Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:43 AM BST

PDB ID	:	1ZPU
Title	:	Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import
Authors	:	Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.
Deposited on	:	2005-05-17
Resolution	:	2.80 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 ①) were used in the production of this report:

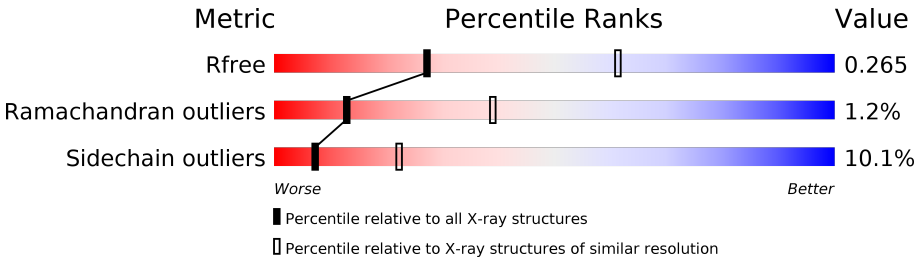
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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%

Mol	Chain	Length	Quality of chain
1	A	534	89% 9% ••
1	B	534	88% 10% •
1	C	534	89% 10% •
1	D	534	88% 10% •
1	E	534	90% 9% •
1	F	534	87% 11% •
2	G	5	100%
2	J	5	100%
2	M	5	20% 80%

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Mol	Chain	Length	Quality of chain
2	O	5	100%
2	S	5	100%
2	U	5	100%
2	Y	5	100%
2	a	5	100%
2	d	5	40% 60%
2	f	5	20% 80%
2	i	5	20% 80%
2	k	5	100%
3	H	6	17% 83%
3	N	6	17% 83%
3	Z	6	100%
3	j	6	100%
4	I	2	100%
4	P	2	50% 50%
4	Q	2	100%
4	V	2	100%
4	b	2	50% 50%
4	g	2	100%
5	K	3	100%
5	L	3	100%
5	W	3	100%
5	X	3	100%
5	c	3	33% 67%
5	h	3	100%

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Mol	Chain	Length	Quality of chain
5	l	3	100%
6	R	4	100%
7	T	7	14% 86%
7	e	7	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	a	1	X	-	-	-
2	NAG	f	1	X	-	-	-
3	NAG	H	1	X	-	-	-
3	NAG	N	1	X	-	-	-
3	NAG	Z	1	X	-	-	-
3	NAG	j	1	X	-	-	-
4	NAG	b	1	X	-	-	-
5	NAG	L	1	X	-	-	-
5	NAG	X	1	X	-	-	-
5	NAG	c	1	X	-	-	-
5	NAG	h	1	X	-	-	-
5	NAG	l	1	X	-	-	-
6	NAG	R	1	X	-	-	-
7	NAG	T	1	X	-	-	-
7	NAG	e	1	X	-	-	-
8	NAG	A	2006	X	-	-	-
8	NAG	A	2012	X	-	-	-
8	NAG	A	2018	X	-	-	-
8	NAG	B	2006	X	-	-	-
8	NAG	B	2012	X	-	-	-
8	NAG	B	2018	X	-	-	-
8	NAG	C	2012	X	-	-	-
8	NAG	C	2018	X	-	-	-
8	NAG	D	2006	X	-	-	-
8	NAG	E	2012	X	-	-	-
8	NAG	F	2005	X	-	-	-
8	NAG	F	2006	X	-	-	-
8	NAG	F	2009	X	-	-	-
8	NAG	F	2012	X	-	-	-

2 Entry composition

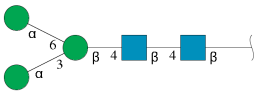
There are 9 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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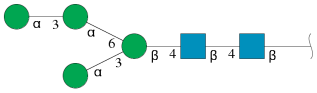
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	U	5	Total C N O 61 34 2 25	0	0	0
2	Y	5	Total C N O 61 34 2 25	0	0	0
2	a	5	Total C N O 61 34 2 25	0	0	0
2	d	5	Total C N O 61 34 2 25	0	0	0
2	f	5	Total C N O 61 34 2 25	0	0	0
2	i	5	Total C N O 61 34 2 25	0	0	0
2	k	5	Total C N O 61 34 2 25	0	0	0

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

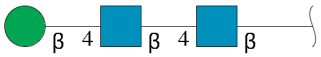


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	H	6	Total C N O 72 40 2 30	0	0	0
3	N	6	Total C N O 72 40 2 30	0	0	0
3	Z	6	Total C N O 72 40 2 30	0	0	0
3	j	6	Total C N O 72 40 2 30	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	Q	2	Total C N O 28 16 2 10	0	0	0
4	V	2	Total C N O 28 16 2 10	0	0	0
4	b	2	Total C N O 28 16 2 10	0	0	0
4	g	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 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.

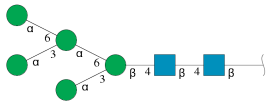


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	3	Total C N O 39 22 2 15	0	0	0
5	L	3	Total C N O 39 22 2 15	0	0	0
5	W	3	Total C N O 39 22 2 15	0	0	0
5	X	3	Total C N O 39 22 2 15	0	0	0
5	c	3	Total C N O 39 22 2 15	0	0	0
5	h	3	Total C N O 39 22 2 15	0	0	0
5	l	3	Total C N O 39 22 2 15	0	0	0

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

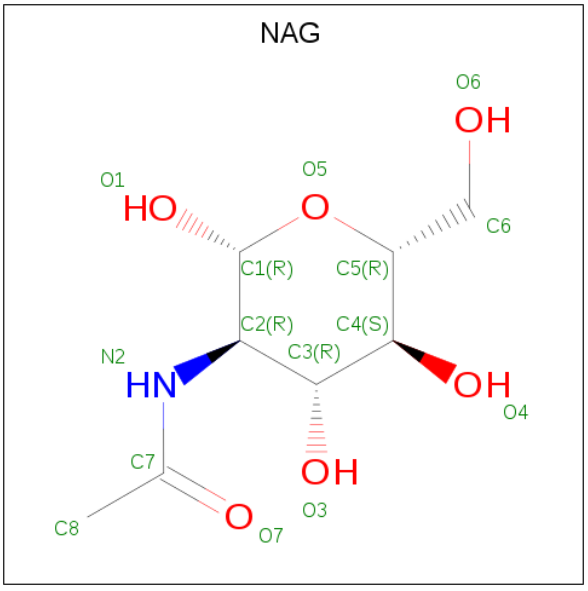
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	e	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C N O 14 8 1 5	0	0
8	E	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

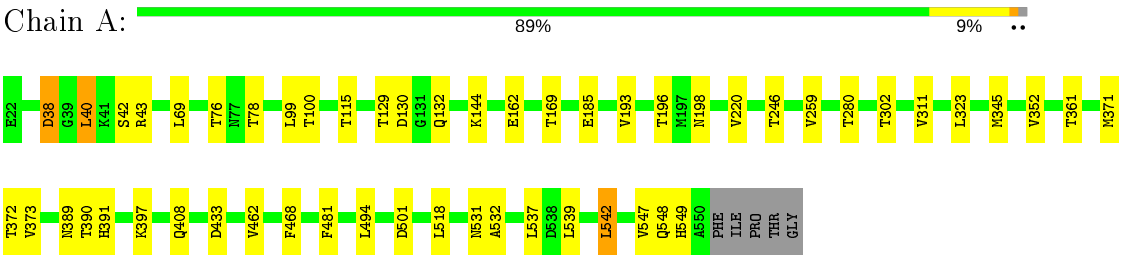
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	4	Total Cu 4 4	0	0
9	E	4	Total Cu 4 4	0	0
9	B	4	Total Cu 4 4	0	0
9	C	4	Total Cu 4 4	0	0
9	A	4	Total Cu 4 4	0	0
9	F	4	Total Cu 4 4	0	0

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. 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. 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.

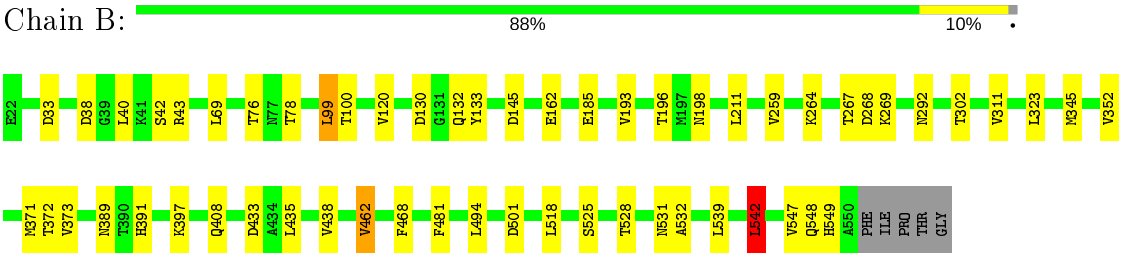
- Molecule 1: Iron transport multicopper oxidase FET3

Chain A:



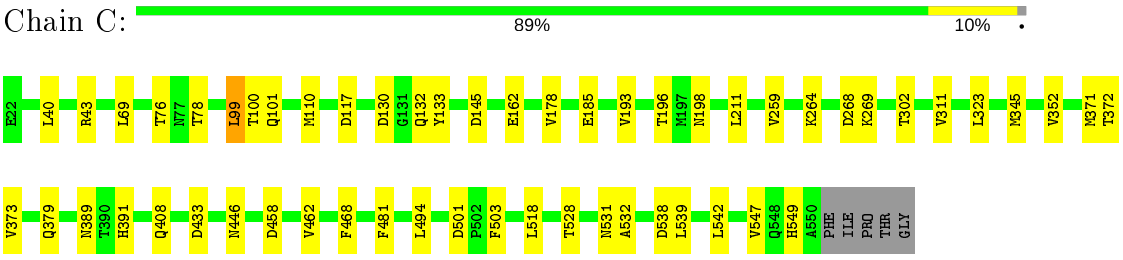
- Molecule 1: Iron transport multicopper oxidase FET3

Chain B:



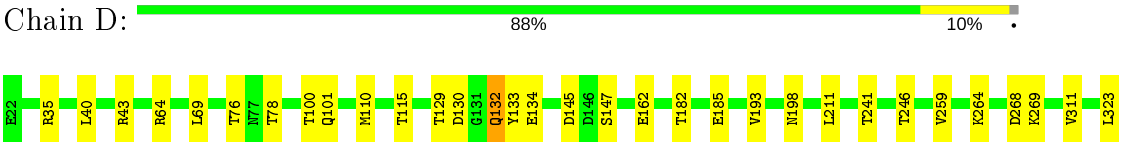
- Molecule 1: Iron transport multicopper oxidase FET3

Chain C:



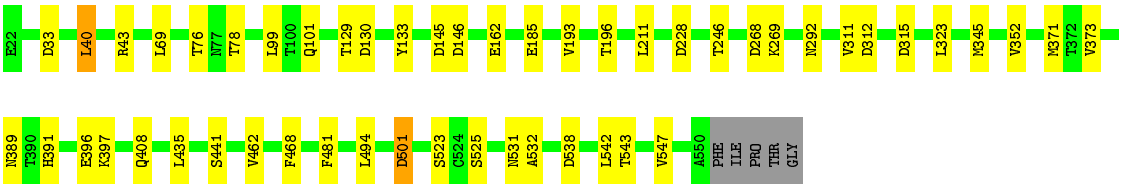
- Molecule 1: Iron transport multicopper oxidase FET3

Chain D:



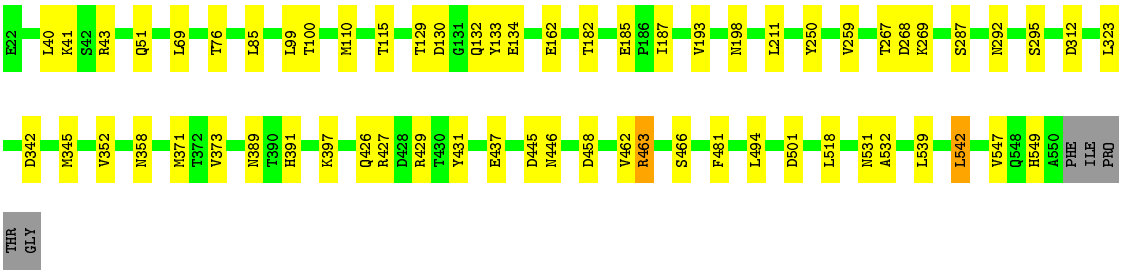
• Molecule 1: Iron transport multicopper oxidase FET3

Chain E:



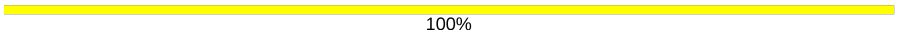
• Molecule 1: Iron transport multicopper oxidase FET3

Chain F:



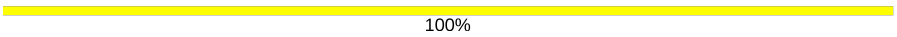
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



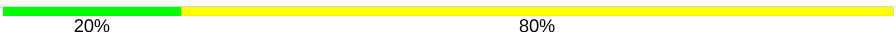
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

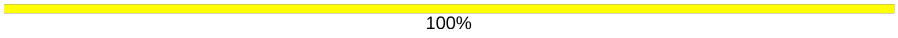


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

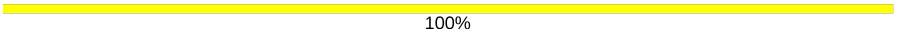
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

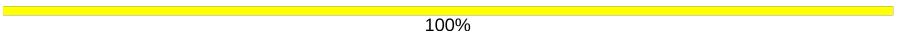


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

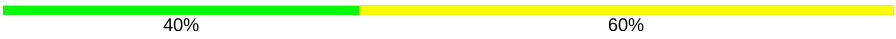
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

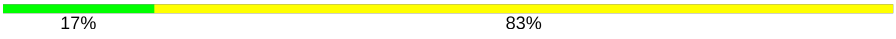
Chain i:

• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

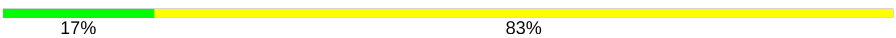
• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

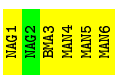
Chain H:



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

Chain N:

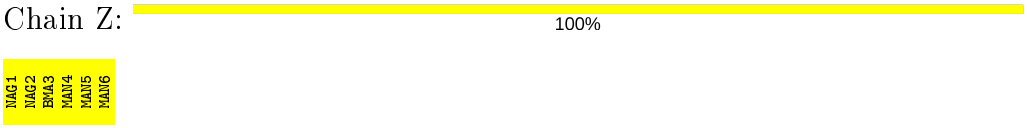




• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam

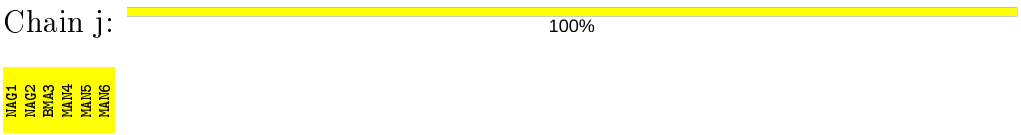
ido-2-deoxy-beta-D-glucopyranose

Chain Z:



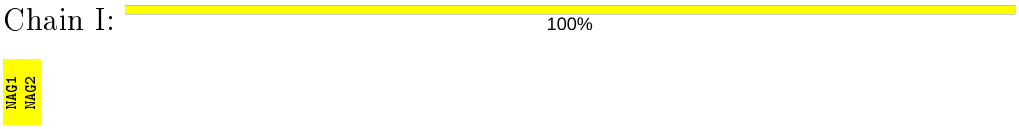
• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



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

Chain I:

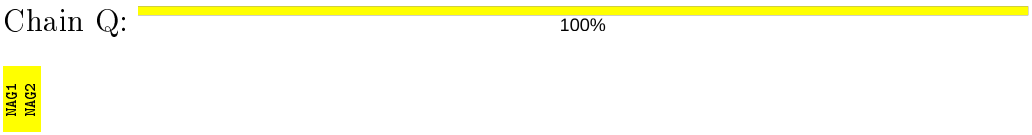


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

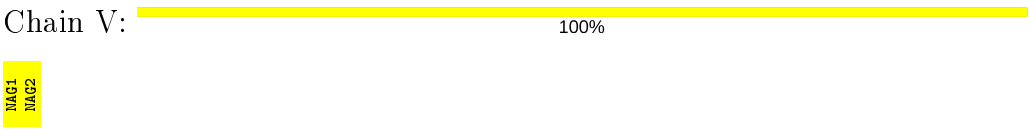
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain V:



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

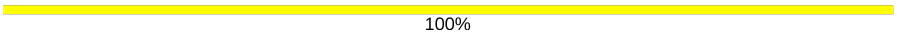
Chain b:

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

Chain K:



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

Chain L:

• Molecule 5: 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

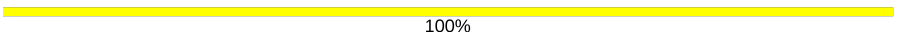
Chain X:

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

Chain c:

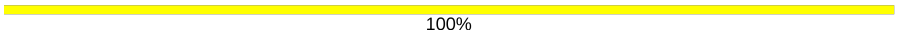
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



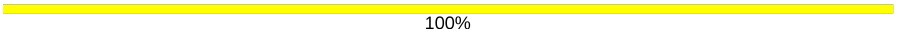
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



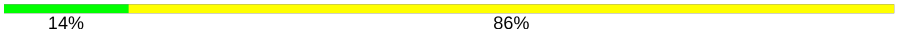
• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 36.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (36.72-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.257 0.235 , 0.265	Depositor DCC
R_{free} test set	6726 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BMA, NAG, CU1, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.50	0/4373	0.66	2/5981 (0.0%)
1	B	0.50	0/4373	0.66	3/5981 (0.1%)
1	C	0.55	5/4373 (0.1%)	0.64	2/5981 (0.0%)
1	D	0.51	3/4373 (0.1%)	0.60	2/5981 (0.0%)
1	E	0.44	1/4373 (0.0%)	0.58	1/5981 (0.0%)
1	F	0.99	20/4373 (0.5%)	0.77	11/5981 (0.2%)
All	All	0.61	29/26238 (0.1%)	0.65	21/35886 (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	F	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	40.06	1.85	1.33
1	F	250	TYR	CE2-CZ	15.67	1.58	1.38
1	F	250	TYR	CG-CD2	15.35	1.59	1.39
1	D	515	GLU	CD-OE1	13.48	1.40	1.25
1	F	250	TYR	CE1-CZ	13.27	1.55	1.38
1	F	250	TYR	CG-CD1	11.36	1.53	1.39
1	F	358	ASN	CG-OD1	10.61	1.47	1.24
1	F	445	ASP	CG-OD2	9.77	1.47	1.25
1	F	431	TYR	CE1-CZ	9.44	1.50	1.38
1	C	538	ASP	CG-OD2	9.41	1.47	1.25
1	D	515	GLU	CD-OE2	8.80	1.35	1.25
1	D	35	ARG	CZ-NH1	8.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	431	TYR	CG-CD2	7.97	1.49	1.39
1	F	312	ASP	CG-OD2	7.86	1.43	1.25
1	F	431	TYR	CG-CD1	7.78	1.49	1.39
1	F	426	GLN	CD-OE1	7.58	1.40	1.24
1	F	446	ASN	CG-OD1	7.40	1.40	1.24
1	C	379	GLN	CG-CD	7.34	1.68	1.51
1	C	538	ASP	CB-CG	7.01	1.66	1.51
1	F	429	ARG	NE-CZ	6.76	1.41	1.33
1	C	503	PHE	CD2-CE2	6.44	1.52	1.39
1	F	463	ARG	CD-NE	6.35	1.57	1.46
1	F	312	ASP	CG-OD1	6.22	1.39	1.25
1	F	463	ARG	NE-CZ	5.97	1.40	1.33
1	F	445	ASP	CG-OD1	5.95	1.39	1.25
1	F	437	GLU	CD-OE1	5.86	1.32	1.25
1	F	437	GLU	CD-OE2	5.60	1.31	1.25
1	C	379	GLN	CD-NE2	5.29	1.46	1.32
1	E	396	GLU	CD-OE1	5.10	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	463	ARG	NE-CZ-NH2	-25.91	107.34	120.30
1	F	463	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	F	445	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	F	429	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	F	463	ARG	NH1-CZ-NH2	-8.13	110.46	119.40
1	F	250	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	C	458	ASP	CB-CA-C	-7.02	96.35	110.40
1	F	250	TYR	CD1-CG-CD2	6.90	125.49	117.90
1	D	542	LEU	CA-CB-CG	6.81	130.96	115.30
1	B	542	LEU	CA-CB-CG	6.34	129.88	115.30
1	F	312	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	F	431	TYR	CG-CD2-CE2	-5.88	116.60	121.30
1	F	250	TYR	CG-CD1-CE1	-5.71	116.73	121.30
1	B	462	VAL	CB-CA-C	-5.59	100.79	111.40
1	E	40	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	38	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	D	35	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	99	LEU	CA-CB-CG	5.43	127.79	115.30
1	F	250	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	40	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	99	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	12	36
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	14	41
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	17	46
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	10	33
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	14	41
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	14	41
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	13	39

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP
1	E	531	ASN
1	F	130	ASP
1	A	531	ASN

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Mol	Chain	Res	Type
1	B	130	ASP
1	B	542	LEU
1	C	531	ASN
1	D	531	ASN
1	D	542	LEU
1	F	531	ASN
1	A	542	LEU
1	C	542	LEU
1	E	542	LEU
1	F	542	LEU
1	A	132	GLN
1	A	501	ASP
1	B	501	ASP
1	B	532	ALA
1	C	501	ASP
1	D	501	ASP
1	E	501	ASP
1	E	532	ALA
1	F	501	ASP
1	B	132	GLN
1	C	532	ALA
1	D	129	THR
1	D	132	GLN
1	D	397	LYS
1	D	532	ALA
1	E	129	THR
1	F	532	ALA
1	A	129	THR
1	A	532	ALA
1	F	129	THR

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	477/481 (99%)	430 (90%)	47 (10%)	8 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	477/481 (99%)	425 (89%)	52 (11%)	6 19
1	C	477/481 (99%)	431 (90%)	46 (10%)	8 24
1	D	477/481 (99%)	425 (89%)	52 (11%)	6 19
1	E	477/481 (99%)	432 (91%)	45 (9%)	8 26
1	F	477/481 (99%)	429 (90%)	48 (10%)	7 22
All	All	2862/2886 (99%)	2572 (90%)	290 (10%)	7 22

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	40	LEU
1	A	42	SER
1	A	43	ARG
1	A	69	LEU
1	A	76	THR
1	A	78	THR
1	A	99	LEU
1	A	100	THR
1	A	115	THR
1	A	144	LYS
1	A	162	GLU
1	A	169	THR
1	A	185	GLU
1	A	193	VAL
1	A	196	THR
1	A	198	ASN
1	A	220	VAL
1	A	246	THR
1	A	259	VAL
1	A	280	THR
1	A	302	THR
1	A	311	VAL
1	A	323	LEU
1	A	345	MET
1	A	352	VAL
1	A	361	THR
1	A	371	MET
1	A	372	THR
1	A	373	VAL

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Mol	Chain	Res	Type
1	A	389	ASN
1	A	390	THR
1	A	391	HIS
1	A	397	LYS
1	A	408	GLN
1	A	433	ASP
1	A	462	VAL
1	A	468	PHE
1	A	481	PHE
1	A	494	LEU
1	A	518	LEU
1	A	537	LEU
1	A	539	LEU
1	A	542	LEU
1	A	547	VAL
1	A	548	GLN
1	A	549	HIS
1	B	33	ASP
1	B	38	ASP
1	B	40	LEU
1	B	42	SER
1	B	43	ARG
1	B	69	LEU
1	B	76	THR
1	B	78	THR
1	B	99	LEU
1	B	100	THR
1	B	120	VAL
1	B	133	TYR
1	B	145	ASP
1	B	162	GLU
1	B	185	GLU
1	B	193	VAL
1	B	196	THR
1	B	198	ASN
1	B	211	LEU
1	B	259	VAL
1	B	264	LYS
1	B	267	THR
1	B	268	ASP
1	B	269	LYS
1	B	292	ASN

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Mol	Chain	Res	Type
1	B	302	THR
1	B	311	VAL
1	B	323	LEU
1	B	345	MET
1	B	352	VAL
1	B	371	MET
1	B	372	THR
1	B	373	VAL
1	B	389	ASN
1	B	391	HIS
1	B	397	LYS
1	B	408	GLN
1	B	433	ASP
1	B	435	LEU
1	B	438	VAL
1	B	462	VAL
1	B	468	PHE
1	B	481	PHE
1	B	494	LEU
1	B	518	LEU
1	B	525	SER
1	B	528	THR
1	B	539	LEU
1	B	542	LEU
1	B	547	VAL
1	B	548	GLN
1	B	549	HIS
1	C	40	LEU
1	C	43	ARG
1	C	69	LEU
1	C	76	THR
1	C	78	THR
1	C	99	LEU
1	C	100	THR
1	C	101	GLN
1	C	110	MET
1	C	117	ASP
1	C	132	GLN
1	C	133	TYR
1	C	145	ASP
1	C	162	GLU
1	C	178	VAL

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Mol	Chain	Res	Type
1	C	185	GLU
1	C	193	VAL
1	C	196	THR
1	C	198	ASN
1	C	211	LEU
1	C	259	VAL
1	C	264	LYS
1	C	268	ASP
1	C	269	LYS
1	C	302	THR
1	C	311	VAL
1	C	323	LEU
1	C	345	MET
1	C	352	VAL
1	C	371	MET
1	C	372	THR
1	C	373	VAL
1	C	389	ASN
1	C	391	HIS
1	C	408	GLN
1	C	433	ASP
1	C	446	ASN
1	C	462	VAL
1	C	468	PHE
1	C	481	PHE
1	C	494	LEU
1	C	518	LEU
1	C	528	THR
1	C	539	LEU
1	C	547	VAL
1	C	549	HIS
1	D	40	LEU
1	D	43	ARG
1	D	64	ARG
1	D	69	LEU
1	D	76	THR
1	D	78	THR
1	D	100	THR
1	D	101	GLN
1	D	110	MET
1	D	115	THR
1	D	132	GLN

