



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:09 PM UTC

PDB ID : 8BES / pdb_00008bes
Title : Structure of D188A-fructofuranosidase from *Rhodotorula dairenensis* in complex with fructose
Authors : Jimenez-Ortega, E.; Sanz-Aparicio, J.
Deposited on : 2022-10-21
Resolution : 1.86 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

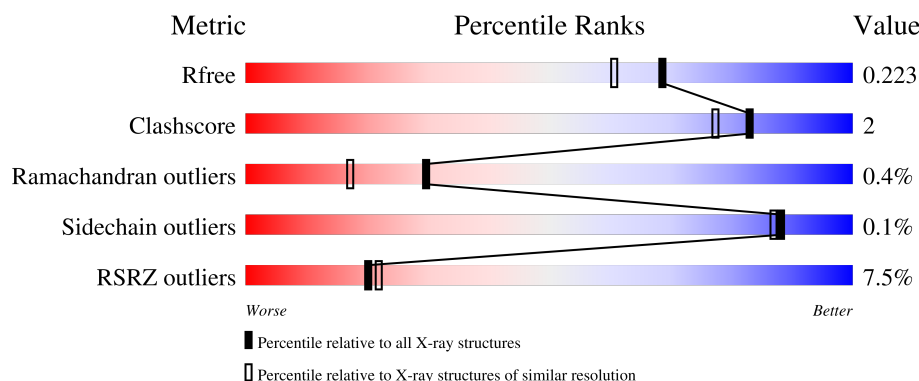
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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.



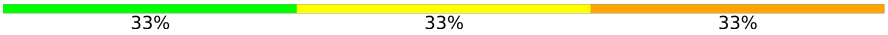
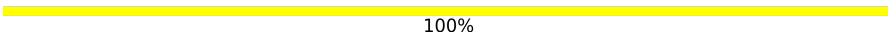
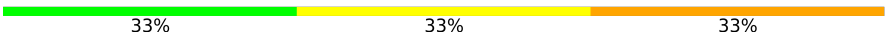
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	2% 74% • 22%
1	B	675	4% 74% • 22%
1	C	675	4% 75% • 22%
1	D	675	13% 73% • 22%
2	E	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 33% 33%
3	K	3	 67% 33%
4	G	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 100%
4	L	2	 50% 50%
5	H	6	 33% 33% 33%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 19127 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	526	Total	C	N	O	S	0	7	0
			4085	2599	665	810	11			
1	B	526	Total	C	N	O	S	0	2	0
			4052	2579	659	803	11			
1	C	524	Total	C	N	O	S	0	1	0
			4034	2570	657	796	11			
1	D	524	Total	C	N	O	S	0	0	0
			4026	2566	655	794	11			

There are 4 discrepancies between the modelled and reference sequences:

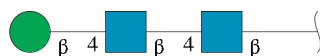
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
B	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
C	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
D	188	ALA	ASP	engineered mutation	UNP A0A856TAI5

- 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.



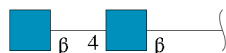
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



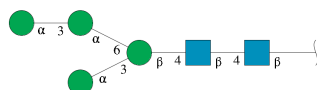
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

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



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

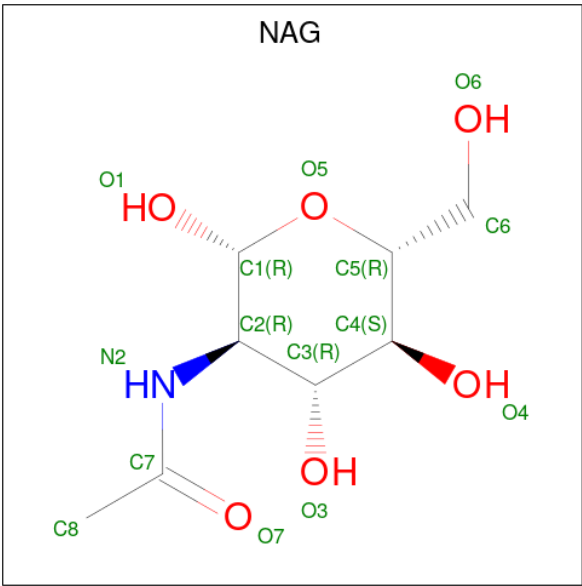
- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



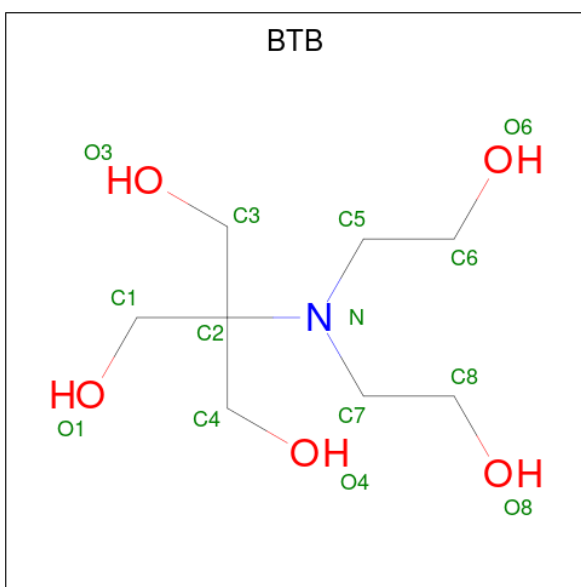
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1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

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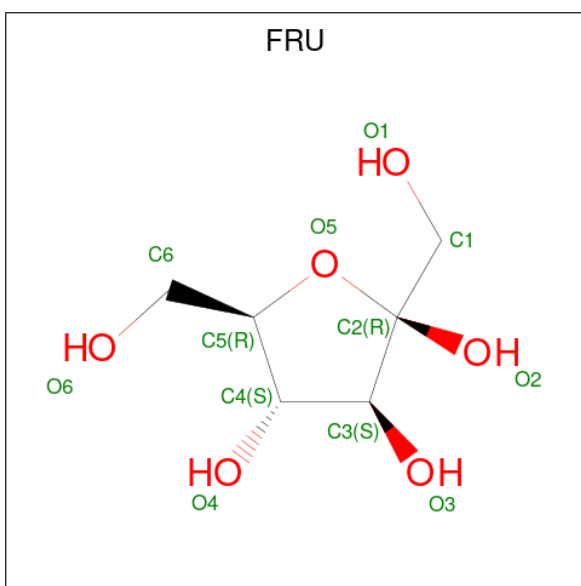
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



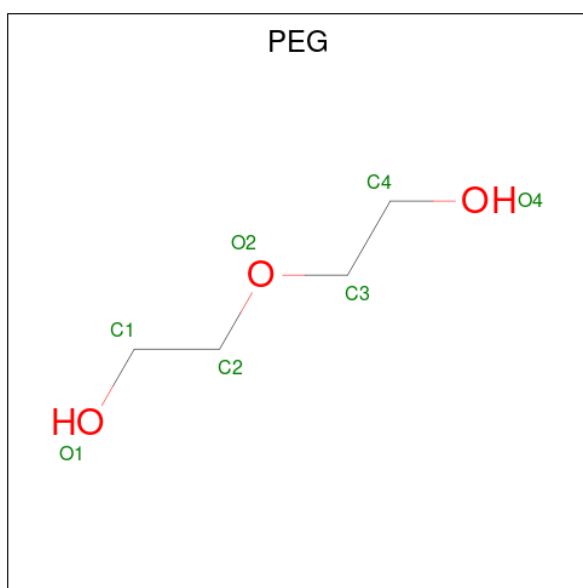
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is beta-D-fructofuranose (CCD ID: FRU) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			12	6	6		
9	B	1	Total	C	O	0	0
			12	6	6		
9	C	1	Total	C	O	0	0
			12	6	6		
9	D	1	Total	C	O	0	0
			12	6	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			7	4	3		

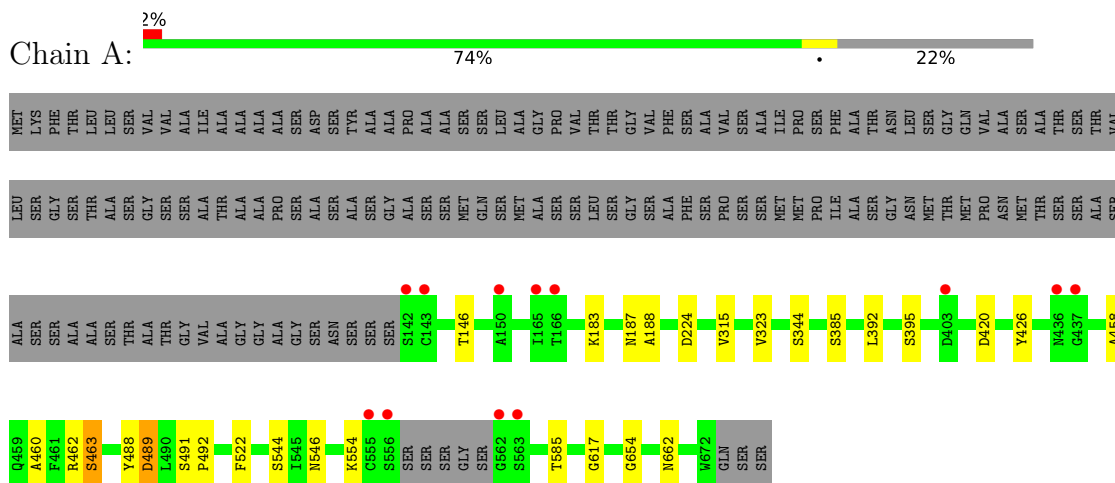
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	572	Total	O	0	0
			572	572		
11	B	502	Total	O	0	0
			502	502		
11	C	446	Total	O	0	0
			446	446		
11	D	452	Total	O	0	0
			452	452		

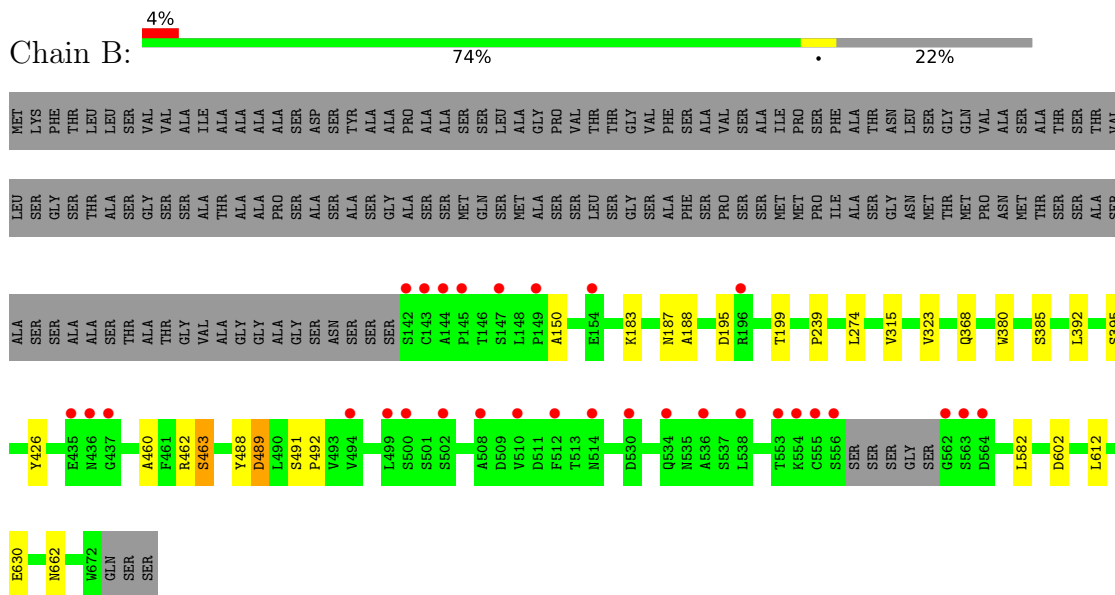
3 Residue-property plots

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

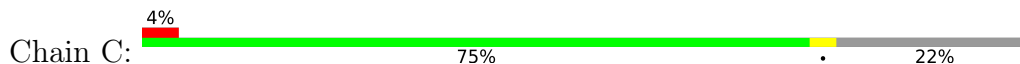
- Molecule 1: Beta-fructofuranosidase

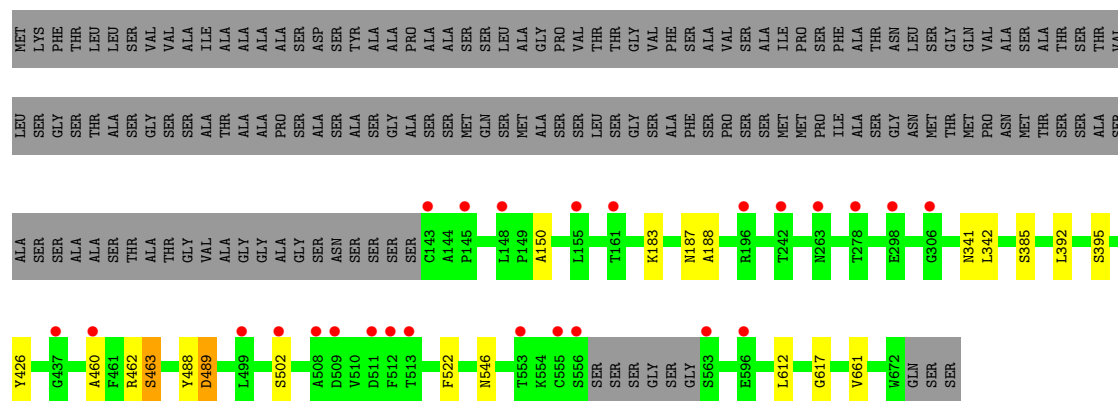


- Molecule 1: Beta-fructofuranosidase

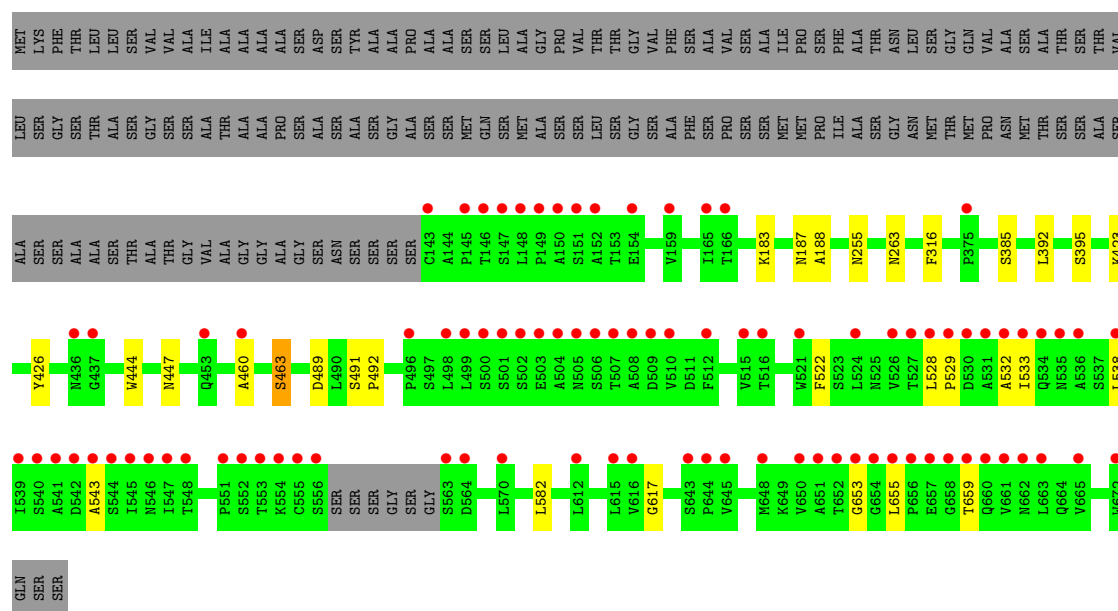
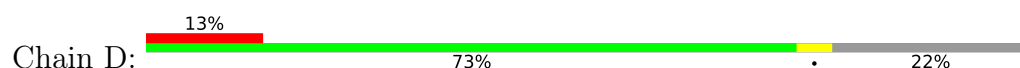


- Molecule 1: Beta-fructofuranosidase





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



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

Chain K:  67% 33%


MAG1
MAG2
BMA3

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

Chain G:  50% 50%

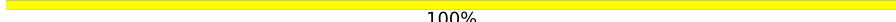

MAG1
MAG2

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

Chain I:  50% 50%


MAG1
MAG2

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

Chain J:  100%

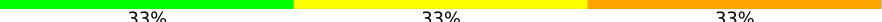

MAG1
MAG2

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

Chain L:  50% 50%


MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.85Å 112.69Å 139.62Å 90.00° 104.90° 90.00°	Depositor
Resolution (Å)	45.74 – 1.86 45.74 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.74-1.86) 99.9 (45.74-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.217 0.192 , 0.223	Depositor DCC
R_{free} test set	10109 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19127	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: BMA, NAG, MAN, FRU, PEG, BTB

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	0.95	0/4216	1.14	1/5797 (0.0%)
1	B	0.95	0/4180	1.15	1/5748 (0.0%)
1	C	0.95	0/4162	1.16	0/5724
1	D	0.96	0/4154	1.17	0/5713
All	All	0.95	0/16712	1.16	2/22982 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	602	ASP	CA-CB-CG	5.17	117.77	112.60

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	4085	0	3794	21	0
1	B	4052	0	3762	20	0
1	C	4034	0	3748	15	0
1	D	4026	0	3747	20	0
2	E	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	39	0	34	1	0
3	K	39	0	34	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	1	0
4	L	28	0	25	0	0
5	H	72	0	61	1	0
6	A	33	0	30	2	0
6	B	22	0	20	1	0
6	C	55	0	50	1	0
6	D	33	0	30	0	0
7	A	126	0	117	7	0
7	B	84	0	78	5	0
7	C	98	0	91	1	0
7	D	84	0	78	1	0
8	A	14	0	19	0	0
8	B	14	0	19	1	0
8	C	14	0	19	0	0
8	D	14	0	19	1	0
9	A	12	0	12	0	0
9	B	12	0	12	0	0
9	C	12	0	12	0	0
9	D	12	0	12	0	0
10	D	7	0	10	1	0
11	A	572	0	0	0	0
11	B	502	0	0	3	0
11	C	446	0	0	0	0
11	D	452	0	0	3	0
All	All	19127	0	15951	80	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 2.

