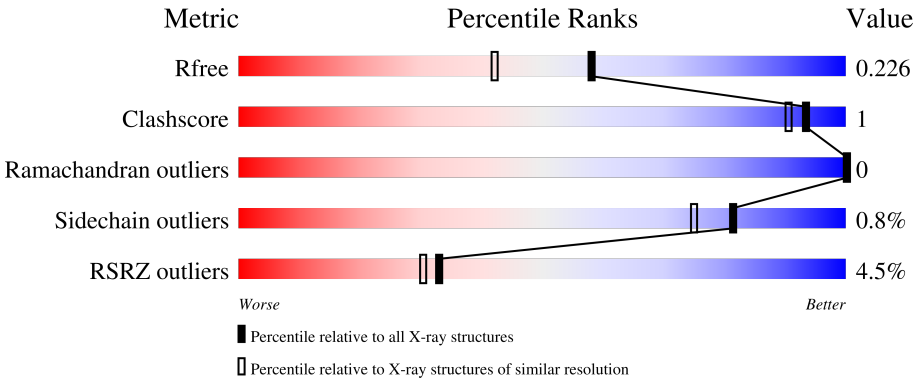
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	617	3% 91% · 5%
1	BBB	617	6% 91% · 5%
2	AlA	3	33% 67%
2	BkB	3	100%
3	AmA	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	AnA	2	100%
3	AoA	2	100%
3	AqA	2	50% 50%
3	BmB	2	100%
3	BoB	2	100%
3	BpB	2	50% 50%
3	BvB	2	100%
3	BwB	2	50% 50%
4	AsA	4	75% 25%
4	BqB	4	100%
5	AwA	3	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	AlA	3	X	-	-	-
2	BMA	BkB	3	X	-	-	-
3	NAG	AmA	2	X	-	-	-
3	NAG	AnA	2	X	-	-	-
3	NAG	AoA	2	X	-	-	-
3	NAG	AqA	2	X	-	-	X
3	NAG	BoB	2	X	-	-	-
3	NAG	BpB	2	X	-	-	-
3	NAG	BvB	2	X	-	-	X
3	NAG	BwB	2	X	-	-	-
4	NAG	BqB	3	X	-	-	-
5	FUC	AwA	2	-	-	-	X
5	NAG	AwA	3	X	-	-	X
7	NAG	AAA	712	-	-	-	X
7	NAG	AAA	714	-	-	-	X
7	NAG	BBB	711	-	-	-	X
7	NAG	BBB	712	-	-	-	X
7	NAG	BBB	713	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10222 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 Receptor-like protein kinase HSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	589	Total	C	N	O	S	0	7	0
			4496	2839	746	895	16			
1	BBB	585	Total	C	N	O	S	0	6	0
			4411	2789	730	878	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	12	GLY	-	expression tag	UNP Q9SGP2
AAA	13	SER	-	expression tag	UNP Q9SGP2
AAA	14	SER	-	expression tag	UNP Q9SGP2
AAA	15	MET	-	expression tag	UNP Q9SGP2
AAA	16	ASP	-	expression tag	UNP Q9SGP2
AAA	619	LEU	-	expression tag	UNP Q9SGP2
AAA	620	GLU	-	expression tag	UNP Q9SGP2
AAA	621	GLY	-	expression tag	UNP Q9SGP2
AAA	622	SER	-	expression tag	UNP Q9SGP2
AAA	623	GLU	-	expression tag	UNP Q9SGP2
AAA	624	ASN	-	expression tag	UNP Q9SGP2
AAA	625	LEU	-	expression tag	UNP Q9SGP2
AAA	626	TYR	-	expression tag	UNP Q9SGP2
AAA	627	PHE	-	expression tag	UNP Q9SGP2
AAA	628	GLN	-	expression tag	UNP Q9SGP2
BBB	12	GLY	-	expression tag	UNP Q9SGP2
BBB	13	SER	-	expression tag	UNP Q9SGP2
BBB	14	SER	-	expression tag	UNP Q9SGP2
BBB	15	MET	-	expression tag	UNP Q9SGP2
BBB	16	ASP	-	expression tag	UNP Q9SGP2
BBB	619	LEU	-	expression tag	UNP Q9SGP2
BBB	620	GLU	-	expression tag	UNP Q9SGP2
BBB	621	GLY	-	expression tag	UNP Q9SGP2
BBB	622	SER	-	expression tag	UNP Q9SGP2
BBB	623	GLU	-	expression tag	UNP Q9SGP2

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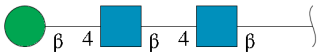
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	624	ASN	-	expression tag	UNP Q9SGP2
BBB	625	LEU	-	expression tag	UNP Q9SGP2
BBB	626	TYR	-	expression tag	UNP Q9SGP2
BBB	627	PHE	-	expression tag	UNP Q9SGP2
BBB	628	GLN	-	expression tag	UNP Q9SGP2

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	AlA	3	Total C N O 39 22 2 15	0	0	0
2	BkB	3	Total C N O 39 22 2 15	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	AmA	2	Total C N O 28 16 2 10	0	0	0
3	AnA	2	Total C N O 28 16 2 10	0	0	0
3	AoA	2	Total C N O 28 16 2 10	0	0	0
3	AqA	2	Total C N O 28 16 2 10	0	0	0
3	BmB	2	Total C N O 28 16 2 10	0	0	0
3	BoB	2	Total C N O 28 16 2 10	0	0	0
3	BpB	2	Total C N O 28 16 2 10	0	0	0

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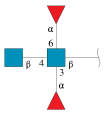
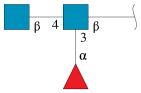
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	BvB	2	Total C N O 28 16 2 10	0	0	0
3	BwB	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



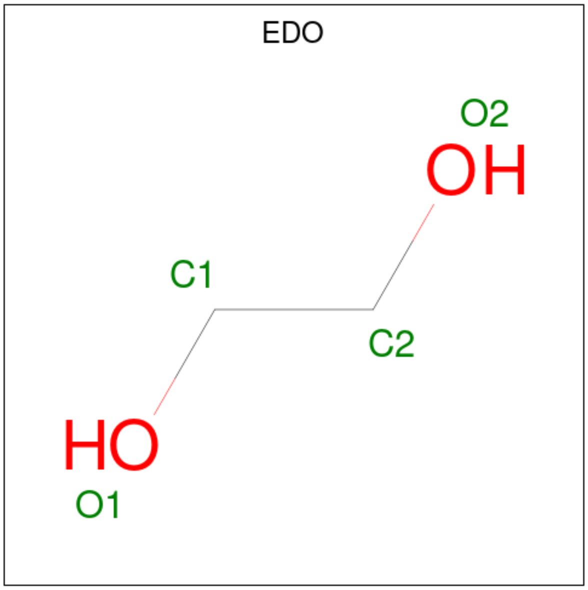
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	AsA	4	Total C N O 48 28 2 18	0	0	0
4	BqB	4	Total C N O 48 28 2 18	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	AwA	3	Total C N O 38 22 2 14	0	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	AAA	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0

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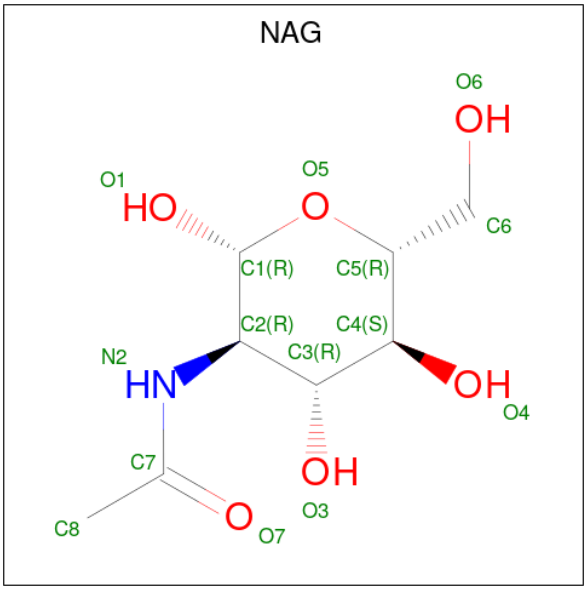
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0
6	BBB	1	Total C O 4 2 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C N O 14 8 1 5	0	0
7	AAA	1	Total C N O 14 8 1 5	0	0
7	AAA	1	Total C N O 14 8 1 5	0	0
7	BBB	1	Total C N O 14 8 1 5	0	0

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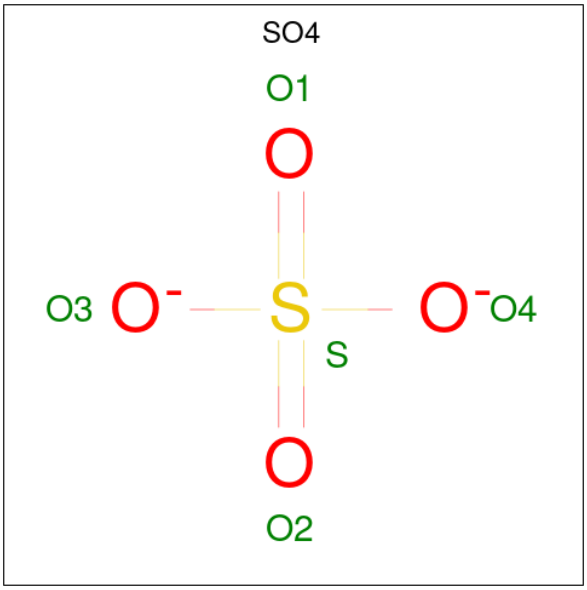
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	BBB	1	Total C N O 14 8 1 5	0	0
7	BBB	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total O S 5 4 1	0	0
8	BBB	1	Total O S 5 4 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	BBB	1	Total Na 1 1	0	0

- Molecule 10 is water.

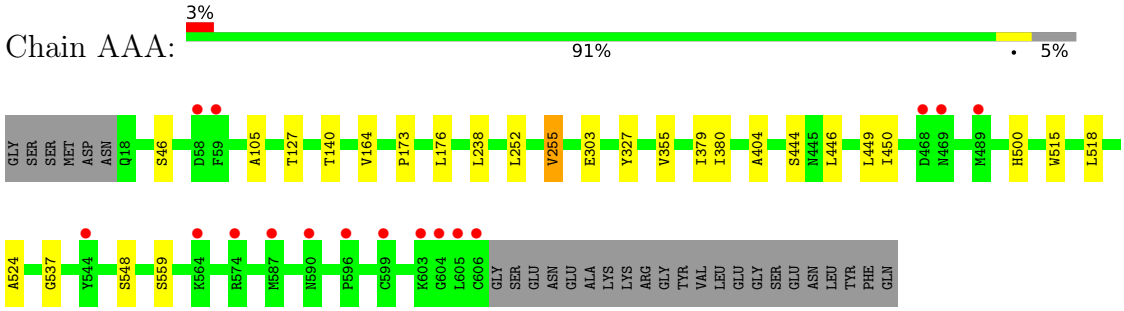
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	355	Total O 355 355	0	0
10	BBB	317	Total O 317 317	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

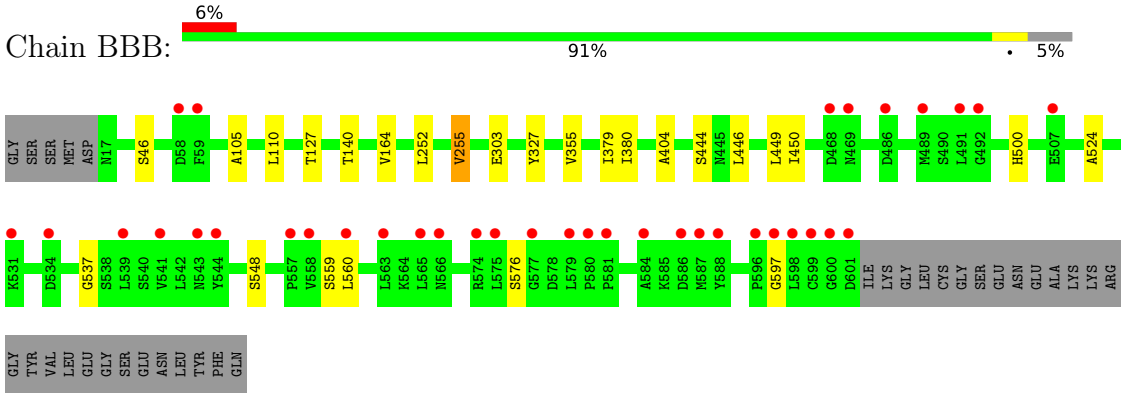
• Molecule 1: Receptor-like protein kinase HSL1

Chain AAA:



• Molecule 1: Receptor-like protein kinase HSL1

Chain BBB:

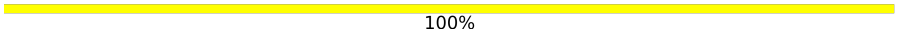


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AlA:

• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BkB:

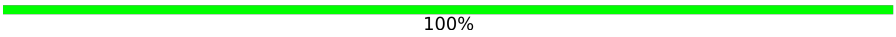


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AmA:

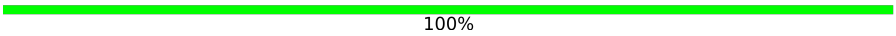
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AnA:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AoA:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AqA:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BmB:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

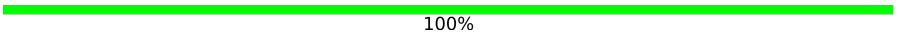
Chain BoB:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BpB:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BvB:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

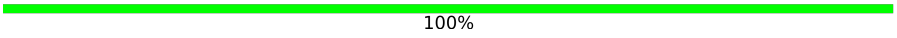
Chain BwB:

• Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AsA:

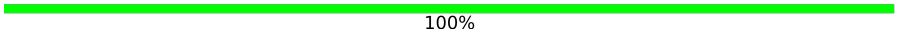
• Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BqB:



• Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AwA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.54Å 84.00Å 89.06Å 99.18° 113.73° 108.41°	Depositor
Resolution (Å)	47.08 – 1.83 47.08 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.08-1.83) 94.4 (47.08-1.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.216 0.212 , 0.226	Depositor DCC
R_{free} test set	7798 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10222	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: FUC, NA, NAG, BMA, SO4, EDO

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	0.62	0/4582	0.63	0/6241
1	BBB	0.63	0/4497	0.63	0/6136
All	All	0.62	0/9079	0.63	0/12377

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4496	0	4414	13	0
1	BBB	4411	0	4279	13	0
2	AlA	39	0	34	0	0
2	BkB	39	0	34	0	0
3	AmA	28	0	25	0	0
3	AnA	28	0	25	0	0
3	AoA	28	0	25	0	0
3	AqA	28	0	25	0	0
3	BmB	28	0	25	0	0
3	BoB	28	0	25	0	0
3	BpB	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BvB	28	0	25	0	0
3	BwB	28	0	25	0	0
4	AsA	48	0	43	0	0
4	BqB	48	0	43	0	0
5	AwA	38	0	34	0	0
6	AAA	44	0	66	1	0
6	BBB	40	0	60	0	0
7	AAA	42	0	39	0	0
7	BBB	42	0	39	0	0
8	AAA	5	0	0	0	0
8	BBB	5	0	0	0	0
9	BBB	1	0	0	0	0
10	AAA	355	0	0	0	0
10	BBB	317	0	0	0	0
All	All	10222	0	9310	26	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 (26) 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:AAA:537:GLY:HA3	1:AAA:559:SER:HB2	1.85	0.58
1:AAA:105:ALA:HB2	1:AAA:127:THR:HB	1.87	0.56
1:BBB:537:GLY:HA3	1:BBB:559:SER:HB2	1.88	0.55
1:BBB:105:ALA:HB2	1:BBB:127:THR:HB	1.89	0.54
1:BBB:576:SER:HA	1:BBB:597:GLY:HA3	1.92	0.50
1:BBB:355:VAL:HG22	1:BBB:379:ILE:HG22	1.96	0.48
1:AAA:173:PRO:HG2	1:AAA:176:LEU:HG	1.94	0.48
1:AAA:355:VAL:HG22	1:AAA:379:ILE:HG22	1.96	0.47
1:BBB:303:GLU:HB3	1:BBB:327:TYR:CE2	2.50	0.46
1:AAA:303:GLU:HB3	1:AAA:327:TYR:CE2	2.50	0.46
1:AAA:524:ALA:HA	1:AAA:548:SER:O	2.17	0.45
1:BBB:524:ALA:HA	1:BBB:548:SER:O	2.17	0.44
1:BBB:380:ILE:HA	1:BBB:404:ALA:O	2.18	0.44
1:BBB:560:LEU:HD23	1:BBB:560:LEU:HA	1.89	0.43
1:BBB:252:LEU:HB3	1:BBB:255:VAL:HB	2.01	0.43
1:AAA:380:ILE:HA	1:AAA:404:ALA:O	2.18	0.42
1:BBB:446:LEU:HD21	1:BBB:449:LEU:HD13	2.01	0.42
1:AAA:140:THR:HA	1:AAA:164:VAL:O	2.20	0.42
1:AAA:252:LEU:HB3	1:AAA:255:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:500:HIS:HA	1:BBB:524:ALA:O	2.20	0.41
1:AAA:446:LEU:HD21	1:AAA:449:LEU:HD13	2.03	0.41
1:AAA:500:HIS:HA	1:AAA:524:ALA:O	2.20	0.41
1:BBB:140:THR:HA	1:BBB:164:VAL:O	2.21	0.41
1:AAA:238:LEU:HA	6:AAA:704:EDO:H11	2.03	0.40
1:BBB:110:LEU:HD12	1:BBB:110:LEU:HA	1.92	0.40
1:AAA:515:TRP:HB3	1:AAA:518:LEU:HB2	2.04	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	594/617 (96%)	585 (98%)	9 (2%)	0	100	100
1	BBB	589/617 (96%)	580 (98%)	9 (2%)	0	100	100
All	All	1183/1234 (96%)	1165 (98%)	18 (2%)	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	514/540 (95%)	510 (99%)	4 (1%)	81	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BBB	495/540 (92%)	491 (99%)	4 (1%)	81 75
All	All	1009/1080 (93%)	1001 (99%)	8 (1%)	81 75

