



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2022 – 06:33 pm GMT

PDB ID : 8BEU
Title : Structure of D188A-fructofuranosidase from *Rhodotorula dairenensis* in complex with raffinose
Authors : Jimenez-Ortega, E.; Sanz-Aparicio, J.
Deposited on : 2022-10-21
Resolution : 2.27 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

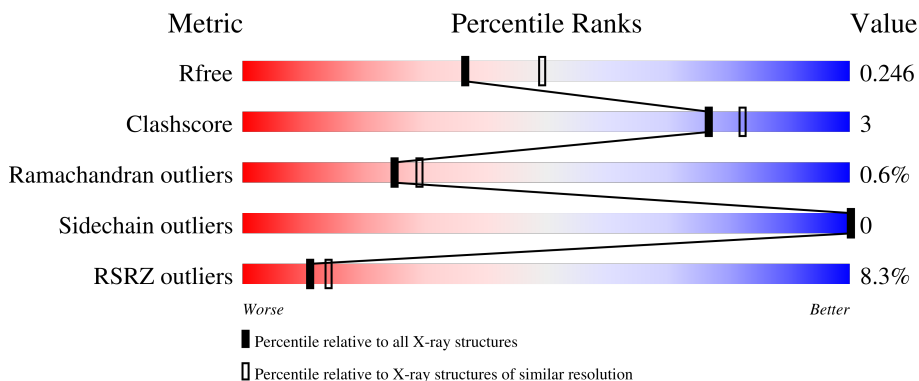
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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.




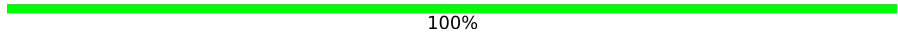

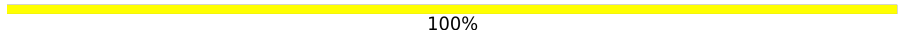
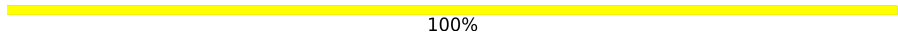
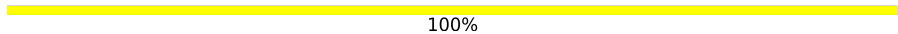



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	675	 0% 75% 22%
1	B	675	 5% 74% 22%
1	C	675	 3% 74% 22%
1	D	675	 16% 70% 23%
2	E	4	 25% 75%

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Mol	Chain	Length	Quality of chain
2	K	4	 25% 75%
3	F	2	 100%
3	I	2	 50% 50%
4	G	3	 100%
4	J	3	 100%
4	L	3	 100%
4	N	3	 33% 67%
5	H	5	 60% 40%
6	M	3	 67% 33%

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
7	MAN	D	702	-	-	X	-

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 17609 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-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	Total 4047	C 2577	N 659	O 800	S 11	0	0	0
1	B	526	Total 4038	C 2572	N 657	O 798	S 11	0	0	0
1	C	526	Total 4038	C 2572	N 657	O 799	S 10	0	0	0
1	D	521	Total 4010	C 2556	N 653	O 790	S 11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
B	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
C	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
D	188	ALA	ASP	engineered mutation	UNP A0A856TAI5

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



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

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

cetamido-2-deoxy-beta-D-glucopyranose.



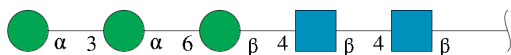
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose.



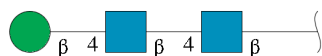
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	G	3	34	18	16	0	0	0
4	J	3	34	18	16	0	0	0
4	L	3	34	18	16	0	0	0
4	N	3	34	18	16	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



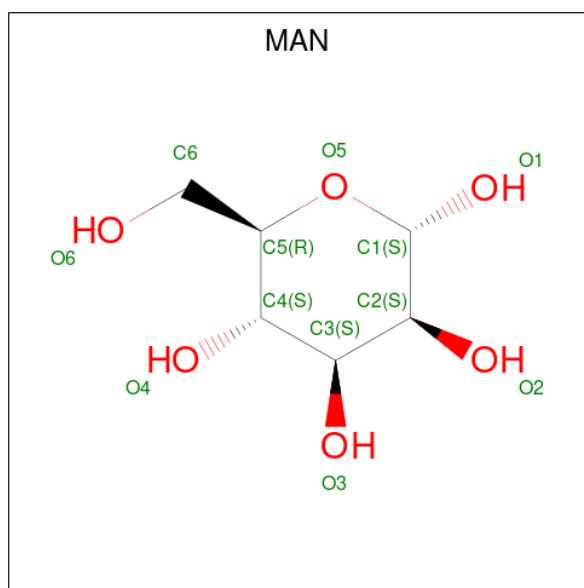
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	5	61	34	2	25	0	0	0

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



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

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



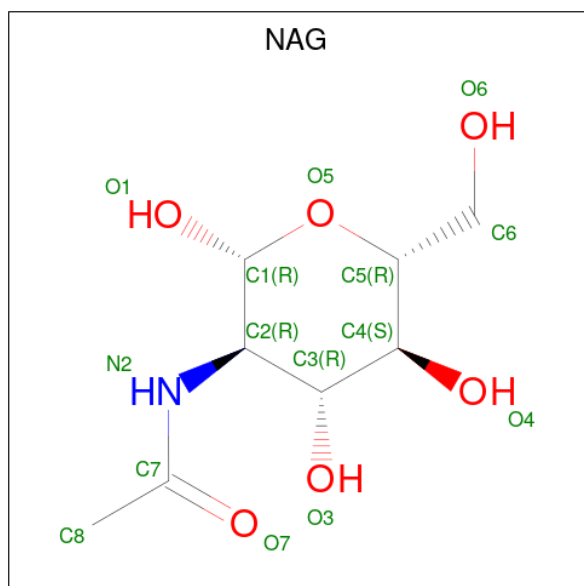
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	11	6	5	0	0
7	A	1	11	6	5	0	0
7	A	1	11	6	5	0	0
7	A	1	11	6	5	0	0
7	A	1	11	6	5	0	0
7	B	1	11	6	5	0	0
7	B	1	11	6	5	0	0
7	C	1	11	6	5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		

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



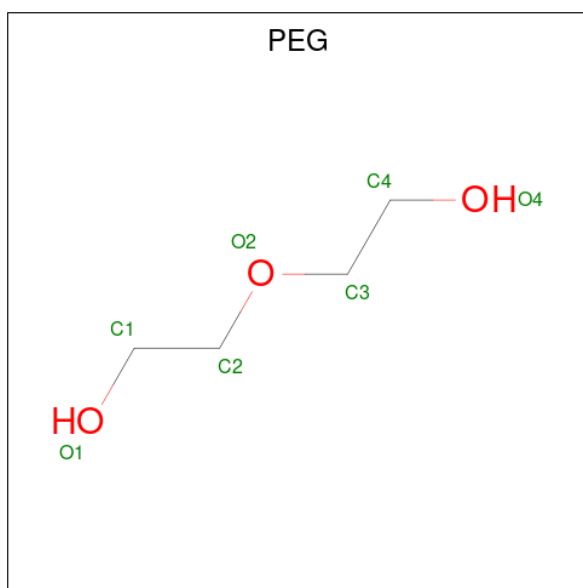
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C O	0	0
			7	4 3		

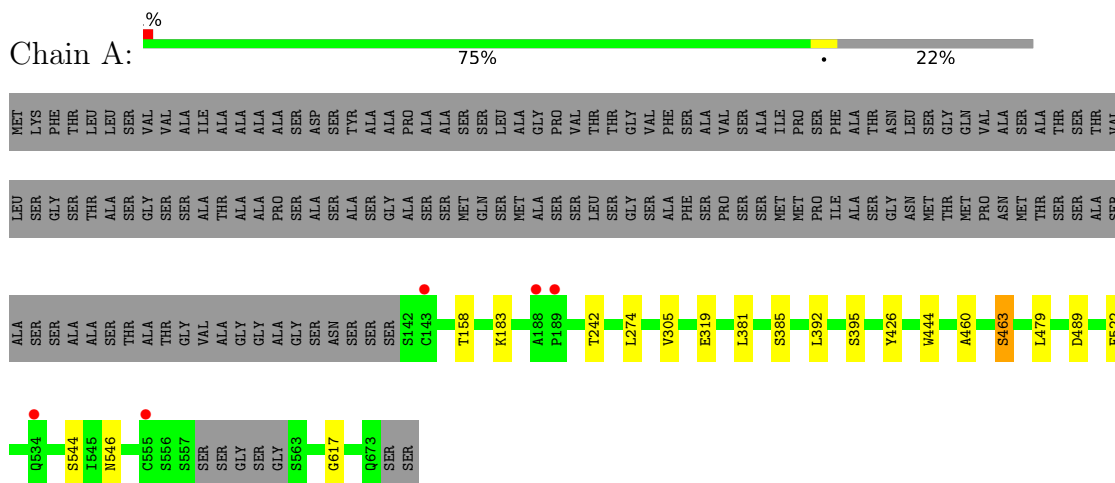
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	213	Total	O	0	0
			213	213		
10	B	139	Total	O	0	0
			139	139		
10	C	130	Total	O	0	0
			130	130		
10	D	74	Total	O	0	0
			74	74		

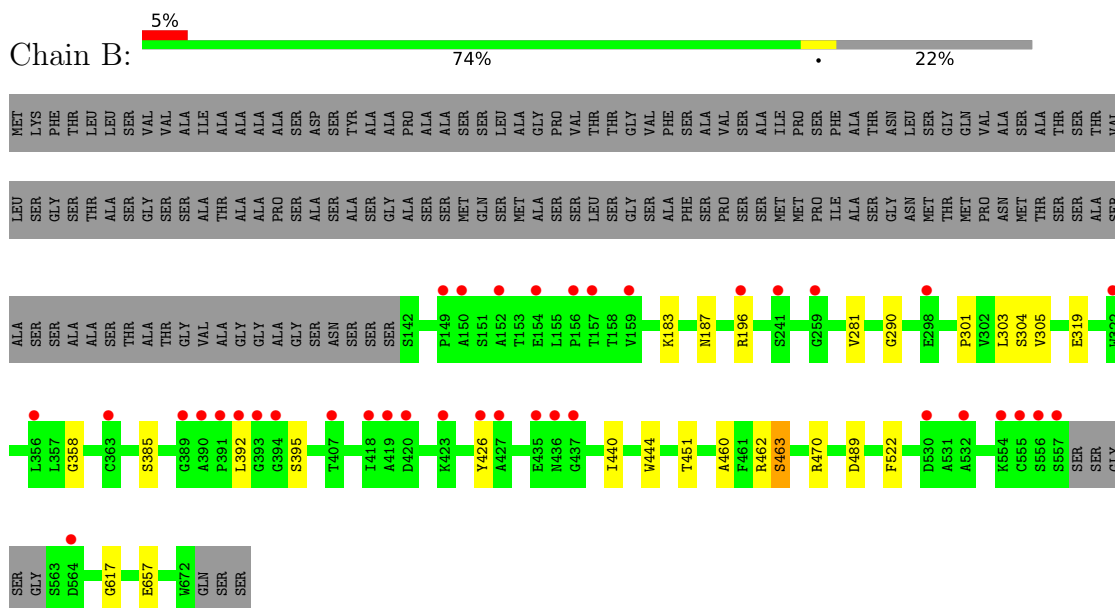
3 Residue-property plots (i)

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-fructofuranosidase



- Molecule 1: Beta-fructofuranosidase



- Molecule 1: Beta-fructofuranosidase



MAG1
MAG2
BMA3
MAN4

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

Chain F:  100%

MAG1
MAG2

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

Chain I:  50%

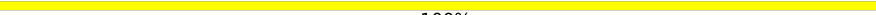
MAG1
MAG2

- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain G:  100%


FRU1
GLC2
GLA3

- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain J:  100%

FRU1
GLC2
GLA3

- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain L:  100%

FRU1
GLC2
GLA3

- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain N:  33%

FRU1
GLC2
GLA3

- Molecule 5: 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

nose

Chain H:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain M:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.01Å 114.54Å 139.16Å 90.00° 104.58° 90.00°	Depositor
Resolution (Å)	46.29 – 2.27 46.25 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-2.27) 99.8 (46.25-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.27Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.247 0.208 , 0.246	Depositor DCC
R_{free} test set	5731 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17609	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: PEG, NAG, FRU, MAN, GLA, BMA, GLC

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	0.64	0/4175	0.78	0/5741
1	B	0.64	0/4166	0.77	0/5729
1	C	0.64	0/4165	0.77	0/5726
1	D	0.66	0/4136	0.77	0/5685
All	All	0.65	0/16642	0.77	0/22881

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	4047	0	3760	18	0
1	B	4038	0	3758	24	0
1	C	4038	0	3758	17	0
1	D	4010	0	3732	36	0
2	E	50	0	43	0	0
2	K	50	0	43	0	0
3	F	28	0	25	0	0
3	I	28	0	25	1	0
4	G	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	34	0	30	0	0
4	L	34	0	30	0	0
4	N	34	0	30	2	0
5	H	61	0	52	0	0
6	M	39	0	34	0	0
7	A	55	0	50	1	0
7	B	22	0	20	0	0
7	C	33	0	30	0	0
7	D	33	0	30	6	0
8	A	126	0	117	4	0
8	B	84	0	78	1	0
8	C	98	0	91	4	0
8	D	70	0	65	1	0
9	B	7	0	10	0	0
10	A	213	0	0	1	0
10	B	139	0	0	1	0
10	C	130	0	0	1	0
10	D	74	0	0	3	0
All	All	17609	0	15841	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 3.

