wwPDB X-ray Structure Validation Summary Report (i)

Jan 22, 2024 – 04:56 pm GMT

PDB ID	:	8CGW
Title	:	Insulin-regulated aminopeptidase (IRAP) in complex with an allosteric benzopyran-based inhibitor
Authors	:	Mpakali, A.; Stratikos, E.; Giastas, P.
Deposited on	:	2023-02-06
Resolution	:	3.03 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

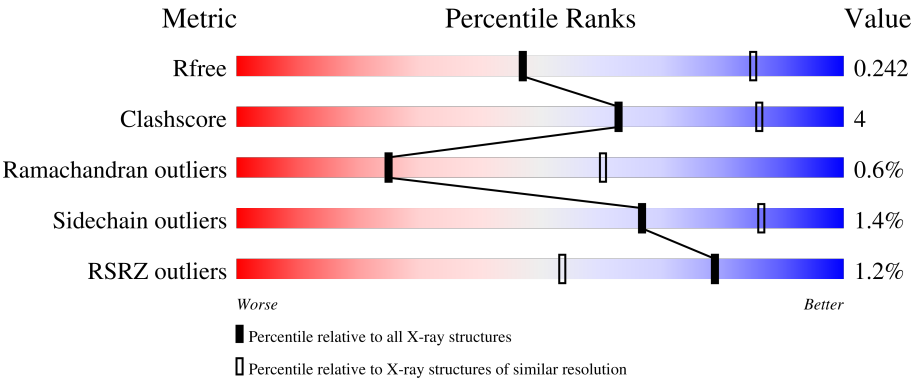
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	A	873	85% 13%
1	B	873	83% 14%
2	C	3	100%
2	D	3	67% 33%
2	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	I	3	33% 67%
2	L	3	100%
3	E	6	33% 33% 33%
4	F	2	50% 50%
4	K	2	100%
4	M	2	50% 50%
4	N	2	100%
5	G	4	50% 50%
5	J	4	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
5	BMA	G	3	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 14531 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.

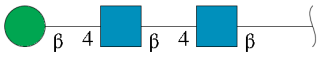
- Molecule 1 is a protein called Leucyl-cystinyl aminopeptidase, pregnancy serum form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	0	2	0
			6926	4483	1120	1297	26			
1	B	853	Total	C	N	O	S	0	0	0
			6837	4430	1114	1267	26			

There are 4 discrepancies between the modelled and reference sequences:

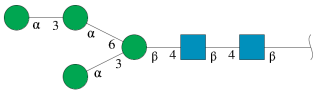
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6

- 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	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

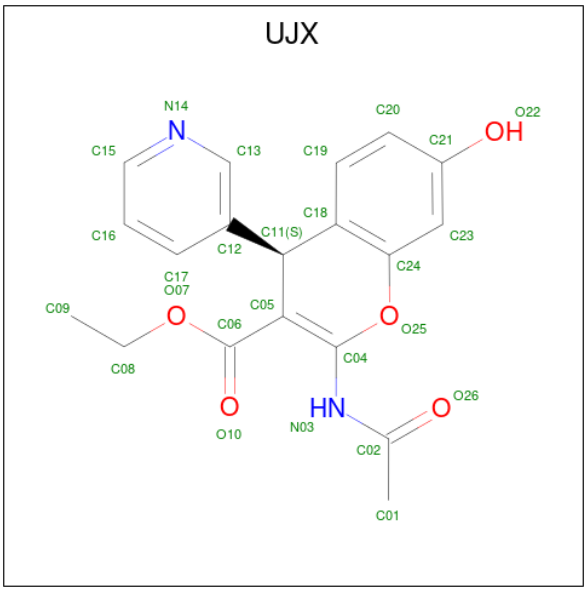
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

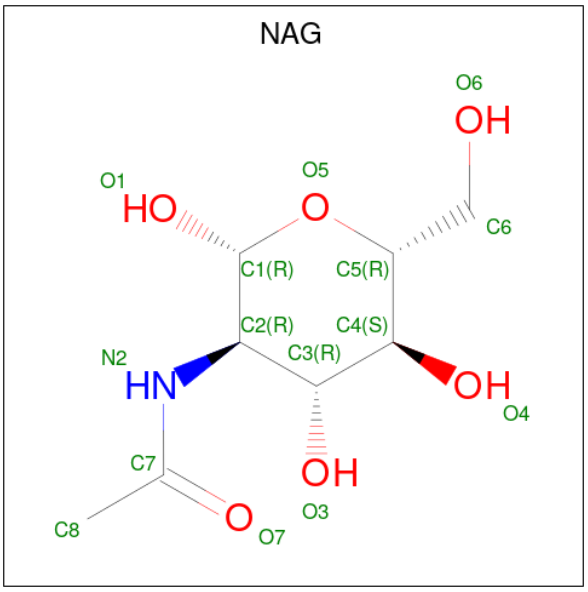
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0

- Molecule 7 is ethyl 2-acetamido-7-hydroxy-4-(pyridin-3-yl)-4H-chromene-3-carboxy late (three-letter code: UJX) (formula: $C_{19}H_{18}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



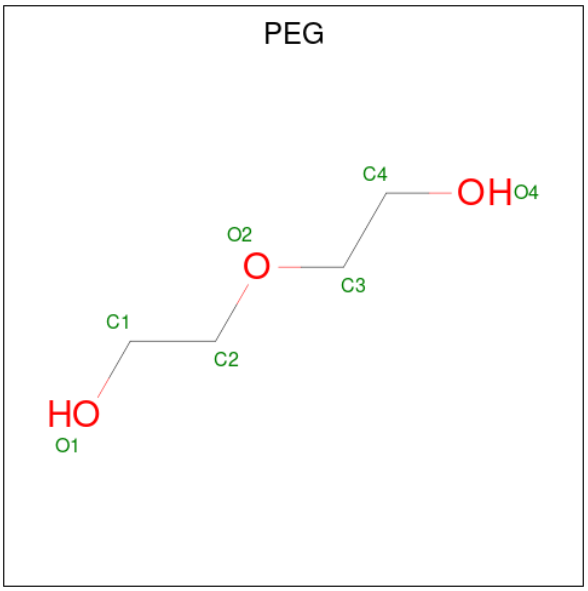
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 26 19 2 5	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



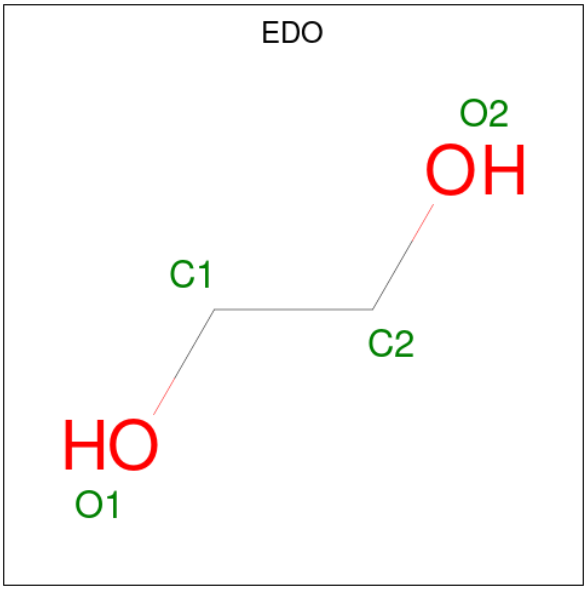
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



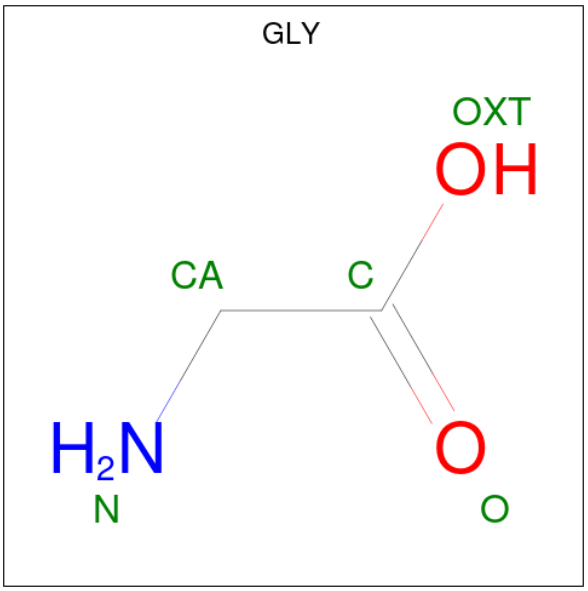
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 5 2 1 2	0	0
11	A	1	Total C N O 5 2 1 2	0	0
11	B	1	Total C N O 5 2 1 2	0	0
11	B	1	Total C N O 5 2 1 2	0	0

- Molecule 12 is water.

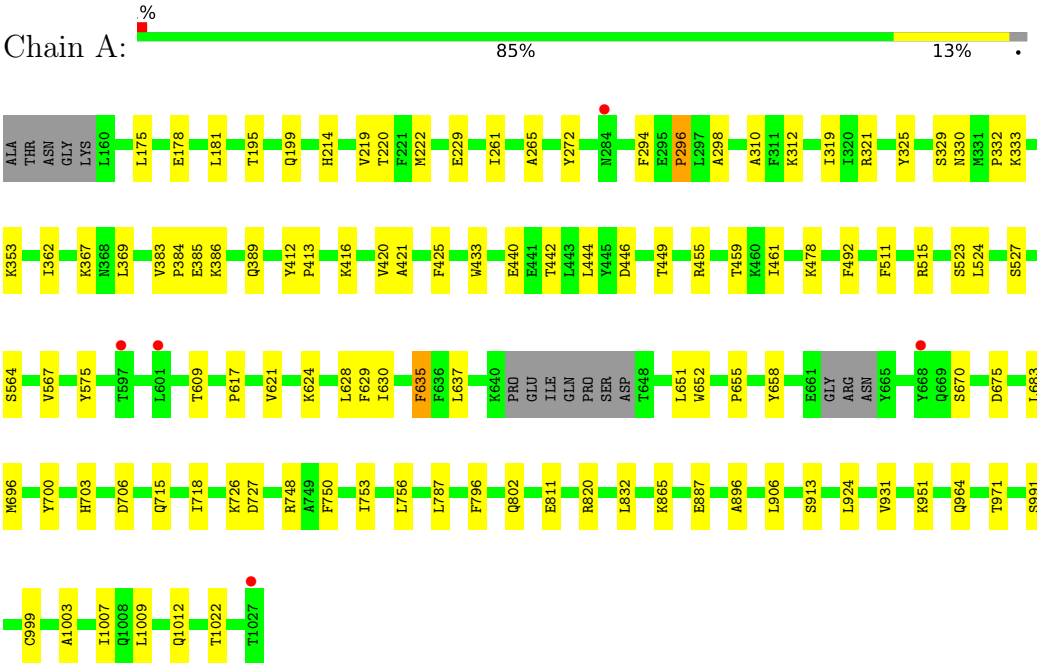
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	44	Total O 44 44	0	0
12	B	28	Total O 28 28	0	0

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.

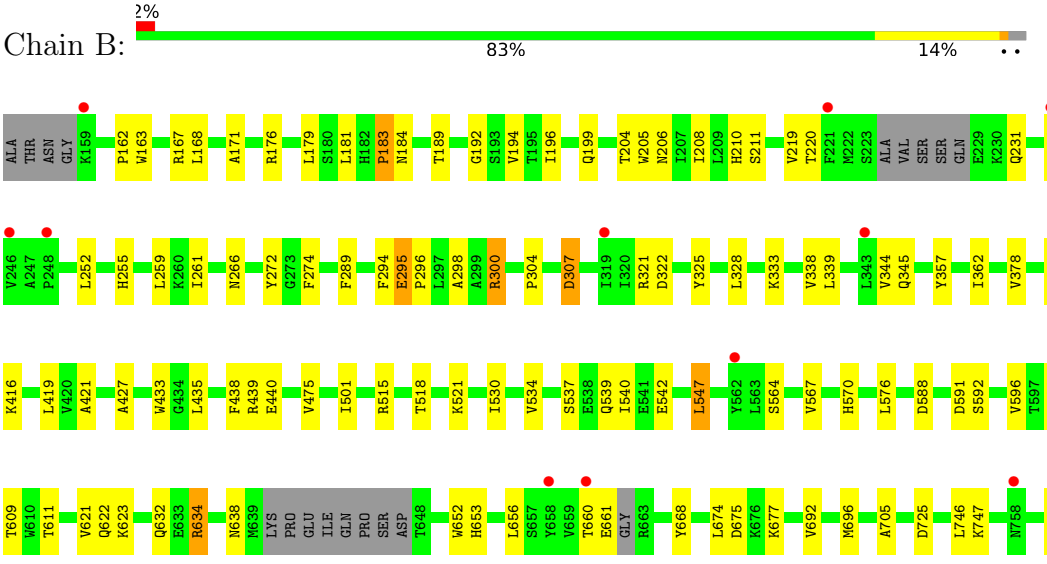
• Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form

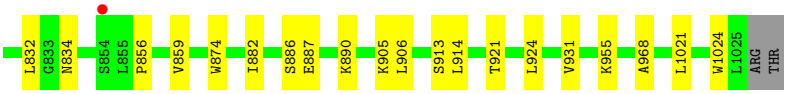
Chain A:



• Molecule 1: Leucyl-cystinyl aminopeptidase, pregnancy serum form

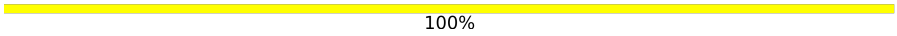
Chain B:





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

Chain C:



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

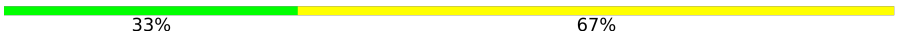
Chain D:

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

Chain H:

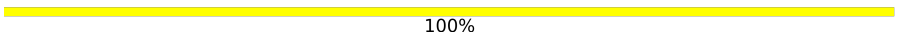
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



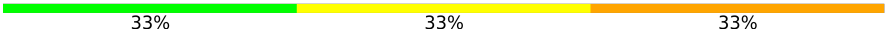
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

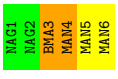
Chain L:



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

Chain E:



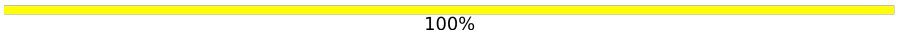


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain K:

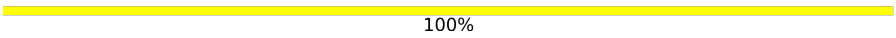


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain N:

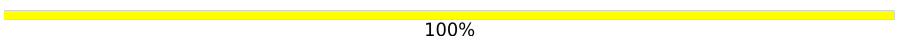


• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.38Å 257.68Å 73.49Å 90.00° 110.44° 90.00°	Depositor
Resolution (Å)	51.36 – 3.03 51.36 – 3.03	Depositor EDS
% Data completeness (in resolution range)	92.7 (51.36-3.03) 92.7 (51.36-3.03)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.242 0.203 , 0.242	Depositor DCC
R_{free} test set	2063 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14531	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NAG, UJX, EDO, ZN, PEG, BMA, MAN

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	A	0.33	0/7102	0.59	2/9640 (0.0%)
1	B	0.35	1/7005 (0.0%)	0.59	4/9515 (0.0%)
All	All	0.34	1/14107 (0.0%)	0.59	6/19155 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ASP	C-N	-6.55	1.19	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	651	LEU	CB-CG-CD1	8.76	125.89	111.00
1	B	339	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	183	PRO	C-N-CA	5.18	134.64	121.70
1	B	300	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	651	LEU	CB-CG-CD2	-5.05	102.41	111.00

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	A	6926	0	6746	60	0
1	B	6837	0	6635	61	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	L	39	0	34	0	0
3	E	72	0	61	1	0
4	F	28	0	25	1	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
5	G	50	0	43	0	0
5	J	50	0	43	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	26	0	0	0	0
8	A	84	0	78	0	0
8	B	70	0	65	0	0
9	A	7	0	10	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
11	A	10	0	4	0	0
11	B	10	0	4	1	0
12	A	44	0	0	0	0
12	B	28	0	0	0	0
All	All	14531	0	13971	122	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 4.

The worst 5 of 122 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:B:609:THR:HG21	1:B:653:HIS:H	1.51	0.75
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.82	0.61
1:A:492:PHE:HZ	1:A:560:LYS:HD3	1.66	0.61
1:A:446:ASP:HB3	1:A:449:THR:HG22	1.84	0.59
1:A:964:GLN:HG2	1:A:999:CYS:HB3	1.85	0.57

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	A	854/873 (98%)	817 (96%)	35 (4%)	2 (0%)	47 80
1	B	845/873 (97%)	790 (94%)	46 (5%)	9 (1%)	14 47
All	All	1699/1746 (97%)	1607 (95%)	81 (5%)	11 (1%)	25 60

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	B	598	ASN
1	A	296	PRO
1	A	635	PHE
1	B	183	PRO

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	A	754/782 (96%)	748 (99%)	6 (1%)	81 92
1	B	734/782 (94%)	719 (98%)	15 (2%)	55 81
All	All	1488/1564 (95%)	1467 (99%)	21 (1%)	67 86

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	592	SER

Continued on next page...

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Mol	Chain	Res	Type
1	B	634	ARG
1	B	797	LYS
1	B	668	TYR
1	B	623	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	GLN
1	B	703	HIS
1	B	801	ASN
1	B	805	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

37 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	C	1	1,2	14,14,15	0.63	1 (7%)	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.72	1 (5%)
2	BMA	C	3	2	11,11,12	0.84	0	15,15,17	1.13	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.16	0	17,19,21	0.58	0
2	NAG	D	2	2	14,14,15	0.59	0	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	D	3	2	11,11,12	0.79	0	15,15,17	0.82	0
3	NAG	E	1	1,3	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	E	2	3	14,14,15	0.41	0	17,19,21	0.53	0
3	BMA	E	3	3	11,11,12	1.00	1 (9%)	15,15,17	0.85	0
3	MAN	E	4	3	11,11,12	1.09	2 (18%)	15,15,17	1.79	3 (20%)
3	MAN	E	5	3	11,11,12	0.93	0	15,15,17	0.97	1 (6%)
3	MAN	E	6	3	11,11,12	0.85	1 (9%)	15,15,17	1.43	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.33	0	17,19,21	1.22	3 (17%)
4	NAG	F	2	4	14,14,15	0.78	0	17,19,21	0.71	0
5	NAG	G	1	1,5	14,14,15	0.44	0	17,19,21	0.59	1 (5%)
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.63	0
5	BMA	G	3	5	11,11,12	0.92	0	15,15,17	0.87	0
5	MAN	G	4	5	11,11,12	1.07	1 (9%)	15,15,17	1.00	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	H	2	2	14,14,15	0.34	0	17,19,21	0.81	0
2	BMA	H	3	2	11,11,12	0.87	0	15,15,17	0.94	1 (6%)
2	NAG	I	1	1,2	14,14,15	0.40	0	17,19,21	0.53	0
2	NAG	I	2	2	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
2	BMA	I	3	2	11,11,12	1.34	2 (18%)	15,15,17	1.01	1 (6%)
5	NAG	J	1	1,5	14,14,15	0.20	0	17,19,21	0.64	1 (5%)
5	NAG	J	2	5	14,14,15	0.33	0	17,19,21	1.62	3 (17%)
5	BMA	J	3	5	11,11,12	0.78	0	15,15,17	1.02	1 (6%)
5	MAN	J	4	5	11,11,12	0.77	0	15,15,17	1.08	2 (13%)
4	NAG	K	1	1,4	14,14,15	1.37	1 (7%)	17,19,21	2.07	2 (11%)
4	NAG	K	2	4	14,14,15	1.29	1 (7%)	17,19,21	1.74	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
2	NAG	L	2	2	14,14,15	1.29	2 (14%)	17,19,21	1.41	3 (17%)
2	BMA	L	3	2	11,11,12	1.12	1 (9%)	15,15,17	1.29	3 (20%)
4	NAG	M	1	1,4	14,14,15	1.32	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	M	2	4	14,14,15	0.59	0	17,19,21	0.71	0
4	NAG	N	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.78	1 (5%)
4	NAG	N	2	4	14,14,15	0.81	1 (7%)	17,19,21	1.08	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	1/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1
3	MAN	E	6	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	1/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C1	-4.71	1.36	1.43
4	K	2	NAG	C1-C2	4.63	1.59	1.52
4	K	1	NAG	O5-C1	-3.86	1.37	1.43
2	L	2	NAG	O5-C1	3.47	1.49	1.43
2	L	2	NAG	C1-C2	2.80	1.56	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1	NAG	C2-N2-C7	7.09	133.00	122.90
3	E	4	MAN	C1-O5-C5	5.61	119.79	112.19
4	K	2	NAG	C2-N2-C7	5.41	130.61	122.90
5	J	2	NAG	C1-O5-C5	4.28	117.99	112.19
3	E	6	MAN	C1-O5-C5	4.27	117.98	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2

All (1) ring outliers are listed below:

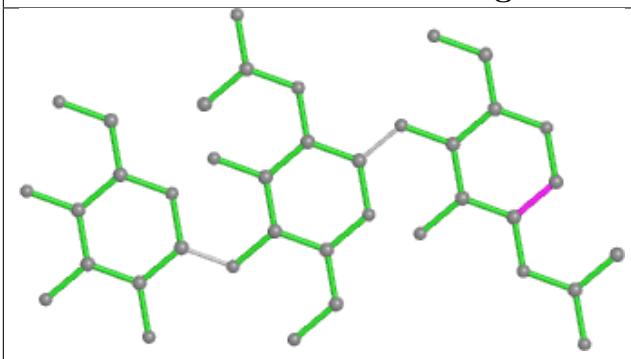
Mol	Chain	Res	Type	Atoms
3	E	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

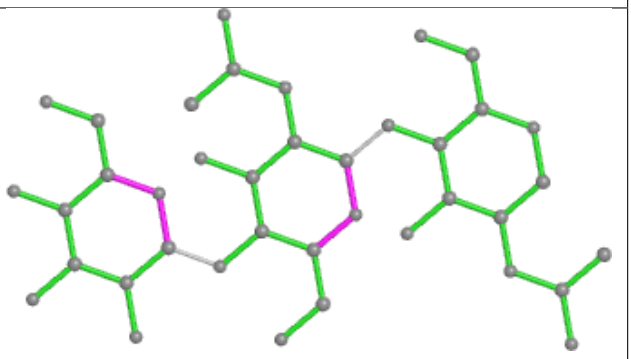
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
3	E	4	MAN	1	0
3	E	3	BMA	1	0

