



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 10:31 AM EDT

PDB ID : 6DRU
Title : Xylosidase from *Aspergillus niger*
Authors : Cao, H.; Xu, W.; Betancourt, M.; Walton, J.D.; Brumm, P.; Phillips Jr., G.N.;
Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2018-06-13
Resolution : 2.70 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 : 2.14.6
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) : 2.14.6

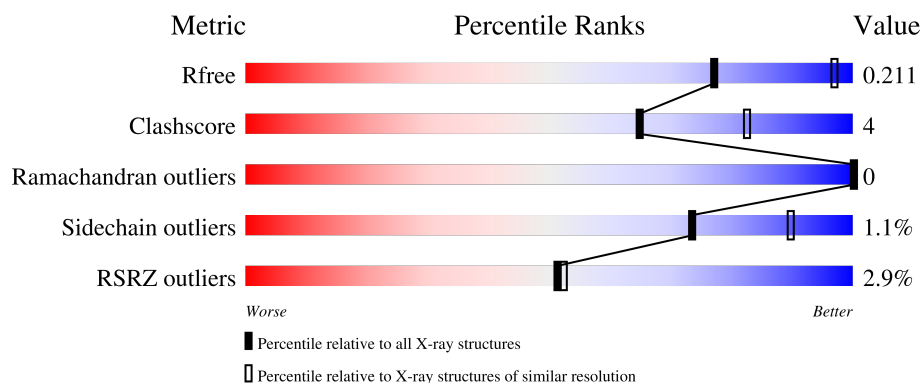
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.




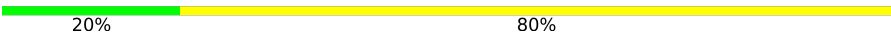
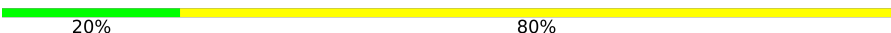

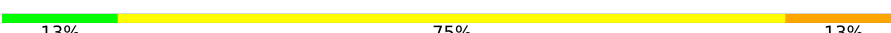
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	718	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	B	718	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
2	C	6	<div> <div>17%</div> <div> <div></div> <div>67%</div> <div>17%</div> </div> </div>
3	D	9	<div> <div>78%</div> <div>22%</div> </div>
4	E	10	<div> <div>10%</div> <div>90%</div> </div>

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Mol	Chain	Length	Quality of chain
4	I	10	 10%90%
5	F	5	 20%80%
5	J	5	 20%80%
6	G	4	 50%50%
7	H	8	 13%75%13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	A	828	-	-	-	X

2 Entry composition [i](#)

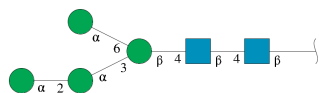
There are 11 unique types of molecules in this entry. The entry contains 12553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycosyl hydrolases family 31 family protein.

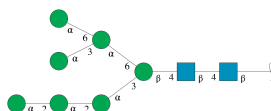
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	1	0
			5724	3659	961	1084	20			
1	B	717	Total	C	N	O	S	0	1	0
			5718	3654	960	1084	20			

- Molecule 2 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
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

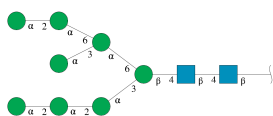
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			105	58	2	45			

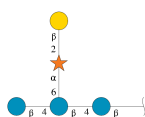
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra

nose-(1-6)-[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.



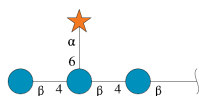
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	10	Total	C	N	O	0	0	0
			116	64	2	50			
4	I	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-4)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



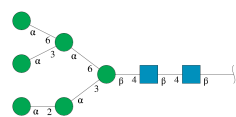
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	F	5	Total	C	O	0	0	0
			54	29	25			
5	J	5	Total	C	O	0	0	0
			54	29	25			

- Molecule 6 is an oligosaccharide called beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



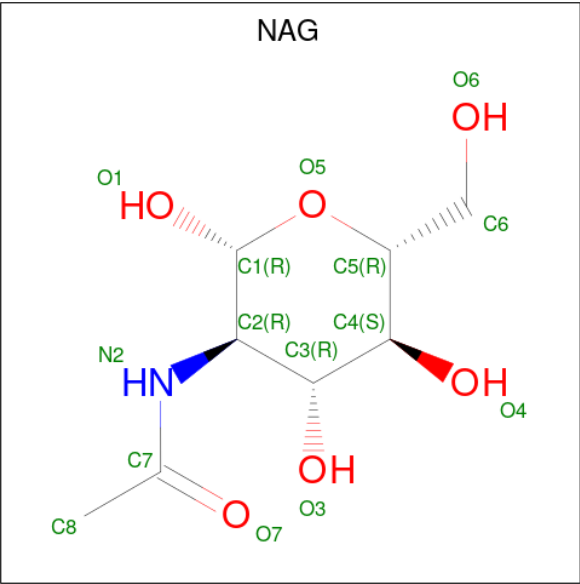
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	G	4	Total	C	O	0	0	0
			43	23	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	H	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



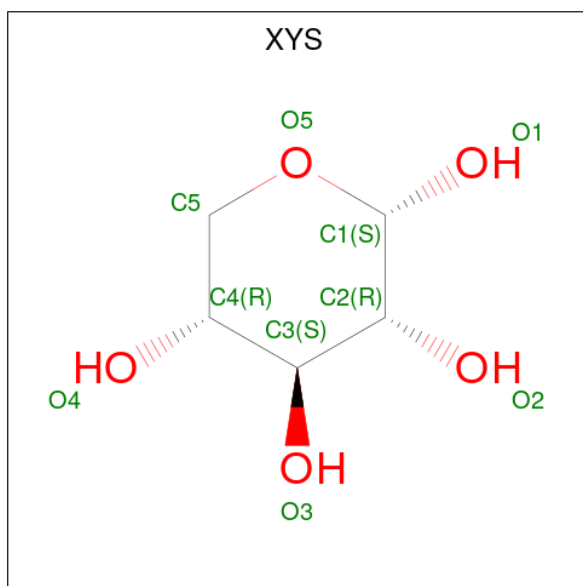
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is alpha-D-xylopyranose (three-letter code: XYZ) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	5	5		
9	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		

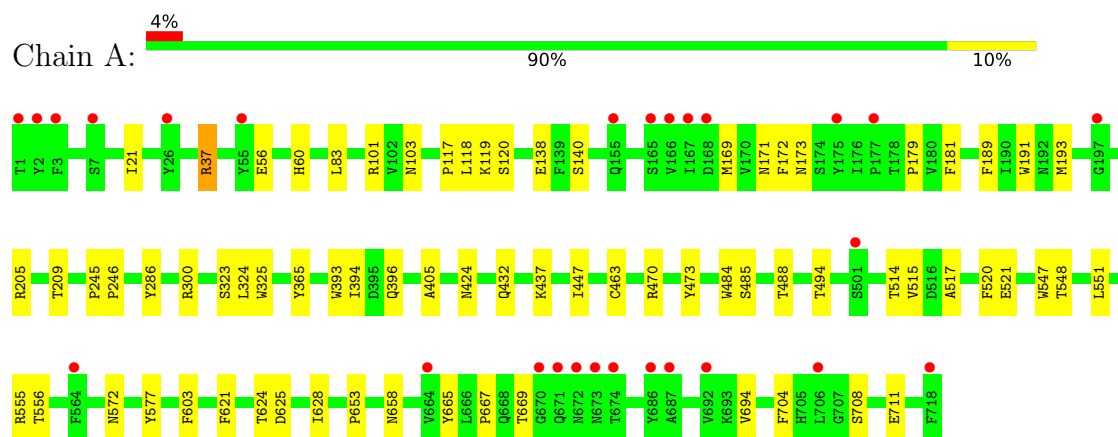
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	153	Total	O	0	0
			153	153		
11	B	140	Total	O	0	0
			140	140		

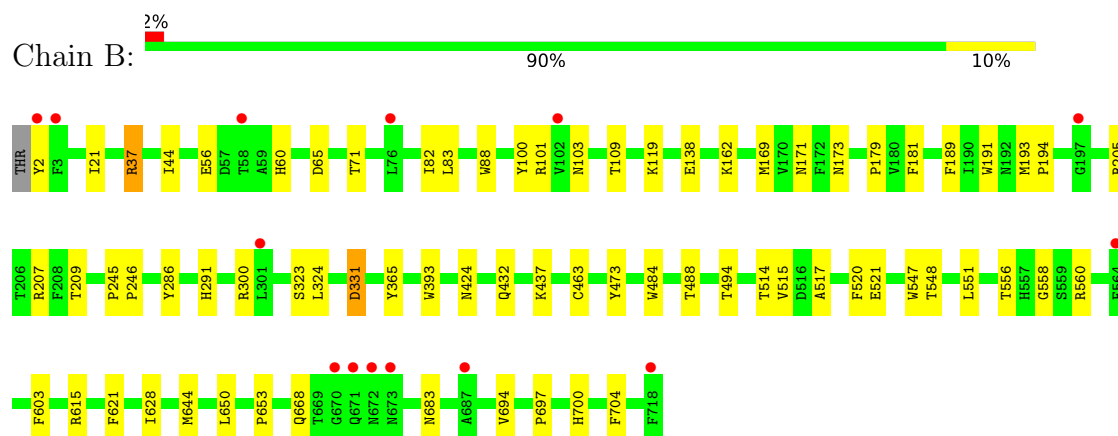
3 Residue-property plots

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: Glycosyl hydrolases family 31 family protein




- Molecule 1: Glycosyl hydrolases family 31 family protein



- Molecule 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



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

Chain D:  78% 22%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

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

Chain E:  10% 90%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain I:  10% 90%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 5: β -D-galactopyranose-(1-2)- α -D-xylopyranose-(1-6)-[β -D-glucopyranose-(1-4)] β -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain F:  20% 80%

BGC1
BGC2
XTS3
GAL4
BGC5

- Molecule 5: β -D-galactopyranose-(1-2)- α -D-xylopyranose-(1-6)-[β -D-glucopyranose-(1-4)] β -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain J:  20% 80%

BGC1
BGC2
XTS3
GAL4
BGC5

- Molecule 6: β -D-glucopyranose-(1-4)-[α -D-xylopyranose-(1-6)] β -D-glucopyranose-(1-4)- β -D-glucopyranose

Chain G:  50% 50%

BGC1
BGC2
BGC3
XTS4

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

Chain H:  13% 75% 13%

MAG1
MAG2
ENA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.13Å 146.13Å 220.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 2.70 47.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.91-2.70) 84.2 (47.92-2.70)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.181 , 0.212 0.180 , 0.211	Depositor DCC
R_{free} test set	1992 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12553	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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: GOL, BGC, NAG, GAL, BMA, XYS, 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	0.25	0/5906	0.44	0/8073
1	B	0.25	0/5900	0.45	0/8064
All	All	0.25	0/11806	0.44	0/16137

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5724	0	5401	49	0
1	B	5718	0	5386	48	0
2	C	72	0	61	2	0
3	D	105	0	88	3	0
4	E	116	0	97	0	0
4	I	116	0	97	0	0
5	F	54	0	46	0	0
5	J	54	0	46	0	0
6	G	43	0	37	0	0
7	H	94	0	79	1	0
8	A	56	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	70	0	65	1	0
9	A	10	0	10	0	0
9	B	10	0	10	0	0
10	A	6	0	8	0	0
10	B	12	0	16	1	0
11	A	153	0	0	6	0
11	B	140	0	0	3	0
All	All	12553	0	11499	97	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 4.

