wwPDB X-ray Structure Validation Summary Report (i)

Nov 29, 2022 – 12:16 am GMT

PDB ID	:	5M8P
Title	:	Crystal structure of human tyrosinase related protein 1 in complex with tyrosine
Authors	:	Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on	:	2016-10-29
Resolution	:	2.80 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:

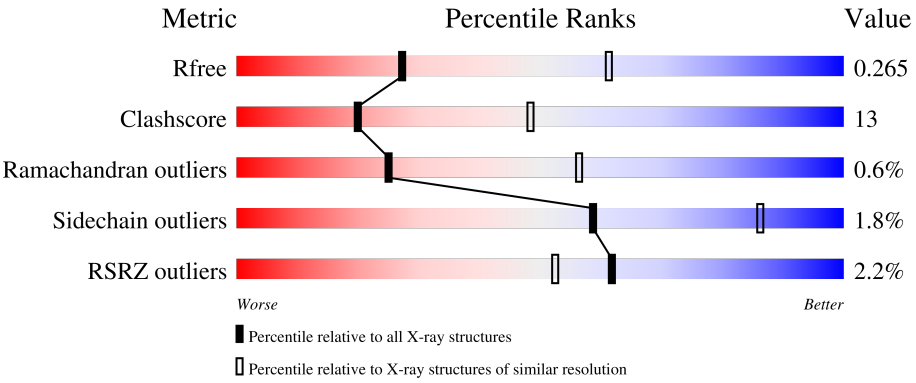
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	446	82% 17%
1	B	446	79% 20%
1	C	446	4% 70% 28%
1	D	446	3% 73% 27%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	J	3	67% 33%
2	O	3	67% 33%
2	U	3	33% 33% 33%
3	F	2	100%
3	K	2	50% 50%
3	Q	2	50% 50%
4	G	2	100%
4	H	2	100%
4	I	2	50% 50%
4	N	2	50% 50%
4	P	2	50% 50%
4	R	2	50% 50%
4	W	2	50% 50%
4	Y	2	50% 50%
5	L	3	100%
6	M	5	80% 20%
6	X	5	20% 40% 40%
7	S	2	50% 50%
8	T	3	67% 33%
9	V	4	25% 75%

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
3	NAG	Q	1	-	-	X	-
4	NAG	H	2	-	-	-	X
4	NAG	Y	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	T	2	-	-	-	X
8	MAN	T	3	-	-	-	X

2 Entry composition (i)

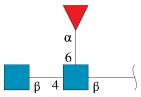
There are 14 unique types of molecules in this entry. The entry contains 15116 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	B	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	C	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	D	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			

- Molecule 2 is an oligosaccharide called 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
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	O	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	U	3	Total	C	N	O	0	0	0
			38	22	2	14			

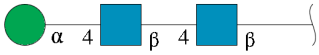
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 24 14 1 9	0	0	0
3	K	2	Total C N O 24 14 1 9	0	0	0
3	Q	2	Total C N O 24 14 1 9	0	0	0

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

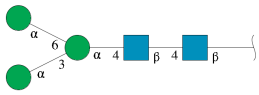
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 28 16 2 10	0	0	0
4	H	2	Total C N O 28 16 2 10	0	0	0
4	I	2	Total C N O 28 16 2 10	0	0	0
4	N	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	R	2	Total C N O 28 16 2 10	0	0	0
4	W	2	Total C N O 28 16 2 10	0	0	0
4	Y	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-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	L	3	Total C N O 39 22 2 15	0	0	0

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

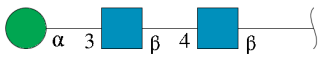


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

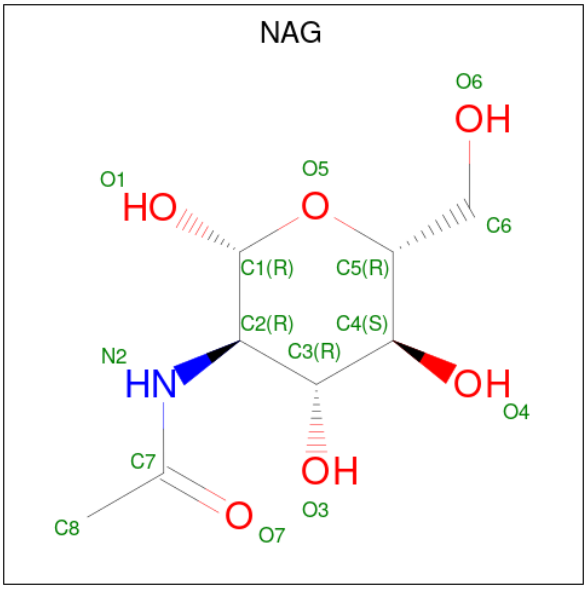


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(5-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

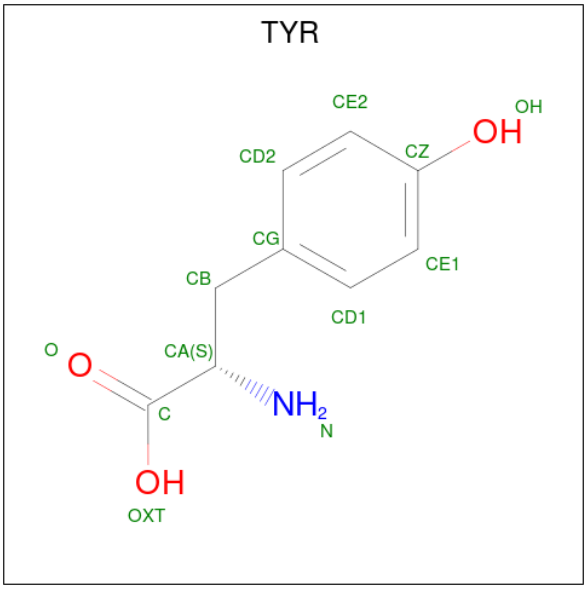
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	V	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			13	9	1	3		

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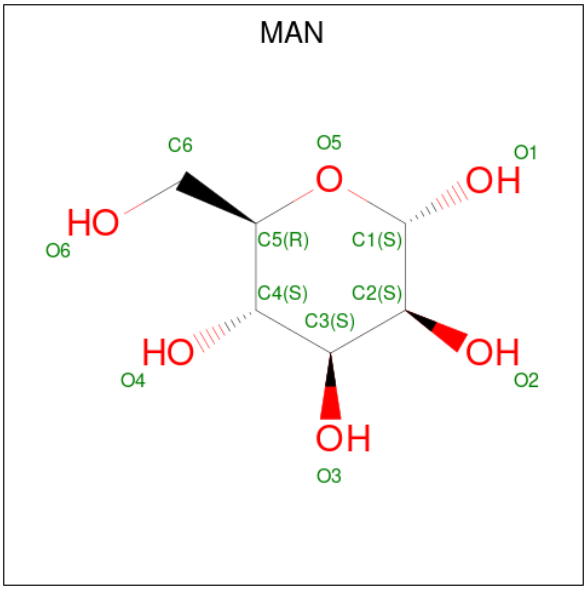
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O 13 9 1 3	0	0
11	C	1	Total C N O 13 9 1 3	0	0
11	D	1	Total C N O 13 9 1 3	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total Zn 3 3	0	0
12	B	2	Total Zn 2 2	0	0
12	C	2	Total Zn 2 2	0	0
12	D	2	Total Zn 2 2	0	0

- Molecule 13 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 11 6 5	0	0

- Molecule 14 is water.

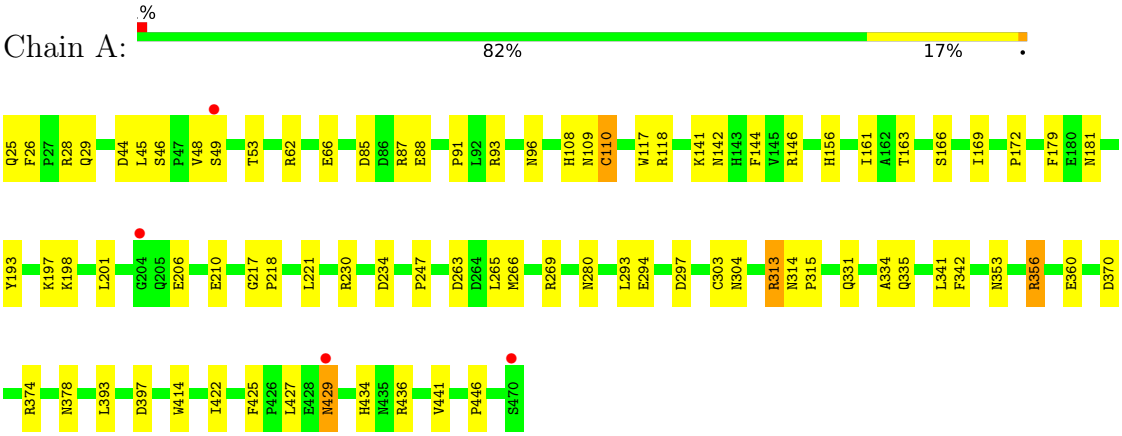
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	21	Total O 21 21	0	0
14	B	24	Total O 24 24	0	0
14	C	10	Total O 10 10	0	0
14	D	10	Total O 10 10	0	0

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.

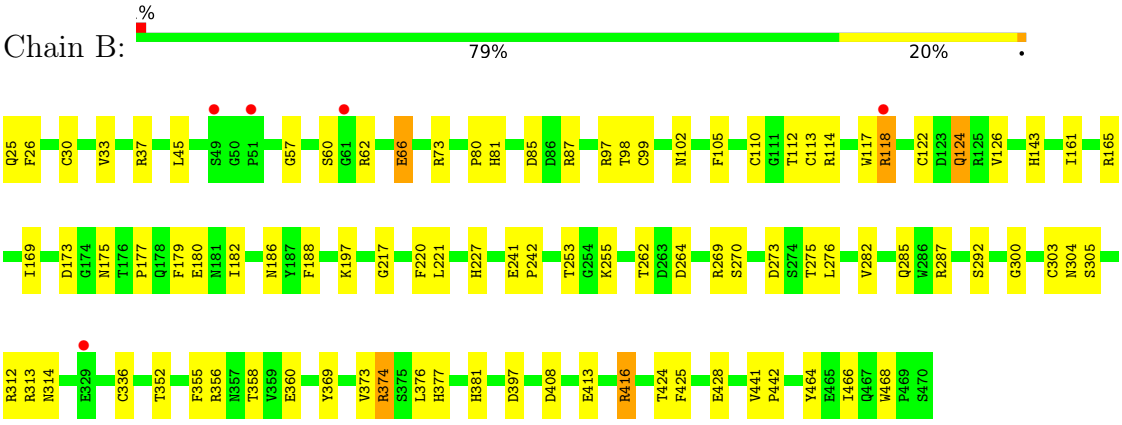
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain A:



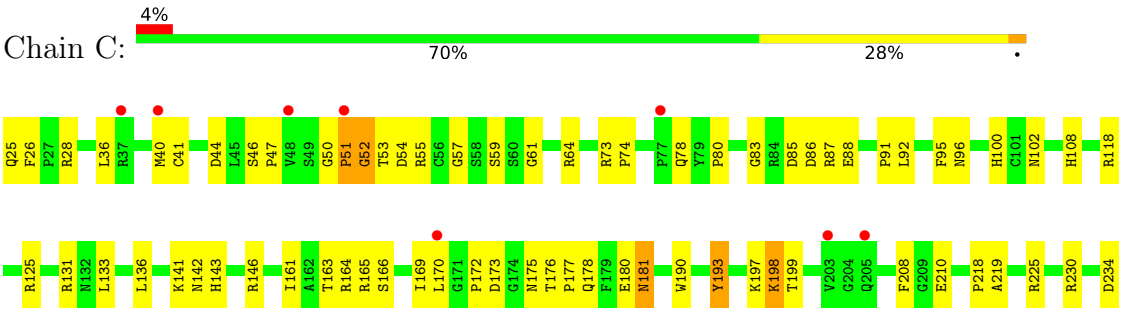
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

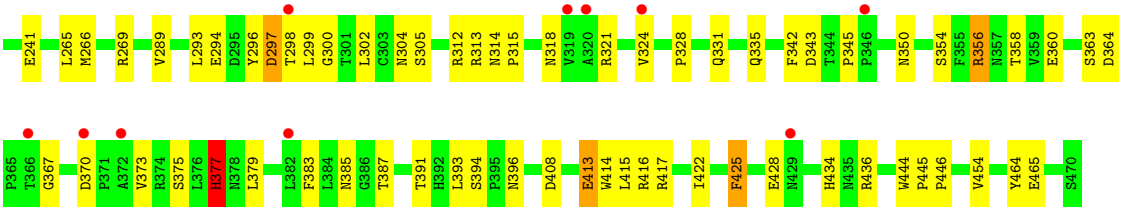
Chain B:



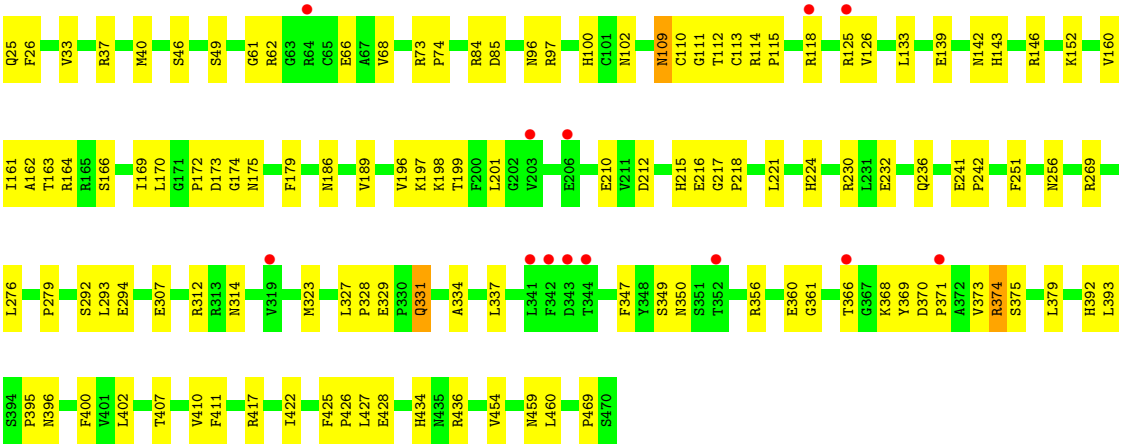
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain C:





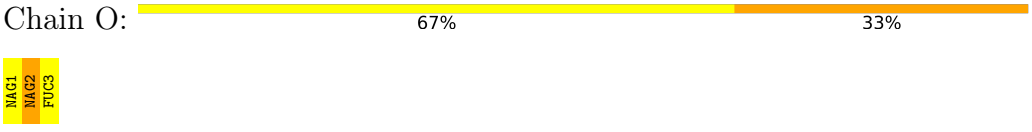
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



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

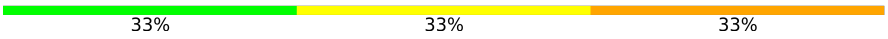
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

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



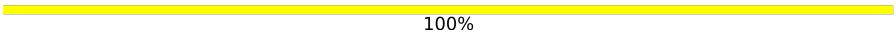
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain F:



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

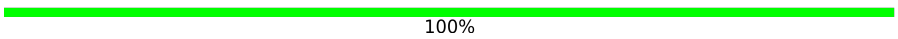
Chain K:

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

Chain Q:

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

Chain G:



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

Chain H:

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

Chain I:

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

Chain N:

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

Chain P:

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

Chain R:

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

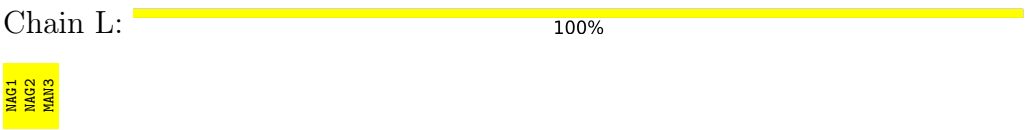
Chain W:

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

Chain Y:

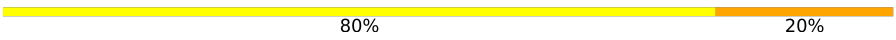
• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



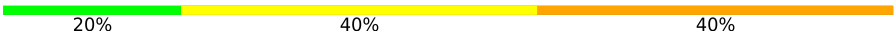
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain X:

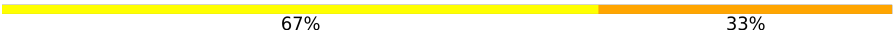


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(5-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.52Å 140.32Å 191.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.80 47.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.92-2.80) 90.9 (47.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.205 , 0.262 0.209 , 0.265	Depositor DCC
R_{free} test set	2997 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15116	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, ZN, MAN, NAG

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	0.70	3/3667 (0.1%)	0.70	3/4998 (0.1%)
1	B	0.64	3/3667 (0.1%)	0.64	1/4998 (0.0%)
1	C	0.78	10/3667 (0.3%)	0.77	8/4998 (0.2%)
1	D	0.61	1/3667 (0.0%)	0.62	0/4998
All	All	0.68	17/14668 (0.1%)	0.69	12/19992 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	HIS	CB-CG	-16.28	1.20	1.50
1	C	377	HIS	C-O	15.03	1.51	1.23
1	C	377	HIS	C-N	-11.09	1.08	1.34
1	D	46	SER	C-N	-10.49	1.14	1.34
1	C	356	ARG	CZ-NH2	-7.54	1.23	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	377	HIS	CA-C-N	13.11	146.05	117.20
1	C	377	HIS	O-C-N	-11.00	105.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	297	ASP	CB-CG-OD1	-9.80	109.48	118.30
1	C	297	ASP	CB-CG-OD2	8.29	125.76	118.30
1	C	377	HIS	CA-C-O	-8.19	102.91	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	377	HIS	Peptide,Mainchain
1	D	109	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3560	0	3325	59	0
1	B	3560	0	3325	72	0
1	C	3560	0	3326	128	1
1	D	3560	0	3325	95	0
2	E	38	0	34	2	0
2	J	38	0	34	1	0
2	O	38	0	34	2	0
2	U	38	0	34	1	0
3	F	24	0	22	0	0
3	K	24	0	22	0	0
3	Q	24	0	22	7	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0
4	I	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	3	0
4	R	28	0	25	0	0
4	W	28	0	24	0	0
4	Y	28	0	25	1	0
5	L	39	0	34	0	0
6	M	61	0	52	1	0
6	X	61	0	52	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	28	0	25	1	0
8	T	39	0	34	1	0
9	V	49	0	42	2	0
10	A	14	0	12	0	0
11	A	13	0	8	2	0
11	B	13	0	8	2	0
11	C	13	0	8	3	0
11	D	13	0	8	2	0
12	A	3	0	0	0	0
12	B	2	0	0	0	0
12	C	2	0	0	0	0
12	D	2	0	0	0	0
13	C	11	0	10	1	0
14	A	21	0	0	2	0
14	B	24	0	0	4	0
14	C	10	0	0	1	0
14	D	10	0	0	4	0
All	All	15116	0	13995	366	1

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 13.