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

Mol	Chain	Res	Type
1	AAA	46	SER
1	AAA	255	VAL
1	AAA	444	SER
1	AAA	450	ILE
1	BBB	46	SER
1	BBB	255	VAL
1	BBB	444	SER
1	BBB	450	ILE

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)

35 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	AlA	1	2,1	14,14,15	0.29	0	17,19,21	1.03	2 (11%)
2	NAG	AlA	2	2	14,14,15	0.31	0	17,19,21	0.70	0
2	BMA	AlA	3	2	11,11,12	0.31	0	15,15,17	1.04	2 (13%)
3	NAG	AmA	1	3,1	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	AmA	2	3	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
3	NAG	AnA	1	3,1	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	AnA	2	3	14,14,15	0.30	0	17,19,21	0.71	0
3	NAG	AoA	1	3,1	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	AoA	2	3	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	AqA	1	3,1	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
3	NAG	AqA	2	3	14,14,15	0.32	0	17,19,21	0.70	0
4	NAG	AsA	1	1,4	14,14,15	0.31	0	17,19,21	0.71	0
4	FUC	AsA	2	4	10,10,11	0.35	0	14,14,16	0.65	0
4	NAG	AsA	3	4	14,14,15	0.26	0	17,19,21	0.77	1 (5%)
4	FUC	AsA	4	4	10,10,11	0.32	0	14,14,16	0.61	0
5	NAG	AwA	1	5,1	14,14,15	0.34	0	17,19,21	0.69	0
5	FUC	AwA	2	5	10,10,11	0.29	0	14,14,16	0.62	0
5	NAG	AwA	3	5	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	BkB	1	2,1	14,14,15	0.29	0	17,19,21	0.96	1 (5%)
2	NAG	BkB	2	2	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
2	BMA	BkB	3	2	11,11,12	0.33	0	15,15,17	0.95	2 (13%)
3	NAG	BmB	1	3,1	14,14,15	0.27	0	17,19,21	0.60	0
3	NAG	BmB	2	3	14,14,15	0.28	0	17,19,21	0.79	0
3	NAG	BoB	1	3,1	14,14,15	0.32	0	17,19,21	0.63	0
3	NAG	BoB	2	3	14,14,15	0.31	0	17,19,21	0.70	0
3	NAG	BpB	1	3,1	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
3	NAG	BpB	2	3	14,14,15	0.37	0	17,19,21	0.71	0
4	NAG	BqB	1	1,4	14,14,15	0.29	0	17,19,21	0.66	0
4	FUC	BqB	2	4	10,10,11	0.34	0	14,14,16	0.59	0
4	NAG	BqB	3	4	14,14,15	0.28	0	17,19,21	0.67	0
4	FUC	BqB	4	4	10,10,11	0.31	0	14,14,16	0.70	0
3	NAG	BvB	1	3,1	14,14,15	0.28	0	17,19,21	0.65	0
3	NAG	BvB	2	3	14,14,15	0.34	0	17,19,21	0.77	0
3	NAG	BwB	1	3,1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	BwB	2	3	14,14,15	0.30	0	17,19,21	0.83	1 (5%)

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	AlA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AlA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AlA	3	2	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	AmA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AmA	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	AnA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AnA	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	AoA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AoA	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	AqA	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	AqA	2	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	AsA	1	1,4	-	1/6/23/26	0/1/1/1
4	FUC	AsA	2	4	-	-	0/1/1/1
4	NAG	AsA	3	4	-	0/6/23/26	0/1/1/1
4	FUC	AsA	4	4	-	-	0/1/1/1
5	NAG	AwA	1	5,1	-	0/6/23/26	0/1/1/1
5	FUC	AwA	2	5	-	-	0/1/1/1
5	NAG	AwA	3	5	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	BkB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BkB	2	2	-	0/6/23/26	0/1/1/1
2	BMA	BkB	3	2	1/1/4/5	1/2/19/22	0/1/1/1
3	NAG	BmB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BmB	2	3	-	0/6/23/26	0/1/1/1
3	NAG	BoB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BoB	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	BpB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BpB	2	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	BqB	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	BqB	2	4	-	-	0/1/1/1
4	NAG	BqB	3	4	1/1/5/7	0/6/23/26	0/1/1/1
4	FUC	BqB	4	4	-	-	0/1/1/1
3	NAG	BvB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BvB	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	BwB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BwB	2	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AlA	3	BMA	C1-O5-C5	2.93	116.17	112.19
2	AlA	1	NAG	O5-C1-C2	-2.53	107.29	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BkB	3	BMA	C1-C2-C3	2.50	112.74	109.67
2	BkB	1	NAG	O5-C1-C2	-2.38	107.54	111.29
2	AlA	1	NAG	C1-O5-C5	2.32	115.34	112.19
3	BpB	1	NAG	C1-O5-C5	2.32	115.33	112.19
2	BkB	3	BMA	C1-O5-C5	2.19	115.16	112.19
3	AmA	2	NAG	O5-C5-C6	2.16	110.59	107.20
2	AlA	3	BMA	C1-C2-C3	2.10	112.24	109.67
2	BkB	2	NAG	C1-O5-C5	2.07	115.00	112.19
3	BwB	2	NAG	C1-O5-C5	2.04	114.96	112.19
3	AqA	1	NAG	C1-O5-C5	2.02	114.93	112.19
4	AsA	3	NAG	C1-O5-C5	2.02	114.93	112.19

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AlA	3	BMA	C1
2	BkB	3	BMA	C1
3	AmA	2	NAG	C1
3	AnA	2	NAG	C1
3	AoA	2	NAG	C1
3	AqA	2	NAG	C1
3	BoB	2	NAG	C1
3	BpB	2	NAG	C1
3	BvB	2	NAG	C1
3	BwB	2	NAG	C1
4	BqB	3	NAG	C1
5	AwA	3	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AmA	2	NAG	O5-C5-C6-O6
3	AmA	2	NAG	C4-C5-C6-O6
3	BvB	2	NAG	C4-C5-C6-O6
2	BkB	3	BMA	O5-C5-C6-O6
3	BvB	2	NAG	O5-C5-C6-O6
4	AsA	1	NAG	C4-C5-C6-O6

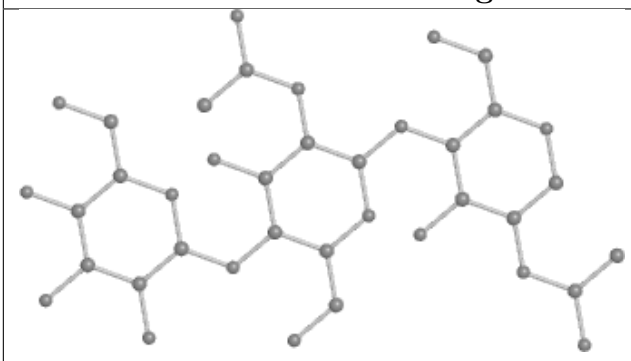
There are no ring outliers.

No monomer is involved in short contacts.

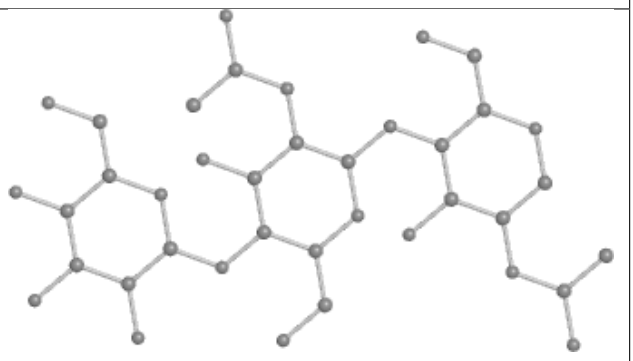
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

