



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 PM UTC

PDB ID : 8BEU / pdb_00008beu
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

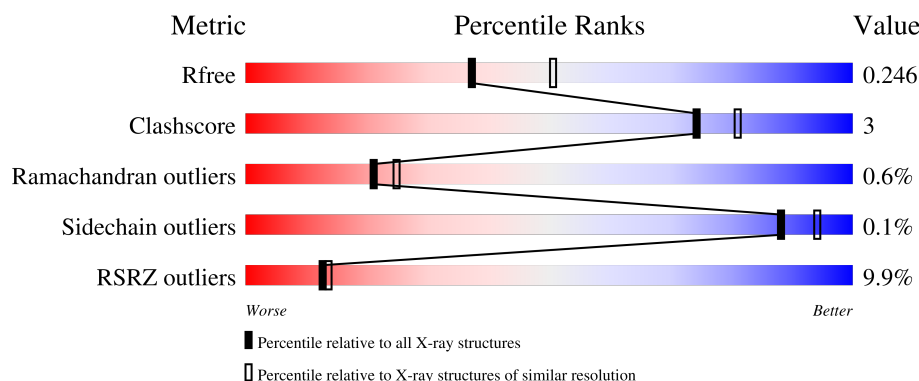
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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.



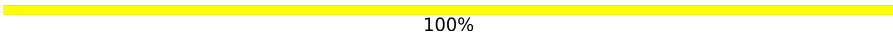
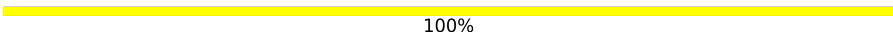
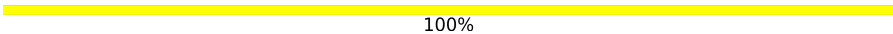
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	4% 73% 22%
1	D	675	21% 70% 7% 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	 80% 20%
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

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

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
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

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



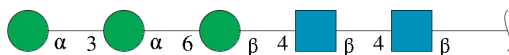
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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
4	G	3	Total	C	O	0	0	0
			34	18	16			
4	J	3	Total	C	O	0	0	0
			34	18	16			
4	L	3	Total	C	O	0	0	0
			34	18	16			
4	N	3	Total	C	O	0	0	0
			34	18	16			

- 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.



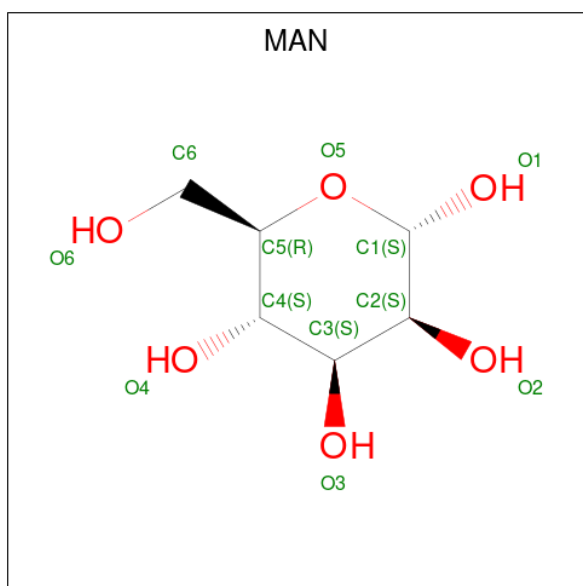
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



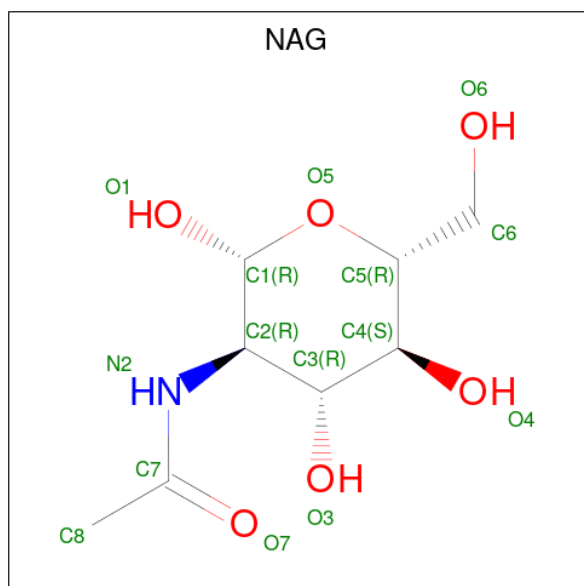
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		

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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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



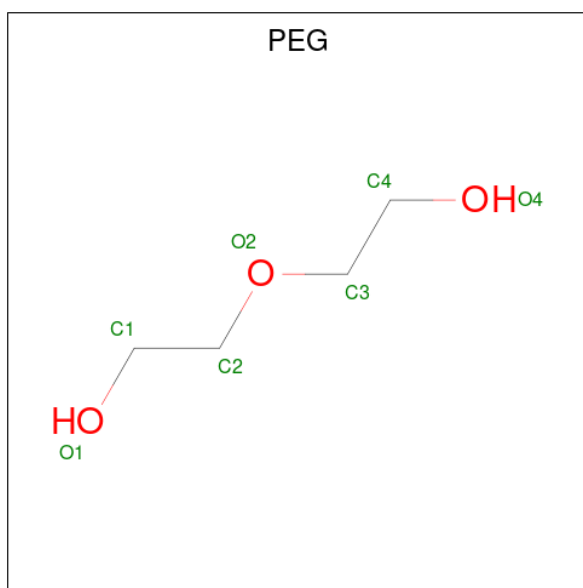
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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	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		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

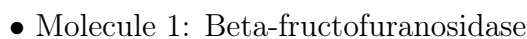
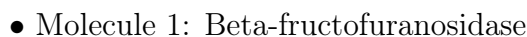


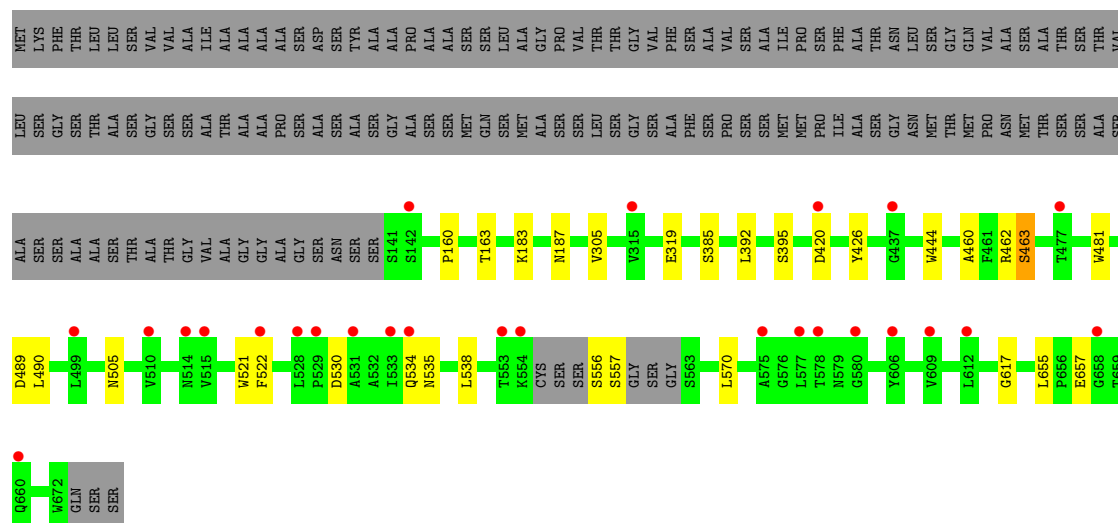
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

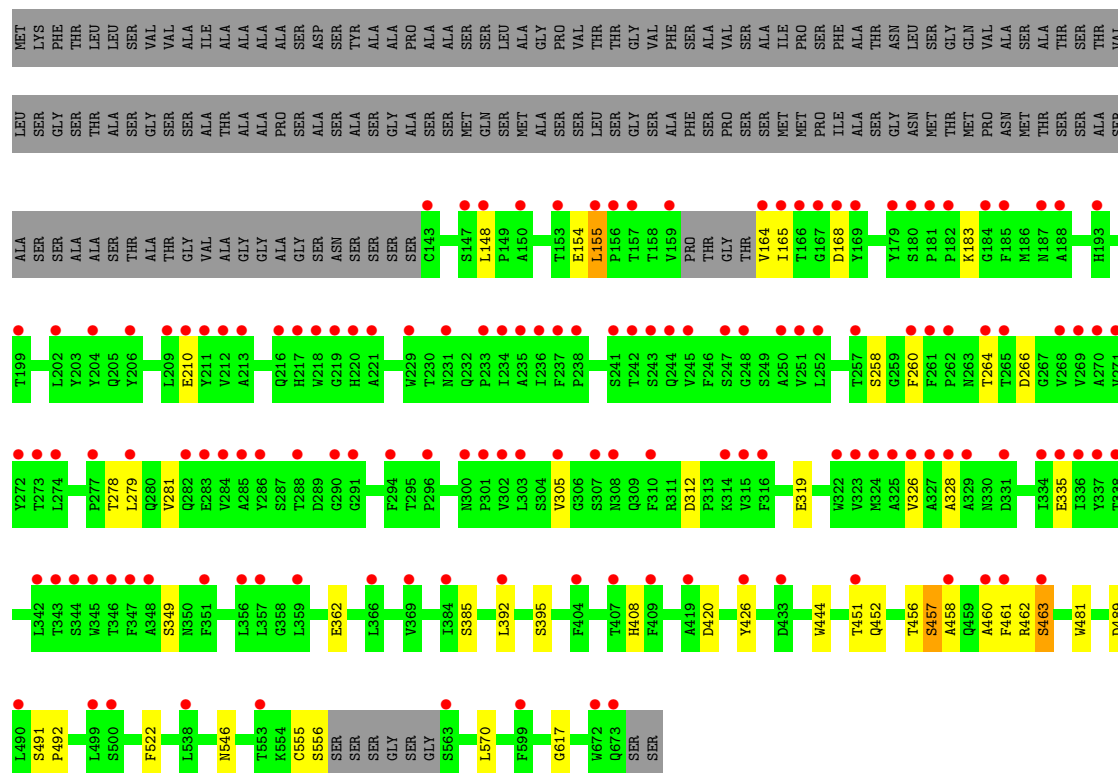
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	213	Total	O	0	0
			213	213		
10	B	139	Total	O	0	0
			139	139		
10	C	130	Total	O	0	0
			130	130		
10	D	74	Total	O	0	0
			74	74		

- Molecule 1: Beta-fructofuranosidase

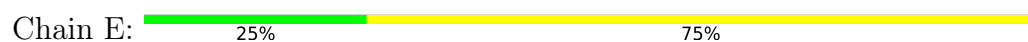




• Molecule 1: Beta-fructofuranosidase



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

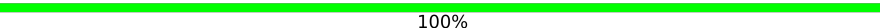


- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  25% 75%



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

Chain F:  100%

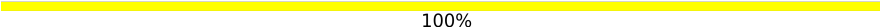


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

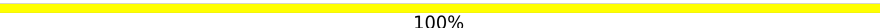


- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain G:  100%

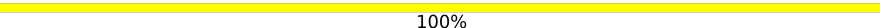


- Molecule 4: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain J:  100%



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

Chain L:  100%



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

Chain N:  33% 67%



- 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

Chain H:  80% 20%



- 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%



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 46.29 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-2.27) 99.8 (46.29-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.27Å)	Xtriage
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	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
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

Xtriage'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: MAN, PEG, BMA, NAG, FRU, GLA, 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	0.98	0/4175	1.20	3/5741 (0.1%)
1	B	1.00	0/4166	1.22	1/5729 (0.0%)
1	C	0.99	0/4165	1.21	2/5726 (0.0%)
1	D	1.02	0/4136	1.22	3/5685 (0.1%)
All	All	1.00	0/16642	1.21	9/22881 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	420	ASP	CA-CB-CG	6.22	118.83	112.60
1	D	420	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	420	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	457	SER	N-CA-C	-5.87	102.74	110.43
1	A	305	VAL	N-CA-C	-5.23	107.61	112.43
1	D	457	SER	CA-C-O	-5.15	116.20	121.87
1	A	436	ASN	CB-CA-C	-5.04	109.80	115.79
1	C	505	ASN	CB-CA-C	-5.00	104.50	111.80