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

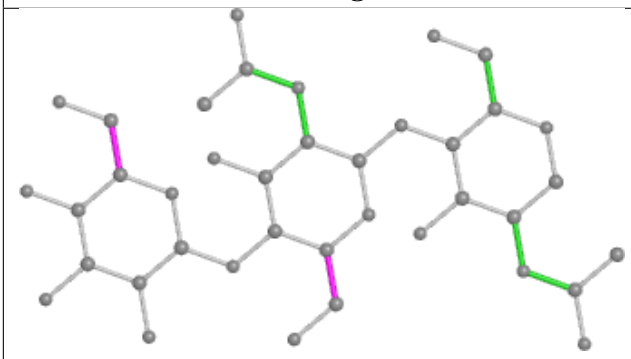
Oligosaccharide Chain C



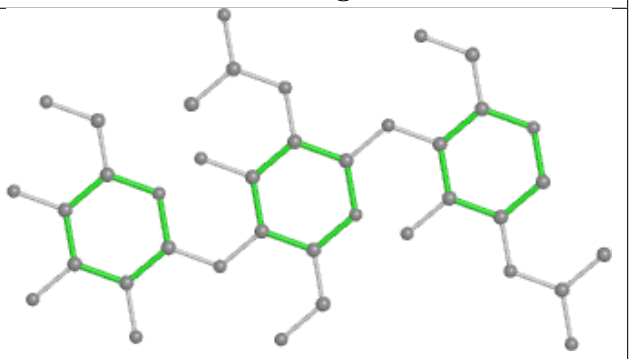
Bond lengths



Bond angles

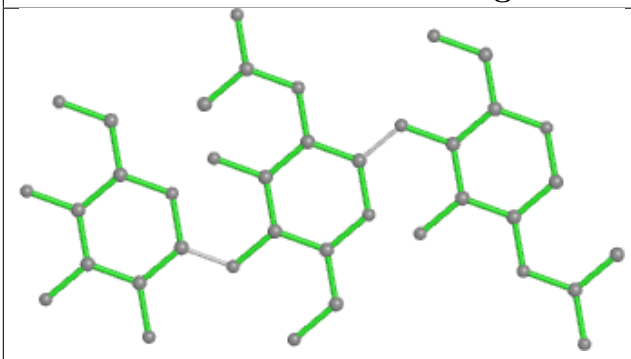


Torsions

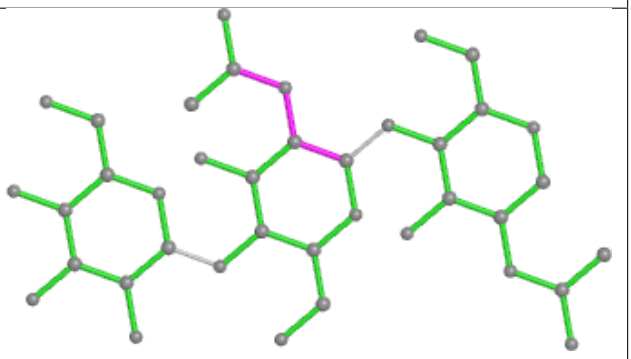


Rings

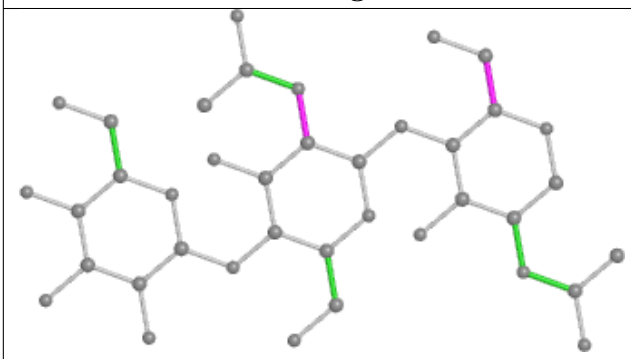
Oligosaccharide Chain D



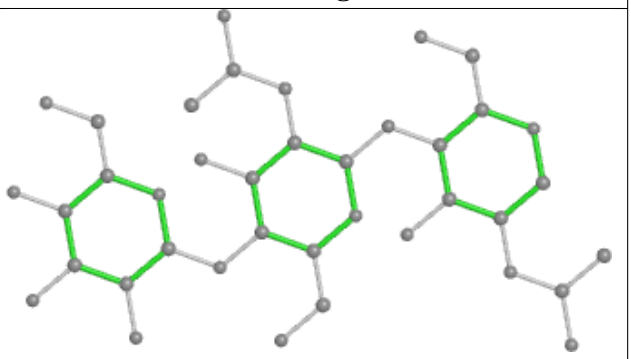
Bond lengths



Bond angles

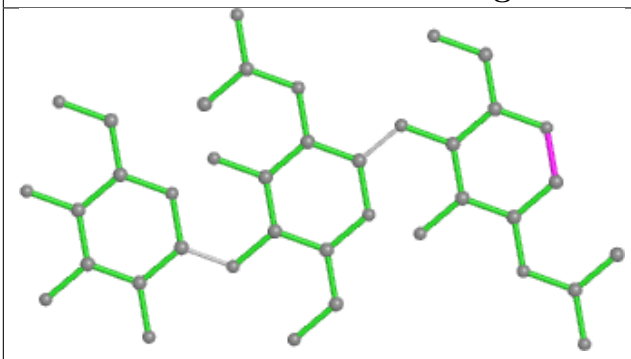


Torsions

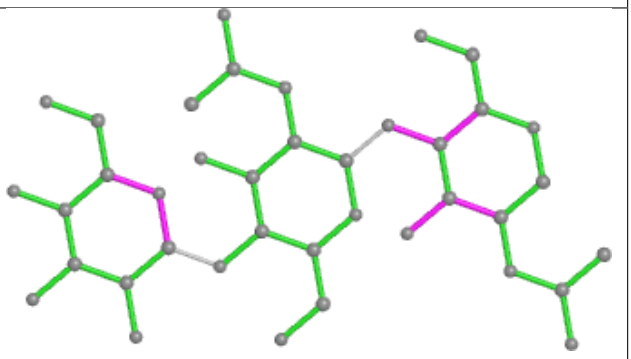


Rings

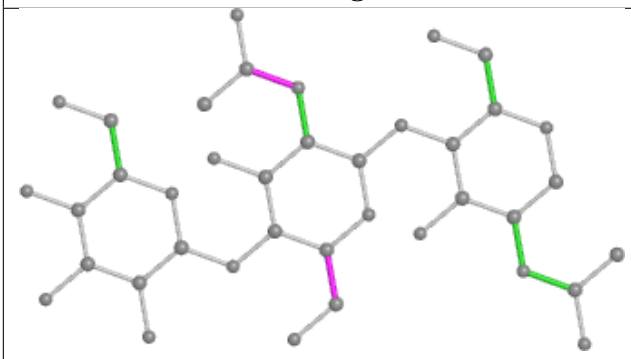
Oligosaccharide Chain H



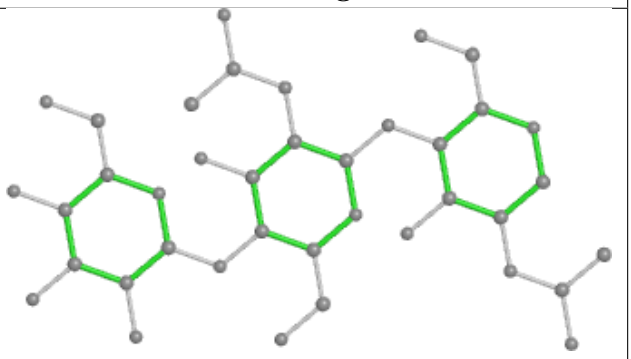
Bond lengths



Bond angles

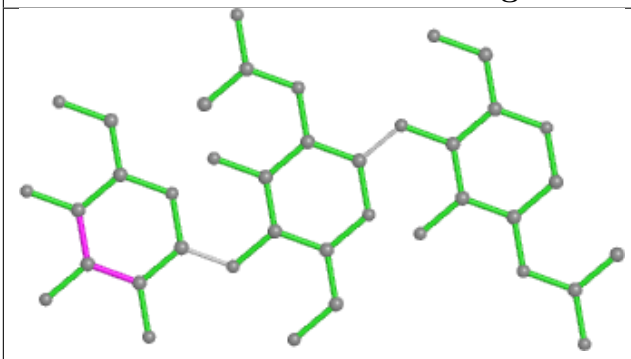


Torsions

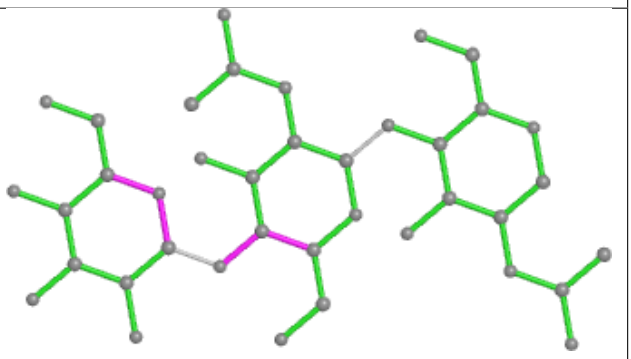


Rings

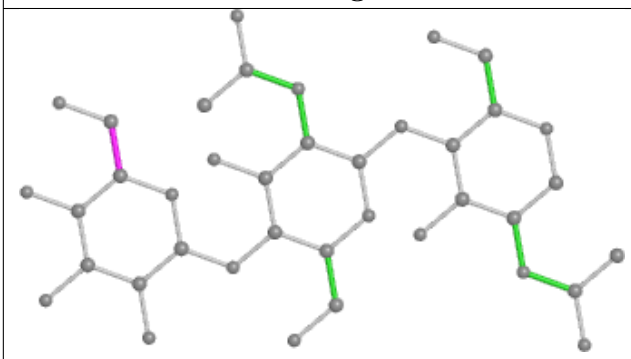
Oligosaccharide Chain I



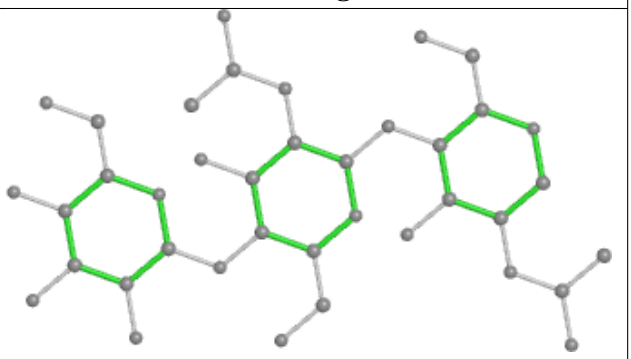
Bond lengths



Bond angles

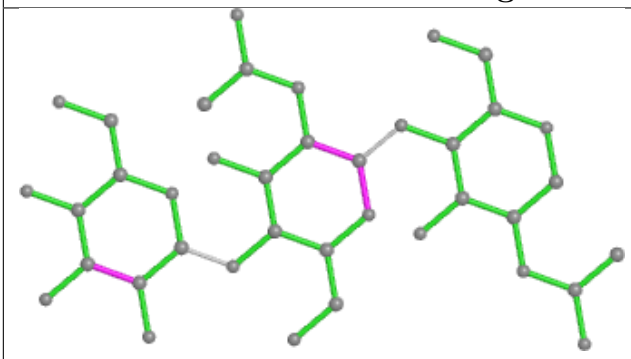


Torsions

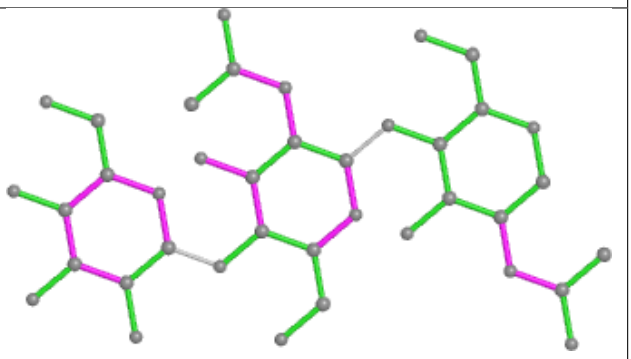


Rings

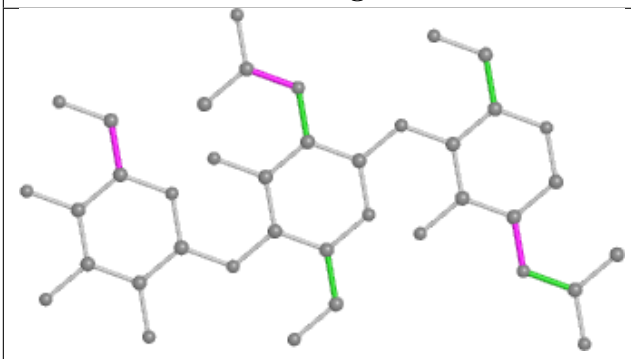
Oligosaccharide Chain L



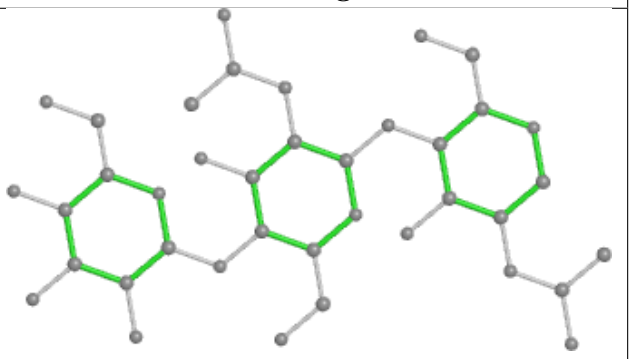
Bond lengths



Bond angles

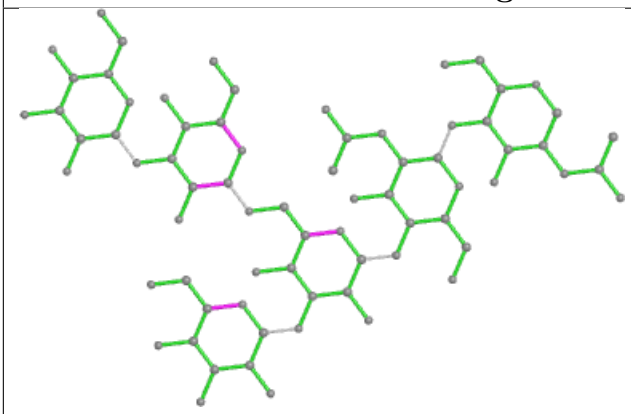


Torsions

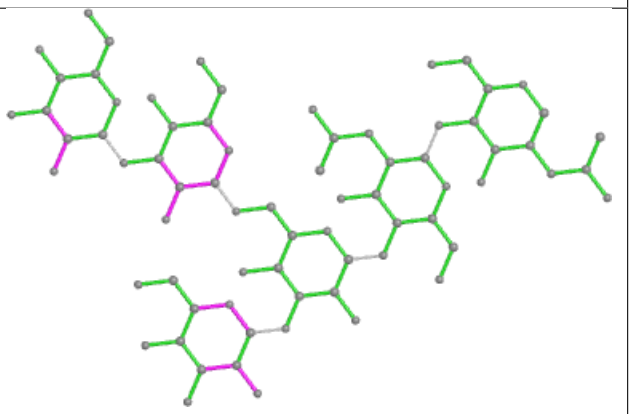


Rings

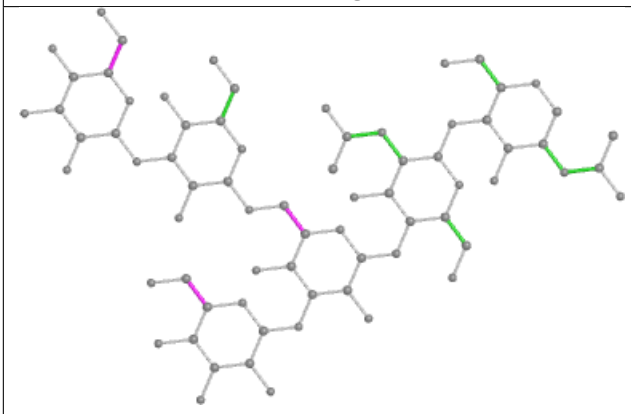
Oligosaccharide Chain E



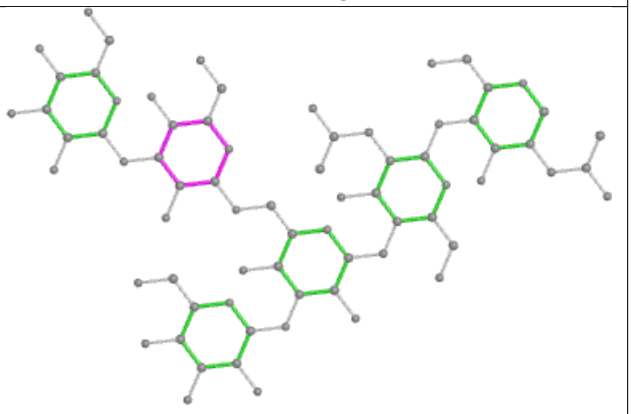
Bond lengths



Bond angles

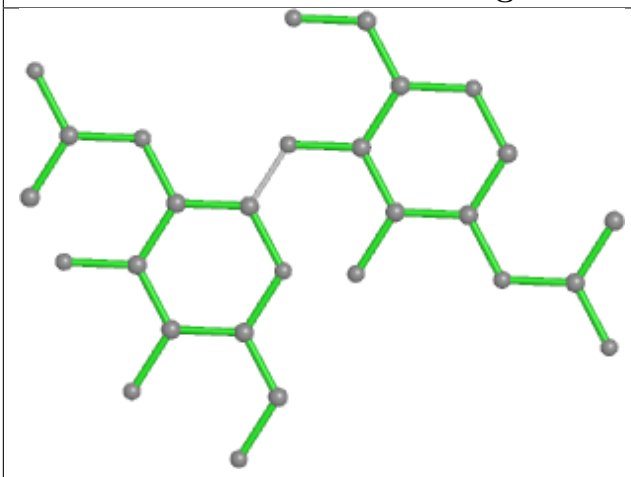


Torsions

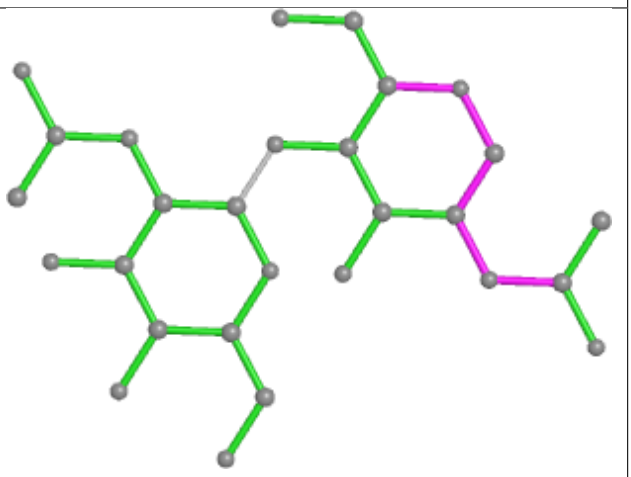


Rings

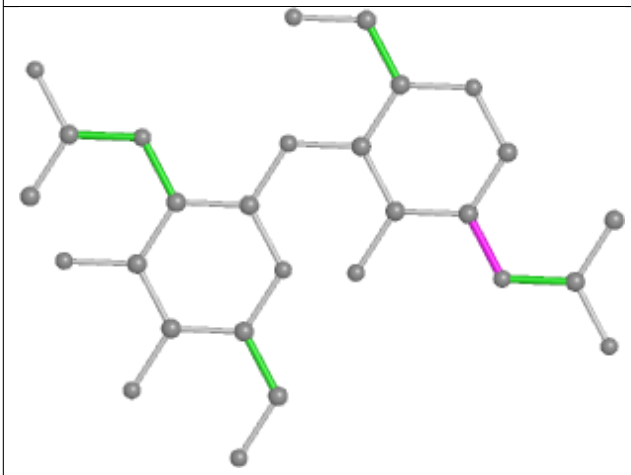
Oligosaccharide Chain F



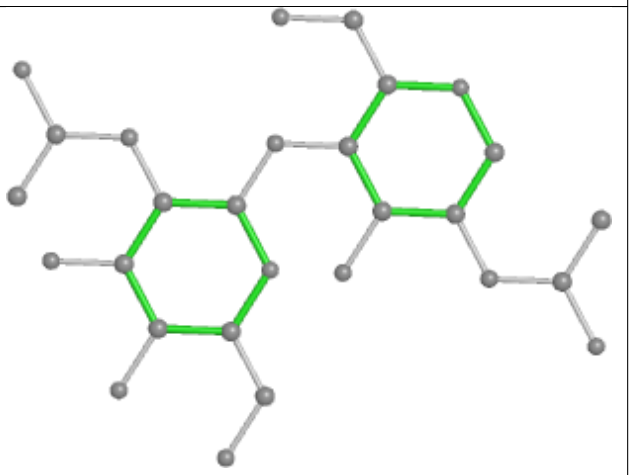
Bond lengths



Bond angles

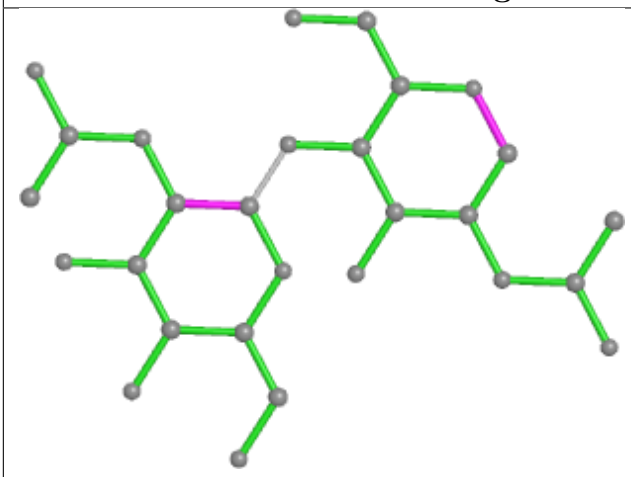


Torsions

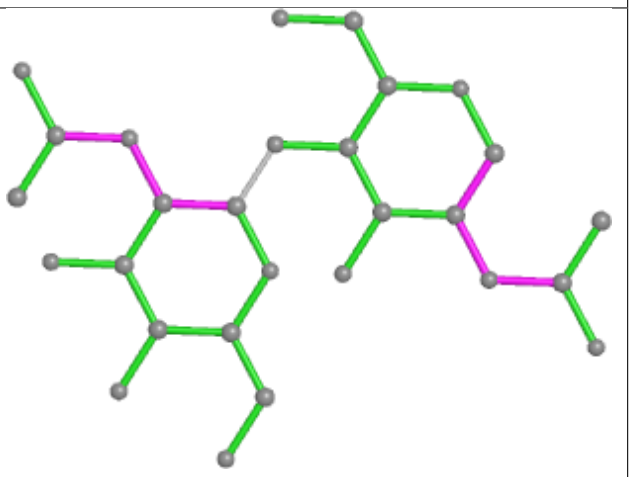


