



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 01:36 am GMT

PDB ID : 6FJG
Title : Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with fructose and 4-nitrophenol
Authors : Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on : 2018-01-22
Resolution : 1.73 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

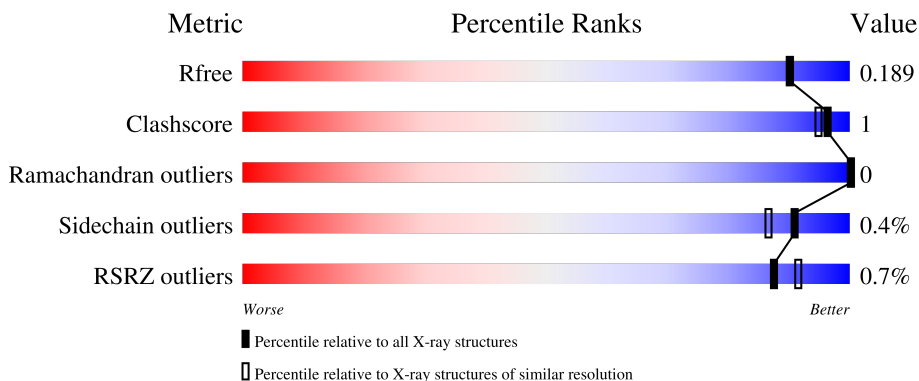
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



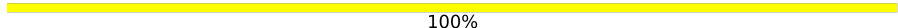


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	665	 92% • 6%
1	B	665	 92% • 6%
2	C	6	 83% 17%
2	F	6	 33% 67%
3	D	10	 40% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	H	2	 50% 50%
5	G	9	 56% 44%

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
3	MAN	D	6	-	-	-	X
8	EDO	A	1014	-	-	-	X
8	EDO	A	1015	-	-	-	X
8	EDO	B	1011	-	-	X	X
8	EDO	B	1012	-	-	-	X
9	NAG	B	1215	-	-	-	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 12173 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

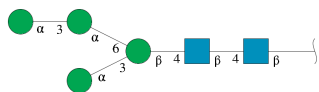
- Molecule 1 is a protein called Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	624	Total	C	N	O	S	0	3	0
			4822	3072	788	955	7			
1	B	624	Total	C	N	O	S	0	3	0
			4822	3072	788	955	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	ILE	conflict	UNP J7HDY4
A	80	ALA	ASP	engineered mutation	UNP J7HDY4
A	663	ALA	SER	conflict	UNP J7HDY4
A	665	TYR	ARG	conflict	UNP J7HDY4
B	2	VAL	ILE	conflict	UNP J7HDY4
B	80	ALA	ASP	engineered mutation	UNP J7HDY4
B	663	ALA	SER	conflict	UNP J7HDY4
B	665	TYR	ARG	conflict	UNP J7HDY4

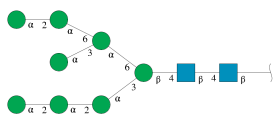
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

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



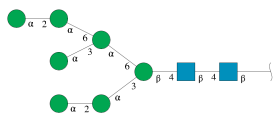
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	10	116	64	2	50	0	0	0

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



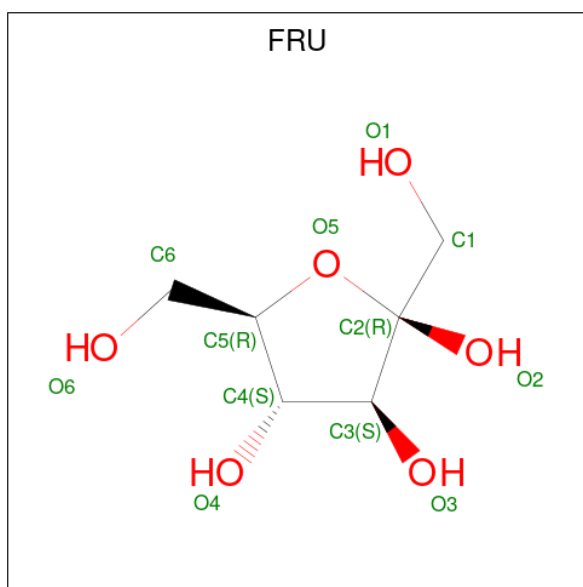
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0
4	H	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.



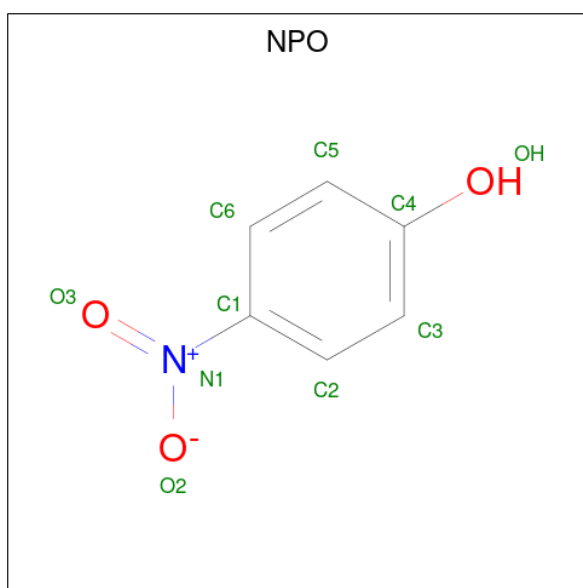
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	9	105	58	2	45	0	0	0

- Molecule 6 is beta-D-fructofuranose (three-letter code: FRU) (formula: C₆H₁₂O₆).



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

- Molecule 7 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



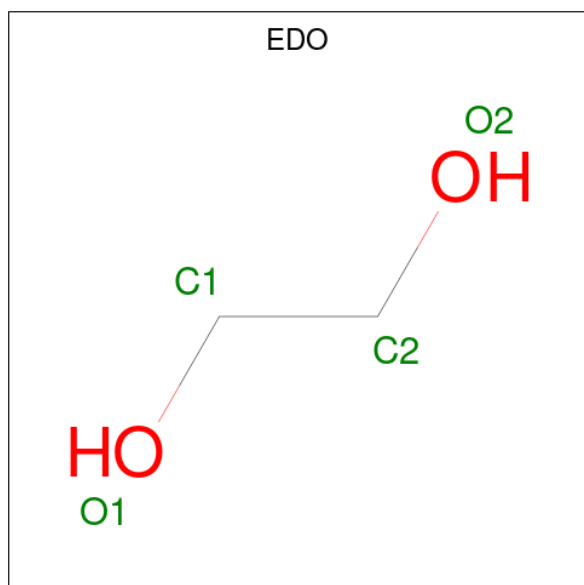
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			10	6	1	3		
7	A	1	Total	C	N	O	0	0
			10	6	1	3		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	1
			28	16	2	10		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	850	Total	O	0	0
			850	850		
10	B	696	Total	O	0	0
			696	696		

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

Chain D:  40% 60%



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

Chain E:  100%



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

Chain H:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 G:  56% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.50Å 205.65Å 146.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.33 – 1.73 84.17 – 1.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (119.33-1.73) 99.9 (84.17-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.163 , 0.178 0.174 , 0.189	Depositor DCC
R_{free} test set	11750 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtrriage
Anisotropy	0.591	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12173	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% 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, NPO, FRU, NAG, EDO, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/4957	0.66	0/6777
1	B	0.39	0/4957	0.65	0/6777
All	All	0.40	0/9914	0.65	0/13554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4822	0	4511	6	0
1	B	4822	0	4514	10	1
2	C	72	0	61	1	0
2	F	72	0	61	0	0
3	D	116	0	97	0	1
4	E	28	0	25	0	0
4	H	28	0	25	0	0
5	G	105	0	88	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	20	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	20	0	9	0	0
8	A	52	0	78	1	0
8	B	40	0	60	7	1
9	A	224	0	208	3	0
9	B	182	0	169	1	0
10	A	850	0	0	2	0
10	B	696	0	0	1	0
All	All	12173	0	9938	20	2

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 1.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:THR:HB	8:B:1011:EDO:H21	1.55	0.87
1:B:618:THR:HB	8:B:1011:EDO:C2	2.27	0.65
1:B:619:ALA:HB3	8:B:1011:EDO:H12	1.85	0.58
1:A:237:THR:HG23	10:A:2556:HOH:O	2.07	0.55
1:B:429:PRO:HB3	9:B:1444:NAG:H62	1.89	0.54
1:B:150:ILE:HG12	1:B:224:VAL:HG11	1.93	0.51
10:A:2108:HOH:O	2:C:2:NAG:H83	2.11	0.51
1:A:169:PRO:HD3	8:A:1003:EDO:H21	1.92	0.50
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.94	0.49
1:B:618:THR:CB	8:B:1011:EDO:H21	2.37	0.46
1:A:525:GLU:H	9:A:1606:NAG:H81	1.81	0.45
8:B:1012:EDO:H11	10:B:2023:HOH:O	2.17	0.44
1:B:662:PHE:O	8:B:1009:EDO:H22	2.17	0.44
1:B:578:THR:HG21	8:B:1006:EDO:H12	1.99	0.44
9:A:1606:NAG:H3	9:A:1606:NAG:H83	2.00	0.44
1:A:393:TRP:CZ2	1:A:395:TYR:HB3	2.55	0.42
1:B:393:TRP:CZ2	1:B:395:TYR:HB3	2.54	0.42
9:A:1471[A]:NAG:H83	9:A:1471[A]:NAG:H2	1.94	0.41
1:A:145:PHE:HB2	1:A:163:THR:HB	2.03	0.41
1:B:145:PHE:HB2	1:B:163:THR:HB	2.03	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLU:OE2	8:B:1011:EDO:O2[4_545]	1.80	0.40
3:D:8:MAN:O4	3:D:8:MAN:O4[2_555]	2.03	0.17

