Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:29 AM BST

PDB ID	:	3W9T
Title	:	pore-forming CEL-III
Authors	:	Unno, H.; Goda, S.; Hatakeyama, T.
Deposited on	:	2013-04-16
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

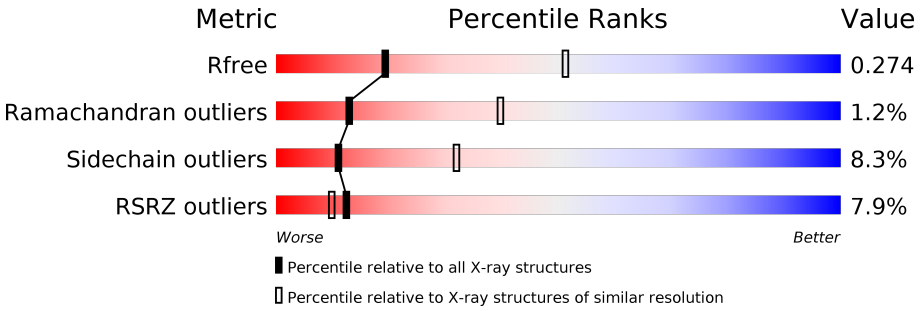
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	7% 92% 7%
1	B	432	7% 90% 9%
1	C	432	6% 91% 7%
1	D	432	7% 91% 9%
1	E	432	8% 91% 8%
1	F	432	9% 91% 8%
1	G	432	11% 91% 9%

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Mol	Chain	Length	Quality of chain
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	100%
2	K	2	50% 50%
2	L	2	100%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	100%
2	R	2	100%
2	S	2	50% 50%
2	T	2	50% 50%
2	U	2	100%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 50%
2	Y	2	50% 50%
2	Z	2	50% 50%
2	a	2	50% 50%
2	b	2	100%
2	c	2	50% 50%
2	d	2	50% 50%
2	e	2	100%
2	f	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	g	2	100%
2	h	2	50% 50%
2	i	2	50% 50%
2	j	2	100%
2	k	2	50% 50%
2	l	2	50% 50%
2	m	2	50% 50%
2	n	2	50% 50%
2	o	2	100%
2	p	2	50% 50%
2	q	2	50% 50%
2	r	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	V	1	-	-	-	X
2	FRU	l	1	-	-	-	X
3	CA	C	1014	-	-	X	-

2 Entry composition

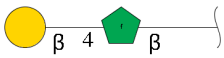
There are 5 unique types of molecules in this entry. The entry contains 24175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	C	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	G	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	B	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	F	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	E	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	D	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	M	2	Total C O 23 12 11	0	0	0
2	N	2	Total C O 23 12 11	0	0	0
2	O	2	Total C O 23 12 11	0	0	0
2	P	2	Total C O 23 12 11	0	0	0
2	Q	2	Total C O 23 12 11	0	0	0
2	R	2	Total C O 23 12 11	0	0	0
2	S	2	Total C O 23 12 11	0	0	0
2	T	2	Total C O 23 12 11	0	0	0
2	U	2	Total C O 23 12 11	0	0	0
2	V	2	Total C O 23 12 11	0	0	0
2	W	2	Total C O 23 12 11	0	0	0
2	X	2	Total C O 23 12 11	0	0	0
2	Y	2	Total C O 23 12 11	0	0	0
2	Z	2	Total C O 23 12 11	0	0	0
2	a	2	Total C O 23 12 11	0	0	0
2	b	2	Total C O 23 12 11	0	0	0
2	c	2	Total C O 23 12 11	0	0	0
2	d	2	Total C O 23 12 11	0	0	0
2	e	2	Total C O 23 12 11	0	0	0
2	f	2	Total C O 23 12 11	0	0	0
2	g	2	Total C O 23 12 11	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	h	2	Total C O 23 12 11	0	0	0
2	i	2	Total C O 23 12 11	0	0	0
2	j	2	Total C O 23 12 11	0	0	0
2	k	2	Total C O 23 12 11	0	0	0
2	l	2	Total C O 23 12 11	0	0	0
2	m	2	Total C O 23 12 11	0	0	0
2	n	2	Total C O 23 12 11	0	0	0
2	o	2	Total C O 23 12 11	0	0	0
2	p	2	Total C O 23 12 11	0	0	0
2	q	2	Total C O 23 12 11	0	0	0
2	r	2	Total C O 23 12 11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	6	Total Ca 6 6	0	0
3	D	6	Total Ca 6 6	0	0
3	E	7	Total Ca 7 7	0	0
3	B	6	Total Ca 6 6	0	0
3	C	7	Total Ca 7 7	0	0
3	A	6	Total Ca 6 6	0	0
3	F	6	Total Ca 6 6	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is water.

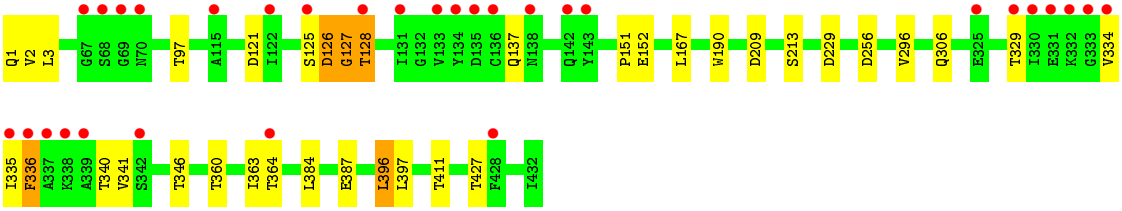
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	C	9	Total O 9 9	0	0
5	G	5	Total O 5 5	0	0
5	B	14	Total O 14 14	0	0
5	F	13	Total O 13 13	0	0
5	E	10	Total O 10 10	0	0
5	D	14	Total O 14 14	0	0

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.

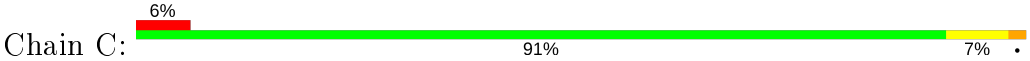
- Molecule 1: Hemolytic lectin CEL-III

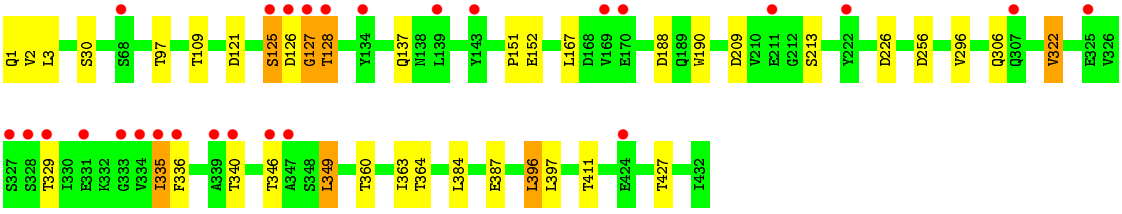
Chain A:



- Molecule 1: Hemolytic lectin CEL-III

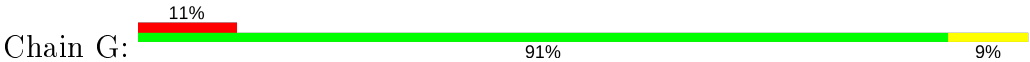
Chain C:

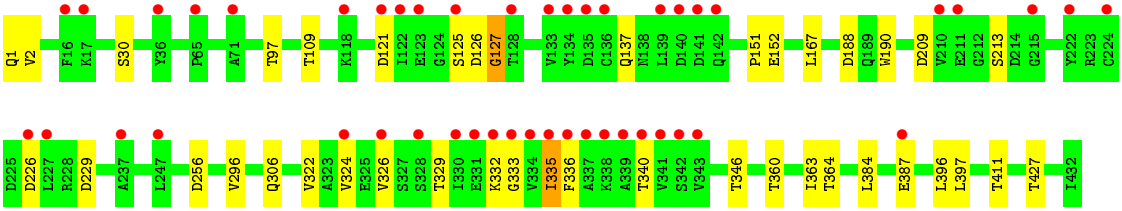




- Molecule 1: Hemolytic lectin CEL-III

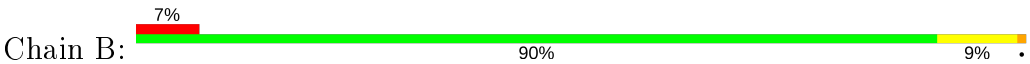
Chain G:

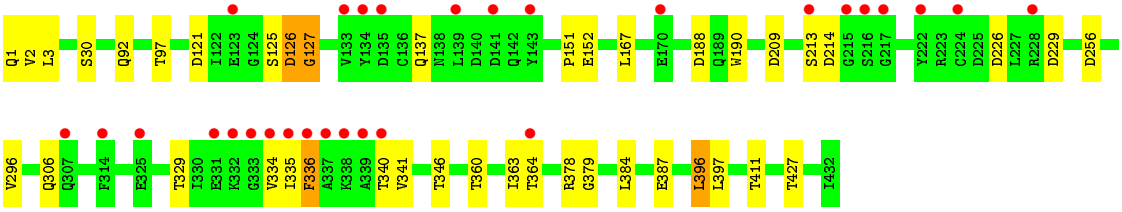




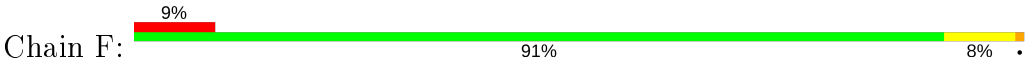
- Molecule 1: Hemolytic lectin CEL-III

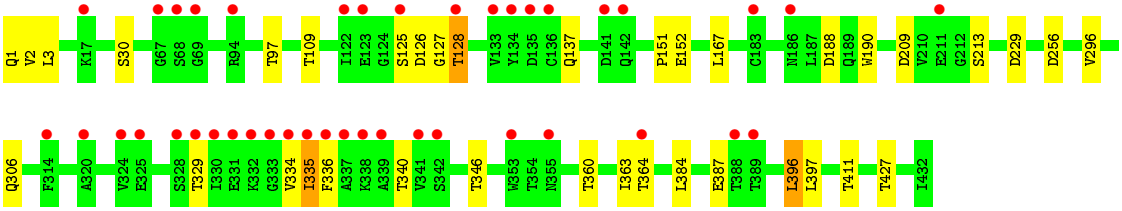
Chain B:



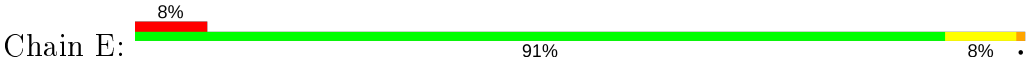


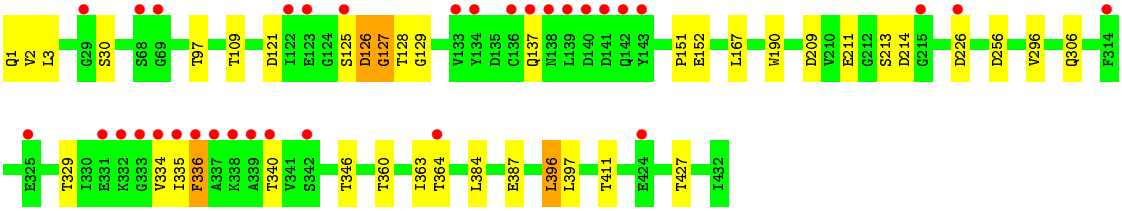
• Molecule 1: Hemolytic lectin CEL-III



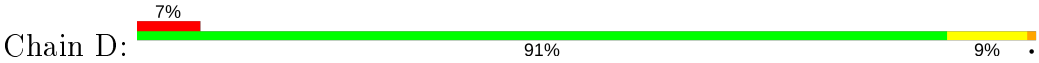


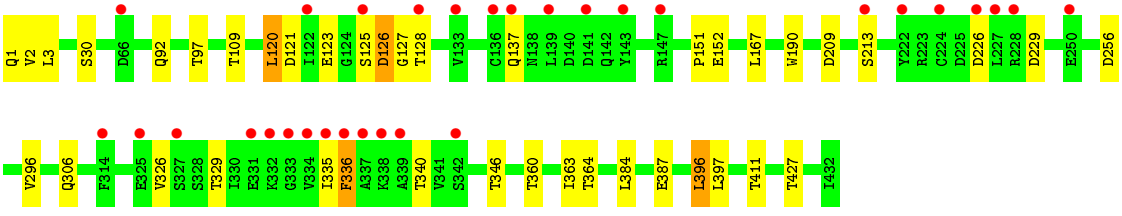
• Molecule 1: Hemolytic lectin CEL-III





• Molecule 1: Hemolytic lectin CEL-III





• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

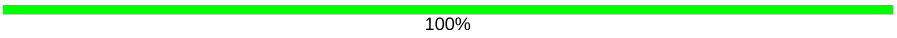
Chain J:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain K:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain L:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain M:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain N:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain O:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

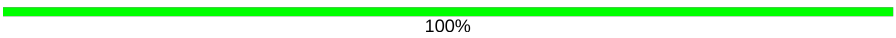
Chain P:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Q:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain R:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

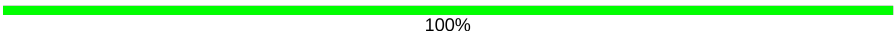
Chain S:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain T:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain U:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain V:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain W:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain X:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Y:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

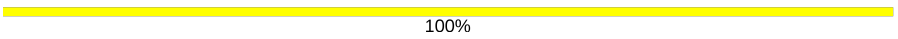
Chain Z:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain a:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain b:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

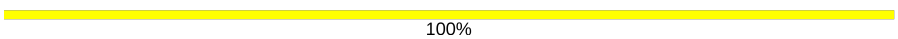
Chain c:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain d:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain e:

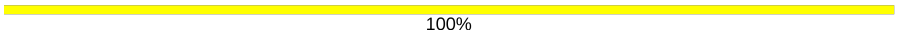


• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain f:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain g:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain h:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain i:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain j:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain k:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain l:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

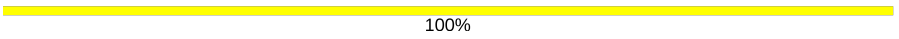
Chain m:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain n:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain o:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain p:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain q:

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain r:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.80Å 228.65Å 133.02Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.90) 98.4 (48.20-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.273 0.239 , 0.274	Depositor DCC
R_{free} test set	5691 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24175	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% 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: MG, GAL, PCA, CA, FRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	1/3366 (0.0%)	0.70	3/4566 (0.1%)
1	B	0.47	1/3366 (0.0%)	0.72	4/4566 (0.1%)
1	C	0.46	0/3366	0.71	5/4566 (0.1%)
1	D	0.45	0/3366	0.68	2/4566 (0.0%)
1	E	0.47	0/3366	0.69	2/4566 (0.0%)
1	F	0.49	0/3366	0.70	2/4566 (0.0%)
1	G	0.45	0/3366	0.71	1/4566 (0.0%)
All	All	0.47	2/23562 (0.0%)	0.70	19/31962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CG-OD2	-7.12	1.08	1.25
1	B	379	GLY	N-CA	-5.95	1.37	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	128	THR	N-CA-C	-10.58	82.44	111.00
1	B	378	ARG	C-N-CA	9.70	142.68	122.30
1	A	126	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	B	378	ARG	CA-C-N	7.94	132.07	116.20
1	C	349	LEU	CA-CB-CG	6.93	131.23	115.30
1	E	129	GLY	N-CA-C	6.81	130.11	113.10
1	B	378	ARG	O-C-N	-6.64	111.91	123.20
1	C	349	LEU	CB-CG-CD1	6.01	121.23	111.00
1	D	120	LEU	CB-CG-CD2	5.99	121.17	111.00
1	E	396	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	396	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	396	LEU	CA-CB-CG	5.26	127.40	115.30
1	G	2	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	F	2	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	F	396	LEU	CA-CB-CG	5.08	127.00	115.30
1	C	322	VAL	CG1-CB-CG2	5.02	118.94	110.90

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PRO	Peptide
1	A	335	ILE	Peptide
1	B	126	ASP	Peptide
1	B	127	GLY	Peptide
1	B	151	PRO	Peptide
1	B	335	ILE	Peptide
1	C	125	SER	Peptide
1	C	127	GLY	Peptide
1	C	151	PRO	Peptide
1	C	335	ILE	Peptide
1	D	126	ASP	Peptide
1	D	127	GLY	Peptide
1	D	151	PRO	Peptide
1	D	335	ILE	Peptide
1	E	126	ASP	Peptide
1	E	127	GLY	Peptide
1	E	151	PRO	Peptide
1	E	335	ILE	Peptide
1	F	127	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	F	151	PRO	Peptide
1	F	335	ILE	Peptide
1	G	127	GLY	Peptide
1	G	151	PRO	Peptide
1	G	332	LYS	Peptide
1	G	335	ILE	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/432 (100%)	407 (95%)	18 (4%)	5 (1%)	13	40
1	B	430/432 (100%)	410 (95%)	16 (4%)	4 (1%)	17	48
1	C	430/432 (100%)	410 (95%)	13 (3%)	7 (2%)	9	32
1	D	430/432 (100%)	411 (96%)	15 (4%)	4 (1%)	17	48
1	E	430/432 (100%)	408 (95%)	17 (4%)	5 (1%)	13	40
1	F	430/432 (100%)	410 (95%)	15 (4%)	5 (1%)	13	40
1	G	430/432 (100%)	411 (96%)	12 (3%)	7 (2%)	9	32
All	All	3010/3024 (100%)	2867 (95%)	106 (4%)	37 (1%)	13	40

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	ASP
1	C	128	THR
1	C	336	PHE
1	G	126	ASP

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Mol	Chain	Res	Type
1	G	336	PHE
1	B	126	ASP
1	F	126	ASP
1	F	128	THR
1	F	336	PHE
1	E	126	ASP
1	E	127	GLY
1	D	126	ASP
1	A	127	GLY
1	A	336	PHE
1	C	127	GLY
1	G	127	GLY
1	B	336	PHE
1	E	336	PHE
1	D	336	PHE
1	C	152	GLU
1	B	226	ASP
1	E	152	GLU
1	D	152	GLU
1	D	226	ASP
1	A	126	ASP
1	A	128	THR
1	C	226	ASP
1	G	152	GLU
1	G	226	ASP
1	G	333	GLY
1	B	152	GLU
1	F	152	GLU
1	A	152	GLU
1	G	335	ILE
1	E	226	ASP
1	C	335	ILE
1	F	335	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	340 (92%)	30 (8%)	11 33
1	B	370/370 (100%)	337 (91%)	33 (9%)	9 29
1	C	370/370 (100%)	340 (92%)	30 (8%)	11 33
1	D	370/370 (100%)	337 (91%)	33 (9%)	9 29
1	E	370/370 (100%)	339 (92%)	31 (8%)	11 31
1	F	370/370 (100%)	341 (92%)	29 (8%)	12 34
1	G	370/370 (100%)	340 (92%)	30 (8%)	11 33
All	All	2590/2590 (100%)	2374 (92%)	216 (8%)	11 32

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	LEU
1	A	97	THR
1	A	121	ASP
1	A	125	SER
1	A	128	THR
1	A	137	GLN
1	A	167	LEU
1	A	190	TRP
1	A	209	ASP
1	A	213	SER
1	A	229	ASP
1	A	256	ASP
1	A	296	VAL
1	A	306	GLN
1	A	329	THR
1	A	334	VAL
1	A	336	PHE
1	A	340	THR
1	A	341	VAL
1	A	346	THR
1	A	360	THR
1	A	363	ILE
1	A	364	THR
1	A	384	LEU
1	A	387	GLU
1	A	396	LEU
1	A	397	LEU
1	A	411	THR

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Mol	Chain	Res	Type
1	A	427	THR
1	C	2	VAL
1	C	3	LEU
1	C	30	SER
1	C	97	THR
1	C	109	THR
1	C	121	ASP
1	C	125	SER
1	C	137	GLN
1	C	167	LEU
1	C	188	ASP
1	C	190	TRP
1	C	209	ASP
1	C	213	SER
1	C	256	ASP
1	C	296	VAL
1	C	306	GLN
1	C	322	VAL
1	C	329	THR
1	C	340	THR
1	C	346	THR
1	C	349	LEU
1	C	360	THR
1	C	363	ILE
1	C	364	THR
1	C	384	LEU
1	C	387	GLU
1	C	396	LEU
1	C	397	LEU
1	C	411	THR
1	C	427	THR
1	G	30	SER
1	G	97	THR
1	G	109	THR
1	G	121	ASP
1	G	125	SER
1	G	137	GLN
1	G	167	LEU
1	G	188	ASP
1	G	190	TRP
1	G	209	ASP
1	G	213	SER

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Mol	Chain	Res	Type
1	G	229	ASP
1	G	256	ASP
1	G	296	VAL
1	G	306	GLN
1	G	322	VAL
1	G	324	VAL
1	G	326	VAL
1	G	329	THR
1	G	340	THR
1	G	346	THR
1	G	360	THR
1	G	363	ILE
1	G	364	THR
1	G	384	LEU
1	G	387	GLU
1	G	396	LEU
1	G	397	LEU
1	G	411	THR
1	G	427	THR
1	B	2	VAL
1	B	3	LEU
1	B	30	SER
1	B	92	GLN
1	B	97	THR
1	B	121	ASP
1	B	125	SER
1	B	137	GLN
1	B	167	LEU
1	B	188	ASP
1	B	190	TRP
1	B	209	ASP
1	B	213	SER
1	B	214	ASP
1	B	229	ASP
1	B	256	ASP
1	B	296	VAL
1	B	306	GLN
1	B	329	THR
1	B	334	VAL
1	B	336	PHE
1	B	340	THR
1	B	341	VAL

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Mol	Chain	Res	Type
1	B	346	THR
1	B	360	THR
1	B	363	ILE
1	B	364	THR
1	B	384	LEU
1	B	387	GLU
1	B	396	LEU
1	B	397	LEU
1	B	411	THR
1	B	427	THR
1	F	3	LEU
1	F	30	SER
1	F	97	THR
1	F	109	THR
1	F	125	SER
1	F	128	THR
1	F	137	GLN
1	F	167	LEU
1	F	188	ASP
1	F	190	TRP
1	F	209	ASP
1	F	213	SER
1	F	229	ASP
1	F	256	ASP
1	F	296	VAL
1	F	306	GLN
1	F	329	THR
1	F	334	VAL
1	F	340	THR
1	F	346	THR
1	F	360	THR
1	F	363	ILE
1	F	364	THR
1	F	384	LEU
1	F	387	GLU
1	F	396	LEU
1	F	397	LEU
1	F	411	THR
1	F	427	THR
1	E	2	VAL
1	E	3	LEU
1	E	30	SER

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Mol	Chain	Res	Type
1	E	97	THR
1	E	109	THR
1	E	121	ASP
1	E	125	SER
1	E	128	THR
1	E	137	GLN
1	E	167	LEU
1	E	190	TRP
1	E	209	ASP
1	E	213	SER
1	E	214	ASP
1	E	256	ASP
1	E	296	VAL
1	E	306	GLN
1	E	329	THR
1	E	334	VAL
1	E	336	PHE
1	E	340	THR
1	E	346	THR
1	E	360	THR
1	E	363	ILE
1	E	364	THR
1	E	384	LEU
1	E	387	GLU
1	E	396	LEU
1	E	397	LEU
1	E	411	THR
1	E	427	THR
1	D	2	VAL
1	D	3	LEU
1	D	30	SER
1	D	92	GLN
1	D	97	THR
1	D	109	THR
1	D	120	LEU
1	D	121	ASP
1	D	125	SER
1	D	128	THR
1	D	137	GLN
1	D	167	LEU
1	D	190	TRP
1	D	209	ASP

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Mol	Chain	Res	Type
1	D	213	SER
1	D	229	ASP
1	D	256	ASP
1	D	296	VAL
1	D	306	GLN
1	D	326	VAL
1	D	329	THR
1	D	336	PHE
1	D	340	THR
1	D	346	THR
1	D	360	THR
1	D	363	ILE
1	D	364	THR
1	D	384	LEU
1	D	387	GLU
1	D	396	LEU
1	D	397	LEU
1	D	411	THR
1	D	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	270	GLN
1	A	301	ASN
1	A	306	GLN
1	C	32	ASN
1	C	270	GLN
1	C	301	ASN
1	C	306	GLN
1	G	32	ASN
1	G	301	ASN
1	G	306	GLN
1	B	32	ASN
1	B	301	ASN
1	B	306	GLN
1	F	32	ASN
1	F	138	ASN
1	F	270	GLN
1	F	301	ASN
1	F	306	GLN