All (97) 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:A:396:GLN:HE21	1:A:470:ARG:HH12	1.18	0.90
1:A:101:ARG:NH1	1:A:103:ASN:OD1	2.08	0.86
1:B:101:ARG:NH1	1:B:103:ASN:OD1	2.18	0.76
1:B:103:ASN:HD21	1:B:109:THR:HG23	1.54	0.70
1:A:171:ASN:OD1	1:A:437:LYS:NZ	2.25	0.69
1:B:162:LYS:NZ	11:B:901:HOH:O	2.26	0.68
1:B:621:PHE:HB2	1:B:628:ILE:HD12	1.76	0.66
1:B:179:PRO:HB2	1:B:191:TRP:HB3	1.76	0.66
1:A:173:ASN:HB3	1:B:119:LYS:HD2	1.77	0.65
1:B:44:ILE:HB	1:B:194:PRO:HG3	1.77	0.65
1:B:615:ARG:HB2	1:B:644:MET:HB2	1.78	0.64
1:B:21:ILE:HG21	1:B:83:LEU:HD22	1.80	0.64
2:C:1:NAG:H82	3:D:4:MAN:H3	1.80	0.63
1:A:119:LYS:HD2	1:B:173:ASN:HB3	1.79	0.63
1:A:179:PRO:HB2	1:A:191:TRP:HB3	1.79	0.62
1:A:246:PRO:HD3	1:A:463:CYS:HB2	1.81	0.61
1:A:658:ASN:ND2	11:A:908:HOH:O	2.32	0.61
1:B:644:MET:HE1	1:B:650:LEU:HB2	1.82	0.59
1:B:171:ASN:OD1	1:B:437:LYS:NZ	2.36	0.58
1:B:246:PRO:HD3	1:B:463:CYS:HB2	1.85	0.58
1:A:488:THR:HB	1:A:494:THR:HG21	1.87	0.57
1:B:300:ARG:NH2	7:H:2:NAG:O3	2.38	0.57
1:A:572:ASN:OD1	1:A:577:TYR:OH	2.24	0.55
1:B:488:THR:HB	1:B:494:THR:HG21	1.89	0.55
1:B:205:ARG:HH12	1:B:207:ARG:CZ	2.20	0.55
1:A:621:PHE:HB2	1:A:628:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:HA	1:B:432:GLN:HB3	1.89	0.54
1:B:82:ILE:HG12	1:B:100:TYR:HB2	1.90	0.54
1:A:325:TRP:CZ2	1:A:396:GLN:HG3	2.43	0.54
1:B:37:ARG:H	1:B:37:ARG:HD2	1.73	0.54
11:A:912:HOH:O	1:B:207:ARG:NH1	2.42	0.53
1:A:555:ARG:NH1	11:A:901:HOH:O	2.13	0.53
1:B:668:GLN:NE2	11:B:907:HOH:O	2.32	0.52
2:C:1:NAG:H81	3:D:3:BMA:O2	2.10	0.52
1:A:119:LYS:NZ	11:A:916:HOH:O	2.40	0.51
1:A:56:GLU:HG2	1:A:60:HIS:NE2	2.26	0.50
1:B:56:GLU:HG2	1:B:60:HIS:NE2	2.27	0.50
1:B:694:VAL:HG11	1:B:704:PHE:HZ	1.75	0.50
1:A:21:ILE:HG21	1:A:83:LEU:HD22	1.93	0.50
1:A:694:VAL:HG11	1:A:704:PHE:CZ	2.46	0.50
1:A:517:ALA:HB2	1:A:548:THR:HG21	1.93	0.50
1:B:2:TYR:N	11:B:914:HOH:O	2.46	0.49
1:B:71:THR:HB	10:B:830:GOL:H31	1.94	0.49
1:A:694:VAL:HG11	1:A:704:PHE:HZ	1.76	0.49
1:A:424:ASN:HA	1:A:432:GLN:HB3	1.95	0.49
1:B:138:GLU:HG2	1:B:209:THR:HG22	1.95	0.49
1:A:394:ILE:HD13	1:A:447:ILE:HD13	1.94	0.48
1:A:138:GLU:HG2	1:A:209:THR:HG22	1.95	0.48
1:B:291:HIS:CD2	1:B:331[B]:ASP:HB3	2.49	0.48
1:B:694:VAL:HG11	1:B:704:PHE:CZ	2.49	0.47
1:B:517:ALA:HB2	1:B:548:THR:HG21	1.96	0.47
1:A:169:MET:HB3	1:A:437:LYS:HE2	1.96	0.47
1:B:437:LYS:HE3	1:B:473:TYR:CE1	2.50	0.47
1:B:37:ARG:HD2	1:B:37:ARG:N	2.29	0.46
1:A:396:GLN:HE21	1:A:470:ARG:NH1	2.00	0.46
1:B:191:TRP:CE2	1:B:193:MET:HG3	2.51	0.46
1:B:245:PRO:HG3	1:B:603:PHE:CD1	2.51	0.46
1:B:520:PHE:CD2	1:B:521:GLU:HG3	2.50	0.46
1:A:181:PHE:CE2	1:A:189:PHE:HB3	2.50	0.45
1:A:437:LYS:HE3	1:A:473:TYR:CE1	2.51	0.45
1:A:37:ARG:HD2	1:A:37:ARG:H	1.82	0.45
1:B:547:TRP:CD1	1:B:653:PRO:HG3	2.51	0.45
1:A:117:PRO:HG2	1:A:120:SER:HB3	1.98	0.45
1:A:708:SER:HB3	1:A:711:GLU:HG3	1.97	0.45
1:A:191:TRP:CE2	1:A:193:MET:HG3	2.52	0.45
1:A:520:PHE:HD2	1:A:521:GLU:HG3	1.81	0.45
1:B:205:ARG:HH12	1:B:207:ARG:NE	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:SER:HA	1:B:393:TRP:HB3	1.98	0.44
1:A:548:THR:HA	1:A:551:LEU:HD12	1.98	0.44
1:B:169:MET:HB3	1:B:437:LYS:HE2	2.00	0.44
1:A:517:ALA:HB3	1:A:556:THR:HA	1.99	0.44
1:A:520:PHE:CD2	1:A:521:GLU:HG3	2.53	0.44
1:B:205:ARG:NH1	1:B:207:ARG:NE	2.66	0.44
1:A:323:SER:HA	1:A:393:TRP:HB3	1.99	0.44
1:A:628:ILE:HD11	1:A:667:PRO:HB3	1.99	0.43
1:A:625:ASP:OD2	1:A:665:TYR:OH	2.29	0.43
1:A:245:PRO:HG3	1:A:603:PHE:CD1	2.54	0.43
1:B:520:PHE:HD2	1:B:521:GLU:HG3	1.84	0.43
1:A:624:THR:HG21	1:A:669:THR:C	2.39	0.43
1:B:517:ALA:HB3	1:B:556:THR:HA	2.00	0.42
1:A:37:ARG:HD2	1:A:37:ARG:N	2.34	0.42
1:B:514:THR:OG1	1:B:515:VAL:N	2.52	0.42
1:B:548:THR:HA	1:B:551:LEU:HD12	2.01	0.42
1:B:683:ASN:HD22	8:B:820:NAG:H83	1.84	0.42
1:B:697:PRO:HD2	1:B:700:HIS:HB2	2.01	0.42
1:A:547:TRP:CD1	1:A:653:PRO:HG3	2.55	0.42
1:A:394:ILE:HG21	1:A:447:ILE:HD11	2.02	0.41
1:A:118:LEU:HG	1:A:119:LYS:HE2	2.01	0.41
1:A:514:THR:OG1	1:A:515:VAL:N	2.53	0.41
1:B:621:PHE:CZ	1:B:644:MET:HE3	2.55	0.41
1:A:140:SER:HB3	1:A:205:ARG:HD2	2.02	0.41
1:A:172:PHE:CG	1:A:405:ALA:HB2	2.55	0.41
1:A:300:ARG:NH2	3:D:2:NAG:O3	2.54	0.41
1:A:485:SER:HB2	11:A:972:HOH:O	2.20	0.41
1:B:181:PHE:CE2	1:B:189:PHE:HB3	2.56	0.41
1:A:555:ARG:HD3	11:A:901:HOH:O	2.21	0.40
1:B:558:GLY:HA3	1:B:560:ARG:NH1	2.37	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	717/718 (100%)	688 (96%)	29 (4%)	0	100	100
1	B	716/718 (100%)	686 (96%)	30 (4%)	0	100	100
All	All	1433/1436 (100%)	1374 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	607/606 (100%)	602 (99%)	5 (1%)	81	93
1	B	606/606 (100%)	597 (98%)	9 (2%)	65	86
All	All	1213/1212 (100%)	1199 (99%)	14 (1%)	73	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	286	TYR
1	A	324	LEU
1	A	365	TYR
1	A	484	TRP
1	B	37	ARG
1	B	65	ASP
1	B	88	TRP
1	B	286	TYR
1	B	324	LEU
1	B	331[A]	ASP
1	B	331[B]	ASP
1	B	365	TYR
1	B	484	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	396	GLN
1	A	445	GLN
1	B	156	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 ⓘ