The worst 5 of 366 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:C:181:ASN:HD21	3:Q:1:NAG:C1	1.17	1.50
1:C:181:ASN:ND2	3:Q:1:NAG:C1	1.85	1.40
1:D:118:ARG:HH11	1:D:242:PRO:CB	1.44	1.30
1:D:118:ARG:NH1	1:D:242:PRO:CB	1.95	1.29
1:C:198:LYS:HD2	1:C:297:ASP:OD1	1.30	1.27

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:OG	6:X:5:MAN:O3[1_655]	2.13	0.07

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	444/446 (100%)	413 (93%)	30 (7%)	1 (0%)	47 78
1	B	444/446 (100%)	411 (93%)	31 (7%)	2 (0%)	29 61
1	C	444/446 (100%)	413 (93%)	26 (6%)	5 (1%)	14 41
1	D	444/446 (100%)	407 (92%)	34 (8%)	3 (1%)	22 53
All	All	1776/1784 (100%)	1644 (93%)	121 (7%)	11 (1%)	25 56

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	GLY
1	C	51	PRO
1	C	377	HIS
1	C	172	PRO
1	D	172	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	395/395 (100%)	390 (99%)	5 (1%)	69 91
1	B	395/395 (100%)	385 (98%)	10 (2%)	47 80
1	C	395/395 (100%)	388 (98%)	7 (2%)	59 86
1	D	395/395 (100%)	389 (98%)	6 (2%)	65 89
All	All	1580/1580 (100%)	1552 (98%)	28 (2%)	59 86

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	425	PHE
1	D	425	PHE
1	C	193	TYR
1	D	292	SER
1	C	181	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	175	ASN
1	D	353	ASN
1	B	124	GLN
1	B	175	ASN
1	C	181	ASN

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)

56 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	E	1	1,2	14,14,15	1.06	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	E	2	2	14,14,15	0.66	1 (7%)	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FUC	E	3	2	10,10,11	0.69	0	14,14,16	2.66	6 (42%)
3	NAG	F	1	1,3	14,14,15	1.42	2 (14%)	17,19,21	1.33	2 (11%)
3	FUC	F	2	3	10,10,11	1.19	2 (20%)	14,14,16	1.25	2 (14%)
4	NAG	G	1	1,4	14,14,15	0.57	0	17,19,21	0.51	0
4	NAG	G	2	4	14,14,15	0.47	0	17,19,21	0.44	0
4	NAG	H	1	1,4	14,14,15	0.81	1 (7%)	17,19,21	0.62	0
4	NAG	H	2	4	14,14,15	1.52	1 (7%)	17,19,21	1.09	2 (11%)
4	NAG	I	1	1,4	14,14,15	0.75	1 (7%)	17,19,21	0.51	0
4	NAG	I	2	4	14,14,15	0.22	0	17,19,21	0.57	0
2	NAG	J	1	1,2	14,14,15	0.92	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	J	2	2	14,14,15	0.33	0	17,19,21	0.61	0
2	FUC	J	3	2	10,10,11	1.20	1 (10%)	14,14,16	1.00	0
3	NAG	K	1	1,3	14,14,15	0.32	0	17,19,21	0.77	0
3	FUC	K	2	3	10,10,11	1.54	2 (20%)	14,14,16	1.61	3 (21%)
5	NAG	L	1	1,5	14,14,15	2.16	2 (14%)	17,19,21	1.02	2 (11%)
5	NAG	L	2	5	14,14,15	1.76	1 (7%)	17,19,21	1.07	2 (11%)
5	MAN	L	3	5	11,11,12	1.13	1 (9%)	15,15,17	0.95	1 (6%)
6	NAG	M	1	1,6	14,14,15	0.82	1 (7%)	17,19,21	0.78	0
6	NAG	M	2	6	14,14,15	0.71	0	17,19,21	0.64	0
6	MAN	M	3	6	11,11,12	1.97	2 (18%)	15,15,17	2.00	4 (26%)
6	MAN	M	4	6	11,11,12	1.08	1 (9%)	15,15,17	1.20	0
6	MAN	M	5	6	11,11,12	1.47	1 (9%)	15,15,17	2.43	3 (20%)
4	NAG	N	1	1,4	14,14,15	0.51	0	17,19,21	0.53	0
4	NAG	N	2	4	14,14,15	0.18	0	17,19,21	0.92	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.26	0	17,19,21	0.85	0
2	NAG	O	2	2	14,14,15	0.33	0	17,19,21	1.42	2 (11%)
2	FUC	O	3	2	10,10,11	1.00	1 (10%)	14,14,16	1.80	4 (28%)
4	NAG	P	1	1,4	14,14,15	0.68	1 (7%)	17,19,21	0.88	0
4	NAG	P	2	4	14,14,15	1.23	2 (14%)	17,19,21	2.19	3 (17%)
3	NAG	Q	1	3	14,14,15	0.42	0	17,19,21	1.63	2 (11%)
3	FUC	Q	2	3	10,10,11	1.79	1 (10%)	14,14,16	1.55	4 (28%)
4	NAG	R	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	0.65	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.60	0
7	NAG	S	1	7	14,14,15	0.26	0	17,19,21	1.21	3 (17%)
7	NAG	S	2	7	14,14,15	0.44	0	17,19,21	0.51	0
8	NAG	T	1	1,8	14,14,15	2.40	1 (7%)	17,19,21	2.63	1 (5%)
8	NAG	T	2	8	14,14,15	0.79	1 (7%)	17,19,21	1.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	T	3	8	11,11,12	1.34	2 (18%)	15,15,17	2.27	3 (20%)
2	NAG	U	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	0.77	0
2	NAG	U	2	2	14,14,15	0.42	0	17,19,21	0.37	0
2	FUC	U	3	2	10,10,11	1.01	0	14,14,16	2.29	8 (57%)
9	NAG	V	1	1,9	14,14,15	1.07	2 (14%)	17,19,21	0.87	0
9	NAG	V	2	9	14,14,15	1.29	1 (7%)	17,19,21	0.98	1 (5%)
9	MAN	V	3	9	11,11,12	1.55	1 (9%)	15,15,17	1.08	1 (6%)
9	FUC	V	4	9	10,10,11	0.57	0	14,14,16	1.42	2 (14%)
4	NAG	W	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	0.75	1 (5%)
4	NAG	W	2	4	14,14,15	0.38	0	17,19,21	0.58	0
6	NAG	X	1	1,6	14,14,15	1.30	1 (7%)	17,19,21	1.27	1 (5%)
6	NAG	X	2	6	14,14,15	0.48	0	17,19,21	0.66	0
6	MAN	X	3	6	11,11,12	1.40	2 (18%)	15,15,17	1.63	3 (20%)
6	MAN	X	4	6	11,11,12	1.27	2 (18%)	15,15,17	1.04	0
6	MAN	X	5	6	11,11,12	1.04	1 (9%)	15,15,17	1.34	3 (20%)
4	NAG	Y	1	1,4	14,14,15	1.45	1 (7%)	17,19,21	1.59	3 (17%)
4	NAG	Y	2	4	14,14,15	0.35	0	17,19,21	0.70	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	J	3	2	-	-	0/1/1/1
3	NAG	K	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	MAN	L	3	5	-	2/2/19/22	1/1/1/1
6	NAG	M	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	MAN	M	3	6	-	2/2/19/22	1/1/1/1
6	MAN	M	4	6	-	0/2/19/22	1/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	6/6/23/26	0/1/1/1
2	FUC	O	3	2	-	-	0/1/1/1
4	NAG	P	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	5/6/23/26	0/1/1/1
3	FUC	Q	2	3	-	-	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
7	NAG	S	1	7	-	3/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	MAN	T	3	8	-	0/2/19/22	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	FUC	U	3	2	-	-	0/1/1/1
9	NAG	V	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	V	2	9	-	3/6/23/26	0/1/1/1
9	MAN	V	3	9	-	2/2/19/22	1/1/1/1
9	FUC	V	4	9	-	-	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	MAN	X	3	6	-	2/2/19/22	1/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	MAN	X	5	6	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	4/6/23/26	0/1/1/1

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	1	NAG	O5-C1	8.82	1.57	1.43
5	L	1	NAG	O5-C1	-7.70	1.31	1.43
5	L	2	NAG	O5-C1	-6.49	1.33	1.43
6	M	3	MAN	C2-C3	-5.51	1.44	1.52
4	H	2	NAG	C1-C2	5.12	1.60	1.52

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	1	NAG	C1-O5-C5	10.50	126.42	112.19
4	P	2	NAG	C2-N2-C7	7.40	133.44	122.90
6	M	5	MAN	C1-O5-C5	7.34	122.13	112.19
2	E	3	FUC	O5-C5-C4	6.13	120.51	109.52
8	T	2	NAG	C1-O5-C5	6.11	120.47	112.19

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	2	NAG	C3-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
2	E	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	MAN	C1-C2-C3-C4-C5-O5
6	M	3	MAN	C1-C2-C3-C4-C5-O5

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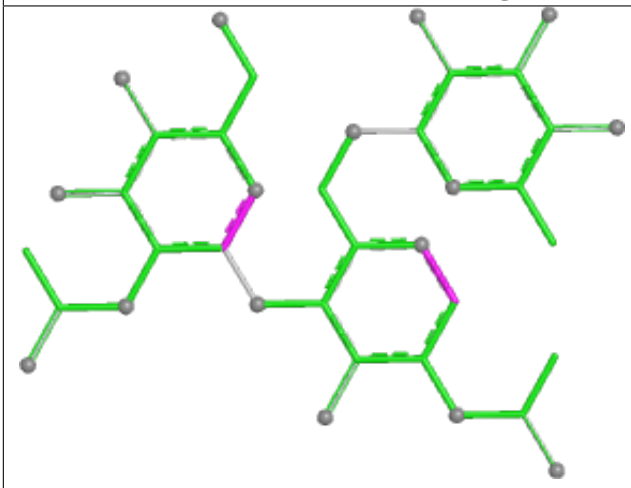
Mol	Chain	Res	Type	Atoms
6	X	3	MAN	C1-C2-C3-C4-C5-O5
9	V	3	MAN	C1-C2-C3-C4-C5-O5
6	M	4	MAN	C1-C2-C3-C4-C5-O5

21 monomers are involved in 27 short contacts:

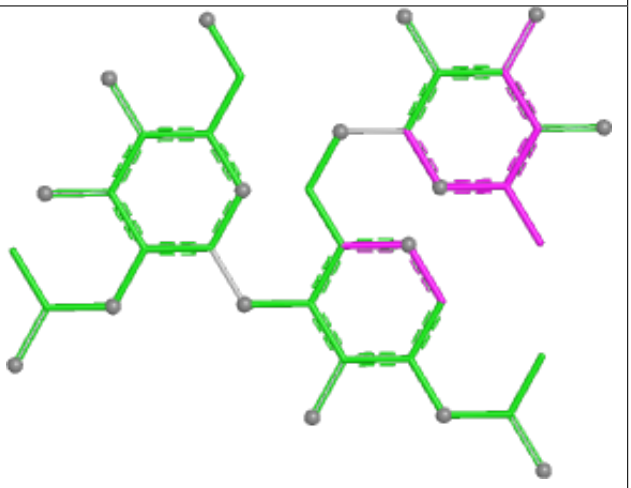
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	1	0
3	Q	1	NAG	7	0
2	E	2	NAG	1	0
6	X	5	MAN	0	1
2	J	2	NAG	1	0
2	E	1	NAG	2	0
6	X	1	NAG	3	0
7	S	1	NAG	1	0
9	V	1	NAG	1	0
9	V	3	MAN	1	0
9	V	4	FUC	1	0
4	P	2	NAG	3	0
2	O	2	NAG	2	0
6	M	3	MAN	1	0
2	J	1	NAG	1	0
4	H	1	NAG	1	0
4	H	2	NAG	1	0
2	U	1	NAG	1	0
8	T	1	NAG	1	0
2	O	1	NAG	1	0
6	M	2	NAG	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.