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Mol	Chain	Res	Type
1	E	32	ASN
1	E	138	ASN
1	E	270	GLN
1	E	301	ASN
1	E	306	GLN
1	D	32	ASN
1	D	270	GLN
1	D	301	ASN
1	D	306	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	F	1	1	7,8,9	0.51	0	9,10,12	2.24	4 (44%)
1	PCA	G	1	1	7,8,9	0.64	0	9,10,12	2.18	3 (33%)
1	PCA	E	1	1	7,8,9	0.47	0	9,10,12	2.35	3 (33%)
1	PCA	C	1	1	7,8,9	0.51	0	9,10,12	2.28	4 (44%)
1	PCA	A	1	1	7,8,9	0.56	0	9,10,12	2.29	3 (33%)
1	PCA	B	1	1	7,8,9	0.50	0	9,10,12	2.12	2 (22%)
1	PCA	D	1	1	7,8,9	0.63	0	9,10,12	2.22	2 (22%)

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
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	PCA	CB-CA-C	5.00	119.59	112.70
1	E	1	PCA	CB-CA-C	4.90	119.45	112.70
1	C	1	PCA	CB-CA-C	4.48	118.87	112.70
1	A	1	PCA	CB-CA-C	4.36	118.70	112.70
1	F	1	PCA	CA-N-CD	-4.32	98.79	113.58
1	B	1	PCA	CB-CA-C	4.25	118.55	112.70
1	G	1	PCA	CB-CA-C	4.13	118.38	112.70
1	A	1	PCA	CA-N-CD	-3.93	100.12	113.58
1	C	1	PCA	CA-N-CD	-3.73	100.80	113.58
1	E	1	PCA	CA-N-CD	-3.73	100.81	113.58
1	B	1	PCA	CA-N-CD	-3.66	101.05	113.58
1	G	1	PCA	CA-N-CD	-3.62	101.19	113.58
1	D	1	PCA	CA-N-CD	-3.48	101.65	113.58
1	F	1	PCA	CB-CA-C	3.38	117.36	112.70
1	F	1	PCA	OE-CD-CG	-2.45	122.48	126.76
1	A	1	PCA	OE-CD-CG	-2.32	122.71	126.76
1	F	1	PCA	CB-CG-CD	-2.28	100.73	104.40
1	G	1	PCA	OE-CD-CG	-2.25	122.83	126.76
1	E	1	PCA	OE-CD-CG	-2.20	122.92	126.76
1	C	1	PCA	OE-CD-CG	-2.10	123.09	126.76
1	C	1	PCA	CB-CG-CD	-2.03	101.13	104.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

74 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	FRU	H	1	2	11,12,12	0.71	0	10,18,18	0.88	0
2	GAL	H	2	3,2	11,11,12	0.32	0	15,15,17	1.49	2 (13%)
2	FRU	I	1	2	11,12,12	0.65	0	10,18,18	0.88	0
2	GAL	I	2	3,2	11,11,12	0.73	0	15,15,17	2.12	3 (20%)
2	FRU	J	1	2	11,12,12	0.72	1 (9%)	10,18,18	1.02	0
2	GAL	J	2	3,2	11,11,12	0.39	0	15,15,17	1.01	1 (6%)
2	FRU	K	1	2	11,12,12	0.61	0	10,18,18	0.72	0
2	GAL	K	2	3,2	11,11,12	0.29	0	15,15,17	1.01	1 (6%)
2	FRU	L	1	2	11,12,12	0.57	0	10,18,18	0.84	0
2	GAL	L	2	3,2	11,11,12	0.34	0	15,15,17	0.85	0
2	FRU	M	1	2	11,12,12	0.78	0	10,18,18	1.03	0
2	GAL	M	2	3,2	11,11,12	0.75	0	15,15,17	1.83	3 (20%)
2	FRU	N	1	2	11,12,12	0.70	0	10,18,18	0.70	0
2	GAL	N	2	3,2	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	FRU	O	1	2	11,12,12	0.67	0	10,18,18	0.82	0
2	GAL	O	2	3,2	11,11,12	0.34	0	15,15,17	1.64	5 (33%)
2	FRU	P	1	2	11,12,12	0.75	0	10,18,18	0.64	0
2	GAL	P	2	3,2	11,11,12	0.56	0	15,15,17	1.34	3 (20%)
2	FRU	Q	1	2	11,12,12	0.72	0	10,18,18	1.06	1 (10%)
2	GAL	Q	2	3,2	11,11,12	0.37	0	15,15,17	1.09	1 (6%)
2	FRU	R	1	2	11,12,12	0.63	0	10,18,18	0.98	0
2	GAL	R	2	3,2	11,11,12	0.37	0	15,15,17	0.47	0
2	FRU	S	1	2	11,12,12	0.71	0	10,18,18	0.65	0
2	GAL	S	2	3,2	11,11,12	0.31	0	15,15,17	1.21	2 (13%)
2	FRU	T	1	2	11,12,12	0.65	0	10,18,18	0.90	0
2	GAL	T	2	3,2	11,11,12	0.40	0	15,15,17	2.16	3 (20%)
2	FRU	U	1	2	11,12,12	0.65	0	10,18,18	0.83	0
2	GAL	U	2	3,2	11,11,12	0.33	0	15,15,17	0.92	0
2	FRU	V	1	2	11,12,12	0.65	0	10,18,18	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	V	2	3,2	11,11,12	0.44	0	15,15,17	2.04	3 (20%)
2	FRU	W	1	2	11,12,12	0.78	0	10,18,18	1.45	1 (10%)
2	GAL	W	2	3,2	11,11,12	0.34	0	15,15,17	0.86	0
2	FRU	X	1	2	11,12,12	0.79	0	10,18,18	0.91	0
2	GAL	X	2	3,2	11,11,12	0.73	0	15,15,17	2.12	5 (33%)
2	FRU	Y	1	2	11,12,12	0.67	0	10,18,18	0.75	0
2	GAL	Y	2	3,2	11,11,12	0.29	0	15,15,17	0.91	1 (6%)
2	FRU	Z	1	2	11,12,12	0.73	0	10,18,18	0.81	0
2	GAL	Z	2	3,2	11,11,12	0.36	0	15,15,17	2.73	6 (40%)
2	FRU	a	1	2	11,12,12	0.56	0	10,18,18	1.10	0
2	GAL	a	2	3,2	11,11,12	0.45	0	15,15,17	1.88	1 (6%)
2	FRU	b	1	2	11,12,12	0.96	1 (9%)	10,18,18	1.20	0
2	GAL	b	2	2	11,11,12	0.57	0	15,15,17	3.12	6 (40%)
2	FRU	c	1	2	11,12,12	0.85	0	10,18,18	1.04	1 (10%)
2	GAL	c	2	3,2	11,11,12	0.39	0	15,15,17	0.84	0
2	FRU	d	1	2	11,12,12	0.78	1 (9%)	10,18,18	0.55	0
2	GAL	d	2	3,2	11,11,12	0.31	0	15,15,17	0.83	0
2	FRU	e	1	2	11,12,12	0.96	1 (9%)	10,18,18	0.93	0
2	GAL	e	2	3,2	11,11,12	0.72	0	15,15,17	2.10	2 (13%)
2	FRU	f	1	2	11,12,12	0.65	0	10,18,18	0.57	0
2	GAL	f	2	3,2	11,11,12	0.42	0	15,15,17	1.25	2 (13%)
2	FRU	g	1	2	11,12,12	1.01	0	10,18,18	1.12	1 (10%)
2	GAL	g	2	2	11,11,12	0.69	0	15,15,17	2.25	8 (53%)
2	FRU	h	1	2	11,12,12	0.61	0	10,18,18	0.97	0
2	GAL	h	2	3,2	11,11,12	0.59	0	15,15,17	1.44	2 (13%)
2	FRU	i	1	2	11,12,12	0.60	0	10,18,18	0.88	0
2	GAL	i	2	3,2	11,11,12	0.41	0	15,15,17	1.30	1 (6%)
2	FRU	j	1	2	11,12,12	0.77	1 (9%)	10,18,18	0.84	0
2	GAL	j	2	3,2	11,11,12	0.52	0	15,15,17	1.28	2 (13%)
2	FRU	k	1	2	11,12,12	0.69	0	10,18,18	0.84	0
2	GAL	k	2	3,2	11,11,12	0.54	0	15,15,17	1.31	1 (6%)
2	FRU	l	1	2	11,12,12	0.64	0	10,18,18	0.82	0
2	GAL	l	2	3,2	11,11,12	0.65	0	15,15,17	1.96	3 (20%)
2	FRU	m	1	2	11,12,12	0.76	0	10,18,18	1.09	0
2	GAL	m	2	2	11,11,12	0.48	0	15,15,17	2.26	4 (26%)
2	FRU	n	1	2	11,12,12	0.70	1 (9%)	10,18,18	1.13	0
2	GAL	n	2	3,2	11,11,12	0.42	0	15,15,17	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FRU	o	1	2	11,12,12	0.70	0	10,18,18	0.96	1 (10%)
2	GAL	o	2	3,2	11,11,12	0.46	0	15,15,17	1.64	2 (13%)
2	FRU	p	1	2	11,12,12	0.69	0	10,18,18	0.80	0
2	GAL	p	2	3,2	11,11,12	0.59	0	15,15,17	1.30	2 (13%)
2	FRU	q	1	2	11,12,12	0.68	0	10,18,18	0.85	0
2	GAL	q	2	3,2	11,11,12	0.41	0	15,15,17	2.23	2 (13%)
2	FRU	r	1	2	11,12,12	0.53	0	10,18,18	0.97	0
2	GAL	r	2	3,2	11,11,12	0.34	0	15,15,17	1.75	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	H	1	2	-	5/5/24/24	0/1/1/1
2	GAL	H	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	I	1	2	-	2/5/24/24	0/1/1/1
2	GAL	I	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	J	1	2	-	4/5/24/24	0/1/1/1
2	GAL	J	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	K	1	2	-	2/5/24/24	0/1/1/1
2	GAL	K	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	L	1	2	-	3/5/24/24	0/1/1/1
2	GAL	L	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	M	1	2	-	0/5/24/24	0/1/1/1
2	GAL	M	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	N	1	2	-	3/5/24/24	0/1/1/1
2	GAL	N	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	O	1	2	-	3/5/24/24	0/1/1/1
2	GAL	O	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	P	1	2	-	3/5/24/24	0/1/1/1
2	GAL	P	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	Q	1	2	-	4/5/24/24	0/1/1/1
2	GAL	Q	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	R	1	2	-	3/5/24/24	0/1/1/1
2	GAL	R	2	3,2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	S	1	2	-	0/5/24/24	0/1/1/1
2	GAL	S	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	T	1	2	-	3/5/24/24	0/1/1/1
2	GAL	T	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	U	1	2	-	3/5/24/24	0/1/1/1
2	GAL	U	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	V	1	2	-	5/5/24/24	0/1/1/1
2	GAL	V	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	W	1	2	-	2/5/24/24	0/1/1/1
2	GAL	W	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	X	1	2	-	5/5/24/24	0/1/1/1
2	GAL	X	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	Y	1	2	-	2/5/24/24	0/1/1/1
2	GAL	Y	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	Z	1	2	-	2/5/24/24	0/1/1/1
2	GAL	Z	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	a	1	2	-	2/5/24/24	0/1/1/1
2	GAL	a	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	b	1	2	-	3/5/24/24	0/1/1/1
2	GAL	b	2	2	-	2/2/19/22	0/1/1/1
2	FRU	c	1	2	-	0/5/24/24	0/1/1/1
2	GAL	c	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	d	1	2	-	1/5/24/24	0/1/1/1
2	GAL	d	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	e	1	2	-	2/5/24/24	0/1/1/1
2	GAL	e	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	f	1	2	-	2/5/24/24	0/1/1/1
2	GAL	f	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	g	1	2	-	3/5/24/24	0/1/1/1
2	GAL	g	2	2	-	0/2/19/22	0/1/1/1
2	FRU	h	1	2	-	2/5/24/24	0/1/1/1
2	GAL	h	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	i	1	2	-	3/5/24/24	0/1/1/1
2	GAL	i	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	j	1	2	-	3/5/24/24	0/1/1/1
2	GAL	j	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	k	1	2	-	2/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	k	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	l	1	2	-	3/5/24/24	0/1/1/1
2	GAL	l	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	m	1	2	-	2/5/24/24	0/1/1/1
2	GAL	m	2	2	-	0/2/19/22	0/1/1/1
2	FRU	n	1	2	-	2/5/24/24	0/1/1/1
2	GAL	n	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	o	1	2	-	5/5/24/24	0/1/1/1
2	GAL	o	2	3,2	-	0/2/19/22	0/1/1/1
2	FRU	p	1	2	-	3/5/24/24	0/1/1/1
2	GAL	p	2	3,2	-	2/2/19/22	0/1/1/1
2	FRU	q	1	2	-	5/5/24/24	0/1/1/1
2	GAL	q	2	3,2	-	1/2/19/22	0/1/1/1
2	FRU	r	1	2	-	4/5/24/24	0/1/1/1
2	GAL	r	2	3,2	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	1	FRU	O2-C2	2.13	1.44	1.40
2	j	1	FRU	O2-C2	2.12	1.44	1.40
2	J	1	FRU	O2-C2	2.09	1.44	1.40
2	b	1	FRU	O2-C2	2.08	1.44	1.40
2	n	1	FRU	O2-C2	2.07	1.44	1.40
2	d	1	FRU	O2-C2	2.00	1.44	1.40

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	2	GAL	C1-O5-C5	-9.61	99.17	112.19
2	q	2	GAL	C1-O5-C5	7.60	122.50	112.19
2	T	2	GAL	C1-O5-C5	6.55	121.06	112.19
2	I	2	GAL	C1-O5-C5	6.39	120.85	112.19
2	a	2	GAL	C1-O5-C5	6.08	120.43	112.19
2	Z	2	GAL	C1-O5-C5	6.02	120.34	112.19
2	V	2	GAL	C1-O5-C5	5.89	120.17	112.19
2	e	2	GAL	C1-C2-C3	5.56	116.50	109.67
2	N	2	GAL	C1-O5-C5	5.44	119.57	112.19
2	l	2	GAL	C1-O5-C5	5.33	119.41	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	o	2	GAL	C1-O5-C5	5.19	119.23	112.19
2	X	2	GAL	C1-O5-C5	5.09	119.09	112.19
2	Z	2	GAL	C1-C2-C3	4.69	115.44	109.67
2	M	2	GAL	C3-C4-C5	4.68	118.60	110.24
2	m	2	GAL	O3-C3-C2	-4.68	101.03	109.99
2	m	2	GAL	C1-C2-C3	-4.60	104.02	109.67
2	e	2	GAL	C1-O5-C5	4.45	118.22	112.19
2	Z	2	GAL	C2-C3-C4	4.40	118.51	110.89
2	b	2	GAL	O5-C5-C6	4.32	113.98	107.20
2	M	2	GAL	C1-O5-C5	4.24	117.93	112.19
2	l	2	GAL	O5-C5-C6	4.14	113.69	107.20
2	g	2	GAL	C1-C2-C3	-4.08	104.65	109.67
2	Z	2	GAL	C3-C4-C5	3.92	117.23	110.24
2	H	2	GAL	O5-C5-C6	3.84	113.23	107.20
2	P	2	GAL	C1-O5-C5	3.79	117.33	112.19
2	m	2	GAL	O5-C5-C6	3.76	113.10	107.20
2	k	2	GAL	O5-C5-C6	3.63	112.90	107.20
2	g	2	GAL	O3-C3-C2	-3.43	103.42	109.99
2	r	2	GAL	C1-C2-C3	3.38	113.82	109.67
2	g	2	GAL	O5-C5-C6	3.30	112.39	107.20
2	X	2	GAL	C1-C2-C3	3.21	113.61	109.67
2	N	2	GAL	O5-C5-C4	3.20	118.61	110.83
2	V	2	GAL	C1-C2-C3	3.16	113.55	109.67
2	r	2	GAL	C1-O5-C5	3.11	116.41	112.19
2	g	2	GAL	O5-C5-C4	-3.10	103.29	110.83
2	r	2	GAL	O5-C5-C6	3.09	112.04	107.20
2	O	2	GAL	C1-C2-C3	3.07	113.43	109.67
2	X	2	GAL	O4-C4-C5	3.06	116.90	109.30
2	I	2	GAL	C1-C2-C3	3.06	113.42	109.67
2	N	2	GAL	C3-C4-C5	3.05	115.69	110.24
2	h	2	GAL	C1-O5-C5	3.01	116.27	112.19
2	W	1	FRU	O4-C4-C3	-3.00	103.16	112.15
2	j	2	GAL	O5-C5-C6	2.93	111.80	107.20
2	h	2	GAL	O5-C1-C2	2.87	115.20	110.77
2	i	2	GAL	C1-C2-C3	2.85	113.17	109.67
2	g	2	GAL	C1-O5-C5	-2.84	108.34	112.19
2	m	2	GAL	O5-C5-C4	-2.77	104.08	110.83
2	b	2	GAL	C1-C2-C3	-2.76	106.27	109.67
2	b	2	GAL	O5-C5-C4	-2.73	104.17	110.83
2	g	1	FRU	C6-C5-C4	-2.66	108.67	115.09
2	V	2	GAL	O5-C5-C6	2.64	111.34	107.20
2	I	2	GAL	O5-C5-C6	2.59	111.27	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	r	2	GAL	C3-C4-C5	-2.59	105.63	110.24
2	Z	2	GAL	O5-C5-C6	2.56	111.22	107.20
2	p	2	GAL	O5-C5-C6	2.55	111.21	107.20
2	j	2	GAL	O3-C3-C4	-2.52	104.53	110.35
2	f	2	GAL	O5-C1-C2	-2.43	107.02	110.77
2	O	2	GAL	C3-C4-C5	-2.42	105.92	110.24
2	S	2	GAL	C1-C2-C3	2.41	112.63	109.67
2	Z	2	GAL	O5-C1-C2	2.39	114.46	110.77
2	O	2	GAL	O4-C4-C5	2.37	115.19	109.30
2	J	2	GAL	O5-C5-C6	2.37	110.92	107.20
2	b	2	GAL	O5-C1-C2	-2.37	107.11	110.77
2	Q	1	FRU	C6-C5-C4	-2.36	109.39	115.09
2	g	2	GAL	O2-C2-C3	2.32	114.78	110.14
2	K	2	GAL	C1-O5-C5	2.31	115.32	112.19
2	f	2	GAL	C3-C4-C5	2.30	114.34	110.24
2	Q	2	GAL	O5-C5-C6	2.28	110.78	107.20
2	b	2	GAL	O3-C3-C4	-2.27	105.10	110.35
2	O	2	GAL	C1-O5-C5	2.27	115.26	112.19
2	M	2	GAL	O5-C5-C4	2.26	116.33	110.83
2	O	2	GAL	O5-C5-C6	2.24	110.72	107.20
2	Y	2	GAL	O5-C5-C6	2.21	110.66	107.20
2	H	2	GAL	C1-C2-C3	2.20	112.37	109.67
2	q	2	GAL	O5-C1-C2	2.19	114.15	110.77
2	S	2	GAL	O5-C5-C6	2.17	110.61	107.20
2	P	2	GAL	C1-C2-C3	2.16	112.32	109.67
2	X	2	GAL	O5-C1-C2	2.14	114.07	110.77
2	P	2	GAL	O5-C5-C6	2.13	110.54	107.20
2	g	2	GAL	O2-C2-C1	2.11	113.47	109.15
2	T	2	GAL	O5-C1-C2	2.07	113.96	110.77
2	o	1	FRU	O4-C4-C3	-2.05	106.01	112.15
2	X	2	GAL	O5-C5-C4	2.04	115.80	110.83
2	g	2	GAL	O4-C4-C3	-2.04	105.63	110.35
2	c	1	FRU	C6-C5-C4	-2.03	110.18	115.09
2	T	2	GAL	O5-C5-C4	2.03	115.76	110.83
2	o	2	GAL	O5-C5-C6	2.02	110.38	107.20
2	p	2	GAL	O5-C1-C2	-2.01	107.67	110.77
2	l	2	GAL	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	1	FRU	O5-C5-C6-O6
2	I	1	FRU	O1-C1-C2-O2
2	n	1	FRU	O5-C5-C6-O6
2	l	1	FRU	O1-C1-C2-C3
2	l	1	FRU	O1-C1-C2-O2
2	l	1	FRU	O1-C1-C2-O5
2	i	1	FRU	O1-C1-C2-C3
2	i	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O1-C1-C2-C3
2	J	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O1-C1-C2-O5
2	r	1	FRU	O1-C1-C2-O2
2	q	1	FRU	O1-C1-C2-O2
2	g	1	FRU	O1-C1-C2-C3
2	g	1	FRU	O1-C1-C2-O2
2	H	1	FRU	O1-C1-C2-C3
2	H	1	FRU	O1-C1-C2-O2
2	H	1	FRU	O1-C1-C2-O5
2	X	1	FRU	O1-C1-C2-C3
2	X	1	FRU	O1-C1-C2-O2
2	O	1	FRU	O1-C1-C2-C3
2	O	1	FRU	O1-C1-C2-O2
2	O	1	FRU	O1-C1-C2-O5
2	U	1	FRU	O1-C1-C2-C3
2	U	1	FRU	O1-C1-C2-O2
2	U	1	FRU	O1-C1-C2-O5
2	h	1	FRU	O1-C1-C2-O2
2	N	1	FRU	O1-C1-C2-C3
2	N	1	FRU	O1-C1-C2-O2
2	N	1	FRU	O1-C1-C2-O5
2	b	1	FRU	O1-C1-C2-C3
2	b	1	FRU	O1-C1-C2-O2
2	b	1	FRU	O1-C1-C2-O5
2	R	1	FRU	O5-C5-C6-O6
2	r	1	FRU	O5-C5-C6-O6
2	H	1	FRU	O5-C5-C6-O6
2	P	1	FRU	O5-C5-C6-O6
2	a	1	FRU	C4-C5-C6-O6
2	H	1	FRU	C4-C5-C6-O6
2	p	1	FRU	O5-C5-C6-O6
2	K	1	FRU	O5-C5-C6-O6
2	Z	1	FRU	O5-C5-C6-O6
2	J	2	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	n	1	FRU	C4-C5-C6-O6
2	r	1	FRU	C4-C5-C6-O6
2	P	1	FRU	C4-C5-C6-O6
2	b	2	GAL	O5-C5-C6-O6
2	Q	1	FRU	O5-C5-C6-O6
2	q	1	FRU	O5-C5-C6-O6
2	Y	1	FRU	O5-C5-C6-O6
2	V	1	FRU	O5-C5-C6-O6
2	L	1	FRU	O5-C5-C6-O6
2	o	1	FRU	C4-C5-C6-O6
2	p	1	FRU	C4-C5-C6-O6
2	Q	1	FRU	C4-C5-C6-O6
2	R	1	FRU	C4-C5-C6-O6
2	Y	1	FRU	C4-C5-C6-O6
2	V	1	FRU	C4-C5-C6-O6
2	L	1	FRU	C4-C5-C6-O6
2	l	2	GAL	O5-C5-C6-O6
2	V	2	GAL	O5-C5-C6-O6
2	r	2	GAL	O5-C5-C6-O6
2	j	2	GAL	O5-C5-C6-O6
2	b	2	GAL	C4-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	f	2	GAL	O5-C5-C6-O6
2	l	2	GAL	C4-C5-C6-O6
2	Z	1	FRU	C4-C5-C6-O6
2	U	2	GAL	O5-C5-C6-O6
2	J	2	GAL	C4-C5-C6-O6
2	V	2	GAL	C4-C5-C6-O6
2	c	2	GAL	O5-C5-C6-O6
2	j	2	GAL	C4-C5-C6-O6
2	n	2	GAL	C4-C5-C6-O6
2	p	2	GAL	O5-C5-C6-O6
2	c	2	GAL	C4-C5-C6-O6
2	r	2	GAL	C4-C5-C6-O6
2	N	2	GAL	O5-C5-C6-O6
2	k	2	GAL	O5-C5-C6-O6
2	k	2	GAL	C4-C5-C6-O6
2	f	2	GAL	C4-C5-C6-O6
2	N	2	GAL	C4-C5-C6-O6
2	n	2	GAL	O5-C5-C6-O6
2	H	2	GAL	C4-C5-C6-O6
2	U	2	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	W	2	GAL	C4-C5-C6-O6
2	R	2	GAL	C4-C5-C6-O6
2	o	1	FRU	O5-C5-C6-O6
2	P	2	GAL	O5-C5-C6-O6
2	Y	2	GAL	O5-C5-C6-O6
2	i	1	FRU	O1-C1-C2-O5
2	g	1	FRU	O1-C1-C2-O5
2	X	1	FRU	O1-C1-C2-O5
2	K	1	FRU	C4-C5-C6-O6
2	q	1	FRU	C4-C5-C6-O6
2	q	2	GAL	C4-C5-C6-O6
2	k	1	FRU	C4-C5-C6-O6
2	X	1	FRU	O5-C5-C6-O6
2	X	2	GAL	C4-C5-C6-O6
2	R	2	GAL	O5-C5-C6-O6
2	p	2	GAL	C4-C5-C6-O6
2	e	1	FRU	O5-C5-C6-O6
2	o	1	FRU	O1-C1-C2-C3
2	Z	2	GAL	O5-C5-C6-O6
2	q	1	FRU	O1-C1-C2-O5
2	M	2	GAL	O5-C5-C6-O6
2	W	1	FRU	O5-C5-C6-O6
2	O	2	GAL	C4-C5-C6-O6
2	T	2	GAL	C4-C5-C6-O6
2	e	2	GAL	O5-C5-C6-O6
2	p	1	FRU	O1-C1-C2-O2
2	T	1	FRU	O1-C1-C2-O2
2	d	1	FRU	O5-C5-C6-O6
2	T	1	FRU	O1-C1-C2-O5
2	P	2	GAL	C4-C5-C6-O6
2	W	2	GAL	O5-C5-C6-O6
2	X	1	FRU	C4-C5-C6-O6
2	f	1	FRU	O1-C1-C2-C3
2	V	1	FRU	O1-C1-C2-C3
2	j	1	FRU	O1-C1-C2-C3
2	V	1	FRU	O1-C1-C2-O5
2	j	1	FRU	O1-C1-C2-O5
2	Y	2	GAL	C4-C5-C6-O6
2	k	1	FRU	O5-C5-C6-O6
2	O	2	GAL	O5-C5-C6-O6
2	h	1	FRU	O1-C1-C2-O5
2	o	1	FRU	O1-C1-C2-O2