57 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	1.17	2 (14%)	17,19,21	1.11	1 (5%)
2	NAG	C	2	2	14,14,15	1.20	2 (14%)	17,19,21	1.09	1 (5%)
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	0.68	0
2	MAN	C	4	2	11,11,12	0.76	0	15,15,17	0.95	1 (6%)
2	MAN	C	5	2	11,11,12	0.72	0	15,15,17	0.98	1 (6%)
2	MAN	C	6	2	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
3	NAG	D	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	1.11	1 (5%)
3	NAG	D	2	3	14,14,15	1.19	2 (14%)	17,19,21	1.07	1 (5%)
3	BMA	D	3	3	11,11,12	0.59	0	15,15,17	0.70	0
3	MAN	D	4	3	11,11,12	0.78	0	15,15,17	1.07	1 (6%)
3	MAN	D	5	3	11,11,12	0.75	0	15,15,17	1.18	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	6	3	11,11,12	0.77	0	15,15,17	1.03	1 (6%)
3	MAN	D	7	3	11,11,12	0.76	0	15,15,17	1.13	2 (13%)
3	MAN	D	8	3	11,11,12	0.80	0	15,15,17	1.11	1 (6%)
3	MAN	D	9	3	11,11,12	0.78	0	15,15,17	1.15	1 (6%)
4	NAG	E	1	1,4	14,14,15	1.18	2 (14%)	17,19,21	1.18	1 (5%)
4	MAN	E	10	4	11,11,12	0.79	0	15,15,17	1.10	1 (6%)
4	NAG	E	2	4	14,14,15	1.19	2 (14%)	17,19,21	1.06	1 (5%)
4	BMA	E	3	4	11,11,12	0.59	0	15,15,17	0.76	0
4	MAN	E	4	4	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
4	MAN	E	5	4	11,11,12	0.83	0	15,15,17	1.29	1 (6%)
4	MAN	E	6	4	11,11,12	0.77	0	15,15,17	0.97	1 (6%)
4	MAN	E	7	4	11,11,12	0.76	0	15,15,17	1.00	1 (6%)
4	MAN	E	8	4	11,11,12	0.78	0	15,15,17	1.06	1 (6%)
4	MAN	E	9	4	11,11,12	0.77	0	15,15,17	1.04	1 (6%)
5	BGC	F	1	5	12,12,12	0.85	0	17,17,17	0.89	1 (5%)
5	BGC	F	2	5	11,11,12	1.05	1 (9%)	15,15,17	1.02	1 (6%)
5	XYS	F	3	5	9,9,10	0.69	0	10,12,14	0.75	0
5	GAL	F	4	5	11,11,12	2.75	1 (9%)	15,15,17	2.36	3 (20%)
5	BGC	F	5	5	11,11,12	1.03	1 (9%)	15,15,17	0.99	1 (6%)
6	BGC	G	1	6	12,12,12	0.83	0	17,17,17	0.95	1 (5%)
6	BGC	G	2	6	11,11,12	0.27	0	15,15,17	0.63	0
6	BGC	G	3	6	11,11,12	0.99	0	15,15,17	0.95	1 (6%)
6	XYS	G	4	6	9,9,10	0.22	0	10,12,14	0.53	0
7	NAG	H	1	1,7	14,14,15	1.19	2 (14%)	17,19,21	1.03	1 (5%)
7	NAG	H	2	7	14,14,15	1.20	2 (14%)	17,19,21	1.05	1 (5%)
7	BMA	H	3	7	11,11,12	0.59	0	15,15,17	0.79	0
7	MAN	H	4	7	11,11,12	0.75	0	15,15,17	1.01	1 (6%)
7	MAN	H	5	7	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
7	MAN	H	6	7	11,11,12	0.77	0	15,15,17	1.17	2 (13%)
7	MAN	H	7	7	11,11,12	0.81	0	15,15,17	1.10	1 (6%)
7	MAN	H	8	7	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
4	NAG	I	1	1,4	14,14,15	1.17	2 (14%)	17,19,21	1.14	2 (11%)
4	MAN	I	10	4	11,11,12	0.79	0	15,15,17	0.98	1 (6%)
4	NAG	I	2	4	14,14,15	1.22	2 (14%)	17,19,21	1.18	2 (11%)
4	BMA	I	3	4	11,11,12	0.60	0	15,15,17	0.73	0
4	MAN	I	4	4	11,11,12	0.76	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	I	5	4	11,11,12	0.82	0	15,15,17	1.11	1 (6%)
4	MAN	I	6	4	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
4	MAN	I	7	4	11,11,12	0.79	0	15,15,17	0.97	1 (6%)
4	MAN	I	8	4	11,11,12	0.79	0	15,15,17	1.08	1 (6%)
4	MAN	I	9	4	11,11,12	0.76	0	15,15,17	1.06	1 (6%)
5	BGC	J	1	5	12,12,12	0.83	0	17,17,17	0.84	1 (5%)
5	BGC	J	2	5	11,11,12	1.00	1 (9%)	15,15,17	0.89	1 (6%)
5	XYS	J	3	5	9,9,10	0.70	0	10,12,14	0.72	0
5	GAL	J	4	5	11,11,12	2.80	1 (9%)	15,15,17	2.19	3 (20%)
5	BGC	J	5	5	11,11,12	1.01	1 (9%)	15,15,17	0.94	1 (6%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	MAN	D	8	3	-	2/2/19/22	0/1/1/1
3	MAN	D	9	3	-	1/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	MAN	E	10	4	-	2/2/19/22	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	GAL	C2-C3	-8.96	1.39	1.52
5	F	4	GAL	C2-C3	-8.80	1.39	1.52
7	H	2	NAG	C7-N2	2.39	1.42	1.34
7	H	1	NAG	C7-N2	2.38	1.42	1.34
3	D	2	NAG	C7-N2	2.34	1.42	1.34
4	E	1	NAG	C7-N2	2.33	1.42	1.34
4	I	2	NAG	C7-N2	2.33	1.42	1.34
4	I	1	NAG	C7-N2	2.32	1.42	1.34
3	D	1	NAG	C7-N2	2.31	1.42	1.34
2	C	2	NAG	C7-N2	2.30	1.42	1.34
4	E	2	NAG	C7-N2	2.30	1.42	1.34
2	C	1	NAG	C7-N2	2.22	1.42	1.34
4	E	1	NAG	C2-N2	-2.22	1.42	1.46
4	E	2	NAG	C2-N2	-2.22	1.42	1.46
4	I	2	NAG	C2-N2	-2.21	1.42	1.46
3	D	1	NAG	C2-N2	-2.20	1.42	1.46
2	C	2	NAG	C2-N2	-2.20	1.42	1.46
3	D	2	NAG	C2-N2	-2.19	1.42	1.46
2	C	1	NAG	C2-N2	-2.19	1.42	1.46
4	I	1	NAG	C2-N2	-2.16	1.42	1.46
5	F	2	BGC	C2-C3	-2.14	1.49	1.52
5	F	5	BGC	C2-C3	-2.13	1.49	1.52
5	J	5	BGC	C2-C3	-2.12	1.49	1.52
7	H	2	NAG	C2-N2	-2.10	1.42	1.46
7	H	1	NAG	C2-N2	-2.09	1.42	1.46
5	J	2	BGC	C2-C3	-2.06	1.49	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	4	GAL	C1-C2-C3	7.73	119.16	109.67
5	J	4	GAL	C1-C2-C3	6.80	118.03	109.67
4	E	5	MAN	C1-O5-C5	-3.92	106.88	112.19
3	D	5	MAN	C1-O5-C5	-3.57	107.35	112.19
3	D	9	MAN	C1-O5-C5	-3.53	107.41	112.19
4	I	5	MAN	C1-O5-C5	-3.37	107.62	112.19
3	D	4	MAN	C1-O5-C5	-3.36	107.65	112.19
4	I	6	MAN	C1-O5-C5	-3.34	107.67	112.19
7	H	6	MAN	C1-O5-C5	-3.24	107.80	112.19
5	J	4	GAL	O3-C3-C4	3.18	117.70	110.35
4	I	8	MAN	C1-O5-C5	-3.17	107.89	112.19
7	H	8	MAN	C1-O5-C5	-3.13	107.95	112.19
7	H	7	MAN	C1-O5-C5	-3.12	107.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	MAN	C1-O5-C5	-3.12	107.97	112.19
4	E	10	MAN	C1-O5-C5	-3.11	107.98	112.19
6	G	1	BGC	C1-O5-C5	-3.11	107.80	113.66
4	E	9	MAN	C1-O5-C5	-3.11	107.98	112.19
3	D	8	MAN	C1-O5-C5	-3.10	107.99	112.19
4	I	9	MAN	C1-O5-C5	-3.10	107.99	112.19
5	F	4	GAL	O3-C3-C4	3.05	117.39	110.35
7	H	4	MAN	C1-O5-C5	-3.00	108.12	112.19
4	E	8	MAN	C1-O5-C5	-2.90	108.27	112.19
2	C	6	MAN	C1-O5-C5	-2.89	108.28	112.19
4	E	6	MAN	C1-O5-C5	-2.82	108.37	112.19
4	I	10	MAN	C1-O5-C5	-2.78	108.42	112.19
5	F	2	BGC	C1-O5-C5	-2.74	108.47	112.19
5	F	1	BGC	C1-O5-C5	-2.74	108.49	113.66
3	D	6	MAN	C1-O5-C5	-2.73	108.49	112.19
4	I	7	MAN	C1-O5-C5	-2.71	108.52	112.19
7	H	5	MAN	C1-O5-C5	-2.69	108.54	112.19
2	C	4	MAN	C1-O5-C5	-2.65	108.60	112.19
6	G	3	BGC	C1-O5-C5	-2.64	108.62	112.19
2	C	1	NAG	C2-N2-C7	-2.63	119.16	122.90
4	E	4	MAN	C1-O5-C5	-2.61	108.66	112.19
5	J	1	BGC	C1-O5-C5	-2.58	108.79	113.66
4	I	4	MAN	C1-O5-C5	-2.55	108.74	112.19
4	E	7	MAN	C1-O5-C5	-2.54	108.75	112.19
5	J	5	BGC	C1-O5-C5	-2.53	108.76	112.19
5	F	4	GAL	C1-O5-C5	-2.48	108.83	112.19
7	H	2	NAG	C8-C7-N2	2.44	120.24	116.10
4	I	2	NAG	C8-C7-N2	2.43	120.21	116.10
4	E	1	NAG	C8-C7-N2	2.40	120.16	116.10
2	C	5	MAN	O5-C5-C6	2.39	110.96	107.20
5	F	5	BGC	C1-O5-C5	-2.39	108.95	112.19
2	C	2	NAG	C8-C7-N2	2.35	120.08	116.10
4	I	2	NAG	C2-N2-C7	-2.27	119.66	122.90
4	E	2	NAG	C8-C7-N2	2.27	119.94	116.10
4	I	1	NAG	C8-C7-N2	2.21	119.84	116.10
7	H	6	MAN	O5-C5-C6	2.18	110.63	107.20
3	D	2	NAG	C8-C7-N2	2.18	119.79	116.10
3	D	7	MAN	O5-C5-C6	2.16	110.60	107.20
5	J	4	GAL	C1-O5-C5	-2.16	109.26	112.19
5	J	2	BGC	C1-O5-C5	-2.16	109.27	112.19
3	D	1	NAG	C8-C7-N2	2.16	119.75	116.10
4	I	1	NAG	C1-O5-C5	2.14	115.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1	NAG	C8-C7-N2	2.11	119.67	116.10

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	8	MAN	C4-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
7	H	5	MAN	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
6	G	2	BGC	O5-C5-C6-O6
6	G	3	BGC	O5-C5-C6-O6
6	G	2	BGC	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	E	9	MAN	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	D	8	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
7	H	8	MAN	O5-C5-C6-O6
5	F	1	BGC	O5-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6
4	E	8	MAN	O5-C5-C6-O6
7	H	5	MAN	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
6	G	3	BGC	C4-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	E	9	MAN	C4-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
4	E	8	MAN	C4-C5-C6-O6
5	F	1	BGC	C4-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

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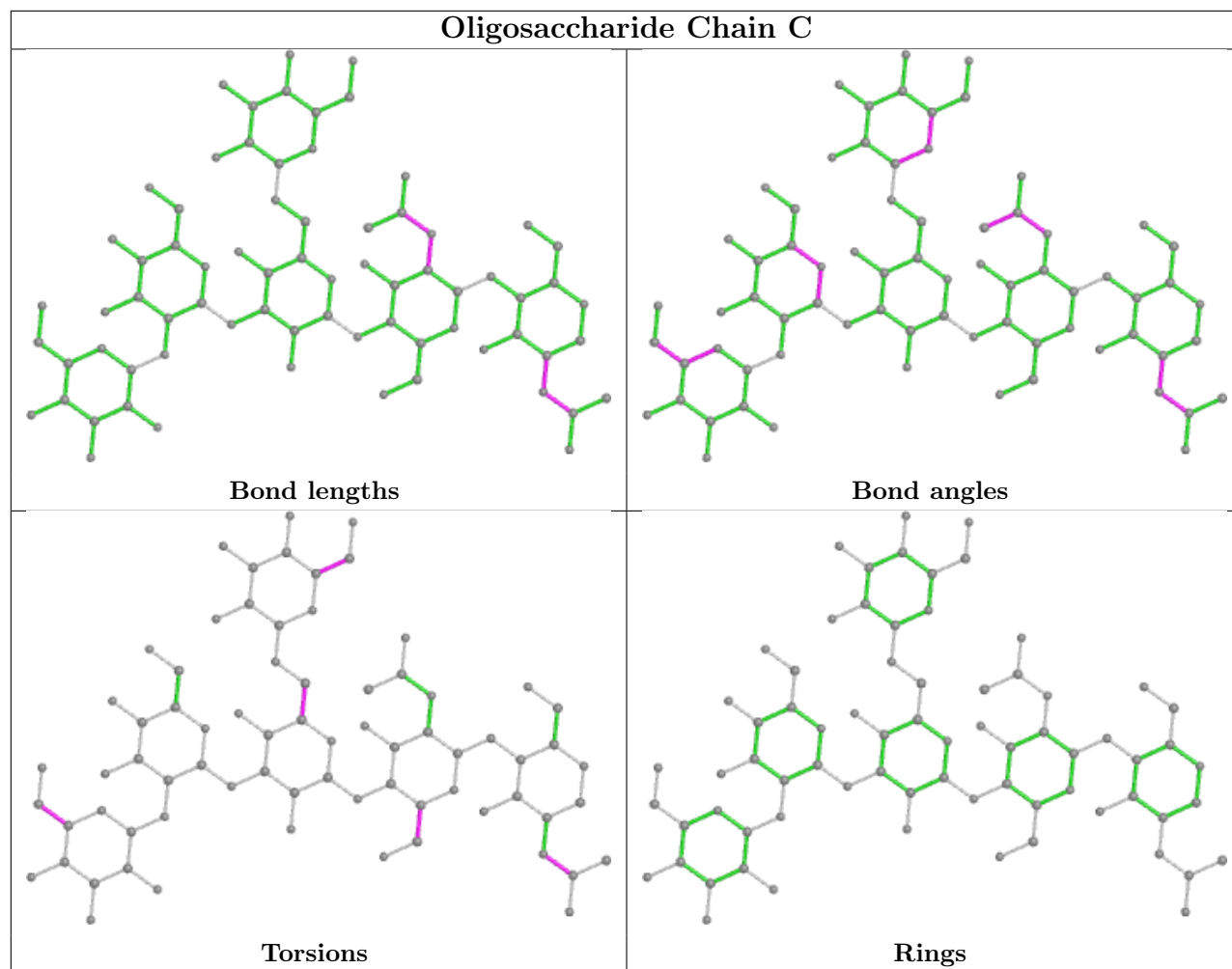
Mol	Chain	Res	Type	Atoms
7	H	1	NAG	O5-C5-C6-O6
7	H	8	MAN	C4-C5-C6-O6
4	E	5	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
7	H	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	E	10	MAN	O5-C5-C6-O6
4	I	8	MAN	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	E	10	MAN	C4-C5-C6-O6
4	I	8	MAN	C4-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	I	10	MAN	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
4	I	10	MAN	C4-C5-C6-O6
6	G	1	BGC	C4-C5-C6-O6
6	G	1	BGC	O5-C5-C6-O6
3	D	9	MAN	O5-C5-C6-O6
5	J	5	BGC	O5-C5-C6-O6
7	H	3	BMA	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
7	H	6	MAN	C4-C5-C6-O6
5	F	5	BGC	O5-C5-C6-O6
7	H	6	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