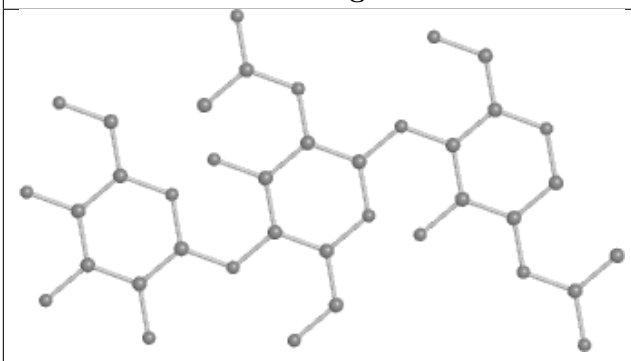
Oligosaccharide Chain AlA



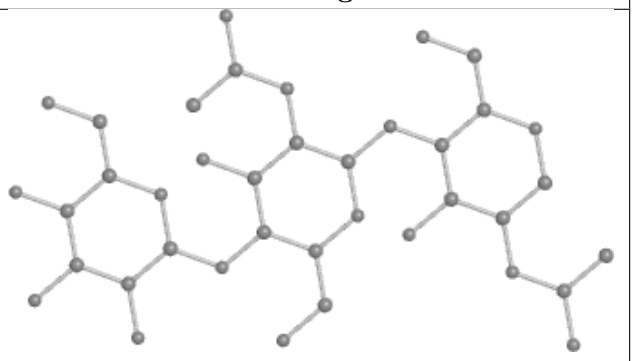
Bond lengths



Bond angles

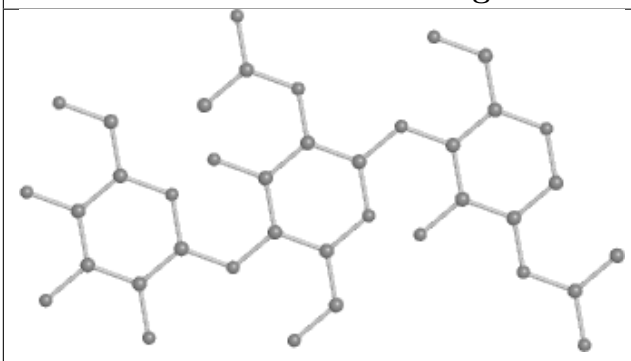


Torsions

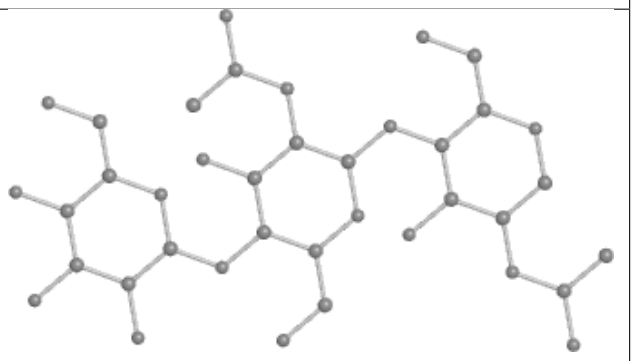


Rings

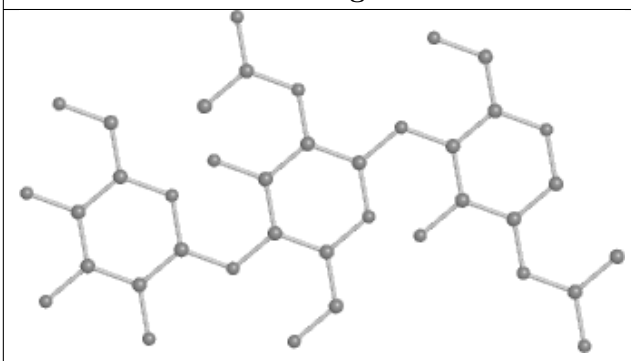
Oligosaccharide Chain BkB



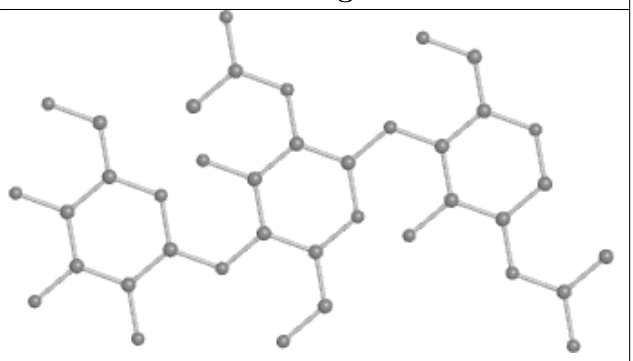
Bond lengths



Bond angles

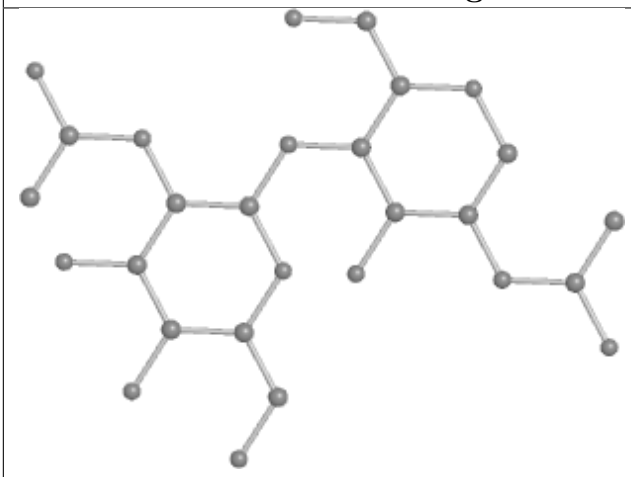


Torsions

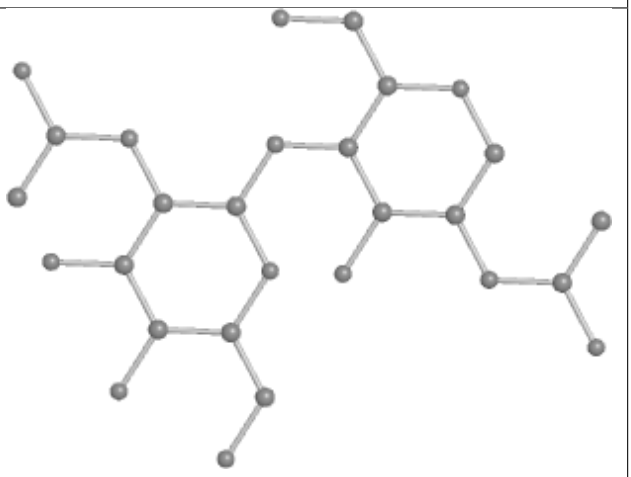


Rings

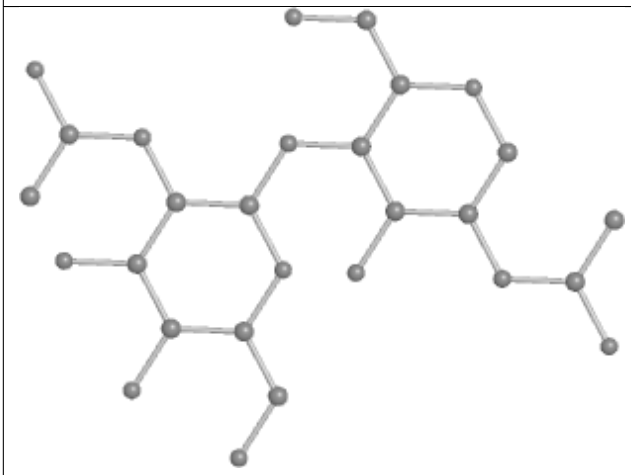
Oligosaccharide Chain AmA



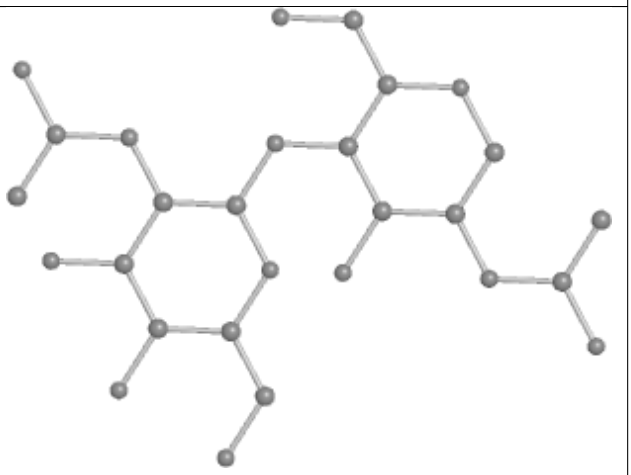
Bond lengths



Bond angles

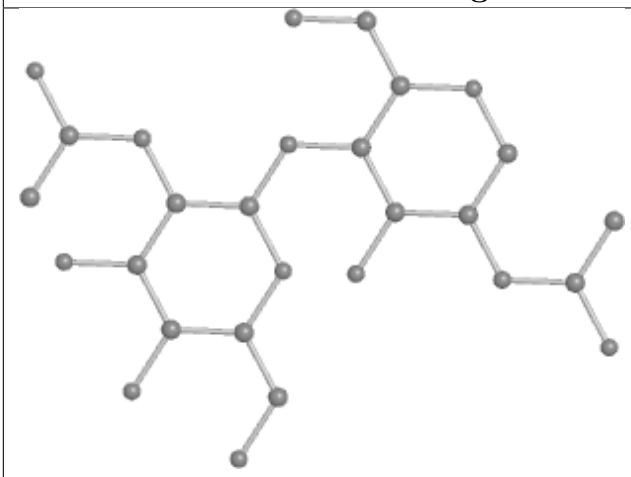


Torsions

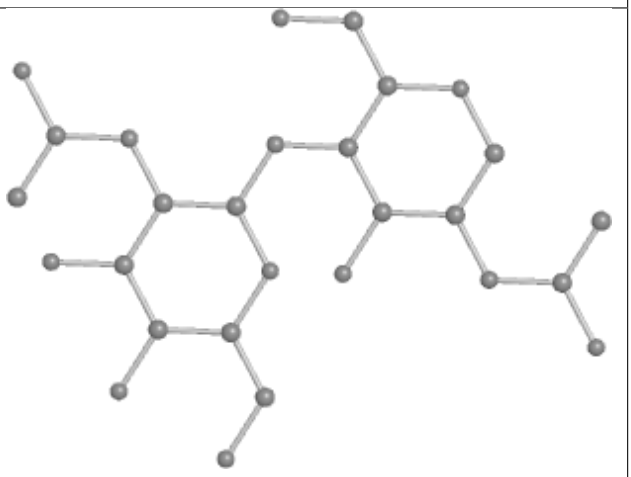


Rings

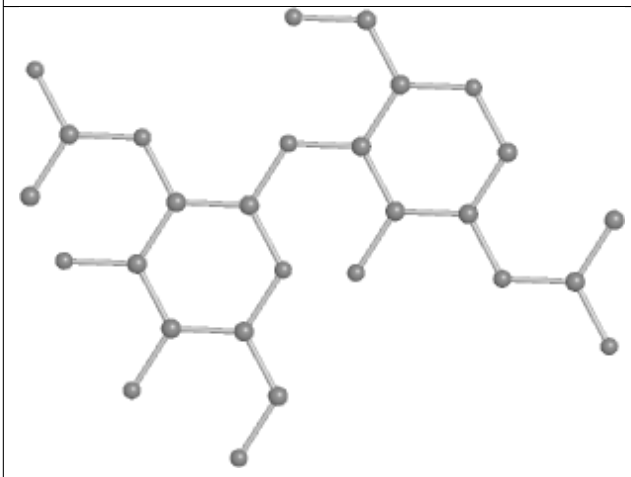
Oligosaccharide Chain AnA



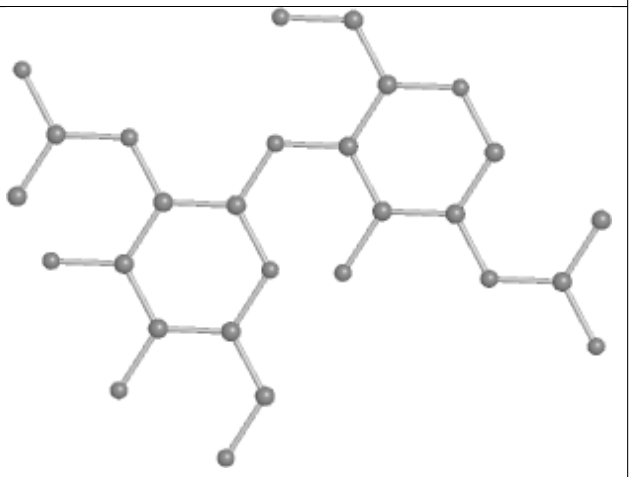
Bond lengths



Bond angles

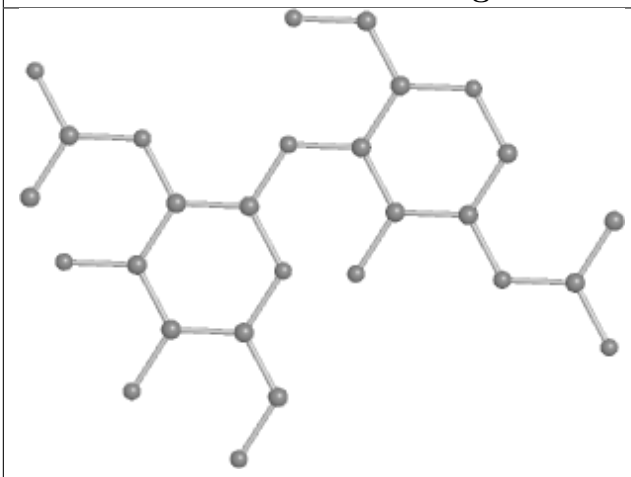


Torsions

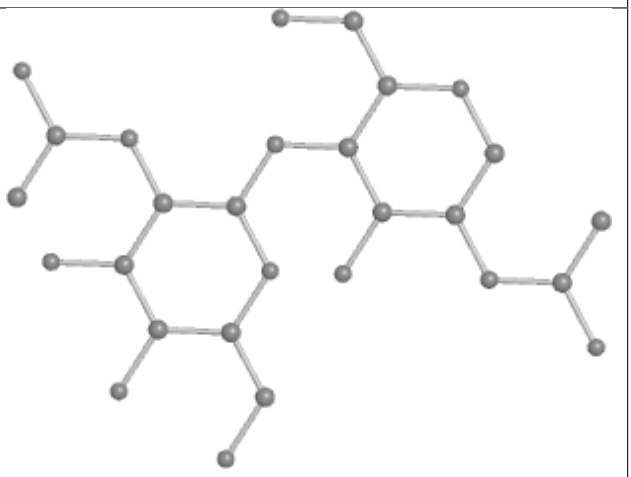


Rings

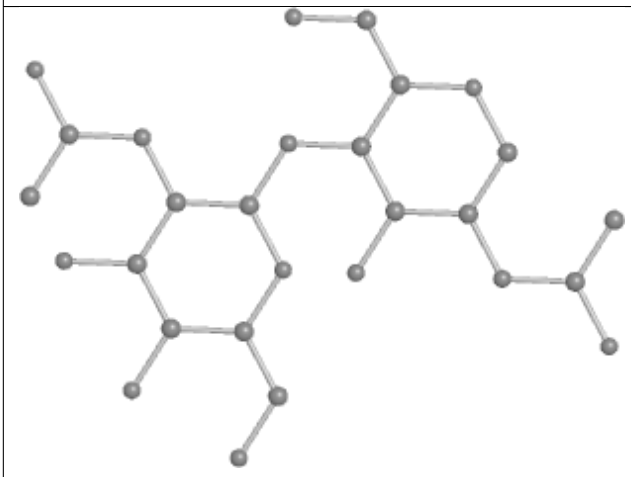
Oligosaccharide Chain AoA



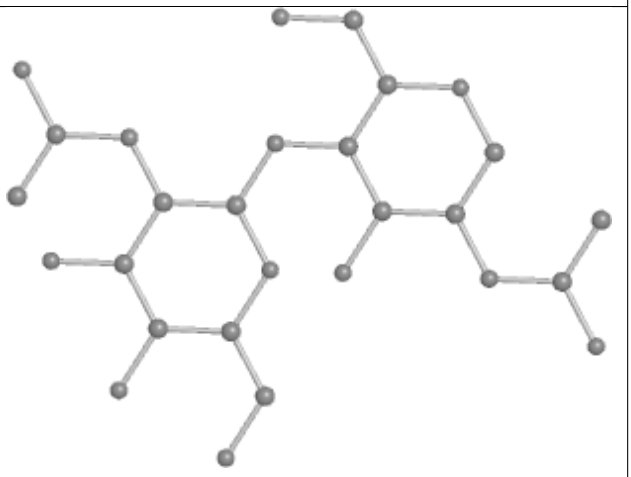
Bond lengths



Bond angles