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:D:165:ILE:CG2	1:D:183:LYS:HE2	2.05	0.86
7:D:702:MAN:H3	7:D:703:MAN:H61	1.61	0.81
1:D:148:LEU:HD13	1:D:168:ASP:HB3	1.64	0.79
7:D:702:MAN:H3	7:D:703:MAN:C6	2.12	0.78
7:D:702:MAN:C3	7:D:703:MAN:H61	2.19	0.72
1:D:326:VAL:HG13	1:D:335:GLU:HG2	1.72	0.69
1:A:392:LEU:HD23	1:B:392:LEU:HD23	1.74	0.68
1:A:158:THR:HG23	7:A:703:MAN:H2	1.75	0.67
1:D:165:ILE:HG23	1:D:183:LYS:HE2	1.78	0.65
1:C:530:ASP:O	1:C:534:GLN:HG2	1.98	0.64
1:B:196:ARG:O	1:B:196:ARG:NH1	2.32	0.62
1:C:655:LEU:O	8:C:708:NAG:H5	1.99	0.62
1:D:385:SER:HB3	1:D:426:TYR:CE1	2.36	0.60
1:C:183:LYS:HA	1:C:460:ALA:O	2.01	0.60
1:B:183:LYS:HA	1:B:460:ALA:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HA	1:A:460:ALA:O	2.02	0.58
1:D:326:VAL:HG13	1:D:335:GLU:CG	2.35	0.57
1:B:440:ILE:HD11	1:B:470:ARG:HD3	1.87	0.57
1:B:281:VAL:HG13	1:B:303:LEU:O	2.06	0.55
1:B:385:SER:HB3	1:B:426:TYR:CE1	2.42	0.55
1:A:385:SER:HB3	1:A:426:TYR:CE1	2.41	0.55
1:B:281:VAL:CG1	1:B:303:LEU:O	2.55	0.55
1:A:479:LEU:HD21	1:B:358:GLY:O	2.07	0.54
1:A:242:THR:HG23	10:A:909:HOH:O	2.07	0.54
1:D:281:VAL:HG22	10:D:859:HOH:O	2.08	0.54
1:C:385:SER:HB3	1:C:426:TYR:CE1	2.43	0.54
1:A:395:SER:HB2	1:A:426:TYR:CD1	2.43	0.53
1:A:546:ASN:HD22	8:A:713:NAG:C7	2.21	0.53
1:D:395:SER:HB2	1:D:426:TYR:CD1	2.43	0.53
1:D:264:THR:HG22	1:D:266:ASP:H	1.73	0.53
1:D:328:ALA:HB2	1:D:335:GLU:OE2	2.08	0.53
1:B:395:SER:HB2	1:B:426:TYR:CD1	2.44	0.52
1:B:281:VAL:CG1	1:B:301:PRO:HB2	2.39	0.52
1:B:281:VAL:HG11	1:B:301:PRO:CB	2.40	0.52
1:C:395:SER:HB2	1:C:426:TYR:CD1	2.44	0.52
1:D:457:SER:O	1:D:458:ALA:HB3	2.09	0.52
1:D:349:SER:OG	1:D:408:HIS:CD2	2.63	0.52
1:C:444:TRP:HE1	1:C:463:SER:HB3	1.75	0.51
8:C:708:NAG:H61	10:C:921:HOH:O	2.11	0.50
1:D:362:GLU:OE1	4:N:2:GLC:H3	2.11	0.49
1:A:274:LEU:HD21	8:A:706:NAG:H62	1.93	0.49
1:D:278:THR:HG22	1:D:279:LEU:HG	1.95	0.48
1:C:490:LEU:HD23	1:C:521:TRP:CD1	2.49	0.48
1:D:148:LEU:O	7:D:702:MAN:H5	2.13	0.48
1:D:462:ARG:O	1:D:463:SER:HB2	2.14	0.48
1:A:444:TRP:HE1	1:A:463:SER:HB3	1.79	0.48
1:B:657:GLU:HG2	8:B:707:NAG:O3	2.14	0.48
1:D:210:GLU:HB2	10:D:867:HOH:O	2.14	0.48
1:A:392:LEU:HD23	1:B:392:LEU:CD2	2.44	0.48
1:C:160:PRO:HB2	1:C:163:THR:CG2	2.43	0.48
1:D:305:VAL:HG12	1:D:305:VAL:O	2.13	0.48
1:B:444:TRP:HE1	1:B:463:SER:HB3	1.79	0.48
1:B:281:VAL:HG11	1:B:301:PRO:HB2	1.95	0.47
7:D:702:MAN:C3	7:D:703:MAN:C6	2.86	0.46
7:D:702:MAN:H3	7:D:703:MAN:H62	1.95	0.46
1:D:444:TRP:HE1	1:D:463:SER:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.82	0.45
1:D:456:THR:HB	1:D:461:PHE:CZ	2.51	0.45
1:D:481:TRP:CZ2	8:D:706:NAG:H3	2.51	0.45
1:C:522:PHE:CE1	1:C:617:GLY:HA3	2.51	0.45
1:D:148:LEU:HD22	1:D:168:ASP:OD2	2.17	0.45
1:A:305:VAL:O	1:A:305:VAL:HG12	2.17	0.45
1:A:392:LEU:CD2	1:B:392:LEU:HD23	2.45	0.45
1:D:522:PHE:CE1	1:D:617:GLY:HA3	2.52	0.44
1:C:305:VAL:HG12	1:C:305:VAL:O	2.18	0.44
1:D:154:GLU:O	1:D:155:LEU:HB2	2.17	0.44
1:B:462:ARG:O	1:B:463:SER:HB2	2.17	0.44
1:D:165:ILE:HG21	1:D:183:LYS:HG3	1.99	0.44
1:A:522:PHE:CE1	1:A:617:GLY:HA3	2.52	0.44
1:D:258:SER:HB2	1:D:260:PHE:CE2	2.53	0.44
1:D:456:THR:HB	1:D:461:PHE:CE1	2.52	0.44
1:B:522:PHE:CZ	1:B:617:GLY:HA3	2.53	0.43
1:D:555:CYS:O	1:D:556:SER:HB2	2.18	0.43
1:C:462:ARG:O	1:C:463:SER:HB2	2.18	0.43
1:A:546:ASN:ND2	8:A:713:NAG:C7	2.81	0.43
1:C:481:TRP:CZ2	8:C:707:NAG:H3	2.54	0.43
1:C:522:PHE:CZ	1:C:617:GLY:HA3	2.54	0.42
1:D:183:LYS:HA	1:D:460:ALA:O	2.18	0.42
1:B:444:TRP:HZ2	1:B:451:THR:HG1	1.64	0.42
1:B:290:GLY:N	10:B:805:HOH:O	2.40	0.42
1:D:154:GLU:HB3	1:D:155:LEU:H	1.44	0.42
1:D:546:ASN:ND2	10:D:801:HOH:O	2.27	0.42
1:B:305:VAL:HG12	1:B:305:VAL:O	2.20	0.42
1:D:312:ASP:OD1	4:N:1:FRU:O4	2.26	0.42
1:B:281:VAL:HG13	1:B:304:SER:HB2	2.00	0.41
1:D:522:PHE:CZ	1:D:617:GLY:HA3	2.55	0.41
1:D:451:THR:HG23	1:D:452:GLN:HG3	2.02	0.41
3:I:1:NAG:H61	3:I:2:NAG:N2	2.35	0.41
1:C:657:GLU:HG2	8:C:708:NAG:O3	2.20	0.41
1:B:522:PHE:CE1	1:B:617:GLY:HA3	2.55	0.41
1:A:544:SER:OG	8:A:713:NAG:N2	2.49	0.41
1:C:187:ASN:HA	1:C:444:TRP:NE1	2.36	0.41
1:A:522:PHE:CZ	1:A:617:GLY:HA3	2.55	0.41
1:B:187:ASN:HA	1:B:444:TRP:NE1	2.36	0.41
1:D:491:SER:N	1:D:492:PRO:CD	2.84	0.40
1:C:392:LEU:HD23	1:D:392:LEU:HD23	2.04	0.40
1:C:556:SER:O	1:C:557:SER:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/675 (78%)	503 (96%)	17 (3%)	3 (1%)	25	29
1	B	522/675 (77%)	501 (96%)	18 (3%)	3 (1%)	25	29
1	C	520/675 (77%)	500 (96%)	17 (3%)	3 (1%)	25	29
1	D	515/675 (76%)	485 (94%)	26 (5%)	4 (1%)	19	22
All	All	2080/2700 (77%)	1989 (96%)	78 (4%)	13 (1%)	25	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	155	LEU
1	A	463	SER
1	A	489	ASP
1	B	319	GLU
1	B	463	SER
1	B	489	ASP
1	C	319	GLU
1	C	463	SER
1	C	489	ASP
1	D	463	SER
1	D	489	ASP
1	A	319	GLU
1	D	319	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	443/545 (81%)	443 (100%)	0	100	100
1	B	442/545 (81%)	442 (100%)	0	100	100
1	C	442/545 (81%)	442 (100%)	0	100	100
1	D	438/545 (80%)	438 (100%)	0	100	100
All	All	1765/2180 (81%)	1765 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

32 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	0.60	0	17,19,21	0.98	1 (5%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	1.04	0
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	1.29	3 (20%)
2	MAN	E	4	2	11,11,12	0.38	0	15,15,17	1.09	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.52	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	2	3	14,14,15	0.52	0	17,19,21	0.98	0
4	FRU	G	1	4	11,12,12	0.79	1 (9%)	10,18,18	1.11	1 (10%)
4	GLC	G	2	4	11,11,12	1.11	1 (9%)	15,15,17	1.24	1 (6%)
4	GLA	G	3	4	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.51	0	17,19,21	0.95	0
5	NAG	H	2	5	14,14,15	0.40	0	17,19,21	1.09	1 (5%)
5	BMA	H	3	5	11,11,12	0.34	0	15,15,17	0.72	0
5	MAN	H	4	5	11,11,12	0.37	0	15,15,17	0.65	0
5	MAN	H	5	5	11,11,12	0.48	0	15,15,17	1.25	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.60	0	17,19,21	0.61	0
3	NAG	I	2	3	14,14,15	0.34	0	17,19,21	1.11	2 (11%)
4	FRU	J	1	4	11,12,12	0.76	1 (9%)	10,18,18	1.27	1 (10%)
4	GLC	J	2	4	11,11,12	0.78	1 (9%)	15,15,17	1.17	1 (6%)
4	GLA	J	3	4	11,11,12	0.94	0	15,15,17	1.39	2 (13%)
2	NAG	K	1	2,1	14,14,15	0.58	0	17,19,21	1.22	2 (11%)
2	NAG	K	2	2	14,14,15	0.51	0	17,19,21	0.65	0
2	BMA	K	3	2	11,11,12	0.54	0	15,15,17	1.04	2 (13%)
2	MAN	K	4	2	11,11,12	0.67	0	15,15,17	1.20	1 (6%)
4	FRU	L	1	4	11,12,12	0.76	0	10,18,18	1.43	1 (10%)
4	GLC	L	2	4	11,11,12	0.86	1 (9%)	15,15,17	0.85	0
4	GLA	L	3	4	11,11,12	0.81	0	15,15,17	1.67	2 (13%)
6	NAG	M	1	1,6	14,14,15	0.76	0	17,19,21	1.28	1 (5%)
6	NAG	M	2	6	14,14,15	0.37	0	17,19,21	0.69	0
6	BMA	M	3	6	11,11,12	0.50	0	15,15,17	0.75	0
4	FRU	N	1	4	11,12,12	1.17	1 (9%)	10,18,18	0.92	1 (10%)
4	GLC	N	2	4	11,11,12	0.97	0	15,15,17	1.29	2 (13%)
4	GLA	N	3	4	11,11,12	0.71	0	15,15,17	1.40	2 (13%)