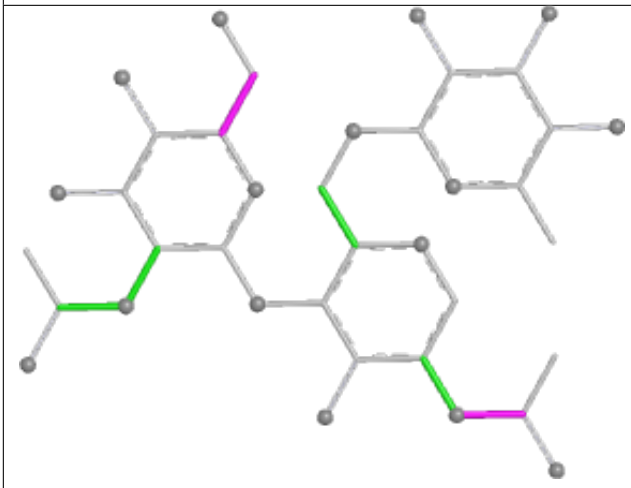
Oligosaccharide Chain E



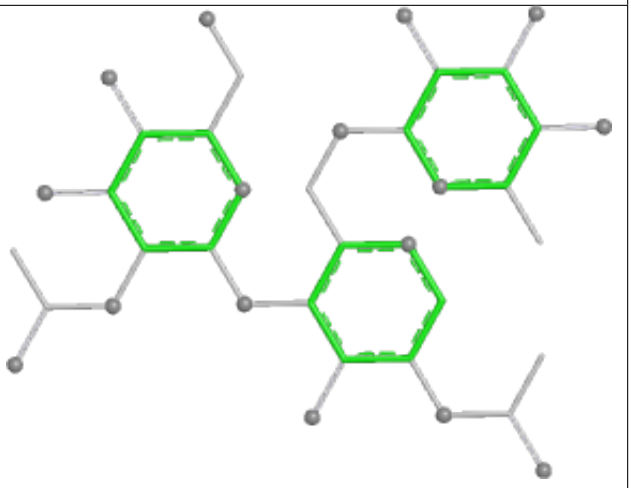
Bond lengths



Bond angles

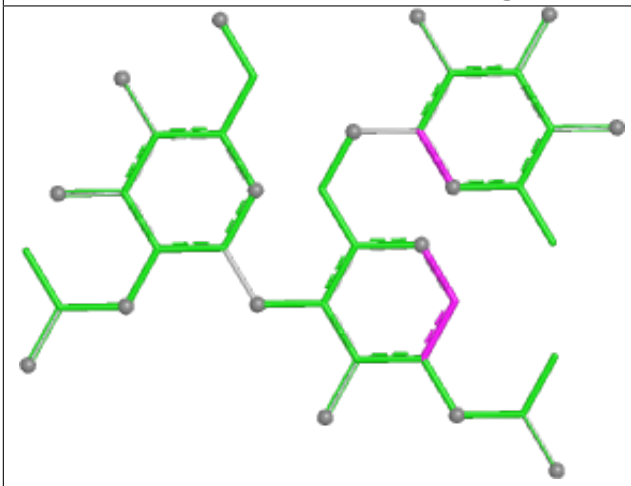


Torsions

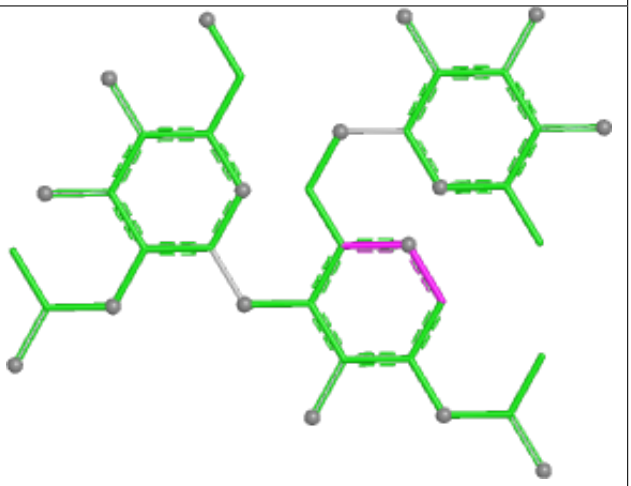


Rings

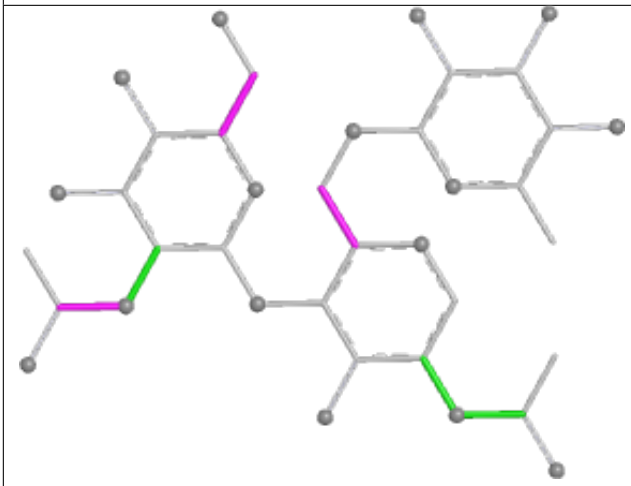
Oligosaccharide Chain J



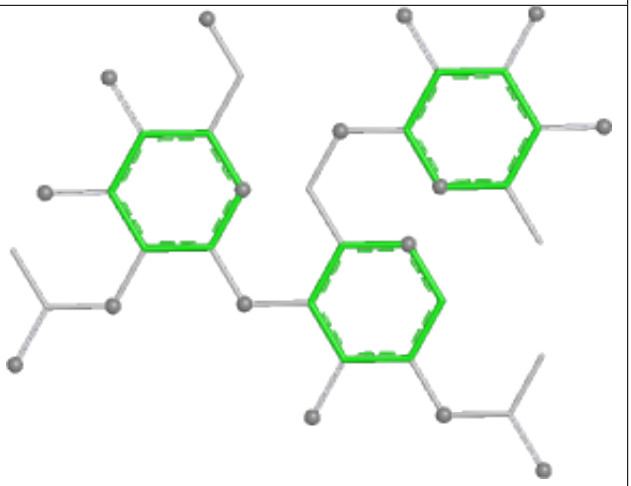
Bond lengths



Bond angles

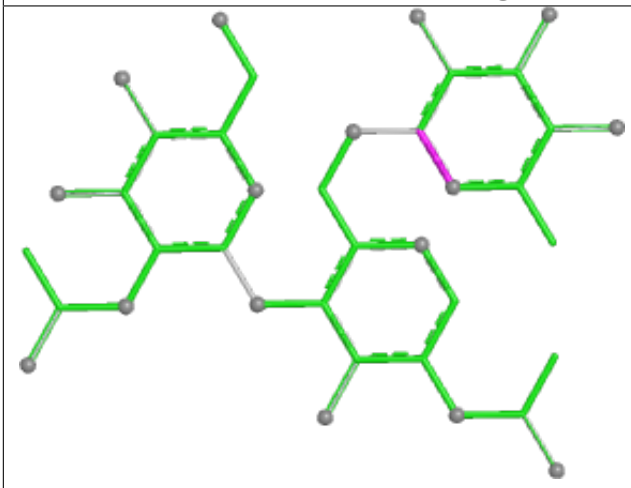


Torsions

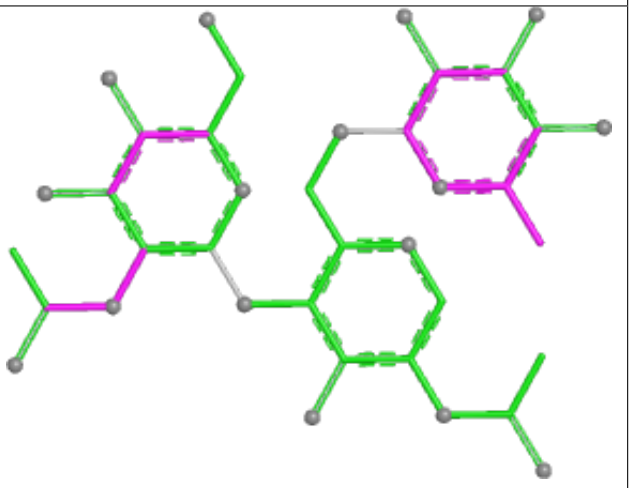


Rings

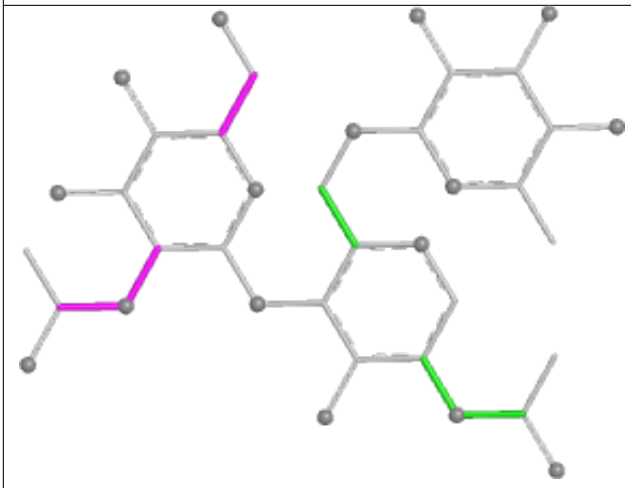
Oligosaccharide Chain O



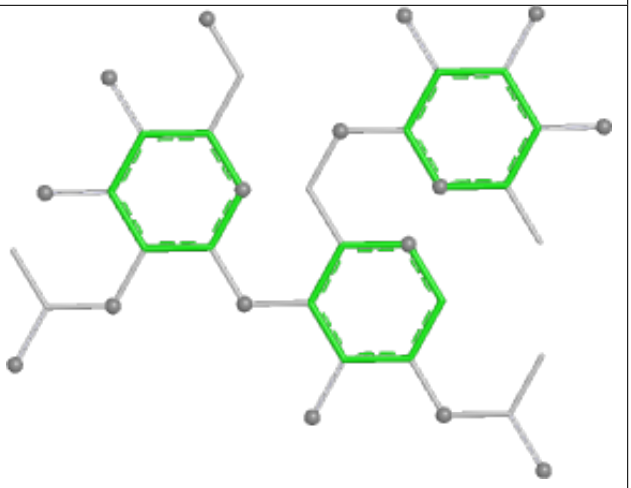
Bond lengths



Bond angles

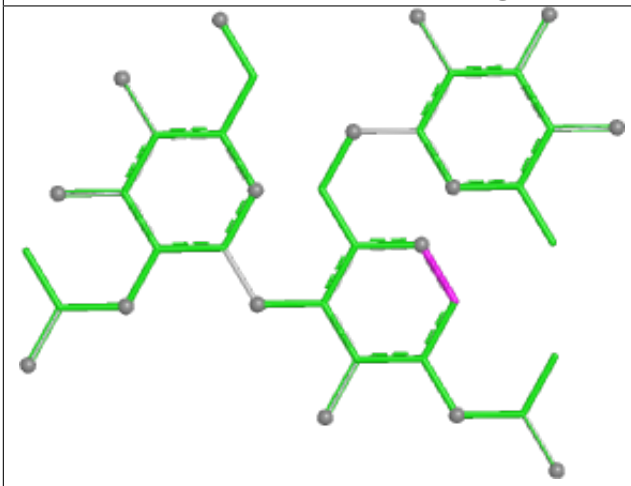


Torsions

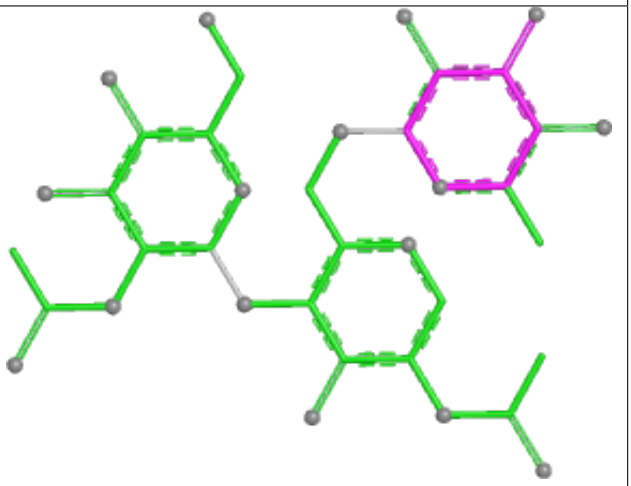


Rings

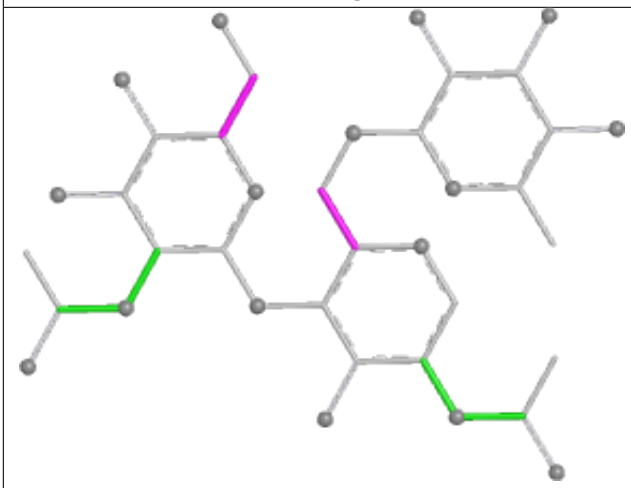
Oligosaccharide Chain U



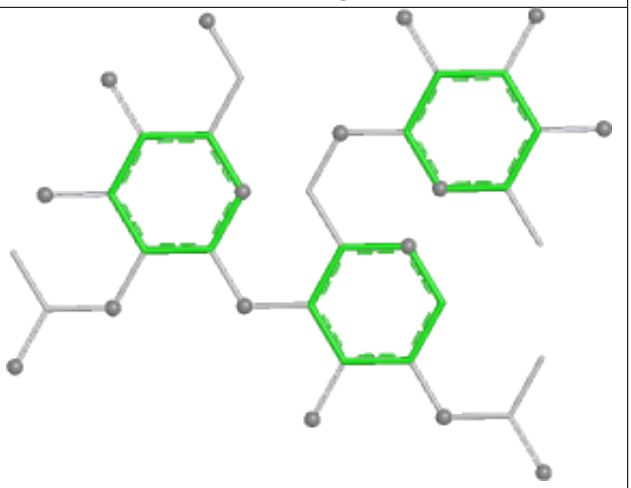
Bond lengths



Bond angles

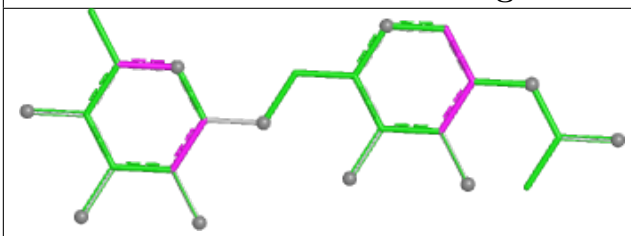


Torsions

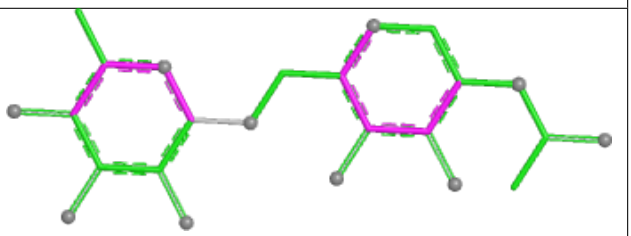


Rings

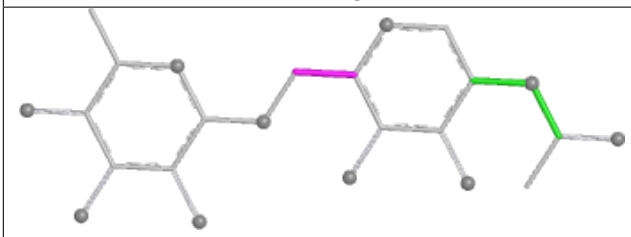
Oligosaccharide Chain F



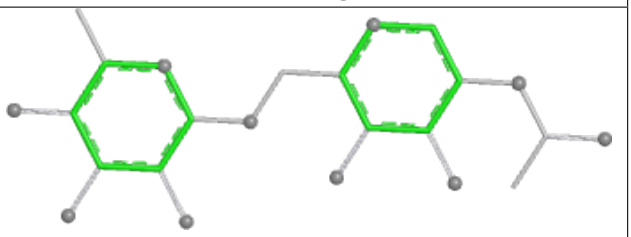
Bond lengths



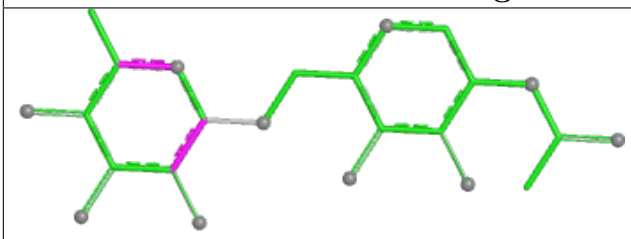
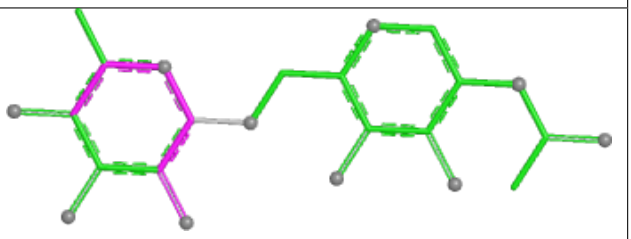
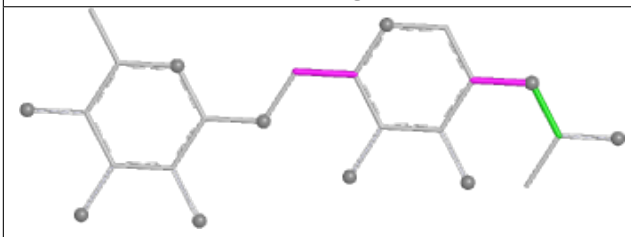
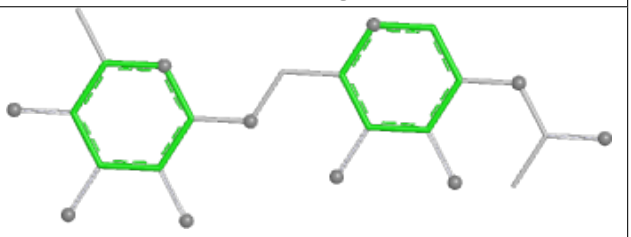
Bond angles

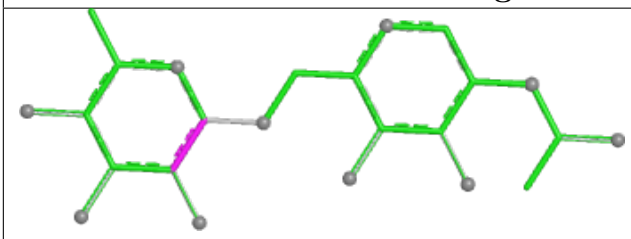
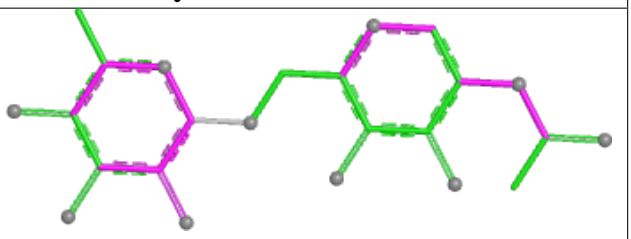
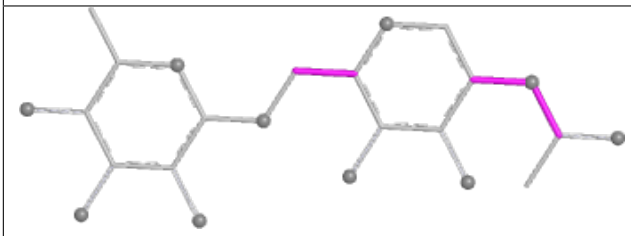
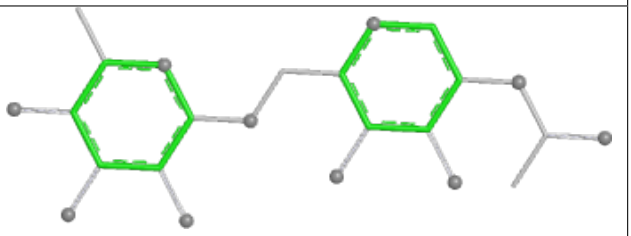


Torsions

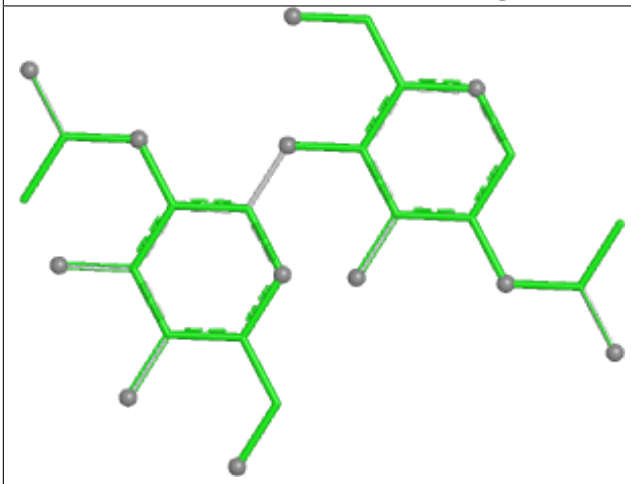


Rings

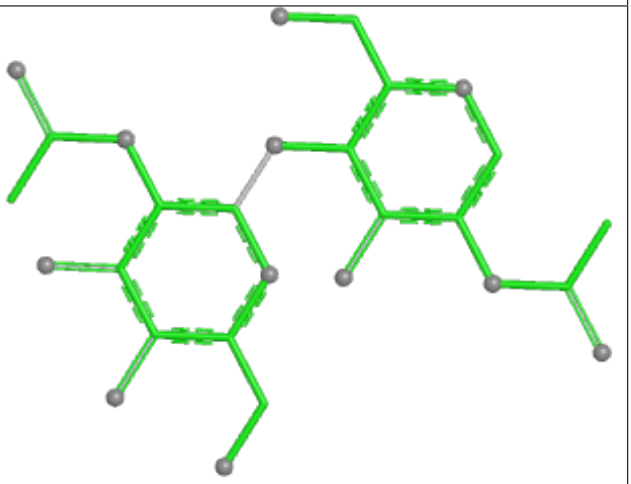
Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