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Mol	Chain	Res	Type
1	D	133	TYR
1	D	134	GLU
1	D	145	ASP
1	D	147	SER
1	D	162	GLU
1	D	182	THR
1	D	185	GLU
1	D	193	VAL
1	D	198	ASN
1	D	211	LEU
1	D	241	THR
1	D	246	THR
1	D	259	VAL
1	D	264	LYS
1	D	268	ASP
1	D	269	LYS
1	D	311	VAL
1	D	323	LEU
1	D	345	MET
1	D	371	MET
1	D	372	THR
1	D	373	VAL
1	D	389	ASN
1	D	390	THR
1	D	391	HIS
1	D	397	LYS
1	D	430	THR
1	D	433	ASP
1	D	435	LEU
1	D	462	VAL
1	D	466	SER
1	D	468	PHE
1	D	481	PHE
1	D	491	LEU
1	D	494	LEU
1	D	518	LEU
1	D	539	LEU
1	D	542	LEU
1	D	547	VAL
1	D	548	GLN
1	D	549	HIS
1	E	33	ASP

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Mol	Chain	Res	Type
1	E	40	LEU
1	E	43	ARG
1	E	69	LEU
1	E	76	THR
1	E	78	THR
1	E	99	LEU
1	E	101	GLN
1	E	133	TYR
1	E	145	ASP
1	E	146	ASP
1	E	162	GLU
1	E	185	GLU
1	E	193	VAL
1	E	196	THR
1	E	211	LEU
1	E	228	ASP
1	E	246	THR
1	E	268	ASP
1	E	269	LYS
1	E	292	ASN
1	E	311	VAL
1	E	312	ASP
1	E	315	ASP
1	E	323	LEU
1	E	345	MET
1	E	352	VAL
1	E	371	MET
1	E	373	VAL
1	E	389	ASN
1	E	391	HIS
1	E	397	LYS
1	E	408	GLN
1	E	435	LEU
1	E	441	SER
1	E	462	VAL
1	E	468	PHE
1	E	481	PHE
1	E	494	LEU
1	E	501	ASP
1	E	523	SER
1	E	525	SER
1	E	538	ASP

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Mol	Chain	Res	Type
1	E	543	THR
1	E	547	VAL
1	F	40	LEU
1	F	41	LYS
1	F	43	ARG
1	F	51	GLN
1	F	69	LEU
1	F	76	THR
1	F	85	LEU
1	F	99	LEU
1	F	100	THR
1	F	110	MET
1	F	115	THR
1	F	132	GLN
1	F	133	TYR
1	F	134	GLU
1	F	162	GLU
1	F	182	THR
1	F	185	GLU
1	F	187	ILE
1	F	193	VAL
1	F	198	ASN
1	F	211	LEU
1	F	259	VAL
1	F	267	THR
1	F	268	ASP
1	F	269	LYS
1	F	287	SER
1	F	292	ASN
1	F	295	SER
1	F	323	LEU
1	F	342	ASP
1	F	345	MET
1	F	352	VAL
1	F	371	MET
1	F	373	VAL
1	F	389	ASN
1	F	391	HIS
1	F	397	LYS
1	F	427	ARG
1	F	458	ASP
1	F	462	VAL

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Mol	Chain	Res	Type
1	F	466	SER
1	F	481	PHE
1	F	494	LEU
1	F	518	LEU
1	F	539	LEU
1	F	542	LEU
1	F	547	VAL
1	F	549	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	255	GLN
1	B	222	GLN
1	B	255	GLN
1	B	275	GLN
1	B	324	GLN
1	B	517	HIS
1	C	51	GLN
1	C	66	GLN
1	C	517	HIS
1	D	324	GLN
1	E	195	ASN
1	E	382	ASN
1	E	549	HIS
1	F	309	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

135 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	G	1	1,2	14,14,15	0.72	0	17,19,21	1.36	3 (17%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	1.06	2 (11%)
2	BMA	G	3	2	11,11,12	0.83	0	15,15,17	1.88	3 (20%)
2	MAN	G	4	2	11,11,12	0.60	0	15,15,17	1.37	1 (6%)
2	MAN	G	5	2	11,11,12	0.74	0	15,15,17	2.18	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.79	0	17,19,21	2.04	4 (23%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.85	0
3	BMA	H	3	3	11,11,12	0.76	0	15,15,17	1.95	3 (20%)
3	MAN	H	4	3	11,11,12	0.61	0	15,15,17	1.10	1 (6%)
3	MAN	H	5	3	11,11,12	0.72	0	15,15,17	1.13	1 (6%)
3	MAN	H	6	3	11,11,12	0.68	0	15,15,17	1.75	3 (20%)
4	NAG	I	1	1,4	14,14,15	0.64	0	17,19,21	2.13	5 (29%)
4	NAG	I	2	4	14,14,15	1.05	1 (7%)	17,19,21	1.35	3 (17%)
2	NAG	J	1	1,2	14,14,15	0.71	0	17,19,21	1.80	4 (23%)
2	NAG	J	2	2	14,14,15	0.63	0	17,19,21	1.99	3 (17%)
2	BMA	J	3	2	11,11,12	0.73	0	15,15,17	1.51	3 (20%)
2	MAN	J	4	2	11,11,12	0.73	0	15,15,17	1.85	3 (20%)
2	MAN	J	5	2	11,11,12	0.70	0	15,15,17	1.76	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.51	0	17,19,21	1.95	4 (23%)
5	NAG	K	2	5	14,14,15	0.48	0	17,19,21	1.00	1 (5%)
5	BMA	K	3	5	11,11,12	0.94	0	15,15,17	1.19	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.50	0	17,19,21	1.88	4 (23%)
5	NAG	L	2	5	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
5	BMA	L	3	5	11,11,12	0.64	0	15,15,17	2.08	2 (13%)
2	NAG	M	1	1,2	14,14,15	0.73	0	17,19,21	1.01	0
2	NAG	M	2	2	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
2	BMA	M	3	2	11,11,12	0.77	0	15,15,17	1.00	2 (13%)
2	MAN	M	4	2	11,11,12	0.71	0	15,15,17	2.81	7 (46%)
2	MAN	M	5	2	11,11,12	0.45	0	15,15,17	1.47	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	N	1	1,3	14,14,15	0.68	0	17,19,21	1.50	4 (23%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.04	0
3	BMA	N	3	3	11,11,12	0.78	0	15,15,17	1.51	3 (20%)
3	MAN	N	4	3	11,11,12	0.62	0	15,15,17	2.07	2 (13%)
3	MAN	N	5	3	11,11,12	0.56	0	15,15,17	1.27	1 (6%)
3	MAN	N	6	3	11,11,12	0.57	0	15,15,17	1.19	2 (13%)
2	NAG	O	1	1,2	14,14,15	0.55	0	17,19,21	1.73	3 (17%)
2	NAG	O	2	2	14,14,15	0.74	0	17,19,21	1.27	2 (11%)
2	BMA	O	3	2	11,11,12	0.76	0	15,15,17	1.70	5 (33%)
2	MAN	O	4	2	11,11,12	0.62	0	15,15,17	2.11	5 (33%)
2	MAN	O	5	2	11,11,12	1.69	2 (18%)	15,15,17	2.30	4 (26%)
4	NAG	P	1	1,4	14,14,15	0.56	0	17,19,21	1.00	0
4	NAG	P	2	4	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.47	0	17,19,21	1.79	3 (17%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.19	1 (5%)
6	NAG	R	1	1,6	14,14,15	0.74	0	17,19,21	1.61	1 (5%)
6	NAG	R	2	6	14,14,15	0.64	0	17,19,21	1.26	3 (17%)
6	BMA	R	3	6	11,11,12	0.55	0	15,15,17	1.13	2 (13%)
6	MAN	R	4	6	11,11,12	0.55	0	15,15,17	2.23	5 (33%)
2	NAG	S	1	1,2	14,14,15	0.73	0	17,19,21	1.34	4 (23%)
2	NAG	S	2	2	14,14,15	0.63	0	17,19,21	1.34	3 (17%)
2	BMA	S	3	2	11,11,12	0.57	0	15,15,17	2.13	4 (26%)
2	MAN	S	4	2	11,11,12	0.57	0	15,15,17	1.52	3 (20%)
2	MAN	S	5	2	11,11,12	0.63	0	15,15,17	1.48	4 (26%)
7	NAG	T	1	1,7	14,14,15	0.91	1 (7%)	17,19,21	2.07	7 (41%)
7	NAG	T	2	7	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
7	BMA	T	3	7	11,11,12	0.59	0	15,15,17	1.91	3 (20%)
7	MAN	T	4	7	11,11,12	0.61	0	15,15,17	1.29	1 (6%)
7	MAN	T	5	7	11,11,12	0.72	0	15,15,17	0.78	0
7	MAN	T	6	7	11,11,12	0.57	0	15,15,17	2.15	3 (20%)
7	MAN	T	7	7	11,11,12	0.77	0	15,15,17	2.01	4 (26%)
2	NAG	U	1	1,2	14,14,15	0.48	0	17,19,21	1.96	2 (11%)
2	NAG	U	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.25	4 (23%)
2	BMA	U	3	2	11,11,12	0.70	0	15,15,17	1.31	2 (13%)
2	MAN	U	4	2	11,11,12	0.78	0	15,15,17	1.68	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	U	5	2	11,11,12	0.60	0	15,15,17	1.65	2 (13%)
4	NAG	V	1	1,4	14,14,15	0.52	0	17,19,21	1.14	1 (5%)
4	NAG	V	2	4	14,14,15	1.20	2 (14%)	17,19,21	1.48	2 (11%)
5	NAG	W	1	1,5	14,14,15	1.98	3 (21%)	17,19,21	0.93	0
5	NAG	W	2	5	14,14,15	1.75	3 (21%)	17,19,21	2.18	4 (23%)
5	BMA	W	3	5	11,11,12	2.47	1 (9%)	15,15,17	1.82	4 (26%)
5	NAG	X	1	1,5	14,14,15	0.49	0	17,19,21	1.79	5 (29%)
5	NAG	X	2	5	14,14,15	0.43	0	17,19,21	1.20	2 (11%)
5	BMA	X	3	5	11,11,12	0.68	0	15,15,17	1.03	1 (6%)
2	NAG	Y	1	1,2	14,14,15	0.55	0	17,19,21	0.94	1 (5%)
2	NAG	Y	2	2	14,14,15	0.59	0	17,19,21	1.23	3 (17%)
2	BMA	Y	3	2	11,11,12	0.59	0	15,15,17	1.50	3 (20%)
2	MAN	Y	4	2	11,11,12	0.58	0	15,15,17	1.38	2 (13%)
2	MAN	Y	5	2	11,11,12	0.64	0	15,15,17	1.24	1 (6%)
3	NAG	Z	1	1,3	14,14,15	0.63	0	17,19,21	1.70	3 (17%)
3	NAG	Z	2	3	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
3	BMA	Z	3	3	11,11,12	0.73	0	15,15,17	1.85	4 (26%)
3	MAN	Z	4	3	11,11,12	0.60	0	15,15,17	1.17	2 (13%)
3	MAN	Z	5	3	11,11,12	0.63	0	15,15,17	0.96	1 (6%)
3	MAN	Z	6	3	11,11,12	1.07	1 (9%)	15,15,17	2.06	4 (26%)
2	NAG	a	1	1,2	14,14,15	0.41	0	17,19,21	1.26	2 (11%)
2	NAG	a	2	2	14,14,15	0.59	0	17,19,21	1.00	2 (11%)
2	BMA	a	3	2	11,11,12	0.68	0	15,15,17	1.22	2 (13%)
2	MAN	a	4	2	11,11,12	0.55	0	15,15,17	1.75	4 (26%)
2	MAN	a	5	2	11,11,12	0.62	0	15,15,17	1.54	2 (13%)
4	NAG	b	1	1,4	14,14,15	1.38	2 (14%)	17,19,21	1.59	3 (17%)
4	NAG	b	2	4	14,14,15	0.51	0	17,19,21	0.72	0
5	NAG	c	1	1,5	14,14,15	0.53	0	17,19,21	1.36	2 (11%)
5	NAG	c	2	5	14,14,15	0.55	0	17,19,21	0.85	0
5	BMA	c	3	5	11,11,12	0.56	0	15,15,17	0.98	2 (13%)
2	NAG	d	1	1,2	14,14,15	0.60	0	17,19,21	1.15	1 (5%)
2	NAG	d	2	2	14,14,15	0.56	0	17,19,21	0.82	0
2	BMA	d	3	2	11,11,12	0.78	0	15,15,17	2.15	4 (26%)
2	MAN	d	4	2	11,11,12	0.60	0	15,15,17	0.69	0
2	MAN	d	5	2	11,11,12	0.55	0	15,15,17	1.40	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	e	1	1,7	14,14,15	0.58	0	17,19,21	1.05	1 (5%)
7	NAG	e	2	7	14,14,15	0.50	0	17,19,21	1.26	2 (11%)
7	BMA	e	3	7	11,11,12	0.63	0	15,15,17	1.53	3 (20%)
7	MAN	e	4	7	11,11,12	0.63	0	15,15,17	1.55	4 (26%)
7	MAN	e	5	7	11,11,12	0.56	0	15,15,17	1.06	1 (6%)
7	MAN	e	6	7	11,11,12	0.71	0	15,15,17	1.61	2 (13%)
7	MAN	e	7	7	11,11,12	0.53	0	15,15,17	1.56	1 (6%)
2	NAG	f	1	1,2	14,14,15	0.55	0	17,19,21	1.47	3 (17%)
2	NAG	f	2	2	14,14,15	0.51	0	17,19,21	0.94	0
2	BMA	f	3	2	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
2	MAN	f	4	2	11,11,12	0.57	0	15,15,17	1.44	3 (20%)
2	MAN	f	5	2	11,11,12	0.58	0	15,15,17	1.48	3 (20%)
4	NAG	g	1	1,4	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
4	NAG	g	2	4	14,14,15	0.59	0	17,19,21	1.06	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.59	0	17,19,21	1.64	4 (23%)
5	NAG	h	2	5	14,14,15	0.61	0	17,19,21	1.10	1 (5%)
5	BMA	h	3	5	11,11,12	0.88	0	15,15,17	1.98	5 (33%)
2	NAG	i	1	1,2	14,14,15	0.62	0	17,19,21	0.94	0
2	NAG	i	2	2	14,14,15	0.61	0	17,19,21	1.17	1 (5%)
2	BMA	i	3	2	11,11,12	0.66	0	15,15,17	1.41	3 (20%)
2	MAN	i	4	2	11,11,12	0.65	0	15,15,17	1.87	4 (26%)
2	MAN	i	5	2	11,11,12	0.49	0	15,15,17	1.63	2 (13%)
3	NAG	j	1	1,3	14,14,15	0.63	0	17,19,21	1.45	3 (17%)
3	NAG	j	2	3	14,14,15	0.73	0	17,19,21	1.52	3 (17%)
3	BMA	j	3	3	11,11,12	0.80	0	15,15,17	0.97	2 (13%)
3	MAN	j	4	3	11,11,12	1.18	1 (9%)	15,15,17	1.45	2 (13%)
3	MAN	j	5	3	11,11,12	0.95	1 (9%)	15,15,17	0.94	1 (6%)
3	MAN	j	6	3	11,11,12	0.60	0	15,15,17	1.68	2 (13%)
2	NAG	k	1	1,2	14,14,15	0.51	0	17,19,21	1.31	2 (11%)
2	NAG	k	2	2	14,14,15	0.56	0	17,19,21	1.06	2 (11%)
2	BMA	k	3	2	11,11,12	0.71	0	15,15,17	1.34	1 (6%)
2	MAN	k	4	2	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
2	MAN	k	5	2	11,11,12	1.57	1 (9%)	15,15,17	1.81	2 (13%)
5	NAG	l	1	1,5	14,14,15	0.50	0	17,19,21	1.10	1 (5%)
5	NAG	l	2	5	14,14,15	0.58	0	17,19,21	1.48	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	l	3	5	11,11,12	1.85	2 (18%)	15,15,17	1.07	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1
3	MAN	N	6	3	-	2/2/19/22	0/1/1/1
2	NAG	O	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	2/2/19/22	0/1/1/1
2	MAN	O	5	2	-	2/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
6	NAG	R	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	BMA	S	3	2	-	2/2/19/22	0/1/1/1
2	MAN	S	4	2	-	1/2/19/22	0/1/1/1
2	MAN	S	5	2	-	1/2/19/22	0/1/1/1
7	NAG	T	1	1,7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	MAN	T	4	7	-	0/2/19/22	0/1/1/1
7	MAN	T	5	7	-	0/2/19/22	0/1/1/1
7	MAN	T	6	7	-	2/2/19/22	0/1/1/1
7	MAN	T	7	7	-	2/2/19/22	0/1/1/1
2	NAG	U	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	U	2	2	-	4/6/23/26	0/1/1/1
2	BMA	U	3	2	-	2/2/19/22	0/1/1/1
2	MAN	U	4	2	-	2/2/19/22	0/1/1/1
2	MAN	U	5	2	-	2/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
5	NAG	X	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Y	4	2	-	2/2/19/22	0/1/1/1
2	MAN	Y	5	2	-	1/2/19/22	0/1/1/1
3	NAG	Z	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	4	3	-	0/2/19/22	0/1/1/1
3	MAN	Z	5	3	-	2/2/19/22	0/1/1/1
3	MAN	Z	6	3	-	2/2/19/22	0/1/1/1
2	NAG	a	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	BMA	a	3	2	-	2/2/19/22	0/1/1/1
2	MAN	a	4	2	-	1/2/19/22	0/1/1/1
2	MAN	a	5	2	-	2/2/19/22	0/1/1/1
4	NAG	b	1	1,4	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
5	NAG	c	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
2	BMA	d	3	2	-	2/2/19/22	0/1/1/1
2	MAN	d	4	2	-	2/2/19/22	0/1/1/1
2	MAN	d	5	2	-	2/2/19/22	0/1/1/1
7	NAG	e	1	1,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	e	2	7	-	4/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
7	MAN	e	4	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	e	5	7	-	0/2/19/22	0/1/1/1
7	MAN	e	6	7	-	2/2/19/22	0/1/1/1
7	MAN	e	7	7	-	2/2/19/22	0/1/1/1
2	NAG	f	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1
2	BMA	f	3	2	-	2/2/19/22	0/1/1/1
2	MAN	f	4	2	-	1/2/19/22	1/1/1/1
2	MAN	f	5	2	-	2/2/19/22	0/1/1/1
4	NAG	g	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	g	2	4	-	0/6/23/26	0/1/1/1
5	NAG	h	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
5	BMA	h	3	5	-	2/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	i	2	2	-	4/6/23/26	0/1/1/1
2	BMA	i	3	2	-	0/2/19/22	0/1/1/1
2	MAN	i	4	2	-	1/2/19/22	0/1/1/1
2	MAN	i	5	2	-	1/2/19/22	1/1/1/1
3	NAG	j	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	j	2	3	-	5/6/23/26	0/1/1/1
3	BMA	j	3	3	-	2/2/19/22	0/1/1/1
3	MAN	j	4	3	-	2/2/19/22	0/1/1/1
3	MAN	j	5	3	-	1/2/19/22	0/1/1/1
3	MAN	j	6	3	-	2/2/19/22	0/1/1/1
2	NAG	k	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	k	2	2	-	5/6/23/26	0/1/1/1
2	BMA	k	3	2	-	0/2/19/22	0/1/1/1
2	MAN	k	4	2	-	2/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	1/1/1/1
5	NAG	l	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
5	BMA	l	3	5	-	2/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	O6-C6	7.74	1.75	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	5	MAN	O6-C6	4.87	1.63	1.42
5	l	3	BMA	O6-C6	4.79	1.62	1.42
5	W	1	NAG	C8-C7	4.59	1.60	1.50
5	W	2	NAG	C8-C7	4.54	1.60	1.50
5	W	1	NAG	O7-C7	4.43	1.33	1.23
4	b	1	NAG	C8-C7	4.04	1.58	1.50
2	O	5	MAN	O6-C6	3.81	1.58	1.42
3	j	4	MAN	O6-C6	3.52	1.57	1.42
5	W	2	NAG	O7-C7	3.37	1.30	1.23
2	O	5	MAN	C2-C3	3.28	1.57	1.52
5	W	1	NAG	O6-C6	3.10	1.55	1.42
3	Z	6	MAN	O6-C6	2.81	1.54	1.42
5	W	2	NAG	C7-N2	2.73	1.43	1.34
4	V	2	NAG	C8-C7	2.60	1.55	1.50
3	j	5	MAN	O6-C6	2.60	1.53	1.42
4	V	2	NAG	O7-C7	2.59	1.29	1.23
5	l	3	BMA	C4-C3	2.57	1.58	1.52
4	b	1	NAG	O7-C7	2.52	1.28	1.23
4	I	2	NAG	C1-C2	2.30	1.55	1.52
7	T	1	NAG	O5-C1	-2.26	1.40	1.43
2	U	2	NAG	O7-C7	2.00	1.27	1.23