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	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	FRU	G	1	4	-	1/5/24/24	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1
4	GLA	G	3	4	-	0/2/19/22	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	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
4	FRU	J	1	4	-	0/5/24/24	0/1/1/1
4	GLC	J	2	4	-	0/2/19/22	0/1/1/1
4	GLA	J	3	4	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	MAN	K	4	2	-	2/2/19/22	0/1/1/1
4	FRU	L	1	4	-	3/5/24/24	0/1/1/1
4	GLC	L	2	4	-	0/2/19/22	0/1/1/1
4	GLA	L	3	4	-	2/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
4	FRU	N	1	4	-	0/5/24/24	0/1/1/1
4	GLC	N	2	4	-	2/2/19/22	0/1/1/1
4	GLA	N	3	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	GLC	O5-C1	-3.34	1.38	1.43
4	N	1	FRU	O2-C2	3.15	1.46	1.40
4	L	2	GLC	O5-C1	-2.47	1.39	1.43
4	J	1	FRU	O2-C2	2.26	1.44	1.40
4	J	2	GLC	O5-C1	-2.12	1.40	1.43
4	G	1	FRU	O2-C2	2.10	1.44	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	4.05	117.67	112.19
4	L	3	GLA	C1-C2-C3	-3.93	104.84	109.67
2	K	1	NAG	O5-C1-C2	-3.50	105.76	111.29
4	G	3	GLA	C1-C2-C3	-3.33	105.58	109.67
4	L	3	GLA	C1-O5-C5	-3.23	107.81	112.19
4	L	1	FRU	O1-C1-C2	-3.11	105.24	111.86
4	J	1	FRU	O1-C1-C2	-3.01	105.46	111.86
2	E	1	NAG	C1-O5-C5	3.00	116.26	112.19
5	H	5	MAN	O5-C1-C2	2.99	115.39	110.77
5	H	2	NAG	C1-O5-C5	-2.95	108.19	112.19
4	N	3	GLA	C2-C3-C4	2.82	115.77	110.89
2	E	3	BMA	O5-C5-C6	2.80	111.60	107.20
4	G	2	GLC	C1-O5-C5	-2.71	108.53	112.19
4	J	2	GLC	O5-C1-C2	2.70	114.93	110.77
4	N	3	GLA	C3-C4-C5	2.67	115.00	110.24
2	K	4	MAN	C3-C4-C5	2.64	114.94	110.24
4	N	2	GLC	C1-C2-C3	-2.58	106.50	109.67
2	E	3	BMA	C1-C2-C3	2.49	112.73	109.67
4	N	2	GLC	O5-C1-C2	2.43	114.52	110.77
3	I	2	NAG	O5-C5-C6	2.41	110.98	107.20
3	I	2	NAG	C2-N2-C7	-2.30	119.63	122.90
2	E	4	MAN	C1-O5-C5	-2.29	109.10	112.19
4	J	3	GLA	C3-C4-C5	2.25	114.26	110.24
5	H	5	MAN	C1-C2-C3	2.23	112.40	109.67
2	K	3	BMA	C1-C2-C3	2.22	112.39	109.67
4	G	1	FRU	O1-C1-C2	-2.17	107.25	111.86
2	K	1	NAG	O5-C5-C4	-2.16	105.56	110.83
4	N	1	FRU	O4-C4-C5	2.14	117.25	111.05
4	J	3	GLA	C1-C2-C3	-2.10	107.09	109.67
2	K	3	BMA	C3-C4-C5	2.06	113.91	110.24
2	E	3	BMA	C6-C5-C4	-2.01	108.30	113.00

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	FRU	O1-C1-C2-C3
4	L	1	FRU	O1-C1-C2-O2
4	L	1	FRU	O1-C1-C2-O5
3	F	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C8-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
2	K	4	MAN	C4-C5-C6-O6

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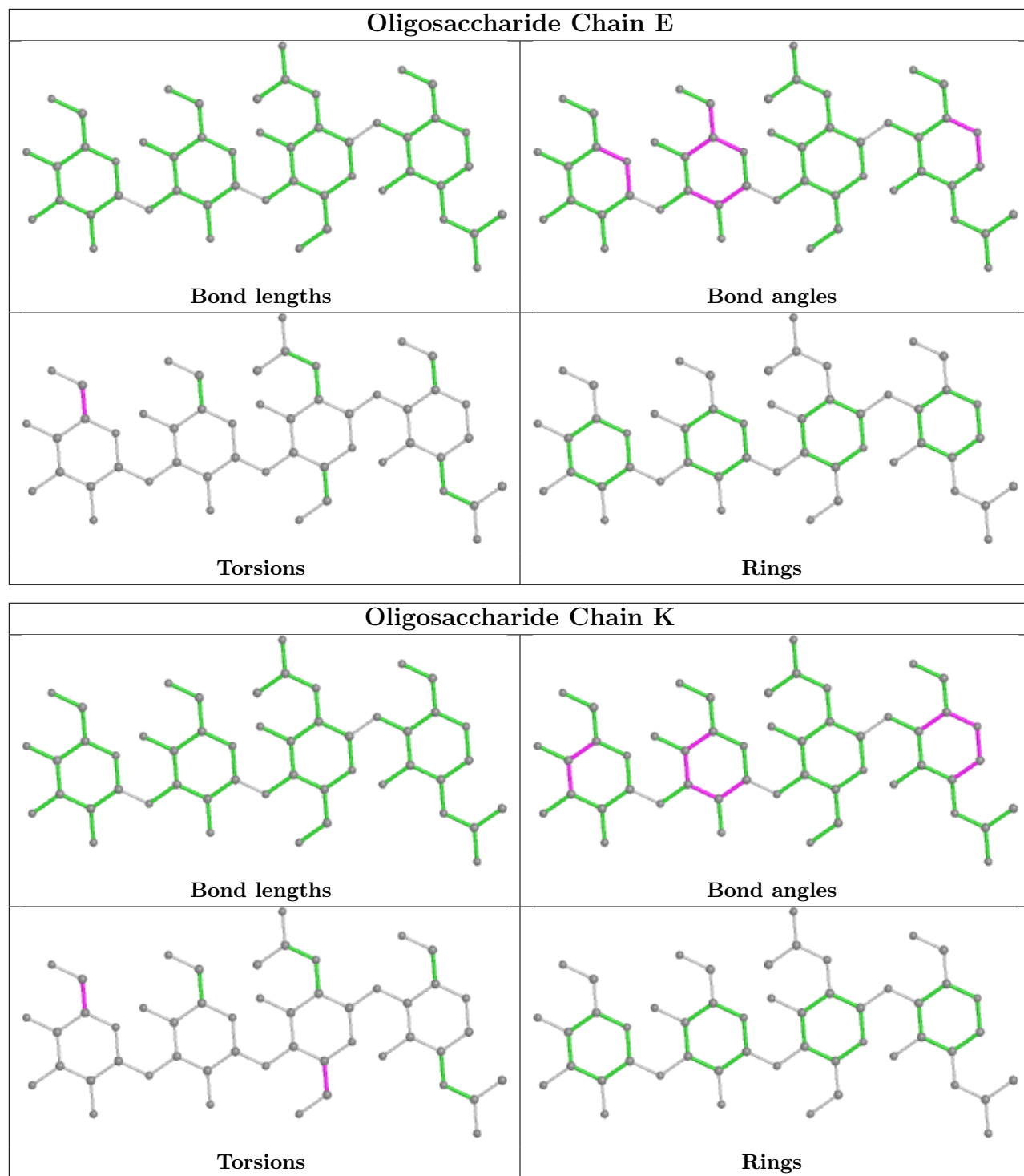
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
4	L	3	GLA	O5-C5-C6-O6
2	K	4	MAN	O5-C5-C6-O6
5	H	2	NAG	O7-C7-N2-C2
6	M	3	BMA	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	N	2	GLC	O5-C5-C6-O6
4	N	2	GLC	C4-C5-C6-O6
4	G	1	FRU	O1-C1-C2-C3
4	L	3	GLA	C4-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6

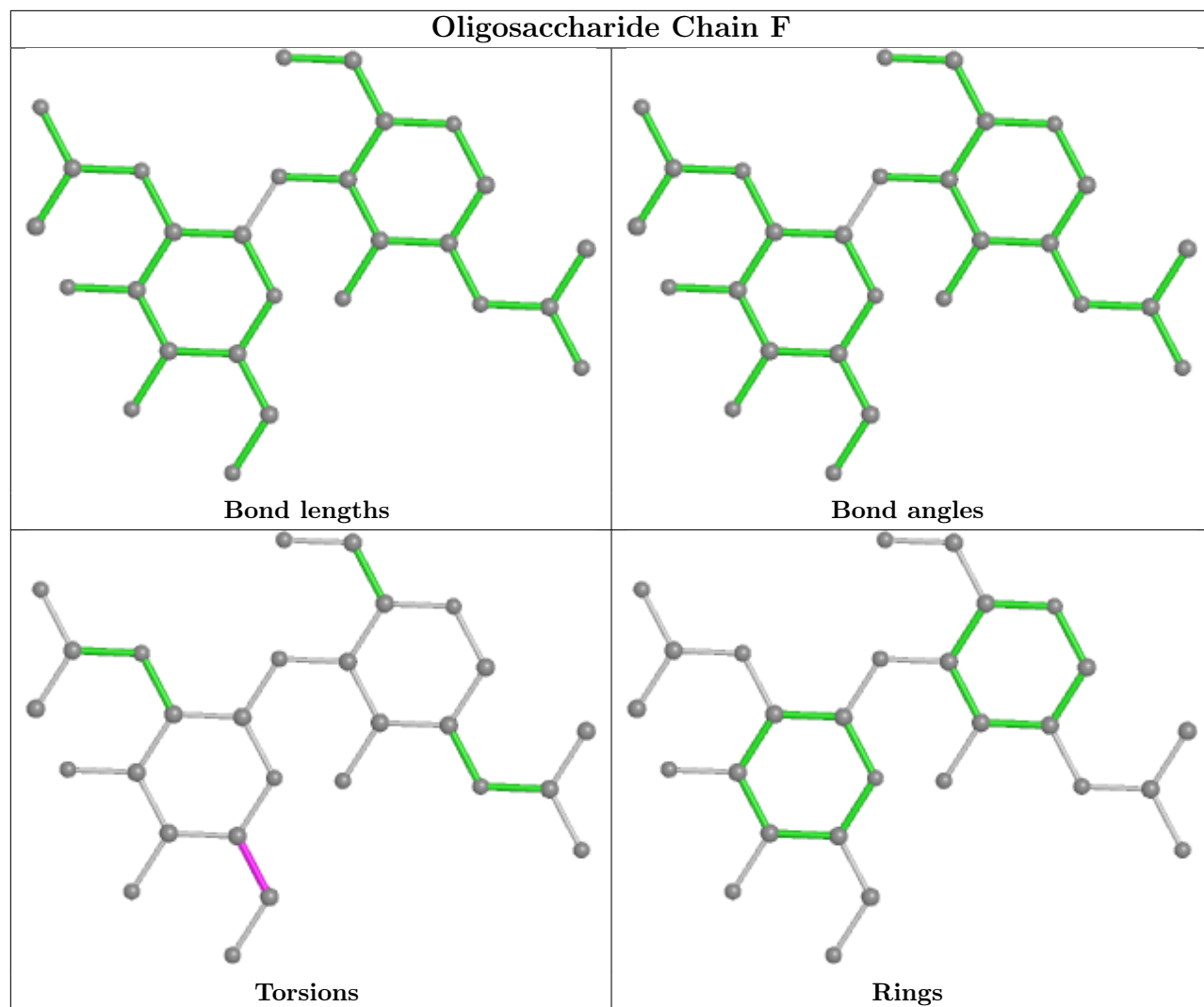
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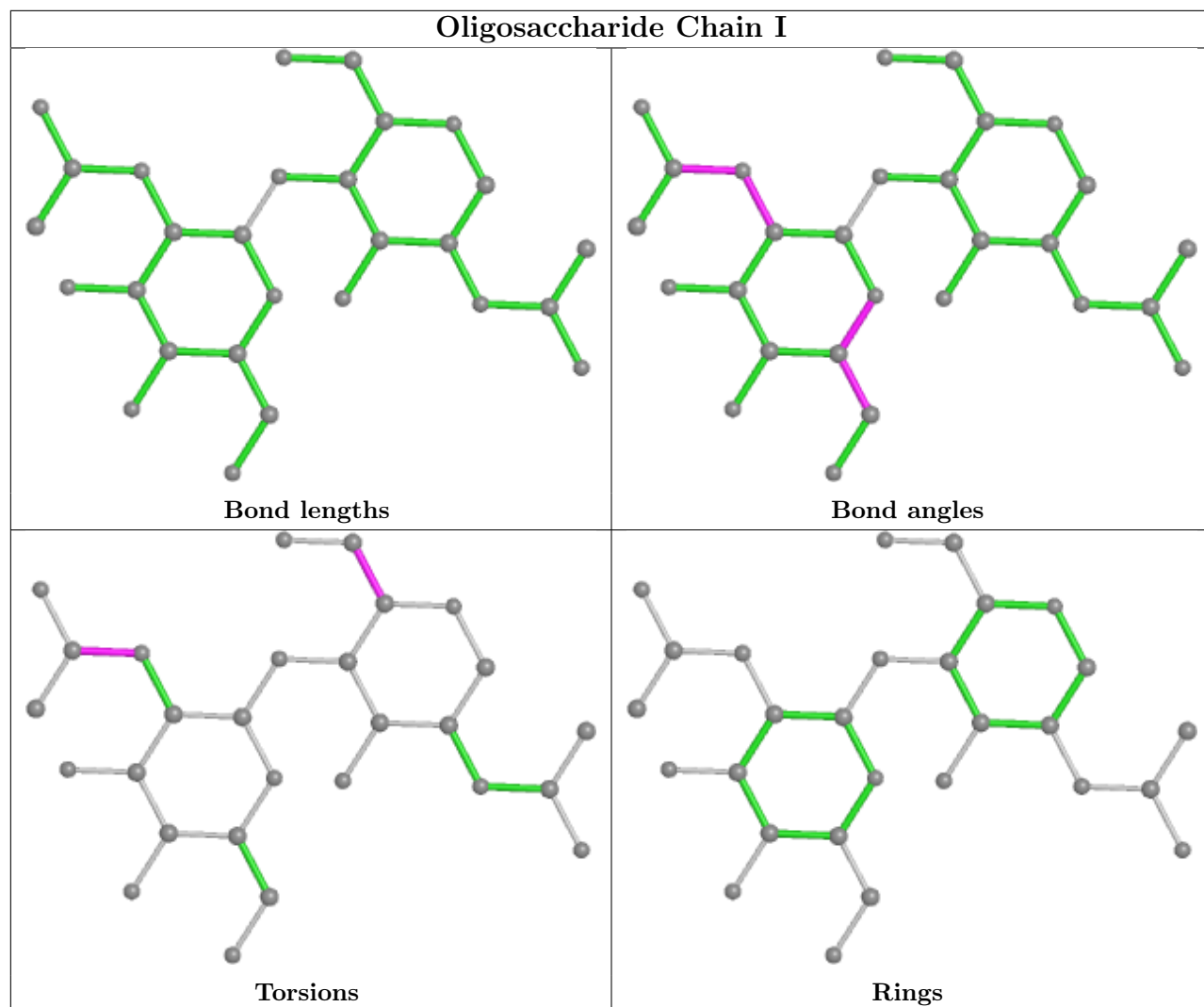
4 monomers are involved in 3 short contacts:

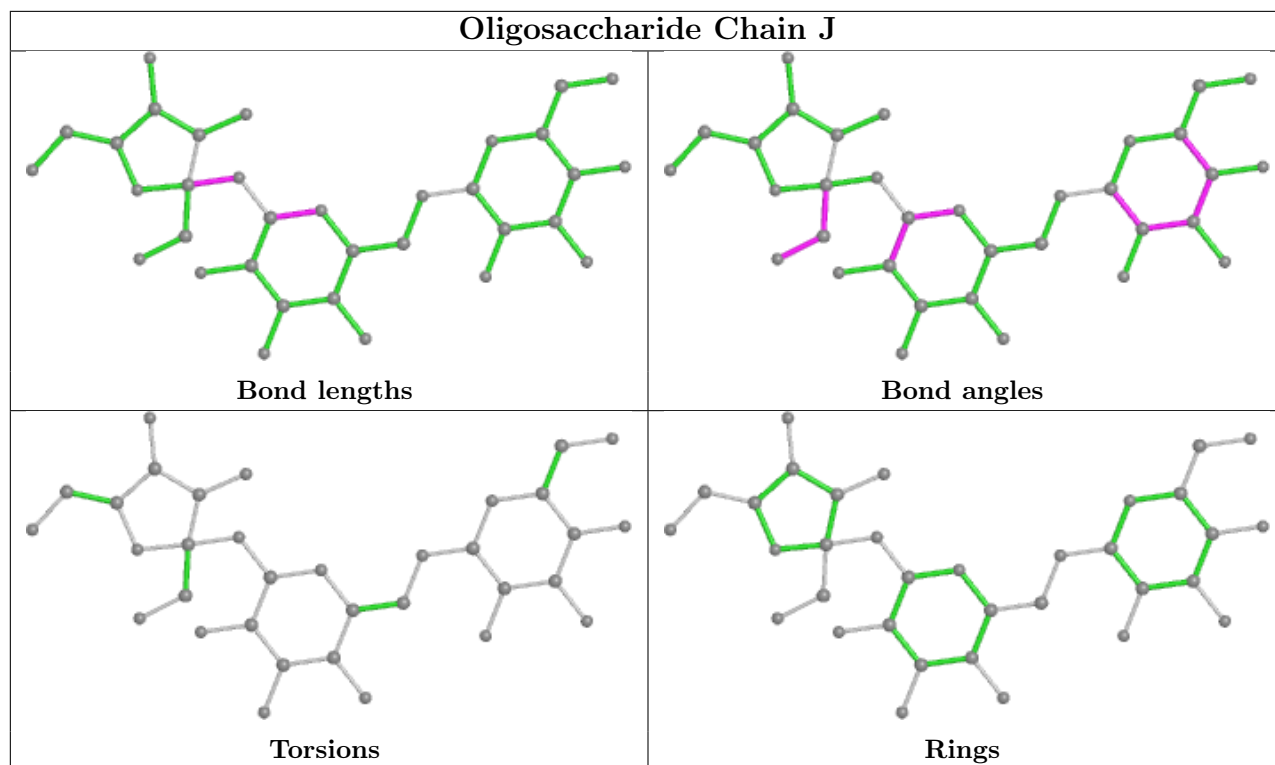
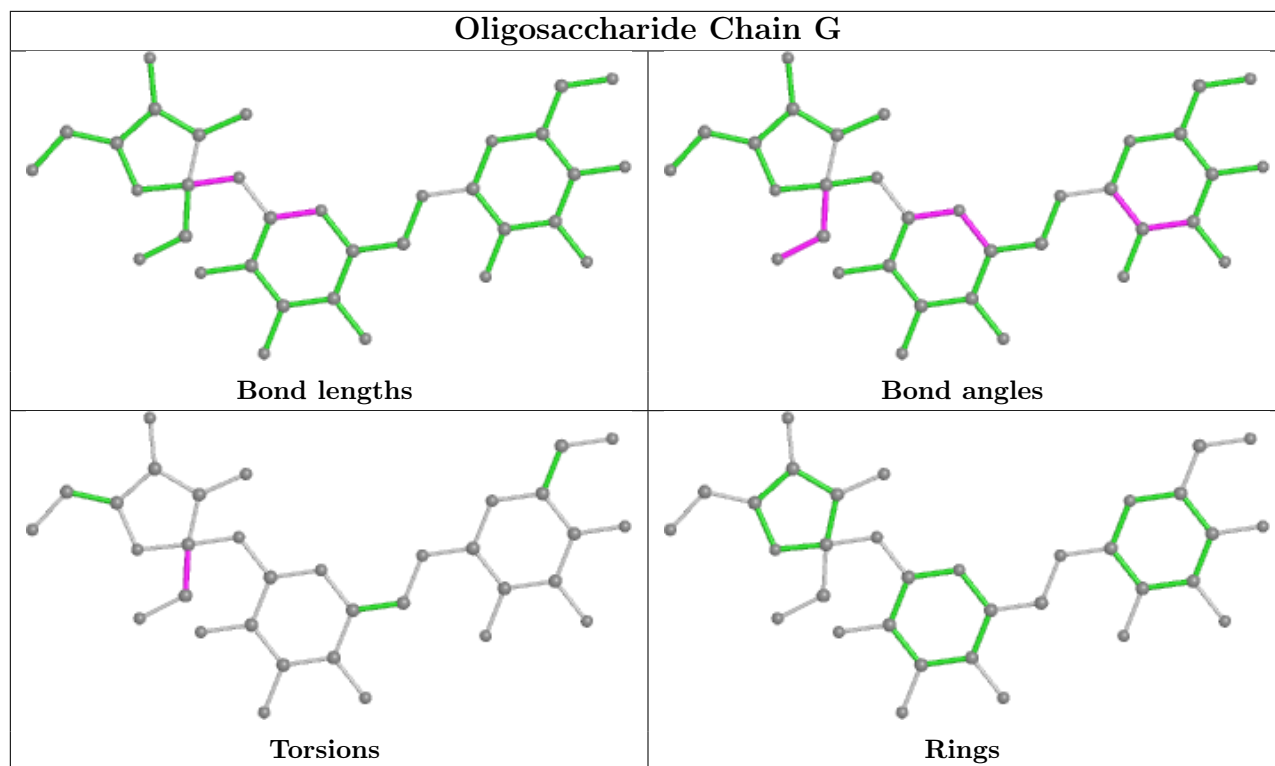
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	GLC	1	0
3	I	2	NAG	1	0
3	I	1	NAG	1	0
4	N	1	FRU	1	0

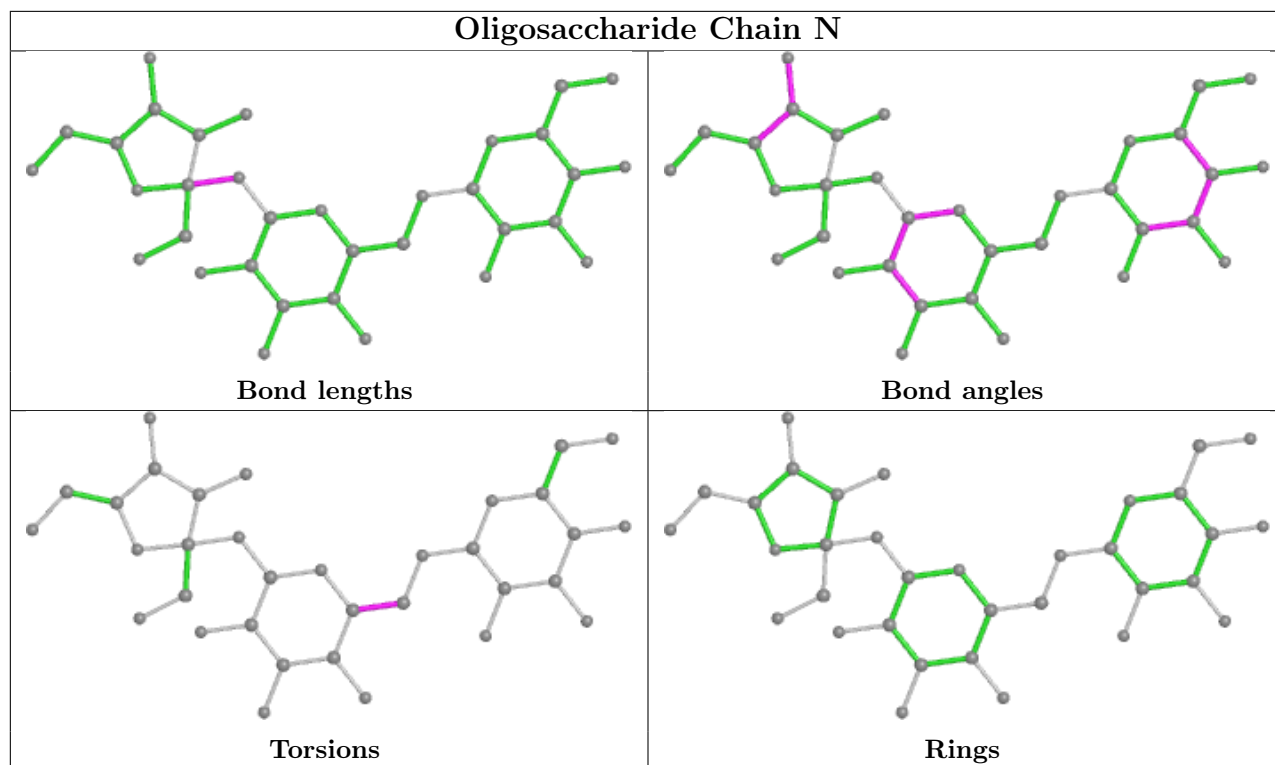
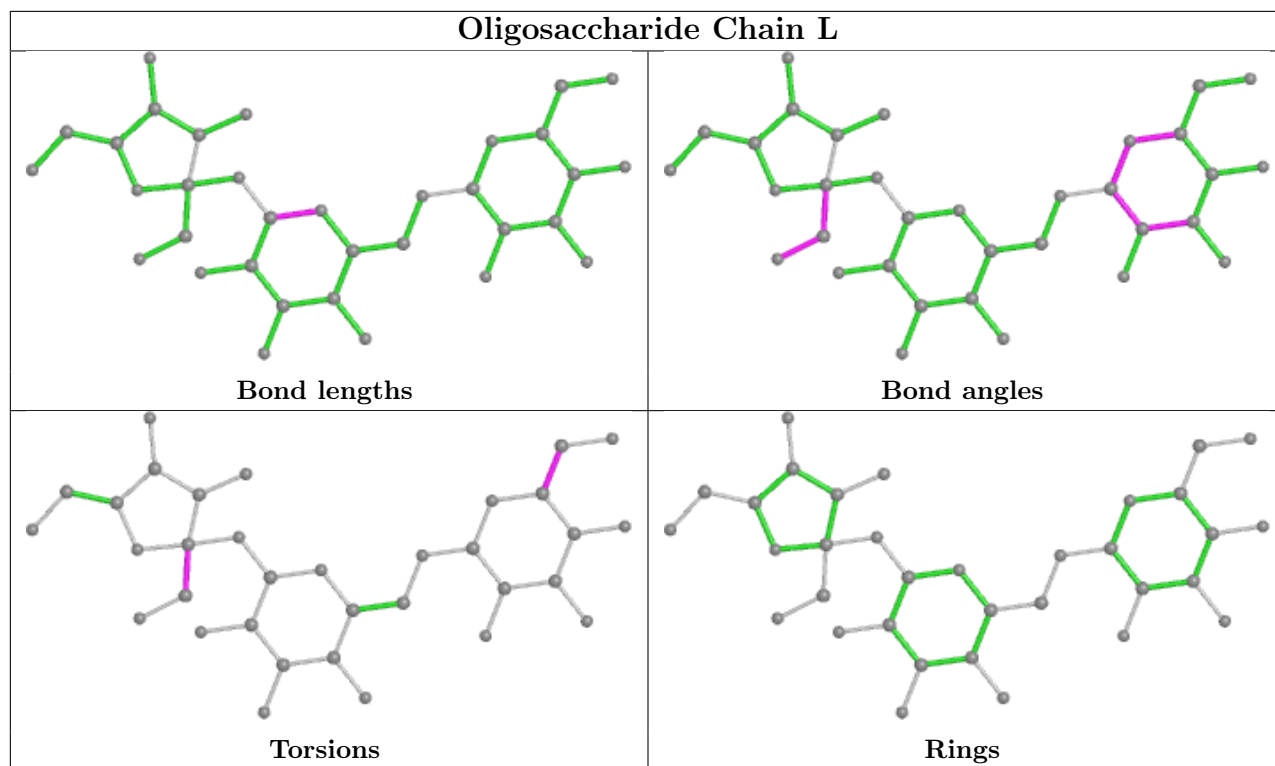
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