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	19	0
1	B	4038	0	3758	24	0
1	C	4038	0	3758	19	0
1	D	4010	0	3732	37	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
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	101	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 (101) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:312:ASP:OD1	4:N:1:FRU:O4	2.26	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:305:VAL:HG12	1:D:305:VAL:O	2.13	0.47
1:D:462:ARG:O	1:D:463:SER:HB2	2.14	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
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: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:A:570:LEU:C	1:A:570:LEU:HD23	2.45	0.42
1:D:546:ASN:ND2	10:D:801:HOH:O	2.27	0.42
1:B:570:LEU:C	1:B:570:LEU:HD23	2.45	0.42
1:B:305:VAL:HG12	1:B:305:VAL:O	2.20	0.42
1:B:281:VAL:HG13	1:B:304:SER:HB2	2.00	0.41
1:D:570:LEU:HD23	1:D:570:LEU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:570:LEU:C	1:C:570:LEU:HD23	2.45	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:C:535:ASN:CG	1:C:538:LEU:HD13	2.46	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

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	523/675 (78%)	503 (96%)	17 (3%)	3 (1%)	21	25
1	B	522/675 (77%)	501 (96%)	18 (3%)	3 (1%)	21	25
1	C	520/675 (77%)	500 (96%)	17 (3%)	3 (1%)	21	25
1	D	515/675 (76%)	485 (94%)	26 (5%)	4 (1%)	16	18
All	All	2080/2700 (77%)	1989 (96%)	78 (4%)	13 (1%)	21	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	155	LEU
1	A	463	SER
1	A	489	ASP

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Mol	Chain	Res	Type
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%)	442 (100%)	1 (0%)	87	93
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%)	437 (100%)	1 (0%)	87	93
All	All	1765/2180 (81%)	1763 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	THR
1	D	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	299	ASN
1	A	436	ASN
1	A	471	ASN

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Mol	Chain	Res	Type
1	A	673	GLN
1	B	187	ASN
1	B	263	ASN
1	B	299	ASN
1	B	308	ASN
1	B	471	ASN
1	B	664	GLN
1	B	666	ASN
1	C	187	ASN
1	C	308	ASN
1	C	471	ASN
1	D	187	ASN
1	D	299	ASN
1	D	308	ASN
1	D	471	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	0.62	0	17,19,21	1.00	1 (5%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	1.01	0
2	BMA	E	3	2	11,11,12	0.66	0	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	E	4	2	11,11,12	0.38	0	15,15,17	1.01	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.51	0	17,19,21	0.89	0
3	NAG	F	2	3	14,14,15	0.56	0	17,19,21	0.94	0
4	FRU	G	1	4	11,12,12	0.81	1 (9%)	10,18,18	1.07	0
4	GLC	G	2	4	11,11,12	1.06	1 (9%)	15,15,17	1.19	1 (6%)
4	GLA	G	3	4	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.52	0	17,19,21	0.96	0
5	NAG	H	2	5	14,14,15	0.41	0	17,19,21	1.08	1 (5%)
5	BMA	H	3	5	11,11,12	0.33	0	15,15,17	0.65	0
5	MAN	H	4	5	11,11,12	0.37	0	15,15,17	0.56	0
5	MAN	H	5	5	11,11,12	0.48	0	15,15,17	1.02	0
3	NAG	I	1	1,3	14,14,15	0.59	0	17,19,21	0.59	0
3	NAG	I	2	3	14,14,15	0.35	0	17,19,21	1.06	1 (5%)
4	FRU	J	1	4	11,12,12	0.75	1 (9%)	10,18,18	1.21	1 (10%)
4	GLC	J	2	4	11,11,12	0.75	1 (9%)	15,15,17	1.01	0
4	GLA	J	3	4	11,11,12	0.92	0	15,15,17	1.28	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.59	0	17,19,21	1.24	2 (11%)
2	NAG	K	2	2	14,14,15	0.50	0	17,19,21	0.65	0
2	BMA	K	3	2	11,11,12	0.53	0	15,15,17	0.94	1 (6%)
2	MAN	K	4	2	11,11,12	0.65	0	15,15,17	1.07	1 (6%)
4	FRU	L	1	4	11,12,12	0.77	0	10,18,18	1.38	1 (10%)
4	GLC	L	2	4	11,11,12	0.82	1 (9%)	15,15,17	0.82	0
4	GLA	L	3	4	11,11,12	0.79	0	15,15,17	1.55	2 (13%)
6	NAG	M	1	6,1	14,14,15	0.76	0	17,19,21	1.30	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	0.48	0	15,15,17	0.63	0
4	FRU	N	1	4	11,12,12	1.09	1 (9%)	10,18,18	0.92	1 (10%)
4	GLC	N	2	4	11,11,12	0.95	0	15,15,17	1.08	1 (6%)
4	GLA	N	3	4	11,11,12	0.71	0	15,15,17	1.29	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	NAG	F	1	1,3	-	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	1,3	-	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	-	1/5/24/24	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	1,2	-	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	6,1	-	1/6/23/26	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	-	1/5/24/24	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	-3.16	1.38	1.43
4	N	1	FRU	O2-C2	3.12	1.46	1.40
4	L	2	GLC	O5-C1	-2.33	1.39	1.43
4	J	1	FRU	O2-C2	2.25	1.44	1.40
4	G	1	FRU	O2-C2	2.09	1.44	1.40
4	J	2	GLC	O5-C1	-2.00	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	4.09	117.67	112.19
2	K	1	NAG	O5-C1-C2	-3.57	105.76	111.29
4	L	3	GLA	C1-C2-C3	-3.30	104.84	109.64
4	L	3	GLA	C1-O5-C5	-3.27	107.81	112.19
2	E	1	NAG	C1-O5-C5	3.04	116.26	112.19
5	H	2	NAG	C1-O5-C5	-2.98	108.19	112.19
4	L	1	FRU	O1-C1-C2	-2.91	105.24	111.67
4	J	1	FRU	O1-C1-C2	-2.81	105.46	111.67
4	G	3	GLA	C1-C2-C3	-2.79	105.58	109.64
4	N	3	GLA	C2-C3-C4	2.79	115.77	110.86
4	G	2	GLC	C1-O5-C5	-2.73	108.53	112.19
4	N	3	GLA	C3-C4-C5	2.63	115.00	110.23
2	K	4	MAN	C3-C4-C5	2.60	114.94	110.23
3	I	2	NAG	C2-N2-C7	-2.44	119.63	122.90
2	E	4	MAN	C1-O5-C5	-2.31	109.10	112.19
4	J	3	GLA	C3-C4-C5	2.22	114.26	110.23
2	K	1	NAG	O5-C5-C4	-2.16	105.56	110.83
4	N	2	GLC	C1-C2-C3	-2.16	106.50	109.64
4	N	1	FRU	O4-C4-C5	2.15	117.25	111.08
2	E	3	BMA	C1-C2-C3	2.12	112.73	109.64
2	K	3	BMA	C3-C4-C5	2.03	113.91	110.23
2	E	3	BMA	O5-C5-C6	2.02	111.60	107.66

There are no chirality outliers.

All (27) 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	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
2	K	4	MAN	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

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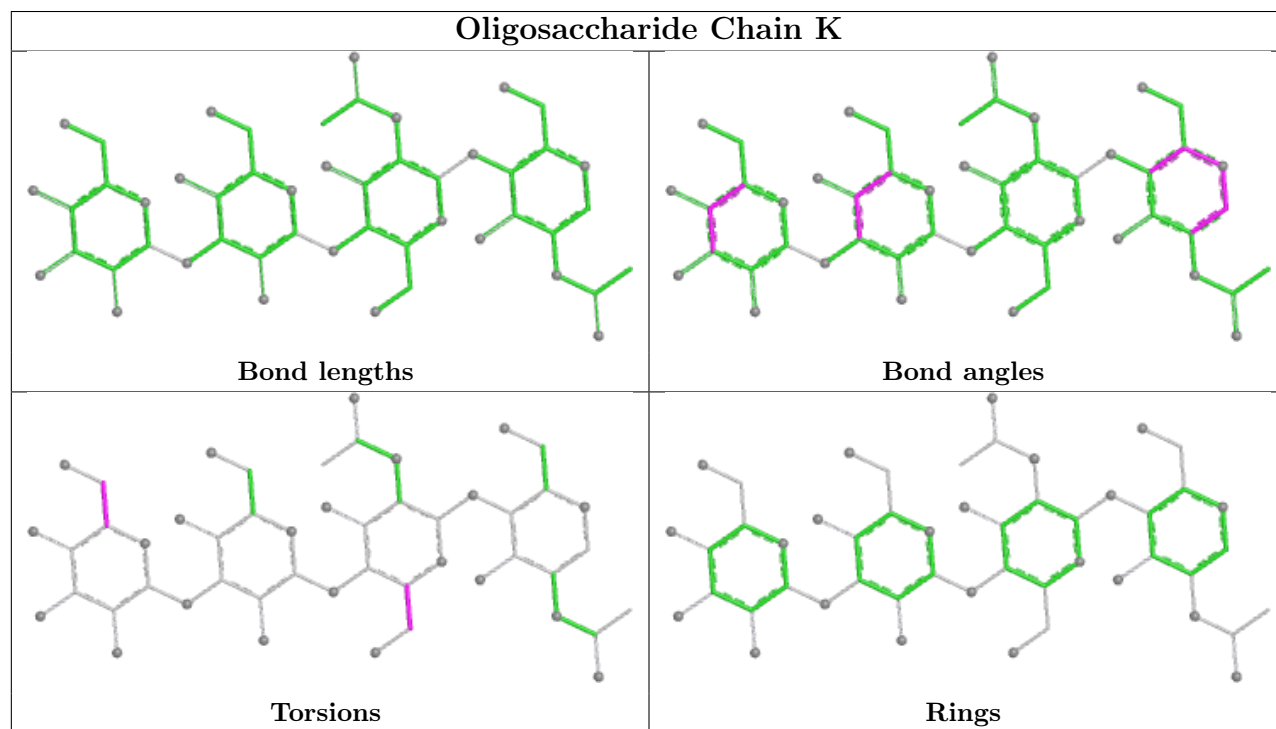
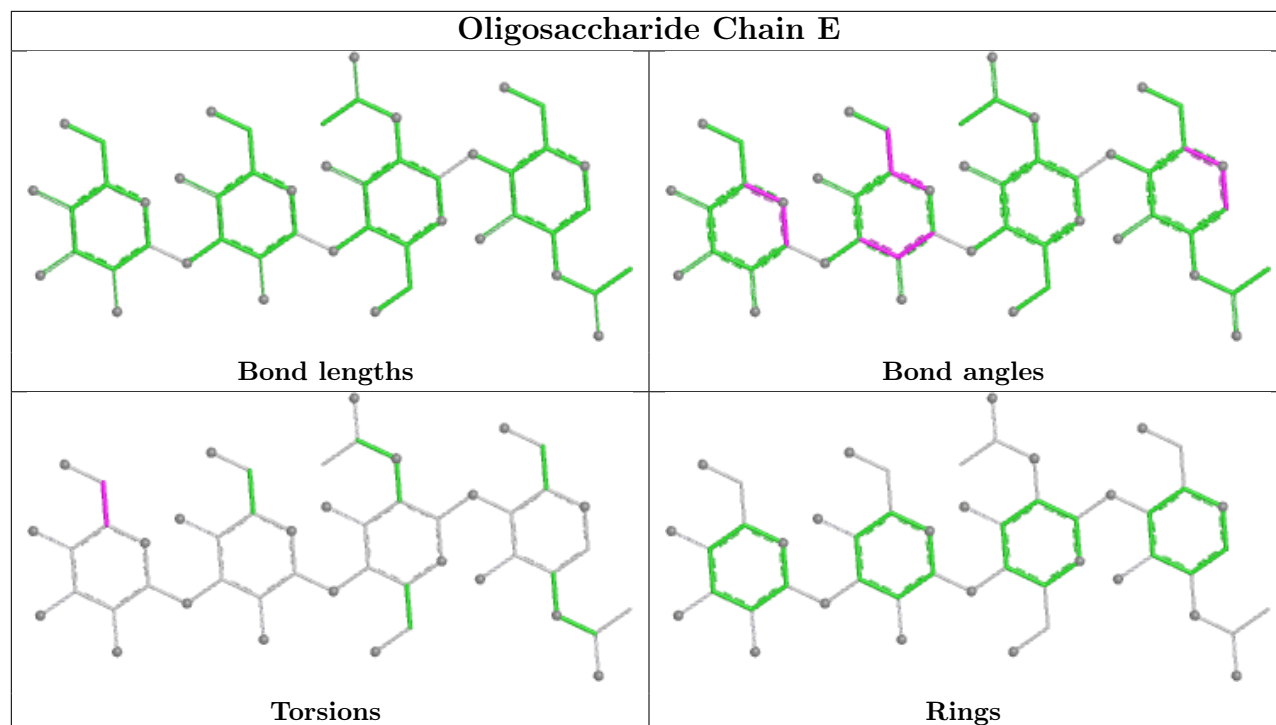
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
4	N	2	GLC	O5-C5-C6-O6
4	N	2	GLC	C4-C5-C6-O6
6	M	1	NAG	C1-C2-N2-C7
4	G	1	FRU	O1-C1-C2-C3
4	L	3	GLA	C4-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
4	J	1	FRU	O1-C1-C2-C3
4	N	1	FRU	O1-C1-C2-C3

