Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2024 – 10:12 pm BST

PDB ID	:	9EY8
Title	:	Crystal structure of human tyrosinase-related protein 1 (TYRP1) in complex with (s)-amino-L-tyrosine
Authors	:	Ng, Y.M.; Soler-Lopez, M.
Deposited on	:	2024-04-09
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

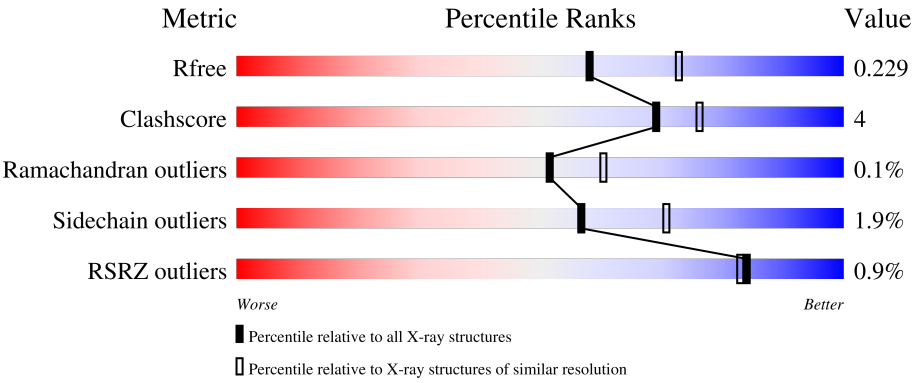
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	AA	450	91% 9%
1	BA	450	% 90% 9%
1	CA	450	% 90% 9%
1	DA	450	2% 89% 11%
2	A	6	17% 50% 33%

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Mol	Chain	Length	Quality of chain
2	C	6	17% 50% 33%
2	L	6	17% 83%
2	T	6	100%
3	B	5	100%
3	H	5	100%
4	D	3	33% 67%
4	W	3	100%
5	E	4	100%
5	G	4	100%
5	S	4	50% 50%
6	F	2	100%
6	J	2	100%
6	K	2	50% 50%
6	M	2	50% 50%
6	Q	2	50% 50%
6	U	2	100%
6	V	2	100%
7	I	3	100%
8	N	7	86% 14%
9	O	7	100%
10	P	6	100%
11	R	2	50% 50%
11	X	2	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
12	NAG	DA	502	-	-	-	X
2	MAN	C	4	-	-	-	X
2	MAN	C	5	-	-	-	X
3	MAN	B	5	-	-	-	X
6	NAG	J	2	-	-	-	X
8	MAN	N	4	-	-	-	X
8	MAN	N	5	-	-	-	X
8	MAN	N	6	-	-	-	X
9	MAN	O	6	-	-	-	X
9	MAN	O	7	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16585 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.

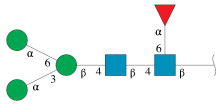
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	447	Total	C	N	O	S	0	1	0
			3578	2244	638	673	23			
1	BA	447	Total	C	N	O	S	0	1	0
			3582	2245	640	674	23			
1	CA	447	Total	C	N	O	S	0	0	0
			3571	2239	636	673	23			
1	DA	450	Total	C	N	O	S	0	1	0
			3603	2259	642	679	23			

There are 12 discrepancies between the modelled and reference sequences:

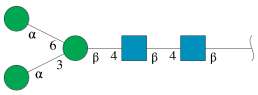
Chain	Residue	Modelled	Actual	Comment	Reference
AA	472	GLU	-	expression tag	UNP P17643
AA	473	ASN	-	expression tag	UNP P17643
AA	474	LEU	-	expression tag	UNP P17643
BA	472	GLU	-	expression tag	UNP P17643
BA	473	ASN	-	expression tag	UNP P17643
BA	474	LEU	-	expression tag	UNP P17643
CA	472	GLU	-	expression tag	UNP P17643
CA	473	ASN	-	expression tag	UNP P17643
CA	474	LEU	-	expression tag	UNP P17643
DA	472	GLU	-	expression tag	UNP P17643
DA	473	ASN	-	expression tag	UNP P17643
DA	474	LEU	-	expression tag	UNP P17643

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



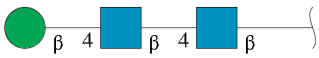
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	A	6	Total C N O 71 40 2 29	0	0	0
2	C	6	Total C N O 71 40 2 29	0	0	0
2	L	6	Total C N O 71 40 2 29	0	0	0
2	T	6	Total C N O 71 40 2 29	0	0	0

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



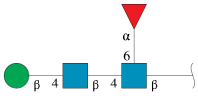
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	B	5	Total C N O 61 34 2 25	0	0	0
3	H	5	Total C N O 61 34 2 25	0	0	0

- Molecule 4 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
4	D	3	Total C N O 39 22 2 15	0	0	0
4	W	3	Total C N O 39 22 2 15	0	0	0

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

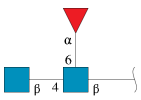


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	4	Total C N O 49 28 2 19	0	0	0
5	G	4	Total C N O 49 28 2 19	0	0	0
5	S	4	Total C N O 49 28 2 19	0	0	0

- Molecule 6 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
6	F	2	Total C N O 28 16 2 10	0	0	0
6	J	2	Total C N O 28 16 2 10	0	0	0
6	K	2	Total C N O 28 16 2 10	0	0	0
6	M	2	Total C N O 28 16 2 10	0	0	0
6	Q	2	Total C N O 28 16 2 10	0	0	0
6	U	2	Total C N O 28 16 2 10	0	0	0
6	V	2	Total C N O 28 16 2 10	0	0	0

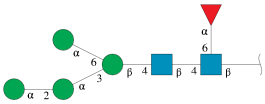
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

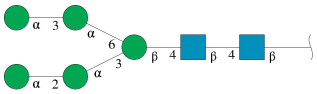
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

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



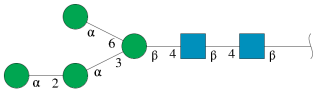
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	7	Total	C	N	O	0	0	0
			82	46	2	34			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]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
9	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

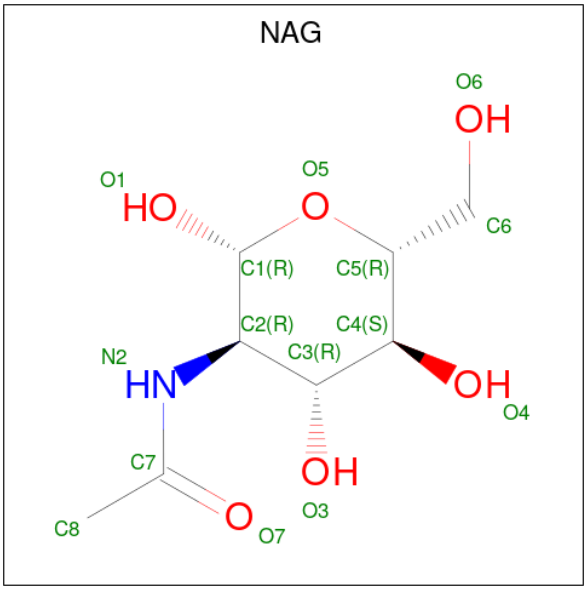


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

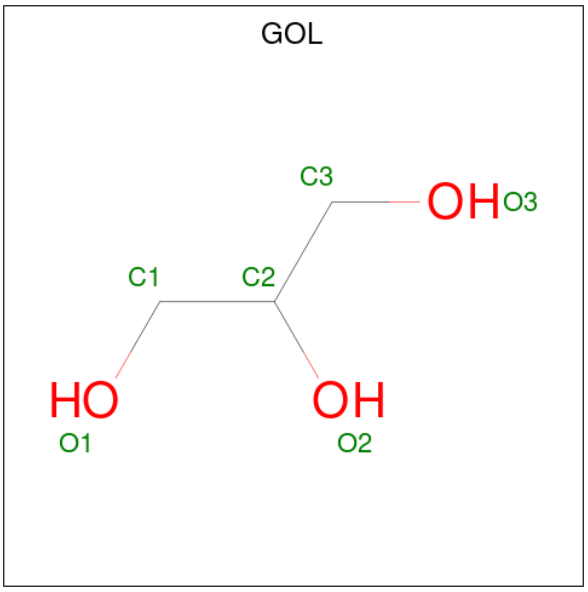
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	R	2	Total C N O 24 14 1 9	0	0	0
11	X	2	Total C N O 24 14 1 9	0	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	AA	1	Total C N O 14 8 1 5	0	0
12	CA	1	Total C N O 14 8 1 5	0	0
12	DA	1	Total C N O 14 8 1 5	0	0
12	DA	1	Total C N O 14 8 1 5	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

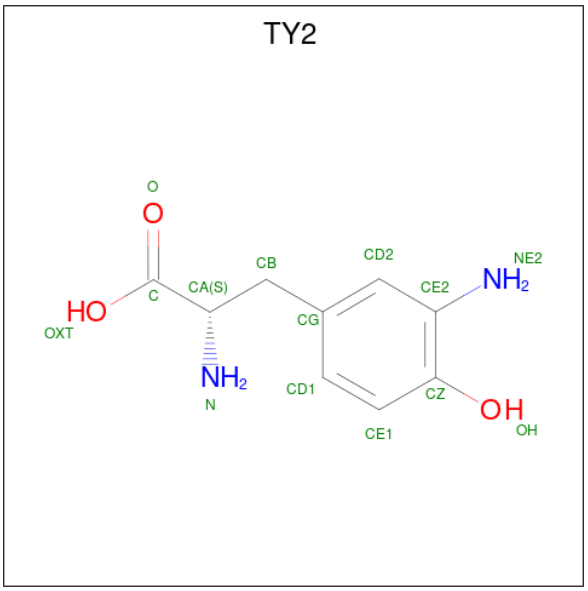


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	AA	1	Total C O 6 3 3	0	0
13	BA	1	Total C O 6 3 3	0	0
13	CA	1	Total C O 6 3 3	0	0
13	DA	1	Total C O 6 3 3	0	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	AA	2	Total Zn 2 2	0	0
14	BA	2	Total Zn 2 2	0	0
14	CA	2	Total Zn 2 2	0	0
14	DA	2	Total Zn 2 2	0	0

- Molecule 15 is 3-AMINO-L-TYROSINE (three-letter code: TY2) (formula: $C_9H_{12}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	CA	1	Total C N O 14 9 2 3	0	0

- Molecule 16 is water.

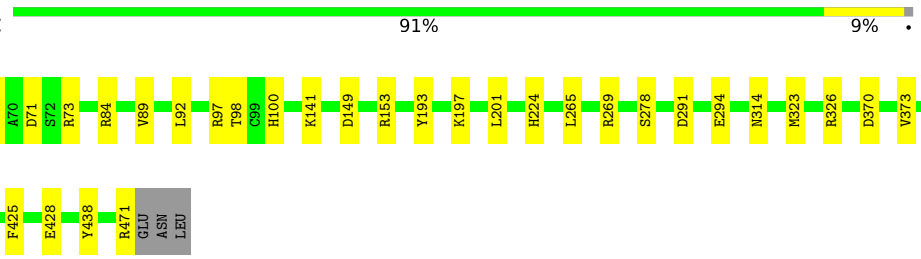
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	AA	313	Total O 313 313	0	0
16	BA	261	Total O 261 261	0	0
16	CA	229	Total O 229 229	0	0
16	DA	196	Total O 196 196	0	0

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.

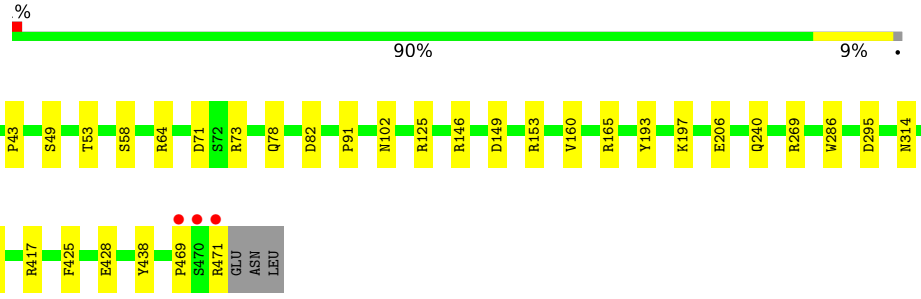
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain AA:



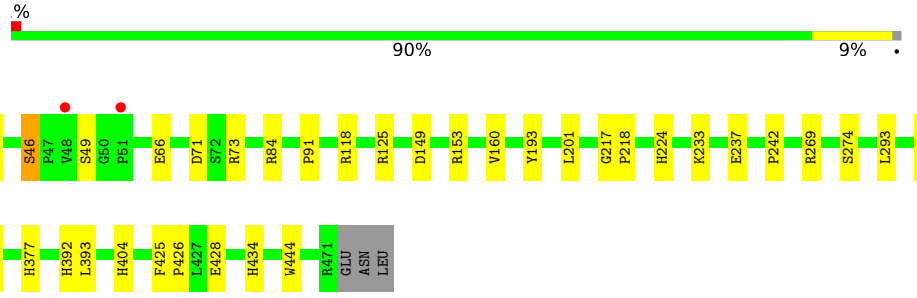
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain BA:



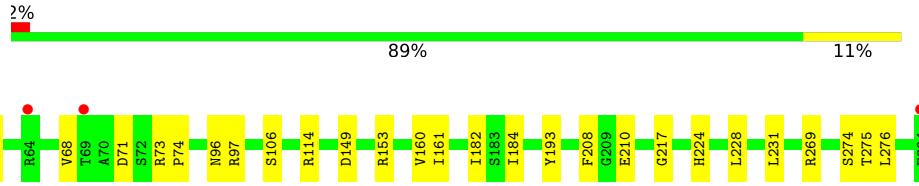
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain CA:



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

Chain DA:

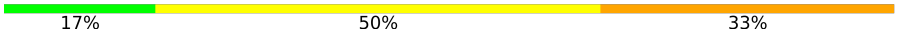


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

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

Chain C:

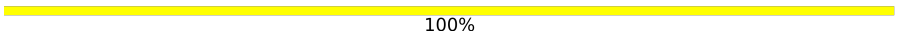


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

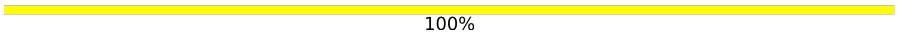
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



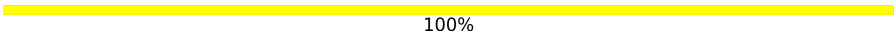
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



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

Chain H:

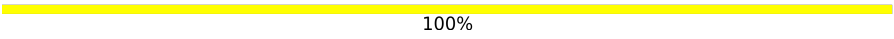


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

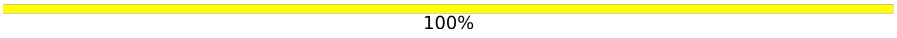
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



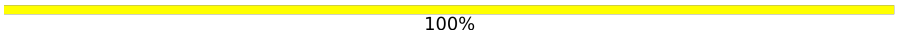
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain G:

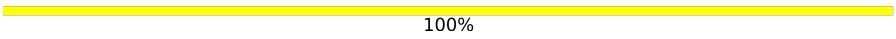


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

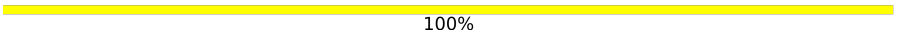
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

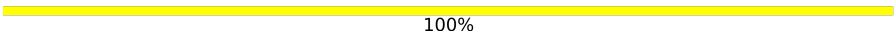
Chain M:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

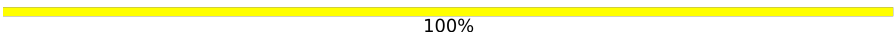
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



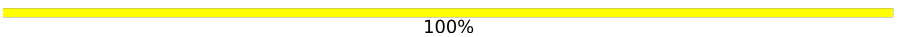
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



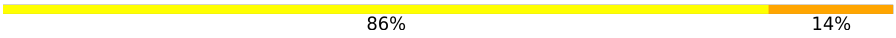
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



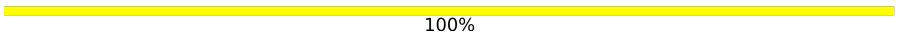
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



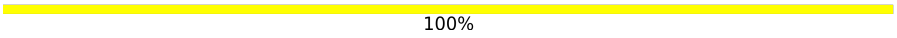
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

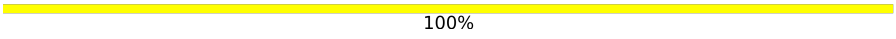


• Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.97Å 126.97Å 212.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.20 47.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.26-2.20) 99.5 (47.26-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.189 , 0.233 0.185 , 0.229	Depositor DCC
R_{free} test set	6089 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.2	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	0.95	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TY2, GOL, MAN, BMA, NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.43	0/3689	0.63	0/5027
1	BA	0.45	0/3689	0.63	0/5026
1	CA	0.44	0/3678	0.63	0/5012
1	DA	0.40	0/3714	0.61	0/5061
All	All	0.43	0/14770	0.63	0/20126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3578	0	3343	26	0
1	BA	3582	0	3349	26	0
1	CA	3571	0	3337	26	0
1	DA	3603	0	3366	31	0
2	A	71	0	61	2	0
2	C	71	0	61	1	0
2	L	71	0	61	0	0
2	T	71	0	61	0	0
3	B	61	0	52	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	61	0	52	0	0
4	D	39	0	34	0	0
4	W	39	0	34	0	0
5	E	49	0	43	0	0
5	G	49	0	43	0	0
5	S	49	0	43	0	0
6	F	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	1	0
6	M	28	0	25	0	0
6	Q	28	0	25	1	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
7	I	38	0	34	0	0
8	N	82	0	70	1	0
9	O	83	0	70	0	0
10	P	72	0	61	0	0
11	R	24	0	22	2	0
11	X	24	0	22	0	0
12	AA	14	0	13	0	0
12	CA	14	0	13	0	0
12	DA	28	0	26	0	0
13	AA	6	0	8	0	0
13	BA	6	0	8	1	0
13	CA	6	0	8	1	0
13	DA	6	0	8	0	0
14	AA	2	0	0	0	0
14	BA	2	0	0	0	0
14	CA	2	0	0	0	0
14	DA	2	0	0	0	0
15	CA	14	0	11	0	0
16	AA	313	0	0	10	0
16	BA	261	0	0	10	0
16	CA	229	0	0	3	1
16	DA	196	0	0	9	0
All	All	16585	0	14489	111	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 4.

All (111) 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:DA:74:PRO:O	16:DA:601:HOH:O	1.92	0.87
1:BA:125:ARG:NH1	16:BA:603:HOH:O	2.08	0.86
1:BA:25:GLN:N	1:BA:25:GLN:OE1	2.10	0.84
1:BA:269:ARG:NH1	1:BA:314:ASN:OD1	2.11	0.84
1:CA:149:ASP:OD2	1:CA:153:ARG:NH1	2.11	0.83
1:DA:471:ARG:NH1	16:DA:604:HOH:O	2.13	0.80
1:DA:25:GLN:N	1:DA:25:GLN:OE1	2.15	0.79
1:BA:78:GLN:OE1	16:BA:601:HOH:O	2.00	0.79
1:AA:25:GLN:N	1:AA:25:GLN:OE1	2.16	0.78
1:CA:25:GLN:OE1	1:CA:25:GLN:N	2.18	0.76
1:AA:97:ARG:NH1	16:AA:601:HOH:O	2.19	0.75
1:CA:218:PRO:HD2	1:CA:434:HIS:HB3	1.70	0.74
1:AA:25:GLN:NE2	16:AA:602:HOH:O	2.22	0.73
1:CA:29:GLN:HG3	1:CA:43:PRO:HB3	1.74	0.69
1:DA:413:GLU:OE2	16:DA:603:HOH:O	2.11	0.67
1:BA:165:ARG:NH1	16:BA:602:HOH:O	2.01	0.67
1:CA:444:TRP:O	16:CA:601:HOH:O	2.13	0.66
1:DA:345:PRO:HG3	8:N:1:NAG:H83	1.76	0.66
1:DA:184:ILE:O	16:DA:605:HOH:O	2.14	0.65
16:AA:903:HOH:O	2:A:6:FUC:O2	2.14	0.65
1:BA:34:GLU:OE2	1:BA:37:ARG:NH1	2.31	0.64
1:BA:146:ARG:NH1	16:BA:606:HOH:O	2.26	0.64
1:DA:269:ARG:NH1	1:DA:314:ASN:OD1	2.31	0.63
1:CA:46:SER:OG	1:CA:46:SER:O	2.16	0.62
1:DA:417:ARG:NH1	16:DA:602:HOH:O	2.10	0.62
1:CA:71:ASP:HB3	16:CA:754:HOH:O	1.99	0.61
1:CA:73:ARG:NH1	1:CA:428:GLU:OE1	2.35	0.60
2:C:2:NAG:O4	2:C:5:MAN:H2	2.04	0.58
1:DA:149:ASP:OD2	1:DA:153:ARG:NH1	2.38	0.57
1:BA:71:ASP:O	16:BA:604:HOH:O	2.17	0.57
1:AA:100[B]:HIS:ND1	16:AA:606:HOH:O	2.33	0.56
1:DA:106:SER:HB2	1:DA:114:ARG:HG2	1.89	0.55
1:AA:471:ARG:NH1	16:AA:611:HOH:O	2.40	0.54
1:CA:293:LEU:HD13	1:CA:392:HIS:CD2	2.42	0.54
13:CA:502:GOL:H11	16:CA:763:HOH:O	2.07	0.54
1:BA:29:GLN:HG3	1:BA:43:PRO:HB3	1.90	0.54
1:BA:64[A]:ARG:NH1	1:BA:102:ASN:OD1	2.41	0.54
1:AA:141:LYS:HD3	1:AA:265:LEU:HD21	1.89	0.53
1:DA:25:GLN:N	1:DA:160:VAL:O	2.41	0.53
1:CA:217:GLY:O	1:CA:356:ARG:HD3	2.09	0.53
1:AA:49:SER:HB2	1:AA:53:THR:HG21	1.90	0.53
1:AA:291:ASP:HB2	1:AA:393:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:269:ARG:HD3	1:DA:274:SER:HB2	1.92	0.52
1:BA:149:ASP:OD2	1:BA:153:ARG:NH1	2.44	0.51
1:DA:97:ARG:NH2	16:DA:608:HOH:O	2.26	0.50
1:AA:89:VAL:HG23	1:AA:92:LEU:HB2	1.93	0.50
1:BA:25:GLN:N	1:BA:160:VAL:O	2.45	0.50
1:CA:392:HIS:CD2	1:CA:393:LEU:HG	2.47	0.50
1:AA:224:HIS:CD2	1:AA:404:HIS:CE1	3.00	0.50
1:DA:322:PRO:HA	1:DA:325:GLN:HG3	1.93	0.49
1:CA:118:ARG:HD2	1:CA:242:PRO:HB3	1.94	0.49
1:DA:231:LEU:HA	16:DA:728:HOH:O	2.11	0.49
1:AA:71:ASP:HB3	16:AA:619:HOH:O	2.12	0.48
1:CA:28:ARG:NH1	11:R:1:NAG:H82	2.28	0.48
1:BA:71:ASP:HA	16:BA:810:HOH:O	2.13	0.48
1:AA:416:ARG:HH11	1:AA:416:ARG:HG2	1.79	0.48
1:AA:269:ARG:NH1	1:AA:314:ASN:OD1	2.46	0.47
1:CA:224:HIS:CD2	1:CA:404:HIS:CE1	3.02	0.47
1:DA:224:HIS:CD2	1:DA:404:HIS:CE1	3.02	0.47
1:AA:149:ASP:O	1:AA:153:ARG:HG3	2.15	0.46
1:BA:73:ARG:NH1	1:BA:428:GLU:OE1	2.48	0.46
1:BA:295:ASP:OD2	6:K:2:NAG:H5	2.15	0.46
1:CA:25:GLN:N	1:CA:160:VAL:O	2.48	0.46
1:AA:323:MET:HE2	16:AA:819:HOH:O	2.15	0.46
1:CA:28:ARG:HH12	11:R:1:NAG:H82	1.80	0.45
1:DA:208:PHE:CZ	1:DA:210:GLU:HB2	2.51	0.45
1:BA:240:GLN:HG2	16:BA:795:HOH:O	2.16	0.45
1:DA:217:GLY:O	1:DA:356:ARG:HD3	2.16	0.45
1:DA:338:GLU:OE2	1:DA:417:ARG:NH2	2.48	0.45
1:AA:25:GLN:N	1:AA:25:GLN:CD	2.70	0.45
1:BA:331:GLN:OE1	1:BA:471:ARG:HA	2.17	0.45
1:AA:153:ARG:HD3	16:AA:808:HOH:O	2.16	0.44
1:CA:269:ARG:NH1	1:CA:314:ASN:OD1	2.49	0.44
1:BA:82:ASP:OD2	16:BA:605:HOH:O	2.21	0.44
1:DA:161:ILE:HD13	1:DA:182:ILE:HD12	2.00	0.44
1:BA:286:TRP:HA	13:BA:501:GOL:H31	1.99	0.44
1:AA:294:GLU:HG3	16:AA:815:HOH:O	2.17	0.44
1:CA:233:LYS:O	1:CA:237:GLU:HG2	2.18	0.44
1:BA:58:SER:HB3	1:BA:64[B]:ARG:HH11	1.82	0.44
1:CA:392:HIS:NE2	1:CA:393:LEU:HG	2.33	0.44
1:DA:473:ASN:HB2	16:DA:604:HOH:O	2.18	0.43
1:DA:350:ASN:HA	1:DA:369:TYR:CE1	2.53	0.43
1:AA:69:THR:HA	16:AA:668:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:275:THR:OG1	1:DA:312:ARG:NH1	2.50	0.43
1:AA:73:ARG:HD2	1:AA:428:GLU:HB3	2.01	0.43
1:AA:370:ASP:O	1:AA:373:VAL:HG12	2.19	0.43
1:DA:71:ASP:OD1	1:DA:73:ARG:HG3	2.17	0.43
1:DA:68:VAL:HG23	1:DA:96:ASN:C	2.40	0.42
1:BA:389:GLY:HA3	16:BA:641:HOH:O	2.19	0.42
1:CA:233:LYS:HE3	1:CA:237:GLU:OE1	2.18	0.42
1:AA:68:VAL:CG2	1:AA:98:THR:HG23	2.48	0.42
1:AA:84:ARG:NH2	1:AA:201:LEU:O	2.52	0.42
1:AA:387:THR:HG23	1:AA:393:LEU:HD13	2.02	0.42
1:CA:66:GLU:CD	1:DA:436:ARG:HH12	2.22	0.42
1:AA:326:ARG:HB2	1:AA:326:ARG:HH11	1.85	0.42
1:BA:338:GLU:HG2	1:BA:417:ARG:HH22	1.85	0.42
1:BA:165:ARG:HD3	16:BA:602:HOH:O	2.19	0.41
1:BA:392:HIS:CD2	1:BA:393:LEU:HG	2.54	0.41
1:CA:84:ARG:NH2	1:CA:201:LEU:O	2.53	0.41
1:DA:228:LEU:HD11	1:DA:404:HIS:HB3	2.03	0.41
1:CA:118:ARG:CZ	2:A:2:NAG:H62	2.49	0.41
1:DA:393:LEU:HD22	1:DA:396:ASN:HD22	1.85	0.41
1:BA:392:HIS:NE2	1:BA:393:LEU:HG	2.35	0.41
1:CA:125:ARG:HH22	6:Q:1:NAG:H61	1.84	0.41
1:CA:348:TYR:CG	1:CA:349:SER:N	2.89	0.41
1:BA:49:SER:HB2	1:BA:53:THR:HG21	2.03	0.41
1:DA:276:LEU:HD21	1:DA:312:ARG:CZ	2.50	0.41
1:DA:393:LEU:HD22	1:DA:396:ASN:ND2	2.36	0.41
1:DA:71:ASP:HB3	16:DA:700:HOH:O	2.21	0.41
1:AA:201:LEU:HD23	1:AA:201:LEU:HA	1.82	0.41
1:CA:347:PHE:CG	1:CA:426:PRO:HG3	2.56	0.40

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)
3:B:5:MAN:O2	16:CA:665:HOH:O[1_655]	2.04	0.16

