



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:58 AM BST

PDB ID : 5FMC
Title : Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with fructose and BIS-TRIS propane buffer
Authors : Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on : 2015-11-02
Resolution : 1.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

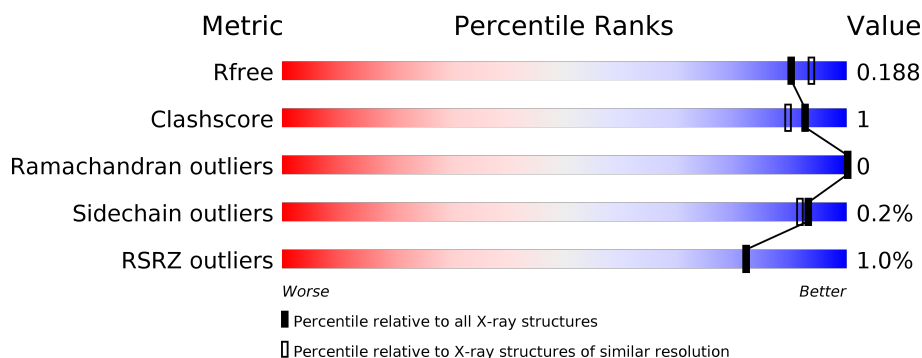
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.




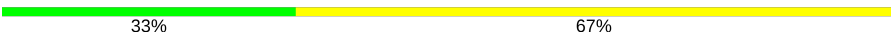
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	663	<div> <div style="width: 90%;"></div> <div style="width: 6%;"></div> </div>
1	B	663	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> </div>
2	C	7	<div> <div style="width: 86%;"></div> <div style="width: 14%;"></div> </div>
3	D	10	<div> <div style="width: 30%;"></div> <div style="width: 70%;"></div> </div>
3	G	10	<div> <div style="width: 40%;"></div> <div style="width: 60%;"></div> </div>
4	E	2	<div> <div style="width: 100%;"></div> </div>

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Mol	Chain	Length	Quality of chain
4	H	2	
5	F	6	

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
2	MAN	C	4	X	-	-	-
2	MAN	C	5	X	-	-	X
3	MAN	D	6	-	-	-	X
3	MAN	G	6	-	-	-	X
3	MAN	G	8	X	-	-	-
5	MAN	F	4	X	-	-	-
8	NAG	A	1215	-	-	-	X
8	NAG	A	1319	-	-	-	X
8	NAG	B	1215	-	-	-	X
8	NAG	B	1236	-	-	-	X
8	NAG	B	1242	-	-	-	X
8	NAG	B	1319	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11999 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.

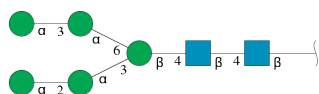
- Molecule 1 is a protein called BETA-FRUCTOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			
1	B	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			

There are 6 discrepancies between the modelled and reference sequences:

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

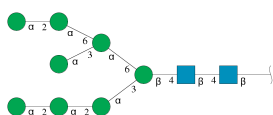
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

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

ucopyranose.



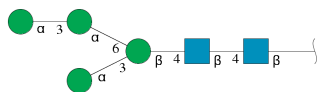
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	0	0	0
			116	64	2	50			
3	G	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



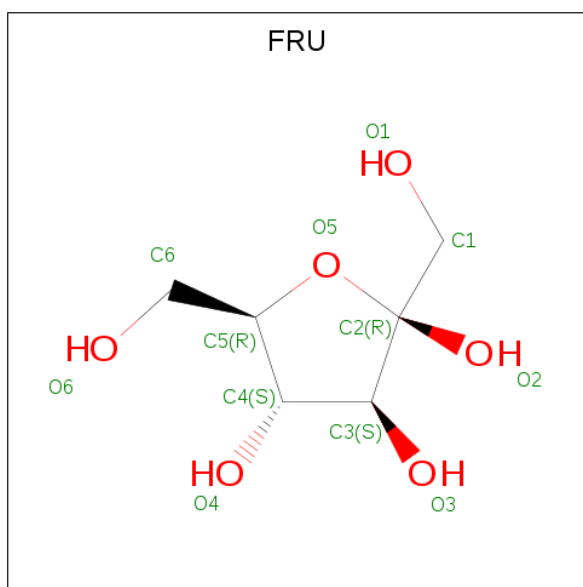
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