All (80) 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:263:ASN:HB3	11:D:1138:HOH:O	1.72	0.89
11:B:1302:HOH:O	3:F:3:BMA:H4	1.70	0.89
1:C:392:LEU:HD23	1:D:392:LEU:HD23	1.67	0.77
1:B:274:LEU:HD21	7:B:703:NAG:H62	1.73	0.70
1:C:150:ALA:HA	6:C:703:MAN:H3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ASN:ND2	7:B:707:NAG:O7	2.25	0.69
1:A:146:THR:HG21	6:A:701:MAN:H5	1.75	0.68
1:A:392:LEU:HD23	1:B:392:LEU:HD23	1.74	0.67
1:D:655:LEU:O	7:D:709:NAG:H3	1.96	0.66
1:B:385:SER:HB3	1:B:426:TYR:CE1	2.34	0.63
1:A:385:SER:HB3	1:A:426:TYR:CE1	2.34	0.63
1:B:274:LEU:HD21	7:B:703:NAG:C6	2.30	0.62
1:D:529:PRO:HD3	1:D:659:THR:OG1	1.99	0.62
1:B:368:GLN:HG3	1:B:380:TRP:CE2	2.35	0.62
1:A:546:ASN:HD22	7:A:712:NAG:H83	1.66	0.61
1:D:395:SER:HB2	1:D:426:TYR:CD1	2.37	0.59
1:D:385:SER:HB3	1:D:426:TYR:CE1	2.39	0.58
1:A:395:SER:HB2	1:A:426:TYR:CD1	2.39	0.58
1:C:395:SER:HB2	1:C:426:TYR:CD1	2.40	0.56
1:C:385:SER:HB3	1:C:426:TYR:CE1	2.40	0.56
1:D:316:PHE:HB2	10:D:701:PEG:H32	1.86	0.56
1:B:395:SER:HB2	1:B:426:TYR:CD1	2.40	0.56
1:A:458:ALA:HA	6:A:702:MAN:H62	1.88	0.56
1:D:528:LEU:HB2	1:D:533:ILE:HD11	1.88	0.55
1:C:183:LYS:HA	1:C:460:ALA:O	2.06	0.55
1:D:187:ASN:ND2	1:D:188:ALA:H	2.06	0.53
1:D:255:ASN:HB3	11:D:871:HOH:O	2.10	0.51
1:A:187:ASN:ND2	1:A:188:ALA:H	2.08	0.51
1:A:224[B]:ASP:C	1:A:224[B]:ASP:OD2	2.55	0.50
1:A:662:ASN:ND2	7:A:710:NAG:O7	2.41	0.49
7:B:704:NAG:H62	11:B:1237:HOH:O	2.12	0.48
1:C:462:ARG:O	1:C:463:SER:HB2	2.12	0.48
1:B:462:ARG:O	1:B:463:SER:HB2	2.13	0.48
1:B:630:GLU:HG3	11:B:1245:HOH:O	2.13	0.48
1:C:522:PHE:CE1	1:C:617:GLY:HA3	2.48	0.47
7:C:711:NAG:H82	7:C:711:NAG:H3	1.95	0.47
1:D:385:SER:HB3	1:D:426:TYR:CZ	2.50	0.47
1:D:255:ASN:CB	11:D:871:HOH:O	2.63	0.47
1:C:488:TYR:O	1:C:489:ASP:C	2.59	0.46
5:H:3:BMA:H4	5:H:4:MAN:H5	1.98	0.46
1:A:462:ARG:O	1:A:463:SER:HB2	2.16	0.46
1:B:150:ALA:HA	6:B:701:MAN:H5	1.98	0.46
1:D:543:ALA:HA	1:D:653:GLY:O	2.16	0.45
1:C:385:SER:HB3	1:C:426:TYR:CZ	2.51	0.45
1:A:183:LYS:HA	1:A:460:ALA:O	2.17	0.45
1:B:385:SER:HB3	1:B:426:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:SER:HB3	1:A:426:TYR:CZ	2.51	0.44
1:D:423:LYS:HG2	1:D:447:ASN:ND2	2.33	0.44
1:B:239:PRO:HG3	7:B:703:NAG:H62	2.00	0.43
1:A:546:ASN:HD22	7:A:712:NAG:C7	2.31	0.43
1:A:546:ASN:HD22	7:A:712:NAG:C8	2.30	0.43
1:B:183:LYS:HA	1:B:460:ALA:O	2.18	0.43
1:C:187:ASN:ND2	1:C:188:ALA:H	2.16	0.43
1:A:522:PHE:CE1	1:A:617:GLY:HA3	2.53	0.43
1:B:488:TYR:O	1:B:489:ASP:C	2.62	0.43
8:B:709:BTB:H72	8:B:709:BTB:O3	2.17	0.42
1:C:546:ASN:HD22	4:J:1:NAG:C7	2.32	0.42
1:B:187:ASN:ND2	1:B:188:ALA:H	2.18	0.42
1:C:341:ASN:O	1:C:342:LEU:HB2	2.19	0.42
1:B:491:SER:N	1:B:492:PRO:CD	2.83	0.42
1:D:491:SER:N	1:D:492:PRO:CD	2.83	0.42
1:A:488:TYR:O	1:A:489:ASP:C	2.63	0.41
1:A:491:SER:N	1:A:492:PRO:CD	2.83	0.41
1:B:195:ASP:OD2	1:B:199:THR:HB	2.20	0.41
1:B:582:LEU:HD23	1:B:582:LEU:C	2.45	0.41
1:C:522:PHE:CZ	1:C:617:GLY:HA3	2.55	0.41
1:D:532:ALA:HA	1:D:538:LEU:HD12	2.02	0.41
1:D:183:LYS:HA	1:D:460:ALA:O	2.20	0.41
1:C:612:LEU:C	1:C:612:LEU:HD23	2.46	0.41
1:A:654:GLY:HA2	7:A:708:NAG:H62	2.03	0.41
1:A:315:VAL:HA	1:A:323:VAL:O	2.21	0.41
1:A:544:SER:OG	7:A:712:NAG:N2	2.34	0.41
1:C:502:SER:HA	1:C:661:VAL:O	2.21	0.41
1:D:582:LEU:C	1:D:582:LEU:HD23	2.45	0.41
8:D:711:BTB:H72	8:D:711:BTB:O3	2.19	0.41
1:A:344:SER:CB	7:A:705:NAG:H5	2.51	0.40
1:B:612:LEU:HD23	1:B:612:LEU:C	2.46	0.40
1:D:444:TRP:HE1	1:D:463:SER:HB3	1.86	0.40
1:B:315:VAL:HA	1:B:323:VAL:O	2.20	0.40
1:D:522:PHE:CE1	1:D:617:GLY:HA3	2.57	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	529/675 (78%)	508 (96%)	19 (4%)	2 (0%)	30	17
1	B	524/675 (78%)	499 (95%)	23 (4%)	2 (0%)	30	17
1	C	521/675 (77%)	499 (96%)	20 (4%)	2 (0%)	30	17
1	D	520/675 (77%)	495 (95%)	23 (4%)	2 (0%)	30	17
All	All	2094/2700 (78%)	2001 (96%)	85 (4%)	8 (0%)	30	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	SER
1	B	463	SER
1	B	489	ASP
1	C	463	SER
1	D	463	SER
1	A	489	ASP
1	C	489	ASP
1	D	489	ASP

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	448/545 (82%)	446 (100%)	2 (0%)	84	82
1	B	443/545 (81%)	443 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	441/545 (81%)	441 (100%)	0	100	100
1	D	440/545 (81%)	440 (100%)	0	100	100
All	All	1772/2180 (81%)	1770 (100%)	2 (0%)	88	87

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

Mol	Chain	Res	Type
1	A	554	LYS
1	A	585	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	354	HIS
1	A	471	ASN
1	A	518	ASN
1	B	187	ASN
1	B	354	HIS
1	B	372	GLN
1	B	449	GLN
1	B	471	ASN
1	B	534	GLN
1	C	187	ASN
1	C	449	GLN
1	C	471	ASN
1	C	518	ASN
1	D	187	ASN
1	D	449	GLN
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 ⓘ

24 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	0.40	0	17,19,21	1.03	1 (5%)
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.98	1 (5%)
2	BMA	E	3	2	11,11,12	0.25	0	15,15,17	0.98	1 (6%)
2	MAN	E	4	2	11,11,12	0.32	0	15,15,17	0.63	0
3	NAG	F	1	3,1	14,14,15	0.34	0	17,19,21	0.91	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	1.11	1 (5%)
3	BMA	F	3	3	11,11,12	0.33	0	15,15,17	1.06	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	1.09	1 (5%)
5	NAG	H	1	5,1	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
5	NAG	H	2	5	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
5	BMA	H	3	5	11,11,12	0.28	0	15,15,17	1.50	1 (6%)
5	MAN	H	4	5	11,11,12	0.40	0	15,15,17	1.12	2 (13%)
5	MAN	H	5	5	11,11,12	0.37	0	15,15,17	0.73	0
5	MAN	H	6	5	11,11,12	0.32	0	15,15,17	0.71	0
4	NAG	I	1	4,1	14,14,15	0.29	0	17,19,21	0.78	0
4	NAG	I	2	4	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	1.05	2 (11%)
3	NAG	K	1	3,1	14,14,15	0.35	0	17,19,21	0.64	0
3	NAG	K	2	3	14,14,15	0.27	0	17,19,21	0.79	0
3	BMA	K	3	3	11,11,12	0.37	0	15,15,17	1.20	1 (6%)
4	NAG	L	1	4,1	14,14,15	0.37	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.29	0	17,19,21	1.04	1 (5%)

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	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	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	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	BMA	C1-O5-C5	4.99	118.87	112.19
3	F	2	NAG	C1-O5-C5	3.82	117.31	112.19
4	L	2	NAG	C1-O5-C5	3.76	117.23	112.19
4	I	2	NAG	C1-O5-C5	3.75	117.21	112.19
3	K	3	BMA	C1-O5-C5	3.65	117.08	112.19
4	G	2	NAG	C1-O5-C5	3.53	116.91	112.19
5	H	2	NAG	C1-O5-C5	3.35	116.68	112.19
2	E	1	NAG	C1-O5-C5	2.90	116.07	112.19
3	F	3	BMA	C1-O5-C5	2.89	116.05	112.19
2	E	2	NAG	C1-O5-C5	2.87	116.03	112.19
2	E	3	BMA	C1-O5-C5	2.71	115.82	112.19
4	J	2	NAG	C1-O5-C5	2.67	115.76	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-O5-C5	2.66	115.75	112.19
3	F	3	BMA	C1-C2-C3	2.31	113.01	109.64
5	H	4	MAN	C1-C2-C3	2.28	112.97	109.64
4	J	2	NAG	C6-C5-C4	-2.27	107.44	113.02
5	H	4	MAN	O5-C5-C6	2.12	111.80	107.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