Rings

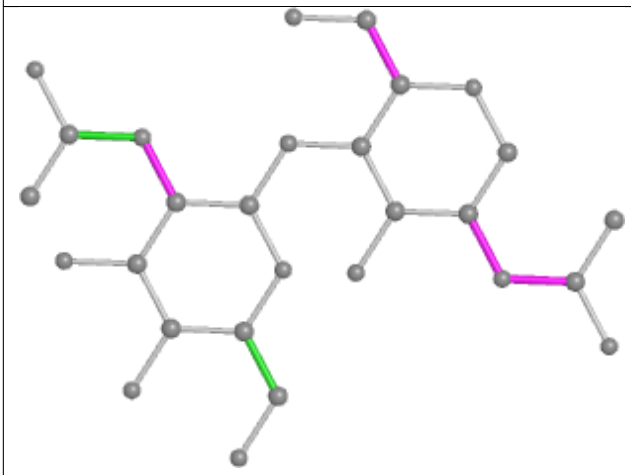
Oligosaccharide Chain K



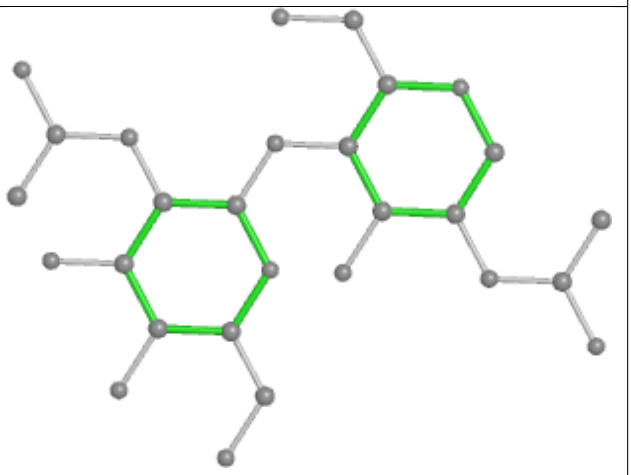
Bond lengths



Bond angles

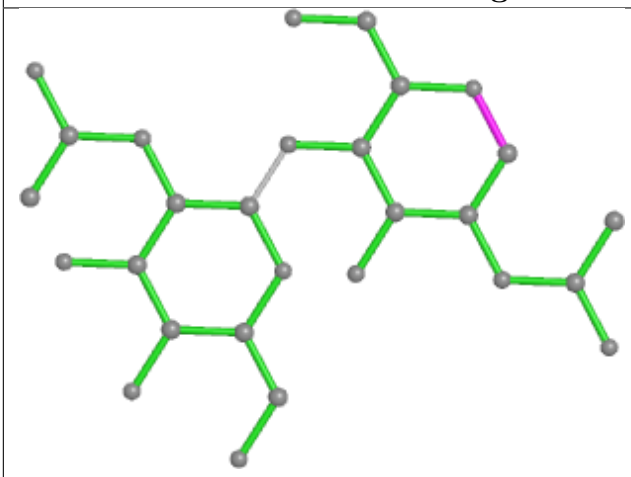


Torsions

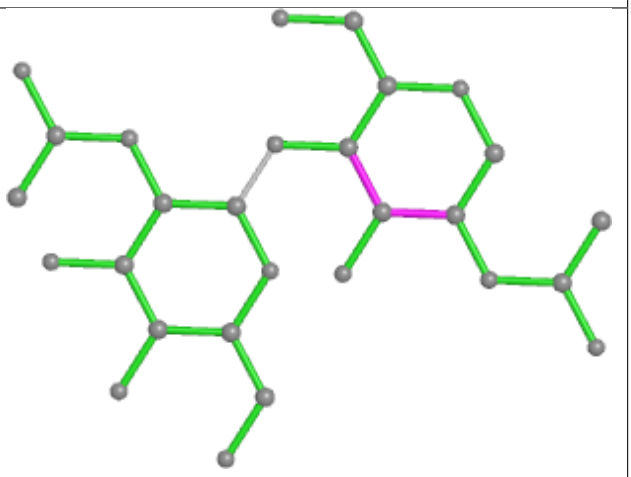


Rings

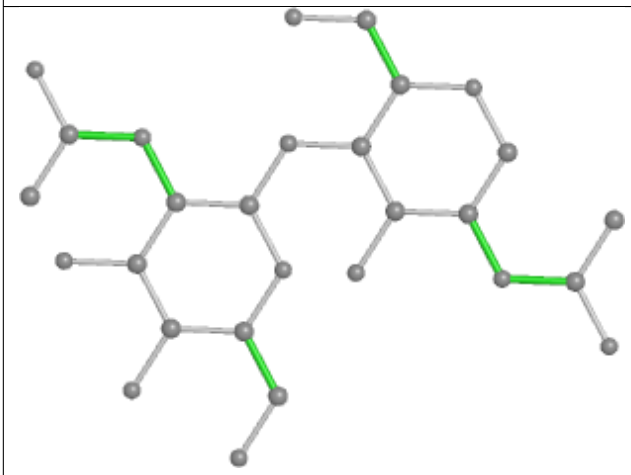
Oligosaccharide Chain M



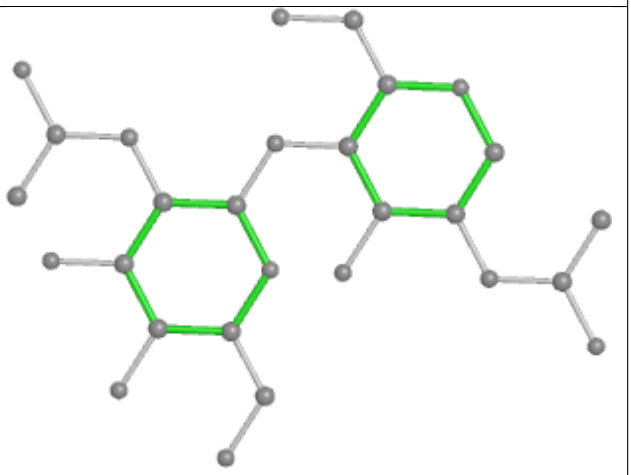
Bond lengths



Bond angles

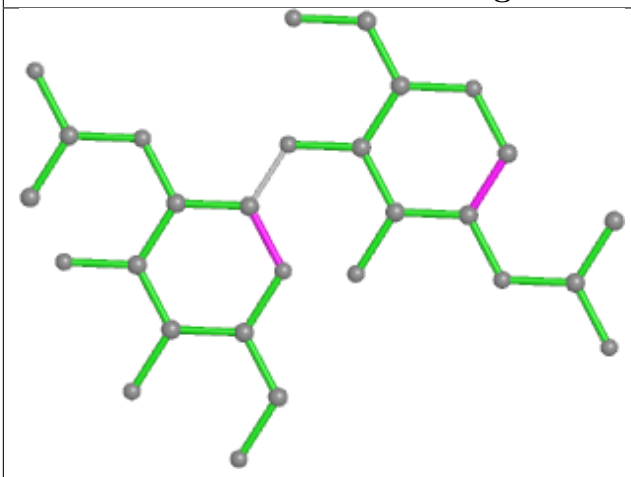


Torsions

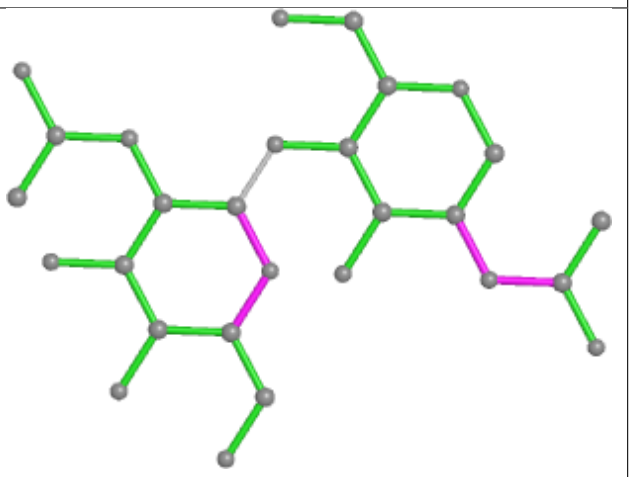


Rings

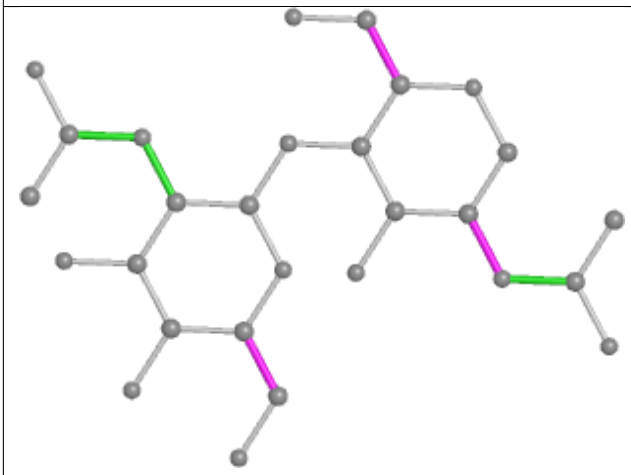
Oligosaccharide Chain N



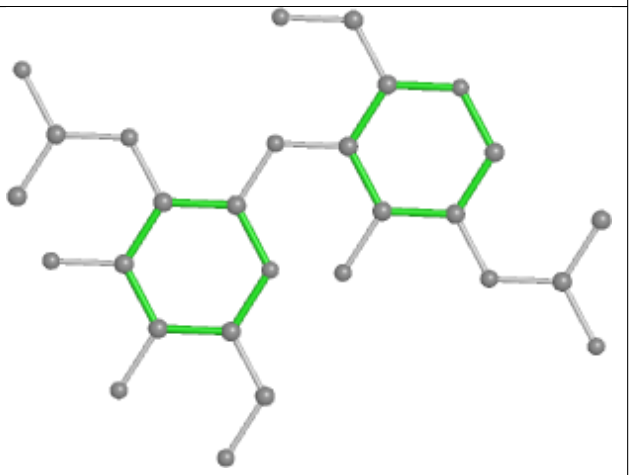
Bond lengths



Bond angles

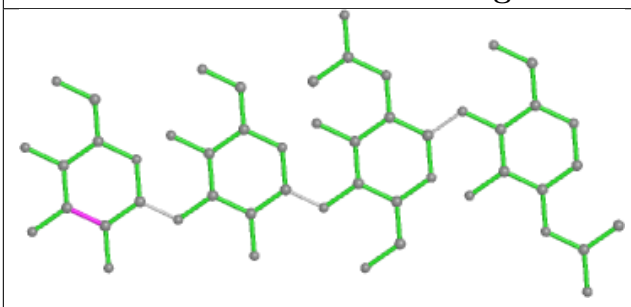


Torsions

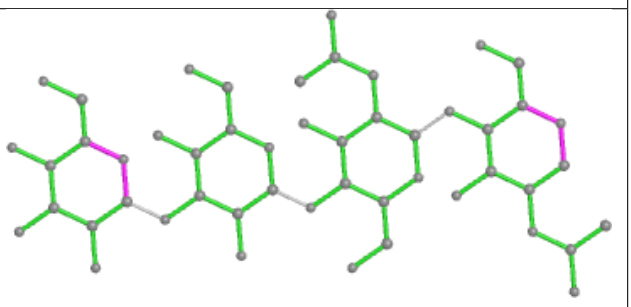


Rings

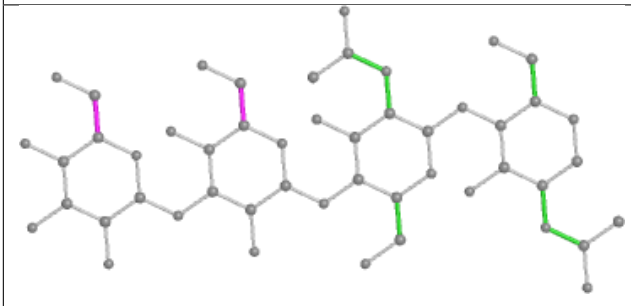
Oligosaccharide Chain G



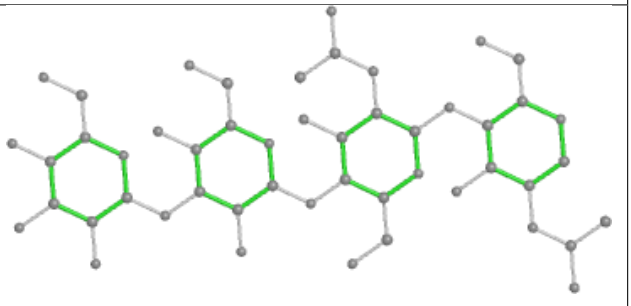
Bond lengths



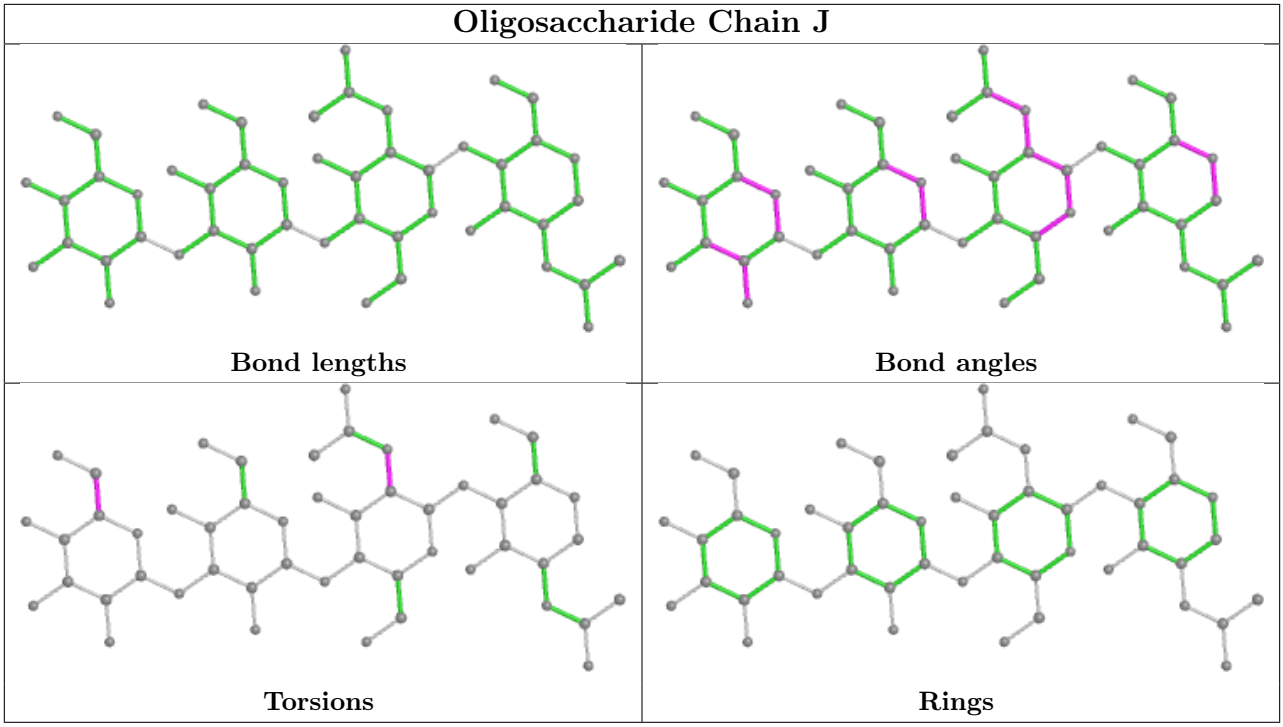
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
10	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.33	0
11	GLY	B	1109	-	4,4,4	1.05	0	3,4,4	1.65	1 (33%)
8	NAG	A	1103	1	14,14,15	0.46	0	17,19,21	0.53	0
8	NAG	A	1104	1	14,14,15	1.21	2 (14%)	17,19,21	1.20	3 (17%)
8	NAG	B	1102	1	14,14,15	0.33	0	17,19,21	0.42	0
8	NAG	A	1105	1	14,14,15	0.58	0	17,19,21	0.79	1 (5%)
8	NAG	B	1104	1	14,14,15	0.57	0	17,19,21	0.51	0
8	NAG	B	1106	1	14,14,15	0.58	0	17,19,21	0.61	1 (5%)
9	PEG	A	1109	-	6,6,6	0.50	0	5,5,5	0.27	0
8	NAG	A	1108	1	14,14,15	0.85	1 (7%)	17,19,21	0.71	0
11	GLY	A	1111	-	4,4,4	1.04	0	3,4,4	1.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	GLY	B	1107	-	4,4,4	1.00	0	3,4,4	1.67	1 (33%)
8	NAG	A	1106	1	14,14,15	0.54	0	17,19,21	0.59	1 (5%)
8	NAG	B	1103	1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