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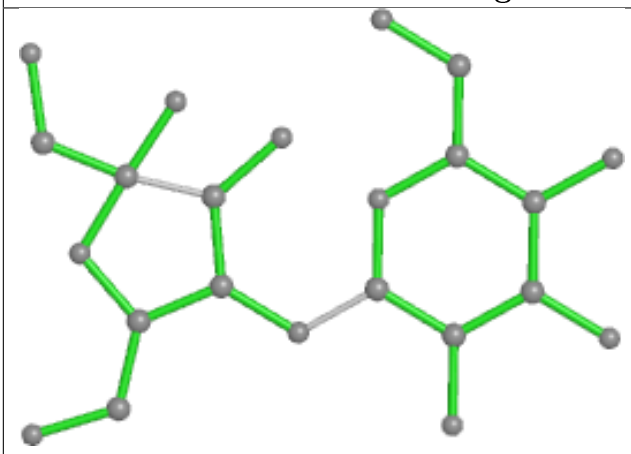
Mol	Chain	Res	Type	Atoms
2	T	1	FRU	O1-C1-C2-C3
2	q	1	FRU	O1-C1-C2-C3
2	m	1	FRU	O5-C5-C6-O6
2	e	1	FRU	C4-C5-C6-O6
2	I	1	FRU	O1-C1-C2-O5
2	m	1	FRU	O1-C1-C2-O5
2	Q	1	FRU	O1-C1-C2-O2
2	V	1	FRU	O1-C1-C2-O2
2	j	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O5-C5-C6-O6
2	o	1	FRU	O1-C1-C2-O5
2	f	1	FRU	O1-C1-C2-O5
2	Q	1	FRU	O1-C1-C2-O5
2	M	2	GAL	C4-C5-C6-O6
2	R	1	FRU	O1-C1-C2-C3
2	L	1	FRU	O1-C1-C2-C3
2	P	1	FRU	O1-C1-C2-C3
2	W	1	FRU	C4-C5-C6-O6
2	r	1	FRU	O1-C1-C2-O5
2	I	2	GAL	C4-C5-C6-O6

There are no ring outliers.

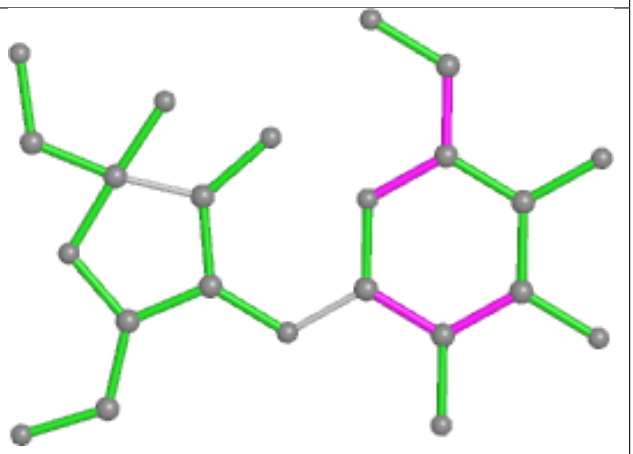
No monomer is involved in short contacts.