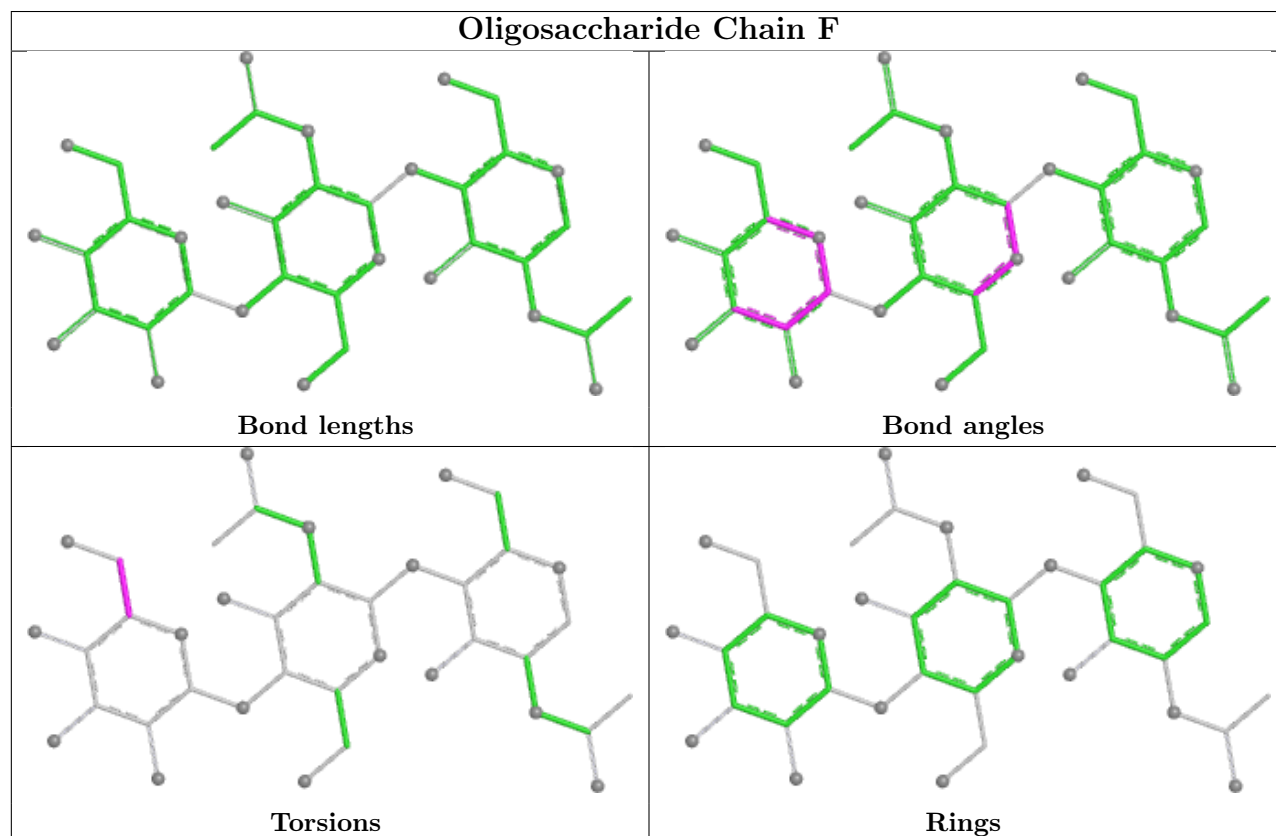
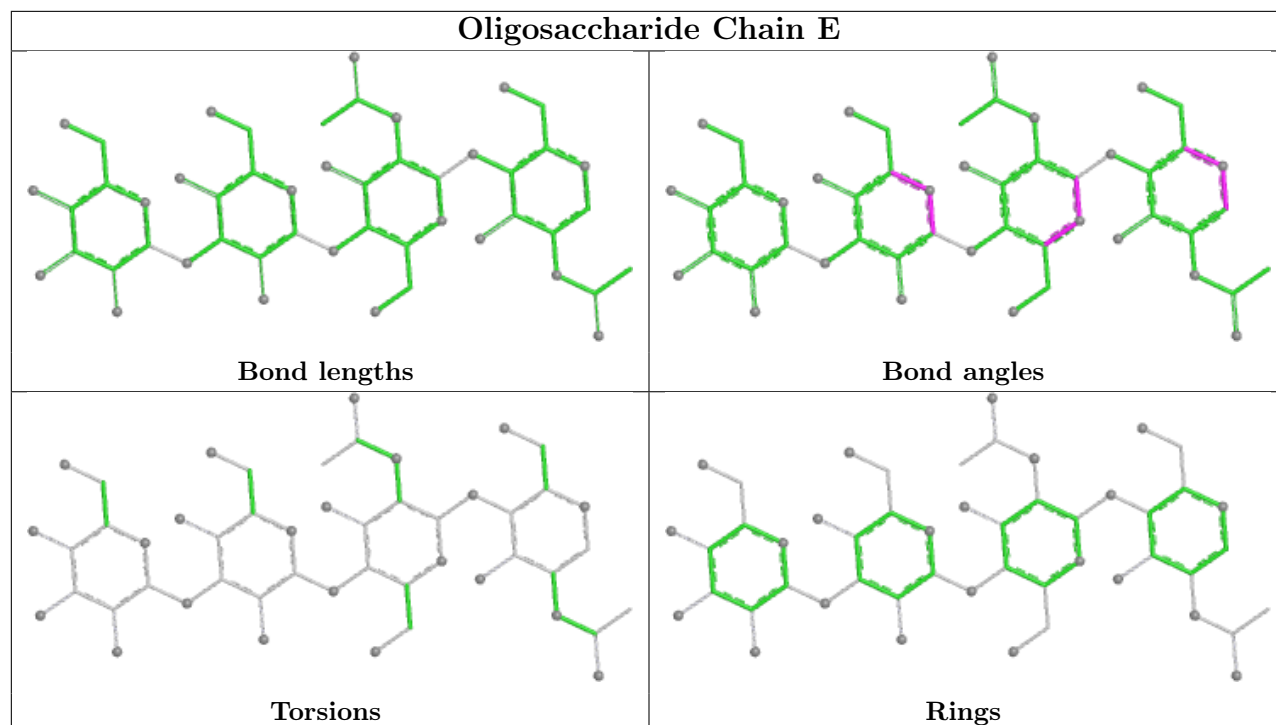
Mol	Chain	Res	Type	Atoms
5	H	5	MAN	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	H	5	MAN	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C1-C2-N2-C7
4	L	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
5	H	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C1-C2-N2-C7
4	J	2	NAG	O5-C5-C6-O6

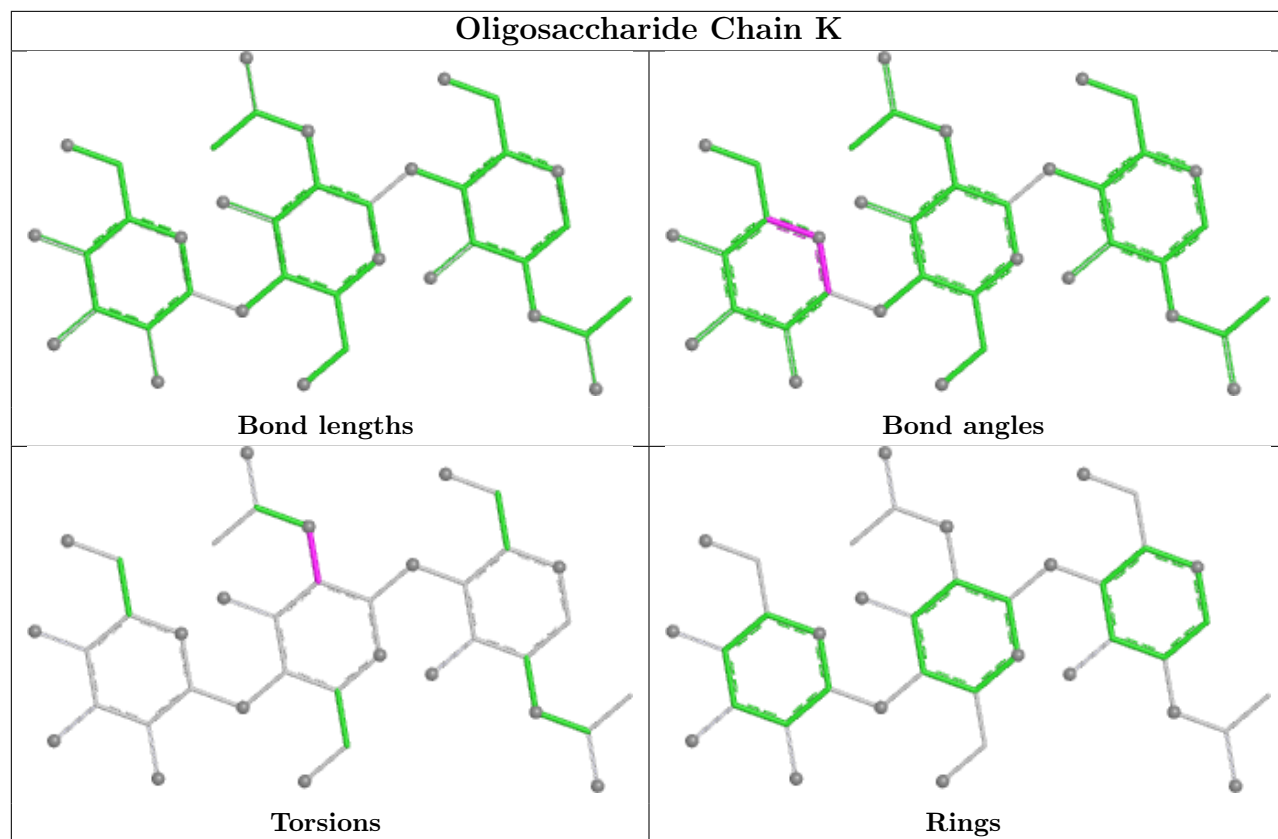
There are no ring outliers.

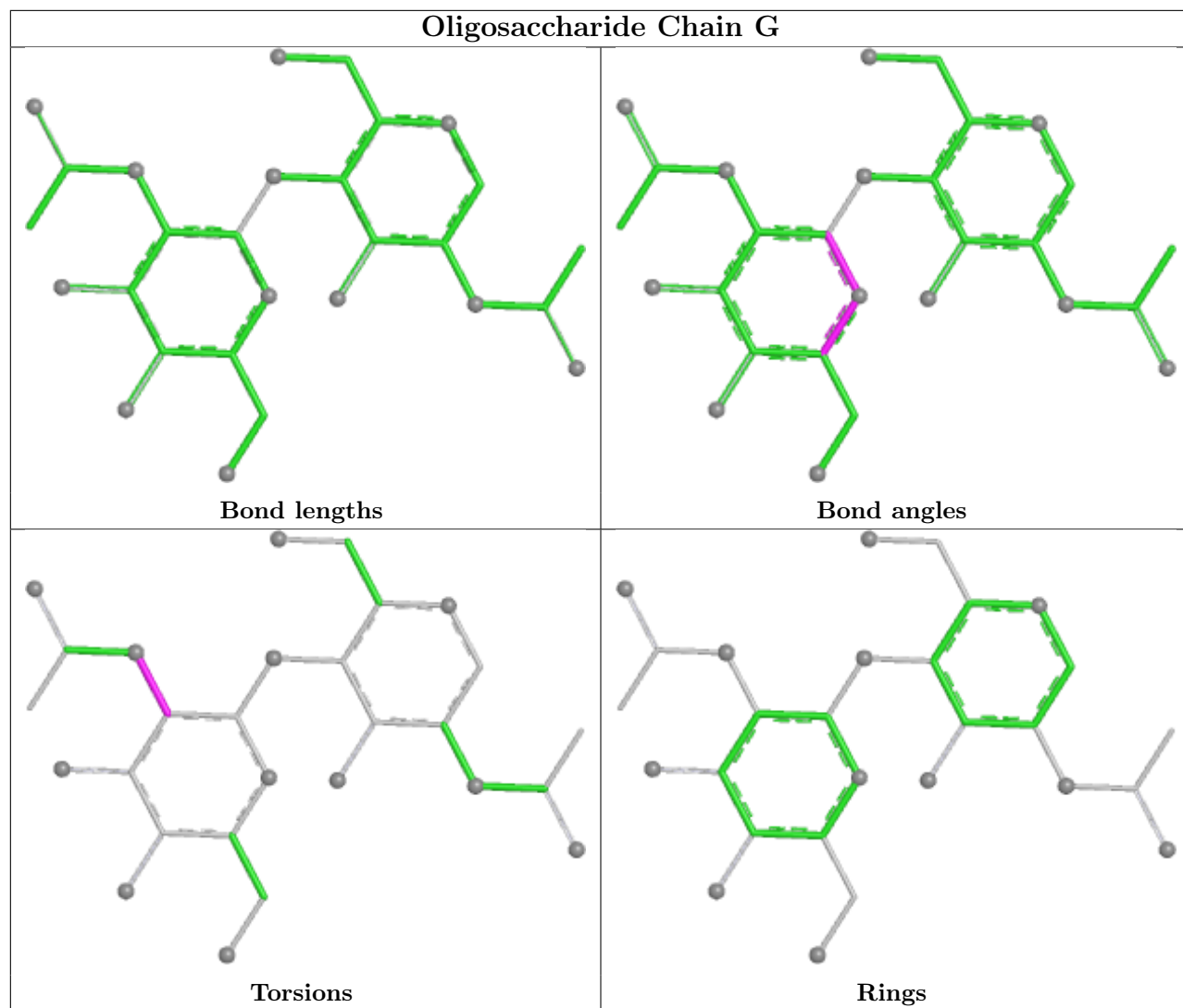
4 monomers are involved in 3 short contacts:

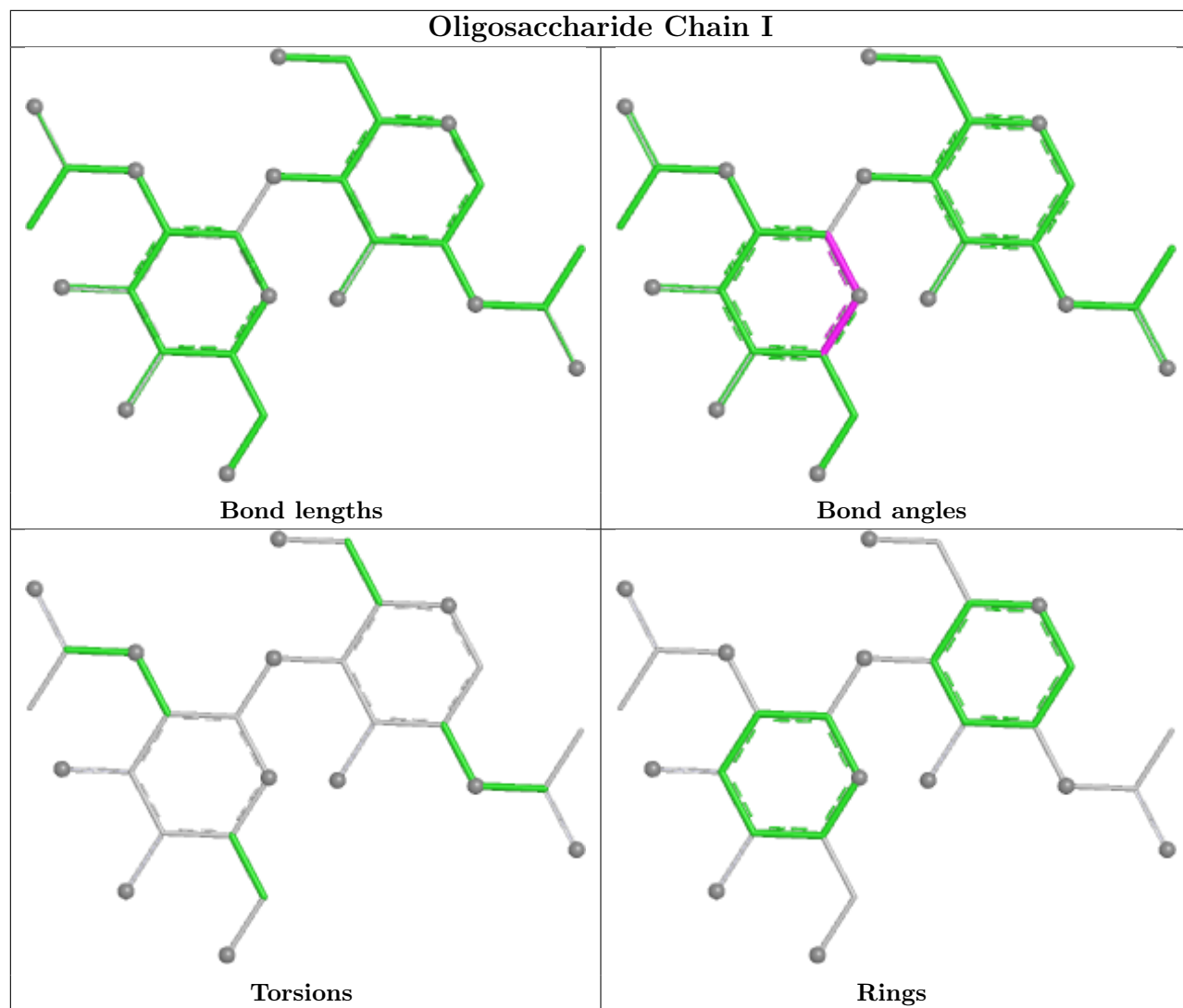
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	1	0
4	J	1	NAG	1	0
5	H	3	BMA	1	0
5	H	4	MAN	1	0