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	AA	446/450 (99%)	428 (96%)	18 (4%)	0	100 100
1	BA	446/450 (99%)	425 (95%)	20 (4%)	1 (0%)	47 55
1	CA	445/450 (99%)	429 (96%)	16 (4%)	0	100 100
1	DA	449/450 (100%)	423 (94%)	26 (6%)	0	100 100
All	All	1786/1800 (99%)	1705 (96%)	80 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BA	469	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	AA	397/399 (100%)	391 (98%)	6 (2%)	65 78
1	BA	397/399 (100%)	390 (98%)	7 (2%)	59 72
1	CA	396/399 (99%)	387 (98%)	9 (2%)	50 63
1	DA	400/399 (100%)	392 (98%)	8 (2%)	55 69
All	All	1590/1596 (100%)	1560 (98%)	30 (2%)	57 71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	193	TYR
1	AA	197	LYS
1	AA	278	SER
1	AA	377	HIS
1	AA	425	PHE
1	AA	438	TYR
1	BA	91	PRO
1	BA	193	TYR
1	BA	197	LYS
1	BA	206	GLU
1	BA	377	HIS
1	BA	425	PHE
1	BA	438	TYR
1	CA	46	SER
1	CA	49	SER
1	CA	91	PRO
1	CA	193	TYR
1	CA	274	SER
1	CA	326	ARG
1	CA	336	CYS
1	CA	377	HIS
1	CA	425	PHE
1	DA	60	SER
1	DA	193	TYR
1	DA	336	CYS
1	DA	363	SER
1	DA	377	HIS
1	DA	425	PHE
1	DA	438	TYR
1	DA	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	25	GLN
1	AA	124	GLN
1	BA	25	GLN
1	BA	240	GLN
1	CA	25	GLN
1	CA	78	GLN
1	DA	25	GLN
1	DA	78	GLN

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)

93 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	A	1	2,1	14,14,15	0.73	0	17,19,21	1.05	0
2	NAG	A	2	2	14,14,15	0.81	0	17,19,21	1.37	3 (17%)
2	BMA	A	3	2	11,11,12	0.94	0	15,15,17	2.25	2 (13%)
2	MAN	A	4	2	11,11,12	0.71	0	15,15,17	1.35	2 (13%)
2	MAN	A	5	2	11,11,12	0.67	0	15,15,17	1.45	2 (13%)
2	FUC	A	6	2	10,10,11	0.99	1 (10%)	14,14,16	2.08	5 (35%)
3	NAG	B	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	1.04	2 (11%)
3	NAG	B	2	3	14,14,15	0.73	0	17,19,21	1.25	2 (11%)
3	BMA	B	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.65	3 (20%)
3	MAN	B	4	3	11,11,12	0.69	0	15,15,17	1.80	2 (13%)
3	MAN	B	5	3	11,11,12	0.82	0	15,15,17	1.07	0
2	NAG	C	1	2,1	14,14,15	0.63	0	17,19,21	1.03	0
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	1.74	3 (17%)
2	BMA	C	3	2	11,11,12	0.96	1 (9%)	15,15,17	3.97	7 (46%)
2	MAN	C	4	2	11,11,12	0.76	0	15,15,17	1.47	1 (6%)
2	MAN	C	5	2	11,11,12	0.61	0	15,15,17	2.74	4 (26%)
2	FUC	C	6	2	10,10,11	0.77	0	14,14,16	1.24	2 (14%)
4	NAG	D	1	1,4	14,14,15	0.70	0	17,19,21	1.06	0
4	NAG	D	2	4	14,14,15	0.78	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	D	3	4	11,11,12	1.05	1 (9%)	15,15,17	2.62	5 (33%)
5	NAG	E	1	1,5	14,14,15	0.90	1 (7%)	17,19,21	1.09	1 (5%)
5	NAG	E	2	5	14,14,15	0.79	0	17,19,21	1.43	2 (11%)
5	BMA	E	3	5	11,11,12	0.93	1 (9%)	15,15,17	2.80	5 (33%)
5	FUC	E	4	5	10,10,11	0.70	0	14,14,16	1.26	1 (7%)
6	NAG	F	1	6,1	14,14,15	0.79	0	17,19,21	2.30	3 (17%)
6	NAG	F	2	6	14,14,15	0.66	0	17,19,21	1.14	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.78	0	17,19,21	1.19	2 (11%)
5	NAG	G	2	5	14,14,15	0.83	0	17,19,21	1.20	1 (5%)
5	BMA	G	3	5	11,11,12	0.96	1 (9%)	15,15,17	2.98	5 (33%)
5	FUC	G	4	5	10,10,11	0.82	0	14,14,16	1.25	1 (7%)
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
3	NAG	H	2	3	14,14,15	0.78	0	17,19,21	1.51	2 (11%)
3	BMA	H	3	3	11,11,12	0.90	0	15,15,17	1.63	4 (26%)
3	MAN	H	4	3	11,11,12	0.58	0	15,15,17	1.64	1 (6%)
3	MAN	H	5	3	11,11,12	0.73	0	15,15,17	2.69	5 (33%)
7	NAG	I	1	1,7	14,14,15	0.79	0	17,19,21	2.26	3 (17%)
7	NAG	I	2	7	14,14,15	0.69	0	17,19,21	1.02	1 (5%)
7	FUC	I	3	7	10,10,11	0.95	1 (10%)	14,14,16	1.10	0
6	NAG	J	1	6,1	14,14,15	0.69	0	17,19,21	1.10	1 (5%)
6	NAG	J	2	6	14,14,15	0.70	0	17,19,21	1.18	2 (11%)
6	NAG	K	1	6,1	14,14,15	0.79	0	17,19,21	1.07	2 (11%)
6	NAG	K	2	6	14,14,15	0.63	0	17,19,21	1.04	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
2	NAG	L	2	2	14,14,15	0.74	0	17,19,21	1.27	3 (17%)
2	BMA	L	3	2	11,11,12	0.97	1 (9%)	15,15,17	1.89	2 (13%)
2	MAN	L	4	2	11,11,12	0.58	0	15,15,17	1.24	1 (6%)
2	MAN	L	5	2	11,11,12	0.63	0	15,15,17	1.20	1 (6%)
2	FUC	L	6	2	10,10,11	0.79	0	14,14,16	1.06	0
6	NAG	M	1	6,1	14,14,15	0.76	0	17,19,21	1.23	1 (5%)
6	NAG	M	2	6	14,14,15	0.74	0	17,19,21	0.90	0
8	NAG	N	1	8,1	14,14,15	0.88	0	17,19,21	1.14	1 (5%)
8	NAG	N	2	8	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
8	BMA	N	3	8	11,11,12	0.78	0	15,15,17	2.94	6 (40%)
8	MAN	N	4	8	11,11,12	0.83	0	15,15,17	1.66	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MAN	N	5	8	11,11,12	0.65	0	15,15,17	2.29	2 (13%)
8	MAN	N	6	8	11,11,12	0.69	0	15,15,17	1.55	2 (13%)
8	FUC	N	7	8	10,10,11	0.77	0	14,14,16	1.21	1 (7%)
9	NAG	O	1	9,1	14,14,15	0.80	0	17,19,21	0.94	1 (5%)
9	NAG	O	2	9	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
9	BMA	O	3	9	11,11,12	0.80	0	15,15,17	2.82	6 (40%)
9	MAN	O	4	9	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
9	MAN	O	5	9	11,11,12	0.60	0	15,15,17	1.51	1 (6%)
9	MAN	O	6	9	11,11,12	0.72	0	15,15,17	1.23	1 (6%)
9	MAN	O	7	9	11,11,12	0.69	0	15,15,17	1.70	2 (13%)
10	NAG	P	1	10,1	14,14,15	0.72	0	17,19,21	1.29	2 (11%)
10	NAG	P	2	10	14,14,15	0.79	0	17,19,21	1.41	3 (17%)
10	BMA	P	3	10	11,11,12	0.94	0	15,15,17	2.67	5 (33%)
10	MAN	P	4	10	11,11,12	0.64	0	15,15,17	2.01	1 (6%)
10	MAN	P	5	10	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
10	MAN	P	6	10	11,11,12	0.77	0	15,15,17	1.75	2 (13%)
6	NAG	Q	1	6,1	14,14,15	0.63	0	17,19,21	1.26	3 (17%)
6	NAG	Q	2	6	14,14,15	0.69	0	17,19,21	1.19	2 (11%)
11	NAG	R	1	11,1	14,14,15	0.85	1 (7%)	17,19,21	2.49	4 (23%)
11	FUC	R	2	11	10,10,11	0.71	0	14,14,16	1.62	3 (21%)
5	NAG	S	1	1,5	14,14,15	0.94	1 (7%)	17,19,21	1.43	2 (11%)
5	NAG	S	2	5	14,14,15	0.80	0	17,19,21	1.04	0
5	BMA	S	3	5	11,11,12	0.96	1 (9%)	15,15,17	2.45	5 (33%)
5	FUC	S	4	5	10,10,11	0.76	0	14,14,16	1.17	0
2	NAG	T	1	2,1	14,14,15	0.80	0	17,19,21	1.02	1 (5%)
2	NAG	T	2	2	14,14,15	0.78	0	17,19,21	0.98	1 (5%)
2	BMA	T	3	2	11,11,12	1.05	1 (9%)	15,15,17	2.16	5 (33%)
2	MAN	T	4	2	11,11,12	0.70	0	15,15,17	1.95	4 (26%)
2	MAN	T	5	2	11,11,12	0.59	0	15,15,17	1.73	2 (13%)
2	FUC	T	6	2	10,10,11	0.84	1 (10%)	14,14,16	1.00	0
6	NAG	U	1	6,1	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
6	NAG	U	2	6	14,14,15	0.72	0	17,19,21	1.26	3 (17%)
6	NAG	V	1	6,1	14,14,15	0.67	0	17,19,21	1.42	3 (17%)
6	NAG	V	2	6	14,14,15	0.69	0	17,19,21	1.23	2 (11%)
4	NAG	W	1	1,4	14,14,15	0.73	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	W	2	4	14,14,15	0.72	0	17,19,21	1.29	1 (5%)
4	BMA	W	3	4	11,11,12	1.04	1 (9%)	15,15,17	2.50	6 (40%)
11	NAG	X	1	11,1	14,14,15	0.76	0	17,19,21	2.67	5 (29%)
11	FUC	X	2	11	10,10,11	0.82	1 (10%)	14,14,16	2.28	5 (35%)

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	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	2/2/19/22	0/1/1/1
2	MAN	A	5	2	-	0/2/19/22	0/1/1/1
2	FUC	A	6	2	-	-	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	MAN	B	5	3	-	2/2/19/22	0/1/1/1
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	FUC	C	6	2	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	FUC	E	4	5	-	-	0/1/1/1
6	NAG	F	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	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	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	G	4	5	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	1/1/1/1
7	NAG	I	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	FUC	I	3	7	-	-	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
2	MAN	L	4	2	-	2/2/19/22	0/1/1/1
2	MAN	L	5	2	-	0/2/19/22	0/1/1/1
2	FUC	L	6	2	-	-	0/1/1/1
6	NAG	M	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
8	NAG	N	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	BMA	N	3	8	-	0/2/19/22	0/1/1/1
8	MAN	N	4	8	-	0/2/19/22	0/1/1/1
8	MAN	N	5	8	-	2/2/19/22	1/1/1/1
8	MAN	N	6	8	-	0/2/19/22	0/1/1/1
8	FUC	N	7	8	-	-	0/1/1/1
9	NAG	O	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	O	2	9	-	1/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
9	MAN	O	4	9	-	2/2/19/22	0/1/1/1
9	MAN	O	5	9	-	0/2/19/22	0/1/1/1
9	MAN	O	6	9	-	2/2/19/22	0/1/1/1
9	MAN	O	7	9	-	2/2/19/22	0/1/1/1
10	NAG	P	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	2/6/23/26	0/1/1/1
10	BMA	P	3	10	-	0/2/19/22	0/1/1/1
10	MAN	P	4	10	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	P	5	10	-	2/2/19/22	0/1/1/1
10	MAN	P	6	10	-	2/2/19/22	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
11	NAG	R	1	11,1	-	5/6/23/26	0/1/1/1
11	FUC	R	2	11	-	-	0/1/1/1
5	NAG	S	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	FUC	S	4	5	-	-	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	0/2/19/22	0/1/1/1
2	MAN	T	5	2	-	2/2/19/22	0/1/1/1
2	FUC	T	6	2	-	-	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
11	NAG	X	1	11,1	-	2/6/23/26	0/1/1/1
11	FUC	X	2	11	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C2-C3	2.68	1.56	1.52
2	T	3	BMA	C2-C3	2.60	1.56	1.52
3	B	3	BMA	C2-C3	2.53	1.56	1.52
4	W	3	BMA	C2-C3	2.49	1.56	1.52
5	G	3	BMA	C2-C3	2.34	1.56	1.52
7	I	3	FUC	O5-C1	-2.27	1.40	1.43
5	S	1	NAG	C1-C2	2.27	1.55	1.52
5	S	3	BMA	C2-C3	2.24	1.55	1.52
2	C	3	BMA	C2-C3	2.23	1.55	1.52
3	B	1	NAG	O5-C1	-2.22	1.40	1.43
11	X	2	FUC	C1-C2	2.21	1.57	1.52
5	E	3	BMA	C2-C3	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	C1-C2	2.07	1.55	1.52
2	L	3	BMA	C2-C3	2.03	1.55	1.52
11	R	1	NAG	C1-C2	2.02	1.55	1.52
2	T	6	FUC	O5-C1	-2.01	1.40	1.43
2	A	6	FUC	O5-C1	-2.00	1.40	1.43

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	C1-O5-C5	11.17	127.32	112.19
5	G	3	BMA	C1-O5-C5	8.91	124.26	112.19
5	E	3	BMA	C1-O5-C5	8.80	124.12	112.19
9	O	3	BMA	C1-O5-C5	8.73	124.02	112.19
2	C	5	MAN	C1-O5-C5	8.37	123.53	112.19
10	P	3	BMA	C1-O5-C5	8.24	123.35	112.19
8	N	3	BMA	C1-O5-C5	8.14	123.23	112.19
6	F	1	NAG	C2-N2-C7	7.76	133.95	122.90
7	I	1	NAG	C2-N2-C7	7.58	133.69	122.90
11	R	1	NAG	C2-N2-C7	7.56	133.67	122.90
4	D	3	BMA	C1-O5-C5	7.35	122.15	112.19
8	N	5	MAN	C1-O5-C5	7.11	121.83	112.19
2	A	3	BMA	C1-O5-C5	7.08	121.79	112.19
5	S	3	BMA	C1-O5-C5	6.96	121.63	112.19
10	P	4	MAN	C1-O5-C5	6.92	121.56	112.19
4	W	3	BMA	C1-O5-C5	6.90	121.54	112.19
11	X	1	NAG	C2-N2-C7	6.77	132.55	122.90
3	H	5	MAN	C3-C4-C5	-6.08	99.39	110.24
2	C	3	BMA	C1-C2-C3	5.98	117.02	109.67
2	L	3	BMA	C1-O5-C5	5.97	120.28	112.19
11	X	1	NAG	C1-C2-N2	5.79	120.37	110.49
11	X	2	FUC	C1-C2-C3	5.59	116.54	109.67
3	B	4	MAN	C1-O5-C5	5.12	119.12	112.19
9	O	5	MAN	C1-O5-C5	5.00	118.97	112.19
3	H	5	MAN	C2-C3-C4	-4.93	102.36	110.89
2	A	6	FUC	C1-C2-C3	-4.88	103.67	109.67
3	H	4	MAN	C1-O5-C5	4.87	118.79	112.19
8	N	6	MAN	C1-O5-C5	4.81	118.72	112.19
2	T	4	MAN	C1-O5-C5	4.79	118.68	112.19
9	O	7	MAN	C1-O5-C5	4.77	118.66	112.19
10	P	6	MAN	C1-O5-C5	4.62	118.45	112.19
2	T	3	BMA	C1-O5-C5	4.58	118.39	112.19
3	H	5	MAN	O3-C3-C4	4.57	120.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	5	MAN	C1-O5-C5	4.52	118.31	112.19
2	C	5	MAN	C1-C2-C3	4.49	115.19	109.67
2	C	3	BMA	O5-C1-C2	4.45	117.65	110.77
2	C	3	BMA	C2-C3-C4	4.37	118.45	110.89
3	H	2	NAG	C1-O5-C5	4.35	118.08	112.19
8	N	3	BMA	O3-C3-C2	-4.29	101.77	109.99
11	R	1	NAG	O5-C5-C6	4.22	113.83	107.20
5	E	2	NAG	C2-N2-C7	4.21	128.89	122.90
2	C	4	MAN	C1-O5-C5	4.20	117.88	112.19
11	X	2	FUC	C1-O5-C5	4.12	122.12	112.78
2	C	2	NAG	C4-C3-C2	-4.09	105.02	111.02
5	G	3	BMA	C3-C4-C5	3.95	117.28	110.24
8	N	4	MAN	C1-O5-C5	3.94	117.53	112.19
11	X	1	NAG	O5-C1-C2	-3.90	105.13	111.29
5	S	3	BMA	C3-C4-C5	3.87	117.14	110.24
8	N	5	MAN	C1-C2-C3	3.83	114.37	109.67
4	W	2	NAG	C2-N2-C7	3.79	128.30	122.90
4	W	3	BMA	C3-C4-C5	3.76	116.94	110.24
4	D	3	BMA	C3-C4-C5	3.74	116.91	110.24
2	A	4	MAN	C1-O5-C5	3.69	117.19	112.19
8	N	4	MAN	O2-C2-C3	3.68	117.50	110.14
2	L	4	MAN	C1-O5-C5	3.65	117.14	112.19
5	S	1	NAG	O4-C4-C3	-3.64	101.92	110.35
2	C	2	NAG	C1-O5-C5	3.61	117.08	112.19
2	C	2	NAG	C3-C4-C5	-3.61	103.81	110.24
2	A	5	MAN	C1-O5-C5	3.57	117.03	112.19
4	D	3	BMA	C2-C3-C4	3.56	117.05	110.89
5	E	3	BMA	C3-C4-C5	3.52	116.51	110.24
10	P	3	BMA	C3-C4-C5	3.51	116.50	110.24
2	C	3	BMA	C3-C4-C5	3.51	116.50	110.24
8	N	3	BMA	C2-C3-C4	3.49	116.94	110.89
9	O	4	MAN	C1-O5-C5	3.47	116.89	112.19
6	V	2	NAG	O5-C1-C2	-3.41	105.90	111.29
6	V	1	NAG	C3-C4-C5	-3.40	104.17	110.24
2	T	3	BMA	C2-C3-C4	3.40	116.78	110.89
9	O	7	MAN	C1-C2-C3	3.38	113.82	109.67
6	F	2	NAG	C1-O5-C5	3.38	116.77	112.19
3	B	3	BMA	C1-O5-C5	3.37	116.76	112.19
11	R	2	FUC	C1-O5-C5	3.37	120.41	112.78
2	T	3	BMA	C1-C2-C3	3.36	113.80	109.67
2	T	4	MAN	C3-C4-C5	-3.30	104.34	110.24
3	H	3	BMA	O6-C6-C5	-3.28	100.05	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	O4-C4-C3	-3.27	102.79	110.35
2	A	6	FUC	O5-C1-C2	-3.27	105.73	110.77
8	N	1	NAG	O3-C3-C2	-3.23	102.78	109.47
11	R	2	FUC	C1-C2-C3	3.20	113.60	109.67
9	O	6	MAN	C1-O5-C5	3.18	116.50	112.19
5	G	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	H	5	MAN	O4-C4-C5	3.17	117.17	109.30
2	T	4	MAN	C1-C2-C3	3.17	113.56	109.67
2	C	5	MAN	O5-C1-C2	3.16	115.65	110.77
9	O	3	BMA	C3-C4-C5	3.13	115.82	110.24
6	F	1	NAG	C8-C7-N2	3.02	121.21	116.10
11	X	1	NAG	O7-C7-N2	3.00	127.46	121.95
2	T	5	MAN	C3-C4-C5	-2.99	104.90	110.24
2	C	3	BMA	O3-C3-C2	-2.98	104.29	109.99
3	B	3	BMA	O5-C5-C6	2.98	111.87	107.20
8	N	3	BMA	C3-C4-C5	2.97	115.54	110.24
11	R	1	NAG	C8-C7-N2	2.97	121.13	116.10
5	G	3	BMA	C2-C3-C4	2.96	116.01	110.89
5	G	3	BMA	O5-C5-C4	2.94	117.98	110.83
2	L	5	MAN	C1-O5-C5	2.93	116.16	112.19
3	B	4	MAN	C1-C2-C3	2.84	113.16	109.67
6	Q	1	NAG	O4-C4-C3	-2.77	103.95	110.35
2	C	3	BMA	O5-C5-C4	2.76	117.55	110.83
8	N	2	NAG	C1-O5-C5	2.76	115.93	112.19
6	V	1	NAG	C1-O5-C5	2.76	115.93	112.19
2	A	6	FUC	O5-C5-C4	2.75	114.46	109.52
10	P	6	MAN	C3-C4-C5	2.75	115.14	110.24
11	X	1	NAG	C8-C7-N2	-2.74	111.46	116.10
2	A	2	NAG	O4-C4-C3	-2.74	104.02	110.35
5	E	4	FUC	C3-C4-C5	-2.74	105.51	109.77
7	I	1	NAG	C3-C4-C5	-2.72	105.39	110.24
10	P	3	BMA	C2-C3-C4	2.70	115.57	110.89
5	G	2	NAG	C4-C3-C2	2.69	114.97	111.02
4	W	3	BMA	O4-C4-C3	-2.69	104.14	110.35
5	G	4	FUC	C1-O5-C5	2.68	118.85	112.78
7	I	1	NAG	C8-C7-N2	2.67	120.62	116.10
3	H	3	BMA	O3-C3-C4	2.67	116.51	110.35
5	S	3	BMA	C2-C3-C4	2.66	115.50	110.89
9	O	3	BMA	O5-C5-C4	2.64	117.24	110.83
8	N	3	BMA	O4-C4-C3	-2.63	104.27	110.35
11	X	2	FUC	C3-C4-C5	-2.62	105.70	109.77
6	U	1	NAG	O5-C1-C2	-2.61	107.17	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	1	NAG	O5-C1-C2	-2.56	107.24	111.29
2	T	3	BMA	O5-C5-C6	2.55	111.21	107.20
4	W	3	BMA	O5-C5-C4	2.53	116.99	110.83
2	L	2	NAG	C1-C2-N2	2.53	114.81	110.49
6	K	1	NAG	C1-O5-C5	2.52	115.61	112.19
11	R	1	NAG	O7-C7-C8	-2.52	117.37	122.06
2	T	2	NAG	O5-C1-C2	-2.50	107.34	111.29
2	A	6	FUC	O3-C3-C4	2.50	116.13	110.35
11	R	2	FUC	O5-C5-C4	2.49	114.00	109.52
6	Q	1	NAG	C2-N2-C7	2.49	126.45	122.90
6	U	2	NAG	C2-N2-C7	2.49	126.45	122.90
6	J	1	NAG	O4-C4-C3	-2.48	104.62	110.35
10	P	3	BMA	O4-C4-C3	-2.48	104.62	110.35
8	N	2	NAG	O4-C4-C3	-2.48	104.63	110.35
11	X	2	FUC	O5-C1-C2	2.46	114.56	110.77
5	S	3	BMA	O5-C5-C4	2.45	116.80	110.83
10	P	2	NAG	O5-C1-C2	-2.44	107.43	111.29
10	P	2	NAG	O5-C5-C6	2.44	111.03	107.20
9	O	1	NAG	O4-C4-C3	-2.44	104.71	110.35
5	E	3	BMA	O5-C5-C4	2.43	116.75	110.83
6	Q	2	NAG	C1-O5-C5	2.43	115.48	112.19
2	C	6	FUC	C1-C2-C3	2.42	112.65	109.67
9	O	3	BMA	C2-C3-C4	2.42	115.08	110.89
2	L	2	NAG	C1-O5-C5	2.41	115.46	112.19
10	P	5	MAN	C1-O5-C5	2.41	115.46	112.19
3	H	3	BMA	C1-O5-C5	2.41	115.45	112.19
3	H	1	NAG	C2-N2-C7	-2.41	119.48	122.90
9	O	3	BMA	O4-C4-C3	-2.40	104.80	110.35
2	L	3	BMA	O3-C3-C4	2.40	115.89	110.35
2	A	2	NAG	O5-C1-C2	-2.39	107.51	111.29
5	E	3	BMA	C2-C3-C4	2.39	115.03	110.89
5	E	3	BMA	O4-C4-C3	-2.38	104.85	110.35
6	K	1	NAG	O4-C4-C3	-2.38	104.85	110.35
4	W	3	BMA	C2-C3-C4	2.36	114.98	110.89
2	A	6	FUC	O4-C4-C5	2.36	114.89	109.67
3	B	2	NAG	O5-C1-C2	-2.35	107.58	111.29
6	V	2	NAG	C1-O5-C5	2.34	115.36	112.19
5	E	2	NAG	O5-C1-C2	-2.34	107.60	111.29
2	A	5	MAN	O2-C2-C1	-2.33	104.39	109.15
2	L	1	NAG	C1-O5-C5	2.32	115.33	112.19
6	J	2	NAG	C3-C4-C5	-2.31	106.12	110.24
9	O	3	BMA	O3-C3-C2	-2.30	105.59	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	1	NAG	C1-C2-N2	2.30	114.41	110.49
9	O	4	MAN	O2-C2-C3	2.29	114.73	110.14
2	C	6	FUC	O3-C3-C2	-2.27	105.65	109.99
4	D	3	BMA	O5-C5-C4	2.26	116.34	110.83
10	P	1	NAG	C1-O5-C5	2.26	115.26	112.19
6	M	1	NAG	C1-O5-C5	2.25	115.24	112.19
9	O	2	NAG	C1-O5-C5	2.25	115.24	112.19
3	B	3	BMA	O3-C3-C4	2.24	115.53	110.35
8	N	3	BMA	O3-C3-C4	2.24	115.52	110.35
2	C	5	MAN	C3-C4-C5	-2.24	106.25	110.24
3	B	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	B	1	NAG	O5-C1-C2	-2.23	107.77	111.29
2	A	2	NAG	O3-C3-C2	-2.22	104.86	109.47
2	T	3	BMA	O4-C4-C3	-2.22	105.21	110.35
6	Q	2	NAG	C2-N2-C7	2.22	126.07	122.90
7	I	2	NAG	C1-O5-C5	2.22	115.20	112.19
5	S	3	BMA	O4-C4-C3	-2.21	105.24	110.35
6	U	2	NAG	O5-C5-C6	2.21	110.66	107.20
2	T	1	NAG	O4-C4-C5	2.19	114.75	109.30
6	K	2	NAG	C1-O5-C5	2.19	115.15	112.19
8	N	6	MAN	C1-C2-C3	2.17	112.33	109.67
8	N	7	FUC	O3-C3-C2	-2.17	105.85	109.99
6	F	1	NAG	O4-C4-C3	-2.16	105.36	110.35
2	L	2	NAG	O5-C1-C2	-2.15	107.89	111.29
10	P	2	NAG	C3-C4-C5	-2.15	106.40	110.24
2	T	4	MAN	O2-C2-C1	-2.14	104.77	109.15
5	E	1	NAG	O5-C1-C2	-2.13	107.92	111.29
2	A	3	BMA	O4-C4-C3	-2.13	105.42	110.35
6	U	2	NAG	C1-O5-C5	2.12	115.06	112.19
11	X	2	FUC	O4-C4-C5	2.11	114.35	109.67
3	H	5	MAN	O2-C2-C3	-2.11	105.91	110.14
6	Q	1	NAG	C4-C3-C2	2.11	114.11	111.02
5	G	3	BMA	C1-C2-C3	2.11	112.26	109.67
4	W	1	NAG	O4-C4-C3	-2.11	105.47	110.35
3	H	3	BMA	O5-C5-C4	2.10	115.93	110.83
10	P	3	BMA	O5-C5-C4	2.09	115.91	110.83
5	G	1	NAG	O4-C4-C3	-2.09	105.53	110.35
2	A	4	MAN	O3-C3-C2	-2.08	106.02	109.99
6	V	1	NAG	O4-C4-C5	2.08	114.45	109.30
3	B	2	NAG	O4-C4-C3	-2.07	105.57	110.35
6	J	2	NAG	O4-C4-C5	2.05	114.38	109.30
4	D	2	NAG	O5-C1-C2	-2.04	108.07	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	3	BMA	O2-C2-C3	2.03	114.21	110.14
4	D	3	BMA	O2-C2-C3	2.01	114.17	110.14