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	5	MAN	C1-O5-C5	7.19	121.93	112.19
2	M	4	MAN	C1-O5-C5	7.07	121.77	112.19
2	O	5	MAN	C1-O5-C5	6.76	121.35	112.19
2	U	1	NAG	C1-O5-C5	6.66	121.22	112.19
7	T	6	MAN	C1-O5-C5	6.53	121.04	112.19
3	N	4	MAN	C1-O5-C5	6.36	120.80	112.19
2	J	2	NAG	C2-N2-C7	6.13	131.63	122.90
2	J	5	MAN	C1-O5-C5	6.10	120.46	112.19
5	W	2	NAG	C2-N2-C7	-5.97	114.40	122.90
3	Z	6	MAN	C1-C2-C3	5.68	116.64	109.67
2	d	3	BMA	C1-C2-C3	5.62	116.58	109.67
7	e	7	MAN	C1-O5-C5	5.52	119.67	112.19
2	k	5	MAN	C1-O5-C5	5.44	119.56	112.19
6	R	4	MAN	C1-O5-C5	5.38	119.48	112.19
2	S	3	BMA	C1-C2-C3	5.24	116.11	109.67
5	L	3	BMA	C1-O5-C5	5.24	119.29	112.19
2	i	5	MAN	C1-O5-C5	5.24	119.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	3	BMA	C1-C2-C3	5.12	115.96	109.67
2	a	4	MAN	C1-C2-C3	-5.02	103.50	109.67
7	T	1	NAG	O5-C1-C2	-5.00	103.40	111.29
2	M	4	MAN	C3-C4-C5	4.93	119.03	110.24
3	H	1	NAG	C2-N2-C7	4.91	129.90	122.90
5	L	1	NAG	C1-O5-C5	4.89	118.81	112.19
4	Q	1	NAG	C2-N2-C7	4.82	129.77	122.90
2	O	1	NAG	C1-O5-C5	4.78	118.67	112.19
2	O	4	MAN	C1-C2-C3	-4.77	103.81	109.67
2	d	5	MAN	C1-O5-C5	4.75	118.63	112.19
2	S	3	BMA	O5-C5-C6	4.73	114.61	107.20
3	Z	1	NAG	C2-N2-C7	4.62	129.48	122.90
2	i	4	MAN	C1-O5-C5	4.59	118.42	112.19
4	I	1	NAG	O5-C1-C2	-4.59	104.04	111.29
3	Z	3	BMA	O3-C3-C2	4.59	118.79	109.99
5	K	1	NAG	C2-N2-C7	4.55	129.38	122.90
4	I	1	NAG	C4-C3-C2	4.54	117.67	111.02
6	R	1	NAG	O5-C1-C2	-4.54	104.13	111.29
7	T	7	MAN	O5-C1-C2	-4.51	103.82	110.77
3	j	6	MAN	C1-O5-C5	4.49	118.27	112.19
7	T	4	MAN	C1-O5-C5	4.47	118.25	112.19
4	b	1	NAG	C2-N2-C7	4.47	129.27	122.90
2	J	4	MAN	C1-C2-C3	-4.45	104.20	109.67
7	T	3	BMA	O3-C3-C2	4.39	118.40	109.99
5	X	1	NAG	O5-C1-C2	-4.37	104.38	111.29
3	j	4	MAN	C1-O5-C5	4.37	118.11	112.19
3	H	3	BMA	O3-C3-C2	4.35	118.32	109.99
5	W	2	NAG	O7-C7-N2	-4.35	113.95	121.95
2	G	3	BMA	C3-C4-C5	4.35	117.99	110.24
2	J	1	NAG	C1-O5-C5	4.31	118.03	112.19
2	U	4	MAN	C1-C2-C3	-4.20	104.50	109.67
2	M	4	MAN	O5-C1-C2	4.17	117.20	110.77
3	H	1	NAG	O5-C1-C2	-4.16	104.72	111.29
4	V	2	NAG	C4-C3-C2	4.14	117.09	111.02
2	U	5	MAN	C1-O5-C5	4.12	117.78	112.19
2	f	5	MAN	C1-O5-C5	4.11	117.76	112.19
5	h	1	NAG	C1-O5-C5	4.10	117.75	112.19
2	a	1	NAG	C1-O5-C5	4.10	117.75	112.19
3	j	1	NAG	O5-C1-C2	-4.07	104.86	111.29
2	J	3	BMA	C1-C2-C3	4.06	114.66	109.67
7	T	7	MAN	C3-C4-C5	4.04	117.45	110.24
6	R	4	MAN	C1-C2-C3	4.03	114.62	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	5	MAN	C1-O5-C5	4.01	117.63	112.19
5	h	3	BMA	C1-C2-C3	4.00	114.58	109.67
2	G	4	MAN	C1-O5-C5	3.98	117.59	112.19
5	K	1	NAG	C1-C2-N2	3.97	117.28	110.49
2	f	4	MAN	C1-O5-C5	3.97	117.57	112.19
3	H	6	MAN	O5-C1-C2	-3.92	104.71	110.77
5	W	3	BMA	C1-C2-C3	3.91	114.48	109.67
2	G	3	BMA	C1-C2-C3	3.89	114.45	109.67
2	k	1	NAG	C1-O5-C5	3.88	117.45	112.19
3	N	1	NAG	O5-C1-C2	-3.85	105.21	111.29
3	j	6	MAN	C1-C2-C3	3.85	114.40	109.67
7	e	6	MAN	C3-C4-C5	3.85	117.10	110.24
2	i	4	MAN	C3-C4-C5	3.85	117.10	110.24
2	J	1	NAG	O5-C5-C6	3.83	113.20	107.20
2	O	3	BMA	O3-C3-C2	-3.80	102.71	109.99
3	j	2	NAG	C4-C3-C2	3.78	116.56	111.02
5	h	3	BMA	C3-C4-C5	3.75	116.93	110.24
3	N	3	BMA	O3-C3-C2	3.71	117.10	109.99
3	N	4	MAN	C3-C4-C5	3.69	116.81	110.24
5	c	1	NAG	O5-C1-C2	-3.67	105.50	111.29
2	i	2	NAG	C1-O5-C5	3.63	117.11	112.19
4	I	2	NAG	C2-N2-C7	3.60	128.03	122.90
3	N	5	MAN	C1-O5-C5	3.56	117.01	112.19
3	H	3	BMA	O3-C3-C4	3.55	118.56	110.35
5	W	3	BMA	O6-C6-C5	-3.55	99.13	111.29
4	Q	1	NAG	O5-C1-C2	-3.52	105.73	111.29
2	Y	4	MAN	C3-C4-C5	3.46	116.42	110.24
7	T	3	BMA	C1-O5-C5	3.46	116.89	112.19
5	X	2	NAG	C1-O5-C5	3.44	116.85	112.19
3	H	6	MAN	C3-C4-C5	3.42	116.34	110.24
5	K	1	NAG	O5-C1-C2	-3.39	105.94	111.29
5	h	3	BMA	C2-C3-C4	3.38	116.75	110.89
6	R	4	MAN	O5-C5-C6	3.38	112.50	107.20
2	Y	3	BMA	O5-C5-C6	3.35	112.45	107.20
2	S	2	NAG	O4-C4-C3	-3.33	102.65	110.35
2	M	5	MAN	C1-O5-C5	3.32	116.69	112.19
7	e	4	MAN	C1-O5-C5	3.31	116.68	112.19
2	d	3	BMA	C2-C3-C4	3.30	116.61	110.89
5	K	3	BMA	C1-C2-C3	3.30	113.72	109.67
2	O	1	NAG	O5-C5-C6	3.29	112.37	107.20
2	O	1	NAG	C2-N2-C7	-3.22	118.31	122.90
2	S	4	MAN	C3-C4-C5	3.22	115.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	f	1	NAG	C4-C3-C2	3.22	115.74	111.02
2	S	5	MAN	C1-C2-C3	-3.22	105.71	109.67
2	k	3	BMA	C3-C4-C5	3.21	115.97	110.24
4	V	1	NAG	C1-O5-C5	3.20	116.53	112.19
3	H	3	BMA	C3-C4-C5	-3.20	104.53	110.24
2	O	4	MAN	C1-O5-C5	3.17	116.49	112.19
3	Z	4	MAN	C1-O5-C5	3.17	116.49	112.19
2	G	5	MAN	O5-C5-C6	3.16	112.16	107.20
3	Z	1	NAG	C1-O5-C5	3.16	116.47	112.19
2	U	5	MAN	C3-C4-C5	3.16	115.87	110.24
2	a	5	MAN	C3-C4-C5	3.14	115.84	110.24
5	l	2	NAG	C1-O5-C5	3.14	116.44	112.19
5	X	1	NAG	C8-C7-N2	3.12	121.38	116.10
2	J	2	NAG	C8-C7-N2	3.12	121.38	116.10
7	e	3	BMA	C1-C2-C3	-3.11	105.85	109.67
2	M	5	MAN	O5-C5-C6	3.10	112.07	107.20
4	I	1	NAG	C2-N2-C7	3.08	127.29	122.90
2	O	5	MAN	C3-C4-C5	3.07	115.72	110.24
2	M	2	NAG	C1-O5-C5	3.05	116.33	112.19
2	O	4	MAN	C3-C4-C5	3.05	115.68	110.24
2	J	4	MAN	O2-C2-C1	3.05	115.39	109.15
7	e	4	MAN	C1-C2-C3	3.04	113.40	109.67
2	i	3	BMA	C1-C2-C3	3.04	113.40	109.67
7	e	3	BMA	O3-C3-C2	3.03	115.79	109.99
3	H	5	MAN	C1-O5-C5	3.03	116.29	112.19
2	d	3	BMA	C3-C4-C5	3.02	115.63	110.24
3	j	2	NAG	C2-N2-C7	3.02	127.20	122.90
2	Y	2	NAG	C1-O5-C5	3.00	116.26	112.19
3	Z	6	MAN	C2-C3-C4	3.00	116.08	110.89
2	O	5	MAN	C1-C2-C3	3.00	113.35	109.67
2	Y	3	BMA	C1-C2-C3	2.97	113.32	109.67
5	L	1	NAG	C3-C4-C5	-2.97	104.95	110.24
4	b	1	NAG	C1-C2-N2	2.96	115.55	110.49
2	G	1	NAG	C1-O5-C5	2.94	116.18	112.19
2	O	3	BMA	O5-C5-C6	2.94	111.81	107.20
7	T	1	NAG	C2-N2-C7	2.94	127.09	122.90
2	d	3	BMA	O5-C5-C6	2.94	111.81	107.20
2	k	4	MAN	O5-C5-C6	2.93	111.79	107.20
2	k	5	MAN	C1-C2-C3	2.92	113.25	109.67
2	S	2	NAG	C2-N2-C7	-2.91	118.76	122.90
4	g	2	NAG	C4-C3-C2	2.90	115.27	111.02
4	Q	2	NAG	C1-O5-C5	2.90	116.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	W	2	NAG	O7-C7-C8	2.89	127.42	122.06
2	J	2	NAG	O5-C1-C2	-2.88	106.75	111.29
3	H	6	MAN	C1-O5-C5	2.87	116.08	112.19
2	U	3	BMA	C1-C2-C3	2.87	113.19	109.67
3	Z	3	BMA	C3-C4-C5	-2.85	105.15	110.24
2	M	4	MAN	O5-C5-C4	2.84	117.74	110.83
7	e	6	MAN	C1-O5-C5	2.84	116.04	112.19
2	O	4	MAN	O2-C2-C1	2.83	114.93	109.15
2	a	3	BMA	O3-C3-C2	-2.83	104.58	109.99
7	e	2	NAG	C1-O5-C5	2.82	116.02	112.19
5	X	1	NAG	C3-C4-C5	-2.82	105.22	110.24
2	U	4	MAN	O5-C5-C6	2.81	111.61	107.20
7	T	3	BMA	O3-C3-C4	2.80	116.82	110.35
2	U	1	NAG	C2-N2-C7	-2.80	118.92	122.90
7	e	5	MAN	C1-O5-C5	2.80	115.98	112.19
5	l	2	NAG	O5-C1-C2	-2.78	106.90	111.29
2	k	1	NAG	O5-C5-C6	2.77	111.55	107.20
3	H	4	MAN	C1-O5-C5	2.76	115.94	112.19
5	h	3	BMA	O5-C5-C6	2.76	111.53	107.20
6	R	3	BMA	O5-C5-C6	2.76	111.53	107.20
7	T	1	NAG	C4-C3-C2	2.76	115.06	111.02
5	h	1	NAG	C2-N2-C7	2.75	126.82	122.90
2	S	5	MAN	O5-C5-C6	2.74	111.50	107.20
3	j	5	MAN	C1-O5-C5	2.71	115.86	112.19
2	k	2	NAG	C4-C3-C2	2.70	114.97	111.02
5	h	2	NAG	C4-C3-C2	2.70	114.97	111.02
2	a	3	BMA	O3-C3-C4	2.69	116.57	110.35
2	i	3	BMA	C1-O5-C5	2.69	115.83	112.19
7	T	1	NAG	C3-C4-C5	-2.69	105.45	110.24
3	Z	3	BMA	O3-C3-C4	2.68	116.55	110.35
2	J	3	BMA	O3-C3-C2	-2.68	104.86	109.99
2	U	2	NAG	C1-C2-N2	2.66	115.03	110.49
2	U	3	BMA	O3-C3-C2	-2.65	104.92	109.99
2	S	5	MAN	O5-C1-C2	-2.65	106.68	110.77
2	G	3	BMA	O5-C5-C6	2.64	111.34	107.20
6	R	4	MAN	C3-C4-C5	2.64	114.95	110.24
4	I	1	NAG	C8-C7-N2	2.64	120.56	116.10
7	T	1	NAG	C6-C5-C4	2.63	119.15	113.00
2	i	3	BMA	C3-C4-C5	2.61	114.89	110.24
5	l	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	b	1	NAG	O5-C1-C2	-2.60	107.18	111.29
5	L	1	NAG	O5-C1-C2	-2.60	107.18	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	2	NAG	C1-O5-C5	2.60	115.72	112.19
2	M	4	MAN	C2-C3-C4	2.60	115.39	110.89
5	l	2	NAG	C2-N2-C7	-2.59	119.21	122.90
3	Z	6	MAN	C1-O5-C5	2.59	115.70	112.19
2	d	1	NAG	O5-C1-C2	-2.58	107.21	111.29
3	Z	5	MAN	C1-O5-C5	2.58	115.69	112.19
2	O	2	NAG	C4-C3-C2	2.57	114.78	111.02
4	Q	1	NAG	C1-O5-C5	2.55	115.64	112.19
7	T	7	MAN	O5-C5-C6	2.54	111.19	107.20
2	G	2	NAG	C1-O5-C5	2.54	115.64	112.19
2	J	4	MAN	O5-C5-C6	2.54	111.19	107.20
5	h	1	NAG	C8-C7-N2	2.53	120.38	116.10
6	R	3	BMA	C1-C2-C3	2.52	112.76	109.67
2	O	2	NAG	O7-C7-N2	2.52	126.58	121.95
3	Z	3	BMA	C1-O5-C5	2.51	115.59	112.19
2	M	5	MAN	C2-C3-C4	-2.50	106.57	110.89
6	R	2	NAG	O4-C4-C3	-2.50	104.58	110.35
2	O	3	BMA	O3-C3-C4	2.49	116.11	110.35
7	T	2	NAG	O5-C5-C6	2.48	111.09	107.20
5	X	3	BMA	O5-C5-C6	2.47	111.08	107.20
5	W	3	BMA	C2-C3-C4	2.47	115.16	110.89
5	X	1	NAG	O7-C7-C8	-2.45	117.50	122.06
2	G	1	NAG	C6-C5-C4	-2.44	107.28	113.00
4	I	2	NAG	O5-C5-C6	2.44	111.03	107.20
2	J	3	BMA	O5-C5-C6	2.44	111.02	107.20
3	j	1	NAG	C8-C7-N2	2.43	120.22	116.10
2	f	1	NAG	C3-C4-C5	2.42	114.56	110.24
2	i	4	MAN	O5-C5-C6	2.42	111.00	107.20
2	S	4	MAN	C1-C2-C3	-2.42	106.69	109.67
2	S	1	NAG	O7-C7-C8	-2.42	117.57	122.06
7	e	3	BMA	O3-C3-C4	2.41	115.92	110.35
3	j	1	NAG	C2-N2-C7	2.41	126.33	122.90
3	j	3	BMA	C1-C2-C3	2.40	112.61	109.67
2	a	2	NAG	O5-C1-C2	-2.38	107.52	111.29
2	S	1	NAG	O5-C1-C2	-2.38	107.53	111.29
7	e	4	MAN	O5-C5-C6	2.38	110.93	107.20
2	U	4	MAN	O2-C2-C1	2.38	114.01	109.15
3	H	1	NAG	C8-C7-N2	2.37	120.12	116.10
2	Y	1	NAG	O5-C1-C2	-2.36	107.56	111.29
3	j	2	NAG	O5-C5-C6	2.35	110.89	107.20
7	T	1	NAG	C8-C7-N2	2.35	120.08	116.10
7	e	4	MAN	C3-C4-C5	2.35	114.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	l	2	NAG	C4-C3-C2	-2.34	107.59	111.02
4	V	2	NAG	C3-C4-C5	2.33	114.39	110.24
7	e	1	NAG	O5-C1-C2	-2.31	107.64	111.29
2	Y	5	MAN	C3-C4-C5	2.29	114.33	110.24
2	Y	4	MAN	O5-C5-C6	2.29	110.80	107.20
2	U	2	NAG	C1-O5-C5	2.29	115.30	112.19
2	U	2	NAG	O5-C1-C2	-2.29	107.67	111.29
2	S	1	NAG	C4-C3-C2	2.28	114.36	111.02
7	T	1	NAG	O5-C5-C4	-2.28	105.28	110.83
2	J	1	NAG	C1-C2-N2	2.27	114.36	110.49
5	X	1	NAG	C1-O5-C5	2.27	115.26	112.19
2	i	5	MAN	O5-C5-C6	2.26	110.75	107.20
5	c	1	NAG	C8-C7-N2	2.26	119.93	116.10
2	M	4	MAN	O5-C5-C6	2.26	110.75	107.20
2	S	3	BMA	O5-C1-C2	2.26	114.26	110.77
4	P	2	NAG	C3-C4-C5	2.26	114.27	110.24
2	S	2	NAG	C1-O5-C5	2.25	115.25	112.19
5	W	3	BMA	C1-O5-C5	2.24	115.23	112.19
6	R	2	NAG	C1-O5-C5	-2.24	109.16	112.19
2	G	2	NAG	O5-C1-C2	-2.24	107.75	111.29
2	a	4	MAN	O5-C5-C6	2.23	110.70	107.20
3	N	6	MAN	C1-O5-C5	2.23	115.21	112.19
3	Z	2	NAG	C1-O5-C5	2.22	115.21	112.19
2	O	5	MAN	O5-C5-C4	2.21	116.21	110.83
2	Y	2	NAG	O4-C4-C3	-2.21	105.25	110.35
3	N	3	BMA	O3-C3-C4	2.21	115.45	110.35
2	f	1	NAG	C1-C2-N2	-2.20	106.72	110.49
4	g	1	NAG	C2-N2-C7	2.20	126.04	122.90
2	f	5	MAN	O5-C5-C6	2.20	110.65	107.20
2	a	4	MAN	O2-C2-C1	2.19	113.63	109.15
2	i	4	MAN	O5-C5-C4	2.19	116.14	110.83
2	M	3	BMA	C1-O5-C5	2.18	115.15	112.19
3	N	1	NAG	C2-N2-C7	2.18	126.01	122.90
3	Z	1	NAG	O5-C1-C2	-2.17	107.86	111.29
5	X	2	NAG	O5-C1-C2	-2.17	107.86	111.29
7	T	7	MAN	C2-C3-C4	2.17	114.65	110.89
2	S	4	MAN	O5-C1-C2	-2.17	107.42	110.77
7	T	6	MAN	O2-C2-C1	2.17	113.58	109.15
2	f	3	BMA	O3-C3-C2	-2.15	105.87	109.99
2	a	4	MAN	O5-C1-C2	-2.15	107.45	110.77
2	k	2	NAG	C2-N2-C7	2.15	125.97	122.90
4	I	1	NAG	O4-C4-C3	-2.15	105.38	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	4	MAN	O5-C5-C6	2.14	110.56	107.20
2	f	5	MAN	C1-C2-C3	2.14	112.30	109.67
2	O	4	MAN	O3-C3-C2	-2.14	105.90	109.99
5	L	1	NAG	O7-C7-C8	-2.13	118.09	122.06
6	R	2	NAG	O5-C5-C6	2.13	110.55	107.20
5	h	1	NAG	O7-C7-C8	-2.13	118.11	122.06
2	S	3	BMA	O3-C3-C2	-2.13	105.92	109.99
2	O	3	BMA	C3-C4-C5	2.12	114.03	110.24
2	a	2	NAG	C3-C4-C5	2.12	114.02	110.24
3	j	3	BMA	C1-O5-C5	2.12	115.06	112.19
5	L	2	NAG	O5-C1-C2	-2.11	107.96	111.29
3	j	4	MAN	C3-C4-C5	2.11	114.00	110.24
2	f	4	MAN	C1-C2-C3	-2.11	107.08	109.67
5	c	3	BMA	C1-C2-C3	2.09	112.24	109.67
3	H	1	NAG	C3-C4-C5	-2.09	106.50	110.24
2	Y	3	BMA	O3-C3-C2	-2.09	105.99	109.99
5	K	2	NAG	O5-C5-C6	2.09	110.48	107.20
7	e	2	NAG	C3-C4-C5	2.09	113.97	110.24
2	M	4	MAN	C1-C2-C3	2.09	112.23	109.67
2	J	1	NAG	C2-N2-C7	-2.07	119.96	122.90
4	g	1	NAG	C1-C2-N2	2.07	114.02	110.49
3	N	6	MAN	O5-C1-C2	-2.07	107.58	110.77
2	U	2	NAG	C2-N2-C7	2.06	125.84	122.90
5	h	3	BMA	O5-C1-C2	-2.06	107.59	110.77
2	a	1	NAG	O5-C5-C6	2.06	110.43	107.20
2	S	5	MAN	O2-C2-C1	2.06	113.36	109.15
2	O	3	BMA	C1-C2-C3	2.05	112.19	109.67
4	I	2	NAG	C4-C3-C2	2.05	114.02	111.02
2	S	1	NAG	O4-C4-C3	-2.04	105.63	110.35
3	Z	6	MAN	O5-C1-C2	2.04	113.92	110.77
3	N	1	NAG	C8-C7-N2	2.04	119.56	116.10
7	T	6	MAN	C1-C2-C3	-2.04	107.16	109.67
2	f	4	MAN	O5-C5-C6	2.03	110.39	107.20
5	c	3	BMA	C1-O5-C5	2.03	114.95	112.19
6	R	4	MAN	O5-C1-C2	2.03	113.91	110.77
2	G	1	NAG	O5-C1-C2	-2.03	108.08	111.29
3	N	1	NAG	C1-O5-C5	2.02	114.93	112.19
2	M	3	BMA	O5-C1-C2	-2.02	107.65	110.77
5	W	2	NAG	C1-O5-C5	2.01	114.92	112.19
2	Y	2	NAG	C4-C3-C2	2.01	113.96	111.02
5	K	1	NAG	C3-C4-C5	2.01	113.82	110.24
3	N	3	BMA	O5-C1-C2	-2.00	107.68	110.77

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	T	1	NAG	C1
5	L	1	NAG	C1
3	N	1	NAG	C1
2	a	1	NAG	C1
5	h	1	NAG	C1
7	e	1	NAG	C1
4	b	1	NAG	C1
2	f	1	NAG	C1
3	Z	1	NAG	C1
5	l	1	NAG	C1
6	R	1	NAG	C1
3	H	1	NAG	C1
3	j	1	NAG	C1
5	X	1	NAG	C1
5	c	1	NAG	C1

All (247) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	k	2	NAG	C3-C2-N2-C7
2	k	2	NAG	C8-C7-N2-C2
2	k	2	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	W	2	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
2	k	1	NAG	C8-C7-N2-C2
2	k	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
2	J	4	MAN	C4-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	U	4	MAN	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6
3	Z	6	MAN	O5-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
2	U	4	MAN	C4-C5-C6-O6
2	d	4	MAN	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
7	e	4	MAN	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
2	a	5	MAN	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
2	S	3	BMA	O5-C5-C6-O6
2	d	5	MAN	O5-C5-C6-O6
5	h	3	BMA	O5-C5-C6-O6
2	Y	4	MAN	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
7	T	7	MAN	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
3	j	3	BMA	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
3	N	6	MAN	O5-C5-C6-O6
2	f	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	k	4	MAN	O5-C5-C6-O6
2	d	5	MAN	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
3	Z	6	MAN	C4-C5-C6-O6
7	T	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
7	T	6	MAN	O5-C5-C6-O6
7	e	6	MAN	O5-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C1-C2-N2-C7
2	J	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	j	3	BMA	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
2	d	3	BMA	C4-C5-C6-O6
3	N	6	MAN	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
2	i	4	MAN	O5-C5-C6-O6
5	l	3	BMA	C4-C5-C6-O6
2	Y	4	MAN	C4-C5-C6-O6
2	S	3	BMA	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
7	T	1	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	Y	3	BMA	C4-C5-C6-O6
2	d	4	MAN	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
2	U	5	MAN	C4-C5-C6-O6
2	O	5	MAN	C4-C5-C6-O6
3	j	4	MAN	C4-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
3	Z	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	e	7	MAN	O5-C5-C6-O6
2	k	4	MAN	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
7	T	6	MAN	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
3	j	6	MAN	O5-C5-C6-O6
2	a	4	MAN	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
2	f	5	MAN	O5-C5-C6-O6
2	f	3	BMA	C4-C5-C6-O6
3	j	4	MAN	O5-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
7	e	4	MAN	C4-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
5	h	3	BMA	C4-C5-C6-O6
2	U	3	BMA	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
2	a	5	MAN	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
4	g	1	NAG	C1-C2-N2-C7
4	P	2	NAG	C8-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
2	i	2	NAG	C8-C7-N2-C2
5	l	3	BMA	O5-C5-C6-O6
2	M	4	MAN	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
3	Z	5	MAN	O5-C5-C6-O6
7	T	7	MAN	C4-C5-C6-O6
2	O	4	MAN	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	S	5	MAN	O5-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	M	5	MAN	O5-C5-C6-O6
2	Y	5	MAN	O5-C5-C6-O6
4	P	2	NAG	O7-C7-N2-C2
2	J	5	MAN	O5-C5-C6-O6
2	U	5	MAN	O5-C5-C6-O6
5	W	1	NAG	O7-C7-N2-C2
7	e	2	NAG	O5-C5-C6-O6
5	l	1	NAG	C8-C7-N2-C2
2	i	5	MAN	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
2	f	4	MAN	O5-C5-C6-O6
2	S	4	MAN	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
2	i	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C3-C2-N2-C7
5	c	2	NAG	C8-C7-N2-C2
2	f	3	BMA	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
5	l	1	NAG	O7-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
3	H	4	MAN	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
7	e	7	MAN	C4-C5-C6-O6
2	a	3	BMA	C4-C5-C6-O6
5	K	1	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
3	j	2	NAG	C3-C2-N2-C7
3	j	5	MAN	C4-C5-C6-O6
3	j	6	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	K	2	NAG	O7-C7-N2-C2
6	R	4	MAN	O5-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	O	4	MAN	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
7	e	6	MAN	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
2	U	3	BMA	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6

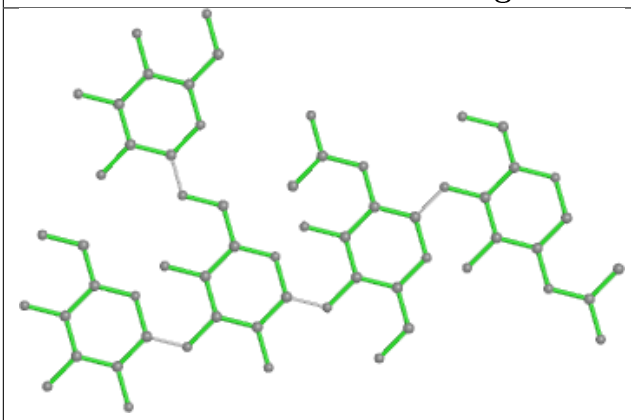
All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	5	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	f	4	MAN	C1-C2-C3-C4-C5-O5
2	i	5	MAN	C1-C2-C3-C4-C5-O5
2	M	5	MAN	C1-C2-C3-C4-C5-O5

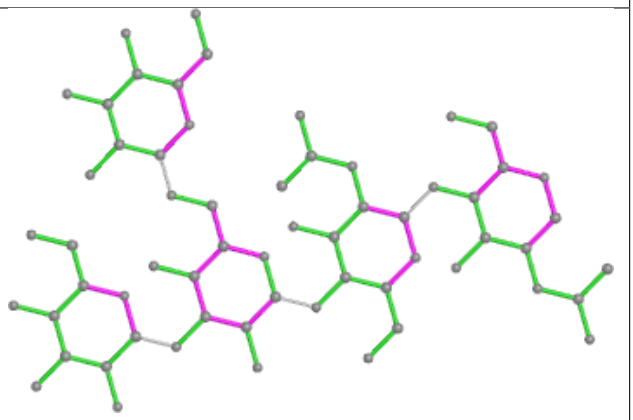
No monomer is involved in short contacts.