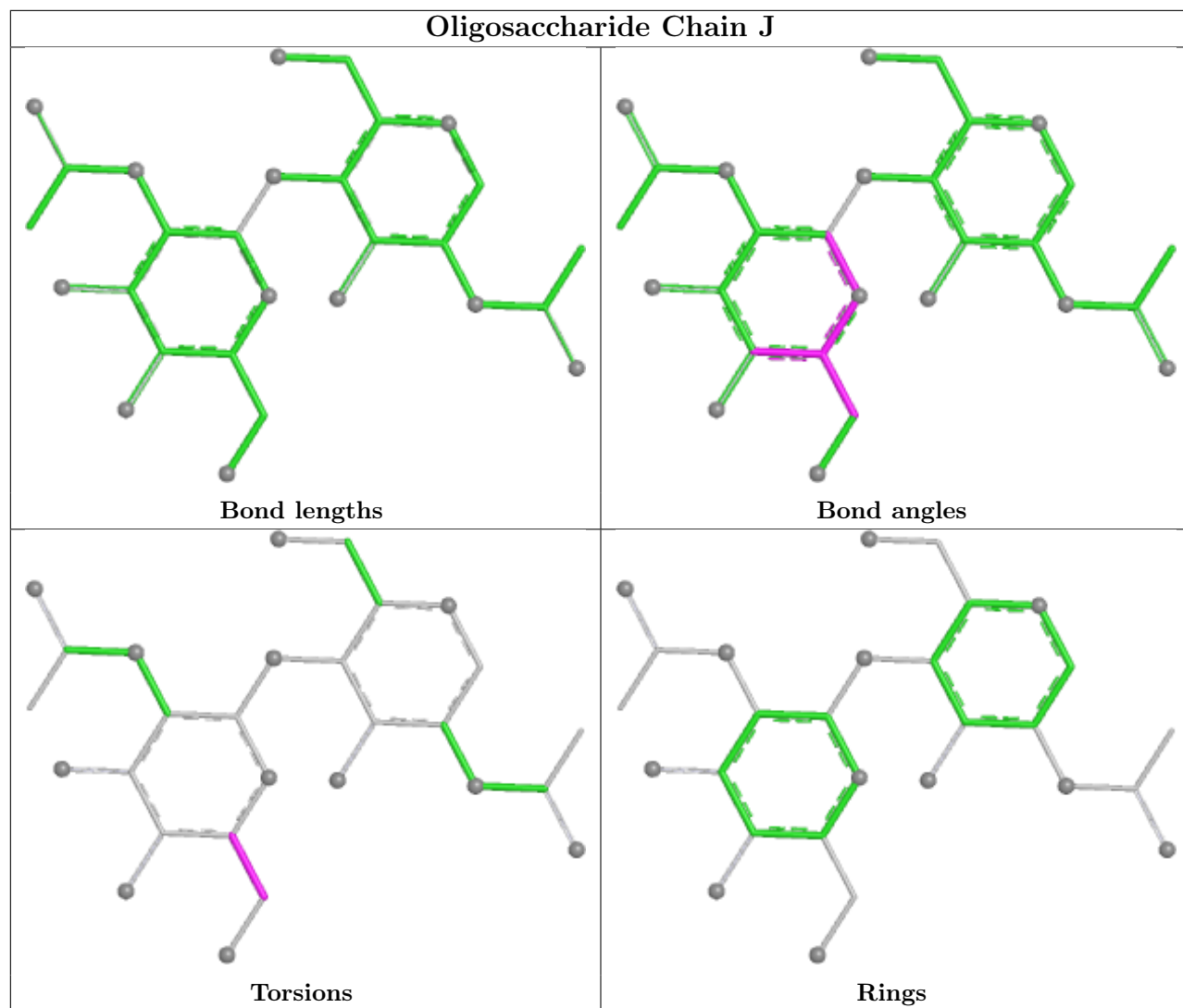
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

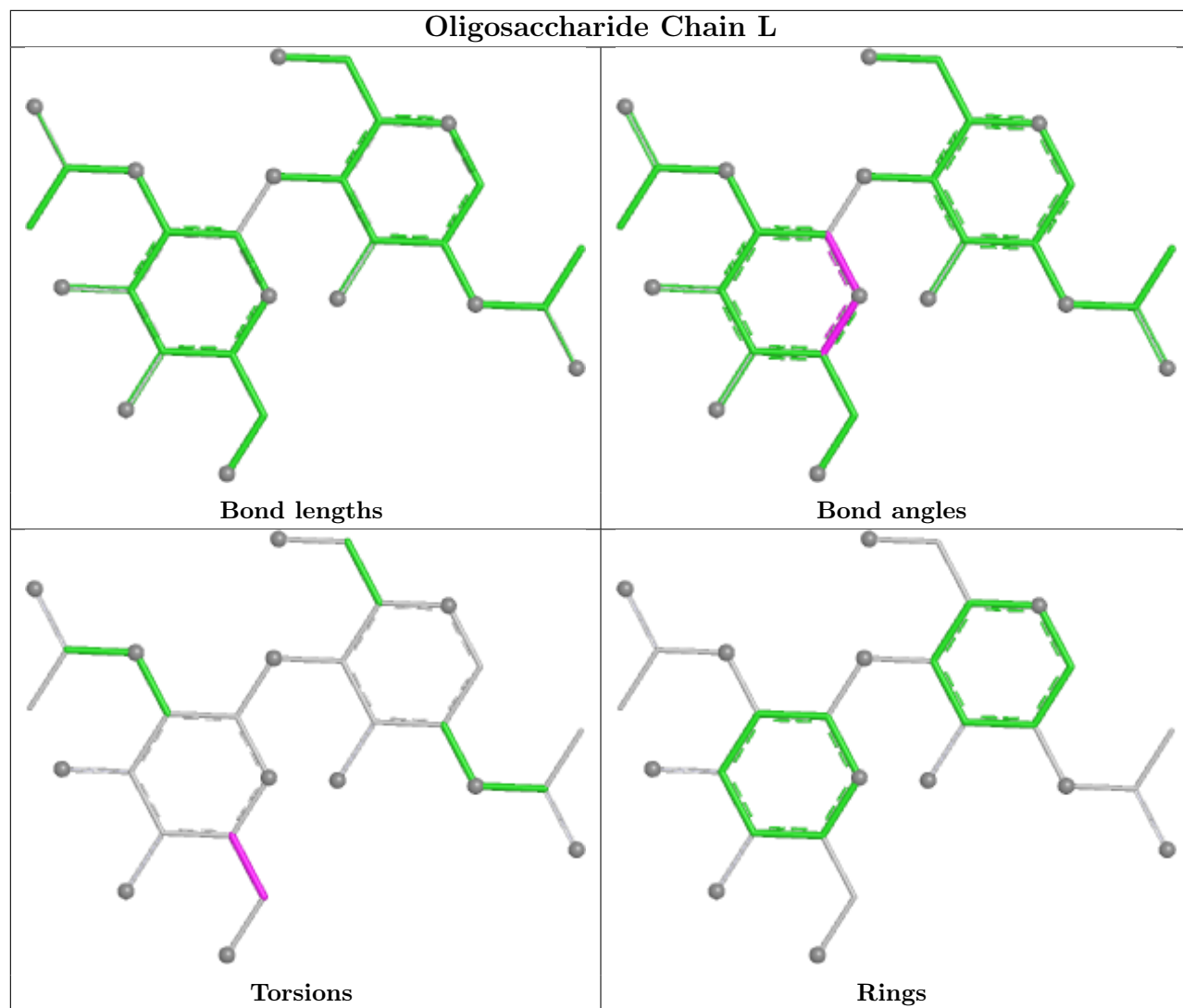


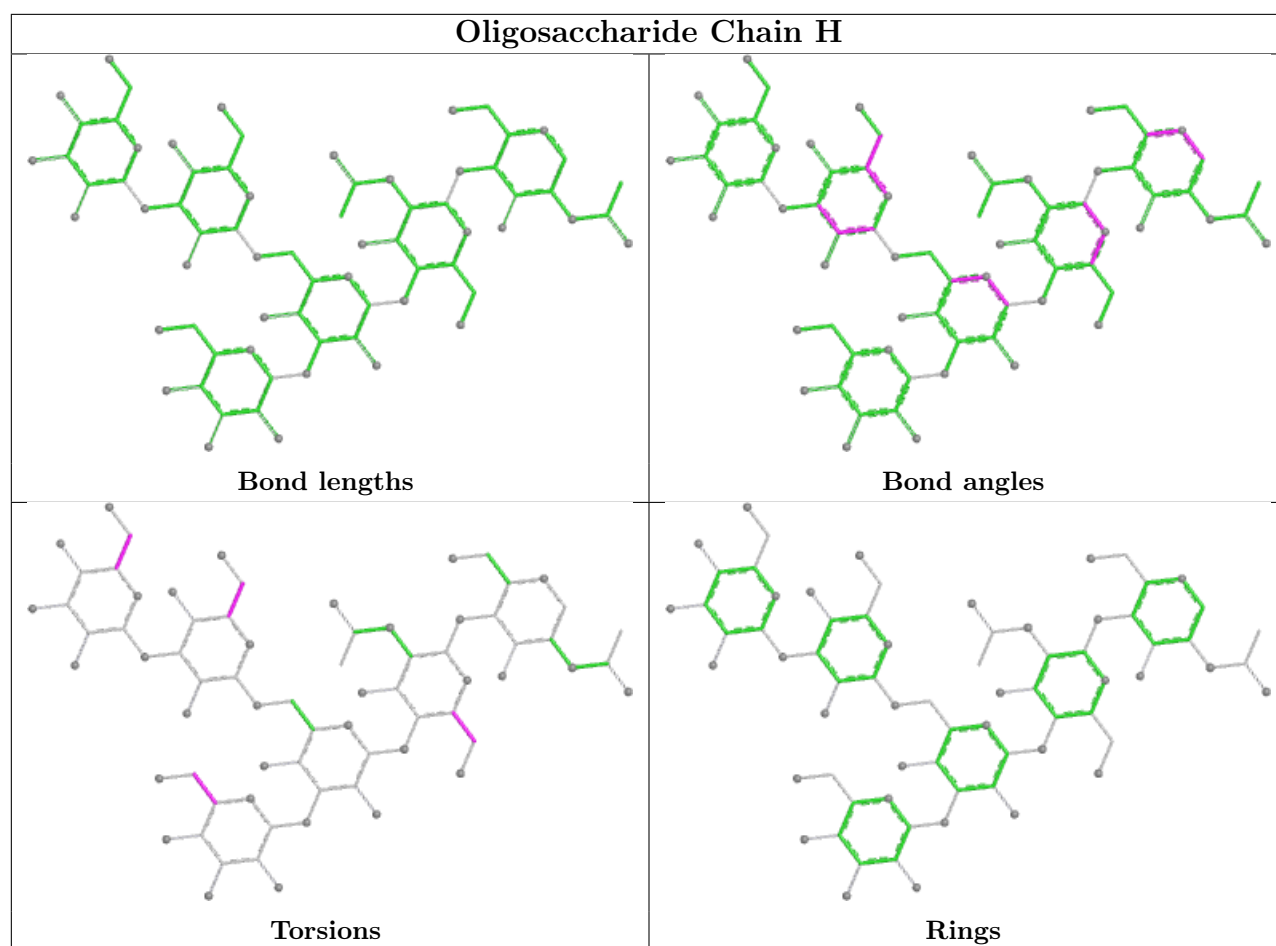












5.6 Ligand geometry [i](#)

50 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	BTB	D	711	-	13,13,13	1.01	1 (7%)	7,16,16	0.34	0
7	NAG	A	706	1	14,14,15	0.34	0	17,19,21	0.85	0
7	NAG	C	711	1	14,14,15	0.61	0	17,19,21	1.62	2 (11%)
7	NAG	B	704	1	14,14,15	0.23	0	17,19,21	0.97	0
6	MAN	A	702	1	11,11,12	0.26	0	15,15,17	0.72	0
7	NAG	C	709	1	14,14,15	0.40	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	710	1	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
7	NAG	A	709	1	14,14,15	0.42	0	17,19,21	0.71	0
7	NAG	D	706	1	14,14,15	0.47	0	17,19,21	1.23	3 (17%)
10	PEG	D	701	-	6,6,6	0.24	0	5,5,5	0.17	0
7	NAG	B	707	1	14,14,15	0.52	0	17,19,21	1.85	5 (29%)
7	NAG	A	712	1	14,14,15	0.31	0	17,19,21	1.04	2 (11%)
6	MAN	D	702	1	11,11,12	0.31	0	15,15,17	0.64	0
7	NAG	B	705	1	14,14,15	0.43	0	17,19,21	0.94	1 (5%)
6	MAN	D	703	1	11,11,12	0.26	0	15,15,17	0.66	0
8	BTB	C	713	-	13,13,13	1.08	1 (7%)	7,16,16	0.29	0
6	MAN	A	703	1	11,11,12	0.42	0	15,15,17	0.58	0
6	MAN	B	701	1	11,11,12	0.31	0	15,15,17	0.69	0
7	NAG	D	709	1	14,14,15	0.67	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	A	711	1	14,14,15	0.38	0	17,19,21	0.85	0
7	NAG	D	710	1	14,14,15	0.33	0	17,19,21	0.63	0
7	NAG	A	710	1	14,14,15	0.38	0	17,19,21	1.44	2 (11%)
8	BTB	B	709	-	13,13,13	0.99	1 (7%)	7,16,16	0.47	0
7	NAG	D	705	1	14,14,15	0.29	0	17,19,21	0.78	0
9	FRU	B	710	-	11,12,12	0.75	0	10,18,18	1.00	1 (10%)
6	MAN	A	701	1	11,11,12	0.33	0	15,15,17	1.08	1 (6%)
7	NAG	B	708	1	14,14,15	0.42	0	17,19,21	0.84	0
7	NAG	C	707	1	14,14,15	0.50	0	17,19,21	1.30	3 (17%)
6	MAN	C	703	1	11,11,12	0.35	0	15,15,17	0.83	0
7	NAG	B	706	1	14,14,15	0.30	0	17,19,21	0.92	1 (5%)
9	FRU	C	714	-	11,12,12	0.61	0	10,18,18	0.68	0
7	NAG	B	703	1	14,14,15	0.43	0	17,19,21	1.34	3 (17%)
7	NAG	D	707	1	14,14,15	0.25	0	17,19,21	0.61	0
7	NAG	A	707	1	14,14,15	0.39	0	17,19,21	0.72	0
6	MAN	B	702	1	11,11,12	0.29	0	15,15,17	0.67	0
6	MAN	D	704	1	11,11,12	0.35	0	15,15,17	0.65	0
7	NAG	C	712	1	14,14,15	0.22	0	17,19,21	0.77	0
9	FRU	D	712	-	11,12,12	0.78	1 (9%)	10,18,18	0.88	0
6	MAN	C	701	1	11,11,12	0.28	0	15,15,17	0.55	0
6	MAN	C	702	1	11,11,12	0.35	0	15,15,17	0.70	0
9	FRU	A	714	-	11,12,12	0.59	0	10,18,18	0.81	0
8	BTB	A	713	-	13,13,13	1.00	1 (7%)	7,16,16	0.34	0
7	NAG	A	704	1	14,14,15	0.20	0	17,19,21	1.09	2 (11%)
6	MAN	C	705	1	11,11,12	0.39	0	15,15,17	0.62	0
7	NAG	A	705	1	14,14,15	0.28	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	706	1	14,14,15	0.26	0	17,19,21	0.67	0
7	NAG	C	708	1	14,14,15	0.36	0	17,19,21	0.78	0
7	NAG	D	708	1	14,14,15	0.28	0	17,19,21	0.71	0
7	NAG	A	708	1	14,14,15	0.28	0	17,19,21	1.06	0
6	MAN	C	704	1	11,11,12	0.35	0	15,15,17	0.70	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	BTB	D	711	-	-	1/21/21/21	-
7	NAG	A	706	1	-	0/6/23/26	0/1/1/1
7	NAG	C	711	1	-	4/6/23/26	0/1/1/1
7	NAG	B	704	1	-	0/6/23/26	0/1/1/1
6	MAN	A	702	1	-	0/2/19/22	0/1/1/1
7	NAG	C	709	1	-	0/6/23/26	0/1/1/1
7	NAG	C	710	1	-	0/6/23/26	0/1/1/1
7	NAG	A	709	1	-	0/6/23/26	0/1/1/1
7	NAG	D	706	1	-	1/6/23/26	0/1/1/1
10	PEG	D	701	-	-	4/4/4/4	-
7	NAG	B	707	1	-	3/6/23/26	0/1/1/1
7	NAG	A	712	1	-	4/6/23/26	0/1/1/1
6	MAN	D	702	1	-	0/2/19/22	0/1/1/1
7	NAG	B	705	1	-	0/6/23/26	0/1/1/1
6	MAN	D	703	1	-	0/2/19/22	0/1/1/1
8	BTB	C	713	-	-	0/21/21/21	-
6	MAN	A	703	1	-	1/2/19/22	0/1/1/1
6	MAN	B	701	1	-	0/2/19/22	0/1/1/1
7	NAG	D	709	1	-	4/6/23/26	0/1/1/1
7	NAG	A	711	1	-	0/6/23/26	0/1/1/1
7	NAG	D	710	1	-	0/6/23/26	0/1/1/1
7	NAG	A	710	1	-	4/6/23/26	0/1/1/1
8	BTB	B	709	-	-	1/21/21/21	-
7	NAG	D	705	1	-	0/6/23/26	0/1/1/1
9	FRU	B	710	-	-	4/5/24/24	0/1/1/1
6	MAN	A	701	1	-	2/2/19/22	0/1/1/1
7	NAG	B	708	1	-	1/6/23/26	0/1/1/1
7	NAG	C	707	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	C	703	1	-	2/2/19/22	0/1/1/1
7	NAG	B	706	1	-	0/6/23/26	0/1/1/1
9	FRU	C	714	-	-	5/5/24/24	0/1/1/1
7	NAG	B	703	1	-	1/6/23/26	0/1/1/1
7	NAG	D	707	1	-	0/6/23/26	0/1/1/1
7	NAG	A	707	1	-	0/6/23/26	0/1/1/1
6	MAN	B	702	1	-	0/2/19/22	0/1/1/1
6	MAN	D	704	1	-	2/2/19/22	0/1/1/1
7	NAG	C	712	1	-	0/6/23/26	0/1/1/1
9	FRU	D	712	-	-	3/5/24/24	0/1/1/1
6	MAN	C	701	1	-	1/2/19/22	0/1/1/1
6	MAN	C	702	1	-	1/2/19/22	0/1/1/1
9	FRU	A	714	-	-	2/5/24/24	0/1/1/1
8	BTB	A	713	-	-	1/21/21/21	-
7	NAG	A	704	1	-	1/6/23/26	0/1/1/1
6	MAN	C	705	1	-	0/2/19/22	0/1/1/1
7	NAG	A	705	1	-	0/6/23/26	0/1/1/1
7	NAG	C	706	1	-	1/6/23/26	0/1/1/1
7	NAG	C	708	1	-	1/6/23/26	0/1/1/1
7	NAG	D	708	1	-	0/6/23/26	0/1/1/1
7	NAG	A	708	1	-	0/6/23/26	0/1/1/1
6	MAN	C	704	1	-	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)
8	C	713	BTB	C2-N	2.44	1.53	1.48
9	D	712	FRU	O2-C2	2.40	1.44	1.40
7	D	709	NAG	O7-C7	2.23	1.28	1.23
8	D	711	BTB	C2-N	2.21	1.52	1.48
8	B	709	BTB	C5-N	2.08	1.50	1.48
8	A	713	BTB	C2-N	2.06	1.52	1.48

