



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 12:38 AM JST

PDB ID : 6JBS
Title : Bifunctional xylosidase/glucosidase LXYL
Authors : Gong, W.M.; Yang, L.Y.
Deposited on : 2019-01-26
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

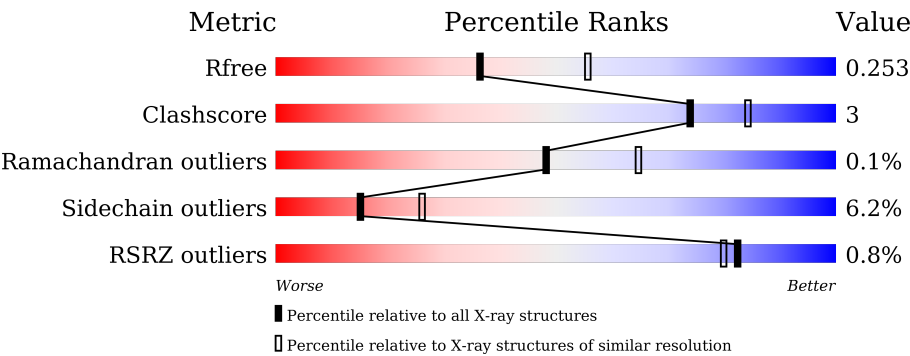
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



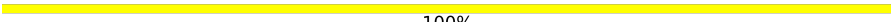


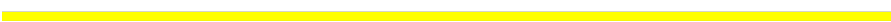






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	809	<div><div></div><div>85%7% • 6%</div></div>
1	B	809	<div><div>%</div><div>84%8% • 6%</div></div>
1	C	809	<div><div>%</div><div>84%9% • 6%</div></div>
1	D	809	<div><div>%</div><div>86%7% • 6%</div></div>
2	E	3	<div><div></div><div>100%</div></div>
2	N	3	<div><div></div><div>100%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	7	 100%
4	G	6	 33% 67%
5	H	3	 100%
5	K	3	 100%
6	I	7	 14% 86%
6	L	7	 14% 86%
6	O	7	 14% 86%
7	J	2	 50% 50%
8	M	5	 100%
9	P	7	 29% 71%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25512 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-D-xylosidase/beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	1	0
			5752	3640	963	1132	17			
1	B	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			
1	C	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			
1	D	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	804	HIS	-	expression tag	UNP G8GLP2
A	805	HIS	-	expression tag	UNP G8GLP2
A	806	HIS	-	expression tag	UNP G8GLP2
A	807	HIS	-	expression tag	UNP G8GLP2
A	808	HIS	-	expression tag	UNP G8GLP2
A	809	HIS	-	expression tag	UNP G8GLP2
B	804	HIS	-	expression tag	UNP G8GLP2
B	805	HIS	-	expression tag	UNP G8GLP2
B	806	HIS	-	expression tag	UNP G8GLP2
B	807	HIS	-	expression tag	UNP G8GLP2
B	808	HIS	-	expression tag	UNP G8GLP2
B	809	HIS	-	expression tag	UNP G8GLP2
C	804	HIS	-	expression tag	UNP G8GLP2
C	805	HIS	-	expression tag	UNP G8GLP2
C	806	HIS	-	expression tag	UNP G8GLP2
C	807	HIS	-	expression tag	UNP G8GLP2
C	808	HIS	-	expression tag	UNP G8GLP2
C	809	HIS	-	expression tag	UNP G8GLP2
D	804	HIS	-	expression tag	UNP G8GLP2
D	805	HIS	-	expression tag	UNP G8GLP2
D	806	HIS	-	expression tag	UNP G8GLP2

Continued on next page...

Continued from previous page...

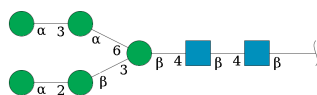
Chain	Residue	Modelled	Actual	Comment	Reference
D	807	HIS	-	expression tag	UNP G8GLP2
D	808	HIS	-	expression tag	UNP G8GLP2
D	809	HIS	-	expression tag	UNP G8GLP2

- Molecule 2 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.



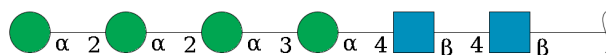
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

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



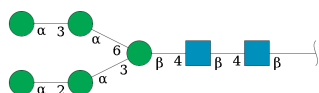
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

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



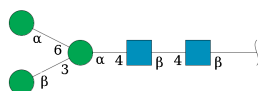
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	L	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



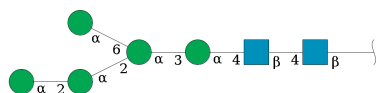
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



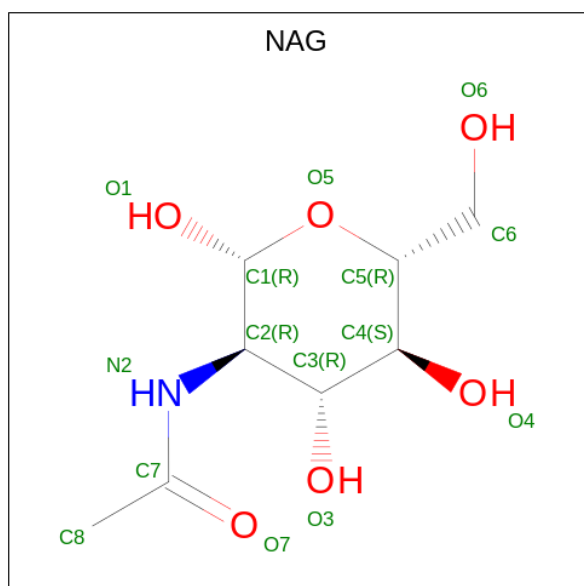
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



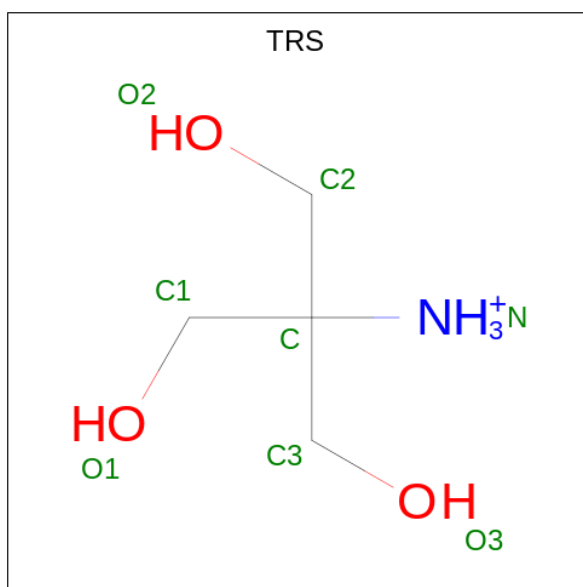
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			13	8	1	4		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			13	8	1	4		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			13	8	1	4		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			13	8	1	4		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			8	4	1	3		
11	B	1	Total	C	N	O	0	0
			8	4	1	3		
11	C	1	Total	C	N	O	0	0
			8	4	1	3		
11	D	1	Total	C	N	O	0	0
			8	4	1	3		

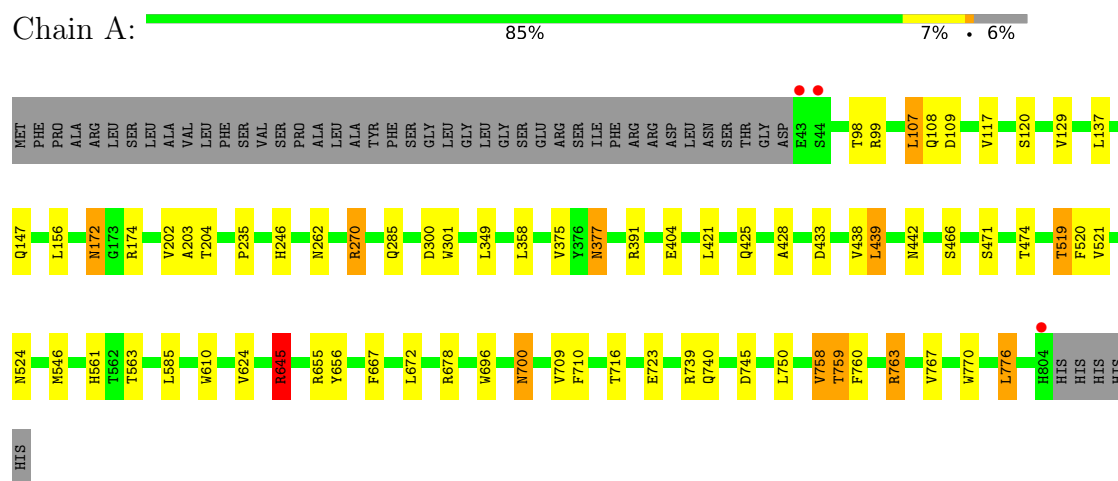
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	402	Total	O	0	0
			402	402		
12	B	311	Total	O	0	0
			311	311		
12	C	398	Total	O	0	0
			398	398		
12	D	433	Total	O	0	0
			433	433		

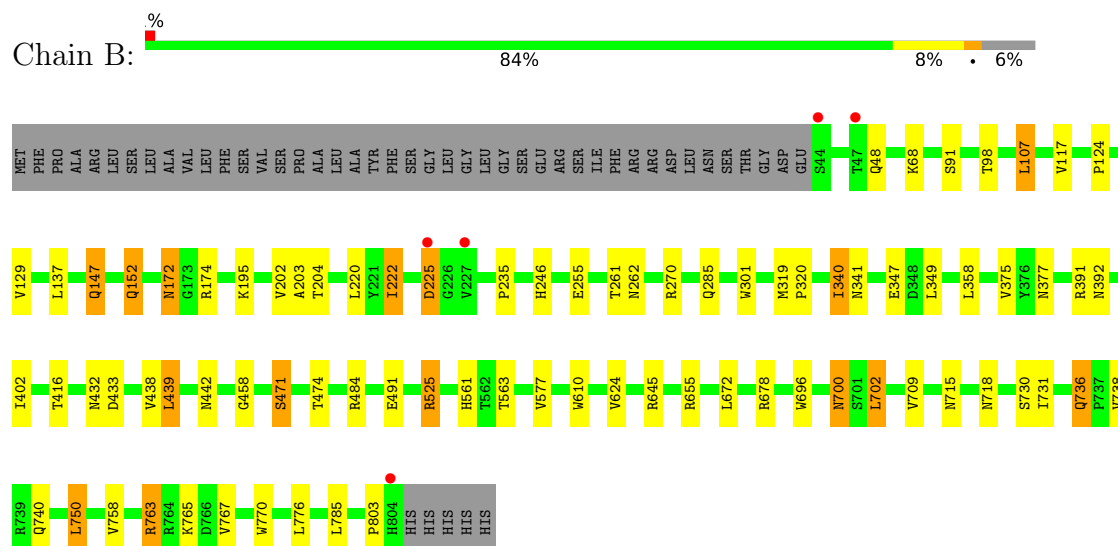
3 Residue-property plots [i](#)

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.

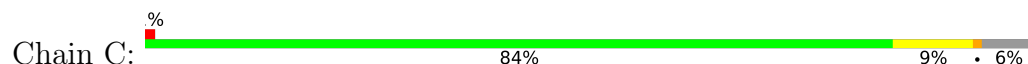
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

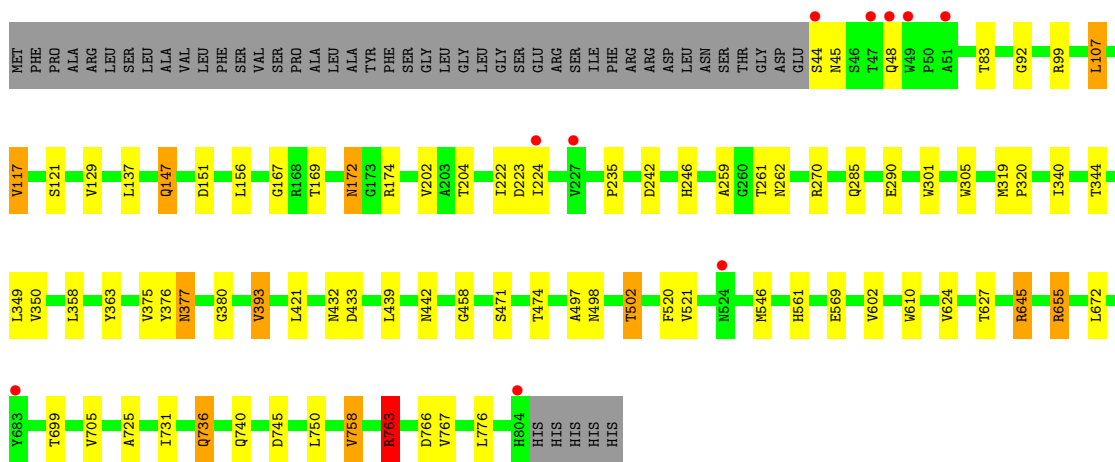


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

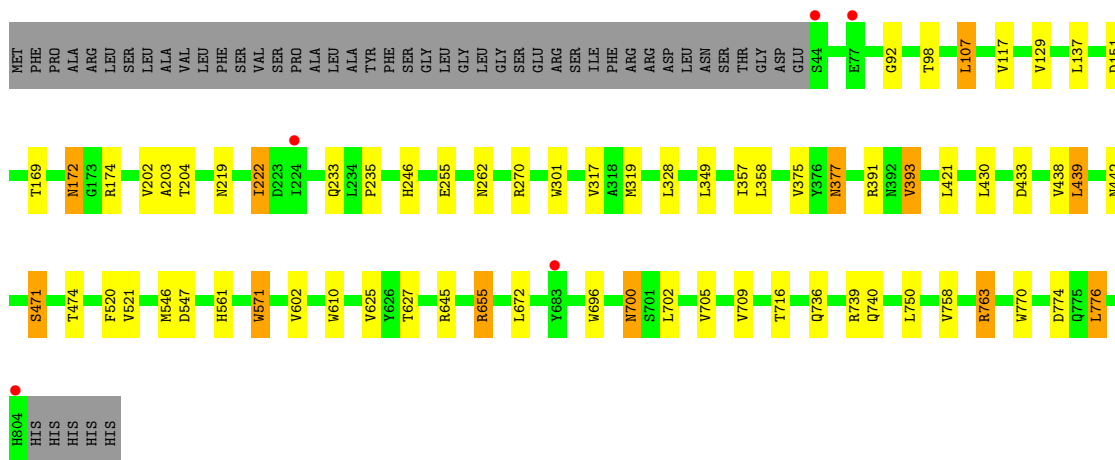
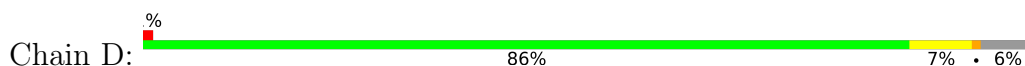


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

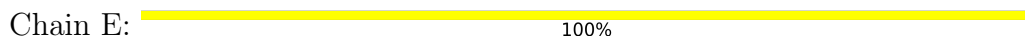




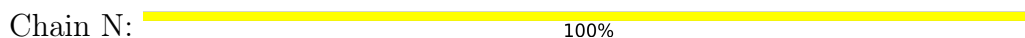
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



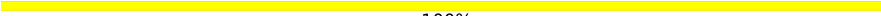
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain F:  100%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

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

Chain G:  33% 67%


MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

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

Chain H:  100%


MAG1
MAG2
MAN3

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

Chain K:  100%


MAG1
MAG2
MAN3

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

Chain I:  14% 86%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7


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

Chain L:  14% 86%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

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

Chain O:  14% 86%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



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

Chain M:  100%



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

Chain P:  29% 71%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.91Å 131.91Å 385.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.40) 99.7 (50.00-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.251 0.190 , 0.253	Depositor DCC
R_{free} test set	6893 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25512	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% 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

5.1 Standard geometry

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

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	0.48	0/5896	0.71	4/8067 (0.0%)
1	B	0.47	0/5885	0.70	5/8052 (0.1%)
1	C	0.49	0/5885	0.71	2/8052 (0.0%)
1	D	0.48	0/5885	0.70	5/8052 (0.1%)
All	All	0.48	0/23551	0.71	16/32223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	763	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	645	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	763	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	D	391	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	776	LEU	CA-CB-CG	5.75	128.54	115.30
1	A	391	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	484	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	655	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	391	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	655	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	484	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	391	ARG	NE-CZ-NH2	-5.27	117.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	99	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	107	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	763	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	259	ALA	Peptide
1	C	699	THR	Peptide

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	5752	0	5533	37	0
1	B	5744	0	5526	35	0
1	C	5744	0	5526	38	0
1	D	5744	0	5526	31	0
2	E	39	0	34	0	0
2	N	39	0	34	0	0
3	F	83	0	70	0	0
4	G	72	0	61	0	0
5	H	39	0	34	0	0
5	K	39	0	34	0	0
6	I	83	0	70	0	0
6	L	83	0	70	0	0
6	O	83	0	70	0	0
7	J	28	0	25	0	0
8	M	61	0	52	0	0
9	P	83	0	69	0	0
10	A	55	0	50	0	0
10	B	55	0	50	1	0
10	C	55	0	50	0	0
10	D	55	0	50	0	0
11	A	8	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	8	0	12	0	0
11	C	8	0	12	0	0
11	D	8	0	12	0	0
12	A	402	0	0	2	0
12	B	311	0	0	5	0
12	C	398	0	0	3	0
12	D	433	0	0	0	0
All	All	25512	0	22982	139	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 3.