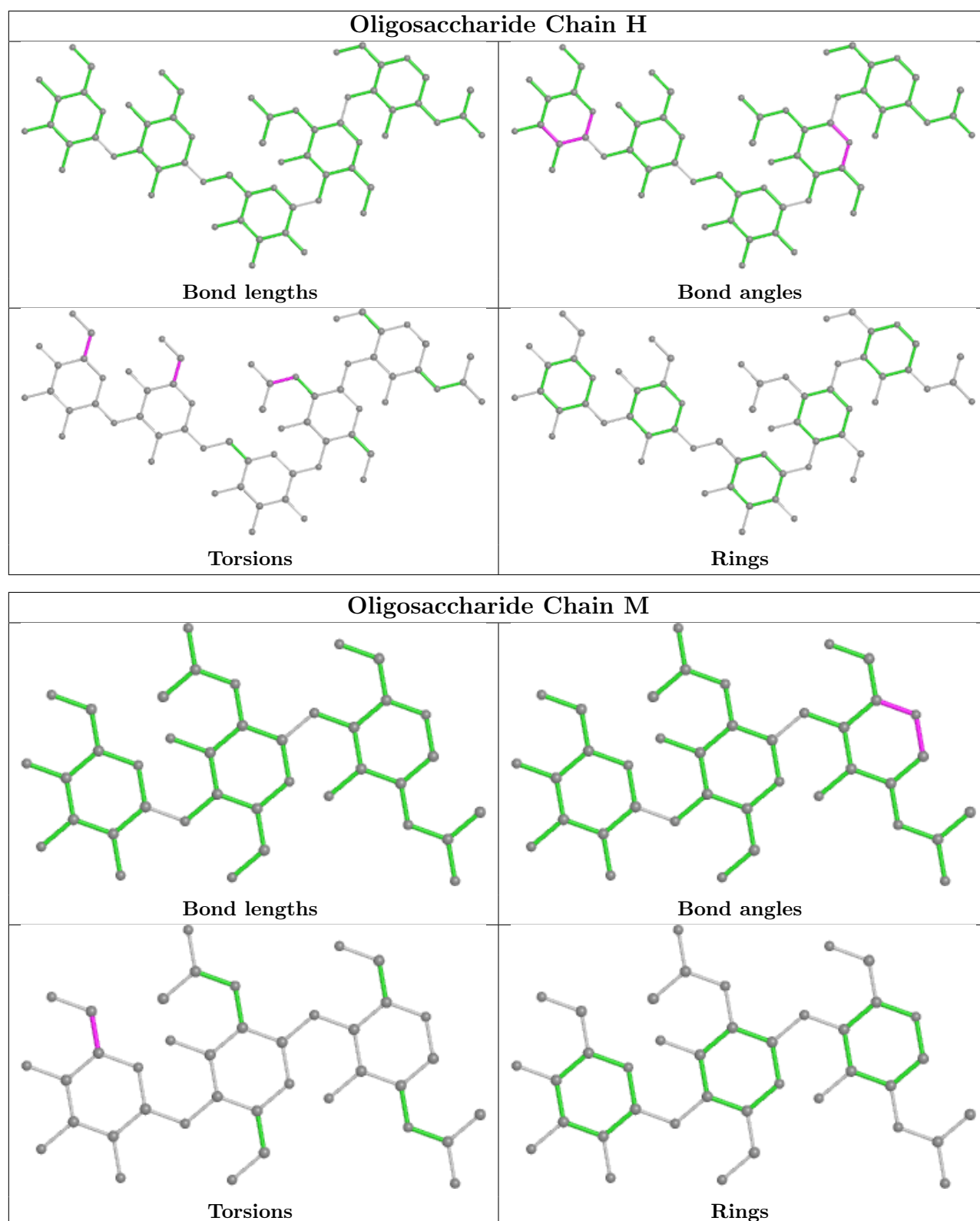












5.6 Ligand geometry [i](#)

41 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
8	NAG	D	708	1	14,14,15	0.38	0	17,19,21	1.01	1 (5%)
7	MAN	C	702	1	11,11,12	0.48	0	15,15,17	1.55	4 (26%)
8	NAG	A	711	1	14,14,15	0.39	0	17,19,21	0.79	0
7	MAN	A	701	1	11,11,12	0.44	0	15,15,17	1.89	4 (26%)
8	NAG	B	705	1	14,14,15	0.33	0	17,19,21	1.28	2 (11%)
8	NAG	A	707	1	14,14,15	0.57	0	17,19,21	0.99	2 (11%)
8	NAG	D	704	1	14,14,15	0.62	0	17,19,21	0.97	0
7	MAN	A	703	1	11,11,12	0.46	0	15,15,17	0.93	1 (6%)
8	NAG	C	704	1	14,14,15	0.43	0	17,19,21	0.75	0
8	NAG	D	705	1	14,14,15	0.38	0	17,19,21	1.21	3 (17%)
8	NAG	A	708	1	14,14,15	0.41	0	17,19,21	1.05	1 (5%)
8	NAG	D	706	1	14,14,15	0.46	0	17,19,21	1.02	1 (5%)
7	MAN	A	704	1	11,11,12	0.37	0	15,15,17	1.72	4 (26%)
8	NAG	C	710	1	14,14,15	0.57	0	17,19,21	1.11	1 (5%)
7	MAN	C	701	1	11,11,12	0.37	0	15,15,17	1.43	2 (13%)
8	NAG	B	709	1	14,14,15	0.28	0	17,19,21	0.90	1 (5%)
8	NAG	C	708	1	14,14,15	0.78	0	17,19,21	1.50	3 (17%)
8	NAG	A	712	1	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
8	NAG	A	709	1	14,14,15	0.44	0	17,19,21	0.91	0
7	MAN	D	703	1	11,11,12	1.51	2 (18%)	15,15,17	1.16	1 (6%)
8	NAG	A	714	1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
7	MAN	D	702	1	11,11,12	0.66	0	15,15,17	1.61	4 (26%)
7	MAN	C	703	1	11,11,12	0.59	0	15,15,17	1.46	3 (20%)
8	NAG	B	704	1	14,14,15	0.36	0	17,19,21	0.83	0
8	NAG	D	707	1	14,14,15	0.36	0	17,19,21	0.89	0
8	NAG	C	709	1	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
8	NAG	A	706	1	14,14,15	0.37	0	17,19,21	0.91	0
8	NAG	B	706	1	14,14,15	0.28	0	17,19,21	1.24	3 (17%)
8	NAG	B	707	1	14,14,15	0.30	0	17,19,21	0.87	0
7	MAN	B	701	1	11,11,12	0.33	0	15,15,17	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	713	1	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
8	NAG	A	710	1	14,14,15	0.44	0	17,19,21	1.02	1 (5%)
7	MAN	D	701	1	11,11,12	0.28	0	15,15,17	1.35	2 (13%)
7	MAN	B	703	1	11,11,12	0.35	0	15,15,17	1.46	1 (6%)
8	NAG	C	706	1	14,14,15	0.30	0	17,19,21	0.78	0
8	NAG	B	708	1	14,14,15	0.50	0	17,19,21	1.18	1 (5%)
8	NAG	C	705	1	14,14,15	0.61	0	17,19,21	1.37	2 (11%)
7	MAN	A	702	1	11,11,12	0.38	0	15,15,17	0.73	0
8	NAG	C	707	1	14,14,15	0.62	0	17,19,21	0.77	0
7	MAN	A	705	1	11,11,12	0.62	0	15,15,17	2.24	3 (20%)
9	PEG	B	702	-	6,6,6	0.25	0	5,5,5	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	708	1	-	1/6/23/26	0/1/1/1
7	MAN	C	702	1	-	2/2/19/22	0/1/1/1
8	NAG	A	711	1	-	0/6/23/26	0/1/1/1
7	MAN	A	701	1	-	2/2/19/22	0/1/1/1
8	NAG	B	705	1	-	2/6/23/26	0/1/1/1
8	NAG	A	707	1	-	1/6/23/26	0/1/1/1
8	NAG	D	704	1	-	4/6/23/26	0/1/1/1
7	MAN	A	703	1	-	0/2/19/22	0/1/1/1
8	NAG	C	704	1	-	2/6/23/26	0/1/1/1
8	NAG	D	705	1	-	2/6/23/26	0/1/1/1
8	NAG	A	708	1	-	2/6/23/26	0/1/1/1
8	NAG	D	706	1	-	2/6/23/26	0/1/1/1
7	MAN	A	704	1	-	1/2/19/22	0/1/1/1
8	NAG	C	710	1	-	3/6/23/26	0/1/1/1
7	MAN	C	701	1	-	2/2/19/22	0/1/1/1
8	NAG	B	709	1	-	0/6/23/26	0/1/1/1
8	NAG	C	708	1	-	5/6/23/26	0/1/1/1
8	NAG	A	712	1	-	2/6/23/26	0/1/1/1
8	NAG	A	709	1	-	2/6/23/26	0/1/1/1
7	MAN	D	703	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	714	1	-	2/6/23/26	0/1/1/1
7	MAN	D	702	1	-	0/2/19/22	0/1/1/1
7	MAN	C	703	1	-	0/2/19/22	0/1/1/1
8	NAG	B	704	1	-	0/6/23/26	0/1/1/1
8	NAG	D	707	1	-	2/6/23/26	0/1/1/1
8	NAG	C	709	1	-	2/6/23/26	0/1/1/1
8	NAG	A	706	1	-	1/6/23/26	0/1/1/1
8	NAG	B	706	1	-	0/6/23/26	0/1/1/1
8	NAG	B	707	1	-	1/6/23/26	0/1/1/1
7	MAN	B	701	1	-	0/2/19/22	0/1/1/1
8	NAG	A	713	1	-	4/6/23/26	0/1/1/1
8	NAG	A	710	1	-	1/6/23/26	0/1/1/1
7	MAN	D	701	1	-	0/2/19/22	0/1/1/1
7	MAN	B	703	1	-	1/2/19/22	0/1/1/1
8	NAG	C	706	1	-	0/6/23/26	0/1/1/1
8	NAG	B	708	1	-	1/6/23/26	0/1/1/1
8	NAG	C	705	1	-	4/6/23/26	0/1/1/1
7	MAN	A	702	1	-	2/2/19/22	0/1/1/1
8	NAG	C	707	1	-	0/6/23/26	0/1/1/1
7	MAN	A	705	1	-	2/2/19/22	0/1/1/1
9	PEG	B	702	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	703	MAN	C2-C3	-3.07	1.48	1.52
7	D	703	MAN	C4-C5	-2.03	1.48	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	MAN	O5-C1-C2	-7.11	99.79	110.77
7	B	703	MAN	O5-C1-C2	-5.03	103.01	110.77
7	A	701	MAN	C1-O5-C5	-4.71	105.81	112.19
8	C	705	NAG	C2-N2-C7	-4.49	116.51	122.90
7	C	701	MAN	O5-C1-C2	-3.95	104.68	110.77
8	C	708	NAG	C1-O5-C5	-3.73	107.14	112.19
7	D	702	MAN	C1-O5-C5	3.69	117.19	112.19
7	A	704	MAN	O5-C1-C2	-3.66	105.12	110.77
7	C	702	MAN	O5-C1-C2	-3.61	105.19	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	709	NAG	C2-N2-C7	-3.61	117.77	122.90
8	B	708	NAG	C1-O5-C5	-3.50	107.45	112.19
7	A	704	MAN	C1-C2-C3	-3.47	105.40	109.67
7	C	703	MAN	O5-C1-C2	-3.41	105.50	110.77
8	B	705	NAG	O5-C1-C2	-3.38	105.95	111.29
8	C	708	NAG	O5-C5-C6	3.14	112.12	107.20
7	A	701	MAN	O5-C1-C2	-3.06	106.05	110.77
7	D	701	MAN	C1-C2-C3	3.02	113.37	109.67
7	A	705	MAN	C3-C4-C5	3.00	115.59	110.24
7	A	705	MAN	C1-O5-C5	-2.98	108.15	112.19
7	A	701	MAN	C3-C4-C5	2.87	115.35	110.24
7	B	701	MAN	O5-C1-C2	-2.85	106.37	110.77
8	A	714	NAG	O5-C1-C2	-2.84	106.81	111.29
8	A	713	NAG	C1-O5-C5	-2.81	108.38	112.19
8	D	705	NAG	C2-N2-C7	2.73	126.80	122.90
8	D	706	NAG	C1-O5-C5	-2.72	108.50	112.19
7	D	702	MAN	O5-C5-C6	2.67	111.39	107.20
8	C	710	NAG	C1-C2-N2	-2.64	105.98	110.49
8	A	708	NAG	C4-C3-C2	-2.63	107.17	111.02
8	B	706	NAG	C2-N2-C7	-2.63	119.16	122.90
7	C	702	MAN	C1-C2-C3	-2.60	106.47	109.67
8	B	706	NAG	C4-C3-C2	-2.60	107.21	111.02
7	A	703	MAN	O5-C1-C2	-2.52	106.88	110.77
7	D	701	MAN	C1-O5-C5	2.46	115.52	112.19
7	C	703	MAN	O2-C2-C1	2.45	114.17	109.15
7	D	702	MAN	O5-C1-C2	2.44	114.53	110.77
8	B	706	NAG	O5-C1-C2	-2.43	107.45	111.29
7	A	701	MAN	O4-C4-C5	-2.43	103.28	109.30
7	C	702	MAN	C1-O5-C5	-2.42	108.92	112.19
7	C	701	MAN	C1-O5-C5	-2.39	108.96	112.19
8	A	710	NAG	O5-C5-C6	2.38	110.93	107.20
8	A	712	NAG	C2-N2-C7	-2.30	119.62	122.90
8	C	705	NAG	C1-C2-N2	-2.29	106.58	110.49
8	B	705	NAG	C3-C4-C5	2.26	114.27	110.24
7	A	704	MAN	C1-O5-C5	-2.23	109.17	112.19