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	711	NAG	C2-N2-C7	-5.13	116.03	122.90
7	B	707	NAG	C2-N2-C7	-5.05	116.14	122.90
7	A	710	NAG	C1-C2-N2	-3.88	104.33	110.43
6	A	701	MAN	C1-O5-C5	3.62	117.04	112.19
7	C	710	NAG	C1-O5-C5	3.35	116.68	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	703	NAG	O5-C1-C2	-2.81	106.94	111.29
7	A	704	NAG	C1-C2-N2	2.78	114.82	110.43
7	D	706	NAG	C1-O5-C5	2.76	115.88	112.19
7	C	711	NAG	C1-C2-N2	2.74	114.75	110.43
7	A	710	NAG	C8-C7-N2	2.62	120.47	116.12
7	B	705	NAG	C1-O5-C5	2.62	115.69	112.19
7	B	703	NAG	C1-O5-C5	2.61	115.69	112.19
7	B	707	NAG	C4-C3-C2	2.55	114.76	111.02
7	A	704	NAG	O5-C1-C2	-2.53	107.37	111.29
7	C	707	NAG	O5-C1-C2	-2.46	107.48	111.29
7	B	707	NAG	C1-O5-C5	2.44	115.46	112.19
7	C	707	NAG	C1-O5-C5	2.41	115.42	112.19
7	B	707	NAG	C1-C2-N2	-2.38	106.68	110.43
7	D	709	NAG	C8-C7-N2	2.35	120.02	116.12
7	B	703	NAG	O5-C5-C6	2.35	112.24	107.66
7	C	707	NAG	C4-C3-C2	-2.31	107.63	111.02
7	A	712	NAG	C2-N2-C7	2.27	125.95	122.90
7	B	706	NAG	C1-O5-C5	2.27	115.23	112.19
7	B	707	NAG	O5-C1-C2	2.25	114.77	111.29
7	A	712	NAG	C1-C2-N2	-2.23	106.93	110.43
7	D	706	NAG	C1-C2-N2	2.20	113.89	110.43
7	A	705	NAG	C1-O5-C5	2.14	115.06	112.19
9	B	710	FRU	C6-C5-C4	-2.09	110.17	115.10
7	D	706	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	710	NAG	C8-C7-N2-C2
7	A	710	NAG	O7-C7-N2-C2
7	B	707	NAG	C8-C7-N2-C2
7	B	707	NAG	O7-C7-N2-C2
7	C	711	NAG	C1-C2-N2-C7
7	C	711	NAG	C8-C7-N2-C2
7	C	711	NAG	O7-C7-N2-C2
7	D	706	NAG	C1-C2-N2-C7
7	D	709	NAG	C8-C7-N2-C2
7	D	709	NAG	O7-C7-N2-C2
6	C	703	MAN	O5-C5-C6-O6
7	A	712	NAG	O7-C7-N2-C2
10	D	701	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	C	703	MAN	C4-C5-C6-O6
7	A	712	NAG	O5-C5-C6-O6
7	A	710	NAG	C4-C5-C6-O6
7	A	712	NAG	C4-C5-C6-O6
7	A	712	NAG	C8-C7-N2-C2
6	D	704	MAN	O5-C5-C6-O6
6	A	701	MAN	O5-C5-C6-O6
7	A	710	NAG	O5-C5-C6-O6
7	D	709	NAG	O5-C5-C6-O6
9	C	714	FRU	O1-C1-C2-O5
9	C	714	FRU	O5-C5-C6-O6
9	C	714	FRU	C4-C5-C6-O6
9	B	710	FRU	C4-C5-C6-O6
6	C	701	MAN	O5-C5-C6-O6
10	D	701	PEG	O2-C3-C4-O4
9	B	710	FRU	O5-C5-C6-O6
9	A	714	FRU	O1-C1-C2-O5
6	A	703	MAN	O5-C5-C6-O6
6	C	702	MAN	O5-C5-C6-O6
10	D	701	PEG	O1-C1-C2-O2
7	B	707	NAG	O5-C5-C6-O6
7	C	706	NAG	O5-C5-C6-O6
9	D	712	FRU	O1-C1-C2-O5
6	D	704	MAN	C4-C5-C6-O6
9	A	714	FRU	O1-C1-C2-C3
9	C	714	FRU	O1-C1-C2-C3
9	D	712	FRU	O1-C1-C2-C3
7	C	708	NAG	C4-C5-C6-O6
9	B	710	FRU	O1-C1-C2-O5
10	D	701	PEG	C4-C3-O2-C2
6	A	701	MAN	C4-C5-C6-O6
7	D	709	NAG	C4-C5-C6-O6
7	A	704	NAG	C8-C7-N2-C2
9	B	710	FRU	O1-C1-C2-C3
7	C	707	NAG	C3-C2-N2-C7
8	B	709	BTB	N-C7-C8-O8
9	D	712	FRU	O5-C5-C6-O6
7	B	703	NAG	C1-C2-N2-C7
7	B	708	NAG	C1-C2-N2-C7
7	C	707	NAG	C1-C2-N2-C7
7	C	711	NAG	C4-C5-C6-O6
8	A	713	BTB	N-C5-C6-O6

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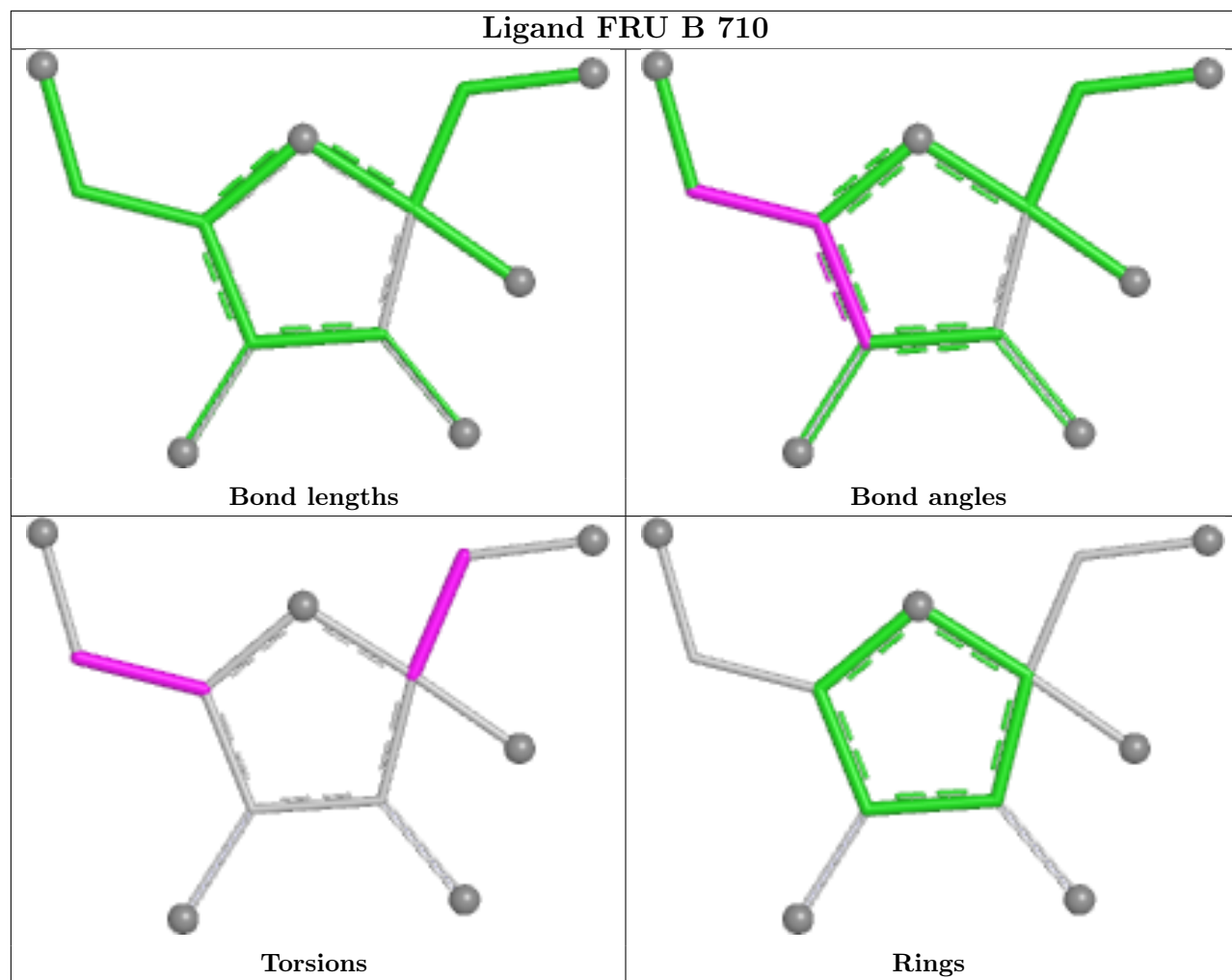
Mol	Chain	Res	Type	Atoms
9	C	714	FRU	O1-C1-C2-O2
8	D	711	BTB	N-C7-C8-O8

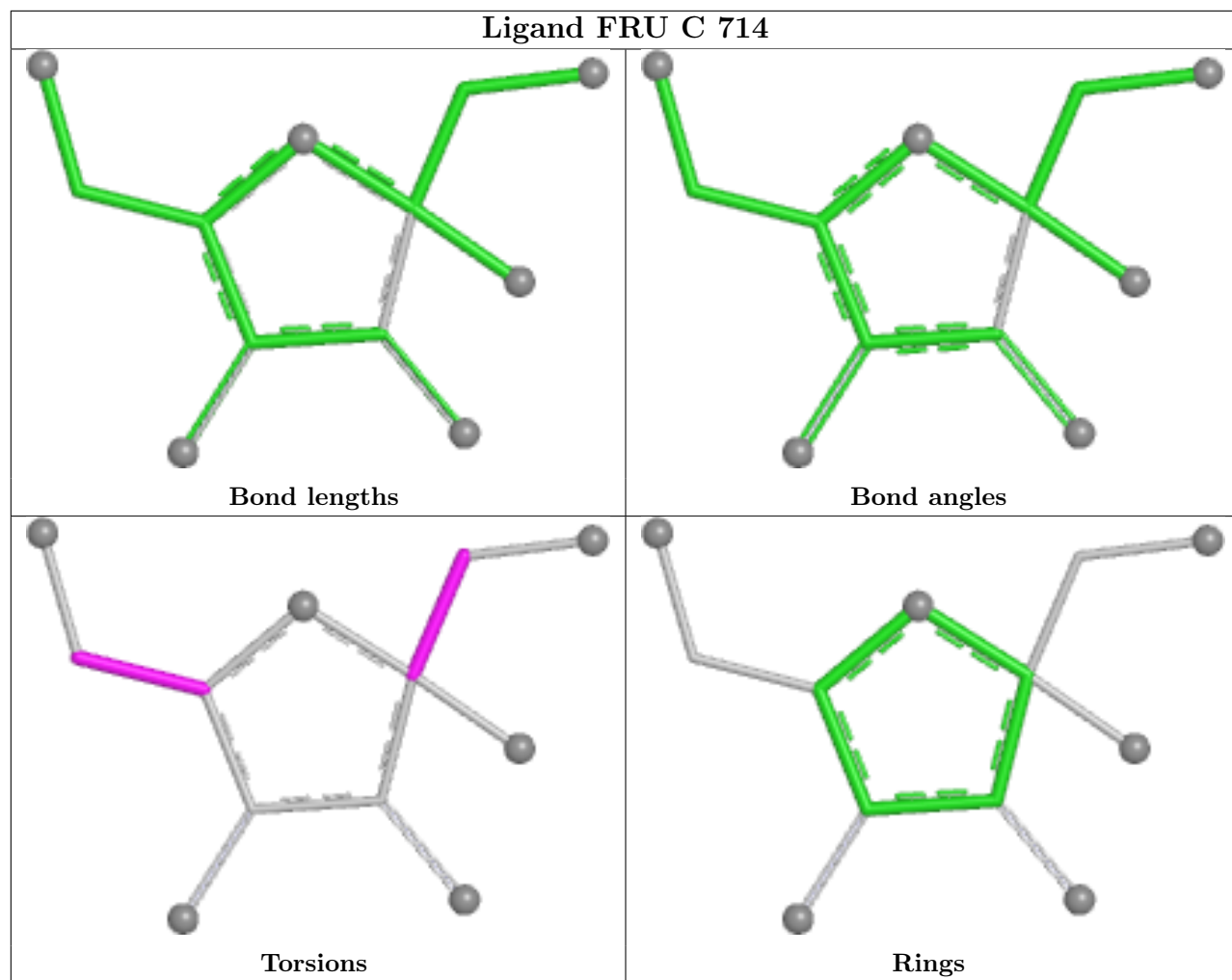
There are no ring outliers.