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	625/665 (94%)	597 (96%)	28 (4%)	0	100	100
1	B	625/665 (94%)	598 (96%)	27 (4%)	0	100	100
All	All	1250/1330 (94%)	1195 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	500/529 (94%)	498 (100%)	2 (0%)	91	86
1	B	500/529 (94%)	498 (100%)	2 (0%)	91	86
All	All	1000/1058 (94%)	996 (100%)	4 (0%)	91	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	503	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	142	ARG
1	B	503	LEU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

35 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	1.29	2 (11%)
2	BMA	C	3	2	11,11,12	0.36	0	15,15,17	1.22	1 (6%)
2	MAN	C	4	2	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
2	MAN	C	5	2	11,11,12	0.42	0	15,15,17	0.83	1 (6%)
2	MAN	C	6	2	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.86	1 (7%)	17,19,21	0.73	0
3	MAN	D	10	3	11,11,12	0.42	0	15,15,17	0.73	0
3	NAG	D	2	3	14,14,15	0.41	0	17,19,21	0.95	0
3	BMA	D	3	3	11,11,12	0.48	0	15,15,17	0.89	0
3	MAN	D	4	3	11,11,12	0.28	0	15,15,17	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	5	3	11,11,12	0.38	0	15,15,17	1.48	1 (6%)
3	MAN	D	6	3	11,11,12	0.36	0	15,15,17	0.87	1 (6%)
3	MAN	D	7	3	11,11,12	0.42	0	15,15,17	0.84	0
3	MAN	D	8	3	11,11,12	0.33	0	15,15,17	0.81	0
3	MAN	D	9	3	11,11,12	0.46	0	15,15,17	1.06	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
4	NAG	E	2	4	14,14,15	0.35	0	17,19,21	1.41	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.35	0	17,19,21	1.10	3 (17%)
2	NAG	F	2	2	14,14,15	0.51	0	17,19,21	0.73	0
2	BMA	F	3	2	11,11,12	0.35	0	15,15,17	1.10	1 (6%)
2	MAN	F	4	2	11,11,12	0.56	0	15,15,17	0.87	0
2	MAN	F	5	2	11,11,12	0.35	0	15,15,17	0.83	1 (6%)
2	MAN	F	6	2	11,11,12	0.43	0	15,15,17	1.00	1 (6%)
5	NAG	G	1	5,1	14,14,15	0.79	1 (7%)	17,19,21	0.83	0
5	NAG	G	2	5	14,14,15	0.37	0	17,19,21	0.89	0
5	BMA	G	3	5	11,11,12	0.41	0	15,15,17	0.74	0
5	MAN	G	4	5	11,11,12	0.34	0	15,15,17	0.92	0
5	MAN	G	5	5	11,11,12	0.33	0	15,15,17	0.86	0
5	MAN	G	6	5	11,11,12	0.52	0	15,15,17	0.91	1 (6%)
5	MAN	G	7	5	11,11,12	0.30	0	15,15,17	0.81	0
5	MAN	G	8	5	11,11,12	0.38	0	15,15,17	0.93	1 (6%)
5	MAN	G	9	5	11,11,12	0.45	0	15,15,17	0.71	1 (6%)
4	NAG	H	1	4,1	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
4	NAG	H	2	4	14,14,15	0.41	0	17,19,21	0.98	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	2/2/19/22	0/1/1/1
2	MAN	F	6	2	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
5	MAN	G	7	5	-	0/2/19/22	0/1/1/1
5	MAN	G	8	5	-	2/2/19/22	0/1/1/1
5	MAN	G	9	5	-	2/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	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)
5	G	1	NAG	C1-C2	2.61	1.56	1.52
3	D	1	NAG	C1-C2	2.40	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	4.79	118.68	112.19
4	E	2	NAG	C8-C7-N2	3.07	121.30	116.10
2	C	1	NAG	O5-C1-C2	-3.01	106.53	111.29
5	G	8	MAN	C1-O5-C5	2.90	116.12	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C2-N2-C7	2.86	126.97	122.90
2	C	2	NAG	C2-N2-C7	2.85	126.97	122.90
3	D	9	MAN	O5-C5-C6	2.70	111.44	107.20
2	F	3	BMA	C1-O5-C5	2.69	115.84	112.19
2	F	1	NAG	C1-O5-C5	2.53	115.62	112.19
2	C	4	MAN	C1-C2-C3	2.52	112.77	109.67
3	D	4	MAN	C1-O5-C5	2.49	115.57	112.19
2	C	5	MAN	C1-O5-C5	2.48	115.55	112.19
2	F	1	NAG	O4-C4-C5	2.40	115.26	109.30
3	D	6	MAN	C1-O5-C5	2.36	115.39	112.19
4	E	1	NAG	O4-C4-C3	-2.35	104.92	110.35
2	F	5	MAN	C1-O5-C5	2.31	115.32	112.19
2	F	6	MAN	O5-C5-C6	2.29	110.79	107.20
2	C	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	D	4	MAN	O2-C2-C1	-2.26	104.53	109.15
5	G	6	MAN	C1-O5-C5	2.16	115.12	112.19
5	G	9	MAN	C1-O5-C5	2.15	115.11	112.19
4	H	1	NAG	C1-C2-N2	-2.14	106.83	110.49
2	C	2	NAG	C1-O5-C5	2.12	115.06	112.19
2	C	4	MAN	C1-O5-C5	2.11	115.05	112.19
2	F	1	NAG	O5-C1-C2	-2.10	107.98	111.29
2	C	3	BMA	C1-O5-C5	2.04	114.96	112.19
2	C	6	MAN	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

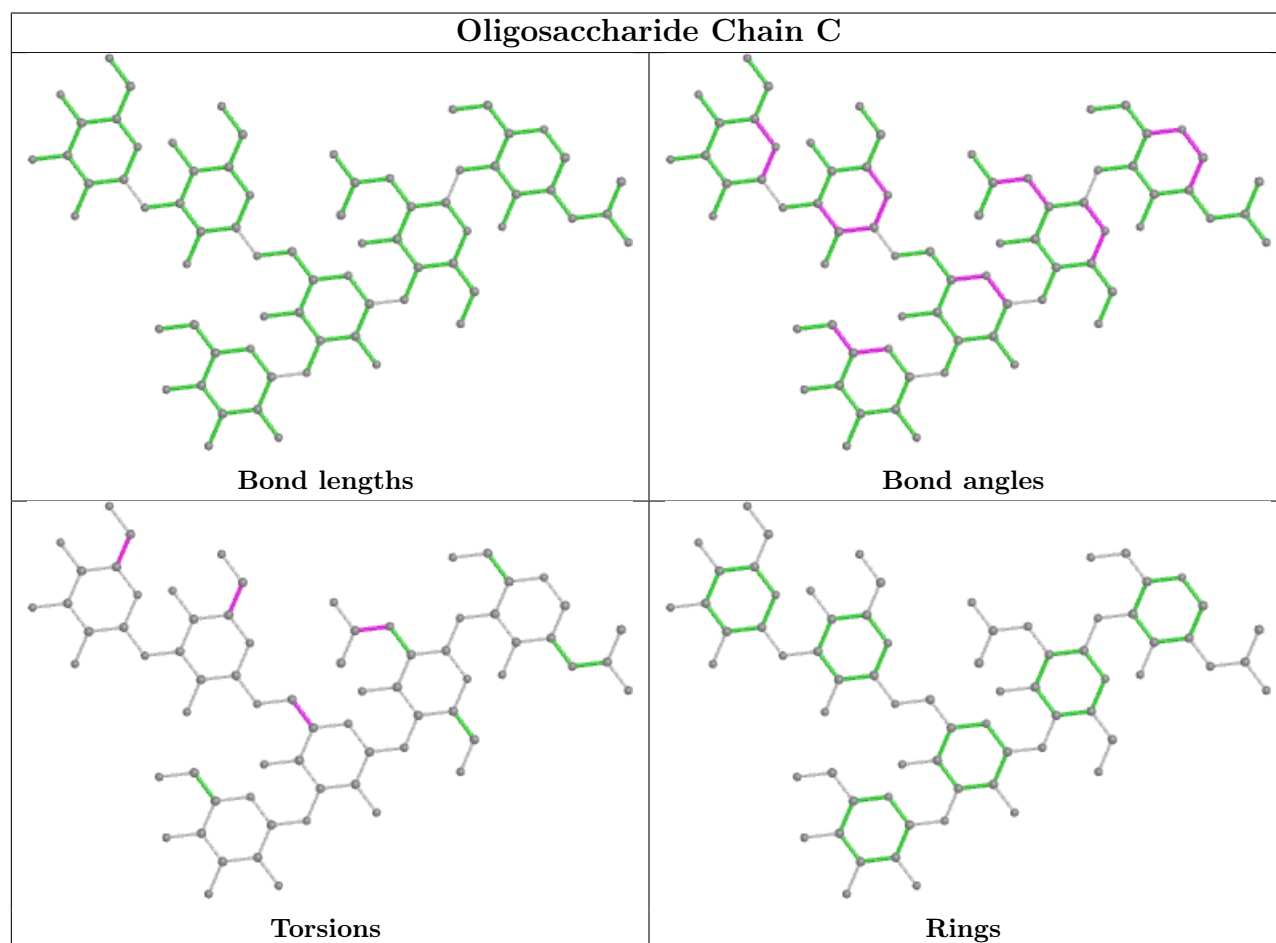
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
5	G	8	MAN	C4-C5-C6-O6