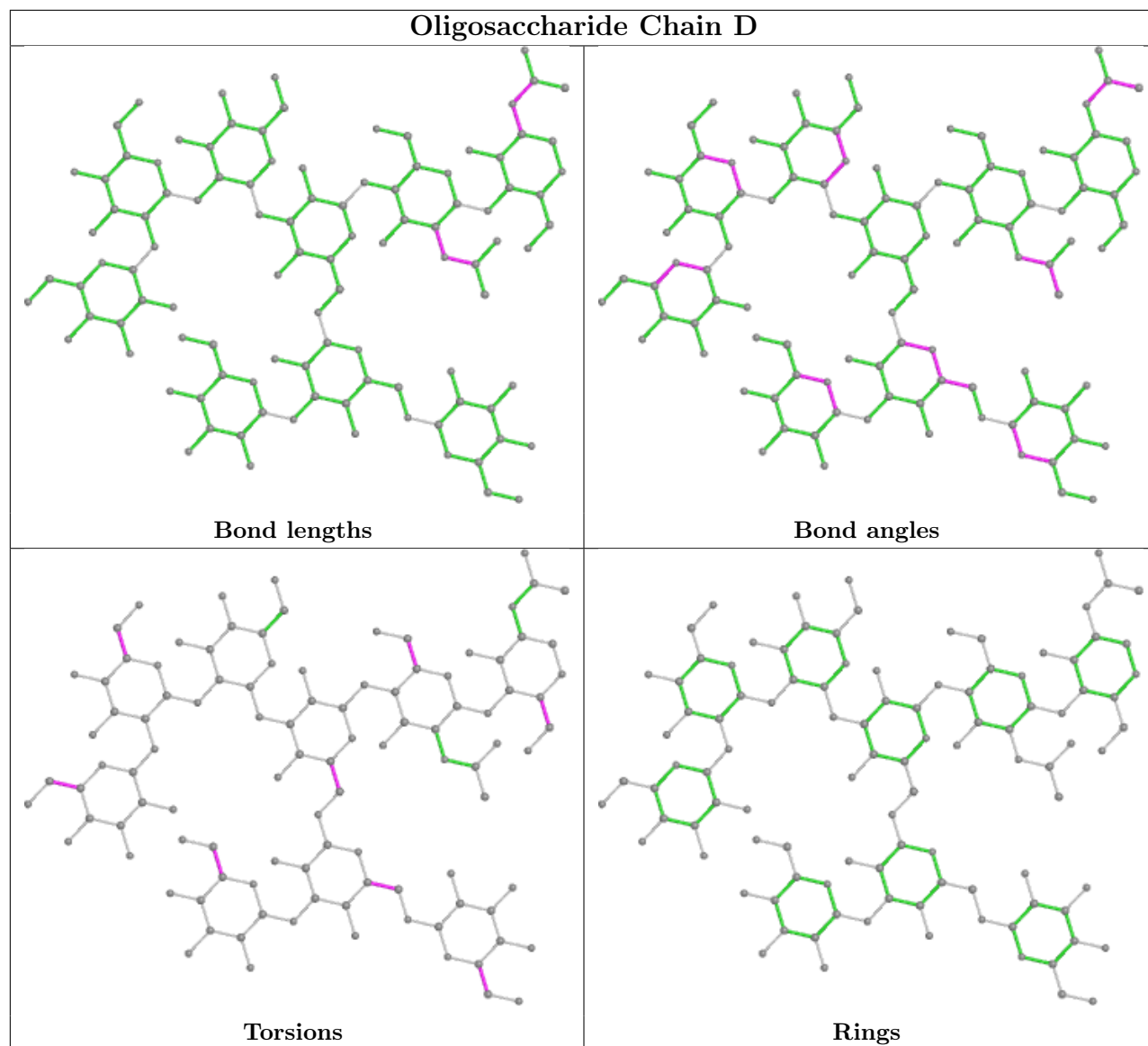
There are no ring outliers.

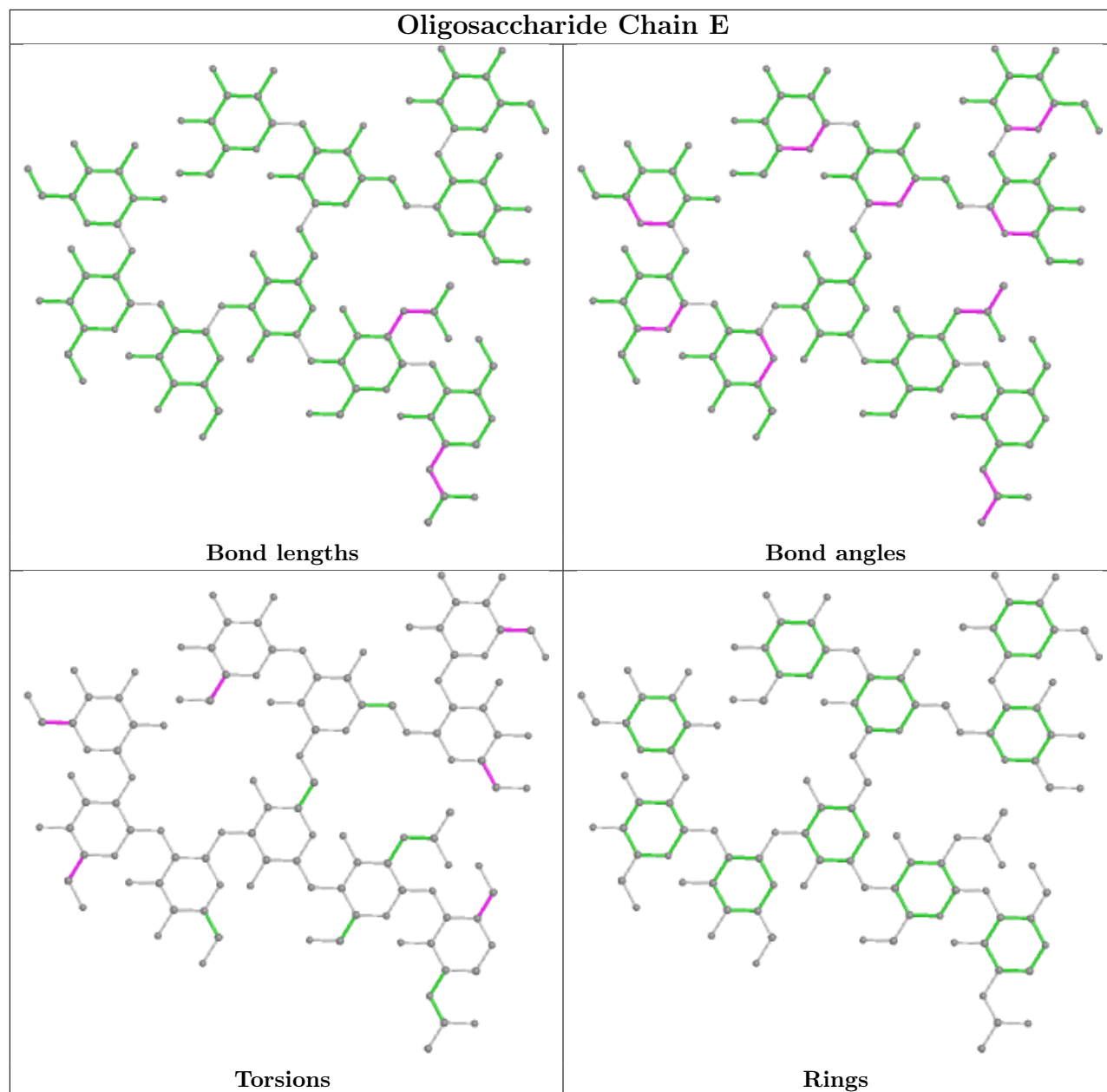
5 monomers are involved in 4 short contacts:

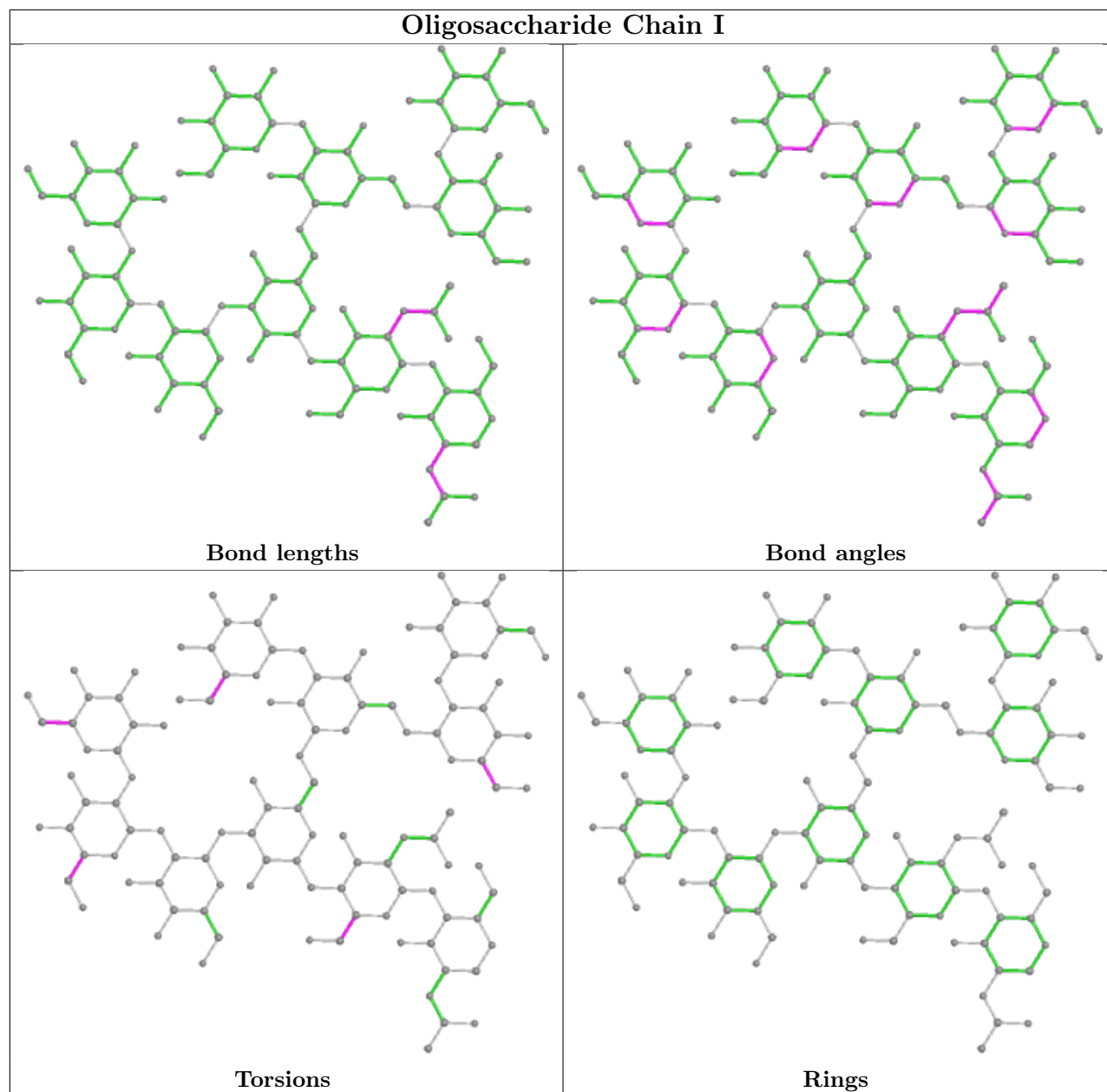
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	D	4	MAN	1	0
2	C	1	NAG	2	0
7	H	2	NAG	1	0
3	D	3	BMA	1	0