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

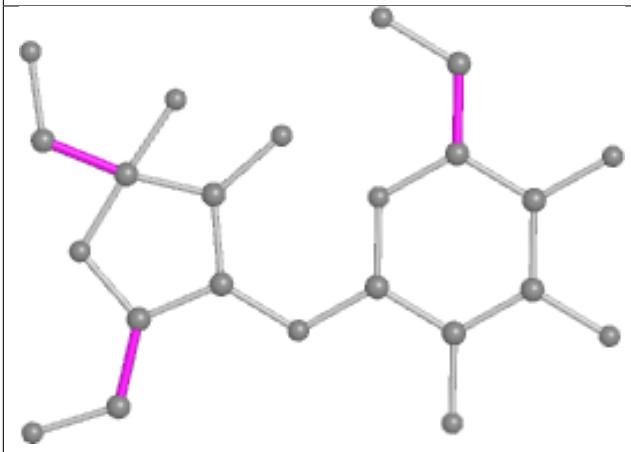
Oligosaccharide Chain H



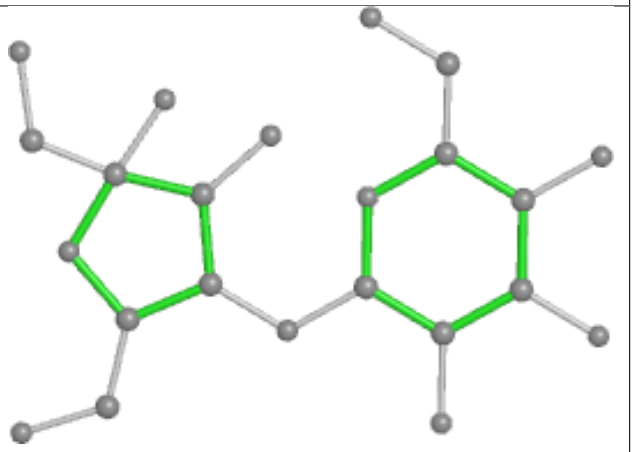
Bond lengths



Bond angles

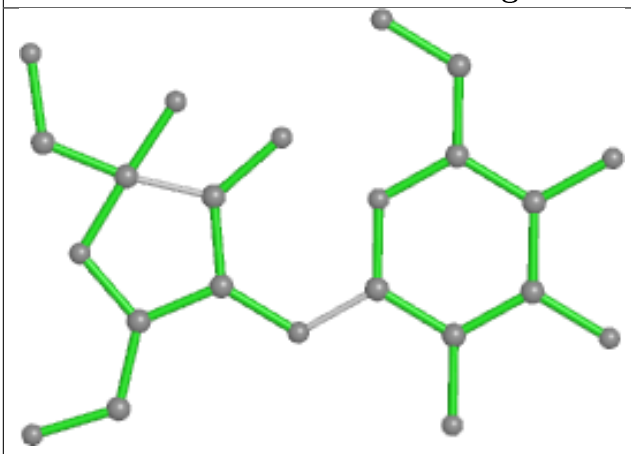


Torsions

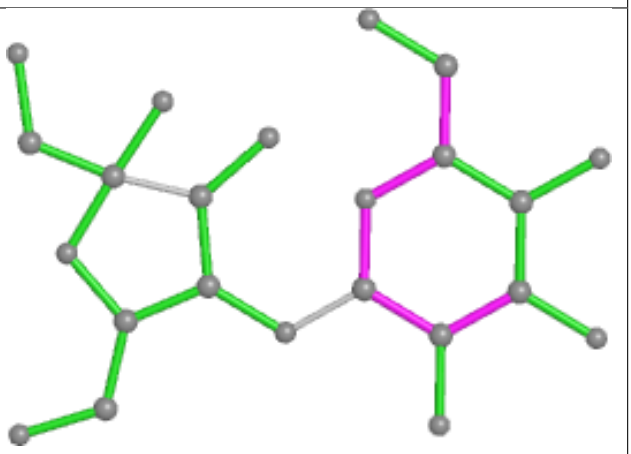


Rings

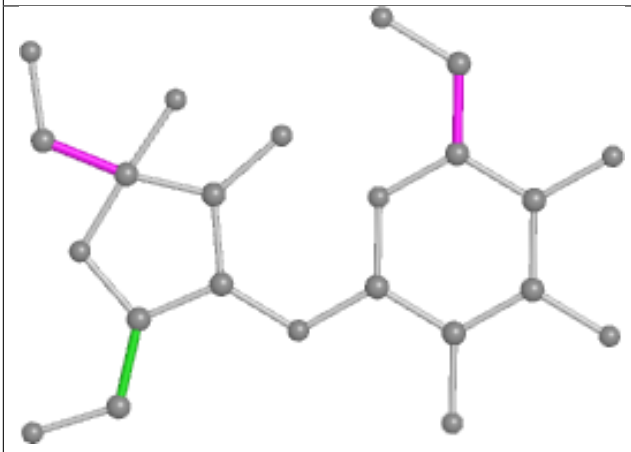
Oligosaccharide Chain I



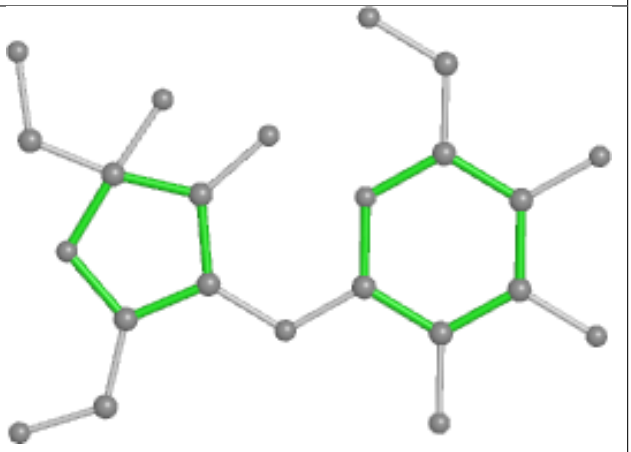
Bond lengths



Bond angles

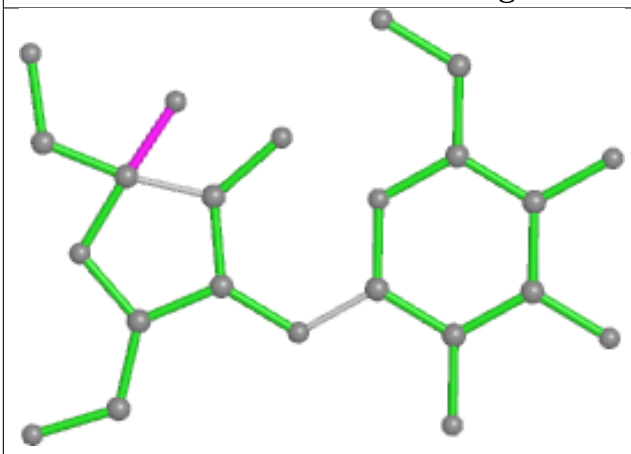


Torsions

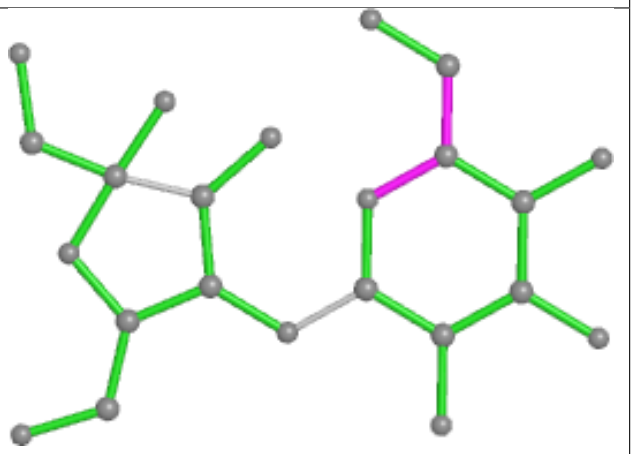


Rings

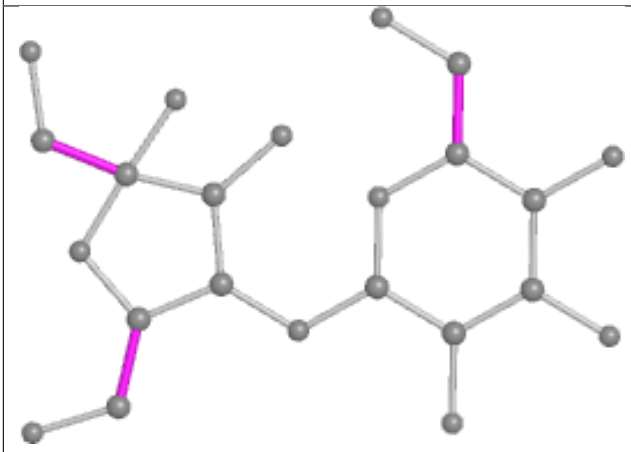
Oligosaccharide Chain J



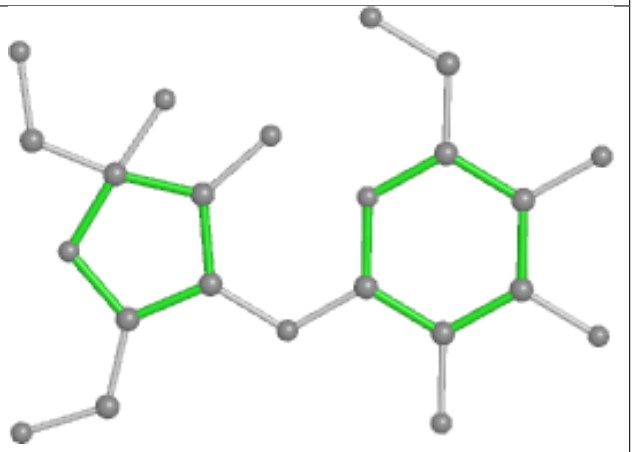
Bond lengths



Bond angles

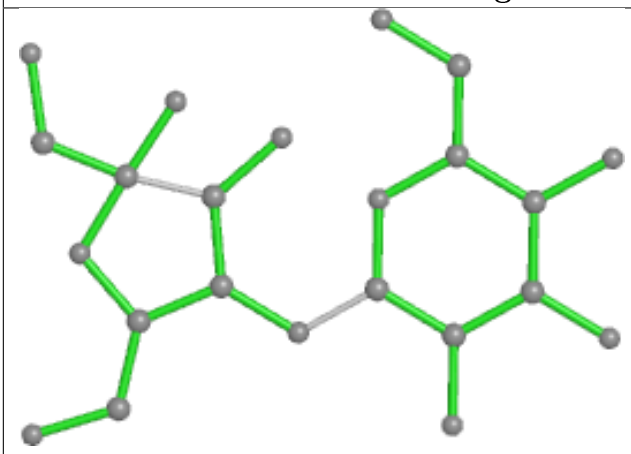


Torsions

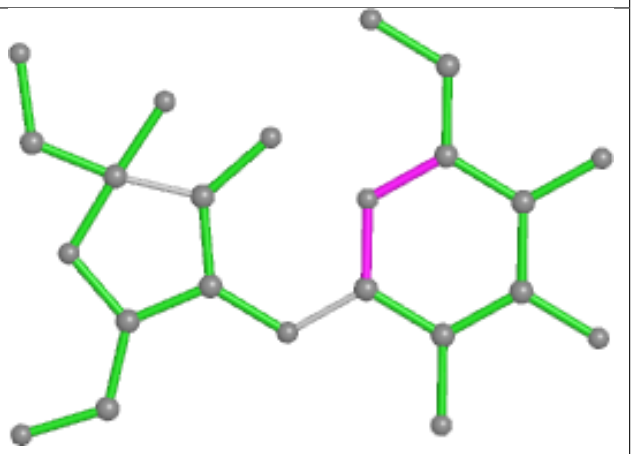


Rings

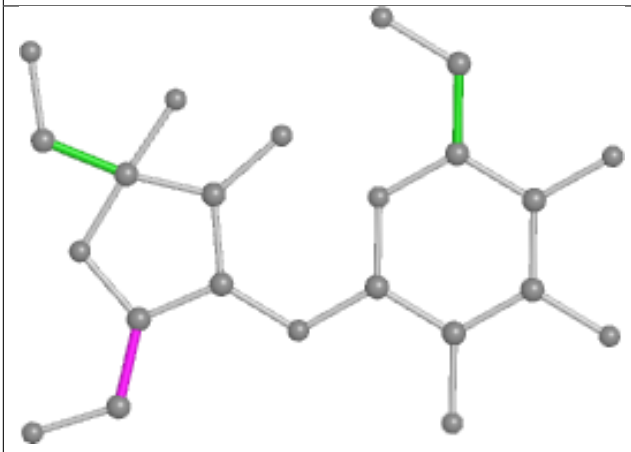
Oligosaccharide Chain K



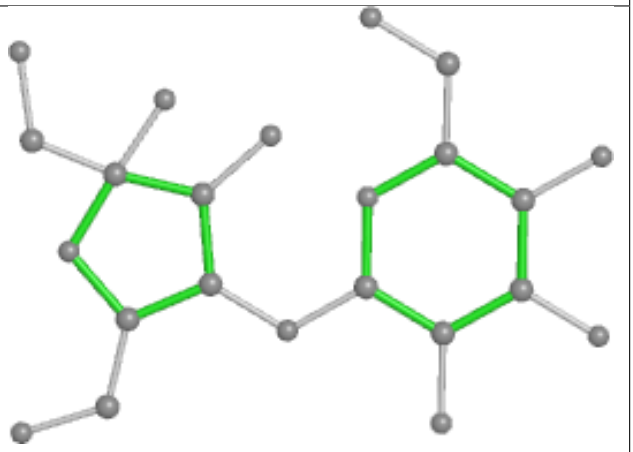
Bond lengths



Bond angles

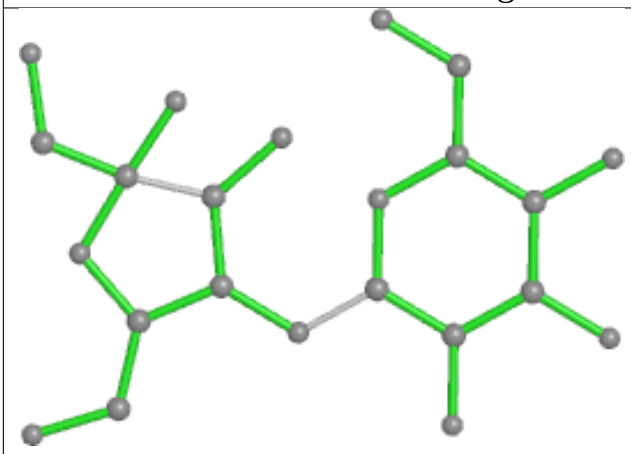


Torsions

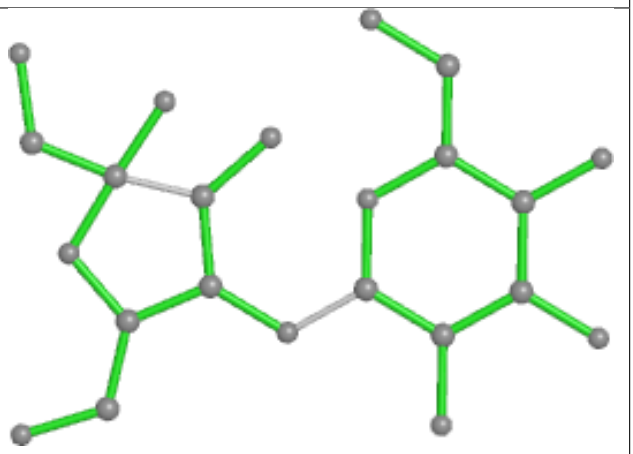


Rings

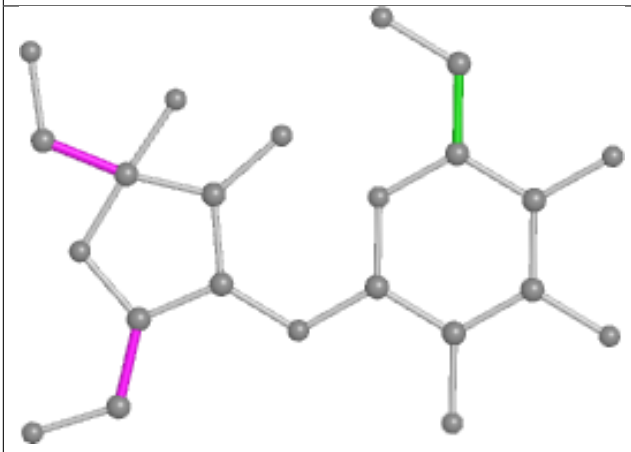
Oligosaccharide Chain L



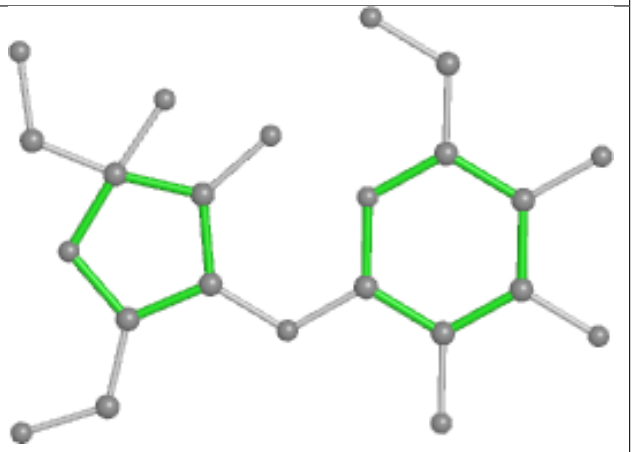
Bond lengths



Bond angles

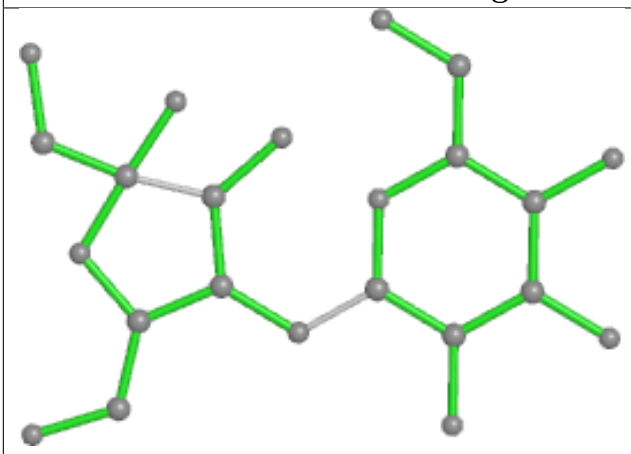


Torsions

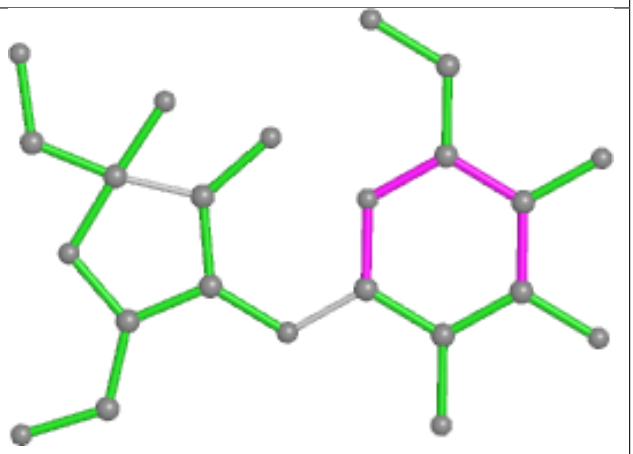


Rings

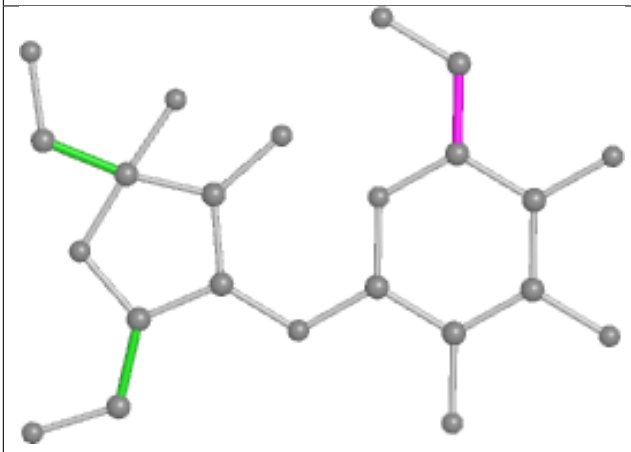
Oligosaccharide Chain M



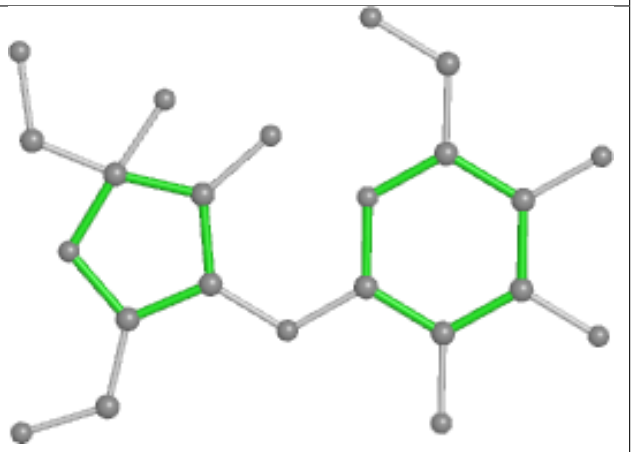
Bond lengths



Bond angles

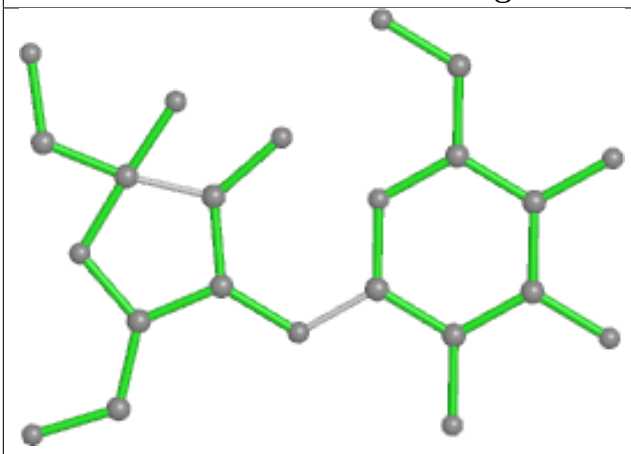


Torsions

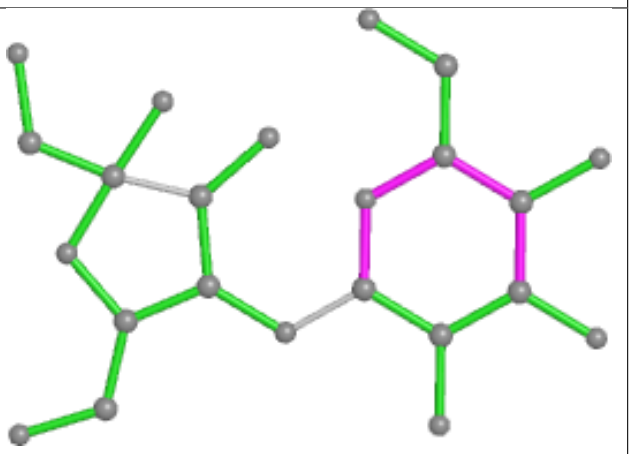


Rings

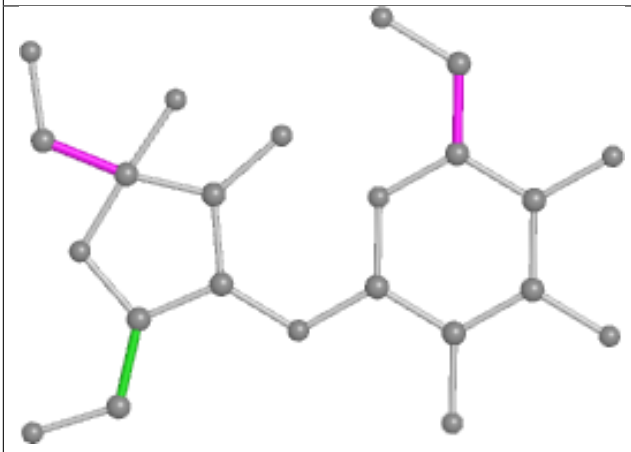
Oligosaccharide Chain N



Bond lengths



Bond angles



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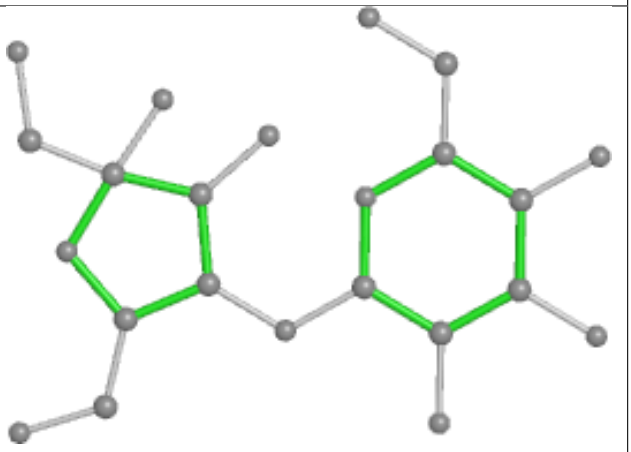
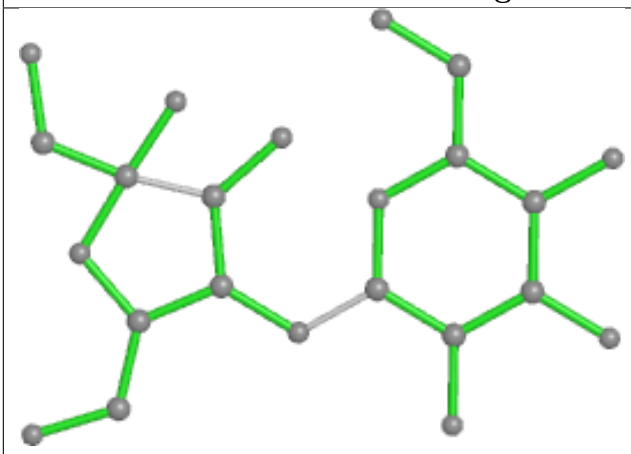
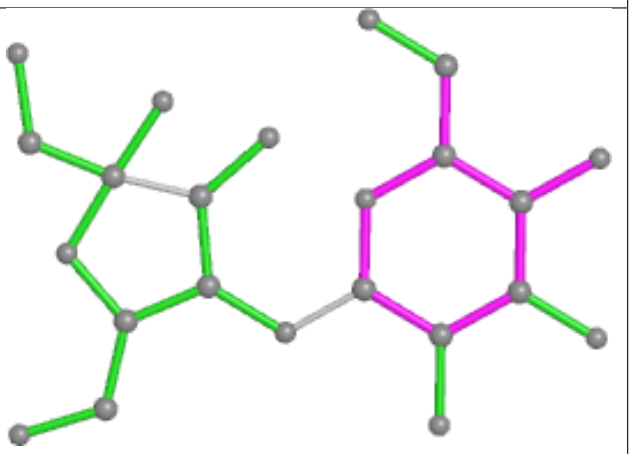