7	UJX	A	1102	-	27,28,28	4.37	15 (55%)	35,39,39	2.78	18 (51%)
8	NAG	A	1107	1	14,14,15	0.30	0	17,19,21	0.44	0
10	EDO	B	1108	-	3,3,3	0.46	0	2,2,2	0.34	0
8	NAG	B	1105	1	14,14,15	1.96	3 (21%)	17,19,21	1.70	4 (23%)
11	GLY	A	1112	-	4,4,4	1.04	0	3,4,4	1.74	1 (33%)

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
10	EDO	A	1110	-	-	0/1/1/1	-
11	GLY	B	1109	-	-	1/2/2/2	-
8	NAG	A	1103	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1104	1	-	3/6/23/26	0/1/1/1
8	NAG	B	1102	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1104	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1106	1	-	0/6/23/26	0/1/1/1
9	PEG	A	1109	-	-	2/4/4/4	-
8	NAG	A	1108	1	-	3/6/23/26	0/1/1/1
11	GLY	A	1111	-	-	2/2/2/2	-
11	GLY	B	1107	-	-	2/2/2/2	-
8	NAG	A	1106	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1103	1	-	0/6/23/26	0/1/1/1
7	UJX	A	1102	-	-	6/13/31/31	0/3/3/3
8	NAG	A	1107	1	-	1/6/23/26	0/1/1/1
10	EDO	B	1108	-	-	0/1/1/1	-
8	NAG	B	1105	1	-	2/6/23/26	0/1/1/1
11	GLY	A	1112	-	-	2/2/2/2	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1102	UJX	C11-C05	11.35	1.67	1.52
7	A	1102	UJX	C12-C11	9.59	1.65	1.52
7	A	1102	UJX	O25-C04	9.00	1.41	1.35
7	A	1102	UJX	C02-N03	6.97	1.50	1.37
8	B	1105	NAG	C1-C2	5.64	1.60	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1102	UJX	C01-C02-N03	6.76	127.00	115.29
7	A	1102	UJX	C12-C11-C05	5.94	119.37	111.47
7	A	1102	UJX	O07-C06-O10	-4.41	115.39	123.34
7	A	1102	UJX	C06-C05-C04	4.33	121.49	118.56
7	A	1102	UJX	O07-C06-C05	3.93	119.32	112.31

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1102	UJX	C04-C05-C06-O07
7	A	1102	UJX	C04-C05-C06-O10
7	A	1102	UJX	C05-C06-O07-C08
7	A	1102	UJX	O10-C06-O07-C08
11	A	1111	GLY	O-C-CA-N

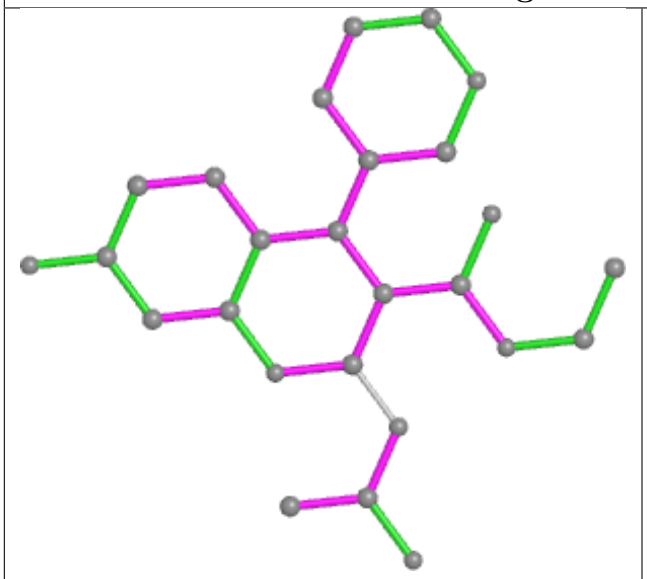
There are no ring outliers.