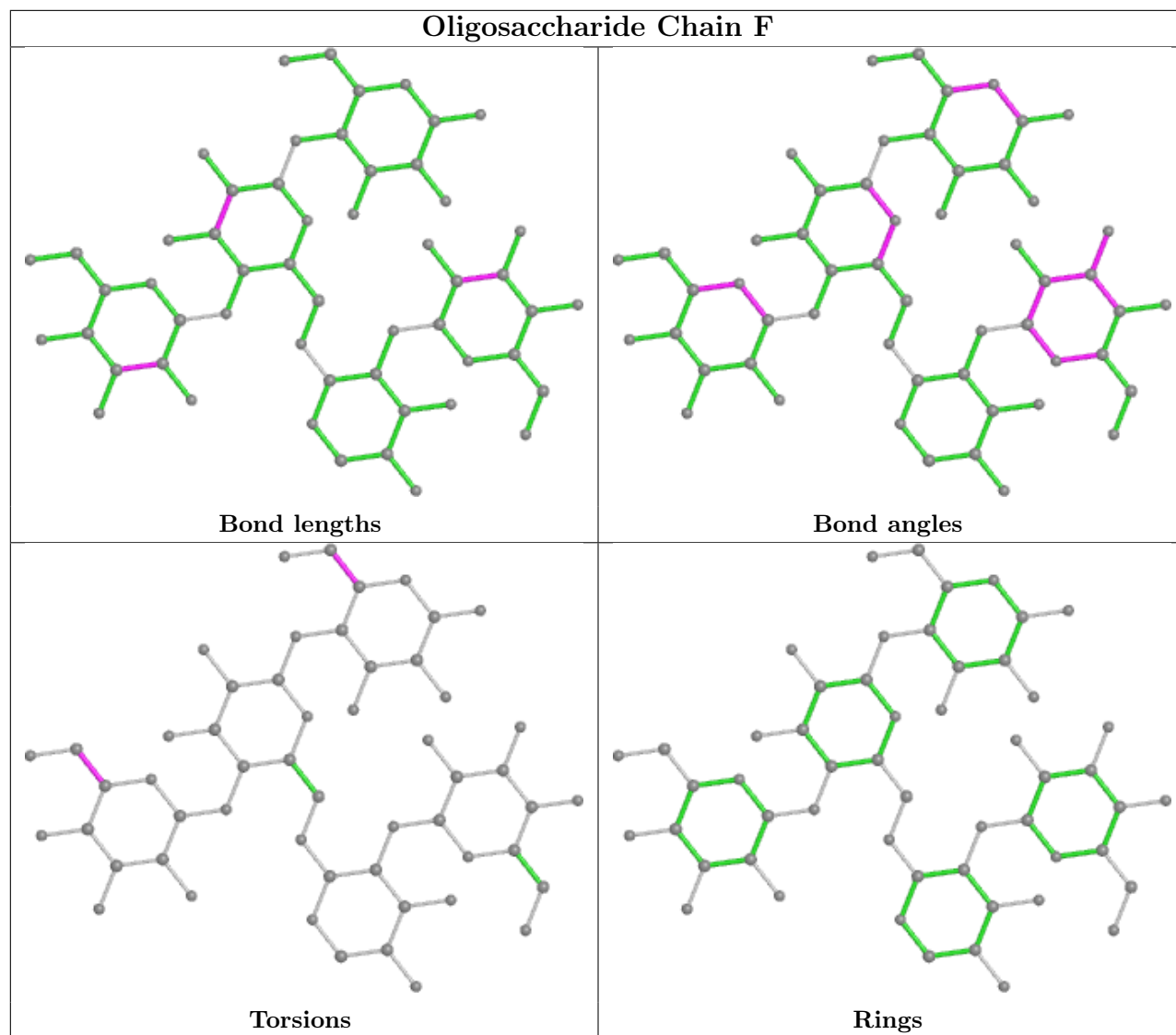
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

