



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:43 PM BST

PDB ID : 4IIF
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with castanospermine
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.45 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

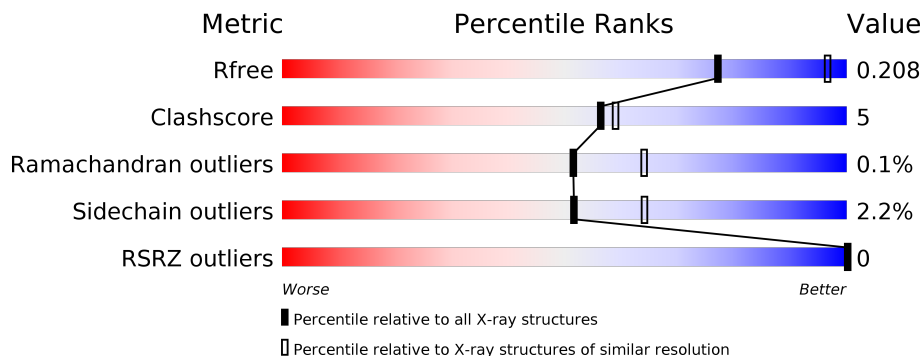
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



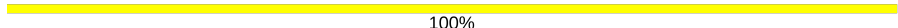

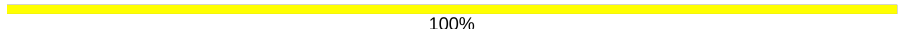
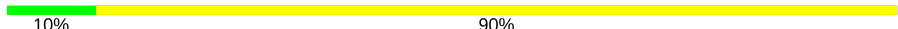
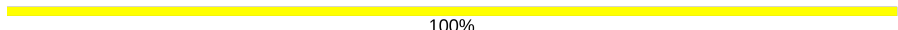
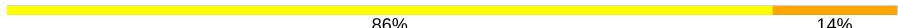

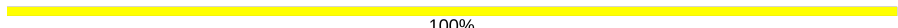
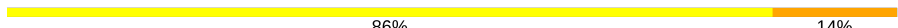
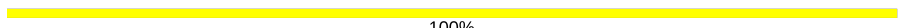
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	
1	B	841	
2	C	4	
2	K	4	
3	D	3	
3	G	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	3	 100%
4	E	2	 50% 50%
4	L	2	 100%
5	F	10	 10% 90%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 86% 14%
7	I	6	 100%
8	J	7	 86% 14%
9	P	8	 100%

2 Entry composition [i](#)

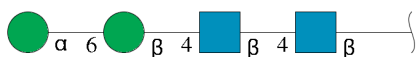
There are 14 unique types of molecules in this entry. The entry contains 14647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	833	6378	4026	1095	1239	18	0	0	0
1	B	832	6375	4023	1095	1239	18	0	0	0

- Molecule 2 is an oligosaccharide called 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
			Total	C	N	O			
2	C	4	50	28	2	20	0	0	0
2	K	4	50	28	2	20	0	0	0

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

Continued on next page...

Continued from previous page...

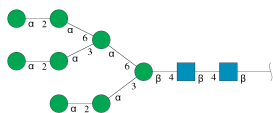
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	N	3	39	22	2	15	0	0	0

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



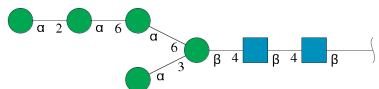
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0
4	L	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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
			Total	C	N	O			
5	F	10	116	64	2	50	0	0	0
5	M	10	116	64	2	50	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



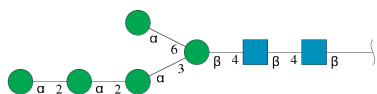
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



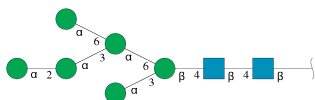
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



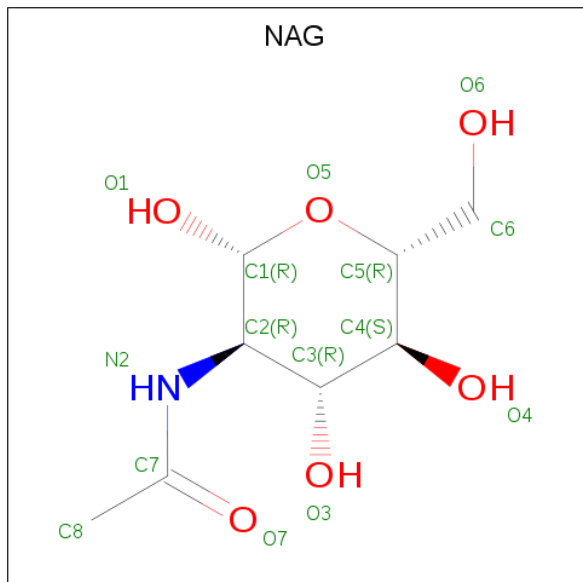
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



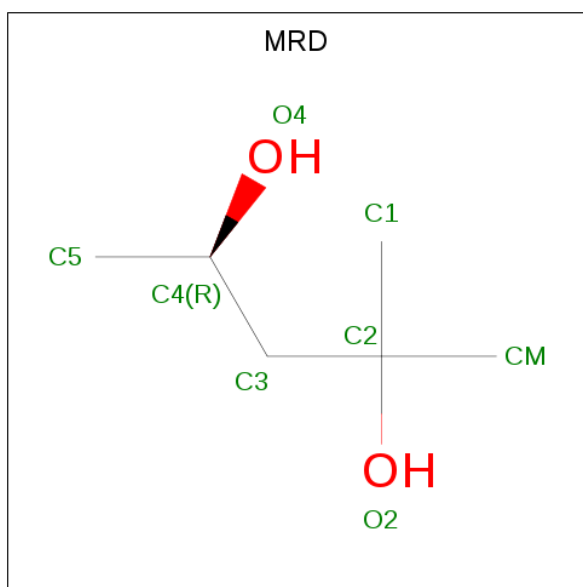
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



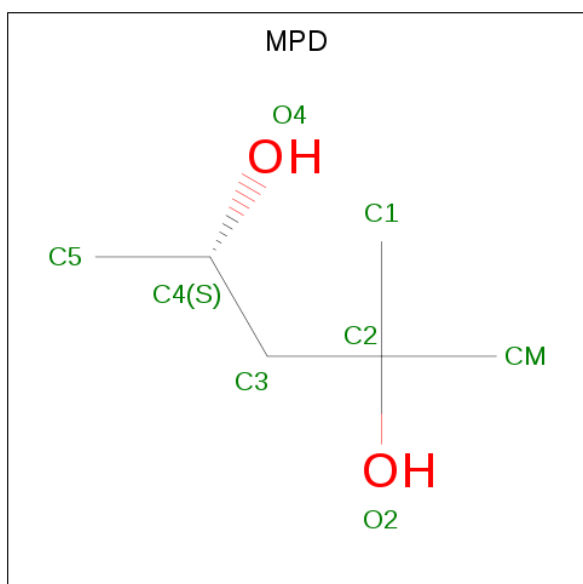
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	Total 14	C 8	N 1	O 5	0	0
10	A	1	Total 14	C 8	N 1	O 5	0	0
10	B	1	Total 14	C 8	N 1	O 5	0	0
10	B	1	Total 14	C 8	N 1	O 5	0	0
10	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 11 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



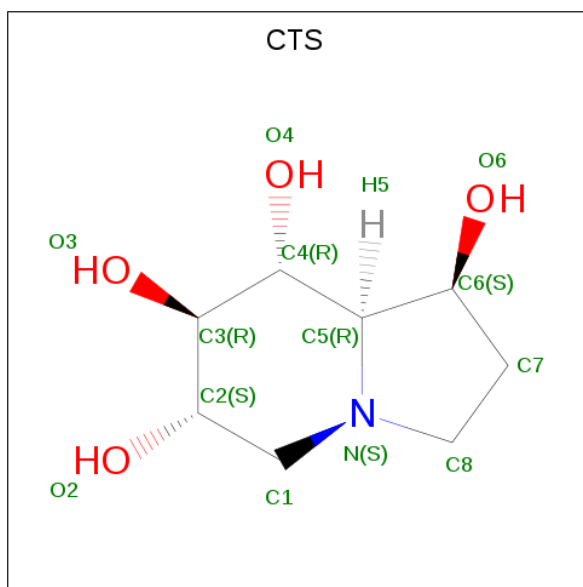
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			8	6	2		
11	B	1	Total	C	O	0	0
			8	6	2		
11	B	1	Total	C	O	0	0
			8	6	2		
11	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0

- Molecule 13 is CASTANOSPERMINE (three-letter code: CTS) (formula: $C_8H_{15}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C N O 13 8 1 4	0	0
13	B	1	Total C N O 13 8 1 4	0	0

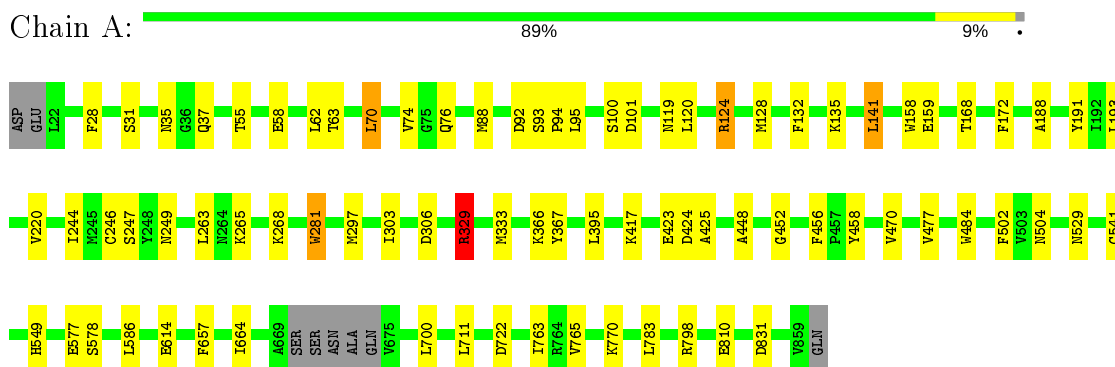
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	380	Total O 380 380	0	0
14	B	450	Total O 450 450	0	0

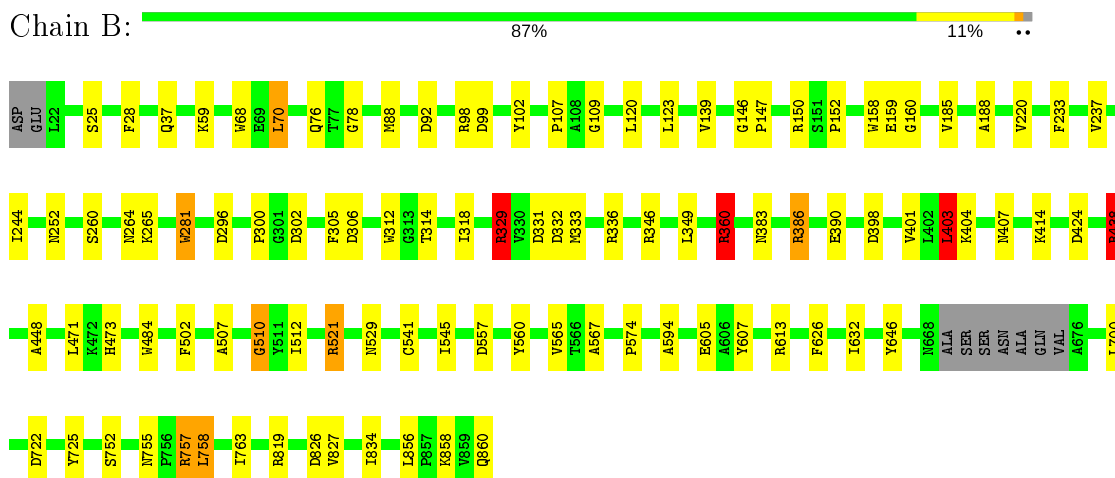
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

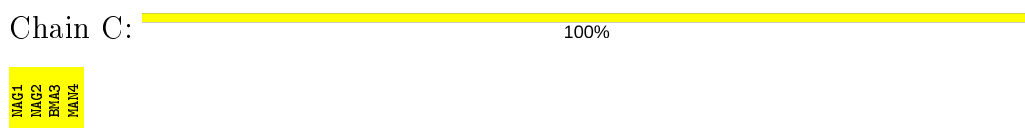
- Molecule 1: Beta-glucosidase 1



- Molecule 1: Beta-glucosidase 1



- Molecule 2: 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



- Molecule 2: 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:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain D:  100%

MAG1
MAG2
BMA3

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

Chain G:  100%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain E:  50% 50%

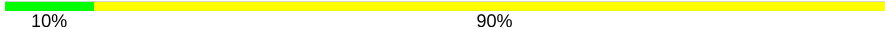
MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 F:  10% 90%

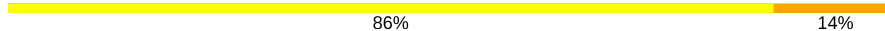
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 M:  100%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 6: alpha-D-mannopyranose-(1-2)-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 H:  86% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 6: alpha-D-mannopyranose-(1-2)-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 O:  86% 14%