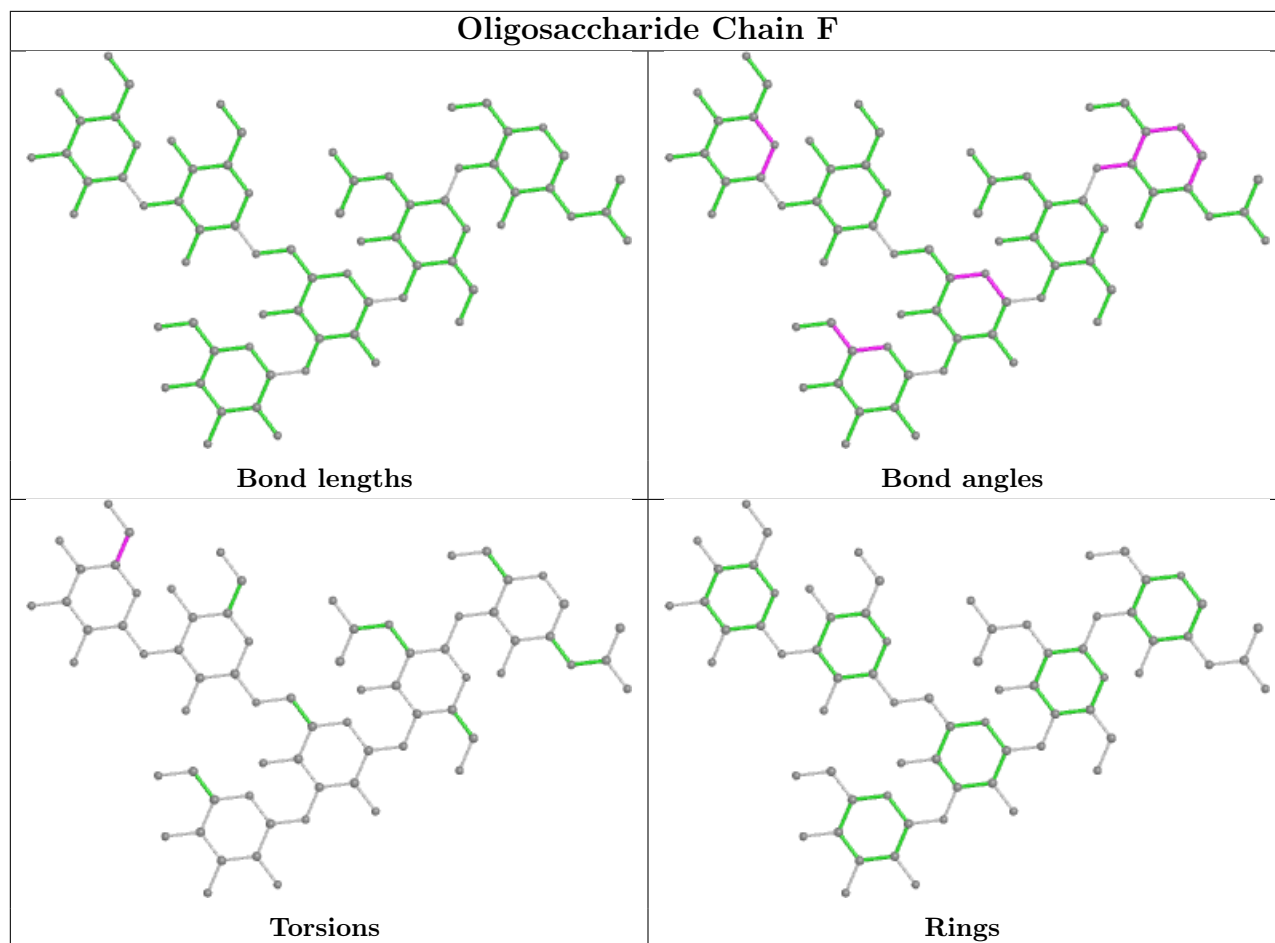
There are no ring outliers.

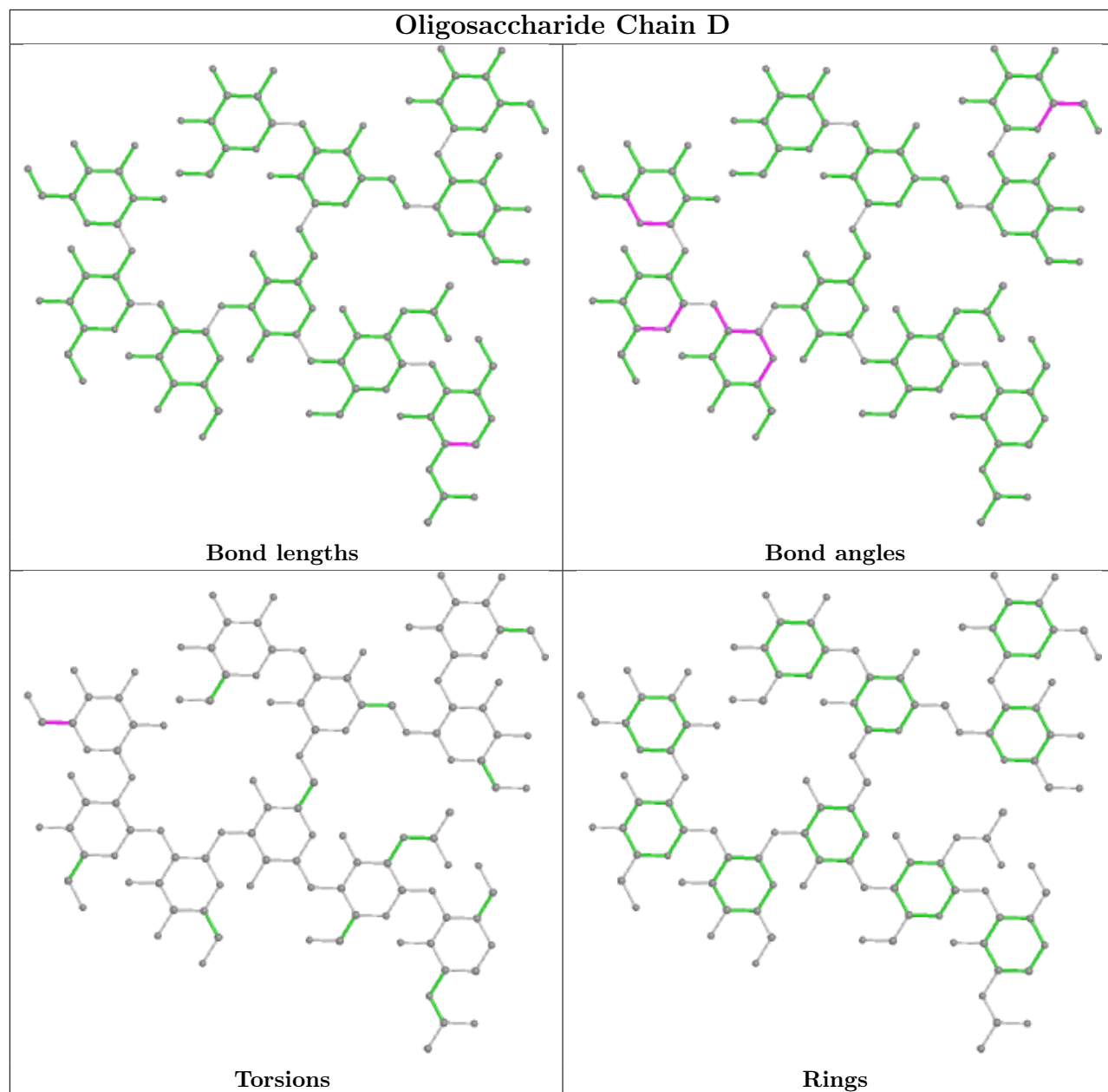
2 monomers are involved in 2 short contacts:

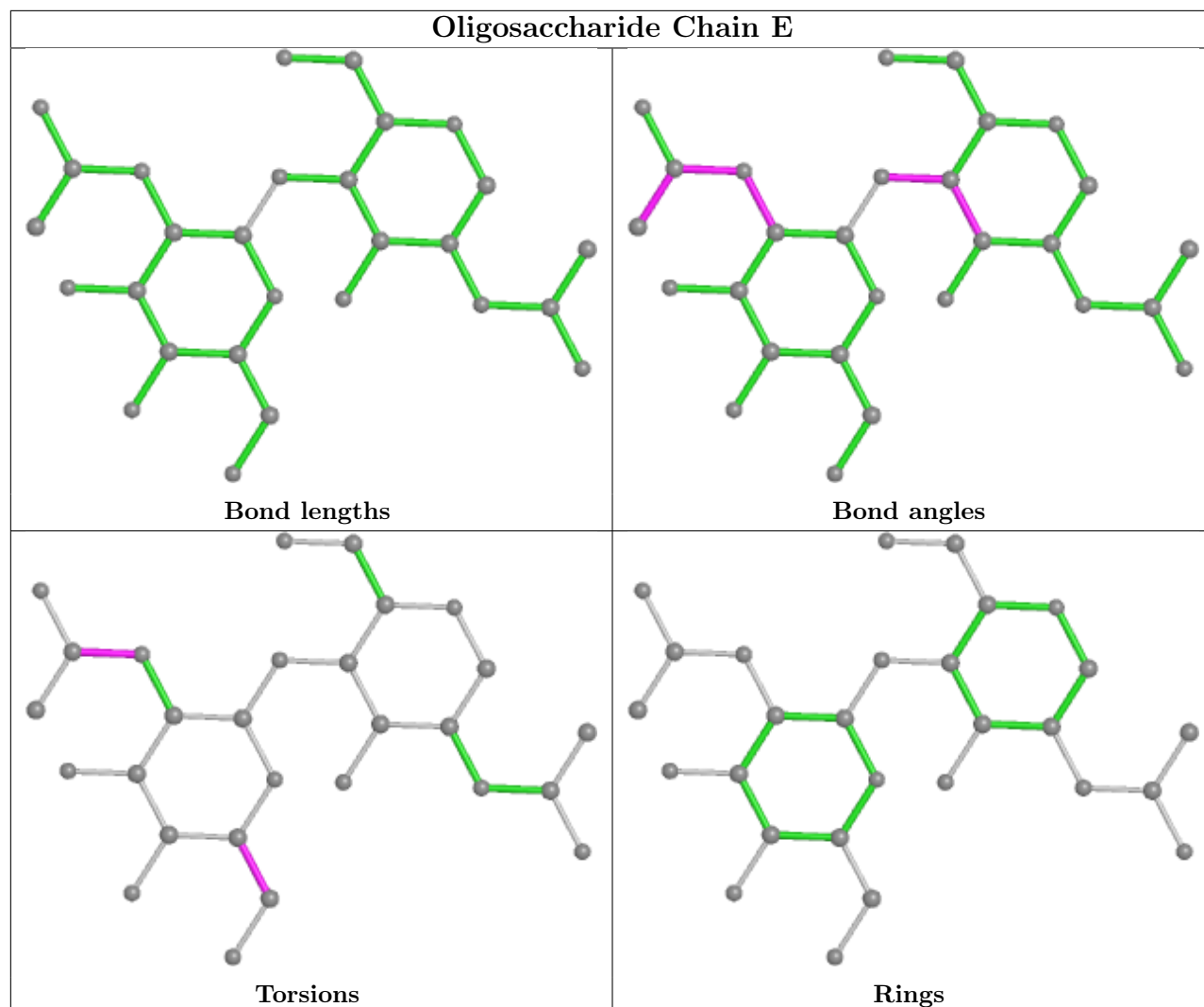
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
3	D	8	MAN	0	1

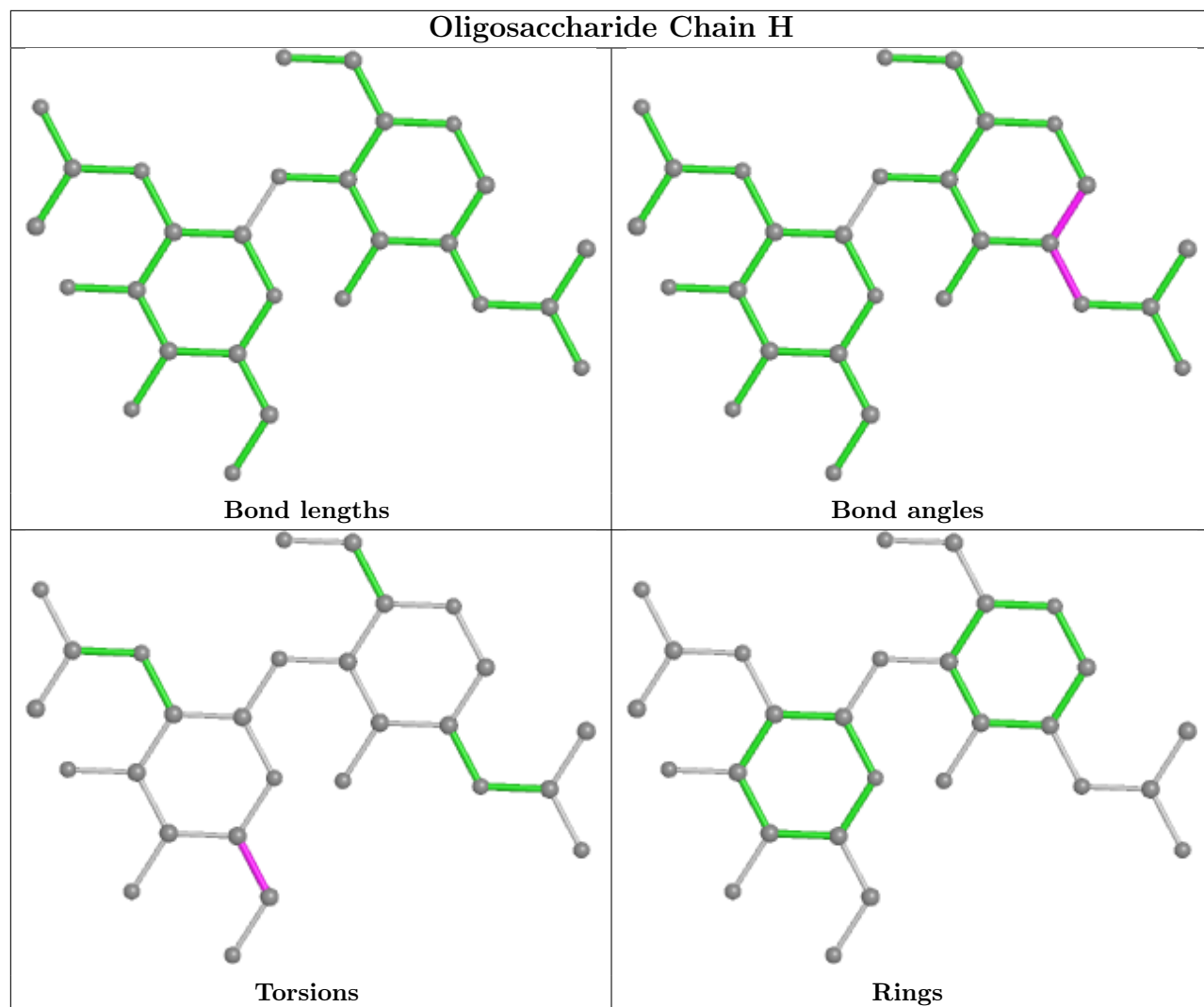
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