All (139) 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:525:ARG:NH2	12:B:1001:HOH:O	1.99	0.95
1:C:319:MET:SD	12:C:1344:HOH:O	2.26	0.92
1:C:497:ALA:HB1	1:C:502:THR:HG21	1.59	0.85
1:B:696:TRP:HA	1:B:700:ASN:HD21	1.43	0.83
1:D:92:GLY:HA3	1:D:319:MET:HE2	1.64	0.78
1:D:645:ARG:HH11	1:D:740:GLN:HE21	1.34	0.74
1:D:92:GLY:HA3	1:D:319:MET:CE	2.21	0.69
1:B:491:GLU:OE1	12:B:1002:HOH:O	2.10	0.69
1:B:235:PRO:O	1:B:270:ARG:NH1	2.26	0.69
1:D:235:PRO:O	1:D:270:ARG:NH1	2.25	0.69
1:D:696:TRP:HA	1:D:700:ASN:HD21	1.59	0.66
1:B:577:VAL:HG23	12:B:1024:HOH:O	1.98	0.64
1:A:645:ARG:NH1	1:A:740:GLN:HE21	1.96	0.63
1:A:433:ASP:OD2	1:A:561:HIS:HD2	1.81	0.63
1:D:442:ASN:HD21	1:D:471:SER:H	1.47	0.62
1:A:235:PRO:HD2	1:A:270:ARG:HD2	1.81	0.61
1:A:645:ARG:HD3	12:A:1313:HOH:O	2.01	0.61
1:C:421:LEU:HD11	1:C:520:PHE:HZ	1.66	0.61
1:A:172:ASN:HD22	1:A:174:ARG:H	1.51	0.59
1:B:442:ASN:HD21	1:B:471:SER:H	1.49	0.58
1:A:442:ASN:HD21	1:A:471:SER:H	1.51	0.58
1:B:433:ASP:OD2	1:B:561:HIS:HD2	1.86	0.58
1:D:521:VAL:HG11	1:D:546:MET:CE	2.33	0.58
1:A:428:ALA:HB3	1:A:519:THR:HB	1.86	0.57
1:C:521:VAL:HG11	1:C:546:MET:CE	2.34	0.57
1:C:442:ASN:HD21	1:C:471:SER:H	1.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ASN:HD22	1:D:174:ARG:H	1.53	0.57
1:D:433:ASP:OD2	1:D:561:HIS:HD2	1.87	0.57
1:A:696:TRP:HA	1:A:700:ASN:HD21	1.70	0.56
1:A:204:THR:H	1:A:262:ASN:HD22	1.54	0.55
1:A:421:LEU:HD11	1:A:520:PHE:HZ	1.71	0.55
1:C:433:ASP:OD2	1:C:561:HIS:HD2	1.90	0.55
1:C:172:ASN:HD22	1:C:174:ARG:H	1.53	0.55
1:D:521:VAL:HG11	1:D:546:MET:HE2	1.89	0.55
1:B:731:ILE:O	1:B:736:GLN:HG2	2.08	0.54
1:C:246:HIS:HE1	1:C:290:GLU:OE2	1.92	0.53
1:A:521:VAL:HG11	1:A:546:MET:HE2	1.90	0.53
1:B:147:GLN:HG2	12:B:1299:HOH:O	2.09	0.52
1:B:340:ILE:HD11	1:B:347:GLU:CA	2.39	0.52
1:A:466:SER:CB	11:A:921:TRS:H32	2.40	0.52
1:B:340:ILE:HD11	1:B:347:GLU:HB2	1.92	0.52
1:D:421:LEU:HD11	1:D:520:PHE:HZ	1.75	0.51
1:B:172:ASN:HD22	1:B:174:ARG:H	1.58	0.51
1:C:377:ASN:HD21	1:C:380:GLY:H	1.58	0.51
1:B:340:ILE:HD11	1:B:347:GLU:CB	2.40	0.51
1:C:147:GLN:HG2	12:C:1325:HOH:O	2.10	0.51
1:D:204:THR:H	1:D:262:ASN:HD22	1.60	0.50
1:C:204:THR:H	1:C:262:ASN:HD22	1.60	0.50
1:B:525:ARG:NH1	1:B:563:THR:OG1	2.45	0.50
1:C:521:VAL:HG11	1:C:546:MET:HE2	1.93	0.50
1:B:432:ASN:HD21	1:B:458:GLY:H	1.59	0.50
1:B:438:VAL:HG23	1:B:439:LEU:HD13	1.92	0.50
1:D:222:ILE:HG23	1:D:328:LEU:HD23	1.93	0.50
1:A:235:PRO:O	1:A:270:ARG:HD3	2.13	0.49
1:D:438:VAL:HG13	1:D:439:LEU:HD13	1.93	0.49
1:C:319:MET:HE3	1:C:320:PRO:HA	1.94	0.49
1:C:377:ASN:C	1:C:377:ASN:HD22	2.15	0.49
1:C:745:ASP:HB3	1:C:758:VAL:HG22	1.95	0.49
1:A:521:VAL:HG11	1:A:546:MET:CE	2.43	0.49
1:C:731:ILE:O	1:C:736:GLN:HG2	2.13	0.48
1:A:700:ASN:C	1:A:700:ASN:HD22	2.17	0.48
1:C:498:ASN:O	1:C:502:THR:HG23	2.13	0.48
1:D:219:ASN:HD21	1:D:233:GLN:HE21	1.62	0.48
1:D:645:ARG:HH11	1:D:740:GLN:NE2	2.08	0.48
1:A:655:ARG:HG2	1:A:656:TYR:CD2	2.49	0.48
1:D:700:ASN:HD22	1:D:700:ASN:C	2.16	0.48
1:C:377:ASN:ND2	1:C:380:GLY:H	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ASN:HD21	1:C:458:GLY:H	1.61	0.47
1:A:377:ASN:HD22	1:A:377:ASN:C	2.17	0.47
1:C:45:ASN:HD22	1:C:48:GLN:HB2	1.79	0.47
1:D:219:ASN:HD21	1:D:233:GLN:NE2	2.12	0.47
1:D:246:HIS:CE1	1:D:770:TRP:CZ2	3.02	0.47
1:B:416:THR:HG22	1:B:416:THR:O	2.14	0.47
1:D:547:ASP:OD1	1:D:571:TRP:HZ3	1.98	0.47
1:D:645:ARG:NH1	1:D:740:GLN:HE21	2.07	0.46
1:C:736:GLN:HE21	1:C:736:GLN:HA	1.80	0.46
1:A:425:GLN:HE21	1:B:392:ASN:HD22	1.64	0.45
1:B:246:HIS:CE1	1:B:770:TRP:CZ2	3.04	0.45
1:B:255:GLU:OE2	1:B:763:ARG:NH2	2.49	0.45
1:D:317:VAL:HG22	1:D:357:ILE:HD11	1.97	0.45
1:D:442:ASN:HD21	1:D:471:SER:N	2.11	0.45
1:D:774:ASP:HB2	1:D:776:LEU:HD22	1.98	0.45
1:C:763:ARG:HD3	1:C:766:ASP:OD2	2.17	0.45
1:A:300:ASP:OD1	11:A:921:TRS:N	2.50	0.45
1:A:442:ASN:HD21	1:A:471:SER:N	2.15	0.45
1:C:645:ARG:NH1	1:C:740:GLN:HE21	2.15	0.45
1:D:203:ALA:HA	1:D:262:ASN:ND2	2.32	0.45
1:B:220:LEU:HD12	1:B:222:ILE:HG13	1.98	0.45
1:C:44:SER:N	12:C:1014:HOH:O	2.50	0.45
1:B:702:LEU:HD22	1:B:765:LYS:HB2	1.99	0.44
1:A:421:LEU:HD11	1:A:520:PHE:CZ	2.52	0.44
1:A:203:ALA:HA	1:A:262:ASN:ND2	2.33	0.44
1:B:730:SER:HB3	1:B:738:VAL:O	2.18	0.44
1:D:377:ASN:HD22	1:D:377:ASN:C	2.20	0.44
1:A:563:THR:HG22	1:A:585:LEU:HD11	1.99	0.44
1:A:524:ASN:HA	1:A:561:HIS:O	2.18	0.43
1:B:203:ALA:HA	1:B:262:ASN:ND2	2.32	0.43
1:A:108:GLN:HG3	1:A:109:ASP:O	2.19	0.43
1:A:438:VAL:HG23	1:A:439:LEU:HD13	2.01	0.43
1:A:710:PHE:CD1	1:A:759:THR:HB	2.53	0.43
1:B:645:ARG:HH22	1:B:740:GLN:HE21	1.67	0.43
1:A:107:LEU:HD22	1:A:156:LEU:HD22	2.01	0.43
1:D:255:GLU:OE2	1:D:763:ARG:NH2	2.52	0.43
1:A:758:VAL:HG13	1:A:760:PHE:CE2	2.54	0.42
1:B:319:MET:HE3	1:B:320:PRO:HA	1.99	0.42
10:B:911:NAG:H3	10:B:911:NAG:H83	2.02	0.42
1:D:151:ASP:HB3	1:D:393:VAL:HG22	2.00	0.42
1:A:678:ARG:NH1	1:C:363:TYR:O	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASP:CB	1:C:393:VAL:CG2	2.97	0.42
1:A:645:ARG:HH11	1:A:740:GLN:HE21	1.65	0.42
1:B:442:ASN:ND2	1:B:471:SER:H	2.16	0.42
1:C:92:GLY:HA3	1:C:319:MET:HE1	2.02	0.42
1:C:151:ASP:HB3	1:C:393:VAL:CG2	2.50	0.42
1:A:745:ASP:HB3	1:A:758:VAL:HG22	2.01	0.42
1:B:124:PRO:HD3	1:B:402:ILE:HG23	2.01	0.42
1:C:421:LEU:HD11	1:C:520:PHE:CZ	2.52	0.42
1:C:725:ALA:CB	1:C:758:VAL:HG21	2.50	0.42
1:A:561:HIS:HE1	12:A:1064:HOH:O	2.02	0.41
1:C:92:GLY:CA	1:C:319:MET:HE1	2.51	0.41
1:C:242:ASP:O	1:C:246:HIS:HD2	2.04	0.41
1:A:246:HIS:CE1	1:A:770:TRP:CZ2	3.08	0.41
1:B:416:THR:HG21	12:B:1042:HOH:O	2.20	0.41
1:B:702:LEU:HD22	1:B:765:LYS:CB	2.50	0.41
1:C:117:VAL:HG22	1:C:376:TYR:CD2	2.55	0.41
1:C:497:ALA:HB2	1:D:438:VAL:HG22	2.03	0.41
1:D:776:LEU:O	1:D:776:LEU:HD23	2.20	0.41
1:A:433:ASP:OD2	1:A:561:HIS:CD2	2.69	0.40
1:B:204:THR:H	1:B:262:ASN:HD22	1.68	0.40
1:B:715:ASN:HB2	1:B:750:LEU:HD13	2.03	0.40
1:C:107:LEU:HD22	1:C:156:LEU:HD22	2.03	0.40
1:C:235:PRO:HD3	1:C:305:TRP:CZ2	2.56	0.40
1:C:569:GLU:OE1	1:C:655:ARG:NH1	2.53	0.40
1:A:758:VAL:HG13	1:A:760:PHE:CZ	2.56	0.40
1:A:667:PHE:CE2	1:A:723:GLU:HB2	2.55	0.40
1:C:340:ILE:HD11	1:C:350:VAL:HG21	2.02	0.40
1:B:340:ILE:HD11	1:B:347:GLU:HA	2.02	0.40
1:B:730:SER:OG	1:B:785:LEU:HB3	2.21	0.40
1:B:152:GLN:HE21	1:B:152:GLN:HA	1.86	0.40
1:D:736:GLN:HA	1:D:736:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	761/809 (94%)	733 (96%)	28 (4%)	0	100	100
1	B	759/809 (94%)	727 (96%)	30 (4%)	2 (0%)	37	51
1	C	759/809 (94%)	729 (96%)	28 (4%)	2 (0%)	37	51
1	D	759/809 (94%)	730 (96%)	29 (4%)	0	100	100
All	All	3038/3236 (94%)	2919 (96%)	115 (4%)	4 (0%)	48	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	803	PRO
1	C	224	ILE
1	B	225	ASP
1	C	167	GLY

5.3.2 Protein sidechains ⓘ

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	613/654 (94%)	578 (94%)	35 (6%)	17	29
1	B	612/654 (94%)	569 (93%)	43 (7%)	12	21
1	C	612/654 (94%)	573 (94%)	39 (6%)	14	24
1	D	612/654 (94%)	577 (94%)	35 (6%)	17	29
All	All	2449/2616 (94%)	2297 (94%)	152 (6%)	15	26

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	99	ARG
1	A	107	LEU
1	A	117	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	SER
1	A	129	VAL
1	A	137	LEU
1	A	147	GLN
1	A	172	ASN
1	A	202	VAL
1	A	270	ARG
1	A	285	GLN
1	A	301	TRP
1	A	349	LEU
1	A	358	LEU
1	A	375	VAL
1	A	377	ASN
1	A	404	GLU
1	A	439	LEU
1	A	474	THR
1	A	519	THR
1	A	610	TRP
1	A	624	VAL
1	A	645	ARG
1	A	672	LEU
1	A	700	ASN
1	A	709	VAL
1	A	716	THR
1	A	739	ARG
1	A	750	LEU
1	A	758	VAL
1	A	759	THR
1	A	763	ARG
1	A	767	VAL
1	A	776	LEU
1	B	48	GLN
1	B	68	LYS
1	B	91	SER
1	B	98	THR
1	B	107	LEU
1	B	117	VAL
1	B	129	VAL
1	B	137	LEU
1	B	147	GLN
1	B	152	GLN
1	B	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	LYS
1	B	202	VAL
1	B	222	ILE
1	B	225	ASP
1	B	261	THR
1	B	285	GLN
1	B	301	TRP
1	B	340	ILE
1	B	341	ASN
1	B	349	LEU
1	B	358	LEU
1	B	375	VAL
1	B	377	ASN
1	B	439	LEU
1	B	471	SER
1	B	474	THR
1	B	525	ARG
1	B	610	TRP
1	B	624	VAL
1	B	655	ARG
1	B	672	LEU
1	B	678	ARG
1	B	700	ASN
1	B	702	LEU
1	B	709	VAL
1	B	718	ASN
1	B	736	GLN
1	B	750	LEU
1	B	758	VAL
1	B	763	ARG
1	B	767	VAL
1	B	776	LEU
1	C	83	THR
1	C	107	LEU
1	C	117	VAL
1	C	121	SER
1	C	129	VAL
1	C	137	LEU
1	C	147	GLN
1	C	169	THR
1	C	172	ASN
1	C	202	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	222	ILE
1	C	223	ASP
1	C	261	THR
1	C	270	ARG
1	C	285	GLN
1	C	301	TRP
1	C	344	THR
1	C	349	LEU
1	C	358	LEU
1	C	375	VAL
1	C	377	ASN
1	C	393	VAL
1	C	439	LEU
1	C	474	THR
1	C	502	THR
1	C	602	VAL
1	C	610	TRP
1	C	624	VAL
1	C	627	THR
1	C	645	ARG
1	C	655	ARG
1	C	672	LEU
1	C	705	VAL
1	C	736	GLN
1	C	750	LEU
1	C	758	VAL
1	C	763	ARG
1	C	767	VAL
1	C	776	LEU
1	D	98	THR
1	D	107	LEU
1	D	117	VAL
1	D	129	VAL
1	D	137	LEU
1	D	169	THR
1	D	172	ASN
1	D	202	VAL
1	D	222	ILE
1	D	301	TRP
1	D	349	LEU
1	D	358	LEU
1	D	375	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	377	ASN
1	D	393	VAL
1	D	430	LEU
1	D	439	LEU
1	D	471	SER
1	D	474	THR
1	D	571	TRP
1	D	602	VAL
1	D	610	TRP
1	D	625	VAL
1	D	627	THR
1	D	655	ARG
1	D	672	LEU
1	D	700	ASN
1	D	702	LEU
1	D	705	VAL
1	D	709	VAL
1	D	716	THR
1	D	739	ARG
1	D	750	LEU
1	D	758	VAL
1	D	776	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	155	HIS
1	A	172	ASN
1	A	229	GLN
1	A	246	HIS
1	A	262	ASN
1	A	377	ASN
1	A	425	GLN
1	A	442	ASN
1	A	561	HIS
1	A	700	ASN
1	A	736	GLN
1	A	740	GLN
1	B	48	GLN
1	B	152	GLN
1	B	155	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	ASN
1	B	246	HIS
1	B	262	ASN
1	B	313	ASN
1	B	341	ASN
1	B	377	ASN
1	B	432	ASN
1	B	442	ASN
1	B	561	HIS
1	B	676	HIS
1	B	700	ASN
1	B	736	GLN
1	B	740	GLN
1	C	45	ASN
1	C	152	GLN
1	C	172	ASN
1	C	229	GLN
1	C	246	HIS
1	C	262	ASN
1	C	377	ASN
1	C	432	ASN
1	C	442	ASN
1	C	561	HIS
1	C	740	GLN
1	D	152	GLN
1	D	155	HIS
1	D	172	ASN
1	D	229	GLN
1	D	233	GLN
1	D	246	HIS
1	D	262	ASN
1	D	377	ASN
1	D	442	ASN
1	D	561	HIS
1	D	676	HIS
1	D	700	ASN
1	D	736	GLN
1	D	740	GLN