7	D	703	MAN	C2-C3-C4	-2.23	107.04	110.89
8	D	708	NAG	C2-N2-C7	-2.21	119.75	122.90
8	A	707	NAG	C8-C7-N2	-2.20	112.38	116.10
7	A	704	MAN	C3-C4-C5	2.19	114.14	110.24
8	B	709	NAG	C2-N2-C7	-2.15	119.84	122.90
8	C	708	NAG	C2-N2-C7	-2.15	119.84	122.90
8	A	707	NAG	O7-C7-N2	2.14	125.89	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	702	MAN	C1-C2-C3	2.13	112.29	109.67
7	C	703	MAN	C3-C4-C5	2.12	114.02	110.24
8	D	705	NAG	C8-C7-N2	2.09	119.63	116.10
8	D	705	NAG	O7-C7-N2	-2.07	118.15	121.95
7	C	702	MAN	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	712	NAG	C8-C7-N2-C2
8	C	705	NAG	C8-C7-N2-C2
8	C	708	NAG	C3-C2-N2-C7
8	C	708	NAG	C8-C7-N2-C2
8	C	708	NAG	O7-C7-N2-C2
8	D	704	NAG	C8-C7-N2-C2
8	D	704	NAG	O7-C7-N2-C2
8	D	707	NAG	C8-C7-N2-C2
8	D	707	NAG	O7-C7-N2-C2
8	A	712	NAG	O7-C7-N2-C2
8	B	705	NAG	O5-C5-C6-O6
7	A	701	MAN	O5-C5-C6-O6
8	A	713	NAG	C8-C7-N2-C2
8	C	705	NAG	O7-C7-N2-C2
8	C	709	NAG	C8-C7-N2-C2
7	A	702	MAN	O5-C5-C6-O6
8	B	705	NAG	C4-C5-C6-O6
7	C	702	MAN	O5-C5-C6-O6
7	A	701	MAN	C4-C5-C6-O6
7	C	702	MAN	C4-C5-C6-O6
8	C	708	NAG	O5-C5-C6-O6
7	D	703	MAN	C4-C5-C6-O6
7	A	705	MAN	O5-C5-C6-O6
8	A	709	NAG	O5-C5-C6-O6
7	C	701	MAN	C4-C5-C6-O6
7	A	705	MAN	C4-C5-C6-O6
8	C	708	NAG	C4-C5-C6-O6
8	D	705	NAG	C8-C7-N2-C2
8	D	705	NAG	O7-C7-N2-C2
8	A	709	NAG	C4-C5-C6-O6
7	A	702	MAN	C4-C5-C6-O6
7	C	701	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	714	NAG	O5-C5-C6-O6
8	D	706	NAG	O5-C5-C6-O6
8	C	709	NAG	O7-C7-N2-C2
9	B	702	PEG	O2-C3-C4-O4
8	A	714	NAG	C4-C5-C6-O6
8	D	706	NAG	C4-C5-C6-O6
8	D	704	NAG	O5-C5-C6-O6
8	C	710	NAG	C1-C2-N2-C7
8	A	708	NAG	C4-C5-C6-O6
7	D	703	MAN	O5-C5-C6-O6
8	A	713	NAG	O7-C7-N2-C2
8	B	708	NAG	O5-C5-C6-O6
8	A	713	NAG	C3-C2-N2-C7
8	D	708	NAG	C8-C7-N2-C2
8	A	707	NAG	O5-C5-C6-O6
8	A	708	NAG	O5-C5-C6-O6
7	A	704	MAN	C4-C5-C6-O6
9	B	702	PEG	C4-C3-O2-C2
8	C	705	NAG	O5-C5-C6-O6
8	C	710	NAG	C8-C7-N2-C2
8	C	704	NAG	O5-C5-C6-O6
8	C	705	NAG	C4-C5-C6-O6
8	A	710	NAG	O5-C5-C6-O6
8	C	704	NAG	C4-C5-C6-O6
8	A	713	NAG	C4-C5-C6-O6
8	A	706	NAG	O5-C5-C6-O6
7	B	703	MAN	C4-C5-C6-O6
8	C	710	NAG	C3-C2-N2-C7
8	D	704	NAG	C4-C5-C6-O6
8	B	707	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	703	MAN	1	0
8	D	706	NAG	1	0
8	C	708	NAG	3	0
7	D	703	MAN	5	0
7	D	702	MAN	6	0
8	A	706	NAG	1	0
8	B	707	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	713	NAG	3	0
8	C	707	NAG	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	527/675 (78%)	0.06	5 (0%) 84 87	23, 37, 62, 93	0
1	B	526/675 (77%)	0.45	37 (7%) 16 20	26, 44, 78, 109	0
1	C	526/675 (77%)	0.35	22 (4%) 36 41	26, 48, 82, 113	0
1	D	521/675 (77%)	1.20	111 (21%) 0 1	35, 62, 94, 118	0
All	All	2100/2700 (77%)	0.51	175 (8%) 11 14	23, 47, 84, 118	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	346	THR	6.3
1	D	673	GLN	5.0
1	D	210	GLU	4.9
1	D	392	LEU	4.8
1	D	344	SER	4.6
1	D	288	THR	4.5
1	D	242	THR	4.5
1	C	534	GLN	4.4
1	D	143	CYS	4.4
1	D	418	ILE	4.3
1	B	555	CYS	4.3
1	A	555	CYS	4.3
1	D	419	ALA	4.2
1	D	184	GLY	4.2
1	D	426	TYR	4.0
1	B	156	PRO	4.0
1	D	149	PRO	4.0
1	D	290	GLY	4.0
1	C	437	GLY	4.0
1	D	261	PHE	4.0
1	D	271	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	259	GLY	3.9
1	B	554	LYS	3.9
1	D	319	GLU	3.9
1	A	143	CYS	3.8
1	D	236	ILE	3.8
1	B	419	ALA	3.8
1	B	407	THR	3.8
1	B	159	VAL	3.7
1	C	143	CYS	3.7
1	D	265	THR	3.7
1	D	436	ASN	3.6
1	D	148	LEU	3.5
1	D	310	PHE	3.5
1	D	512	PHE	3.5
1	B	435	GLU	3.4
1	C	436	ASN	3.4
1	B	418	ILE	3.4
1	B	436	ASN	3.4
1	C	563	SER	3.4
1	D	279	LEU	3.4
1	D	305	VAL	3.3
1	B	152	ALA	3.3
1	D	307	SER	3.3
1	D	329	ALA	3.3
1	D	423	LYS	3.3
1	D	363	CYS	3.3
1	B	390	ALA	3.2
1	B	437	GLY	3.2
1	D	168	ASP	3.2
1	B	557	SER	3.2
1	D	294	PHE	3.2
1	D	233	PRO	3.2
1	D	245	VAL	3.1
1	D	509	ASP	3.1
1	B	150	ALA	3.1
1	B	392	LEU	3.1
1	D	356	LEU	3.1
1	B	564	ASP	3.0
1	D	263	ASN	3.0
1	D	286	TYR	3.0
1	D	296	PRO	3.0
1	C	509	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	425	ASN	2.9
1	C	373	ASP	2.9
1	D	284	VAL	2.9
1	D	393	GLY	2.9
1	D	532	ALA	2.9
1	D	499	LEU	2.9
1	D	328	ALA	2.9
1	D	384	ILE	2.9
1	D	386	ILE	2.9
1	D	302	VAL	2.9
1	D	320	ASP	2.9
1	C	141	SER	2.8
1	C	554	LYS	2.8
1	D	159	VAL	2.8
1	B	157	THR	2.8
1	D	239	PRO	2.8
1	D	151	SER	2.8
1	D	385	SER	2.8
1	D	211	TYR	2.8
1	D	243	SER	2.8
1	D	428	SER	2.8
1	D	498	LEU	2.8
1	B	196	ARG	2.7
1	D	337	TYR	2.7
1	D	235	ALA	2.7
1	D	323	VAL	2.7
1	D	282	GLN	2.7
1	D	427	ALA	2.7
1	D	530	ASP	2.7
1	B	259	GLY	2.7
1	B	426	TYR	2.6
1	D	396	VAL	2.6
1	B	394	GLY	2.6
1	D	552	SER	2.6
1	D	336	ILE	2.6
1	D	500	SER	2.6
1	C	605	SER	2.6
1	D	359	LEU	2.6
1	D	269	VAL	2.6
1	D	152	ALA	2.6
1	D	316	PHE	2.5
1	B	393	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	188	ALA	2.5
1	D	422	ALA	2.5
1	D	338	THR	2.5
1	D	252	LEU	2.5
1	D	510	VAL	2.5
1	C	342	LEU	2.5
1	C	374	ASP	2.5
1	D	272	TYR	2.5
1	B	298	GLU	2.5
1	D	299	ASN	2.5
1	C	317	TRP	2.4
1	D	276	THR	2.4
1	D	444	TRP	2.4
1	C	390	ALA	2.4
1	D	391	PRO	2.4
1	A	188	ALA	2.4
1	D	283	GLU	2.4
1	B	389	GLY	2.3
1	B	149	PRO	2.3
1	C	527	THR	2.3
1	D	237	PHE	2.3
1	B	322	TRP	2.3
1	D	513	THR	2.3
1	D	257	THR	2.3
1	B	154	GLU	2.3
1	C	396	VAL	2.3
1	D	291	GLY	2.3
1	D	554	LYS	2.3
1	D	303	LEU	2.2
1	D	331	ASP	2.2
1	D	357	LEU	2.2
1	D	447	ASN	2.2
1	D	536	ALA	2.2
1	D	155	LEU	2.2
1	B	391	PRO	2.2
1	D	147	SER	2.2
1	D	395	SER	2.2
1	D	179	TYR	2.2
1	B	420	ASP	2.2
1	B	363	CYS	2.2
1	D	154	GLU	2.2
1	A	189	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	217	HIS	2.1
1	B	356	LEU	2.1
1	D	420	ASP	2.1
1	A	534	GLN	2.1
1	B	423	LYS	2.1
1	D	301	PRO	2.1
1	B	530	ASP	2.1
1	D	340	PRO	2.1
1	D	264	THR	2.1
1	D	636	THR	2.1
1	B	556	SER	2.1
1	D	348	ALA	2.1
1	C	378	SER	2.1
1	C	502	SER	2.1
1	C	392	LEU	2.1
1	C	503	GLU	2.1
1	B	241	SER	2.1
1	B	532	ALA	2.1
1	D	390	ALA	2.1
1	D	515	VAL	2.1
1	C	391	PRO	2.1
1	D	254	PRO	2.1
1	D	278	THR	2.0
1	B	427	ALA	2.0
1	C	498	LEU	2.0
1	D	216	GLN	2.0
1	D	166	THR	2.0
1	D	516	THR	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](#)