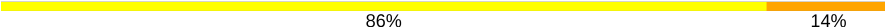
MAG1
MAG2
BMA3
MAN4
MAN5
MAN7

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

Chain I:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain J:  86% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 9: alpha-D-mannopyranose-(1-2)-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 P:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 122.24Å 222.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.45 49.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.08-2.45) 99.4 (49.08-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.205 0.157 , 0.208	Depositor DCC
R_{free} test set	4125 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, CTS, MRD, 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	0.83	3/6541 (0.0%)	0.89	8/8918 (0.1%)
1	B	0.89	2/6538 (0.0%)	0.95	17/8913 (0.2%)
All	All	0.86	5/13079 (0.0%)	0.92	25/17831 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	CYS	CB-SG	6.83	1.93	1.82
1	B	541	CYS	CB-SG	5.52	1.91	1.82
1	B	541	CYS	CA-CB	5.48	1.66	1.53
1	A	423	GLU	CD-OE1	5.33	1.31	1.25
1	A	541	CYS	CA-CB	5.08	1.65	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	B	521	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	B	329	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	B	521	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	438	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	B	329	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	A	329	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	70	LEU	CA-CB-CG	-8.89	94.85	115.30
1	B	360	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	B	70	LEU	CA-CB-CG	-8.56	95.61	115.30
1	B	826	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	124	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	831	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	541	CYS	N-CA-CB	6.90	123.02	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	A	798	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	360	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	101	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	329	ARG	CG-CD-NE	-6.02	99.15	111.80
1	B	438	ARG	CG-CD-NE	-5.66	99.92	111.80
1	B	150	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	403	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	403	LEU	CB-CG-CD1	5.42	120.22	111.00
1	A	722	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	510	GLY	N-CA-C	5.12	125.90	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6378	0	6089	52	0
1	B	6375	0	6082	75	0
2	C	50	0	43	0	0
2	K	50	0	43	3	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	25	2	0
4	L	28	0	25	0	0
5	F	116	0	97	0	0
5	M	116	0	97	0	0
6	H	83	0	70	2	0
6	O	83	0	70	1	0
7	I	72	0	61	0	0
8	J	83	0	70	2	0
9	P	94	0	79	0	0
10	A	28	0	26	0	0
10	B	42	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	8	0	14	1	0
11	B	24	0	42	6	0
12	A	16	0	28	1	0
13	A	13	0	15	2	0
13	B	13	0	15	2	0
14	A	380	0	0	4	0
14	B	450	0	0	7	0
All	All	14647	0	13132	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LEU:HD23	1:B:758:LEU:H	1.22	1.02
1:B:755:ASN:O	1:B:758:LEU:HD23	1.61	0.99
11:B:946:MRD:H1C2	11:B:946:MRD:H5C3	1.47	0.95
1:A:63:THR:HG21	1:A:333:MET:HE2	1.51	0.90
11:B:946:MRD:H1C2	11:B:946:MRD:C5	2.01	0.89
1:B:755:ASN:O	1:B:758:LEU:CD2	2.22	0.87
1:B:758:LEU:HD23	1:B:758:LEU:N	1.90	0.85
1:A:95:LEU:HA	1:A:128:MET:HE1	1.59	0.83
1:B:755:ASN:HB3	1:B:758:LEU:CD2	2.19	0.72
1:B:312:TRP:CH2	1:B:333:MET:HE1	2.24	0.72
1:A:63:THR:CG2	1:A:333:MET:HE2	2.20	0.72
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.26	0.70
1:B:92:ASP:OD2	13:B:948:CTS:O6	2.08	0.69
1:A:124:ARG:CZ	1:A:128:MET:HE3	2.24	0.67
1:B:281:TRP:HB2	13:B:948:CTS:H81	1.75	0.67
1:A:303:ILE:HG21	4:E:2:NAG:H81	1.77	0.65
1:B:755:ASN:HB3	1:B:758:LEU:HD21	1.79	0.64
1:A:770:LYS:HG3	1:A:810:GLU:HG3	1.79	0.64
1:A:159:GLU:HG3	14:A:1021:HOH:O	1.97	0.62
1:B:755:ASN:OD1	1:B:757:ARG:HB2	1.98	0.62
1:B:758:LEU:CD2	1:B:758:LEU:N	2.63	0.61
1:B:312:TRP:CZ3	1:B:333:MET:CE	2.85	0.60
1:B:349:LEU:HD22	14:B:1205:HOH:O	2.02	0.59
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.86	0.57
1:B:386:ARG:HD2	14:B:1314:HOH:O	2.05	0.57
1:B:312:TRP:CZ3	1:B:333:MET:HE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.86	0.57
1:A:159:GLU:CG	14:A:1021:HOH:O	2.51	0.56
1:A:614:GLU:HA	1:A:614:GLU:OE1	2.06	0.56
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.42	0.55
1:B:296:ASP:HA	1:B:333:MET:HG2	1.89	0.55
1:A:63:THR:HB	1:A:333:MET:CE	2.38	0.54
1:B:312:TRP:CH2	1:B:333:MET:CE	2.90	0.54
1:B:99:ASP:O	1:B:360:ARG:NH2	2.41	0.54
1:A:92:ASP:OD2	13:A:941:CTS:O6	2.21	0.53
1:B:260:SER:O	1:B:264:ASN:HB2	2.07	0.53
1:B:139:VAL:HG22	1:B:185:VAL:HB	1.91	0.53
1:B:424:ASP:HB3	1:B:502:PHE:HB3	1.92	0.52
1:B:755:ASN:O	1:B:758:LEU:HD21	2.09	0.51
1:B:827:VAL:HG11	2:K:2:NAG:O3	2.11	0.51
1:A:93:SER:HB2	1:A:452:GLY:HA2	1.92	0.51
1:A:424:ASP:HB3	1:A:502:PHE:HB3	1.92	0.51
1:B:401:VAL:HG12	1:B:403:LEU:HD13	1.93	0.51
1:A:168:THR:O	1:A:172:PHE:HB2	2.11	0.50
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.41	0.50
1:B:755:ASN:HB3	1:B:758:LEU:HD22	1.94	0.49
1:A:28:PHE:CG	1:A:265:LYS:HB2	2.48	0.49
1:B:107:PRO:HG3	1:B:574:PRO:O	2.13	0.49
11:B:947:MRD:O2	11:B:947:MRD:H5C3	2.13	0.49
1:A:281:TRP:CG	13:A:941:CTS:H72	2.48	0.49
1:A:141:LEU:HD21	1:A:281:TRP:CH2	2.48	0.48
1:B:146:GLY:HA2	1:B:147:PRO:C	2.34	0.48
1:B:763:ILE:HD13	1:B:856:LEU:HD22	1.95	0.48
1:B:158:TRP:CE2	1:B:448:ALA:HB3	2.49	0.48
1:B:403:LEU:HG	1:B:646:TYR:CD2	2.48	0.47
1:A:35:ASN:OD1	1:A:37:GLN:HB2	2.15	0.47
1:A:63:THR:CG2	1:A:333:MET:CE	2.92	0.47
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.49	0.47
1:B:448:ALA:HB1	1:B:507:ALA:O	2.14	0.47
1:A:664:ILE:CD1	1:A:765:VAL:HG22	2.44	0.47
11:A:938:MRD:O2	11:A:938:MRD:H5C3	2.14	0.47
1:A:191:TYR:O	1:A:246:CYS:HA	2.16	0.46
4:E:2:NAG:H3	4:E:2:NAG:H83	1.97	0.46
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.98	0.46
1:B:507:ALA:HB2	1:B:521:ARG:HG3	1.98	0.46
1:A:306:ASP:HA	14:A:1012:HOH:O	2.16	0.46
1:B:605:GLU:HB2	14:B:1095:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:946:MRD:H4	11:B:946:MRD:H1C1	1.65	0.46
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.51	0.45
1:B:59:LYS:NZ	1:B:331:ASP:OD1	2.39	0.45
1:A:128:MET:O	1:A:132:PHE:HD2	1.98	0.45
1:A:247:SER:HB2	1:A:249:ASN:OD1	2.17	0.45
1:B:545:ILE:HG12	1:B:567:ALA:HB3	1.97	0.45
1:A:93:SER:HB2	1:A:94:PRO:CD	2.47	0.45
1:B:827:VAL:CG1	2:K:2:NAG:O3	2.65	0.45
1:A:124:ARG:CZ	1:A:128:MET:CE	2.94	0.45
1:A:577:GLU:O	1:A:578:SER:C	2.56	0.45
1:A:664:ILE:HD12	1:A:765:VAL:HG22	1.98	0.44
1:B:159:GLU:HG3	14:B:1015:HOH:O	2.17	0.44
1:A:188:ALA:HB3	1:A:244:ILE:HD13	1.99	0.44
1:B:28:PHE:CG	1:B:265:LYS:HB2	2.52	0.44
1:B:819:ARG:HG3	1:B:834:ILE:HD11	1.99	0.44
1:B:37:GLN:NE2	1:B:752:SER:HB2	2.32	0.44
1:B:473:HIS:HE1	14:B:1122:HOH:O	1.99	0.44
1:B:68:TRP:O	1:B:306:ASP:OD1	2.36	0.44
1:A:484:TRP:CD2	6:H:3:BMA:H62	2.53	0.44
1:B:346:ARG:HA	1:B:346:ARG:HD2	1.90	0.44
1:B:233:PHE:O	1:B:237:VAL:HG23	2.18	0.43
1:B:438:ARG:HA	1:B:438:ARG:HD3	1.59	0.43
1:A:159:GLU:OE2	1:A:452:GLY:HA3	2.18	0.43
1:B:404:LYS:NZ	1:B:565:VAL:O	2.42	0.43
1:B:78:GLY:HA3	8:J:1:NAG:H62	1.99	0.43
1:A:366:LYS:HE2	1:A:367:TYR:OH	2.19	0.43
1:B:755:ASN:CA	1:B:758:LEU:HD21	2.48	0.43
1:A:329:ARG:HA	1:A:329:ARG:HD2	1.72	0.43
1:B:300:PRO:HG2	1:B:302:ASP:OD1	2.19	0.43
1:A:657:PHE:HA	1:A:770:LYS:O	2.19	0.43
1:A:100:SER:OG	1:A:135:LYS:HE3	2.18	0.43
1:B:109:GLY:HA3	1:B:160:GLY:O	2.19	0.43
1:B:332:ASP:O	1:B:336:ARG:HG3	2.19	0.43
1:B:755:ASN:CB	1:B:758:LEU:HD21	2.46	0.43
1:B:819:ARG:NH2	1:B:860:GLN:O	2.51	0.43
1:B:314:THR:HG22	1:B:318:ILE:HD12	2.01	0.42
1:B:722:ASP:HB3	1:B:725:TYR:HB2	2.01	0.42
1:B:37:GLN:HE22	1:B:752:SER:HB2	1.84	0.42
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.54	0.42
1:B:76:GLN:HA	1:B:88:MET:O	2.20	0.42
1:B:557:ASP:HA	1:B:560:TYR:CD2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:OG1	1:A:58:GLU:HG3	2.20	0.42
1:B:438:ARG:HD3	14:B:1102:HOH:O	2.20	0.42
1:A:470:VAL:HG11	1:A:477:VAL:HB	2.02	0.42
11:B:947:MRD:H5C1	2:K:1:NAG:H62	2.02	0.42
1:A:63:THR:O	1:A:297:MET:HA	2.19	0.42
1:A:263:LEU:O	1:A:268:LYS:HG3	2.20	0.41
12:A:939:MPD:HM1	12:A:939:MPD:O4	2.19	0.41
1:B:471:LEU:HA	1:B:471:LEU:HD23	1.85	0.41
1:A:504:ASN:HA	1:A:549:HIS:O	2.20	0.41
1:B:92:ASP:HB2	1:B:98:ARG:HB2	2.00	0.41
1:B:512:ILE:HG21	1:B:512:ILE:HD13	1.83	0.41
1:A:456:PHE:HB3	1:A:458:TYR:O	2.21	0.41
1:A:783:LEU:C	1:A:783:LEU:HD23	2.41	0.41
1:A:425:ALA:HB2	1:A:502:PHE:CD2	2.55	0.41
1:A:76:GLN:HA	1:A:88:MET:O	2.21	0.41
1:A:31:SER:HB3	1:A:329:ARG:HD3	2.01	0.41
1:B:152:PRO:HG3	1:B:607:TYR:CG	2.56	0.41
1:B:305:PHE:HE2	11:B:945:MRD:H1C2	1.86	0.41
1:B:398:ASP:O	1:B:594:ALA:HB2	2.20	0.41
1:B:78:GLY:CA	8:J:1:NAG:H62	2.51	0.41
1:B:329:ARG:HD2	1:B:329:ARG:HA	1.71	0.40
1:B:613:ARG:NH1	14:B:1051:HOH:O	2.26	0.40
1:A:417:LYS:HE3	14:A:1166:HOH:O	2.21	0.40
1:B:25:SER:HB2	1:B:252:ASN:HB2	2.03	0.40
1:B:757:ARG:CG	1:B:757:ARG:HH11	2.34	0.40
1:A:158:TRP:CE2	1:A:448:ALA:HB3	2.56	0.40
1:A:63:THR:CB	1:A:333:MET:CE	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	829/841 (99%)	798 (96%)	31 (4%)	0	100	100
1	B	828/841 (98%)	797 (96%)	30 (4%)	1 (0%)	51	64
All	All	1657/1682 (98%)	1595 (96%)	61 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	510	GLY

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	670/677 (99%)	657 (98%)	13 (2%)	57	69
1	B	670/677 (99%)	653 (98%)	17 (2%)	47	60
All	All	1340/1354 (99%)	1310 (98%)	30 (2%)	52	64

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

Mol	Chain	Res	Type
1	A	62	LEU
1	A	70	LEU
1	A	74	VAL
1	A	119	ASN
1	A	120	LEU
1	A	141	LEU
1	A	281	TRP
1	A	329	ARG
1	A	395	LEU
1	A	586	LEU
1	A	700	LEU
1	A	711	LEU
1	A	763	ILE
1	B	70	LEU
1	B	120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	123	LEU
1	B	281	TRP
1	B	329	ARG
1	B	360	ARG
1	B	386	ARG
1	B	390	GLU
1	B	403	LEU
1	B	407	ASN
1	B	414	LYS
1	B	438	ARG
1	B	632	ILE
1	B	700	LEU
1	B	757	ARG
1	B	758	LEU
1	B	858	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	ASN
1	B	37	GLN
1	B	473	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

76 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
2	NAG	C	2	2	14,14,15	0.75	0	17,19,21	1.81	2 (11%)
2	BMA	C	3	2	11,11,12	1.20	0	15,15,17	2.93	7 (46%)
2	MAN	C	4	2	11,11,12	0.97	0	15,15,17	2.67	7 (46%)
3	NAG	D	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	1.60	3 (17%)
3	NAG	D	2	3	14,14,15	0.65	0	17,19,21	1.32	2 (11%)
3	BMA	D	3	3	11,11,12	0.80	0	15,15,17	2.81	11 (73%)
4	NAG	E	1	1,4	14,14,15	0.62	0	17,19,21	1.82	3 (17%)
4	NAG	E	2	4	14,14,15	0.68	1 (7%)	17,19,21	1.69	4 (23%)
5	NAG	F	1	1,5	14,14,15	0.74	0	17,19,21	1.01	0
5	MAN	F	10	5	11,11,12	1.04	1 (9%)	15,15,17	1.64	2 (13%)
5	NAG	F	2	5	14,14,15	1.00	1 (7%)	17,19,21	1.83	4 (23%)
5	BMA	F	3	5	11,11,12	1.07	1 (9%)	15,15,17	1.11	1 (6%)
5	MAN	F	4	5	11,11,12	0.69	0	15,15,17	1.55	3 (20%)
5	MAN	F	5	5	11,11,12	1.20	2 (18%)	15,15,17	1.93	4 (26%)
5	MAN	F	6	5	11,11,12	0.78	0	15,15,17	1.52	3 (20%)
5	MAN	F	7	5	11,11,12	1.05	1 (9%)	15,15,17	1.50	5 (33%)
5	MAN	F	8	5	11,11,12	0.77	0	15,15,17	1.66	2 (13%)
5	MAN	F	9	5	11,11,12	0.87	0	15,15,17	1.20	2 (13%)
3	NAG	G	1	1,3	14,14,15	0.76	0	17,19,21	1.77	3 (17%)
3	NAG	G	2	3	14,14,15	0.84	0	17,19,21	1.50	5 (29%)
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	1.69	4 (26%)
6	NAG	H	1	1,6	14,14,15	0.75	0	17,19,21	1.40	3 (17%)
6	NAG	H	2	6	14,14,15	0.97	1 (7%)	17,19,21	2.17	6 (35%)
6	BMA	H	3	6	11,11,12	0.75	0	15,15,17	1.78	3 (20%)
6	MAN	H	4	6	11,11,12	1.08	1 (9%)	15,15,17	1.69	4 (26%)
6	MAN	H	5	6	11,11,12	0.84	1 (9%)	15,15,17	2.31	6 (40%)
6	MAN	H	6	6	11,11,12	0.85	0	15,15,17	1.67	3 (20%)
6	MAN	H	7	6	11,11,12	0.76	0	15,15,17	2.06	5 (33%)
7	NAG	I	1	1,7	14,14,15	0.88	1 (7%)	17,19,21	2.25	5 (29%)
7	NAG	I	2	7	14,14,15	0.88	1 (7%)	17,19,21	1.37	1 (5%)
7	BMA	I	3	7	11,11,12	0.69	0	15,15,17	1.90	4 (26%)
7	MAN	I	4	7	11,11,12	1.11	0	15,15,17	2.36	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	I	5	7	11,11,12	1.31	1 (9%)	15,15,17	2.09	6 (40%)
7	MAN	I	6	7	11,11,12	0.78	0	15,15,17	1.37	2 (13%)
8	NAG	J	1	1,8	14,14,15	1.20	1 (7%)	17,19,21	1.51	2 (11%)
8	NAG	J	2	8	14,14,15	0.87	0	17,19,21	1.63	3 (17%)
8	BMA	J	3	8	11,11,12	0.84	0	15,15,17	1.79	4 (26%)
8	MAN	J	4	8	11,11,12	0.77	0	15,15,17	1.12	1 (6%)
8	MAN	J	5	8	11,11,12	0.76	0	15,15,17	1.66	3 (20%)
8	MAN	J	6	8	11,11,12	0.76	0	15,15,17	1.31	2 (13%)
8	MAN	J	7	8	11,11,12	1.03	1 (9%)	15,15,17	2.09	5 (33%)
2	NAG	K	1	1,2	14,14,15	1.17	3 (21%)	17,19,21	1.66	5 (29%)
2	NAG	K	2	2	14,14,15	0.78	0	17,19,21	1.00	0
2	BMA	K	3	2	11,11,12	0.79	0	15,15,17	1.24	2 (13%)
2	MAN	K	4	2	11,11,12	1.31	1 (9%)	15,15,17	2.24	5 (33%)
4	NAG	L	1	1,4	14,14,15	0.96	1 (7%)	17,19,21	1.65	4 (23%)
4	NAG	L	2	4	14,14,15	0.79	0	17,19,21	1.70	4 (23%)
5	NAG	M	1	1,5	14,14,15	0.81	0	17,19,21	2.00	7 (41%)
5	MAN	M	10	5	11,11,12	1.03	1 (9%)	15,15,17	2.60	8 (53%)
5	NAG	M	2	5	14,14,15	0.78	0	17,19,21	1.38	2 (11%)
5	BMA	M	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.31	4 (26%)
5	MAN	M	4	5	11,11,12	0.74	0	15,15,17	2.14	7 (46%)
5	MAN	M	5	5	11,11,12	0.92	0	15,15,17	1.96	4 (26%)
5	MAN	M	6	5	11,11,12	0.85	0	15,15,17	1.57	2 (13%)
5	MAN	M	7	5	11,11,12	0.89	0	15,15,17	1.68	3 (20%)
5	MAN	M	8	5	11,11,12	0.78	0	15,15,17	1.66	2 (13%)
5	MAN	M	9	5	11,11,12	0.68	0	15,15,17	1.68	4 (26%)
3	NAG	N	1	1,3	14,14,15	0.83	0	17,19,21	1.66	7 (41%)
3	NAG	N	2	3	14,14,15	0.98	1 (7%)	17,19,21	1.21	1 (5%)
3	BMA	N	3	3	11,11,12	0.80	0	15,15,17	2.08	3 (20%)
6	NAG	O	1	1,6	14,14,15	1.08	1 (7%)	17,19,21	1.41	1 (5%)
6	NAG	O	2	6	14,14,15	1.15	2 (14%)	17,19,21	1.84	3 (17%)
6	BMA	O	3	6	11,11,12	0.69	0	15,15,17	1.27	2 (13%)
6	MAN	O	4	6	11,11,12	1.09	0	15,15,17	1.77	3 (20%)
6	MAN	O	5	6	11,11,12	0.70	0	15,15,17	1.70	2 (13%)
6	MAN	O	6	6	11,11,12	0.75	0	15,15,17	1.92	3 (20%)
6	MAN	O	7	6	11,11,12	0.94	0	15,15,17	2.39	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	P	1	1,9	14,14,15	0.98	1 (7%)	17,19,21	1.76	3 (17%)
9	NAG	P	2	9	14,14,15	0.89	1 (7%)	17,19,21	1.59	3 (17%)
9	BMA	P	3	9	11,11,12	1.12	1 (9%)	15,15,17	1.75	3 (20%)
9	MAN	P	4	9	11,11,12	0.67	0	15,15,17	1.76	4 (26%)
9	MAN	P	5	9	11,11,12	0.88	0	15,15,17	1.52	4 (26%)
9	MAN	P	6	9	11,11,12	0.82	0	15,15,17	1.72	2 (13%)
9	MAN	P	7	9	11,11,12	0.86	1 (9%)	15,15,17	2.05	5 (33%)
9	MAN	P	8	9	11,11,12	0.95	0	15,15,17	2.15	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	6/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	2/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
6	MAN	O	7	6	-	2/2/19/22	0/1/1/1
9	NAG	P	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	P	2	9	-	0/6/23/26	0/1/1/1
9	BMA	P	3	9	-	0/2/19/22	0/1/1/1
9	MAN	P	4	9	-	2/2/19/22	0/1/1/1
9	MAN	P	5	9	-	0/2/19/22	0/1/1/1
9	MAN	P	6	9	-	2/2/19/22	0/1/1/1
9	MAN	P	7	9	-	2/2/19/22	0/1/1/1
9	MAN	P	8	9	-	2/2/19/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	O5-C1	-3.11	1.38	1.43
6	O	1	NAG	O5-C1	-2.97	1.39	1.43
3	D	1	NAG	O5-C1	-2.91	1.39	1.43
7	I	5	MAN	O5-C1	-2.88	1.39	1.43
5	F	5	MAN	O5-C1	-2.73	1.39	1.43
6	O	2	NAG	O5-C1	-2.69	1.39	1.43
5	F	2	NAG	O5-C1	-2.69	1.39	1.43
5	M	3	BMA	O5-C1	-2.60	1.39	1.43
9	P	3	BMA	O5-C1	-2.48	1.39	1.43
9	P	1	NAG	O5-C1	-2.47	1.39	1.43
6	O	2	NAG	C2-N2	-2.39	1.42	1.46
2	K	4	MAN	C4-C3	2.38	1.58	1.52
9	P	2	NAG	O5-C1	-2.36	1.39	1.43
5	F	3	BMA	O2-C2	-2.33	1.38	1.43
6	H	4	MAN	O5-C1	-2.31	1.40	1.43
5	F	10	MAN	C2-C3	2.31	1.55	1.52
6	H	2	NAG	O5-C1	-2.30	1.40	1.43
2	K	1	NAG	O5-C1	-2.29	1.40	1.43
5	M	10	MAN	C2-C3	2.27	1.55	1.52
7	I	2	NAG	O5-C1	-2.26	1.40	1.43
6	H	5	MAN	O5-C1	-2.23	1.40	1.43
9	P	7	MAN	C2-C3	2.22	1.55	1.52
5	F	7	MAN	O5-C1	-2.22	1.40	1.43
4	E	2	NAG	O5-C1	-2.20	1.40	1.43
8	J	7	MAN	C4-C5	2.18	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	NAG	C1-C2	2.11	1.55	1.52
4	L	1	NAG	O5-C1	-2.07	1.40	1.43
2	K	1	NAG	C1-C2	2.06	1.55	1.52
5	F	5	MAN	O4-C4	-2.03	1.38	1.43
7	I	1	NAG	C1-C2	-2.01	1.49	1.52
2	K	1	NAG	C2-N2	-2.01	1.42	1.46