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 ⓘ

60 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	1.05	1 (7%)	17,19,21	1.36	1 (5%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.20	2 (11%)
2	BMA	E	3	2	11,11,12	0.64	0	15,15,17	0.84	1 (6%)
3	NAG	F	1	3,1	14,14,15	1.25	1 (7%)	17,19,21	1.12	1 (5%)
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
3	BMA	F	3	3	11,11,12	0.62	0	15,15,17	1.69	2 (13%)
3	BMA	F	4	3	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
3	MAN	F	5	3	11,11,12	0.72	0	15,15,17	1.67	1 (6%)
3	MAN	F	6	3	11,11,12	0.94	0	15,15,17	3.20	5 (33%)
3	MAN	F	7	3	11,11,12	0.25	0	15,15,17	0.89	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.44	0	17,19,21	0.81	0
4	NAG	G	2	4	14,14,15	0.39	0	17,19,21	0.89	0
4	MAN	G	3	4	11,11,12	0.69	0	15,15,17	1.83	3 (20%)
4	MAN	G	4	4	11,11,12	0.68	0	15,15,17	1.78	1 (6%)
4	MAN	G	5	4	11,11,12	0.66	0	15,15,17	2.03	1 (6%)
4	MAN	G	6	4	11,11,12	0.49	0	15,15,17	1.27	2 (13%)
5	NAG	H	1	1,5	14,14,15	1.00	1 (7%)	17,19,21	1.21	2 (11%)
5	NAG	H	2	5	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
5	MAN	H	3	5	11,11,12	0.68	0	15,15,17	1.31	3 (20%)
6	NAG	I	1	1,6	14,14,15	1.11	1 (7%)	17,19,21	1.51	3 (17%)
6	NAG	I	2	6	14,14,15	0.46	0	17,19,21	0.86	0
6	BMA	I	3	6	11,11,12	0.28	0	15,15,17	0.97	1 (6%)
6	MAN	I	4	6	11,11,12	0.48	0	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	I	5	6	11,11,12	0.53	0	15,15,17	1.42	2 (13%)
6	MAN	I	6	6	11,11,12	0.77	0	15,15,17	2.57	5 (33%)
6	MAN	I	7	6	11,11,12	0.39	0	15,15,17	0.95	2 (13%)
7	NAG	J	1	7,1	14,14,15	0.29	0	17,19,21	0.90	0
7	NAG	J	2	7	14,14,15	0.61	0	17,19,21	1.08	2 (11%)
5	NAG	K	1	1,5	14,14,15	1.19	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	K	2	5	14,14,15	0.52	0	17,19,21	1.12	1 (5%)
5	MAN	K	3	5	11,11,12	0.55	0	15,15,17	0.98	1 (6%)
6	NAG	L	1	1,6	14,14,15	1.16	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	L	2	6	14,14,15	0.51	0	17,19,21	1.01	0
6	BMA	L	3	6	11,11,12	0.46	0	15,15,17	1.03	1 (6%)
6	MAN	L	4	6	11,11,12	0.65	0	15,15,17	2.09	3 (20%)
6	MAN	L	5	6	11,11,12	0.70	0	15,15,17	0.93	1 (6%)
6	MAN	L	6	6	11,11,12	0.79	0	15,15,17	3.22	4 (26%)
6	MAN	L	7	6	11,11,12	0.48	0	15,15,17	1.00	2 (13%)
8	NAG	M	1	8,1	14,14,15	0.44	0	17,19,21	1.07	2 (11%)
8	NAG	M	2	8	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
8	MAN	M	3	8	11,11,12	0.54	0	15,15,17	1.72	4 (26%)
8	BMA	M	4	8	11,11,12	0.61	0	15,15,17	1.71	3 (20%)
8	MAN	M	5	8	11,11,12	0.88	0	15,15,17	1.43	3 (20%)
2	NAG	N	1	2,1	14,14,15	0.96	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	N	2	2	14,14,15	0.56	0	17,19,21	1.18	2 (11%)
2	BMA	N	3	2	11,11,12	0.66	0	15,15,17	1.16	2 (13%)
6	NAG	O	1	1,6	14,14,15	1.12	1 (7%)	17,19,21	0.81	0
6	NAG	O	2	6	14,14,15	0.28	0	17,19,21	0.71	0
6	BMA	O	3	6	11,11,12	0.37	0	15,15,17	1.28	2 (13%)
6	MAN	O	4	6	11,11,12	0.54	0	15,15,17	1.41	1 (6%)
6	MAN	O	5	6	11,11,12	0.59	0	15,15,17	2.20	4 (26%)
6	MAN	O	6	6	11,11,12	0.69	0	15,15,17	3.10	3 (20%)
6	MAN	O	7	6	11,11,12	0.32	0	15,15,17	1.07	1 (6%)
9	NAG	P	1	9,1	14,14,15	0.39	0	17,19,21	0.96	0
9	NAG	P	2	9	14,14,15	0.44	0	17,19,21	0.92	0
9	MAN	P	3	9	11,11,12	0.66	0	15,15,17	2.30	5 (33%)
9	MAN	P	4	9	11,11,12	0.60	0	15,15,17	2.26	1 (6%)
9	MAN	P	5	9	11,11,12	0.45	0	15,15,17	1.65	2 (13%)
9	MAN	P	6	9	11,11,12	0.31	0	15,15,17	1.31	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	P	7	9	11,11,12	0.89	0	15,15,17	2.47	5 (33%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O4-C4	-4.44	1.32	1.43
6	L	1	NAG	O4-C4	-4.19	1.33	1.43
5	K	1	NAG	O4-C4	-4.17	1.33	1.43
6	O	1	NAG	O4-C4	-3.82	1.34	1.43
6	I	1	NAG	O4-C4	-3.77	1.34	1.43
2	E	1	NAG	O4-C4	-3.72	1.34	1.43
5	H	1	NAG	O4-C4	-3.55	1.34	1.43
2	N	1	NAG	O4-C4	-3.37	1.35	1.43

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	6	MAN	C1-O5-C5	10.08	125.85	112.19
6	O	6	MAN	C1-O5-C5	9.83	125.51	112.19
3	F	6	MAN	C1-O5-C5	9.47	125.02	112.19
9	P	4	MAN	C1-O5-C5	7.87	122.86	112.19
6	I	6	MAN	C1-O5-C5	7.09	121.80	112.19
4	G	5	MAN	C1-O5-C5	6.91	121.55	112.19
6	O	5	MAN	C1-O5-C5	6.50	121.00	112.19
4	G	4	MAN	C1-O5-C5	6.32	120.76	112.19
6	L	4	MAN	C1-O5-C5	6.26	120.68	112.19
9	P	3	MAN	C1-O5-C5	5.83	120.09	112.19
9	P	7	MAN	C1-C2-C3	5.56	116.50	109.67
3	F	5	MAN	C1-O5-C5	5.53	119.68	112.19
9	P	7	MAN	C1-O5-C5	5.48	119.62	112.19
3	F	3	BMA	O3-C3-C2	5.31	120.17	109.99
6	L	6	MAN	O5-C1-C2	4.91	118.34	110.77
9	P	5	MAN	C1-O5-C5	4.85	118.76	112.19
6	O	4	MAN	C1-O5-C5	4.73	118.61	112.19
3	F	6	MAN	O5-C1-C2	4.53	117.77	110.77
6	O	6	MAN	C3-C4-C5	4.41	118.11	110.24
4	G	3	MAN	C1-C2-C3	4.39	115.06	109.67
8	M	4	BMA	C1-C2-C3	-4.27	104.41	109.67
9	P	6	MAN	C1-O5-C5	4.14	117.81	112.19
3	F	6	MAN	C3-C4-C5	4.13	117.61	110.24
2	E	1	NAG	O4-C4-C5	4.12	119.52	109.30
9	P	3	MAN	C1-C2-C3	4.08	114.68	109.67
8	M	3	MAN	C1-O5-C5	3.87	117.44	112.19
6	I	6	MAN	C3-C4-C5	3.86	117.12	110.24
6	I	1	NAG	C1-O5-C5	3.84	117.39	112.19
6	L	6	MAN	C3-C4-C5	3.75	116.92	110.24
9	P	7	MAN	O5-C1-C2	3.66	116.43	110.77
3	F	4	BMA	C1-C2-C3	-3.55	105.31	109.67
6	I	6	MAN	O5-C1-C2	3.53	116.23	110.77
4	G	3	MAN	C3-C4-C5	3.38	116.27	110.24
6	I	5	MAN	C1-O5-C5	3.37	116.76	112.19
6	O	3	BMA	O5-C5-C6	3.26	112.32	107.20
6	O	7	MAN	C1-O5-C5	3.12	116.42	112.19
6	L	4	MAN	O2-C2-C1	-2.93	103.16	109.15
4	G	6	MAN	C1-O5-C5	2.90	116.12	112.19
3	F	6	MAN	C2-C3-C4	2.90	115.91	110.89
2	N	1	NAG	O4-C4-C5	2.89	116.47	109.30
2	N	2	NAG	C1-C2-N2	-2.88	105.57	110.49
6	O	6	MAN	O5-C1-C2	2.86	115.19	110.77
8	M	3	MAN	C1-C2-C3	2.85	113.17	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	5	MAN	O5-C1-C2	2.84	115.15	110.77
6	L	5	MAN	C1-O5-C5	2.79	115.97	112.19
5	H	3	MAN	C1-C2-C3	2.78	113.08	109.67
3	F	1	NAG	O4-C4-C3	2.75	116.72	110.35
8	M	5	MAN	O5-C5-C6	2.73	111.48	107.20
5	H	3	MAN	C1-O5-C5	2.71	115.86	112.19
9	P	3	MAN	O5-C5-C6	2.68	111.41	107.20
2	E	2	NAG	C4-C3-C2	2.67	114.93	111.02
6	I	7	MAN	C1-O5-C5	2.66	115.80	112.19
8	M	2	NAG	O3-C3-C2	-2.63	104.03	109.47
5	K	3	MAN	C1-O5-C5	2.63	115.75	112.19
6	I	4	MAN	C1-O5-C5	2.63	115.75	112.19
6	I	6	MAN	O5-C5-C6	2.61	111.30	107.20
3	F	4	BMA	C3-C4-C5	2.61	114.89	110.24
5	H	3	MAN	O5-C5-C6	2.58	111.25	107.20
6	L	7	MAN	C1-O5-C5	2.56	115.66	112.19
8	M	3	MAN	O3-C3-C4	-2.55	104.46	110.35
6	I	1	NAG	O4-C4-C5	-2.53	103.01	109.30
8	M	4	BMA	O4-C4-C3	-2.52	104.52	110.35
6	L	1	NAG	C1-O5-C5	2.49	115.57	112.19
6	O	3	BMA	C1-O5-C5	2.45	115.51	112.19
5	H	1	NAG	O4-C4-C5	2.43	115.33	109.30
6	L	7	MAN	O5-C5-C6	2.42	111.00	107.20
8	M	1	NAG	O5-C5-C6	2.42	111.00	107.20
9	P	5	MAN	C6-C5-C4	-2.41	107.37	113.00
7	J	2	NAG	O4-C4-C5	2.38	115.20	109.30
8	M	1	NAG	C2-N2-C7	2.35	126.25	122.90
6	L	4	MAN	O2-C2-C3	2.34	114.82	110.14
5	K	2	NAG	O5-C5-C6	2.30	110.81	107.20
8	M	5	MAN	O6-C6-C5	2.30	119.17	111.29
2	N	3	BMA	C1-O5-C5	2.29	115.30	112.19
9	P	7	MAN	C2-C3-C4	2.25	114.79	110.89
5	H	2	NAG	O5-C1-C2	-2.25	107.74	111.29
3	F	2	NAG	O5-C5-C6	2.24	110.72	107.20
4	G	6	MAN	O5-C5-C6	2.24	110.72	107.20
6	I	6	MAN	C2-C3-C4	2.24	114.77	110.89
8	M	4	BMA	C3-C4-C5	2.24	114.23	110.24
6	L	6	MAN	O4-C4-C3	-2.23	105.19	110.35
3	F	7	MAN	C1-O5-C5	2.22	115.20	112.19
6	O	5	MAN	C1-C2-C3	-2.21	106.95	109.67
9	P	3	MAN	O6-C6-C5	2.16	118.71	111.29
6	L	3	BMA	O5-C5-C6	2.16	110.59	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	5	MAN	C3-C4-C5	2.15	114.08	110.24
8	M	3	MAN	C3-C4-C5	2.15	114.08	110.24
6	I	3	BMA	C1-O5-C5	2.13	115.08	112.19
5	K	1	NAG	O4-C4-C5	2.11	114.55	109.30
6	I	4	MAN	O5-C5-C6	2.11	110.52	107.20
2	E	2	NAG	C2-N2-C7	2.11	125.90	122.90
9	P	7	MAN	O3-C3-C4	-2.10	105.50	110.35
6	I	1	NAG	O3-C3-C4	2.09	115.18	110.35
2	N	3	BMA	C3-C4-C5	2.08	113.96	110.24
6	I	7	MAN	O5-C5-C6	2.07	110.45	107.20
2	N	2	NAG	C4-C3-C2	2.06	114.03	111.02
6	I	5	MAN	C3-C4-C5	2.06	113.91	110.24
3	F	6	MAN	O4-C4-C3	-2.05	105.61	110.35
6	O	5	MAN	O2-C2-C3	2.04	114.22	110.14
4	G	3	MAN	C2-C3-C4	2.04	114.42	110.89
3	F	4	BMA	O5-C5-C6	2.04	110.39	107.20
2	E	3	BMA	C1-C2-C3	2.02	112.15	109.67
7	J	2	NAG	C3-C4-C5	-2.02	106.64	110.24
5	H	1	NAG	C1-O5-C5	2.02	114.92	112.19
9	P	3	MAN	O5-C1-C2	2.02	113.88	110.77
3	F	3	BMA	O3-C3-C4	-2.00	105.72	110.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	3	MAN	O5-C5-C6-O6
6	O	6	MAN	O5-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
4	G	6	MAN	C4-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
9	P	6	MAN	O5-C5-C6-O6
6	I	6	MAN	O5-C5-C6-O6
9	P	7	MAN	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
5	K	3	MAN	C4-C5-C6-O6
9	P	7	MAN	C4-C5-C6-O6
9	P	3	MAN	C4-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
9	P	3	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