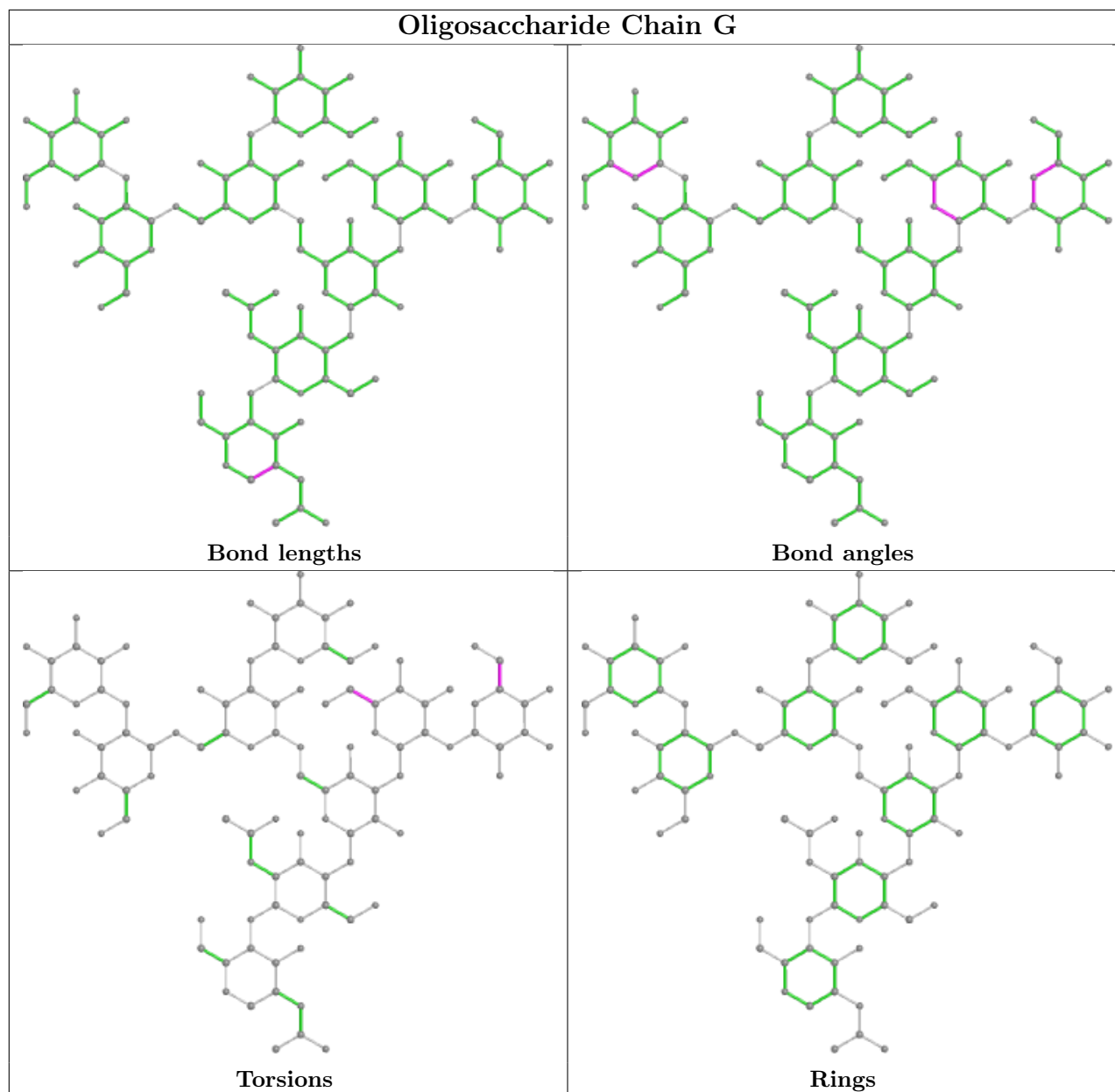












5.6 Ligand geometry [i](#)

58 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
9	NAG	A	1242	1	14,14,15	0.26	0	17,19,21	1.24	2 (11%)
9	NAG	B	1242	1	14,14,15	0.39	0	17,19,21	1.87	4 (23%)
8	EDO	B	1008	-	3,3,3	0.47	0	2,2,2	0.31	0
7	NPO	B	1001	-	9,10,10	0.88	0	11,13,13	0.75	0
9	NAG	A	1444	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
9	NAG	B	1215	1	14,14,15	0.48	0	17,19,21	2.14	3 (17%)
7	NPO	A	1002	-	9,10,10	0.86	0	11,13,13	0.76	0
9	NAG	A	1471[A]	1	14,14,15	0.38	0	17,19,21	1.38	1 (5%)
9	NAG	A	1512	1	14,14,15	0.34	0	17,19,21	1.78	3 (17%)
8	EDO	A	1015	-	3,3,3	0.48	0	2,2,2	0.47	0
9	NAG	A	1319	1	14,14,15	0.38	0	17,19,21	1.23	1 (5%)
9	NAG	A	1483	1	14,14,15	0.33	0	17,19,21	1.29	1 (5%)
9	NAG	A	1555	1	14,14,15	0.26	0	17,19,21	1.10	2 (11%)
9	NAG	A	1052	1	14,14,15	0.27	0	17,19,21	1.18	2 (11%)
8	EDO	A	1013	-	3,3,3	0.44	0	2,2,2	0.27	0
9	NAG	B	1644	1	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
9	NAG	A	1539	1	14,14,15	0.55	0	17,19,21	2.01	1 (5%)
8	EDO	A	1009	-	3,3,3	0.52	0	2,2,2	0.21	0
8	EDO	B	1007	-	3,3,3	0.45	0	2,2,2	0.43	0
8	EDO	A	1007	-	3,3,3	0.53	0	2,2,2	0.03	0
9	NAG	B	1471[A]	1	14,14,15	0.40	0	17,19,21	1.00	2 (11%)
6	FRU	B	1000	-	11,12,12	0.64	0	10,18,18	0.83	0
9	NAG	B	1357	1	14,14,15	0.34	0	17,19,21	0.86	0
9	NAG	B	1483	1	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
8	EDO	A	1008	-	3,3,3	0.46	0	2,2,2	0.21	0
9	NAG	B	1539	1	14,14,15	0.58	0	17,19,21	1.64	2 (11%)
8	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.18	0
9	NAG	A	1236	1	14,14,15	0.53	0	17,19,21	0.92	0
8	EDO	B	1004	-	3,3,3	0.54	0	2,2,2	0.24	0
8	EDO	B	1005	-	3,3,3	0.53	0	2,2,2	0.28	0
8	EDO	B	1010	-	3,3,3	0.54	0	2,2,2	0.23	0
8	EDO	B	1012	-	3,3,3	0.47	0	2,2,2	0.10	0
9	NAG	B	1444	1	14,14,15	0.41	0	17,19,21	1.41	1 (5%)
8	EDO	A	1012	-	3,3,3	0.45	0	2,2,2	0.10	0
9	NAG	B	1555	1	14,14,15	0.48	0	17,19,21	0.89	0
9	NAG	B	1319	1	14,14,15	0.34	0	17,19,21	2.48	2 (11%)
9	NAG	A	1471[B]	1	14,14,15	0.35	0	17,19,21	0.79	0
8	EDO	A	1014	-	3,3,3	0.46	0	2,2,2	0.26	0
8	EDO	B	1011	-	3,3,3	0.36	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	1471[B]	1	14,14,15	0.27	0	17,19,21	0.90	0
8	EDO	A	1003	-	3,3,3	0.62	0	2,2,2	0.60	0
8	EDO	A	1011	-	3,3,3	0.58	0	2,2,2	0.14	0
8	EDO	B	1003	-	3,3,3	0.52	0	2,2,2	0.29	0
9	NAG	A	1606	1	14,14,15	0.44	0	17,19,21	1.74	3 (17%)
8	EDO	A	1010	-	3,3,3	0.59	0	2,2,2	0.33	0
9	NAG	A	1644	1	14,14,15	0.49	0	17,19,21	0.83	0
9	NAG	B	1125	1	14,14,15	0.64	0	17,19,21	2.49	4 (23%)
8	EDO	B	1009	-	3,3,3	0.53	0	2,2,2	0.22	0
9	NAG	A	1357	1	14,14,15	0.26	0	17,19,21	1.36	2 (11%)
6	FRU	A	1000	-	11,12,12	0.61	0	10,18,18	0.79	0
8	EDO	A	1006	-	3,3,3	0.53	0	2,2,2	0.23	0
9	NAG	A	1215	1	14,14,15	0.40	0	17,19,21	1.79	1 (5%)
9	NAG	A	1125	1	14,14,15	0.44	0	17,19,21	1.29	1 (5%)
7	NPO	A	1001	-	9,10,10	0.87	0	11,13,13	0.82	0
8	EDO	A	1004	-	3,3,3	0.58	0	2,2,2	0.26	0
9	NAG	B	1052	1	14,14,15	0.41	0	17,19,21	0.91	0
7	NPO	B	1002	-	9,10,10	0.85	0	11,13,13	0.88	1 (9%)
8	EDO	B	1006	-	3,3,3	0.41	0	2,2,2	0.31	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
9	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1242	1	-	2/6/23/26	0/1/1/1
8	EDO	B	1008	-	-	0/1/1/1	-
7	NPO	B	1001	-	-	0/2/4/4	0/1/1/1
9	NAG	A	1444	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
7	NPO	A	1002	-	-	0/2/4/4	0/1/1/1
9	NAG	A	1471[A]	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1512	1	-	3/6/23/26	0/1/1/1
8	EDO	A	1015	-	-	1/1/1/1	-
9	NAG	A	1319	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1555	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1052	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	1013	-	-	1/1/1/1	-
9	NAG	B	1644	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1539	1	-	1/6/23/26	0/1/1/1
8	EDO	A	1009	-	-	1/1/1/1	-
8	EDO	B	1007	-	-	1/1/1/1	-
8	EDO	A	1007	-	-	0/1/1/1	-
9	NAG	B	1471[A]	1	-	0/6/23/26	0/1/1/1
6	FRU	B	1000	-	-	1/5/24/24	0/1/1/1
9	NAG	B	1357	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
8	EDO	A	1008	-	-	0/1/1/1	-
9	NAG	B	1539	1	-	2/6/23/26	0/1/1/1
8	EDO	A	1005	-	-	0/1/1/1	-
9	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
8	EDO	B	1004	-	-	1/1/1/1	-
8	EDO	B	1005	-	-	1/1/1/1	-
8	EDO	B	1010	-	-	1/1/1/1	-
8	EDO	B	1012	-	-	0/1/1/1	-
9	NAG	B	1444	1	-	2/6/23/26	0/1/1/1
8	EDO	A	1012	-	-	0/1/1/1	-
9	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1319	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1471[B]	1	-	1/6/23/26	0/1/1/1
8	EDO	A	1014	-	-	1/1/1/1	-
8	EDO	B	1011	-	-	0/1/1/1	-
9	NAG	B	1471[B]	1	-	1/6/23/26	0/1/1/1
8	EDO	A	1003	-	-	1/1/1/1	-
8	EDO	A	1011	-	-	0/1/1/1	-
8	EDO	B	1003	-	-	1/1/1/1	-
9	NAG	A	1606	1	-	3/6/23/26	0/1/1/1
8	EDO	A	1010	-	-	1/1/1/1	-
9	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1125	1	-	0/6/23/26	0/1/1/1
8	EDO	B	1009	-	-	1/1/1/1	-
9	NAG	A	1357	1	-	2/6/23/26	0/1/1/1
6	FRU	A	1000	-	-	1/5/24/24	0/1/1/1
8	EDO	A	1006	-	-	1/1/1/1	-
9	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1125	1	-	2/6/23/26	0/1/1/1
7	NPO	A	1001	-	-	0/2/4/4	0/1/1/1
8	EDO	A	1004	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1052	1	-	2/6/23/26	0/1/1/1
7	NPO	B	1002	-	-	0/2/4/4	0/1/1/1
8	EDO	B	1006	-	-	0/1/1/1	-