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O5-C5-C6	-7.12	96.05	107.20
2	C	4	MAN	C1-O5-C5	6.47	120.96	112.19
7	I	1	NAG	C1-O5-C5	6.43	120.90	112.19
6	O	7	MAN	C1-O5-C5	-6.12	103.90	112.19
3	N	3	BMA	C1-O5-C5	5.94	120.23	112.19
9	P	7	MAN	C1-O5-C5	5.66	119.86	112.19
5	M	10	MAN	O2-C2-C1	5.38	120.17	109.15
3	G	1	NAG	C1-O5-C5	5.36	119.46	112.19
6	O	6	MAN	C1-O5-C5	5.34	119.42	112.19
5	M	5	MAN	C1-O5-C5	5.29	119.36	112.19
6	H	2	NAG	C2-N2-C7	-5.24	115.45	122.90
7	I	4	MAN	O5-C5-C6	5.10	115.19	107.20
6	H	7	MAN	O5-C1-C2	-4.87	103.25	110.77
9	P	1	NAG	C1-O5-C5	4.81	118.71	112.19
5	M	8	MAN	C1-O5-C5	4.74	118.61	112.19
4	L	2	NAG	C3-C4-C5	-4.72	101.83	110.24
5	M	10	MAN	O5-C5-C6	4.71	114.58	107.20
7	I	3	BMA	C1-O5-C5	4.70	118.56	112.19
3	D	3	BMA	C3-C4-C5	4.65	118.54	110.24
9	P	3	BMA	O5-C1-C2	-4.62	103.64	110.77
2	C	2	NAG	C3-C4-C5	-4.58	102.06	110.24
6	H	5	MAN	O5-C1-C2	-4.56	103.73	110.77
6	H	5	MAN	C1-O5-C5	4.50	118.29	112.19
3	D	3	BMA	O5-C5-C6	4.49	114.24	107.20
8	J	7	MAN	O4-C4-C3	-4.48	100.00	110.35
3	D	1	NAG	O5-C1-C2	-4.42	104.31	111.29
4	E	1	NAG	C1-O5-C5	4.35	118.09	112.19
5	F	2	NAG	O5-C5-C6	-4.35	100.38	107.20
5	M	9	MAN	C1-O5-C5	4.34	118.08	112.19
8	J	5	MAN	O2-C2-C3	-4.31	101.50	110.14
2	C	4	MAN	O5-C1-C2	4.30	117.42	110.77
2	K	4	MAN	O5-C5-C6	4.30	113.94	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1	NAG	C1-C2-N2	-4.29	103.15	110.49
9	P	4	MAN	O2-C2-C1	-4.28	100.39	109.15
2	C	3	BMA	C3-C4-C5	4.28	117.87	110.24
6	O	4	MAN	C1-O5-C5	4.27	117.98	112.19
2	K	4	MAN	C6-C5-C4	4.17	122.78	113.00
6	H	3	BMA	C1-O5-C5	4.10	117.75	112.19
6	O	7	MAN	O5-C5-C6	4.08	113.60	107.20
9	P	8	MAN	C3-C4-C5	4.04	117.44	110.24
2	C	4	MAN	C3-C4-C5	4.04	117.44	110.24
6	O	5	MAN	C1-O5-C5	4.01	117.63	112.19
6	O	2	NAG	O5-C1-C2	-4.01	104.96	111.29
6	H	4	MAN	O3-C3-C4	3.98	119.54	110.35
8	J	2	NAG	C1-O5-C5	3.97	117.57	112.19
5	F	4	MAN	O6-C6-C5	-3.97	97.69	111.29
5	M	5	MAN	O6-C6-C5	-3.93	97.82	111.29
5	F	10	MAN	O2-C2-C3	3.93	118.00	110.14
6	H	6	MAN	O5-C5-C6	3.91	113.34	107.20
2	C	3	BMA	C1-C2-C3	3.88	114.44	109.67
2	K	4	MAN	O3-C3-C4	3.87	119.31	110.35
8	J	1	NAG	C1-O5-C5	3.85	117.41	112.19
8	J	3	BMA	C1-C2-C3	-3.85	104.94	109.67
6	H	2	NAG	O5-C1-C2	-3.80	105.29	111.29
5	M	2	NAG	C1-C2-N2	-3.78	104.03	110.49
6	H	7	MAN	C1-C2-C3	-3.77	105.03	109.67
3	D	3	BMA	C1-C2-C3	3.75	114.28	109.67
5	M	10	MAN	C6-C5-C4	-3.74	104.25	113.00
9	P	2	NAG	C2-N2-C7	-3.73	117.59	122.90
7	I	2	NAG	C1-O5-C5	3.73	117.24	112.19
4	E	1	NAG	C2-N2-C7	3.71	128.19	122.90
6	O	1	NAG	C2-N2-C7	-3.70	117.63	122.90
7	I	5	MAN	C6-C5-C4	3.67	121.59	113.00
9	P	8	MAN	C1-C2-C3	3.65	114.16	109.67
5	M	6	MAN	C1-O5-C5	3.64	117.13	112.19
5	M	4	MAN	O3-C3-C2	3.61	116.90	109.99
8	J	5	MAN	O5-C5-C6	3.60	112.84	107.20
9	P	6	MAN	O5-C5-C6	3.60	112.84	107.20
7	I	5	MAN	O2-C2-C3	-3.58	102.96	110.14
6	O	2	NAG	C3-C4-C5	-3.57	103.87	110.24
6	O	2	NAG	C2-N2-C7	-3.53	117.88	122.90
3	D	3	BMA	O2-C2-C3	-3.50	103.12	110.14
5	M	4	MAN	C1-O5-C5	3.49	116.92	112.19
4	L	1	NAG	C1-O5-C5	3.48	116.91	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O5-C5-C4	3.48	119.28	110.83
5	F	10	MAN	C2-C3-C4	3.46	116.88	110.89
2	K	1	NAG	C1-O5-C5	3.45	116.87	112.19
4	E	2	NAG	C8-C7-N2	3.41	121.88	116.10
2	K	1	NAG	C4-C3-C2	-3.41	106.02	111.02
3	N	3	BMA	C3-C4-C5	3.41	116.32	110.24
3	G	3	BMA	C1-O5-C5	3.38	116.77	112.19
6	H	3	BMA	C6-C5-C4	-3.37	105.12	113.00
3	G	3	BMA	O2-C2-C1	3.36	116.03	109.15
5	F	2	NAG	C1-C2-N2	-3.36	104.74	110.49
5	F	6	MAN	O5-C5-C6	3.35	112.46	107.20
5	F	5	MAN	C1-O5-C5	3.34	116.72	112.19
9	P	6	MAN	O3-C3-C4	3.32	118.01	110.35
5	M	1	NAG	O4-C4-C5	-3.31	101.09	109.30
2	C	2	NAG	O5-C5-C6	3.29	112.36	107.20
8	J	6	MAN	O5-C5-C6	3.29	112.36	107.20
3	D	1	NAG	O5-C5-C4	-3.28	102.85	110.83
6	H	1	NAG	O3-C3-C2	-3.27	102.70	109.47
2	K	4	MAN	C1-C2-C3	3.24	113.65	109.67
8	J	7	MAN	C6-C5-C4	3.23	120.57	113.00
6	H	1	NAG	C2-N2-C7	-3.22	118.31	122.90
5	M	7	MAN	O2-C2-C3	-3.21	103.71	110.14
9	P	8	MAN	C2-C3-C4	3.19	116.41	110.89
6	O	7	MAN	O5-C1-C2	-3.18	105.86	110.77
9	P	5	MAN	O2-C2-C3	-3.18	103.78	110.14
6	H	3	BMA	O5-C5-C6	3.17	112.17	107.20
5	M	7	MAN	C1-O5-C5	3.16	116.48	112.19
5	F	8	MAN	C1-O5-C5	3.15	116.46	112.19
5	M	4	MAN	C1-C2-C3	-3.15	105.79	109.67
5	M	10	MAN	O2-C2-C3	3.11	116.37	110.14
4	E	2	NAG	C2-N2-C7	3.10	127.31	122.90
6	H	5	MAN	C6-C5-C4	-3.10	105.75	113.00
3	D	2	NAG	C2-N2-C7	-3.09	118.50	122.90
5	M	1	NAG	C3-C4-C5	-3.09	104.72	110.24
9	P	2	NAG	C1-O5-C5	3.09	116.38	112.19
8	J	7	MAN	O6-C6-C5	3.08	121.85	111.29
5	M	1	NAG	C1-C2-N2	-3.06	105.26	110.49
3	N	1	NAG	C1-C2-N2	-3.04	105.30	110.49
6	O	6	MAN	C2-C3-C4	-3.03	105.65	110.89
2	K	4	MAN	O6-C6-C5	3.03	121.69	111.29
3	D	3	BMA	O3-C3-C2	-3.00	104.25	109.99
7	I	4	MAN	O6-C6-C5	2.99	121.54	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	4	MAN	O4-C4-C3	-2.99	103.44	110.35
8	J	2	NAG	O4-C4-C5	-2.99	101.88	109.30
5	F	5	MAN	O6-C6-C5	-2.98	101.06	111.29
2	C	3	BMA	C2-C3-C4	-2.98	105.74	110.89
2	C	4	MAN	O3-C3-C2	-2.97	104.30	109.99
9	P	7	MAN	C3-C4-C5	2.97	115.53	110.24
9	P	8	MAN	O5-C1-C2	2.96	115.34	110.77
3	G	2	NAG	C2-N2-C7	-2.96	118.69	122.90
9	P	2	NAG	O5-C5-C6	2.95	111.83	107.20
6	H	2	NAG	C3-C4-C5	-2.93	105.02	110.24
7	I	5	MAN	C1-O5-C5	2.92	116.14	112.19
8	J	7	MAN	O5-C5-C6	2.92	111.78	107.20
4	L	1	NAG	C6-C5-C4	-2.90	106.22	113.00
7	I	6	MAN	O3-C3-C4	2.89	117.04	110.35
5	F	8	MAN	O3-C3-C2	-2.89	104.45	109.99
6	O	4	MAN	O4-C4-C3	-2.88	103.69	110.35
7	I	4	MAN	C1-O5-C5	2.87	116.08	112.19
5	F	9	MAN	O5-C5-C6	2.86	111.69	107.20
2	C	4	MAN	O3-C3-C4	2.86	116.95	110.35
3	D	3	BMA	O5-C5-C4	-2.84	103.91	110.83
2	C	3	BMA	C1-O5-C5	2.83	116.03	112.19
7	I	1	NAG	C6-C5-C4	-2.82	106.40	113.00
6	O	4	MAN	C1-C2-C3	2.81	113.12	109.67
9	P	3	BMA	O5-C5-C4	-2.81	104.00	110.83
2	K	1	NAG	O5-C1-C2	-2.80	106.86	111.29
3	D	3	BMA	O5-C1-C2	-2.79	106.46	110.77
3	G	2	NAG	C4-C3-C2	2.77	115.08	111.02
7	I	5	MAN	C3-C4-C5	-2.77	105.31	110.24
5	M	10	MAN	O3-C3-C2	2.75	115.26	109.99
3	G	3	BMA	C3-C4-C5	2.73	115.12	110.24
7	I	3	BMA	O5-C1-C2	2.73	114.99	110.77
2	C	3	BMA	O3-C3-C4	2.72	116.65	110.35
3	D	3	BMA	C2-C3-C4	2.71	115.59	110.89
6	H	2	NAG	C1-O5-C5	-2.70	108.53	112.19
8	J	7	MAN	O3-C3-C2	2.69	115.15	109.99
5	M	1	NAG	C8-C7-N2	2.69	120.66	116.10
5	M	3	BMA	C2-C3-C4	-2.68	106.25	110.89
5	M	4	MAN	C2-C3-C4	-2.68	106.25	110.89
3	G	1	NAG	C1-C2-N2	-2.68	105.91	110.49
4	L	1	NAG	O4-C4-C5	-2.67	102.66	109.30
7	I	5	MAN	O4-C4-C3	-2.65	104.22	110.35
8	J	3	BMA	O5-C5-C6	2.64	111.35	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	O5-C1-C2	-2.63	107.13	111.29
4	E	2	NAG	C1-O5-C5	2.62	115.75	112.19
6	H	5	MAN	O6-C6-C5	-2.62	102.31	111.29
5	M	1	NAG	O5-C5-C6	2.62	111.31	107.20
6	H	7	MAN	O2-C2-C3	2.59	115.32	110.14
5	F	7	MAN	C1-O5-C5	-2.58	108.70	112.19
5	F	4	MAN	O3-C3-C4	-2.56	104.42	110.35
9	P	1	NAG	O4-C4-C5	-2.54	102.98	109.30
5	M	6	MAN	O2-C2-C3	2.54	115.23	110.14
2	K	3	BMA	C1-O5-C5	2.54	115.63	112.19
4	L	2	NAG	O6-C6-C5	-2.54	102.58	111.29
5	F	5	MAN	O4-C4-C5	-2.53	103.02	109.30
8	J	3	BMA	O5-C5-C4	-2.52	104.70	110.83
6	H	5	MAN	O2-C2-C3	-2.52	105.10	110.14
3	N	3	BMA	C2-C3-C4	-2.50	106.56	110.89
9	P	4	MAN	O4-C4-C3	-2.48	104.61	110.35
3	N	1	NAG	C1-O5-C5	2.48	115.56	112.19
5	F	4	MAN	O2-C2-C3	-2.47	105.19	110.14
5	F	2	NAG	O5-C1-C2	-2.47	107.39	111.29
9	P	8	MAN	O4-C4-C5	-2.47	103.17	109.30
5	M	1	NAG	C1-O5-C5	-2.46	108.85	112.19
9	P	4	MAN	C1-C2-C3	2.46	112.69	109.67
5	M	4	MAN	O3-C3-C4	-2.46	104.66	110.35
7	I	3	BMA	O3-C3-C4	2.46	116.03	110.35
9	P	1	NAG	O5-C1-C2	-2.44	107.43	111.29
6	H	5	MAN	O2-C2-C1	2.44	114.14	109.15
5	M	7	MAN	O5-C5-C6	2.44	111.03	107.20
3	D	3	BMA	C1-O5-C5	2.44	115.49	112.19
4	L	2	NAG	O4-C4-C5	2.44	115.34	109.30
2	K	3	BMA	C3-C4-C5	2.43	114.58	110.24
5	F	7	MAN	O4-C4-C5	2.43	115.33	109.30
3	D	2	NAG	O5-C5-C6	2.42	111.00	107.20
3	D	1	NAG	C1-C2-N2	2.42	114.63	110.49
3	G	2	NAG	C3-C4-C5	2.42	114.56	110.24
8	J	3	BMA	O6-C6-C5	-2.42	102.99	111.29
7	I	5	MAN	O3-C3-C4	2.41	115.93	110.35
5	F	5	MAN	C6-C5-C4	-2.40	107.37	113.00
6	H	7	MAN	O5-C5-C6	2.40	110.97	107.20
9	P	7	MAN	O2-C2-C3	2.40	114.95	110.14
5	M	9	MAN	O2-C2-C1	2.38	114.02	109.15
5	F	9	MAN	C6-C5-C4	-2.37	107.46	113.00
5	M	3	BMA	O5-C5-C6	2.36	110.90	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	6	MAN	C1-O5-C5	2.35	115.38	112.19
3	N	1	NAG	O4-C4-C5	-2.35	103.46	109.30
3	N	1	NAG	O7-C7-C8	-2.34	117.70	122.06
5	M	4	MAN	O5-C5-C4	-2.34	105.13	110.83
9	P	3	BMA	O2-C2-C1	2.32	113.90	109.15
6	H	4	MAN	O3-C3-C2	2.32	114.44	109.99
5	F	7	MAN	O5-C1-C2	-2.32	107.19	110.77
7	I	3	BMA	O2-C2-C3	2.31	114.77	110.14
5	F	6	MAN	C1-C2-C3	-2.30	106.83	109.67
7	I	1	NAG	O5-C5-C6	2.29	110.79	107.20
3	N	1	NAG	C2-N2-C7	2.29	126.16	122.90
7	I	4	MAN	O4-C4-C5	2.29	114.97	109.30
3	G	2	NAG	C1-O5-C5	2.28	115.29	112.19
5	F	7	MAN	O2-C2-C3	-2.28	105.57	110.14
5	M	4	MAN	O6-C6-C5	-2.28	103.48	111.29
3	G	3	BMA	O3-C3-C4	2.28	115.61	110.35
5	M	5	MAN	O3-C3-C4	-2.27	105.09	110.35
9	P	7	MAN	C1-C2-C3	-2.27	106.87	109.67
3	D	3	BMA	O6-C6-C5	2.27	119.09	111.29
6	H	6	MAN	O3-C3-C4	-2.27	105.09	110.35
5	M	5	MAN	C6-C5-C4	-2.27	107.68	113.00
8	J	2	NAG	O6-C6-C5	-2.27	103.50	111.29
6	H	7	MAN	C2-C3-C4	2.26	114.81	110.89
3	D	3	BMA	O4-C4-C3	-2.26	105.12	110.35
4	L	1	NAG	O5-C5-C6	-2.26	103.67	107.20
6	O	6	MAN	O6-C6-C5	-2.25	103.56	111.29
2	C	4	MAN	O6-C6-C5	2.25	119.01	111.29
8	J	1	NAG	C8-C7-N2	-2.25	112.29	116.10
5	M	1	NAG	C4-C3-C2	2.25	114.31	111.02
7	I	4	MAN	O5-C1-C2	-2.24	107.31	110.77
4	L	2	NAG	C2-N2-C7	2.24	126.10	122.90
5	F	3	BMA	O2-C2-C3	-2.23	105.67	110.14
9	P	8	MAN	O2-C2-C1	2.23	113.71	109.15
6	H	2	NAG	O5-C5-C6	2.23	110.69	107.20
3	N	2	NAG	C2-N2-C7	2.22	126.07	122.90
5	M	2	NAG	C4-C3-C2	2.22	114.27	111.02
5	M	8	MAN	C6-C5-C4	-2.22	107.80	113.00
2	C	4	MAN	O4-C4-C5	-2.22	103.78	109.30
2	K	1	NAG	C8-C7-N2	-2.22	112.34	116.10
2	K	1	NAG	O7-C7-N2	2.21	126.02	121.95
6	H	4	MAN	O5-C1-C2	2.21	114.19	110.77
9	P	4	MAN	O5-C1-C2	-2.21	107.36	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	7	MAN	C6-C5-C4	2.21	118.19	113.00
7	I	4	MAN	C6-C5-C4	2.21	118.19	113.00
7	I	1	NAG	O4-C4-C3	2.17	115.38	110.35
6	O	3	BMA	C3-C4-C5	-2.17	106.37	110.24
5	F	7	MAN	C2-C3-C4	-2.16	107.16	110.89
9	P	5	MAN	O5-C5-C6	2.16	110.59	107.20
9	P	5	MAN	C1-C2-C3	2.15	112.31	109.67
5	M	9	MAN	O2-C2-C3	-2.15	105.83	110.14
3	N	1	NAG	O5-C5-C6	2.15	110.58	107.20
6	H	4	MAN	C2-C3-C4	-2.14	107.19	110.89
5	F	2	NAG	C1-O5-C5	2.14	115.09	112.19
5	F	6	MAN	O4-C4-C3	-2.12	105.45	110.35
3	N	1	NAG	C8-C7-N2	2.12	119.68	116.10
6	H	2	NAG	C6-C5-C4	2.11	117.95	113.00
6	O	5	MAN	C6-C5-C4	-2.11	108.07	113.00
5	M	9	MAN	O5-C1-C2	2.09	114.00	110.77
7	I	6	MAN	O6-C6-C5	-2.08	104.15	111.29
6	O	3	BMA	O3-C3-C2	2.08	113.97	109.99
8	J	4	MAN	C1-C2-C3	-2.07	107.12	109.67
5	M	3	BMA	O3-C3-C4	-2.05	105.60	110.35
8	J	6	MAN	C1-C2-C3	2.05	112.19	109.67
6	O	7	MAN	C3-C4-C5	2.05	113.89	110.24
4	E	2	NAG	O7-C7-C8	-2.04	118.27	122.06
5	M	10	MAN	C1-C2-C3	-2.04	107.16	109.67
9	P	5	MAN	O5-C1-C2	-2.04	107.62	110.77
2	C	1	NAG	O3-C3-C2	-2.03	105.26	109.47
5	M	10	MAN	O5-C1-C2	2.03	113.91	110.77
3	G	1	NAG	O5-C5-C6	-2.02	104.03	107.20
5	M	10	MAN	O4-C4-C5	-2.01	104.29	109.30
5	M	3	BMA	C6-C5-C4	-2.01	108.29	113.00
6	H	1	NAG	C1-O5-C5	2.01	114.92	112.19
8	J	5	MAN	O5-C1-C2	2.01	113.87	110.77
9	P	7	MAN	C2-C3-C4	2.01	114.36	110.89
3	G	2	NAG	C1-C2-N2	-2.00	107.07	110.49