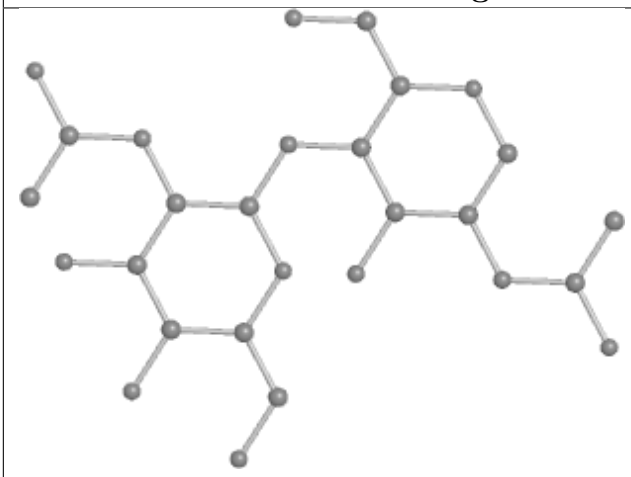


Torsions

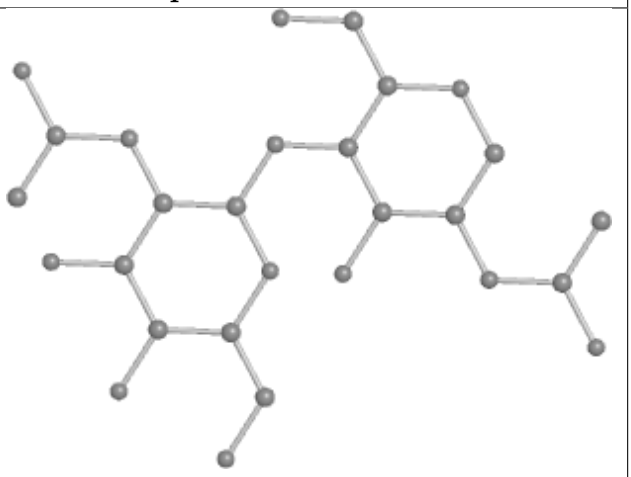


Rings

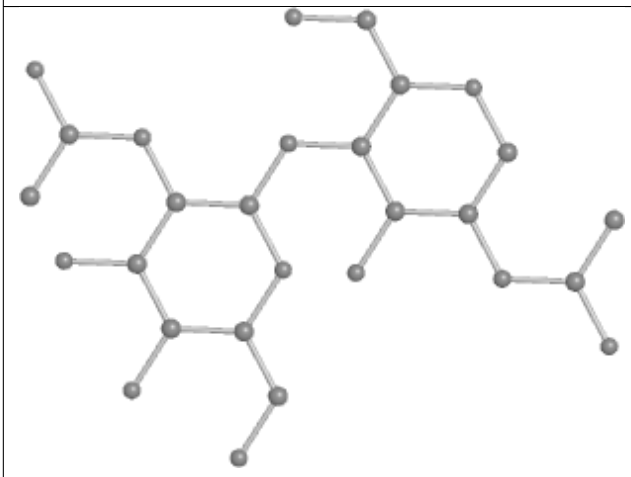
Oligosaccharide Chain AqA



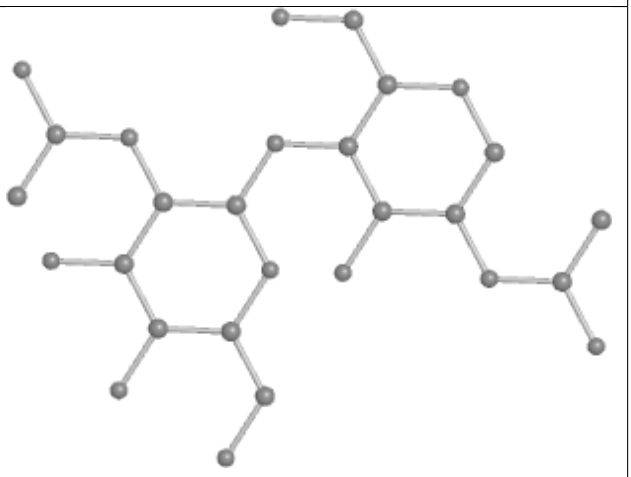
Bond lengths



Bond angles

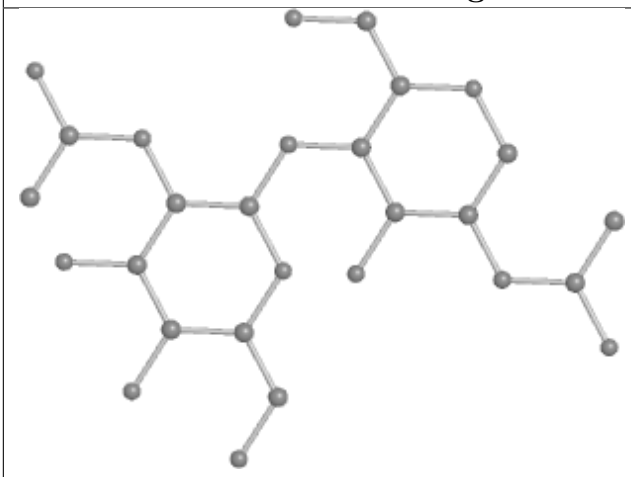


Torsions

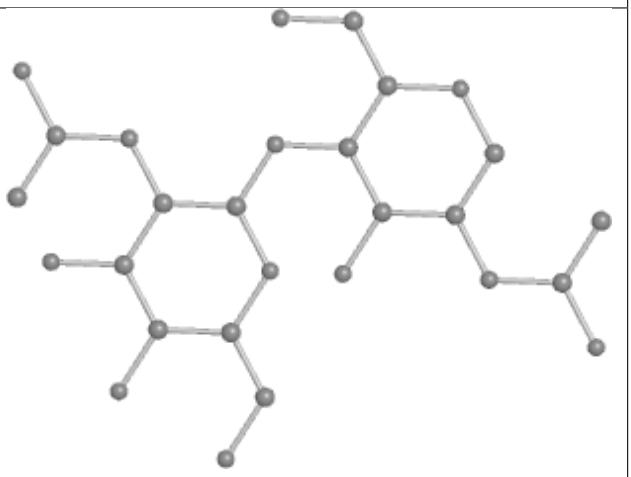


Rings

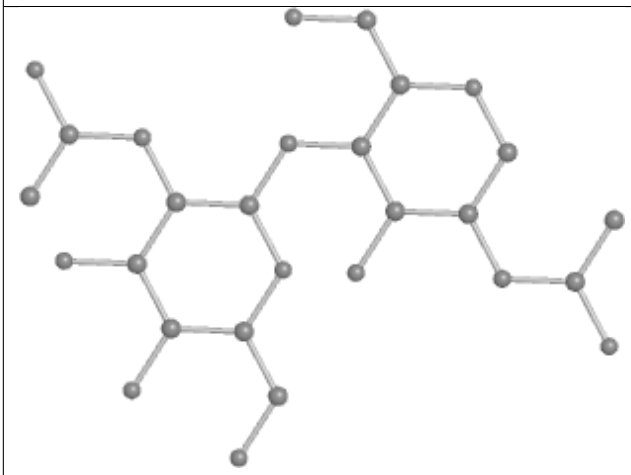
Oligosaccharide Chain BmB



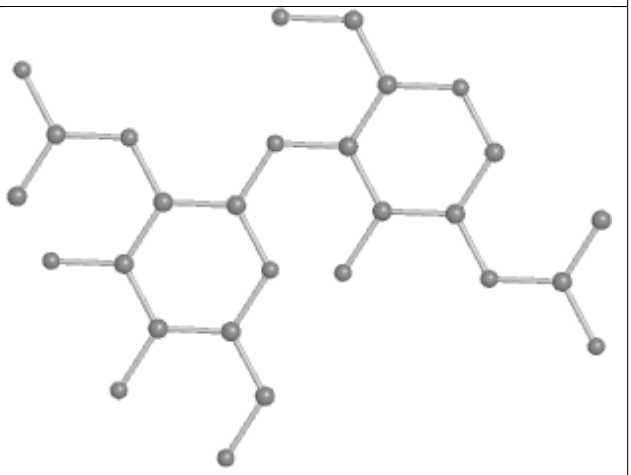
Bond lengths



Bond angles

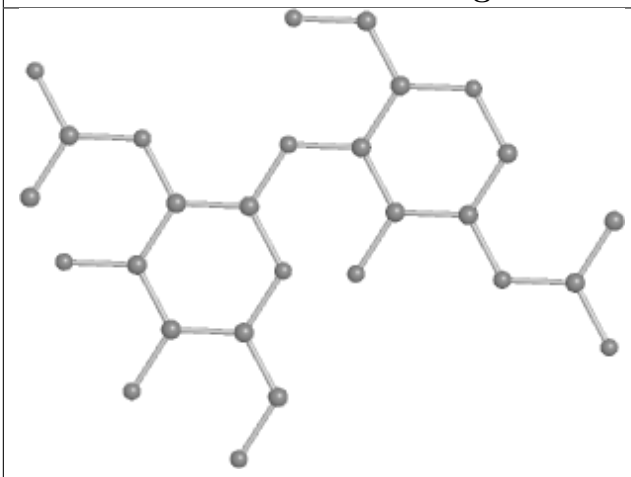


Torsions

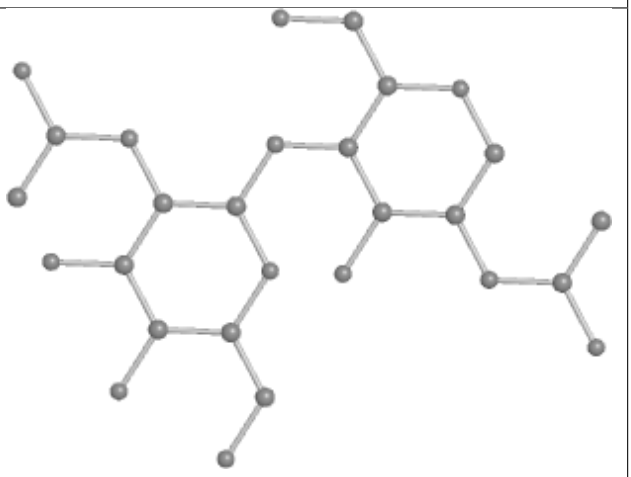


Rings

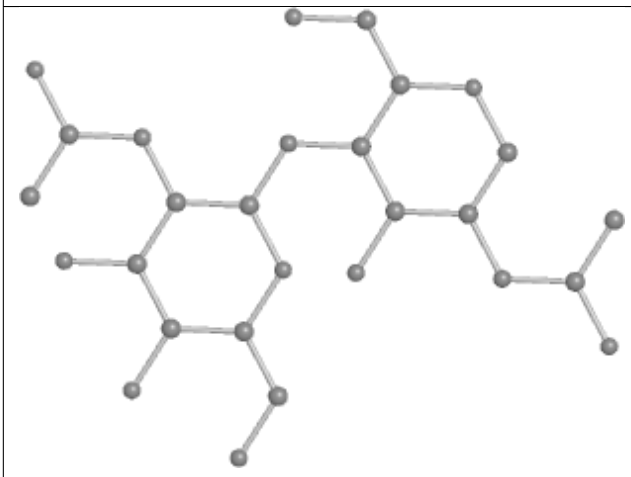
Oligosaccharide Chain BoB



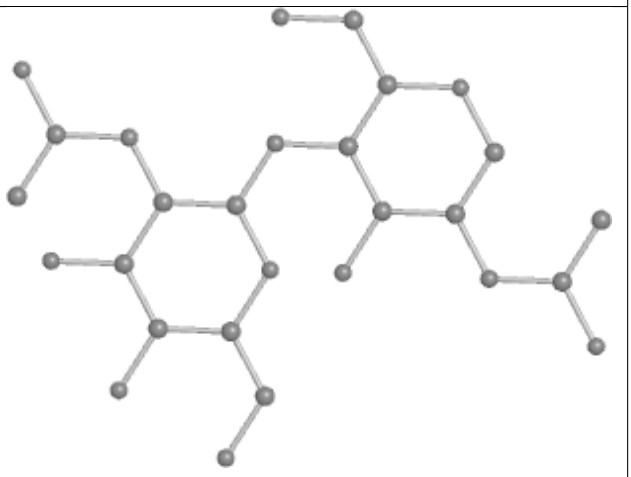
Bond lengths



Bond angles

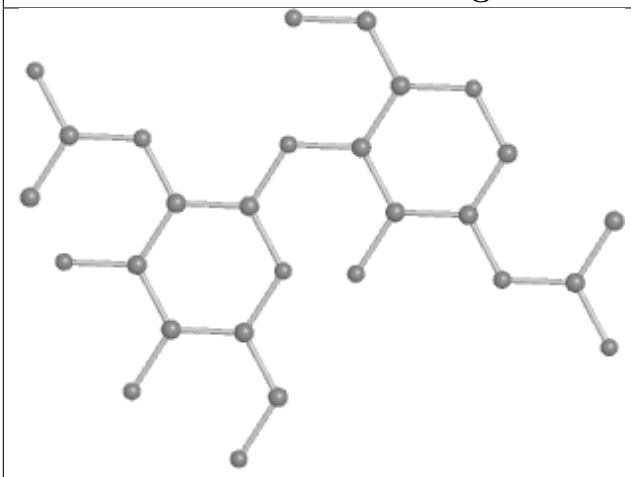


Torsions

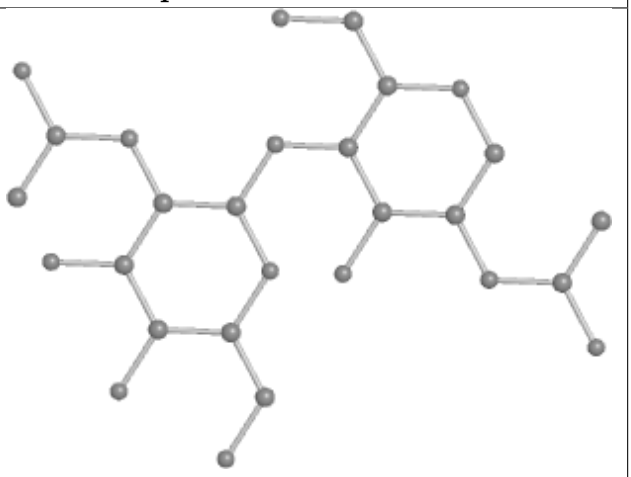


Rings

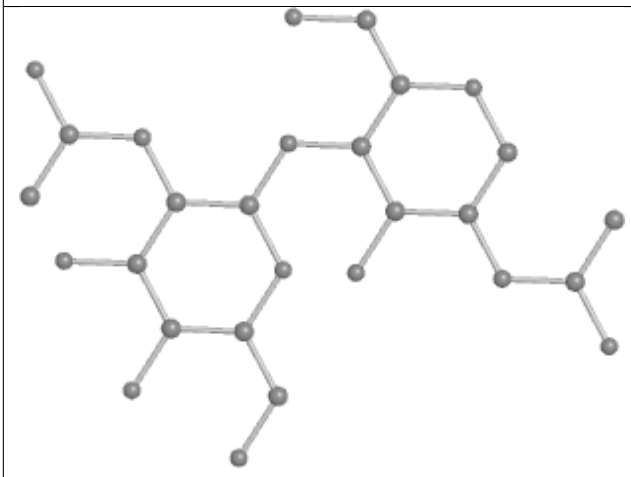
Oligosaccharide Chain BpB



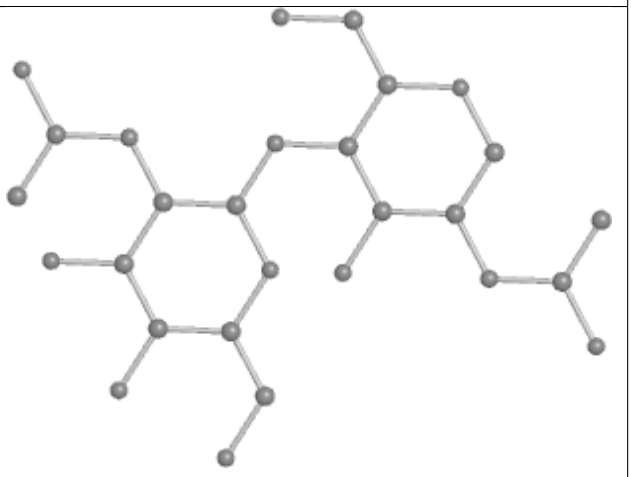
Bond lengths



Bond angles

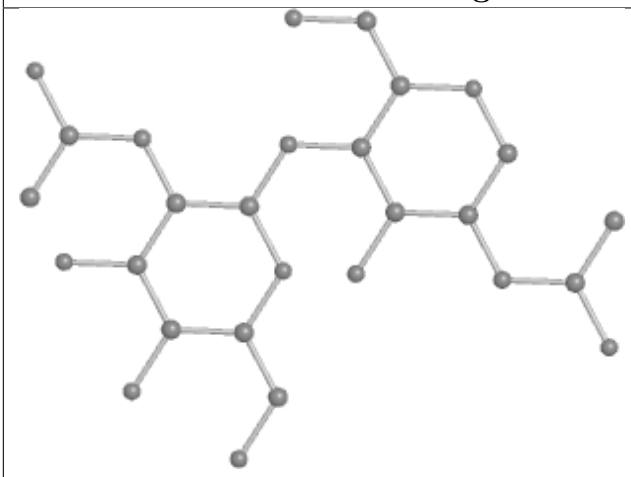


Torsions

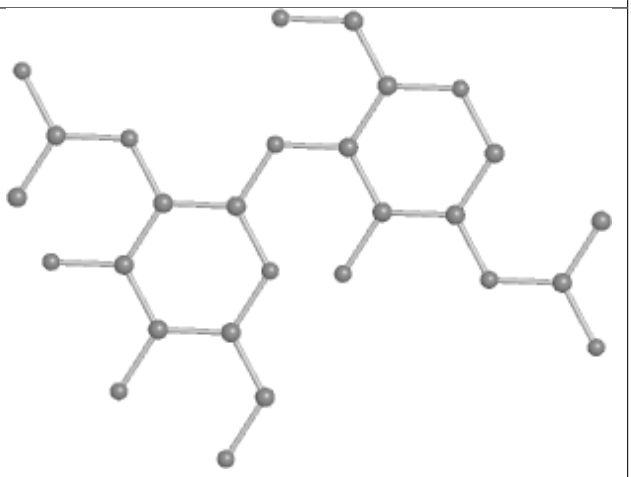


Rings

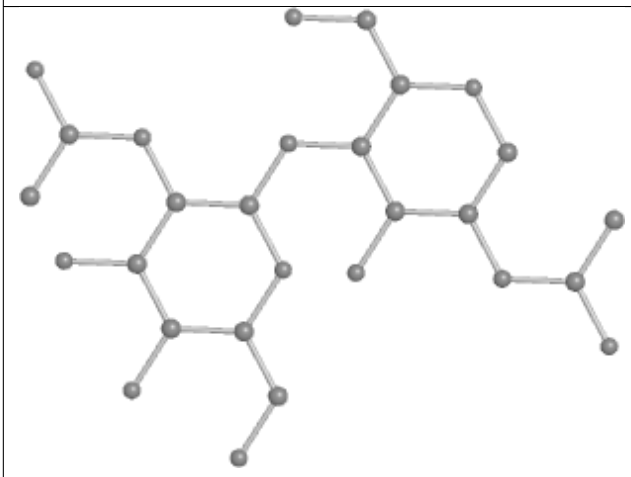