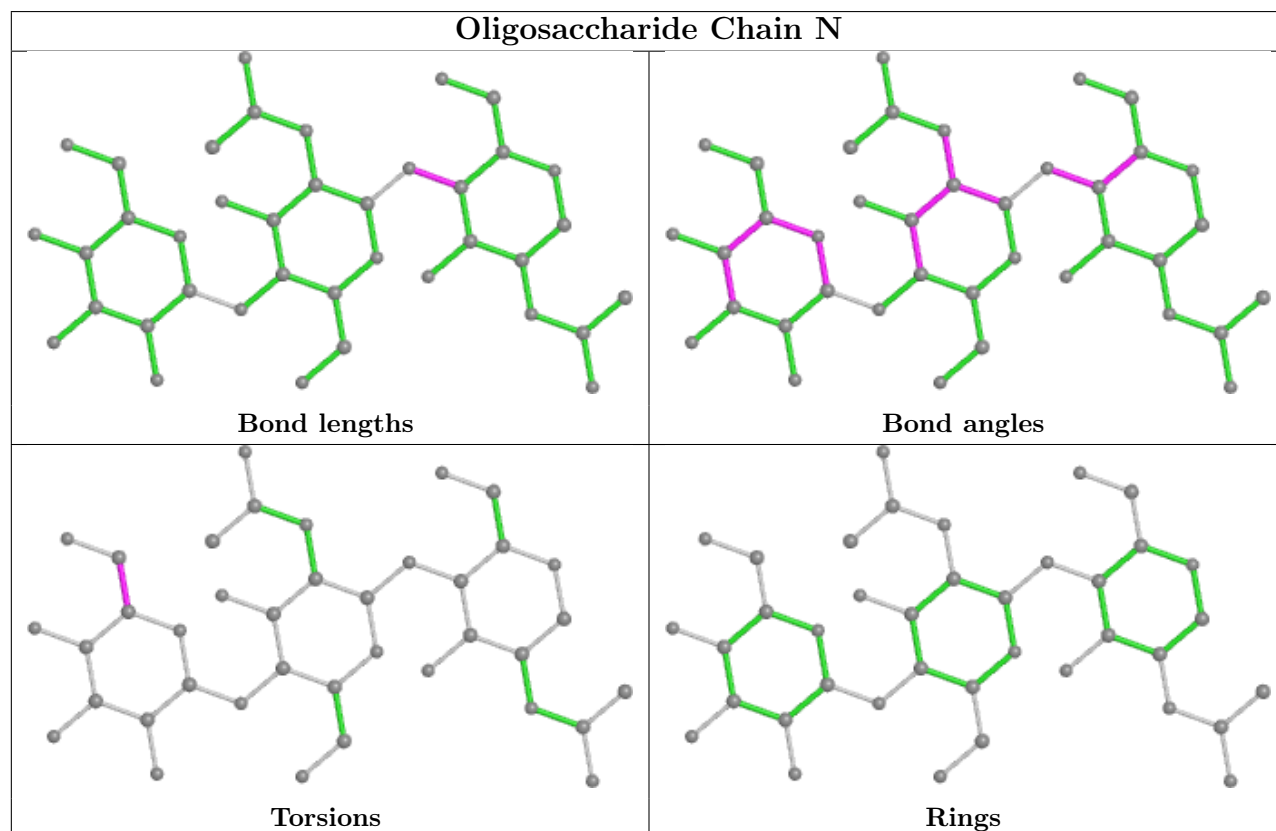
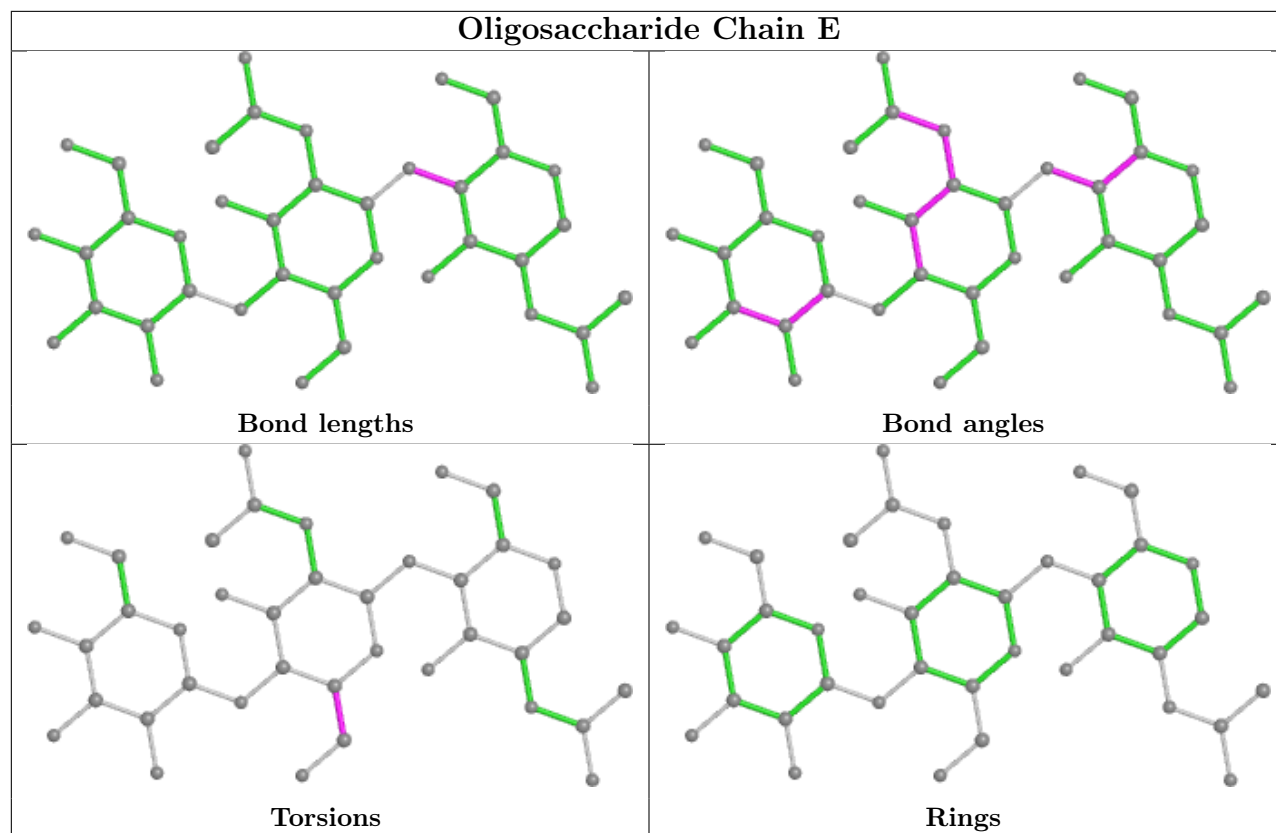
Mol	Chain	Res	Type	Atoms
3	F	6	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	L	6	MAN	O5-C5-C6-O6
6	I	6	MAN	C4-C5-C6-O6
8	M	4	BMA	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
6	O	6	MAN	C4-C5-C6-O6
9	P	6	MAN	C4-C5-C6-O6
4	G	3	MAN	O5-C5-C6-O6
8	M	4	BMA	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
8	M	3	MAN	O5-C5-C6-O6
5	H	3	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
8	M	2	NAG	C4-C5-C6-O6

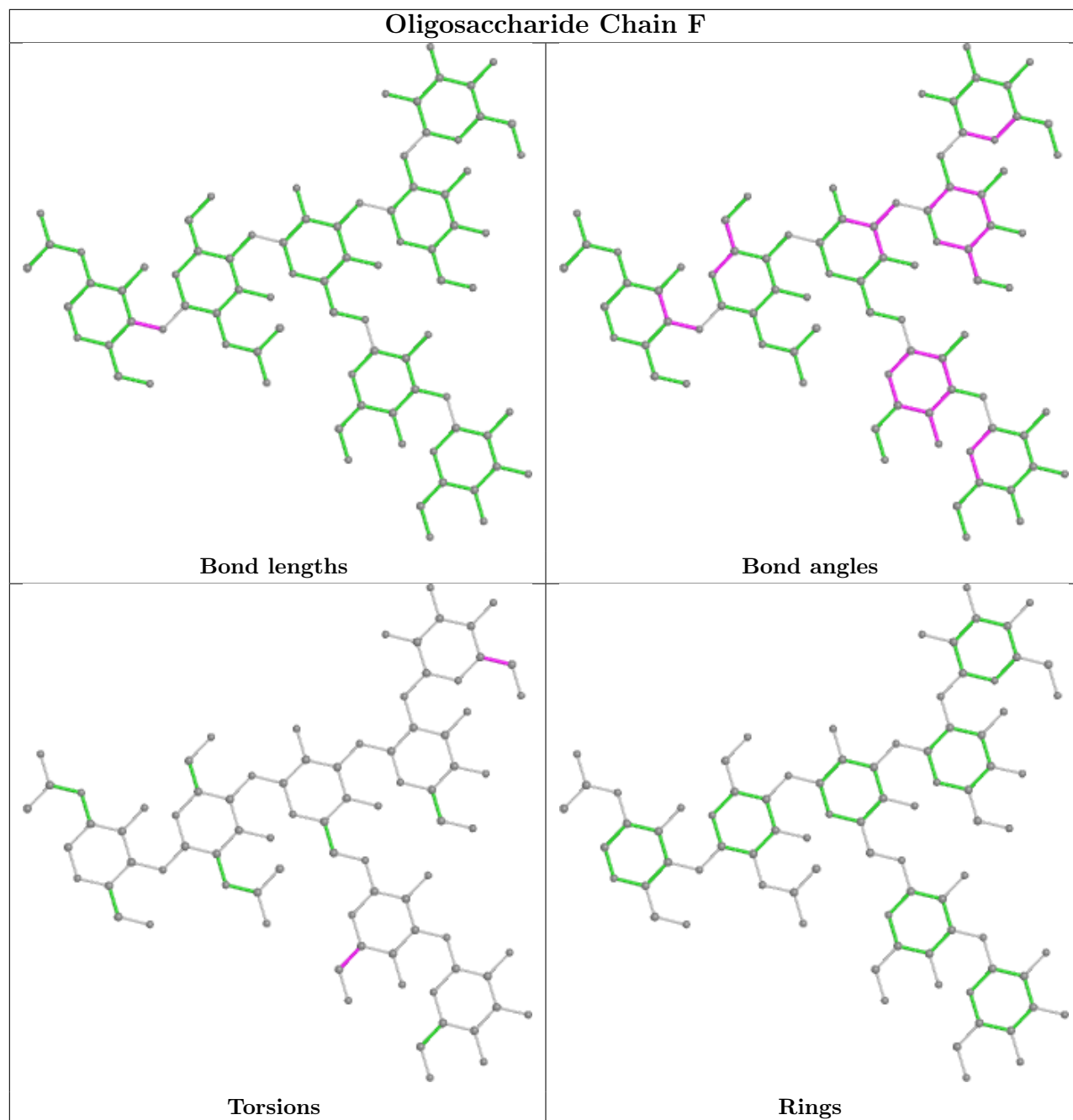
All (2) ring outliers are listed below:

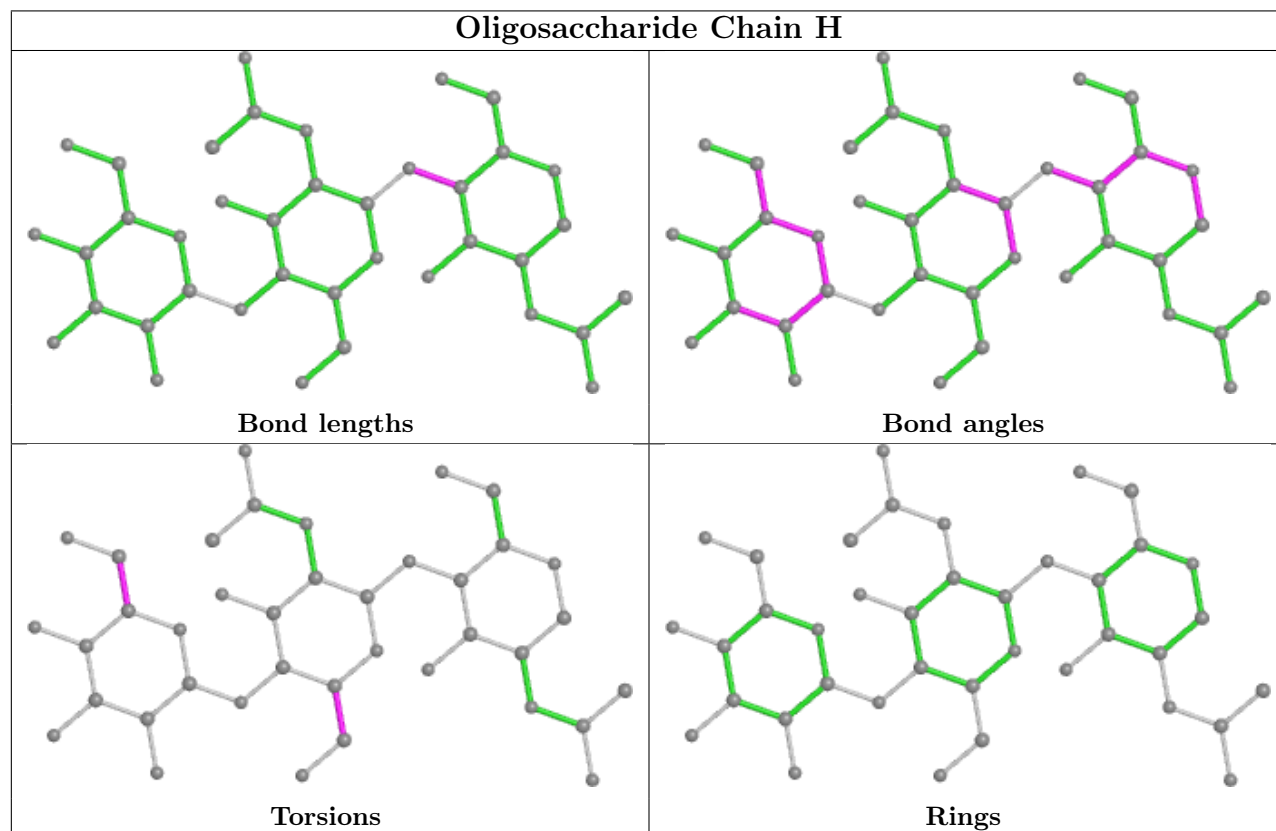
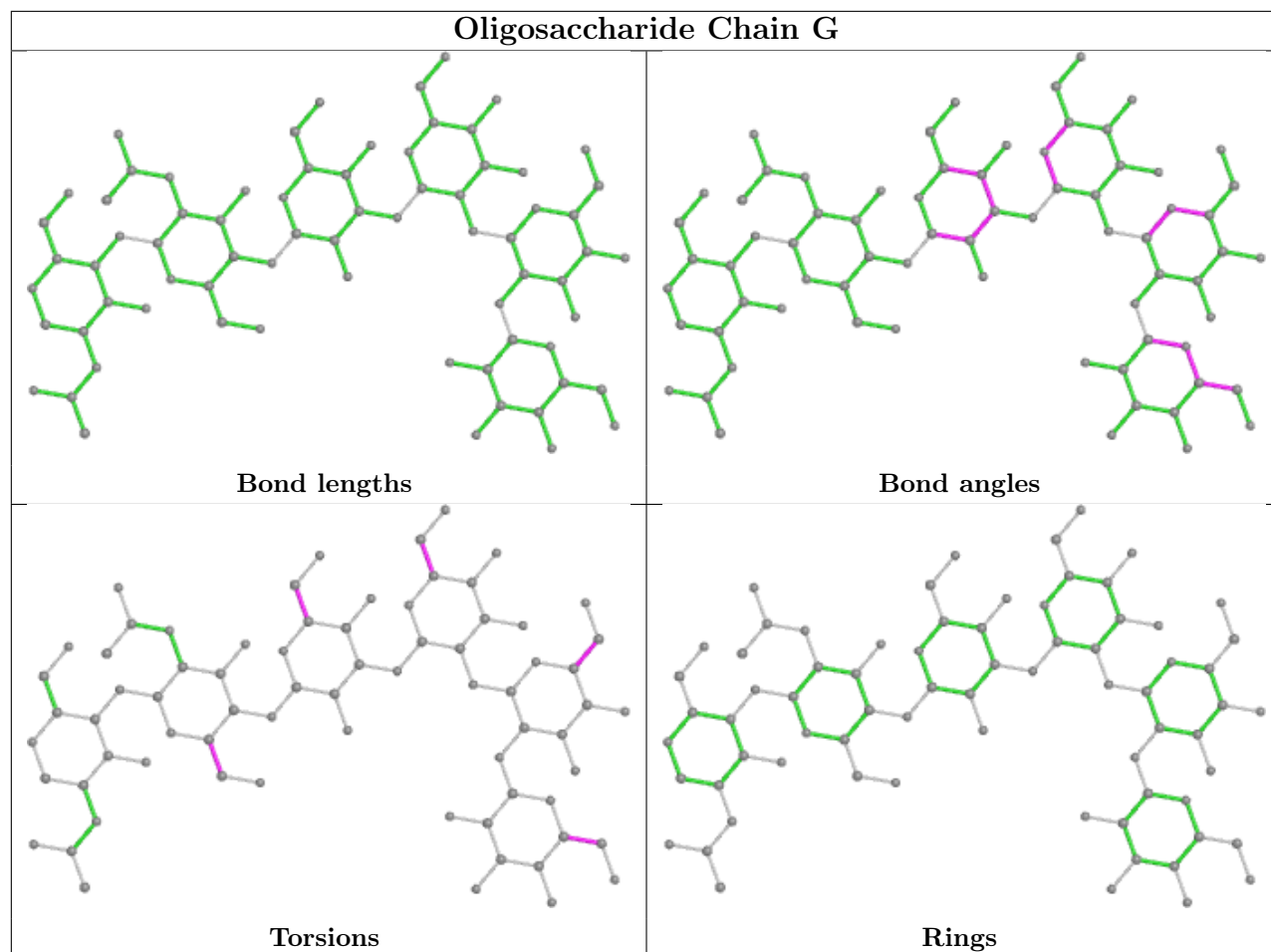
Mol	Chain	Res	Type	Atoms
9	P	3	MAN	C1-C2-C3-C4-C5-O5
5	K	3	MAN	C1-C2-C3-C4-C5-O5

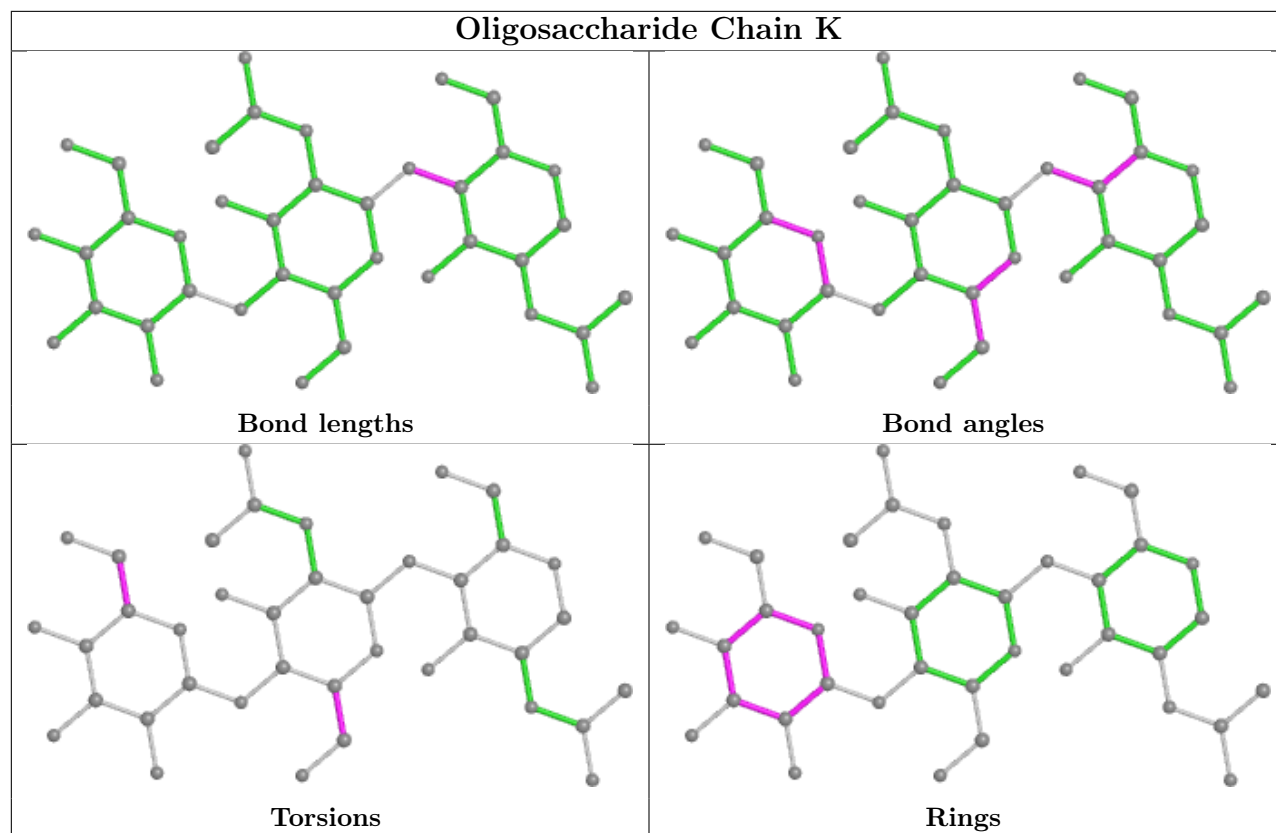
No monomer is involved in short contacts.