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	4	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
9	P	6	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	O	7	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
8	J	6	MAN	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
9	P	8	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
8	J	6	MAN	C4-C5-C6-O6
7	I	6	MAN	C4-C5-C6-O6
5	F	10	MAN	C4-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
6	H	5	MAN	C4-C5-C6-O6
9	P	6	MAN	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
6	O	7	MAN	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
8	J	5	MAN	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
9	P	7	MAN	O5-C5-C6-O6
5	M	10	MAN	O5-C5-C6-O6
9	P	8	MAN	C4-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
9	P	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
5	F	10	MAN	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
9	P	4	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
5	M	10	MAN	C4-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
7	I	5	MAN	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
6	H	3	BMA	C4-C5-C6-O6
8	J	5	MAN	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

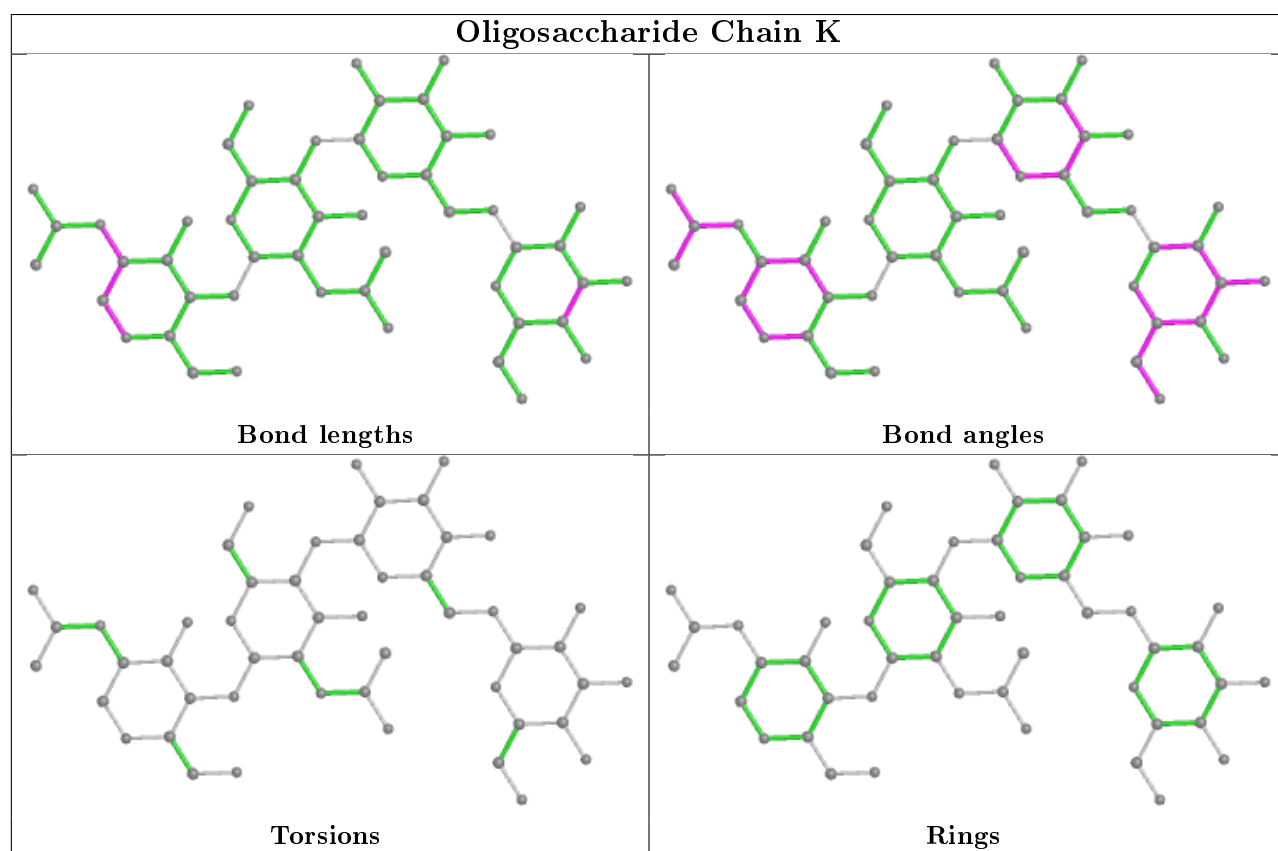
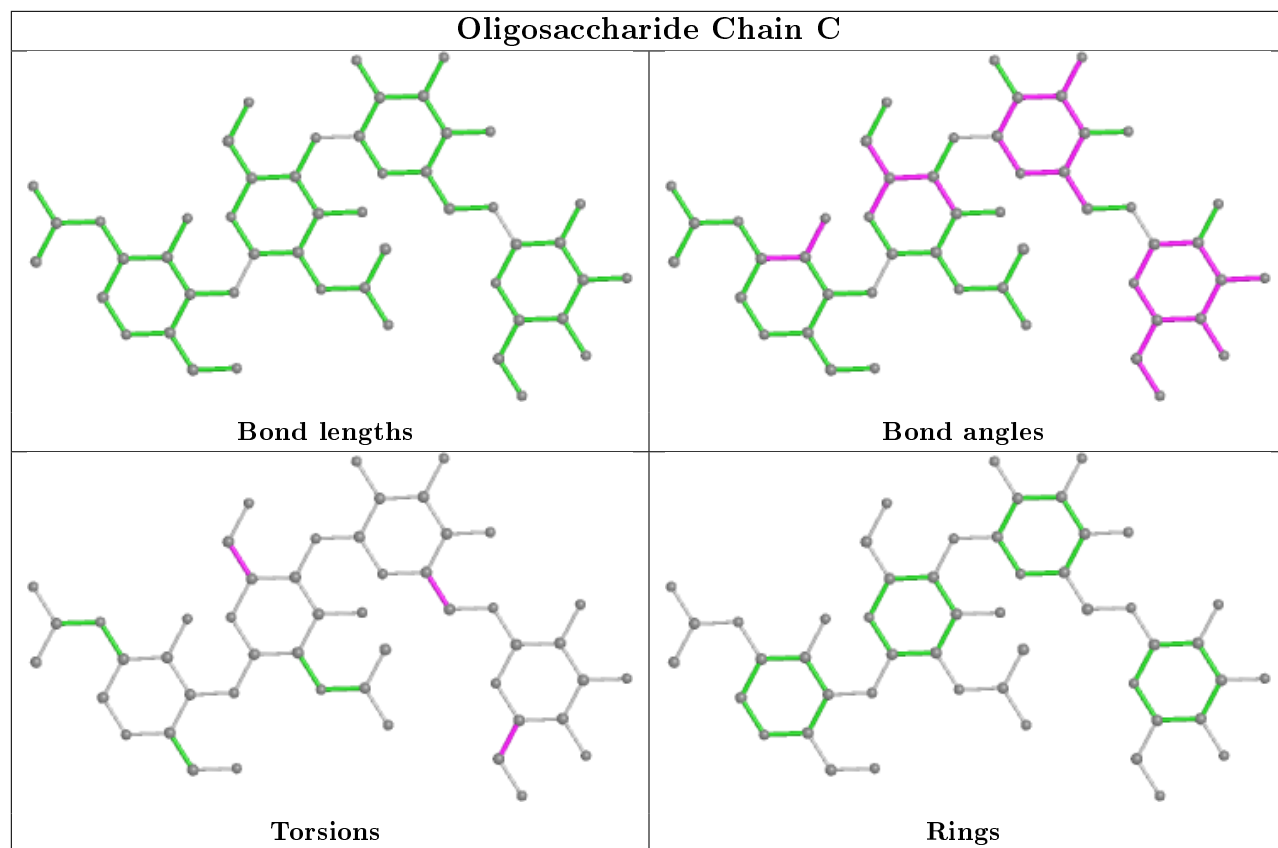
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
9	P	7	MAN	C4-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
9	P	4	MAN	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
8	J	2	NAG	C4-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6

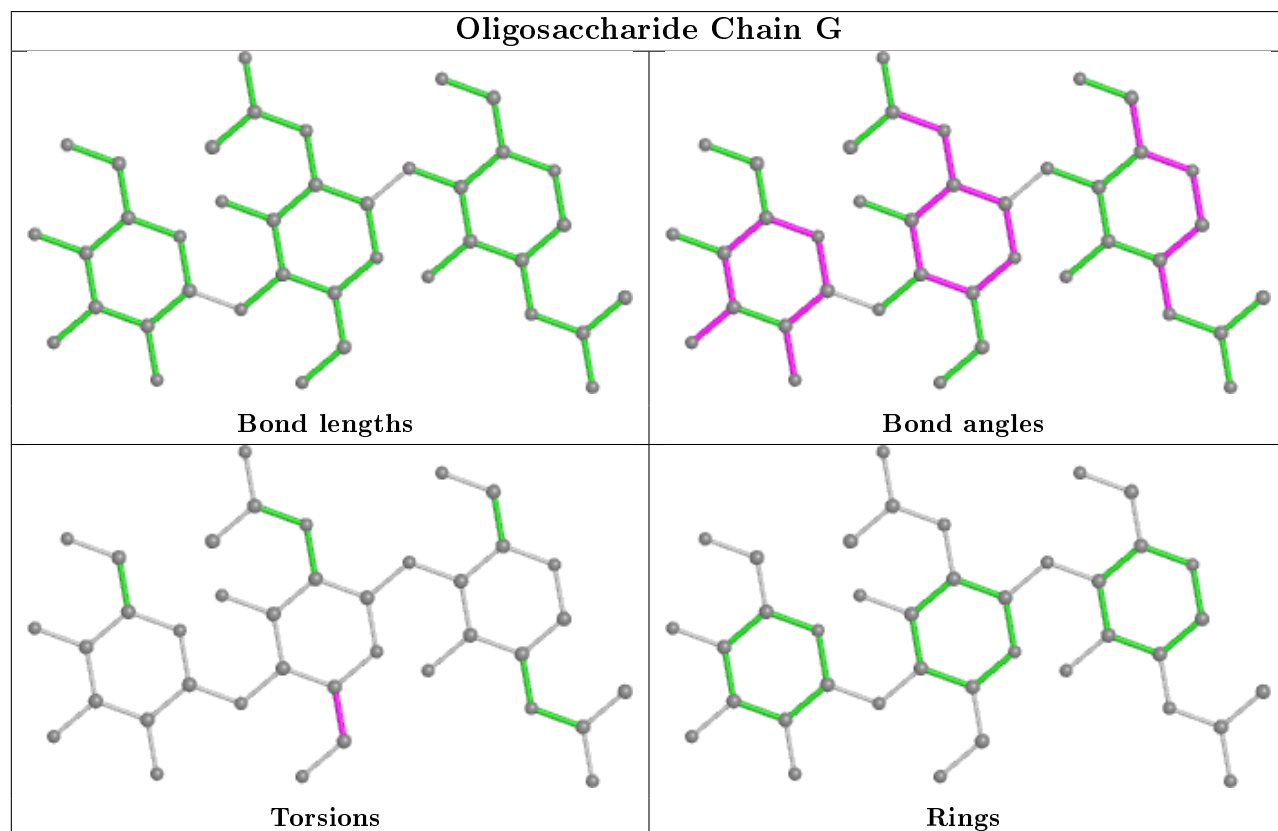
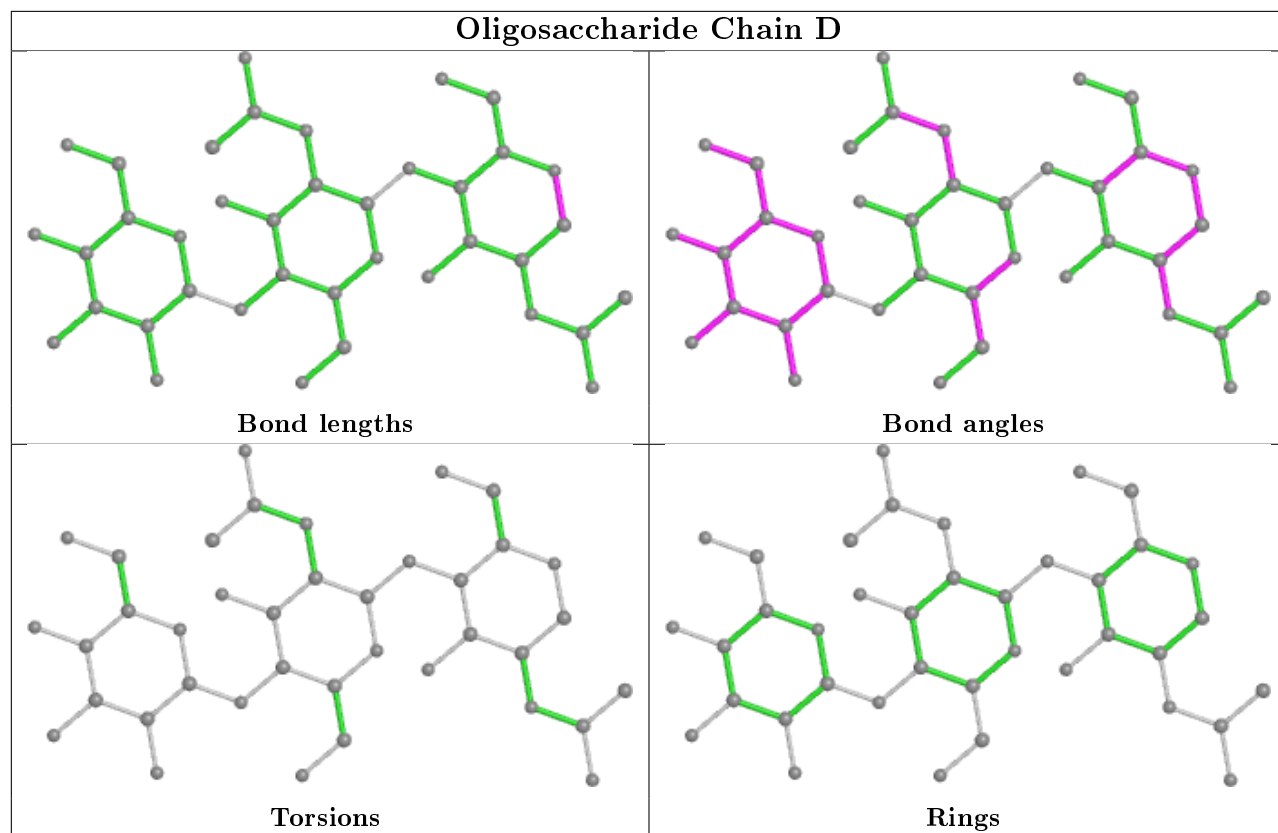
There are no ring outliers.

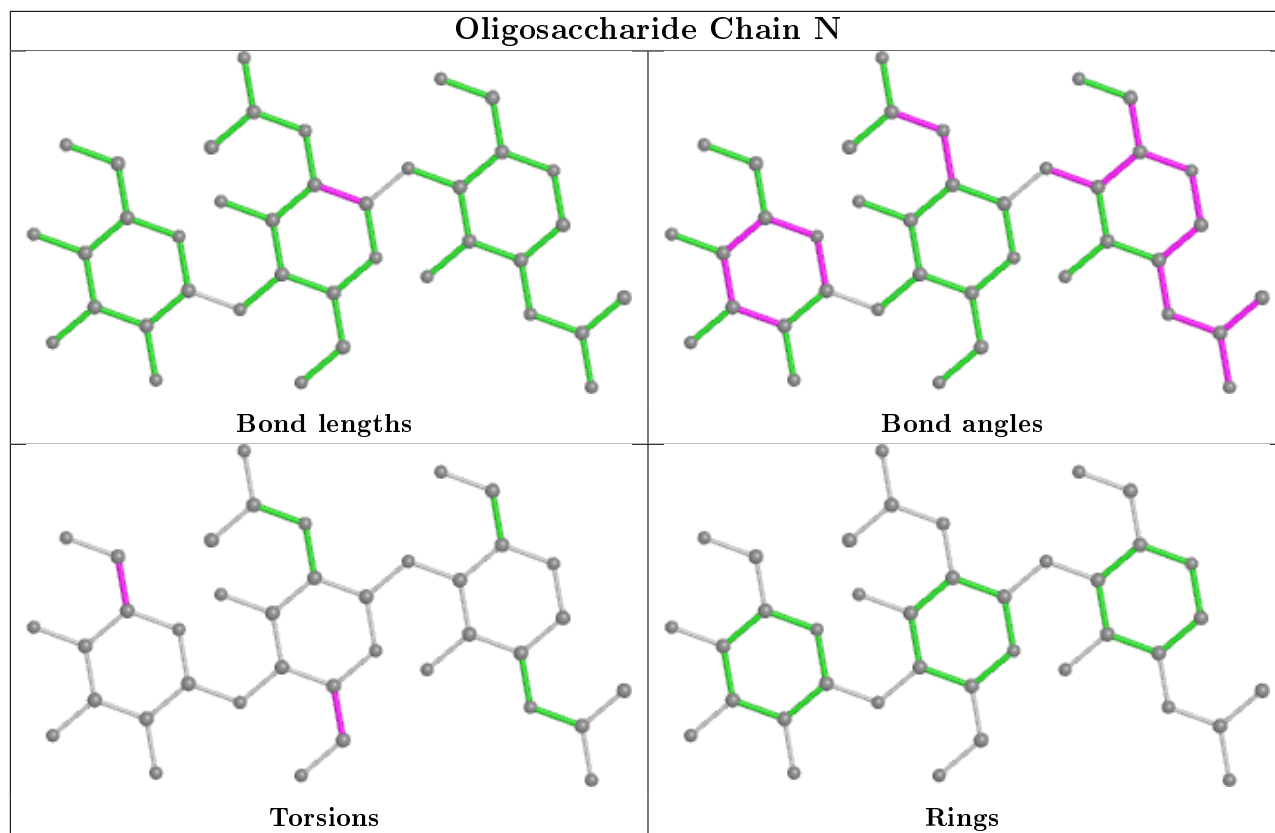
6 monomers are involved in 10 short contacts:

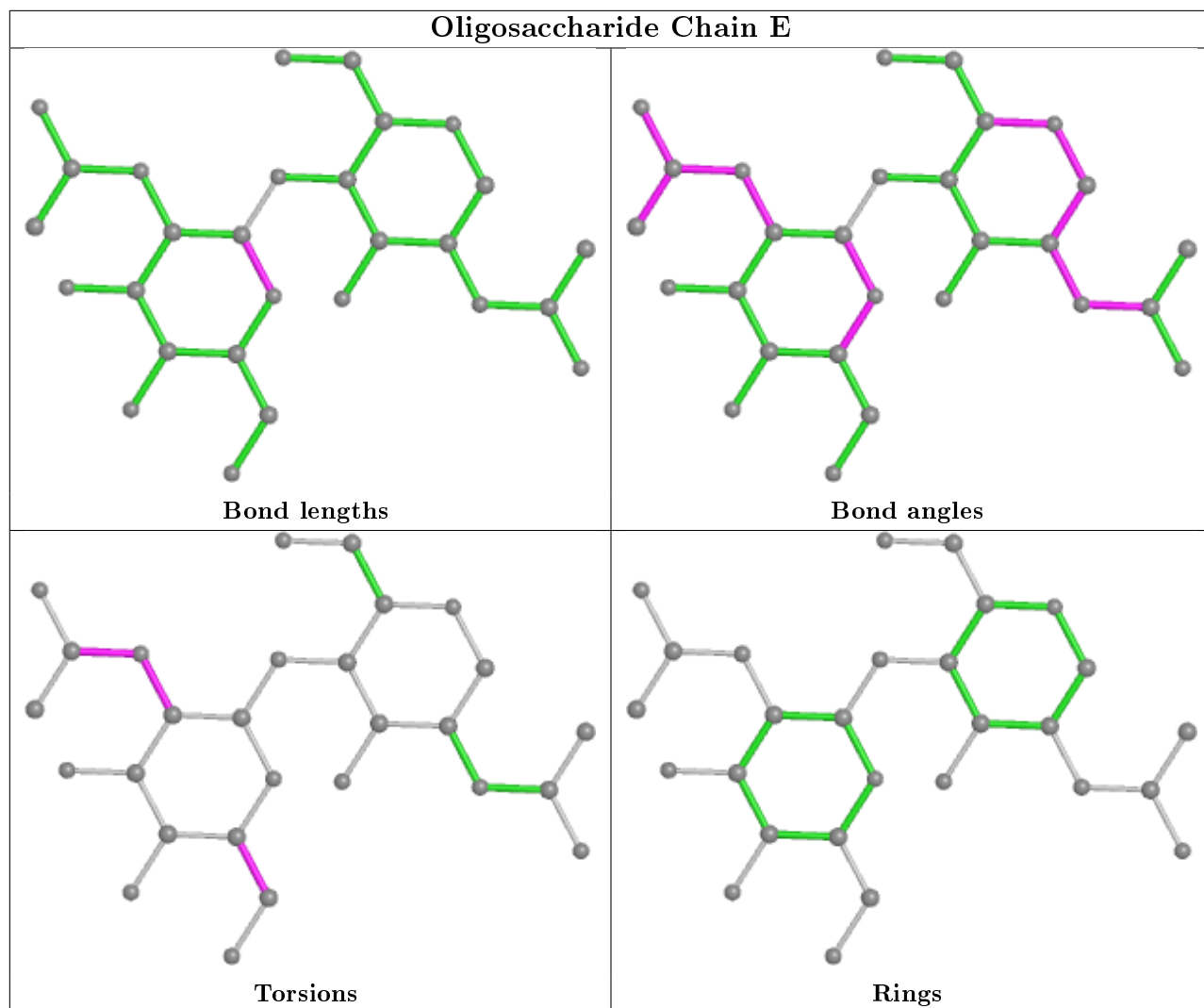
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	3	BMA	1	0
8	J	1	NAG	2	0
2	K	2	NAG	2	0
2	K	1	NAG	1	0
6	H	3	BMA	2	0
4	E	2	NAG	2	0

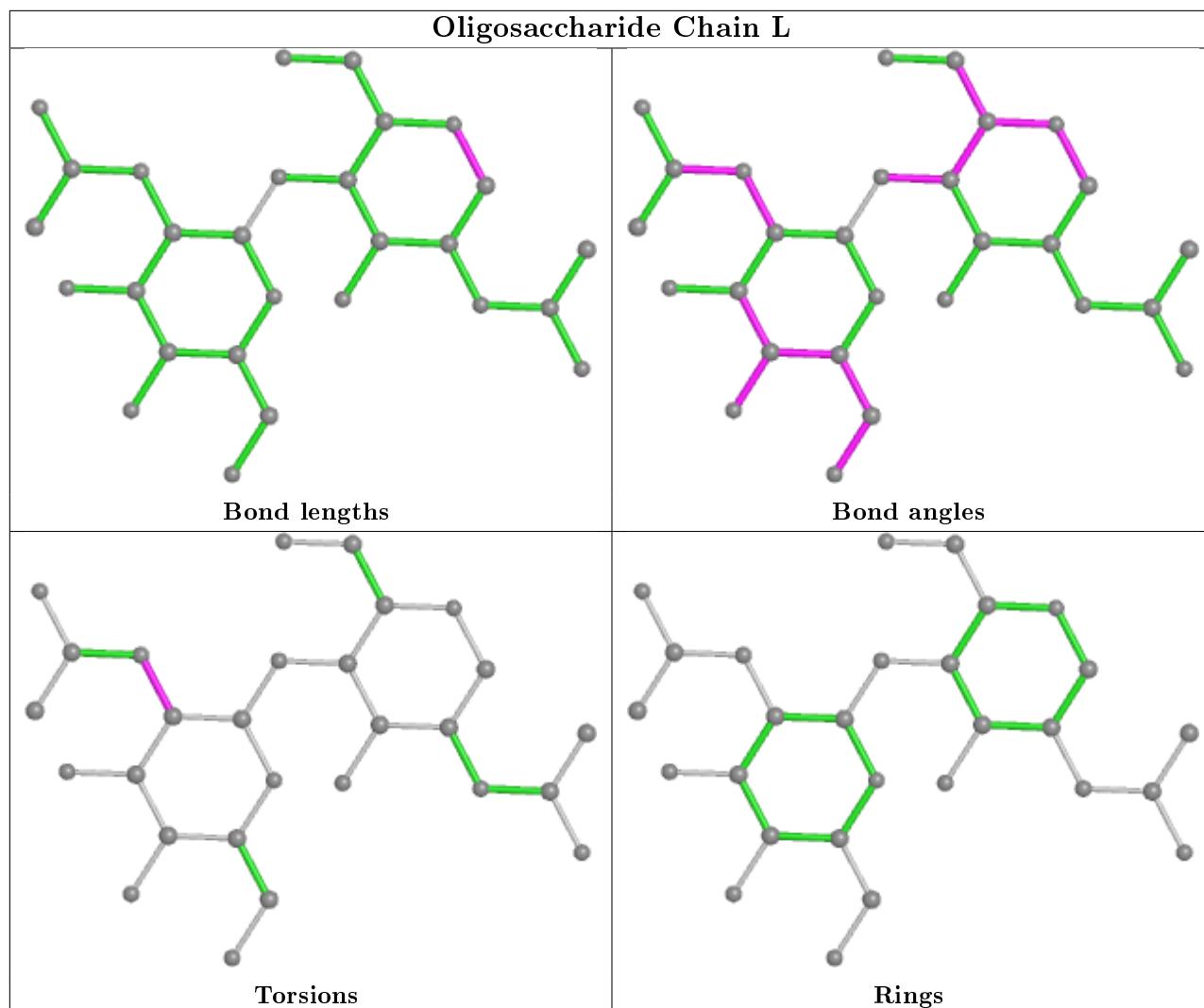
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