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

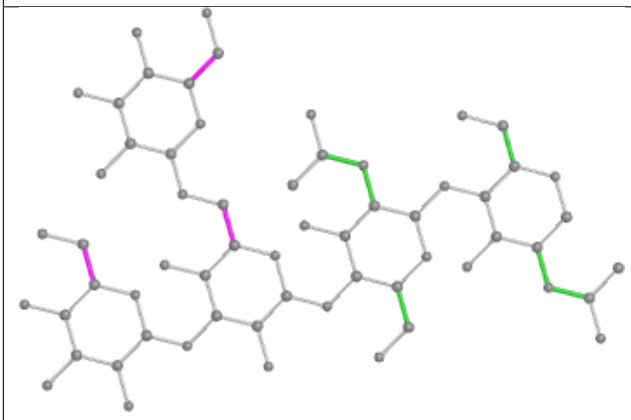
Oligosaccharide Chain G



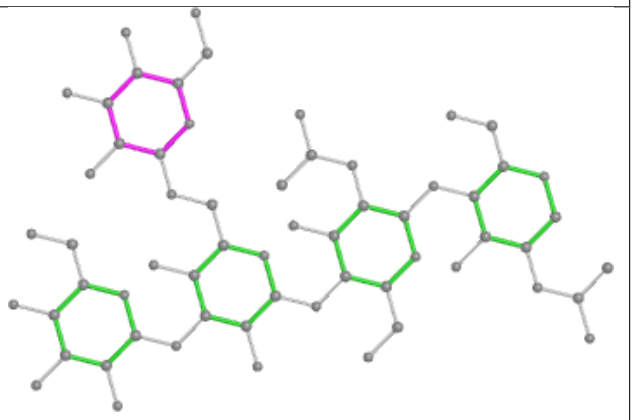
Bond lengths



Bond angles

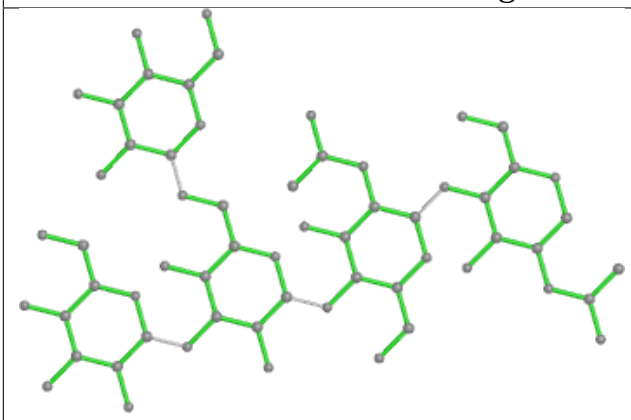


Torsions

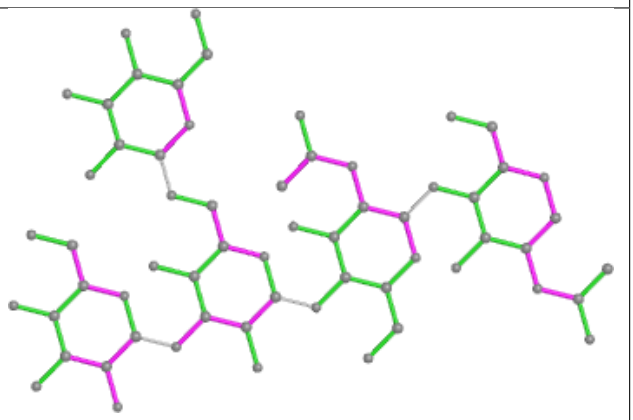


Rings

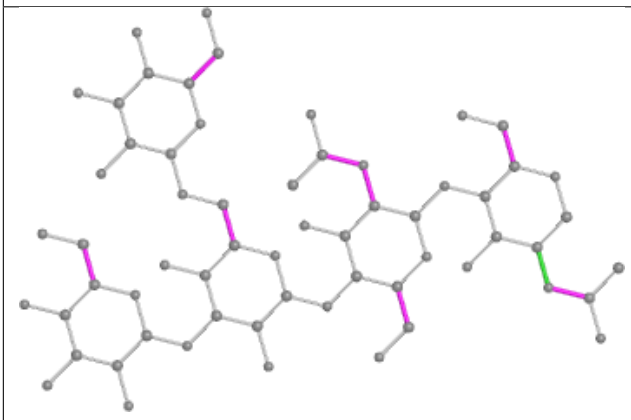
Oligosaccharide Chain J



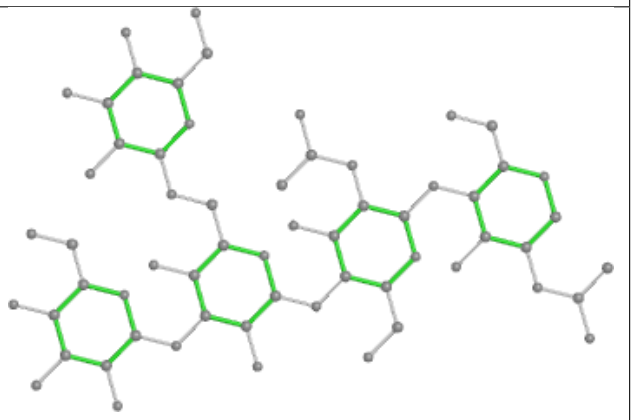
Bond lengths



Bond angles

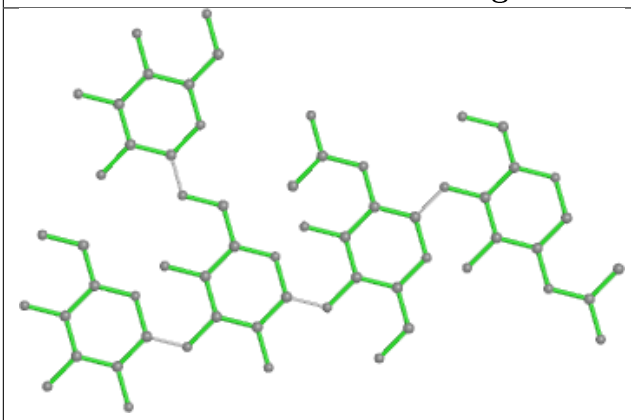


Torsions

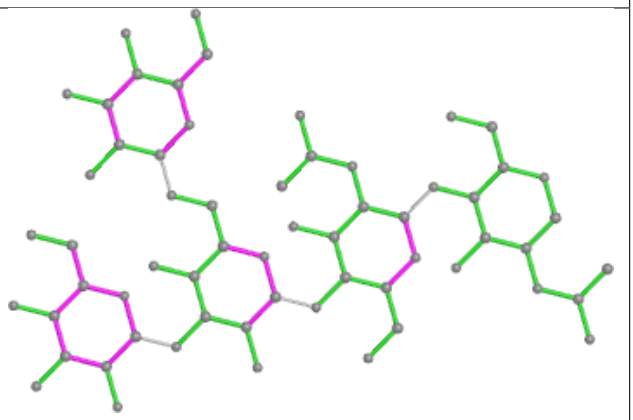


Rings

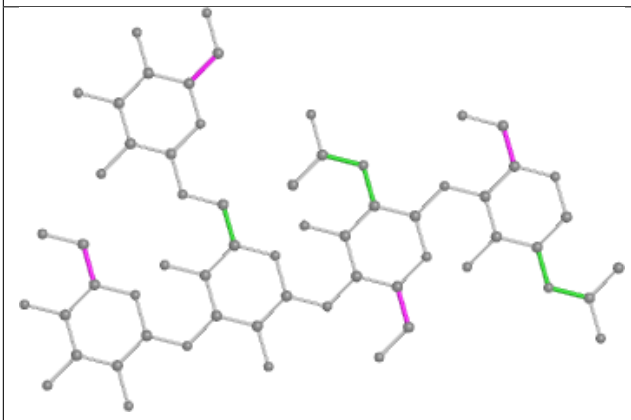
Oligosaccharide Chain M



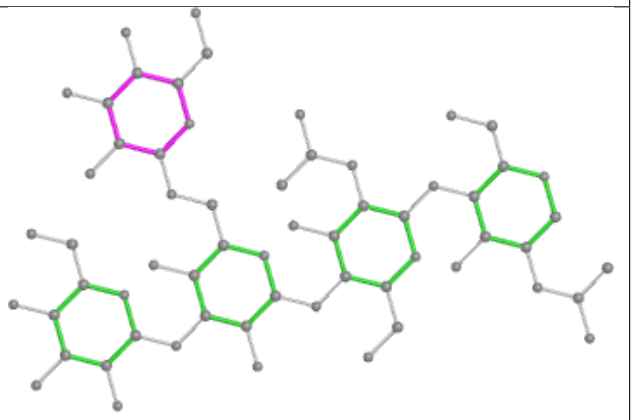
Bond lengths



Bond angles

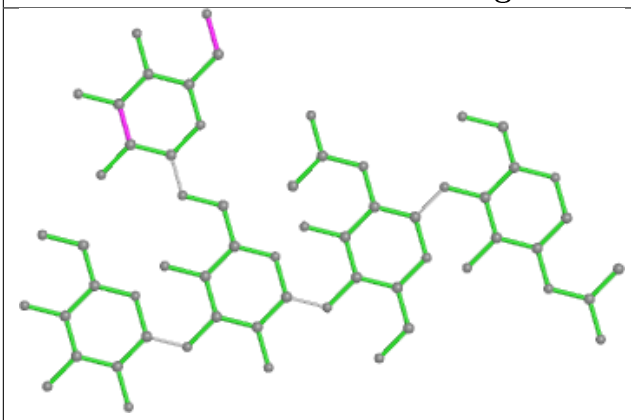


Torsions

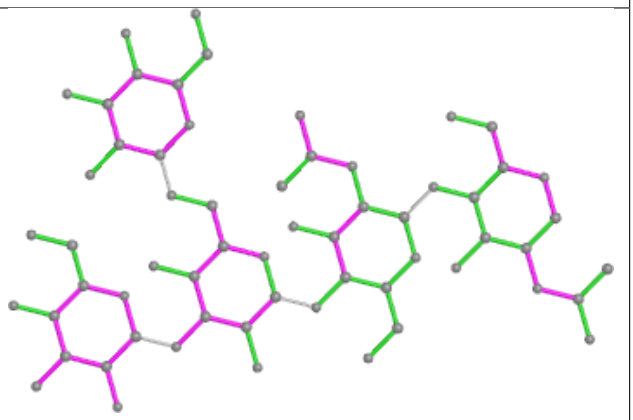


Rings

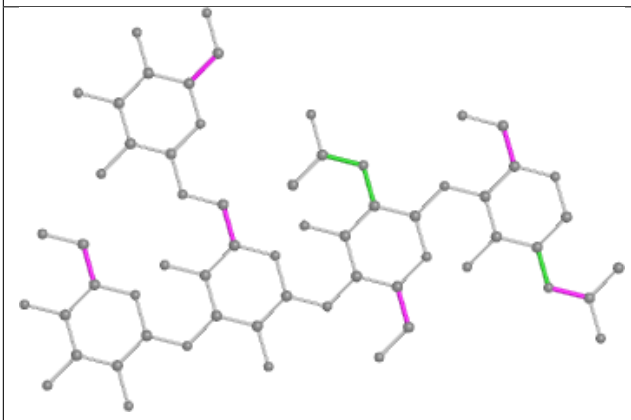
Oligosaccharide Chain O



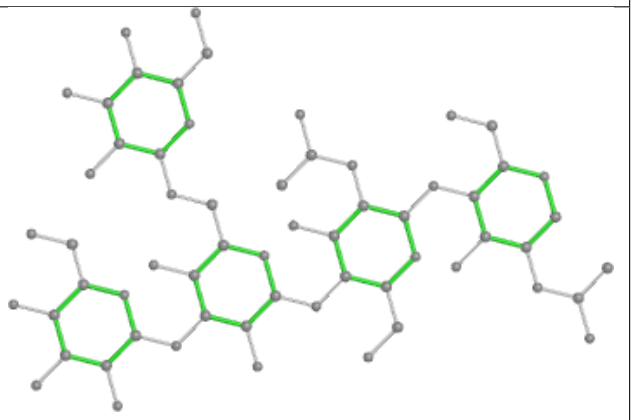
Bond lengths



Bond angles

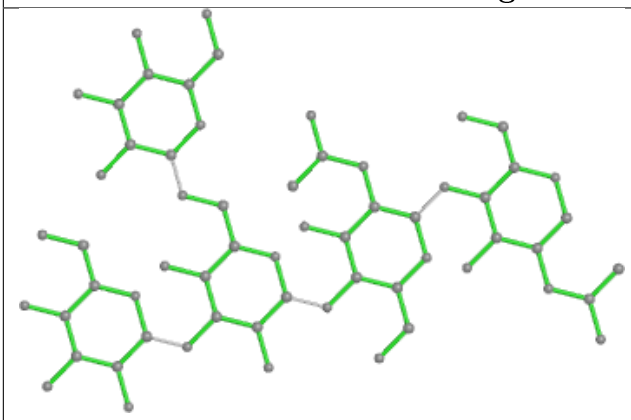


Torsions

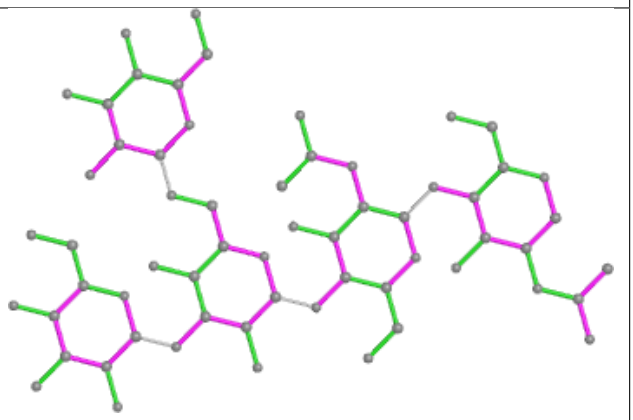


Rings

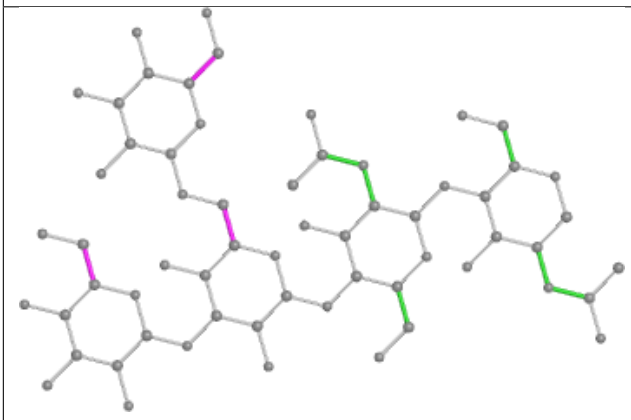
Oligosaccharide Chain S



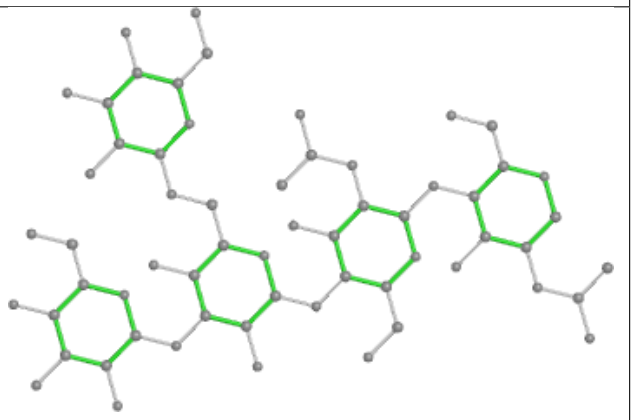
Bond lengths



Bond angles

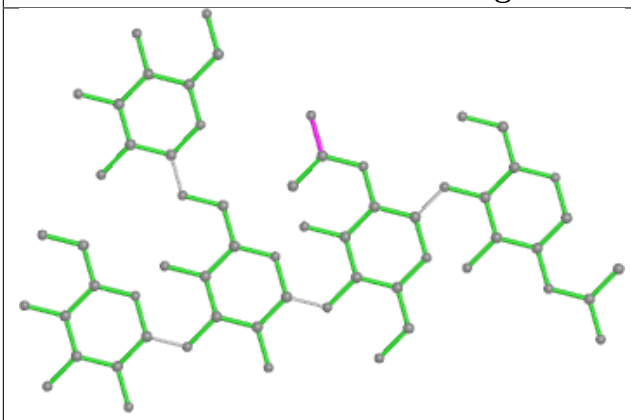


Torsions



Rings

Oligosaccharide Chain U



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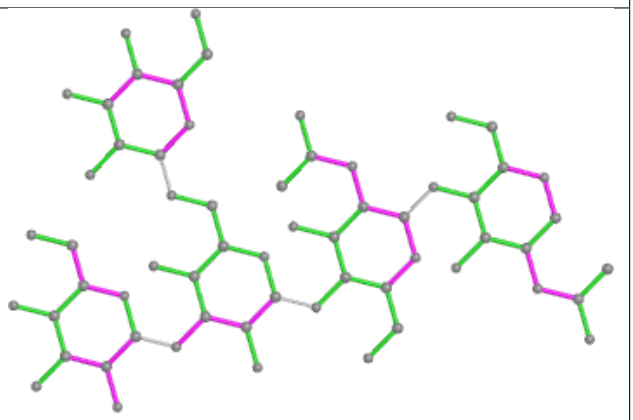
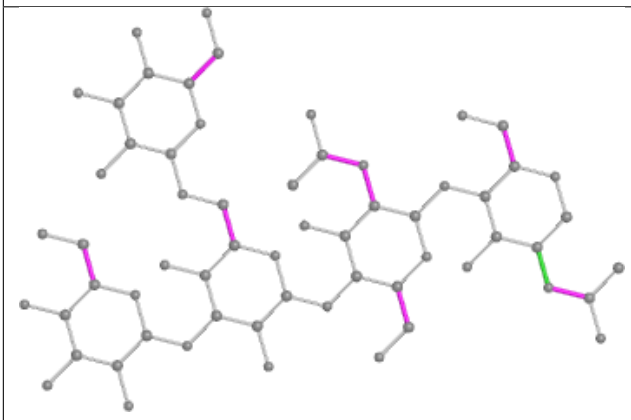


Bond angles



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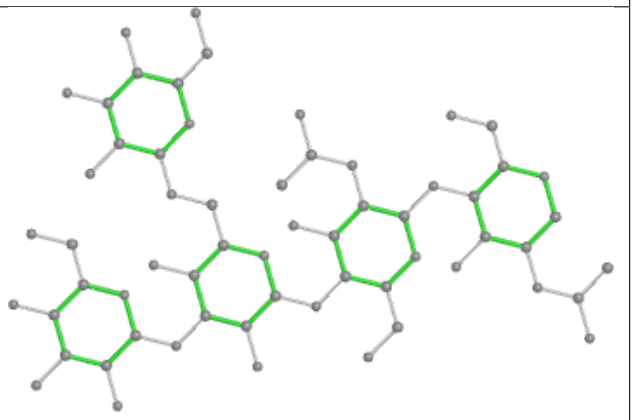
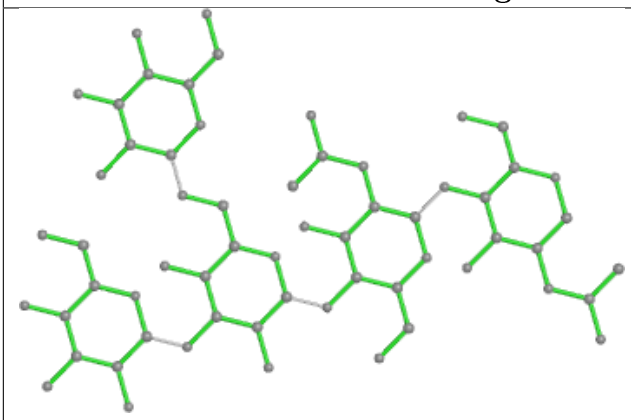


Rings

Oligosaccharide Chain Y



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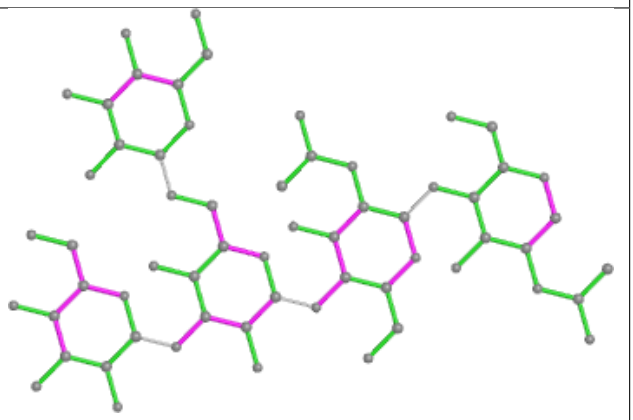
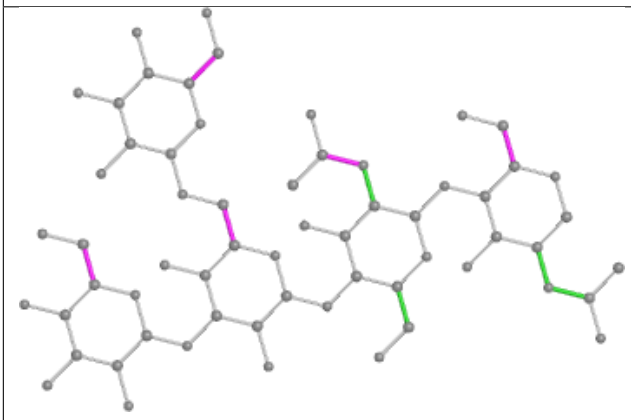
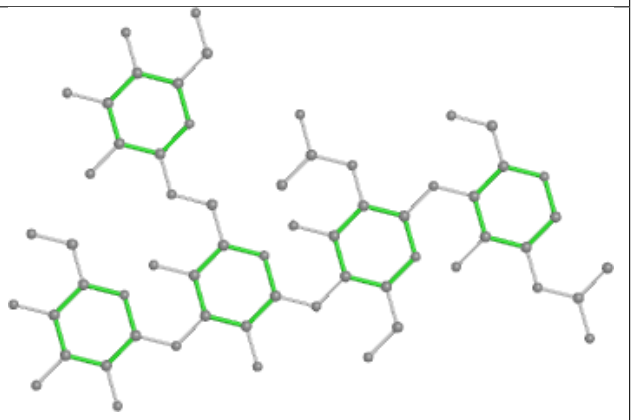


Bond angles

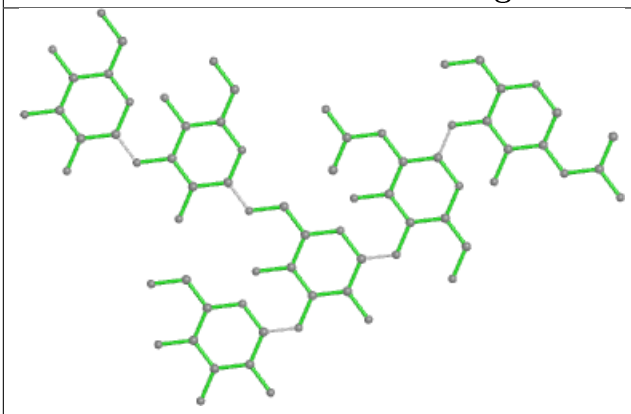


Torsions



Rings

Oligosaccharide Chain H



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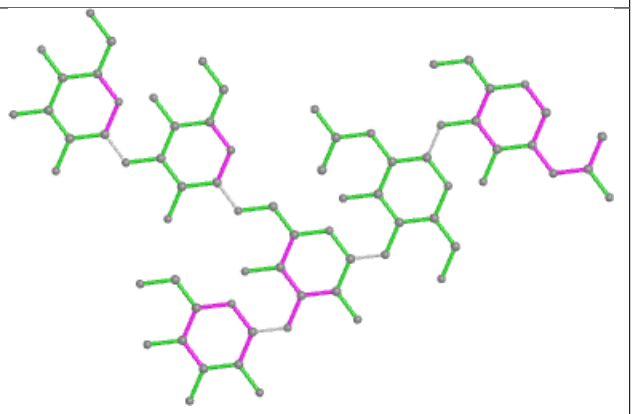
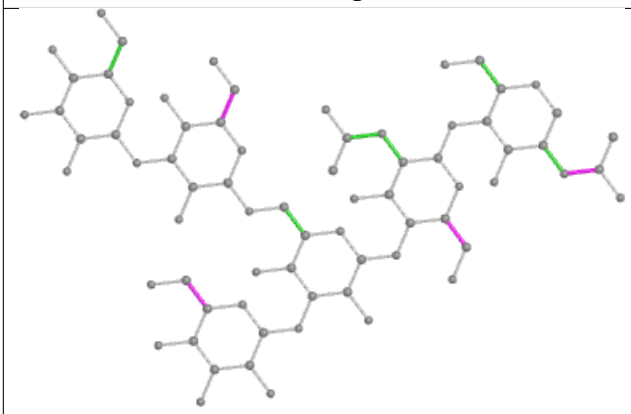


Bond angles



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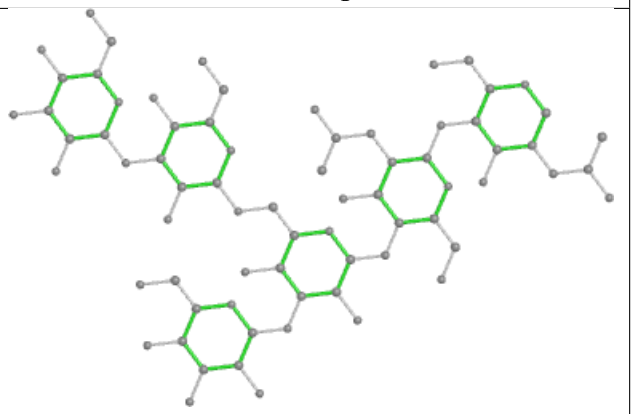
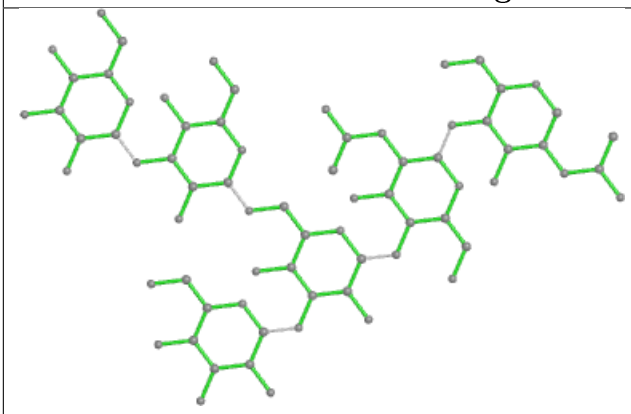


Rings

Oligosaccharide Chain N



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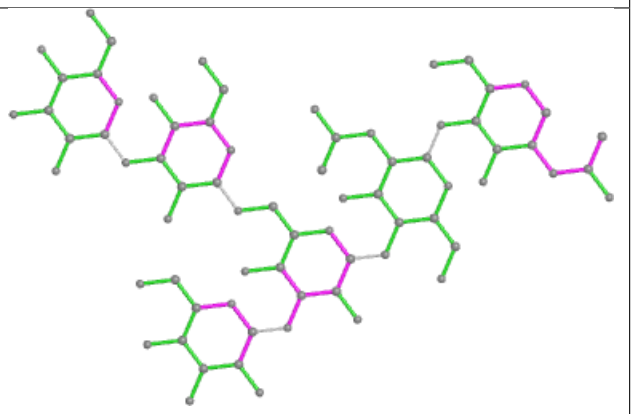
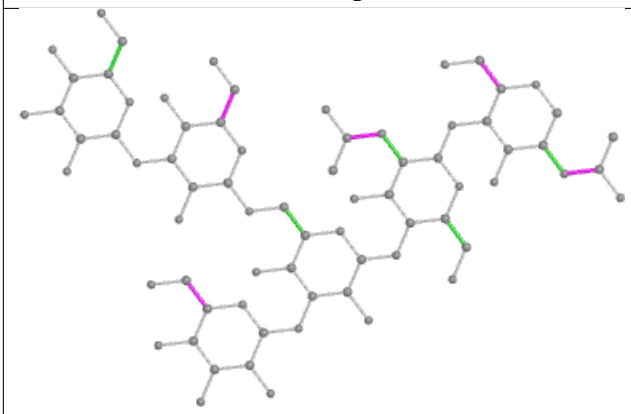


Bond angles



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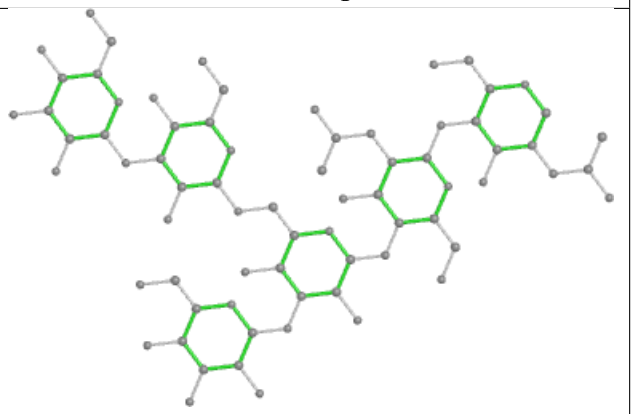
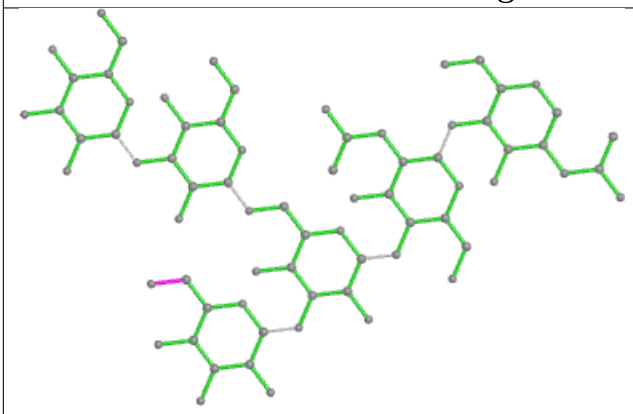