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
3	B	5	MAN	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
11	R	1	NAG	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
8	N	5	MAN	O5-C5-C6-O6
10	P	4	MAN	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
2	T	5	MAN	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
2	T	5	MAN	O5-C5-C6-O6
2	A	4	MAN	C4-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
9	O	4	MAN	O5-C5-C6-O6
3	B	5	MAN	C4-C5-C6-O6
9	O	4	MAN	C4-C5-C6-O6
11	R	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
11	R	1	NAG	C8-C7-N2-C2
11	R	1	NAG	O7-C7-N2-C2
10	P	4	MAN	C4-C5-C6-O6
2	A	4	MAN	O5-C5-C6-O6
9	O	6	MAN	C4-C5-C6-O6
2	L	4	MAN	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
9	O	6	MAN	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
10	P	5	MAN	C4-C5-C6-O6
9	O	7	MAN	C4-C5-C6-O6
11	X	1	NAG	C3-C2-N2-C7
2	L	4	MAN	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
8	N	5	MAN	C4-C5-C6-O6
10	P	5	MAN	O5-C5-C6-O6
11	X	1	NAG	C1-C2-N2-C7
10	P	2	NAG	O5-C5-C6-O6
9	O	7	MAN	O5-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7
6	F	1	NAG	C3-C2-N2-C7
7	I	1	NAG	C3-C2-N2-C7
11	R	1	NAG	C3-C2-N2-C7
9	O	2	NAG	C4-C5-C6-O6
10	P	2	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
6	F	1	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	5	MAN	C1-C2-C3-C4-C5-O5
3	H	5	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
6	K	2	NAG	1	0
11	R	1	NAG	2	0
2	A	6	FUC	1	0
3	B	5	MAN	0	1
2	A	2	NAG	1	0
2	C	5	MAN	1	0
8	N	1	NAG	1	0

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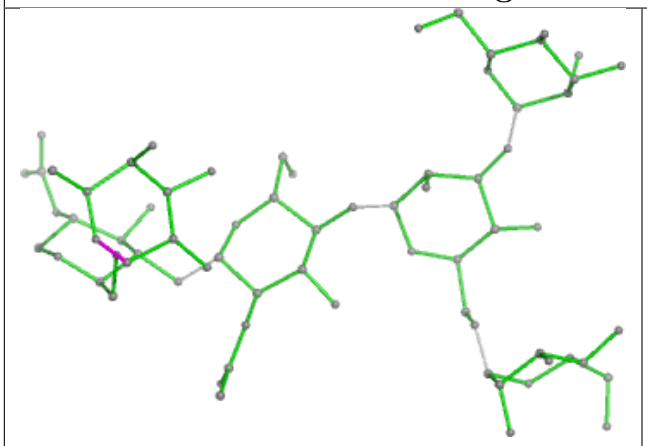
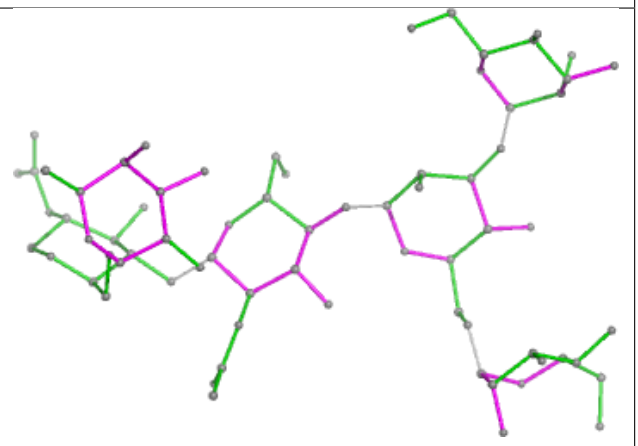
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	1	NAG	1	0

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

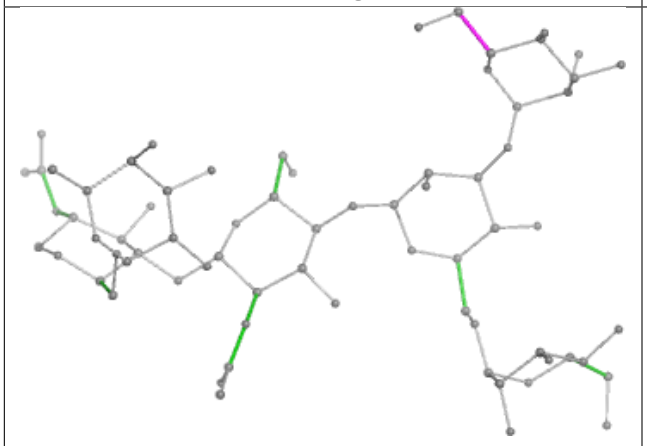
Oligosaccharide Chain A



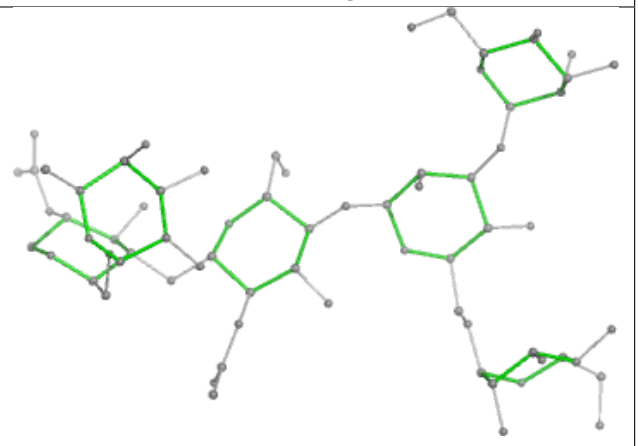
Bond lengths



Bond angles

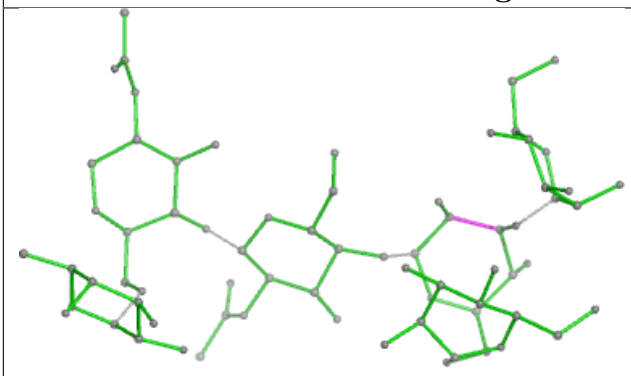


Torsions

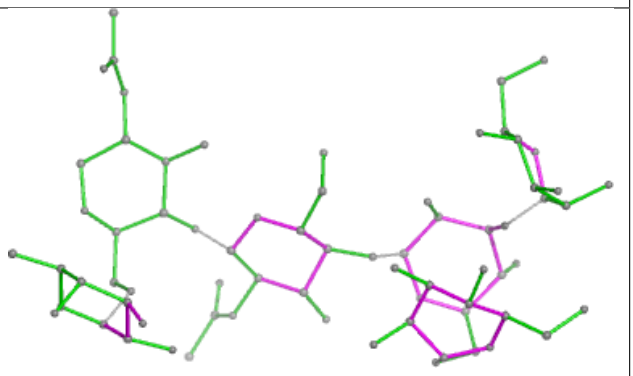


Rings

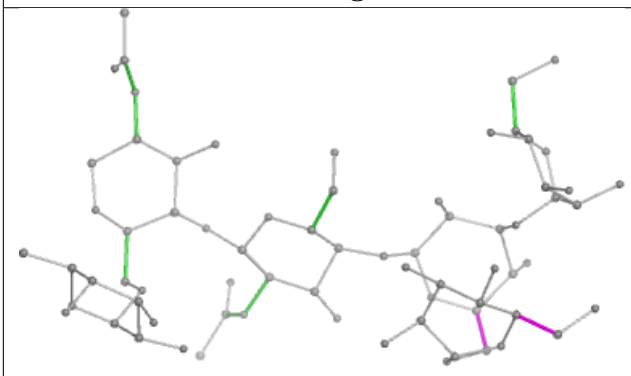
Oligosaccharide Chain C



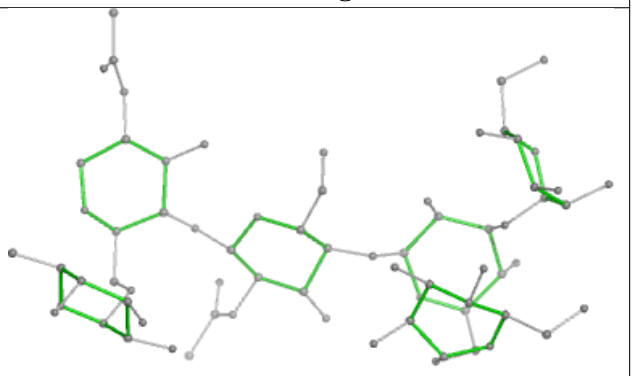
Bond lengths



Bond angles

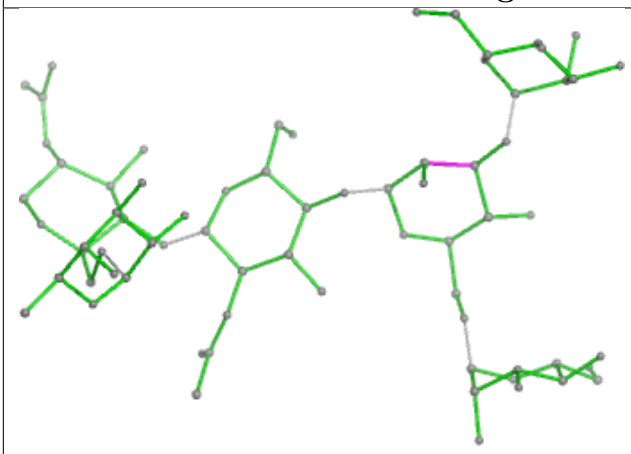


Torsions

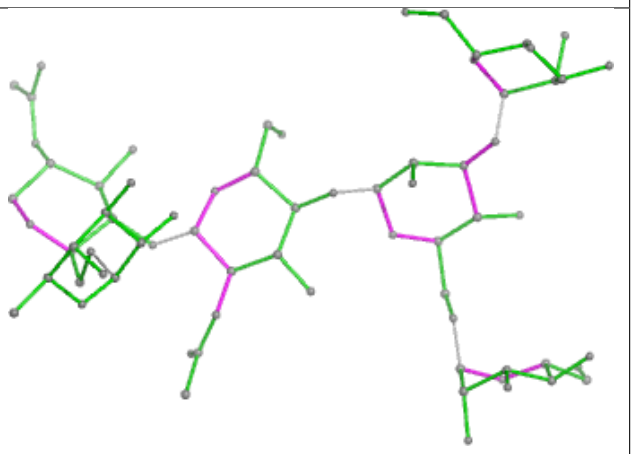


Rings

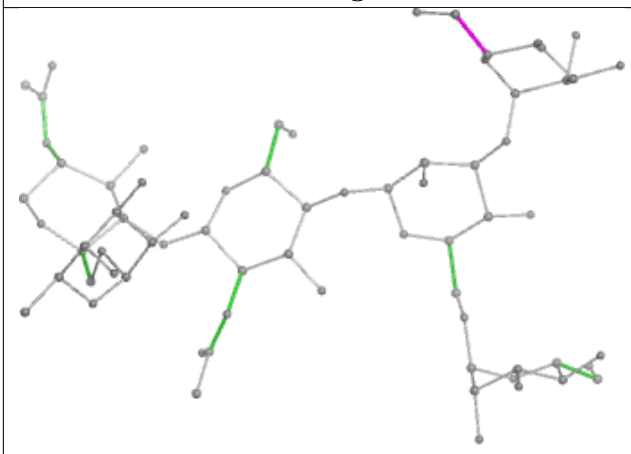
Oligosaccharide Chain L



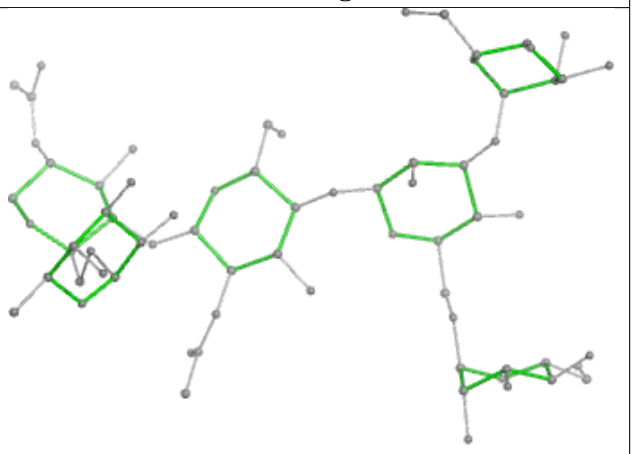
Bond lengths



Bond angles

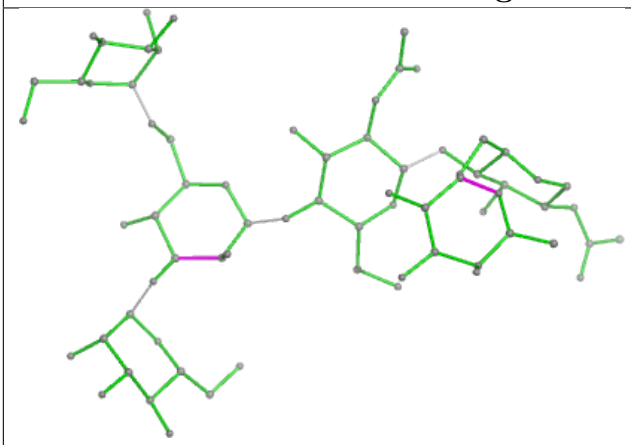


Torsions

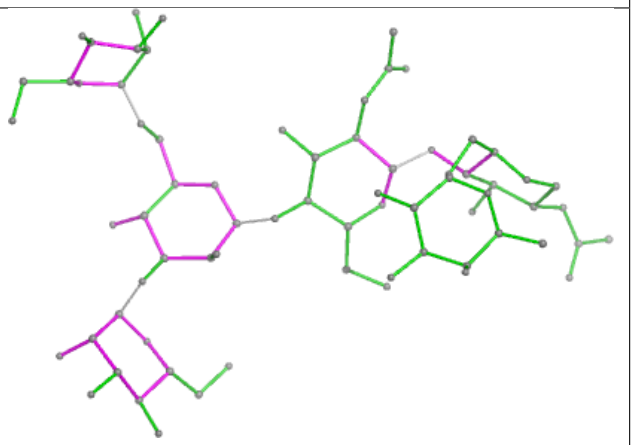


Rings

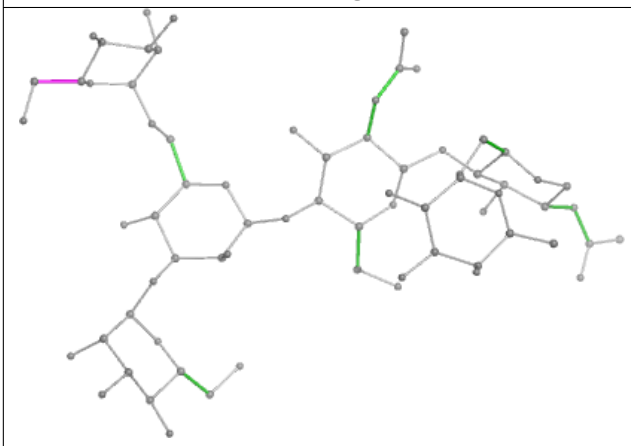
Oligosaccharide Chain T



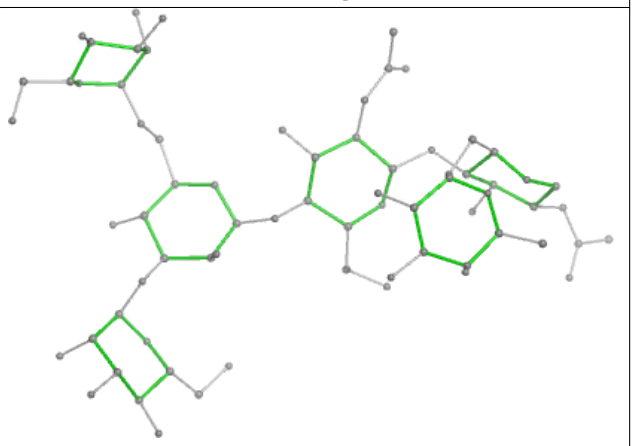
Bond lengths



Bond angles

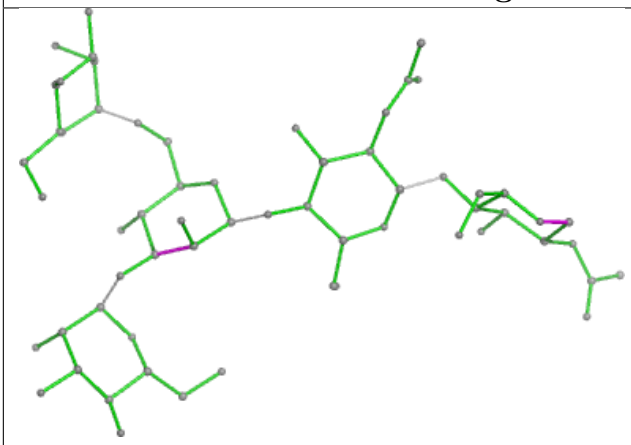


Torsions

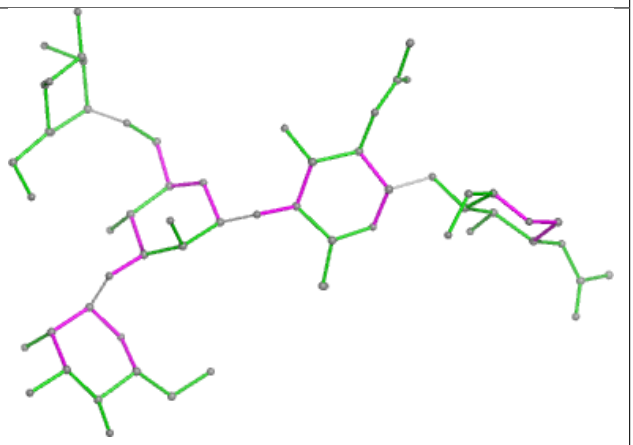


Rings

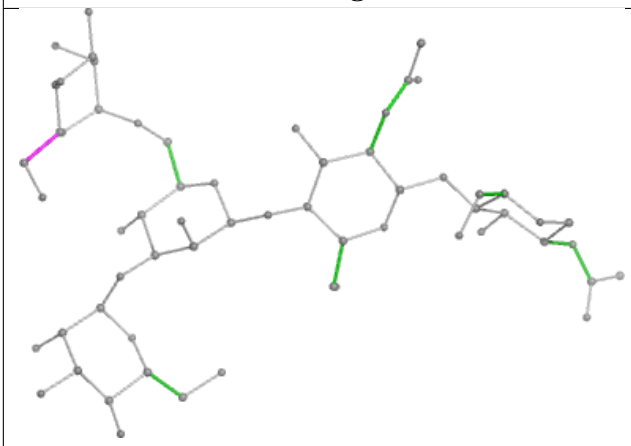
Oligosaccharide Chain B



Bond lengths



Bond angles



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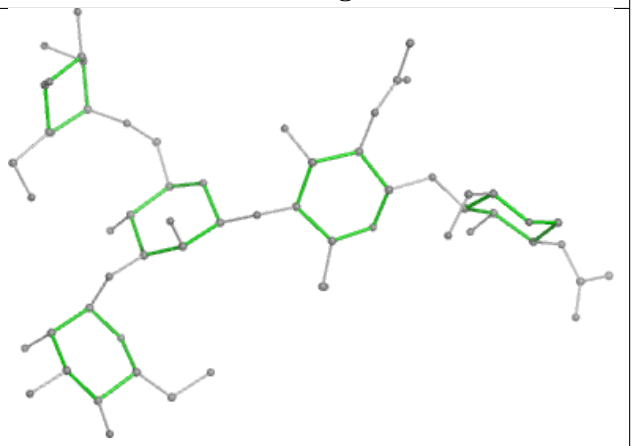
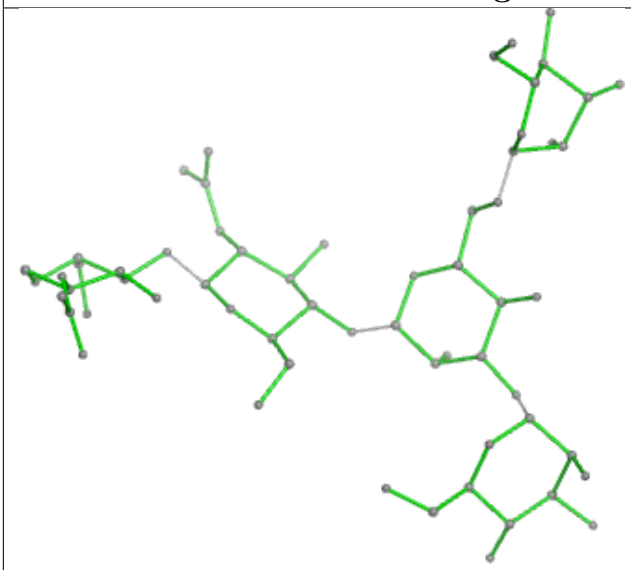
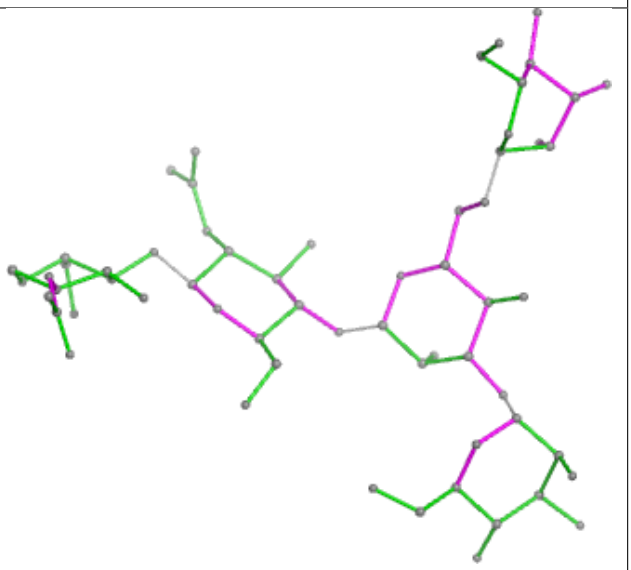