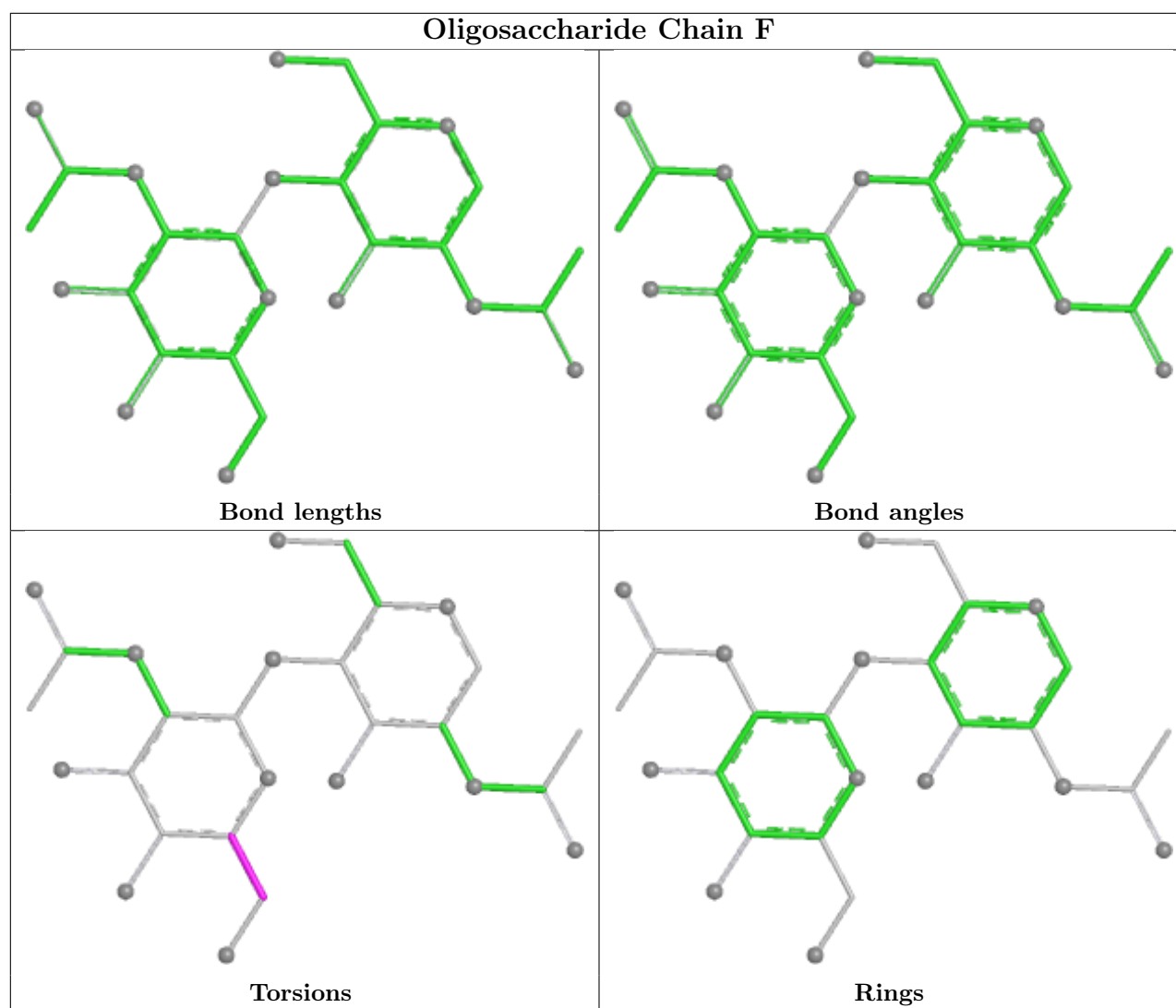
There are no ring outliers.

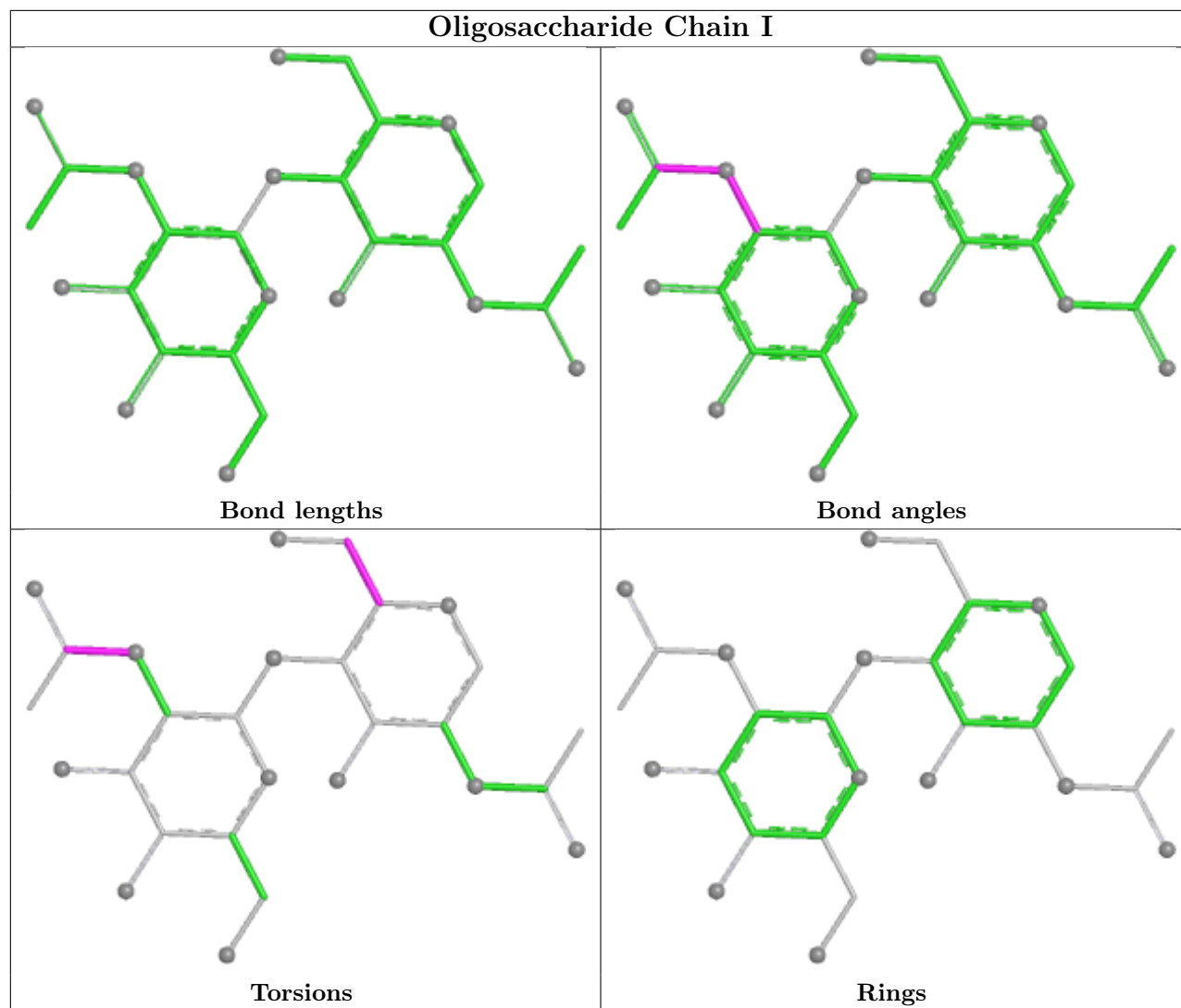
4 monomers are involved in 3 short contacts:

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

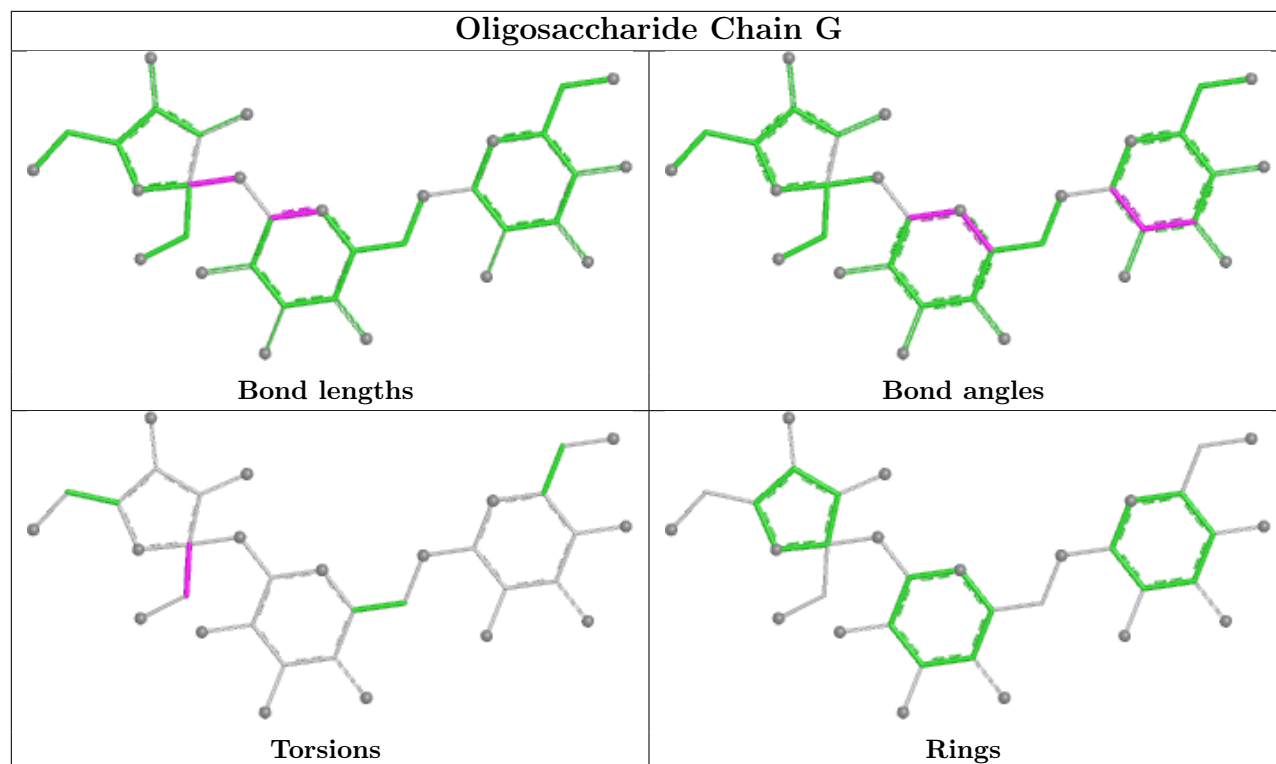
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