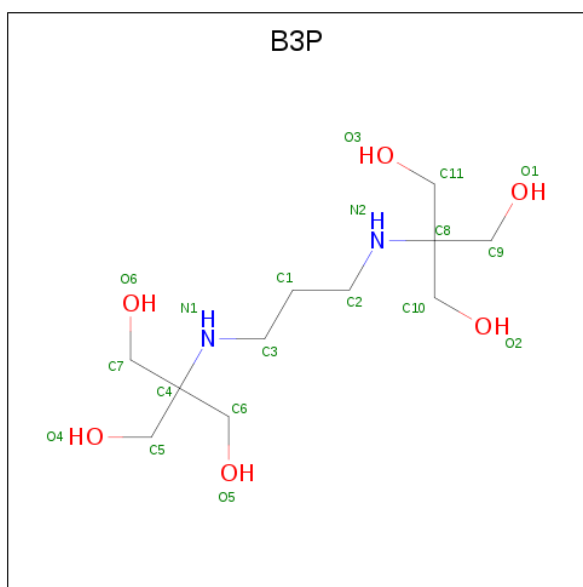
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



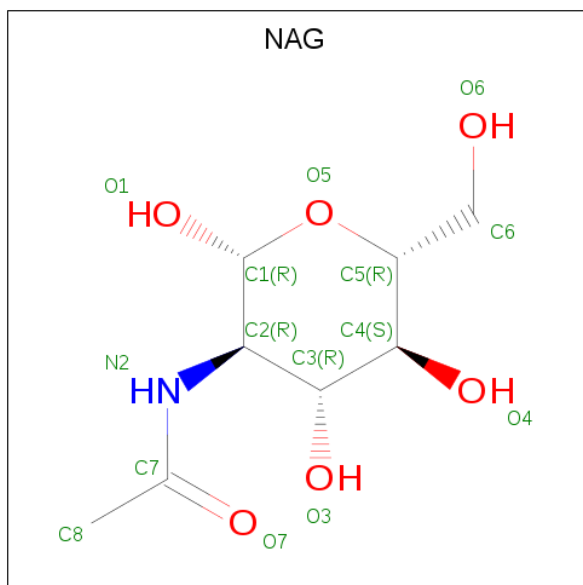
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			19	11	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			19	11	2	6		

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



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

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

- Molecule 9 is water.

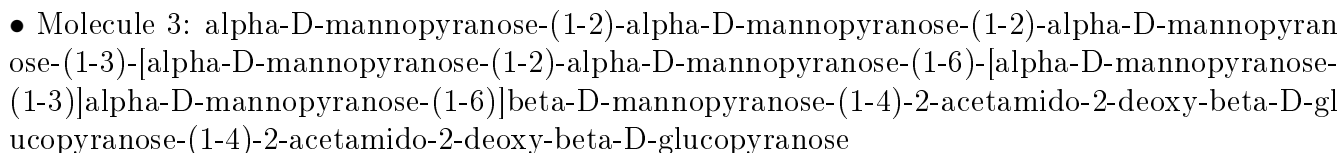
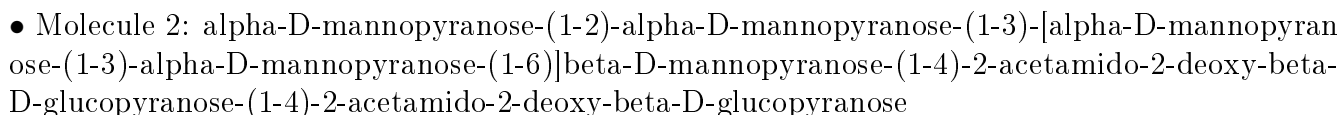
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	852	Total	O	0	0
			852	852		

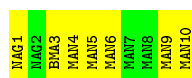
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	640	Total 640	O 640	0	0