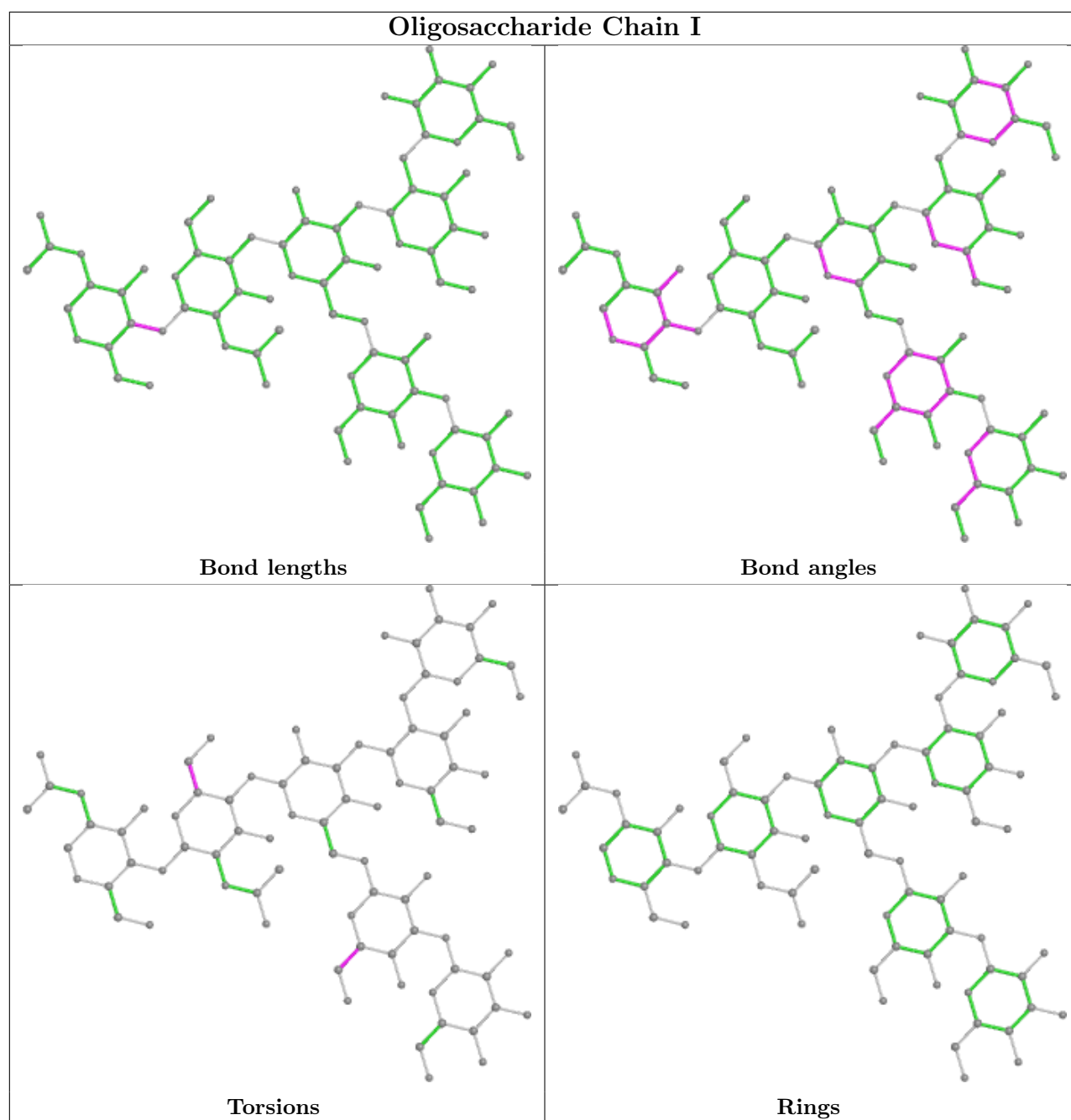
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