Rings

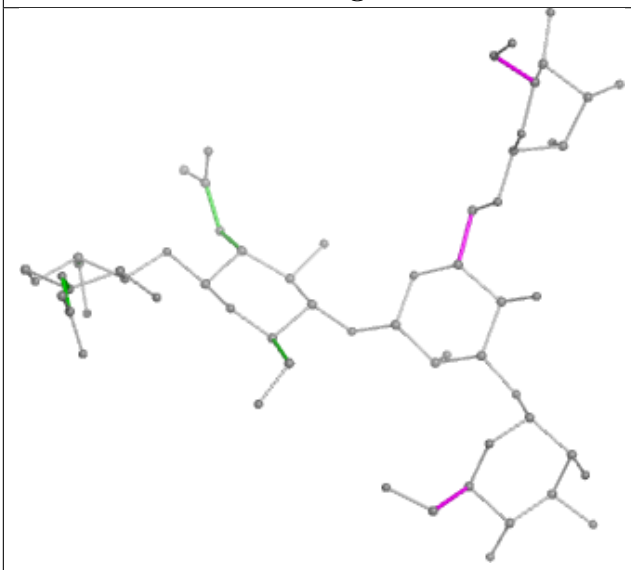
Oligosaccharide Chain H



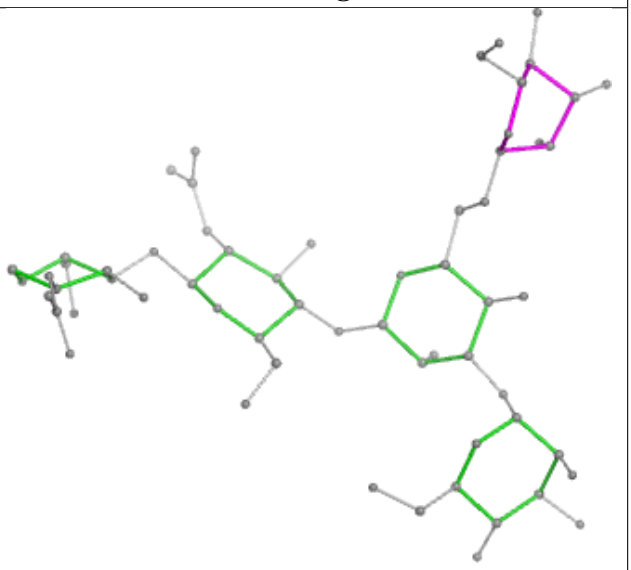
Bond lengths



Bond angles

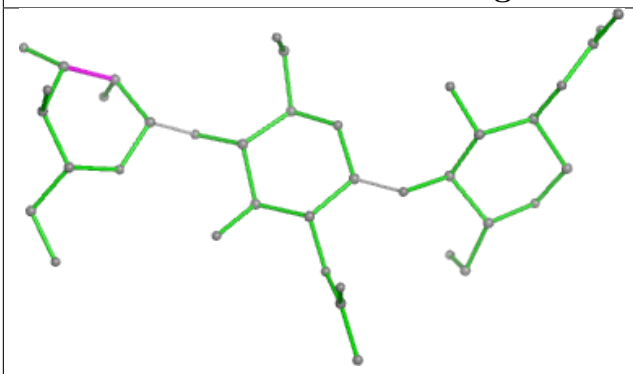


Torsions

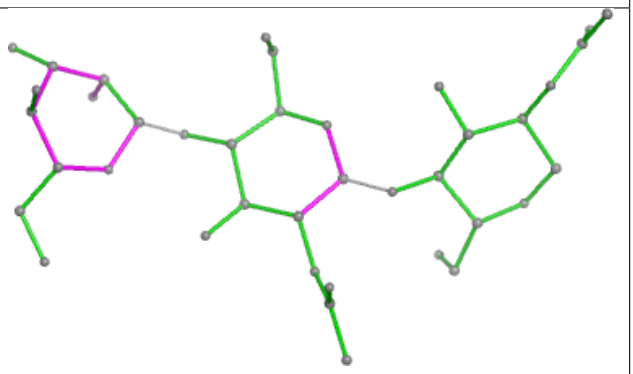


Rings

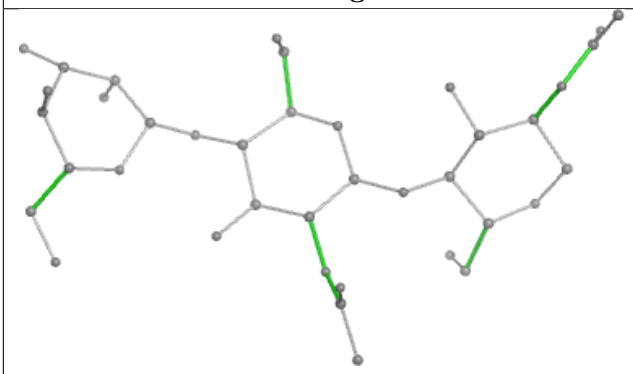
Oligosaccharide Chain D



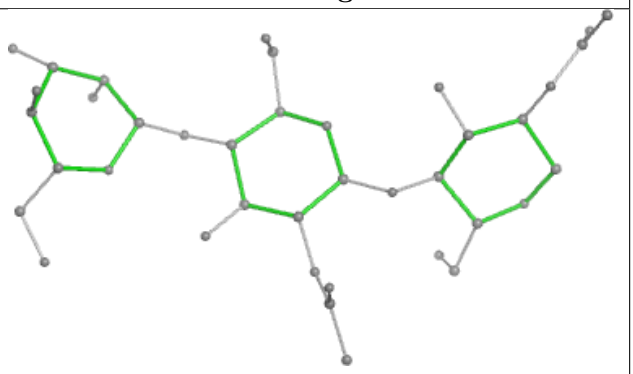
Bond lengths



Bond angles

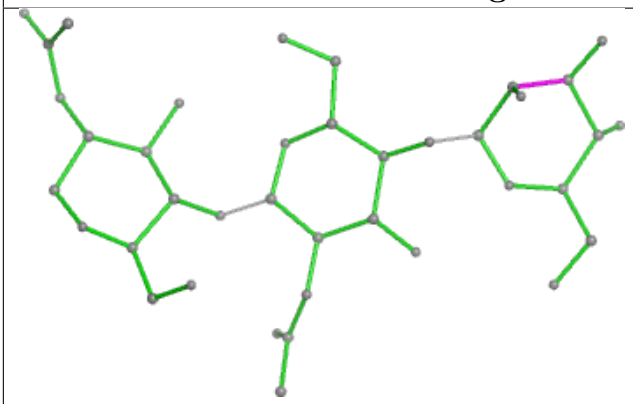


Torsions

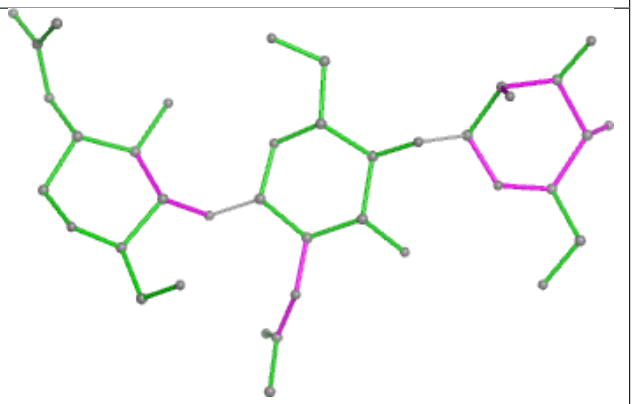


Rings

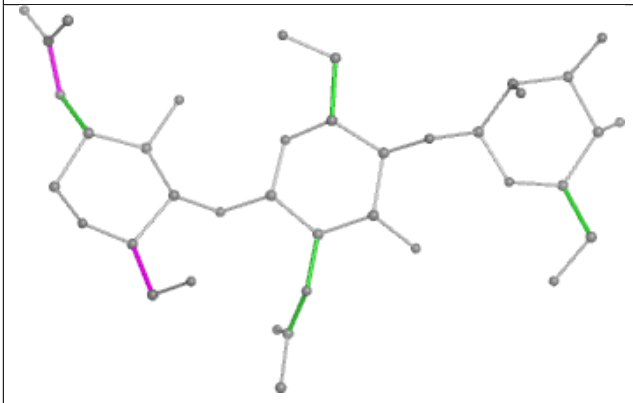
Oligosaccharide Chain W



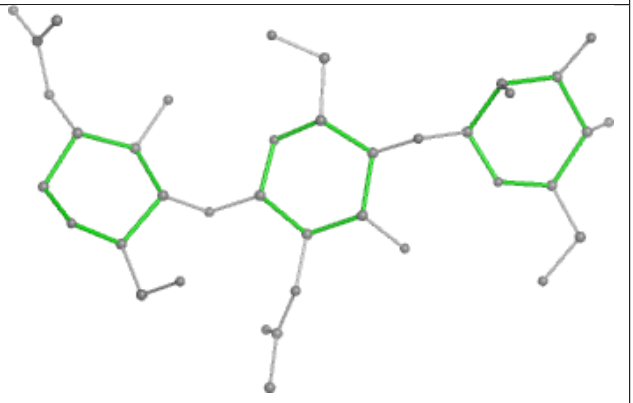
Bond lengths



Bond angles

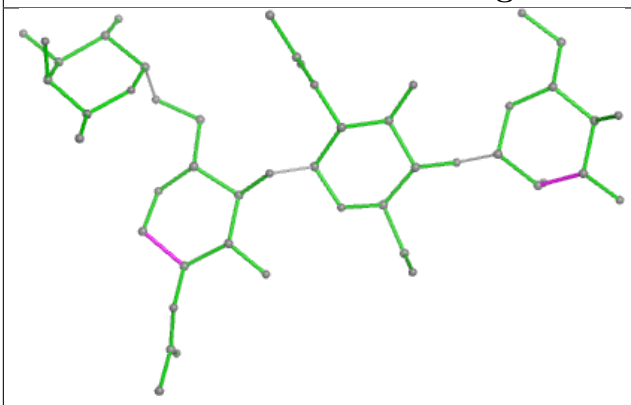


Torsions

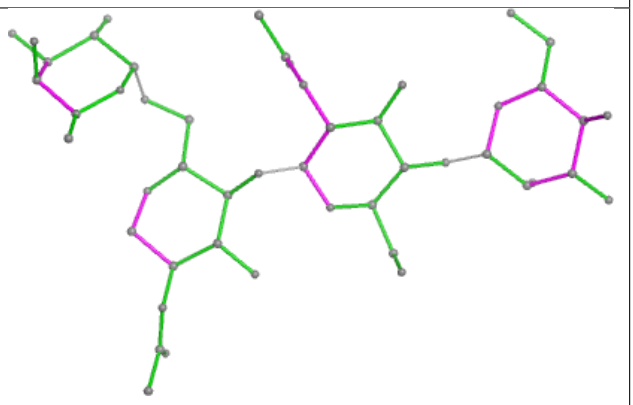


Rings

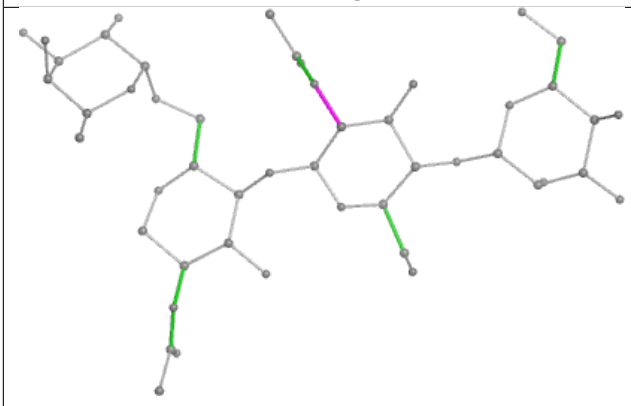
Oligosaccharide Chain E



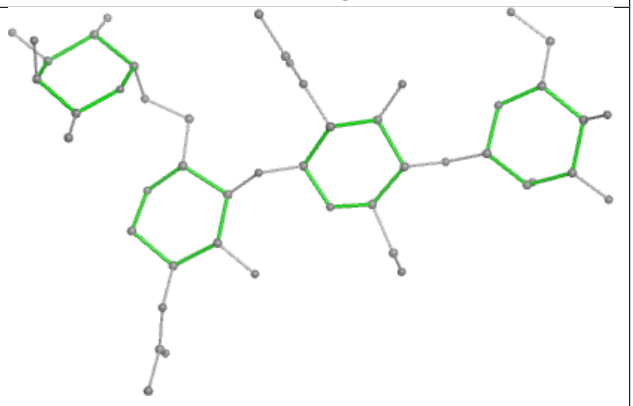
Bond lengths



Bond angles

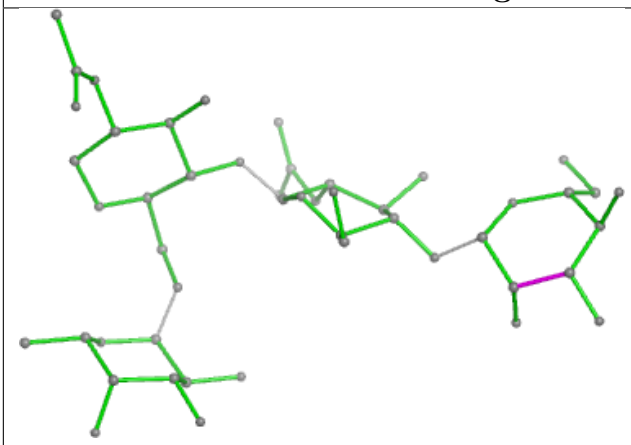


Torsions



Rings

Oligosaccharide Chain G



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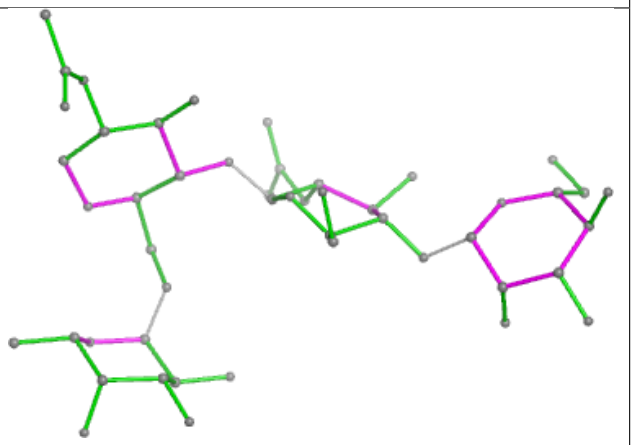
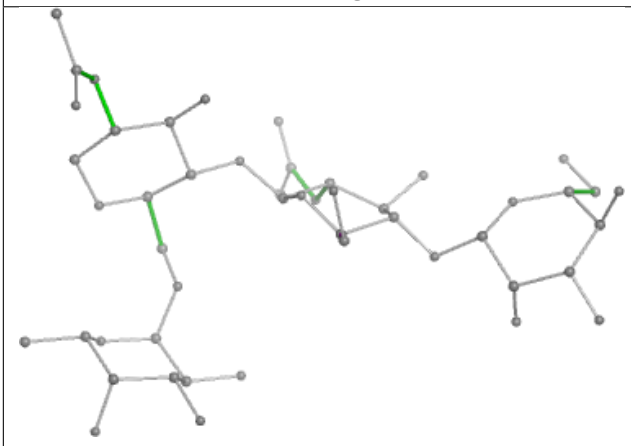
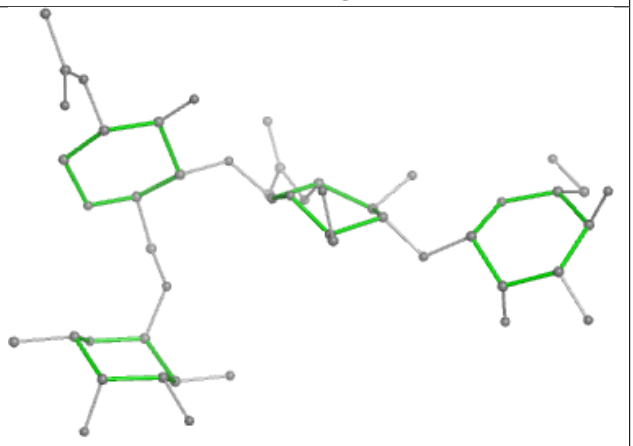


Bond angles

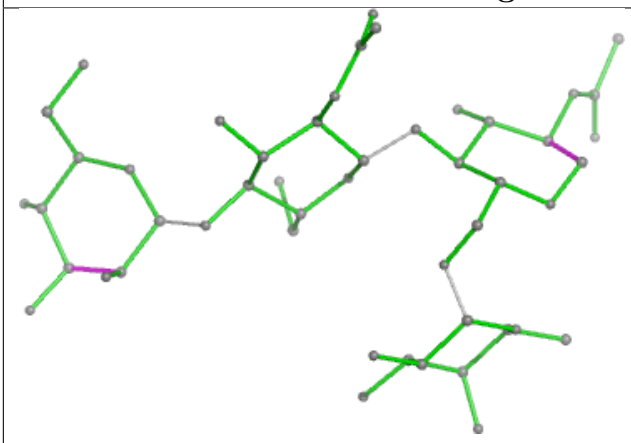


Torsions

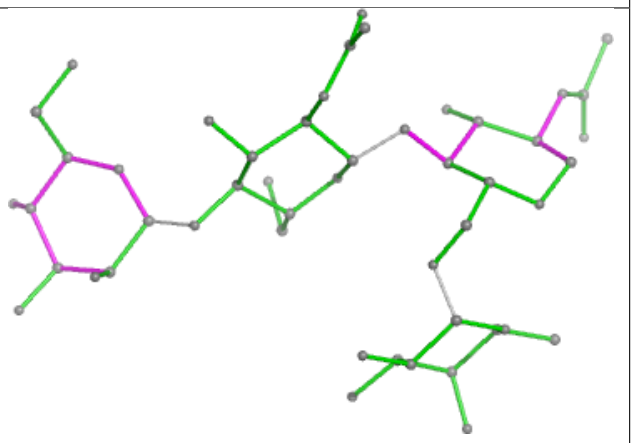


Rings

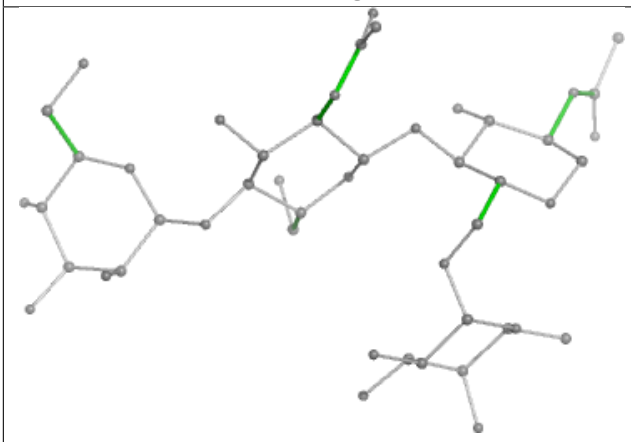
Oligosaccharide Chain S



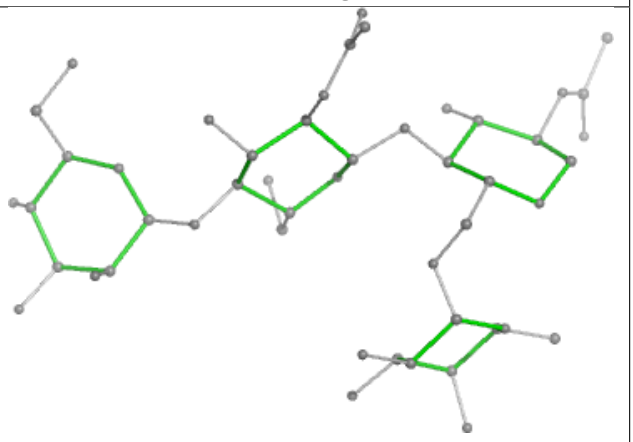
Bond lengths



Bond angles

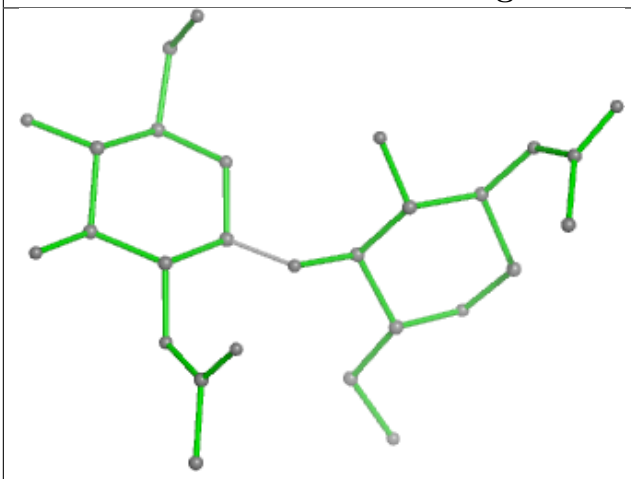


Torsions

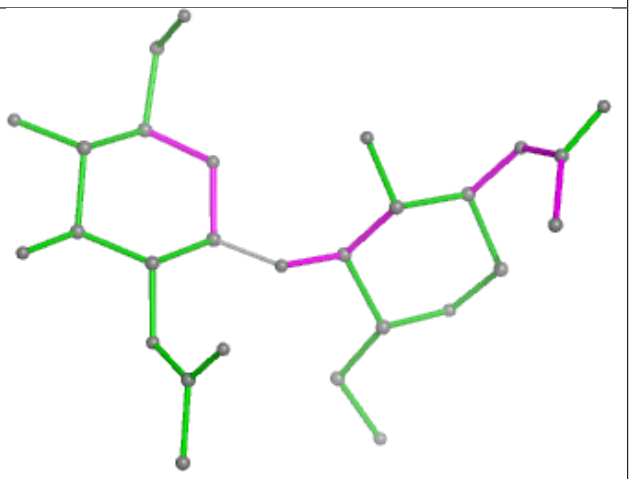


Rings

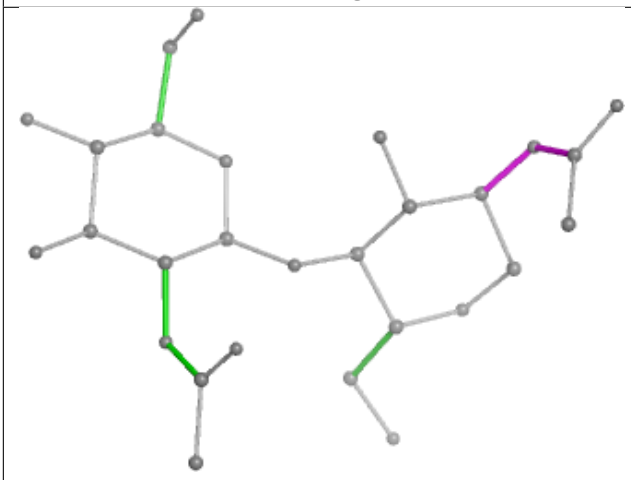
Oligosaccharide Chain F



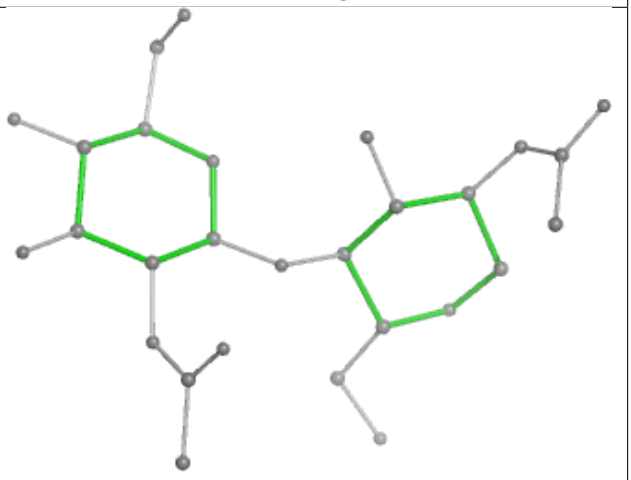
Bond lengths



Bond angles

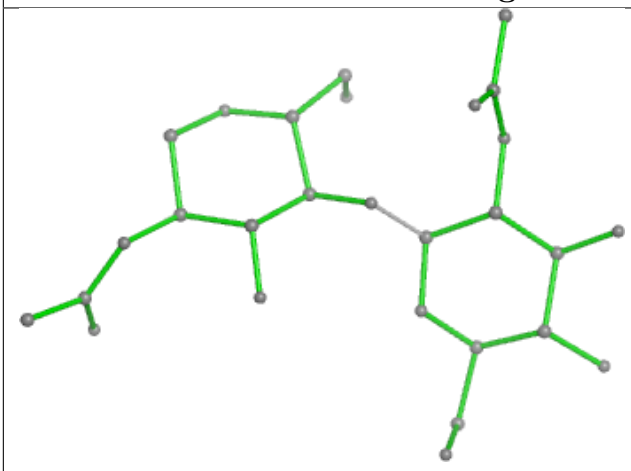


Torsions

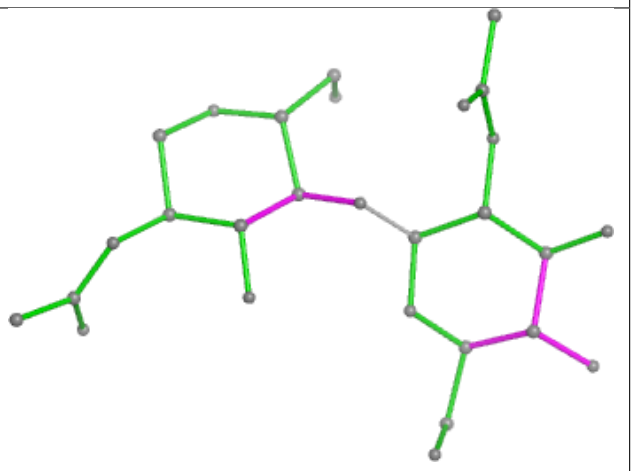


Rings

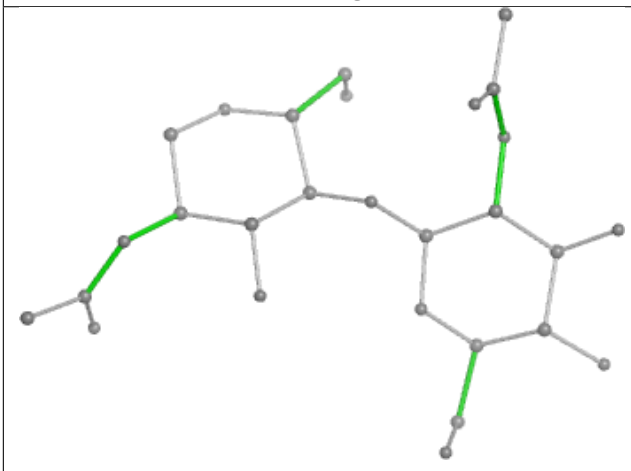
Oligosaccharide Chain J



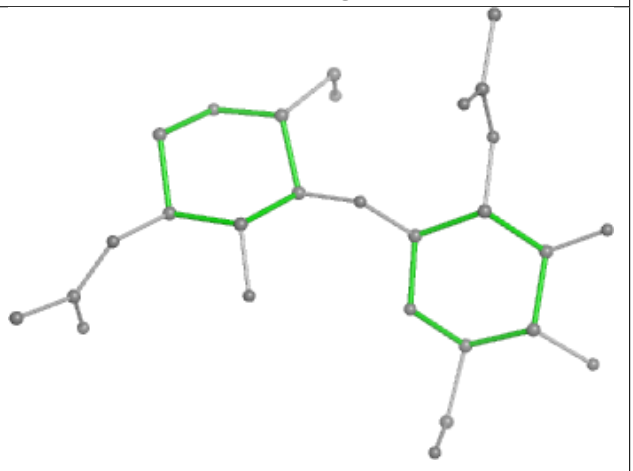
Bond lengths



Bond angles

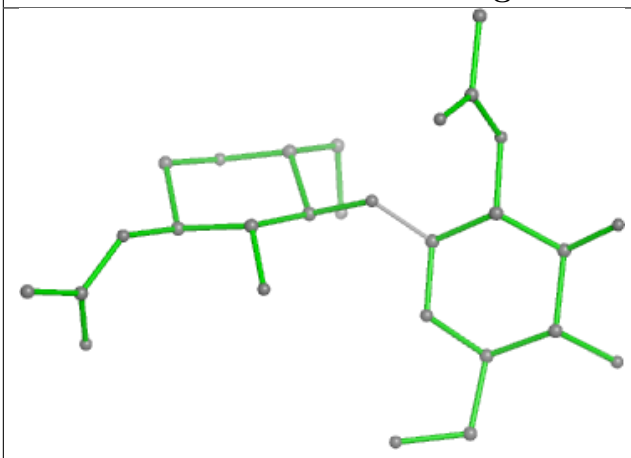


Torsions

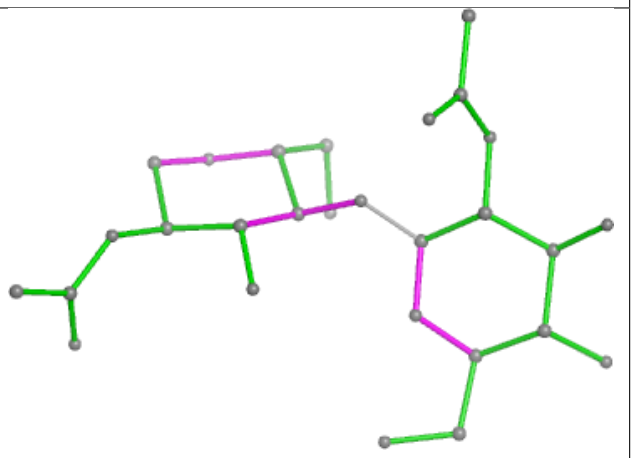


Rings

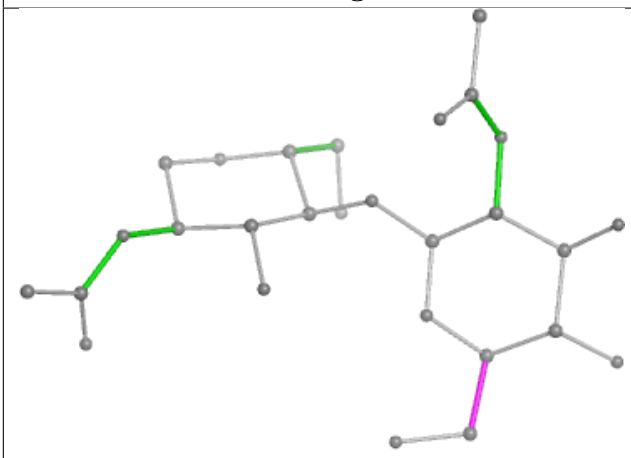
Oligosaccharide Chain K



Bond lengths



Bond angles



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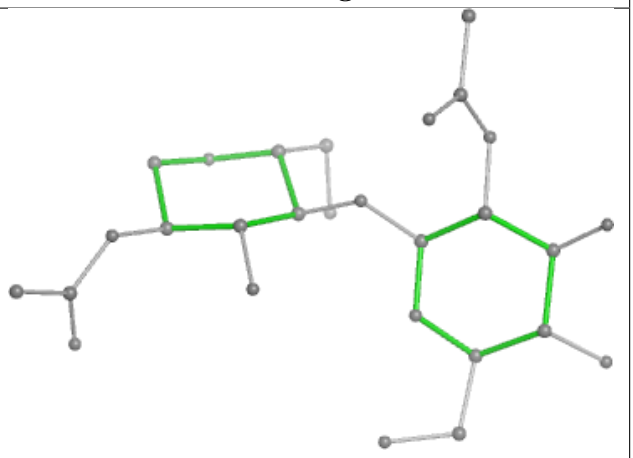
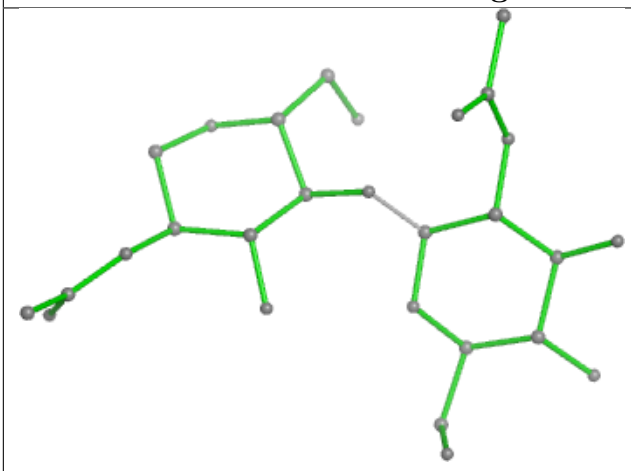


Rings

Oligosaccharide Chain M



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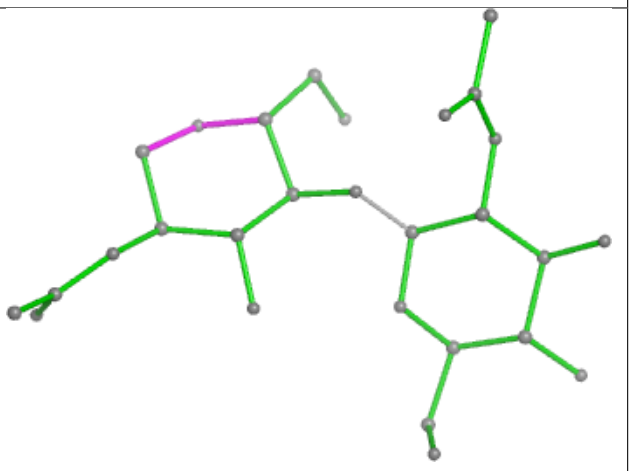
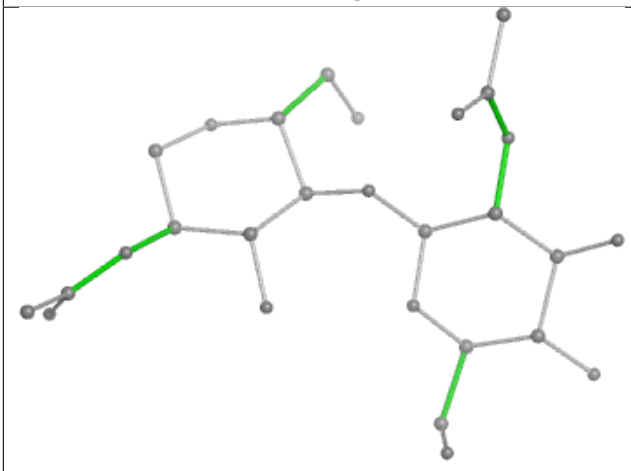
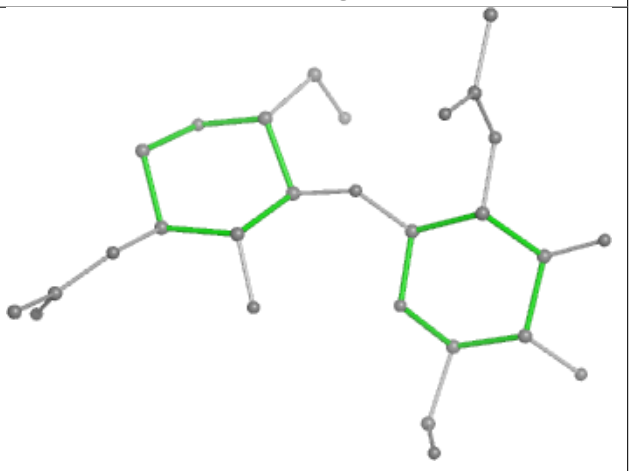