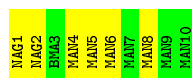
• Molecule 1: BETA-FRUCTOFURANOSIDASE





- 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 G: 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-(1-3)-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 F: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.43Å 204.74Å 145.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.63 – 1.84 48.29 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (118.63-1.84) 99.8 (48.29-1.84)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.163 , 0.179 0.174 , 0.188	Depositor DCC
R_{free} test set	9596 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11999	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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, B3P, NAG, FRU, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	4/4940 (0.1%)	0.72	8/6754 (0.1%)
1	B	0.50	3/4940 (0.1%)	0.73	10/6754 (0.1%)
All	All	0.49	7/9880 (0.1%)	0.72	18/13508 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	590	ALA	C-N	-19.65	0.88	1.34
1	A	590	ALA	C-N	-14.30	1.01	1.34
1	A	93	HIS	C-N	7.79	1.51	1.34
1	A	591	ASN	C-N	-5.48	1.21	1.34
1	B	339	ASP	C-N	-5.32	1.21	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	HIS	O-C-N	12.77	143.13	122.70
1	A	93	HIS	O-C-N	12.61	142.88	122.70
1	B	343	HIS	O-C-N	11.61	141.27	122.70
1	A	343	HIS	O-C-N	10.62	139.69	122.70
1	A	342	ASN	C-N-CA	10.10	146.95	121.70

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	4805	0	4496	13	0
1	B	4805	0	4498	9	0
2	C	83	0	70	1	0
3	D	116	0	97	0	0
3	G	116	0	97	0	0
4	E	28	0	25	0	0
4	H	28	0	25	0	0
5	F	72	0	61	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	19	0	26	1	0
7	B	19	0	26	1	0
8	A	210	0	195	7	0
8	B	182	0	169	1	0
9	A	852	0	0	5	0
9	B	640	0	0	3	0
All	All	11999	0	9809	30	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 1.

The worst 5 of 30 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)
8:A:1319:NAG:H83	9:A:2457:HOH:O	1.37	1.25
1:A:525:GLU:HB2	8:A:1606:NAG:H81	1.76	0.66
1:A:237:THR:HG23	9:A:2332:HOH:O	2.03	0.58
1:B:150:ILE:HG12	1:B:224:VAL:HG11	1.86	0.57
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.87	0.56

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	623/663 (94%)	595 (96%)	28 (4%)	0	100	100
1	B	623/663 (94%)	595 (96%)	28 (4%)	0	100	100
All	All	1246/1326 (94%)	1190 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/527 (94%)	497 (100%)	1 (0%)	93	92
1	B	498/527 (94%)	497 (100%)	1 (0%)	93	92
All	All	996/1054 (94%)	994 (100%)	2 (0%)	93	92

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

Mol	Chain	Res	Type
1	A	142	ARG
1	B	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	B	458	GLN
1	B	268	HIS
1	A	341	GLN
1	B	341	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

37 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.39	0	17,19,21	1.16	2 (11%)
2	NAG	C	2	2	14,14,15	0.63	0	17,19,21	1.41	4 (23%)
2	BMA	C	3	2	11,11,12	0.41	0	15,15,17	1.96	3 (20%)
2	MAN	C	4	2	11,11,12	0.60	0	15,15,17	1.70	3 (20%)
2	MAN	C	5	2	11,11,12	0.58	0	15,15,17	1.25	1 (6%)
2	MAN	C	6	2	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
2	MAN	C	7	2	11,11,12	0.39	0	15,15,17	0.86	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.88	1 (7%)	17,19,21	0.71	0
3	MAN	D	10	3	11,11,12	0.39	0	15,15,17	0.73	1 (6%)
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.88	0
3	BMA	D	3	3	11,11,12	0.37	0	15,15,17	1.42	1 (6%)
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	1.17	1 (6%)
3	MAN	D	5	3	11,11,12	0.37	0	15,15,17	0.91	1 (6%)
3	MAN	D	6	3	11,11,12	0.34	0	15,15,17	0.97	1 (6%)
3	MAN	D	7	3	11,11,12	0.47	0	15,15,17	0.83	0
3	MAN	D	8	3	11,11,12	0.46	0	15,15,17	0.72	0
3	MAN	D	9	3	11,11,12	0.52	0	15,15,17	1.06	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
4	NAG	E	2	4	14,14,15	0.49	0	17,19,21	1.84	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	1	1,5	14,14,15	0.34	0	17,19,21	1.07	3 (17%)
5	NAG	F	2	5	14,14,15	0.52	0	17,19,21	0.76	0
5	BMA	F	3	5	11,11,12	0.37	0	15,15,17	1.65	2 (13%)
5	MAN	F	4	5	11,11,12	0.71	0	15,15,17	1.40	2 (13%)
5	MAN	F	5	5	11,11,12	0.33	0	15,15,17	0.85	1 (6%)
5	MAN	F	6	5	11,11,12	0.37	0	15,15,17	1.03	0
3	NAG	G	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	0.93	0
3	MAN	G	10	3	11,11,12	0.35	0	15,15,17	0.60	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.93	1 (5%)
3	BMA	G	3	3	11,11,12	0.32	0	15,15,17	0.71	0
3	MAN	G	4	3	11,11,12	0.31	0	15,15,17	0.93	1 (6%)
3	MAN	G	5	3	11,11,12	0.39	0	15,15,17	1.35	1 (6%)
3	MAN	G	6	3	11,11,12	0.38	0	15,15,17	0.82	1 (6%)
3	MAN	G	7	3	11,11,12	0.49	0	15,15,17	0.98	0
3	MAN	G	8	3	11,11,12	0.65	0	15,15,17	1.44	2 (13%)
3	MAN	G	9	3	11,11,12	0.52	0	15,15,17	0.86	0
4	NAG	H	1	1,4	14,14,15	0.30	0	17,19,21	1.01	1 (5%)
4	NAG	H	2	4	14,14,15	0.38	0	17,19,21	0.79	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	1,2	-	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	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	C	5	2	1/1/4/5	2/2/19/22	1/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	0/2/19/22	0/1/1/1
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	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	3.04	1.56	1.52
3	G	1	NAG	C1-C2	2.48	1.56	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O3-C3-C2	4.96	119.49	109.99
4	E	2	NAG	C1-O5-C5	4.62	118.46	112.19
5	F	3	BMA	C1-O5-C5	4.56	118.37	112.19
3	D	3	BMA	O3-C3-C4	-4.33	100.33	110.35
2	C	4	MAN	C1-O5-C5	4.17	117.84	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	8	MAN	C1
2	C	5	MAN	C1
2	C	4	MAN	C1
5	F	4	MAN	C1