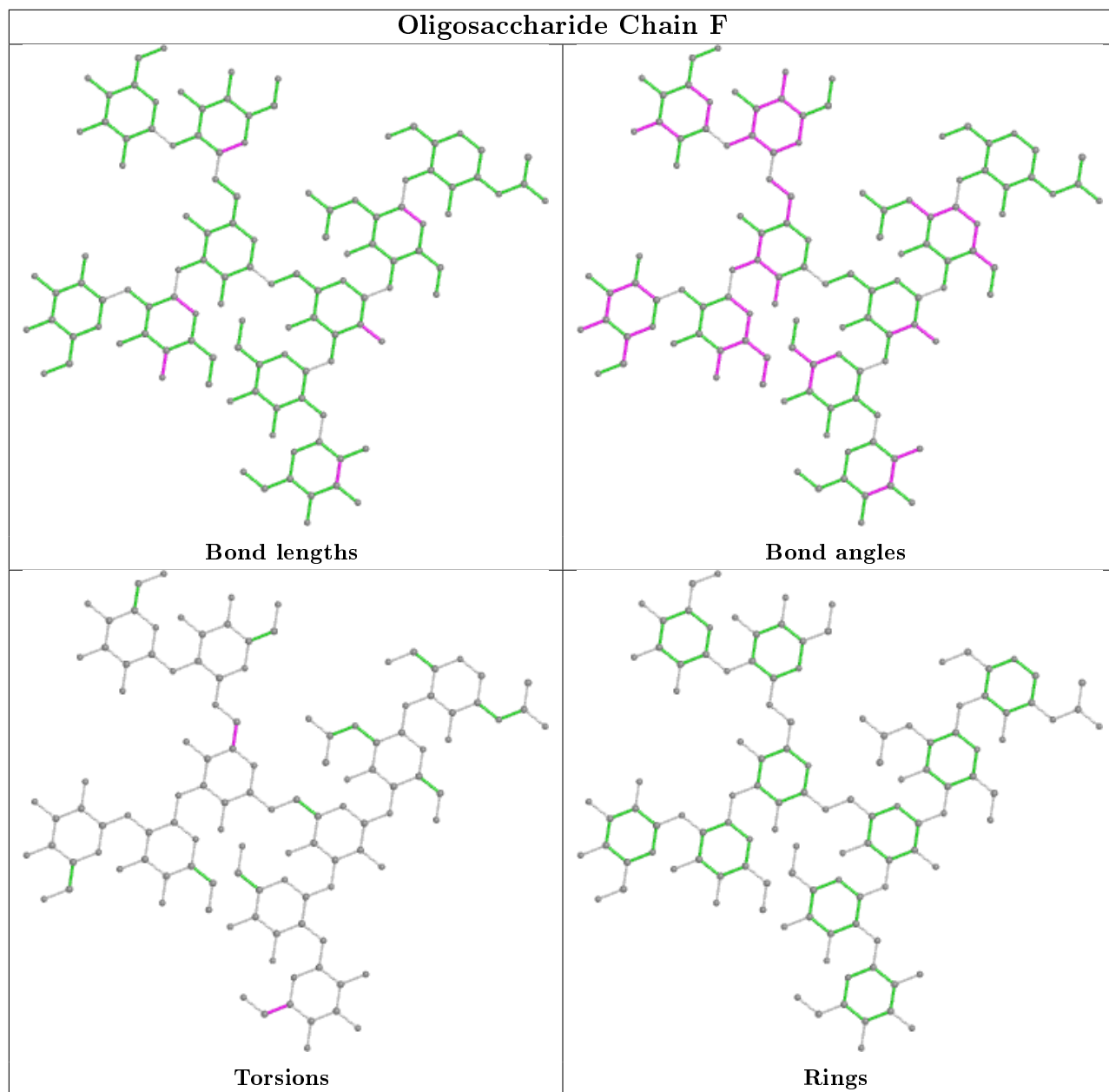


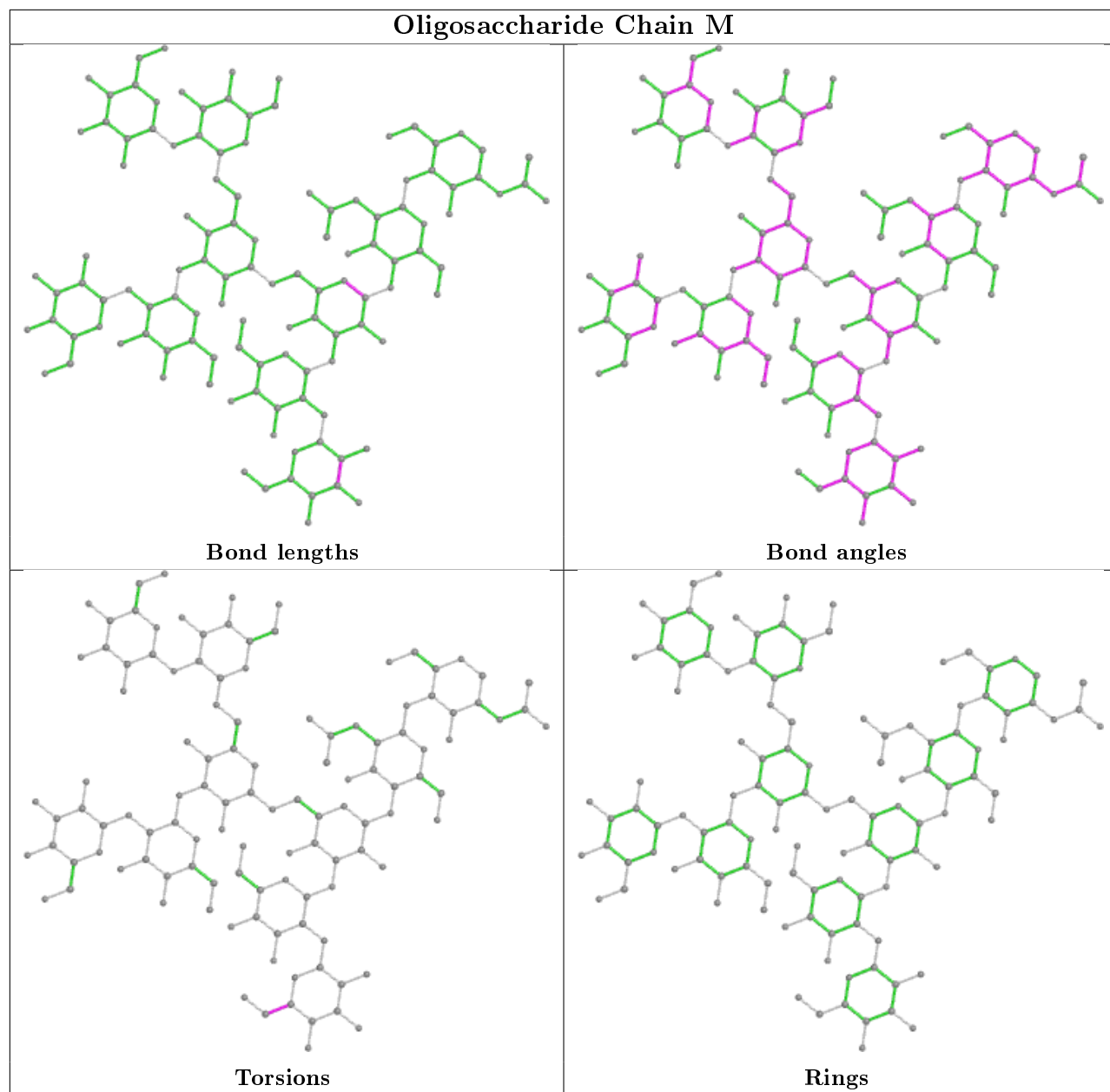


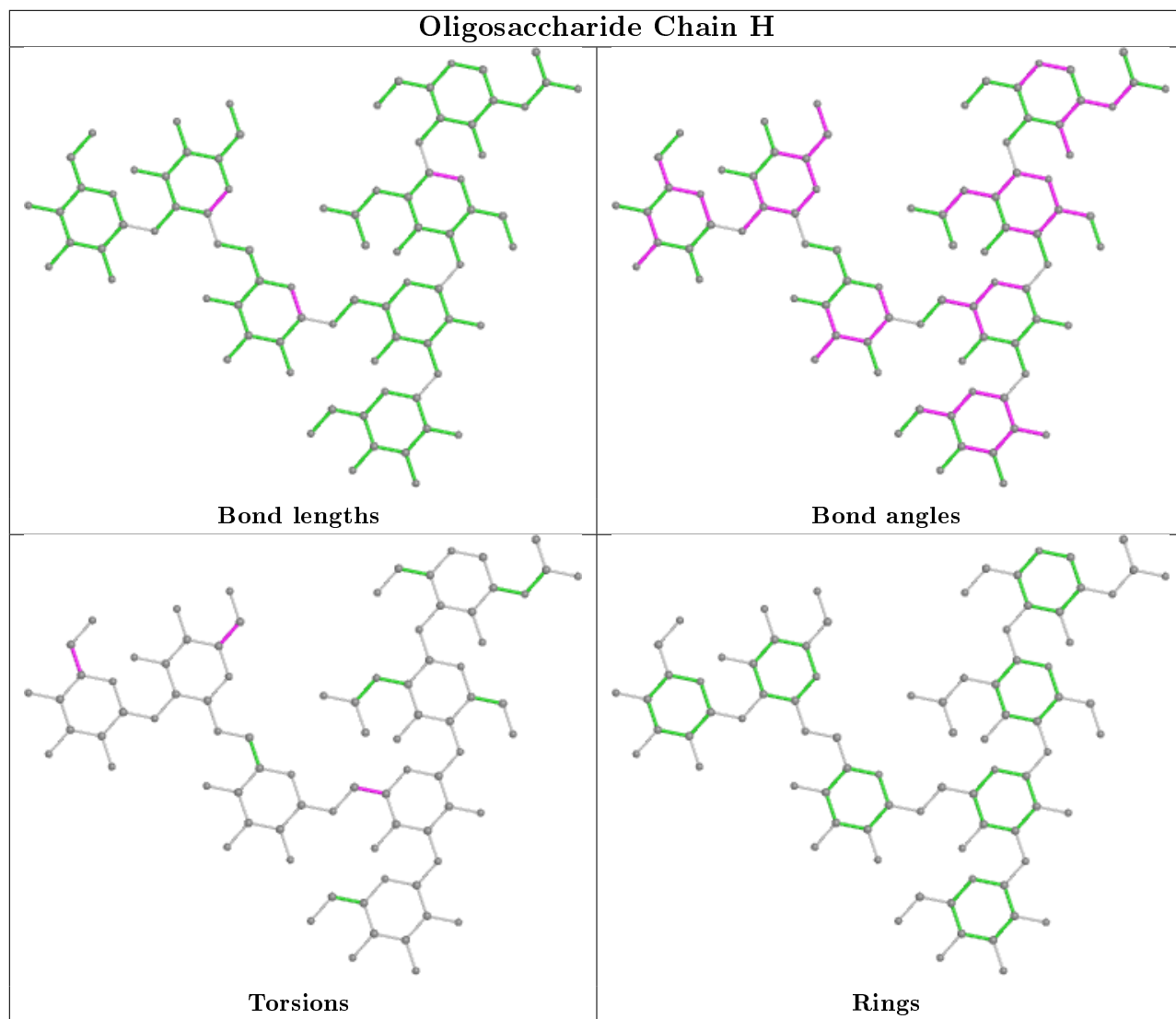


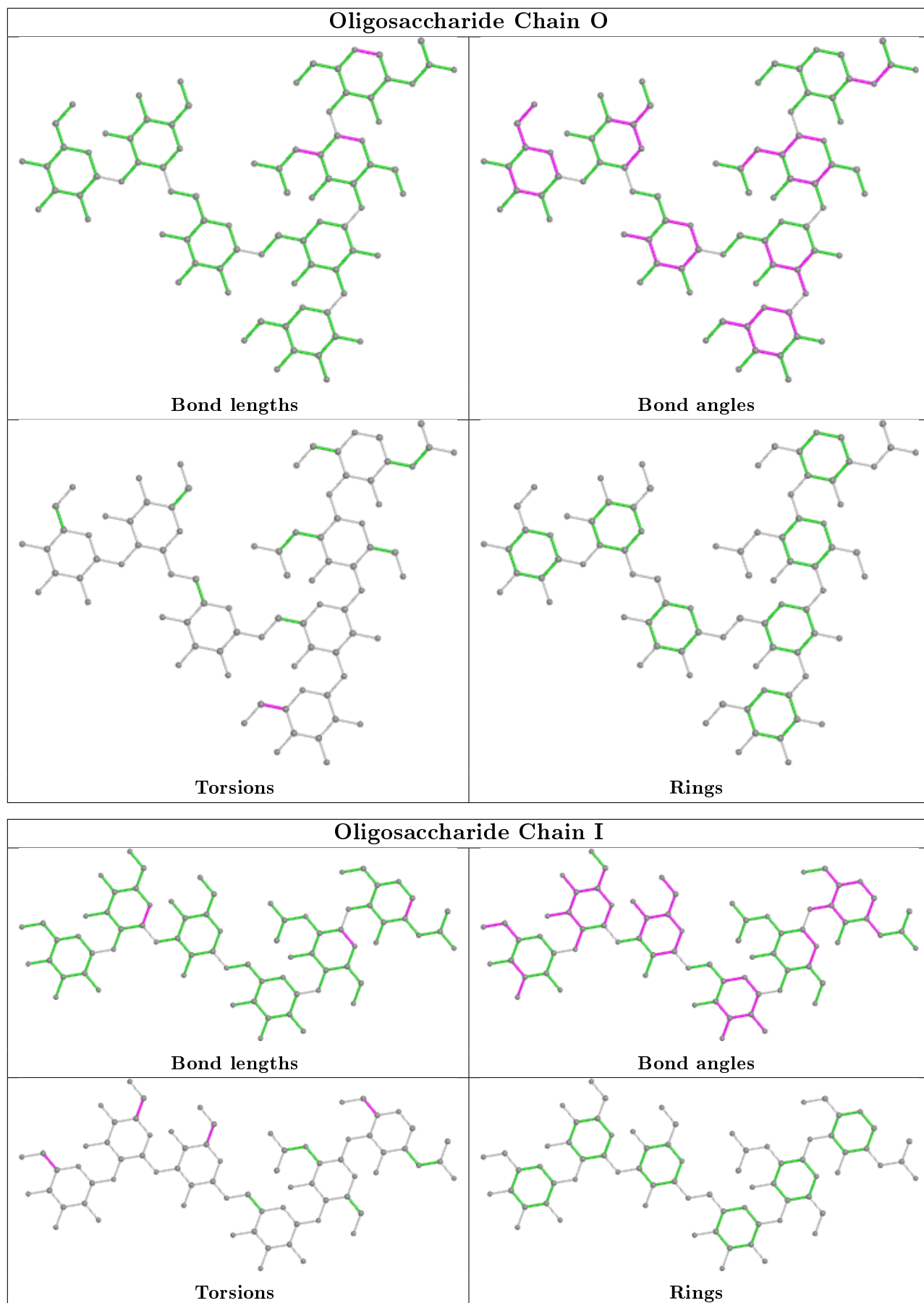


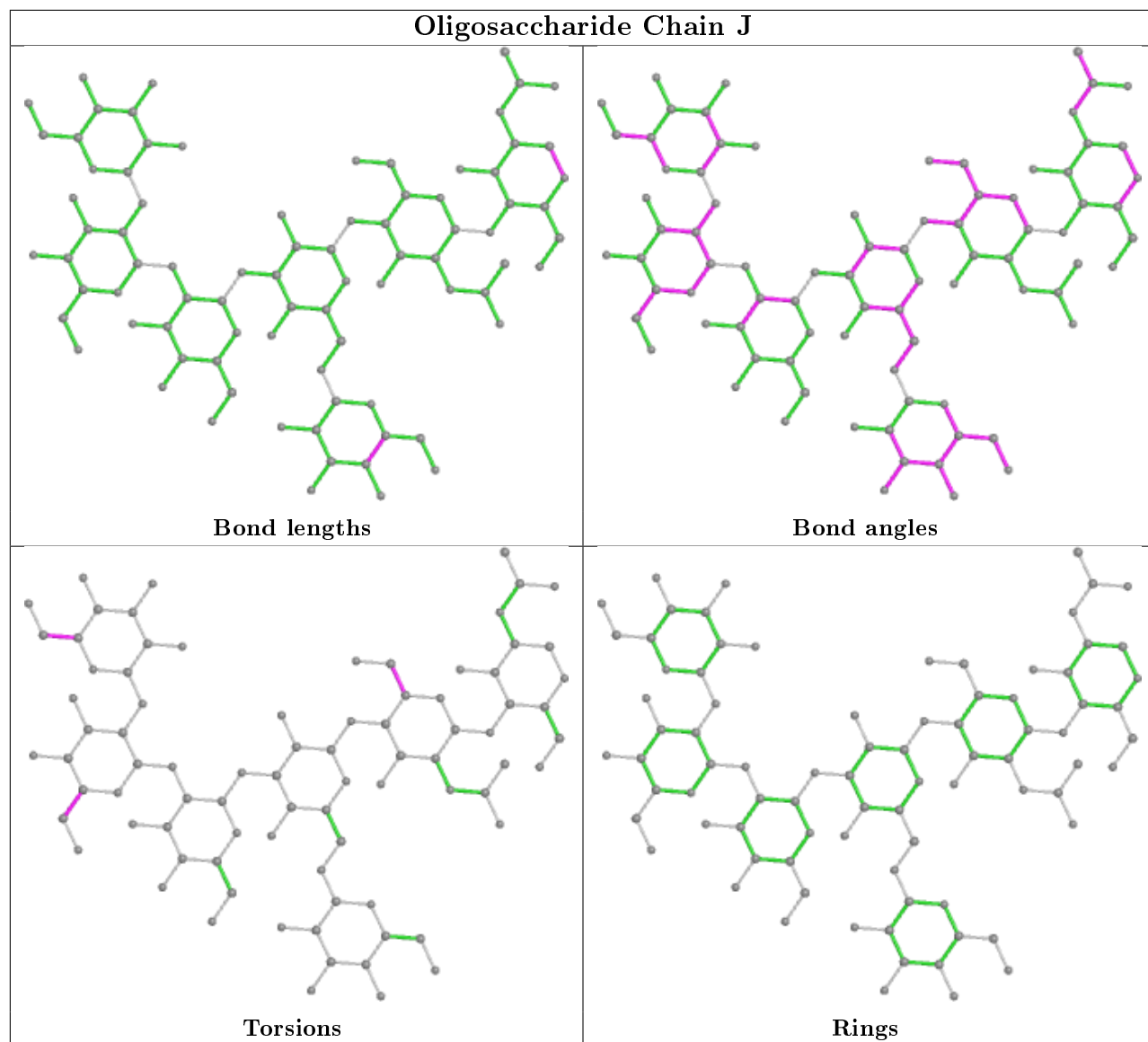


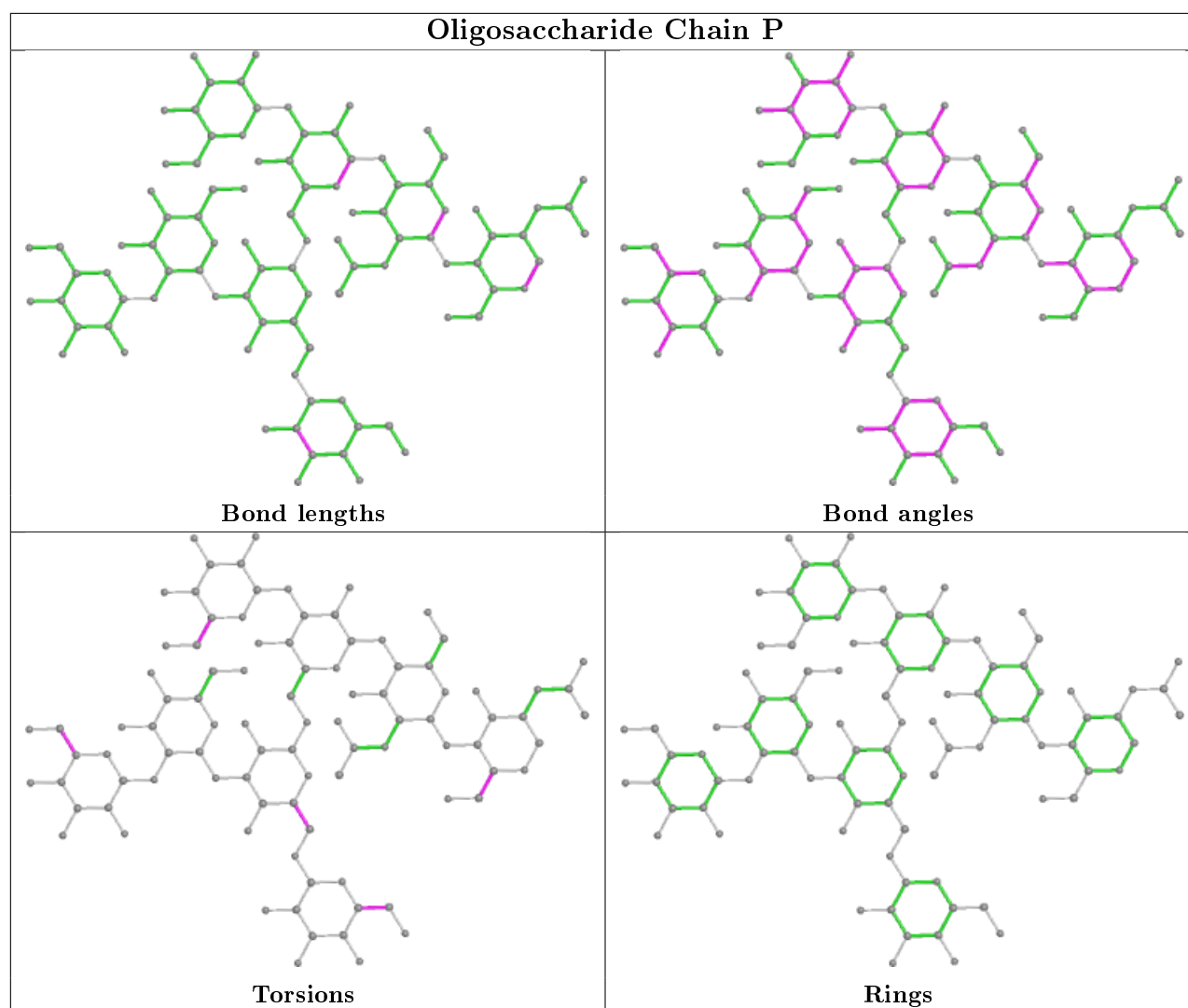












5.6 Ligand geometry [i](#)

13 ligands 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	$\# Z > 2$
11	MRD	B	945	-	7,7,7	0.67	0	9,10,10	0.54	0
13	CTS	B	948	-	14,14,14	1.10	1 (7%)	16,21,21	1.23	1 (6%)
10	NAG	A	905	1	14,14,15	0.75	0	17,19,21	1.50	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	937	1	14,14,15	1.02	0	17,19,21	1.96	7 (41%)
12	MPD	A	939	-	7,7,7	0.34	0	9,10,10	0.59	0
13	CTS	A	941	-	14,14,14	1.42	1 (7%)	16,21,21	1.23	2 (12%)
11	MRD	B	947	-	7,7,7	0.54	0	9,10,10	0.44	0
11	MRD	A	938	-	7,7,7	0.32	0	9,10,10	0.60	0
12	MPD	A	940	-	7,7,7	0.51	0	9,10,10	0.92	0
11	MRD	B	946	-	7,7,7	0.79	0	9,10,10	1.03	1 (11%)
10	NAG	B	908	1	14,14,15	1.09	1 (7%)	17,19,21	1.57	5 (29%)
10	NAG	B	943	1	14,14,15	0.74	0	17,19,21	1.63	2 (11%)
10	NAG	B	944	1	14,14,15	0.71	0	17,19,21	1.48	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MRD	B	945	-	-	1/5/5/5	-
13	CTS	B	948	-	-	-	0/2/2/2
10	NAG	A	905	1	-	0/6/23/26	0/1/1/1
10	NAG	A	937	1	-	0/6/23/26	0/1/1/1
12	MPD	A	939	-	-	3/5/5/5	-
13	CTS	A	941	-	-	-	0/2/2/2
11	MRD	B	947	-	-	1/5/5/5	-
11	MRD	A	938	-	-	1/5/5/5	-
12	MPD	A	940	-	-	2/5/5/5	-
11	MRD	B	946	-	-	4/5/5/5	-
10	NAG	B	908	1	-	1/6/23/26	0/1/1/1
10	NAG	B	943	1	-	1/6/23/26	0/1/1/1
10	NAG	B	944	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	941	CTS	C6-C5	-4.67	1.49	1.54
13	B	948	CTS	C1-C2	3.05	1.56	1.52
10	B	908	NAG	O5-C1	-2.77	1.39	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	943	NAG	C4-C3-C2	4.64	117.82	111.02
10	B	944	NAG	C1-O5-C5	4.40	118.16	112.19
10	A	937	NAG	C2-N2-C7	-4.37	116.68	122.90
10	A	905	NAG	C4-C3-C2	-3.80	105.45	111.02
10	B	943	NAG	O5-C1-C2	-3.33	106.03	111.29
10	A	937	NAG	C1-O5-C5	2.93	116.17	112.19
10	A	937	NAG	C3-C4-C5	-2.87	105.12	110.24
10	A	937	NAG	C1-C2-N2	-2.81	105.68	110.49
10	B	908	NAG	O5-C5-C6	2.76	111.53	107.20
10	B	908	NAG	C2-N2-C7	2.68	126.72	122.90
10	A	905	NAG	O5-C1-C2	2.66	115.49	111.29
10	B	908	NAG	O5-C1-C2	2.52	115.27	111.29
10	A	937	NAG	C8-C7-N2	2.47	120.28	116.10
13	A	941	CTS	O2-C2-C3	-2.36	105.41	110.14
13	A	941	CTS	C1-C2-C3	2.27	112.83	110.24
10	A	937	NAG	O5-C5-C4	-2.27	105.31	110.83
10	B	908	NAG	O5-C5-C4	-2.24	105.37	110.83
10	B	908	NAG	O7-C7-C8	-2.24	117.90	122.06
13	B	948	CTS	C8-N-C5	-2.16	100.08	106.27
11	B	946	MRD	O4-C4-C3	-2.13	102.74	111.36
10	A	937	NAG	C6-C5-C4	2.06	117.84	113.00
10	B	944	NAG	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	939	MPD	O2-C2-C3-C4
12	A	939	MPD	CM-C2-C3-C4
11	A	938	MRD	C2-C3-C4-O4
12	A	940	MPD	C2-C3-C4-O4
11	B	946	MRD	C1-C2-C3-C4
11	B	946	MRD	O2-C2-C3-C4
11	B	946	MRD	C2-C3-C4-O4
10	B	944	NAG	O5-C5-C6-O6
10	B	944	NAG	C4-C5-C6-O6
10	B	908	NAG	C3-C2-N2-C7
12	A	939	MPD	C1-C2-C3-C4
11	B	946	MRD	CM-C2-C3-C4
11	B	945	MRD	O2-C2-C3-C4
10	B	943	NAG	C4-C5-C6-O6
11	B	947	MRD	C2-C3-C4-C5
12	A	940	MPD	C2-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	945	MRD	1	0
13	B	948	CTS	2	0
12	A	939	MPD	1	0
13	A	941	CTS	2	0
11	B	947	MRD	2	0
11	A	938	MRD	1	0
11	B	946	MRD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	833/841 (99%)	-0.55	0 100 100	17, 26, 42, 72	0
1	B	832/841 (98%)	-0.69	0 100 100	16, 23, 35, 58	0
All	All	1665/1682 (98%)	-0.62	0 100 100	16, 24, 39, 72	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.61	0.36	66,80,85,85	0
6	MAN	H	7	11/12	0.77	0.27	60,63,68,68	0
6	MAN	O	7	11/12	0.77	0.28	70,80,84,88	0
2	MAN	C	4	11/12	0.80	0.15	54,63,71,71	0
9	MAN	P	8	11/12	0.83	0.26	62,71,81,81	0
2	BMA	C	3	11/12	0.83	0.13	40,53,60,60	0
2	MAN	K	4	11/12	0.84	0.23	56,69,79,79	0
9	MAN	P	7	11/12	0.85	0.26	53,67,74,75	0
5	MAN	M	10	11/12	0.86	0.15	39,49,55,55	0
3	NAG	G	2	14/15	0.87	0.24	53,63,73,84	0
3	BMA	D	3	11/12	0.89	0.25	39,48,55,56	0

Continued on next page...

Continued from previous page...

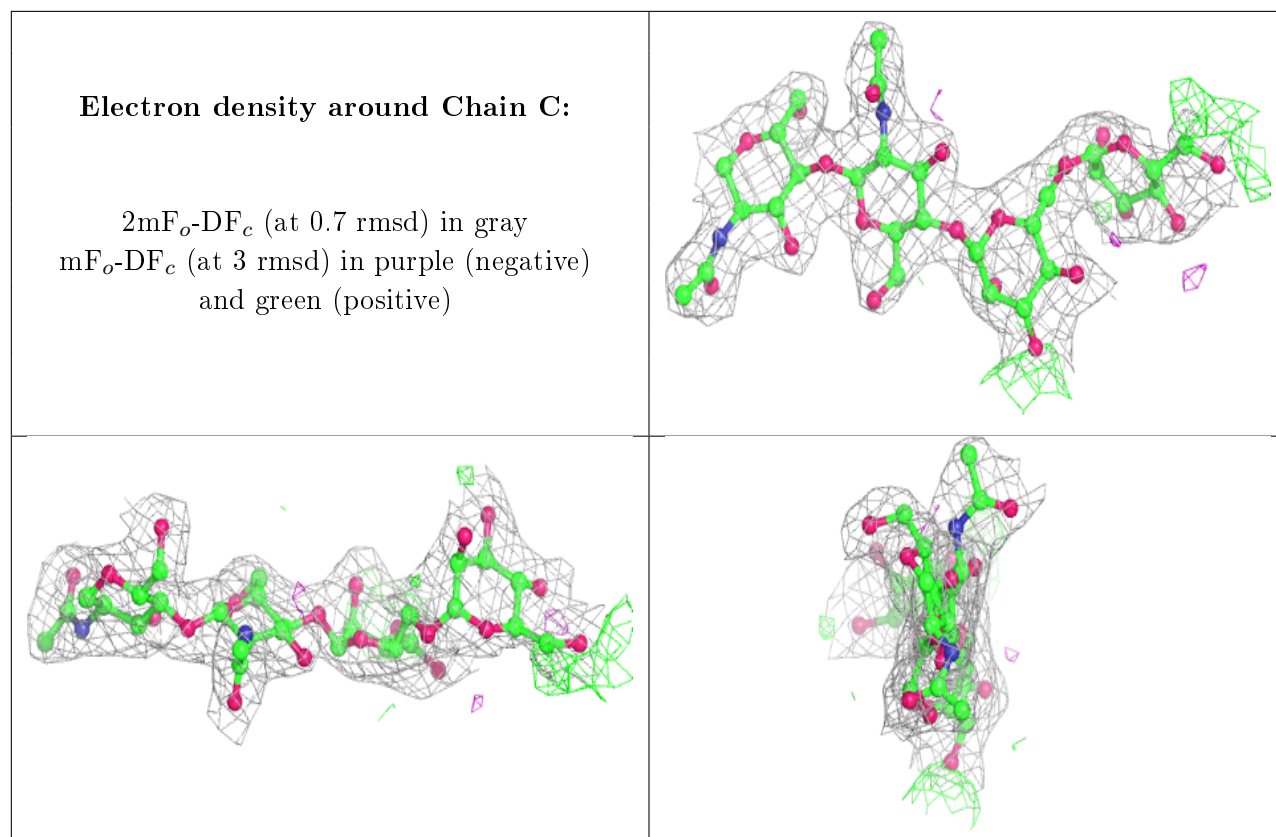
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	N	3	11/12	0.89	0.20	51,63,70,72	0
7	MAN	I	6	11/12	0.89	0.21	50,55,65,70	0
2	BMA	K	3	11/12	0.90	0.13	49,53,58,59	0
8	MAN	J	7	11/12	0.90	0.16	30,38,44,49	0
4	NAG	L	2	14/15	0.91	0.15	30,38,49,52	0
6	BMA	H	3	11/12	0.91	0.16	35,44,50,55	0
6	MAN	O	4	11/12	0.91	0.14	33,35,40,46	0
6	BMA	O	3	11/12	0.92	0.18	40,47,56,68	0
7	BMA	I	3	11/12	0.92	0.13	43,49,55,56	0
5	MAN	F	6	11/12	0.93	0.12	38,41,46,48	0
9	BMA	P	3	11/12	0.93	0.20	42,48,58,67	0
9	MAN	P	6	11/12	0.93	0.29	61,66,71,72	0
7	MAN	I	4	11/12	0.93	0.14	35,37,41,43	0
9	NAG	P	2	14/15	0.93	0.15	29,36,45,45	0
6	NAG	O	2	14/15	0.94	0.16	23,32,39,40	0
5	MAN	M	6	11/12	0.94	0.16	36,41,44,44	0
6	NAG	H	2	14/15	0.94	0.15	27,33,39,42	0
3	NAG	N	2	14/15	0.94	0.10	38,40,45,50	0
5	MAN	F	10	11/12	0.94	0.14	43,49,59,59	0
9	MAN	P	5	11/12	0.94	0.18	39,42,48,50	0
7	MAN	I	5	11/12	0.95	0.13	33,40,46,48	0
6	MAN	H	4	11/12	0.95	0.15	35,40,47,48	0
3	NAG	D	2	14/15	0.95	0.13	27,35,37,37	0
8	MAN	J	6	11/12	0.95	0.19	31,37,41,48	0
3	NAG	G	1	14/15	0.95	0.12	35,39,47,49	0
8	BMA	J	3	11/12	0.95	0.10	32,35,39,40	0
6	NAG	H	1	14/15	0.95	0.15	26,33,47,49	0
6	NAG	O	1	14/15	0.96	0.10	22,33,45,46	0
3	NAG	D	1	14/15	0.96	0.10	26,30,32,34	0
6	MAN	O	6	11/12	0.96	0.15	30,39,43,46	0
3	NAG	N	1	14/15	0.96	0.10	28,33,41,43	0
5	MAN	M	5	11/12	0.96	0.10	27,28,33,37	0
7	NAG	I	2	14/15	0.96	0.17	26,35,48,51	0
4	NAG	E	2	14/15	0.96	0.12	33,38,50,56	0
5	MAN	F	5	11/12	0.96	0.09	29,30,37,45	0
5	MAN	M	9	11/12	0.96	0.10	28,30,33,42	0
2	NAG	K	2	14/15	0.96	0.08	25,34,39,41	0
8	MAN	J	4	11/12	0.96	0.14	38,44,52,56	0
6	MAN	H	6	11/12	0.96	0.12	32,36,44,45	0
5	NAG	F	2	14/15	0.97	0.13	28,31,34,39	0
5	MAN	F	8	11/12	0.97	0.11	28,29,34,35	0
5	NAG	F	1	14/15	0.97	0.16	27,32,39,40	0