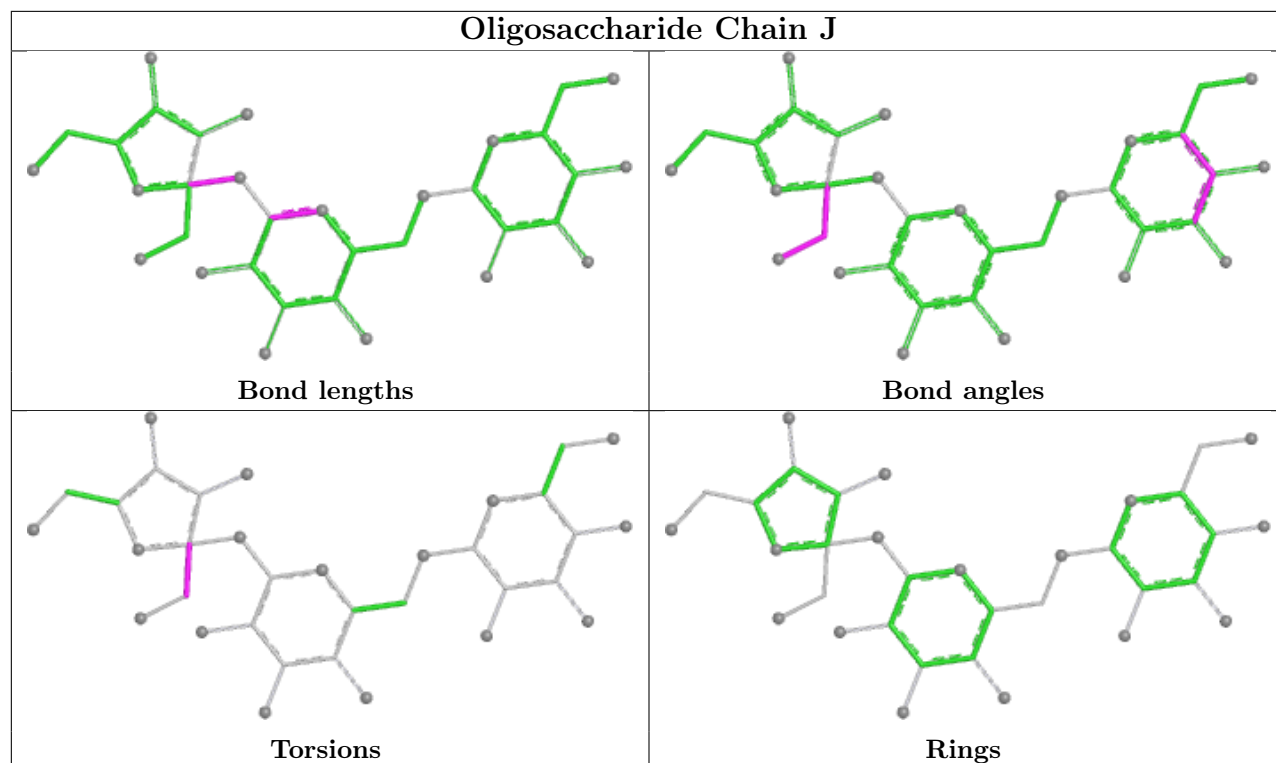


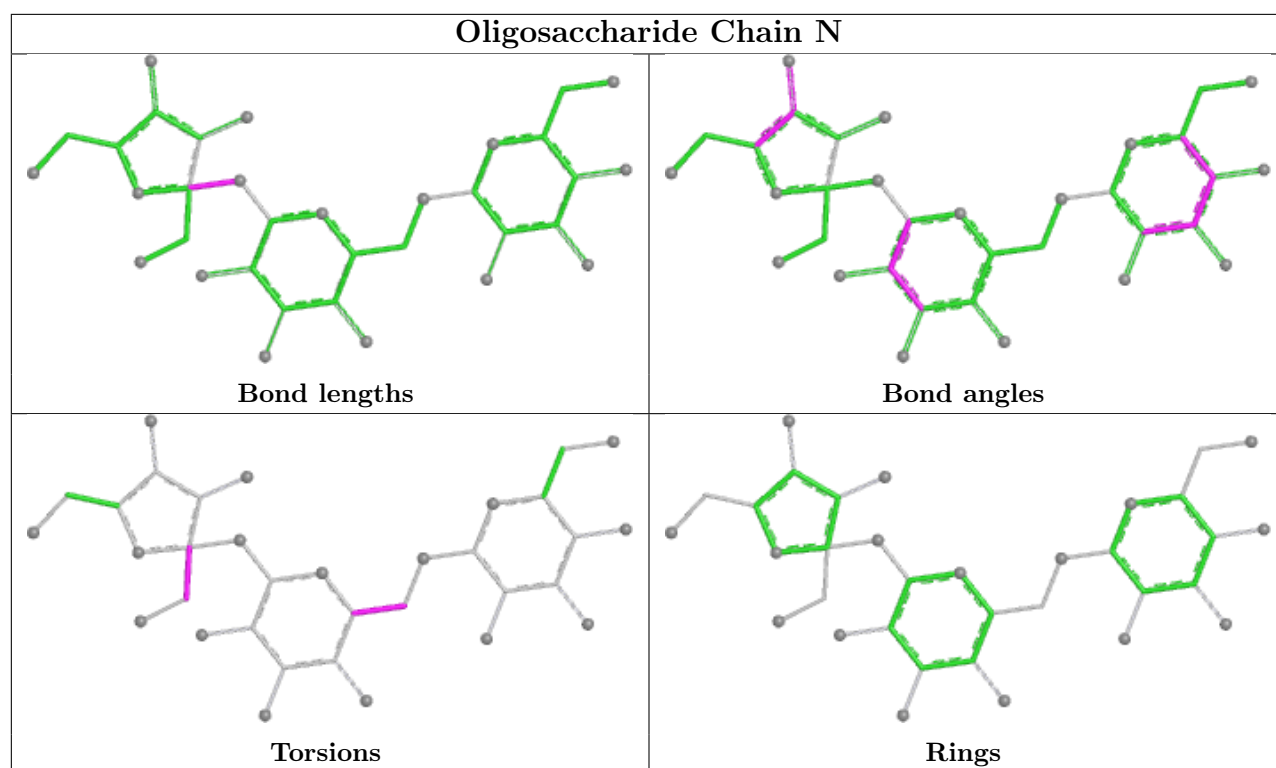
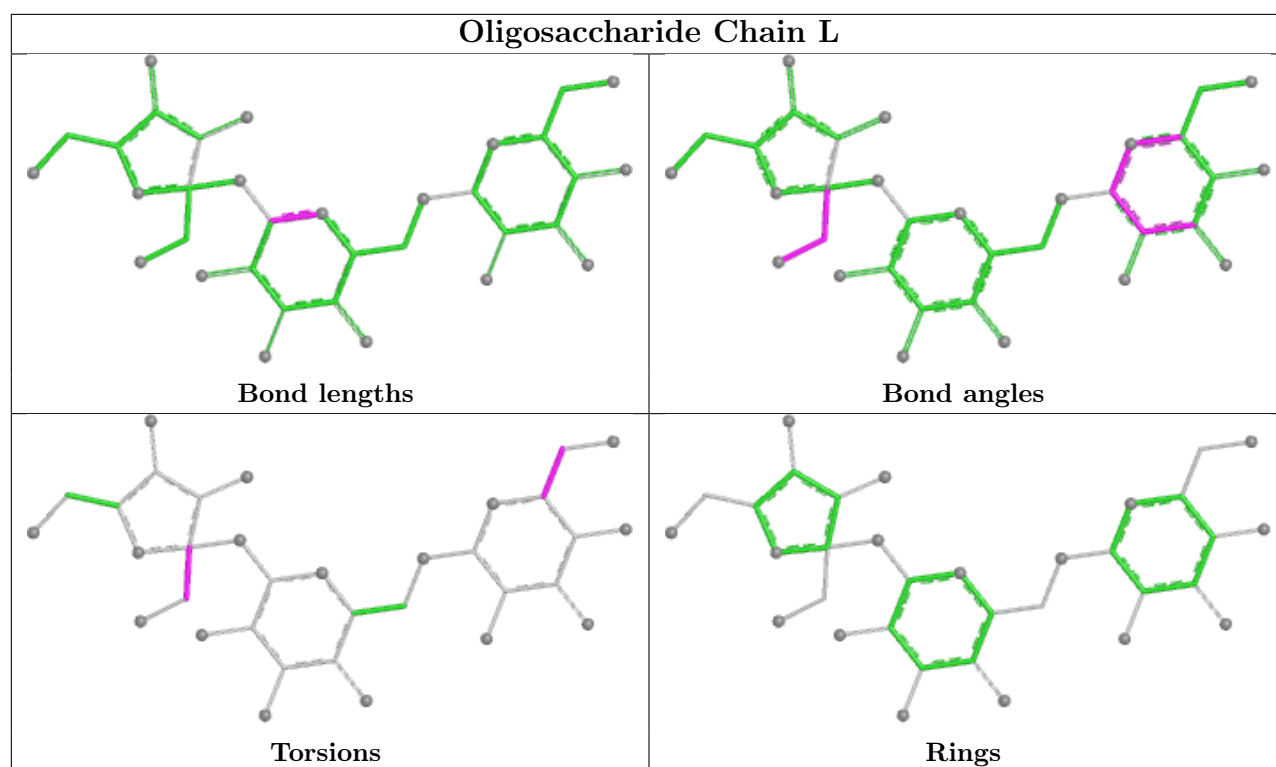