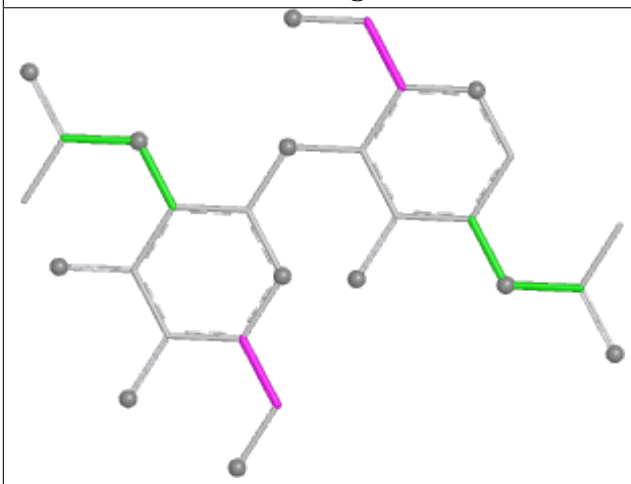
Oligosaccharide Chain G



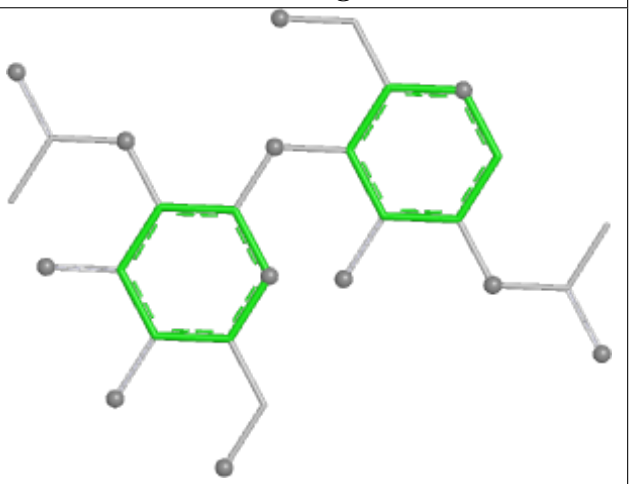
Bond lengths



Bond angles

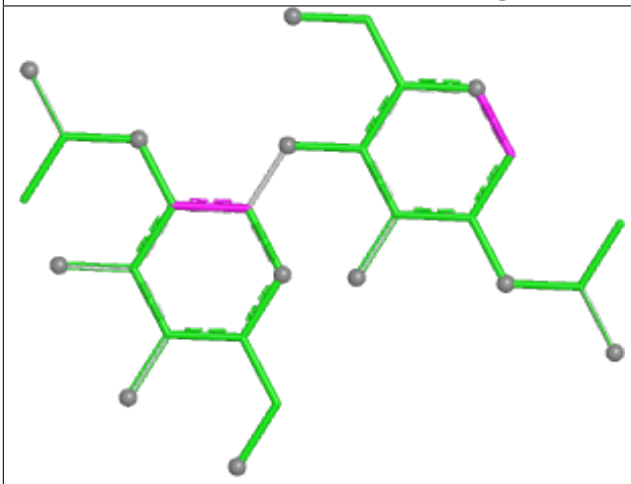


Torsions

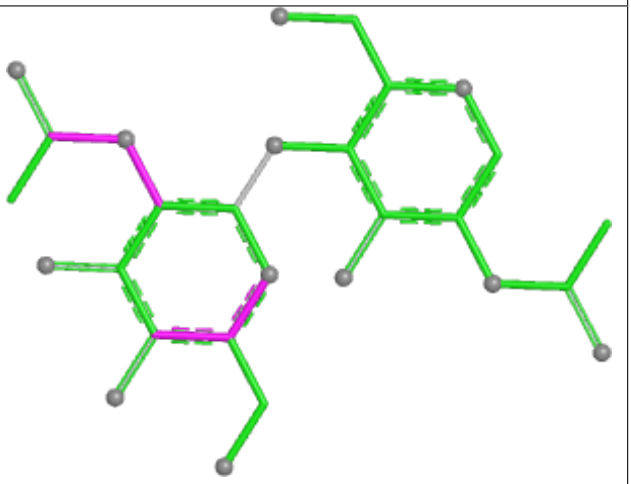


Rings

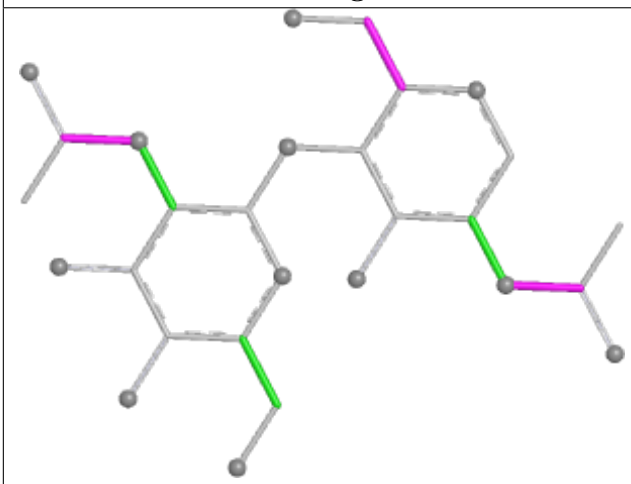
Oligosaccharide Chain H



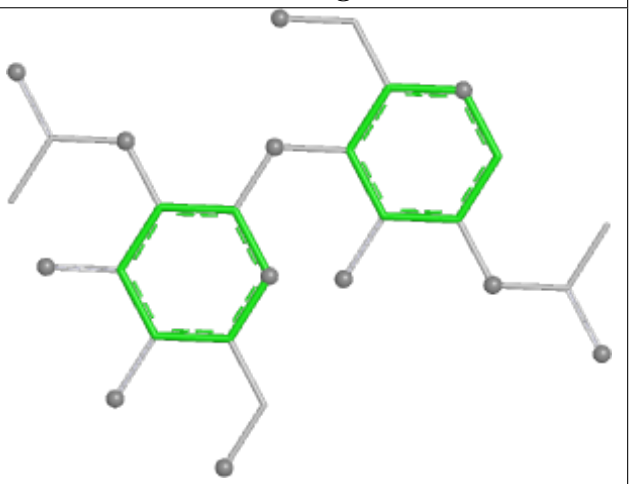
Bond lengths



Bond angles

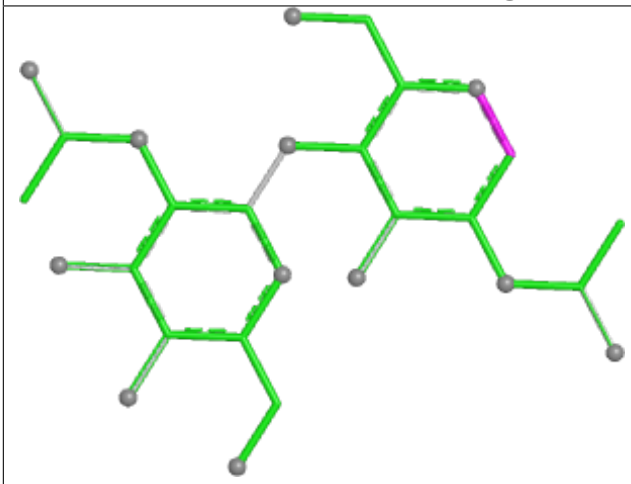


Torsions

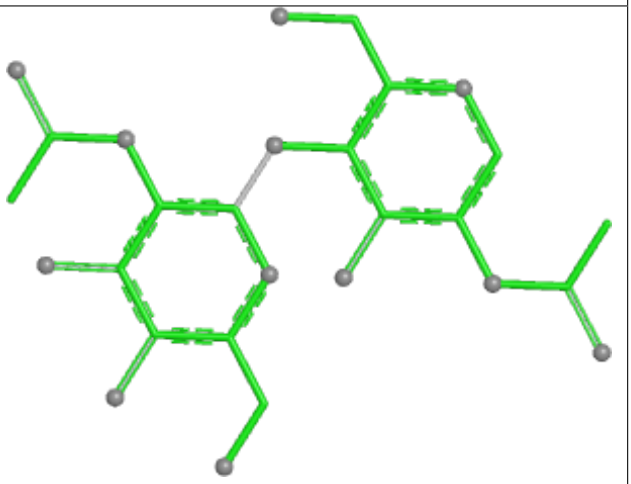


Rings

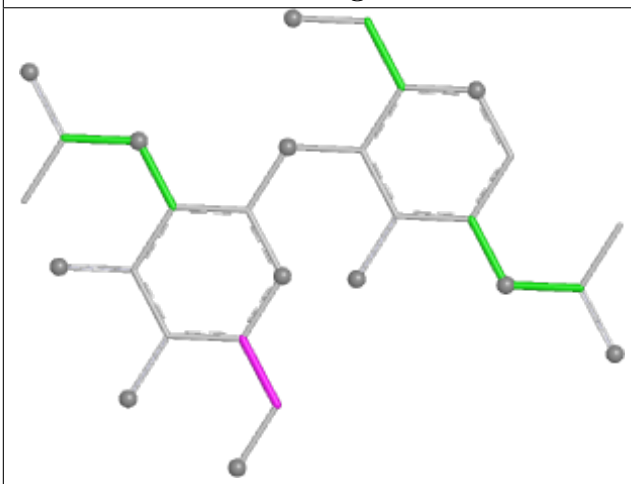
Oligosaccharide Chain I



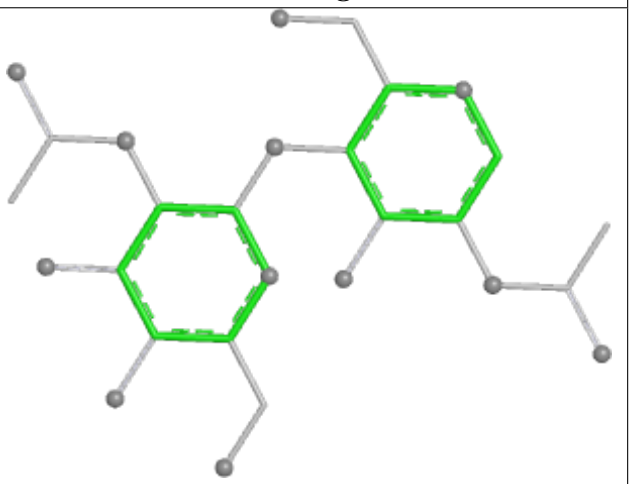
Bond lengths



Bond angles

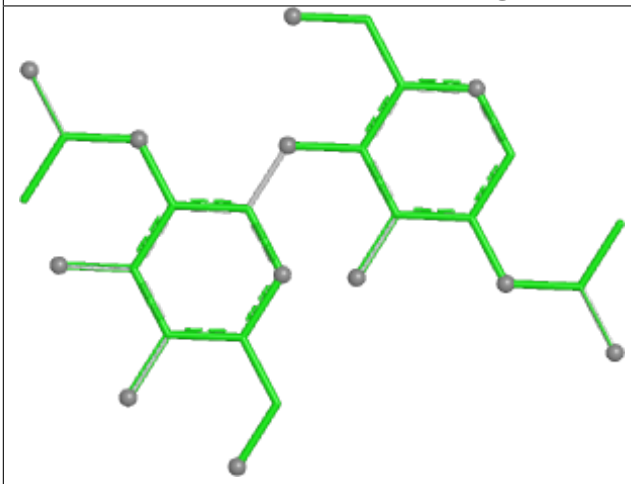


Torsions

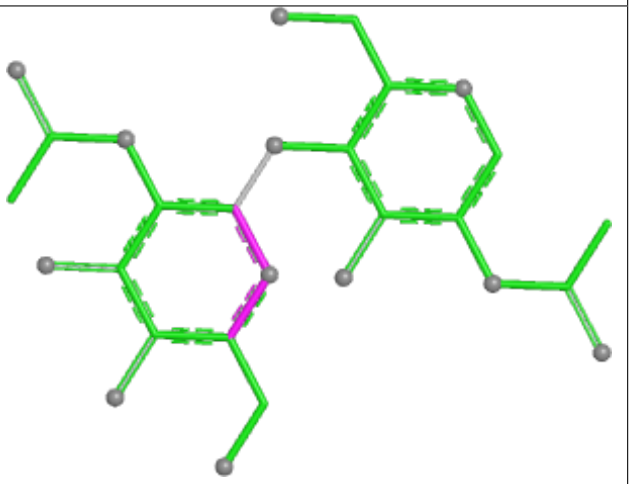


Rings

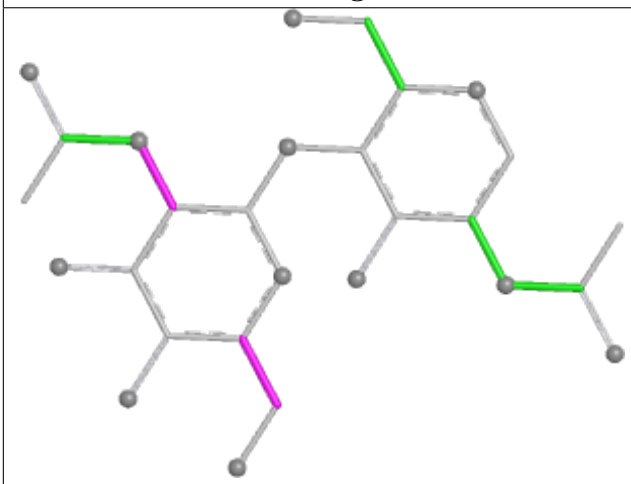
Oligosaccharide Chain N



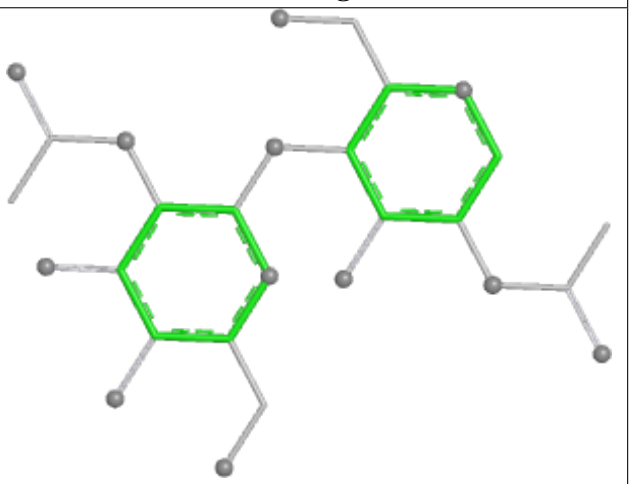
Bond lengths



Bond angles

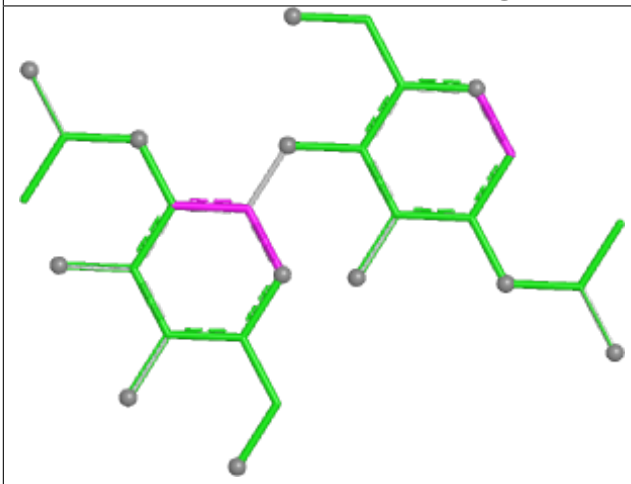


Torsions

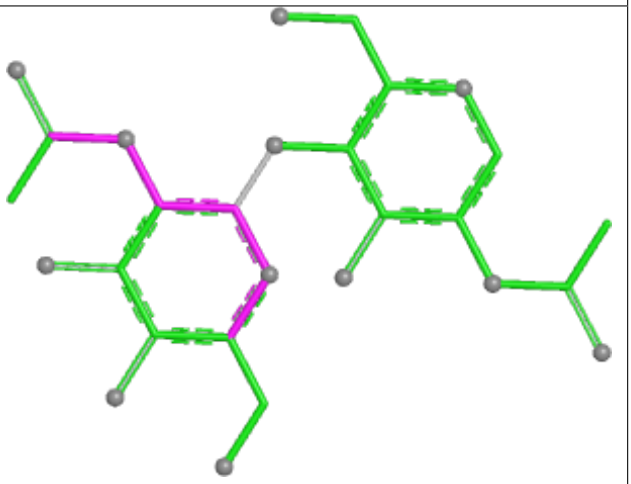


Rings

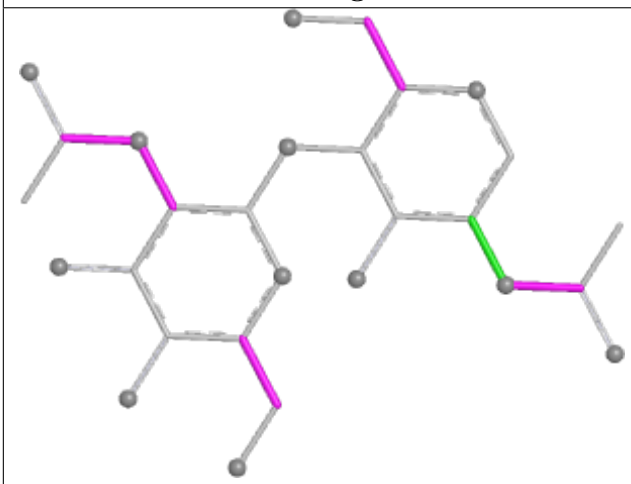
Oligosaccharide Chain P



Bond lengths



Bond angles



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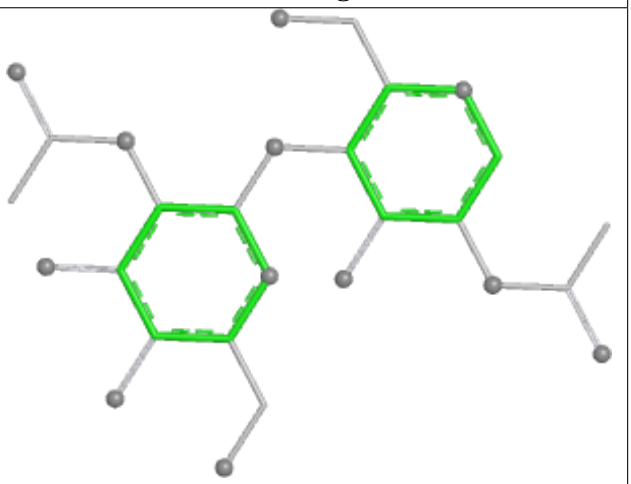
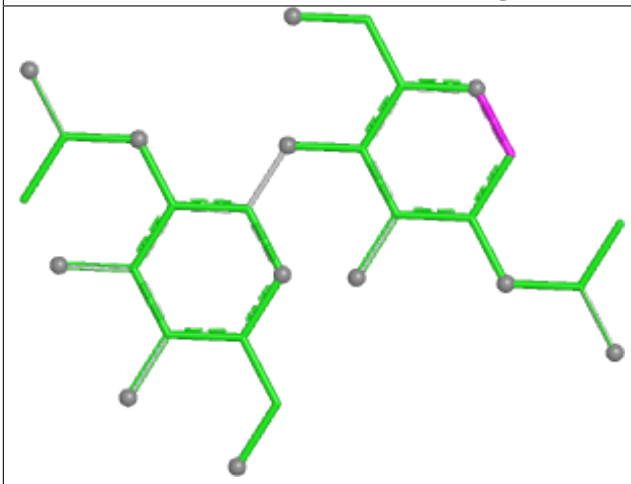
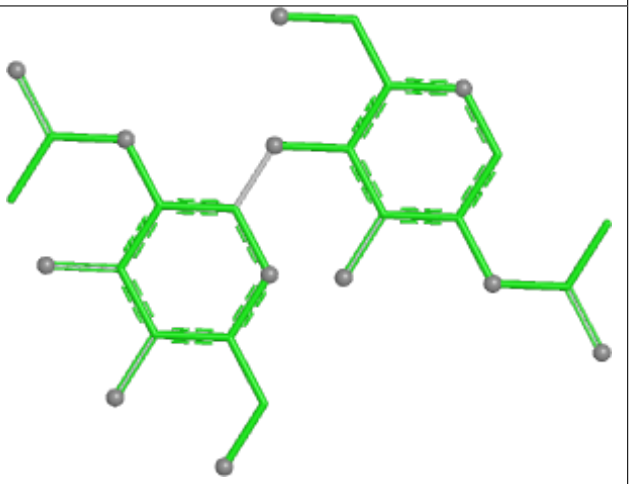