Continued on next page...

Continued from previous page...

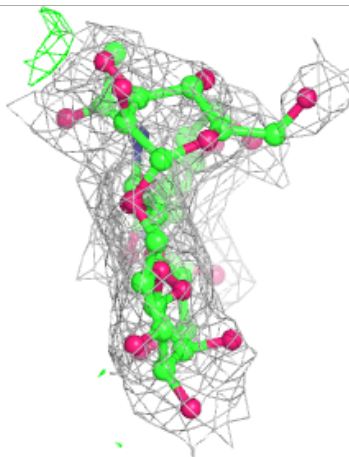
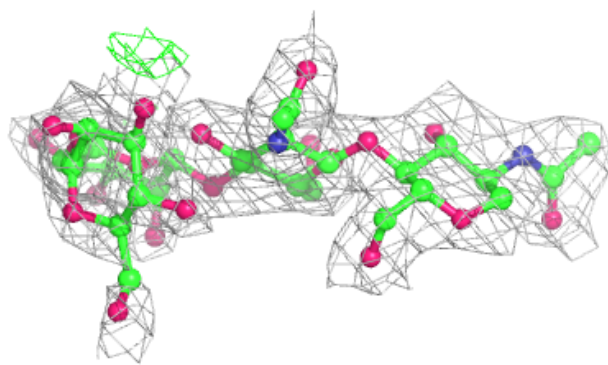
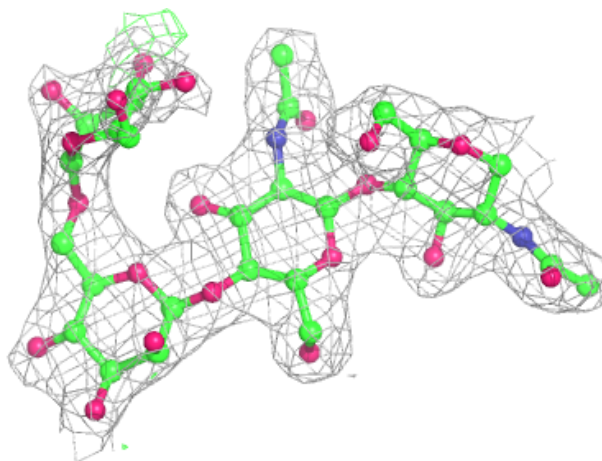
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	1	14/15	0.97	0.11	25,28,32,33	0
2	NAG	C	2	14/15	0.97	0.11	31,41,51,61	0
9	MAN	P	4	11/12	0.97	0.19	30,38,52,60	0
5	NAG	M	2	14/15	0.97	0.11	19,22,26,30	0
5	MAN	F	7	11/12	0.97	0.10	28,31,33,35	0
6	MAN	H	5	11/12	0.97	0.10	26,29,37,43	0
8	MAN	J	5	11/12	0.97	0.17	39,46,51,59	0
5	MAN	F	9	11/12	0.97	0.11	35,38,43,44	0
5	MAN	M	8	11/12	0.97	0.08	26,28,30,31	0
7	NAG	I	1	14/15	0.97	0.12	26,29,33,37	0
6	MAN	O	5	11/12	0.97	0.17	30,34,38,47	0
2	NAG	K	1	14/15	0.97	0.08	22,26,28,32	0
5	BMA	F	3	11/12	0.97	0.10	28,33,34,38	0
9	NAG	P	1	14/15	0.97	0.11	23,25,29,34	0
5	MAN	M	7	11/12	0.98	0.08	19,21,23,24	0
5	NAG	M	1	14/15	0.98	0.10	22,26,29,30	0
5	BMA	M	3	11/12	0.98	0.10	24,25,27,30	0
8	NAG	J	2	14/15	0.98	0.10	21,26,30,31	0
2	NAG	C	1	14/15	0.98	0.09	25,32,35,36	0
4	NAG	L	1	14/15	0.98	0.09	18,22,26,27	0
8	NAG	J	1	14/15	0.99	0.10	19,20,24,28	0
5	MAN	F	4	11/12	0.99	0.08	22,26,28,30	0
5	MAN	M	4	11/12	0.99	0.09	19,21,24,25	0

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



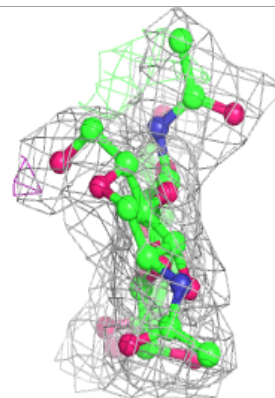
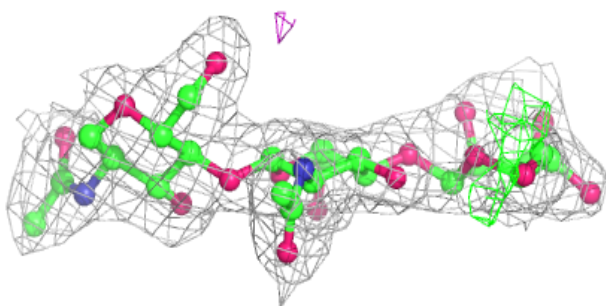
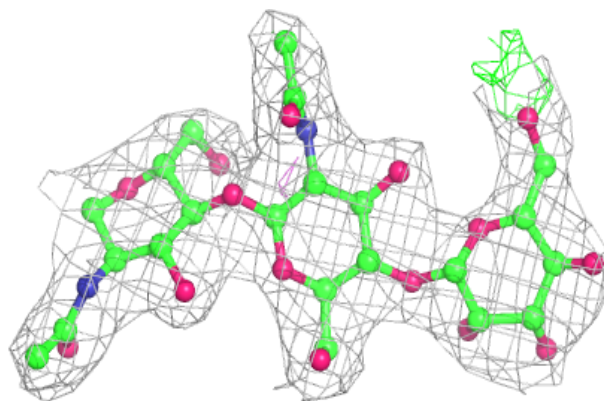
Electron density around Chain K:

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

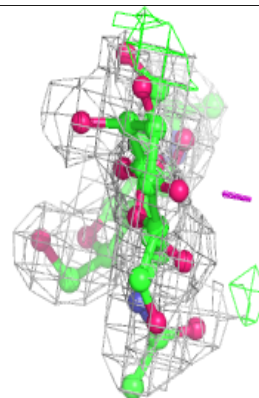
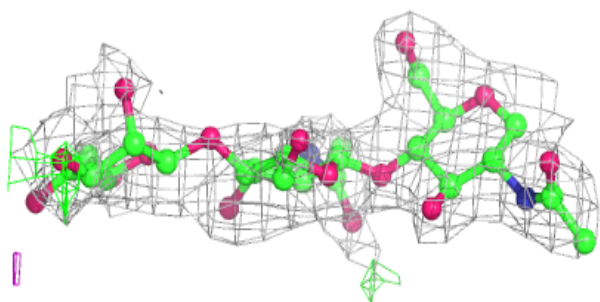
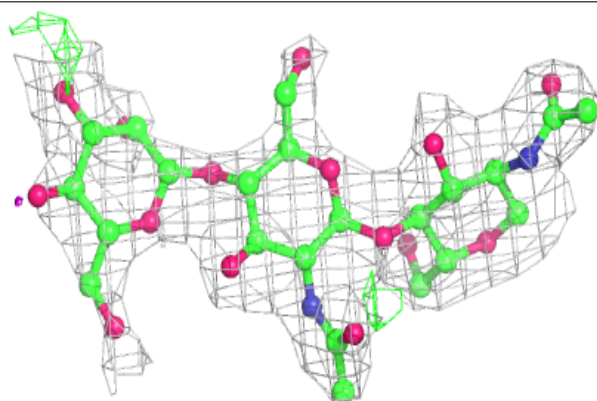


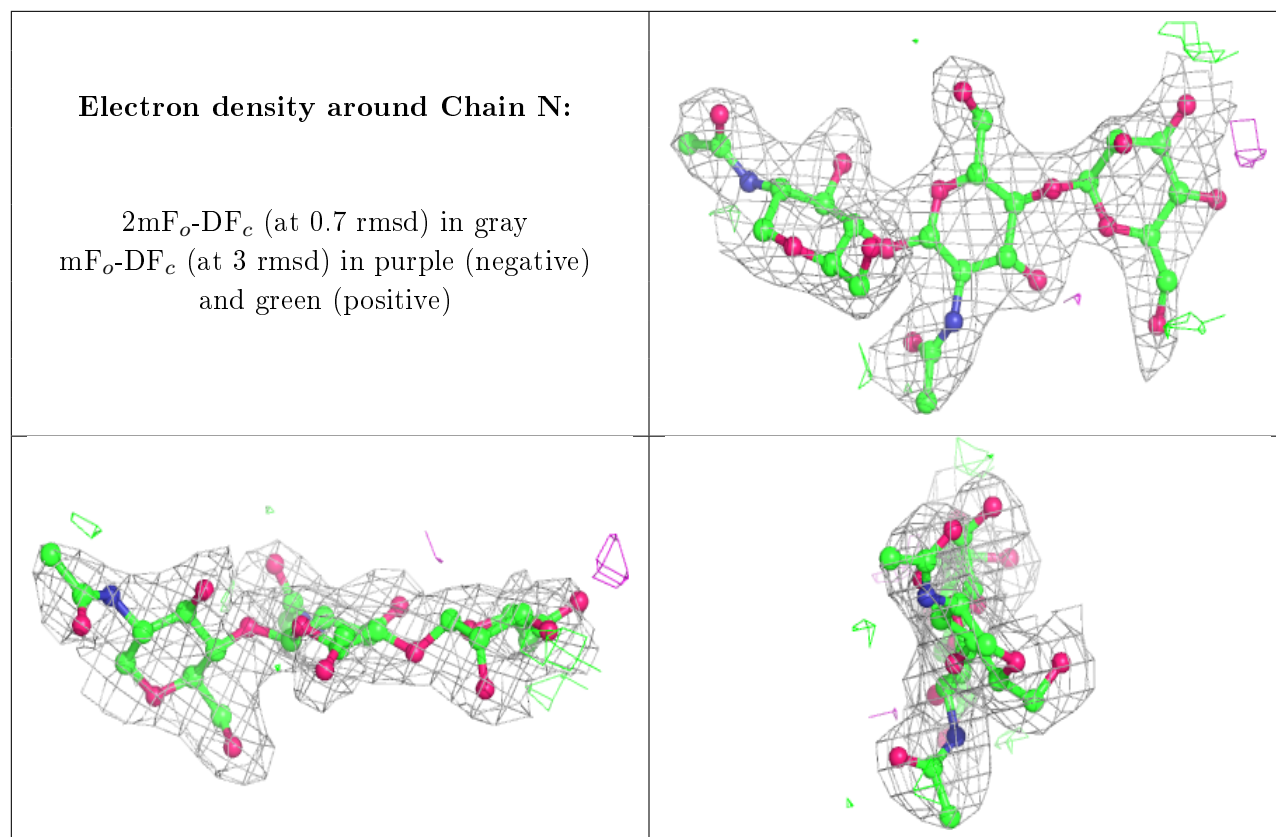
Electron density around Chain D:

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

**Electron density around Chain G:**

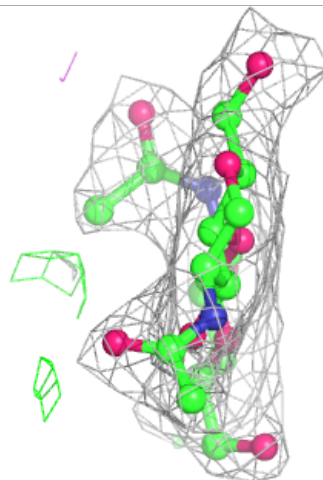
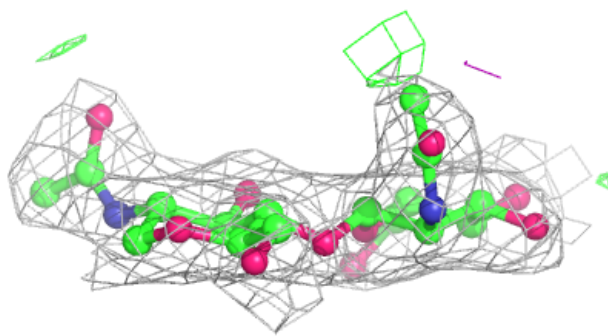
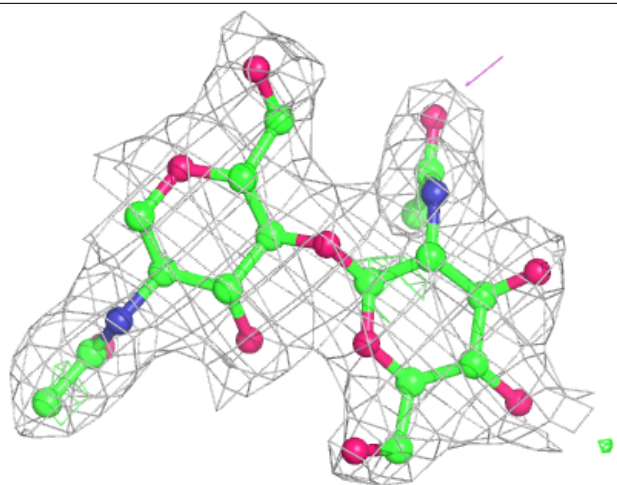
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

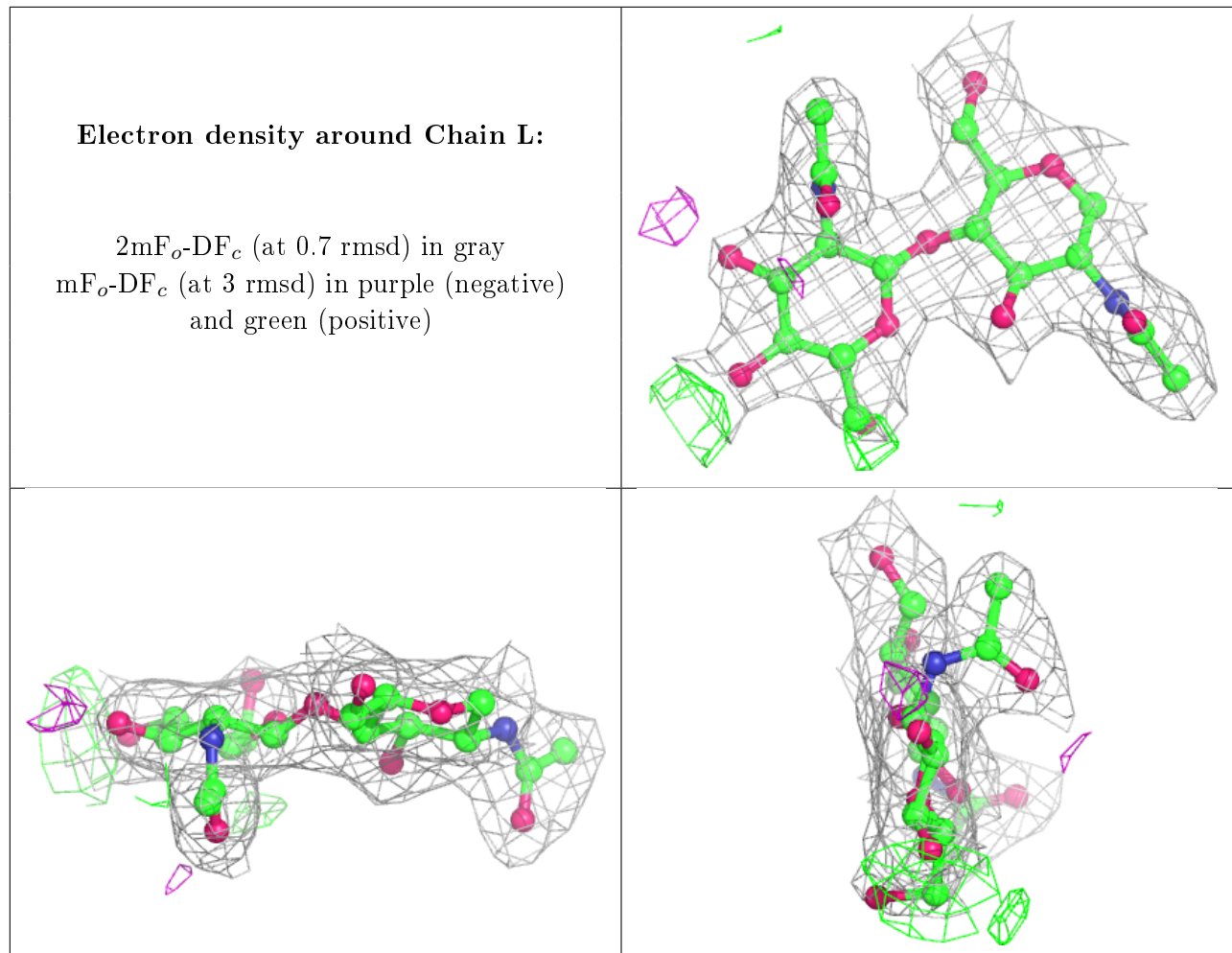




Electron density around Chain E:

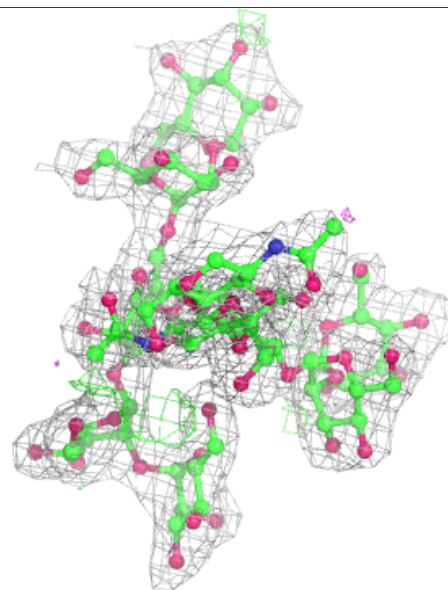
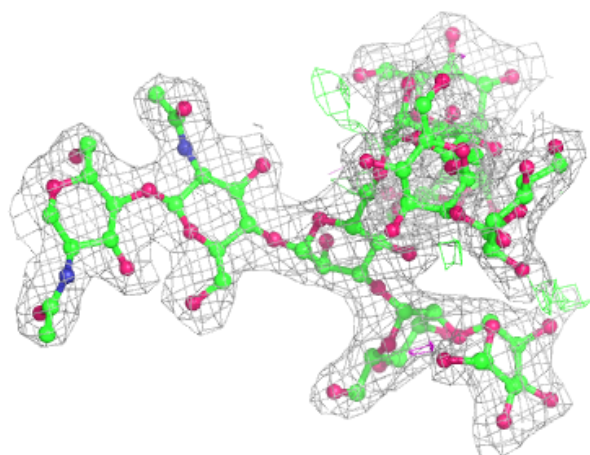
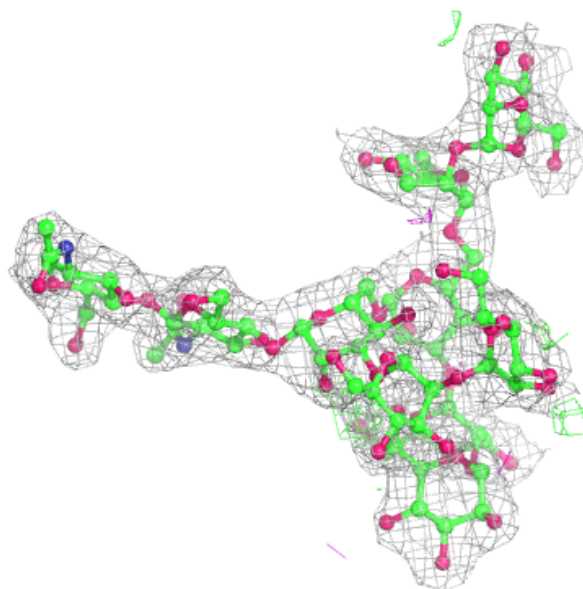
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





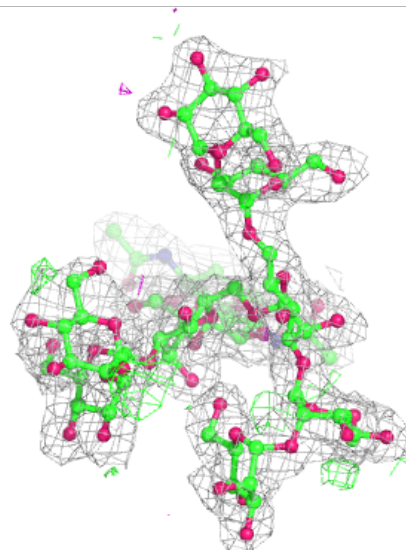
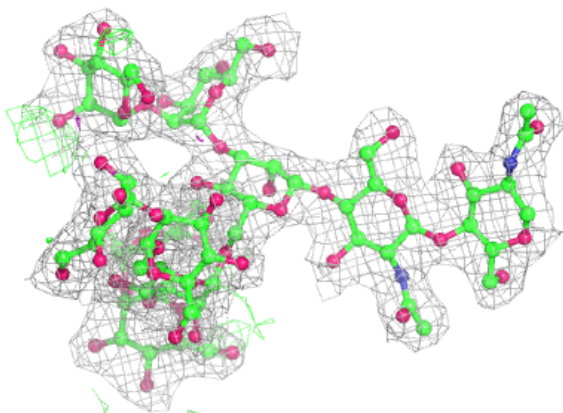
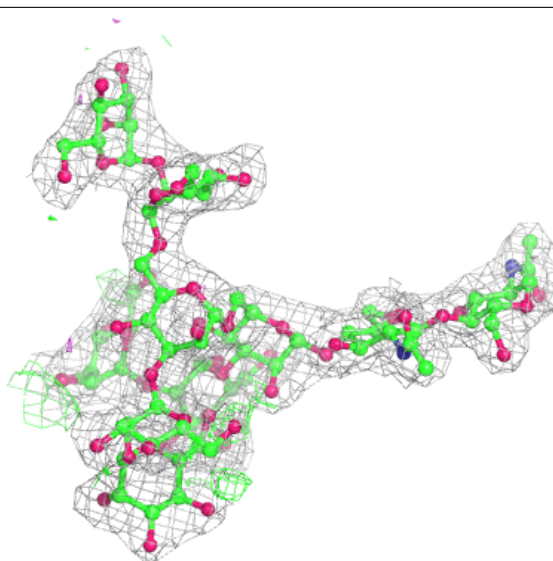
Electron density around Chain F:

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



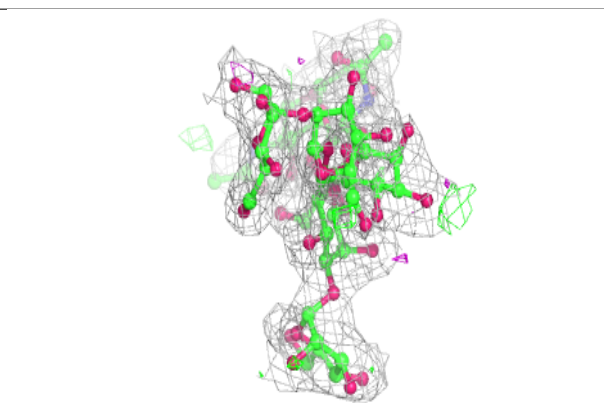
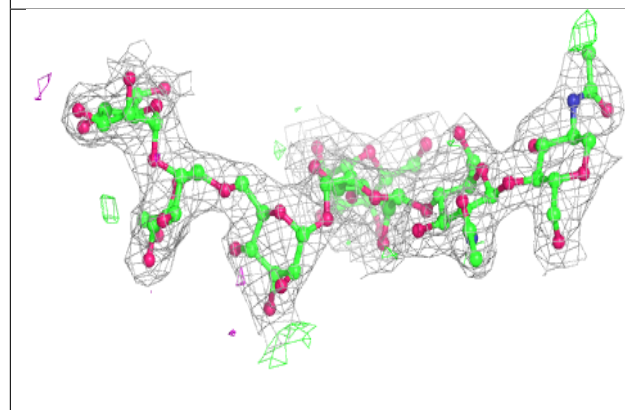
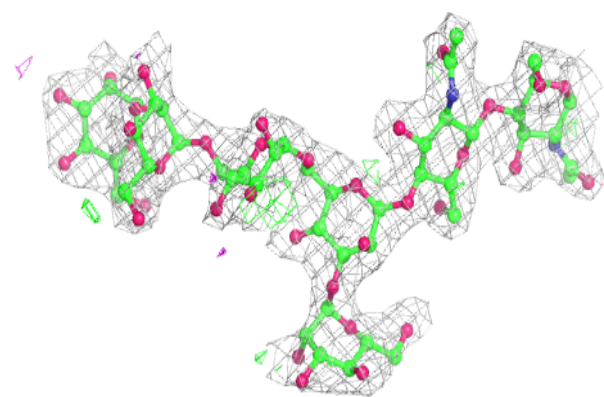
Electron density around Chain M:

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

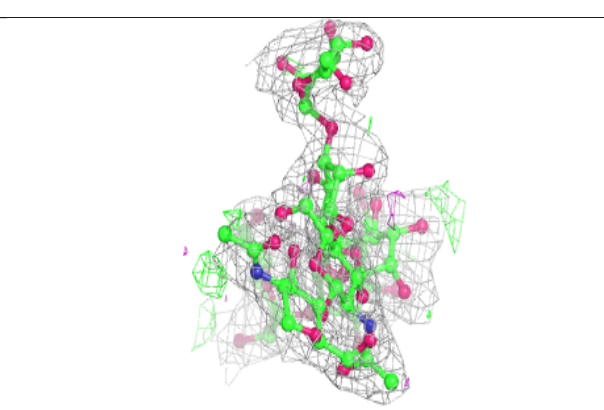
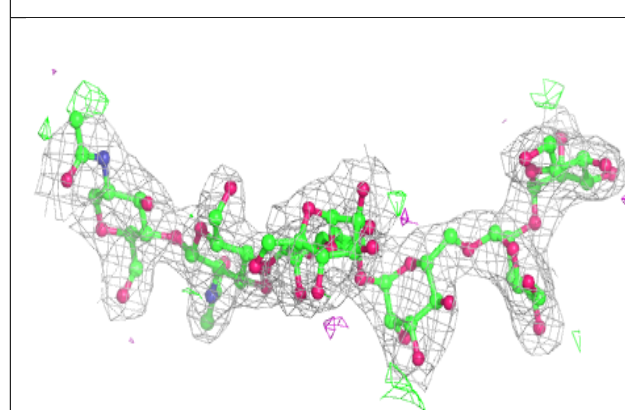
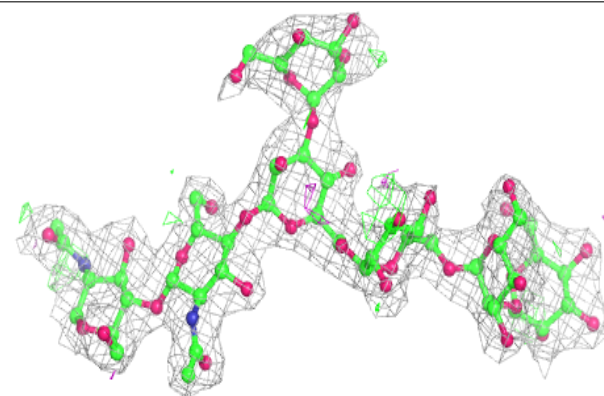


Electron density around Chain H:

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

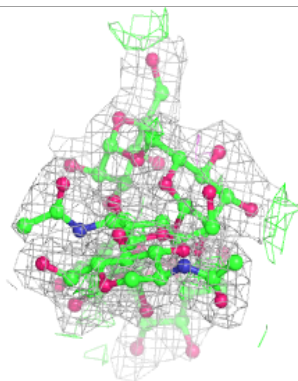
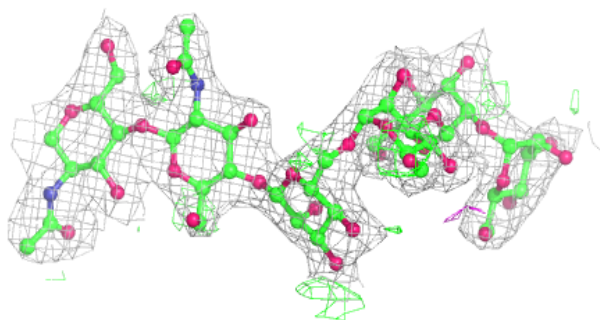
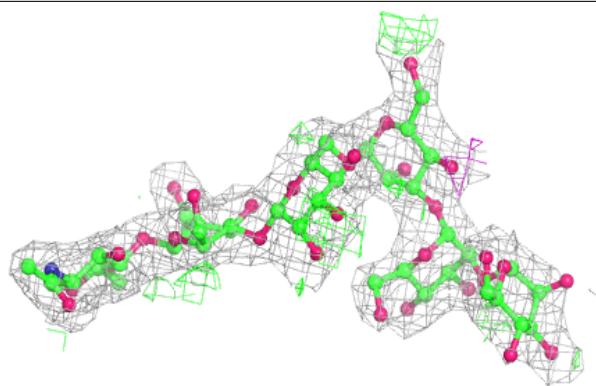
**Electron density around Chain O:**

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

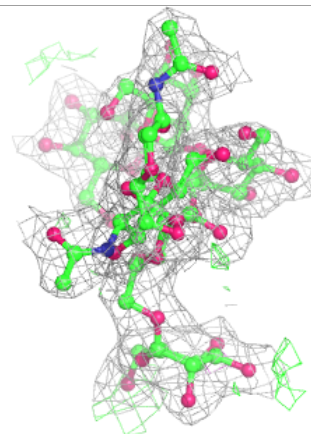
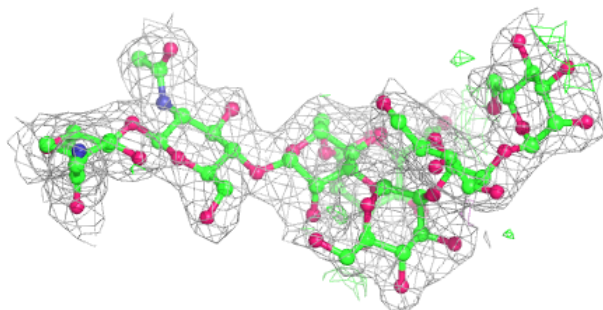
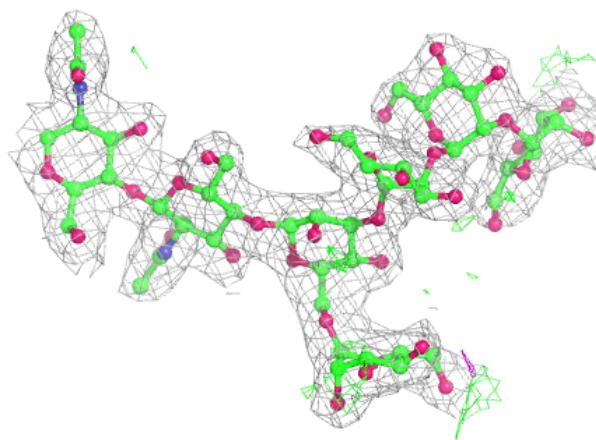


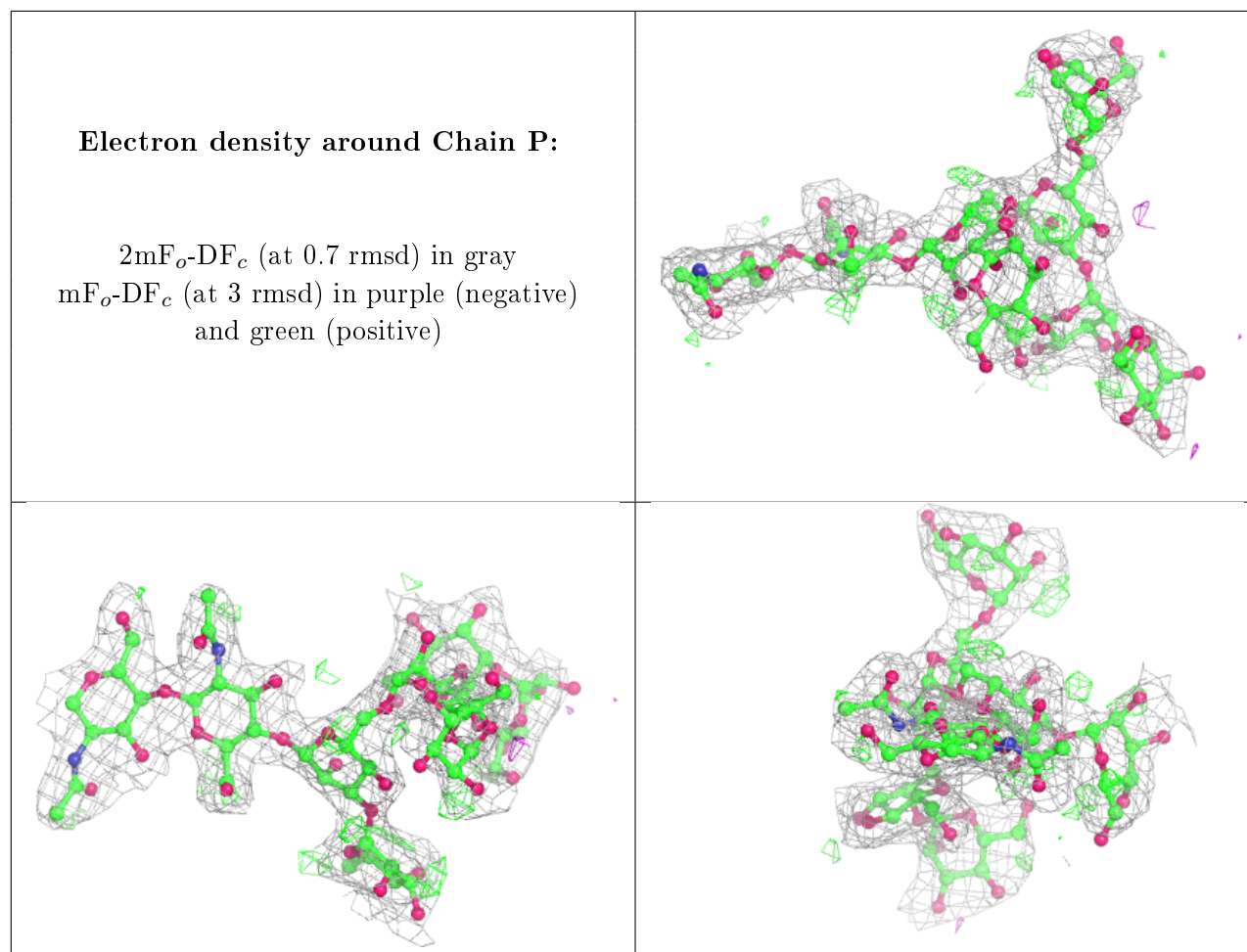
Electron density around Chain I:

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

**Electron density around Chain J:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	MRD	B	945	8/8	0.84	0.29	46,66,73,75	0
12	MPD	A	940	8/8	0.86	0.22	49,58,69,75	0
10	NAG	B	908	14/15	0.87	0.23	50,64,80,82	0
11	MRD	B	947	8/8	0.90	0.18	54,59,63,70	0
10	NAG	B	943	14/15	0.90	0.23	54,68,84,84	0
10	NAG	A	905	14/15	0.91	0.22	55,67,69,75	0
12	MPD	A	939	8/8	0.93	0.19	34,42,48,49	0
11	MRD	B	946	8/8	0.96	0.15	32,38,42,44	0
11	MRD	A	938	8/8	0.96	0.14	38,40,42,43	0
10	NAG	A	937	14/15	0.96	0.24	39,44,47,52	0
10	NAG	B	944	14/15	0.97	0.21	35,39,42,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CTS	A	941	13/13	0.99	0.15	24,26,29,29	0
13	CTS	B	948	13/13	0.99	0.17	20,23,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.