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
3	G	6	MAN	O5-C5-C6-O6
3	G	6	MAN	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6

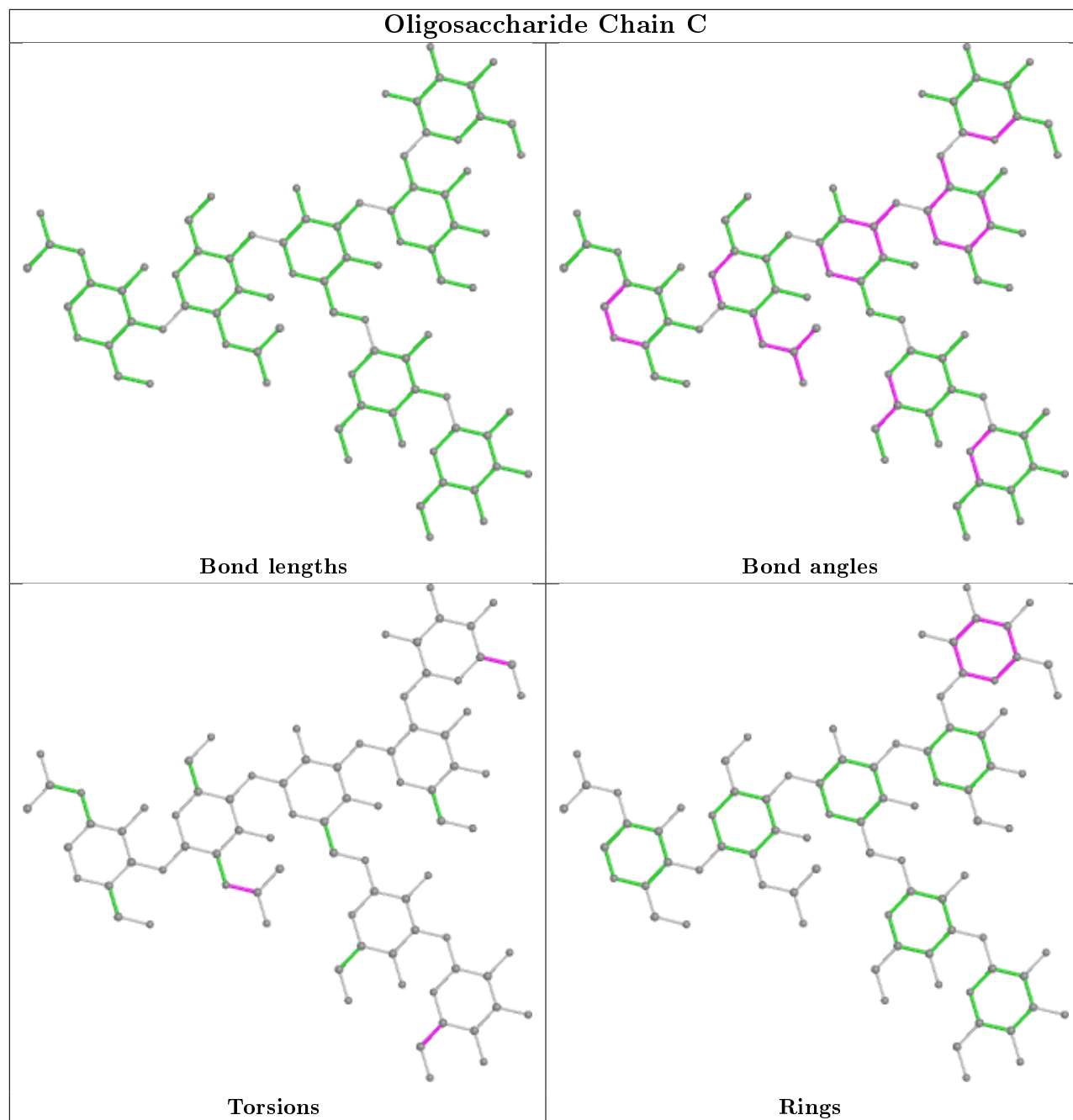
All (1) ring outliers are listed below:

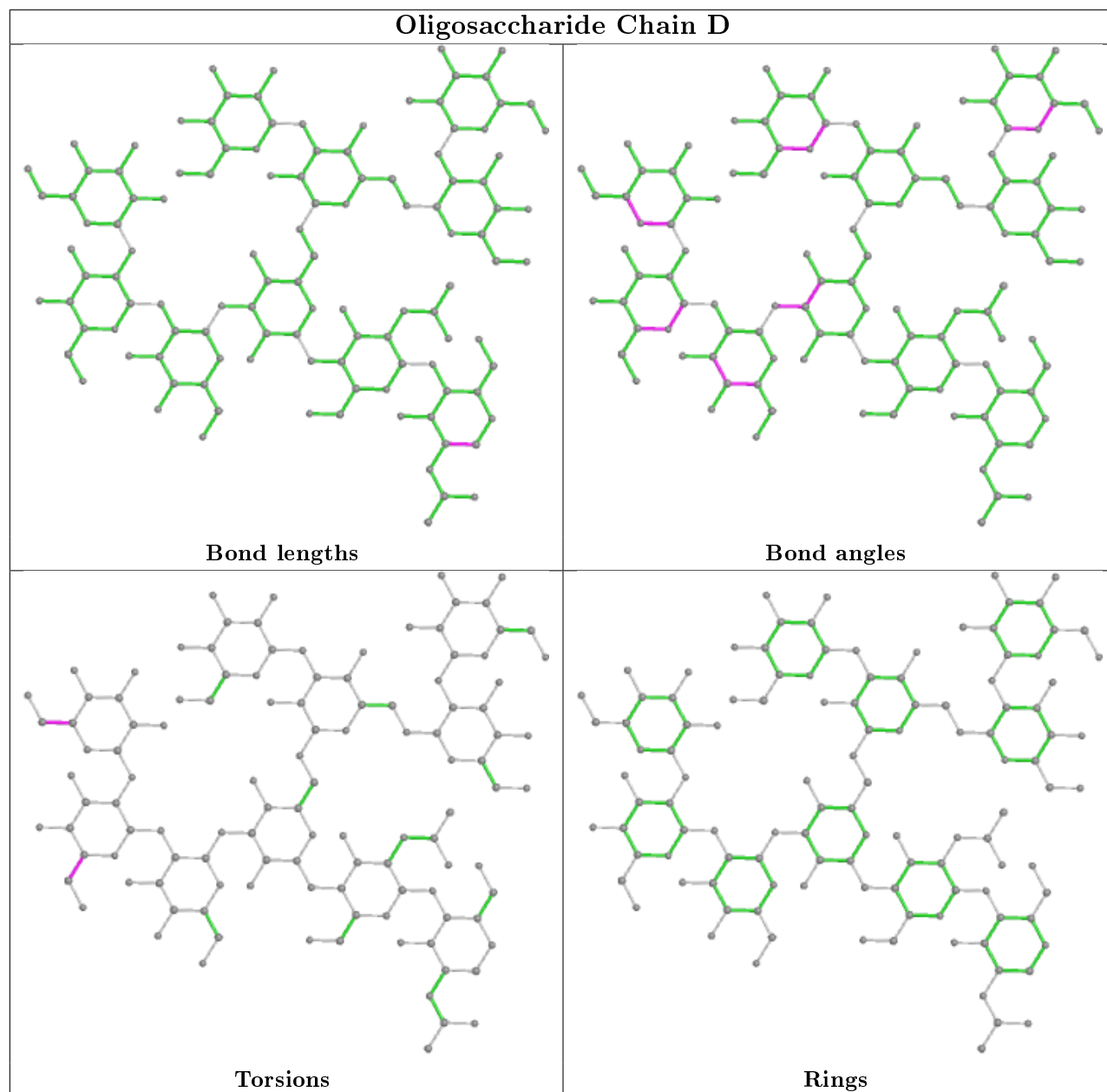
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C1-C2-C3-C4-C5-O5