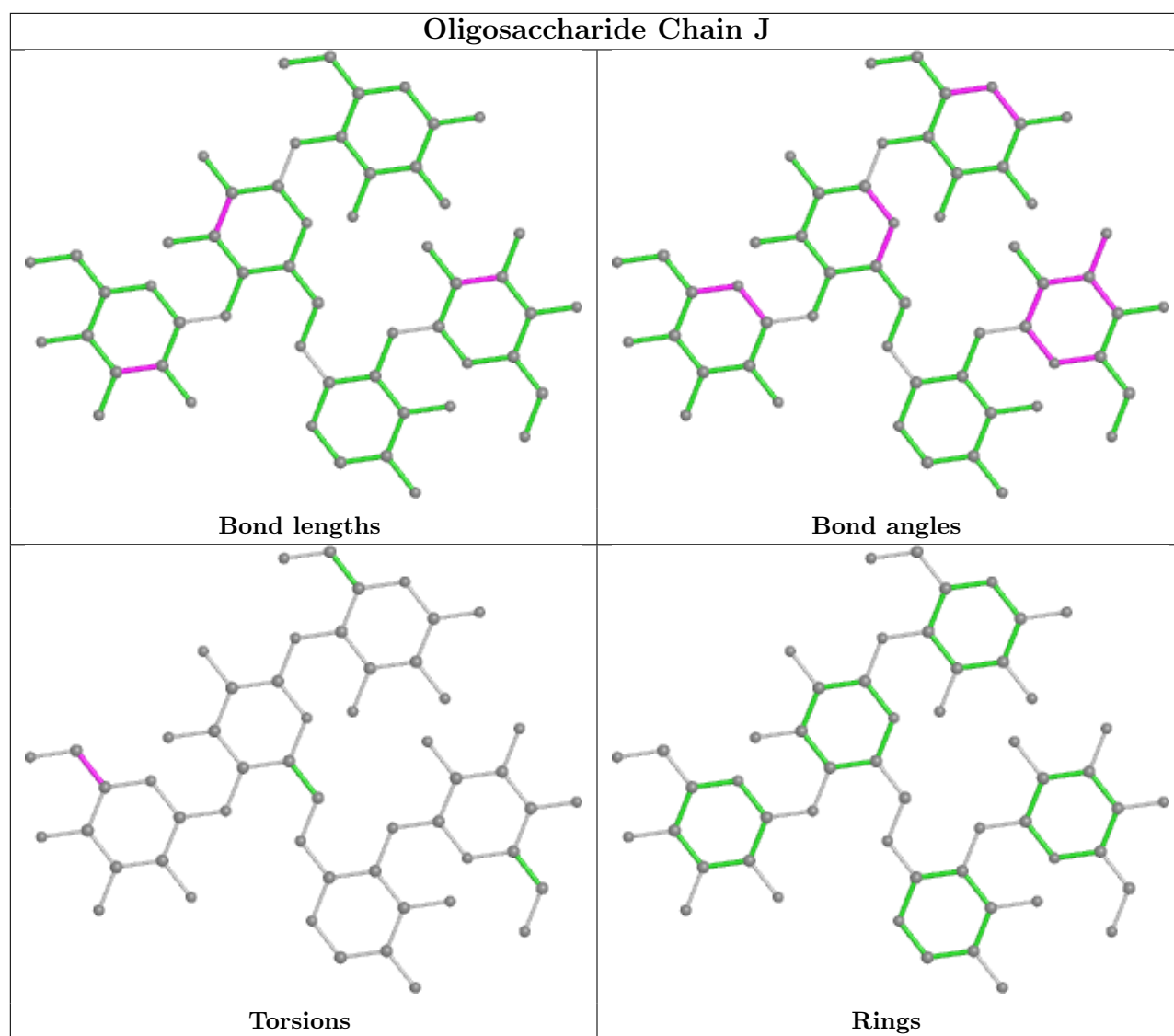


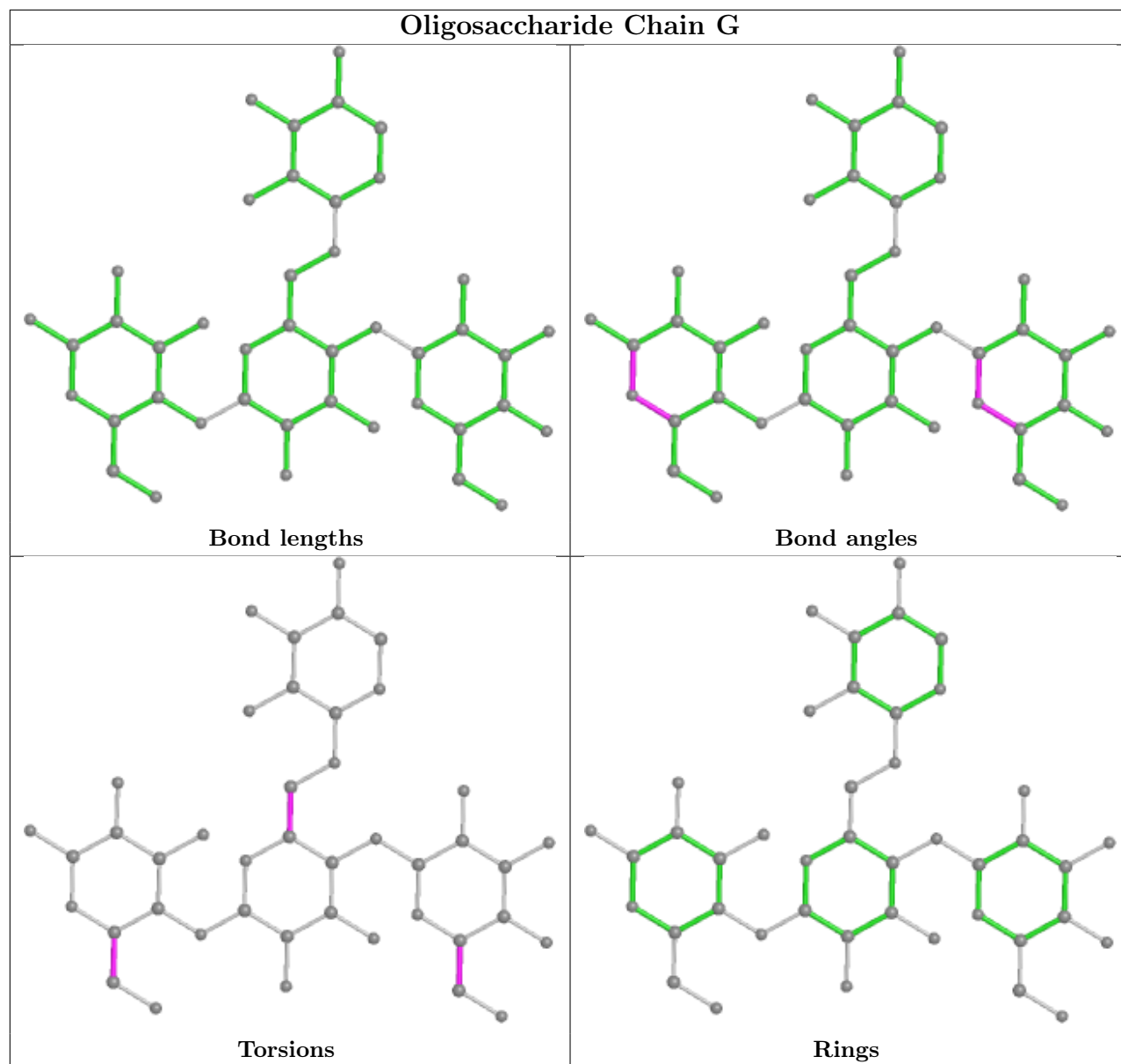


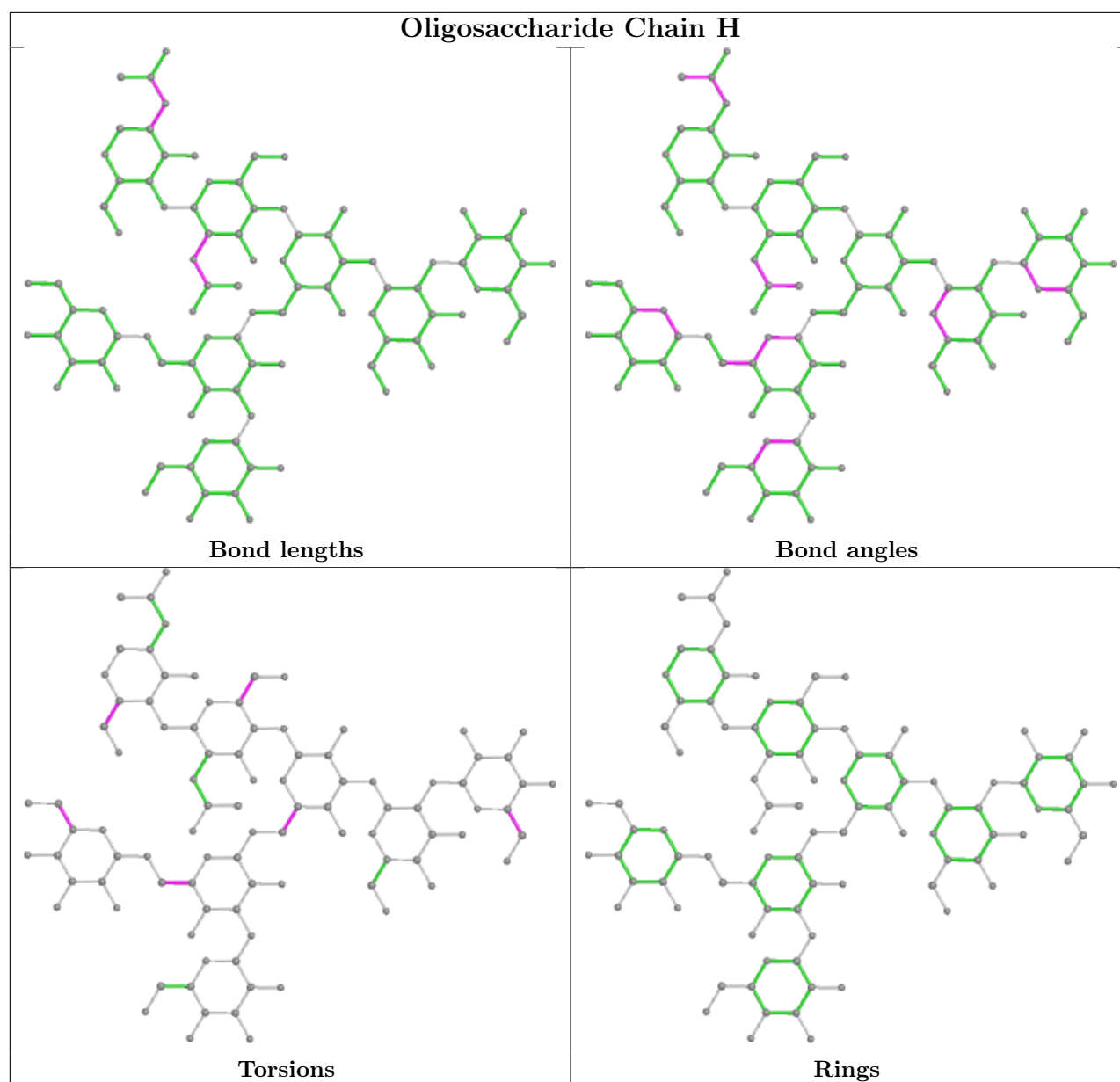












5.6 Ligand geometry [i](#)

14 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	GOL	A	840	-	5,5,5	0.88	0	5,5,5	1.00	0
8	NAG	B	820	1	14,14,15	1.20	2 (14%)	17,19,21	1.16	1 (5%)
8	NAG	B	821	1	14,14,15	1.17	2 (14%)	17,19,21	1.06	1 (5%)
8	NAG	A	827	1	14,14,15	1.15	2 (14%)	17,19,21	1.11	1 (5%)
10	GOL	B	831	-	5,5,5	0.90	0	5,5,5	1.03	0
8	NAG	B	829	1	14,14,15	1.16	2 (14%)	17,19,21	1.37	4 (23%)
8	NAG	B	822	1	14,14,15	1.21	2 (14%)	17,19,21	1.11	1 (5%)
10	GOL	B	830	-	5,5,5	0.88	0	5,5,5	1.01	0
9	XYS	B	828	-	10,10,10	0.79	0	14,14,14	0.83	0
8	NAG	A	835	1	14,14,15	0.30	0	17,19,21	0.61	0
8	NAG	B	801	1	14,14,15	1.16	2 (14%)	17,19,21	1.27	3 (17%)
8	NAG	A	826	1	14,14,15	1.20	2 (14%)	17,19,21	1.11	1 (5%)
8	NAG	A	828	1	14,14,15	1.13	1 (7%)	17,19,21	0.95	0
9	XYS	A	834	-	10,10,10	0.80	0	14,14,14	0.73	1 (7%)

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	GOL	A	840	-	-	2/4/4/4	-
8	NAG	B	820	1	-	3/6/23/26	0/1/1/1
8	NAG	B	821	1	-	2/6/23/26	0/1/1/1
8	NAG	A	827	1	-	2/6/23/26	0/1/1/1
10	GOL	B	831	-	-	2/4/4/4	-
8	NAG	B	829	1	-	1/6/23/26	0/1/1/1
8	NAG	B	822	1	-	4/6/23/26	0/1/1/1
10	GOL	B	830	-	-	2/4/4/4	-
9	XYS	B	828	-	-	-	0/1/1/1
8	NAG	A	835	1	-	0/6/23/26	0/1/1/1
8	NAG	B	801	1	-	0/6/23/26	0/1/1/1
8	NAG	A	826	1	-	2/6/23/26	0/1/1/1
8	NAG	A	828	1	-	1/6/23/26	0/1/1/1
9	XYS	A	834	-	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	828	NAG	C7-N2	2.54	1.43	1.34
8	B	820	NAG	C7-N2	2.39	1.42	1.34
8	B	829	NAG	C7-N2	2.39	1.42	1.34
8	B	821	NAG	C7-N2	2.37	1.42	1.34
8	B	822	NAG	C7-N2	2.35	1.42	1.34
8	A	827	NAG	C7-N2	2.35	1.42	1.34
8	A	826	NAG	C7-N2	2.32	1.42	1.34
8	B	801	NAG	C7-N2	2.32	1.42	1.34
8	B	822	NAG	C2-N2	-2.24	1.42	1.46
8	B	820	NAG	C2-N2	-2.23	1.42	1.46
8	B	801	NAG	C2-N2	-2.21	1.42	1.46
8	A	826	NAG	C2-N2	-2.17	1.42	1.46
8	B	821	NAG	C2-N2	-2.12	1.42	1.46
8	A	827	NAG	C2-N2	-2.11	1.42	1.46
8	B	829	NAG	C2-N2	-2.07	1.42	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	822	NAG	C8-C7-N2	2.79	120.83	116.10
8	B	829	NAG	C1-O5-C5	2.74	115.90	112.19
8	B	820	NAG	C8-C7-N2	2.72	120.70	116.10
8	B	801	NAG	C8-C7-N2	2.54	120.41	116.10
8	B	801	NAG	C2-N2-C7	-2.51	119.33	122.90
8	A	826	NAG	C8-C7-N2	2.49	120.31	116.10
9	A	834	XYS	C5-O5-C1	-2.43	108.63	112.71
8	A	827	NAG	C8-C7-N2	2.28	119.95	116.10
8	B	821	NAG	C8-C7-N2	2.27	119.94	116.10
8	B	829	NAG	C8-C7-N2	2.23	119.88	116.10
8	B	829	NAG	C2-N2-C7	-2.16	119.82	122.90
8	B	801	NAG	C1-O5-C5	2.13	115.07	112.19
8	B	829	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	830	GOL	O1-C1-C2-C3
8	B	822	NAG	O5-C5-C6-O6
8	B	822	NAG	C4-C5-C6-O6
8	B	821	NAG	O5-C5-C6-O6
8	B	820	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	B	820	NAG	O7-C7-N2-C2
8	B	822	NAG	C8-C7-N2-C2
8	B	822	NAG	O7-C7-N2-C2
8	A	826	NAG	C8-C7-N2-C2
8	A	826	NAG	O7-C7-N2-C2
8	B	821	NAG	C4-C5-C6-O6
10	B	831	GOL	O1-C1-C2-O2
10	A	840	GOL	O1-C1-C2-C3
10	B	831	GOL	O1-C1-C2-C3
10	B	830	GOL	O1-C1-C2-O2
8	A	827	NAG	C4-C5-C6-O6
8	B	829	NAG	O5-C5-C6-O6
10	A	840	GOL	O1-C1-C2-O2
8	B	820	NAG	O5-C5-C6-O6
8	A	827	NAG	O5-C5-C6-O6
8	A	828	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	820	NAG	1	0
10	B	830	GOL	1	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	718/718 (100%)	0.20	27 (3%)	40 39	50, 63, 84, 142	0
1	B	717/718 (99%)	0.09	14 (1%)	65 67	50, 63, 85, 137	0
All	All	1435/1436 (99%)	0.15	41 (2%)	51 52	50, 63, 84, 142	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	673	ASN	4.9
1	A	672	ASN	4.6
1	B	672	ASN	4.2
1	A	671	GLN	4.0
1	A	673	ASN	3.8
1	A	3	PHE	3.8
1	A	670	GLY	3.4
1	A	168	ASP	3.3
1	B	564	PHE	3.2
1	B	671	GLN	3.1
1	A	155	GLN	3.1
1	A	55	TYR	3.0
1	B	102	VAL	3.0
1	A	2	TYR	3.0
1	B	3	PHE	2.9
1	A	166	VAL	2.9
1	B	670	GLY	2.8
1	A	692	VAL	2.8
1	A	1	THR	2.8
1	A	167	ILE	2.7
1	B	2	TYR	2.7
1	A	177	PRO	2.7
1	A	165	SER	2.6
1	A	674	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	664	VAL	2.5
1	B	197	GLY	2.4
1	A	686	TYR	2.3
1	A	706	LEU	2.3
1	A	197	GLY	2.3
1	A	564	PHE	2.3
1	A	175	TYR	2.3
1	B	718	PHE	2.2
1	B	301	LEU	2.2
1	B	76	LEU	2.2
1	A	7	SER	2.2
1	A	718	PHE	2.2
1	B	687	ALA	2.1
1	A	687	ALA	2.1
1	B	58	THR	2.0
1	A	501	SER	2.0
1	A	26	TYR	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(\AA^2)	Q<0.9
3	MAN	D	9	11/12	0.79	0.28	93,101,123,130	0
2	MAN	C	5	11/12	0.82	0.18	81,118,131,137	0
7	MAN	H	8	11/12	0.83	0.36	109,123,135,139	0
6	XYS	G	4	9/10	0.83	0.20	93,110,124,124	0
5	GAL	J	4	11/12	0.85	0.15	78,111,127,128	0
2	MAN	C	6	11/12	0.85	0.22	99,112,125,136	0
6	BGC	G	2	11/12	0.86	0.24	97,103,109,114	0
7	MAN	H	5	11/12	0.86	0.24	107,115,126,127	0
5	GAL	F	4	11/12	0.86	0.15	92,118,127,132	0
3	MAN	D	6	11/12	0.86	0.54	118,138,144,153	0
6	BGC	G	1	12/12	0.88	0.38	102,111,131,135	0