Rings

Oligosaccharide Chain Z



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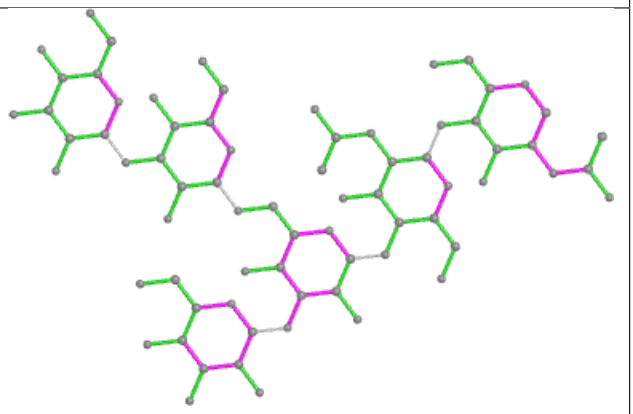
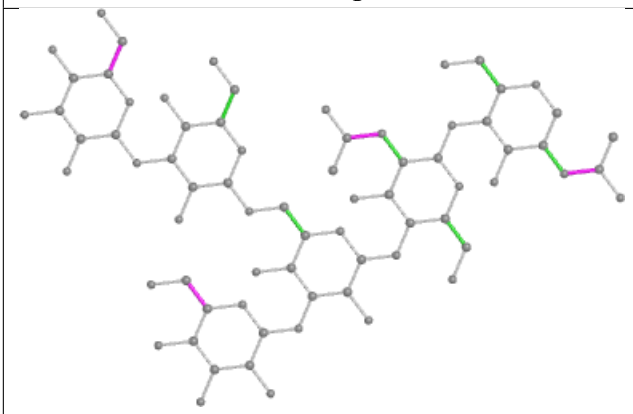


Bond angles



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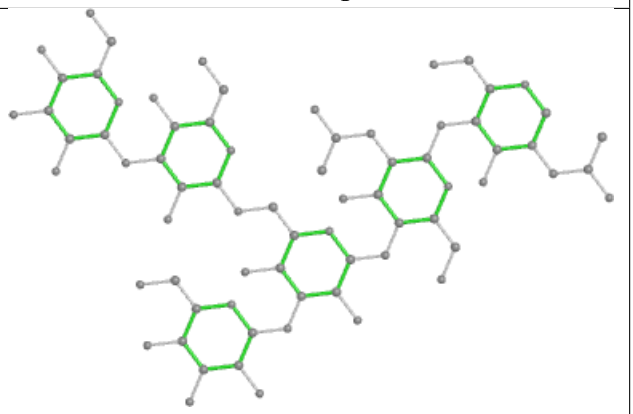
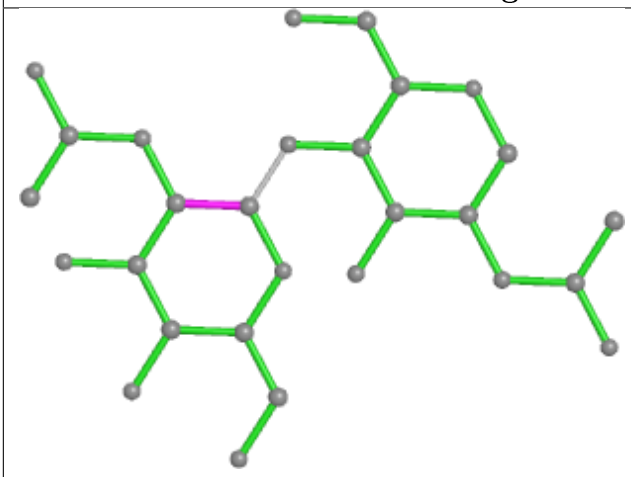


Rings

Oligosaccharide Chain I



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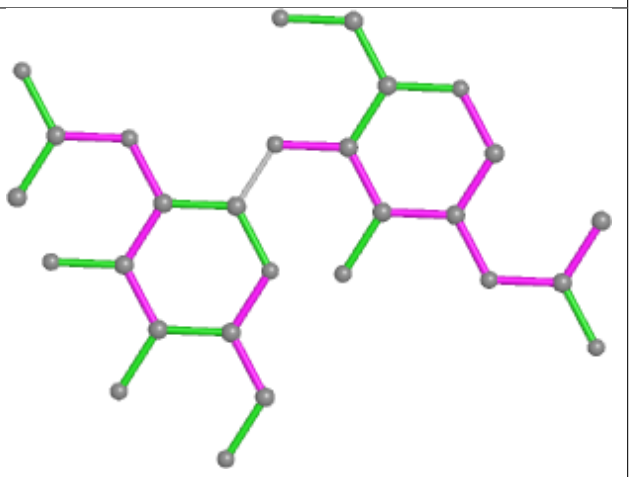
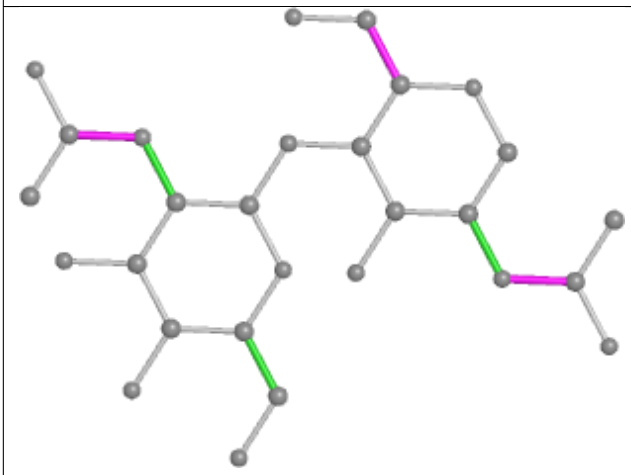


Bond angles



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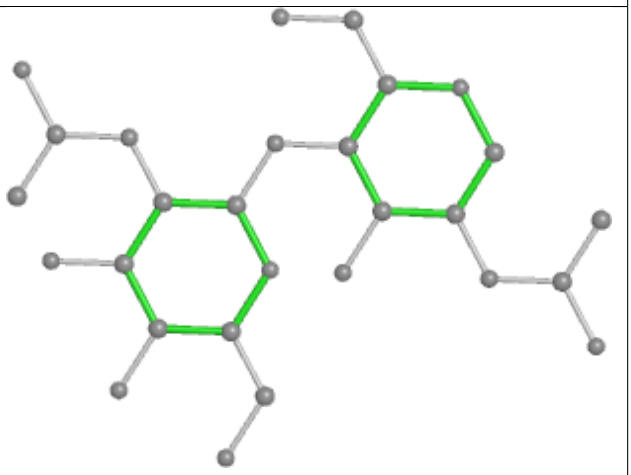
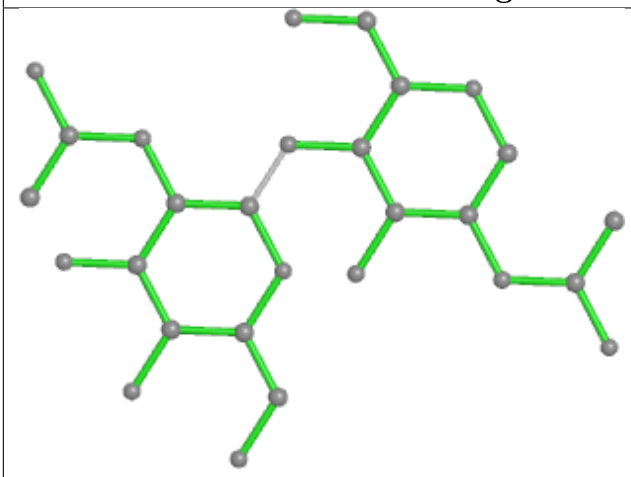


Rings

Oligosaccharide Chain P



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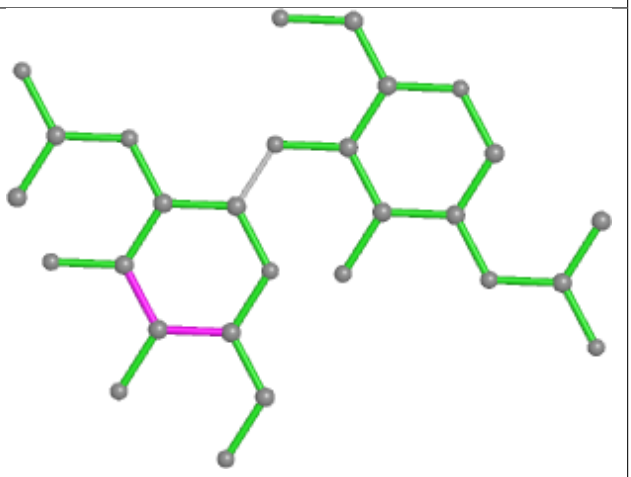

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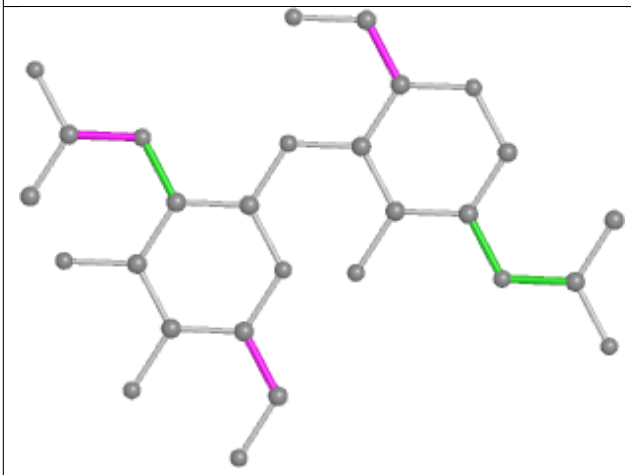

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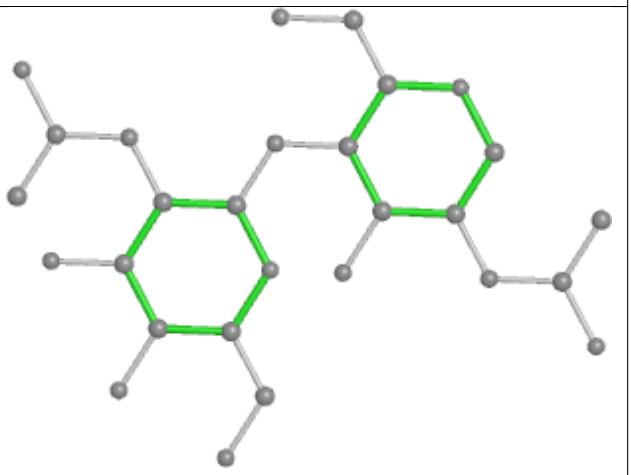
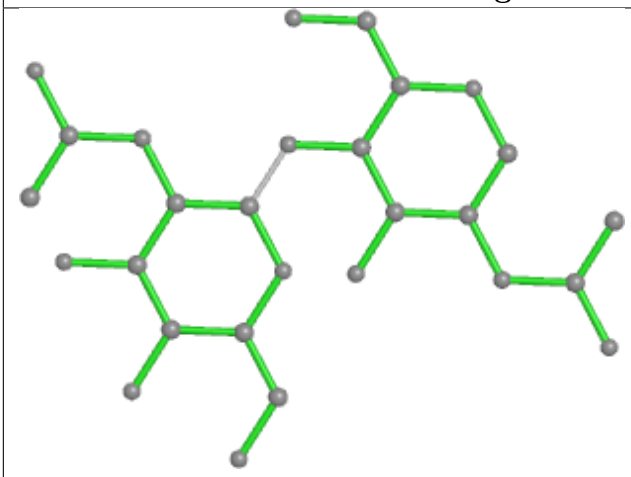


Rings

Oligosaccharide Chain Q



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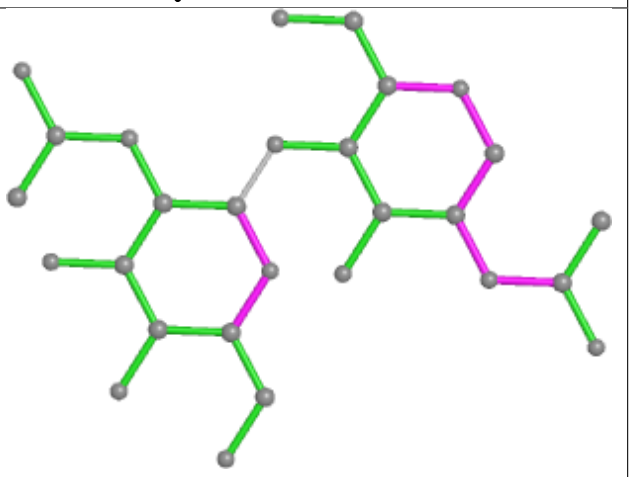
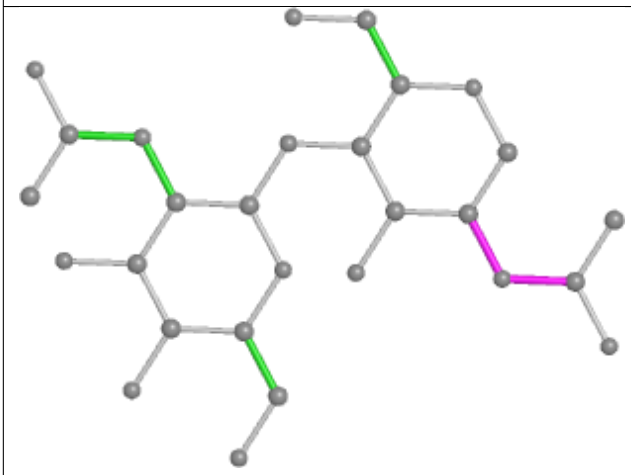
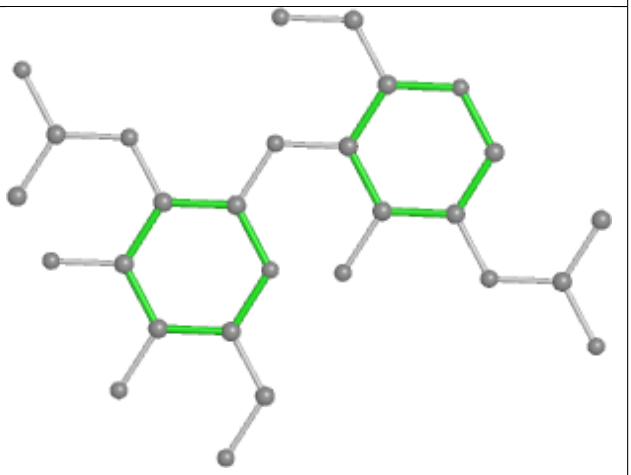


Bond angles

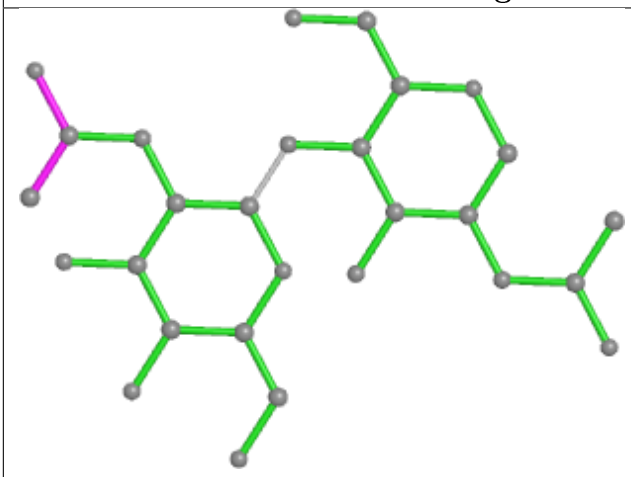


Torsions



Rings

Oligosaccharide Chain V



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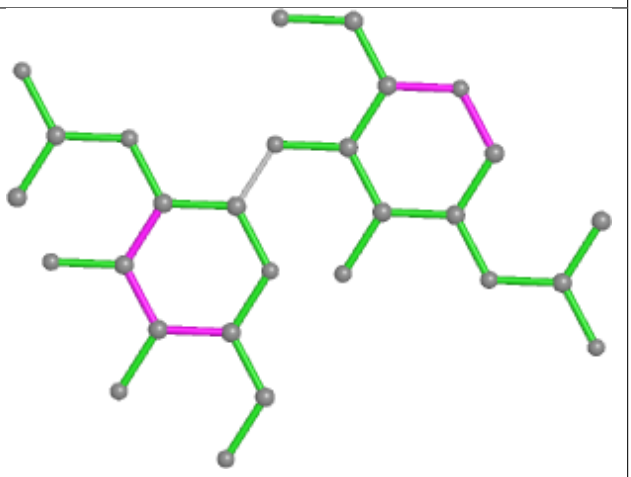
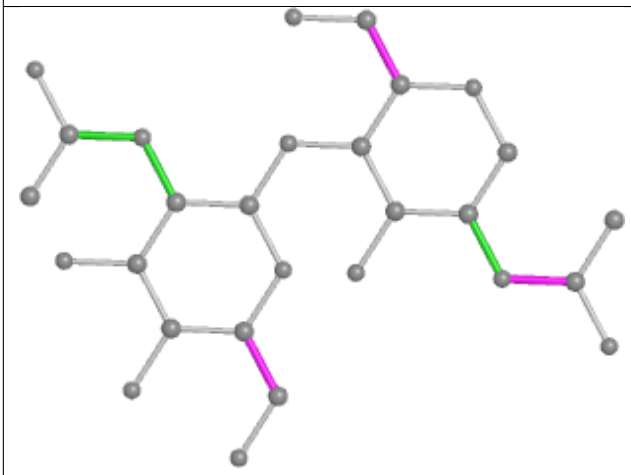


Bond angles



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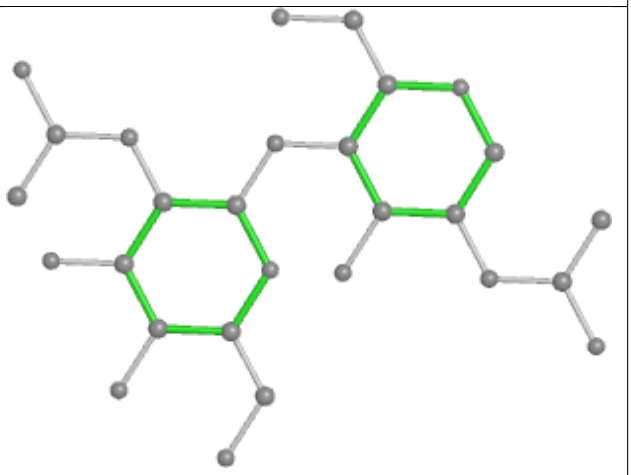
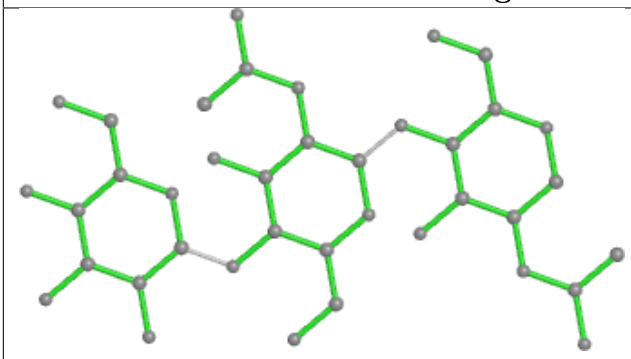


Rings

Oligosaccharide Chain K



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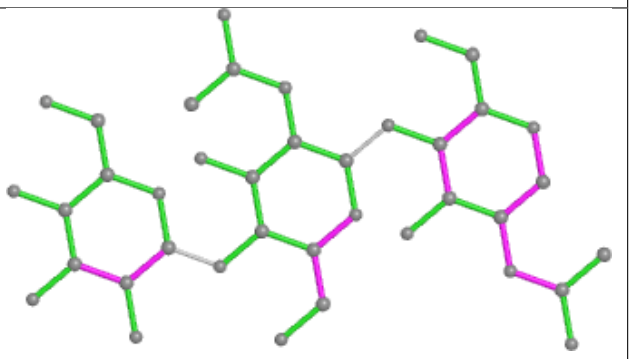
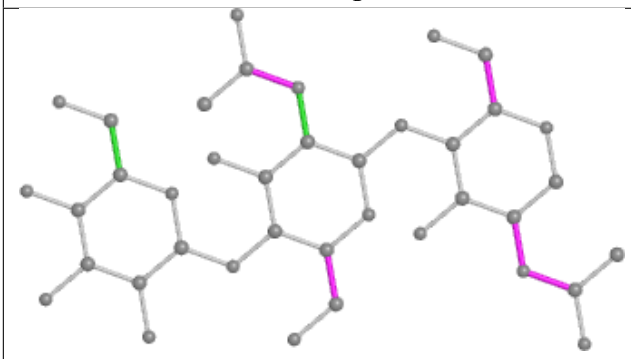


Bond angles



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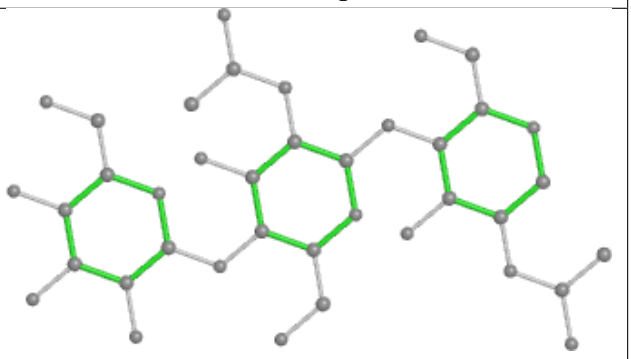
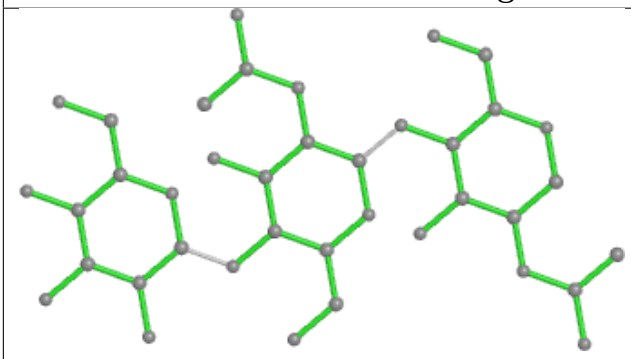
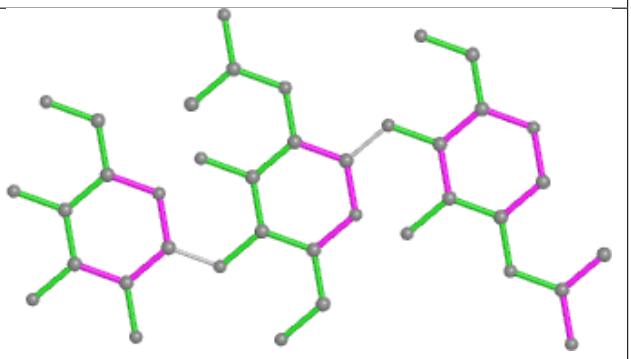


Rings

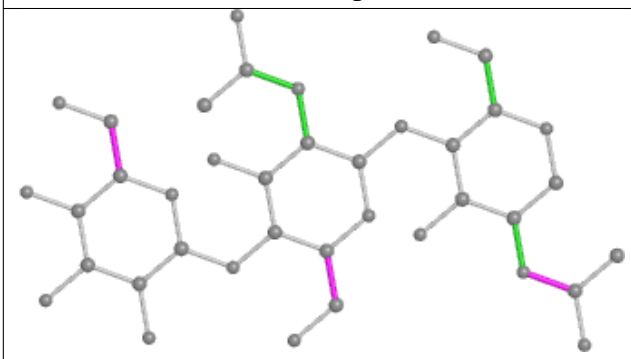
Oligosaccharide Chain L



Bond lengths



Bond angles



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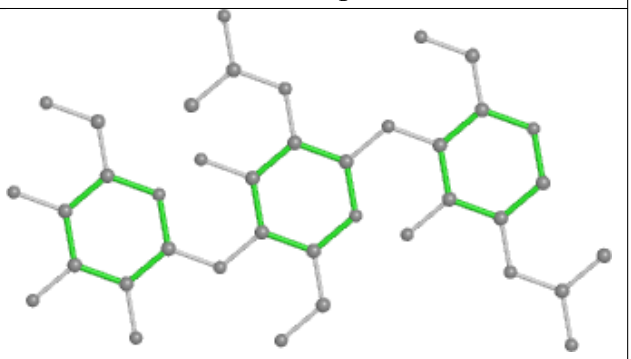
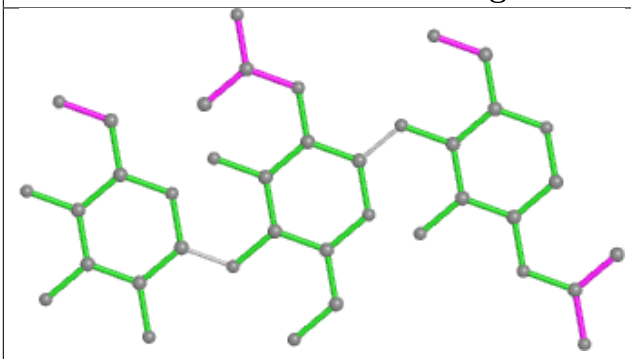