Rings

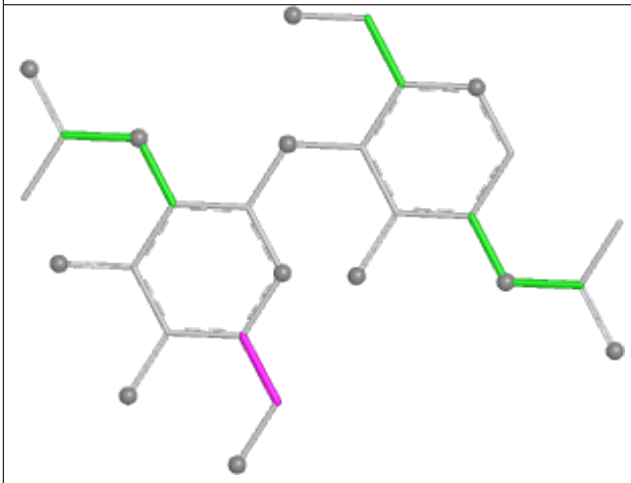
Oligosaccharide Chain R



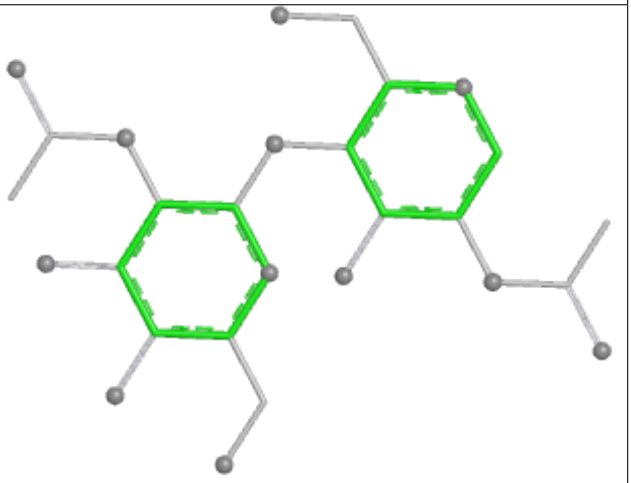
Bond lengths



Bond angles

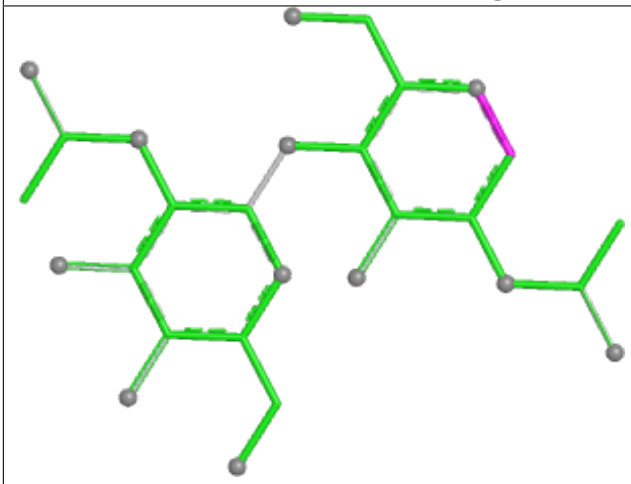


Torsions

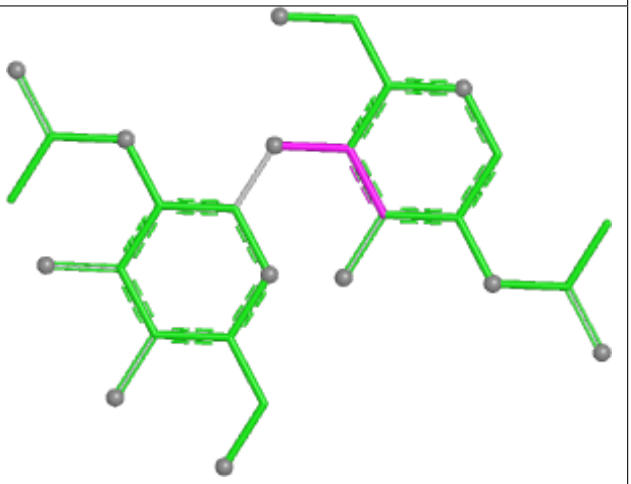


Rings

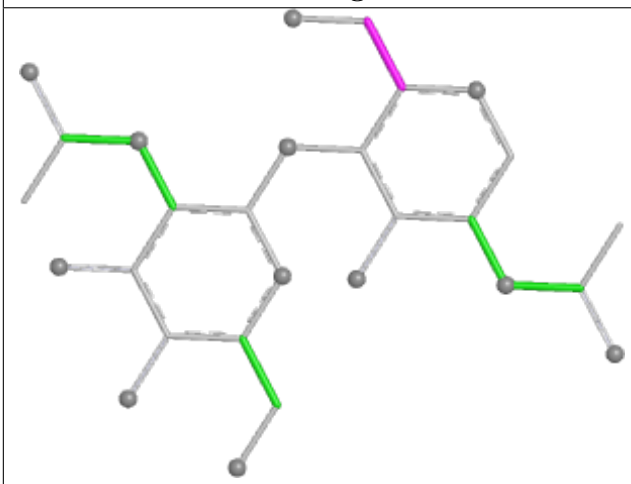
Oligosaccharide Chain W



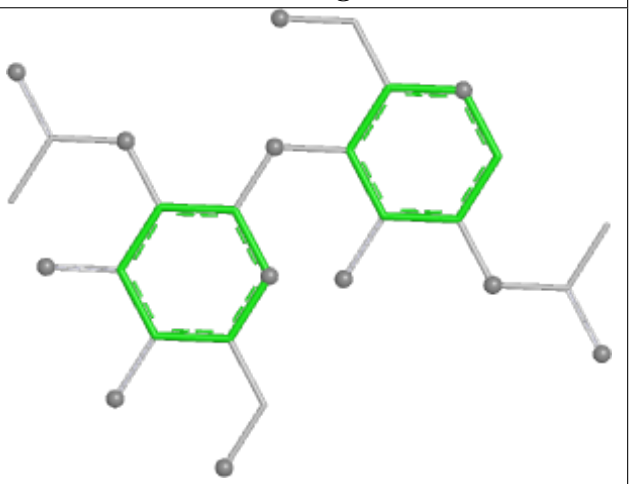
Bond lengths



Bond angles

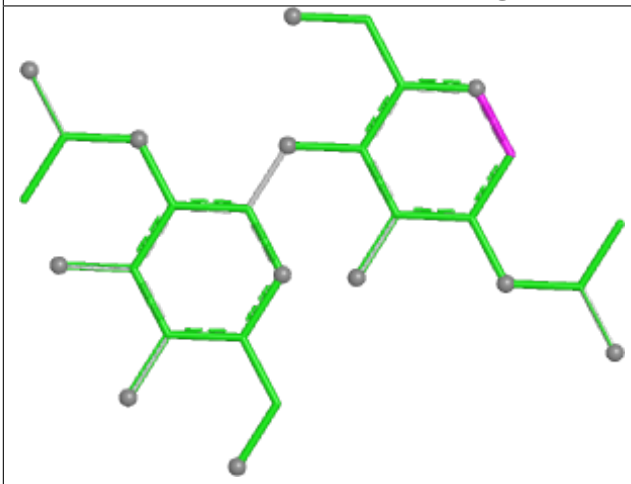


Torsions

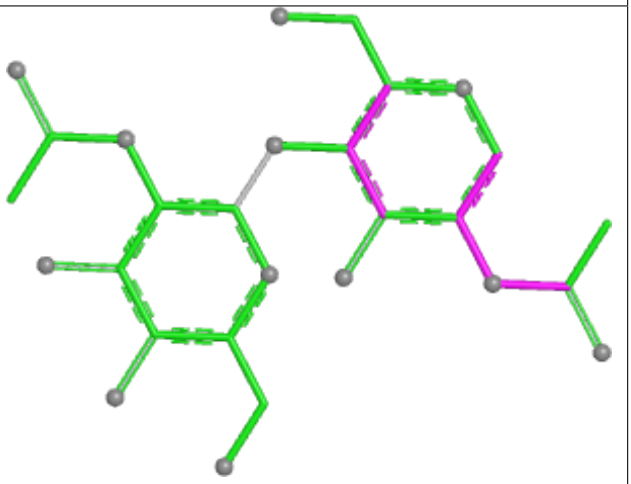


Rings

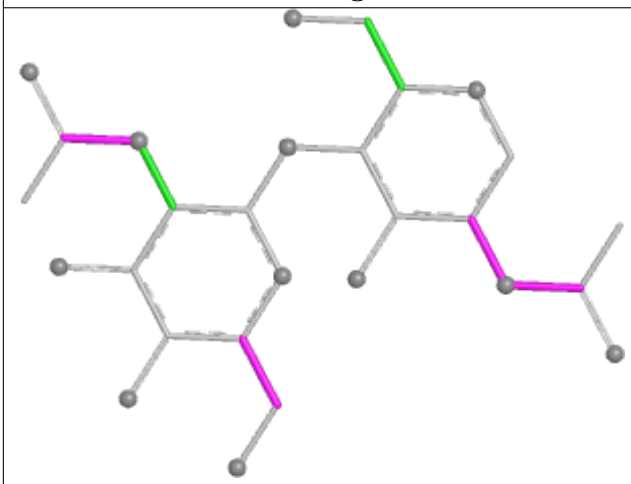
Oligosaccharide Chain Y



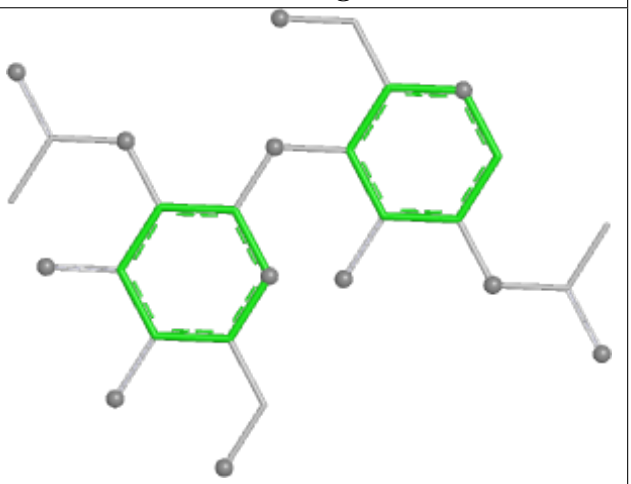
Bond lengths



Bond angles

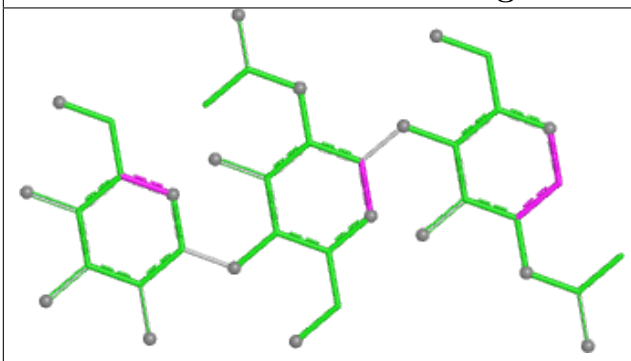


Torsions

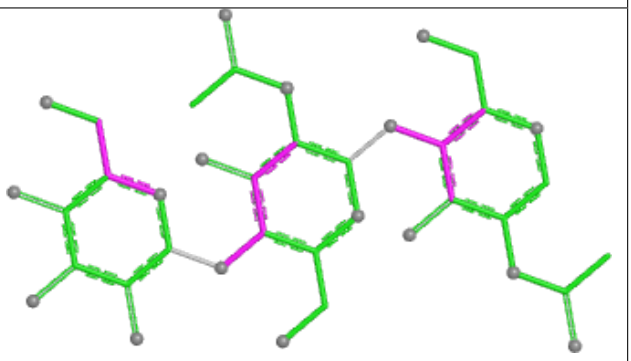


Rings

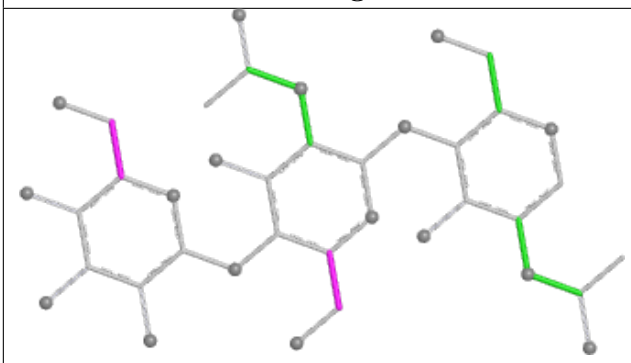
Oligosaccharide Chain L



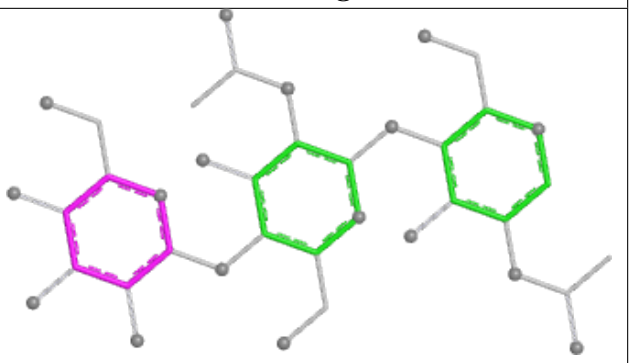
Bond lengths



Bond angles

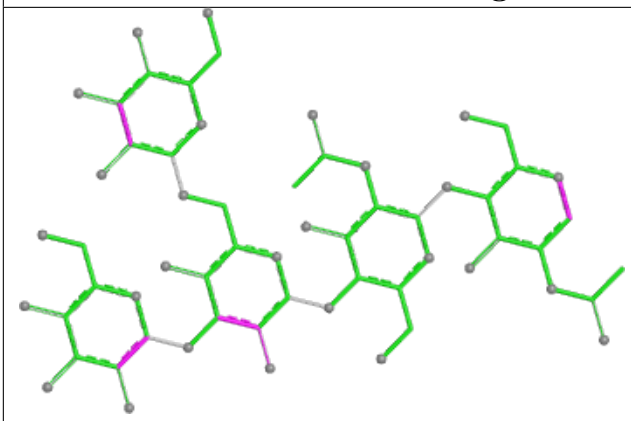


Torsions

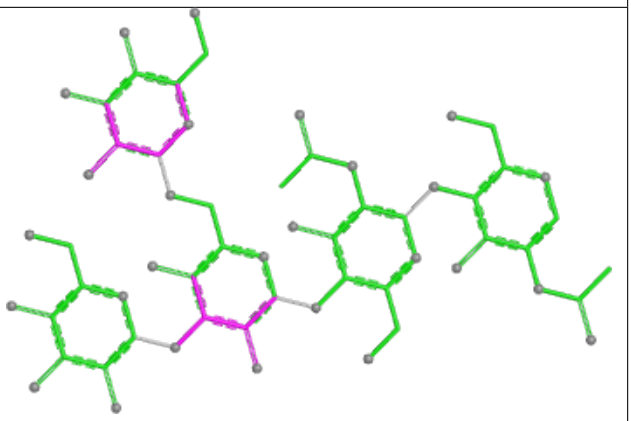


Rings

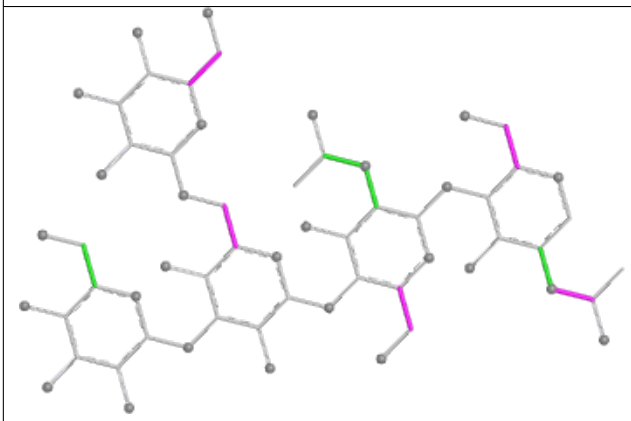
Oligosaccharide Chain M



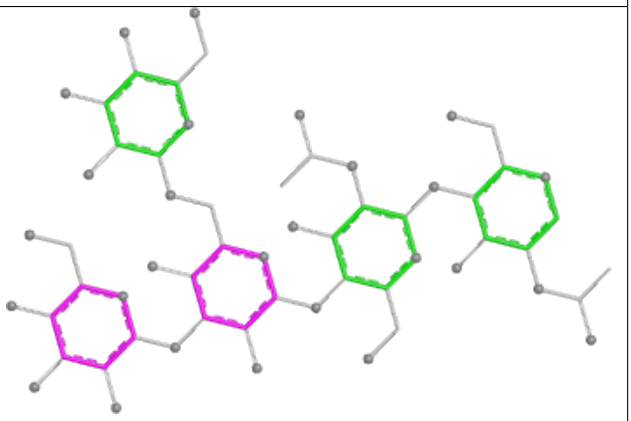
Bond lengths



Bond angles

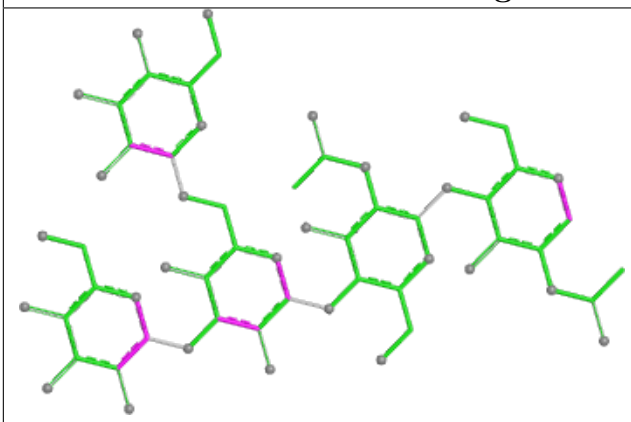


Torsions

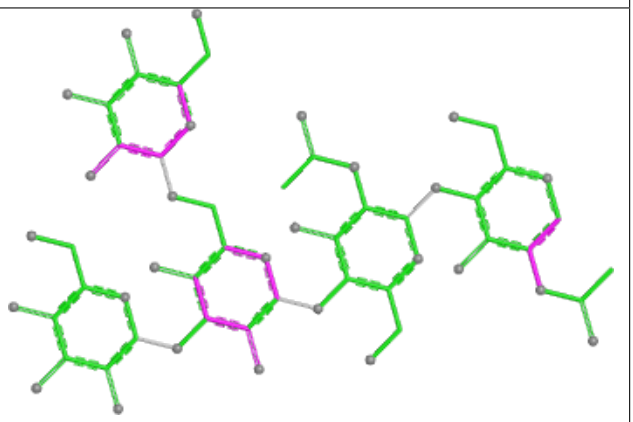


Rings

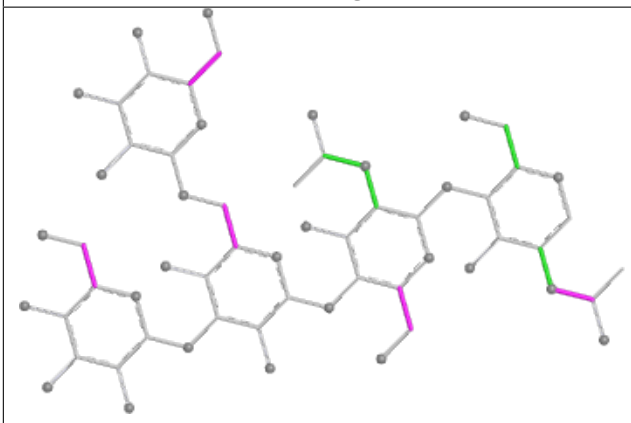
Oligosaccharide Chain X



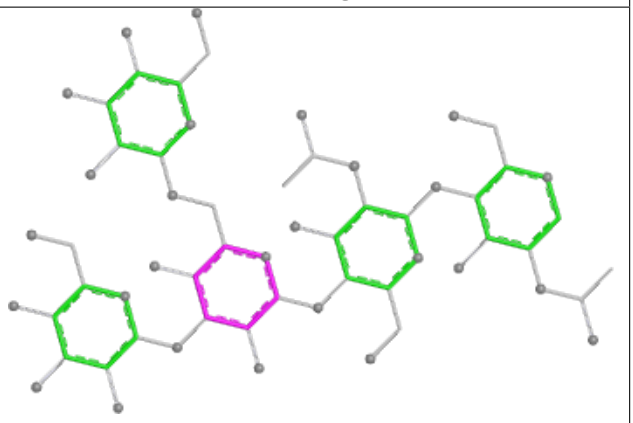
Bond lengths



Bond angles

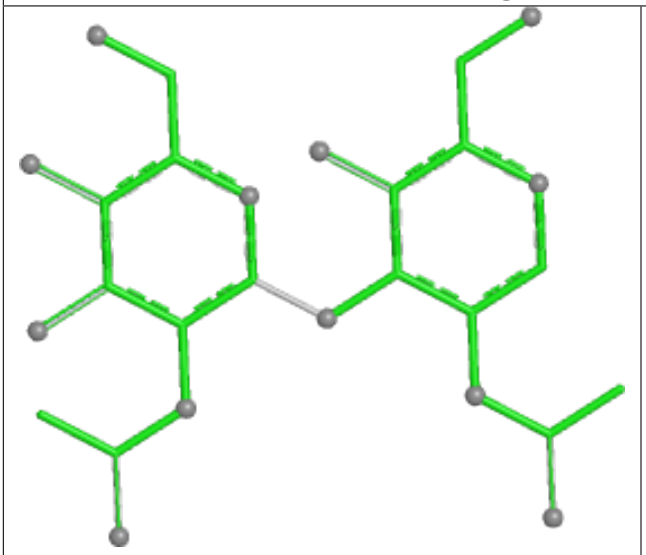


Torsions

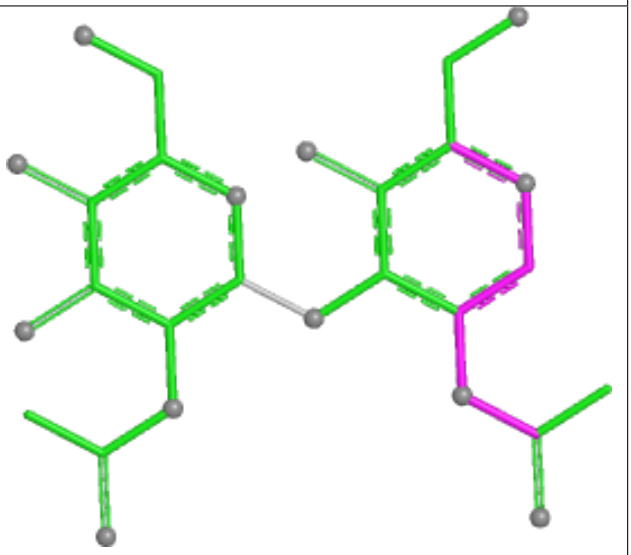


Rings

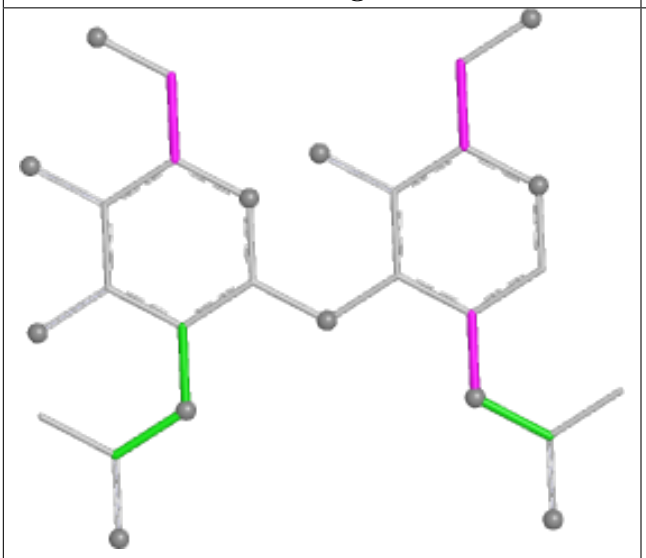
Oligosaccharide Chain S



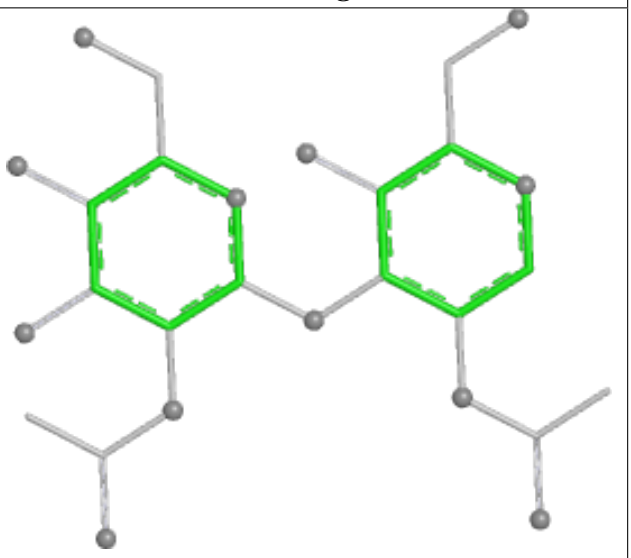
Bond lengths



Bond angles

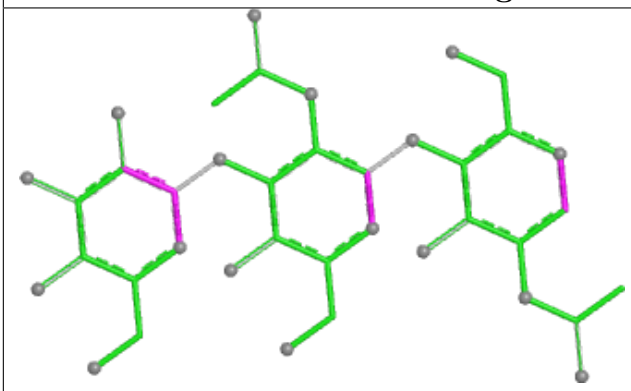


Torsions

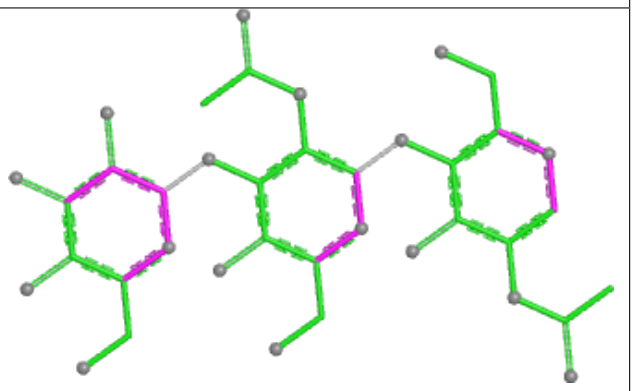


Rings

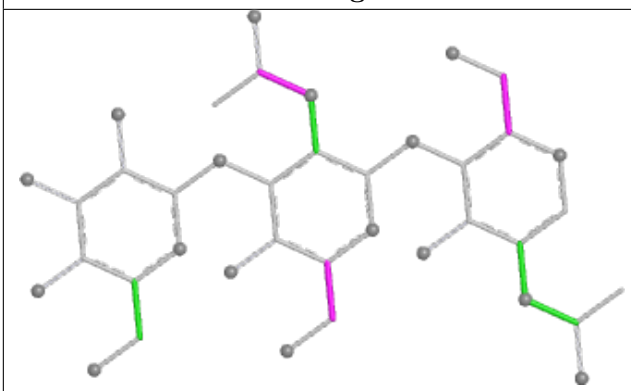
Oligosaccharide Chain T



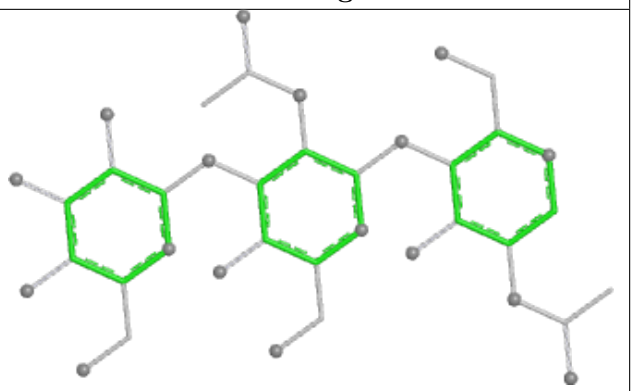
Bond lengths



Bond angles

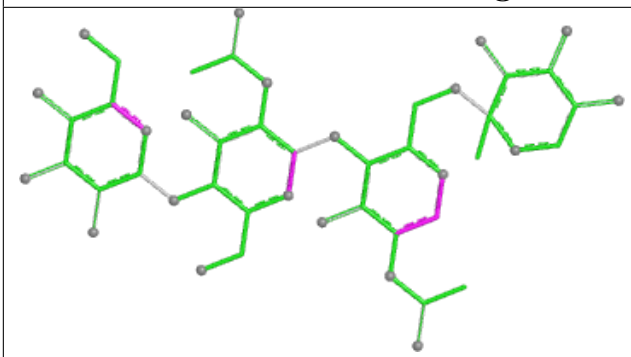


Torsions

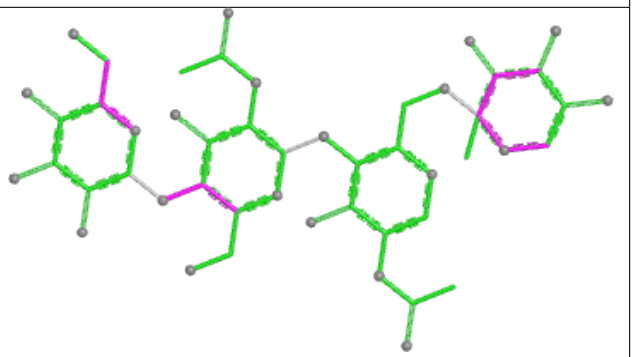


Rings

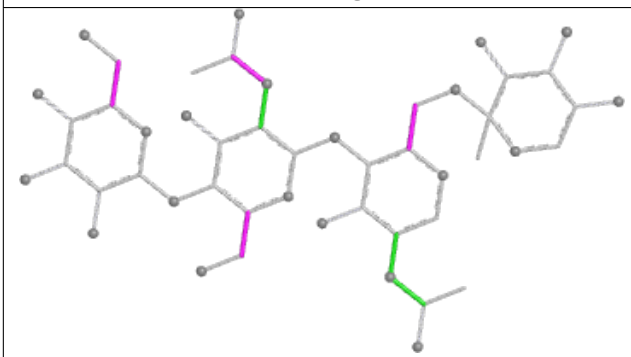
Oligosaccharide Chain V



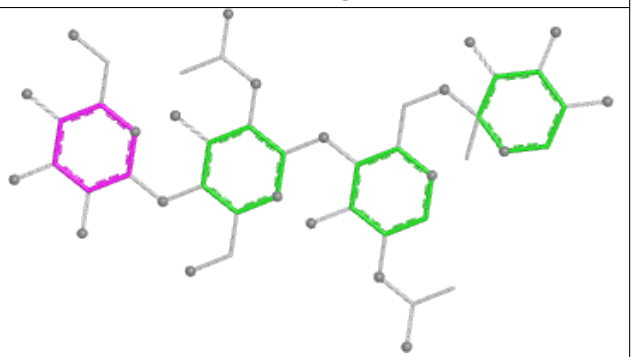
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
11	TYR	D	501	-	12,13,13	1.13	1 (8%)	16,17,17	0.70	0
11	TYR	A	502	-	12,13,13	1.29	1 (8%)	16,17,17	0.67	0
11	TYR	C	502	-	12,13,13	1.13	1 (8%)	16,17,17	1.08	1 (6%)
11	TYR	B	501	-	12,13,13	1.15	1 (8%)	16,17,17	0.82	0
10	NAG	A	501	1	14,14,15	0.56	0	17,19,21	0.71	1 (5%)
13	MAN	C	501	-	11,11,12	2.44	4 (36%)	15,15,17	1.64	4 (26%)