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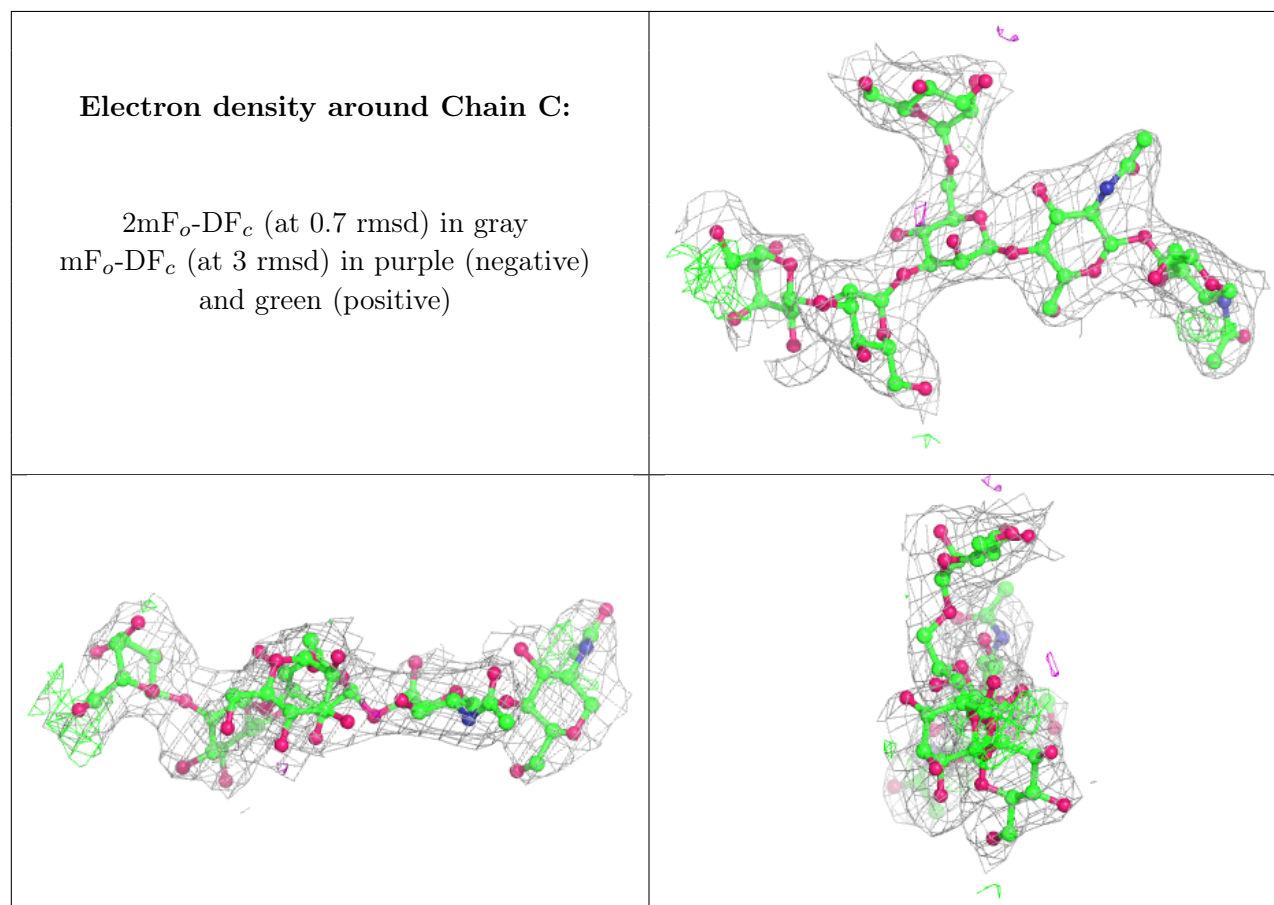
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	BGC	G	3	11/12	0.92	0.26	90,114,119,127	0
5	BGC	F	1	12/12	0.92	0.15	82,91,99,102	0
7	NAG	H	1	14/15	0.92	0.15	66,78,84,97	0
5	BGC	J	1	12/12	0.92	0.15	84,95,100,105	0
3	MAN	D	5	11/12	0.92	0.24	103,110,127,138	0
4	MAN	E	6	11/12	0.93	0.19	94,111,122,123	0
5	XYS	J	3	9/10	0.94	0.12	96,100,106,114	0
3	MAN	D	7	11/12	0.94	0.22	63,77,97,108	0
2	MAN	C	4	11/12	0.95	0.18	81,87,96,110	0
4	MAN	E	7	11/12	0.95	0.12	61,67,74,77	0
3	MAN	D	8	11/12	0.95	0.18	66,68,76,78	0
4	MAN	I	6	11/12	0.95	0.15	87,101,108,111	0
7	NAG	H	2	14/15	0.95	0.22	61,74,76,98	0
5	BGC	J	5	11/12	0.95	0.15	62,67,76,78	0
3	NAG	D	2	14/15	0.96	0.19	61,70,78,88	0
4	MAN	I	5	11/12	0.96	0.13	69,78,83,89	0
5	BGC	J	2	11/12	0.96	0.15	73,79,87,95	0
4	BMA	I	3	11/12	0.96	0.10	54,60,69,69	0
4	MAN	I	4	11/12	0.96	0.11	54,66,72,73	0
4	MAN	I	8	11/12	0.96	0.09	65,71,77,79	0
5	BGC	F	2	11/12	0.96	0.10	74,79,81,88	0
7	MAN	H	6	11/12	0.96	0.28	71,81,97,111	0
4	MAN	E	8	11/12	0.96	0.13	66,72,76,78	0
7	MAN	H	7	11/12	0.96	0.29	73,79,84,88	0
4	NAG	E	1	14/15	0.96	0.13	63,68,74,83	0
4	NAG	I	1	14/15	0.96	0.13	47,65,70,74	0
3	NAG	D	1	14/15	0.96	0.14	58,64,70,86	0
4	MAN	I	9	11/12	0.96	0.11	82,87,95,97	0
5	BGC	F	5	11/12	0.96	0.12	61,73,79,83	0
2	NAG	C	2	14/15	0.96	0.21	49,73,80,84	0
4	MAN	E	10	11/12	0.96	0.18	56,65,71,72	0
7	MAN	H	4	11/12	0.96	0.20	71,84,91,95	0
4	MAN	I	7	11/12	0.96	0.12	61,66,72,73	0
2	NAG	C	1	14/15	0.96	0.20	60,70,78,82	0
5	XYS	F	3	9/10	0.96	0.09	88,93,100,107	0
7	BMA	H	3	11/12	0.97	0.23	66,74,77,80	0
3	BMA	D	3	11/12	0.97	0.16	63,70,75,77	0
4	MAN	I	10	11/12	0.97	0.15	61,64,69,70	0
4	MAN	E	4	11/12	0.97	0.10	65,67,72,74	0
4	NAG	E	2	14/15	0.97	0.13	64,70,83,97	0
4	BMA	E	3	11/12	0.97	0.10	54,60,69,71	0
3	MAN	D	4	11/12	0.97	0.16	66,69,81,85	0

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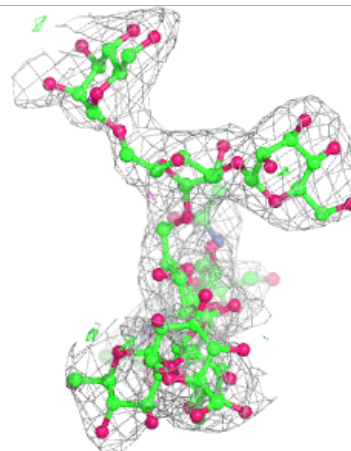
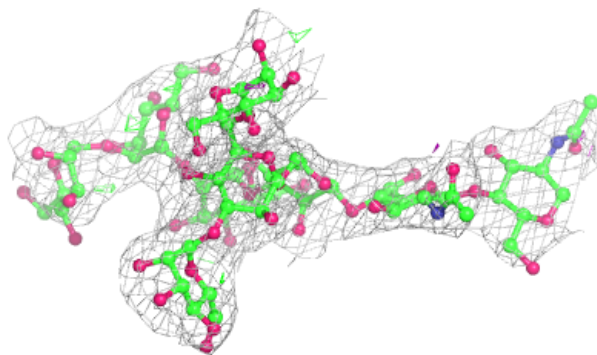
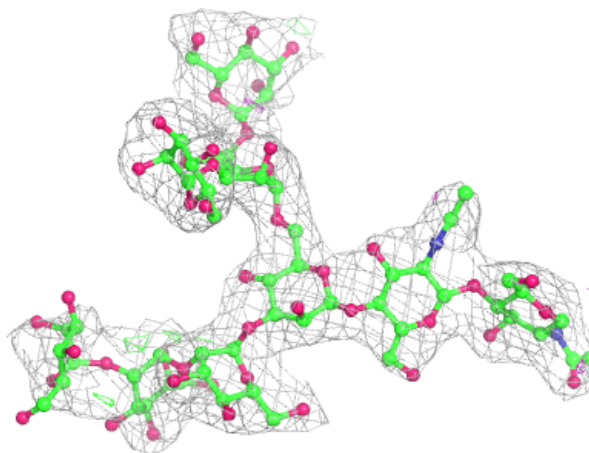
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	I	2	14/15	0.97	0.12	61,67,80,85	0
2	BMA	C	3	11/12	0.97	0.18	66,74,83,91	0
4	MAN	E	5	11/12	0.97	0.10	73,80,92,93	0
4	MAN	E	9	11/12	0.97	0.21	81,86,91,92	0

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.



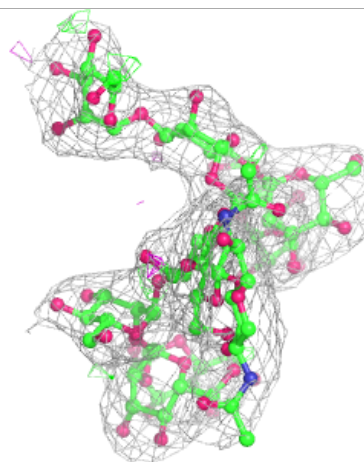
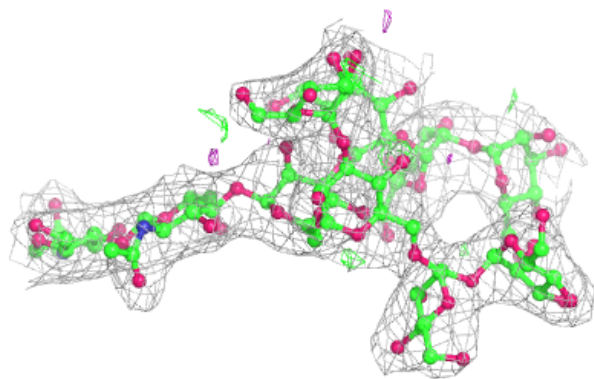
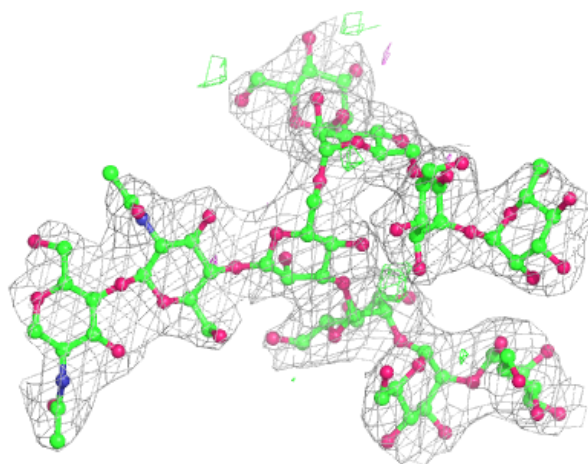
Electron density around Chain D:

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



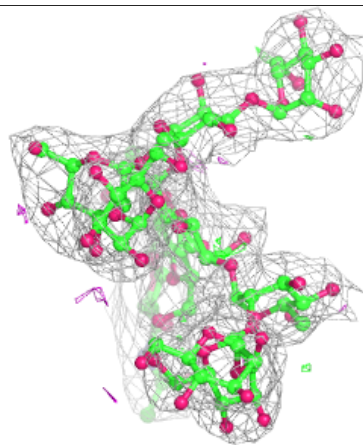
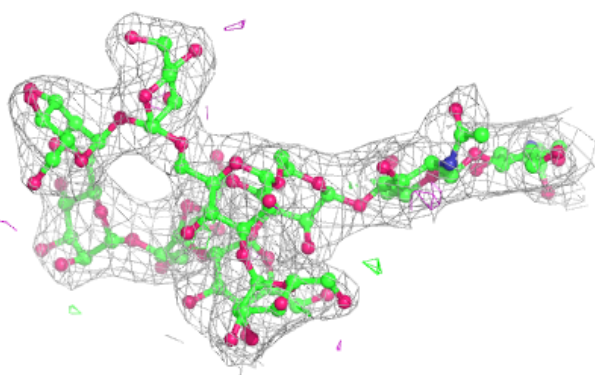
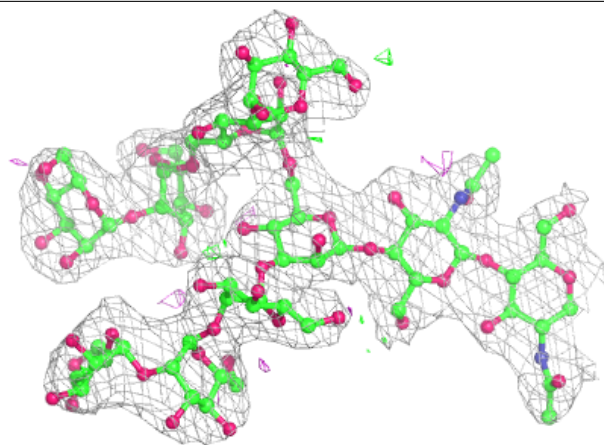
Electron density around Chain E:

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



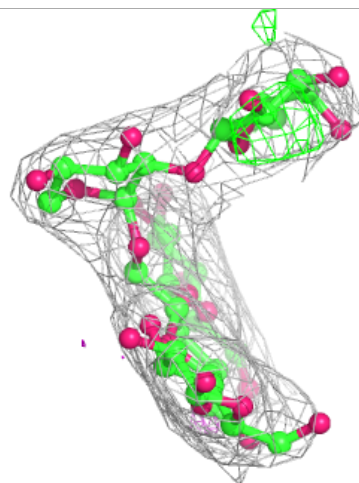
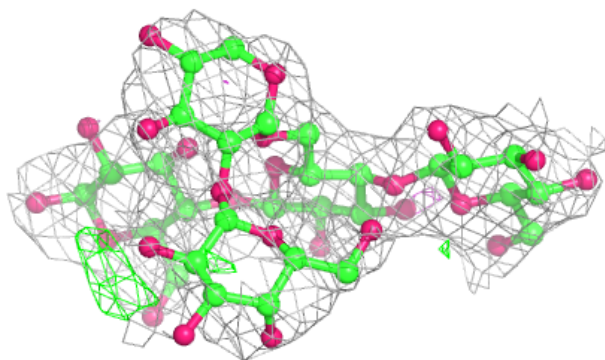
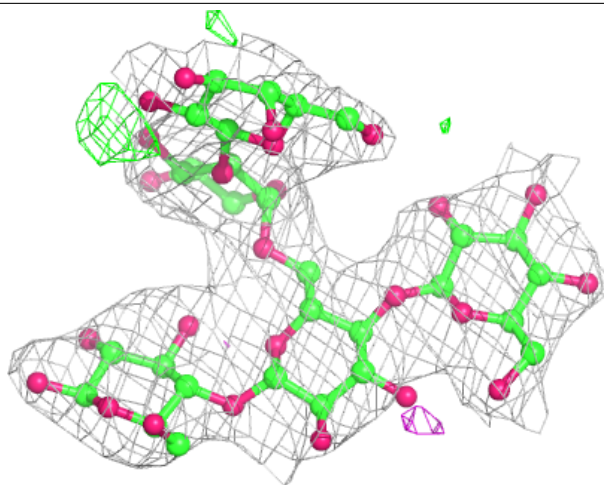
Electron density around Chain I:

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



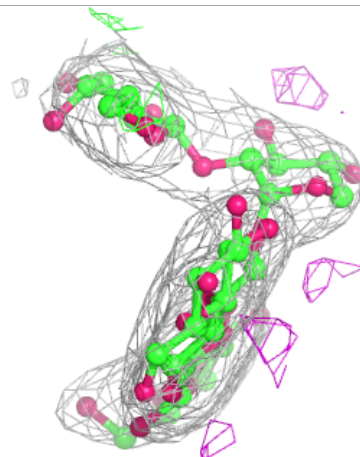
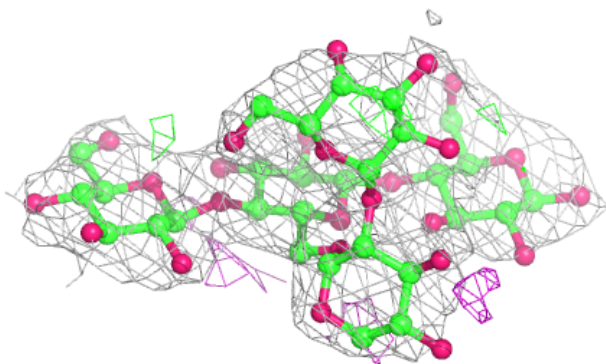
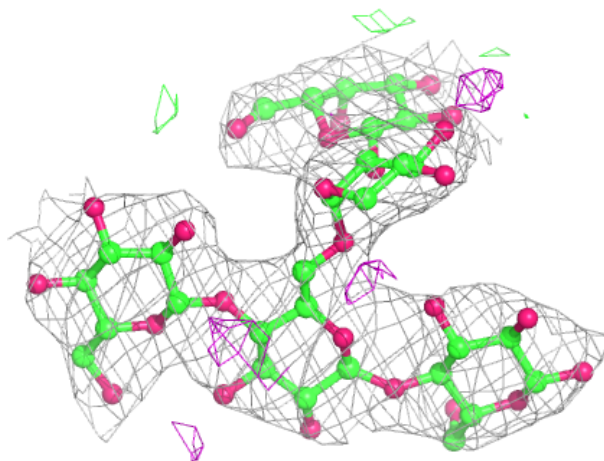
Electron density around Chain F:

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



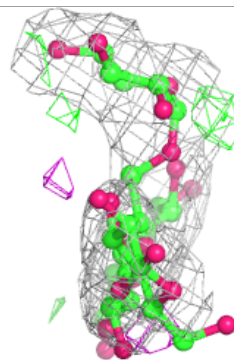
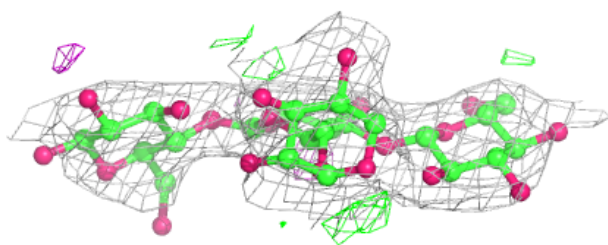
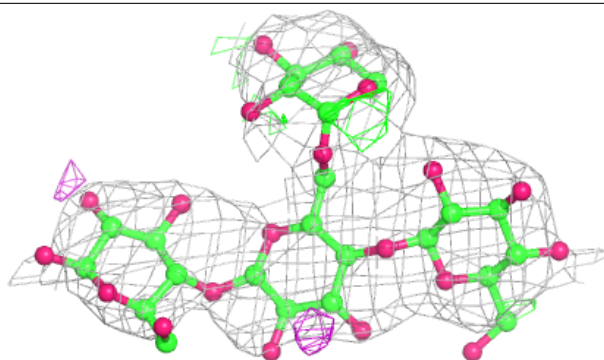
Electron density around Chain J:

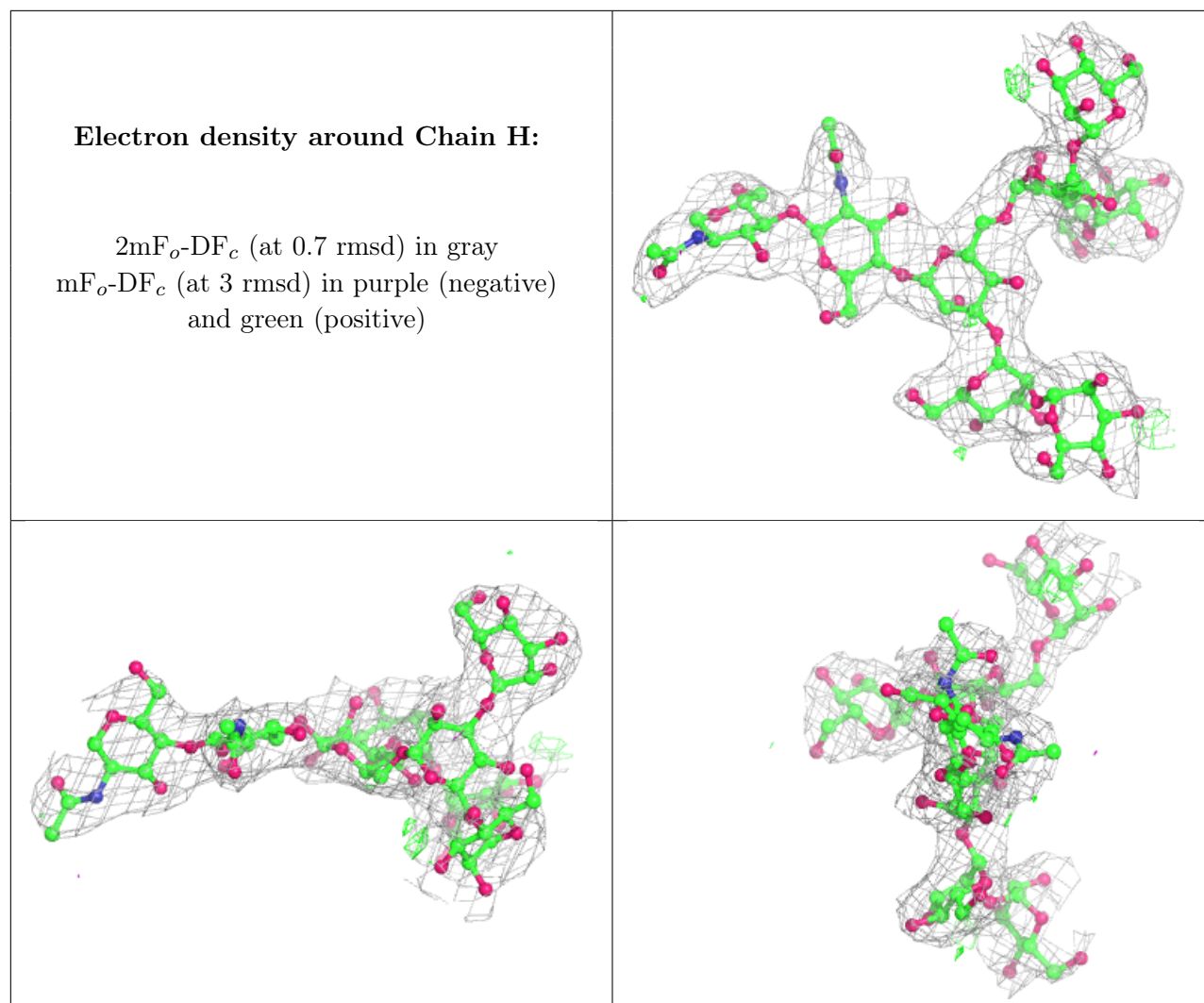
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o - DF_c$ (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
8	NAG	A	828	14/15	0.76	0.52	107,128,133,136	0
8	NAG	B	829	14/15	0.81	0.25	94,114,129,135	0
8	NAG	A	835	14/15	0.86	0.34	88,124,137,142	0
8	NAG	B	822	14/15	0.87	0.48	114,126,133,135	14
8	NAG	B	821	14/15	0.87	0.44	106,122,132,137	0
10	GOL	A	840	6/6	0.87	0.19	51,72,79,84	0
10	GOL	B	831	6/6	0.89	0.12	60,81,89,98	0
10	GOL	B	830	6/6	0.89	0.24	84,92,96,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	A	827	14/15	0.90	0.41	86,114,128,130	0
8	NAG	A	826	14/15	0.93	0.19	76,82,85,86	0
8	NAG	B	820	14/15	0.94	0.16	65,77,90,92	0
8	NAG	B	801	14/15	0.94	0.23	53,69,81,82	0
9	XYS	B	828	10/10	0.96	0.15	54,62,73,75	0
9	XYS	A	834	10/10	0.96	0.15	63,72,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.