Rings

Oligosaccharide Chain W



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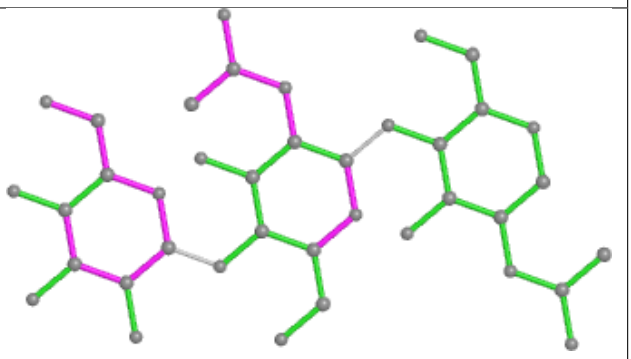
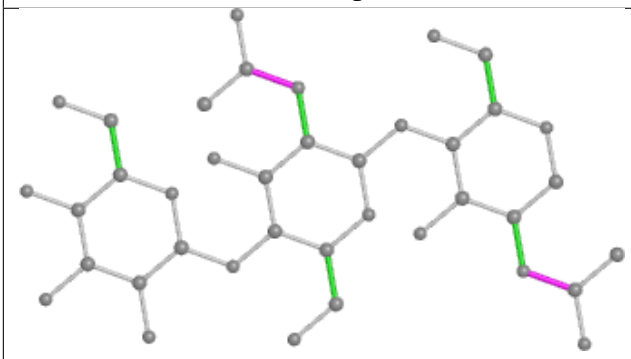


Bond angles



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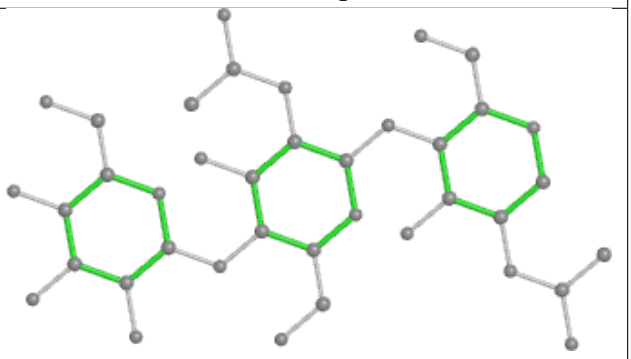
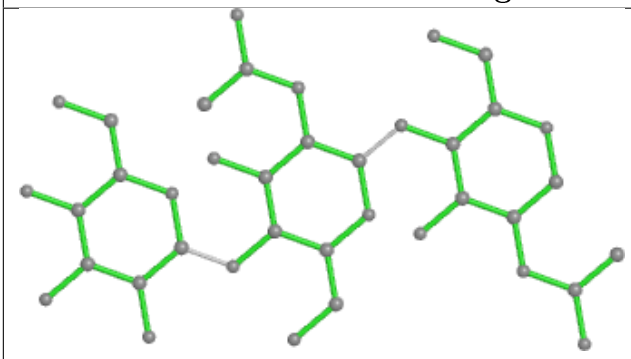
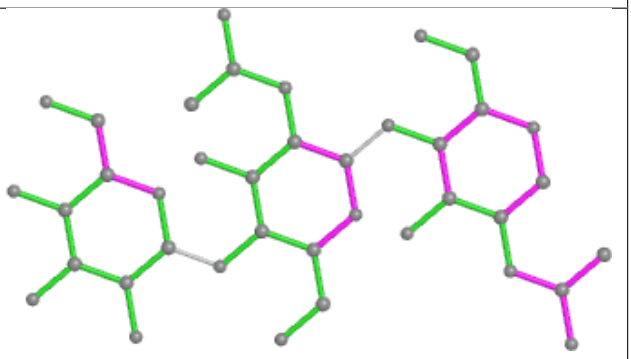


Rings

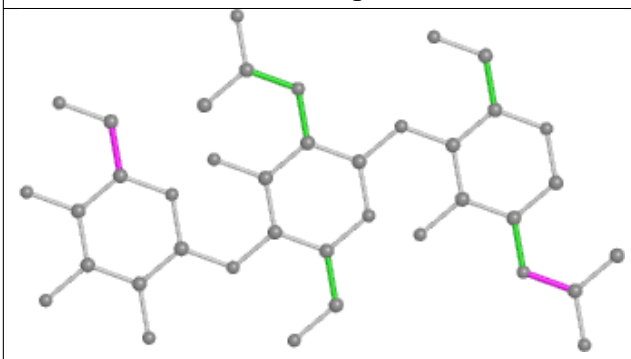
Oligosaccharide Chain X



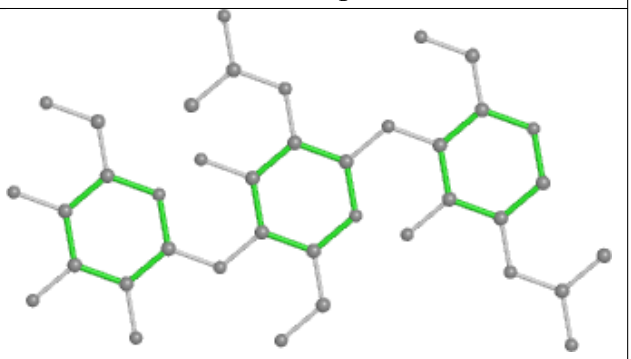
Bond lengths



Bond angles

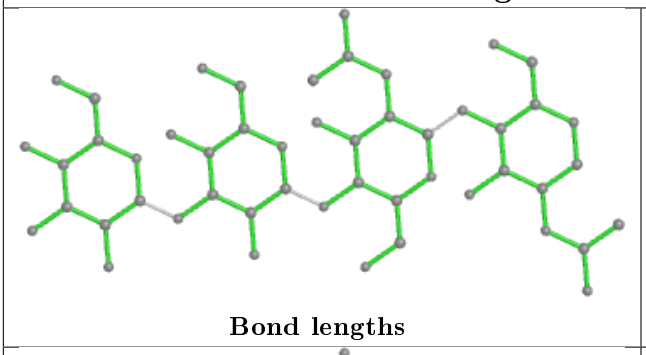


Torsions

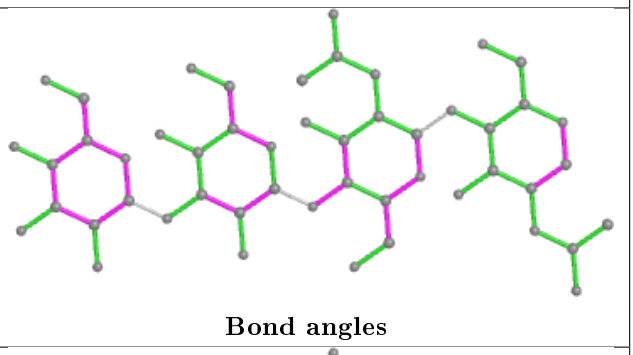


Rings

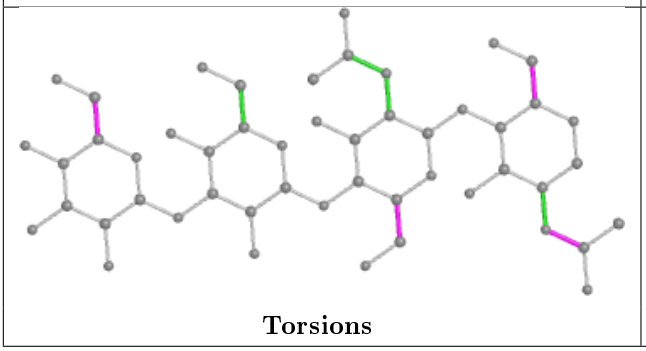
Oligosaccharide Chain R



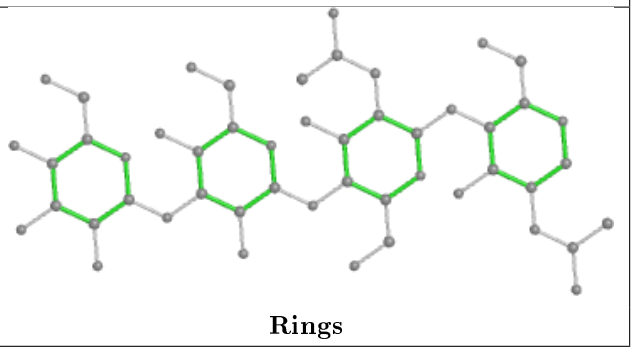
Bond lengths



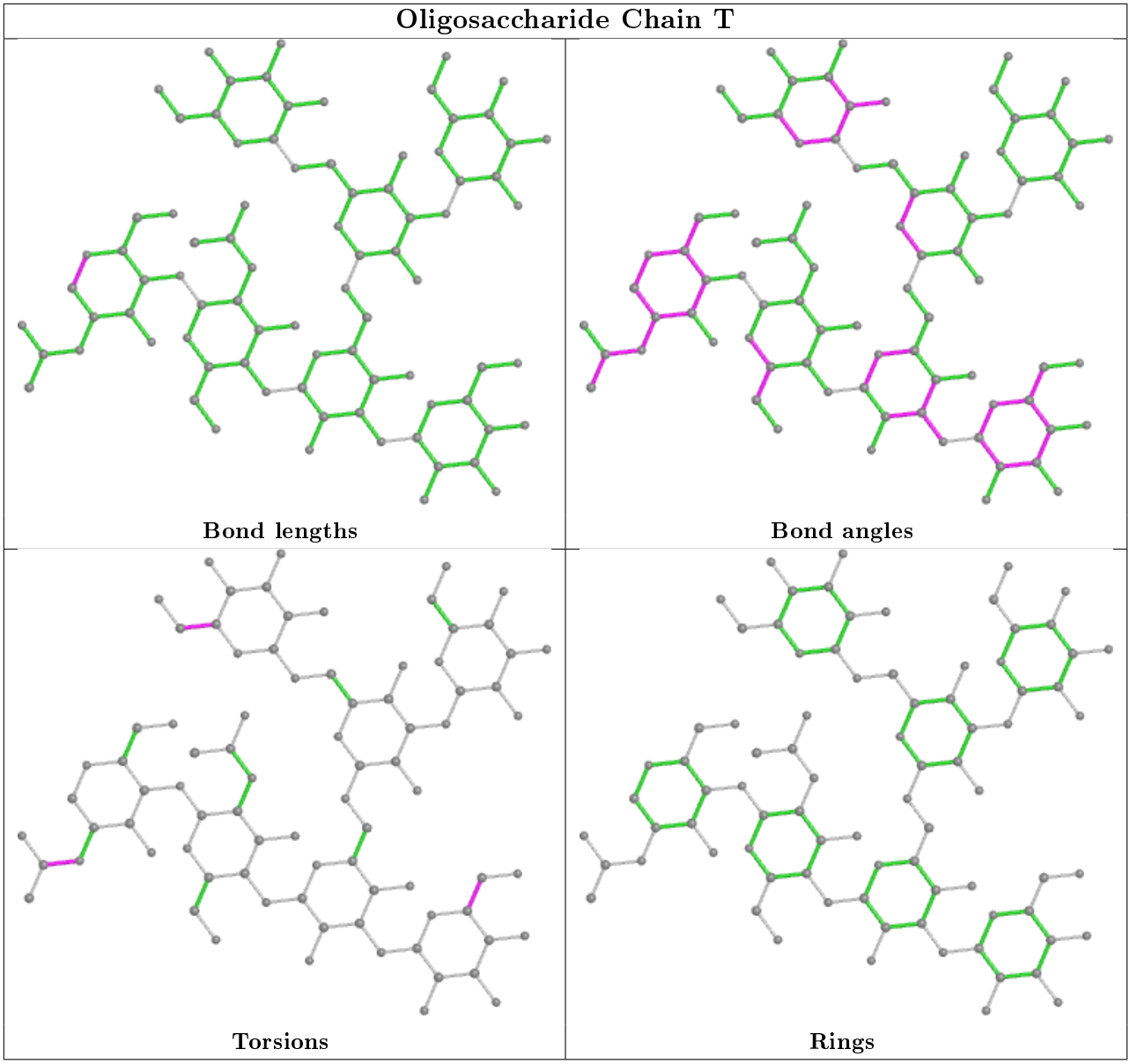
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 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	$\#\|Z\|>2$
8	NAG	A	2012	1	14,14,15	0.55	0	17,19,21	1.22	1 (5%)
8	NAG	B	2012	1	14,14,15	0.54	0	17,19,21	1.23	1 (5%)
8	NAG	F	2012	1	14,14,15	0.49	0	17,19,21	1.39	2 (11%)
8	NAG	A	2008	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
8	NAG	E	2005	1	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
8	NAG	A	2014	1	14,14,15	0.65	0	17,19,21	1.06	0
8	NAG	B	2018	1	14,14,15	0.76	1 (7%)	17,19,21	1.33	2 (11%)
8	NAG	C	2014	1	14,14,15	0.55	0	17,19,21	1.81	3 (17%)
8	NAG	F	2014	1	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
8	NAG	B	2006	1	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
8	NAG	F	2009	1	14,14,15	0.85	0	17,19,21	1.53	4 (23%)
8	NAG	E	2012	1	14,14,15	3.41	2 (14%)	17,19,21	1.52	4 (23%)
8	NAG	C	2006	1	14,14,15	0.46	0	17,19,21	1.45	1 (5%)
8	NAG	D	2005	1	14,14,15	0.54	0	17,19,21	1.21	3 (17%)
8	NAG	C	2018	1	14,14,15	5.03	3 (21%)	17,19,21	2.16	4 (23%)
8	NAG	D	2006	1	14,14,15	3.82	3 (21%)	17,19,21	2.05	5 (29%)
8	NAG	F	2006	1	14,14,15	4.09	4 (28%)	17,19,21	1.92	4 (23%)
8	NAG	E	2014	1	14,14,15	0.48	0	17,19,21	1.84	2 (11%)
8	NAG	B	2014	1	14,14,15	0.47	0	17,19,21	1.97	3 (17%)
8	NAG	D	2014	1	14,14,15	0.53	0	17,19,21	0.90	0
8	NAG	E	2008	1	14,14,15	0.52	0	17,19,21	0.95	0
8	NAG	F	2008	1	14,14,15	0.54	0	17,19,21	1.11	1 (5%)
8	NAG	D	2008	1	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
8	NAG	F	2005	1	14,14,15	4.14	4 (28%)	17,19,21	1.96	5 (29%)
8	NAG	D	2012	1	14,14,15	0.66	0	17,19,21	1.05	0
8	NAG	A	2006	1	14,14,15	0.88	1 (7%)	17,19,21	1.21	3 (17%)
8	NAG	E	2006	1	14,14,15	0.65	0	17,19,21	1.84	4 (23%)
8	NAG	C	2005	1	14,14,15	0.54	0	17,19,21	1.67	4 (23%)
8	NAG	A	2018	1	14,14,15	0.70	0	17,19,21	1.56	2 (11%)
8	NAG	B	2005	1	14,14,15	0.58	0	17,19,21	0.99	2 (11%)
8	NAG	C	2012	1	14,14,15	0.54	0	17,19,21	1.63	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
8	NAG	A	2012	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	B	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	E	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	F	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2006	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2009	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	E	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
8	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	F	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	E	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	E	2008	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2018	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	D	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	F	2005	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2012	1	-	6/6/23/26	0/1/1/1
8	NAG	A	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2006	1	-	3/6/23/26	0/1/1/1
8	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	B	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2012	1	1/1/5/7	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2018	NAG	O7-C7	14.37	1.55	1.23
8	F	2006	NAG	C8-C7	14.35	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	NAG	O7-C7	11.78	1.49	1.23
8	C	2018	NAG	C8-C7	11.44	1.74	1.50
8	E	2012	NAG	C8-C7	10.36	1.72	1.50
8	F	2005	NAG	C8-C7	9.16	1.69	1.50
8	F	2005	NAG	C1-C2	7.70	1.63	1.52
8	F	2005	NAG	O6-C6	7.61	1.74	1.42
8	E	2012	NAG	O7-C7	7.24	1.39	1.23
8	D	2006	NAG	C8-C7	6.63	1.64	1.50
8	F	2005	NAG	C2-N2	5.09	1.55	1.46
8	F	2006	NAG	O7-C7	-3.38	1.15	1.23
8	C	2018	NAG	O6-C6	2.97	1.55	1.42
8	F	2006	NAG	C7-N2	2.80	1.44	1.34
8	D	2006	NAG	C1-C2	2.27	1.55	1.52
8	B	2018	NAG	C1-C2	2.08	1.55	1.52
8	A	2006	NAG	O5-C1	-2.08	1.40	1.43
8	F	2006	NAG	C1-C2	2.03	1.55	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	2014	NAG	C1-O5-C5	6.29	120.71	112.19
8	C	2014	NAG	C1-O5-C5	5.90	120.19	112.19
8	F	2005	NAG	C1-O5-C5	5.40	119.51	112.19
8	D	2006	NAG	C8-C7-N2	-5.19	107.31	116.10
8	B	2014	NAG	C1-O5-C5	5.19	119.22	112.19
8	C	2018	NAG	O7-C7-N2	-4.92	112.90	121.95
8	A	2018	NAG	C4-C3-C2	4.60	117.77	111.02
8	C	2012	NAG	C1-O5-C5	4.59	118.41	112.19
8	E	2006	NAG	C1-O5-C5	4.49	118.28	112.19
8	C	2018	NAG	C4-C3-C2	4.45	117.54	111.02
8	F	2006	NAG	O7-C7-N2	-4.42	113.82	121.95
8	C	2018	NAG	O7-C7-C8	4.20	129.86	122.06
8	B	2018	NAG	C4-C3-C2	4.01	116.89	111.02
8	C	2006	NAG	C1-O5-C5	4.00	117.61	112.19
8	F	2006	NAG	C2-N2-C7	-3.98	117.24	122.90
8	F	2012	NAG	C2-N2-C7	3.70	128.17	122.90
8	C	2005	NAG	C2-N2-C7	3.67	128.13	122.90
8	B	2014	NAG	O5-C1-C2	-3.58	105.64	111.29
8	F	2008	NAG	C1-O5-C5	3.49	116.92	112.19
8	E	2012	NAG	O7-C7-C8	3.46	128.48	122.06
8	F	2005	NAG	O6-C6-C5	-3.42	99.55	111.29
8	C	2005	NAG	C8-C7-N2	3.41	121.88	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	2006	NAG	O5-C1-C2	3.37	116.61	111.29
8	B	2012	NAG	C1-O5-C5	3.36	116.75	112.19
8	F	2009	NAG	C2-N2-C7	3.34	127.66	122.90
8	C	2005	NAG	C1-O5-C5	3.28	116.64	112.19
8	F	2014	NAG	C1-O5-C5	3.20	116.53	112.19
8	D	2006	NAG	C2-N2-C7	-3.13	118.44	122.90
8	A	2012	NAG	C1-O5-C5	3.12	116.42	112.19
8	B	2006	NAG	O5-C1-C2	-3.06	106.45	111.29
8	F	2006	NAG	O5-C1-C2	-2.97	106.60	111.29
8	F	2005	NAG	O7-C7-N2	-2.92	116.59	121.95
8	C	2018	NAG	C3-C4-C5	2.90	115.42	110.24
8	F	2009	NAG	C1-C2-N2	2.90	115.44	110.49
8	F	2006	NAG	O7-C7-C8	2.89	127.43	122.06
8	F	2009	NAG	C1-O5-C5	2.85	116.05	112.19
8	E	2006	NAG	C2-N2-C7	2.83	126.93	122.90
8	D	2008	NAG	O5-C1-C2	-2.60	107.18	111.29
8	E	2006	NAG	C4-C3-C2	2.59	114.81	111.02
8	C	2012	NAG	C4-C3-C2	2.59	114.81	111.02
8	D	2006	NAG	C1-O5-C5	2.57	115.67	112.19
8	F	2012	NAG	C1-O5-C5	2.55	115.64	112.19
8	E	2012	NAG	C1-O5-C5	2.50	115.58	112.19
8	B	2018	NAG	O5-C5-C6	2.49	111.10	107.20
8	E	2012	NAG	C8-C7-N2	-2.47	111.91	116.10
8	A	2006	NAG	O5-C5-C4	-2.44	104.90	110.83
8	A	2018	NAG	C3-C4-C5	2.43	114.58	110.24
8	E	2012	NAG	O5-C5-C6	2.43	111.02	107.20
8	D	2006	NAG	O5-C1-C2	-2.42	107.46	111.29
8	B	2005	NAG	O5-C1-C2	-2.42	107.47	111.29
8	C	2012	NAG	O5-C5-C6	2.41	110.99	107.20
8	C	2014	NAG	O5-C5-C4	2.28	116.38	110.83
8	F	2005	NAG	O5-C1-C2	-2.27	107.70	111.29
8	C	2014	NAG	C6-C5-C4	-2.26	107.71	113.00
8	D	2005	NAG	C8-C7-N2	2.23	119.88	116.10
8	A	2006	NAG	C4-C3-C2	2.23	114.29	111.02
8	E	2014	NAG	C6-C5-C4	-2.23	107.79	113.00
8	A	2008	NAG	O5-C1-C2	-2.22	107.78	111.29
8	D	2005	NAG	O5-C1-C2	-2.17	107.87	111.29
8	F	2014	NAG	O5-C1-C2	-2.16	107.88	111.29
8	A	2006	NAG	O5-C1-C2	-2.11	107.96	111.29
8	D	2005	NAG	O5-C5-C6	2.09	110.49	107.20
8	F	2005	NAG	O5-C5-C6	2.09	110.49	107.20
8	B	2014	NAG	C1-C2-N2	2.08	114.05	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	2009	NAG	O5-C1-C2	-2.07	108.03	111.29
8	C	2005	NAG	O7-C7-C8	-2.06	118.22	122.06
8	B	2005	NAG	C8-C7-N2	2.05	119.58	116.10
8	D	2006	NAG	O5-C5-C6	2.02	110.36	107.20
8	E	2005	NAG	C8-C7-N2	2.01	119.51	116.10

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	2012	NAG	C1
8	B	2012	NAG	C1
8	B	2018	NAG	C1
8	F	2012	NAG	C1
8	B	2006	NAG	C1
8	F	2009	NAG	C1
8	E	2012	NAG	C1
8	C	2018	NAG	C1
8	D	2006	NAG	C1
8	F	2006	NAG	C1
8	A	2018	NAG	C1
8	F	2005	NAG	C1
8	A	2006	NAG	C1
8	C	2012	NAG	C1

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2012	NAG	C8-C7-N2-C2
8	A	2012	NAG	O7-C7-N2-C2
8	B	2012	NAG	O7-C7-N2-C2
8	E	2005	NAG	C8-C7-N2-C2
8	E	2005	NAG	O7-C7-N2-C2
8	A	2014	NAG	O7-C7-N2-C2
8	B	2018	NAG	C8-C7-N2-C2
8	B	2018	NAG	O7-C7-N2-C2
8	F	2014	NAG	C8-C7-N2-C2
8	F	2014	NAG	O7-C7-N2-C2
8	F	2012	NAG	C3-C2-N2-C7
8	F	2012	NAG	C8-C7-N2-C2
8	F	2012	NAG	O7-C7-N2-C2
8	F	2009	NAG	C8-C7-N2-C2
8	F	2009	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	D	2005	NAG	C8-C7-N2-C2
8	D	2005	NAG	O7-C7-N2-C2
8	C	2018	NAG	C8-C7-N2-C2
8	C	2018	NAG	O7-C7-N2-C2
8	D	2006	NAG	C8-C7-N2-C2
8	F	2006	NAG	C8-C7-N2-C2
8	F	2006	NAG	O7-C7-N2-C2
8	B	2014	NAG	C8-C7-N2-C2
8	B	2014	NAG	O7-C7-N2-C2
8	D	2014	NAG	C8-C7-N2-C2
8	D	2014	NAG	O7-C7-N2-C2
8	F	2005	NAG	C3-C2-N2-C7
8	F	2005	NAG	C8-C7-N2-C2
8	F	2005	NAG	O7-C7-N2-C2
8	D	2012	NAG	C8-C7-N2-C2
8	D	2012	NAG	O7-C7-N2-C2
8	E	2006	NAG	C8-C7-N2-C2
8	E	2006	NAG	O7-C7-N2-C2
8	B	2005	NAG	C8-C7-N2-C2
8	B	2005	NAG	O7-C7-N2-C2
8	B	2012	NAG	C8-C7-N2-C2
8	A	2014	NAG	C8-C7-N2-C2
8	D	2006	NAG	O7-C7-N2-C2
8	A	2006	NAG	O7-C7-N2-C2
8	C	2018	NAG	O5-C5-C6-O6
8	E	2014	NAG	O5-C5-C6-O6
8	C	2012	NAG	O5-C5-C6-O6
8	F	2009	NAG	C4-C5-C6-O6
8	D	2014	NAG	C4-C5-C6-O6
8	B	2005	NAG	O5-C5-C6-O6
8	B	2006	NAG	C8-C7-N2-C2
8	B	2006	NAG	O7-C7-N2-C2
8	E	2012	NAG	C8-C7-N2-C2
8	E	2012	NAG	O7-C7-N2-C2
8	C	2006	NAG	C8-C7-N2-C2
8	C	2006	NAG	O7-C7-N2-C2
8	A	2006	NAG	C8-C7-N2-C2
8	B	2014	NAG	O5-C5-C6-O6
8	F	2012	NAG	O5-C5-C6-O6
8	E	2012	NAG	O5-C5-C6-O6
8	C	2014	NAG	O5-C5-C6-O6
8	D	2005	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	2005	NAG	O5-C5-C6-O6
8	B	2018	NAG	O5-C5-C6-O6
8	C	2018	NAG	C4-C5-C6-O6
8	B	2005	NAG	C4-C5-C6-O6
8	C	2012	NAG	C4-C5-C6-O6
8	D	2005	NAG	C4-C5-C6-O6
8	E	2014	NAG	C4-C5-C6-O6
8	F	2009	NAG	O5-C5-C6-O6
8	B	2018	NAG	C4-C5-C6-O6
8	B	2014	NAG	C4-C5-C6-O6
8	C	2005	NAG	C4-C5-C6-O6
8	C	2005	NAG	C8-C7-N2-C2
8	C	2005	NAG	O7-C7-N2-C2
8	D	2014	NAG	O5-C5-C6-O6
8	C	2014	NAG	C4-C5-C6-O6
8	E	2006	NAG	C1-C2-N2-C7
8	E	2008	NAG	O5-C5-C6-O6
8	B	2012	NAG	O5-C5-C6-O6
8	F	2012	NAG	C4-C5-C6-O6
8	A	2006	NAG	C4-C5-C6-O6
8	A	2006	NAG	O5-C5-C6-O6
8	A	2012	NAG	O5-C5-C6-O6
8	F	2006	NAG	C4-C5-C6-O6
8	E	2012	NAG	C4-C5-C6-O6
8	A	2018	NAG	C8-C7-N2-C2
8	E	2008	NAG	C4-C5-C6-O6
8	A	2018	NAG	O7-C7-N2-C2
8	C	2014	NAG	C8-C7-N2-C2
8	F	2006	NAG	O5-C5-C6-O6
8	F	2005	NAG	C1-C2-N2-C7
8	F	2009	NAG	C3-C2-N2-C7
8	C	2014	NAG	O7-C7-N2-C2
8	E	2012	NAG	C1-C2-N2-C7
8	D	2012	NAG	C1-C2-N2-C7
8	A	2018	NAG	C4-C5-C6-O6
8	D	2012	NAG	O5-C5-C6-O6
8	B	2006	NAG	C1-C2-N2-C7
8	D	2012	NAG	C3-C2-N2-C7
8	B	2012	NAG	C4-C5-C6-O6
8	D	2012	NAG	C4-C5-C6-O6