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1125	NAG	C1-O5-C5	8.17	123.26	112.19
9	B	1319	NAG	C1-O5-C5	8.12	123.19	112.19
9	A	1539	NAG	C1-O5-C5	7.59	122.48	112.19
9	A	1215	NAG	C1-O5-C5	6.70	121.27	112.19
9	B	1242	NAG	C1-O5-C5	5.66	119.86	112.19
9	A	1512	NAG	C1-O5-C5	5.40	119.51	112.19
9	B	1539	NAG	C1-O5-C5	5.06	119.05	112.19
9	B	1215	NAG	C1-O5-C5	5.02	119.00	112.19
9	B	1444	NAG	C1-O5-C5	4.99	118.96	112.19
9	A	1483	NAG	C1-O5-C5	4.67	118.52	112.19
9	B	1215	NAG	C4-C3-C2	4.64	117.82	111.02
9	A	1606	NAG	C2-N2-C7	4.45	129.24	122.90
9	B	1215	NAG	C3-C4-C5	4.44	118.15	110.24
9	B	1319	NAG	O5-C1-C2	4.39	118.22	111.29
9	A	1471[A]	NAG	C1-O5-C5	4.32	118.04	112.19
9	A	1606	NAG	C8-C7-N2	3.77	122.47	116.10
9	A	1357	NAG	C2-N2-C7	3.73	128.21	122.90
9	A	1319	NAG	O5-C5-C6	3.60	112.84	107.20
9	B	1125	NAG	C1-C2-N2	3.18	115.91	110.49
9	A	1242	NAG	C1-O5-C5	2.87	116.07	112.19
9	A	1444	NAG	C1-O5-C5	2.85	116.05	112.19
9	A	1125	NAG	C4-C3-C2	2.81	115.13	111.02
9	B	1471[A]	NAG	C1-O5-C5	2.65	115.79	112.19
9	A	1606	NAG	O7-C7-C8	-2.62	117.20	122.06
9	B	1242	NAG	C8-C7-N2	2.60	120.51	116.10
9	A	1242	NAG	C1-C2-N2	2.54	114.82	110.49
9	A	1512	NAG	C8-C7-N2	2.49	120.31	116.10
9	B	1125	NAG	O5-C1-C2	2.43	115.13	111.29
9	A	1357	NAG	C8-C7-N2	2.36	120.10	116.10
9	A	1052	NAG	C8-C7-N2	2.35	120.08	116.10
9	A	1052	NAG	O5-C1-C2	-2.31	107.64	111.29
9	B	1242	NAG	C4-C3-C2	-2.28	107.68	111.02
9	A	1555	NAG	C2-N2-C7	2.26	126.13	122.90
7	B	1002	NPO	O3-N1-C1	2.25	121.99	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1512	NAG	C4-C3-C2	-2.23	107.75	111.02
9	B	1471[A]	NAG	C2-N2-C7	-2.19	119.78	122.90
9	B	1483	NAG	C1-O5-C5	2.16	115.12	112.19
9	B	1644	NAG	C1-C2-N2	-2.14	106.82	110.49
9	B	1125	NAG	C6-C5-C4	-2.10	108.08	113.00
9	A	1555	NAG	C8-C7-N2	2.09	119.63	116.10
9	B	1539	NAG	C1-C2-N2	2.06	114.00	110.49
9	B	1483	NAG	O5-C1-C2	-2.04	108.07	111.29
9	B	1242	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1125	NAG	C4-C5-C6-O6
9	B	1539	NAG	C4-C5-C6-O6
9	A	1319	NAG	O5-C5-C6-O6
9	A	1052	NAG	C8-C7-N2-C2
9	A	1052	NAG	O7-C7-N2-C2
9	A	1357	NAG	C8-C7-N2-C2
9	A	1357	NAG	O7-C7-N2-C2
9	A	1471[A]	NAG	C8-C7-N2-C2
9	A	1471[A]	NAG	O7-C7-N2-C2
9	A	1512	NAG	C8-C7-N2-C2
9	A	1512	NAG	O7-C7-N2-C2
9	A	1555	NAG	C8-C7-N2-C2
9	A	1555	NAG	O7-C7-N2-C2
9	A	1606	NAG	C8-C7-N2-C2
9	A	1606	NAG	O7-C7-N2-C2
9	B	1242	NAG	C8-C7-N2-C2
9	B	1242	NAG	O7-C7-N2-C2
9	A	1125	NAG	O5-C5-C6-O6
9	B	1539	NAG	O5-C5-C6-O6
9	B	1052	NAG	C4-C5-C6-O6
9	A	1319	NAG	C4-C5-C6-O6
9	B	1052	NAG	O5-C5-C6-O6
8	A	1004	EDO	O1-C1-C2-O2
8	A	1006	EDO	O1-C1-C2-O2
8	A	1010	EDO	O1-C1-C2-O2
8	B	1003	EDO	O1-C1-C2-O2
8	B	1004	EDO	O1-C1-C2-O2
8	B	1005	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	1007	EDO	O1-C1-C2-O2
9	B	1319	NAG	C4-C5-C6-O6
9	B	1444	NAG	C4-C5-C6-O6
9	A	1539	NAG	C4-C5-C6-O6
9	B	1357	NAG	C4-C5-C6-O6
8	B	1010	EDO	O1-C1-C2-O2
9	A	1471[B]	NAG	C4-C5-C6-O6
8	A	1003	EDO	O1-C1-C2-O2
8	A	1009	EDO	O1-C1-C2-O2
8	A	1015	EDO	O1-C1-C2-O2
9	B	1444	NAG	O5-C5-C6-O6
9	B	1357	NAG	O5-C5-C6-O6
9	A	1606	NAG	C3-C2-N2-C7
8	B	1009	EDO	O1-C1-C2-O2
9	A	1512	NAG	C4-C5-C6-O6
8	A	1014	EDO	O1-C1-C2-O2
9	A	1052	NAG	C4-C5-C6-O6
8	A	1013	EDO	O1-C1-C2-O2
9	B	1471[B]	NAG	C4-C5-C6-O6
6	A	1000	FRU	O1-C1-C2-C3
6	B	1000	FRU	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1471[A]	NAG	1	0
8	B	1012	EDO	1	0
9	B	1444	NAG	1	0
8	B	1011	EDO	4	1
8	A	1003	EDO	1	0
9	A	1606	NAG	2	0
8	B	1009	EDO	1	0
8	B	1006	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	624/665 (93%)	-0.12	2 (0%) 94 95	12, 20, 31, 45	0
1	B	624/665 (93%)	-0.07	7 (1%) 80 85	14, 26, 41, 50	0
All	All	1248/1330 (93%)	-0.09	9 (0%) 87 91	12, 23, 38, 50	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	TRP	2.8
1	B	622	VAL	2.4
1	B	571	GLU	2.1
1	B	42	CYS	2.1
1	B	569	GLY	2.1
1	A	317	TRP	2.1
1	A	291	TYR	2.0
1	B	619	ALA	2.0
1	B	214	THR	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	F	6	11/12	0.56	0.35	60,67,69,71	0

Continued on next page...

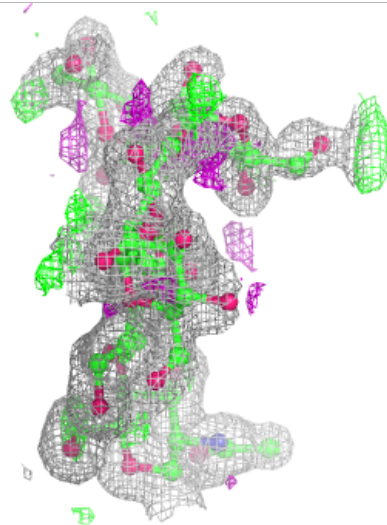
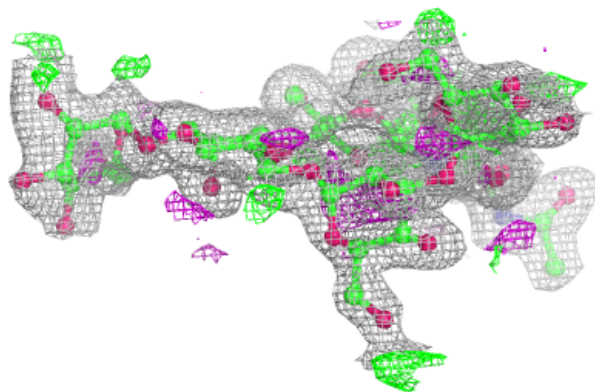
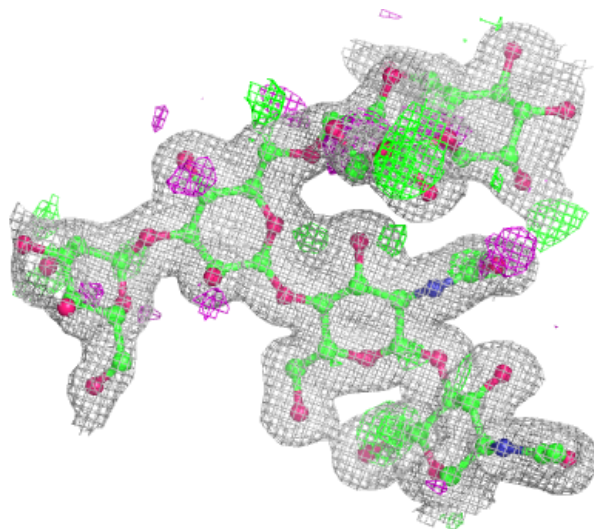
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	G	6	11/12	0.68	0.23	52,55,58,58	0
4	NAG	E	2	14/15	0.69	0.29	71,77,82,83	0
4	NAG	H	2	14/15	0.71	0.30	74,80,87,87	0
3	MAN	D	9	11/12	0.72	0.24	53,56,61,61	0
3	MAN	D	6	11/12	0.73	0.43	72,80,82,83	0
5	MAN	G	9	11/12	0.74	0.19	49,51,53,55	0
2	MAN	C	4	11/12	0.75	0.26	43,45,50,53	0
2	MAN	C	5	11/12	0.76	0.21	43,45,46,47	0
2	MAN	C	6	11/12	0.77	0.24	45,52,55,56	0
2	MAN	F	4	11/12	0.78	0.28	54,57,59,61	0
3	MAN	D	5	11/12	0.78	0.16	48,51,53,61	0
2	MAN	F	5	11/12	0.81	0.23	55,58,59,60	0
3	MAN	D	8	11/12	0.84	0.14	33,36,40,44	0
5	MAN	G	5	11/12	0.85	0.13	36,37,41,45	0
4	NAG	H	1	14/15	0.86	0.17	46,51,57,68	0
5	MAN	G	8	11/12	0.87	0.12	35,41,45,48	0
2	BMA	F	3	11/12	0.87	0.12	35,41,49,50	0
4	NAG	E	1	14/15	0.88	0.16	38,42,49,62	0
3	MAN	D	4	11/12	0.88	0.12	31,38,42,47	0
2	BMA	C	3	11/12	0.92	0.10	26,31,37,39	0
2	NAG	F	2	14/15	0.94	0.09	25,26,28,31	0
5	MAN	G	4	11/12	0.94	0.09	18,20,25,29	0
2	NAG	C	2	14/15	0.95	0.10	18,20,24,31	0
3	MAN	D	7	11/12	0.96	0.09	16,19,24,29	0
3	BMA	D	3	11/12	0.96	0.08	19,19,21,25	0
2	NAG	C	1	14/15	0.96	0.09	16,18,25,25	0
5	BMA	G	3	11/12	0.97	0.07	21,21,24,28	0
3	NAG	D	1	14/15	0.97	0.08	14,14,16,16	0
3	NAG	D	2	14/15	0.97	0.09	15,16,17,18	0
2	NAG	F	1	14/15	0.97	0.07	21,24,31,33	0
3	MAN	D	10	11/12	0.97	0.09	14,14,15,15	0
5	NAG	G	1	14/15	0.97	0.07	17,18,19,19	0
5	NAG	G	2	14/15	0.98	0.07	18,18,20,21	0
5	MAN	G	7	11/12	0.98	0.08	16,16,17,17	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.