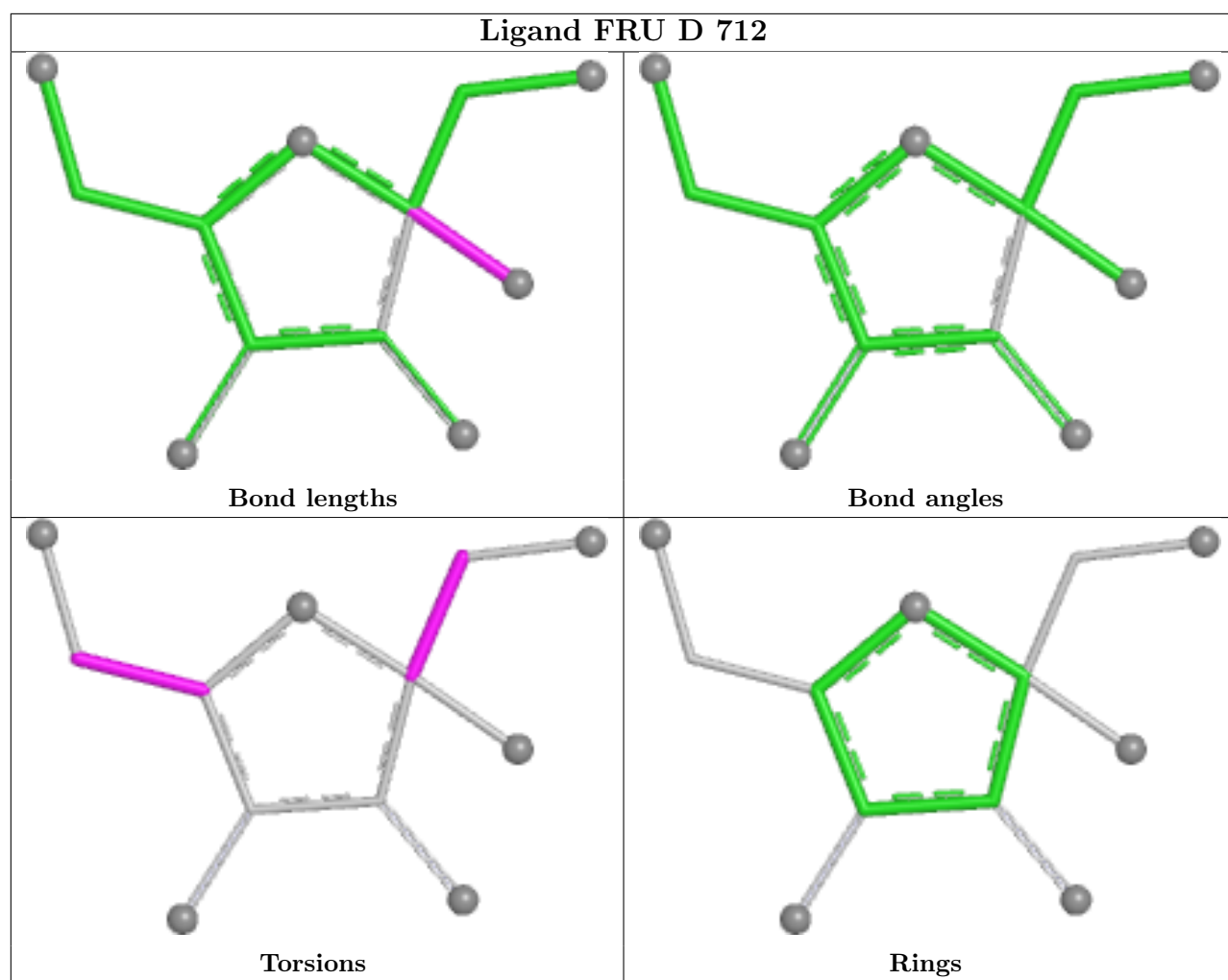
16 monomers are involved in 21 short contacts:

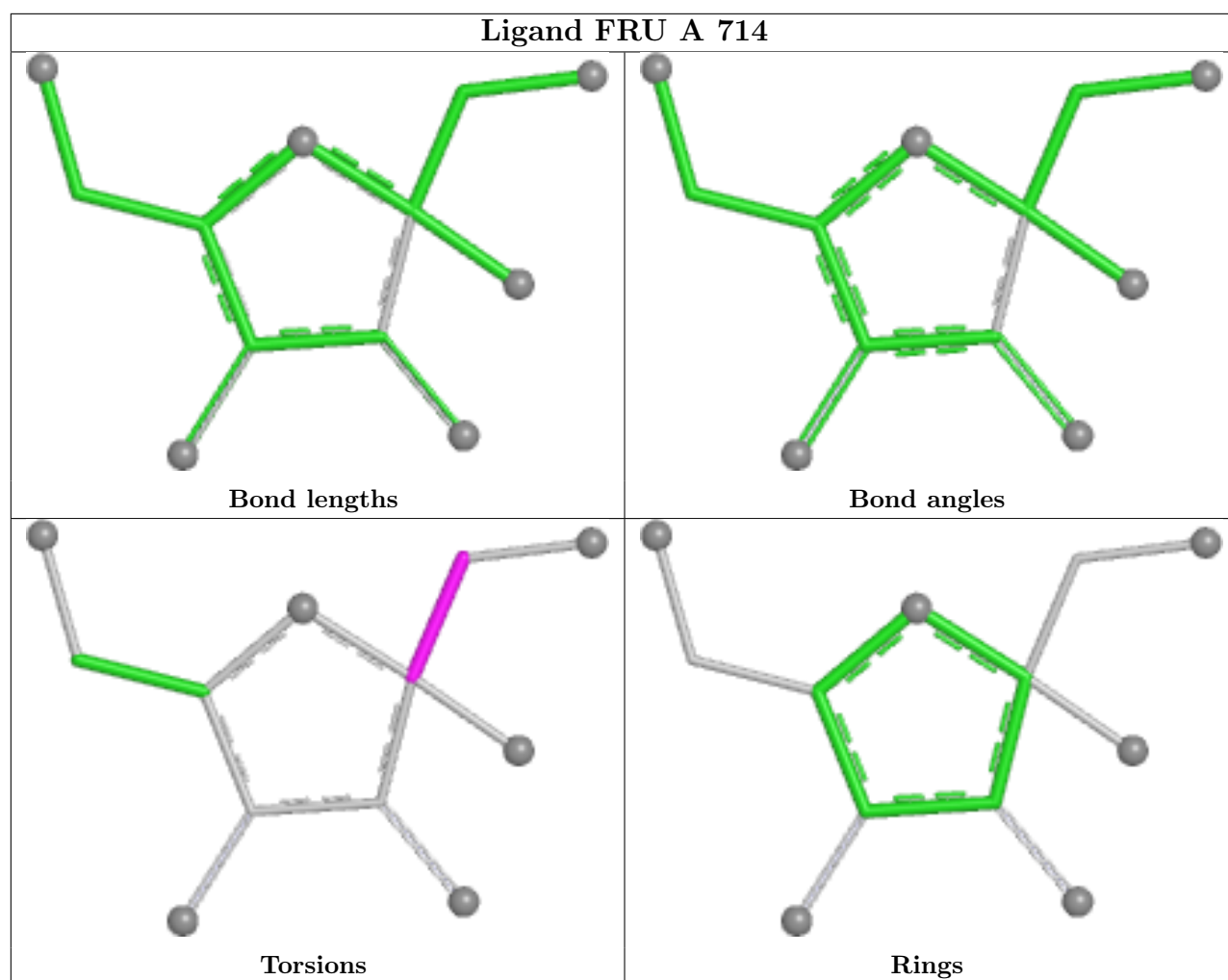
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	711	BTB	1	0
7	C	711	NAG	1	0
7	B	704	NAG	1	0
6	A	702	MAN	1	0
10	D	701	PEG	1	0
7	B	707	NAG	1	0
7	A	712	NAG	4	0
6	B	701	MAN	1	0
7	D	709	NAG	1	0
7	A	710	NAG	1	0
8	B	709	BTB	1	0
6	A	701	MAN	1	0
6	C	703	MAN	1	0
7	B	703	NAG	3	0
7	A	705	NAG	1	0
7	A	708	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	526/675 (77%)	0.03	12 (2%) 61 64	11, 21, 41, 60	7 (1%)
1	B	526/675 (77%)	0.16	30 (5%) 29 32	11, 23, 50, 78	2 (0%)
1	C	524/675 (77%)	0.44	25 (4%) 35 39	15, 27, 47, 69	1 (0%)
1	D	524/675 (77%)	0.83	91 (17%) 4 3	14, 27, 58, 81	0
All	All	2100/2700 (77%)	0.37	158 (7%) 20 22	11, 24, 51, 81	10 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	504	ALA	6.8
1	D	661	VAL	5.9
1	C	143	CYS	4.8
1	D	512	PHE	4.5
1	D	506	SER	4.4
1	D	508	ALA	4.4
1	D	436	ASN	4.4
1	D	655	LEU	4.3
1	D	654	GLY	4.2
1	D	510	VAL	4.0
1	D	663	LEU	3.9
1	D	653	GLY	3.9
1	D	555	CYS	3.9
1	D	437	GLY	3.8
1	A	165	ILE	3.8
1	D	532	ALA	3.7
1	D	499	LEU	3.6
1	D	505	ASN	3.6
1	D	659	THR	3.6
1	D	539	ILE	3.4
1	D	547	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	528	LEU	3.4
1	D	652	THR	3.3
1	D	530	ASP	3.3
1	A	562	GLY	3.3
1	D	656	PRO	3.2
1	D	524	LEU	3.2
1	D	507	THR	3.1
1	D	526	VAL	3.1
1	D	166	THR	3.1
1	D	541	ALA	3.1
1	D	542	ASP	3.1
1	D	650	VAL	3.1
1	B	556	SER	3.1
1	C	437	GLY	3.0
1	A	150	ALA	3.0
1	B	564	ASP	3.0
1	D	545	ILE	3.0
1	D	643	SER	3.0
1	D	665	VAL	3.0
1	A	563	SER	3.0
1	B	553	THR	3.0
1	D	651	ALA	3.0
1	D	556	SER	2.9
1	C	512	PHE	2.9
1	D	145	PRO	2.9
1	A	436	ASN	2.9
1	D	543	ALA	2.9
1	D	502	SER	2.9
1	D	538	LEU	2.9
1	B	143	CYS	2.9
1	D	503	GLU	2.9
1	C	553	THR	2.8
1	D	672	TRP	2.8
1	D	529	PRO	2.8
1	B	142	SER	2.8
1	A	166[A]	THR	2.8
1	C	145	PRO	2.8
1	D	552	SER	2.8
1	D	150	ALA	2.8
1	B	196	ARG	2.8
1	B	562	GLY	2.8
1	D	149	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	556	SER	2.7
1	C	502	SER	2.7
1	D	544	SER	2.7
1	D	531	ALA	2.7
1	C	278	THR	2.7
1	C	148	LEU	2.7
1	D	533	ILE	2.7
1	D	151	SER	2.7
1	B	144	ALA	2.7
1	D	143	CYS	2.7
1	D	460	ALA	2.6
1	B	500	SER	2.6
1	D	553	THR	2.6
1	A	437	GLY	2.6
1	C	161	THR	2.6
1	D	516	THR	2.6
1	B	555	CYS	2.6
1	C	511	ASP	2.6
1	D	165	ILE	2.6
1	A	142	SER	2.6
1	A	143	CYS	2.5
1	D	535	ASN	2.5
1	D	662	ASN	2.5
1	D	648	MET	2.5
1	C	596	GLU	2.5
1	D	546	ASN	2.5
1	D	536	ALA	2.5
1	D	657	GLU	2.5
1	D	554	LYS	2.5
1	A	555	CYS	2.5
1	C	499	LEU	2.5
1	D	658	GLY	2.5
1	C	513	THR	2.5
1	B	514	ASN	2.4
1	D	527	THR	2.4
1	C	563	SER	2.4
1	D	615	LEU	2.4
1	D	509	ASP	2.4
1	C	508	ALA	2.4
1	D	375	PRO	2.4
1	D	515	VAL	2.4
1	D	501	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	499	LEU	2.3
1	D	146	THR	2.3
1	D	660	GLN	2.3
1	B	554	LYS	2.3
1	B	494	VAL	2.3
1	A	403	ASP	2.3
1	D	564	ASP	2.3
1	C	155	LEU	2.3
1	D	540	SER	2.3
1	C	555	CYS	2.3
1	B	149	PRO	2.3
1	B	536	ALA	2.3
1	D	563	SER	2.3
1	D	453	GLN	2.3
1	B	154	GLU	2.2
1	C	460	ALA	2.2
1	B	563	SER	2.2
1	D	147	SER	2.2
1	D	534	GLN	2.2
1	D	644	PRO	2.2
1	C	263	ASN	2.2
1	C	196	ARG	2.2
1	D	645	VAL	2.2
1	B	435	GLU	2.2
1	B	437	GLY	2.2
1	D	551	PRO	2.2
1	D	521	TRP	2.2
1	C	509	ASP	2.2
1	B	538	LEU	2.2
1	B	145	PRO	2.2
1	C	556	SER	2.1
1	D	498	LEU	2.1
1	D	152	ALA	2.1
1	B	512	PHE	2.1
1	D	496	PRO	2.1
1	B	534	GLN	2.1
1	B	502	SER	2.1
1	D	154	GLU	2.1
1	C	306	GLY	2.1
1	D	570	LEU	2.1
1	D	612	LEU	2.1
1	B	530	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	147	SER	2.0
1	C	242	THR	2.0
1	D	548	THR	2.0
1	D	616	VAL	2.0
1	D	148	LEU	2.0
1	B	508	ALA	2.0
1	C	298	GLU	2.0
1	D	500	SER	2.0
1	B	436	ASN	2.0
1	B	510	VAL	2.0
1	D	159	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

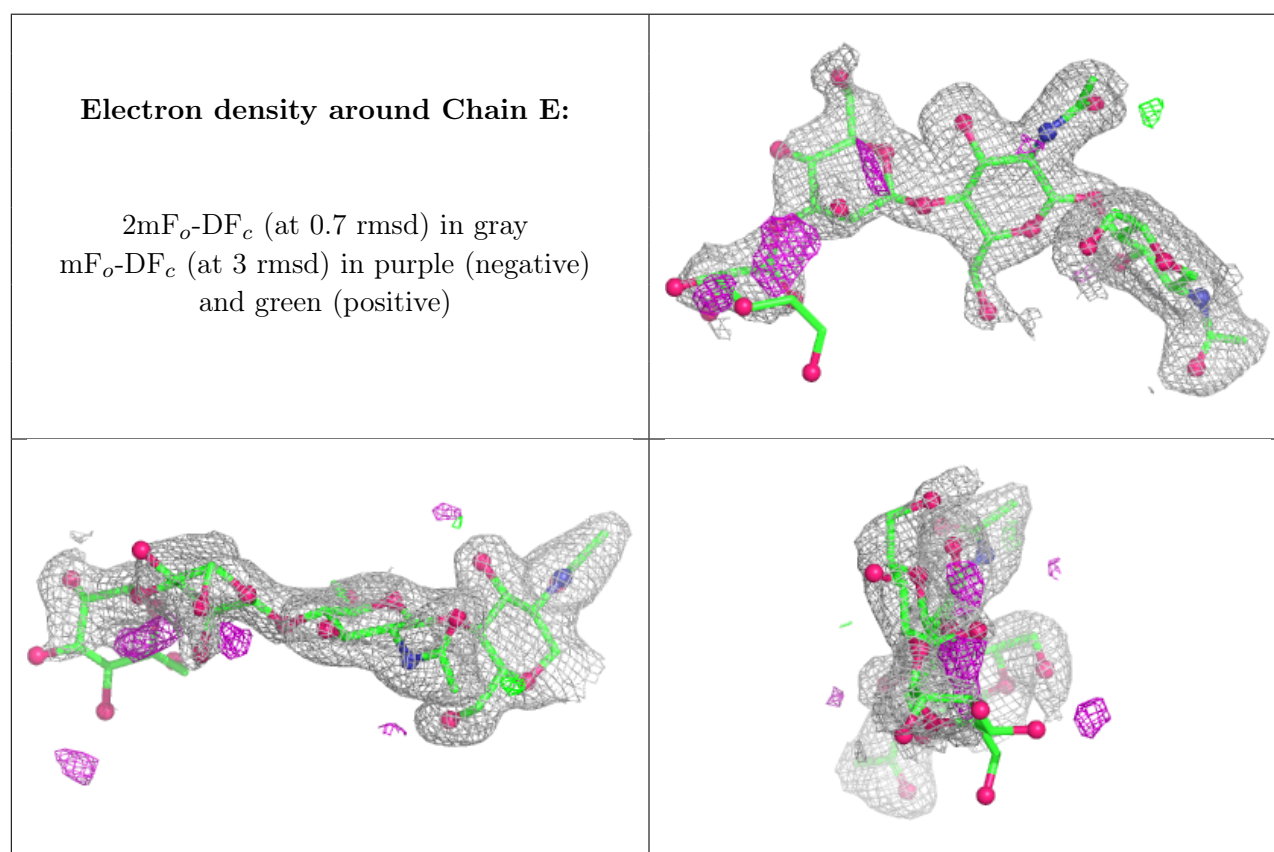
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	F	3	11/12	0.32	0.18	81,86,88,88	0
2	MAN	E	4	11/12	0.45	0.18	88,92,95,97	0
4	NAG	I	2	14/15	0.50	0.19	58,64,72,73	0
3	BMA	K	3	11/12	0.55	0.17	61,63,65,65	0
5	MAN	H	4	11/12	0.56	0.15	77,81,84,84	0
4	NAG	L	2	14/15	0.60	0.17	75,83,87,90	0
4	NAG	G	2	14/15	0.62	0.17	67,77,79,81	0
5	MAN	H	6	11/12	0.64	0.14	75,78,79,80	0
2	BMA	E	3	11/12	0.68	0.14	66,69,73,76	0
5	BMA	H	3	11/12	0.68	0.14	63,69,72,74	0
5	MAN	H	5	11/12	0.70	0.20	53,63,68,68	0
3	NAG	K	2	14/15	0.71	0.15	47,51,57,59	0
4	NAG	J	2	14/15	0.76	0.13	49,52,54,57	0
3	NAG	F	2	14/15	0.83	0.11	42,50,59,60	0
4	NAG	J	1	14/15	0.83	0.11	45,47,51,52	0
2	NAG	E	2	14/15	0.85	0.12	38,41,49,51	0
5	NAG	H	2	14/15	0.88	0.10	41,43,50,54	0