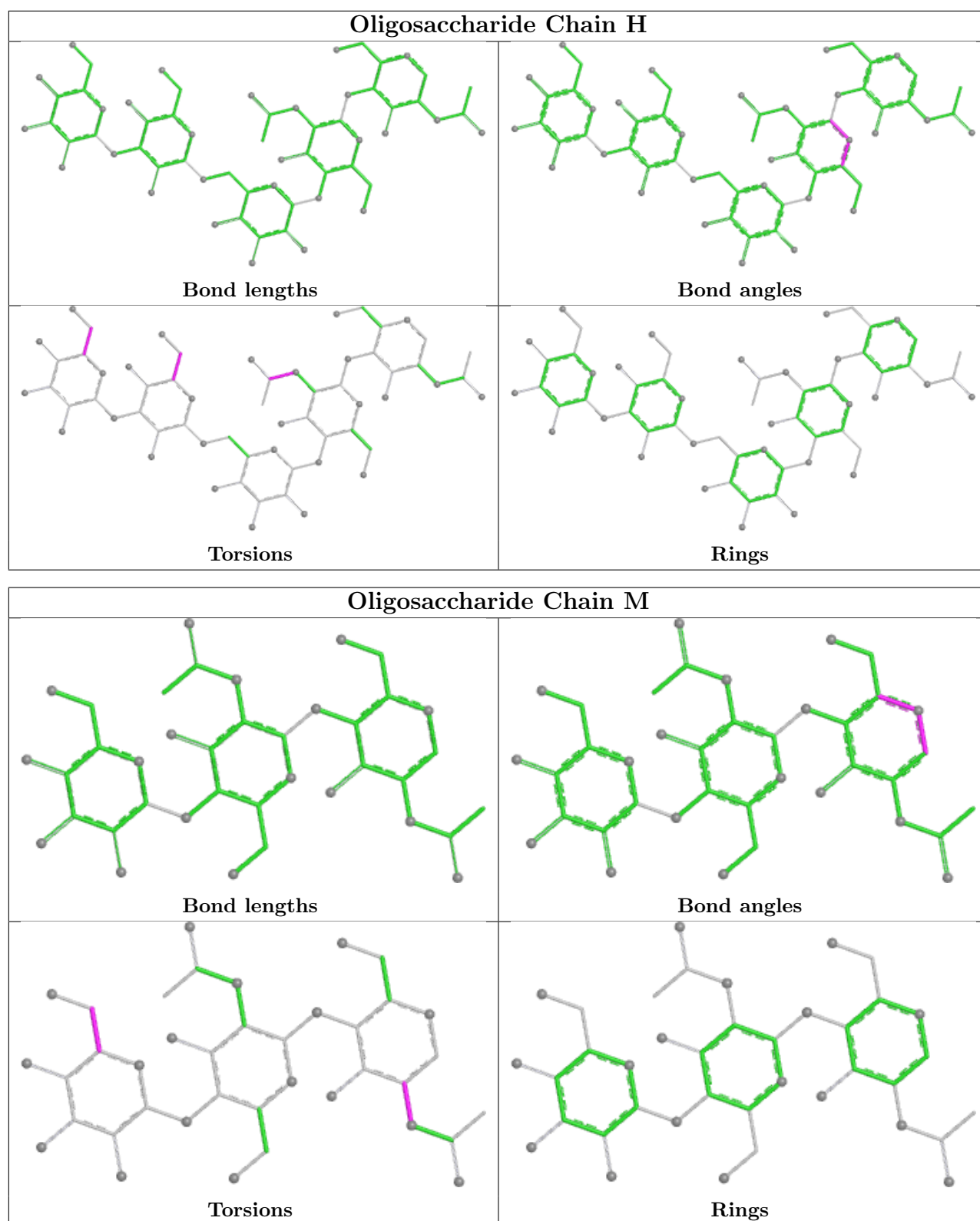
Oligosaccharide Chain G



Oligosaccharide Chain J







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	$\# Z > 2$
7	MAN	C	702	1	11,11,12	0.49	0	15,15,17	1.27	3 (20%)
7	MAN	A	702	1	11,11,12	0.38	0	15,15,17	0.60	0
8	NAG	A	707	1	14,14,15	0.58	0	17,19,21	1.00	2 (11%)
8	NAG	C	708	1	14,14,15	0.80	1 (7%)	17,19,21	1.42	3 (17%)
8	NAG	C	709	1	14,14,15	0.44	0	17,19,21	1.29	1 (5%)
7	MAN	A	705	1	11,11,12	0.62	0	15,15,17	1.73	3 (20%)
8	NAG	D	706	1	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
8	NAG	D	707	1	14,14,15	0.37	0	17,19,21	0.89	0
7	MAN	A	701	1	11,11,12	0.43	0	15,15,17	1.77	3 (20%)
7	MAN	D	702	1	11,11,12	0.64	0	15,15,17	1.42	1 (6%)
8	NAG	A	714	1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
8	NAG	B	707	1	14,14,15	0.30	0	17,19,21	0.86	0
8	NAG	C	704	1	14,14,15	0.43	0	17,19,21	0.75	0
7	MAN	A	703	1	11,11,12	0.45	0	15,15,17	0.73	0
7	MAN	D	701	1	11,11,12	0.27	0	15,15,17	1.24	2 (13%)
8	NAG	B	706	1	14,14,15	0.29	0	17,19,21	1.25	3 (17%)
8	NAG	C	706	1	14,14,15	0.30	0	17,19,21	0.75	0
8	NAG	D	708	1	14,14,15	0.39	0	17,19,21	1.00	2 (11%)
8	NAG	A	710	1	14,14,15	0.44	0	17,19,21	0.94	0
8	NAG	B	709	1	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
8	NAG	A	711	1	14,14,15	0.39	0	17,19,21	0.79	0
8	NAG	C	707	1	14,14,15	0.63	0	17,19,21	0.74	0
7	MAN	B	703	1	11,11,12	0.33	0	15,15,17	1.04	1 (6%)
7	MAN	A	704	1	11,11,12	0.37	0	15,15,17	1.45	4 (26%)
7	MAN	B	701	1	11,11,12	0.32	0	15,15,17	0.73	0
8	NAG	B	708	1	14,14,15	0.49	0	17,19,21	1.14	1 (5%)
8	NAG	A	712	1	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
8	NAG	B	705	1	14,14,15	0.33	0	17,19,21	1.27	2 (11%)
8	NAG	A	709	1	14,14,15	0.45	0	17,19,21	0.87	0
9	PEG	B	702	-	6,6,6	0.25	0	5,5,5	0.17	0
7	MAN	C	703	1	11,11,12	0.57	0	15,15,17	1.21	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	C	701	1	11,11,12	0.35	0	15,15,17	1.15	2 (13%)
8	NAG	C	705	1	14,14,15	0.63	0	17,19,21	1.43	2 (11%)
8	NAG	C	710	1	14,14,15	0.56	0	17,19,21	1.14	1 (5%)
8	NAG	A	708	1	14,14,15	0.43	0	17,19,21	1.07	1 (5%)
8	NAG	A	713	1	14,14,15	0.42	0	17,19,21	1.14	1 (5%)
8	NAG	B	704	1	14,14,15	0.36	0	17,19,21	0.83	0
8	NAG	D	705	1	14,14,15	0.39	0	17,19,21	1.21	3 (17%)
8	NAG	D	704	1	14,14,15	0.64	0	17,19,21	0.95	0
7	MAN	D	703	1	11,11,12	1.45	1 (9%)	15,15,17	1.09	1 (6%)
8	NAG	A	706	1	14,14,15	0.36	0	17,19,21	0.88	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
7	MAN	C	702	1	-	2/2/19/22	0/1/1/1
7	MAN	A	702	1	-	2/2/19/22	0/1/1/1
8	NAG	A	707	1	-	1/6/23/26	0/1/1/1
8	NAG	C	708	1	-	5/6/23/26	0/1/1/1
8	NAG	C	709	1	-	2/6/23/26	0/1/1/1
7	MAN	A	705	1	-	2/2/19/22	0/1/1/1
8	NAG	D	706	1	-	2/6/23/26	0/1/1/1
8	NAG	D	707	1	-	2/6/23/26	0/1/1/1
7	MAN	A	701	1	-	2/2/19/22	0/1/1/1
7	MAN	D	702	1	-	0/2/19/22	0/1/1/1
8	NAG	A	714	1	-	2/6/23/26	0/1/1/1
8	NAG	B	707	1	-	1/6/23/26	0/1/1/1
8	NAG	C	704	1	-	2/6/23/26	0/1/1/1
7	MAN	A	703	1	-	0/2/19/22	0/1/1/1
7	MAN	D	701	1	-	0/2/19/22	0/1/1/1
8	NAG	B	706	1	-	0/6/23/26	0/1/1/1
8	NAG	C	706	1	-	0/6/23/26	0/1/1/1
8	NAG	D	708	1	-	1/6/23/26	0/1/1/1
8	NAG	A	710	1	-	1/6/23/26	0/1/1/1
8	NAG	B	709	1	-	0/6/23/26	0/1/1/1
8	NAG	A	711	1	-	0/6/23/26	0/1/1/1
8	NAG	C	707	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	B	703	1	-	1/2/19/22	0/1/1/1
7	MAN	A	704	1	-	1/2/19/22	0/1/1/1
7	MAN	B	701	1	-	0/2/19/22	0/1/1/1
8	NAG	B	708	1	-	1/6/23/26	0/1/1/1
8	NAG	A	712	1	-	2/6/23/26	0/1/1/1
8	NAG	B	705	1	-	2/6/23/26	0/1/1/1
8	NAG	A	709	1	-	2/6/23/26	0/1/1/1
9	PEG	B	702	-	-	2/4/4/4	-
7	MAN	C	703	1	-	0/2/19/22	0/1/1/1
7	MAN	C	701	1	-	2/2/19/22	0/1/1/1
8	NAG	C	705	1	-	4/6/23/26	0/1/1/1
8	NAG	C	710	1	-	2/6/23/26	0/1/1/1
8	NAG	A	708	1	-	2/6/23/26	0/1/1/1
8	NAG	A	713	1	-	4/6/23/26	0/1/1/1
8	NAG	B	704	1	-	0/6/23/26	0/1/1/1
8	NAG	D	705	1	-	2/6/23/26	0/1/1/1
8	NAG	D	704	1	-	4/6/23/26	0/1/1/1
7	MAN	D	703	1	-	2/2/19/22	0/1/1/1
8	NAG	A	706	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	703	MAN	C2-C3	-2.93	1.48	1.52
8	C	708	NAG	C2-N2	2.08	1.49	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	705	NAG	C2-N2-C7	-4.77	116.51	122.90
7	A	701	MAN	C1-O5-C5	-4.76	105.81	112.19
7	A	705	MAN	O5-C1-C2	-4.61	99.79	110.79
8	C	709	NAG	C2-N2-C7	-3.83	117.77	122.90
8	C	708	NAG	C1-O5-C5	-3.76	107.14	112.19
7	D	702	MAN	C1-O5-C5	3.74	117.19	112.19
8	B	708	NAG	C1-O5-C5	-3.53	107.45	112.19
8	B	705	NAG	O5-C1-C2	-3.45	105.95	111.29
7	B	703	MAN	O5-C1-C2	-3.26	103.01	110.79
7	A	705	MAN	C1-O5-C5	-3.01	108.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	705	MAN	C3-C4-C5	2.96	115.59	110.23
7	A	704	MAN	C1-C2-C3	-2.91	105.40	109.64
8	D	705	NAG	C2-N2-C7	2.91	126.80	122.90
8	A	714	NAG	O5-C1-C2	-2.90	106.81	111.29
8	A	713	NAG	C1-O5-C5	-2.84	108.38	112.19
8	C	710	NAG	C1-C2-N2	-2.83	105.98	110.43
7	A	701	MAN	C3-C4-C5	2.82	115.35	110.23
8	B	706	NAG	C2-N2-C7	-2.79	119.16	122.90
8	D	706	NAG	C1-O5-C5	-2.75	108.50	112.19
8	A	708	NAG	C4-C3-C2	-2.63	107.17	111.02
8	B	706	NAG	C4-C3-C2	-2.60	107.21	111.02
7	D	701	MAN	C1-C2-C3	2.56	113.37	109.64
7	C	701	MAN	O5-C1-C2	-2.56	104.68	110.79
7	D	701	MAN	C1-O5-C5	2.49	115.52	112.19
8	B	706	NAG	O5-C1-C2	-2.48	107.45	111.29
7	A	701	MAN	O4-C4-C5	-2.46	103.28	109.32
8	A	712	NAG	C2-N2-C7	-2.45	119.62	122.90
8	C	705	NAG	C1-C2-N2	-2.44	106.58	110.43
7	C	702	MAN	C1-O5-C5	-2.44	108.92	112.19
7	C	701	MAN	C1-O5-C5	-2.41	108.96	112.19
7	A	704	MAN	O5-C1-C2	-2.38	105.12	110.79
7	C	702	MAN	O5-C1-C2	-2.35	105.19	110.79
8	D	708	NAG	C2-N2-C7	-2.35	119.75	122.90
8	C	708	NAG	O5-C5-C6	2.29	112.12	107.66
8	B	709	NAG	C2-N2-C7	-2.28	119.84	122.90
8	C	708	NAG	C2-N2-C7	-2.28	119.84	122.90
8	A	707	NAG	C8-C7-N2	-2.25	112.38	116.12
7	A	704	MAN	C1-O5-C5	-2.25	109.17	112.19
8	B	705	NAG	C3-C4-C5	2.23	114.27	110.23
7	C	703	MAN	O5-C1-C2	-2.22	105.50	110.79
8	A	707	NAG	O7-C7-N2	2.21	125.89	121.98
7	C	702	MAN	C1-C2-C3	-2.18	106.47	109.64
7	D	703	MAN	C2-C3-C4	-2.17	107.04	110.86
8	D	705	NAG	O7-C7-N2	-2.17	118.15	121.98
7	C	703	MAN	O2-C2-C1	2.16	114.17	109.22
7	A	704	MAN	C3-C4-C5	2.15	114.14	110.23
8	D	705	NAG	C8-C7-N2	2.12	119.63	116.12
7	C	703	MAN	C3-C4-C5	2.09	114.02	110.23
8	D	708	NAG	C1-C2-N2	-2.05	107.21	110.43