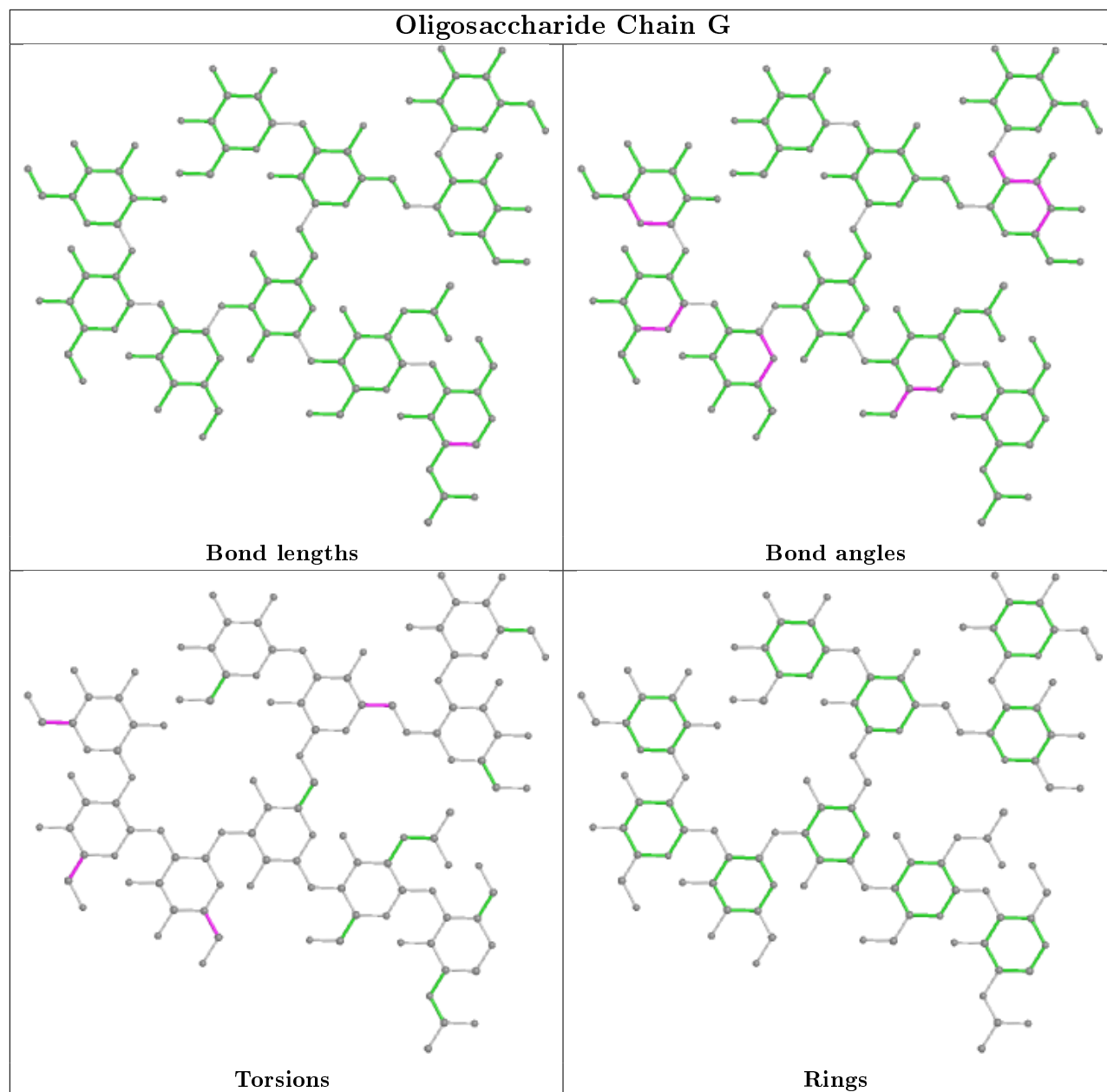
1 monomer is involved in 1 short contact:

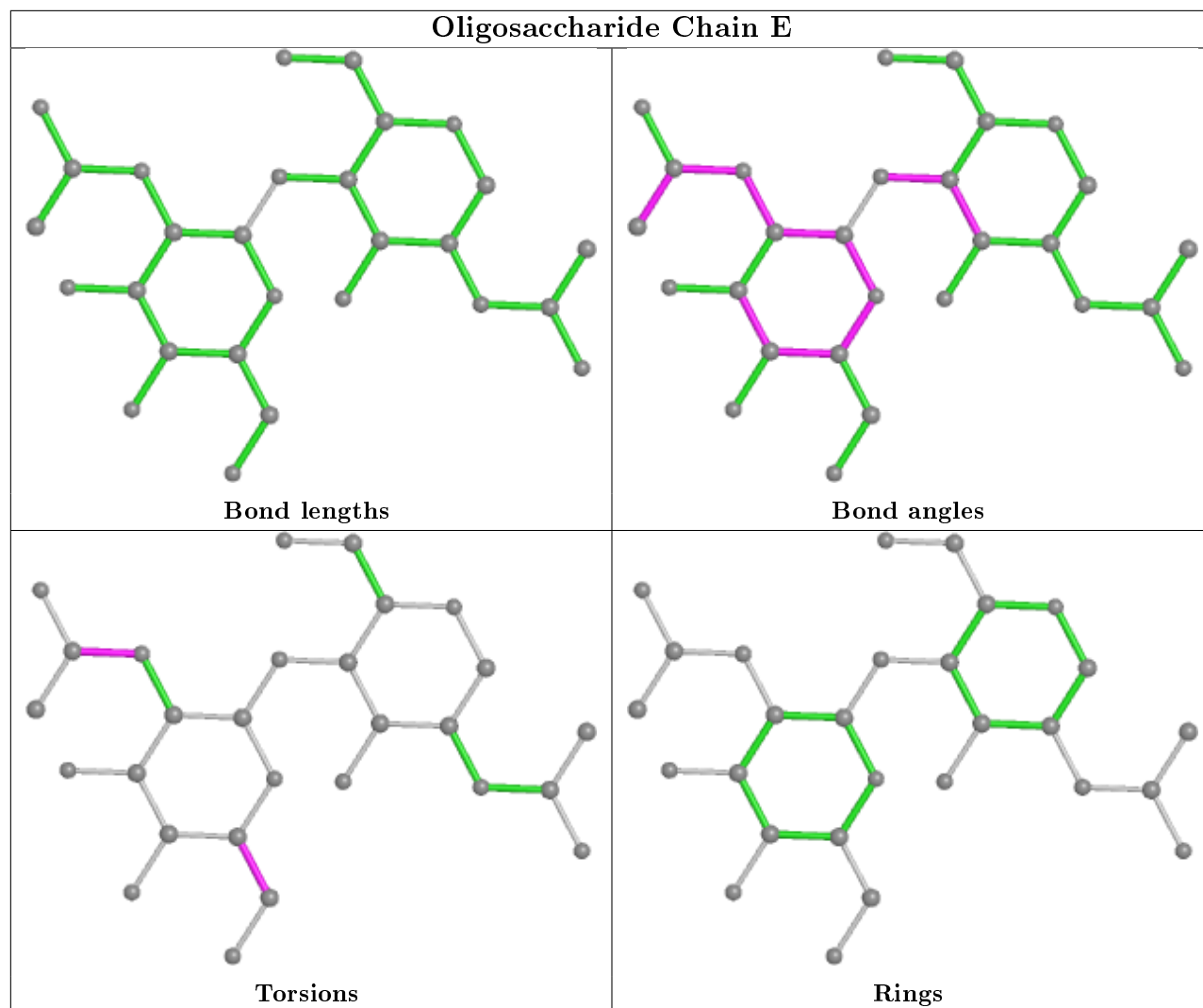
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