Rings

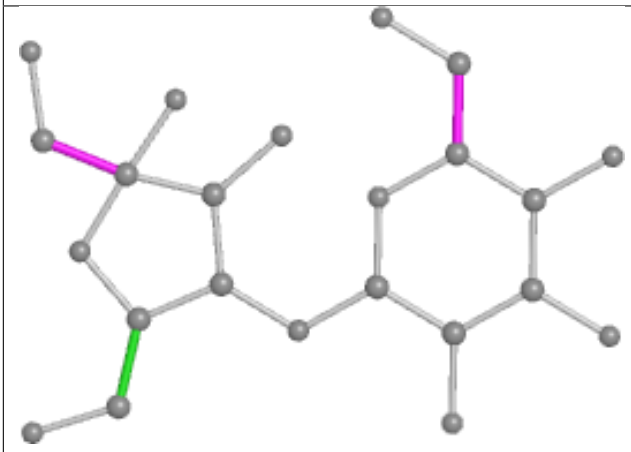
Oligosaccharide Chain O



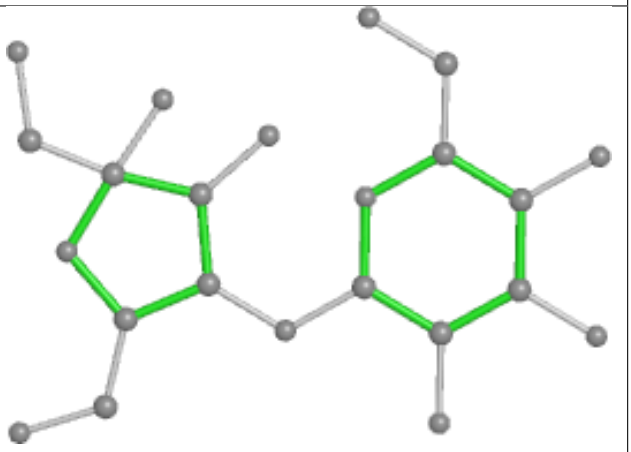
Bond lengths



Bond angles

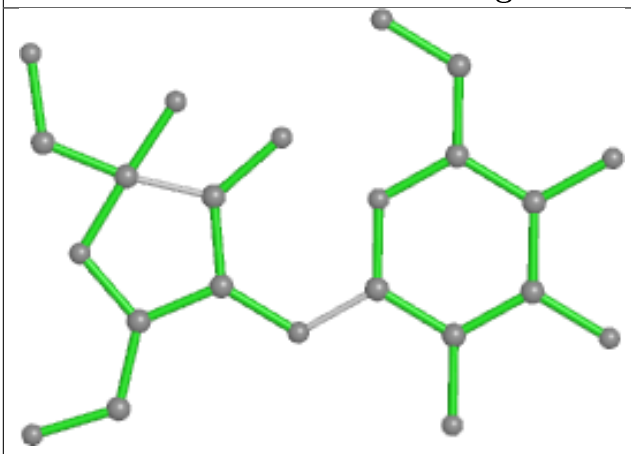


Torsions

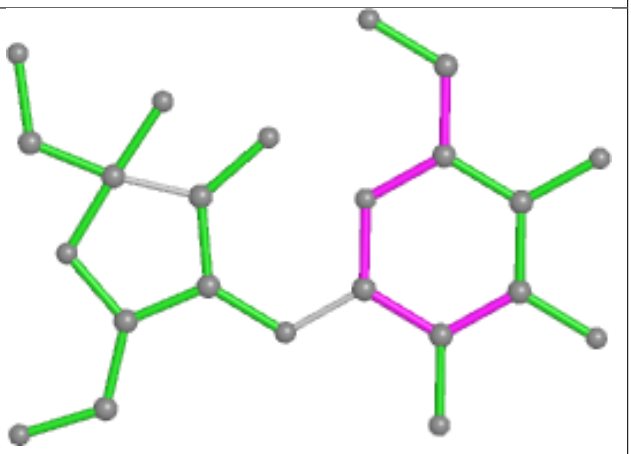


Rings

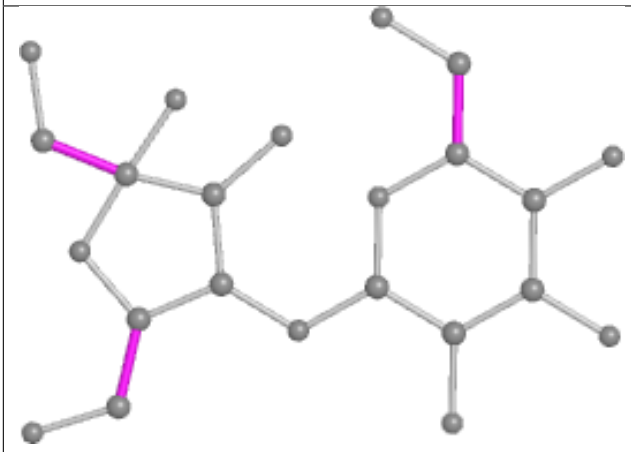
Oligosaccharide Chain P



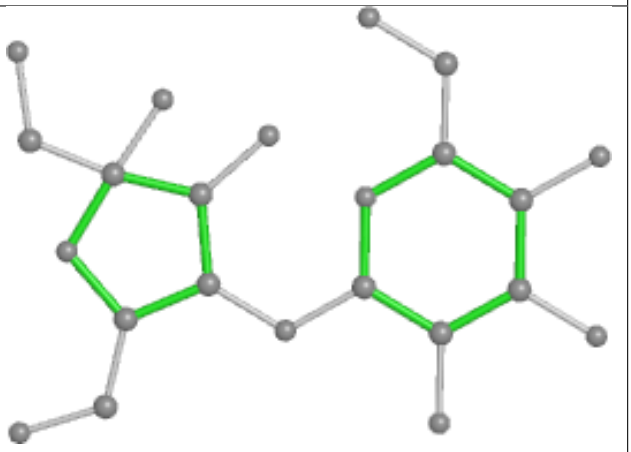
Bond lengths



Bond angles

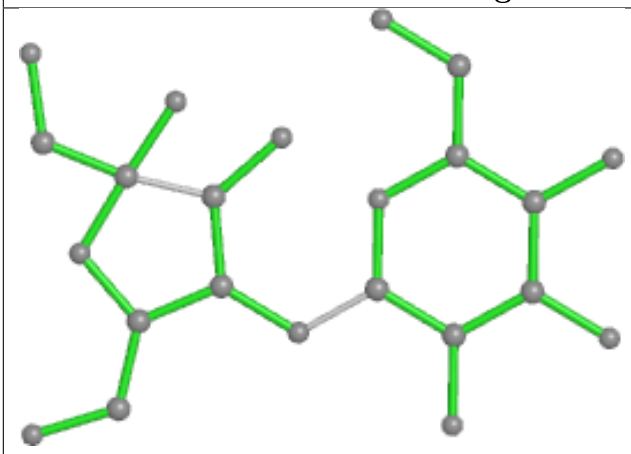


Torsions

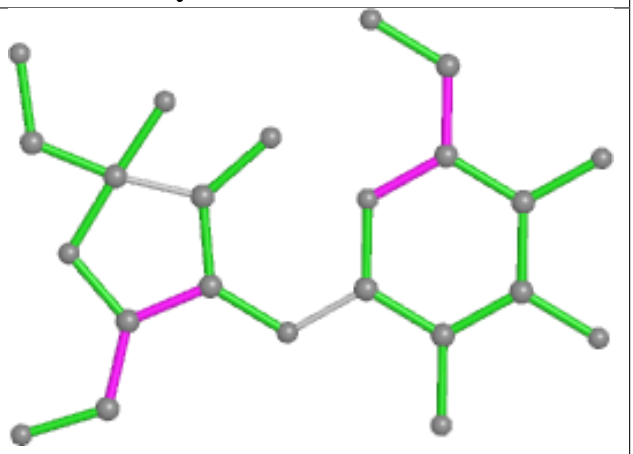


Rings

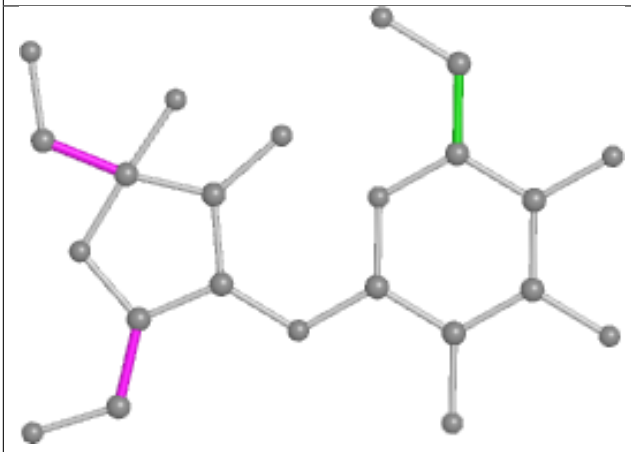
Oligosaccharide Chain Q



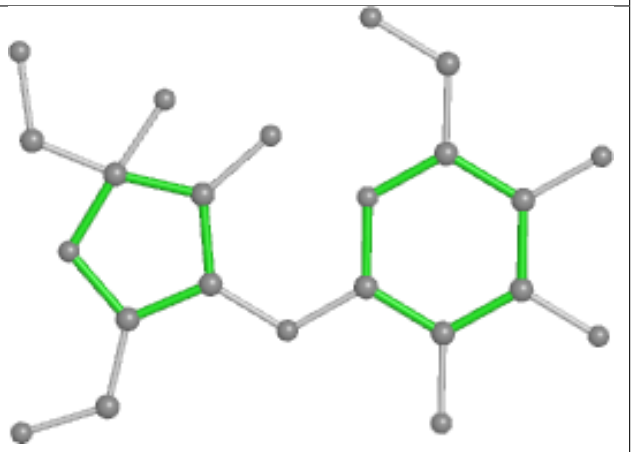
Bond lengths



Bond angles

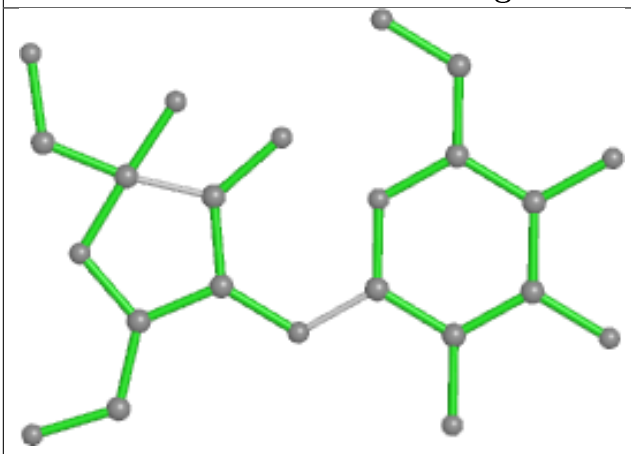


Torsions

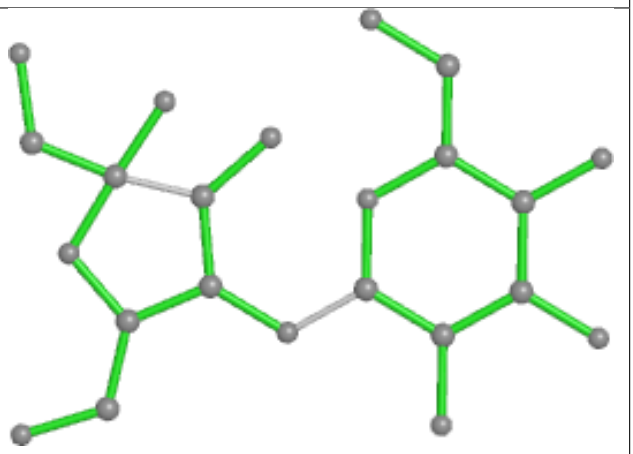


Rings

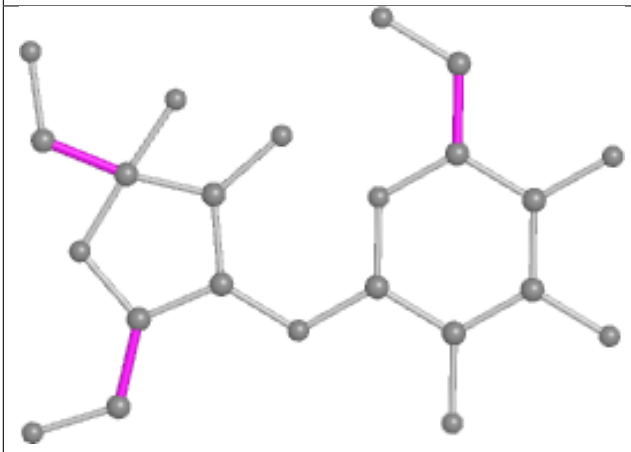
Oligosaccharide Chain R



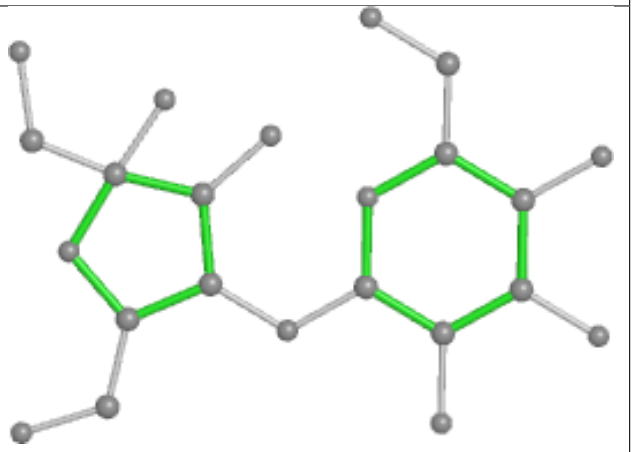
Bond lengths



Bond angles

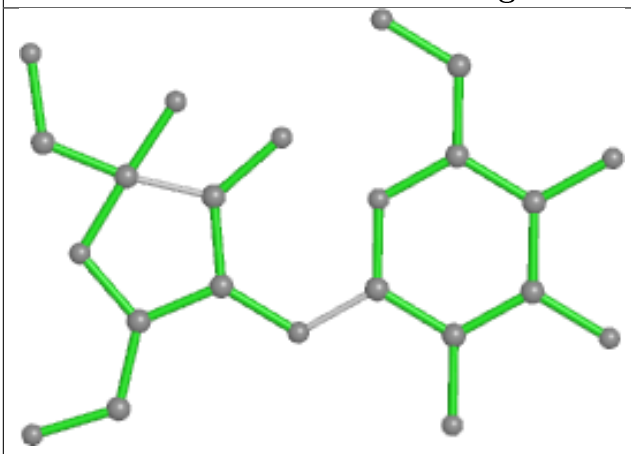


Torsions

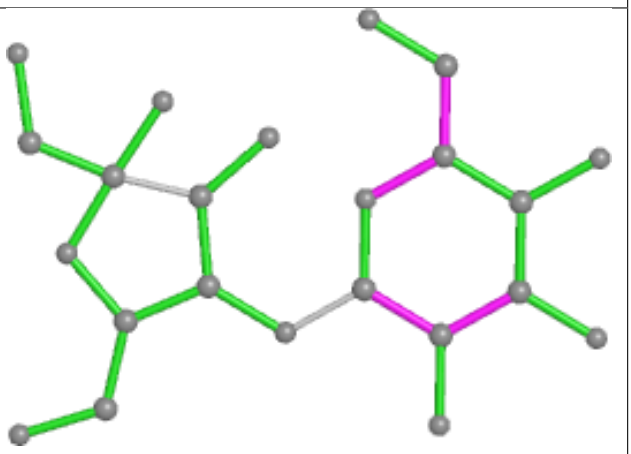


Rings

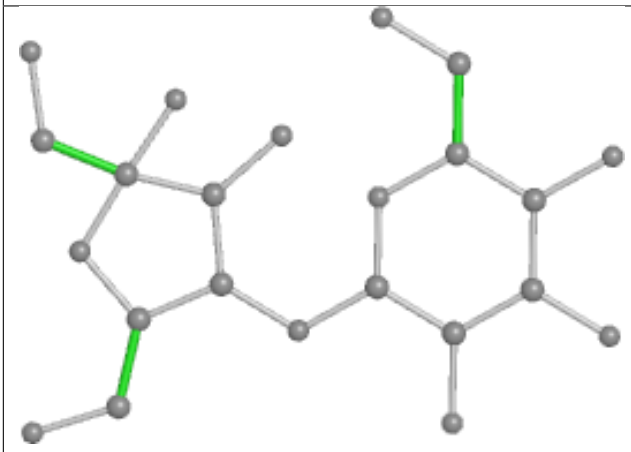
Oligosaccharide Chain S



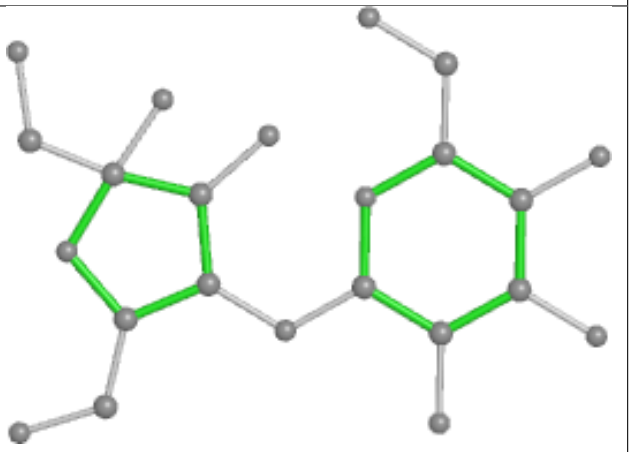
Bond lengths



Bond angles

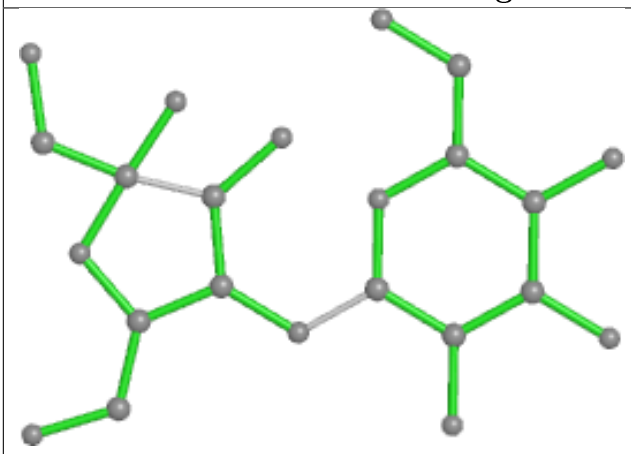


Torsions

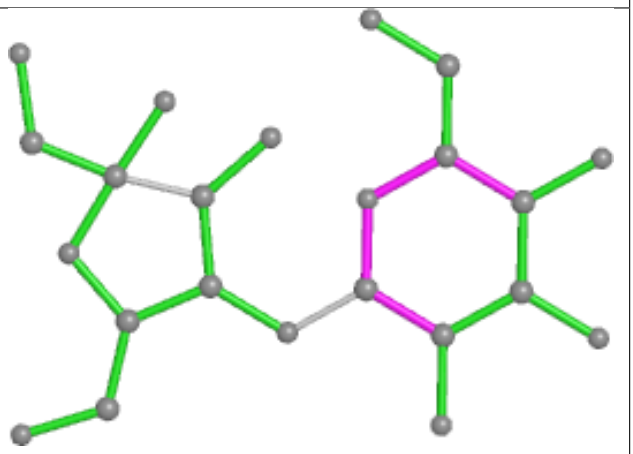


Rings

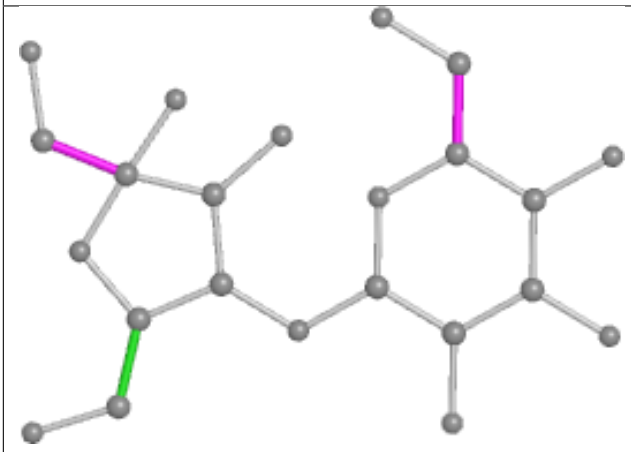
Oligosaccharide Chain T



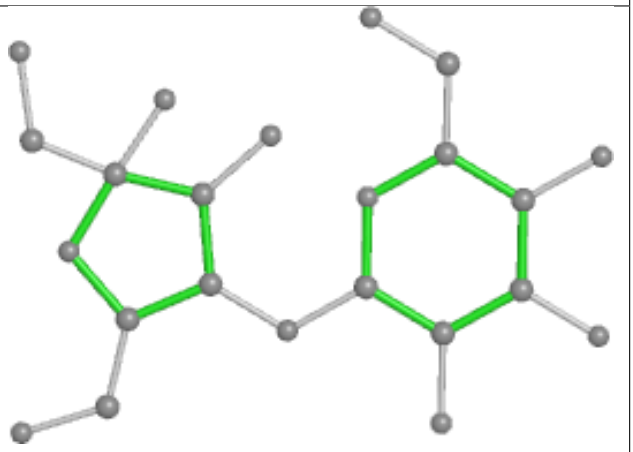
Bond lengths



Bond angles

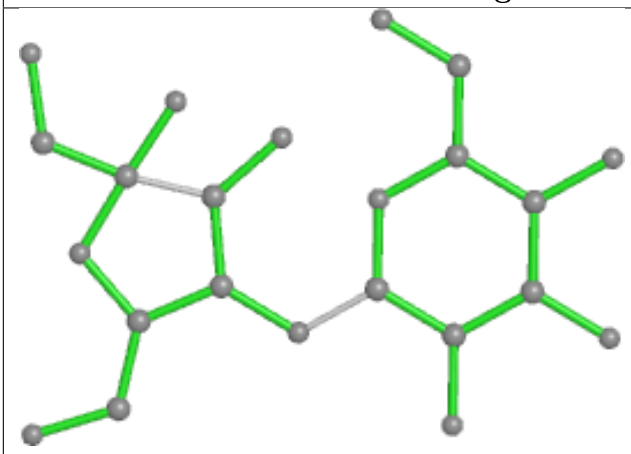


Torsions

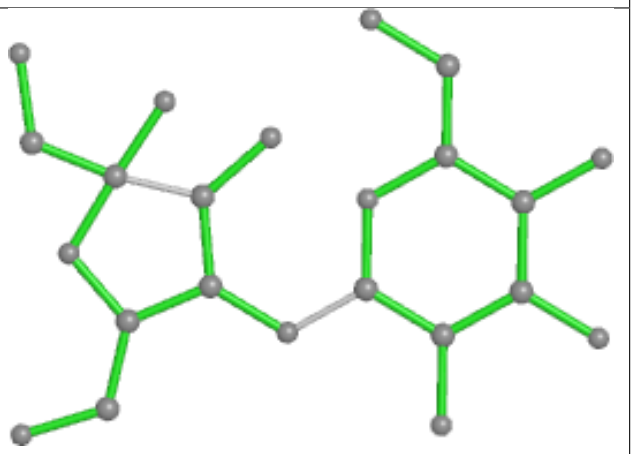


Rings

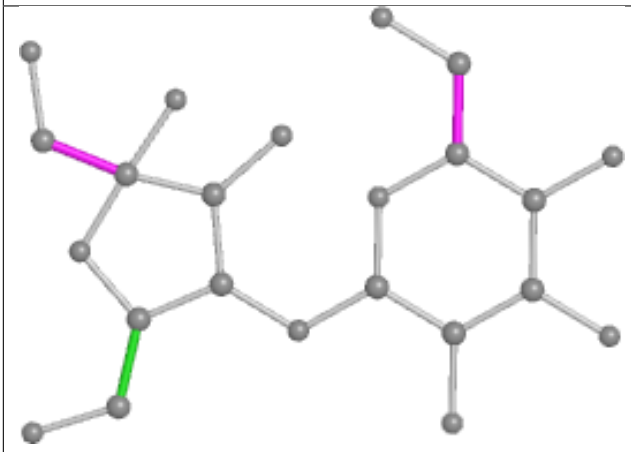
Oligosaccharide Chain U



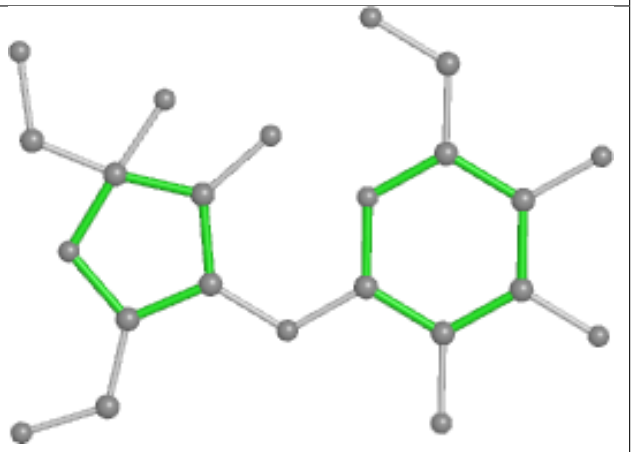
Bond lengths



Bond angles

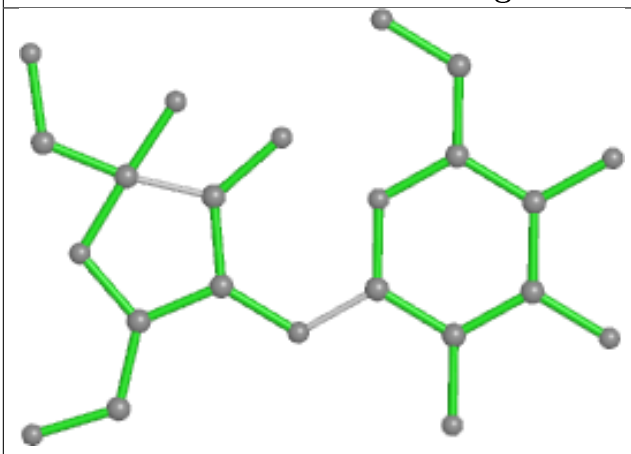


Torsions

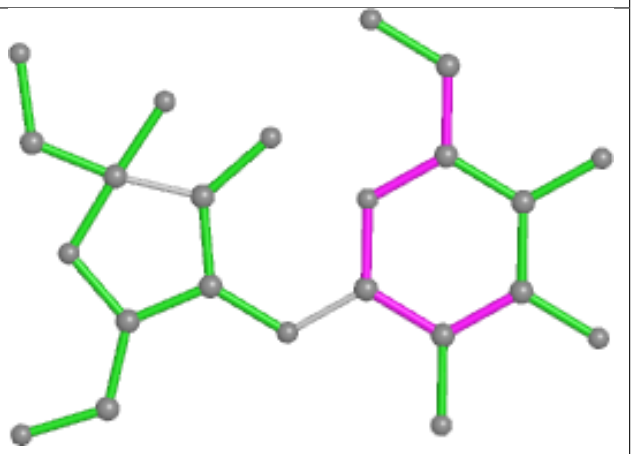


Rings

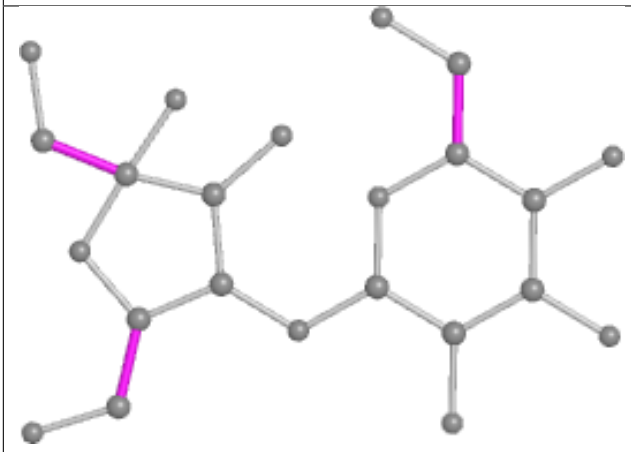
Oligosaccharide Chain V



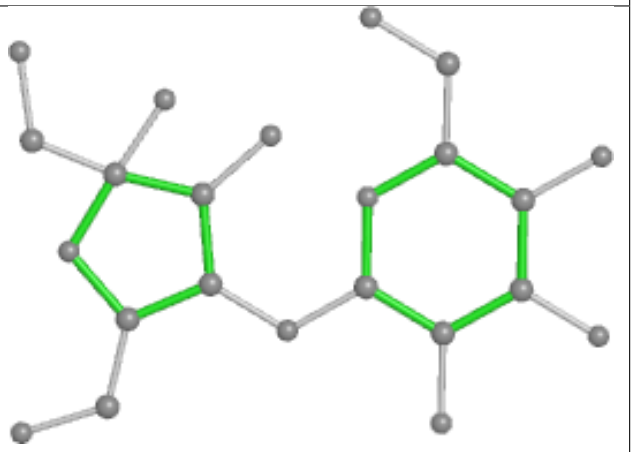
Bond lengths



Bond angles

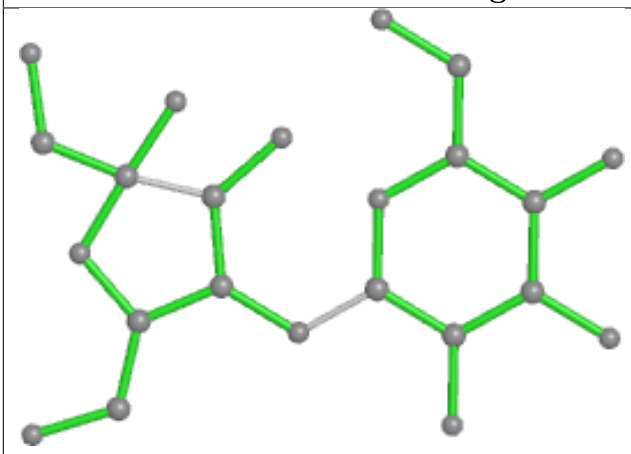


Torsions

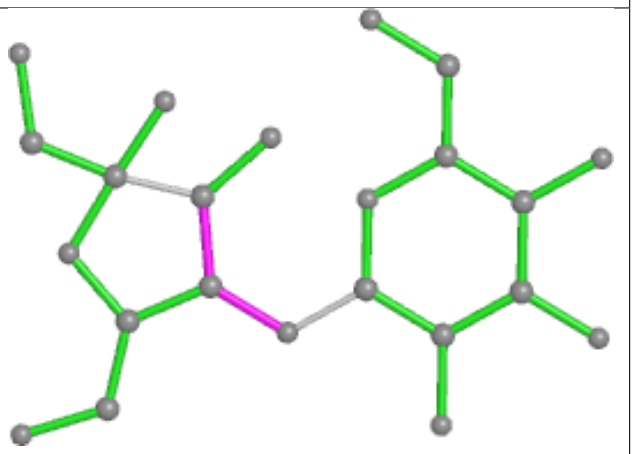


Rings

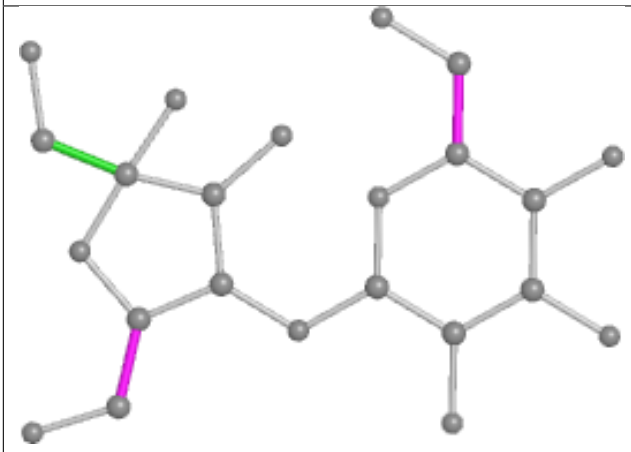
Oligosaccharide Chain W



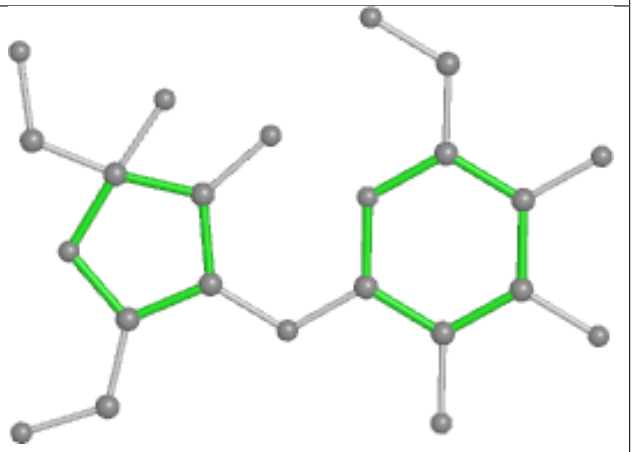
Bond lengths



Bond angles

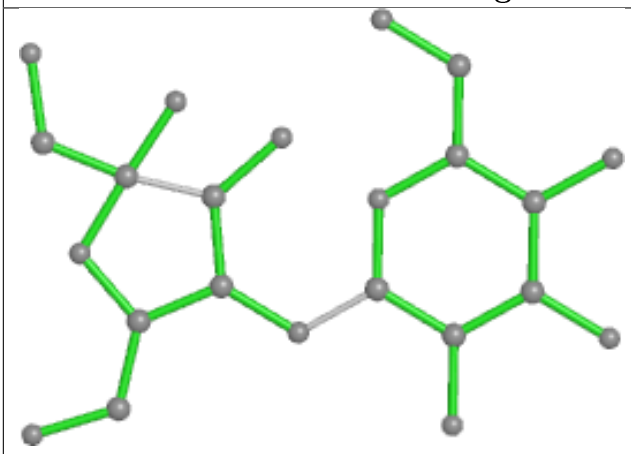


Torsions

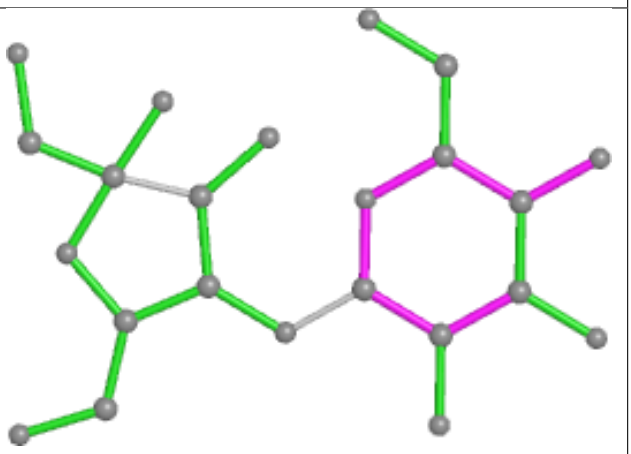


Rings

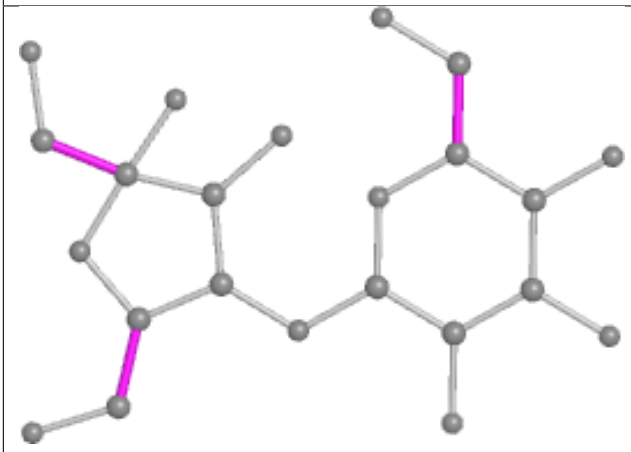
Oligosaccharide Chain X



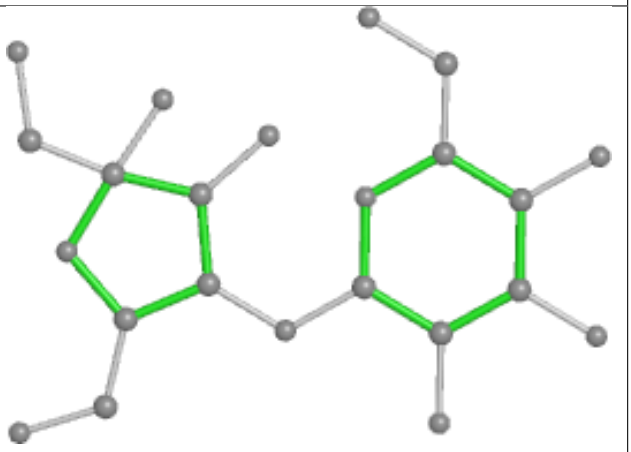
Bond lengths



Bond angles

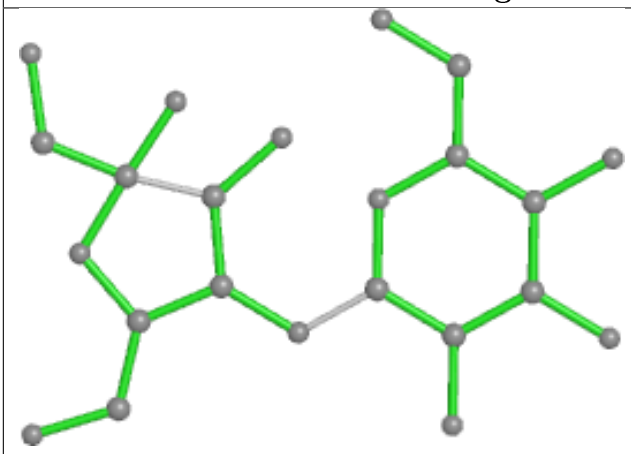


Torsions

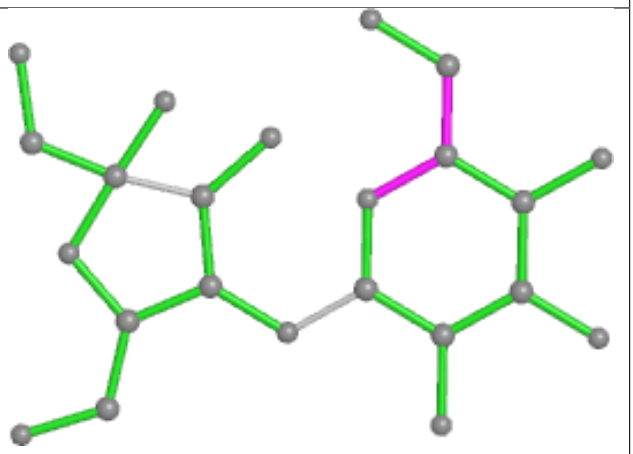


Rings

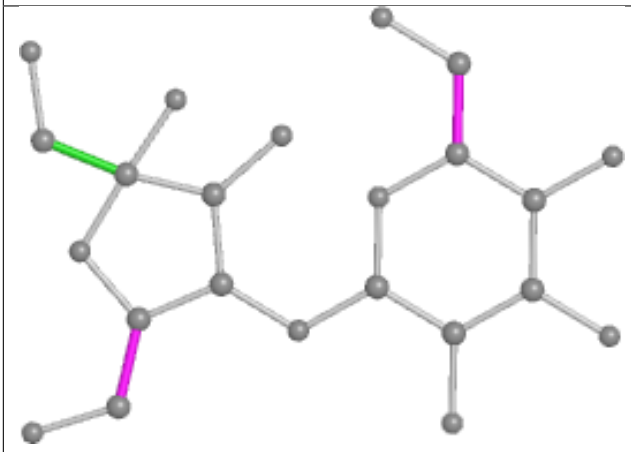
Oligosaccharide Chain Y



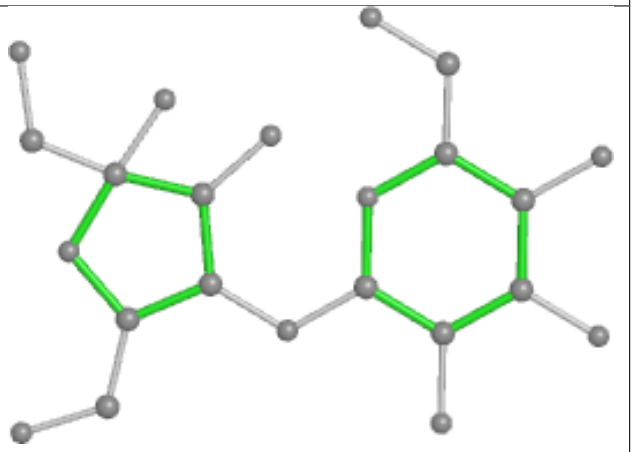
Bond lengths



Bond angles

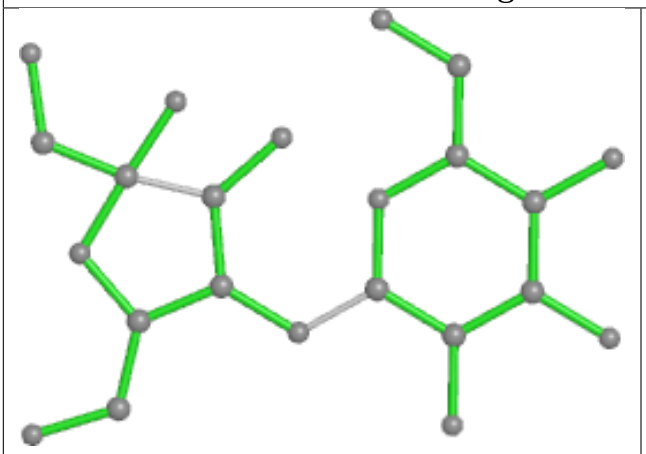


Torsions

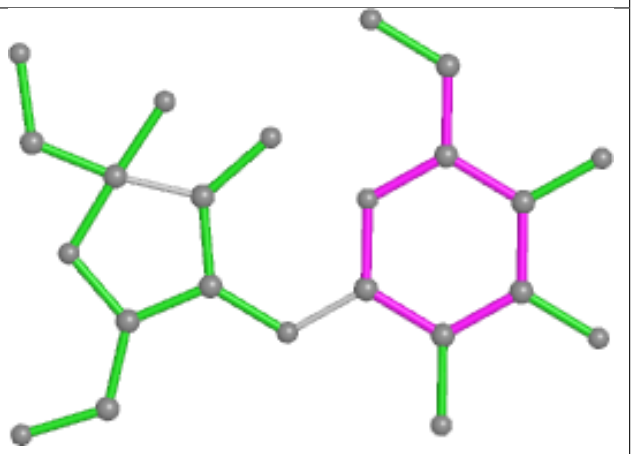


Rings

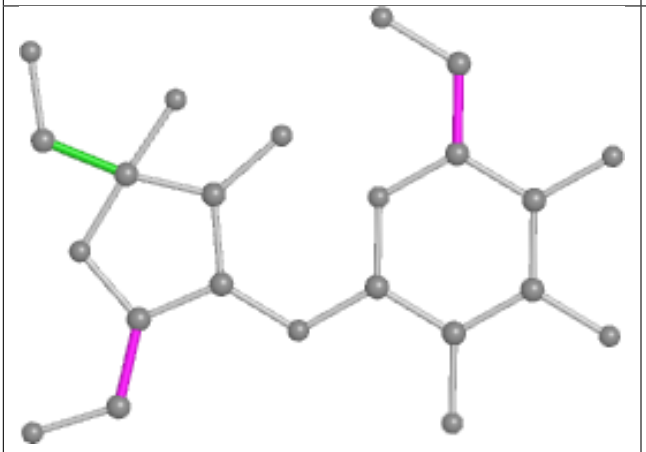
Oligosaccharide Chain Z



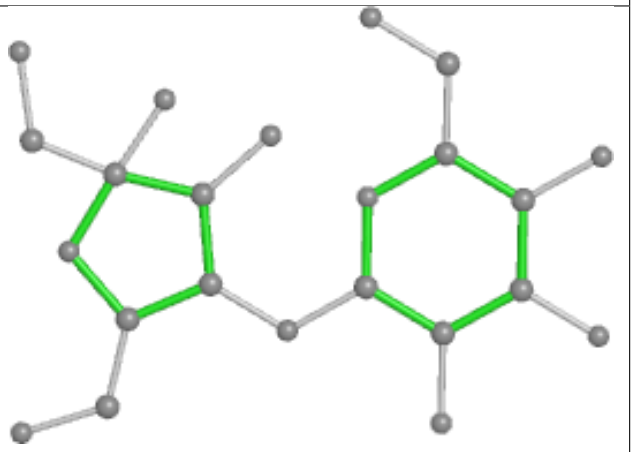
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 58 ligands modelled in this entry, 58 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	431/432 (99%)	0.58	31 (7%) 15 11	42, 73, 121, 211	0
1	B	431/432 (99%)	0.50	29 (6%) 17 13	44, 73, 111, 196	0
1	C	431/432 (99%)	0.48	27 (6%) 20 16	47, 75, 114, 165	0
1	D	431/432 (99%)	0.46	31 (7%) 15 11	43, 77, 119, 218	0
1	E	431/432 (99%)	0.57	33 (7%) 13 10	45, 73, 123, 193	0
1	F	431/432 (99%)	0.66	41 (9%) 8 6	46, 74, 137, 209	0
1	G	431/432 (99%)	0.81	46 (10%) 6 4	43, 77, 138, 211	0
All	All	3017/3024 (99%)	0.58	238 (7%) 12 10	42, 75, 124, 218	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	VAL	12.8
1	G	337	ALA	12.0
1	E	335	ILE	11.4
1	G	334	VAL	11.2
1	G	333	GLY	10.5
1	E	333	GLY	9.7
1	B	336	PHE	8.8
1	G	125	SER	8.3
1	A	334	VAL	7.8
1	A	333	GLY	7.7
1	G	330	ILE	7.7
1	A	335	ILE	7.6
1	G	336	PHE	7.4
1	D	335	ILE	7.2
1	F	334	VAL	7.0
1	A	336	PHE	7.0
1	A	331	GLU	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	333	GLY	7.0
1	B	335	ILE	6.8
1	D	337	ALA	6.7
1	D	226	ASP	6.5
1	F	134	TYR	6.4
1	A	133	VAL	6.3
1	E	136	CYS	6.3
1	G	335	ILE	6.3
1	D	334	VAL	6.3
1	F	333	GLY	6.2
1	E	332	LYS	6.2
1	C	335	ILE	6.2
1	E	338	LYS	5.9
1	E	339	ALA	5.9
1	G	339	ALA	5.8
1	B	337	ALA	5.8
1	A	337	ALA	5.6
1	A	134	TYR	5.6
1	G	328	SER	5.6
1	G	338	LYS	5.5
1	E	336	PHE	5.5
1	A	338	LYS	5.4
1	B	333	GLY	5.4
1	G	332	LYS	5.3
1	D	336	PHE	5.3
1	B	139	LEU	5.1
1	F	337	ALA	5.0
1	B	338	LYS	4.9
1	F	335	ILE	4.9
1	F	133	VAL	4.9
1	B	228	ARG	4.8
1	F	336	PHE	4.6
1	G	140	ASP	4.5
1	G	141	ASP	4.5
1	A	68	SER	4.4
1	A	142	GLN	4.3
1	E	331	GLU	4.3
1	C	333	GLY	4.3
1	E	337	ALA	4.3
1	E	125	SER	4.3
1	F	338	LYS	4.2
1	B	334	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	334	VAL	4.1
1	B	332	LYS	4.0
1	G	341	VAL	4.0
1	A	136	CYS	3.9
1	C	134	TYR	3.9
1	G	123	GLU	3.9
1	F	94	ARG	3.9
1	G	222	TYR	3.9
1	E	142	GLN	3.9
1	E	123	GLU	3.9
1	D	331	GLU	3.9
1	G	135	ASP	3.8
1	A	122	ILE	3.8
1	A	325	GLU	3.8
1	F	142	GLN	3.8
1	G	326	VAL	3.8
1	G	343	VAL	3.8
1	D	338	LYS	3.7
1	G	340	THR	3.7
1	G	331	GLU	3.7
1	C	222	TYR	3.7
1	G	142	GLN	3.6
1	D	137	GLN	3.6
1	C	327	SER	3.6
1	D	339	ALA	3.6
1	A	70	ASN	3.6
1	E	68	SER	3.5
1	G	342	SER	3.5
1	D	213	SER	3.5
1	B	339	ALA	3.5
1	G	122	ILE	3.5
1	A	339	ALA	3.5
1	G	136	CYS	3.5
1	A	67	GLY	3.4
1	F	211	GLU	3.4
1	F	314	PHE	3.4
1	F	342	SER	3.4
1	C	340	THR	3.4
1	F	332	LYS	3.4
1	D	139	LEU	3.4
1	E	325	GLU	3.4
1	F	331	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	330	ILE	3.3
1	A	329	THR	3.3
1	F	389	THR	3.3
1	G	134	TYR	3.2
1	G	237	ALA	3.2
1	B	224	CYS	3.2
1	E	69	GLY	3.2
1	F	341	VAL	3.2
1	D	228	ARG	3.2
1	F	136	CYS	3.1
1	E	342	SER	3.1
1	C	331	GLU	3.1
1	B	222	TYR	3.0
1	D	136	CYS	3.0
1	E	134	TYR	3.0
1	B	216	SER	3.0
1	D	227	LEU	3.0
1	G	133	VAL	3.0
1	C	336	PHE	3.0
1	B	314	PHE	3.0
1	F	69	GLY	3.0
1	F	17	LYS	3.0
1	E	226	ASP	3.0
1	B	331	GLU	3.0
1	C	125	SER	2.9
1	F	364	THR	2.9
1	E	141	ASP	2.9
1	B	364	THR	2.9
1	C	127	GLY	2.9
1	B	143	TYR	2.8
1	D	122	ILE	2.8
1	F	339	ALA	2.8
1	G	211	GLU	2.8
1	D	342	SER	2.8
1	F	141	ASP	2.8
1	B	217	GLY	2.8