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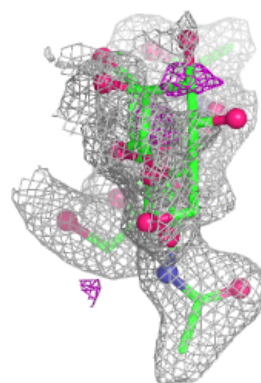
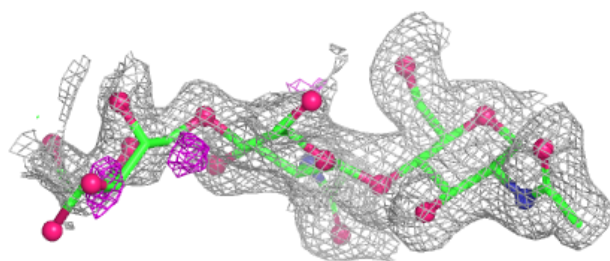
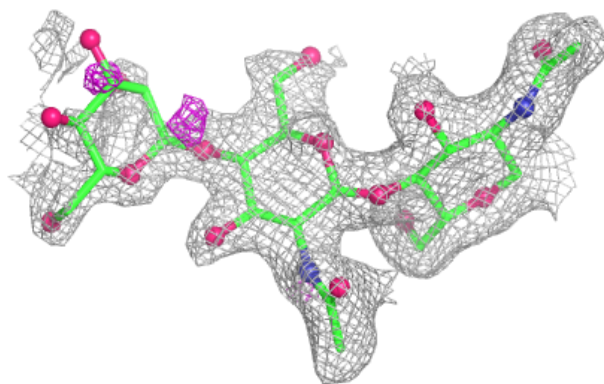
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	L	1	14/15	0.90	0.10	36,39,47,51	0
4	NAG	I	1	14/15	0.92	0.07	23,26,32,34	0
4	NAG	G	1	14/15	0.93	0.07	28,29,37,40	0
3	NAG	K	1	14/15	0.93	0.09	25,28,30,34	0
2	NAG	E	1	14/15	0.93	0.08	28,32,34,35	0
3	NAG	F	1	14/15	0.93	0.08	22,26,29,30	0
5	NAG	H	1	14/15	0.93	0.08	34,38,41,42	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.

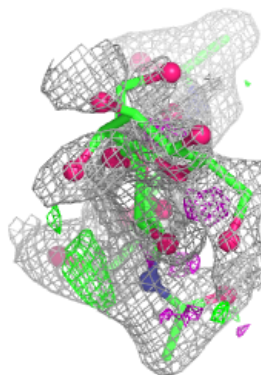
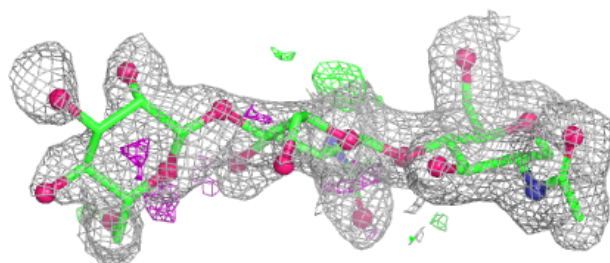
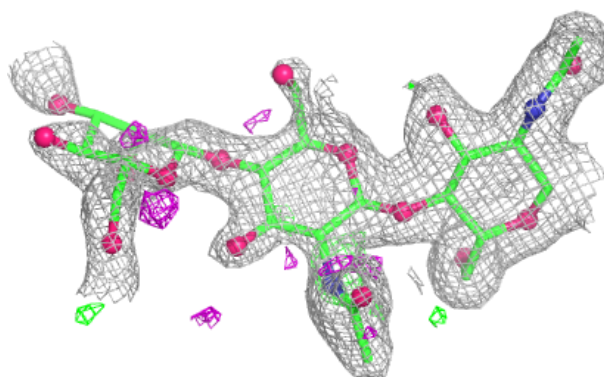


Electron density around Chain F:

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

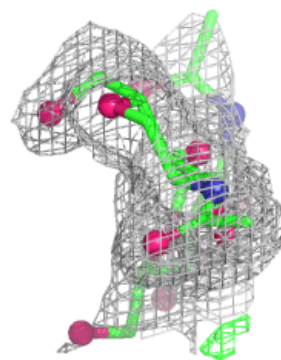
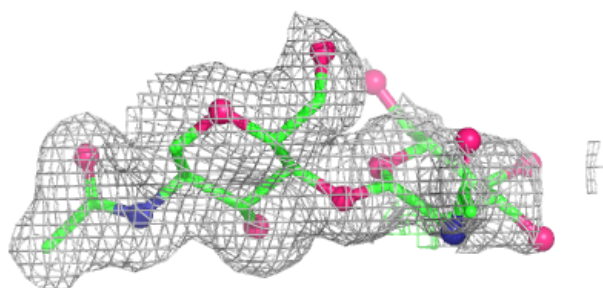
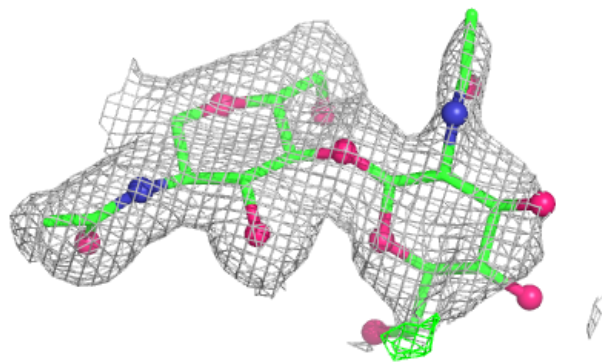
**Electron density around Chain K:**

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



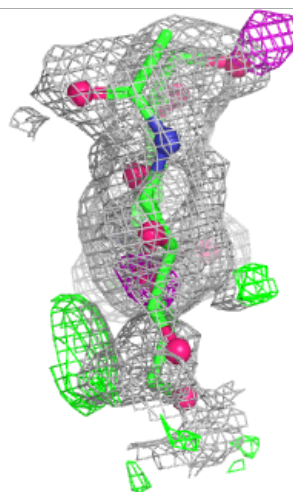
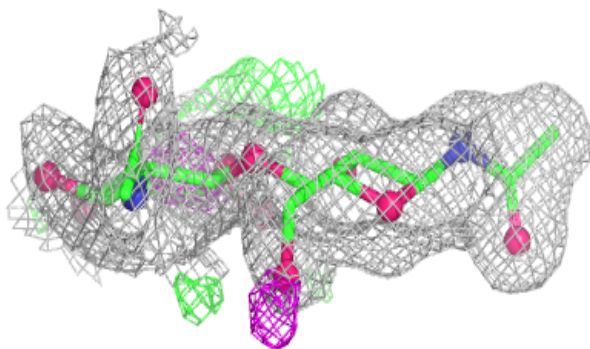
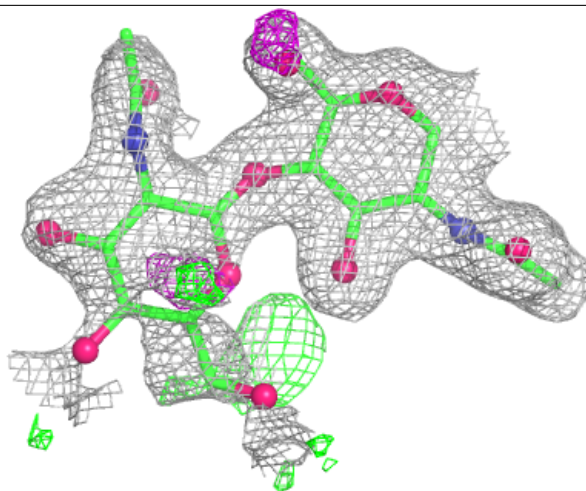
Electron density around Chain G:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



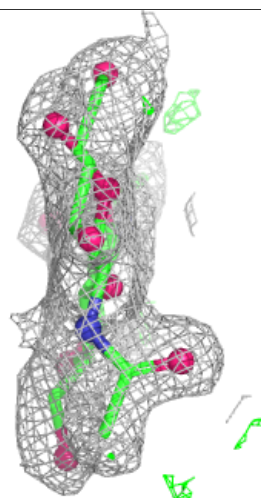
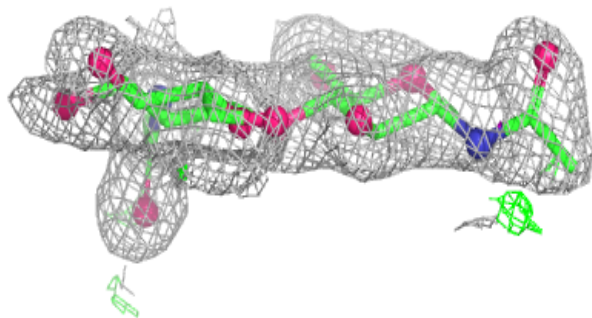
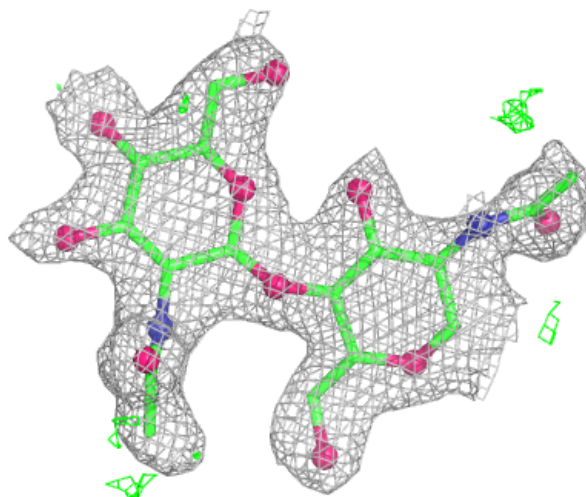
Electron density around Chain I:

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



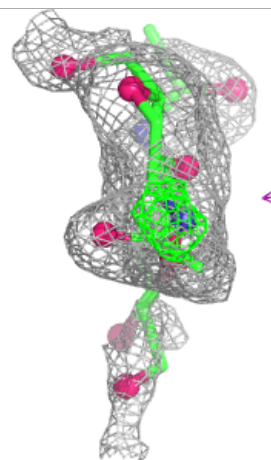
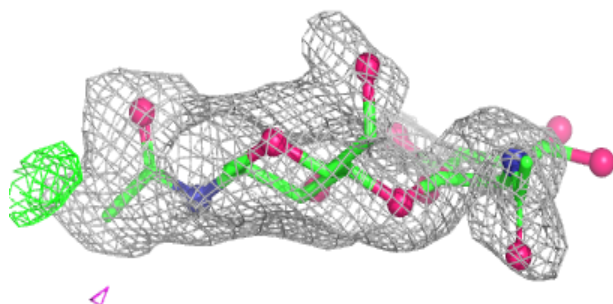
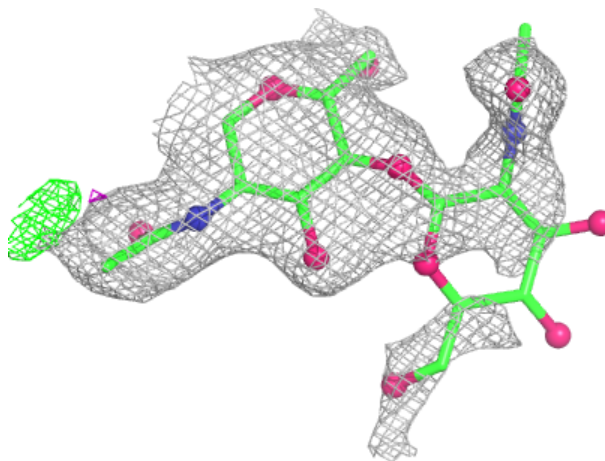
Electron density around Chain J:

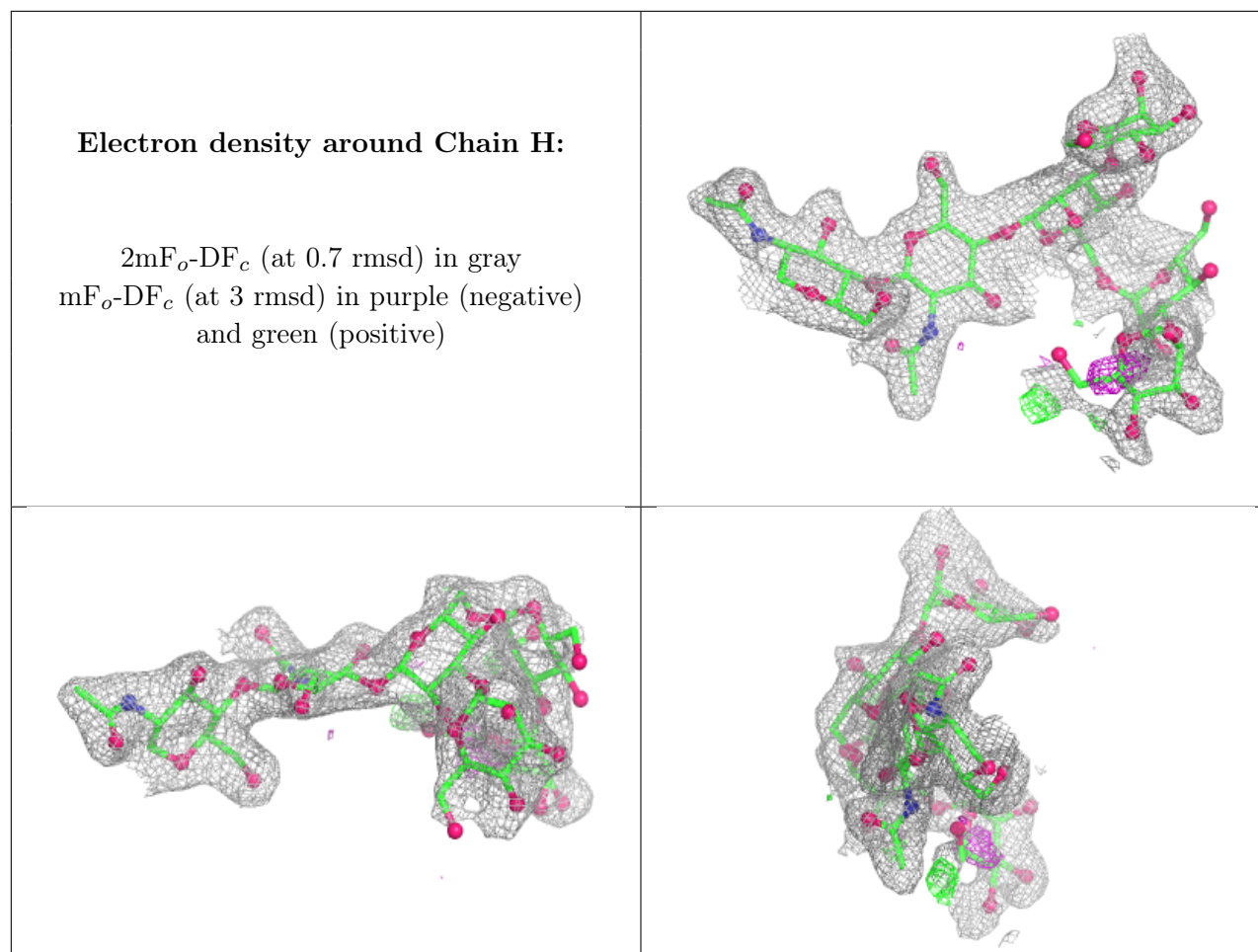
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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($\text{\AA}^2$)	Q<0.9
6	MAN	C	702	11/12	0.48	0.15	74,82,84,86	0
6	MAN	D	702	11/12	0.50	0.17	74,78,80,81	0
6	MAN	A	701	11/12	0.58	0.17	60,65,68,68	0
7	NAG	D	709	14/15	0.60	0.17	76,82,84,85	0
6	MAN	A	702	11/12	0.62	0.15	59,67,70,73	0
6	MAN	B	701	11/12	0.63	0.16	66,75,77,79	0
6	MAN	D	704	11/12	0.64	0.16	64,68,71,72	0
6	MAN	A	703	11/12	0.64	0.17	44,47,49,51	0
7	NAG	B	707	14/15	0.65	0.15	40,42,45,46	0
7	NAG	A	705	14/15	0.65	0.16	51,58,60,62	0
6	MAN	C	704	11/12	0.68	0.16	50,54,60,63	0