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	C	705	NAG	O7-C7-N2-C2
7	A	702	MAN	O5-C5-C6-O6
8	B	705	NAG	C4-C5-C6-O6
7	A	701	MAN	C4-C5-C6-O6
7	C	702	MAN	O5-C5-C6-O6
7	C	702	MAN	C4-C5-C6-O6
8	C	708	NAG	O5-C5-C6-O6
8	A	713	NAG	C8-C7-N2-C2
8	C	709	NAG	C8-C7-N2-C2
7	A	705	MAN	O5-C5-C6-O6
8	A	709	NAG	O5-C5-C6-O6
7	D	703	MAN	C4-C5-C6-O6
7	A	705	MAN	C4-C5-C6-O6
8	C	708	NAG	C4-C5-C6-O6
7	C	701	MAN	C4-C5-C6-O6
8	D	705	NAG	C8-C7-N2-C2
8	D	705	NAG	O7-C7-N2-C2
7	A	702	MAN	C4-C5-C6-O6
7	C	701	MAN	O5-C5-C6-O6
8	A	709	NAG	C4-C5-C6-O6
8	A	714	NAG	O5-C5-C6-O6
8	A	714	NAG	C4-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	D	706	NAG	C4-C5-C6-O6
8	D	704	NAG	O5-C5-C6-O6
8	A	708	NAG	C4-C5-C6-O6
8	A	713	NAG	O7-C7-N2-C2
7	D	703	MAN	O5-C5-C6-O6
8	B	708	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	707	NAG	O5-C5-C6-O6
8	D	708	NAG	C8-C7-N2-C2
7	A	704	MAN	C4-C5-C6-O6
8	A	708	NAG	O5-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	713	NAG	C3-C2-N2-C7
8	C	710	NAG	C3-C2-N2-C7
8	A	706	NAG	O5-C5-C6-O6
7	B	703	MAN	C4-C5-C6-O6
8	D	704	NAG	C4-C5-C6-O6
8	B	707	NAG	O5-C5-C6-O6
8	A	706	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	708	NAG	3	0
8	D	706	NAG	1	0
7	D	702	MAN	6	0
8	B	707	NAG	1	0
7	A	703	MAN	1	0
8	C	707	NAG	1	0
8	A	713	NAG	3	0
7	D	703	MAN	5	0
8	A	706	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%)	0.07	8 (1%) 72 73	23, 37, 62, 93	0
1	B	526/675 (77%)	0.52	31 (5%) 28 29	26, 44, 78, 109	0
1	C	526/675 (77%)	0.50	26 (4%) 35 36	26, 48, 82, 113	0
1	D	521/675 (77%)	1.45	142 (27%) 1 1	35, 62, 94, 118	0
All	All	2100/2700 (77%)	0.63	207 (9%) 13 14	23, 47, 84, 118	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	159	VAL	5.3
1	D	184	GLY	5.1
1	D	294	PHE	4.9
1	D	211	TYR	4.9
1	D	245	VAL	4.8
1	D	219	GLY	4.7
1	D	329	ALA	4.5
1	D	217	HIS	4.4
1	D	271	VAL	4.4
1	D	337	TYR	4.4
1	D	236	ILE	4.3
1	D	296	PRO	4.2
1	D	346	THR	4.1
1	D	264	THR	4.0
1	D	235	ALA	4.0
1	D	269	VAL	3.9
1	D	156	PRO	3.8
1	D	328	ALA	3.7
1	D	288	THR	3.7
1	D	279	LEU	3.6
1	D	426	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	165	ILE	3.6
1	D	290	GLY	3.5
1	D	155	LEU	3.5
1	D	260	PHE	3.5
1	D	277	PRO	3.5
1	D	327	ALA	3.5
1	D	310	PHE	3.5
1	D	272	TYR	3.4
1	D	210	GLU	3.4
1	D	231	ASN	3.4
1	D	461	PHE	3.4
1	D	164	VAL	3.4
1	A	437	GLY	3.3
1	D	336	ILE	3.3
1	D	181	PRO	3.3
1	D	261	PHE	3.3
1	D	243	SER	3.3
1	D	212	VAL	3.3
1	D	268	VAL	3.2
1	D	463	SER	3.1
1	C	437	GLY	3.1
1	D	345	TRP	3.1
1	B	340	PRO	3.1
1	D	359	LEU	3.1
1	D	234	ILE	3.1
1	D	216	GLN	3.1
1	D	284	VAL	3.1
1	D	157	THR	3.1
1	B	437	GLY	3.1
1	C	575	ALA	3.1
1	D	213	ALA	3.1
1	D	460	ALA	3.1
1	B	322	TRP	3.0
1	B	254	PRO	3.0
1	D	209	LEU	3.0
1	A	557	SER	3.0
1	D	307	SER	3.0
1	D	283	GLU	3.0
1	D	179	TYR	3.0
1	D	206	TYR	3.0
1	D	419	ALA	3.0
1	C	534	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLU	3.0
1	D	252	LEU	2.9
1	D	323	VAL	2.9
1	B	433	ASP	2.9
1	D	185	PHE	2.9
1	D	237	PHE	2.9
1	D	672	TRP	2.9
1	C	609	VAL	2.9
1	C	528	LEU	2.9
1	D	168	ASP	2.9
1	D	270	ALA	2.9
1	D	357	LEU	2.8
1	D	347	PHE	2.8
1	D	166	THR	2.8
1	D	282	GLN	2.8
1	C	658	GLY	2.7
1	D	143	CYS	2.7
1	D	325	ALA	2.7
1	D	315	VAL	2.7
1	B	243	SER	2.7
1	D	180	SER	2.7
1	D	500	SER	2.7
1	D	229	TRP	2.7
1	D	242	THR	2.7
1	B	315	VAL	2.7
1	D	302	VAL	2.7
1	B	257	THR	2.7
1	D	331	ASP	2.7
1	B	191	GLY	2.7
1	D	291	GLY	2.7
1	D	334	ILE	2.7
1	B	555	CYS	2.7
1	D	150	ALA	2.6
1	C	522	PHE	2.6
1	D	316	PHE	2.6
1	B	263	ASN	2.6
1	D	433	ASP	2.6
1	B	407	THR	2.6
1	D	182	PRO	2.6
1	A	143	CYS	2.6
1	D	351	PHE	2.6
1	D	305	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	392	LEU	2.6
1	A	555	CYS	2.6
1	D	285	ALA	2.6
1	D	233	PRO	2.6
1	D	188	ALA	2.6
1	D	301	PRO	2.6
1	D	553	THR	2.6
1	D	247	SER	2.6
1	D	244	GLN	2.5
1	D	308	ASN	2.5
1	B	162	GLY	2.5
1	D	241	SER	2.5
1	D	286	TYR	2.5
1	D	499	LEU	2.5
1	C	477	THR	2.5
1	D	409	PHE	2.5
1	B	159	VAL	2.5
1	D	187	ASN	2.5
1	D	300	ASN	2.5
1	C	499	LEU	2.4
1	D	673	GLN	2.4
1	D	407	THR	2.4
1	B	142	SER	2.4
1	D	324	MET	2.4
1	D	303	LEU	2.4
1	D	169	TYR	2.4
1	D	147	SER	2.4
1	D	384	ILE	2.4
1	D	238	PRO	2.4
1	B	306	GLY	2.4
1	C	554	LYS	2.4
1	A	500	SER	2.4
1	C	510	VAL	2.4
1	D	148	LEU	2.4
1	B	532	ALA	2.3
1	B	536	ALA	2.3
1	D	250	ALA	2.3
1	C	578	THR	2.3
1	C	515	VAL	2.3
1	C	577	LEU	2.3
1	C	315	VAL	2.3
1	D	248	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	142	SER	2.3
1	D	563	SER	2.3
1	D	251	VAL	2.3
1	D	265	THR	2.3
1	C	533	ILE	2.3
1	B	305	VAL	2.3
1	D	202	LEU	2.2
1	D	274	LEU	2.2
1	D	326	VAL	2.3
1	B	239	PRO	2.2
1	C	553	THR	2.2
1	D	314	LYS	2.2
1	D	356	LEU	2.2
1	B	610	ASP	2.2
1	D	167	GLY	2.2
1	D	273	THR	2.2
1	D	348	ALA	2.2
1	D	458	ALA	2.2
1	D	322	TRP	2.2
1	C	612	LEU	2.2
1	B	281	VAL	2.2
1	C	420	ASP	2.2
1	C	514	ASN	2.2
1	D	404	PHE	2.2
1	D	153	THR	2.2
1	D	366	LEU	2.1
1	D	599	PHE	2.1
1	D	199	THR	2.1
1	D	338	THR	2.1
1	D	344	SER	2.1
1	B	286	TYR	2.1
1	B	271	VAL	2.1
1	C	529	PRO	2.1
1	B	163	THR	2.1
1	D	335	GLU	2.1
1	D	490	LEU	2.1
1	D	538	LEU	2.1
1	C	660	GLN	2.1
1	A	510	VAL	2.1
1	B	477	THR	2.1
1	B	652	THR	2.1
1	D	451	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	531	ALA	2.1
1	D	193	HIS	2.1
1	D	342	LEU	2.1
1	D	204	TYR	2.1
1	D	369	VAL	2.1
1	C	580	GLY	2.1
1	D	221	ALA	2.0
1	A	534	GLN	2.0
1	D	220	HIS	2.0
1	B	262	PRO	2.0
1	D	262	PRO	2.0
1	C	606	TYR	2.0
1	D	218	TRP	2.0
1	A	563	SER	2.0
1	B	161	THR	2.0
1	D	257	THR	2.0
1	D	343	THR	2.0
1	B	342	LEU	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($\text{\AA}^2$)	Q<0.9
2	MAN	E	4	11/12	0.42	0.17	88,100,106,107	0
5	MAN	H	4	11/12	0.51	0.16	98,111,113,113	0
2	BMA	K	3	11/12	0.56	0.14	80,87,90,97	0
2	MAN	K	4	11/12	0.57	0.13	95,102,105,108	0
6	BMA	M	3	11/12	0.65	0.11	97,104,113,117	0
3	NAG	F	2	14/15	0.67	0.14	92,107,121,121	0
3	NAG	I	2	14/15	0.68	0.13	94,119,124,124	0
5	BMA	H	3	11/12	0.68	0.11	81,84,89,101	0
4	GLA	N	3	11/12	0.69	0.18	81,86,91,92	0
4	GLC	N	2	11/12	0.69	0.17	64,80,84,85	0

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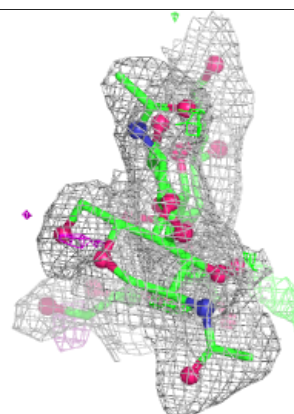
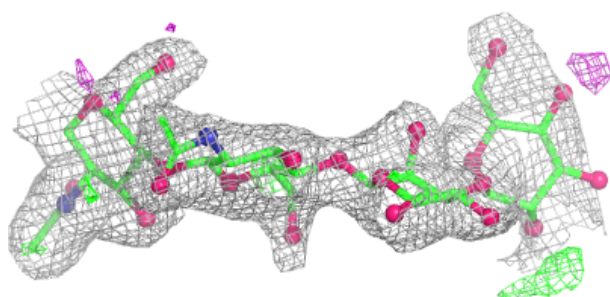
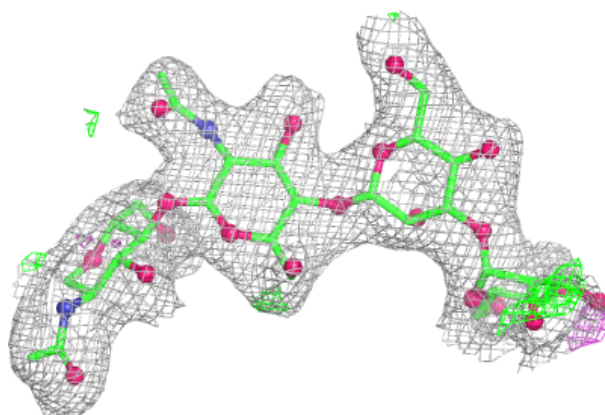
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLA	L	3	11/12	0.73	0.18	70,76,86,88	0
5	MAN	H	5	11/12	0.76	0.17	77,89,99,100	0
4	GLA	J	3	11/12	0.76	0.17	69,75,81,86	0
6	NAG	M	2	14/15	0.79	0.13	78,88,94,95	0
2	NAG	K	2	14/15	0.80	0.12	72,77,81,81	0
6	NAG	M	1	14/15	0.81	0.13	52,66,80,84	0
4	GLA	G	3	11/12	0.82	0.13	55,61,65,66	0
2	BMA	E	3	11/12	0.83	0.10	68,71,72,74	0
4	FRU	N	1	12/12	0.83	0.15	52,65,72,73	0
2	NAG	E	2	14/15	0.86	0.10	51,58,66,72	0
2	NAG	E	1	14/15	0.86	0.10	38,47,51,51	0
2	NAG	K	1	14/15	0.87	0.10	50,55,64,65	0
5	NAG	H	2	14/15	0.87	0.10	68,76,80,81	0
4	GLC	J	2	11/12	0.92	0.08	50,52,58,58	0
3	NAG	F	1	14/15	0.92	0.08	42,50,61,75	0
5	NAG	H	1	14/15	0.92	0.08	46,53,57,67	0
3	NAG	I	1	14/15	0.92	0.08	48,57,64,77	0
4	FRU	J	1	12/12	0.92	0.09	37,43,47,54	0
4	GLC	G	2	11/12	0.94	0.07	33,38,41,50	0
4	GLC	L	2	11/12	0.94	0.07	38,40,46,49	0
4	FRU	L	1	12/12	0.95	0.07	36,38,42,50	0
4	FRU	G	1	12/12	0.97	0.06	27,29,38,44	0