Oligosaccharide Chain BvB



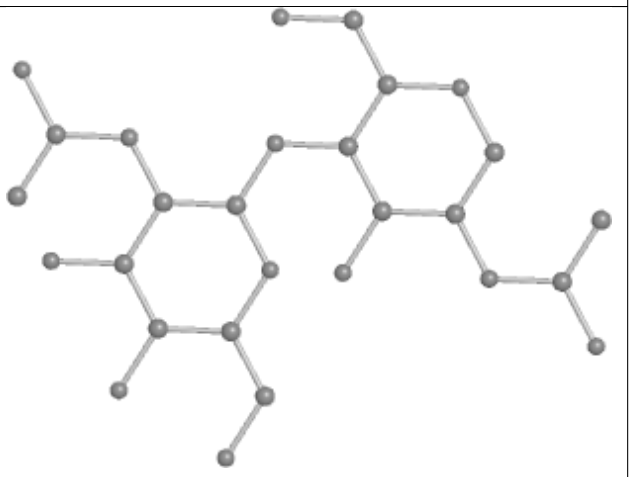
Bond lengths



Bond angles

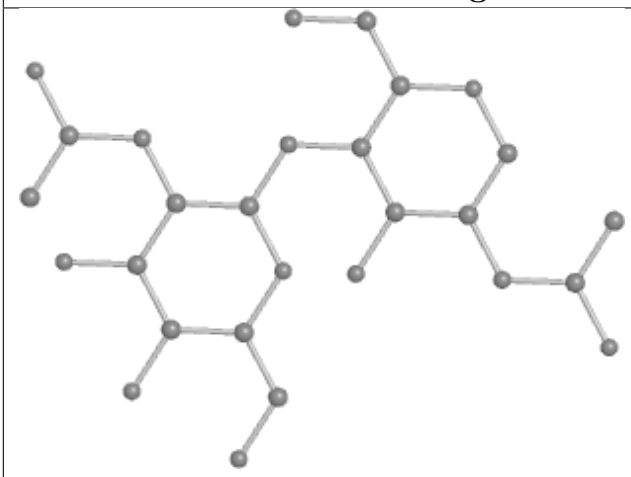


Torsions

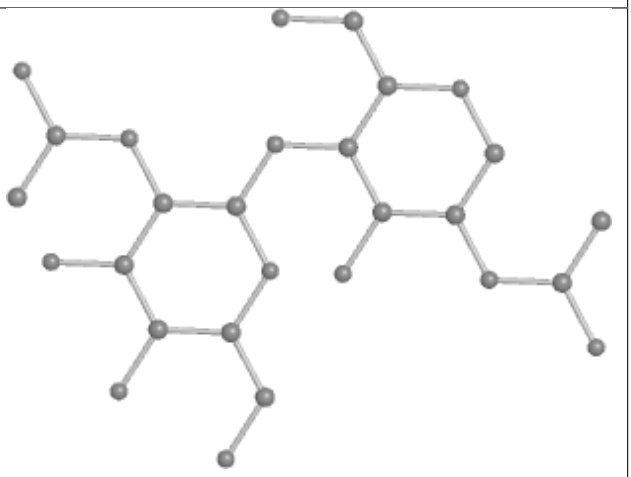


Rings

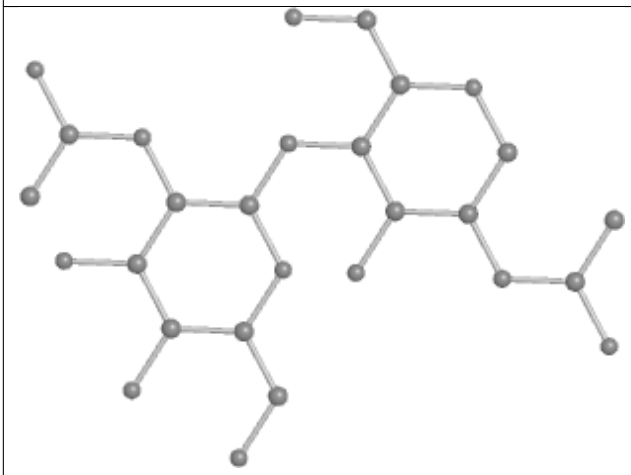
Oligosaccharide Chain BwB



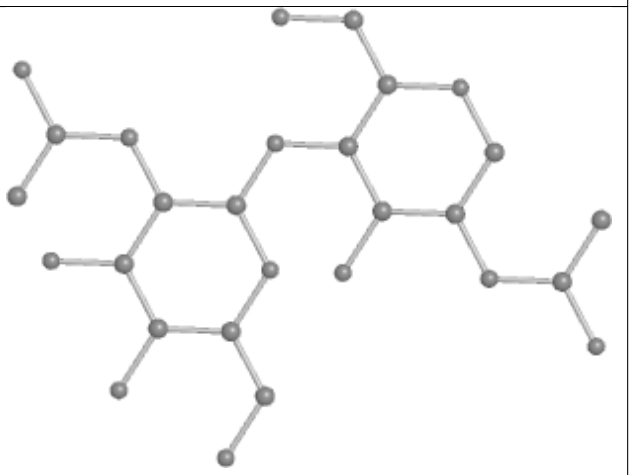
Bond lengths



Bond angles

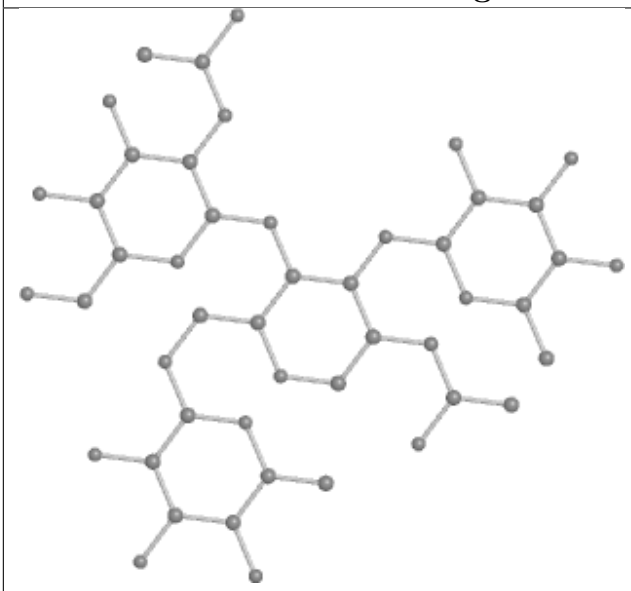


Torsions

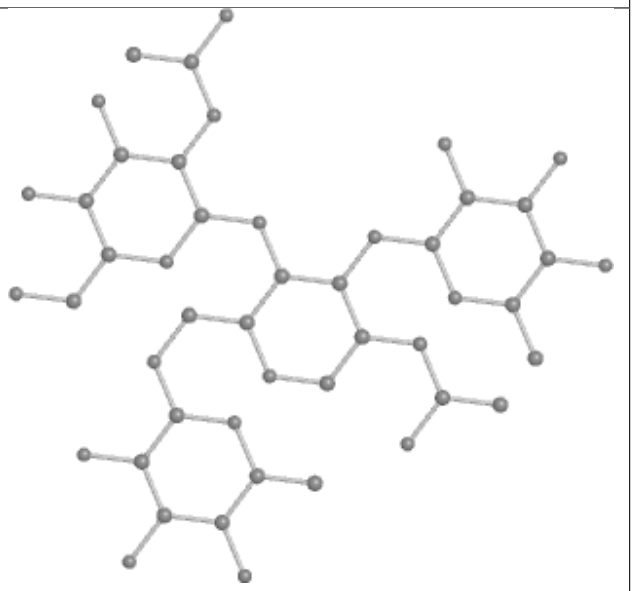


Rings

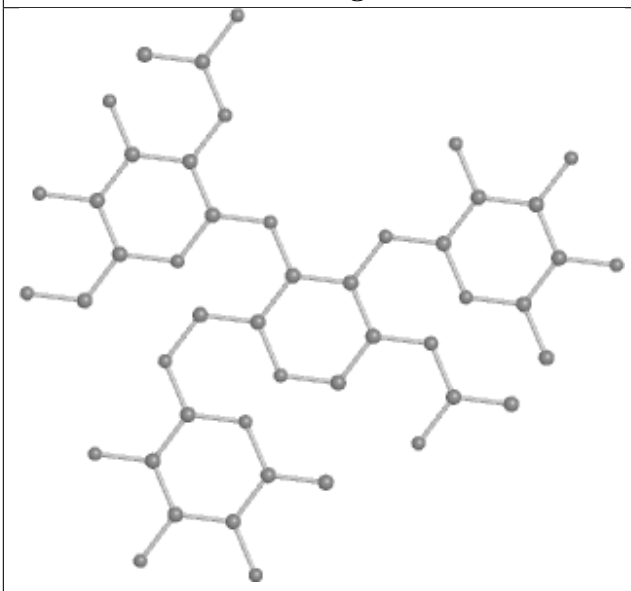
Oligosaccharide Chain AsA



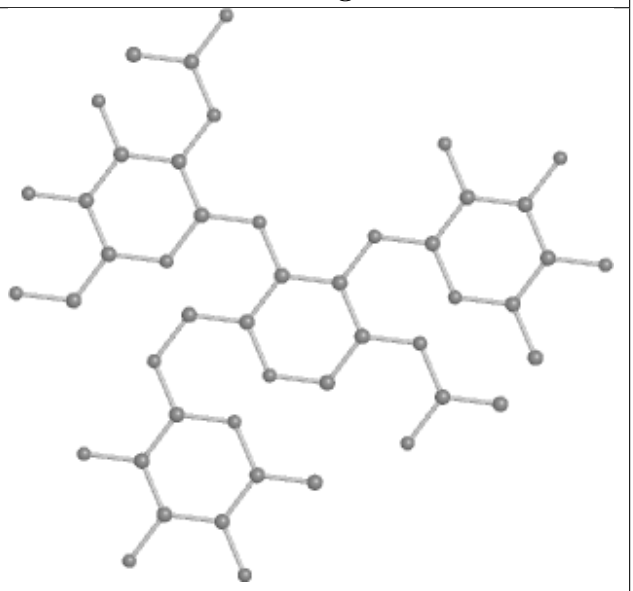
Bond lengths



Bond angles

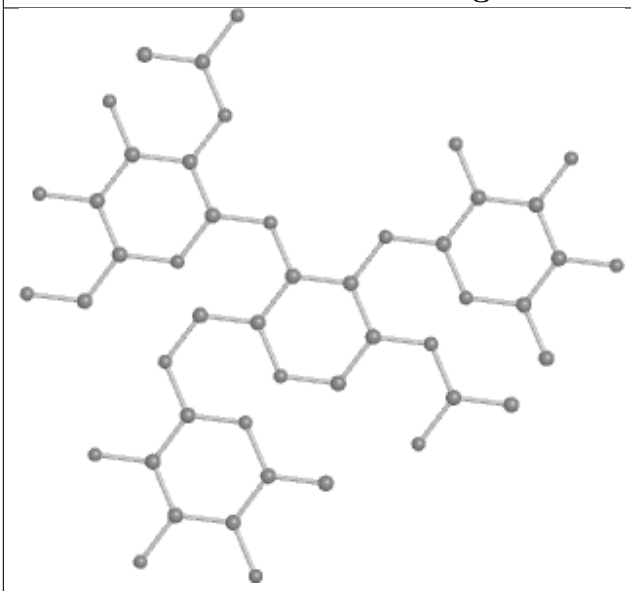


Torsions

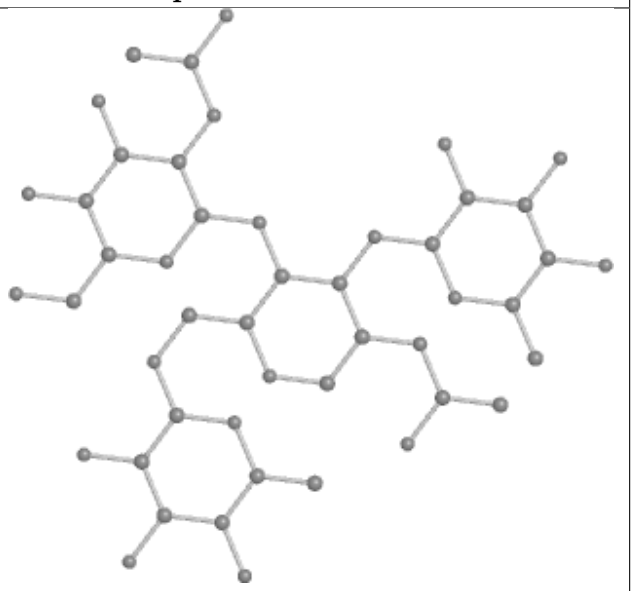


Rings

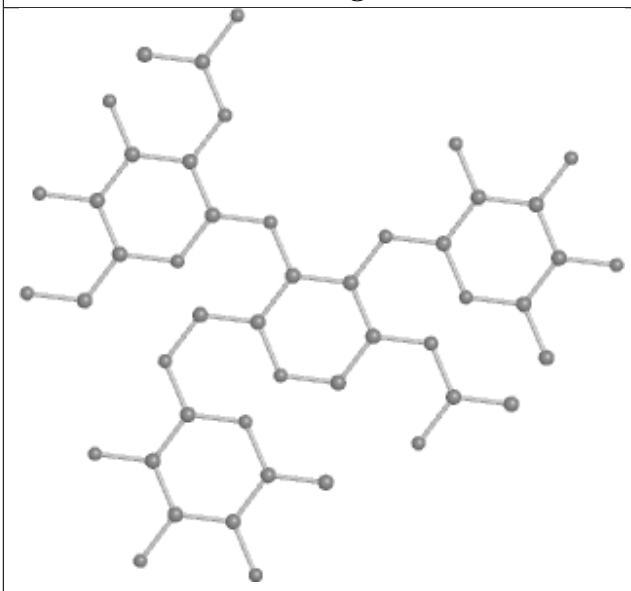
Oligosaccharide Chain BqB



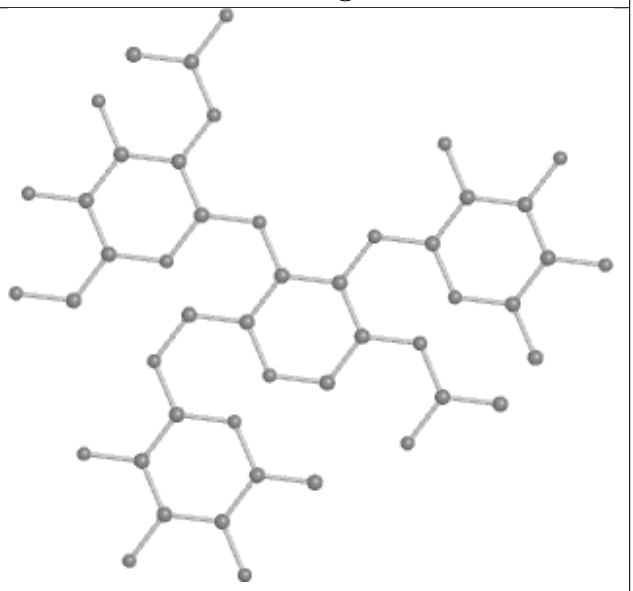
Bond lengths



Bond angles

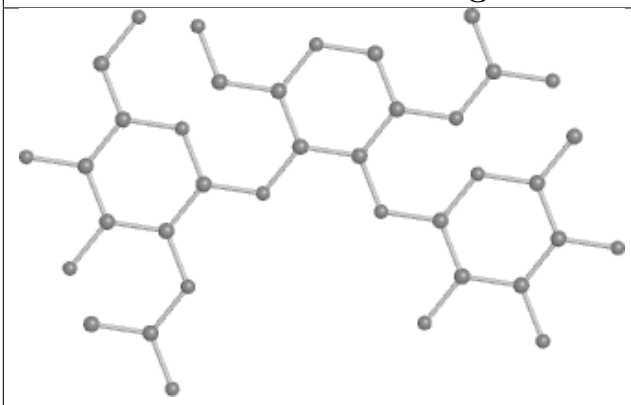


Torsions

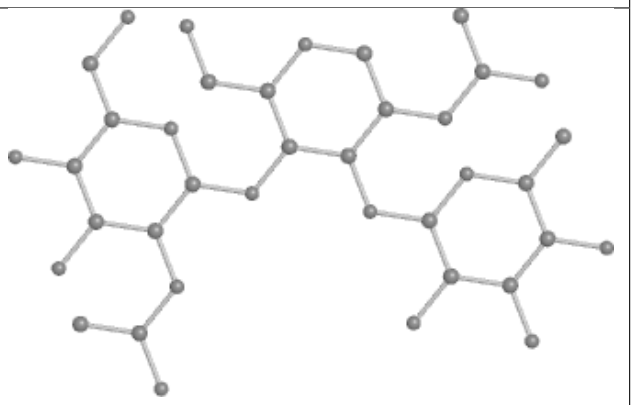


Rings

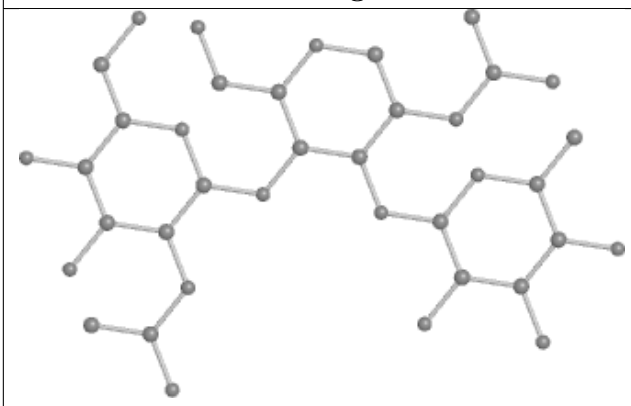
Oligosaccharide Chain AwA



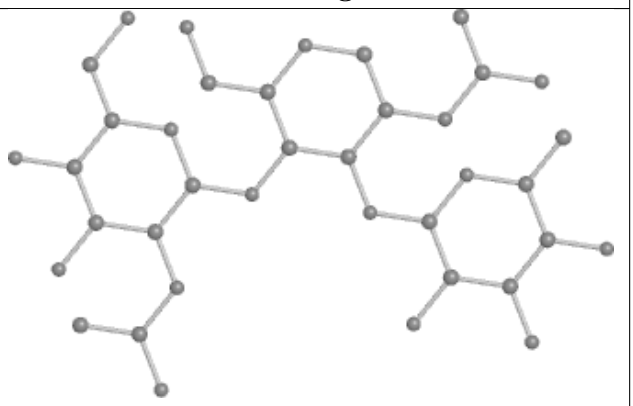
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