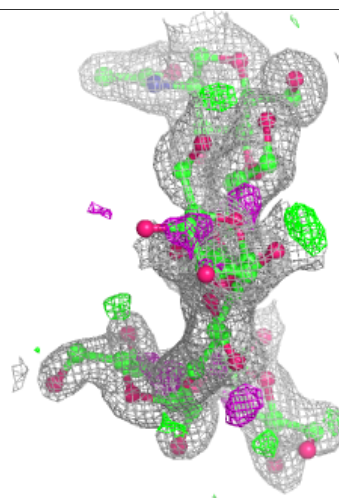
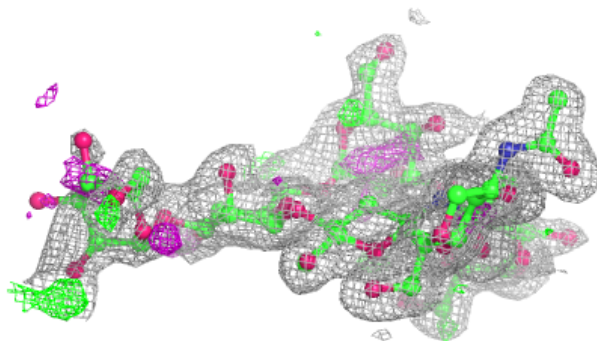
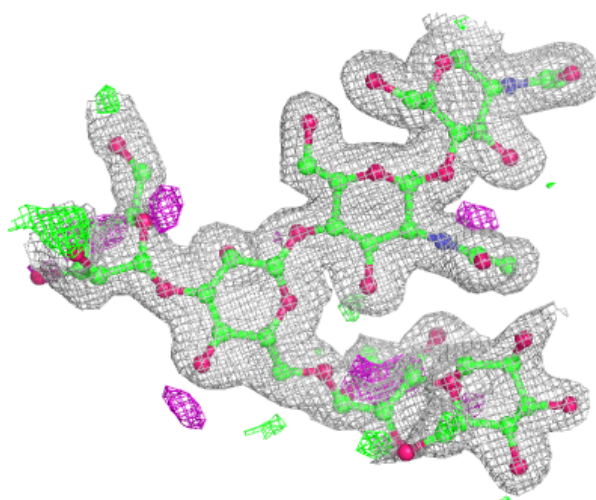
Electron density around Chain C:

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



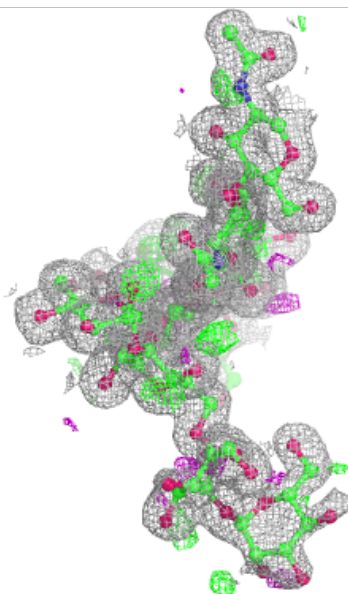
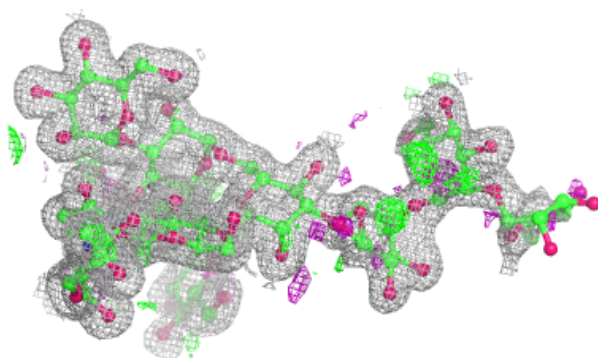
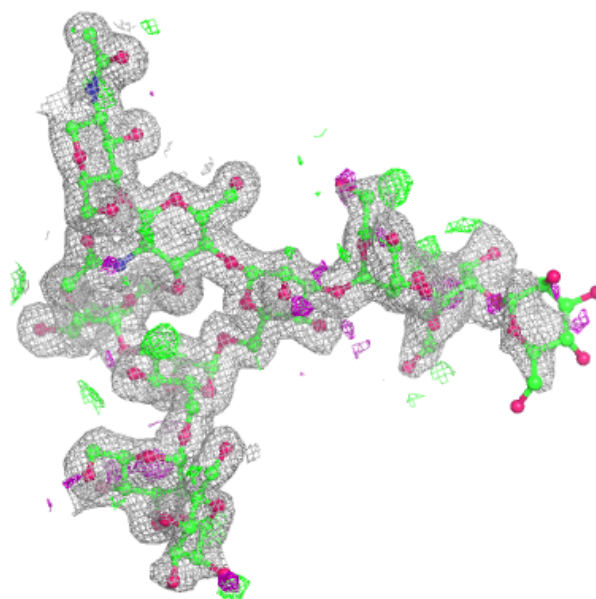
Electron density around Chain F:

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



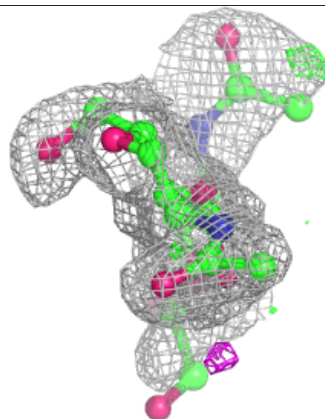
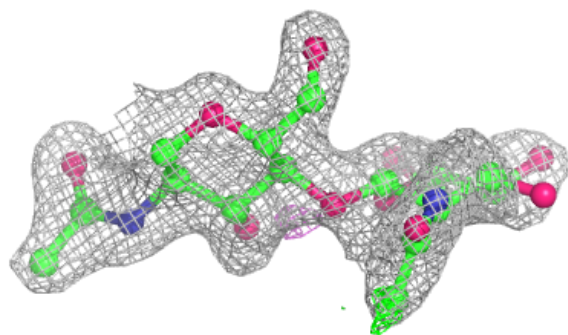
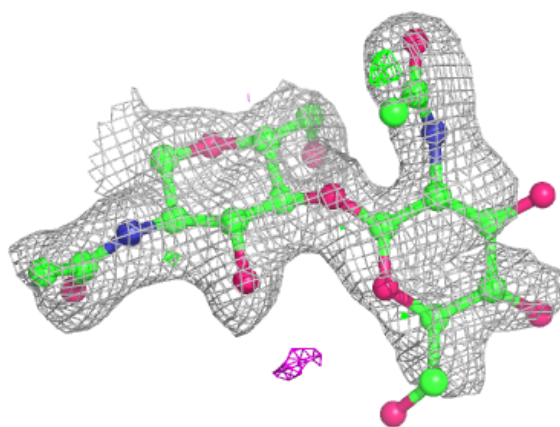
Electron density around Chain D:

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



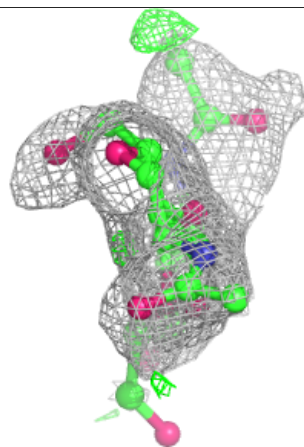
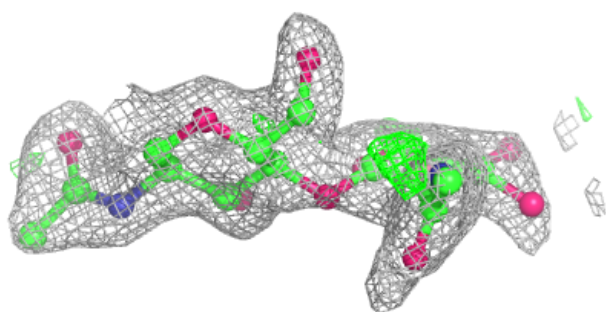
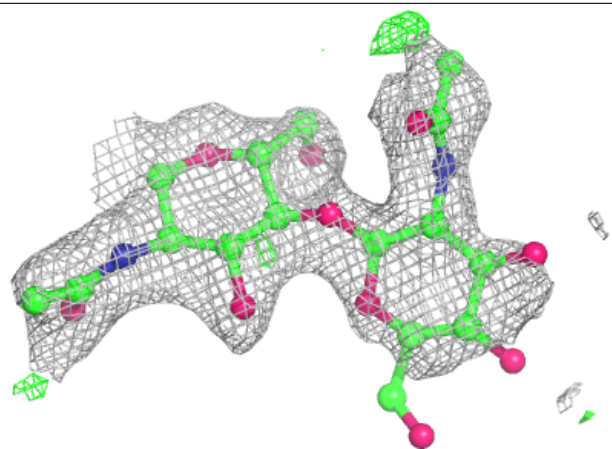
Electron density around Chain E:

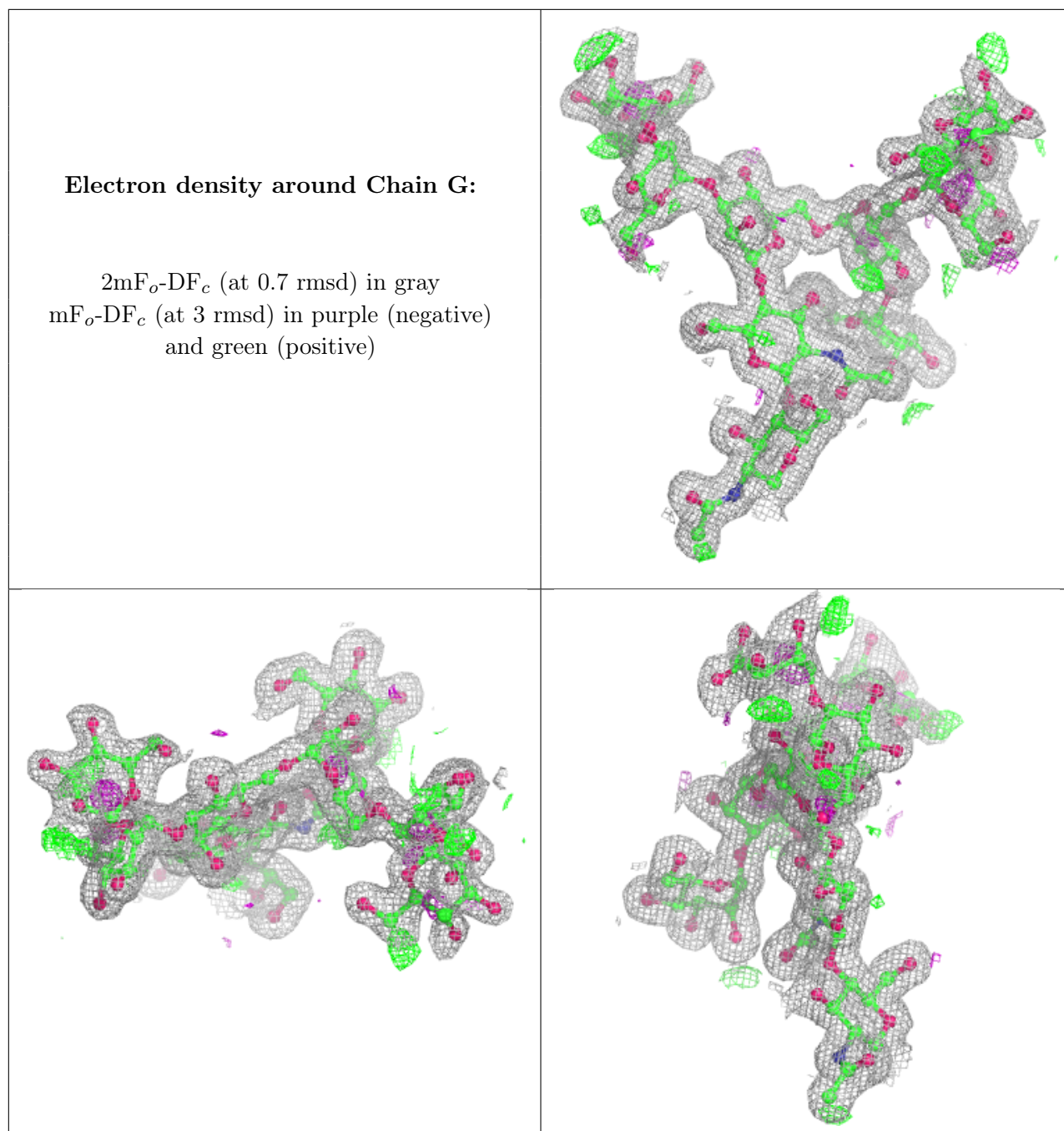
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	A	1014	4/4	0.53	0.43	61,62,63,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	B	1125	14/15	0.54	0.33	54,60,66,69	0
8	EDO	B	1003	4/4	0.55	0.22	58,58,59,60	0
8	EDO	B	1007	4/4	0.60	0.33	51,53,54,54	0
9	NAG	B	1319	14/15	0.62	0.36	75,82,83,83	0
8	EDO	B	1005	4/4	0.63	0.23	73,74,74,75	0
9	NAG	A	1606	14/15	0.67	0.26	45,48,51,55	0
9	NAG	A	1539	14/15	0.68	0.25	44,50,53,54	0
8	EDO	B	1011	4/4	0.68	0.48	54,55,56,57	0
8	EDO	B	1008	4/4	0.69	0.39	63,65,65,66	0
9	NAG	B	1242	14/15	0.69	0.31	70,76,79,79	0
9	NAG	A	1242	14/15	0.69	0.27	54,60,62,64	0
8	EDO	A	1004	4/4	0.71	0.16	50,52,52,55	0
8	EDO	A	1007	4/4	0.71	0.28	61,62,62,63	0
9	NAG	B	1052	14/15	0.73	0.30	58,65,67,68	0
9	NAG	A	1512	14/15	0.73	0.28	52,59,73,78	0
8	EDO	A	1012	4/4	0.75	0.33	63,64,65,65	0
8	EDO	A	1015	4/4	0.75	0.48	56,60,60,62	0
8	EDO	B	1010	4/4	0.75	0.27	60,60,60,61	0
9	NAG	A	1125	14/15	0.77	0.25	50,56,62,66	0
9	NAG	B	1215	14/15	0.77	0.45	66,74,76,77	0
8	EDO	A	1006	4/4	0.77	0.35	69,70,71,71	0
8	EDO	B	1012	4/4	0.77	0.42	47,47,49,52	0
7	NPO	B	1001	10/10	0.78	0.25	43,45,51,52	0
9	NAG	A	1319	14/15	0.78	0.27	58,66,69,70	0
9	NAG	A	1555	14/15	0.78	0.20	48,54,57,58	0
9	NAG	B	1539	14/15	0.78	0.33	50,56,60,60	0
8	EDO	A	1011	4/4	0.79	0.19	43,47,49,50	0
8	EDO	A	1003	4/4	0.79	0.40	44,45,46,46	0
8	EDO	A	1005	4/4	0.79	0.19	59,60,61,61	0
8	EDO	A	1008	4/4	0.80	0.18	67,67,67,68	0
7	NPO	B	1002	10/10	0.81	0.32	55,55,60,62	0
9	NAG	B	1471[A]	14/15	0.82	0.24	20,22,24,25	14
9	NAG	B	1471[B]	14/15	0.82	0.24	26,31,32,32	14
8	EDO	B	1004	4/4	0.82	0.15	50,51,53,53	0
9	NAG	A	1215	14/15	0.83	0.40	53,61,63,66	0
9	NAG	A	1052	14/15	0.83	0.22	44,51,54,55	0
7	NPO	A	1001	10/10	0.83	0.25	34,39,47,49	0
9	NAG	B	1555	14/15	0.83	0.16	39,42,43,44	0
9	NAG	A	1471[A]	14/15	0.84	0.24	17,19,20,23	14
9	NAG	A	1471[B]	14/15	0.84	0.24	27,30,31,32	14
8	EDO	A	1013	4/4	0.84	0.33	48,51,51,54	0
8	EDO	A	1010	4/4	0.85	0.34	44,45,46,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	1483	14/15	0.85	0.19	37,42,45,46	0
8	EDO	A	1009	4/4	0.85	0.20	35,40,42,47	0
7	NPO	A	1002	10/10	0.86	0.22	47,48,53,54	0
9	NAG	A	1236	14/15	0.86	0.13	28,31,35,35	0
8	EDO	B	1006	4/4	0.87	0.23	44,46,48,50	0
8	EDO	B	1009	4/4	0.88	0.38	54,55,56,57	0
9	NAG	B	1483	14/15	0.88	0.24	51,56,58,61	0
9	NAG	B	1357	14/15	0.90	0.16	40,44,48,51	0
9	NAG	B	1644	14/15	0.91	0.10	25,27,33,37	0
9	NAG	B	1444	14/15	0.92	0.11	32,34,35,36	0
9	NAG	A	1644	14/15	0.93	0.08	21,23,29,30	0
9	NAG	A	1444	14/15	0.94	0.09	25,26,29,32	0
9	NAG	A	1357	14/15	0.95	0.10	31,33,37,39	0
6	FRU	A	1000	12/12	0.97	0.07	14,15,18,20	0
6	FRU	B	1000	12/12	0.97	0.07	19,20,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.