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
11	TYR	D	501	-	-	3/8/8/8	0/1/1/1
11	TYR	A	502	-	-	2/8/8/8	0/1/1/1
11	TYR	C	502	-	-	3/8/8/8	0/1/1/1
11	TYR	B	501	-	-	4/8/8/8	0/1/1/1
10	NAG	A	501	1	-	2/6/23/26	0/1/1/1
13	MAN	C	501	-	-	2/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	MAN	O5-C1	-5.61	1.34	1.43
13	C	501	MAN	C2-C3	-3.61	1.47	1.52
13	C	501	MAN	C4-C5	3.09	1.59	1.53
11	B	501	TYR	CE1-CZ	-2.26	1.34	1.38
11	A	502	TYR	CE1-CZ	-2.21	1.34	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	MAN	C3-C4-C5	3.74	116.90	110.24
11	C	502	TYR	CB-CA-N	3.44	124.81	111.46
13	C	501	MAN	O2-C2-C3	-3.34	103.45	110.14
10	A	501	NAG	C1-O5-C5	2.36	115.39	112.19
13	C	501	MAN	O4-C4-C3	-2.09	105.51	110.35

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	502	TYR	N-CA-CB-CG
13	C	501	MAN	O5-C5-C6-O6
10	A	501	NAG	O5-C5-C6-O6
13	C	501	MAN	C4-C5-C6-O6
10	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	501	TYR	2	0
11	A	502	TYR	2	0
11	C	502	TYR	3	0
11	B	501	TYR	2	0
13	C	501	MAN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	46:SER	C	47:PRO	N	1.14
1	C	377:HIS	C	378:ASN	N	1.08

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	446/446 (100%)	-0.23	4 (0%)	84	80	24, 43, 64, 103	0
1	B	446/446 (100%)	-0.16	5 (1%)	80	75	30, 47, 76, 106	0
1	C	446/446 (100%)	0.11	18 (4%)	38	28	36, 61, 93, 115	0
1	D	446/446 (100%)	0.09	13 (2%)	51	41	31, 57, 82, 111	0
All	All	1784/1784 (100%)	-0.05	40 (2%)	62	52	24, 50, 84, 115	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	342	PHE	4.3
1	C	51	PRO	3.3
1	B	118	ARG	3.3
1	D	125	ARG	3.2
1	C	205	GLN	2.9

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
8	MAN	T	3	11/12	0.59	0.45	89,110,115,115	0
9	MAN	V	3	11/12	0.68	0.31	80,89,94,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	P	2	14/15	0.71	0.28	69,83,89,89	0
4	NAG	Y	2	14/15	0.72	0.44	90,96,104,105	0
8	NAG	T	2	14/15	0.73	0.49	95,106,111,116	0
4	NAG	H	2	14/15	0.73	0.49	71,89,100,107	0
6	MAN	X	5	11/12	0.73	0.25	54,72,78,85	0
7	NAG	S	2	14/15	0.74	0.33	111,116,118,119	0
3	NAG	F	1	14/15	0.75	0.21	57,73,81,82	0
3	NAG	Q	1	14/15	0.76	0.21	72,79,83,85	0
2	NAG	O	2	14/15	0.77	0.35	81,92,98,98	0
6	NAG	X	1	14/15	0.78	0.28	62,79,88,89	0
4	NAG	Y	1	14/15	0.79	0.31	72,86,94,103	0
2	NAG	J	2	14/15	0.79	0.28	71,84,89,91	0
2	NAG	U	2	14/15	0.80	0.33	86,90,94,98	0
4	NAG	R	2	14/15	0.82	0.38	90,95,97,102	0
4	NAG	W	1	14/15	0.82	0.17	57,60,74,75	0
6	MAN	M	4	11/12	0.82	0.29	60,69,75,78	0
5	MAN	L	3	11/12	0.84	0.28	73,79,86,89	0
2	FUC	U	3	10/11	0.84	0.26	67,75,83,86	0
4	NAG	I	2	14/15	0.85	0.33	65,72,84,84	0
2	NAG	E	2	14/15	0.85	0.24	78,88,97,104	0
2	NAG	E	1	14/15	0.86	0.15	69,75,83,92	0
6	MAN	M	5	11/12	0.86	0.30	65,72,81,87	0
3	FUC	Q	2	10/11	0.87	0.19	77,86,92,93	0
4	NAG	N	2	14/15	0.87	0.17	60,67,73,77	0
4	NAG	H	1	14/15	0.87	0.21	64,68,92,94	0
3	FUC	F	2	10/11	0.87	0.32	70,80,86,92	0
2	NAG	O	1	14/15	0.88	0.23	68,76,85,86	0
3	NAG	K	1	14/15	0.89	0.16	66,73,77,81	0
4	NAG	R	1	14/15	0.89	0.25	63,74,82,91	0
4	NAG	G	2	14/15	0.89	0.23	63,72,83,85	0
2	NAG	U	1	14/15	0.89	0.23	74,78,92,94	0
4	NAG	P	1	14/15	0.89	0.22	58,67,77,83	0
9	FUC	V	4	10/11	0.89	0.24	61,72,76,85	0
2	FUC	E	3	10/11	0.90	0.20	66,72,80,89	0
2	FUC	O	3	10/11	0.90	0.21	71,81,90,93	0
7	NAG	S	1	14/15	0.90	0.18	82,95,105,109	0
5	NAG	L	1	14/15	0.90	0.19	47,54,59,64	0
8	NAG	T	1	14/15	0.91	0.36	83,94,98,106	0
6	MAN	X	4	11/12	0.91	0.27	63,67,74,79	0
5	NAG	L	2	14/15	0.91	0.20	61,69,75,75	0
9	NAG	V	2	14/15	0.91	0.23	62,75,83,85	0
3	FUC	K	2	10/11	0.91	0.28	70,79,82,82	0

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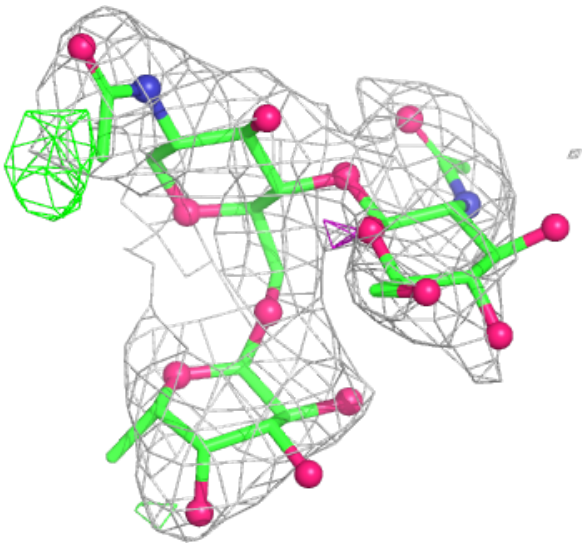
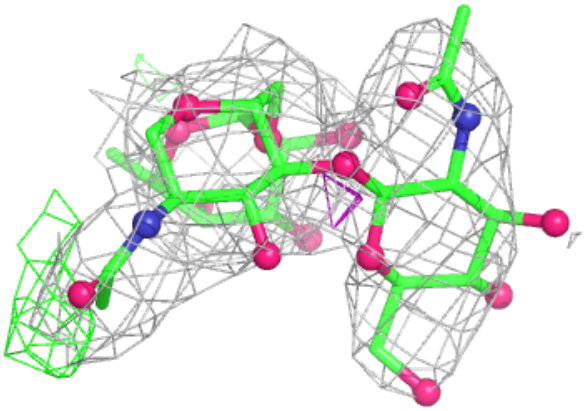
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	M	3	11/12	0.91	0.17	55,58,61,61	0
4	NAG	W	2	14/15	0.92	0.32	71,75,82,88	0
4	NAG	N	1	14/15	0.92	0.21	48,56,62,68	0
6	NAG	X	2	14/15	0.93	0.18	61,69,74,75	0
6	MAN	X	3	11/12	0.93	0.14	58,67,73,73	0
6	NAG	M	1	14/15	0.93	0.16	43,50,62,68	0
2	NAG	J	1	14/15	0.94	0.14	61,67,75,83	0
4	NAG	G	1	14/15	0.94	0.17	48,58,67,69	0
4	NAG	I	1	14/15	0.95	0.23	43,53,57,64	0
2	FUC	J	3	10/11	0.95	0.19	53,66,70,70	0
9	NAG	V	1	14/15	0.96	0.19	46,58,73,79	0
6	NAG	M	2	14/15	0.96	0.15	45,49,55,60	0

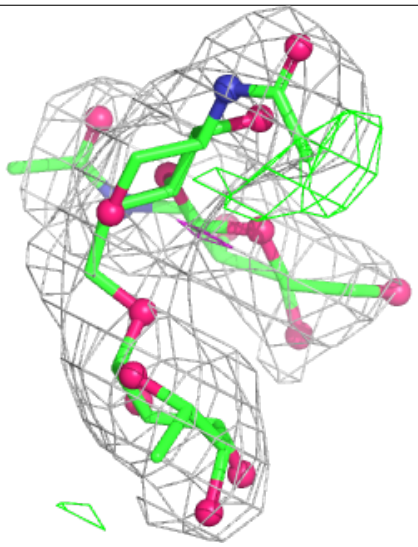
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

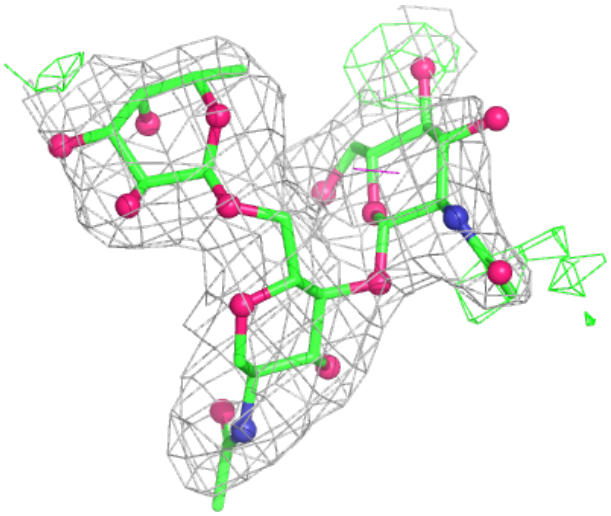


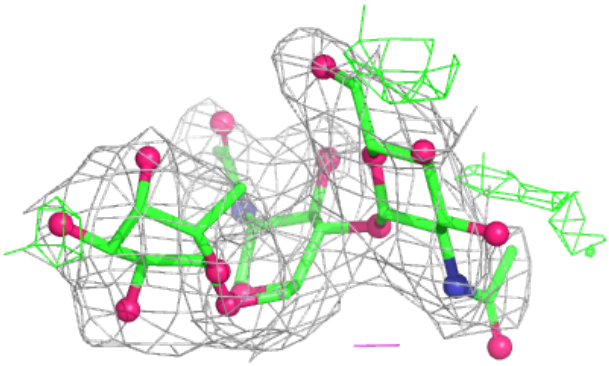


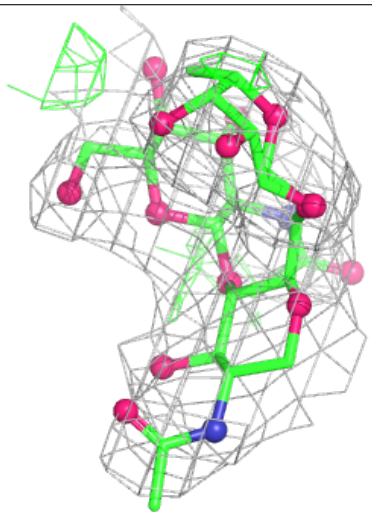


Electron density around Chain J:

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

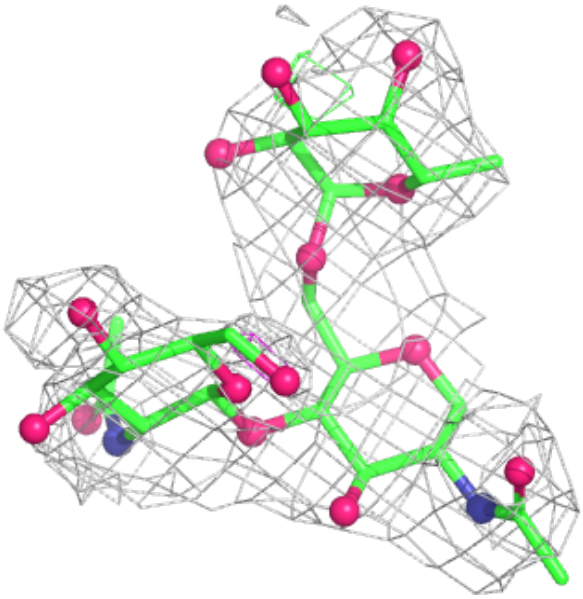


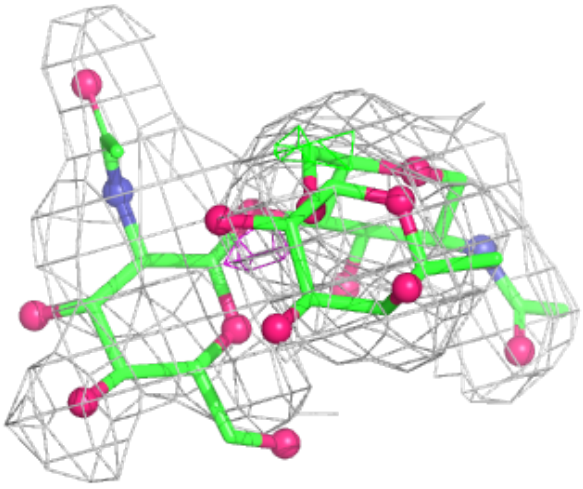


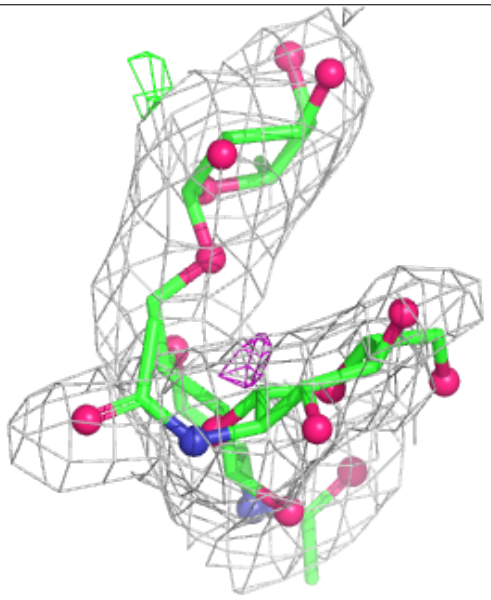


Electron density around Chain O:

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

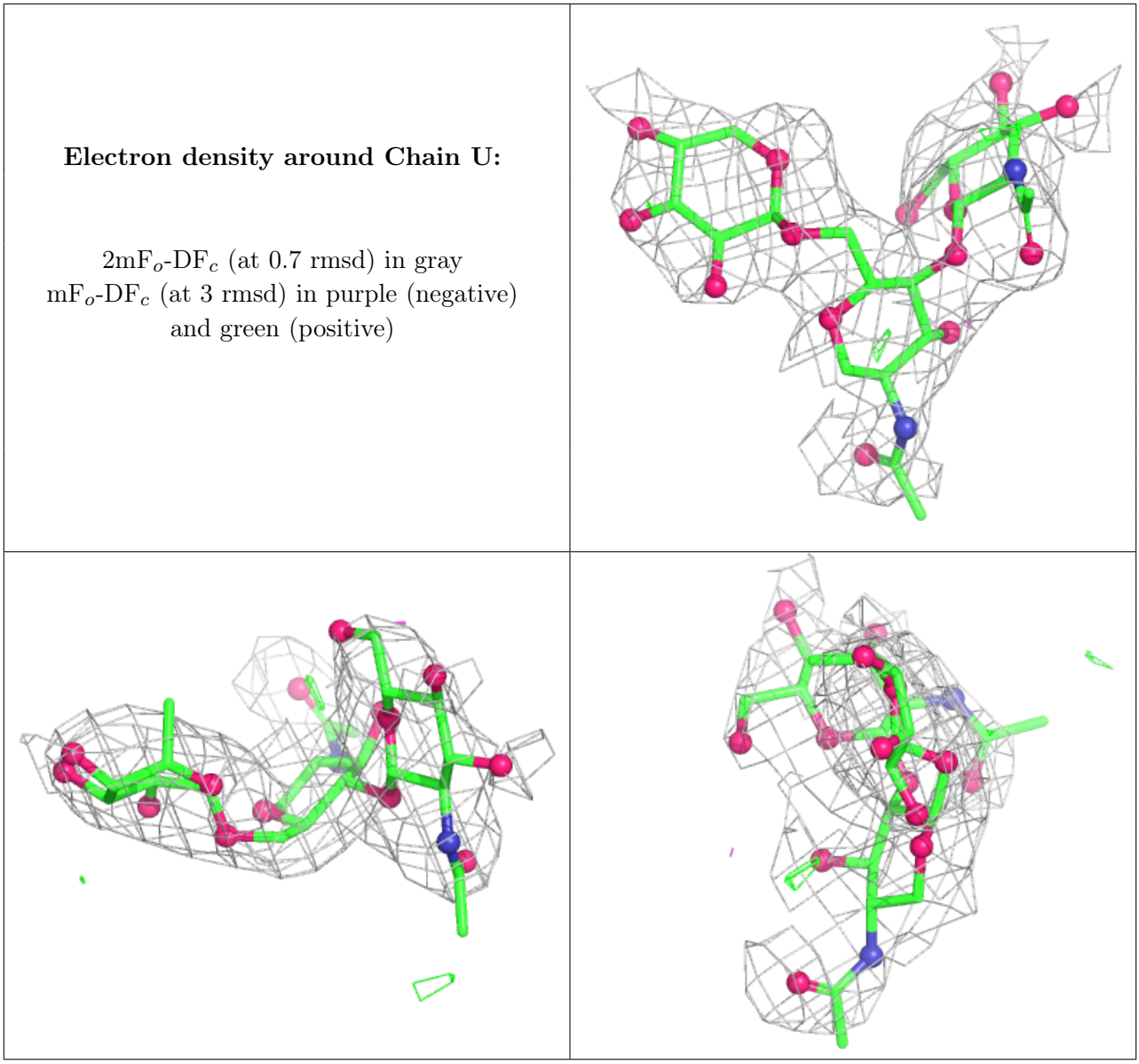






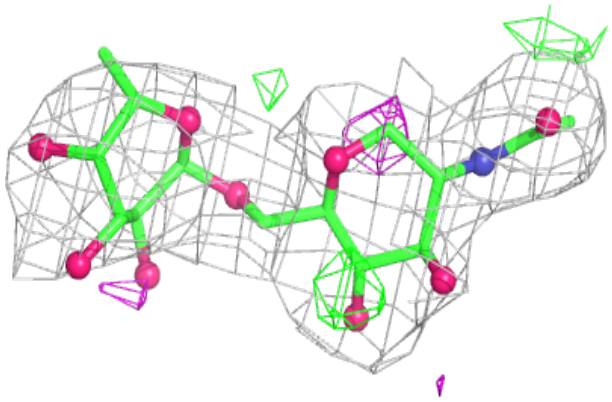
Electron density around Chain U:

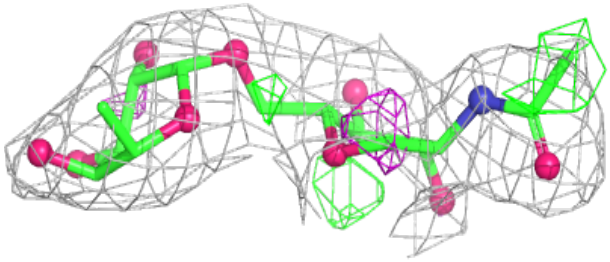
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

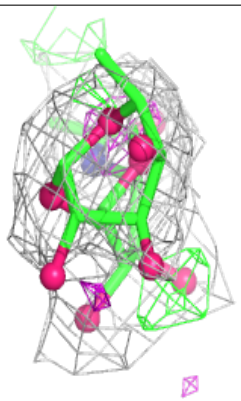


Electron density around Chain F:

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

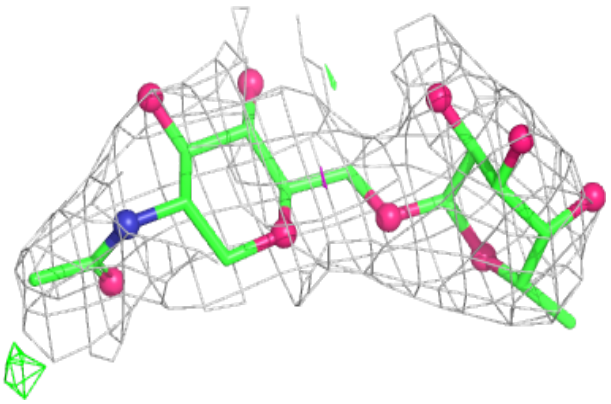


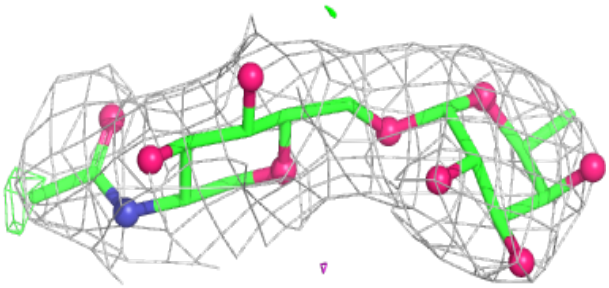


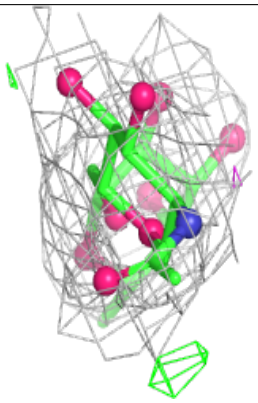


Electron density around Chain K:

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

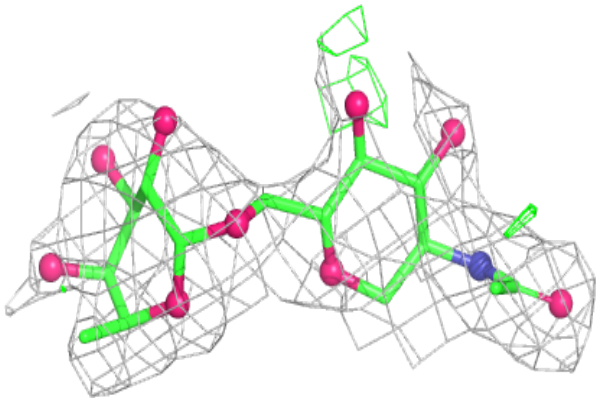


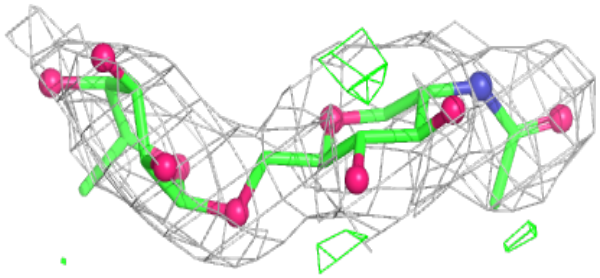


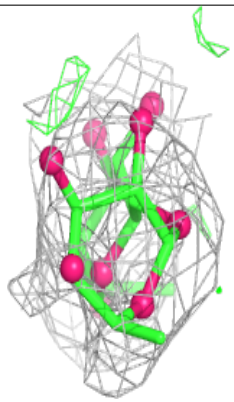


Electron density around Chain Q:

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

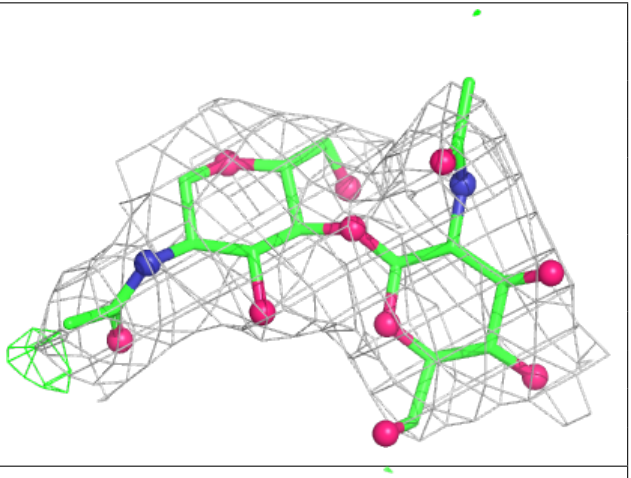


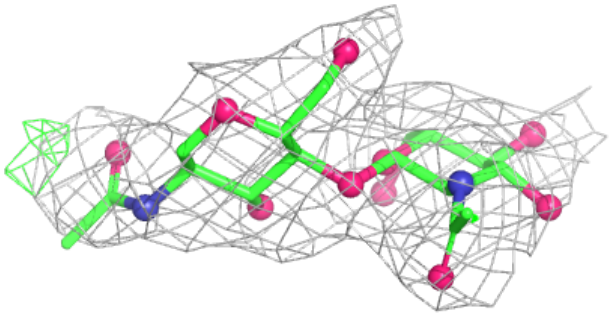


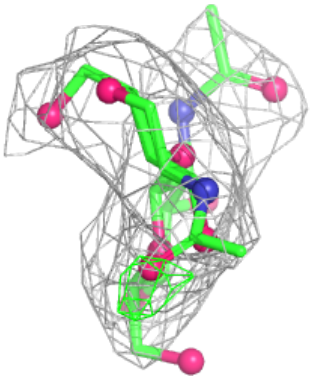


Electron density around Chain G:

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

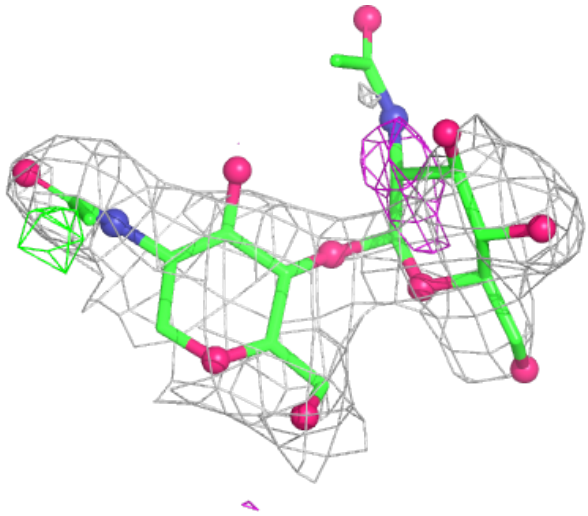


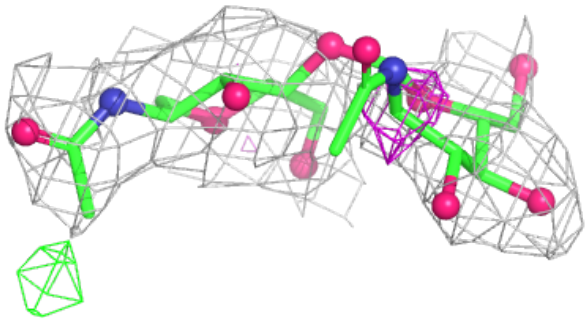


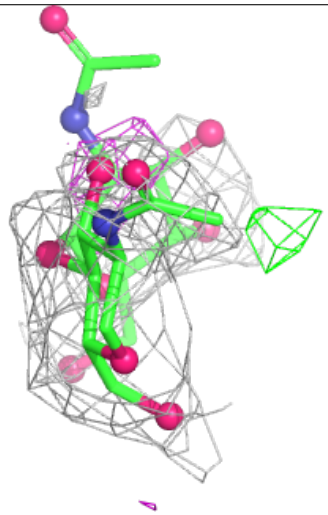


Electron density around Chain H:

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

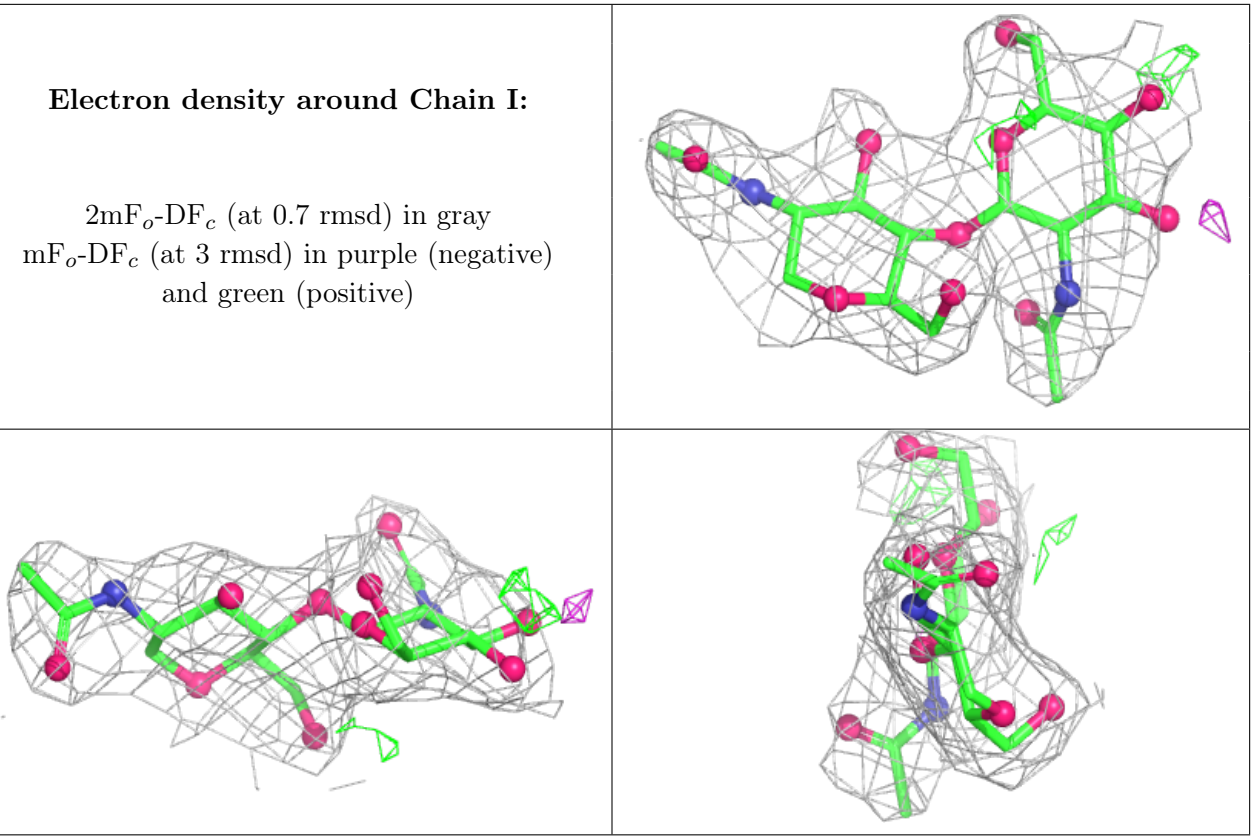






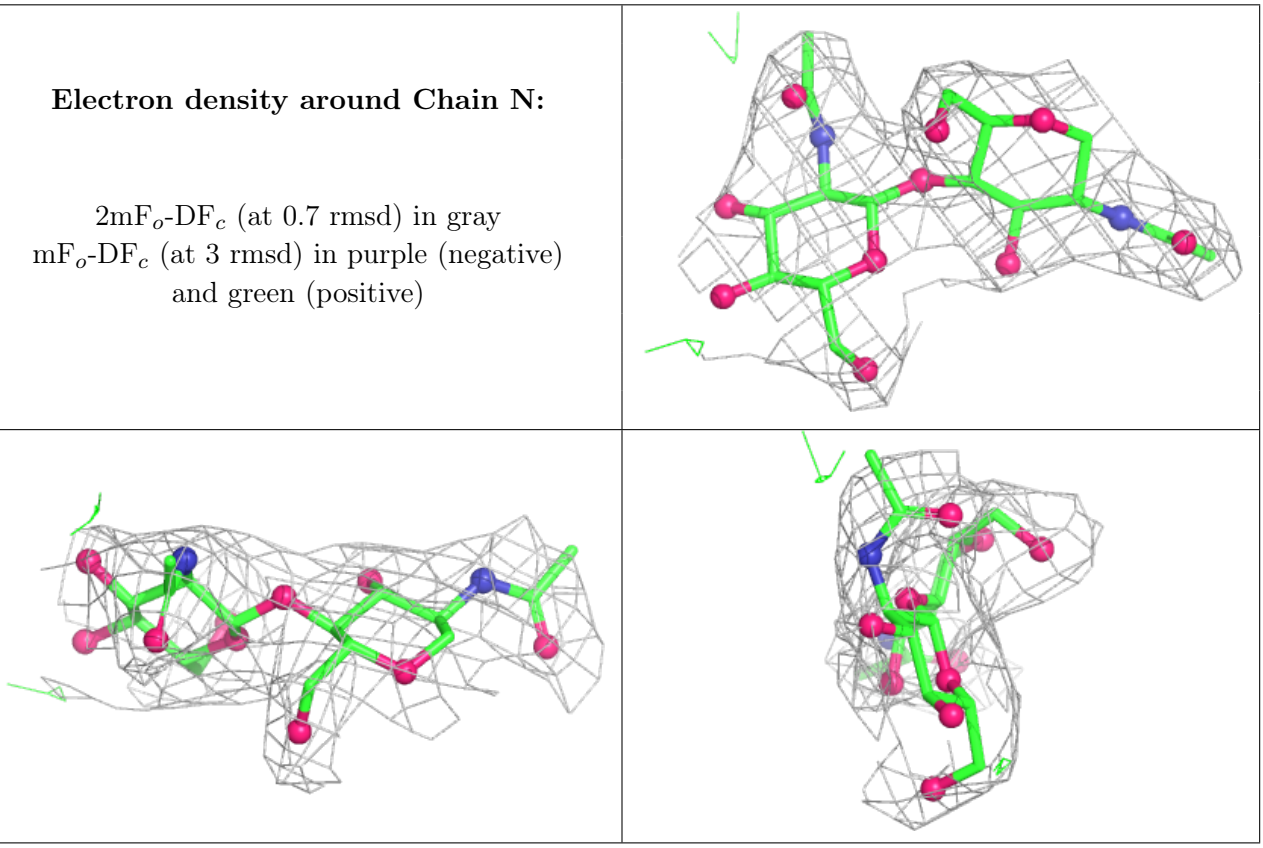
Electron density around Chain I:

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



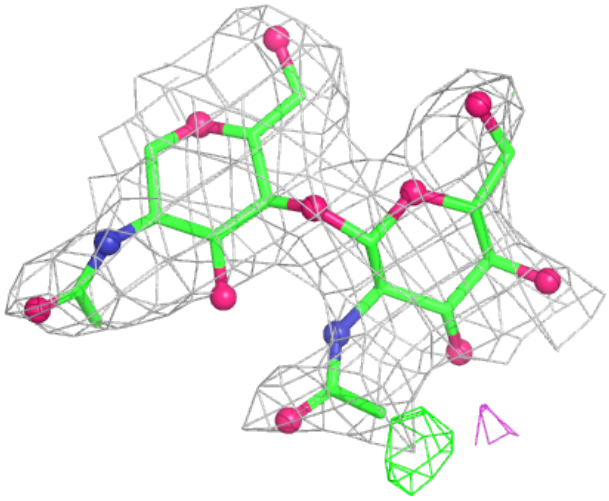
Electron density around Chain N:

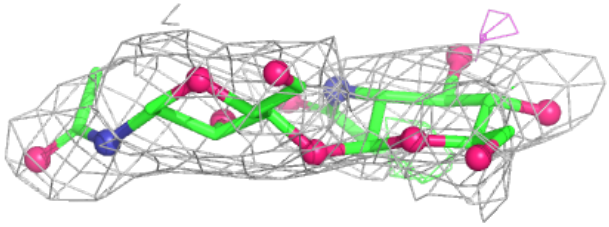
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

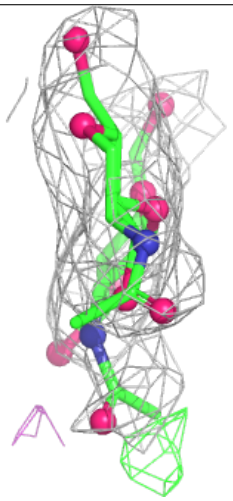


Electron density around Chain P:

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

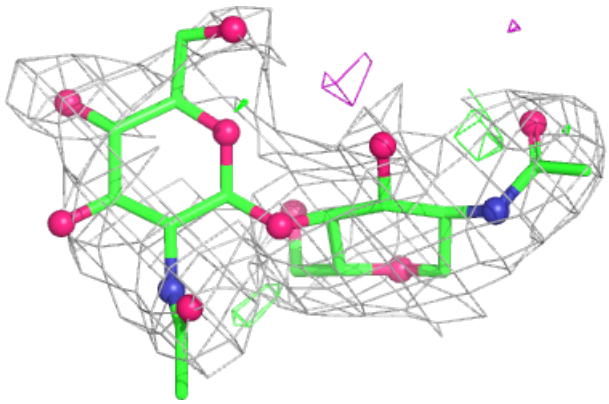


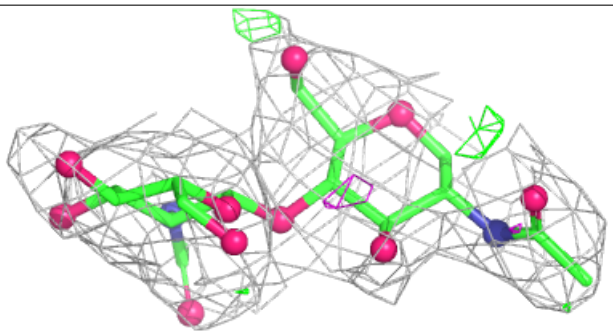


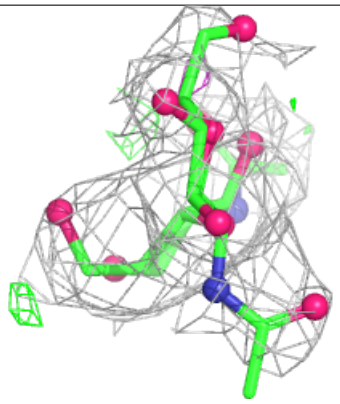


Electron density around Chain R:

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

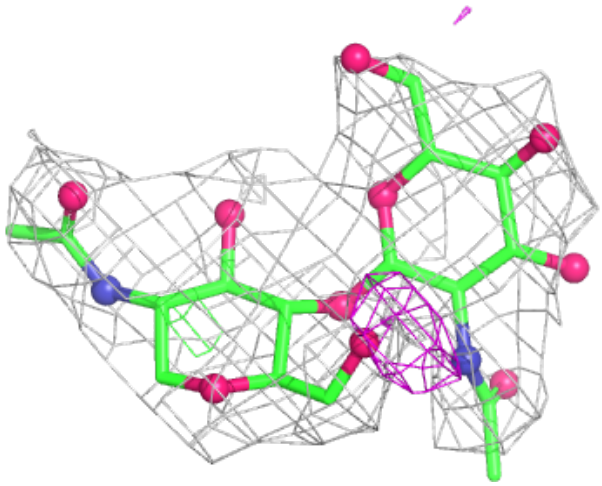


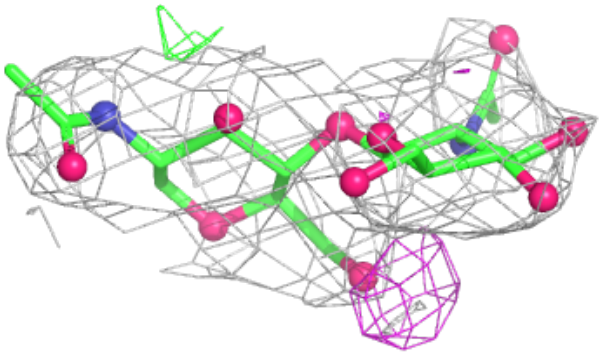


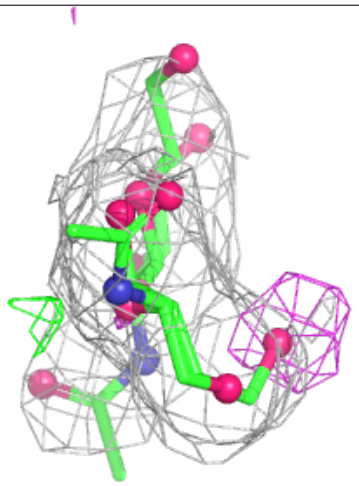


Electron density around Chain W:

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

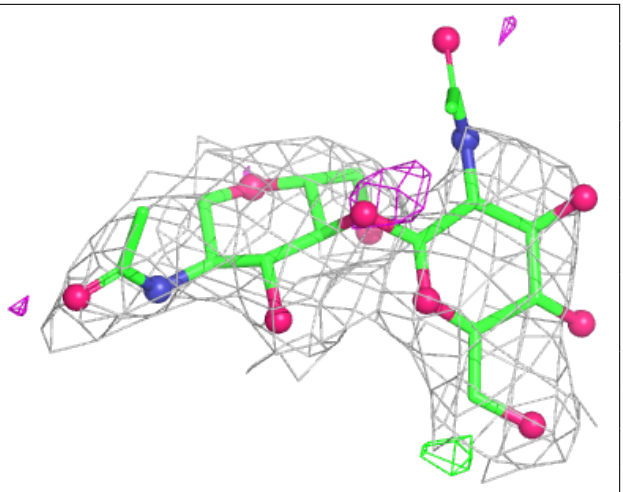


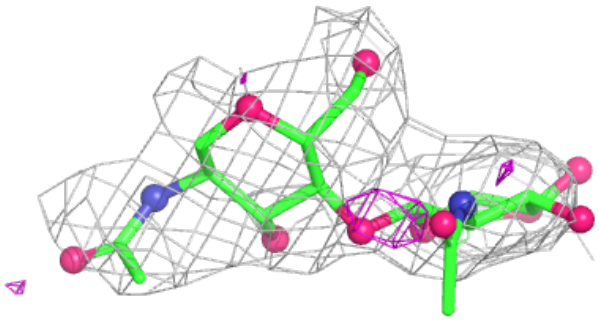


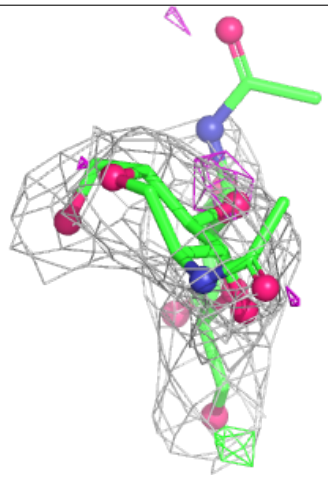


Electron density around Chain Y:

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

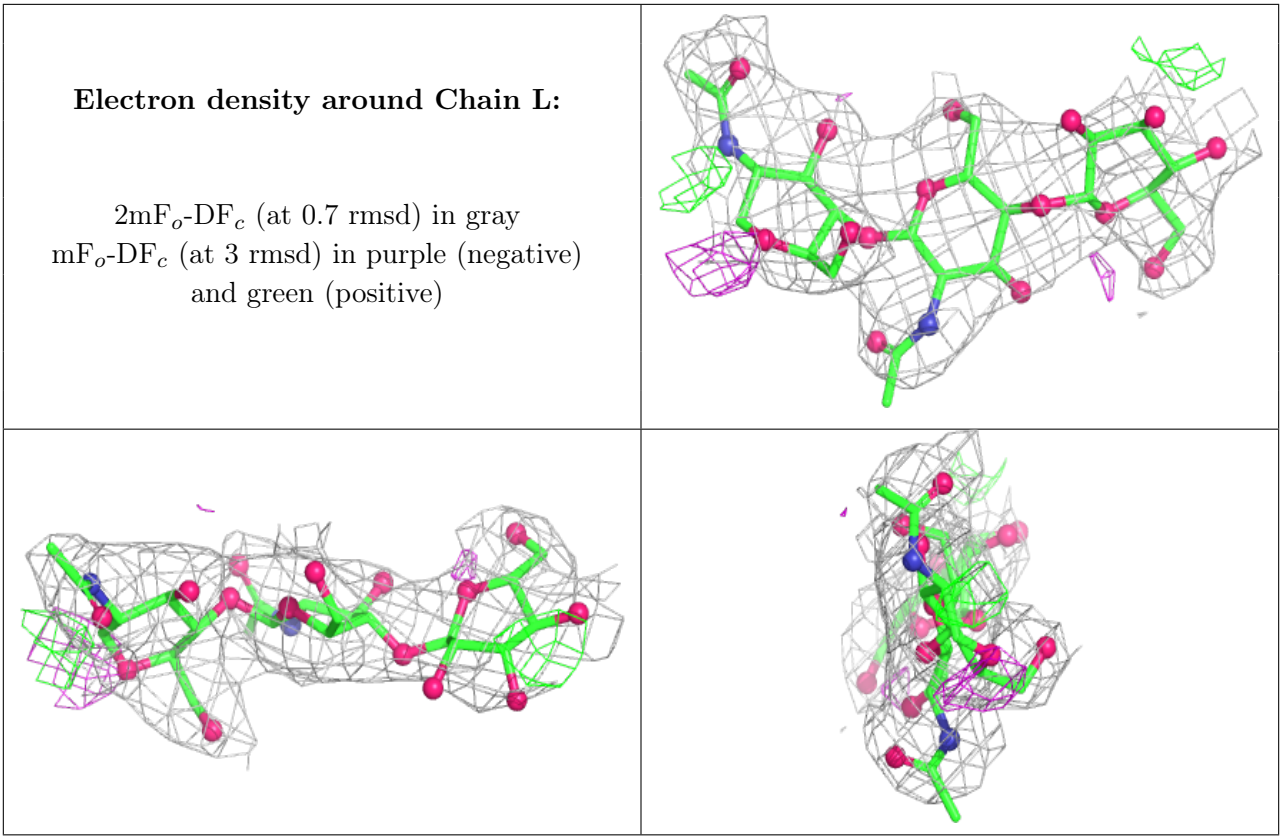






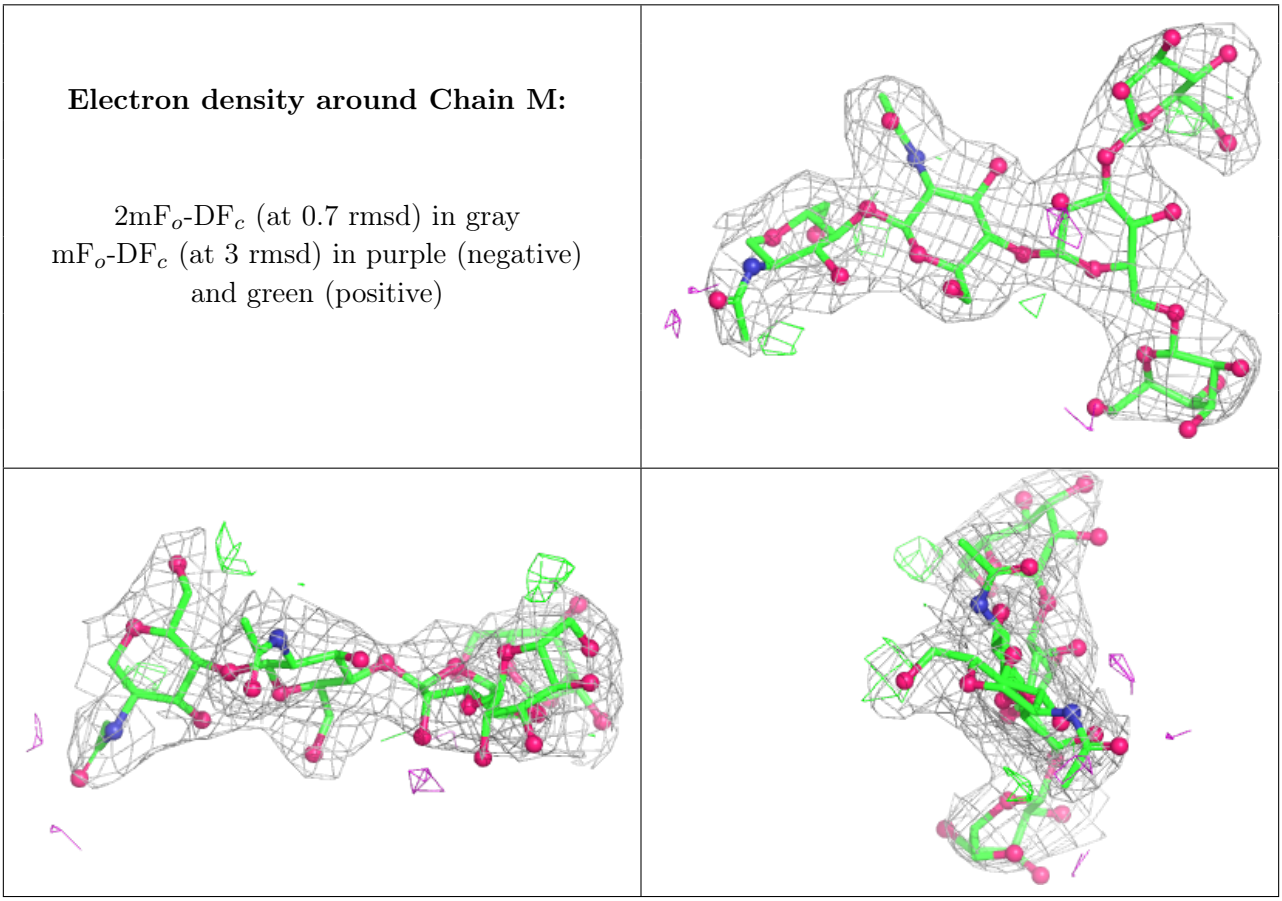
Electron density around Chain L:

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



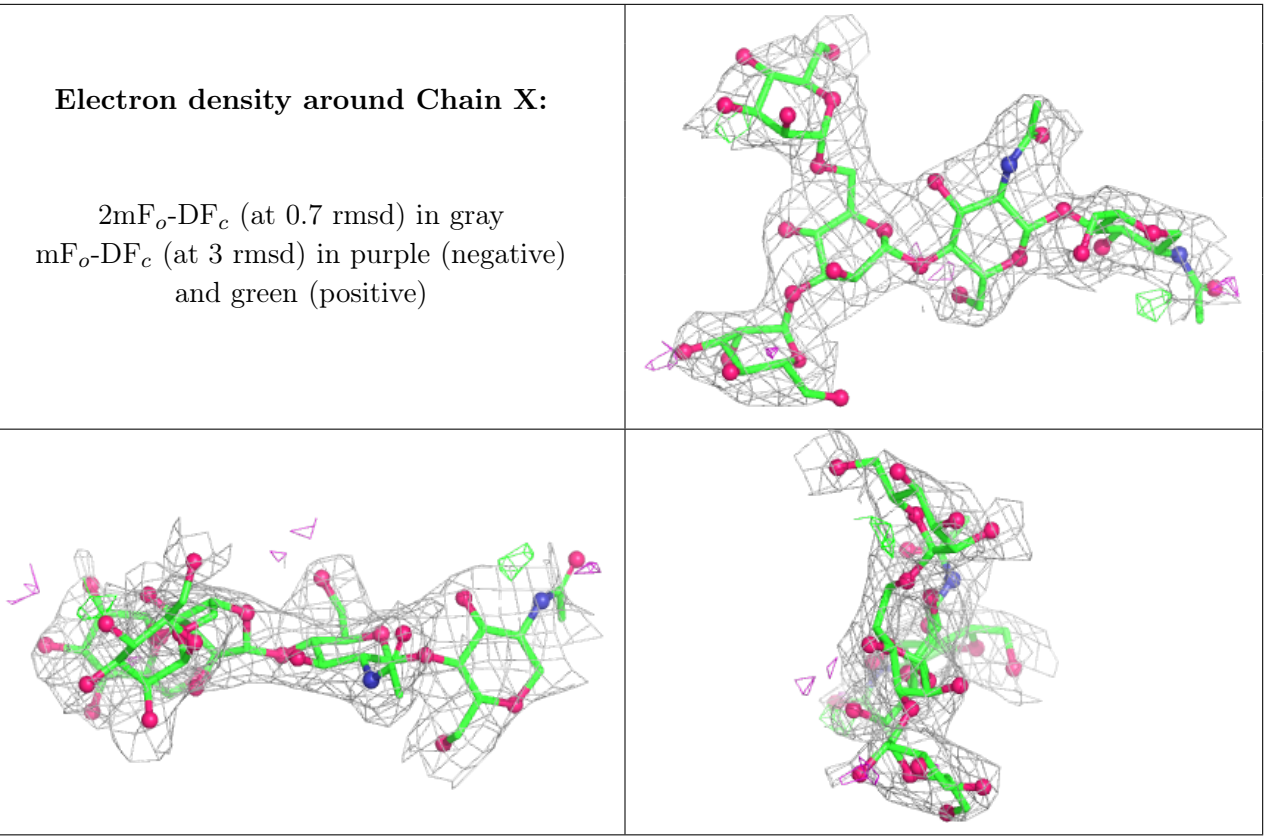
Electron density around Chain M:

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



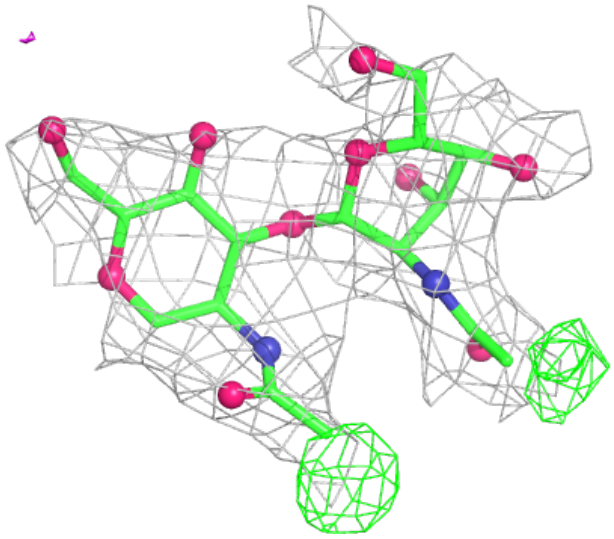
Electron density around Chain X:

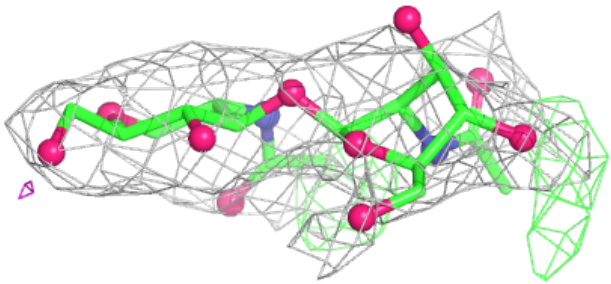
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

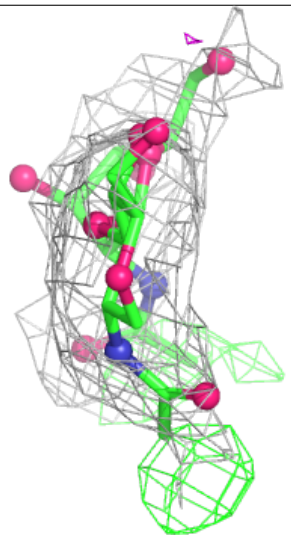


Electron density around Chain S:

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

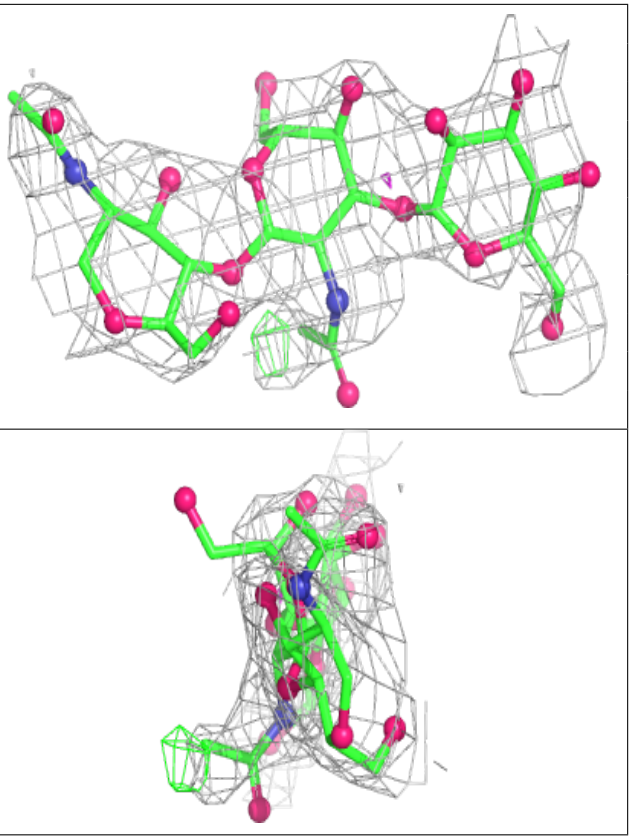






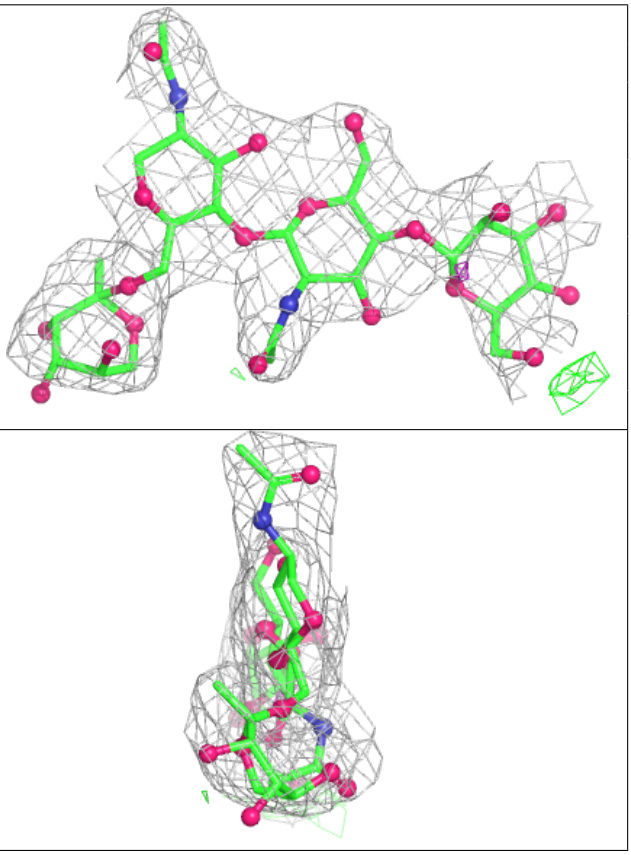
Electron density around Chain T:

$2mF_o$-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 V:

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



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
10	NAG	A	501	14/15	0.67	0.34	86,94,106,107	0
11	TYR	C	502	13/13	0.72	0.37	75,87,96,97	0
11	TYR	D	501	13/13	0.81	0.29	57,67,75,84	0
13	MAN	C	501	11/12	0.89	0.23	84,88,93,93	0
11	TYR	A	502	13/13	0.91	0.23	38,43,56,59	0
11	TYR	B	501	13/13	0.93	0.20	37,47,54,61	0
12	ZN	B	502	1/1	0.96	0.17	46,46,46,46	0
12	ZN	B	503	1/1	0.97	0.12	47,47,47,47	0
12	ZN	C	503	1/1	0.98	0.11	50,50,50,50	0
12	ZN	C	504	1/1	0.98	0.13	63,63,63,63	0
12	ZN	D	503	1/1	0.98	0.10	58,58,58,58	0
12	ZN	A	503	1/1	0.98	0.20	38,38,38,38	0
12	ZN	D	502	1/1	0.99	0.10	48,48,48,48	0
12	ZN	A	504	1/1	0.99	0.16	36,36,36,36	0
12	ZN	A	505	1/1	0.99	0.15	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.