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	$\#\|Z\| > 2$
6	EDO	AAA	702	-	3,3,3	0.06	0	2,2,2	0.16	0
6	EDO	BBB	702	-	3,3,3	0.07	0	2,2,2	0.22	0
6	EDO	BBB	707	-	3,3,3	0.06	0	2,2,2	0.18	0
6	EDO	AAA	709	-	3,3,3	0.05	0	2,2,2	0.17	0
6	EDO	BBB	704	-	3,3,3	0.06	0	2,2,2	0.22	0
8	SO4	BBB	714	-	4,4,4	0.39	0	6,6,6	0.05	0
6	EDO	AAA	705	-	3,3,3	0.07	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	BBB	711	1	14,14,15	0.32	0	17,19,21	0.83	0
6	EDO	AAA	703	-	3,3,3	0.07	0	2,2,2	0.23	0
7	NAG	BBB	712	1	14,14,15	0.29	0	17,19,21	0.72	0
8	SO4	AAA	715	-	4,4,4	0.39	0	6,6,6	0.05	0
6	EDO	AAA	701	-	3,3,3	0.05	0	2,2,2	0.24	0
6	EDO	BBB	709	-	3,3,3	0.07	0	2,2,2	0.20	0
7	NAG	BBB	713	1	14,14,15	0.28	0	17,19,21	0.70	0
6	EDO	AAA	708	-	3,3,3	0.05	0	2,2,2	0.23	0
6	EDO	AAA	704	-	3,3,3	0.04	0	2,2,2	0.24	0
7	NAG	AAA	712	1	14,14,15	0.33	0	17,19,21	0.81	0
6	EDO	BBB	703	-	3,3,3	0.06	0	2,2,2	0.19	0
6	EDO	BBB	701	-	3,3,3	0.05	0	2,2,2	0.13	0
6	EDO	AAA	706	-	3,3,3	0.07	0	2,2,2	0.23	0
6	EDO	BBB	706	-	3,3,3	0.06	0	2,2,2	0.23	0
7	NAG	AAA	714	1	14,14,15	0.27	0	17,19,21	0.65	0
6	EDO	AAA	710	-	3,3,3	0.05	0	2,2,2	0.19	0
6	EDO	BBB	705	-	3,3,3	0.06	0	2,2,2	0.18	0
6	EDO	BBB	710	-	3,3,3	0.07	0	2,2,2	0.22	0
6	EDO	BBB	708	-	3,3,3	0.06	0	2,2,2	0.22	0
6	EDO	AAA	707	-	3,3,3	0.07	0	2,2,2	0.15	0
7	NAG	AAA	713	1	14,14,15	0.31	0	17,19,21	0.83	0
6	EDO	AAA	711	-	3,3,3	0.06	0	2,2,2	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	AAA	702	-	-	0/1/1/1	-
6	EDO	BBB	702	-	-	0/1/1/1	-
6	EDO	BBB	707	-	-	1/1/1/1	-
6	EDO	AAA	709	-	-	0/1/1/1	-
6	EDO	BBB	704	-	-	0/1/1/1	-
6	EDO	AAA	705	-	-	1/1/1/1	-
7	NAG	BBB	711	1	-	0/6/23/26	0/1/1/1
6	EDO	AAA	703	-	-	0/1/1/1	-
7	NAG	BBB	712	1	-	0/6/23/26	0/1/1/1
6	EDO	AAA	701	-	-	1/1/1/1	-
6	EDO	BBB	709	-	-	1/1/1/1	-
7	NAG	BBB	713	1	-	0/6/23/26	0/1/1/1
6	EDO	AAA	708	-	-	0/1/1/1	-
6	EDO	AAA	704	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	AAA	712	1	-	0/6/23/26	0/1/1/1
6	EDO	BBB	703	-	-	1/1/1/1	-
6	EDO	BBB	701	-	-	0/1/1/1	-
6	EDO	AAA	706	-	-	1/1/1/1	-
6	EDO	BBB	706	-	-	1/1/1/1	-
7	NAG	AAA	714	1	-	0/6/23/26	0/1/1/1
6	EDO	AAA	710	-	-	1/1/1/1	-
6	EDO	BBB	705	-	-	1/1/1/1	-
6	EDO	BBB	710	-	-	1/1/1/1	-
6	EDO	BBB	708	-	-	1/1/1/1	-
6	EDO	AAA	707	-	-	1/1/1/1	-
7	NAG	AAA	713	1	-	0/6/23/26	0/1/1/1
6	EDO	AAA	711	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	710	EDO	O1-C1-C2-O2
6	AAA	711	EDO	O1-C1-C2-O2
6	BBB	710	EDO	O1-C1-C2-O2
6	BBB	709	EDO	O1-C1-C2-O2
6	BBB	707	EDO	O1-C1-C2-O2
6	AAA	706	EDO	O1-C1-C2-O2
6	BBB	706	EDO	O1-C1-C2-O2
6	AAA	701	EDO	O1-C1-C2-O2
6	AAA	707	EDO	O1-C1-C2-O2
6	AAA	705	EDO	O1-C1-C2-O2
6	BBB	703	EDO	O1-C1-C2-O2
6	BBB	705	EDO	O1-C1-C2-O2
6	BBB	708	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	704	EDO	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	589/617 (95%)	0.14	16 (2%)	54	52	18, 26, 46, 67	0
1	BBB	585/617 (94%)	0.39	37 (6%)	20	17	18, 28, 62, 80	0
All	All	1174/1234 (95%)	0.26	53 (4%)	33	30	18, 27, 57, 80	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	599	CYS	9.0
1	BBB	598	LEU	6.8
1	BBB	581	PRO	6.1
1	BBB	600	GLY	6.1
1	BBB	580	PRO	4.8
1	BBB	558	VAL	4.5
1	BBB	596	PRO	4.1
1	AAA	606	CYS	4.0
1	BBB	563	LEU	4.0
1	AAA	603	LYS	3.9
1	BBB	544	TYR	3.9
1	BBB	566	ASN	3.8
1	BBB	58	ASP	3.7
1	BBB	574	ARG	3.5
1	BBB	557	PRO	3.5
1	AAA	59	PHE	3.5
1	BBB	489	MET	3.4
1	AAA	58	ASP	3.3
1	BBB	531	LYS	3.2
1	BBB	565	LEU	3.2
1	BBB	492	GLY	3.2
1	BBB	577	GLY	3.1
1	BBB	588	TYR	3.0
1	BBB	597	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	468	ASP	3.0
1	BBB	579	LEU	2.9
1	BBB	59	PHE	2.9
1	BBB	469	ASN	2.9
1	BBB	486	ASP	2.9
1	BBB	575	LEU	2.8
1	AAA	599	CYS	2.7
1	AAA	564	LYS	2.7
1	BBB	541	VAL	2.6
1	BBB	539	LEU	2.6
1	BBB	534	ASP	2.6
1	AAA	605	LEU	2.5
1	BBB	543	ASN	2.5
1	AAA	596	PRO	2.4
1	BBB	584	ALA	2.4
1	AAA	604	GLY	2.4
1	AAA	587	MET	2.4
1	BBB	601	ASP	2.4
1	AAA	574	ARG	2.4
1	BBB	586	ASP	2.3
1	BBB	560	LEU	2.3
1	BBB	587	MET	2.2
1	AAA	544	TYR	2.2
1	AAA	468	ASP	2.2
1	AAA	489	MET	2.1
1	AAA	590	ASN	2.1
1	BBB	507	GLU	2.1
1	AAA	469	ASN	2.1
1	BBB	491	LEU	2.0

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)

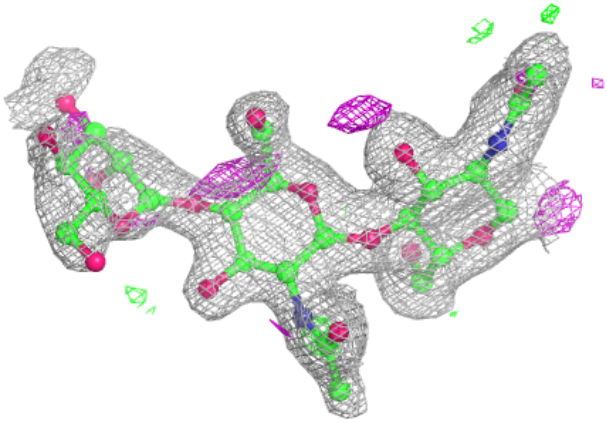
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

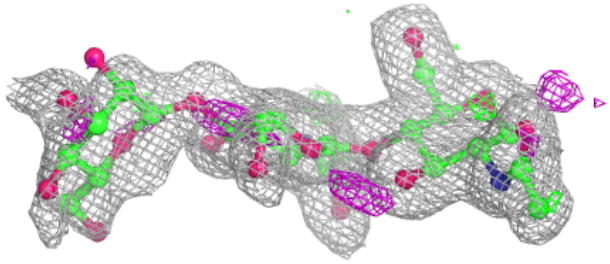
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	BvB	2	14/15	0.43	0.46	79,83,83,84	0
3	NAG	BpB	2	14/15	0.46	0.36	63,66,67,68	0
3	NAG	AqA	2	14/15	0.56	0.50	67,72,74,74	0
3	NAG	BoB	1	14/15	0.64	0.34	65,67,69,72	0
5	NAG	AwA	1	14/15	0.65	0.23	54,57,64,67	0
5	NAG	AwA	3	14/15	0.66	0.45	80,83,84,85	0
3	NAG	BvB	1	14/15	0.67	0.23	52,55,59,64	0
3	NAG	BoB	2	14/15	0.68	0.39	80,82,82,83	0
5	FUC	AwA	2	10/11	0.73	0.48	75,78,79,79	0
2	BMA	BkB	3	11/12	0.74	0.36	63,67,69,70	0
3	NAG	AnA	2	14/15	0.74	0.34	71,73,74,75	0
4	NAG	BqB	3	14/15	0.74	0.32	69,72,73,73	0
4	FUC	BqB	4	10/11	0.77	0.36	66,68,69,70	0
2	BMA	AlA	3	11/12	0.78	0.37	59,64,65,65	0
3	NAG	AmA	2	14/15	0.78	0.31	55,59,62,62	0
3	NAG	AqA	1	14/15	0.80	0.18	37,42,44,50	0
4	FUC	BqB	2	10/11	0.81	0.37	62,63,64,65	0
3	NAG	BmB	2	14/15	0.82	0.18	47,50,52,52	0
3	NAG	AnA	1	14/15	0.82	0.25	55,58,61,63	0
3	NAG	BpB	1	14/15	0.83	0.17	38,43,44,50	0
4	NAG	AsA	3	14/15	0.83	0.23	61,64,66,66	0
4	NAG	BqB	1	14/15	0.83	0.15	45,48,55,57	0
3	NAG	BwB	2	14/15	0.85	0.22	48,50,52,53	0
4	FUC	AsA	4	10/11	0.86	0.29	54,56,57,57	0
4	FUC	AsA	2	10/11	0.87	0.31	54,56,57,57	0
2	NAG	BkB	2	14/15	0.88	0.22	39,42,44,49	0
3	NAG	AoA	2	14/15	0.88	0.26	49,52,53,54	0
3	NAG	BwB	1	14/15	0.89	0.14	32,35,36,40	0
2	NAG	AlA	2	14/15	0.89	0.21	38,40,42,46	0
3	NAG	AoA	1	14/15	0.90	0.13	32,36,37,40	0
4	NAG	AsA	1	14/15	0.90	0.14	41,44,48,51	0
2	NAG	BkB	1	14/15	0.93	0.09	25,26,27,30	0
3	NAG	AmA	1	14/15	0.94	0.10	34,36,38,42	0
3	NAG	BmB	1	14/15	0.94	0.11	31,32,34,38	0
2	NAG	AlA	1	14/15	0.95	0.07	24,25,26,28	0

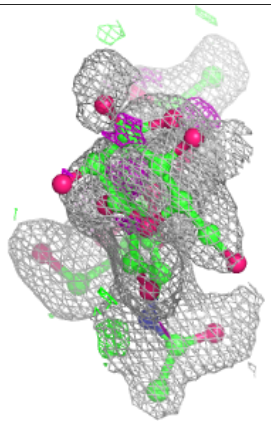
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A1A:

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

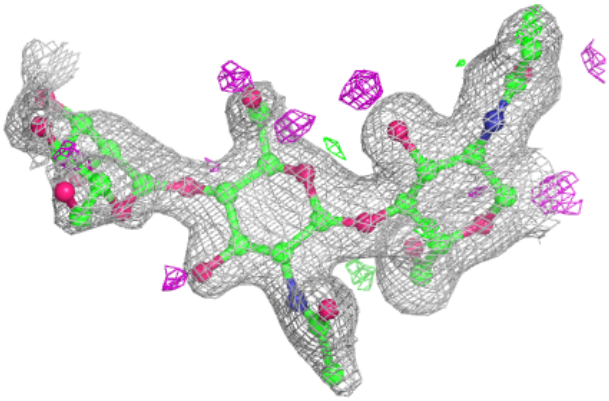


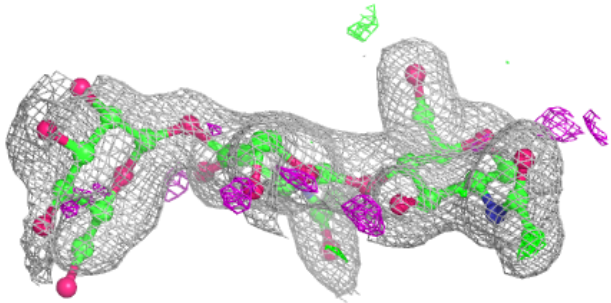


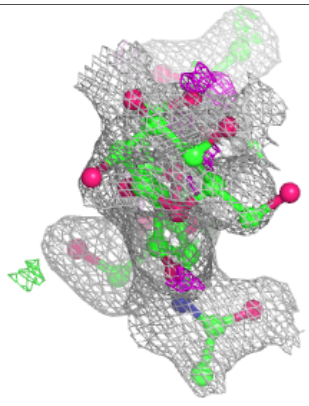


Electron density around Chain BkB:

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

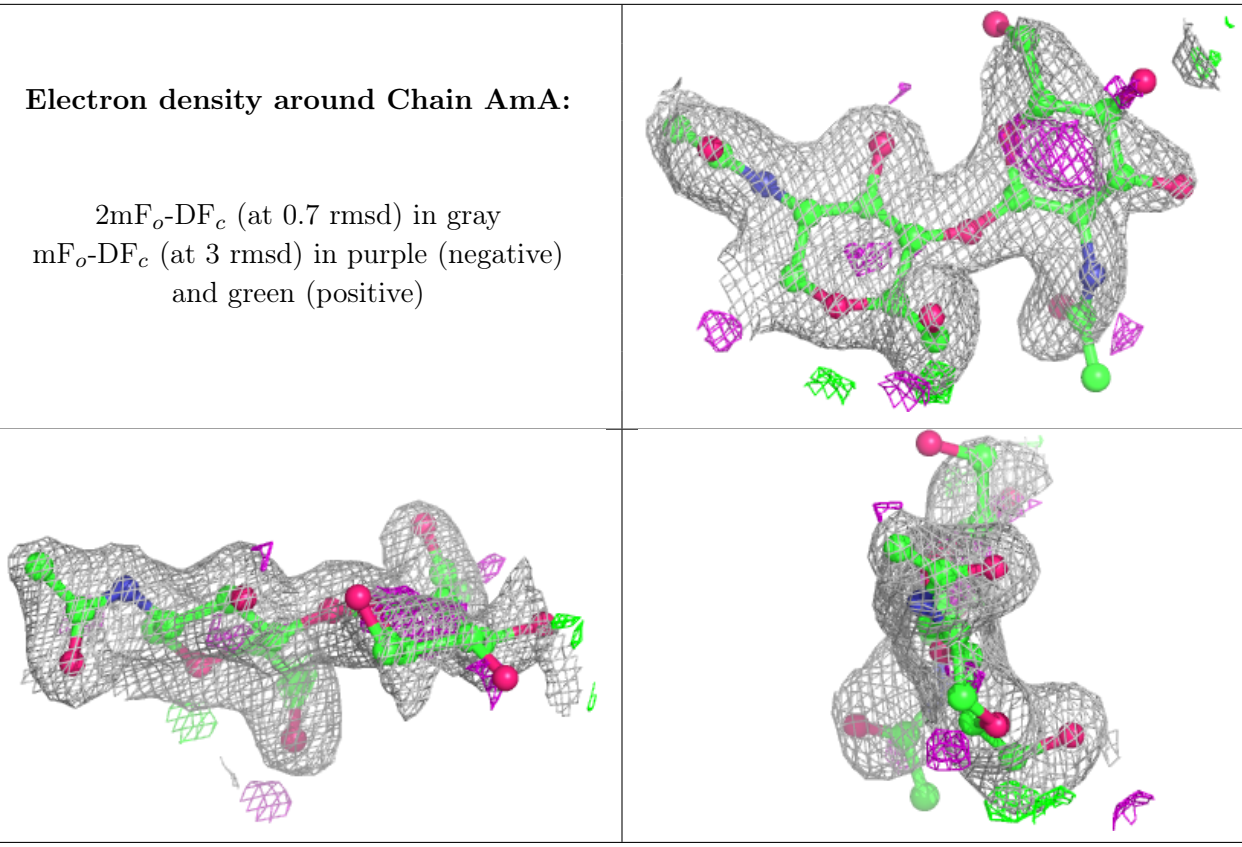






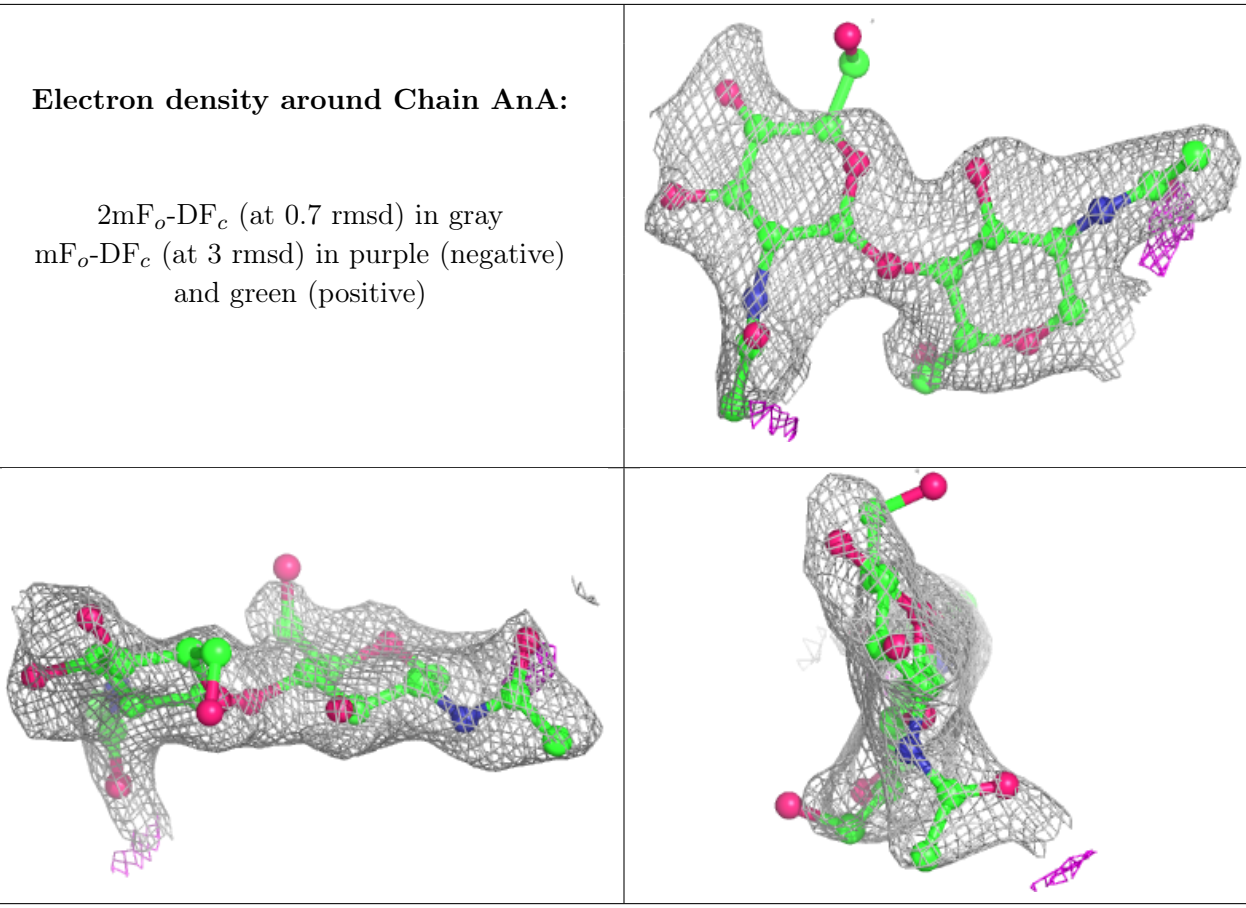
Electron density around Chain AmA:

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



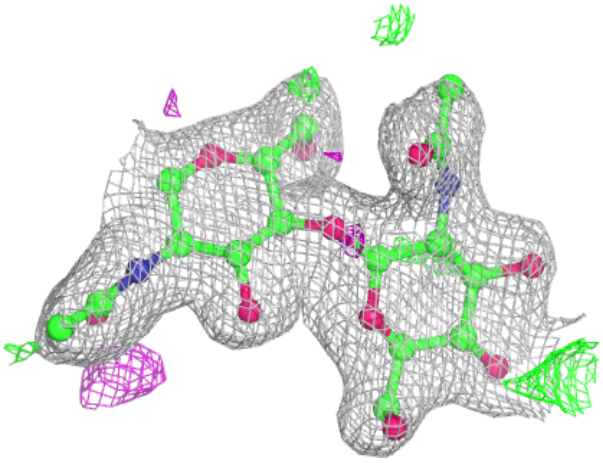
Electron density around Chain AnA:

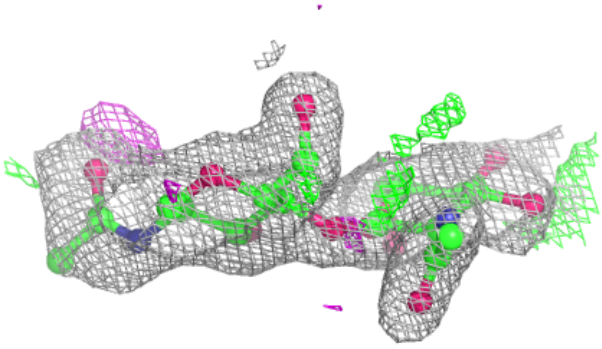
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

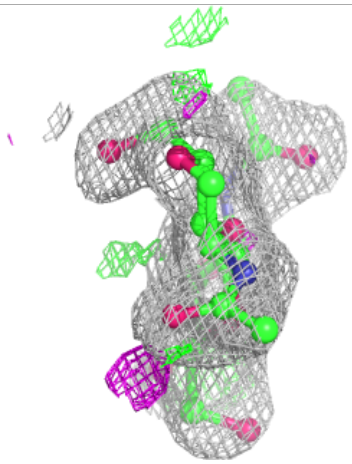


Electron density around Chain AoA:

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

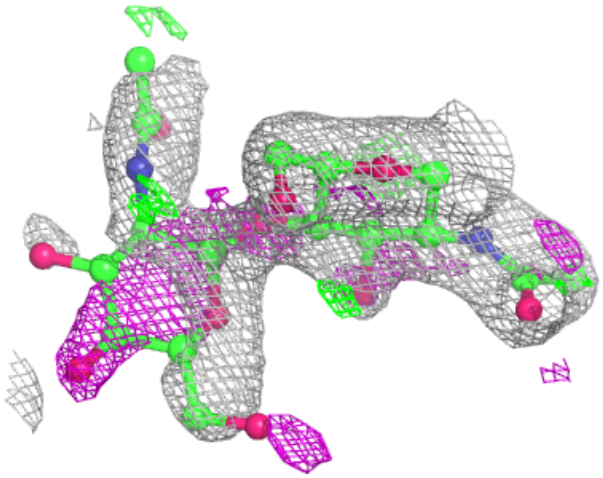


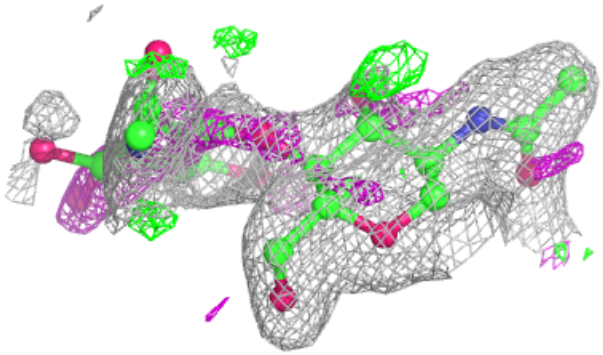


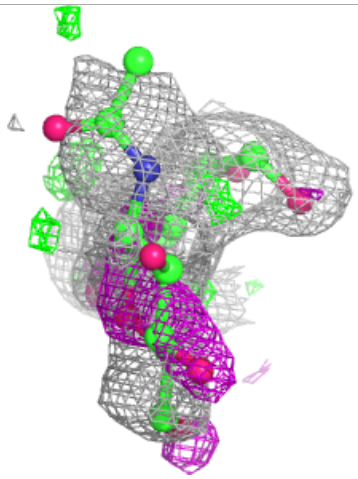


Electron density around Chain AqA:

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

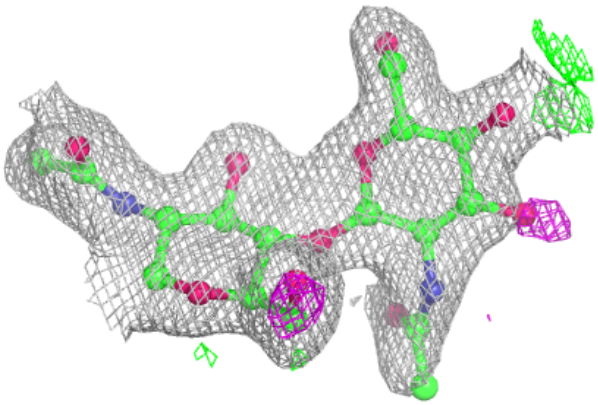


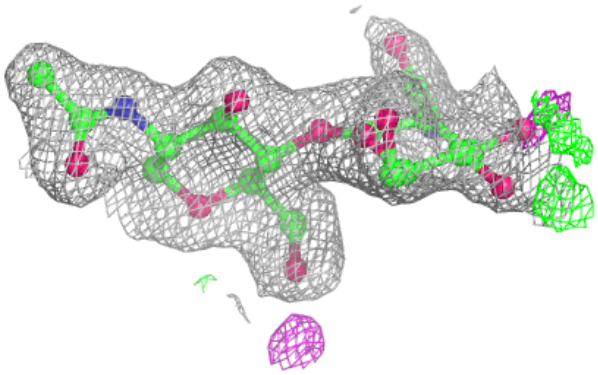


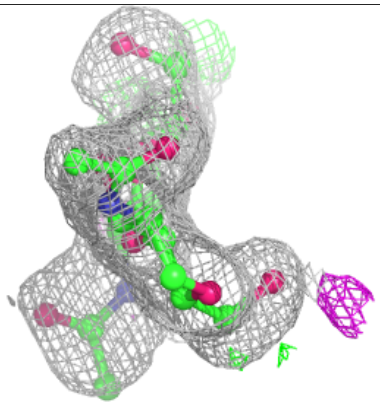


Electron density around Chain BmB:

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

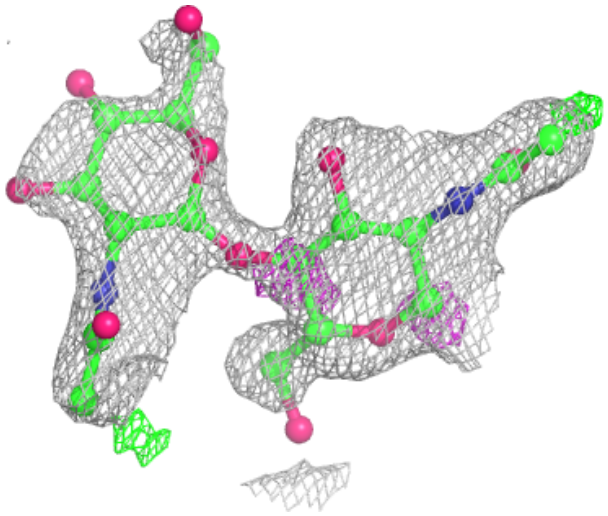


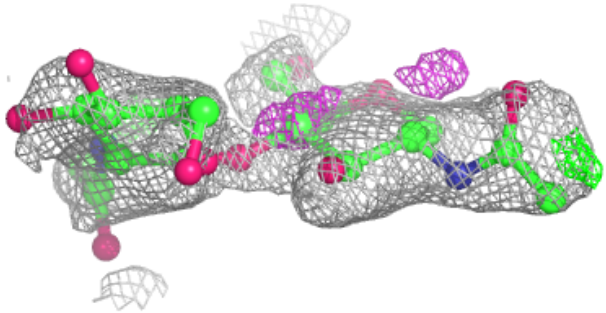


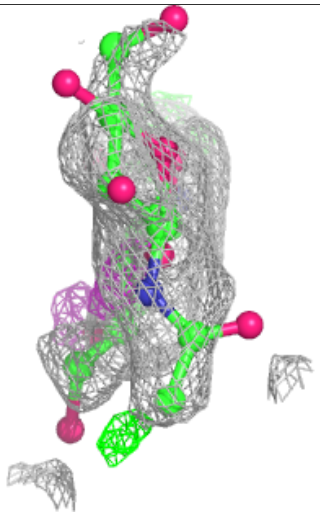


Electron density around Chain BoB:

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

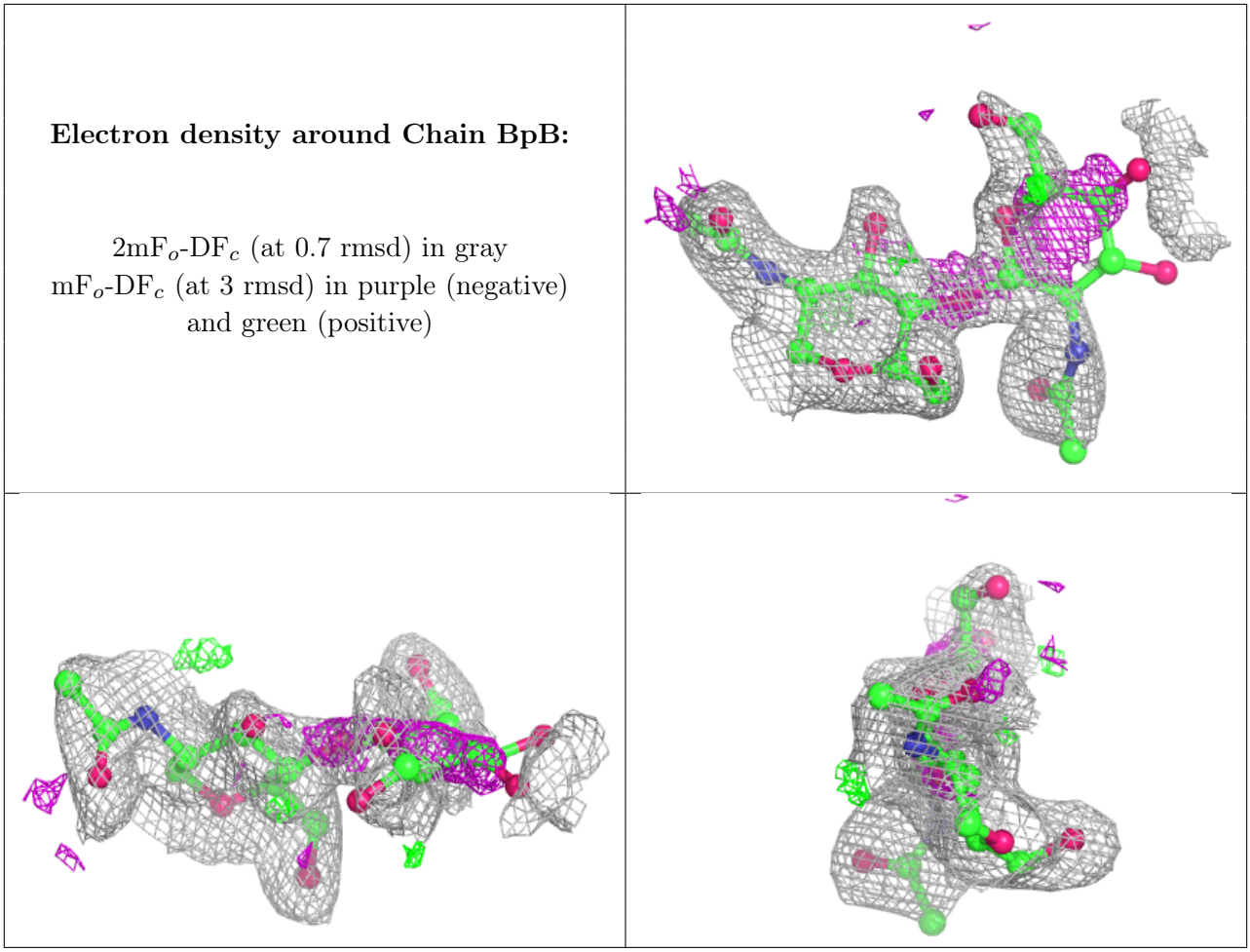






Electron density around Chain BpB:

$2mF_o$-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 BvB:

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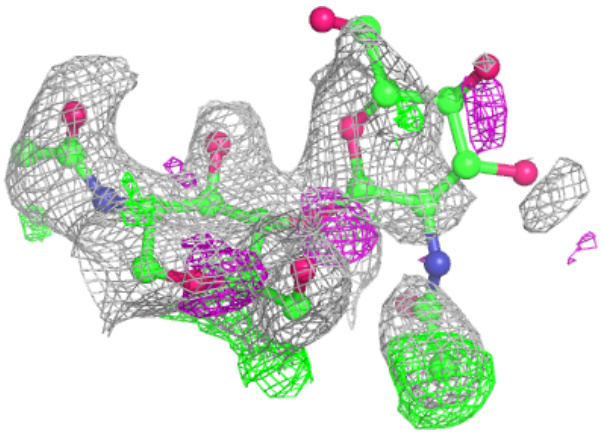
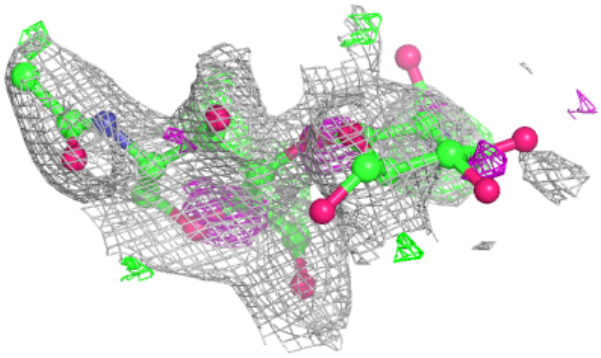
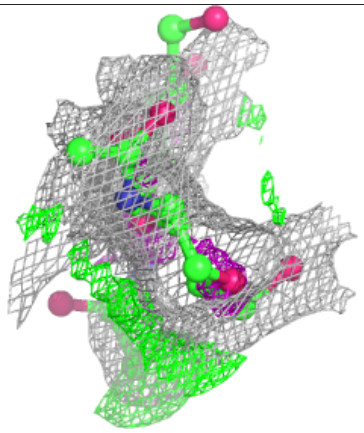
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

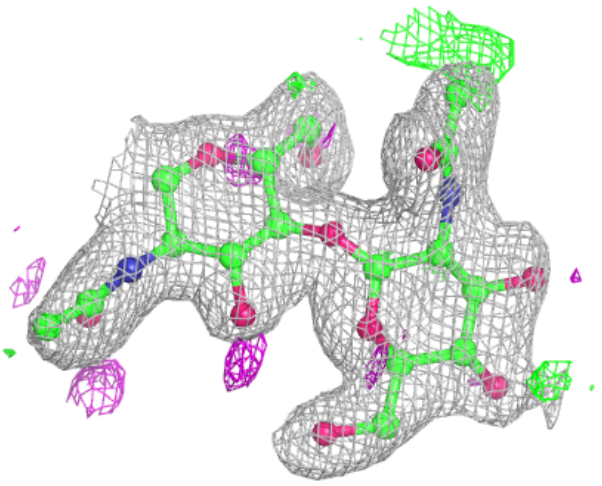


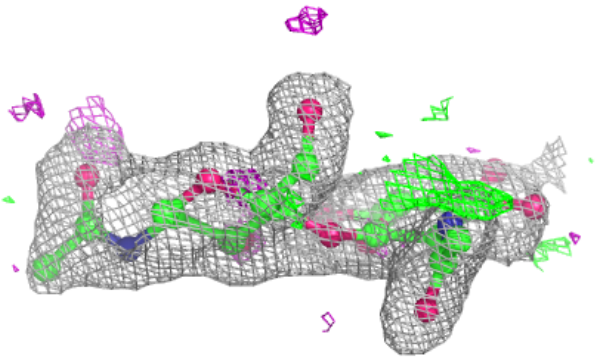


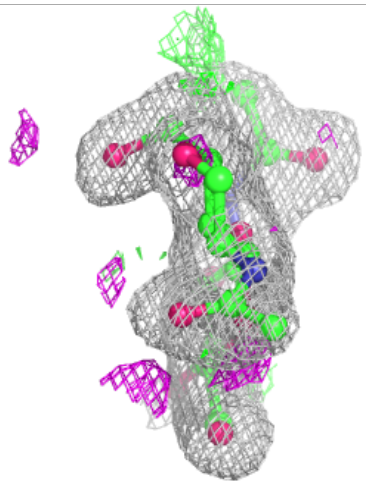


Electron density around Chain BwB:

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

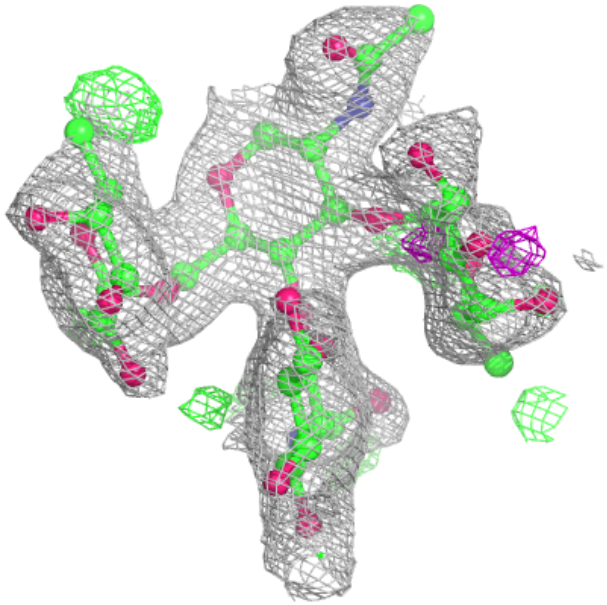


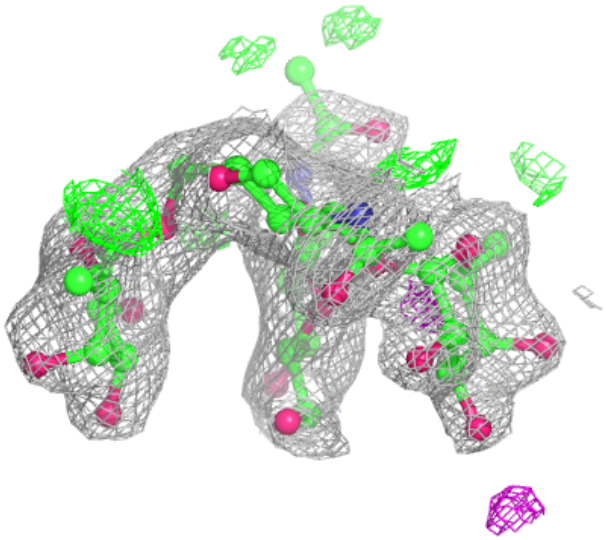


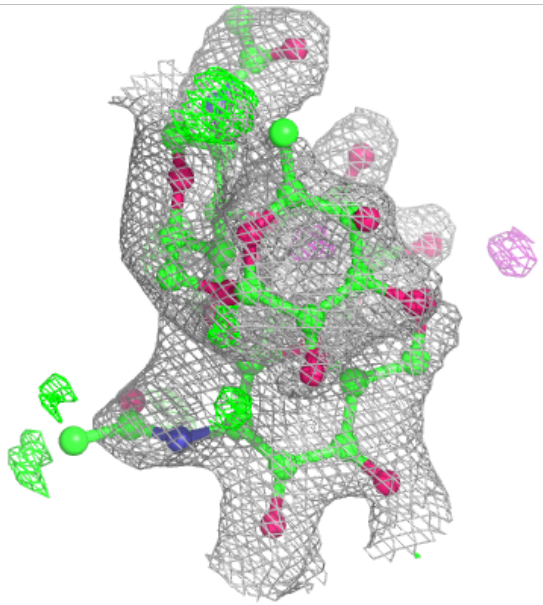


Electron density around Chain AsA:

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

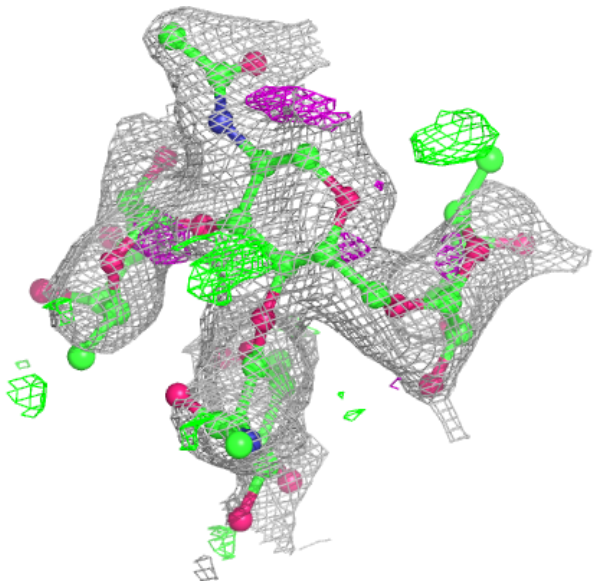


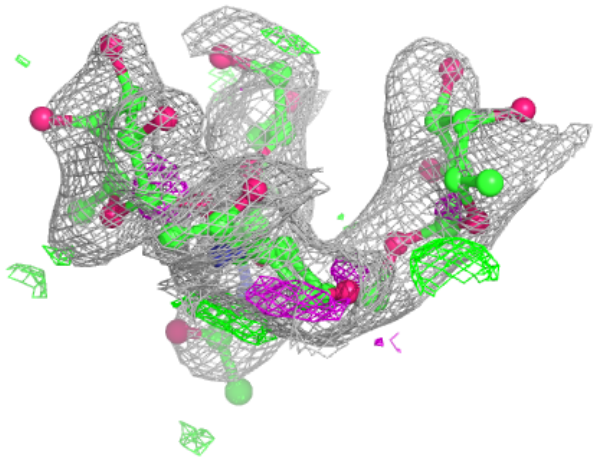


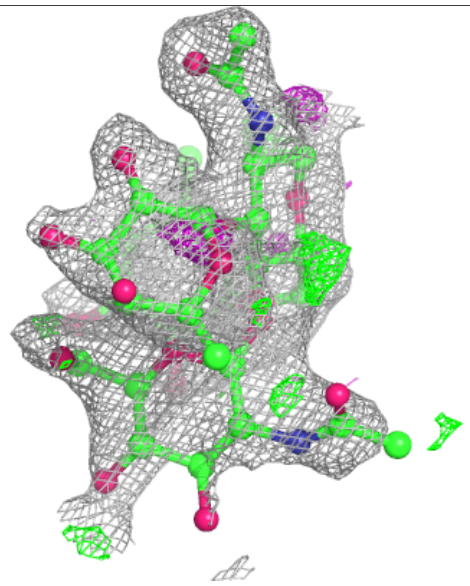


Electron density around Chain BqB:

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

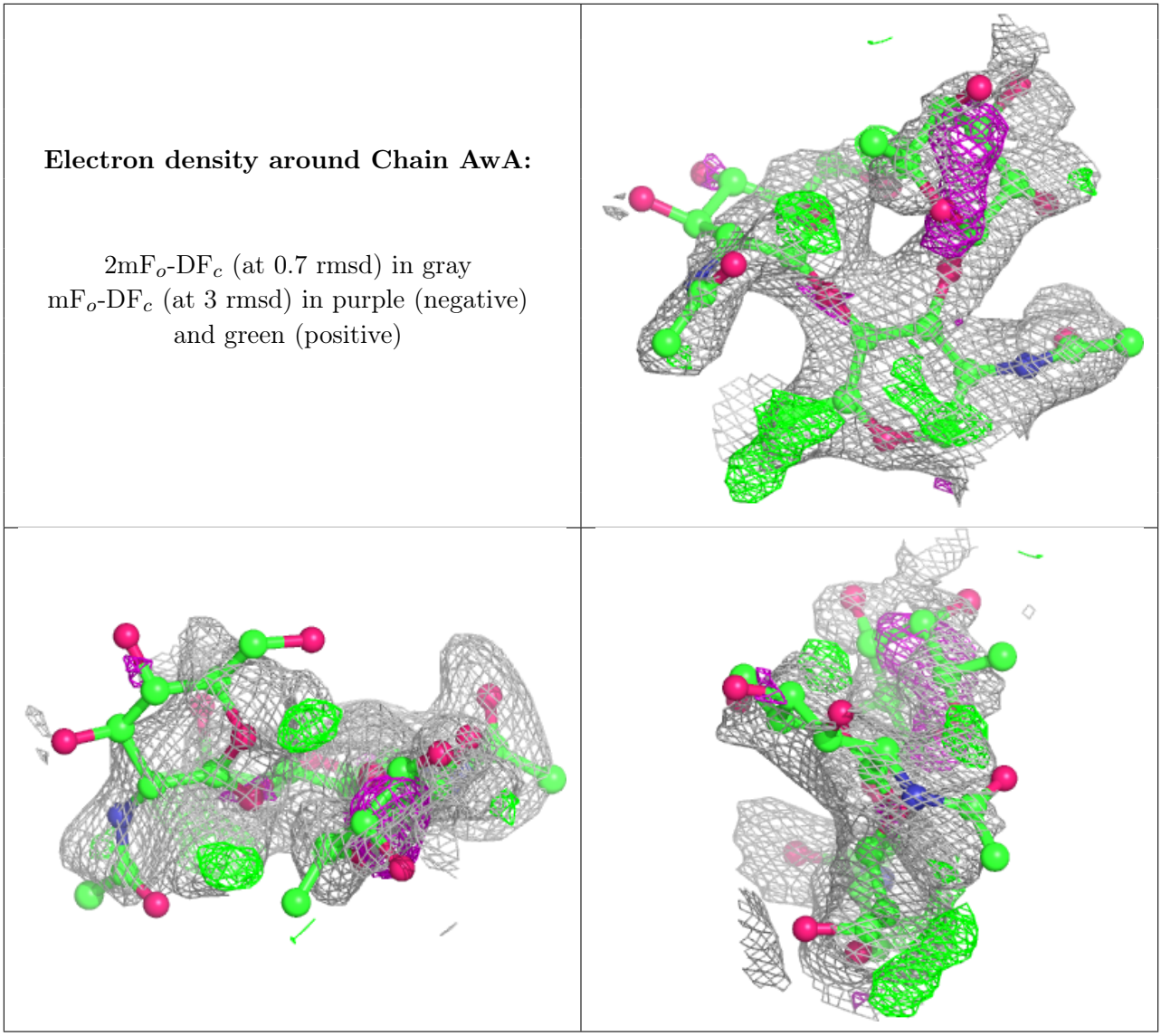






Electron density around Chain AwA:

$2mF_o$-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
9	NA	BBB	715	1/1	0.52	0.38	64,64,64,64	0
7	NAG	BBB	711	14/15	0.56	0.46	51,57,59,60	0
7	NAG	BBB	712	14/15	0.58	0.43	59,61,62,62	0
7	NAG	AAA	712	14/15	0.62	0.46	51,58,59,60	0
7	NAG	AAA	714	14/15	0.68	0.42	43,48,49,49	0
6	EDO	AAA	704	4/4	0.69	0.15	49,50,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	BBB	708	4/4	0.75	0.19	63,63,63,64	0
6	EDO	BBB	709	4/4	0.76	0.24	61,62,62,62	0
7	NAG	AAA	713	14/15	0.76	0.33	49,52,53,53	0
7	NAG	BBB	713	14/15	0.76	0.42	43,47,48,49	0
6	EDO	BBB	710	4/4	0.76	0.36	51,53,53,53	0
6	EDO	AAA	709	4/4	0.78	0.15	64,64,64,64	0
6	EDO	AAA	707	4/4	0.81	0.23	57,57,57,58	0
6	EDO	BBB	707	4/4	0.81	0.12	48,48,49,49	0
6	EDO	AAA	706	4/4	0.82	0.14	52,53,53,53	0
6	EDO	AAA	701	4/4	0.82	0.15	29,30,30,31	0
6	EDO	BBB	705	4/4	0.83	0.34	40,42,42,43	0
6	EDO	AAA	711	4/4	0.83	0.35	51,52,52,53	0
6	EDO	BBB	703	4/4	0.83	0.15	47,49,49,50	0
6	EDO	AAA	702	4/4	0.84	0.20	34,37,37,38	0
6	EDO	BBB	701	4/4	0.85	0.19	37,38,39,40	0
6	EDO	AAA	708	4/4	0.85	0.17	49,49,49,51	0
8	SO4	BBB	714	5/5	0.86	0.19	83,84,85,85	0
6	EDO	AAA	710	4/4	0.87	0.17	50,50,51,51	0
8	SO4	AAA	715	5/5	0.89	0.18	78,79,79,80	0
6	EDO	AAA	703	4/4	0.90	0.17	32,33,33,33	0
6	EDO	AAA	705	4/4	0.91	0.12	46,47,47,47	0
6	EDO	BBB	702	4/4	0.92	0.15	31,32,32,32	0
6	EDO	BBB	704	4/4	0.92	0.14	30,31,31,32	0
6	EDO	BBB	706	4/4	0.93	0.08	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.