1 monomer is involved in 1 short contact:

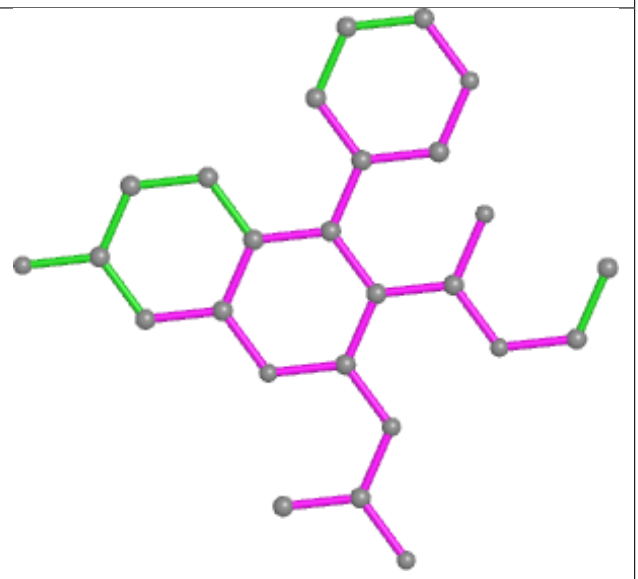
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1109	GLY	1	0

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

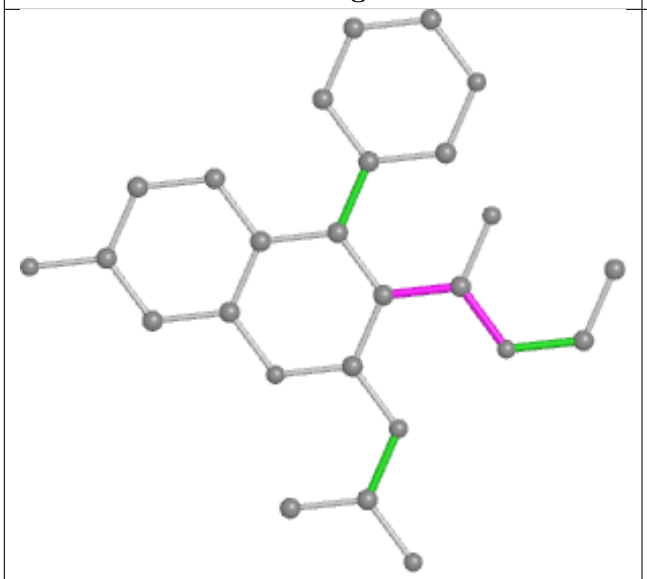
Ligand UJX A 1102



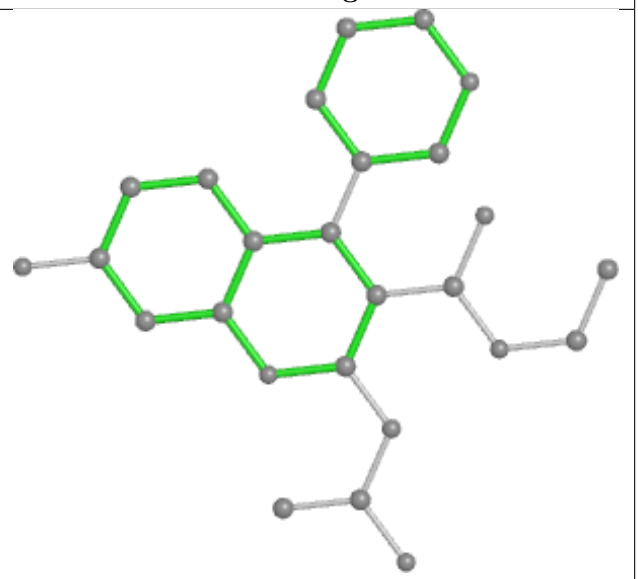
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	307:ASP	C	308:GLU	N	1.19

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	A	858/873 (98%)	-0.33	6 (0%)	87	69	32, 70, 123, 182	0
1	B	853/873 (97%)	-0.14	15 (1%)	68	40	33, 89, 137, 188	0
All	All	1711/1746 (97%)	-0.23	21 (1%)	79	53	32, 81, 130, 188	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	LEU	3.7
1	A	601	LEU	3.1
1	B	245	ILE	2.9
1	B	319	ILE	2.9
1	B	248	PRO	2.7

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	BMA	I	3	11/12	0.58	0.39	155,163,168,173	0
2	BMA	D	3	11/12	0.63	0.21	145,153,158,158	0
2	BMA	L	3	11/12	0.64	0.24	136,152,161,161	0
2	BMA	H	3	11/12	0.70	0.34	168,175,182,183	0
3	MAN	E	6	11/12	0.71	0.28	129,146,153,155	0

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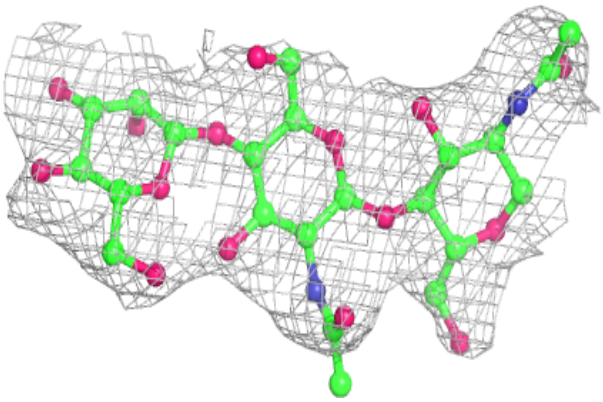
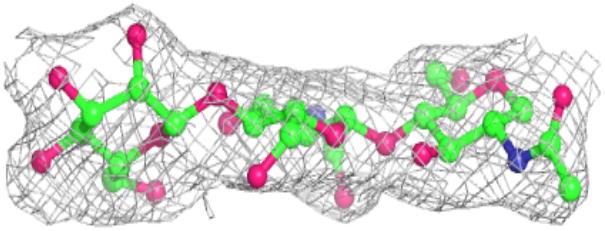
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	J	3	11/12	0.75	0.14	136,143,154,156	0
4	NAG	M	2	14/15	0.77	0.33	119,159,166,167	0
2	NAG	I	2	14/15	0.79	0.37	131,141,151,159	0
3	MAN	E	4	11/12	0.80	0.32	92,130,142,147	0
5	BMA	G	3	11/12	0.80	0.42	103,120,131,132	0
4	NAG	K	2	14/15	0.80	0.42	149,161,168,171	0
4	NAG	N	2	14/15	0.81	0.28	153,165,173,176	0
5	MAN	J	4	11/12	0.81	0.25	145,155,159,160	0
2	BMA	C	3	11/12	0.82	0.19	118,131,138,141	0
4	NAG	N	1	14/15	0.83	0.23	137,153,162,173	0
3	NAG	E	1	14/15	0.84	0.27	135,141,152,156	0
4	NAG	K	1	14/15	0.84	0.28	102,135,141,151	0
2	NAG	D	2	14/15	0.84	0.29	142,153,158,159	0
4	NAG	M	1	14/15	0.85	0.31	153,158,167,175	0
5	MAN	G	4	11/12	0.85	0.43	97,118,125,126	0
2	NAG	D	1	14/15	0.86	0.18	115,126,137,141	0
2	NAG	I	1	14/15	0.86	0.19	106,115,129,139	0
3	BMA	E	3	11/12	0.86	0.35	108,125,139,139	0
3	MAN	E	5	11/12	0.88	0.23	129,145,150,151	0
5	NAG	G	2	14/15	0.88	0.29	117,126,134,136	0
4	NAG	F	2	14/15	0.90	0.16	118,129,138,139	0
2	NAG	H	2	14/15	0.92	0.34	129,141,148,163	0
5	NAG	J	2	14/15	0.92	0.13	102,119,126,139	0
2	NAG	L	1	14/15	0.92	0.24	103,115,123,126	0
2	NAG	L	2	14/15	0.92	0.13	117,125,131,143	0
3	NAG	E	2	14/15	0.93	0.28	139,146,150,152	0
2	NAG	H	1	14/15	0.93	0.21	78,105,114,116	0
4	NAG	F	1	14/15	0.93	0.16	76,97,114,126	0
2	NAG	C	1	14/15	0.93	0.21	100,112,121,127	0
2	NAG	C	2	14/15	0.94	0.22	105,112,119,121	0
5	NAG	G	1	14/15	0.94	0.25	102,114,126,132	0
5	NAG	J	1	14/15	0.95	0.10	107,113,120,124	0

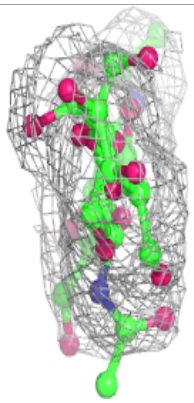
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

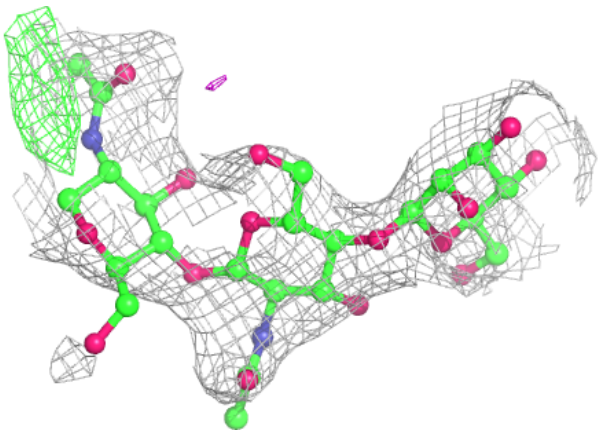


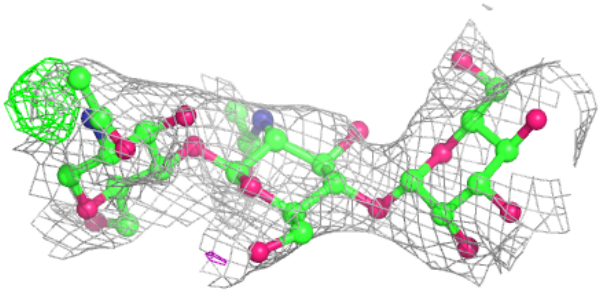


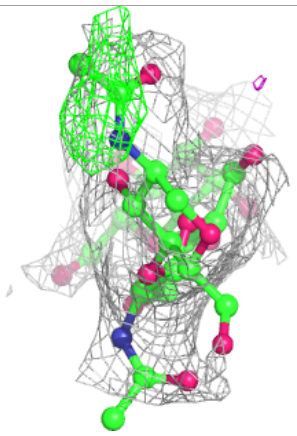


Electron density around Chain D:

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

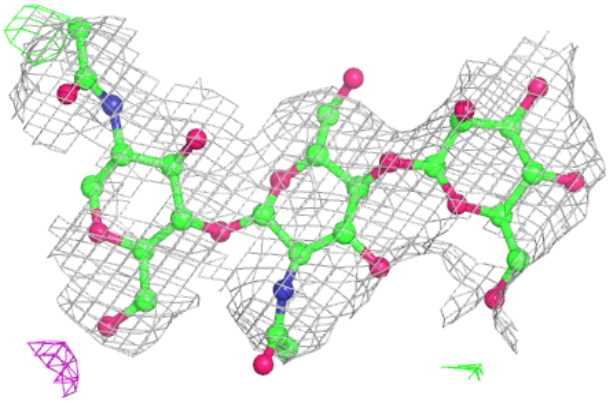


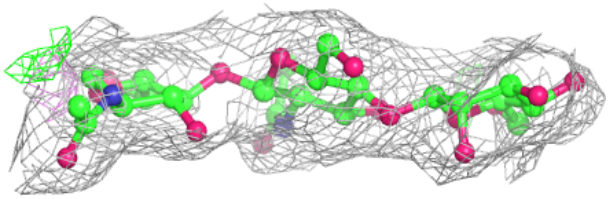


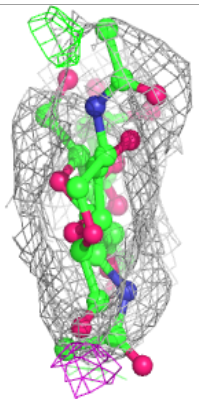


Electron density around Chain H:

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

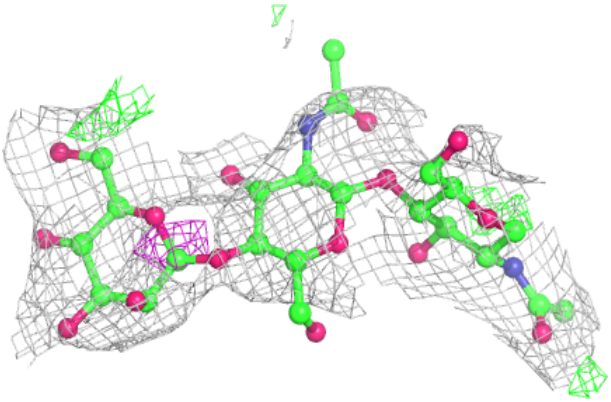


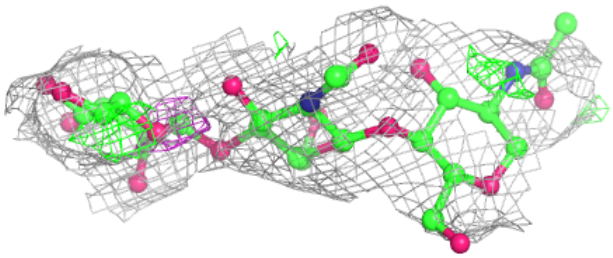


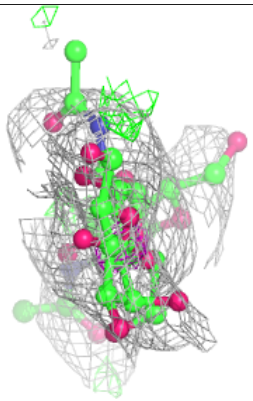


Electron density around Chain I:

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

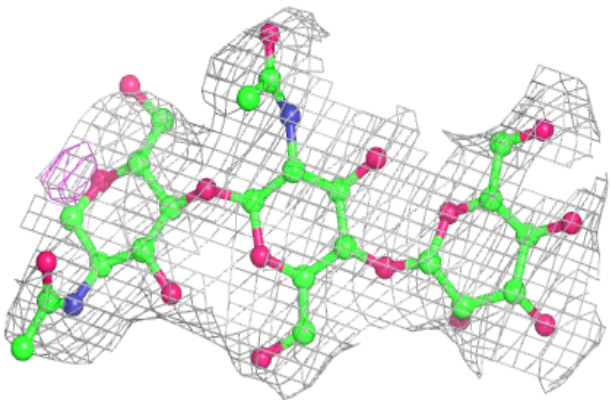


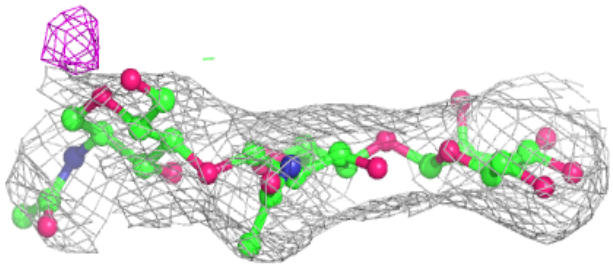


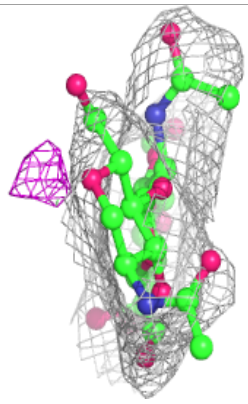


Electron density around Chain L:

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

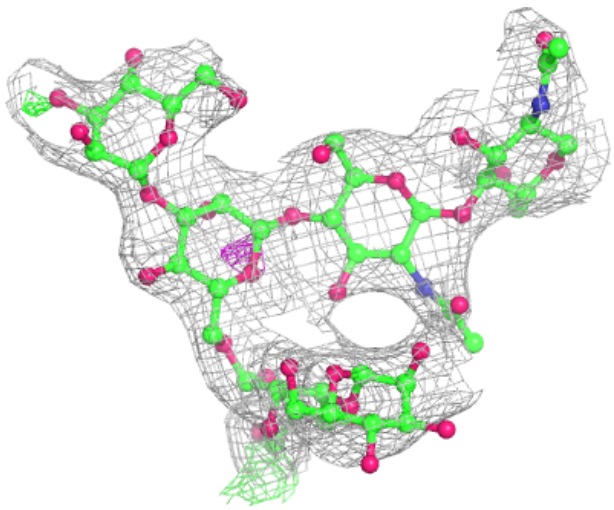


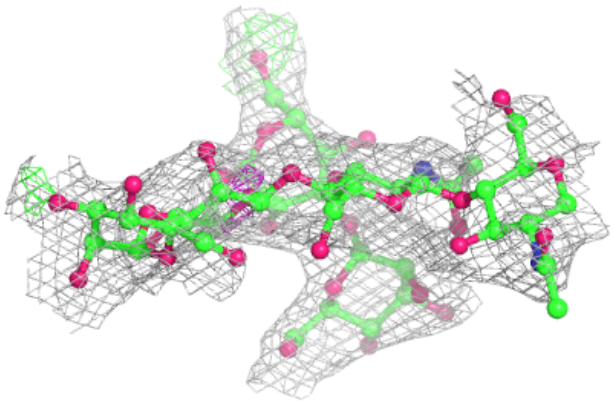


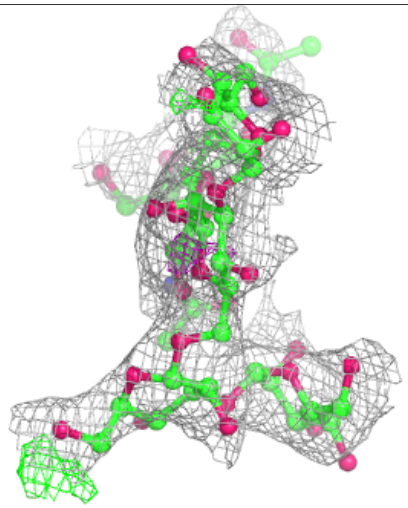


Electron density around Chain E:

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

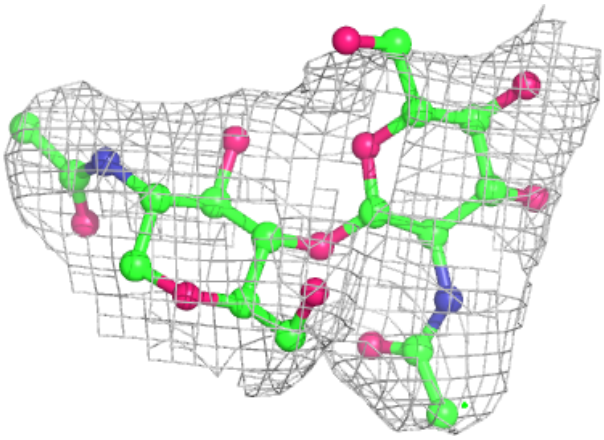


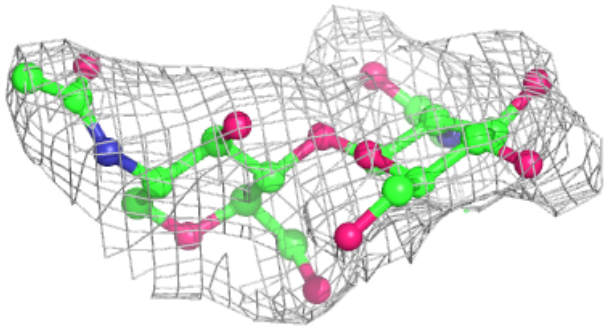


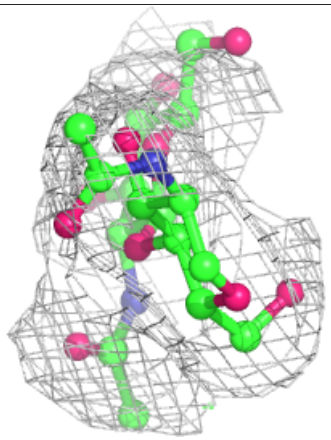


Electron density around Chain F:

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

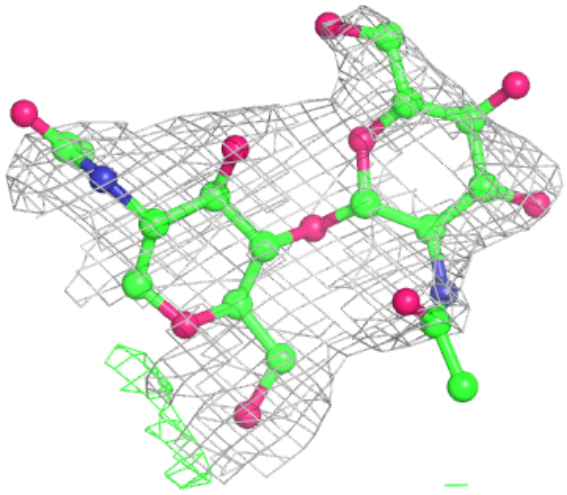


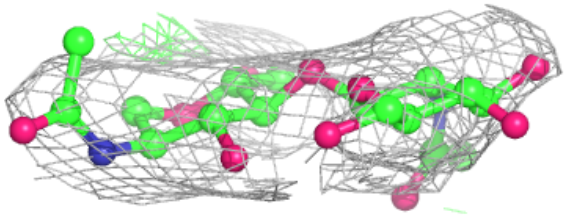


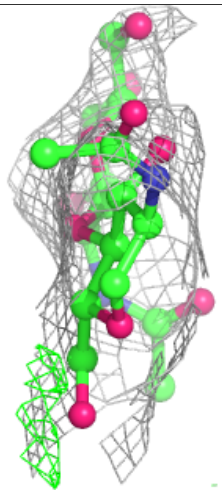


Electron density around Chain K:

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

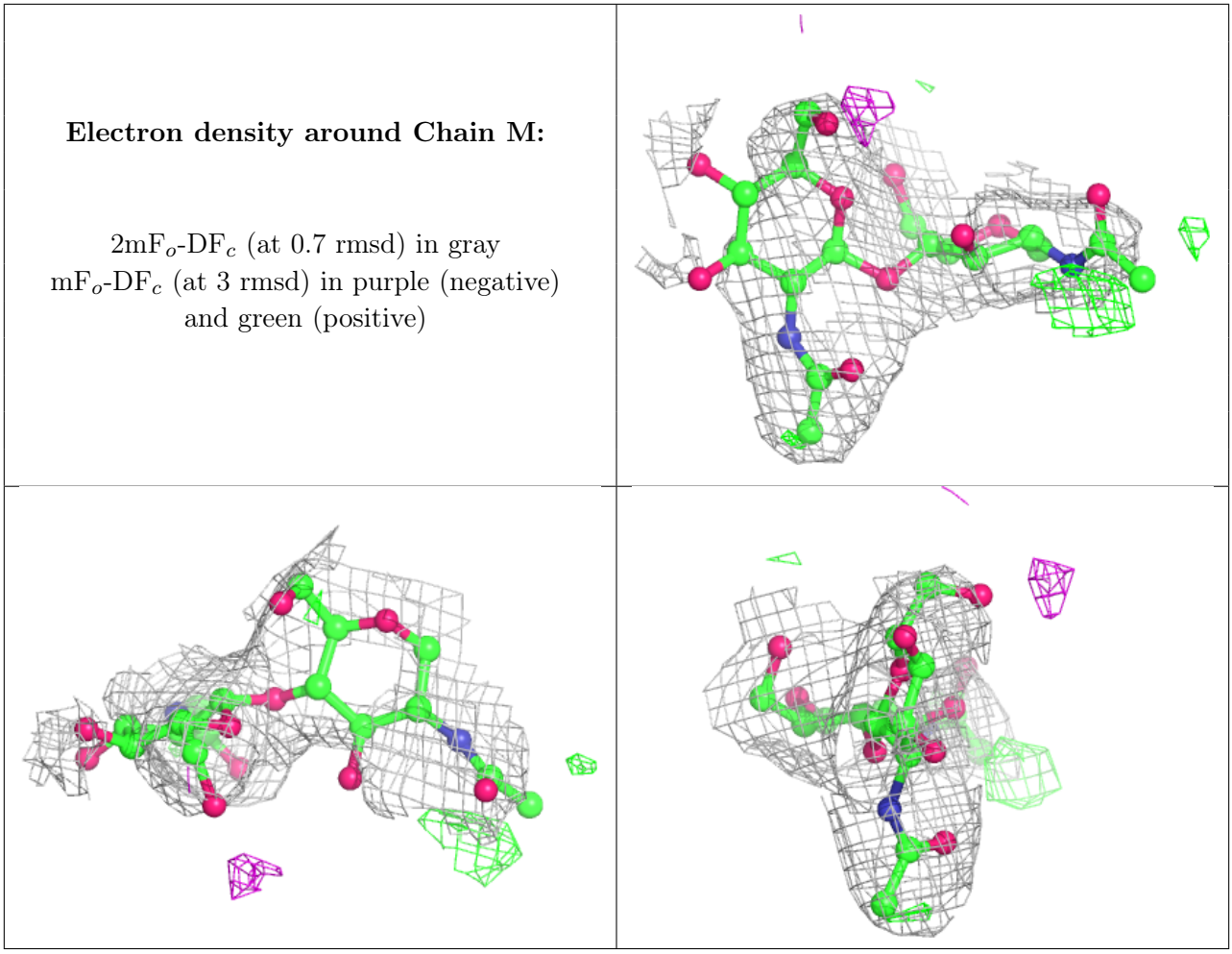






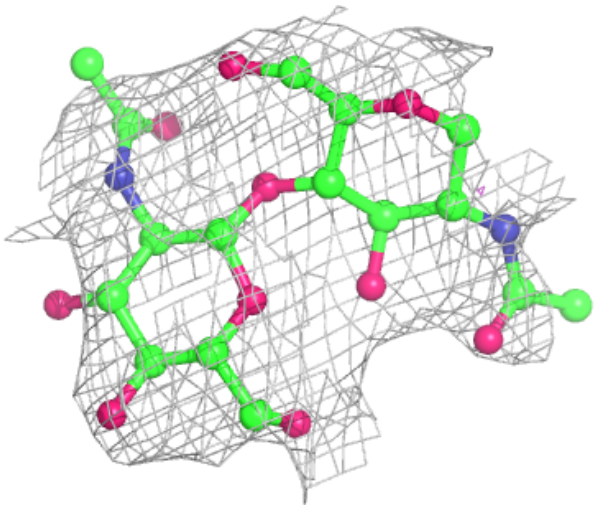
Electron density around Chain M:

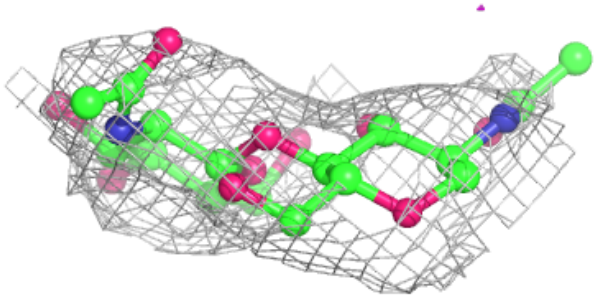
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

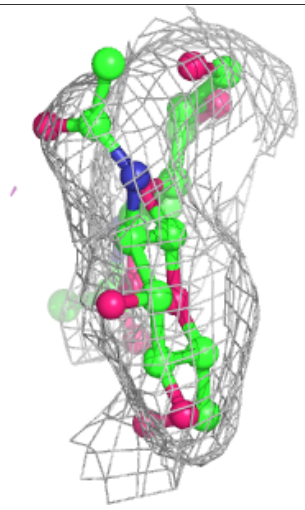


Electron density around Chain N:

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

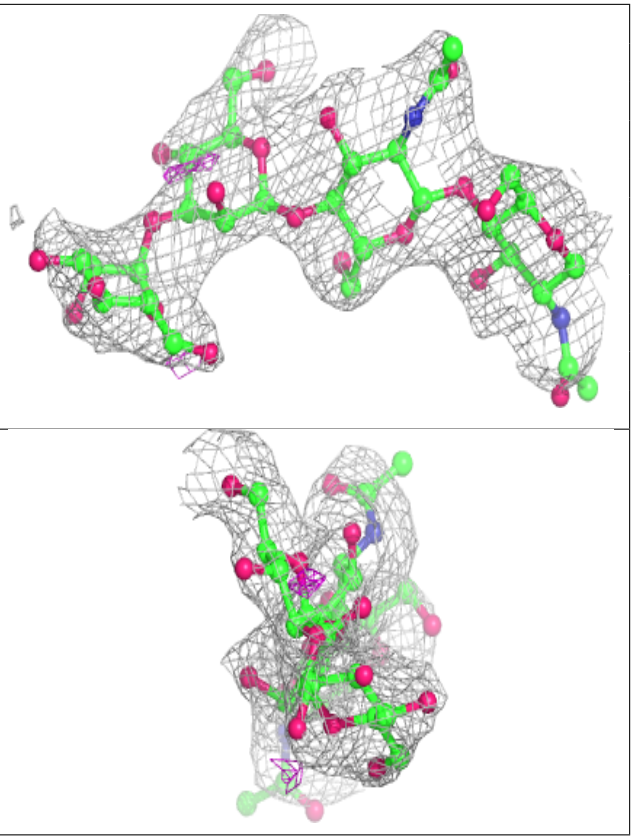


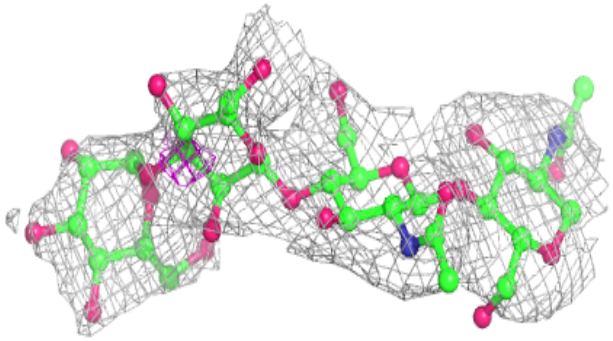




Electron density around Chain G:

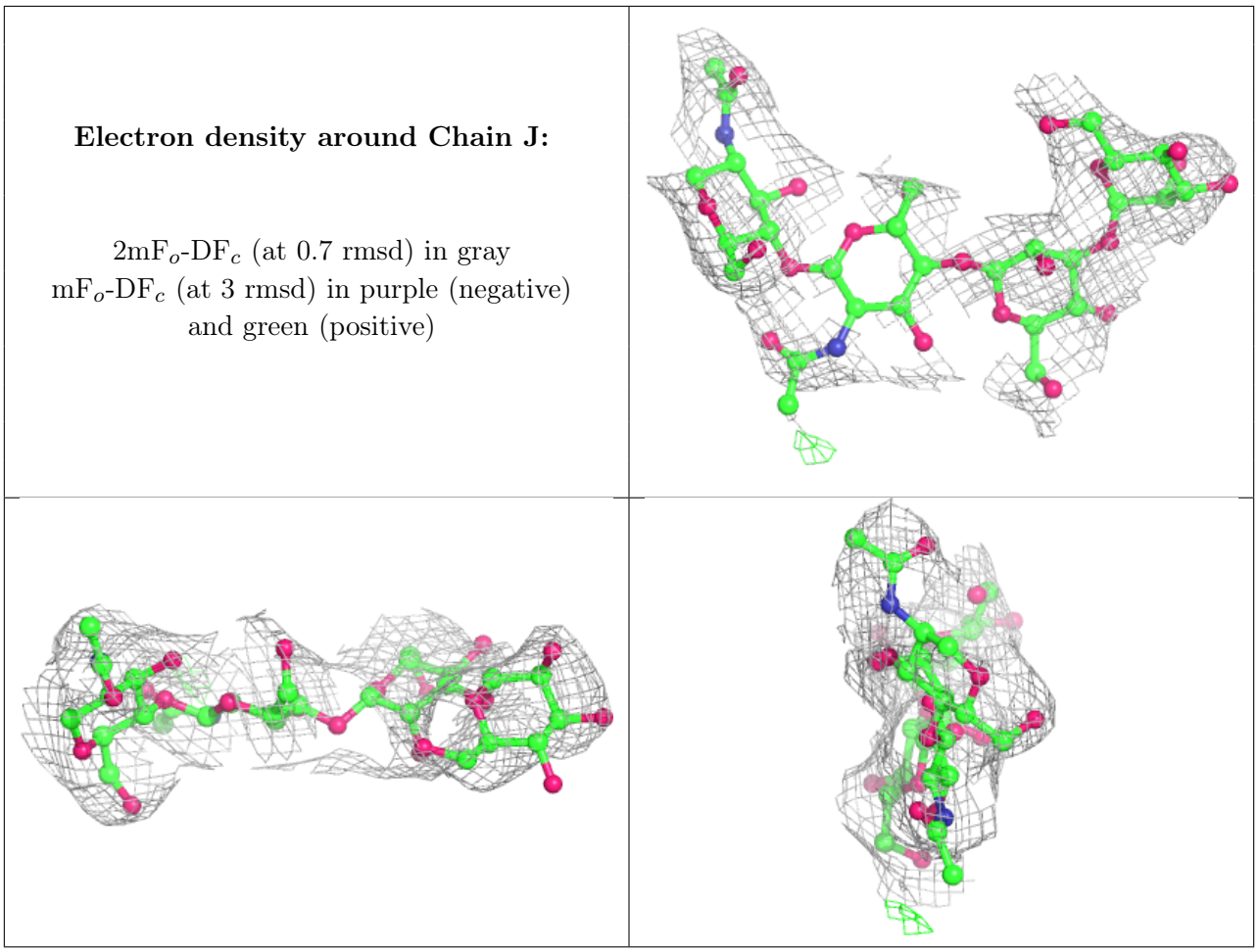
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain J:

$2mF_o$-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
8	NAG	A	1104	14/15	0.72	0.23	148,158,164,171	0
7	UJX	A	1102	26/26	0.74	0.36	122,141,152,153	0
8	NAG	A	1108	14/15	0.74	0.25	148,163,169,171	0
9	PEG	A	1109	7/7	0.76	0.24	84,86,102,104	0
8	NAG	B	1102	14/15	0.77	0.39	154,161,172,175	0
8	NAG	B	1106	14/15	0.81	0.29	109,117,124,129	0
11	GLY	A	1112	5/5	0.81	0.23	82,96,108,109	0
8	NAG	A	1103	14/15	0.82	0.47	120,136,145,147	0
8	NAG	B	1103	14/15	0.82	0.24	147,165,173,177	0
8	NAG	B	1105	14/15	0.82	0.29	121,143,148,153	0
11	GLY	B	1107	5/5	0.85	0.31	111,118,120,121	0

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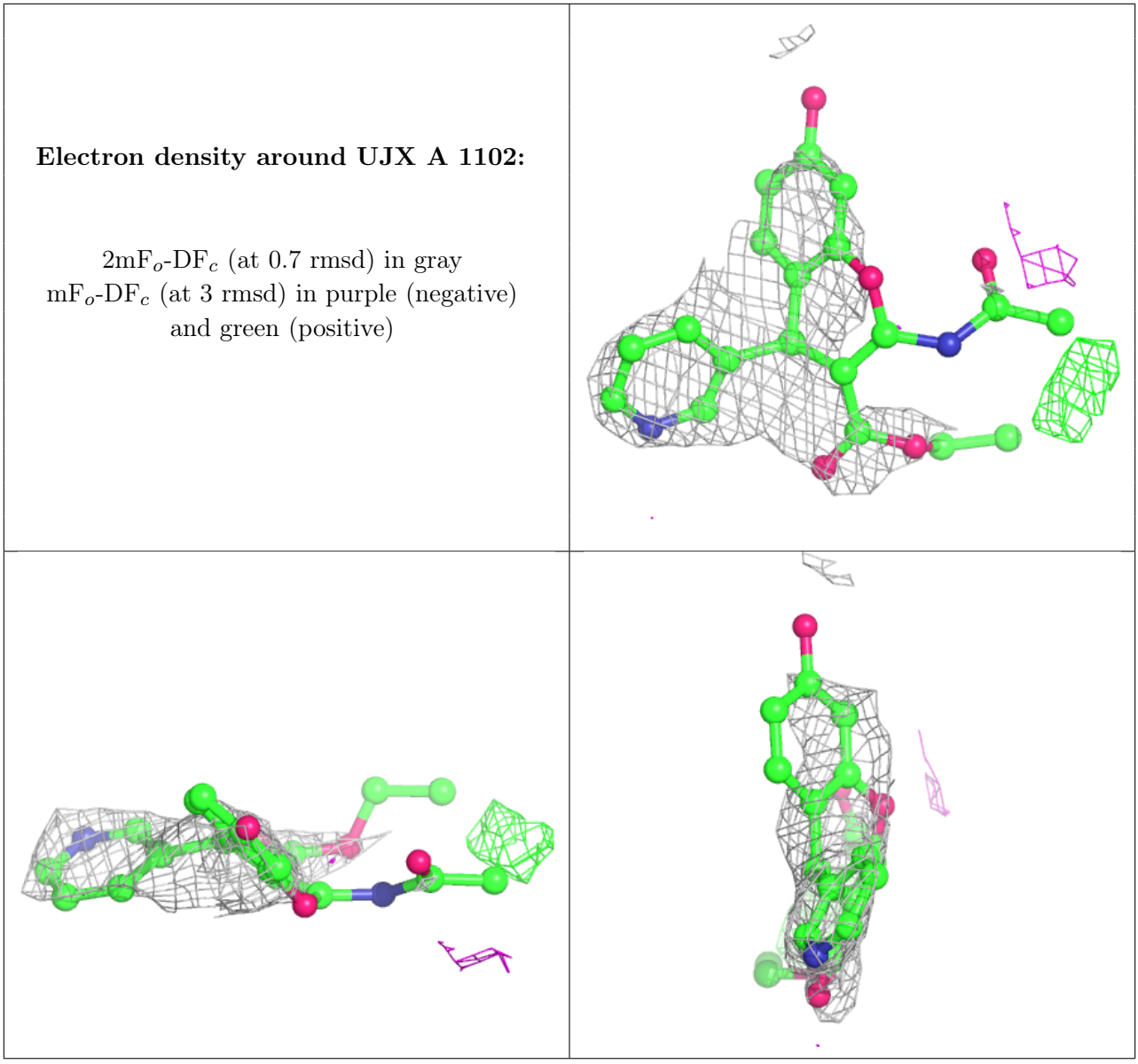
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	A	1106	14/15	0.86	0.15	112,133,140,142	0
8	NAG	A	1105	14/15	0.87	0.14	109,127,137,139	0
8	NAG	A	1107	14/15	0.87	0.36	139,145,150,150	0
10	EDO	A	1110	4/4	0.88	0.36	123,123,124,124	0
8	NAG	B	1104	14/15	0.89	0.25	96,102,109,111	0
11	GLY	A	1111	5/5	0.89	0.16	86,97,105,109	0
10	EDO	B	1108	4/4	0.91	0.20	72,72,78,81	0
11	GLY	B	1109	5/5	0.93	0.48	90,92,93,94	0
6	ZN	B	1101	1/1	0.94	0.20	79,79,79,79	0
6	ZN	A	1101	1/1	0.96	0.25	58,58,58,58	0

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

Electron density around UJX A 1102:

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



6.5 Other polymers

There are no such residues in this entry.