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

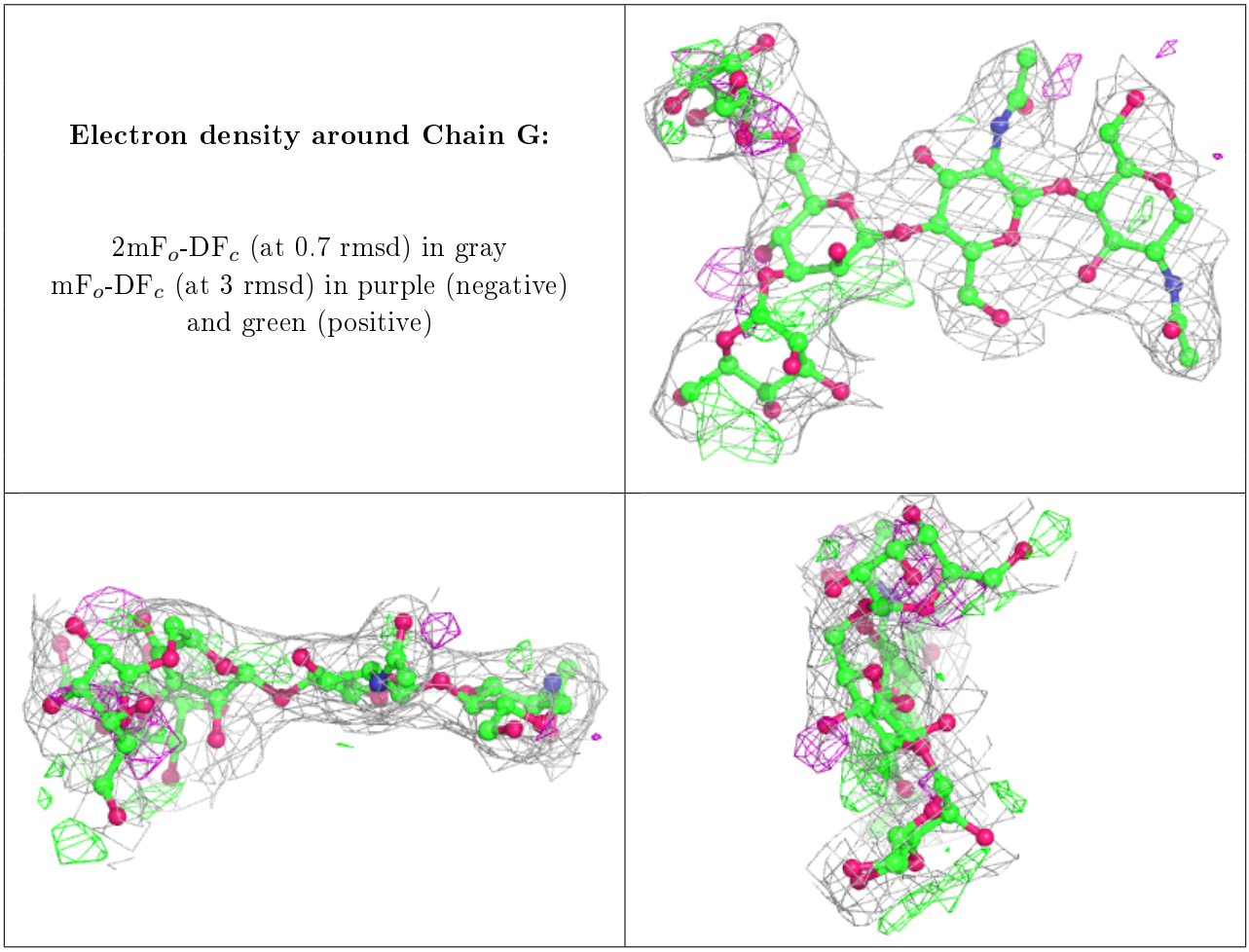
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

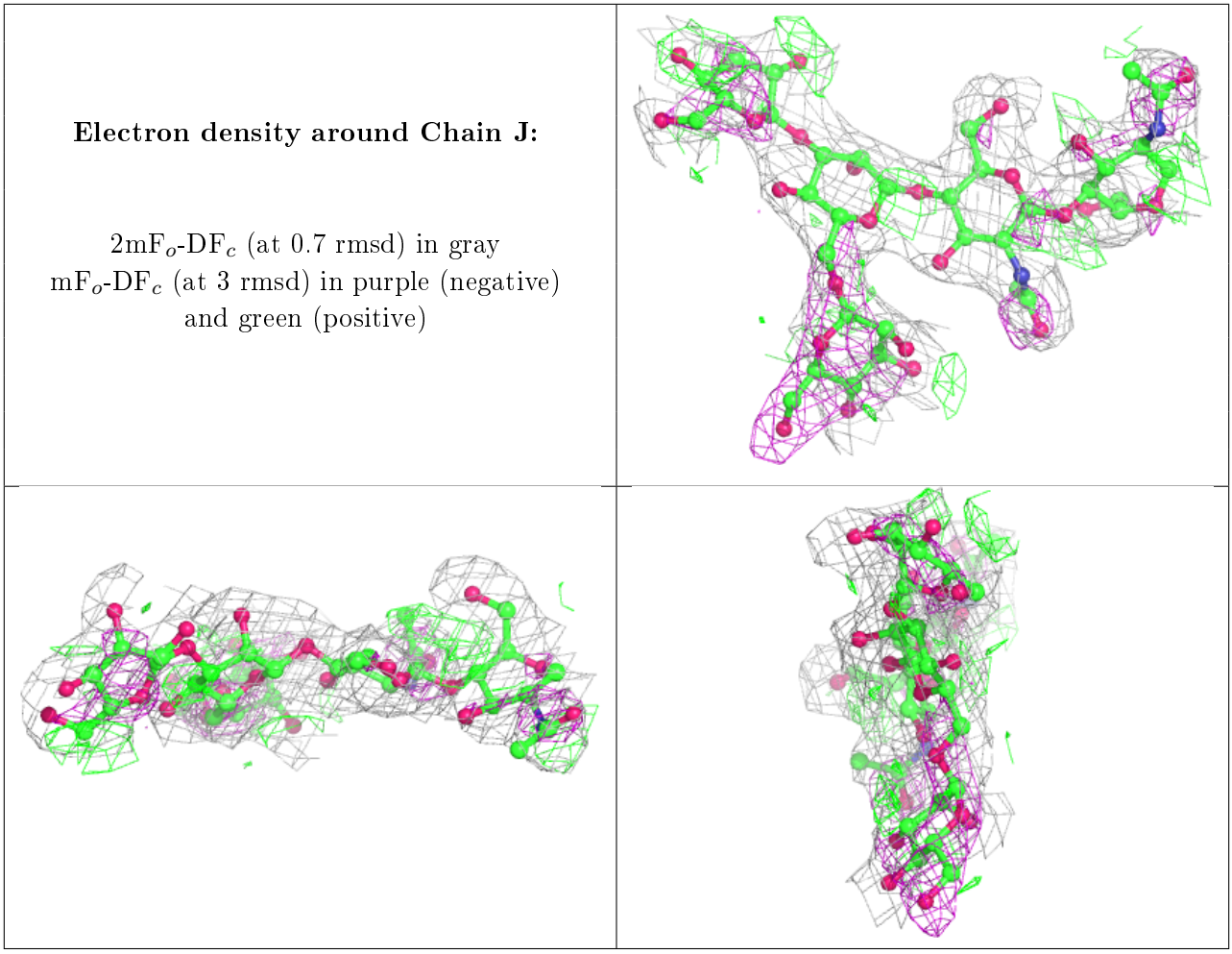
Electron density around Chain G:

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



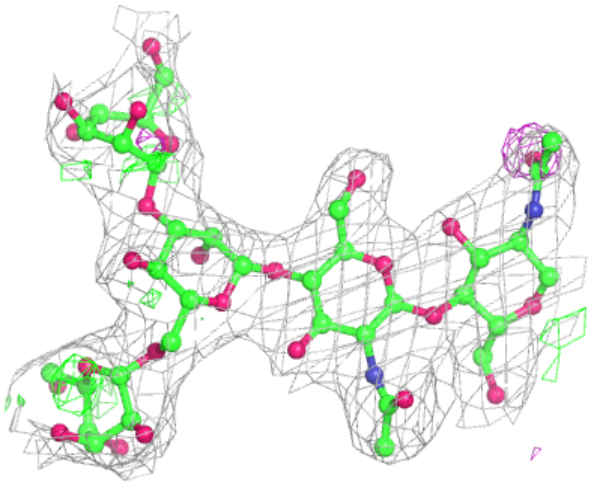
Electron density around Chain J:

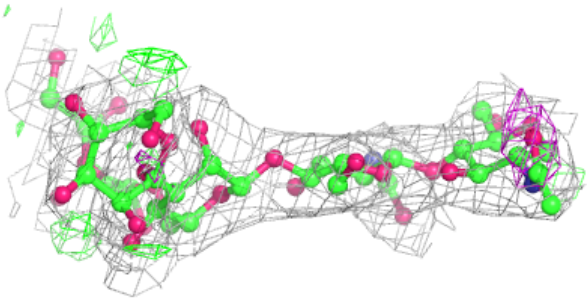
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain M:

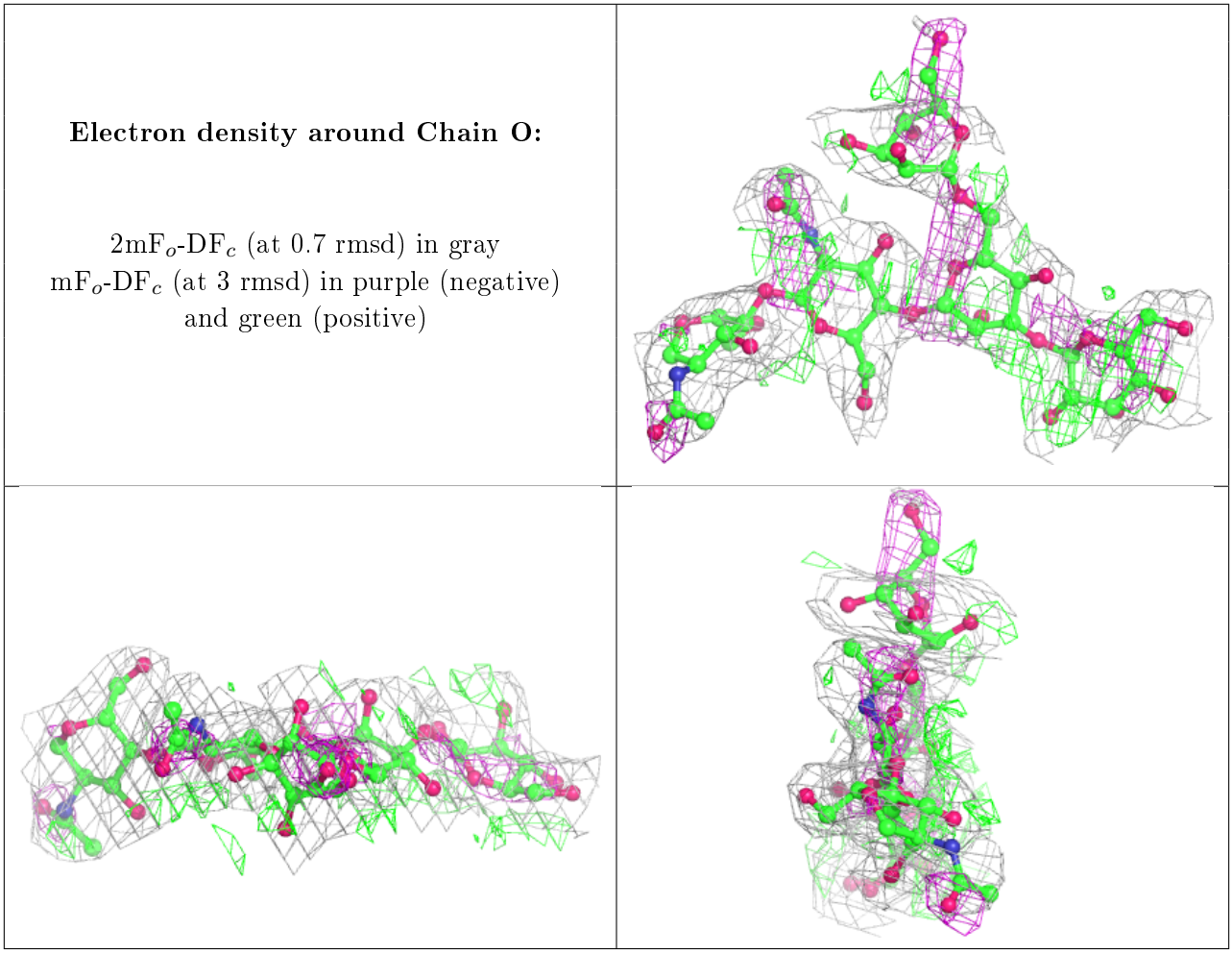
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





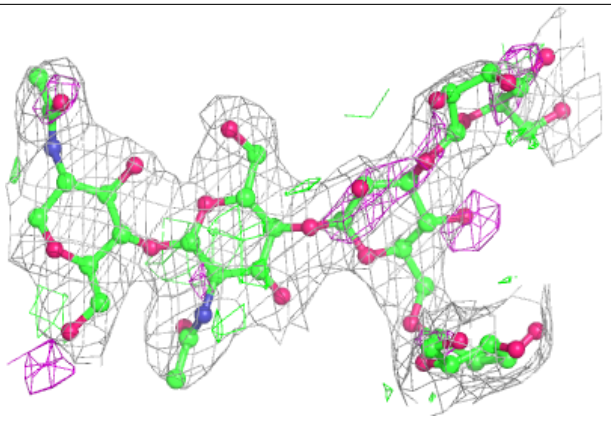
Electron density around Chain O:

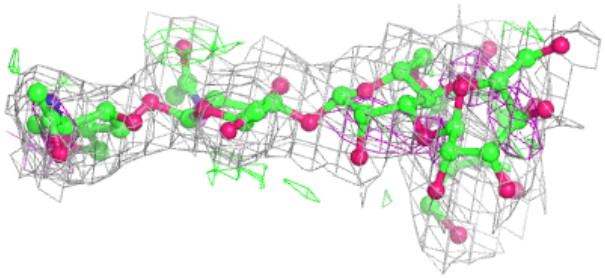
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

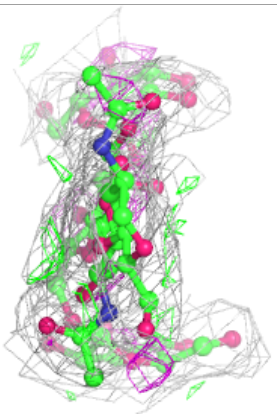


Electron density around Chain S:

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

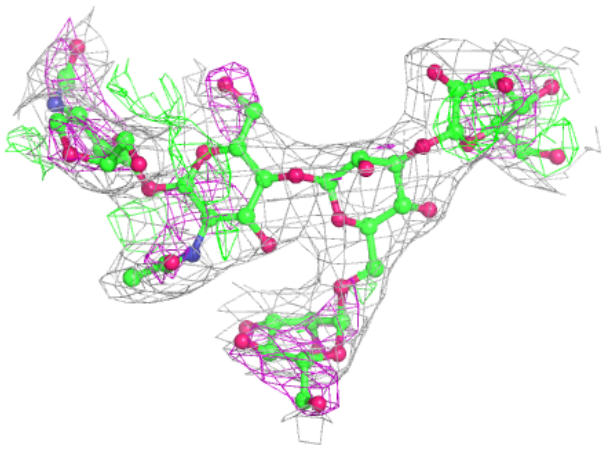


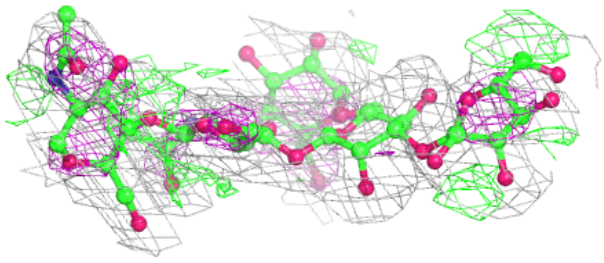


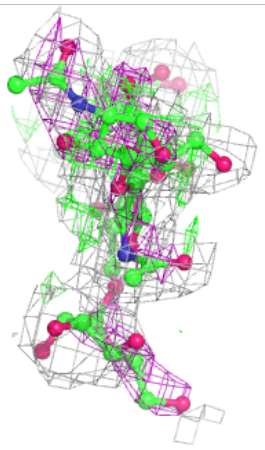


Electron density around Chain U:

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

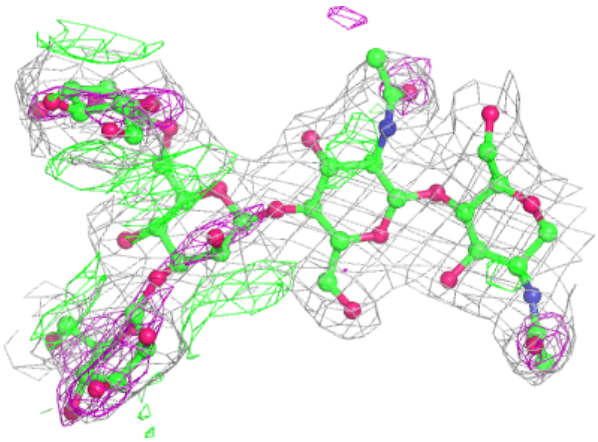


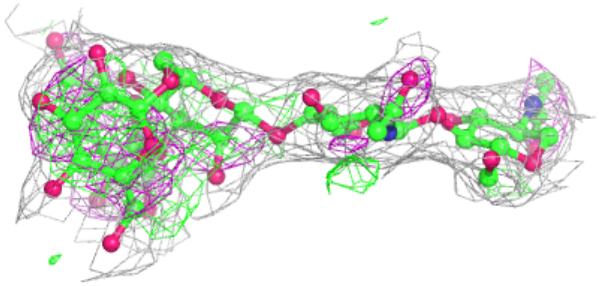


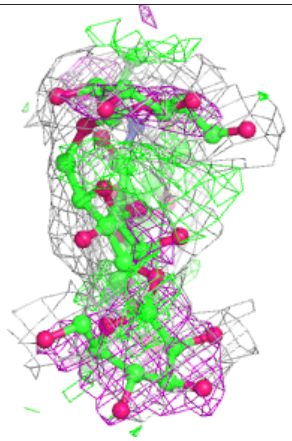


Electron density around Chain Y:

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

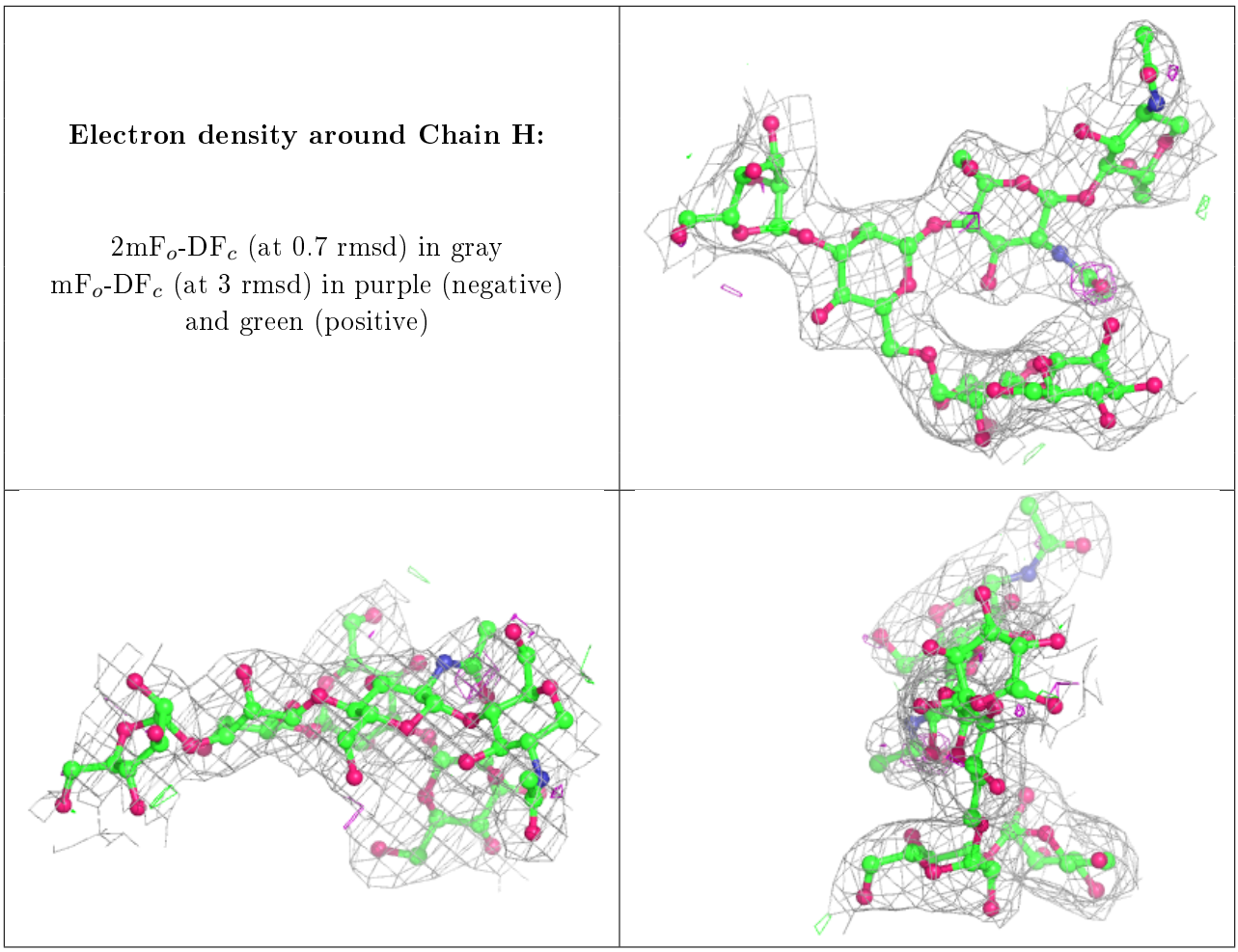






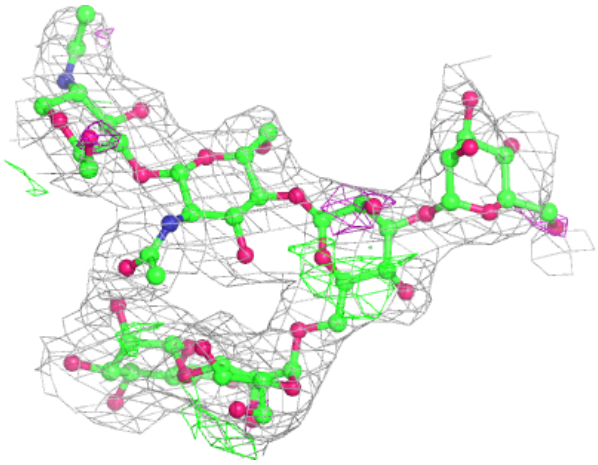
Electron density around Chain H:

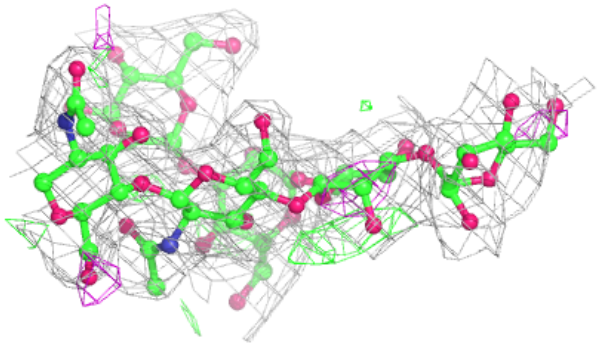
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

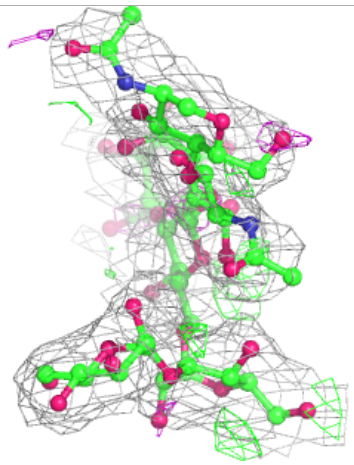


Electron density around Chain N:

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

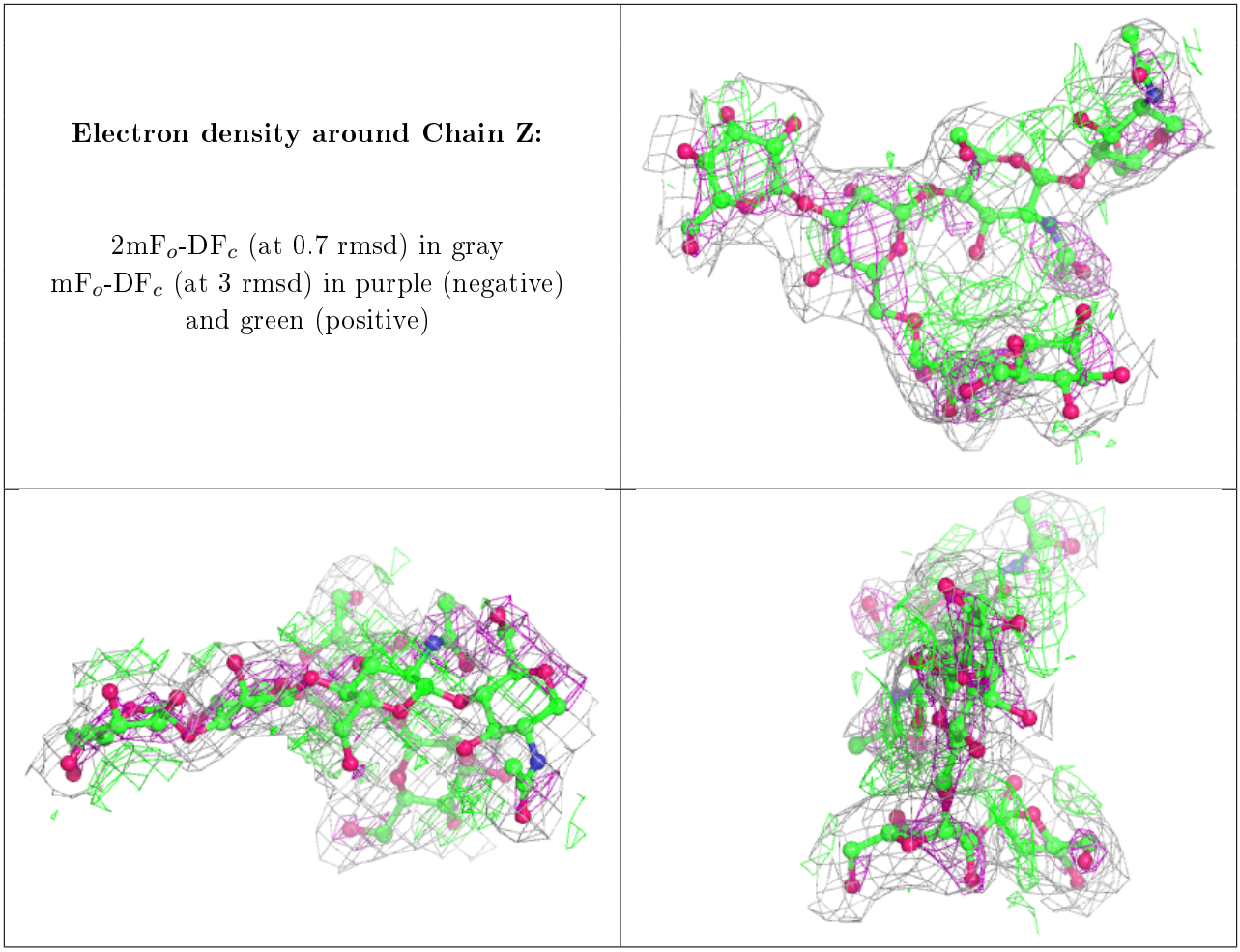






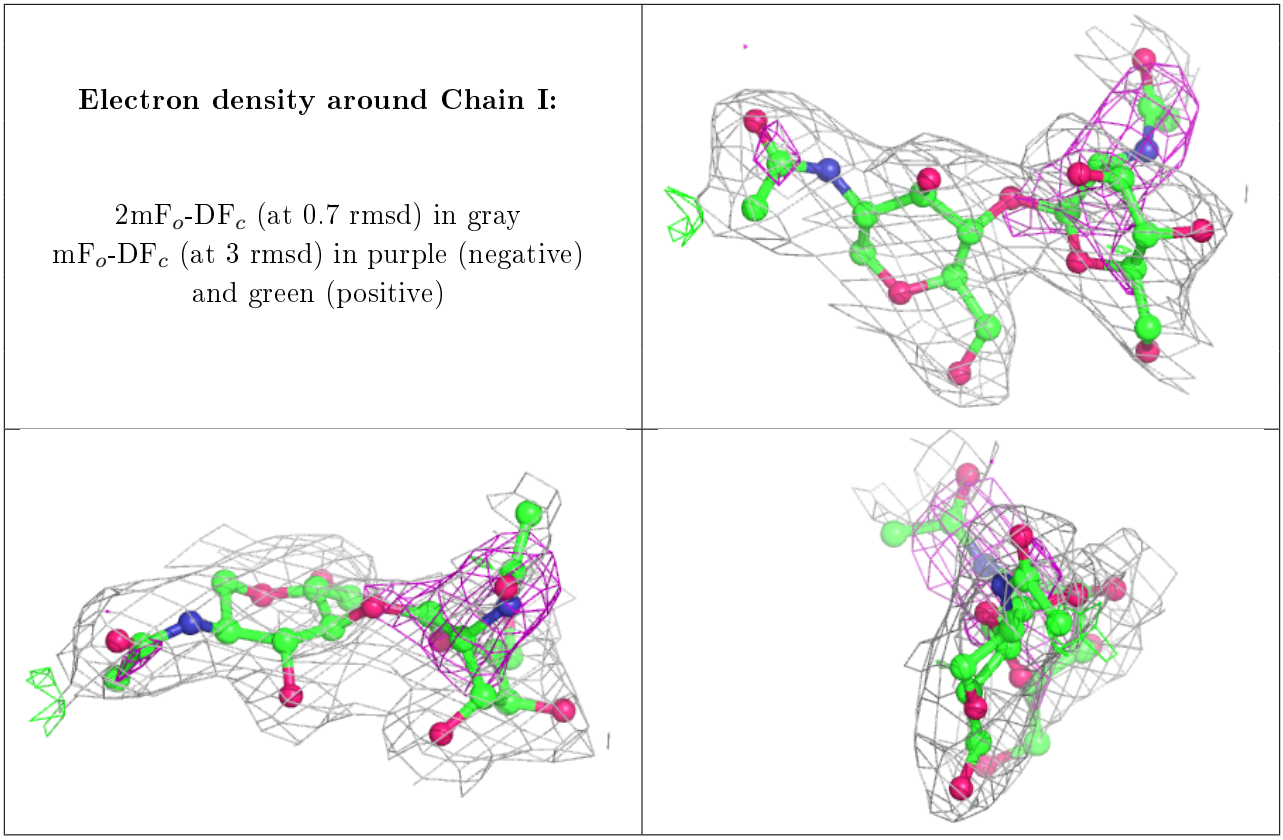
Electron density around Chain Z:

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



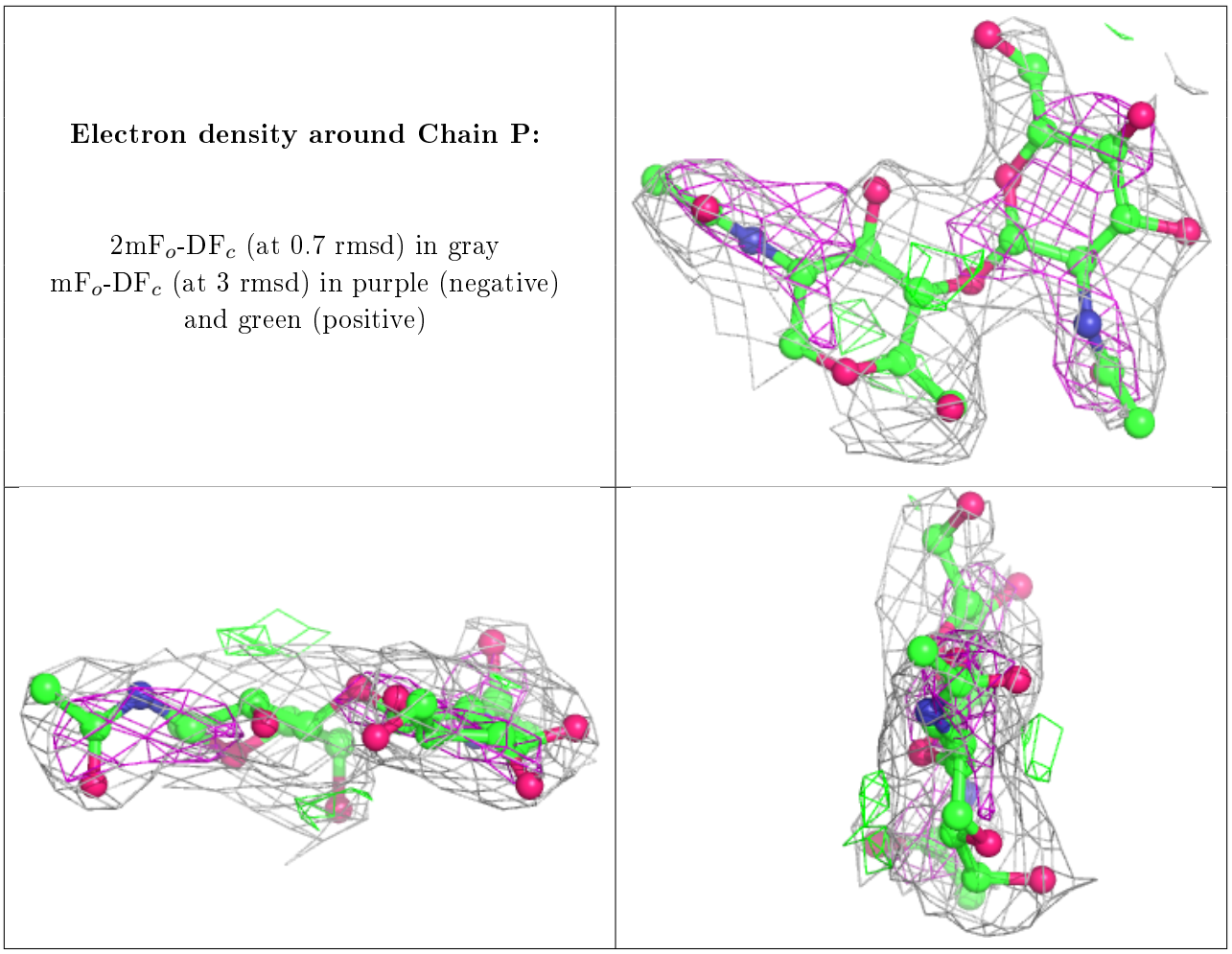
Electron density around Chain I:

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



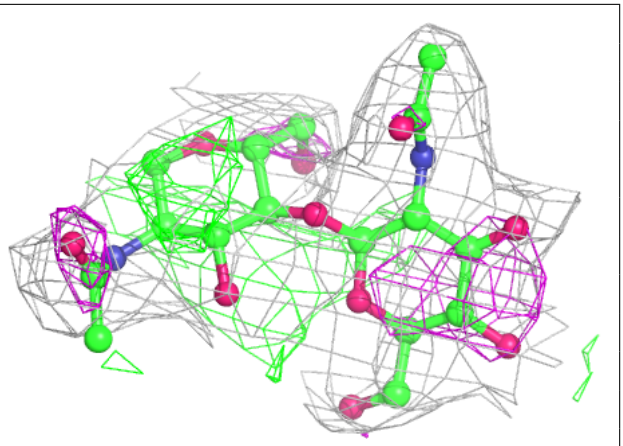
Electron density around Chain P:

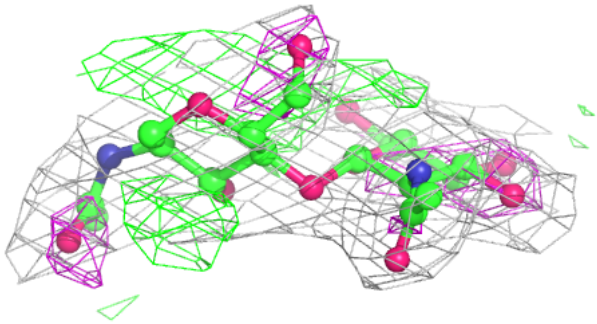
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

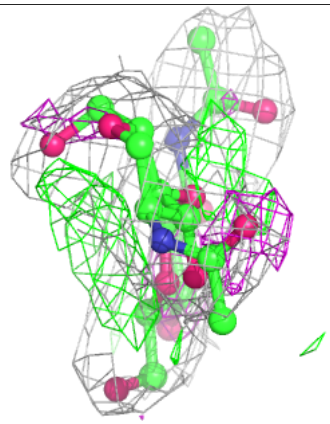


Electron density around Chain Q:

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

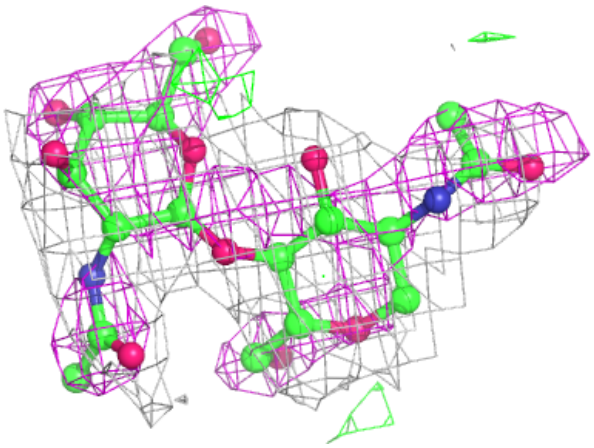


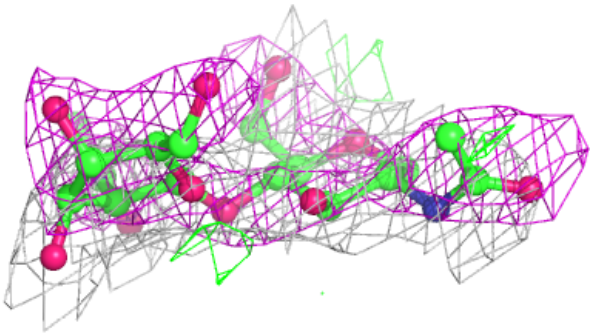


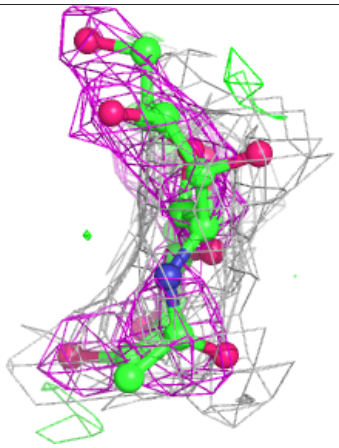


Electron density around Chain V:

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

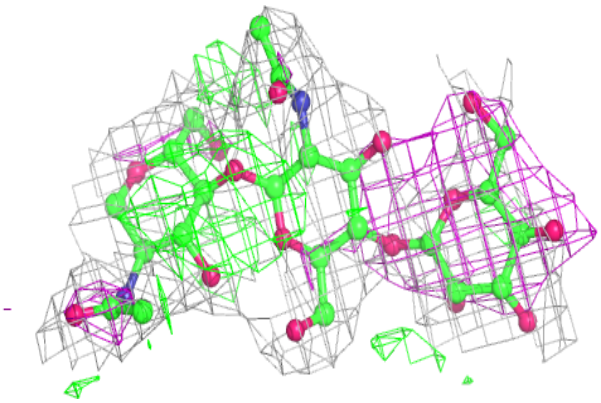


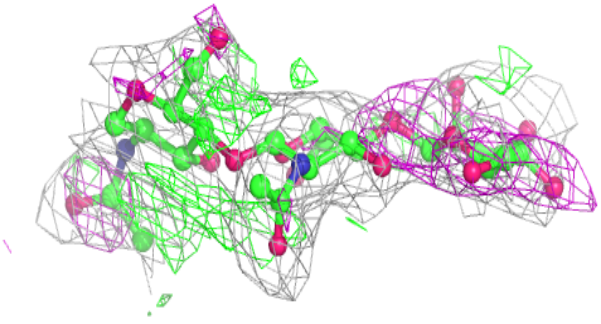


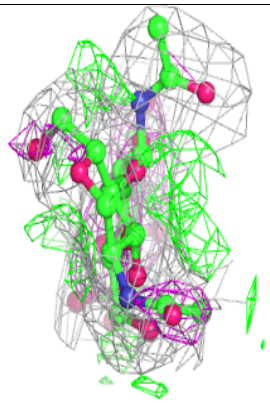


Electron density around Chain K:

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

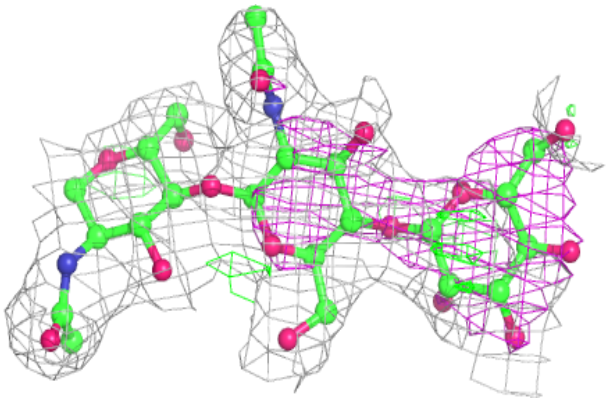


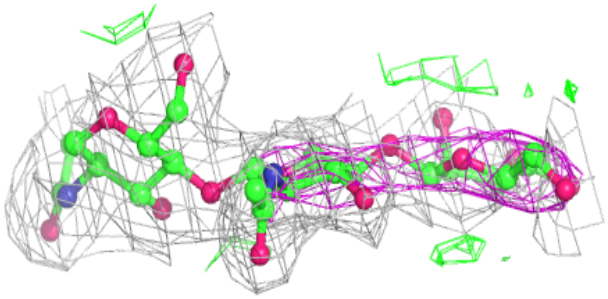


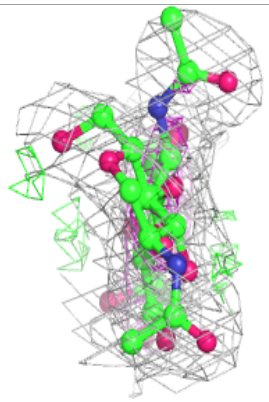


Electron density around Chain L:

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

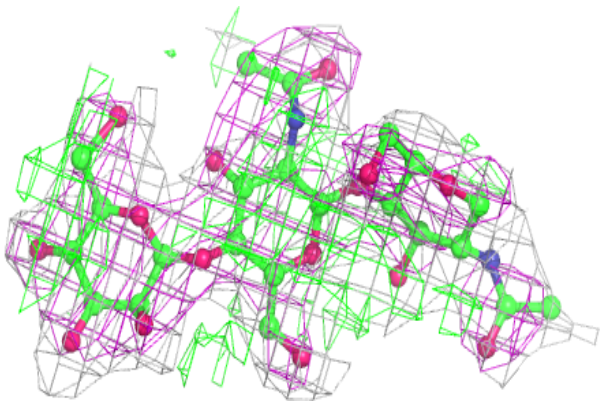


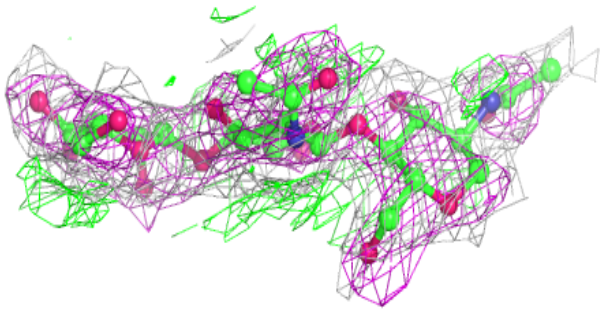


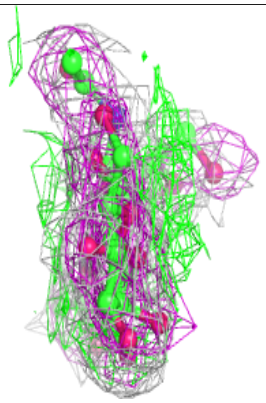


Electron density around Chain W:

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

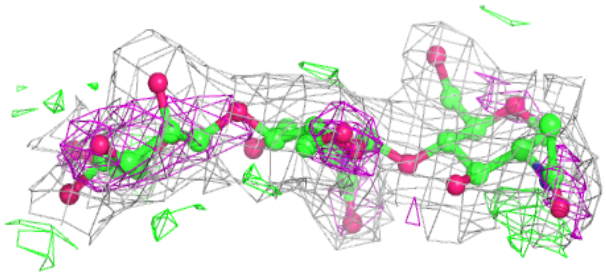


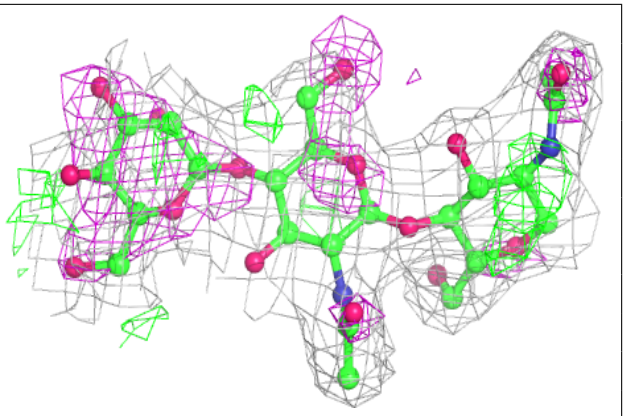


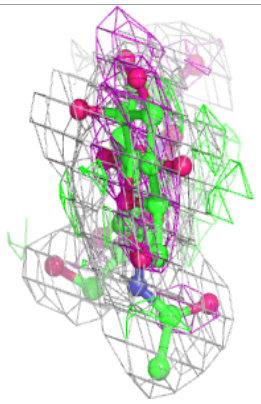


Electron density around Chain X:

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

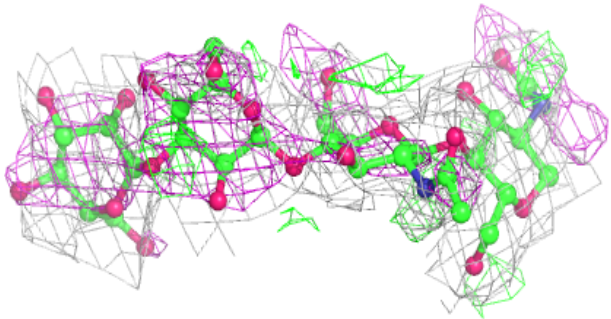


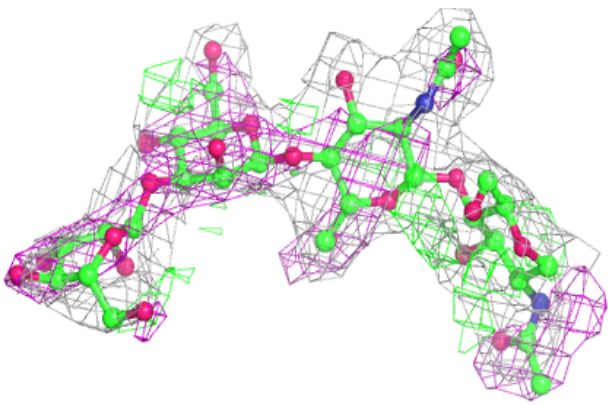


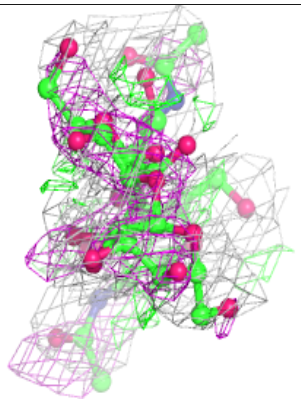


Electron density around Chain R:

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

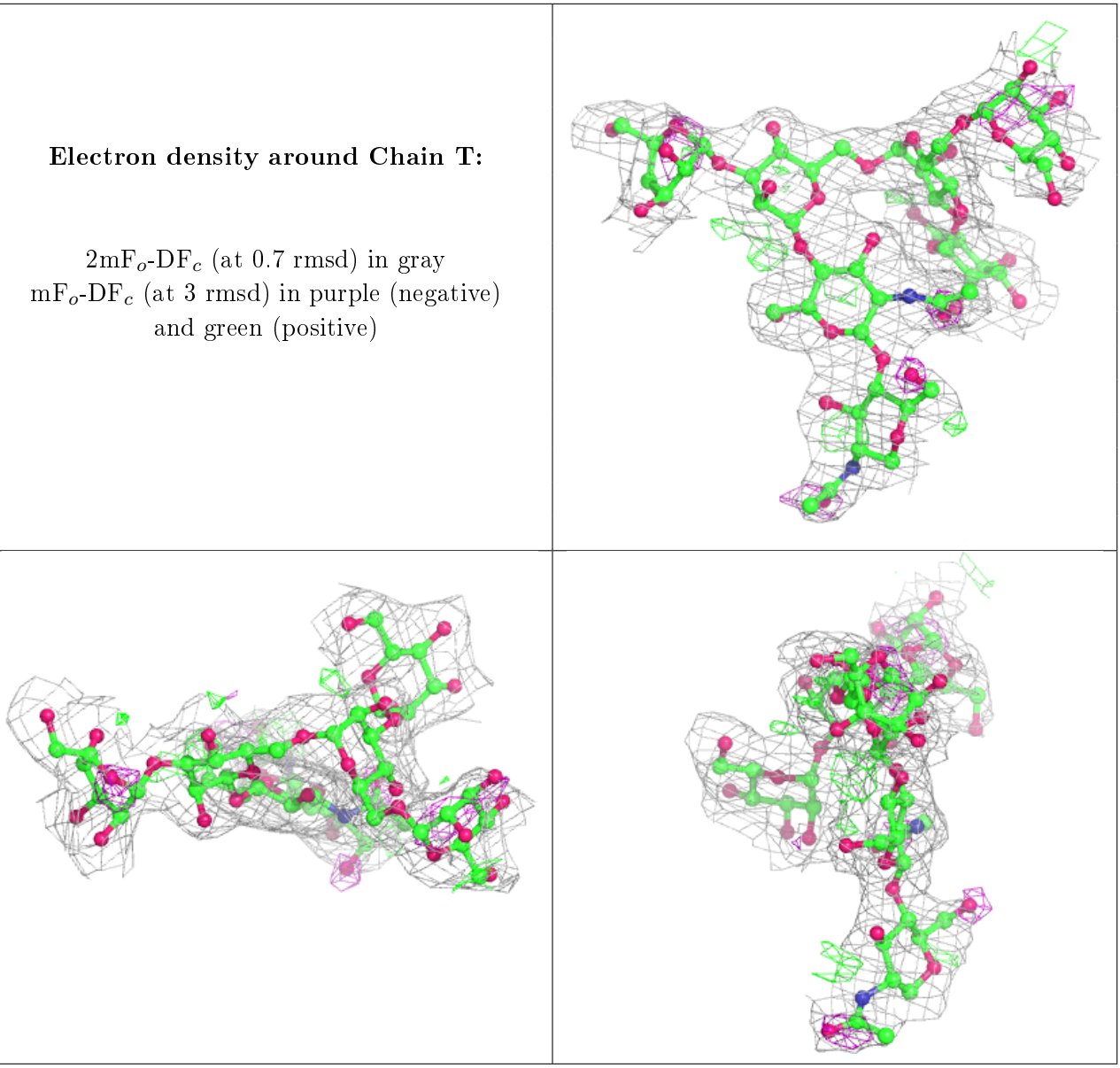






Electron density around Chain T:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.