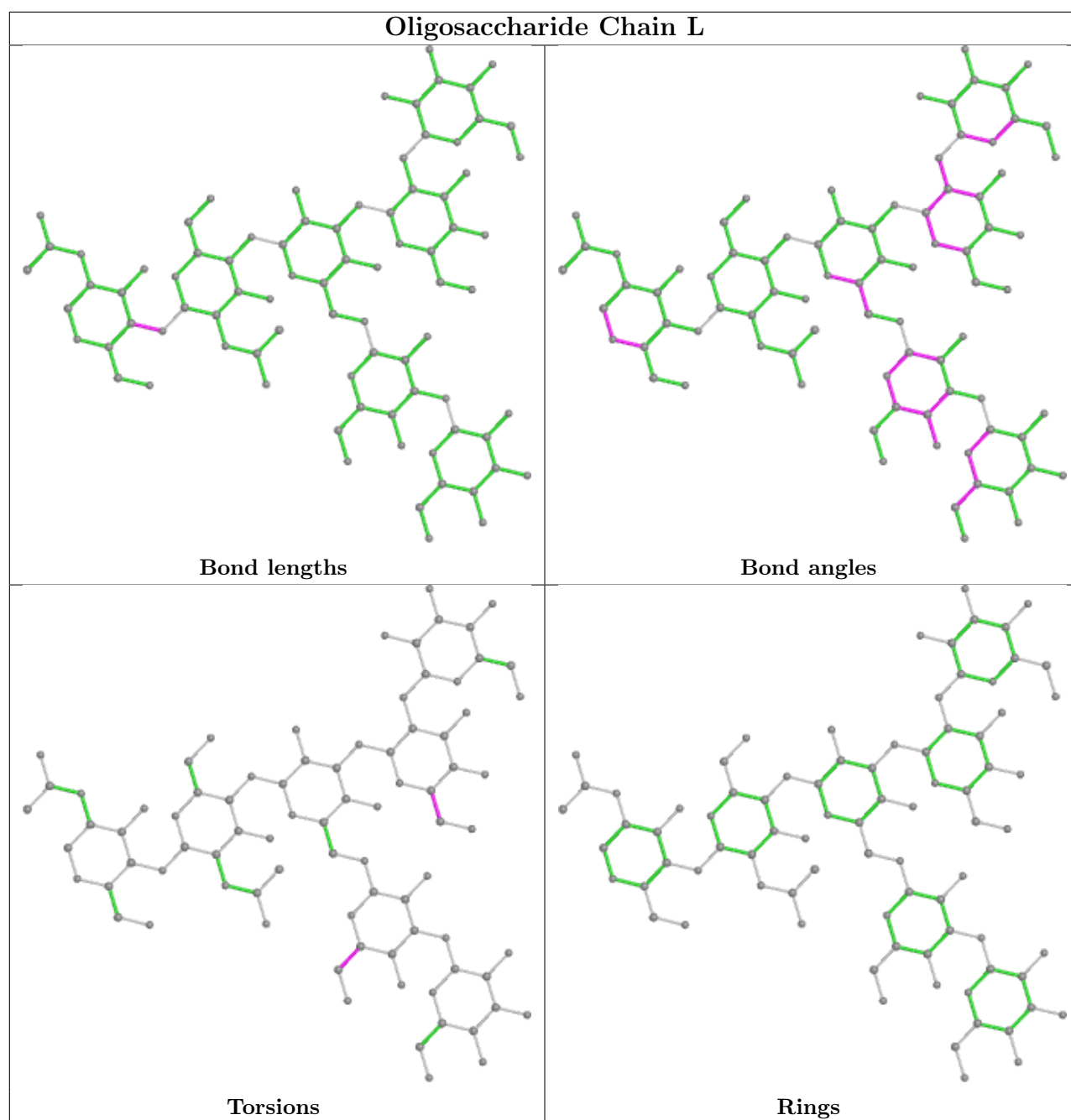


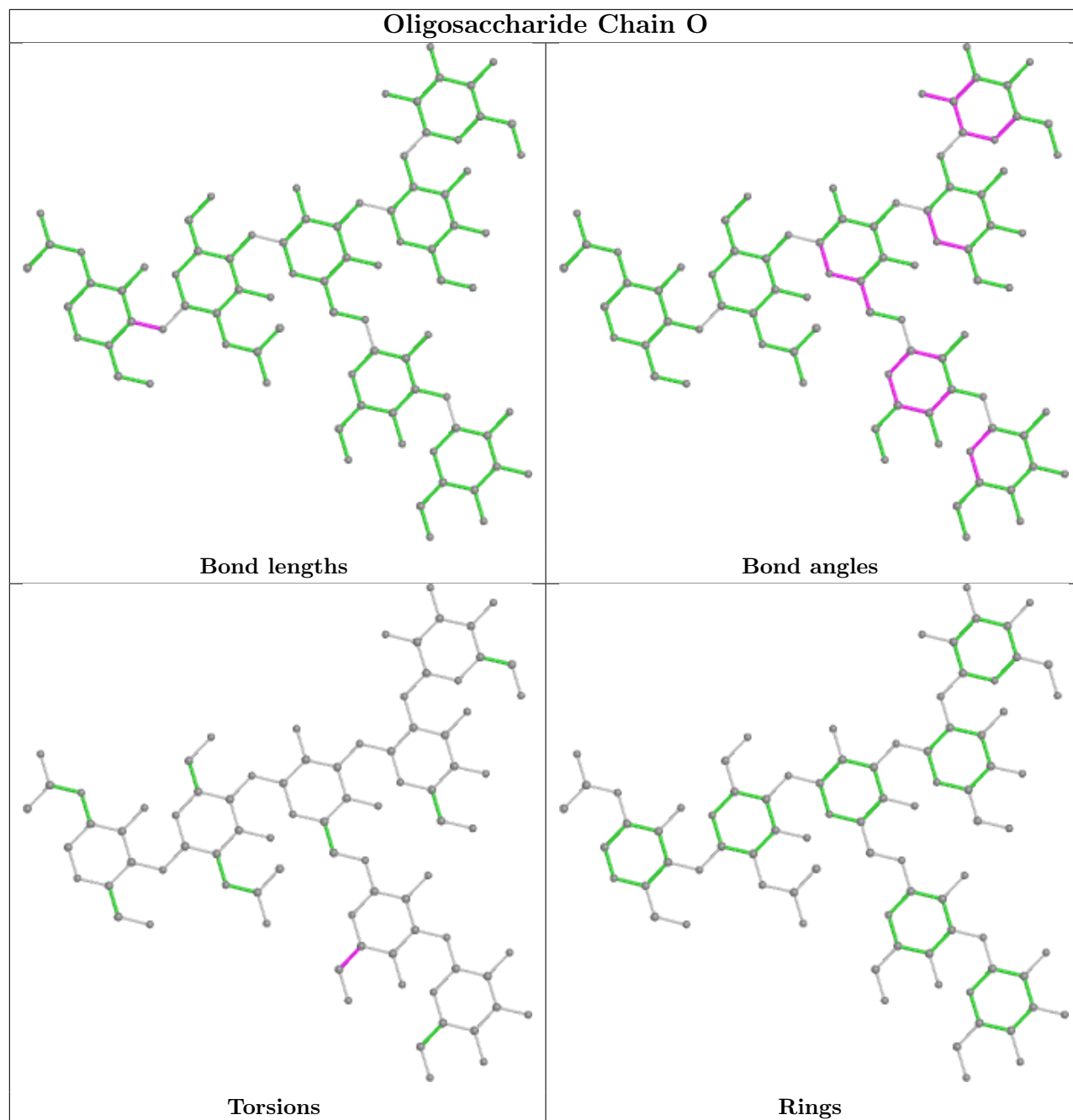


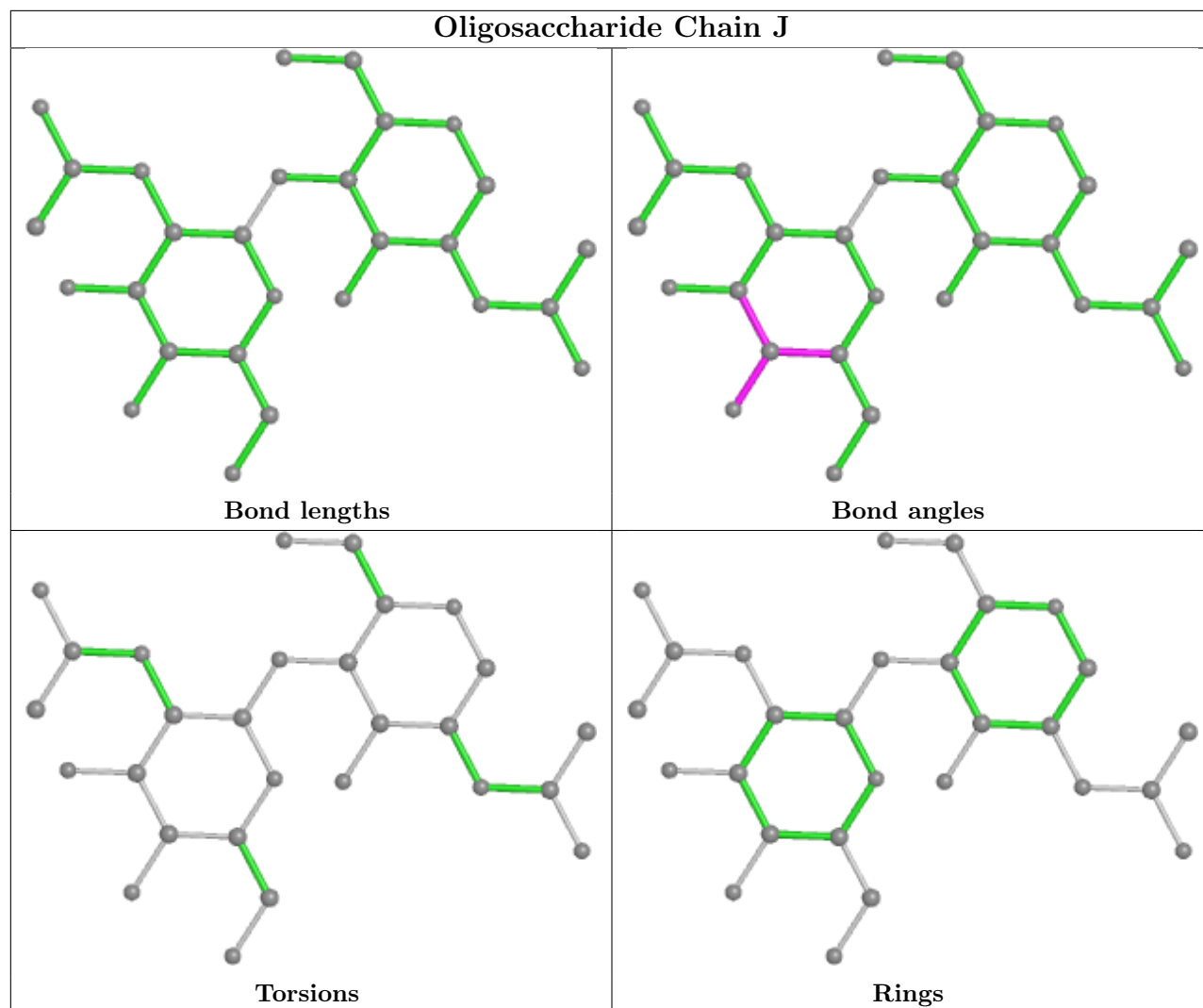


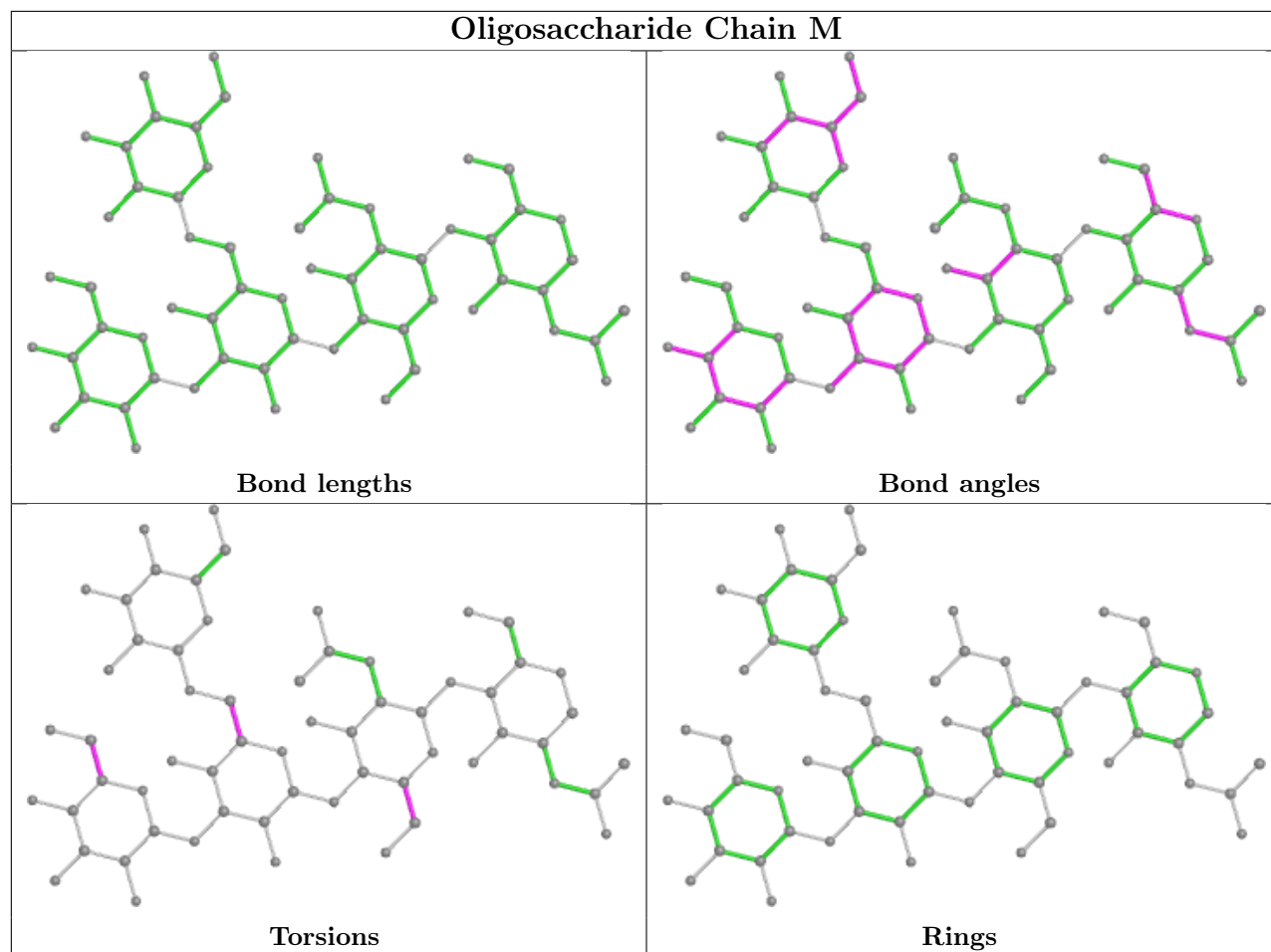


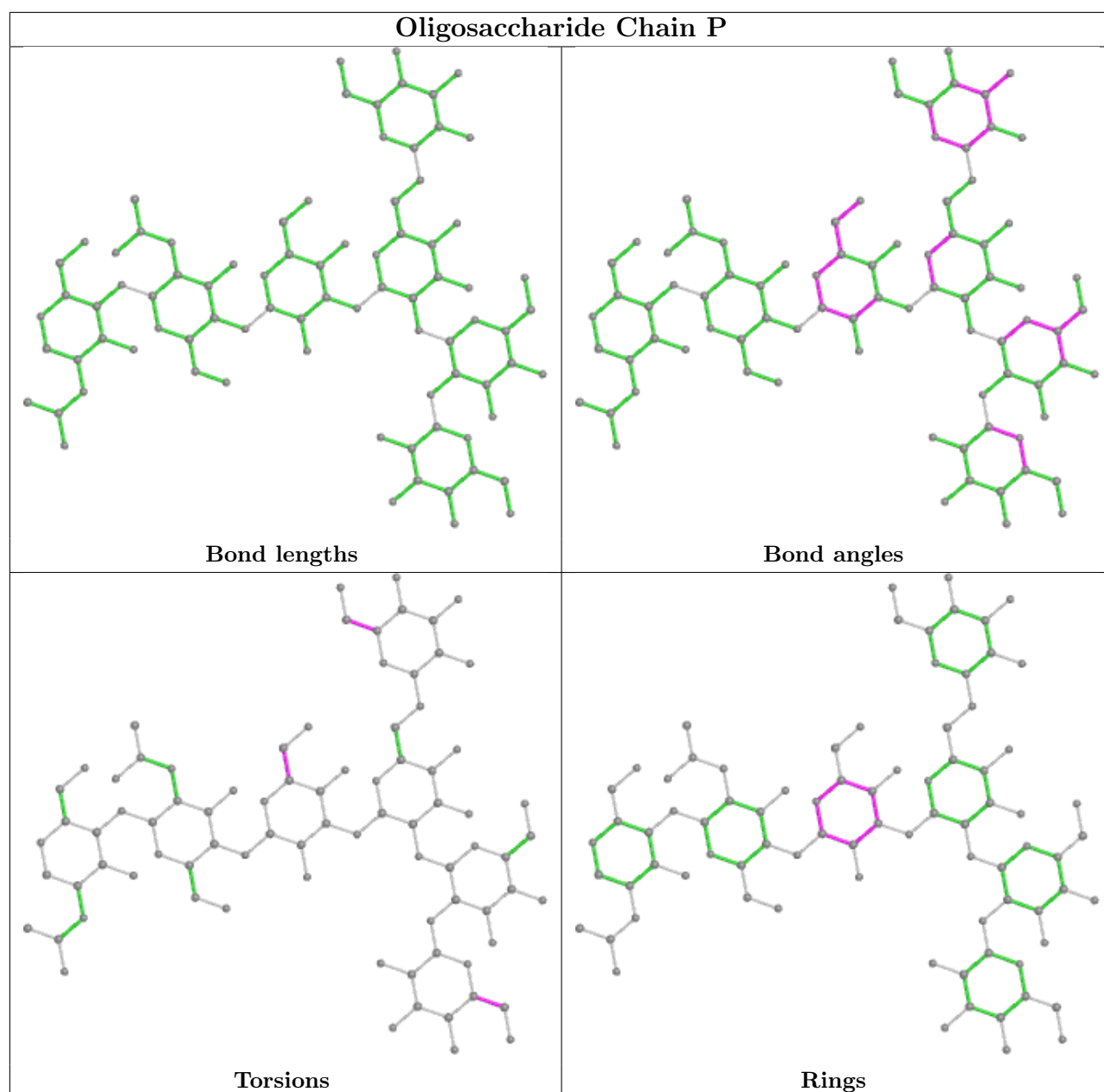












5.6 Ligand geometry [i](#)

20 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
10	NAG	D	911	1	14,14,15	0.35	0	17,19,21	1.19	1 (5%)
10	NAG	B	915	1	14,14,15	0.55	0	17,19,21	1.01	1 (5%)
10	NAG	A	911	1	14,14,15	0.35	0	17,19,21	0.94	2 (11%)
10	NAG	D	912	1	13,13,15	0.85	1 (7%)	16,17,21	1.86	3 (18%)
10	NAG	D	920	1	14,14,15	0.46	0	17,19,21	0.73	0
10	NAG	C	919	1	14,14,15	0.35	0	17,19,21	1.49	3 (17%)
10	NAG	A	912	1	13,13,15	0.97	1 (7%)	16,17,21	1.88	3 (18%)
10	NAG	D	921	1	14,14,15	0.38	0	17,19,21	0.97	1 (5%)
11	TRS	D	922	-	7,7,7	0.51	0	9,9,9	1.11	1 (11%)
10	NAG	A	919	1	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
10	NAG	C	911	1	14,14,15	0.39	0	17,19,21	1.88	3 (17%)
10	NAG	C	918	1	14,14,15	0.31	0	17,19,21	0.79	0
10	NAG	B	911	1	14,14,15	0.48	0	17,19,21	2.15	7 (41%)
10	NAG	A	920	1	14,14,15	0.46	0	17,19,21	1.43	2 (11%)
10	NAG	C	912	1	13,13,15	0.97	1 (7%)	16,17,21	1.70	3 (18%)
11	TRS	B	917	-	7,7,7	0.49	0	9,9,9	0.76	0
11	TRS	A	921	-	7,7,7	0.54	0	9,9,9	1.02	0
10	NAG	B	912	1	13,13,15	0.69	0	16,17,21	1.78	6 (37%)
10	NAG	B	916	1	14,14,15	0.50	0	17,19,21	2.49	3 (17%)
11	TRS	C	920	-	7,7,7	0.61	0	9,9,9	1.04	1 (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
10	NAG	D	911	1	-	0/6/23/26	0/1/1/1
10	NAG	B	915	1	-	0/6/23/26	0/1/1/1
10	NAG	A	911	1	-	2/6/23/26	0/1/1/1
10	NAG	D	912	1	-	4/6/19/26	0/1/1/1
10	NAG	D	920	1	-	0/6/23/26	0/1/1/1
10	NAG	C	919	1	-	0/6/23/26	0/1/1/1
10	NAG	A	912	1	-	0/6/19/26	0/1/1/1
10	NAG	D	921	1	-	0/6/23/26	0/1/1/1
11	TRS	D	922	-	-	0/9/9/9	-
10	NAG	A	919	1	-	0/6/23/26	0/1/1/1
10	NAG	C	911	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	918	1	-	0/6/23/26	0/1/1/1
10	NAG	B	911	1	-	3/6/23/26	0/1/1/1
10	NAG	A	920	1	-	0/6/23/26	0/1/1/1
10	NAG	C	912	1	-	0/6/19/26	0/1/1/1
11	TRS	B	917	-	-	6/9/9/9	-
11	TRS	A	921	-	-	6/9/9/9	-
10	NAG	B	912	1	-	1/6/19/26	0/1/1/1
10	NAG	B	916	1	-	1/6/23/26	0/1/1/1
11	TRS	C	920	-	-	3/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	912	NAG	C1-C2	3.08	1.54	1.51
10	C	912	NAG	C1-C2	3.04	1.54	1.51
10	D	912	NAG	C1-C2	2.53	1.54	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	916	NAG	C1-O5-C5	8.56	123.79	112.19
10	C	911	NAG	C1-O5-C5	6.22	120.62	112.19
10	B	911	NAG	C2-N2-C7	5.09	130.15	122.90
10	A	912	NAG	C3-C2-C1	4.59	113.72	109.50
10	B	911	NAG	C8-C7-N2	4.58	123.85	116.10
10	C	919	NAG	C1-O5-C5	4.19	117.87	112.19
10	D	912	NAG	C3-C2-C1	4.10	113.27	109.50
10	D	912	NAG	C2-N2-C7	3.81	127.80	122.78
10	A	920	NAG	C1-O5-C5	3.68	117.17	112.19
10	B	912	NAG	C3-C2-C1	3.39	112.61	109.50
10	B	916	NAG	C4-C3-C2	-3.32	106.16	111.02
10	A	912	NAG	C3-C4-C5	3.30	115.05	110.77
10	C	912	NAG	C3-C2-C1	3.13	112.37	109.50
10	B	912	NAG	C4-C3-C2	-2.92	108.92	112.53
10	A	919	NAG	C1-O5-C5	2.86	116.07	112.19
10	A	920	NAG	C4-C3-C2	-2.78	106.95	111.02
10	B	912	NAG	C3-C2-N2	-2.77	106.36	110.57
10	B	912	NAG	C1-O5-C5	2.76	115.93	112.19
10	D	911	NAG	O5-C5-C6	2.76	111.53	107.20
10	B	915	NAG	C1-O5-C5	2.67	115.81	112.19
10	D	912	NAG	C8-C7-N2	2.66	120.61	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	911	NAG	O5-C5-C4	2.60	117.15	110.83
10	C	912	NAG	C3-C4-C5	2.58	114.12	110.77
11	C	920	TRS	O2-C2-C	2.56	119.11	111.00
10	B	912	NAG	C6-C5-C4	-2.56	109.97	113.54
10	C	911	NAG	C3-C4-C5	2.46	114.63	110.24
10	C	919	NAG	O5-C5-C6	2.41	110.98	107.20
10	C	912	NAG	C6-C5-C4	-2.40	110.20	113.54
10	D	921	NAG	O5-C5-C6	2.31	110.83	107.20
10	B	916	NAG	O5-C5-C4	2.29	116.41	110.83
10	A	912	NAG	O4-C4-C5	-2.27	105.19	110.01
10	B	911	NAG	C1-O5-C5	2.26	115.25	112.19
10	A	911	NAG	O5-C5-C6	2.25	110.72	107.20
10	B	911	NAG	O7-C7-N2	-2.18	117.94	121.95
10	B	911	NAG	O5-C1-C2	-2.17	107.86	111.29
10	B	912	NAG	O5-C5-C4	2.11	113.19	109.64
11	D	922	TRS	C3-C-C2	2.08	117.27	110.81
10	B	911	NAG	O7-C7-C8	-2.07	118.21	122.06
10	C	919	NAG	C4-C3-C2	-2.03	108.04	111.02
10	A	911	NAG	C4-C3-C2	-2.03	108.05	111.02
10	B	911	NAG	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	911	NAG	C3-C2-N2-C7
11	A	921	TRS	C2-C-C1-O1
11	A	921	TRS	C3-C-C1-O1
11	A	921	TRS	N-C-C1-O1
11	A	921	TRS	C1-C-C2-O2
11	A	921	TRS	N-C-C2-O2
11	B	917	TRS	C3-C-C1-O1
11	B	917	TRS	N-C-C1-O1
11	C	920	TRS	C3-C-C2-O2
11	C	920	TRS	N-C-C2-O2
10	C	911	NAG	O5-C5-C6-O6
10	C	911	NAG	C4-C5-C6-O6
10	B	911	NAG	C8-C7-N2-C2
10	B	911	NAG	O7-C7-N2-C2
10	D	912	NAG	C8-C7-N2-C2
10	D	912	NAG	O7-C7-N2-C2
10	A	911	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	911	NAG	O5-C5-C6-O6
10	D	912	NAG	O5-C5-C6-O6
10	D	912	NAG	C4-C5-C6-O6
10	B	916	NAG	C4-C5-C6-O6
11	A	921	TRS	C3-C-C2-O2
11	B	917	TRS	C2-C-C1-O1
11	B	917	TRS	C2-C-C3-O3
11	B	917	TRS	N-C-C3-O3
11	C	920	TRS	C1-C-C2-O2
10	B	912	NAG	O5-C5-C6-O6
11	B	917	TRS	C1-C-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	911	NAG	1	0
11	A	921	TRS	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	762/809 (94%)	-0.57	3 (0%) 89 87	20, 30, 42, 80	1 (0%)
1	B	761/809 (94%)	-0.30	5 (0%) 84 81	26, 36, 57, 103	0
1	C	761/809 (94%)	-0.44	10 (1%) 74 71	24, 31, 44, 99	0
1	D	761/809 (94%)	-0.49	5 (0%) 84 81	24, 32, 45, 81	0
All	All	3045/3236 (94%)	-0.45	23 (0%) 82 80	20, 32, 49, 103	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	ILE	7.0
1	B	44	SER	5.2
1	A	43	GLU	5.0
1	C	44	SER	5.0
1	D	44	SER	4.9
1	A	44	SER	4.5
1	B	804	HIS	4.5
1	A	804	HIS	3.7
1	C	227	VAL	3.4
1	C	804	HIS	3.2
1	D	224	ILE	3.2
1	D	804	HIS	3.1
1	C	683	TYR	3.1
1	C	49	TRP	3.0
1	B	227	VAL	2.8
1	D	77	GLU	2.4
1	C	48	GLN	2.3
1	C	51	ALA	2.2
1	B	47	THR	2.1
1	C	47	THR	2.1
1	B	225	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	683	TYR	2.0
1	C	524	ASN	2.0

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
5	MAN	H	3	11/12	0.55	0.15	73,77,84,89	0
2	BMA	N	3	11/12	0.57	0.15	69,73,76,78	0
6	MAN	I	5	11/12	0.57	0.15	69,73,83,83	0
3	MAN	F	6	11/12	0.62	0.15	46,48,52,53	0
6	MAN	I	6	11/12	0.63	0.14	54,57,57,59	0
4	MAN	G	5	11/12	0.64	0.14	86,91,95,102	0
3	MAN	F	5	11/12	0.66	0.15	68,75,78,79	0
5	MAN	K	3	11/12	0.66	0.13	69,76,80,82	0
8	MAN	M	5	11/12	0.66	0.15	51,54,57,61	0
2	BMA	E	3	11/12	0.67	0.14	73,76,79,80	0
4	MAN	G	3	11/12	0.67	0.15	71,74,78,79	0
3	BMA	F	4	11/12	0.72	0.13	62,66,70,71	0
4	MAN	G	6	11/12	0.73	0.20	100,106,111,112	0
6	MAN	O	4	11/12	0.74	0.13	60,63,67,67	0
6	MAN	O	5	11/12	0.75	0.12	54,61,69,71	0
6	MAN	L	6	11/12	0.75	0.12	44,46,48,49	0
6	MAN	O	6	11/12	0.76	0.11	47,48,52,52	0
8	BMA	M	4	11/12	0.79	0.13	55,58,62,63	0
4	MAN	G	4	11/12	0.81	0.14	56,67,74,81	0
6	MAN	L	4	11/12	0.82	0.10	51,55,57,63	0
6	MAN	I	4	11/12	0.83	0.10	65,67,74,76	0
6	MAN	L	5	11/12	0.83	0.09	56,62,66,67	0
9	MAN	P	3	11/12	0.83	0.10	42,43,45,46	0
9	MAN	P	5	11/12	0.84	0.11	52,54,55,57	0
7	NAG	J	2	14/15	0.85	0.10	38,41,46,47	0
6	MAN	I	7	11/12	0.87	0.09	52,55,56,59	0

Continued on next page...