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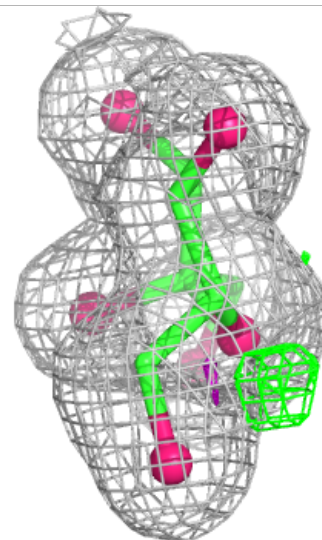
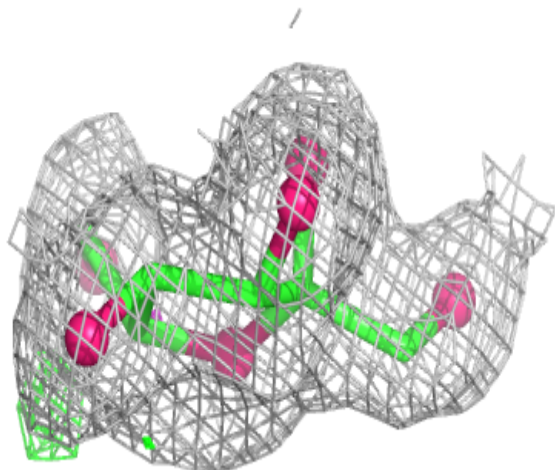
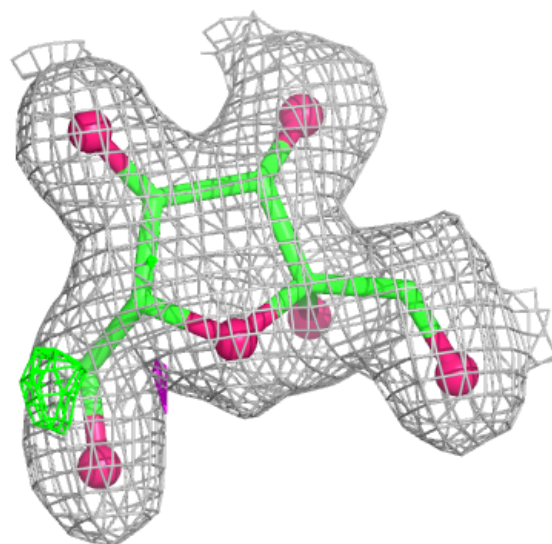
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	C	701	11/12	0.68	0.13	71,74,76,78	0
7	NAG	B	708	14/15	0.69	0.14	38,40,43,43	0
7	NAG	C	708	14/15	0.70	0.16	49,53,54,58	0
7	NAG	A	712	14/15	0.70	0.17	47,52,56,57	0
6	MAN	D	703	11/12	0.71	0.15	66,73,75,76	0
6	MAN	C	703	11/12	0.72	0.15	53,55,57,58	0
7	NAG	B	704	14/15	0.72	0.14	41,47,50,50	0
6	MAN	B	702	11/12	0.73	0.15	59,65,67,67	0
7	NAG	C	711	14/15	0.73	0.14	48,55,60,60	0
7	NAG	A	710	14/15	0.73	0.15	39,46,51,53	0
7	NAG	B	706	14/15	0.75	0.13	53,56,58,59	0
7	NAG	A	704	14/15	0.77	0.13	31,36,40,40	0
6	MAN	C	705	11/12	0.77	0.15	47,49,52,53	0
7	NAG	C	707	14/15	0.77	0.13	38,41,42,44	0
7	NAG	C	706	14/15	0.79	0.14	53,55,63,63	0
7	NAG	D	706	14/15	0.80	0.13	45,47,49,49	0
7	NAG	B	703	14/15	0.81	0.13	43,48,50,51	0
10	PEG	D	701	7/7	0.81	0.16	34,42,47,48	0
7	NAG	A	709	14/15	0.82	0.12	39,41,46,48	0
7	NAG	C	712	14/15	0.83	0.14	37,39,45,47	0
7	NAG	D	710	14/15	0.83	0.11	52,55,58,62	0
7	NAG	C	709	14/15	0.83	0.11	39,44,48,49	0
7	NAG	D	707	14/15	0.84	0.11	37,42,44,44	0
7	NAG	A	711	14/15	0.85	0.13	31,36,41,42	0
7	NAG	A	706	14/15	0.85	0.12	36,42,42,45	0
7	NAG	C	710	14/15	0.86	0.12	39,41,44,45	0
7	NAG	A	708	14/15	0.86	0.12	32,37,41,44	0
7	NAG	D	708	14/15	0.89	0.10	35,40,44,45	0
8	BTB	A	713	14/14	0.89	0.11	30,35,42,44	0
8	BTB	C	713	14/14	0.89	0.11	30,36,38,41	0
7	NAG	A	707	14/15	0.89	0.09	21,24,29,31	0
7	NAG	D	705	14/15	0.90	0.10	39,40,50,52	0
8	BTB	B	709	14/14	0.92	0.09	24,28,33,35	0
9	FRU	A	714	12/12	0.94	0.07	19,23,24,26	0
8	BTB	D	711	14/14	0.94	0.08	23,27,34,34	0
9	FRU	C	714	12/12	0.95	0.07	21,23,25,26	0
9	FRU	D	712	12/12	0.95	0.07	18,19,21,23	0
7	NAG	B	705	14/15	0.95	0.07	20,22,26,27	0
9	FRU	B	710	12/12	0.96	0.06	17,19,22,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

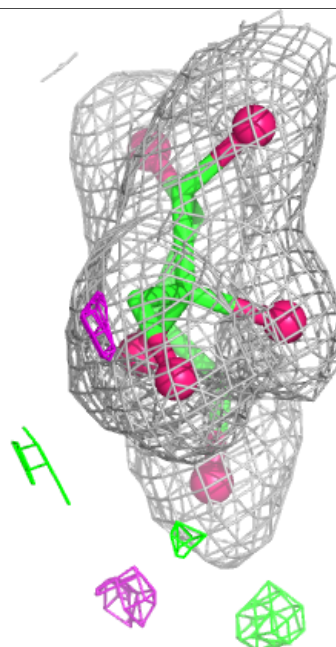
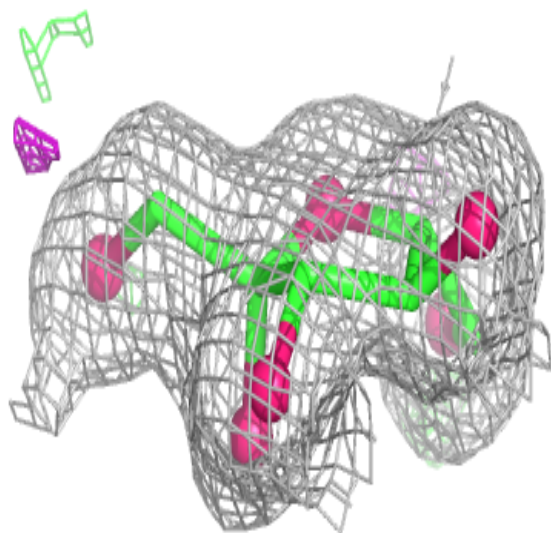
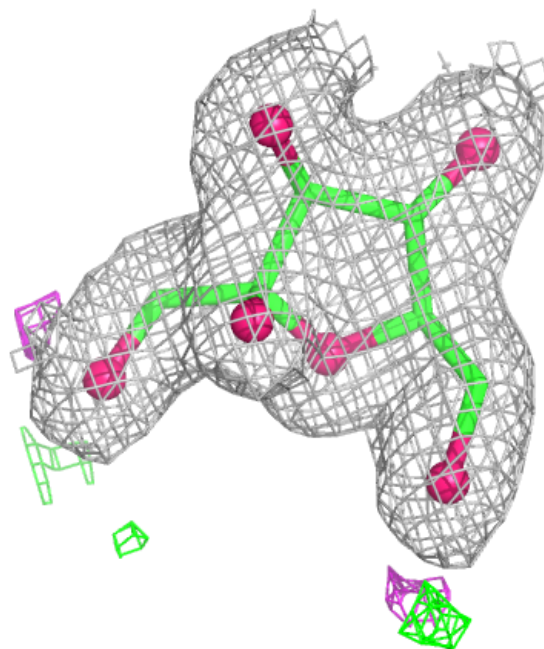
Electron density around FRU A 714:

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



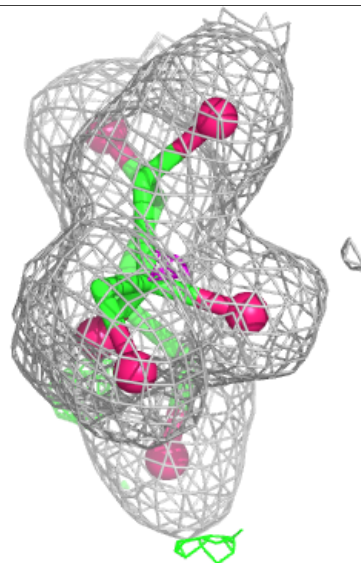
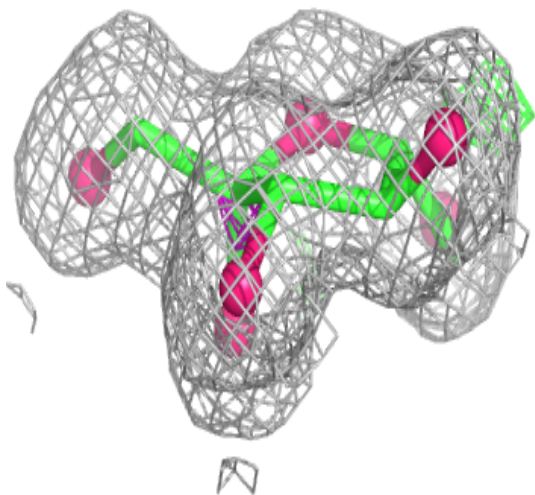
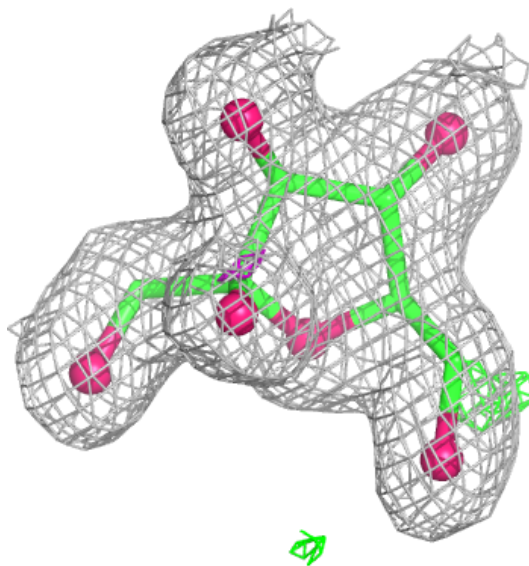
Electron density around FRU C 714:

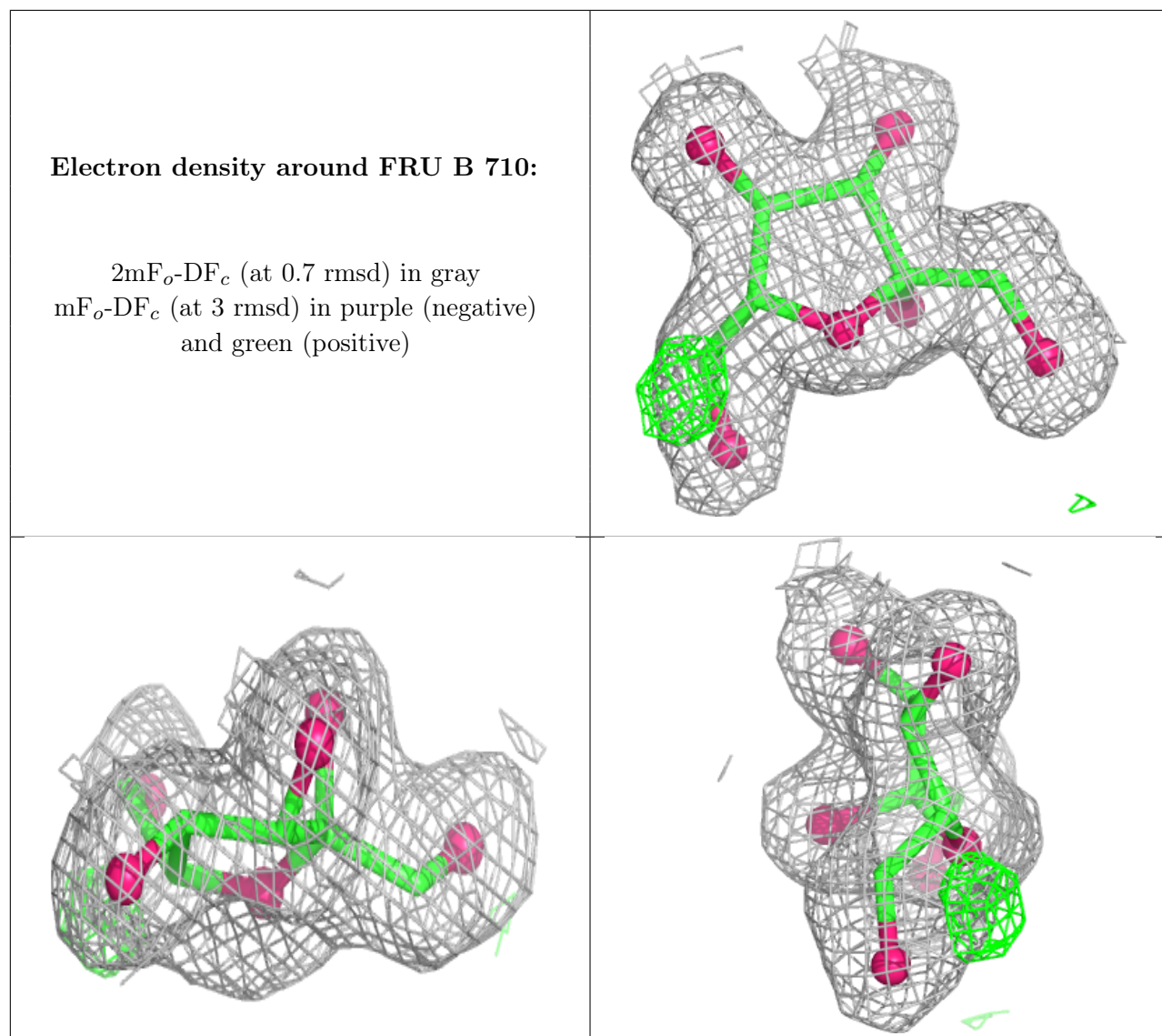
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FRU D 712:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.