Bond angles

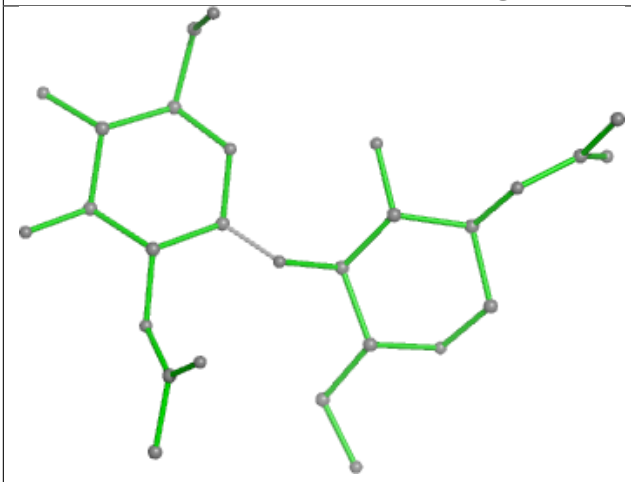


Torsions

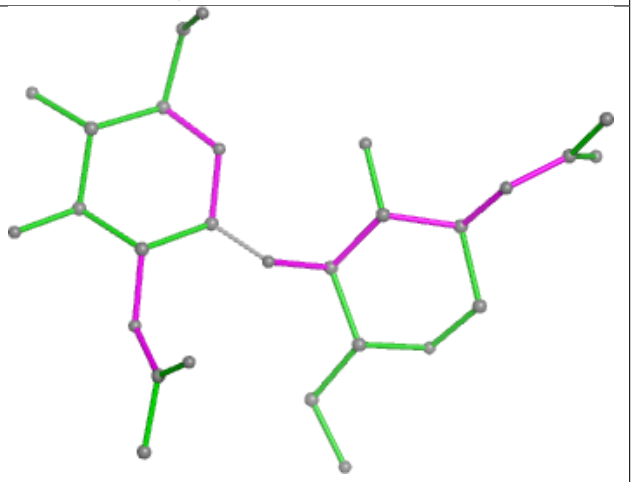


Rings

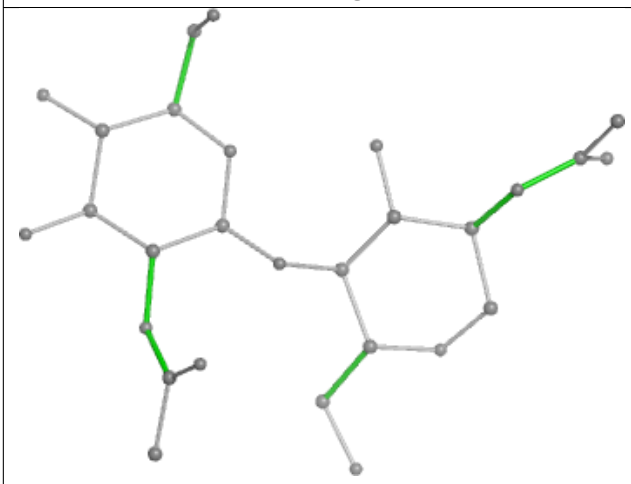
Oligosaccharide Chain Q



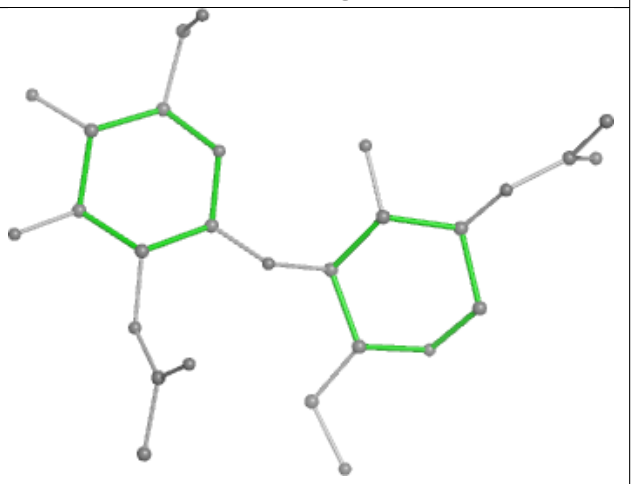
Bond lengths



Bond angles

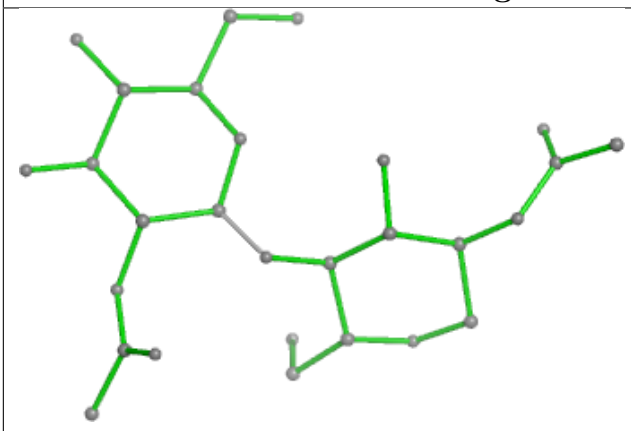


Torsions

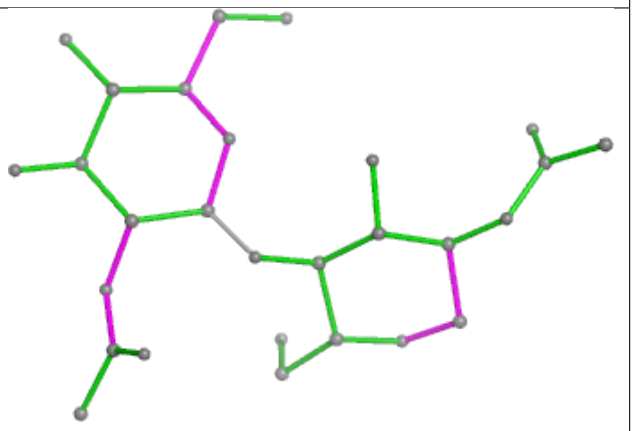


Rings

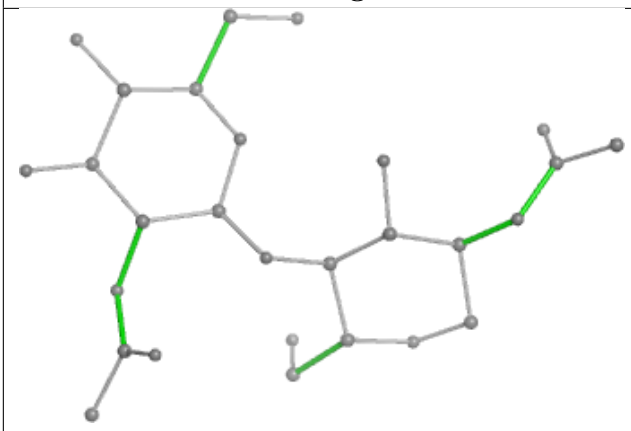
Oligosaccharide Chain U



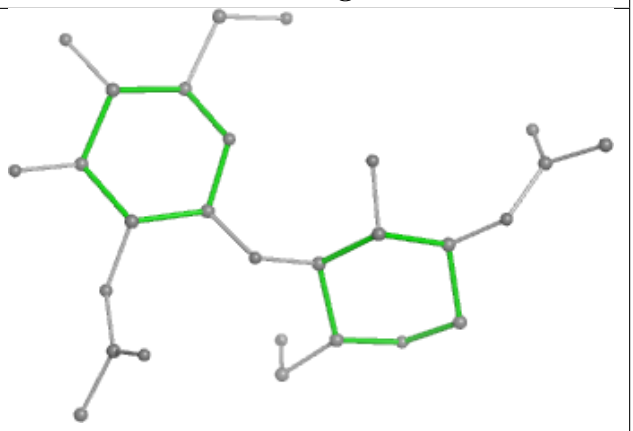
Bond lengths



Bond angles

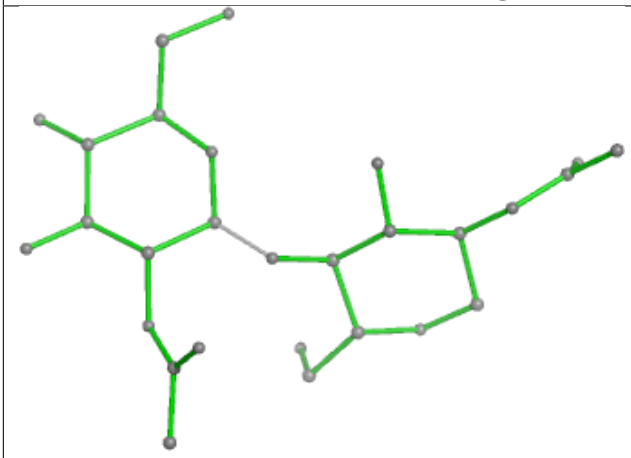


Torsions

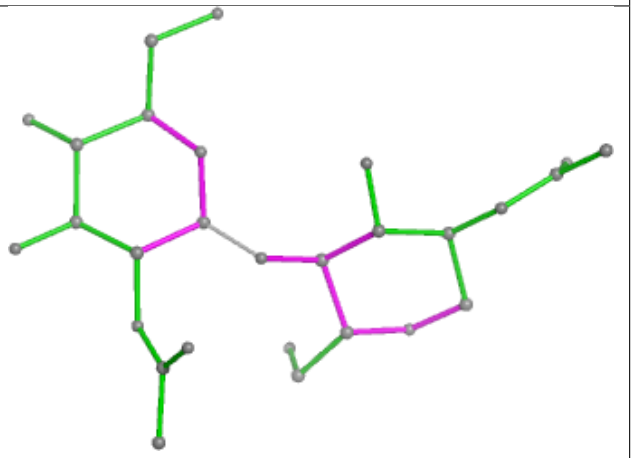


Rings

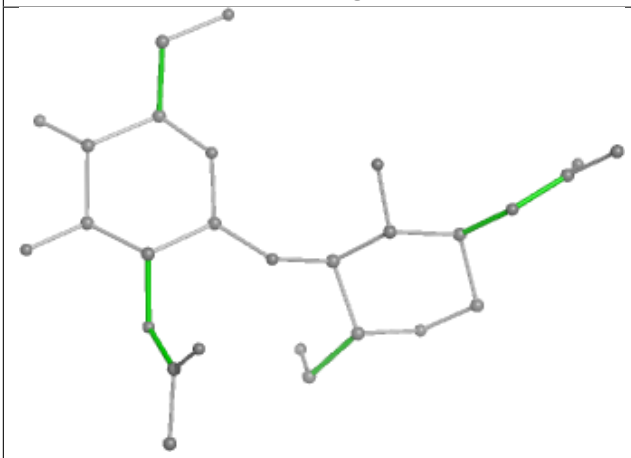
Oligosaccharide Chain V



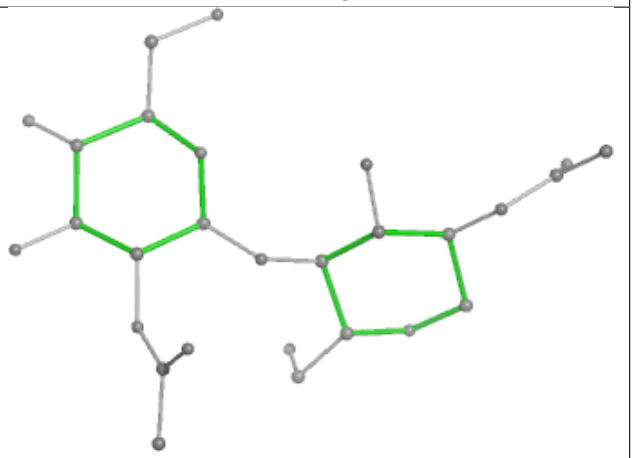
Bond lengths



Bond angles

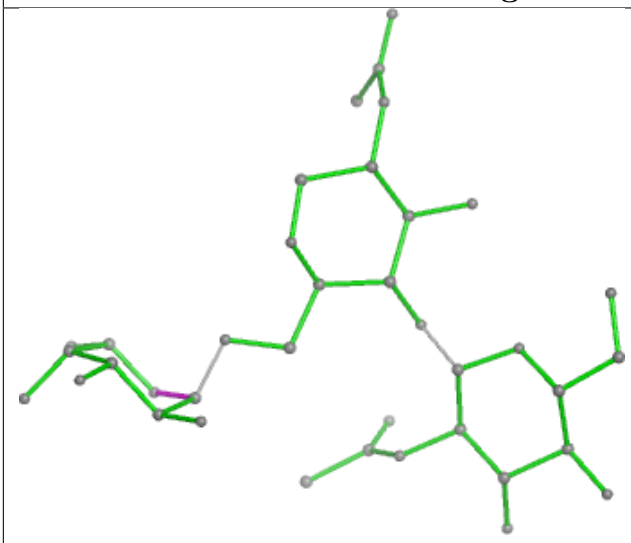


Torsions

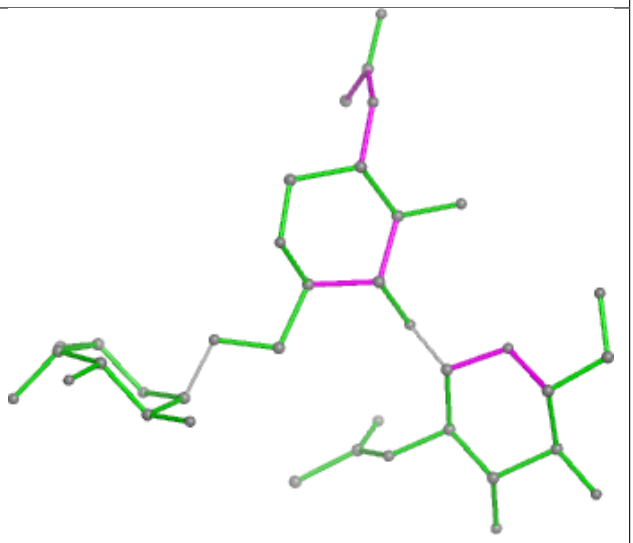


Rings

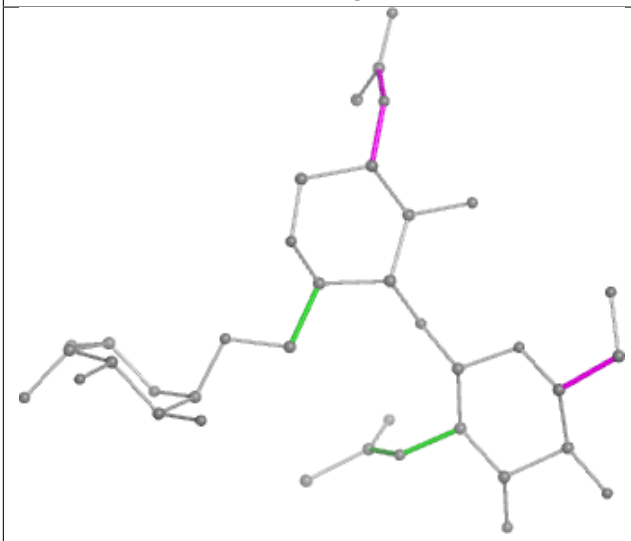
Oligosaccharide Chain I



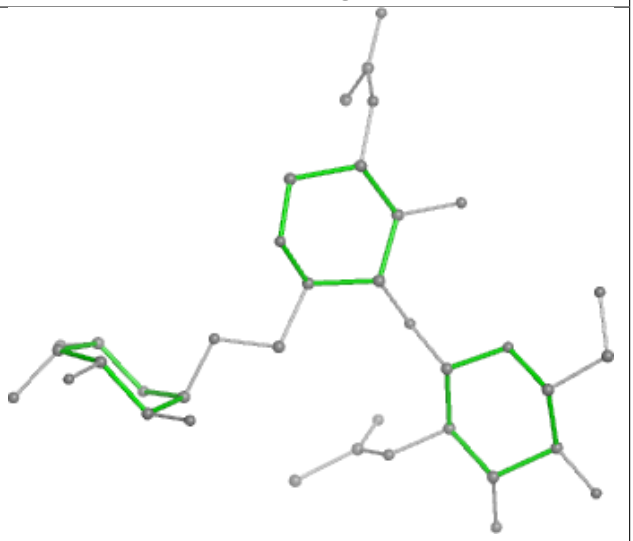
Bond lengths



Bond angles

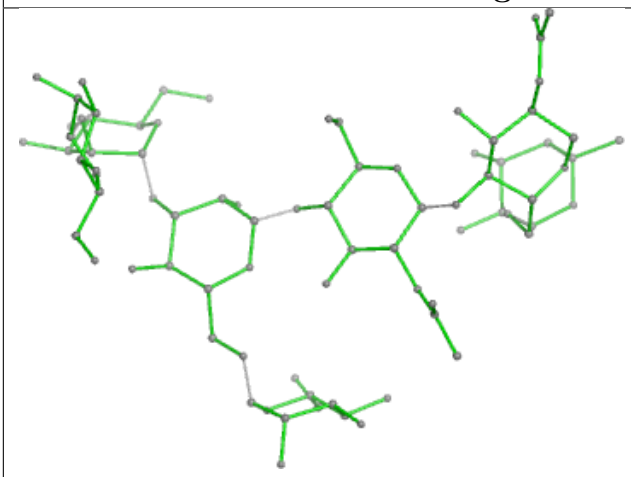


Torsions

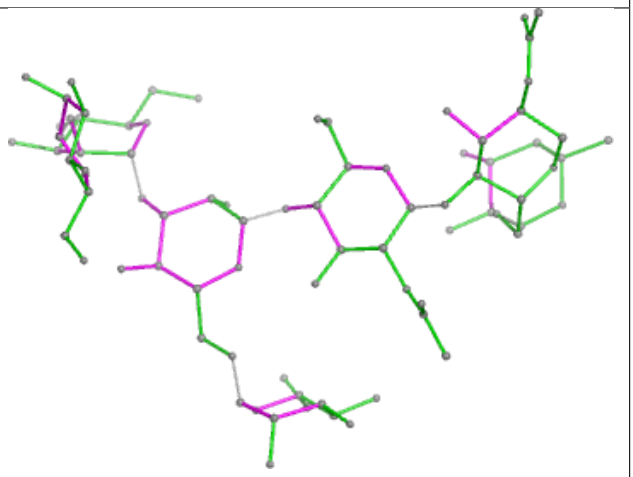


Rings

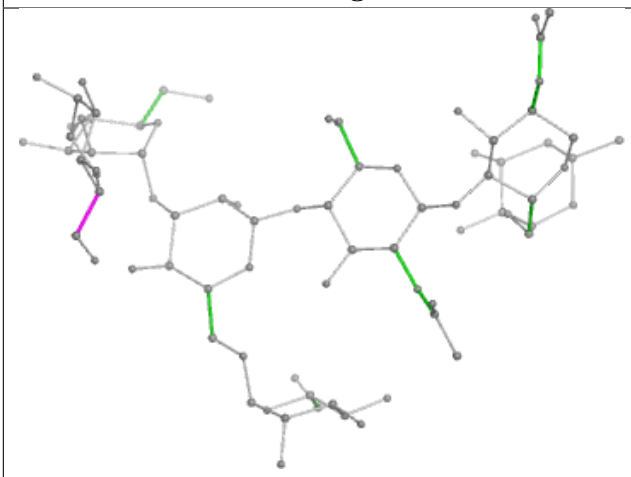
Oligosaccharide Chain N



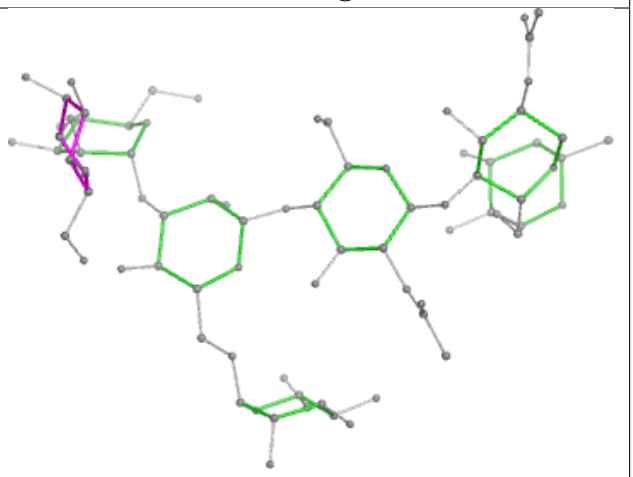
Bond lengths



Bond angles

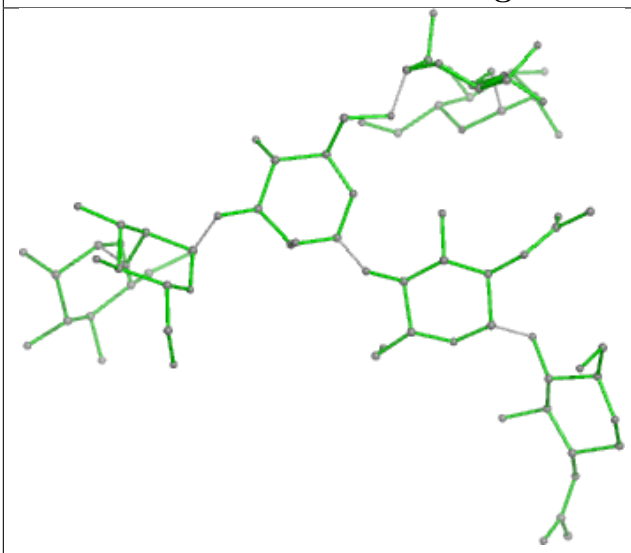


Torsions

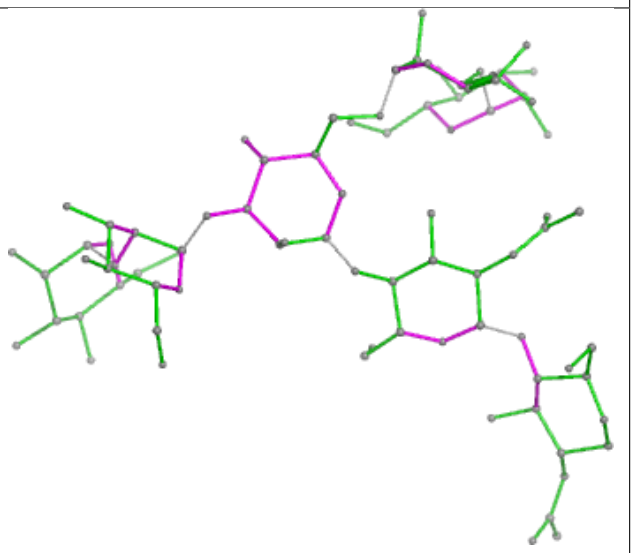


Rings

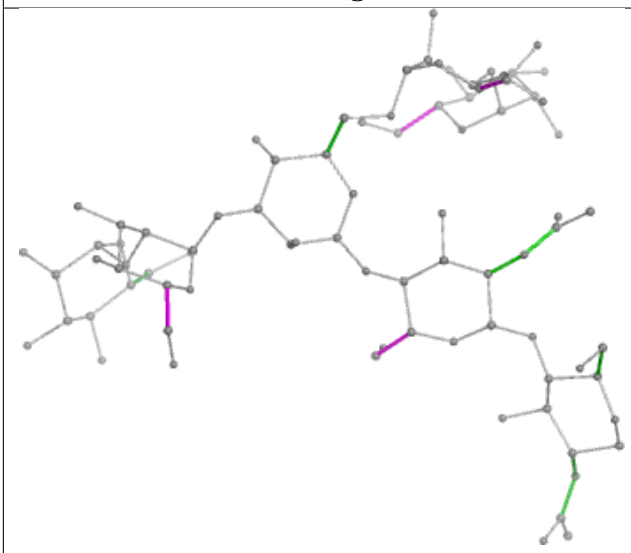
Oligosaccharide Chain O



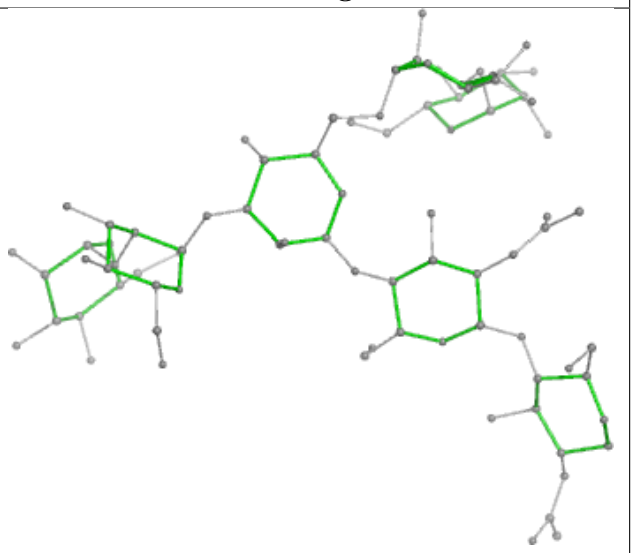
Bond lengths



Bond angles

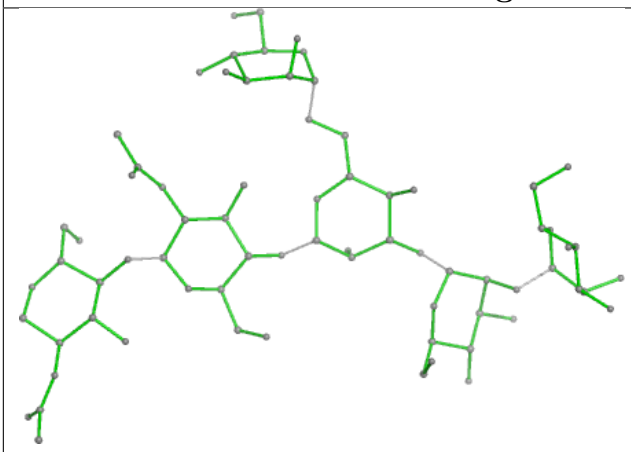


Torsions

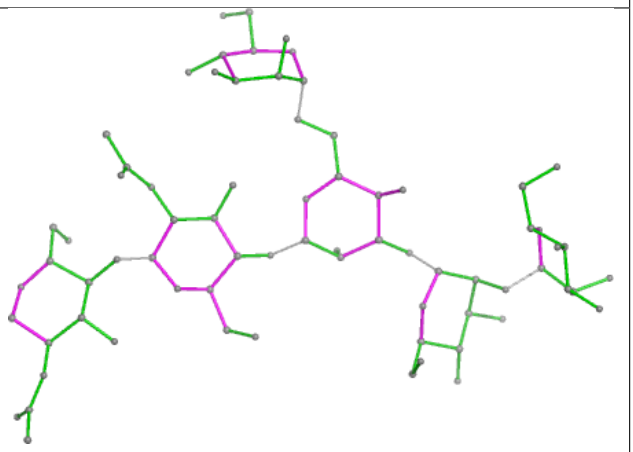


Rings

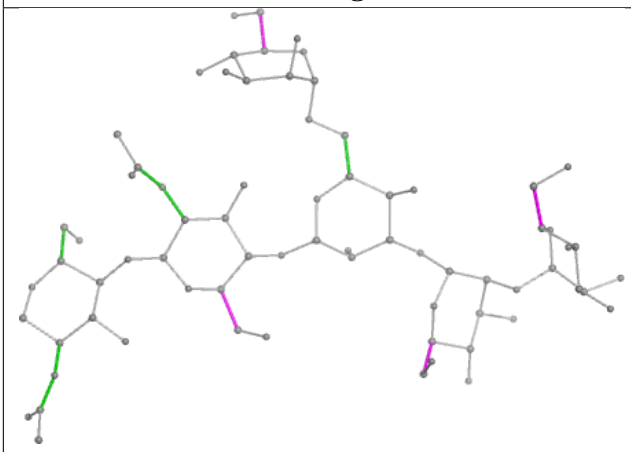
Oligosaccharide Chain P



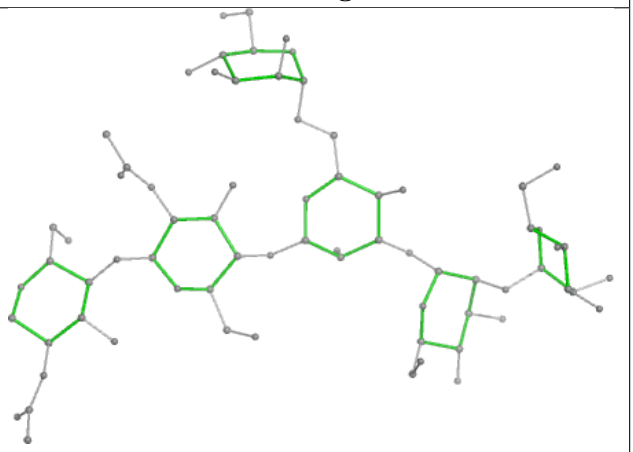
Bond lengths



Bond angles

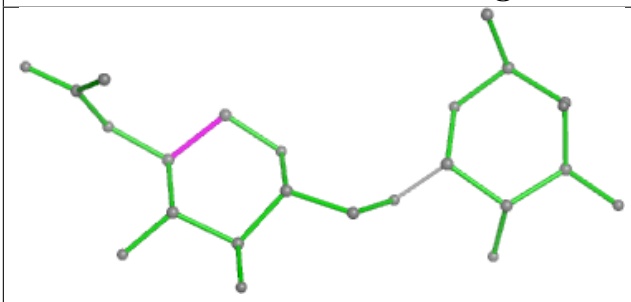


Torsions

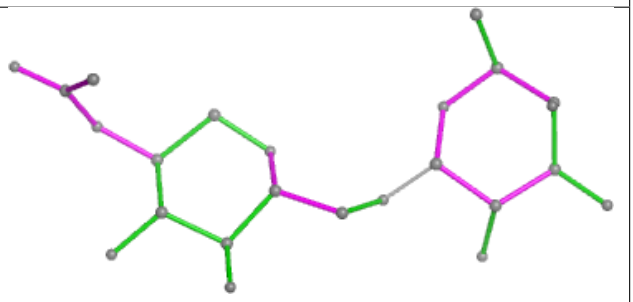


Rings

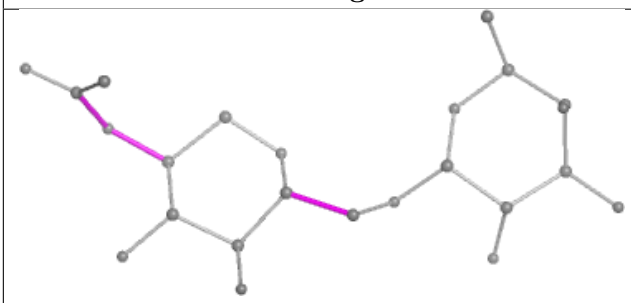
Oligosaccharide Chain R



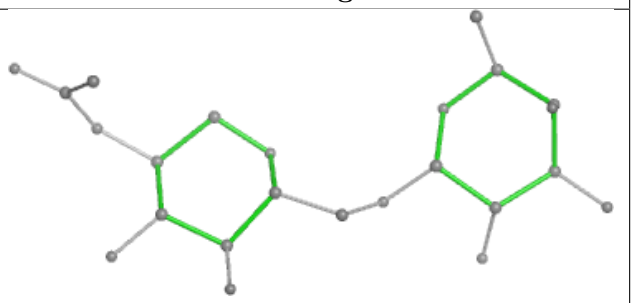
Bond lengths



Bond angles

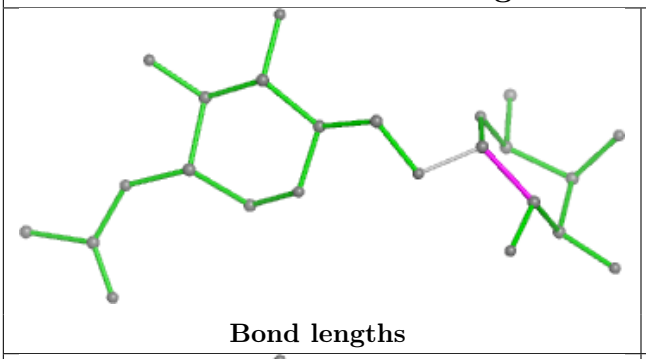


Torsions

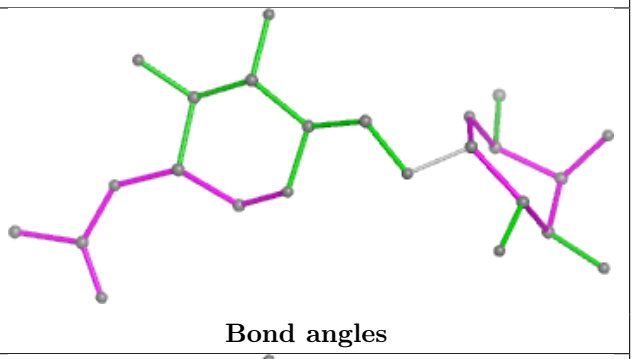


Rings

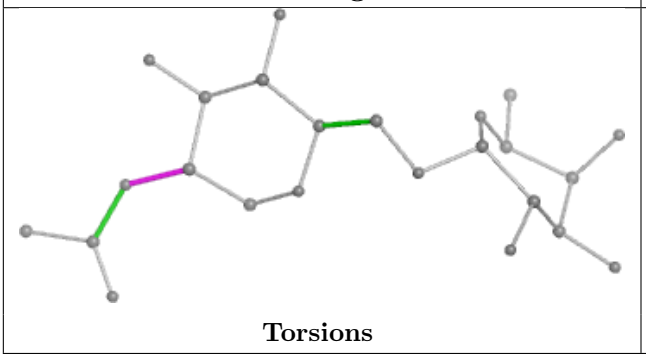
Oligosaccharide Chain X



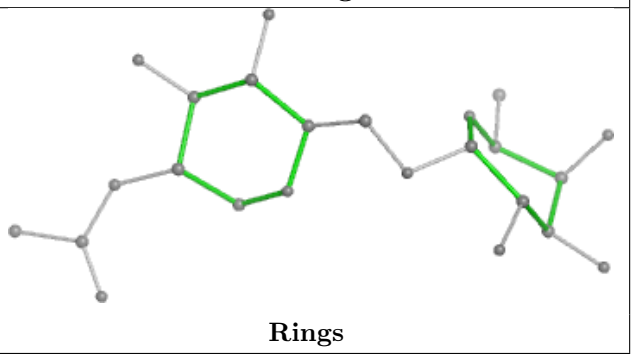
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
12	NAG	AA	501	1	14,14,15	0.92	0	17,19,21	2.27	5 (29%)
13	GOL	BA	501	-	5,5,5	0.27	0	5,5,5	0.31	0
12	NAG	CA	501	1	14,14,15	0.89	1 (7%)	17,19,21	1.55	2 (11%)
15	TY2	CA	503	-	13,14,14	1.16	1 (7%)	18,19,19	2.13	4 (22%)
13	GOL	CA	502	-	5,5,5	0.31	0	5,5,5	0.52	0
13	GOL	AA	502	-	5,5,5	0.22	0	5,5,5	0.51	0
12	NAG	DA	502	1	14,14,15	0.79	0	17,19,21	1.18	1 (5%)
13	GOL	DA	503	-	5,5,5	0.36	0	5,5,5	0.45	0
12	NAG	DA	501	1	14,14,15	0.90	1 (7%)	17,19,21	2.06	3 (17%)

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
12	NAG	AA	501	1	-	3/6/23/26	0/1/1/1
13	GOL	BA	501	-	-	2/4/4/4	-
12	NAG	CA	501	1	-	2/6/23/26	0/1/1/1
15	TY2	CA	503	-	-	2/8/8/8	0/1/1/1
13	GOL	CA	502	-	-	2/4/4/4	-
13	GOL	AA	502	-	-	4/4/4/4	-
12	NAG	DA	502	1	-	2/6/23/26	0/1/1/1
13	GOL	DA	503	-	-	4/4/4/4	-
12	NAG	DA	501	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	CA	501	NAG	C1-C2	2.49	1.56	1.52
12	DA	501	NAG	O5-C1	-2.16	1.40	1.43
15	CA	503	TY2	CE2-NE2	2.16	1.45	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	CA	503	TY2	CE2-CD2-CG	-7.48	118.85	122.18
12	AA	501	NAG	C2-N2-C7	7.10	133.02	122.90
12	DA	501	NAG	C1-O5-C5	-6.79	103.00	112.19
12	CA	501	NAG	C1-O5-C5	4.50	118.29	112.19
12	DA	501	NAG	C1-C2-N2	3.36	116.22	110.49
12	AA	501	NAG	O7-C7-N2	3.11	127.66	121.95
12	CA	501	NAG	C2-N2-C7	3.05	127.25	122.90
12	DA	502	NAG	C1-O5-C5	2.90	116.13	112.19
12	DA	501	NAG	O5-C1-C2	-2.44	107.43	111.29
15	CA	503	TY2	OXT-C-O	-2.22	119.05	124.09
15	CA	503	TY2	CG-CB-CA	-2.21	109.53	114.13
12	AA	501	NAG	O5-C5-C4	-2.19	105.51	110.83
12	AA	501	NAG	C4-C3-C2	2.17	114.19	111.02
12	AA	501	NAG	C1-O5-C5	-2.13	109.31	112.19
15	CA	503	TY2	CD2-CE2-CZ	2.03	121.31	118.94

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AA	501	NAG	C3-C2-N2-C7
13	AA	502	GOL	O1-C1-C2-O2
13	AA	502	GOL	O1-C1-C2-C3
13	AA	502	GOL	C1-C2-C3-O3
13	AA	502	GOL	O2-C2-C3-O3
13	BA	501	GOL	C1-C2-C3-O3
13	BA	501	GOL	O2-C2-C3-O3
13	CA	502	GOL	C1-C2-C3-O3
13	DA	503	GOL	O1-C1-C2-C3
13	DA	503	GOL	C1-C2-C3-O3
12	CA	501	NAG	C8-C7-N2-C2
12	CA	501	NAG	O7-C7-N2-C2
12	DA	501	NAG	C1-C2-N2-C7
15	CA	503	TY2	OXT-C-CA-N
13	CA	502	GOL	O2-C2-C3-O3
13	DA	503	GOL	O1-C1-C2-O2
13	DA	503	GOL	O2-C2-C3-O3
12	AA	501	NAG	O5-C5-C6-O6
12	DA	502	NAG	C4-C5-C6-O6
12	DA	502	NAG	O5-C5-C6-O6
15	CA	503	TY2	O-C-CA-N
12	AA	501	NAG	C4-C5-C6-O6

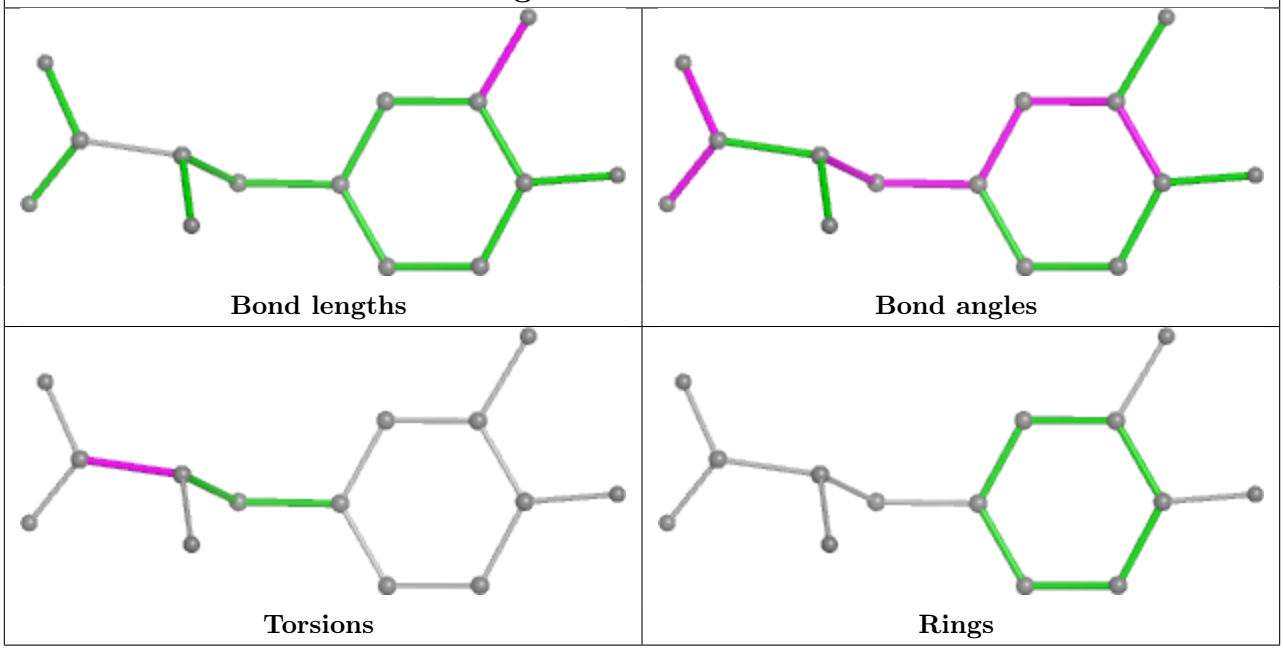
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	BA	501	GOL	1	0
13	CA	502	GOL	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 TY2 CA 503



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	447/450 (99%)	-0.37	0 100 100	25, 37, 53, 73	1 (0%)
1	BA	447/450 (99%)	-0.42	3 (0%) 87 86	27, 38, 52, 80	0
1	CA	447/450 (99%)	-0.35	3 (0%) 87 86	28, 40, 58, 75	0
1	DA	450/450 (100%)	-0.26	10 (2%) 62 59	31, 46, 61, 82	0
All	All	1791/1800 (99%)	-0.35	16 (0%) 84 83	25, 40, 57, 82	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DA	474	LEU	5.9
1	BA	469	PRO	4.0
1	BA	470	SER	4.0
1	CA	48	VAL	4.0