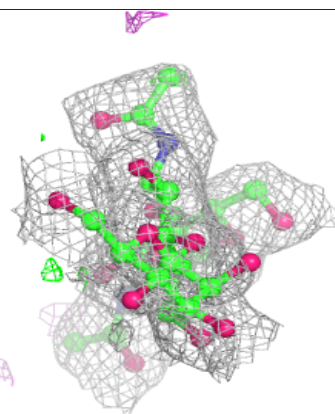
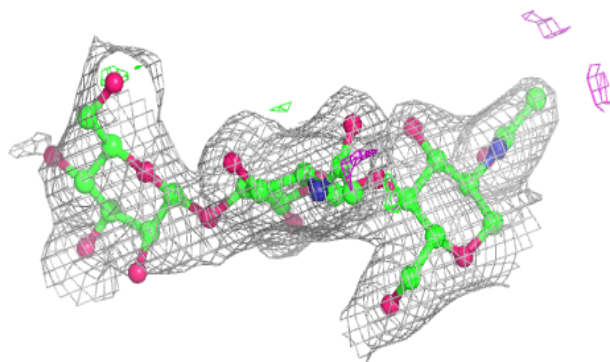
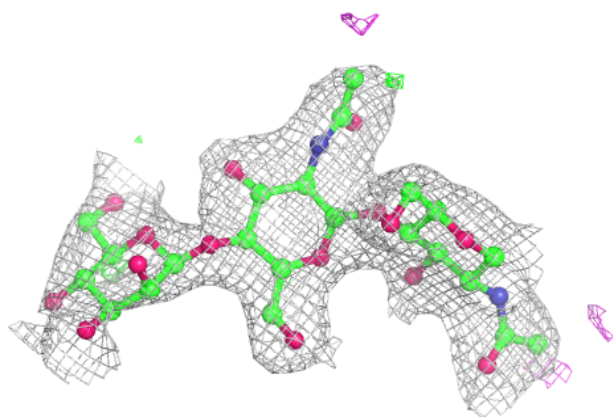
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MAN	P	7	11/12	0.87	0.10	46,52,56,56	0
6	BMA	I	3	11/12	0.88	0.09	52,55,57,63	0
8	MAN	M	3	11/12	0.89	0.08	45,51,54,56	0
5	NAG	K	2	14/15	0.89	0.10	40,49,59,69	0
2	NAG	E	2	14/15	0.89	0.09	43,46,55,66	0
5	NAG	H	2	14/15	0.90	0.09	50,53,59,67	0
6	NAG	L	2	14/15	0.91	0.08	37,39,41,41	0
6	MAN	O	7	11/12	0.91	0.08	44,45,46,46	0
9	MAN	P	6	11/12	0.91	0.09	44,50,52,54	0
4	NAG	G	2	14/15	0.91	0.09	38,43,52,65	0
6	BMA	L	3	11/12	0.92	0.07	40,43,45,50	0
9	MAN	P	4	11/12	0.92	0.07	39,44,49,51	0
6	NAG	I	2	14/15	0.92	0.09	48,51,56,56	0
6	MAN	L	7	11/12	0.92	0.08	41,43,48,51	0
6	NAG	O	2	14/15	0.92	0.09	40,41,44,44	0
6	NAG	I	1	14/15	0.93	0.08	39,43,45,50	0
3	MAN	F	7	11/12	0.93	0.07	41,43,45,45	0
3	BMA	F	3	11/12	0.93	0.07	42,44,47,54	0
2	NAG	N	2	14/15	0.93	0.08	41,46,52,62	0
6	BMA	O	3	11/12	0.93	0.07	40,45,48,57	0
5	NAG	H	1	14/15	0.93	0.09	42,43,47,50	0
9	NAG	P	2	14/15	0.94	0.07	33,35,36,40	0
2	NAG	N	1	14/15	0.94	0.07	27,31,34,41	0
6	NAG	L	1	14/15	0.94	0.07	30,31,35,35	0
4	NAG	G	1	14/15	0.94	0.07	29,32,35,37	0
3	NAG	F	2	14/15	0.94	0.07	35,38,39,41	0
6	NAG	O	1	14/15	0.94	0.07	36,39,41,42	0
8	NAG	M	2	14/15	0.95	0.07	35,37,42,45	0
5	NAG	K	1	14/15	0.95	0.06	32,35,39,43	0
9	NAG	P	1	14/15	0.95	0.06	30,32,33,33	0
8	NAG	M	1	14/15	0.96	0.06	28,29,30,32	0
2	NAG	E	1	14/15	0.96	0.05	31,33,35,40	0
3	NAG	F	1	14/15	0.96	0.06	28,29,31,34	0
7	NAG	J	1	14/15	0.97	0.05	30,33,34,36	0

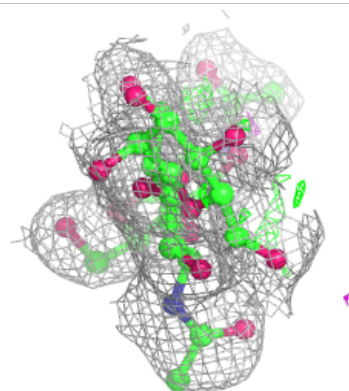
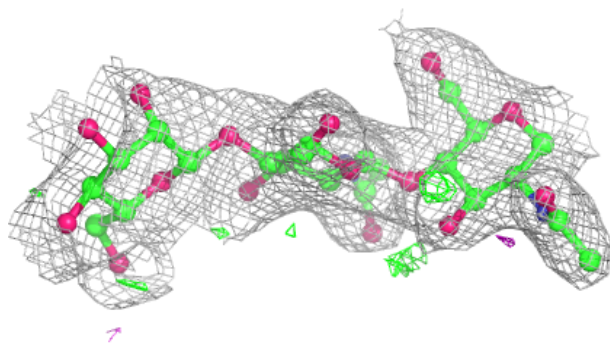
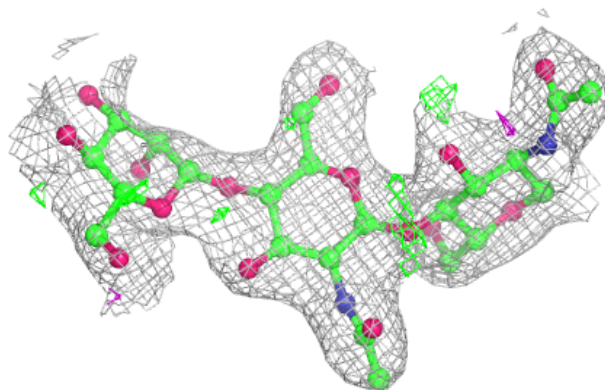
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

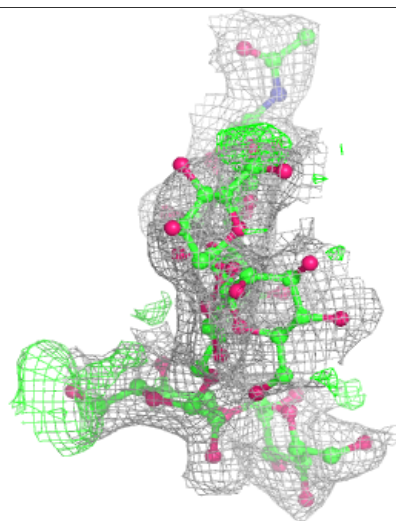
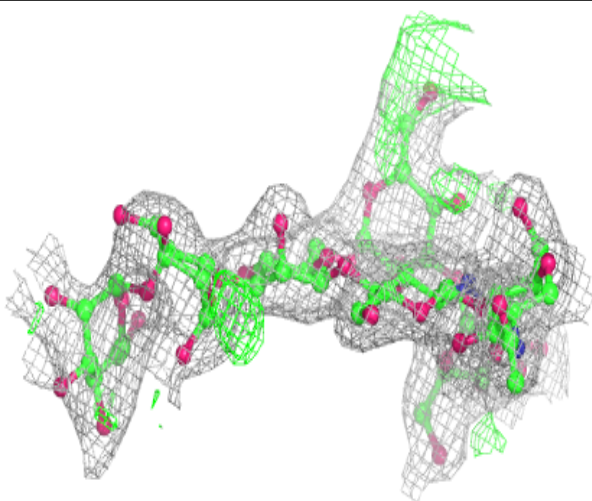
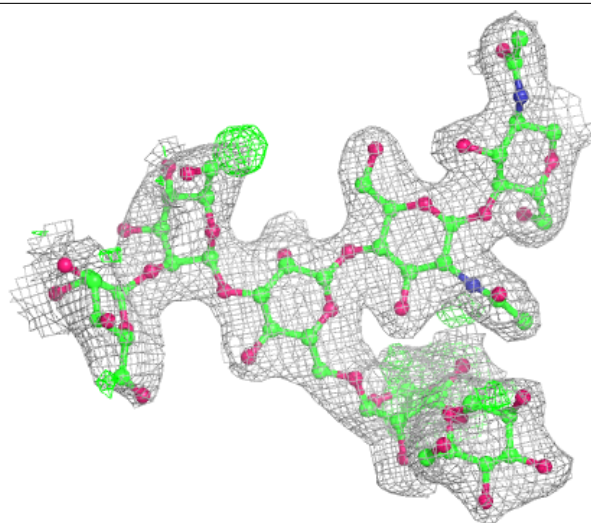
**Electron density around Chain N:**

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



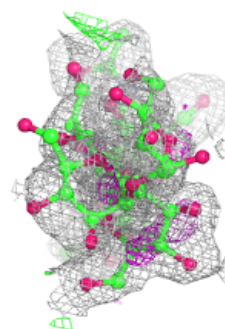
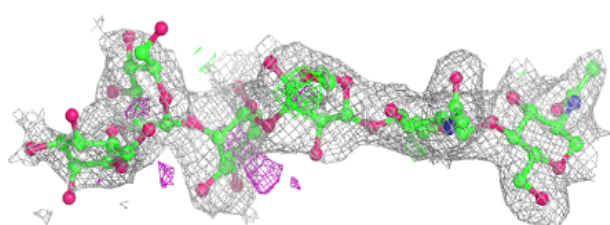
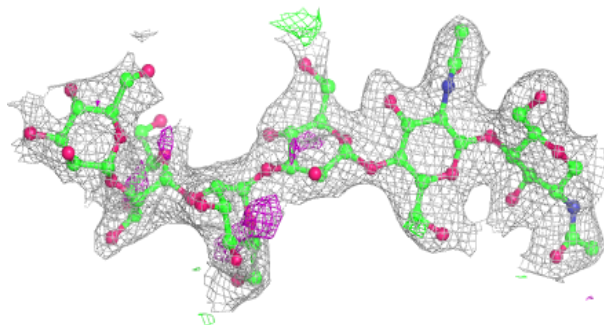
Electron density around Chain F:

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

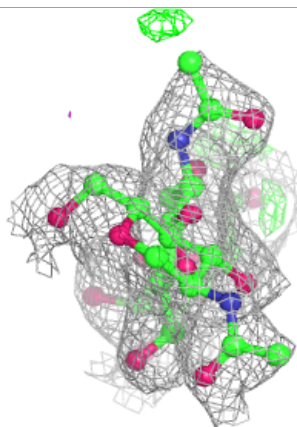
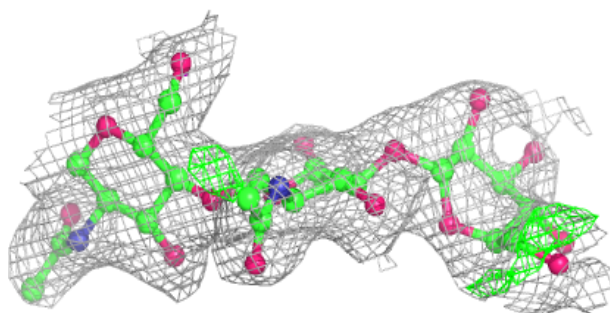
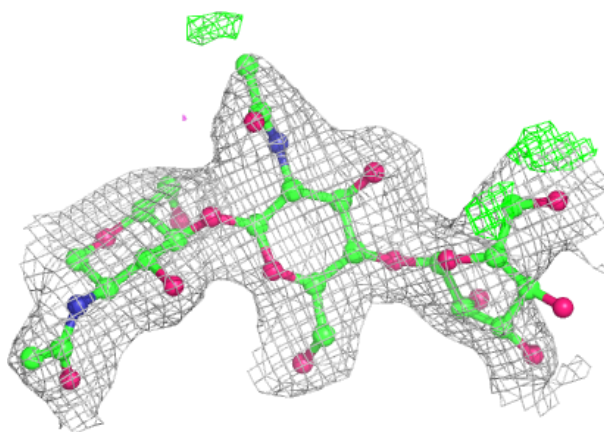


Electron density around Chain G:

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

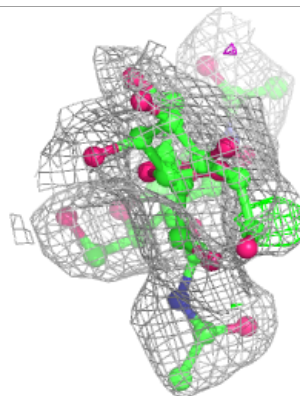
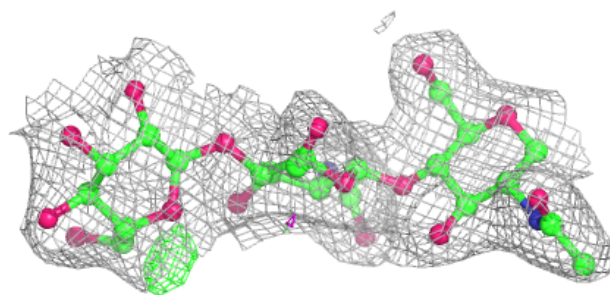
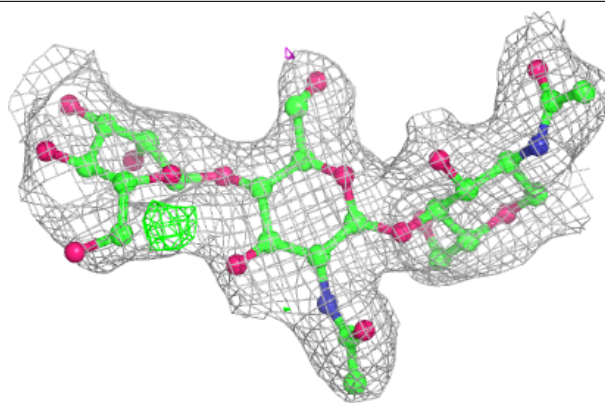
**Electron density around Chain H:**