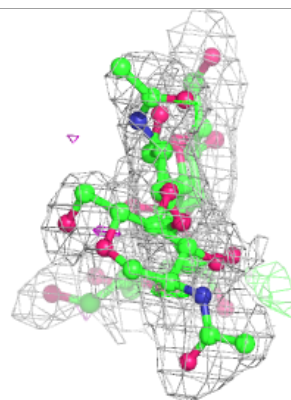
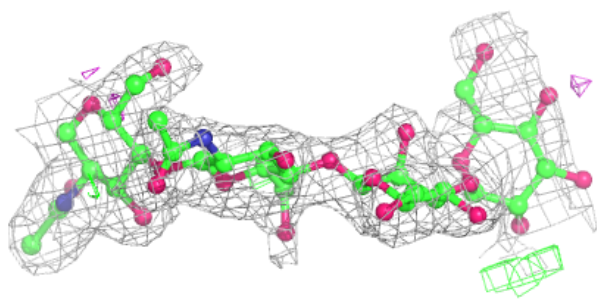
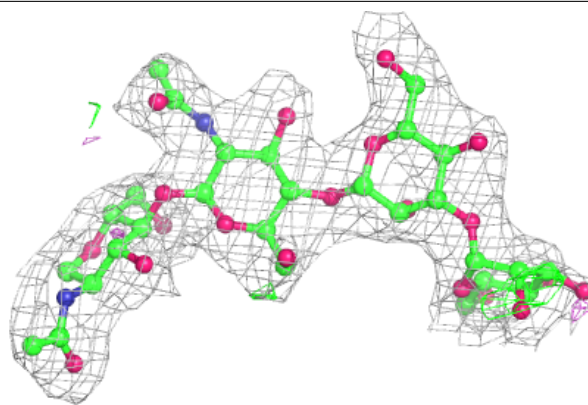
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	H	4	11/12	0.62	0.21	98,111,113,113	0
5	MAN	H	5	11/12	0.69	0.35	77,89,99,100	0
2	MAN	E	4	11/12	0.70	0.27	88,100,106,107	0
4	GLA	N	3	11/12	0.73	0.22	81,86,91,92	0
3	NAG	F	2	14/15	0.75	0.37	92,107,121,121	0
4	GLC	N	2	11/12	0.76	0.20	64,80,84,85	0
4	GLA	L	3	11/12	0.77	0.21	70,76,86,88	0
2	BMA	K	3	11/12	0.79	0.32	80,87,90,97	0
3	NAG	I	2	14/15	0.80	0.44	94,119,124,124	0
2	MAN	K	4	11/12	0.81	0.35	95,102,105,108	0
6	BMA	M	3	11/12	0.82	0.35	97,104,113,117	0
4	GLA	J	3	11/12	0.83	0.26	69,75,81,86	0
5	BMA	H	3	11/12	0.86	0.19	81,84,89,101	0
4	GLA	G	3	11/12	0.87	0.15	55,61,65,66	0
6	NAG	M	1	14/15	0.87	0.20	52,66,80,84	0
4	FRU	N	1	12/12	0.87	0.18	52,65,72,73	0
2	NAG	K	2	14/15	0.88	0.29	72,77,81,81	0
6	NAG	M	2	14/15	0.91	0.26	78,88,94,95	0
2	BMA	E	3	11/12	0.91	0.12	68,71,72,74	0
2	NAG	E	2	14/15	0.92	0.19	51,58,66,72	0
2	NAG	E	1	14/15	0.93	0.15	38,47,51,51	0
5	NAG	H	1	14/15	0.93	0.16	46,53,57,67	0
2	NAG	K	1	14/15	0.93	0.13	50,55,64,65	0
3	NAG	I	1	14/15	0.93	0.14	48,57,64,77	0
4	GLC	J	2	11/12	0.94	0.14	50,52,58,58	0
5	NAG	H	2	14/15	0.94	0.17	68,76,80,81	0
3	NAG	F	1	14/15	0.94	0.14	42,50,61,75	0
4	FRU	J	1	12/12	0.94	0.18	37,43,47,54	0
4	GLC	L	2	11/12	0.96	0.14	38,40,46,49	0
4	GLC	G	2	11/12	0.97	0.14	33,38,41,50	0
4	FRU	L	1	12/12	0.97	0.15	36,38,42,50	0
4	FRU	G	1	12/12	0.97	0.17	27,29,38,44	0

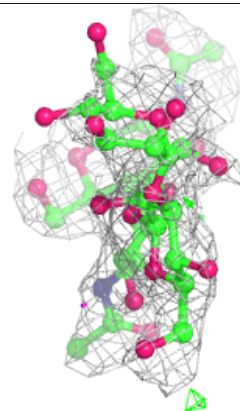
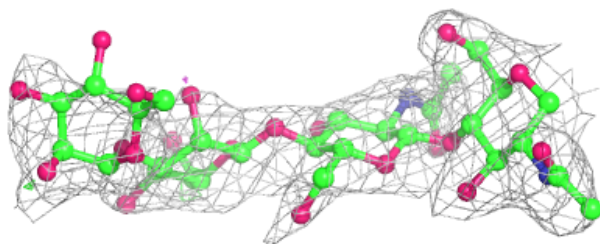
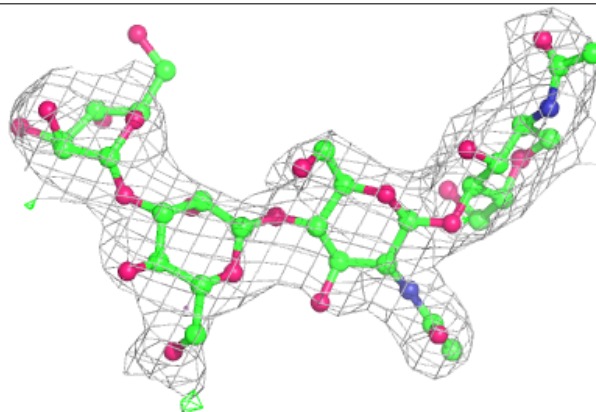
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

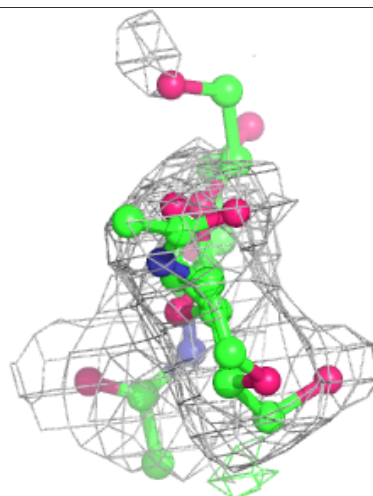
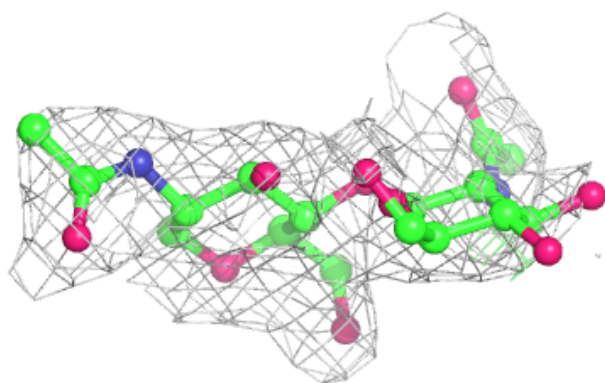
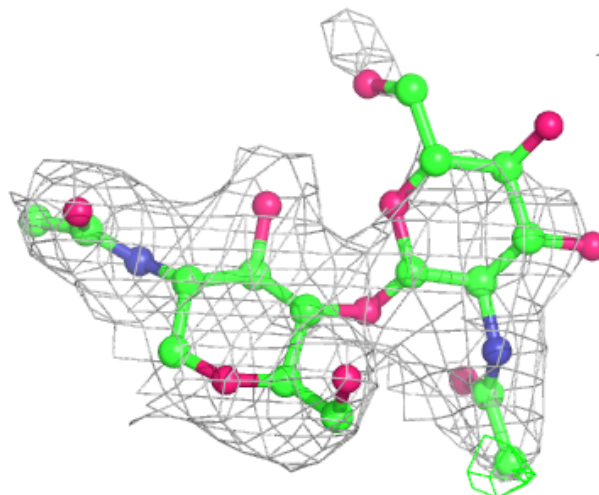
**Electron density around Chain K:**

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



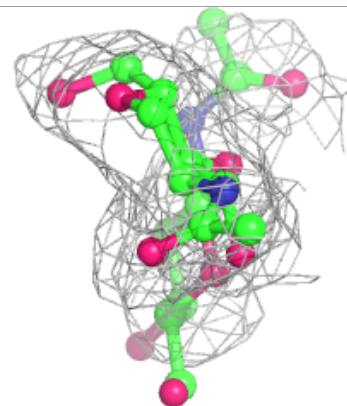
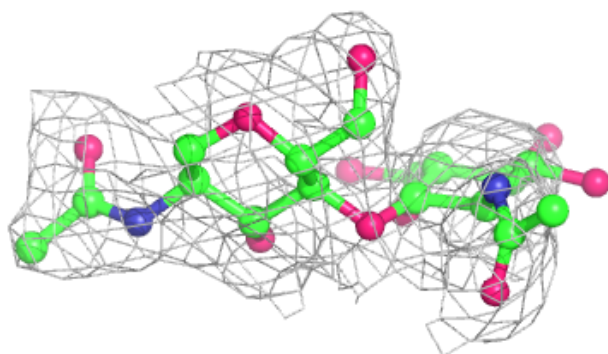
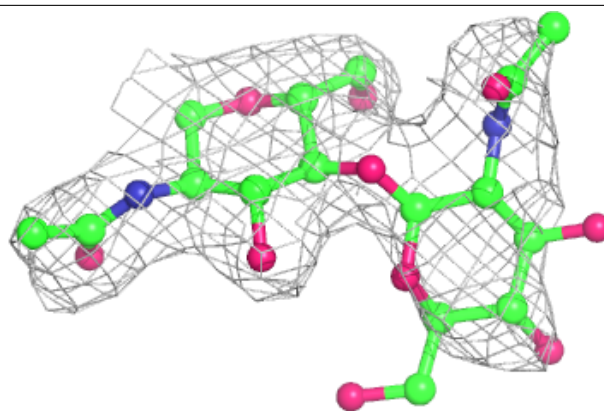
Electron density around Chain F:

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

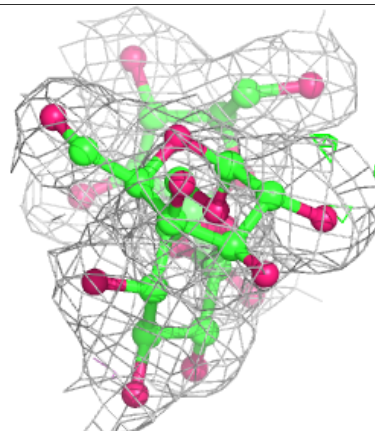
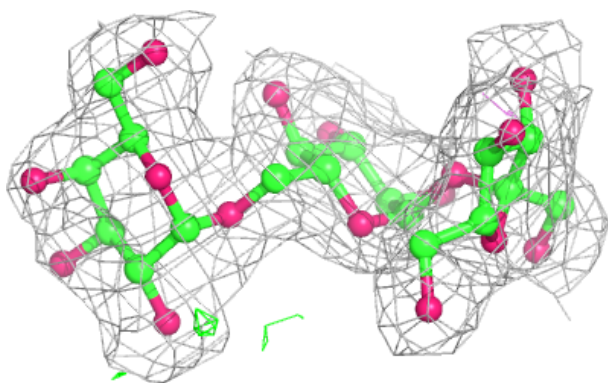
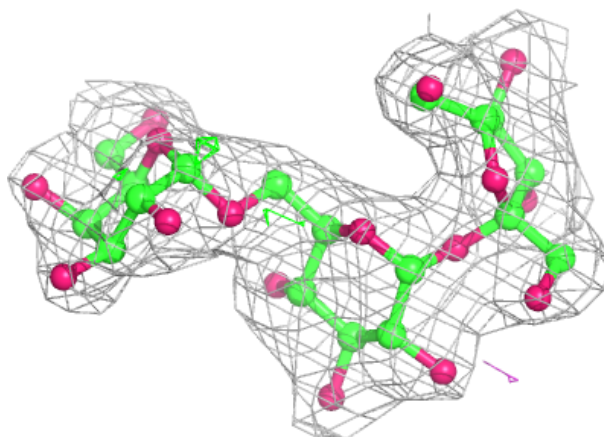


Electron density around Chain I:

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

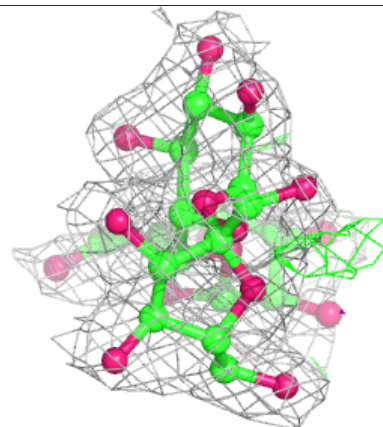
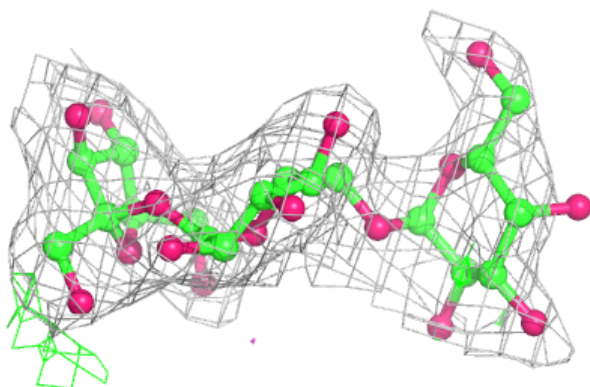
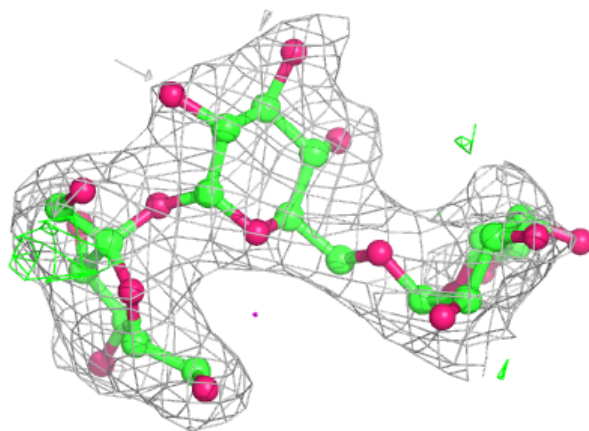
**Electron density around Chain G:**