1	BA	471	ARG	3.8
1	DA	472	GLU	3.4
1	DA	48	VAL	3.1
1	DA	323	MET	2.9
1	CA	37	ARG	2.7
1	DA	69	THR	2.4
1	DA	64	ARG	2.3
1	DA	47	PRO	2.3
1	CA	51	PRO	2.2
1	DA	57	GLY	2.2
1	DA	294	GLU	2.1
1	DA	473	ASN	2.1

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

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

6.3 Carbohydrates (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
2	MAN	C	4	11/12	0.37	0.47	74,101,105,106	0
4	BMA	D	3	11/12	0.37	0.38	89,95,98,99	0
3	MAN	B	5	11/12	0.48	0.42	79,83,88,89	0
3	MAN	B	4	11/12	0.52	0.28	78,87,93,94	0
5	BMA	S	3	11/12	0.57	0.36	87,92,95,97	0
4	BMA	W	3	11/12	0.58	0.37	68,90,95,96	0
10	MAN	P	6	11/12	0.58	0.33	89,95,99,102	0
9	MAN	O	4	11/12	0.61	0.39	95,107,109,109	0
9	MAN	O	7	11/12	0.64	0.62	126,140,143,145	0
8	BMA	N	3	11/12	0.64	0.27	90,94,96,100	0
8	MAN	N	5	11/12	0.65	0.47	106,112,121,123	0
5	FUC	E	4	10/11	0.65	0.34	58,71,81,85	0
8	MAN	N	6	11/12	0.66	0.56	91,94,100,100	0
6	NAG	Q	2	14/15	0.67	0.38	75,91,102,102	0
2	MAN	T	5	11/12	0.69	0.36	74,88,93,94	11
9	MAN	O	6	11/12	0.69	0.53	125,129,132,136	0
2	BMA	C	3	11/12	0.70	0.39	96,101,106,106	0
2	MAN	C	5	11/12	0.71	0.46	95,102,104,105	0
6	NAG	J	1	14/15	0.72	0.32	59,72,81,88	0
6	NAG	Q	1	14/15	0.72	0.24	50,71,79,89	0
11	NAG	R	1	14/15	0.72	0.26	54,69,88,93	0
6	NAG	U	2	14/15	0.73	0.27	66,80,86,89	0
4	NAG	W	2	14/15	0.74	0.33	75,86,90,90	0
6	NAG	F	1	14/15	0.75	0.21	52,63,78,85	0
5	BMA	G	3	11/12	0.75	0.20	77,86,88,91	0
8	MAN	N	4	11/12	0.75	0.47	95,102,110,112	0
9	MAN	O	5	11/12	0.75	0.35	83,97,101,103	0
11	FUC	R	2	10/11	0.75	0.37	79,97,101,103	0
9	BMA	O	3	11/12	0.76	0.31	101,109,116,125	0
4	NAG	W	1	14/15	0.77	0.28	66,75,79,83	0
5	BMA	E	3	11/12	0.77	0.25	68,75,81,82	0
11	NAG	X	1	14/15	0.77	0.31	60,75,88,90	0
11	FUC	X	2	10/11	0.77	0.32	79,82,91,92	0
2	MAN	T	4	11/12	0.78	0.28	96,99,101,102	0
10	BMA	P	3	11/12	0.79	0.26	76,79,90,96	0
3	MAN	H	5	11/12	0.79	0.20	37,54,61,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	J	2	14/15	0.79	0.47	82,91,97,104	0
5	NAG	E	2	14/15	0.80	0.24	68,74,79,79	0
2	MAN	L	5	11/12	0.82	0.20	67,69,72,78	0
6	NAG	F	2	14/15	0.83	0.38	80,87,92,93	0
7	NAG	I	1	14/15	0.84	0.26	56,67,76,83	0
2	BMA	T	3	11/12	0.84	0.17	89,92,94,95	0
3	MAN	H	4	11/12	0.84	0.29	77,80,85,87	0
6	NAG	K	2	14/15	0.84	0.22	65,70,77,83	0
2	FUC	A	6	10/11	0.85	0.27	55,62,69,69	0
7	NAG	I	2	14/15	0.85	0.31	79,82,85,87	0
2	NAG	C	2	14/15	0.85	0.14	57,68,87,93	0
10	NAG	P	2	14/15	0.85	0.13	64,69,79,79	0
6	NAG	V	2	14/15	0.85	0.28	68,74,81,85	0
10	MAN	P	4	11/12	0.86	0.26	68,73,78,79	0
5	NAG	S	2	14/15	0.86	0.20	68,73,81,85	0
3	BMA	B	3	11/12	0.86	0.17	65,73,83,85	0
3	BMA	H	3	11/12	0.87	0.23	51,60,69,76	0
6	NAG	M	2	14/15	0.87	0.26	61,72,79,81	0
7	FUC	I	3	10/11	0.87	0.24	57,72,74,76	0
5	FUC	S	4	10/11	0.87	0.21	65,71,75,79	0
8	NAG	N	2	14/15	0.88	0.19	50,63,77,83	0
2	NAG	T	1	14/15	0.89	0.14	57,62,68,68	0
9	NAG	O	2	14/15	0.89	0.24	73,83,92,94	0
5	NAG	E	1	14/15	0.89	0.12	33,53,70,70	0
6	NAG	M	1	14/15	0.90	0.10	47,54,65,67	0
5	NAG	S	1	14/15	0.90	0.13	56,63,66,66	0
2	FUC	L	6	10/11	0.91	0.24	65,71,73,74	0
5	NAG	G	1	14/15	0.91	0.16	47,54,60,62	0
2	BMA	L	3	11/12	0.91	0.08	44,51,55,68	0
2	MAN	A	5	11/12	0.91	0.20	54,58,66,68	0
2	NAG	C	1	14/15	0.92	0.09	43,51,59,60	0
8	FUC	N	7	10/11	0.92	0.12	37,46,50,53	0
3	NAG	H	1	14/15	0.92	0.11	45,49,52,52	0
4	NAG	D	2	14/15	0.92	0.16	61,68,82,87	0
2	MAN	L	4	11/12	0.92	0.09	51,56,64,70	0
6	NAG	K	1	14/15	0.92	0.11	42,48,56,56	0
6	NAG	V	1	14/15	0.92	0.17	43,60,66,68	0
5	NAG	G	2	14/15	0.92	0.18	62,74,84,88	0
10	MAN	P	5	11/12	0.93	0.13	53,60,66,67	0
3	NAG	B	2	14/15	0.93	0.12	39,48,59,62	0
3	NAG	H	2	14/15	0.93	0.14	48,52,56,60	0
2	NAG	T	2	14/15	0.94	0.16	66,74,79,83	0

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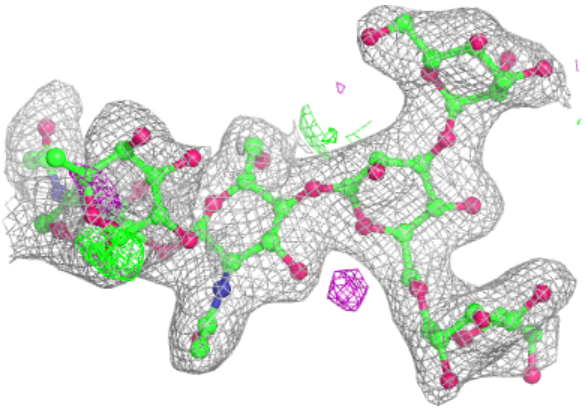
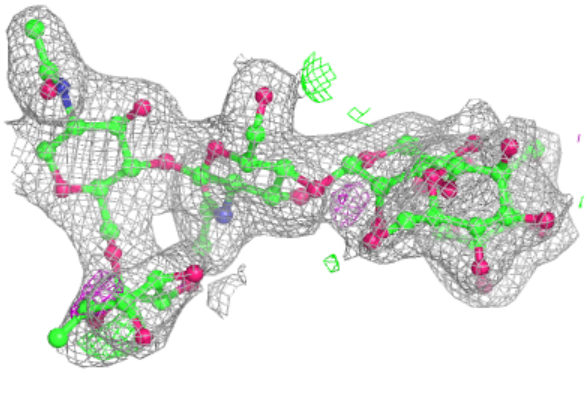
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	U	1	14/15	0.94	0.10	50,57,69,70	0
8	NAG	N	1	14/15	0.94	0.09	40,47,50,51	0
2	NAG	L	2	14/15	0.94	0.08	48,52,58,60	0
4	NAG	D	1	14/15	0.95	0.10	41,47,56,56	0
2	MAN	A	4	11/12	0.95	0.11	45,49,56,58	0
2	FUC	T	6	10/11	0.95	0.14	51,57,61,66	0
3	NAG	B	1	14/15	0.95	0.10	36,41,44,45	0
9	NAG	O	1	14/15	0.96	0.12	42,48,61,64	0
2	NAG	L	1	14/15	0.96	0.10	39,47,51,60	0
5	FUC	G	4	10/11	0.96	0.11	43,50,56,58	0
2	NAG	A	1	14/15	0.96	0.09	34,40,49,51	0
2	BMA	A	3	11/12	0.97	0.09	39,40,47,54	0
2	NAG	A	2	14/15	0.97	0.08	35,43,47,47	0
10	NAG	P	1	14/15	0.97	0.07	45,48,57,63	0
2	FUC	C	6	10/11	0.98	0.07	42,48,54,55	0

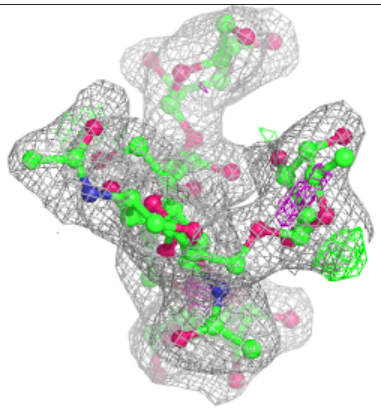
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

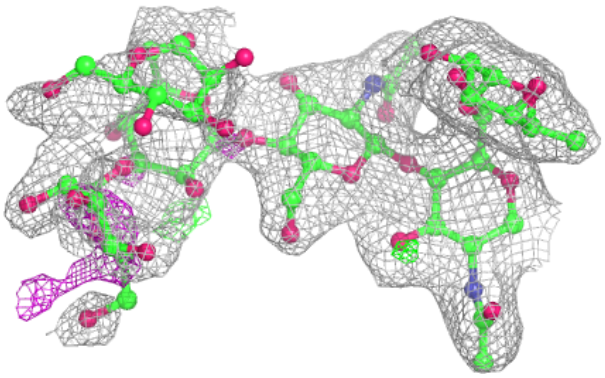


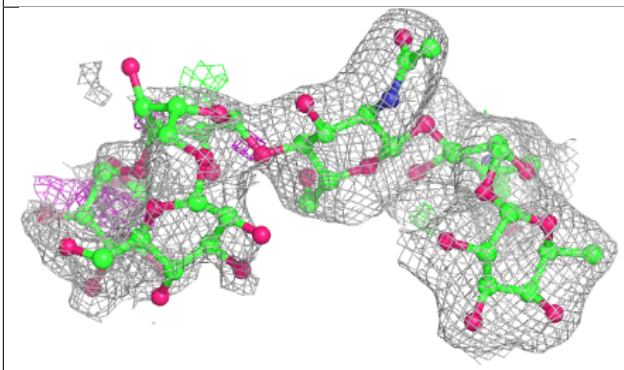


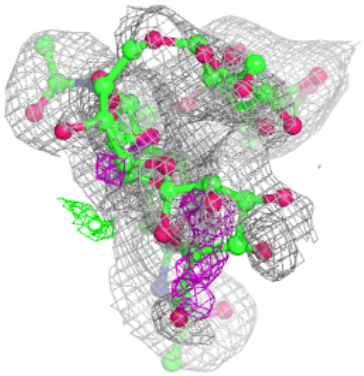


Electron density around Chain C:

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

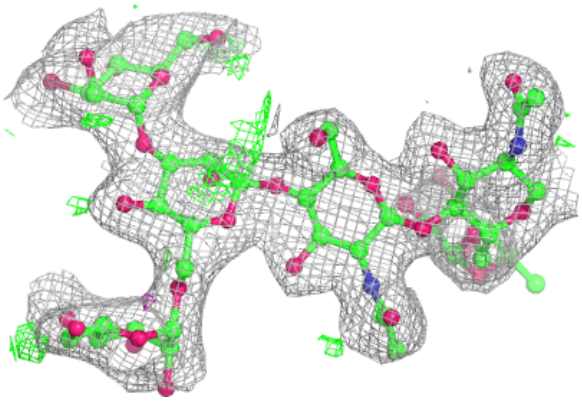


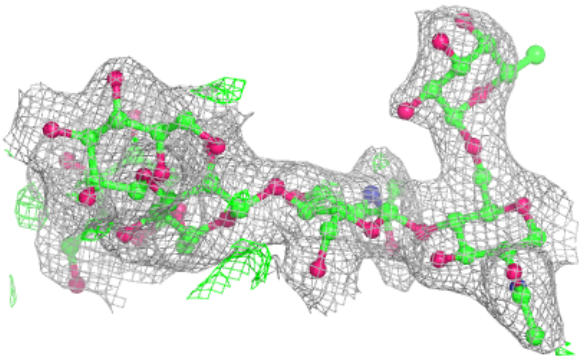


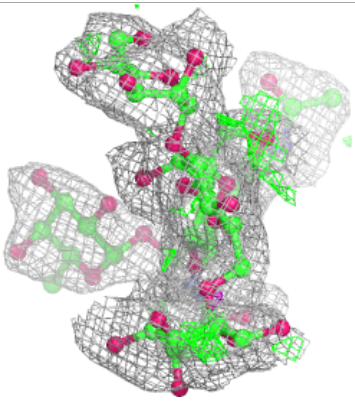


Electron density around Chain L:

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

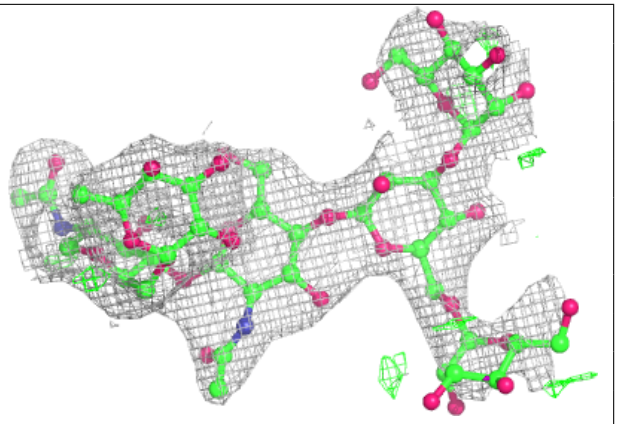


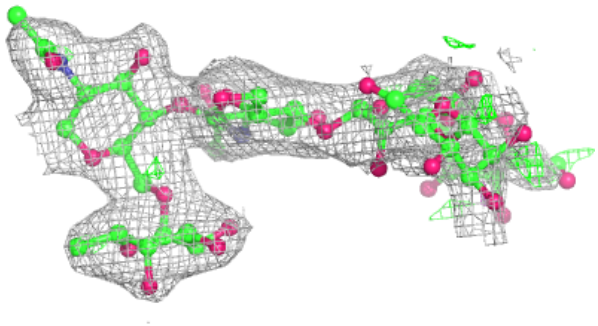


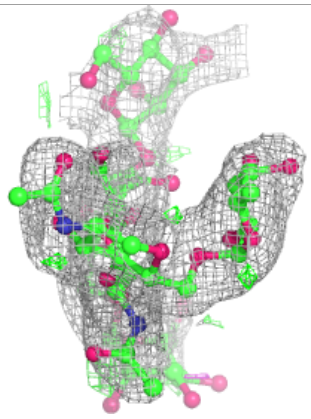


Electron density around Chain T:

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

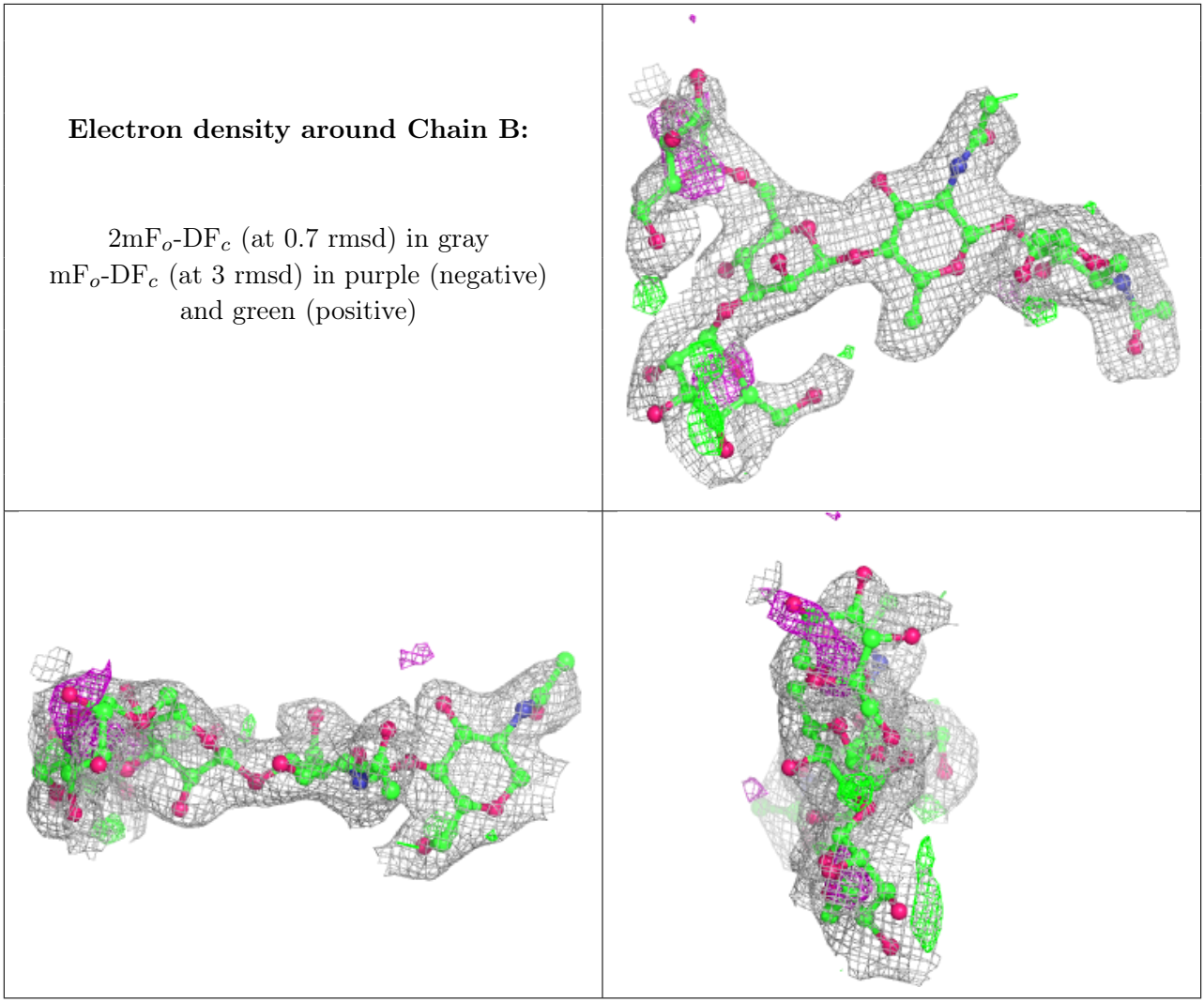






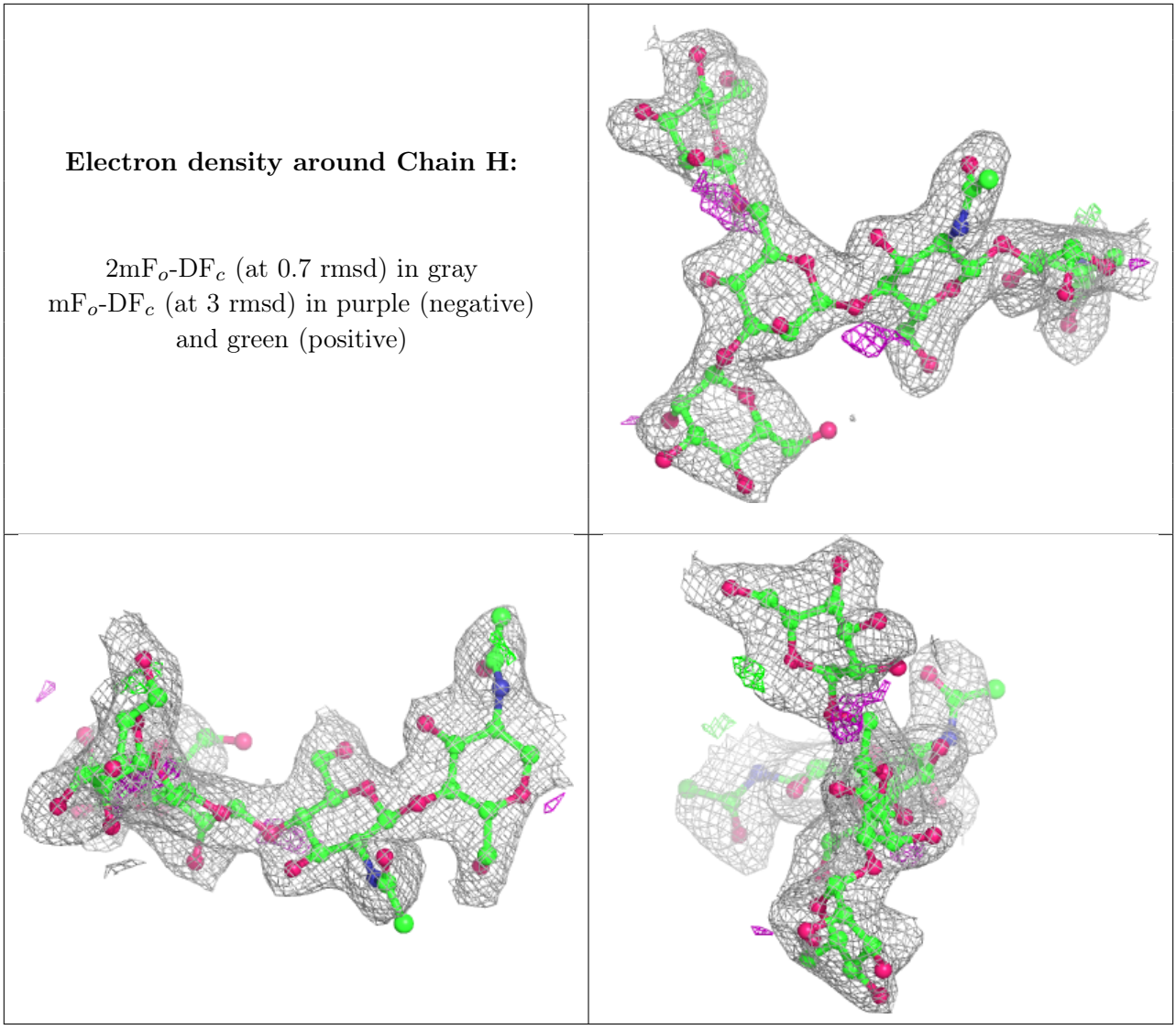
Electron density around Chain B:

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



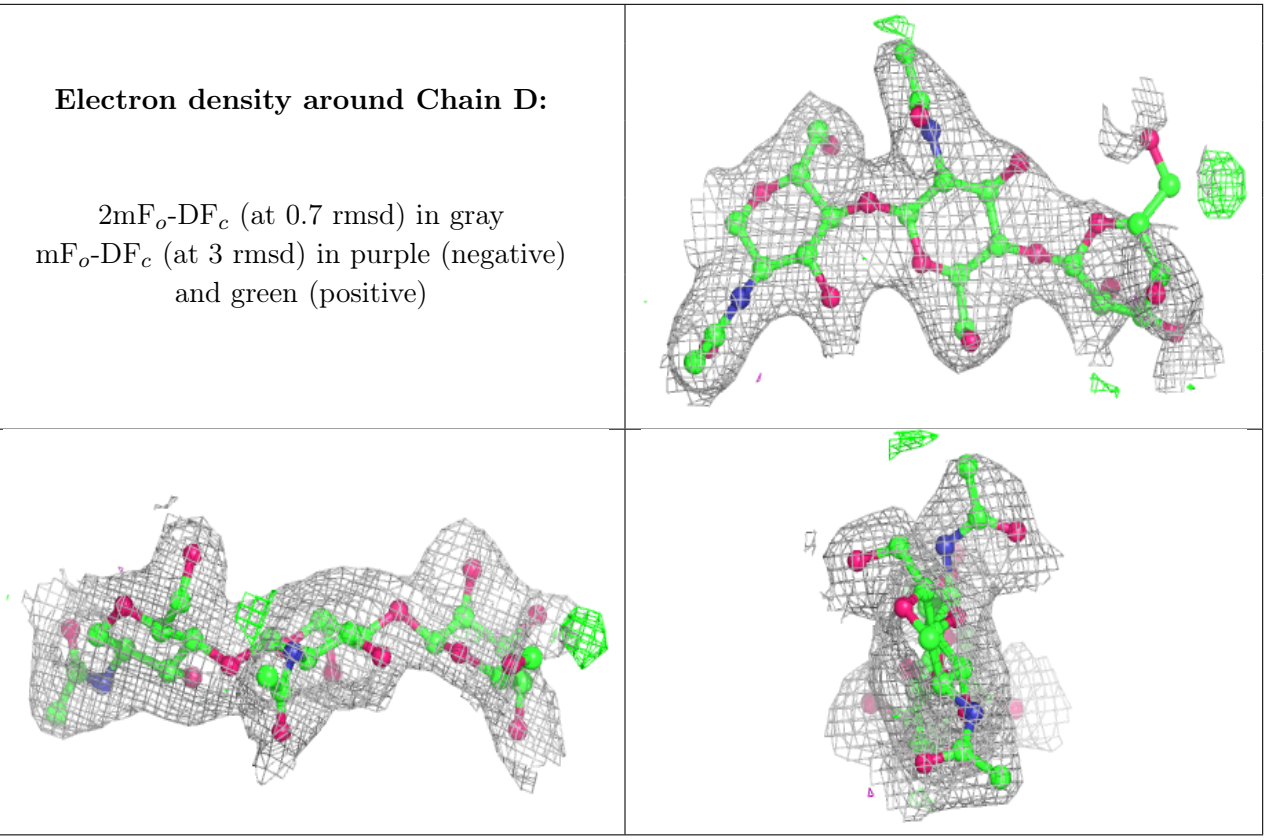
Electron density around Chain H:

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



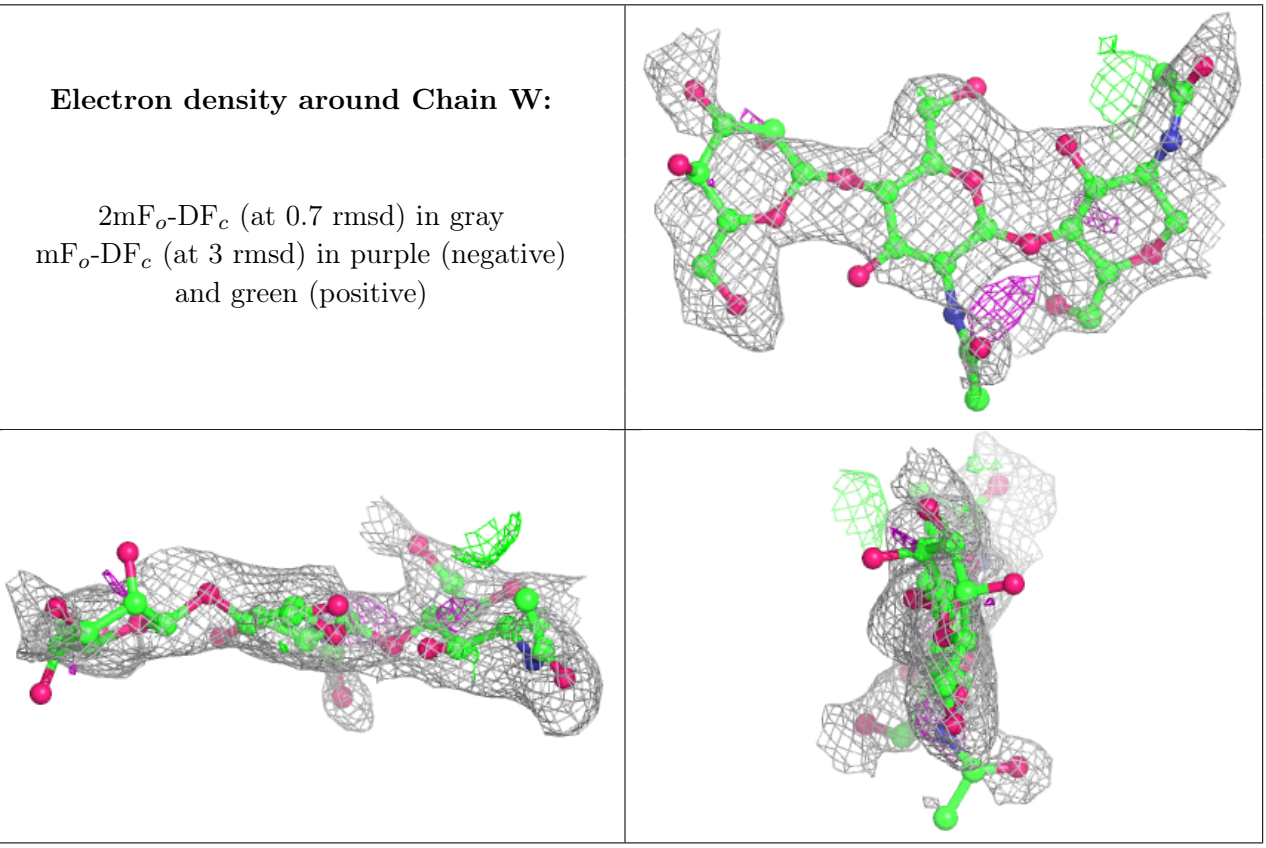
Electron density around Chain D:

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



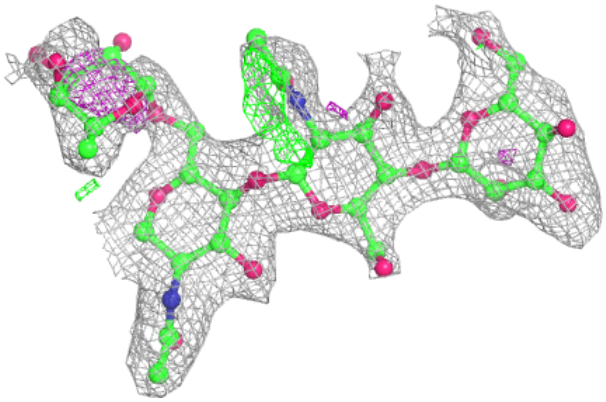
Electron density around Chain W:

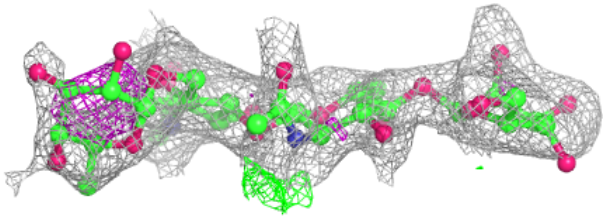
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

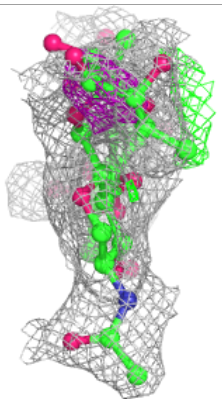


Electron density around Chain E:

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

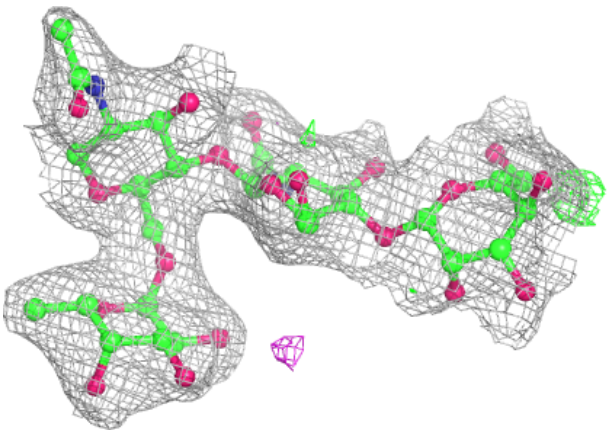


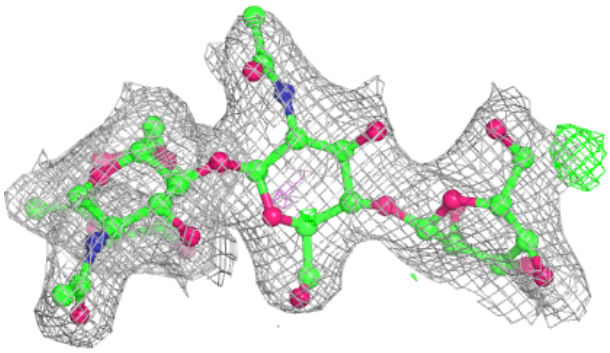


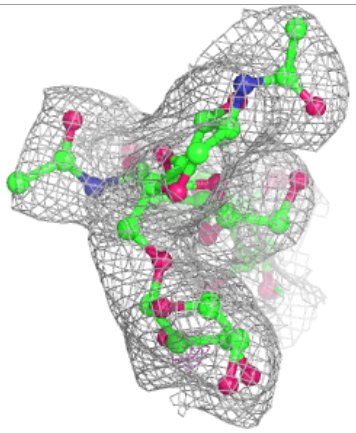


Electron density around Chain G:

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

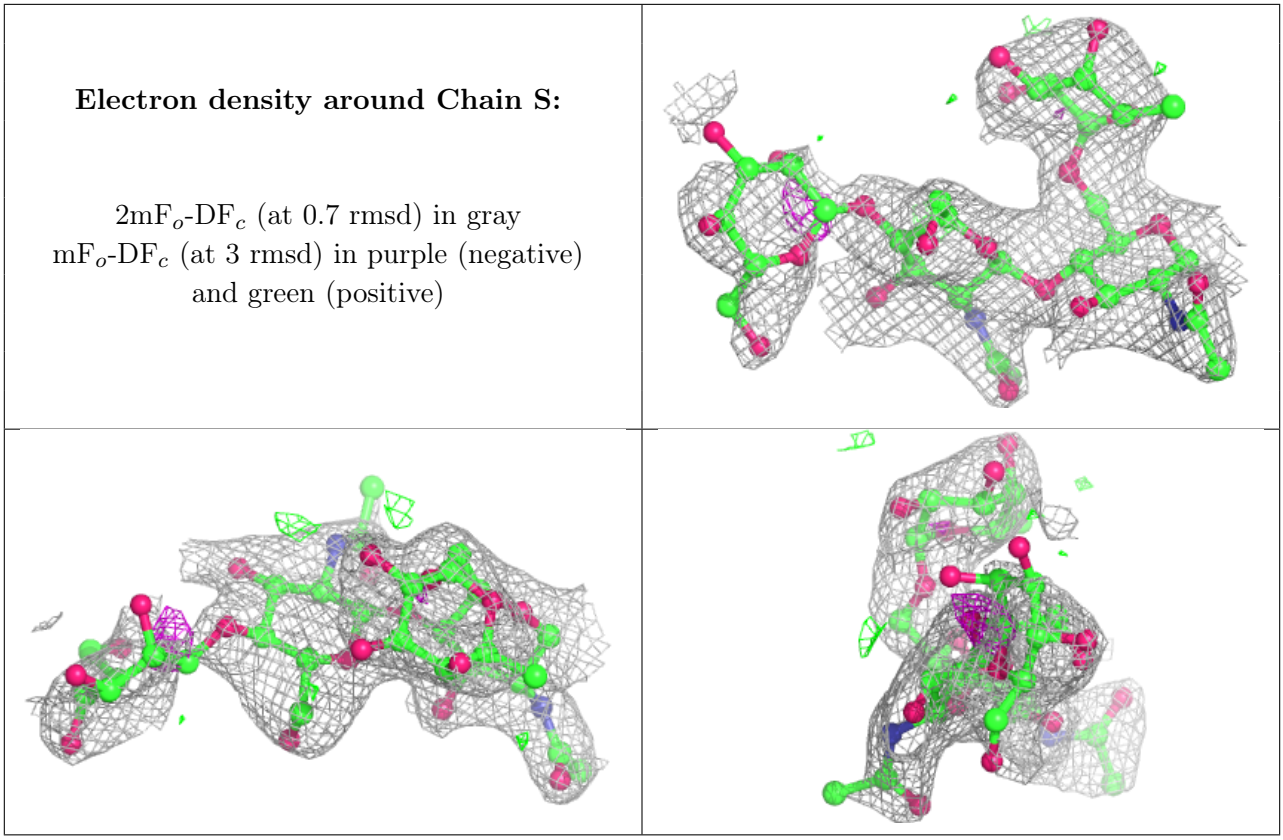






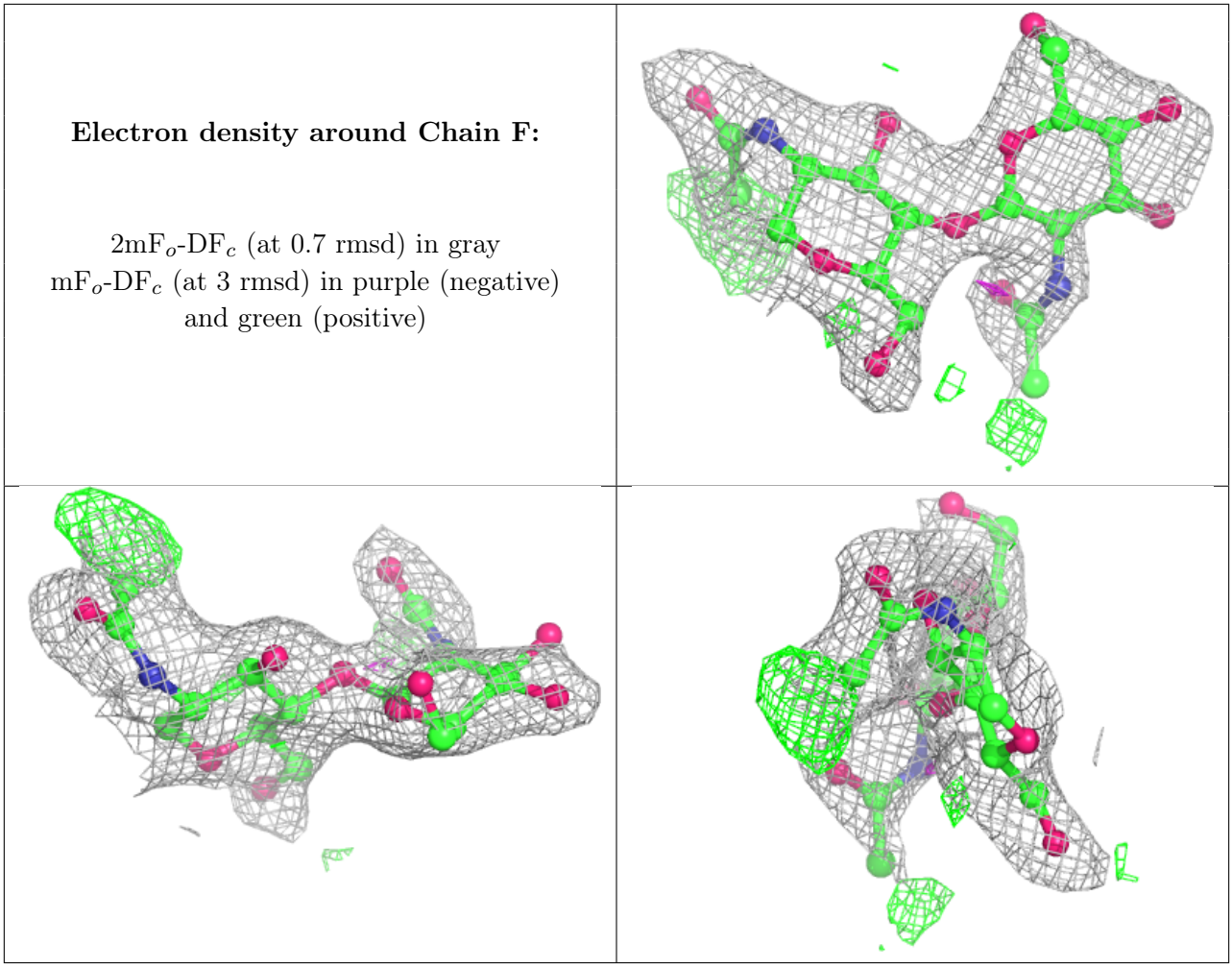
Electron density around Chain S:

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



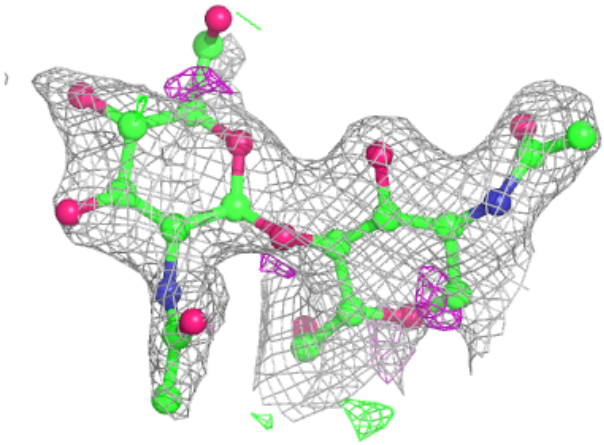
Electron density around Chain F:

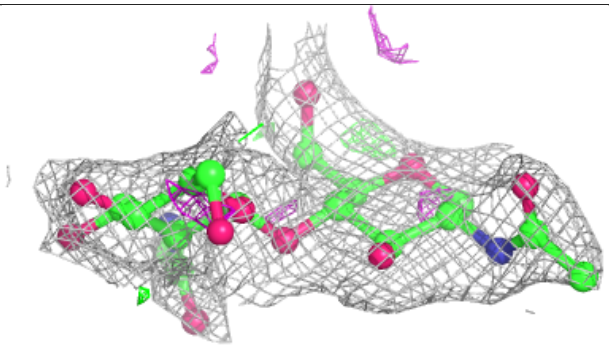
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

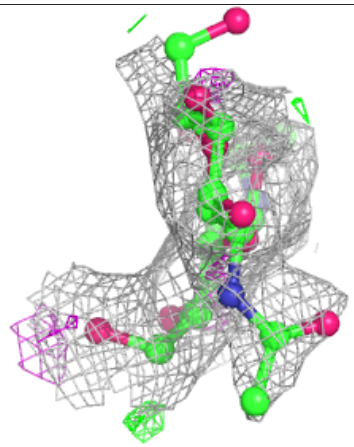


Electron density around Chain J:

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

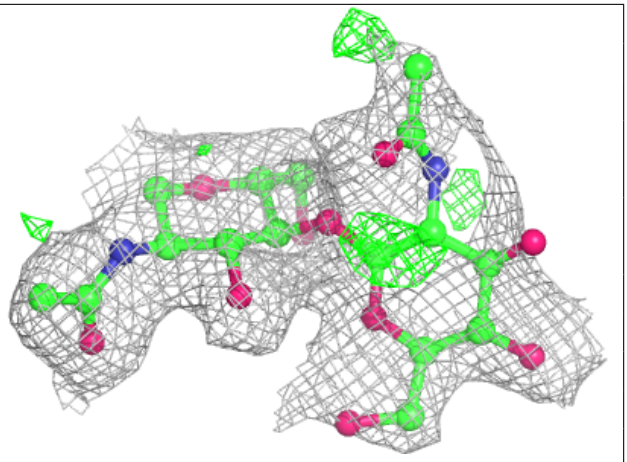


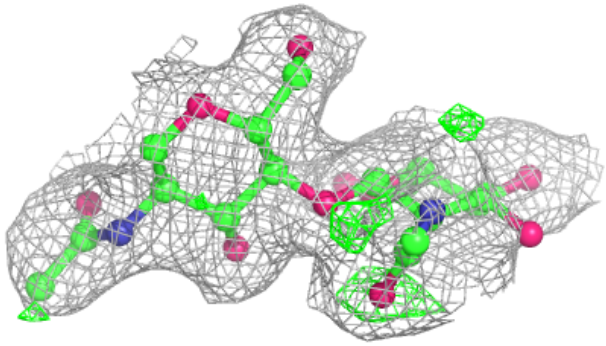


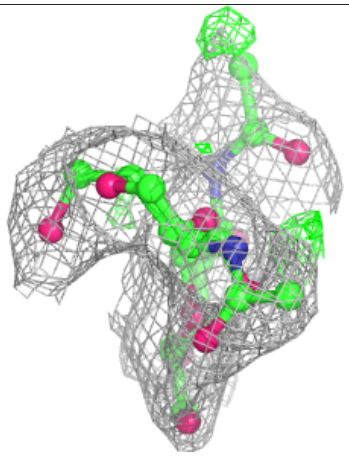


Electron density around Chain K:

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

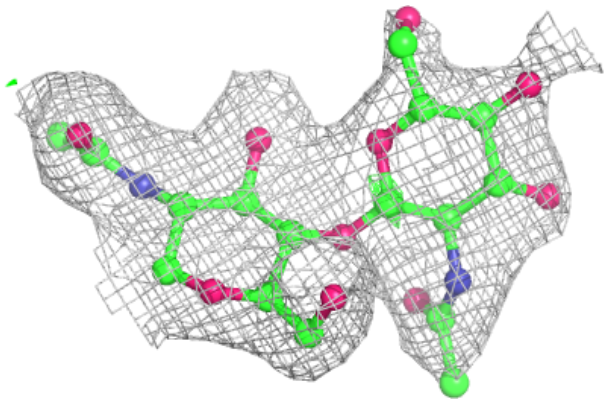


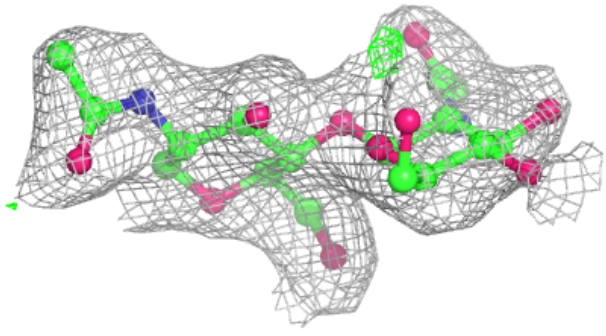


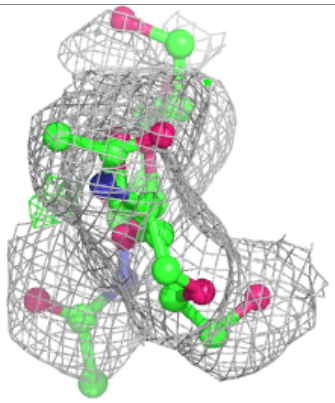


Electron density around Chain M:

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

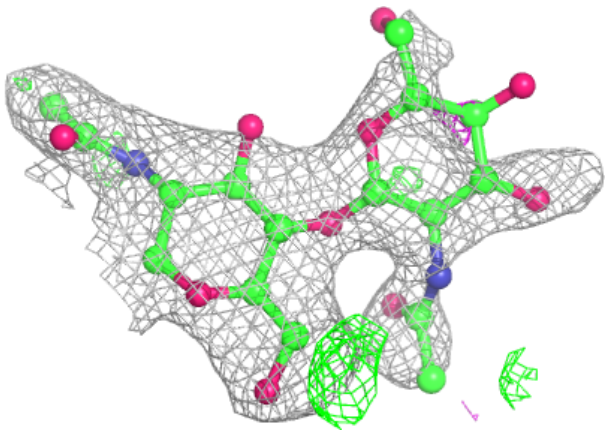


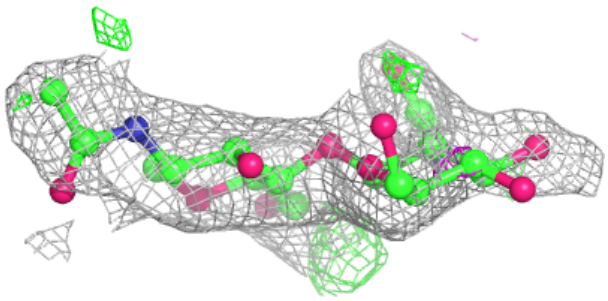


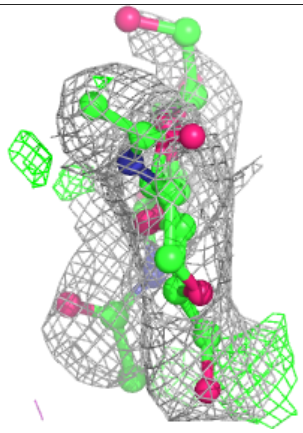


Electron density around Chain Q:

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

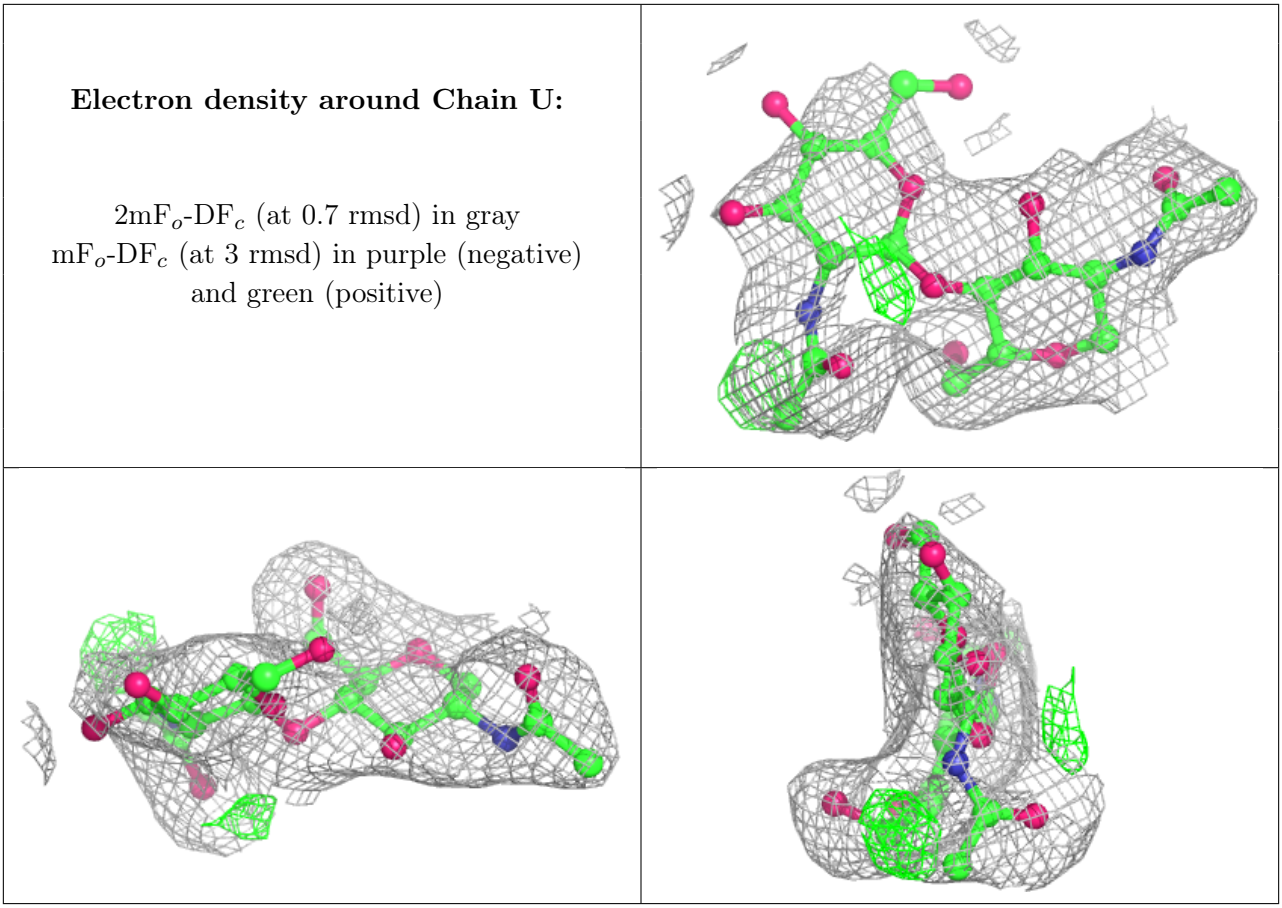






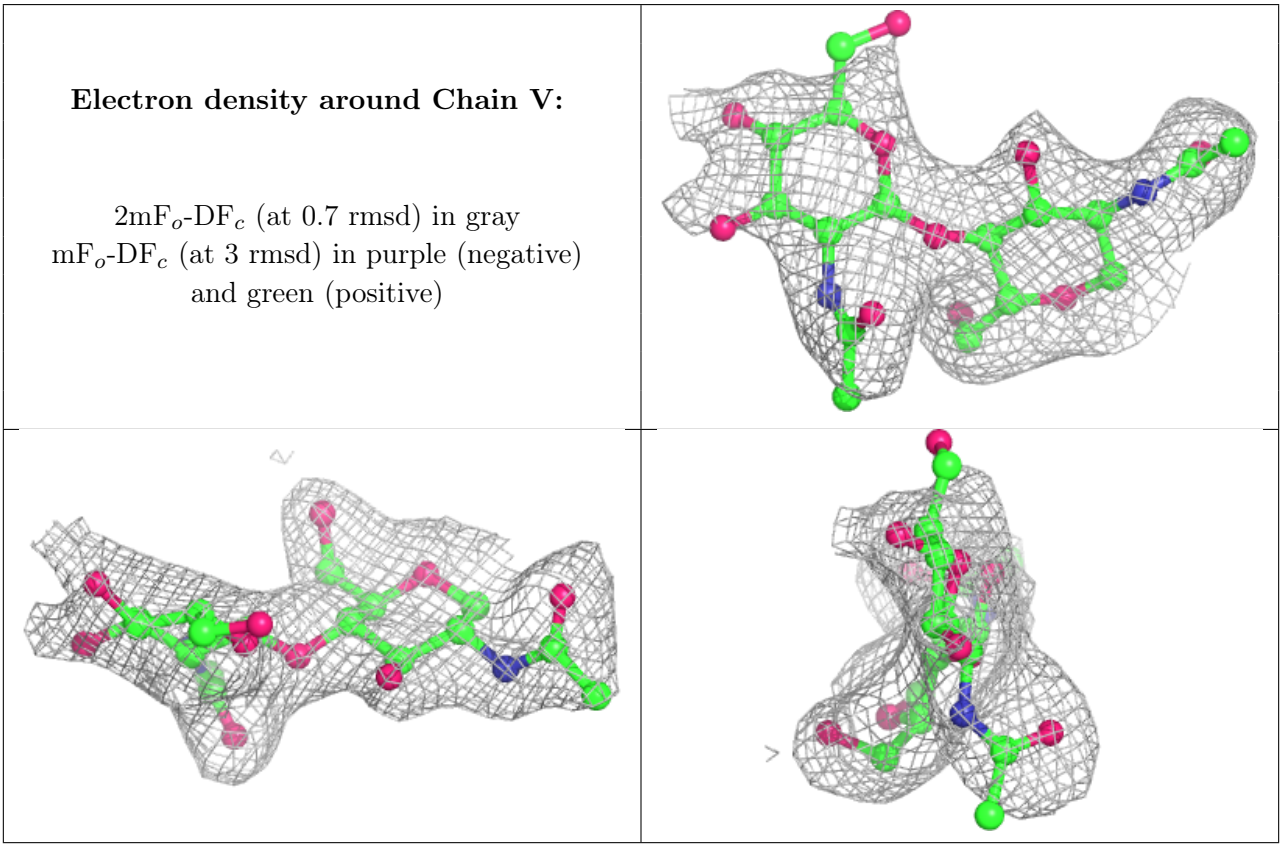
Electron density around Chain U:

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



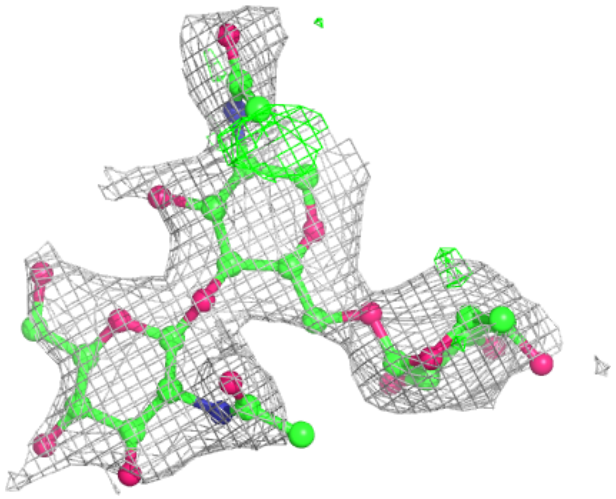
Electron density around Chain V:

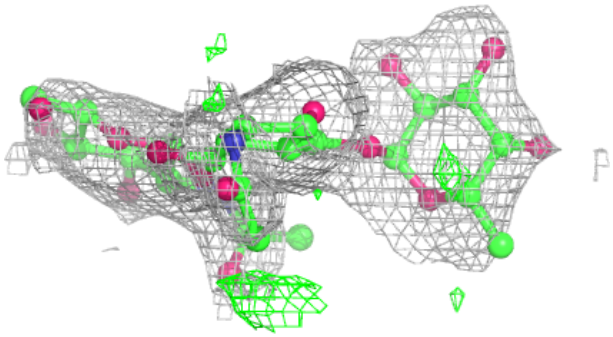
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

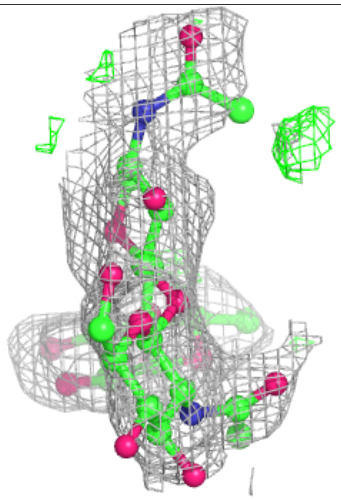


Electron density around Chain I:

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

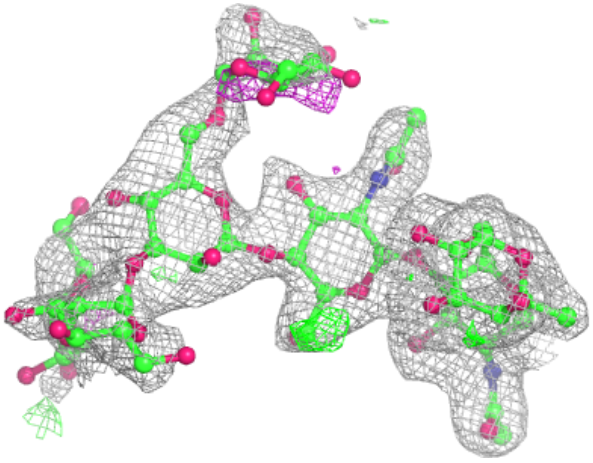


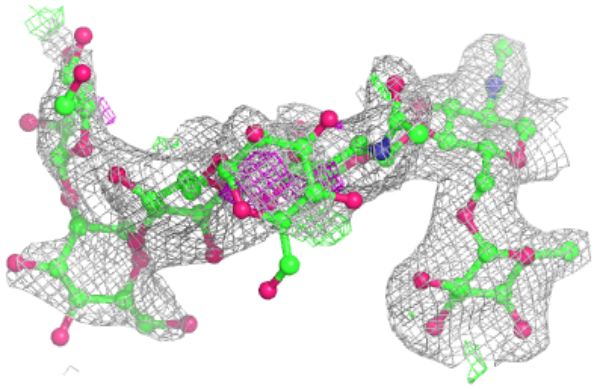




Electron density around Chain N:

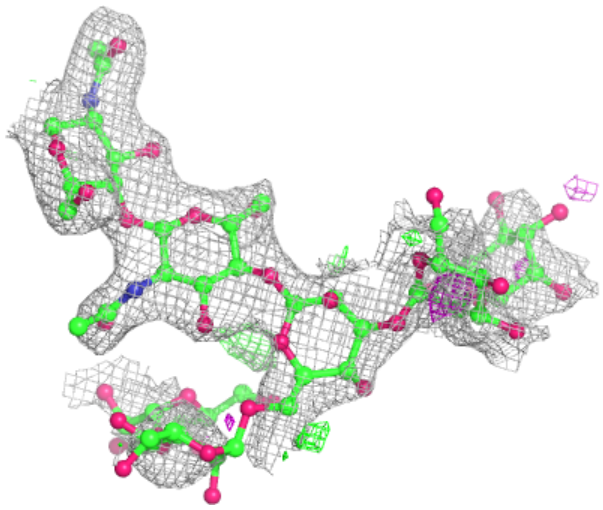
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

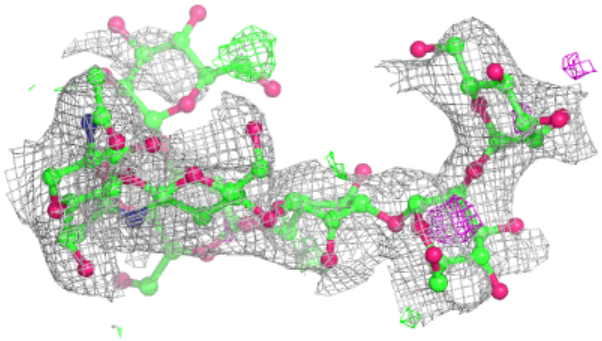


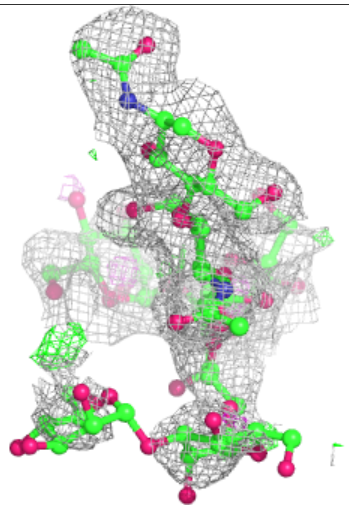


Electron density around Chain O:

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

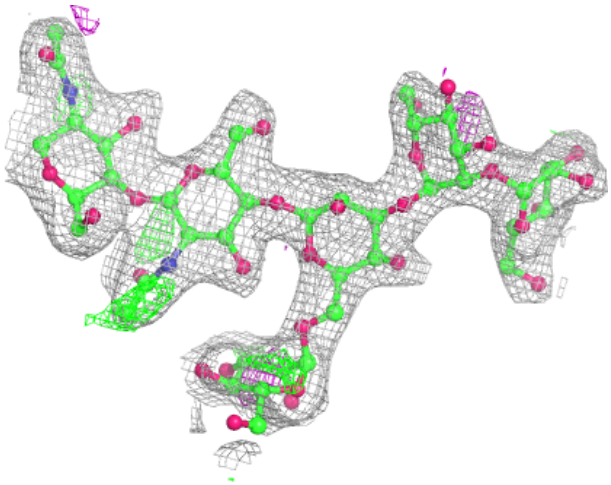


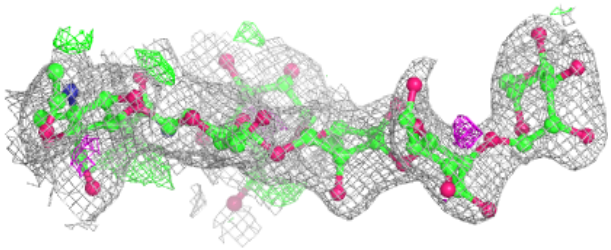


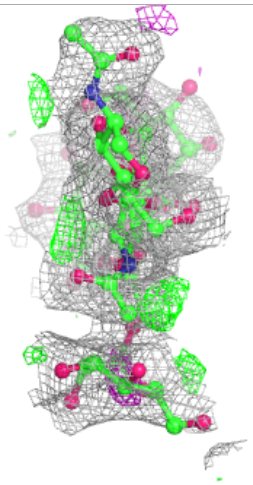


Electron density around Chain P:

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

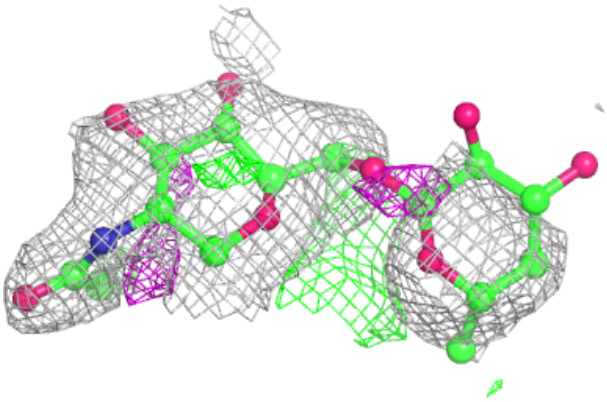


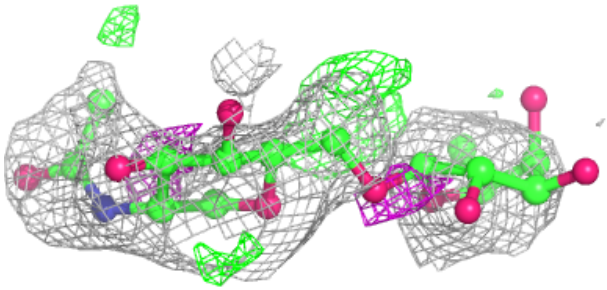


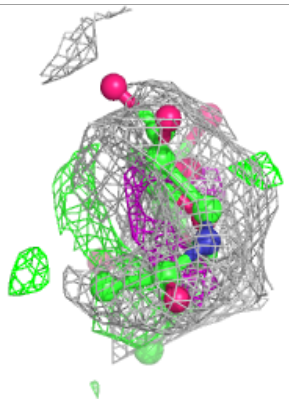


Electron density around Chain R:

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

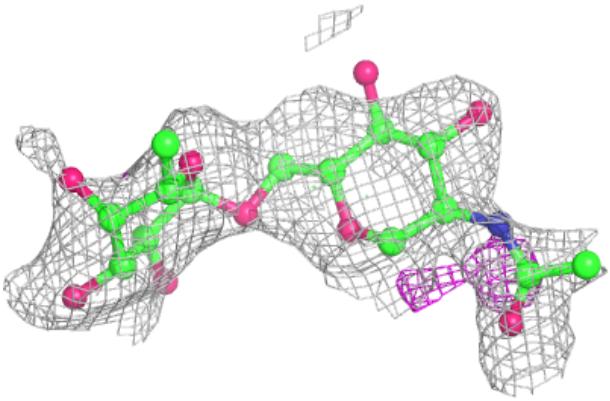


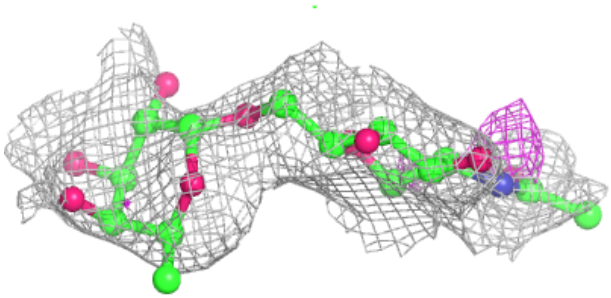


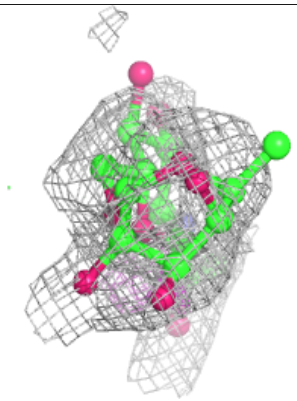


Electron density around Chain X:

$2mF_o$-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)

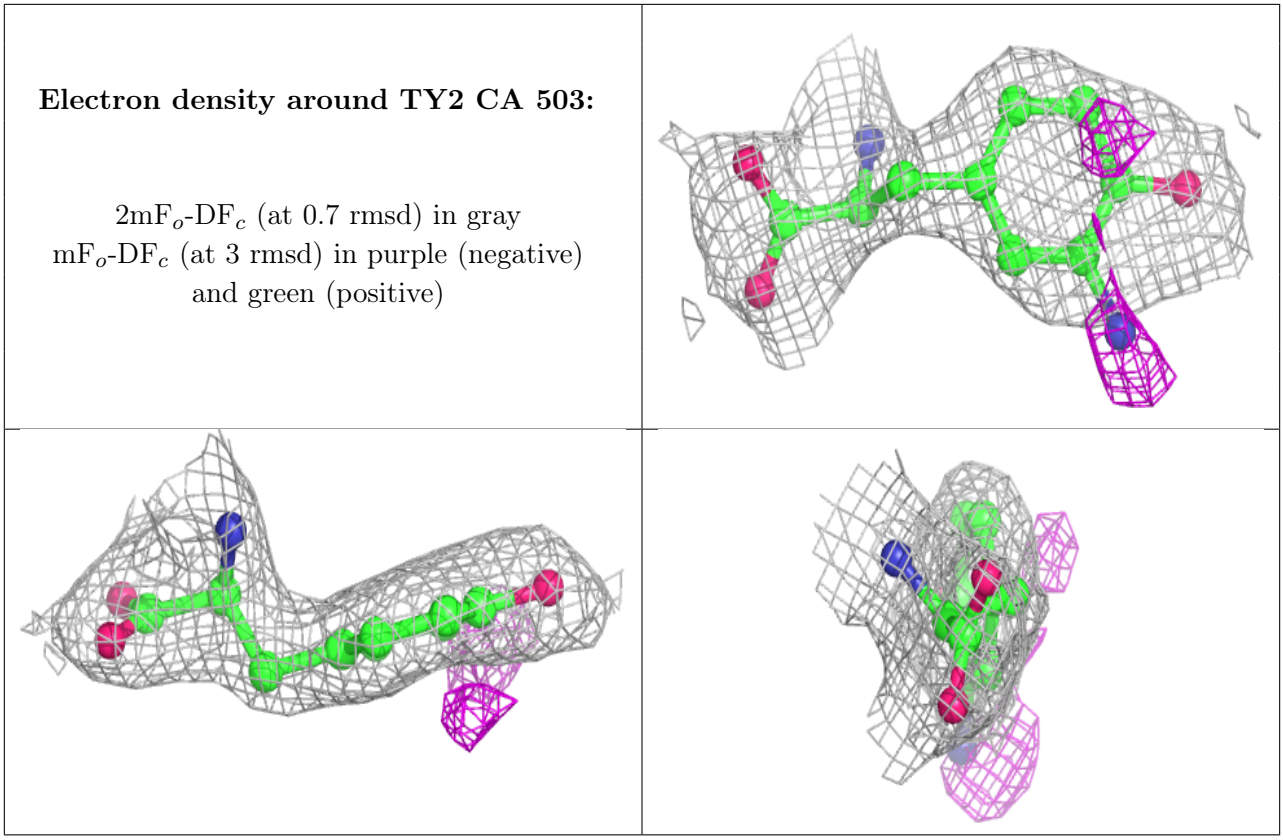
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
12	NAG	DA	502	14/15	0.59	0.45	80,90,98,98	0
12	NAG	CA	501	14/15	0.74	0.35	69,81,91,94	0
12	NAG	DA	501	14/15	0.75	0.28	68,77,85,90	0
12	NAG	AA	501	14/15	0.82	0.30	70,75,78,87	0
13	GOL	DA	503	6/6	0.87	0.21	47,52,59,61	0
13	GOL	BA	501	6/6	0.90	0.13	42,51,59,61	0
13	GOL	AA	502	6/6	0.91	0.13	38,56,63,65	0
13	GOL	CA	502	6/6	0.92	0.11	40,44,56,60	0
15	TY2	CA	503	14/14	0.93	0.15	34,46,56,59	0
14	ZN	CA	504	1/1	0.99	0.13	30,30,30,30	0
14	ZN	CA	505	1/1	0.99	0.17	33,33,33,33	0
14	ZN	BA	503	1/1	0.99	0.17	31,31,31,31	0
14	ZN	AA	504	1/1	1.00	0.14	28,28,28,28	0
14	ZN	BA	502	1/1	1.00	0.13	30,30,30,30	0
14	ZN	DA	504	1/1	1.00	0.14	33,33,33,33	0
14	ZN	DA	505	1/1	1.00	0.12	32,32,32,32	0
14	ZN	AA	503	1/1	1.00	0.17	28,28,28,28	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 TY2 CA 503:

$2mF_o$-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 (i)

There are no such residues in this entry.