1	B	135	ASP	2.8
1	A	138	ASN	2.8
1	E	137	GLN	2.8
1	F	328	SER	2.8
1	G	118	LYS	2.7
1	F	68	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	250	GLU	2.7
1	D	325	GLU	2.7
1	C	169	VAL	2.7
1	E	314	PHE	2.7
1	E	122	ILE	2.7
1	D	327	SER	2.7
1	C	211	GLU	2.7
1	F	329	THR	2.7
1	F	388	THR	2.7
1	G	215	GLY	2.6
1	G	224	CYS	2.6
1	B	133	VAL	2.6
1	B	213	SER	2.6
1	B	141	ASP	2.6
1	G	71	ALA	2.6
1	A	342	SER	2.6
1	G	210	VAL	2.6
1	D	66	ASP	2.6
1	E	140	ASP	2.5
1	E	139	LEU	2.5
1	C	170	GLU	2.5
1	G	247	LEU	2.5
1	D	125	SER	2.5
1	C	424	GLU	2.5
1	G	36	TYR	2.5
1	D	332	LYS	2.5
1	C	329	THR	2.4
1	C	339	ALA	2.4
1	E	215	GLY	2.4
1	F	122	ILE	2.4
1	G	128	THR	2.4
1	E	364	THR	2.4
1	C	325	GLU	2.4
1	F	125	SER	2.4
1	C	307	GLN	2.4
1	F	128	THR	2.4
1	F	135	ASP	2.4
1	A	69	GLY	2.3
1	C	346	THR	2.3
1	A	115	ALA	2.3
1	F	325	GLU	2.3
1	C	126	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	364	THR	2.3
1	A	330	ILE	2.3
1	C	68	SER	2.3
1	C	328	SER	2.3
1	F	183	CYS	2.3
1	G	226	ASP	2.3
1	F	123	GLU	2.3
1	E	340	THR	2.3
1	A	135	ASP	2.3
1	A	332	LYS	2.3
1	G	16	PHE	2.3
1	A	128	THR	2.2
1	B	215	GLY	2.2
1	F	67	GLY	2.2
1	F	320	ALA	2.2
1	D	133	VAL	2.2
1	B	340	THR	2.2
1	D	224	CYS	2.2
1	E	29	GLY	2.2
1	G	387	GLU	2.2
1	C	143	TYR	2.2
1	F	353	TRP	2.2
1	C	347	ALA	2.2
1	E	143	TYR	2.2
1	G	227	LEU	2.2
1	D	141	ASP	2.2
1	D	147	ARG	2.2
1	A	143	TYR	2.2
1	G	324	VAL	2.2
1	C	139	LEU	2.1
1	B	325	GLU	2.1
1	F	324	VAL	2.1
1	E	133	VAL	2.1
1	D	222	TYR	2.1
1	G	17	LYS	2.1
1	E	138	ASN	2.1
1	D	128	THR	2.1
1	A	131	ILE	2.1
1	E	424	GLU	2.1
1	F	355	ASN	2.1
1	B	123	GLU	2.0
1	B	170	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	121	ASP	2.0
1	B	134	TYR	2.0
1	D	143	TYR	2.0
1	A	428	PHE	2.0
1	G	65	PRO	2.0
1	D	314	PHE	2.0
1	A	125	SER	2.0
1	G	139	LEU	2.0
1	B	307	GLN	2.0
1	C	128	THR	2.0
1	F	186	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PCA	F	1	8/9	0.82	0.25	65,67,70,72	0
1	PCA	E	1	8/9	0.84	0.27	86,95,99,101	0
1	PCA	A	1	8/9	0.84	0.24	83,87,93,93	0
1	PCA	C	1	8/9	0.86	0.31	76,88,94,96	0
1	PCA	D	1	8/9	0.88	0.23	76,82,87,88	0
1	PCA	B	1	8/9	0.93	0.24	68,77,80,82	0
1	PCA	G	1	8/9	0.93	0.24	74,76,80,81	0

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	FRU	P	1	12/12	0.74	0.23	108,119,124,125	0
2	FRU	I	1	12/12	0.76	0.43	132,150,157,161	0
2	FRU	V	1	12/12	0.77	0.48	157,164,167,168	0
2	GAL	I	2	11/12	0.79	0.20	100,110,122,126	0
2	GAL	I	2	11/12	0.80	0.39	133,152,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	I	1	12/12	0.80	0.28	110,124,129,132	0
2	FRU	N	1	12/12	0.81	0.39	124,134,137,138	0
2	FRU	e	1	12/12	0.82	0.26	95,100,103,112	0
2	FRU	M	1	12/12	0.82	0.17	109,122,132,143	0
2	FRU	Z	1	12/12	0.84	0.40	116,134,139,148	0
2	FRU	Y	1	12/12	0.86	0.20	100,107,118,121	0
2	GAL	Z	2	11/12	0.86	0.15	92,99,115,116	0
2	FRU	L	1	12/12	0.86	0.20	89,102,110,116	0
2	FRU	O	1	12/12	0.86	0.32	97,111,117,119	0
2	GAL	V	2	11/12	0.87	0.36	140,148,154,157	0
2	FRU	f	1	12/12	0.87	0.15	94,101,104,104	0
2	GAL	e	2	11/12	0.88	0.28	85,96,105,112	0
2	FRU	o	1	12/12	0.88	0.20	123,130,136,139	0
2	FRU	k	1	12/12	0.88	0.20	92,113,121,123	0
2	GAL	M	2	11/12	0.89	0.14	85,97,102,103	0
2	FRU	U	1	12/12	0.89	0.14	96,105,111,112	0
2	FRU	n	1	12/12	0.89	0.23	89,100,103,104	0
2	FRU	T	1	12/12	0.89	0.28	110,125,128,130	0
2	FRU	p	1	12/12	0.89	0.21	118,129,134,137	0
2	FRU	r	1	12/12	0.90	0.17	96,102,107,108	0
2	FRU	i	1	12/12	0.90	0.26	90,100,102,103	0
2	FRU	c	1	12/12	0.90	0.15	88,99,102,102	0
2	GAL	o	2	11/12	0.90	0.26	109,113,121,121	0
2	FRU	K	1	12/12	0.90	0.18	99,114,119,125	0
2	FRU	j	1	12/12	0.90	0.16	87,99,107,107	0
2	FRU	X	1	12/12	0.90	0.26	85,92,99,105	0
2	GAL	P	2	11/12	0.91	0.12	96,102,115,115	0
2	FRU	W	1	12/12	0.91	0.24	94,109,119,120	0
2	FRU	S	1	12/12	0.91	0.21	82,95,101,106	0
2	GAL	N	2	11/12	0.91	0.21	100,110,118,120	0
2	FRU	Q	1	12/12	0.91	0.20	92,110,122,130	0
2	GAL	g	2	11/12	0.92	0.24	72,81,90,91	0
2	FRU	d	1	12/12	0.92	0.22	87,92,100,101	0
2	FRU	q	1	12/12	0.92	0.26	103,111,112,121	0
2	FRU	g	1	12/12	0.92	0.27	68,73,78,82	0
2	FRU	J	1	12/12	0.92	0.21	90,99,108,121	0
2	GAL	f	2	11/12	0.92	0.24	90,98,107,109	0
2	GAL	m	2	11/12	0.93	0.22	78,84,88,89	0
2	GAL	T	2	11/12	0.93	0.16	86,91,100,101	0
2	FRU	H	1	12/12	0.93	0.13	86,95,99,100	0
2	FRU	b	1	12/12	0.93	0.23	66,70,76,86	0
2	FRU	a	1	12/12	0.93	0.20	96,108,116,121	0

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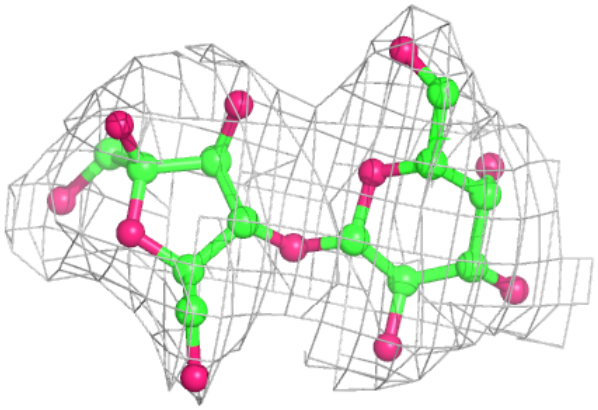
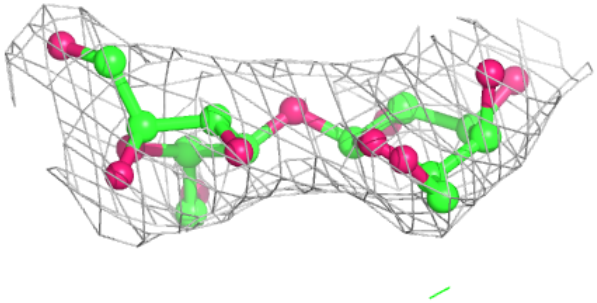
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	Y	2	11/12	0.94	0.22	94,101,110,121	0
2	GAL	k	2	11/12	0.94	0.16	79,83,86,86	0
2	FRU	m	1	12/12	0.94	0.26	82,87,95,102	0
2	GAL	p	2	11/12	0.94	0.16	98,105,109,111	0
2	GAL	i	2	11/12	0.94	0.15	65,73,80,82	0
2	GAL	b	2	11/12	0.94	0.24	61,70,74,76	0
2	GAL	K	2	11/12	0.94	0.17	73,78,85,87	0
2	GAL	j	2	11/12	0.94	0.19	58,67,71,74	0
2	GAL	X	2	11/12	0.94	0.18	69,74,80,81	0
2	GAL	U	2	11/12	0.95	0.13	92,93,95,98	0
2	GAL	a	2	11/12	0.95	0.12	70,84,92,96	0
2	GAL	q	2	11/12	0.95	0.12	69,81,86,90	0
2	FRU	R	1	12/12	0.95	0.15	92,98,101,104	0
2	GAL	J	2	11/12	0.95	0.18	67,73,78,80	0
2	FRU	h	1	12/12	0.95	0.17	72,78,84,88	0
2	GAL	R	2	11/12	0.96	0.12	85,90,95,95	0
2	GAL	W	2	11/12	0.96	0.18	79,82,85,86	0
2	GAL	n	2	11/12	0.96	0.14	75,80,85,86	0
2	GAL	r	2	11/12	0.96	0.18	75,79,86,89	0
2	GAL	O	2	11/12	0.96	0.17	73,77,83,83	0
2	GAL	H	2	11/12	0.96	0.15	79,81,82,83	0
2	GAL	h	2	11/12	0.97	0.16	59,63,67,67	0
2	GAL	Q	2	11/12	0.97	0.15	74,79,86,89	0
2	GAL	d	2	11/12	0.97	0.15	74,79,82,82	0
2	GAL	L	2	11/12	0.97	0.15	72,73,78,79	0
2	GAL	c	2	11/12	0.98	0.17	69,72,74,78	0
2	GAL	S	2	11/12	0.98	0.11	63,67,72,72	0

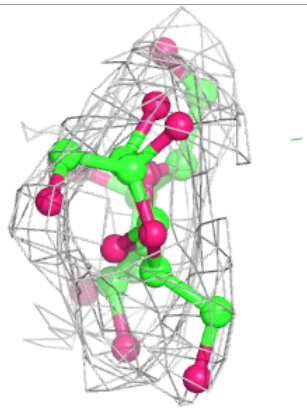
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain H:

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

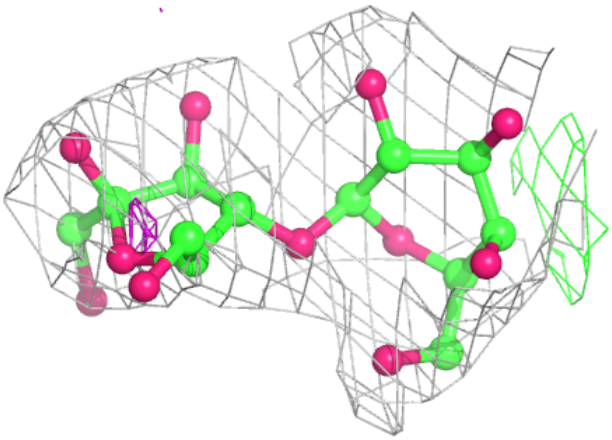


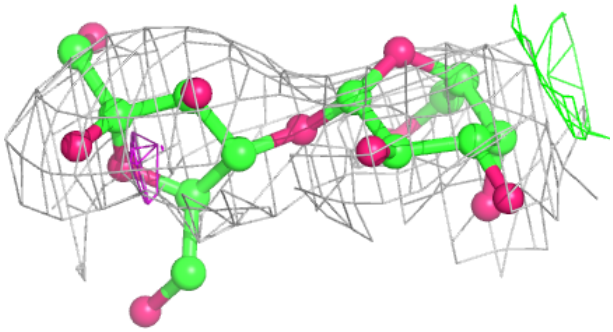


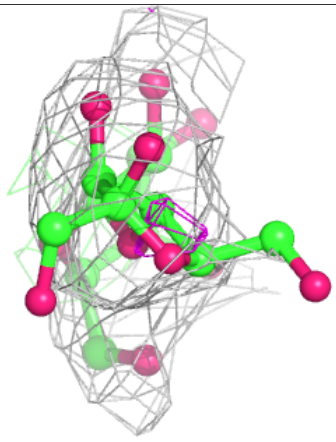


Electron density around Chain I:

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

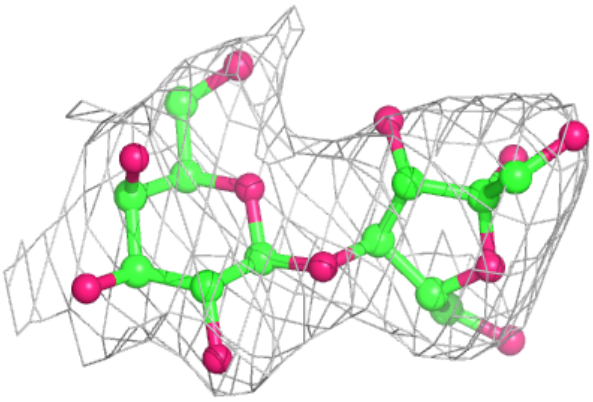


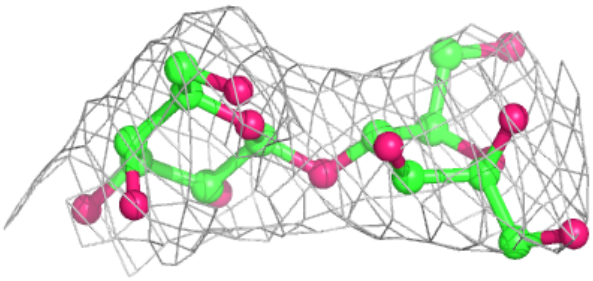


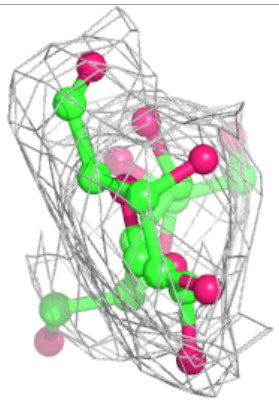


Electron density around Chain J:

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

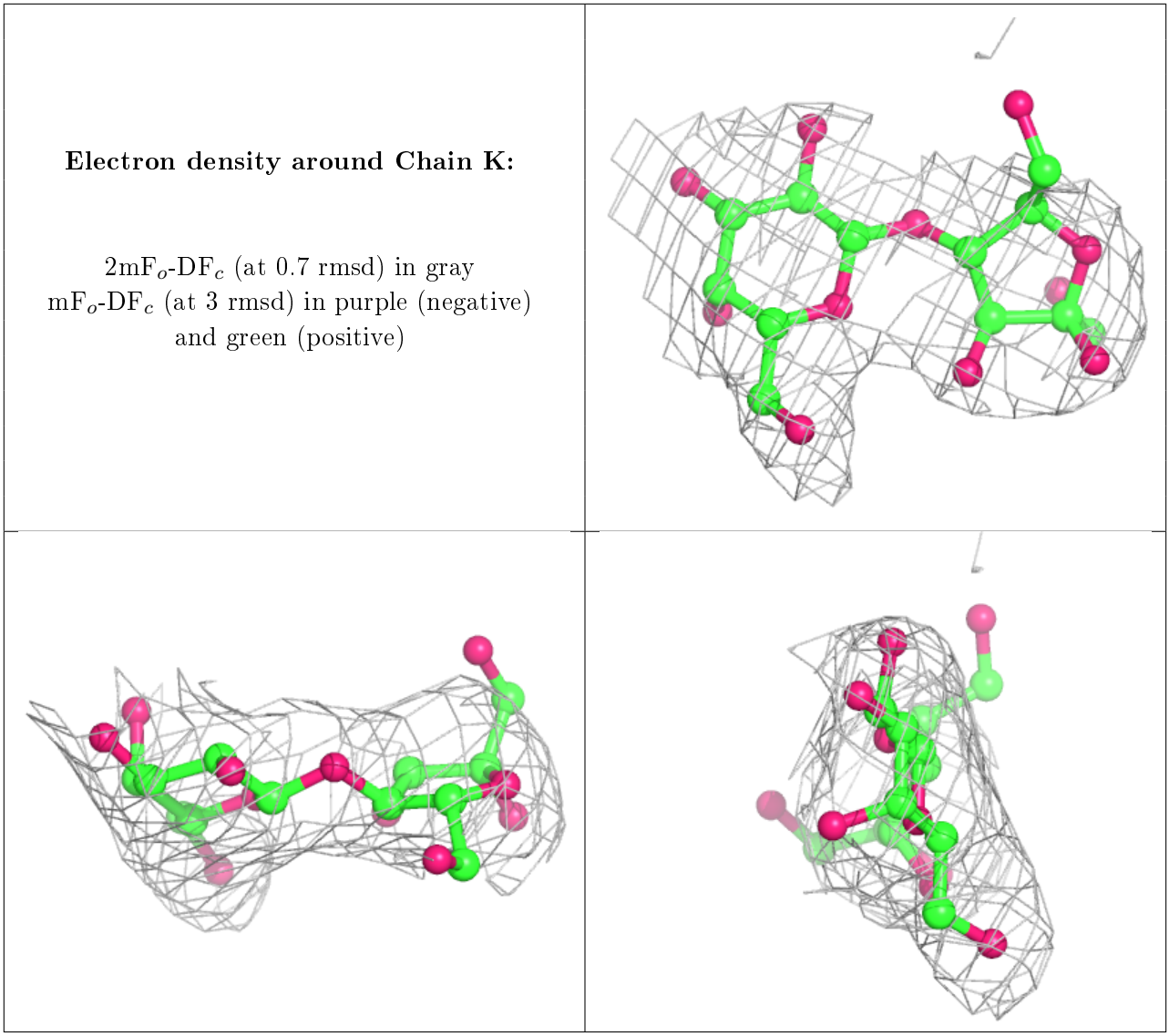






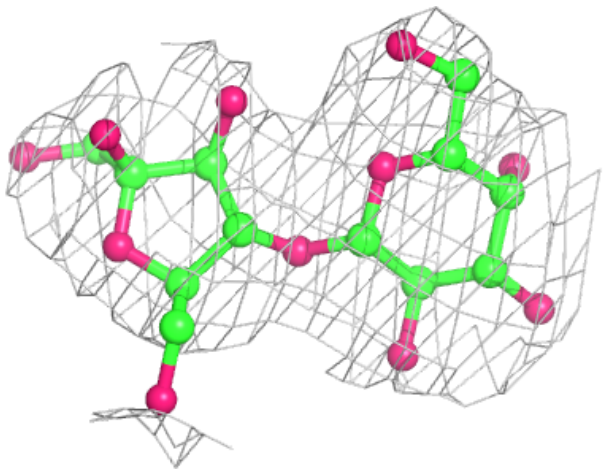
Electron density around Chain K:

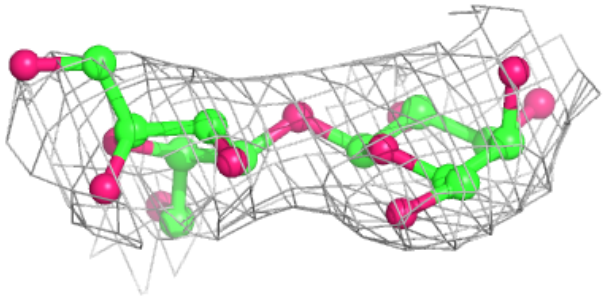
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

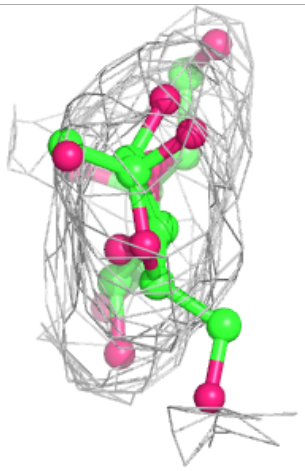


Electron density around Chain L:

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

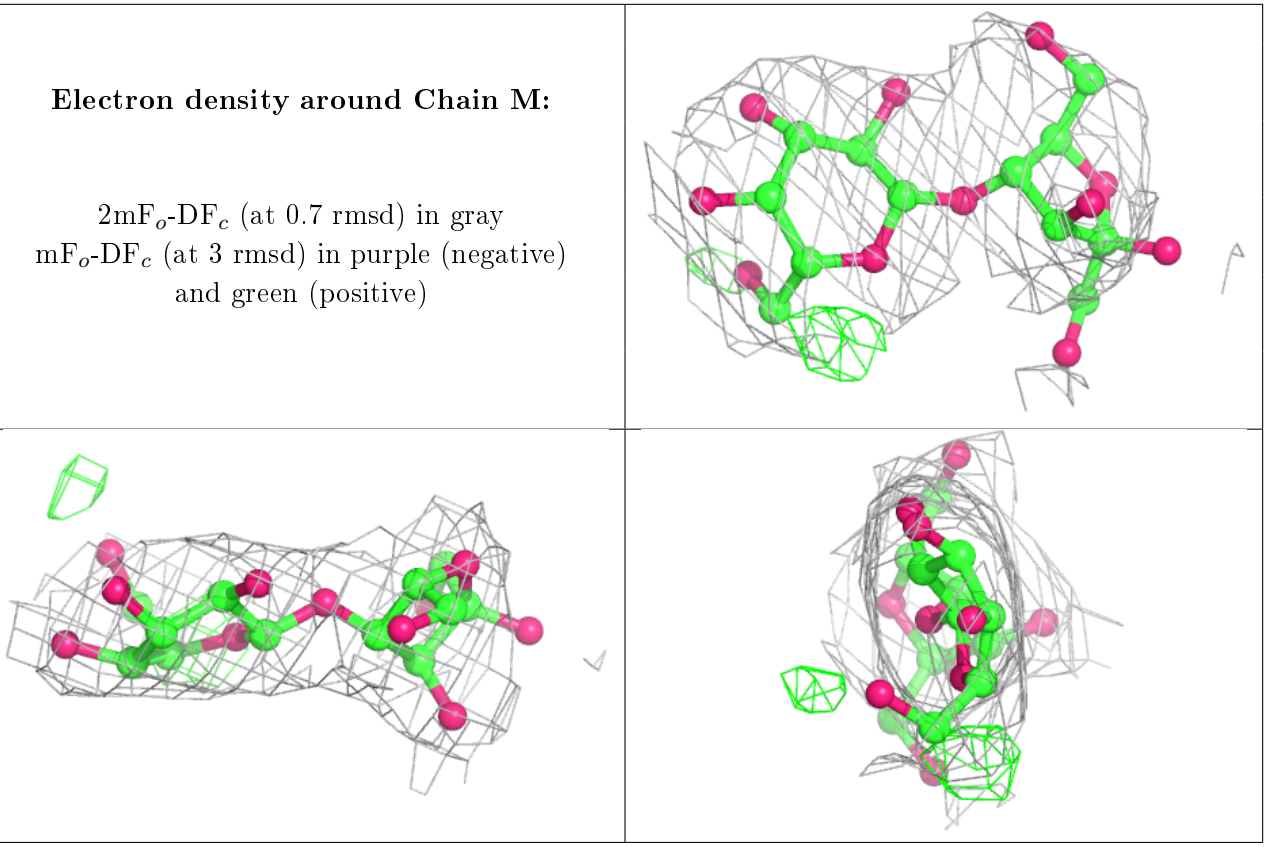






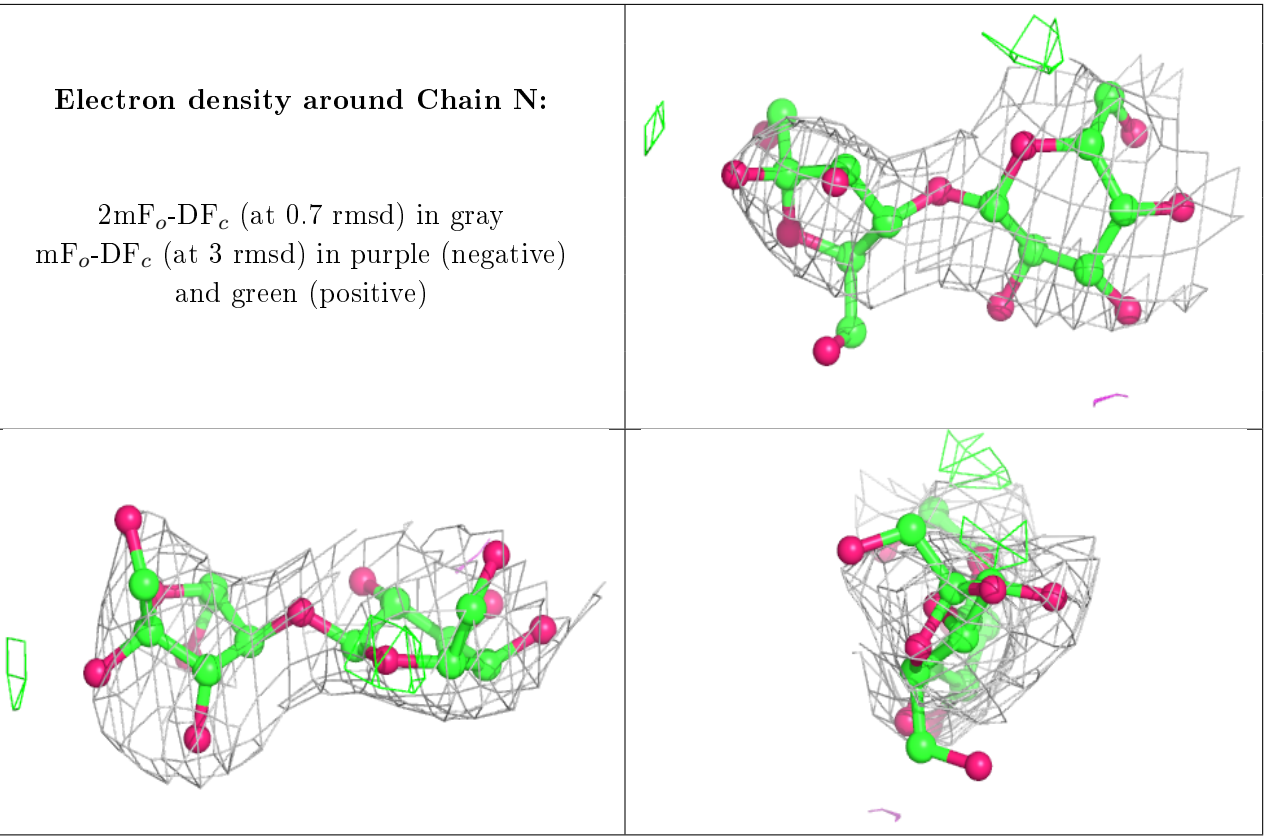
Electron density around Chain M:

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



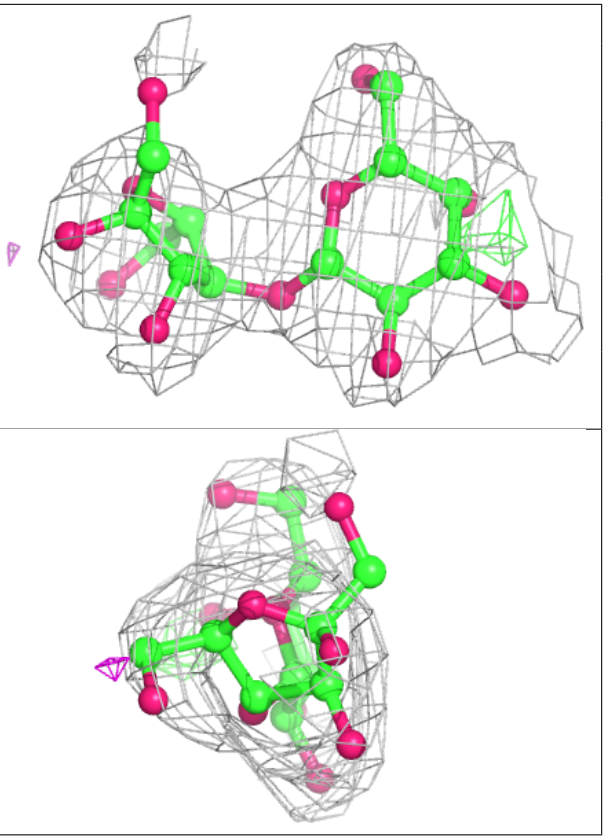
Electron density around Chain N:

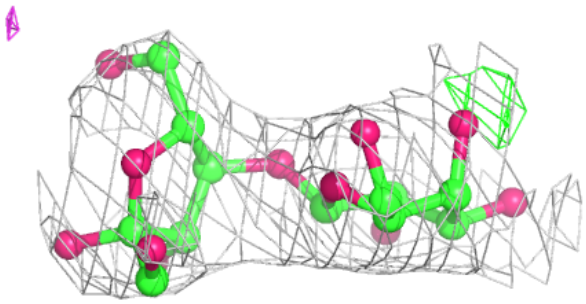
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain O:

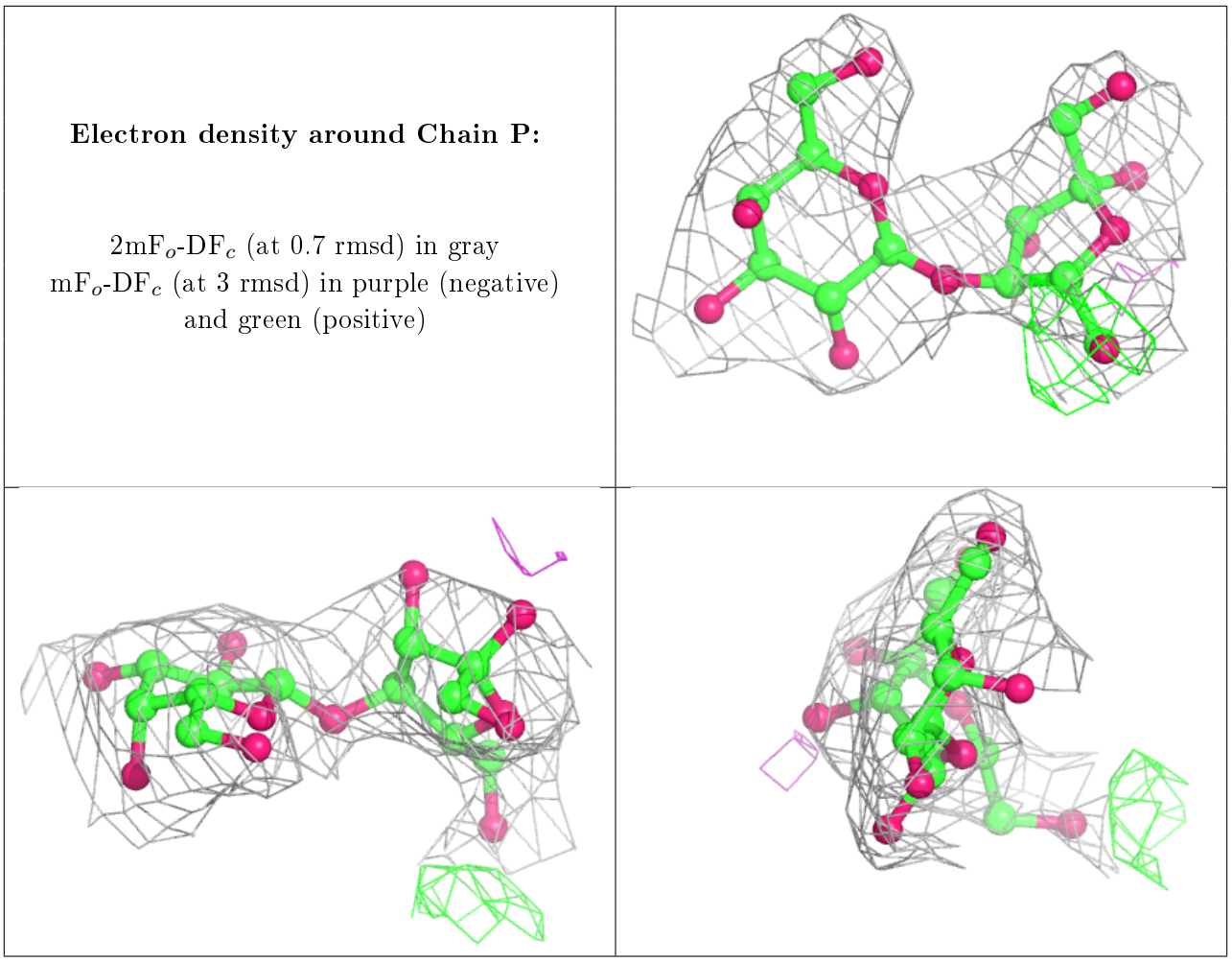
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





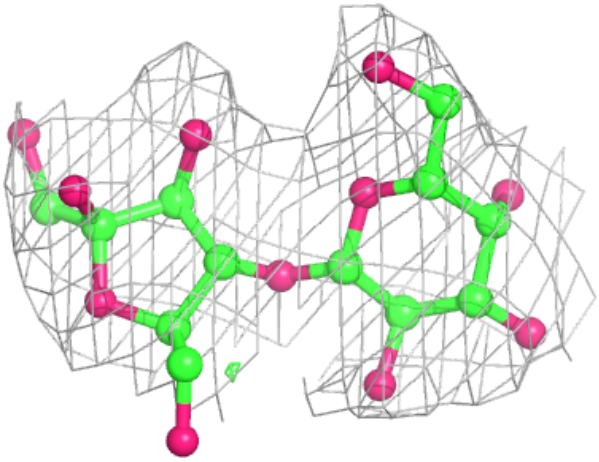
Electron density around Chain P:

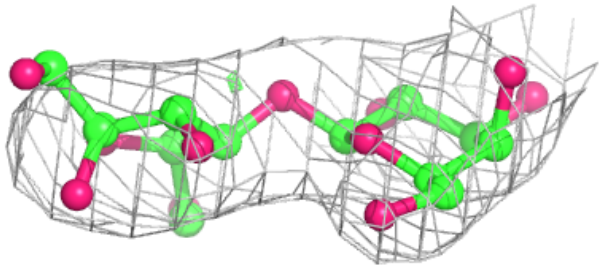
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

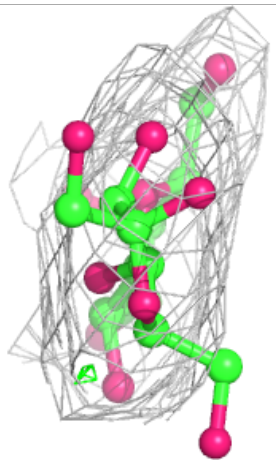


Electron density around Chain Q:

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

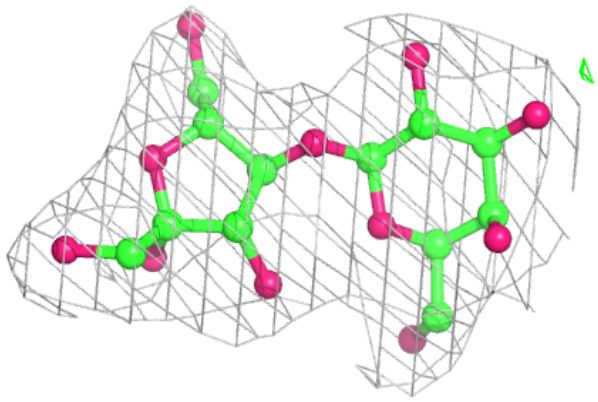


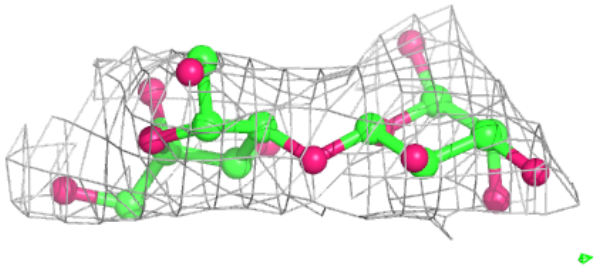


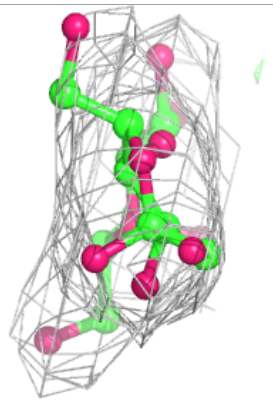


Electron density around Chain R:

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

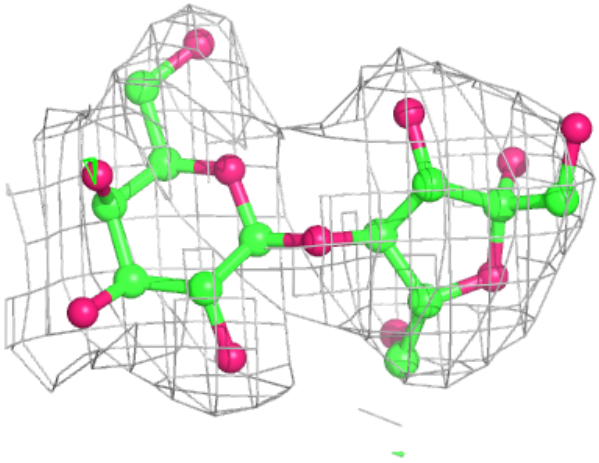


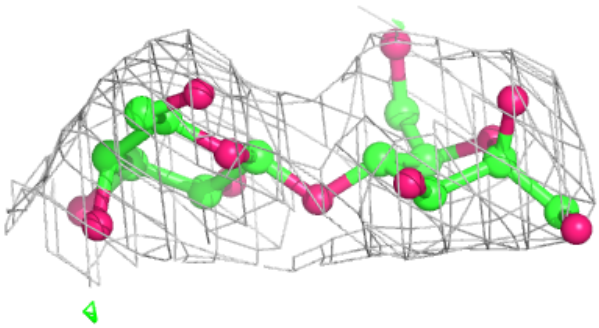


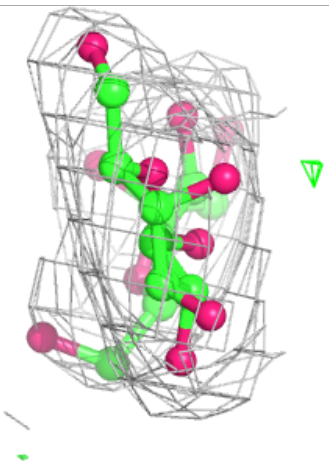


Electron density around Chain S:

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

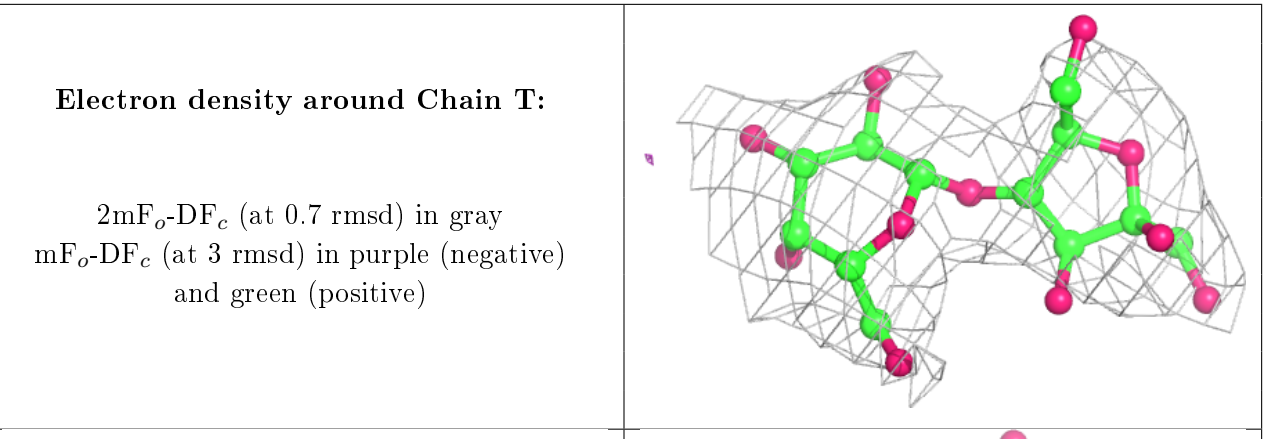






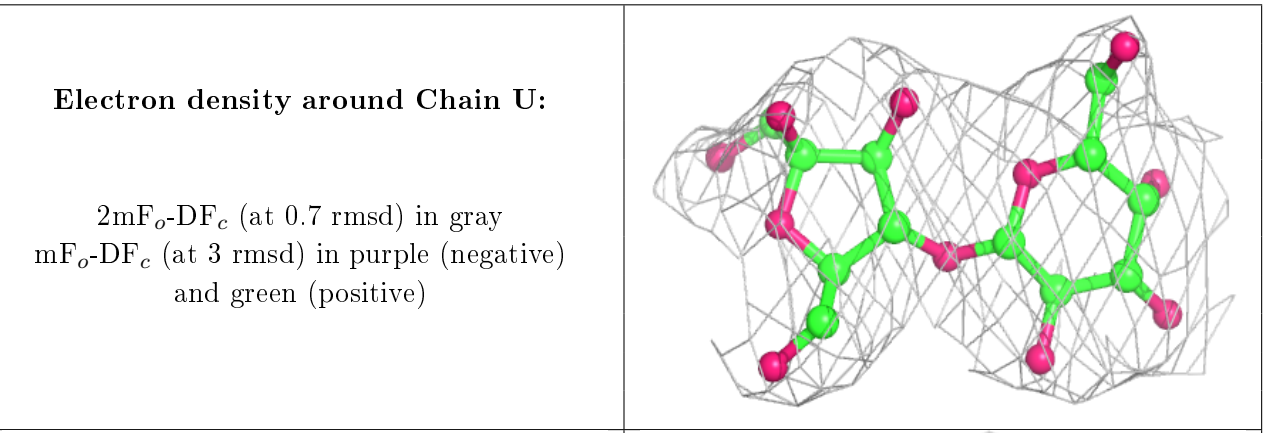
Electron density around Chain T:

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



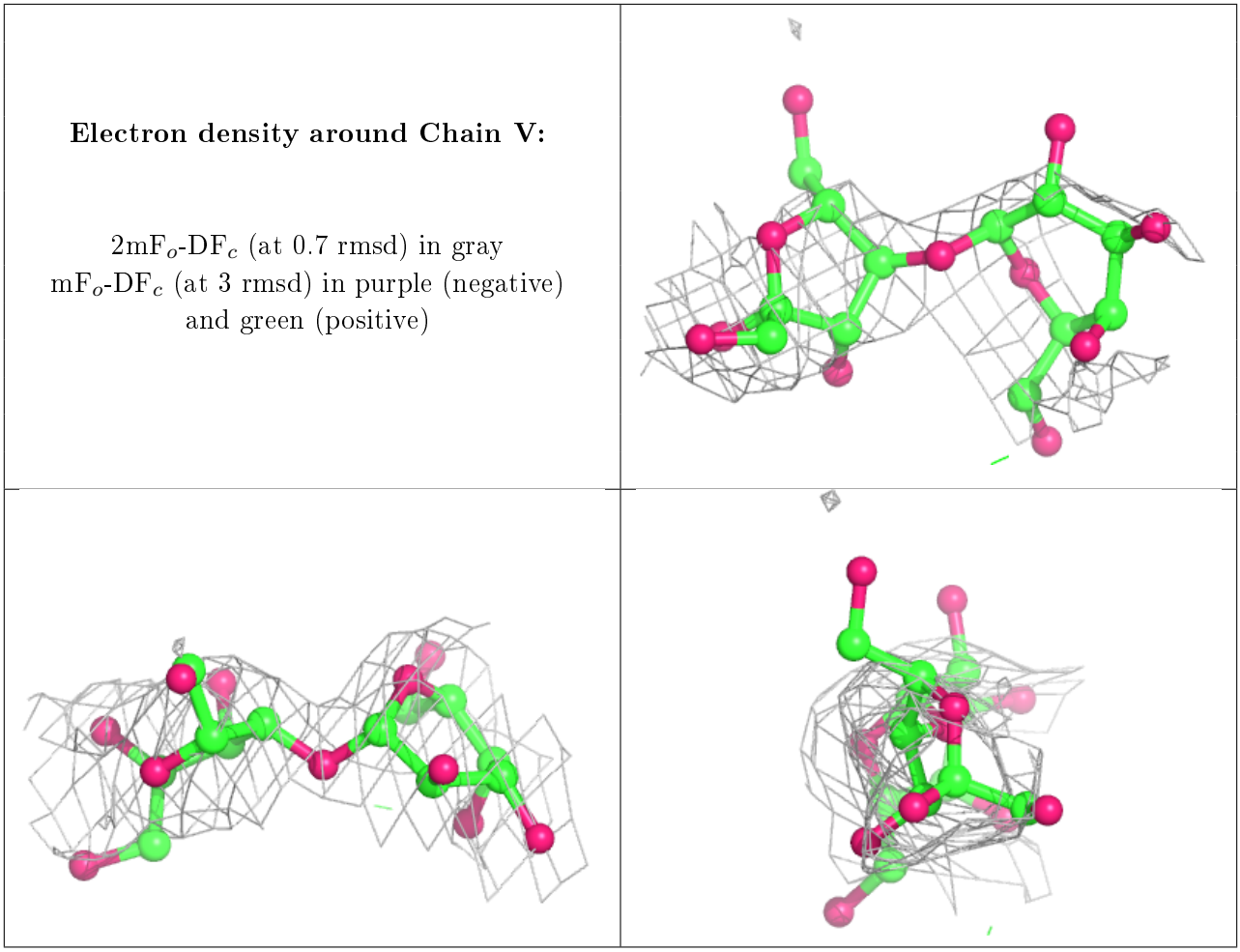
Electron density around Chain U:

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



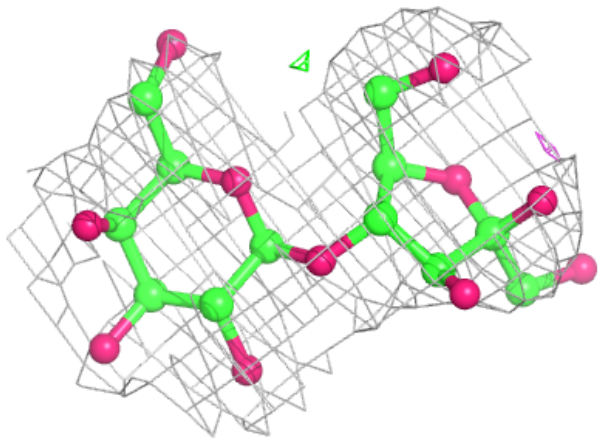
Electron density around Chain V:

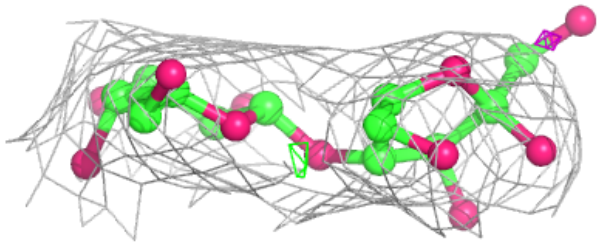
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

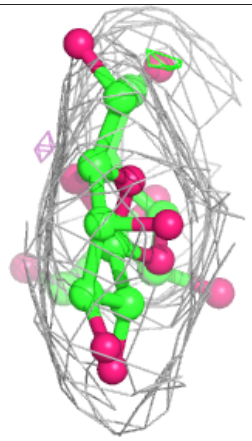


Electron density around Chain W:

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

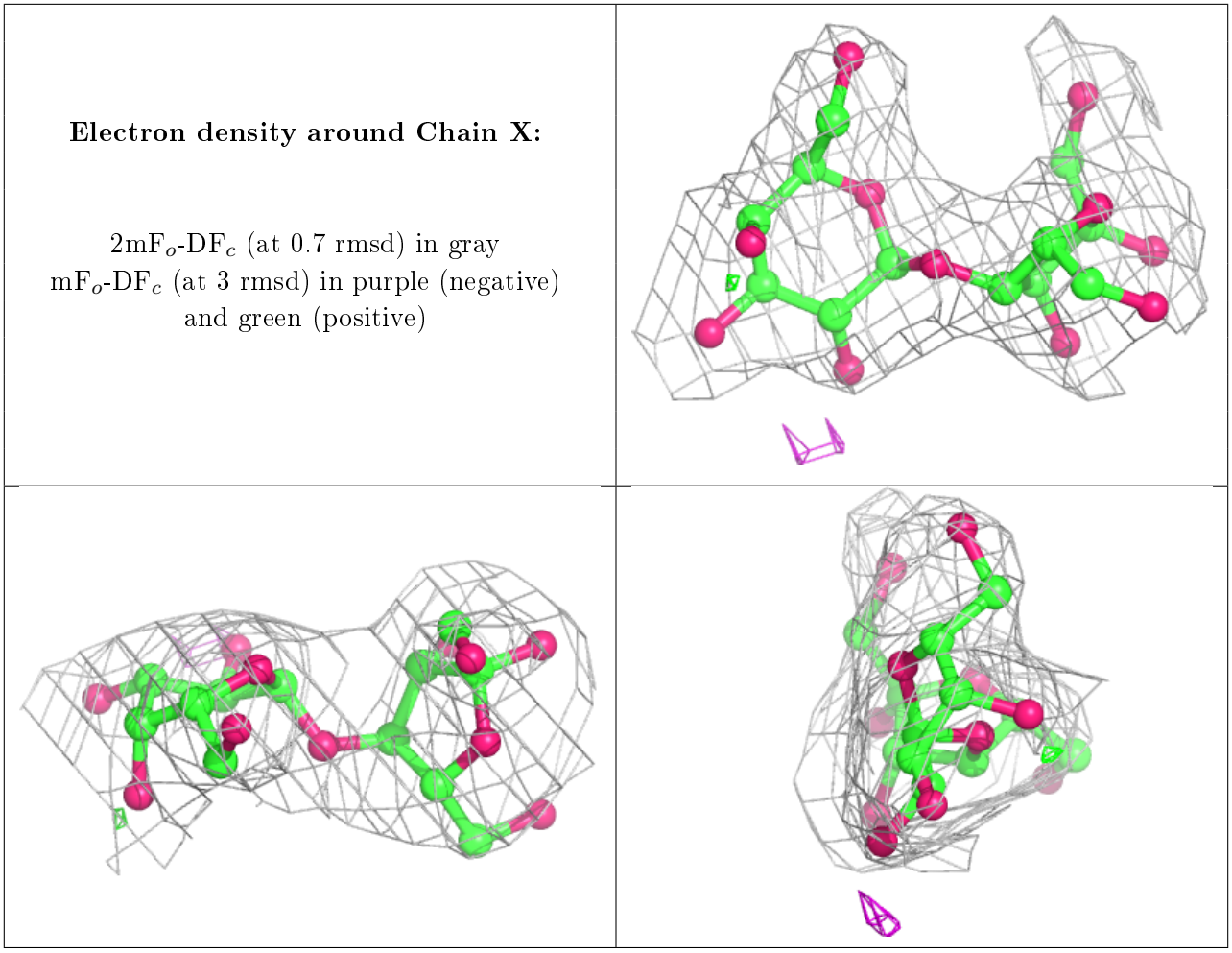






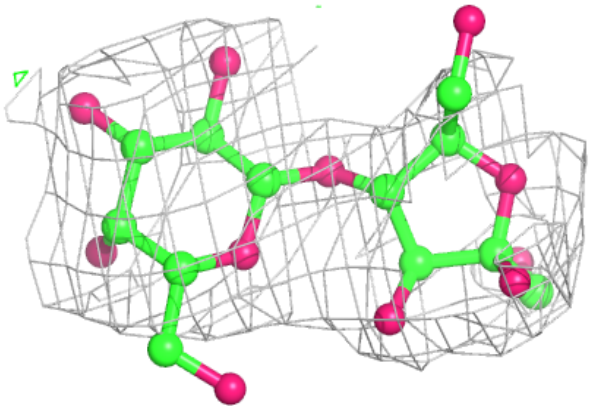
Electron density around Chain X:

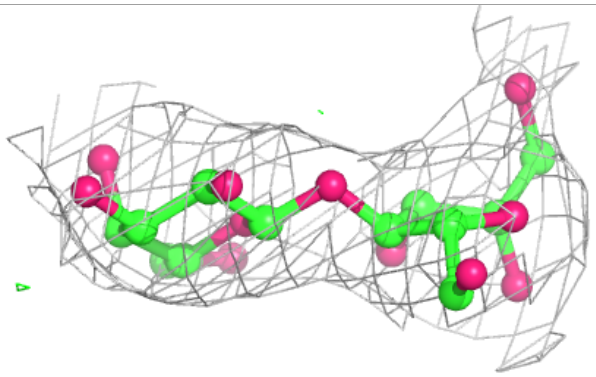
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

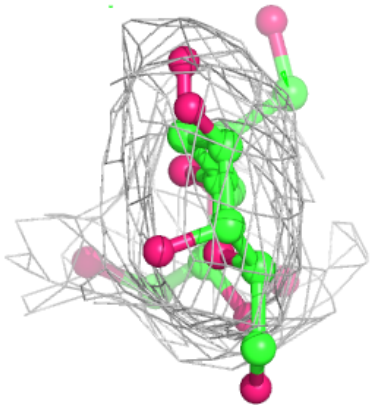


Electron density around Chain Y:

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

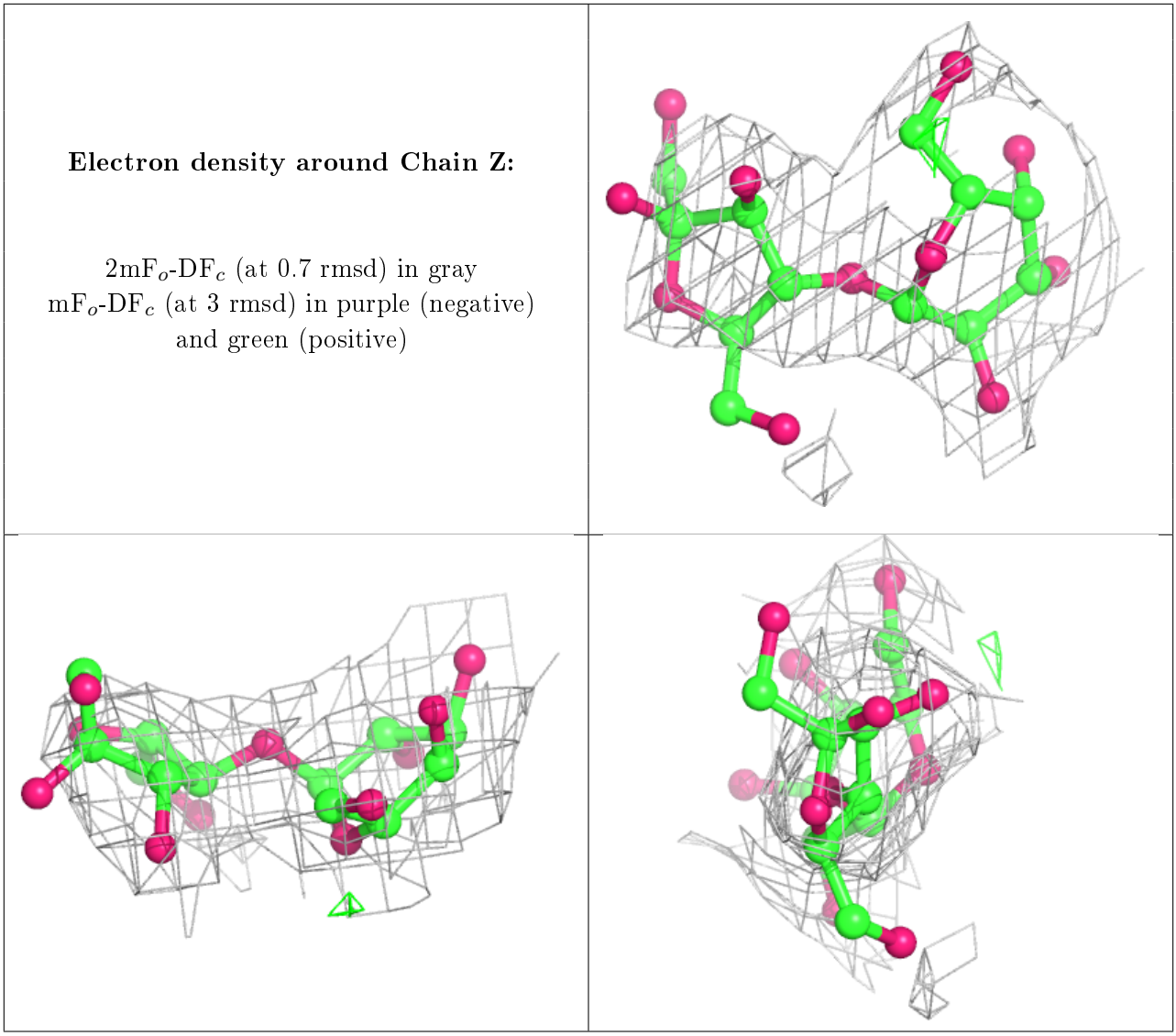






Electron density around Chain Z:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	513	1/1	0.69	0.12	109,109,109,109	0
3	CA	A	1013	1/1	0.76	0.06	96,96,96,96	0
3	CA	E	514	1/1	0.84	0.10	88,88,88,88	0
3	CA	G	513	1/1	0.84	0.05	87,87,87,87	0
3	CA	F	511	1/1	0.85	0.06	127,127,127,127	0
4	MG	D	510	1/1	0.86	0.10	85,85,85,85	0
3	CA	C	1007	1/1	0.88	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1011	1/1	0.88	0.08	72,72,72,72	0
3	CA	G	508	1/1	0.89	0.12	84,84,84,84	0
4	MG	A	1010	1/1	0.90	0.12	59,59,59,59	0
3	CA	D	513	1/1	0.91	0.04	93,93,93,93	0
4	MG	F	510	1/1	0.91	0.10	68,68,68,68	0
3	CA	C	1013	1/1	0.91	0.10	94,94,94,94	0
3	CA	C	1010	1/1	0.91	0.14	91,91,91,91	0
3	CA	F	508	1/1	0.91	0.18	70,70,70,70	0
3	CA	D	503	1/1	0.91	0.11	73,73,73,73	0
3	CA	B	514	1/1	0.92	0.06	88,88,88,88	0
4	MG	B	512	1/1	0.92	0.07	70,70,70,70	0
3	CA	C	1008	1/1	0.93	0.19	69,69,69,69	0
3	CA	D	508	1/1	0.93	0.19	80,80,80,80	0
4	MG	F	509	1/1	0.94	0.10	53,53,53,53	0
3	CA	B	510	1/1	0.94	0.11	85,85,85,85	0
3	CA	E	511	1/1	0.94	0.10	123,123,123,123	0
3	CA	G	506	1/1	0.94	0.06	116,116,116,116	0
3	CA	A	1006	1/1	0.94	0.09	92,92,92,92	0
3	CA	F	513	1/1	0.95	0.07	93,93,93,93	0
4	MG	G	512	1/1	0.95	0.10	108,108,108,108	0
3	CA	B	505	1/1	0.95	0.13	64,64,64,64	0
4	MG	C	1011	1/1	0.95	0.05	86,86,86,86	0
3	CA	A	1007	1/1	0.96	0.12	67,67,67,67	0
3	CA	D	509	1/1	0.96	0.07	97,97,97,97	0
4	MG	B	511	1/1	0.96	0.09	84,84,84,84	0
3	CA	F	505	1/1	0.96	0.19	61,61,61,61	0
3	CA	B	509	1/1	0.96	0.08	96,96,96,96	0
4	MG	C	1012	1/1	0.96	0.07	67,67,67,67	0
3	CA	G	509	1/1	0.96	0.15	66,66,66,66	0
4	MG	D	511	1/1	0.96	0.11	83,83,83,83	0
3	CA	C	1009	1/1	0.96	0.11	75,75,75,75	0
3	CA	E	509	1/1	0.97	0.15	65,65,65,65	0
3	CA	C	1006	1/1	0.97	0.18	65,65,65,65	0
4	MG	E	512	1/1	0.97	0.16	54,54,54,54	0
3	CA	C	1014	1/1	0.97	0.21	60,60,60,60	0
3	CA	B	506	1/1	0.97	0.14	75,75,75,75	0
3	CA	D	505	1/1	0.97	0.17	68,68,68,68	0
3	CA	E	507	1/1	0.97	0.12	60,60,60,60	0
3	CA	E	510	1/1	0.97	0.11	95,95,95,95	0
3	CA	B	508	1/1	0.98	0.17	79,79,79,79	0
3	CA	A	1009	1/1	0.98	0.18	68,68,68,68	0
3	CA	F	506	1/1	0.98	0.14	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	1005	1/1	0.98	0.16	70,70,70,70	0
3	CA	D	504	1/1	0.98	0.05	84,84,84,84	0
3	CA	E	508	1/1	0.98	0.16	55,55,55,55	0
3	CA	G	510	1/1	0.98	0.09	83,83,83,83	0
3	CA	G	507	1/1	0.98	0.11	72,72,72,72	0
3	CA	A	1008	1/1	0.98	0.16	66,66,66,66	0
4	MG	G	511	1/1	0.99	0.09	74,74,74,74	0
3	CA	E	515	1/1	0.99	0.23	37,37,37,37	1
3	CA	F	507	1/1	0.99	0.15	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.