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



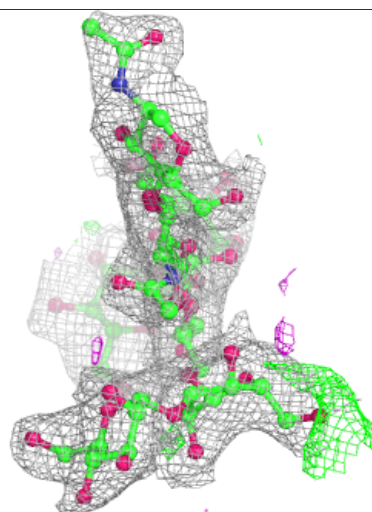
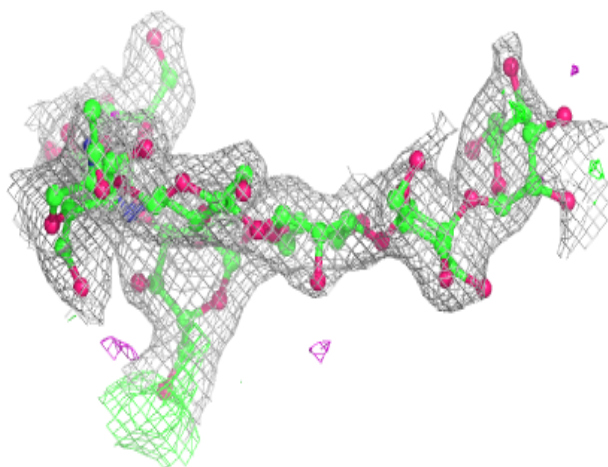
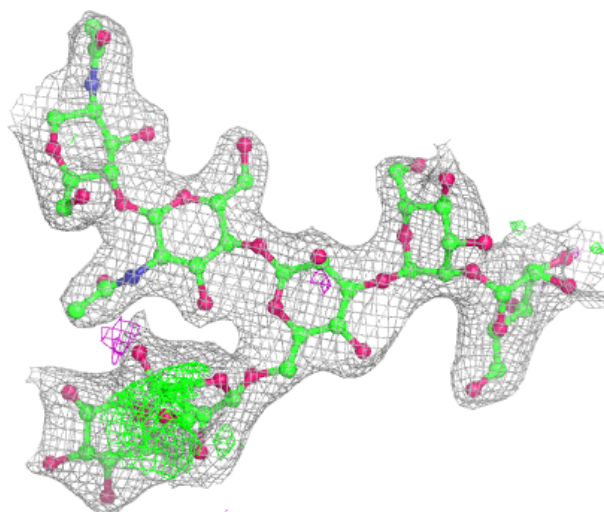
Electron density around Chain K:

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



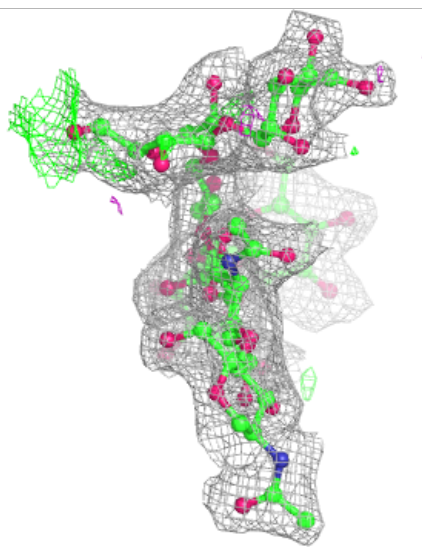
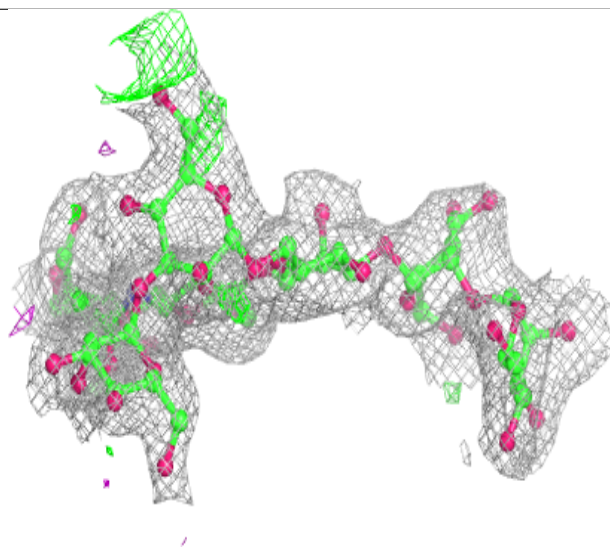
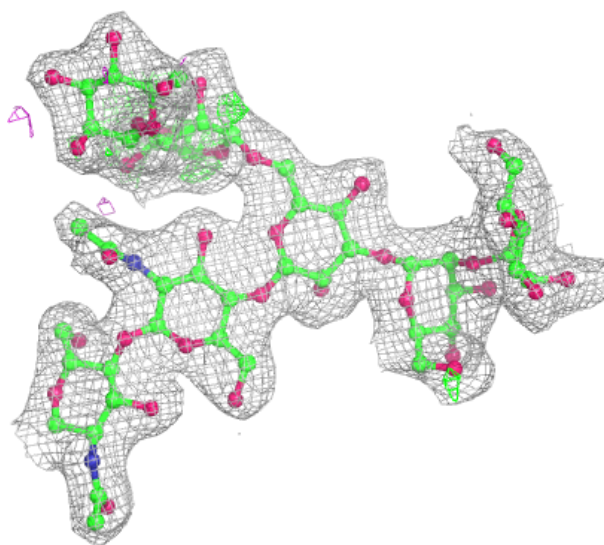
Electron density around Chain I:

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



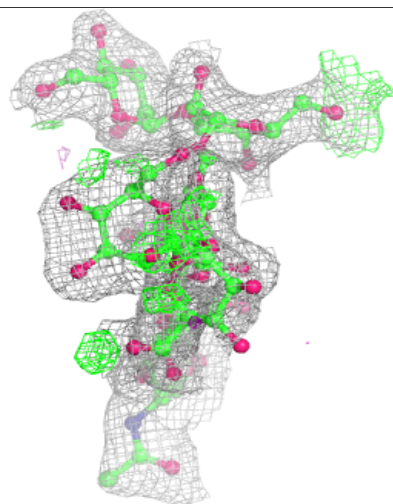
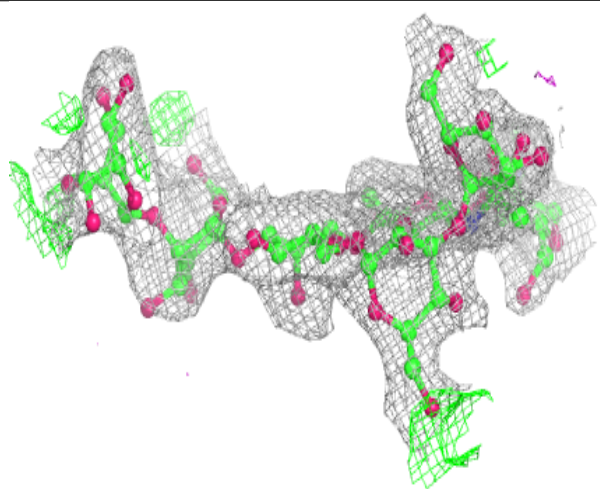
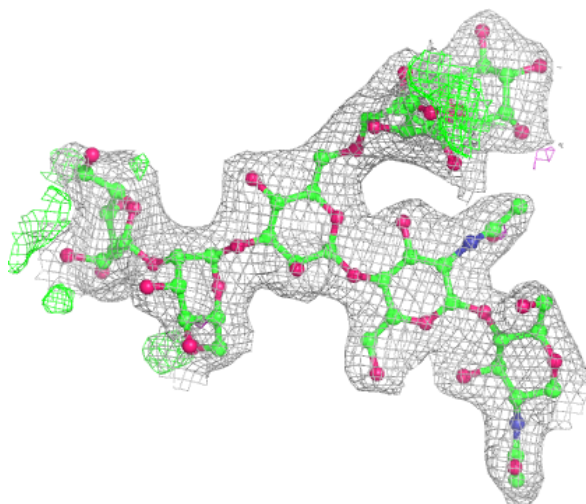
Electron density around Chain L:

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



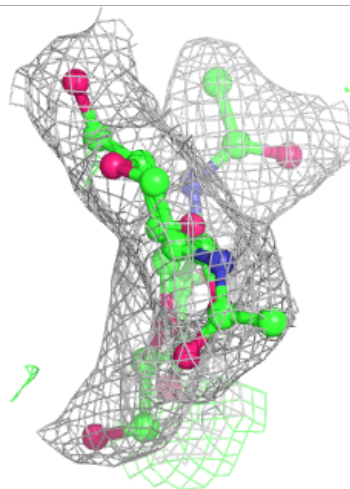
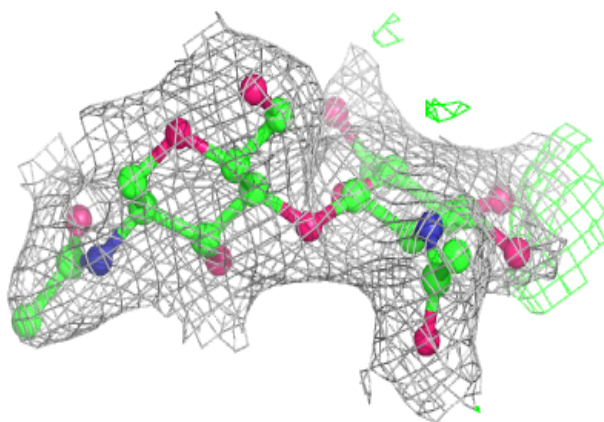
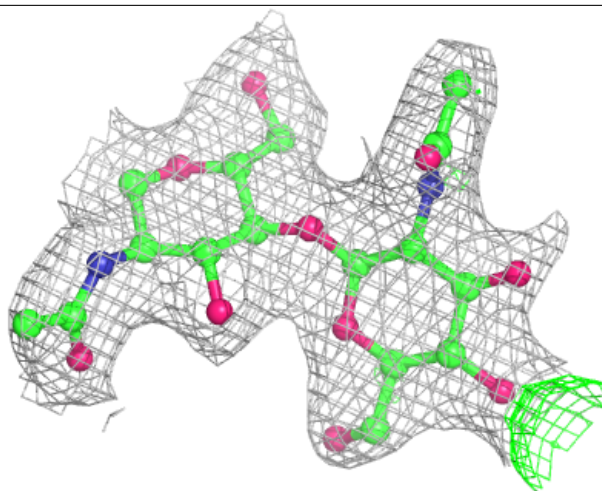
Electron density around Chain O:

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



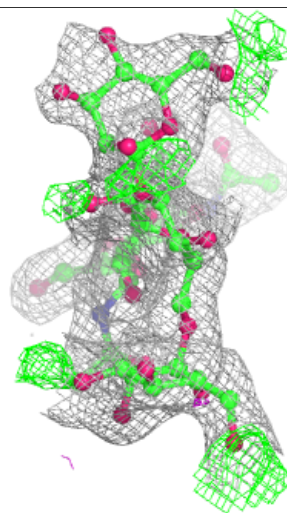
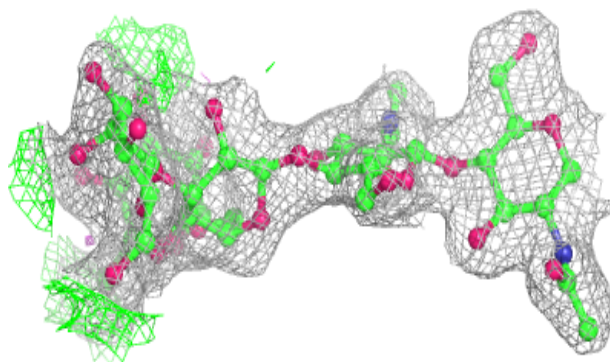
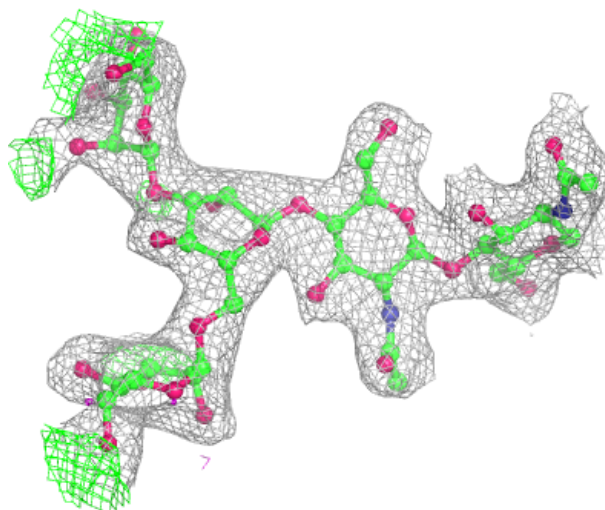
Electron density around Chain J:

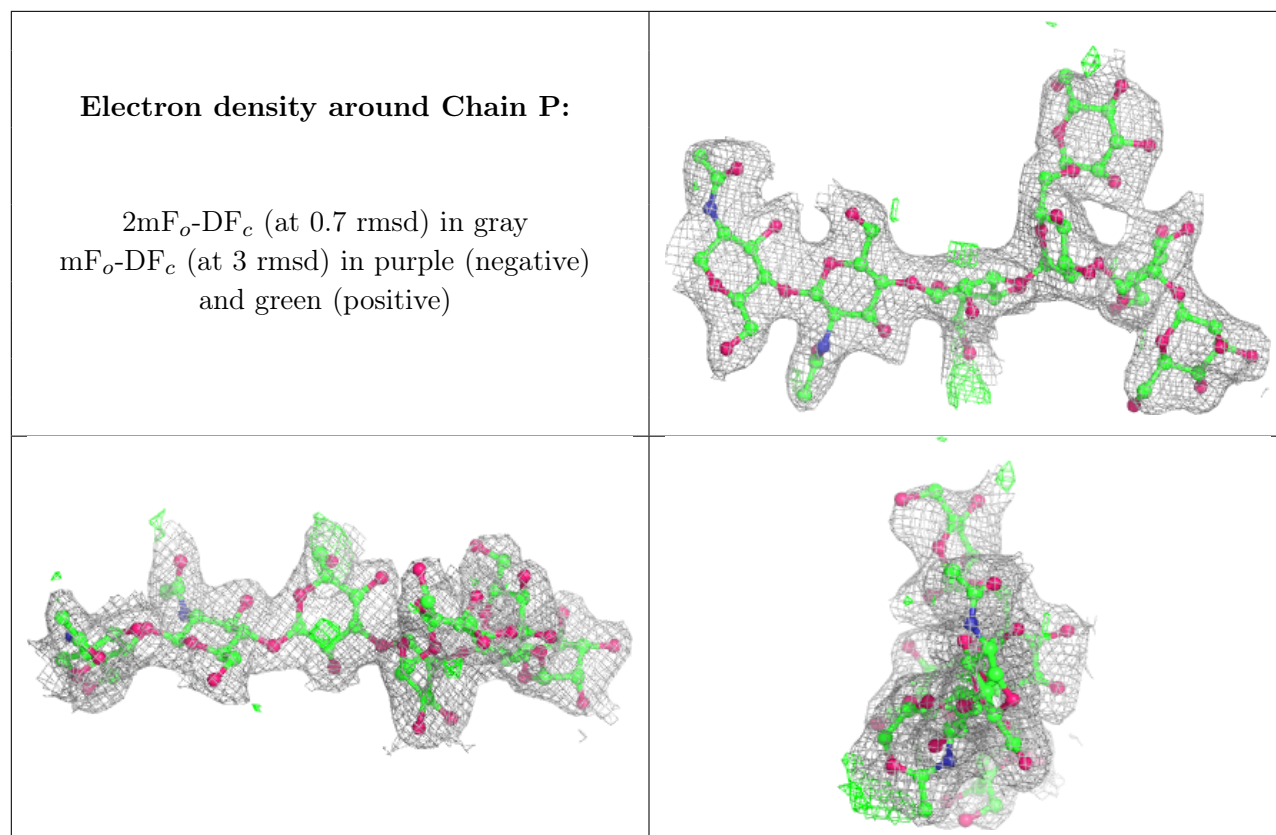
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
10	NAG	A	920	14/15	0.65	0.18	61,77,82,85	0
10	NAG	B	916	14/15	0.69	0.15	70,75,79,83	0
10	NAG	B	911	14/15	0.75	0.11	62,67,69,69	0
10	NAG	C	919	14/15	0.77	0.12	58,64,65,66	0
10	NAG	D	921	14/15	0.78	0.14	48,53,54,55	0
10	NAG	A	911	14/15	0.79	0.12	54,60,68,69	0
10	NAG	D	912	13/15	0.81	0.11	46,47,51,52	0
10	NAG	A	912	13/15	0.81	0.10	43,47,50,51	0
10	NAG	C	912	13/15	0.82	0.10	43,46,49,50	0
10	NAG	C	911	14/15	0.82	0.11	46,50,59,60	0
10	NAG	B	912	13/15	0.85	0.10	47,57,62,67	0
11	TRS	A	921	8/8	0.85	0.14	37,41,47,49	0
11	TRS	C	920	8/8	0.85	0.14	40,43,45,45	0
11	TRS	D	922	8/8	0.86	0.13	35,40,41,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NAG	D	911	14/15	0.87	0.10	47,54,69,69	0
11	TRS	B	917	8/8	0.87	0.12	38,42,44,44	0
10	NAG	D	920	14/15	0.91	0.07	34,35,38,39	0
10	NAG	A	919	14/15	0.94	0.06	32,36,39,41	0
10	NAG	B	915	14/15	0.94	0.07	35,42,43,43	0
10	NAG	C	918	14/15	0.95	0.06	34,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.