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



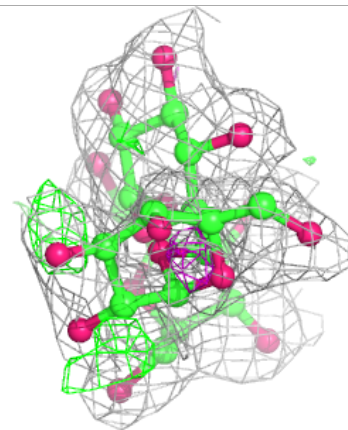
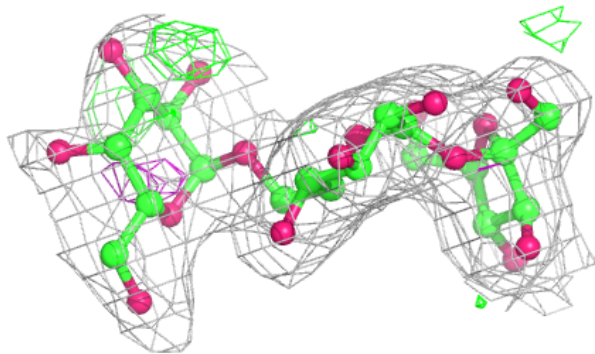
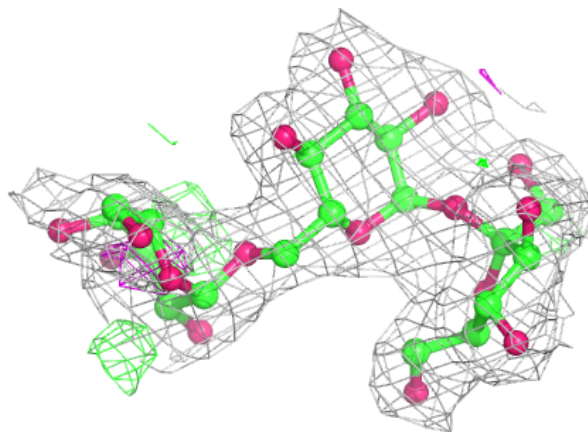
Electron density around Chain J:

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



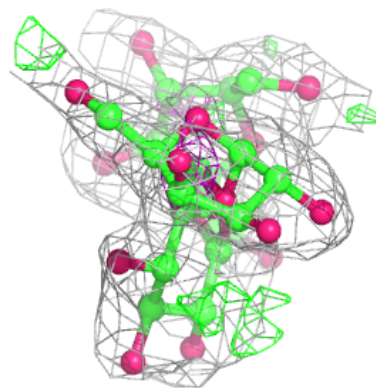
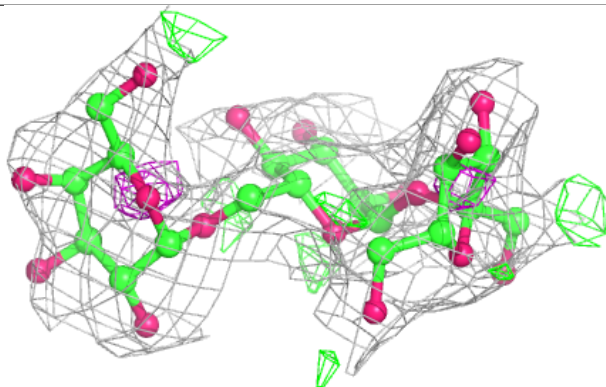
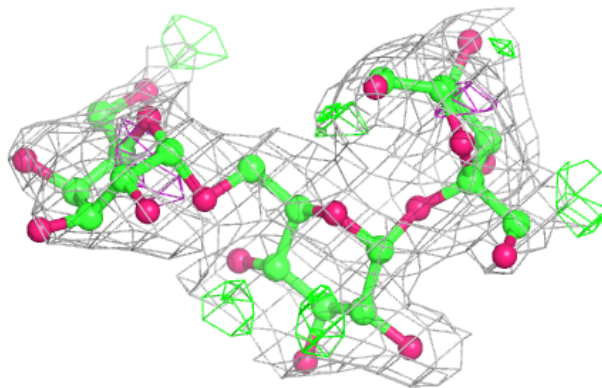
Electron density around Chain L:

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

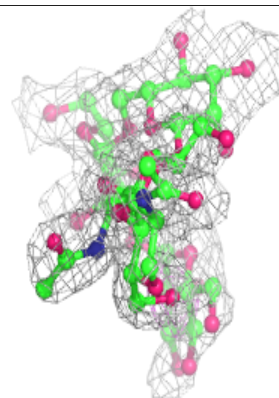
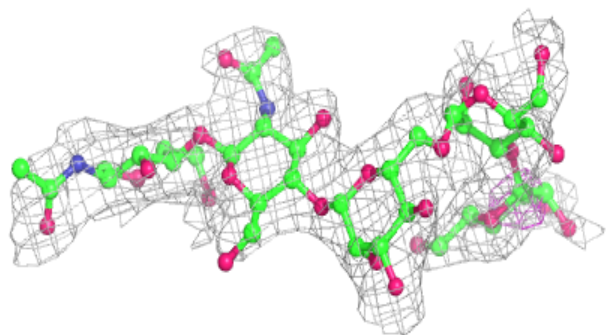
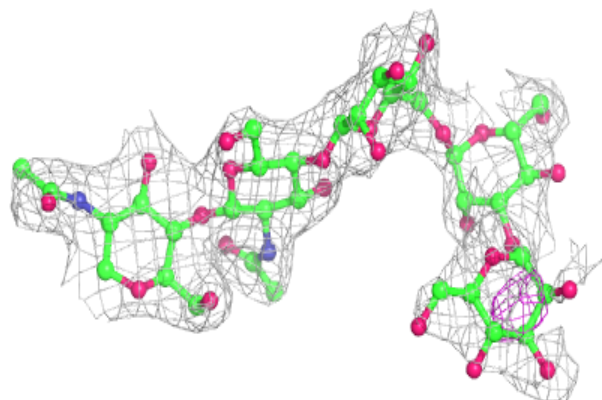


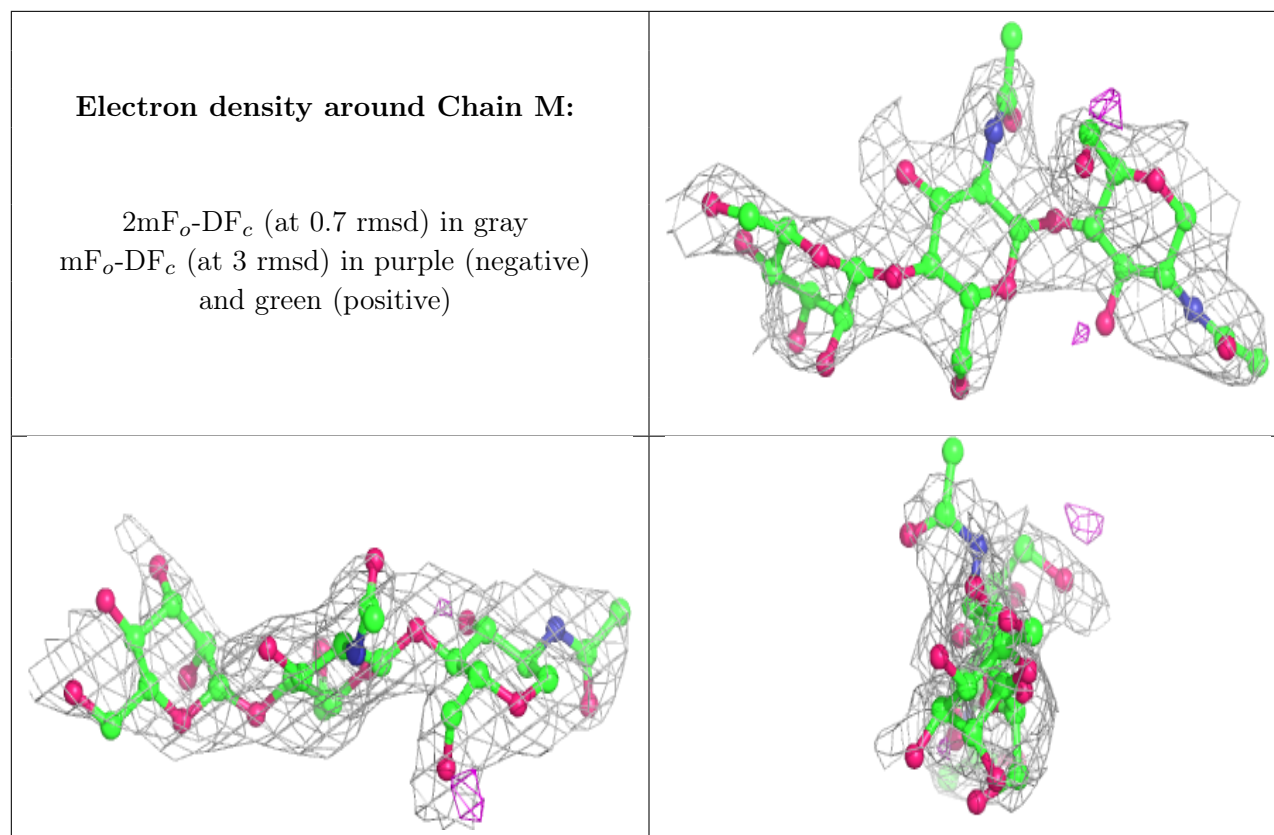
Electron density around Chain N:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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
7	MAN	D	702	11/12	0.63	0.25	97,105,113,116	0
7	MAN	A	702	11/12	0.69	0.22	77,91,94,95	0
8	NAG	B	705	14/15	0.69	0.35	71,85,90,90	14
7	MAN	D	703	11/12	0.74	0.34	27,28,30,31	11
7	MAN	A	705	11/12	0.75	0.25	74,77,82,82	0
8	NAG	A	714	14/15	0.77	0.21	66,78,83,83	0
8	NAG	A	708	14/15	0.77	0.34	63,68,70,71	14
7	MAN	B	703	11/12	0.78	0.30	96,105,113,120	0
8	NAG	C	708	14/15	0.79	0.35	94,101,109,114	0
8	NAG	D	707	14/15	0.79	0.22	78,84,89,93	0
7	MAN	D	701	11/12	0.80	0.28	86,92,94,97	11
8	NAG	D	708	14/15	0.81	0.26	79,93,98,99	0
8	NAG	D	704	14/15	0.82	0.22	76,85,96,97	0
9	PEG	B	702	7/7	0.82	0.14	62,68,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	D	706	14/15	0.83	0.21	53,66,79,83	0
8	NAG	C	705	14/15	0.83	0.39	91,96,100,102	0
8	NAG	B	709	14/15	0.85	0.28	97,106,111,112	0
8	NAG	C	709	14/15	0.85	0.21	69,87,91,92	0
8	NAG	C	710	14/15	0.85	0.24	73,81,83,89	0
7	MAN	A	701	11/12	0.85	0.19	72,76,88,89	0
8	NAG	C	707	14/15	0.87	0.20	51,66,75,79	0
7	MAN	C	703	11/12	0.87	0.21	56,76,81,88	0
8	NAG	B	708	14/15	0.87	0.19	58,76,92,95	0
8	NAG	B	706	14/15	0.88	0.28	76,85,89,91	0
7	MAN	A	703	11/12	0.88	0.22	80,86,89,91	0
8	NAG	C	706	14/15	0.88	0.21	75,82,89,90	0
8	NAG	A	707	14/15	0.89	0.14	53,59,66,66	0
7	MAN	A	704	11/12	0.89	0.12	65,69,75,84	0
8	NAG	A	711	14/15	0.89	0.15	68,80,92,93	0
8	NAG	A	713	14/15	0.89	0.19	67,72,78,79	0
7	MAN	C	701	11/12	0.89	0.25	80,88,94,95	0
8	NAG	B	704	14/15	0.91	0.17	66,80,85,87	0
7	MAN	B	701	11/12	0.91	0.25	86,91,102,103	0
8	NAG	A	709	14/15	0.92	0.20	51,58,71,71	0
8	NAG	A	712	14/15	0.92	0.15	54,59,79,82	0
7	MAN	C	702	11/12	0.93	0.10	54,58,61,67	0
8	NAG	D	705	14/15	0.93	0.16	61,64,68,68	0
8	NAG	B	707	14/15	0.94	0.18	48,56,64,65	0
8	NAG	C	704	14/15	0.94	0.12	53,59,63,64	0
8	NAG	A	710	14/15	0.95	0.13	46,49,53,53	0
8	NAG	A	706	14/15	0.95	0.15	68,77,84,86	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.