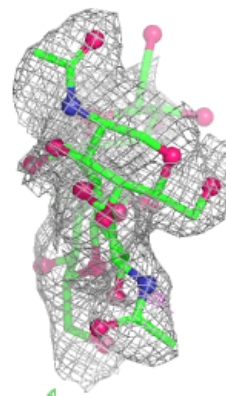
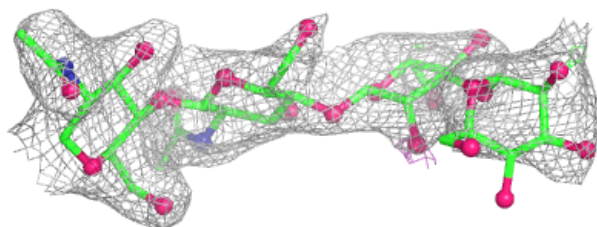
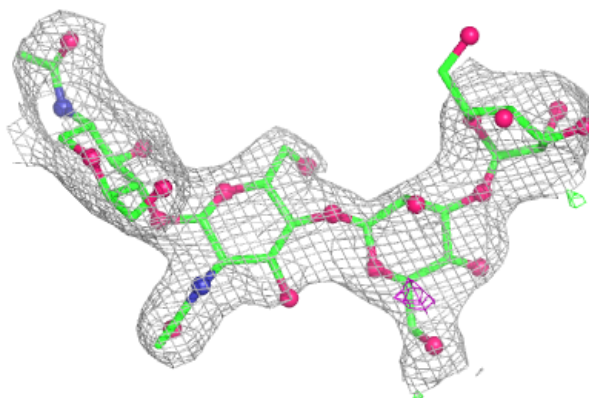
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

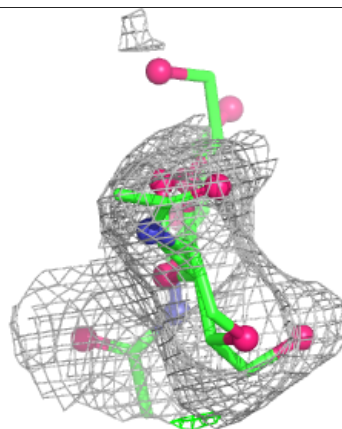
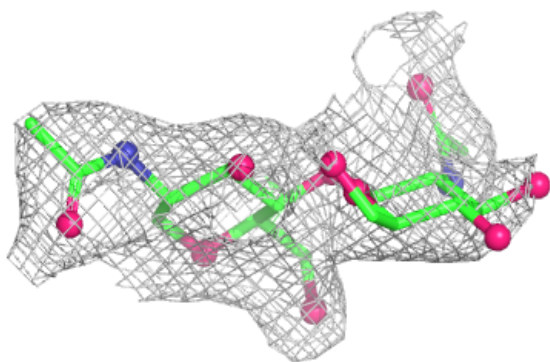
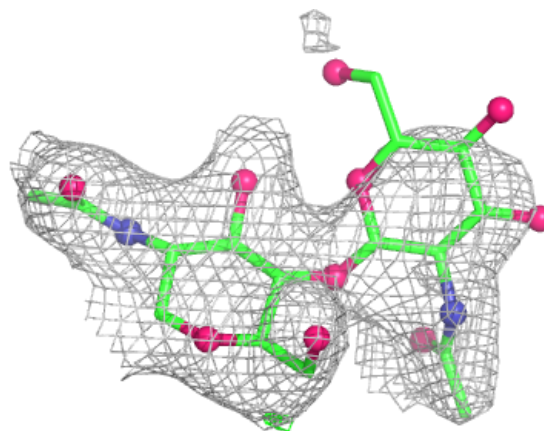
**Electron density around Chain K:**

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

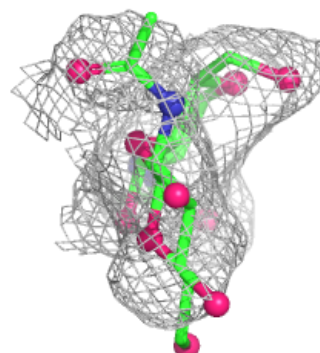
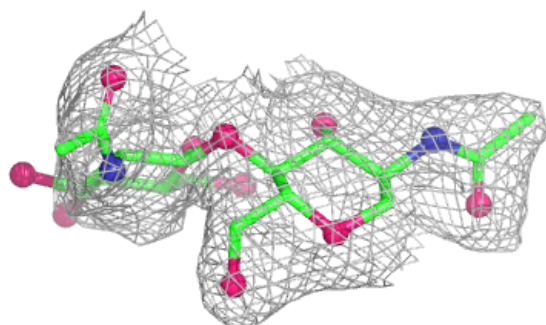
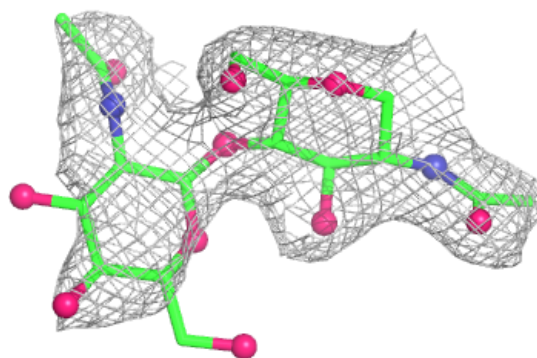


Electron density around Chain F:

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

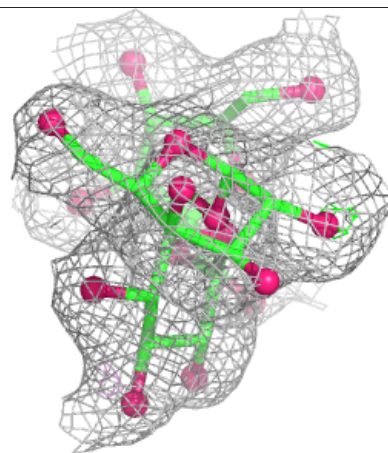
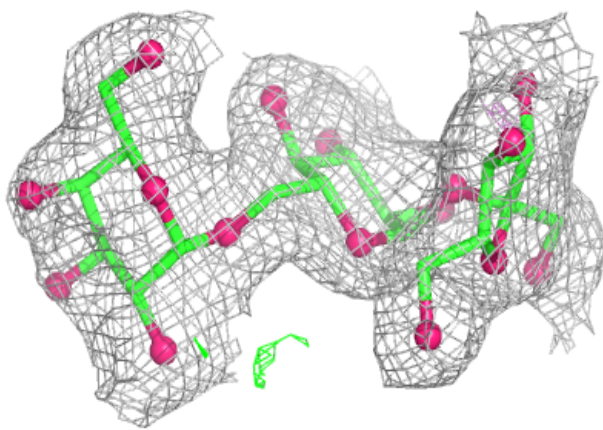
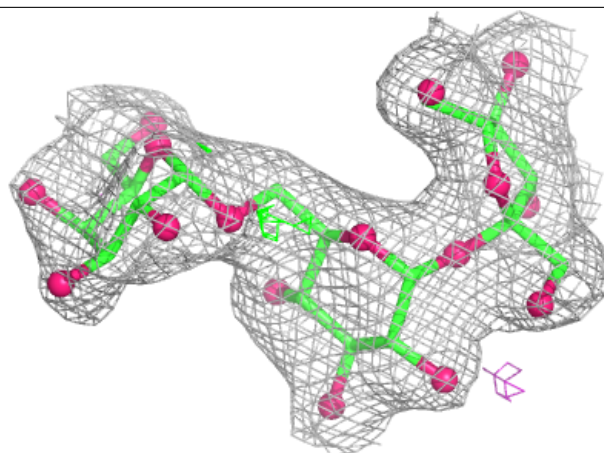
**Electron density around Chain I:**

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



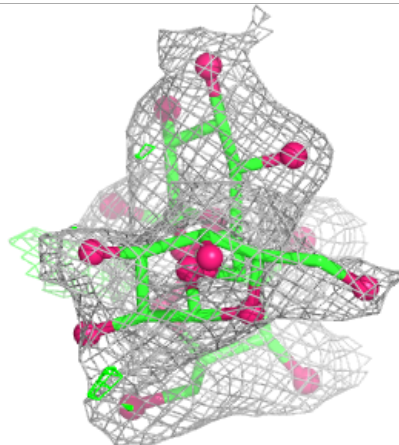
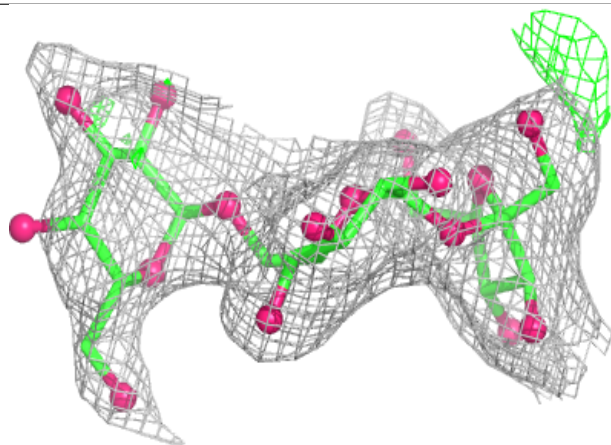
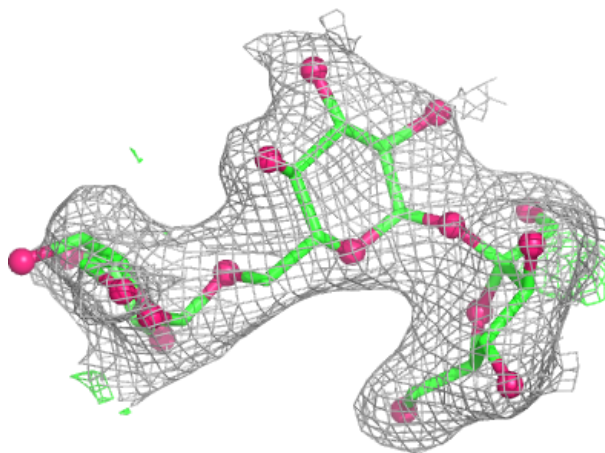
Electron density around Chain G:

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



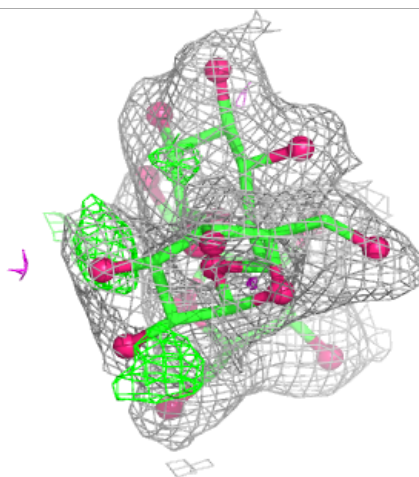
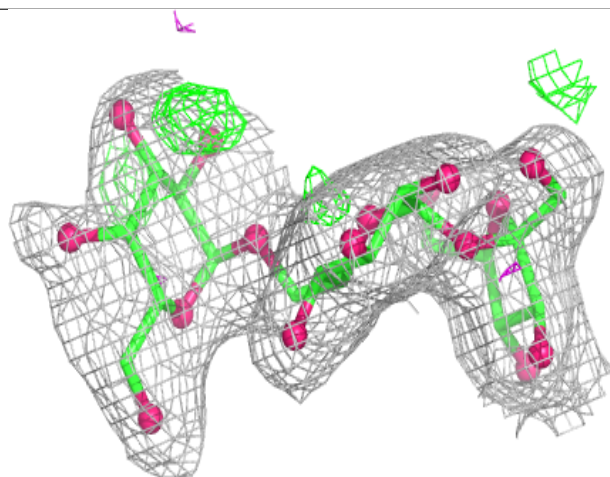
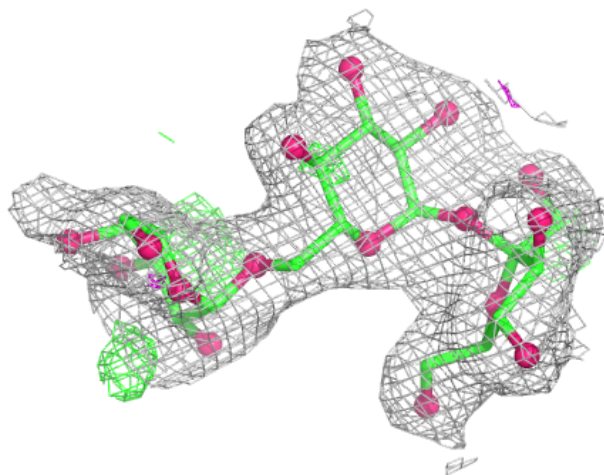
Electron density around Chain J:

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



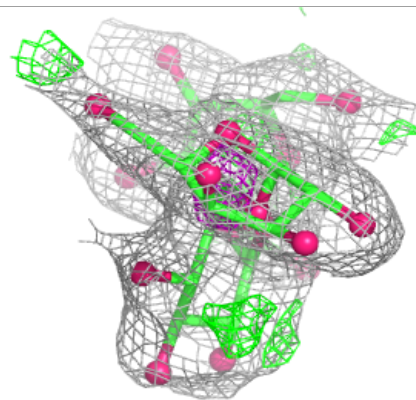
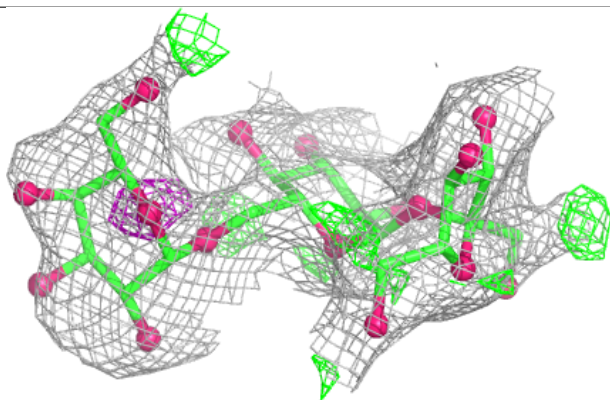
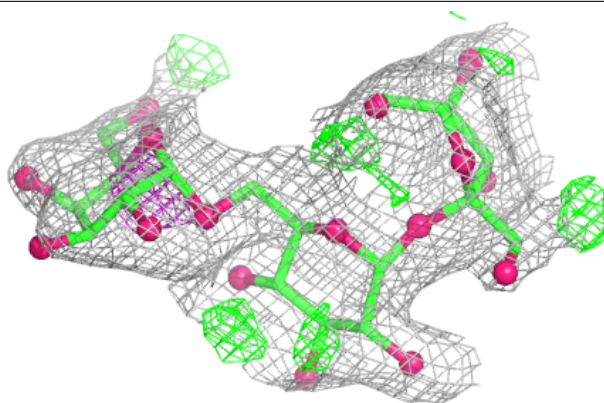
Electron density around Chain L:

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

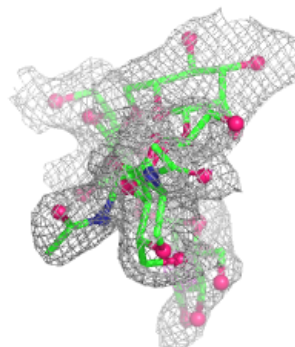
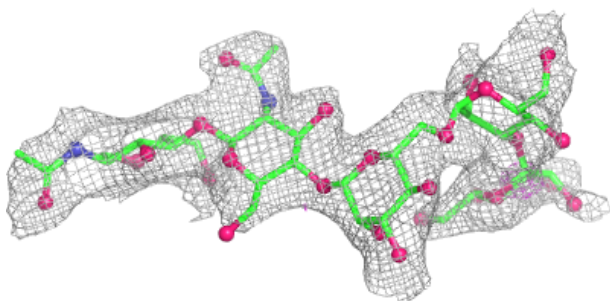
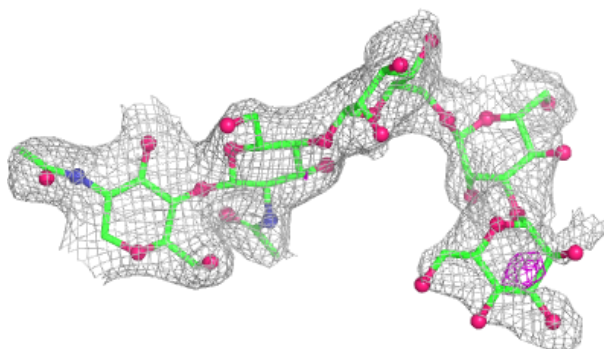


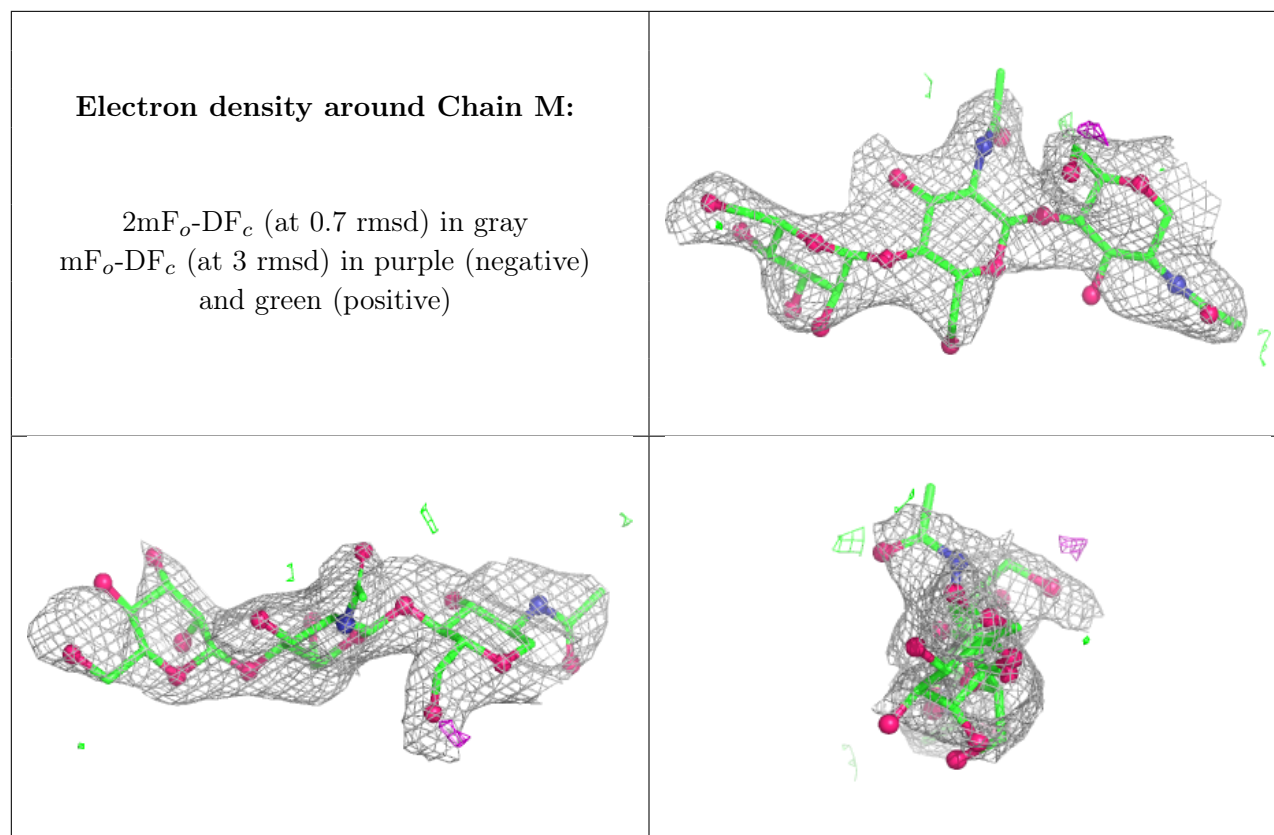
Electron density around Chain N:

$2mF_o-DF_c$ (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 ⓘ

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	A	702	11/12	0.41	0.15	77,91,94,95	0
7	MAN	D	702	11/12	0.47	0.14	97,105,113,116	0
8	NAG	B	705	14/15	0.58	0.20	71,85,90,90	14
7	MAN	D	703	11/12	0.62	0.15	27,28,30,31	11
8	NAG	D	708	14/15	0.65	0.16	79,93,98,99	0
8	NAG	D	704	14/15	0.66	0.15	76,85,96,97	0
7	MAN	D	701	11/12	0.66	0.16	86,92,94,97	11
8	NAG	C	705	14/15	0.67	0.14	91,96,100,102	0
8	NAG	C	708	14/15	0.68	0.14	94,101,109,114	0
8	NAG	C	709	14/15	0.69	0.13	69,87,91,92	0
8	NAG	D	707	14/15	0.70	0.15	78,84,89,93	0
7	MAN	B	703	11/12	0.70	0.13	96,105,113,120	0
8	NAG	B	709	14/15	0.72	0.13	97,106,111,112	0
7	MAN	A	703	11/12	0.74	0.11	80,86,89,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	A	714	14/15	0.74	0.14	66,78,83,83	0
8	NAG	C	710	14/15	0.75	0.14	73,81,83,89	0
8	NAG	A	711	14/15	0.75	0.14	68,80,92,93	0
7	MAN	C	701	11/12	0.76	0.13	80,88,94,95	0
8	NAG	B	708	14/15	0.76	0.13	58,76,92,95	0
7	MAN	B	701	11/12	0.77	0.10	86,91,102,103	0
7	MAN	A	701	11/12	0.77	0.12	72,76,88,89	0
8	NAG	A	708	14/15	0.77	0.17	63,68,70,71	14
8	NAG	B	706	14/15	0.79	0.12	76,85,89,91	0
7	MAN	A	704	11/12	0.80	0.13	65,69,75,84	0
7	MAN	A	705	11/12	0.80	0.15	74,77,82,82	0
7	MAN	C	703	11/12	0.81	0.16	56,76,81,88	0
8	NAG	D	705	14/15	0.81	0.10	61,64,68,68	0
8	NAG	D	706	14/15	0.81	0.12	53,66,79,83	0
8	NAG	A	713	14/15	0.81	0.12	67,72,78,79	0
8	NAG	C	707	14/15	0.81	0.13	51,66,75,79	0
8	NAG	C	706	14/15	0.82	0.12	75,82,89,90	0
8	NAG	A	707	14/15	0.84	0.13	53,59,66,66	0
8	NAG	A	712	14/15	0.85	0.12	54,59,79,82	0
9	PEG	B	702	7/7	0.85	0.16	62,68,70,71	0
8	NAG	C	704	14/15	0.86	0.10	53,59,63,64	0
8	NAG	A	709	14/15	0.87	0.10	51,58,71,71	0
8	NAG	B	704	14/15	0.88	0.09	66,80,85,87	0
8	NAG	A	706	14/15	0.88	0.12	68,77,84,86	0
8	NAG	B	707	14/15	0.91	0.08	48,56,64,65	0
8	NAG	A	710	14/15	0.92	0.08	46,49,53,53	0
7	MAN	C	702	11/12	0.92	0.09	54,58,61,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.