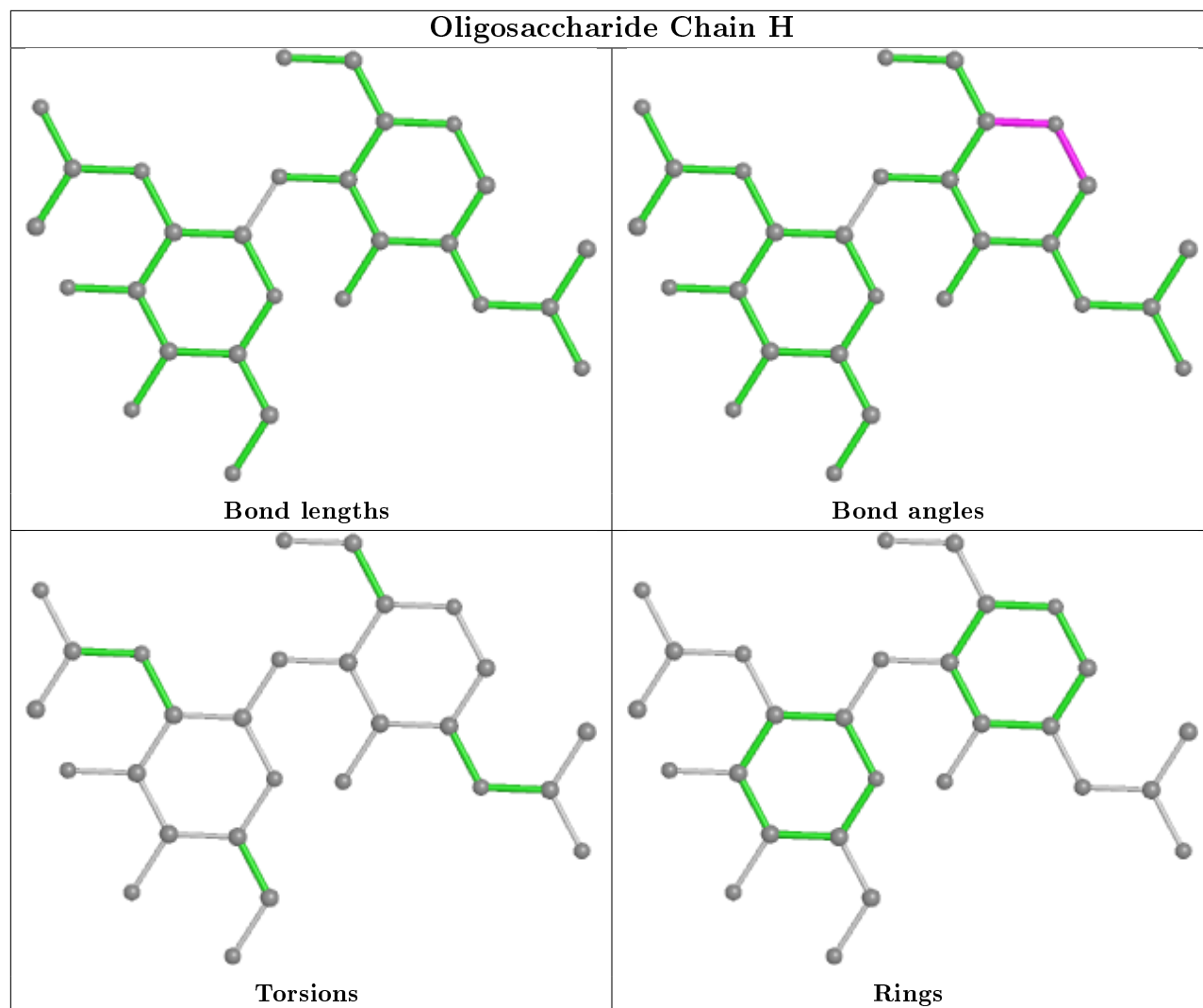
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

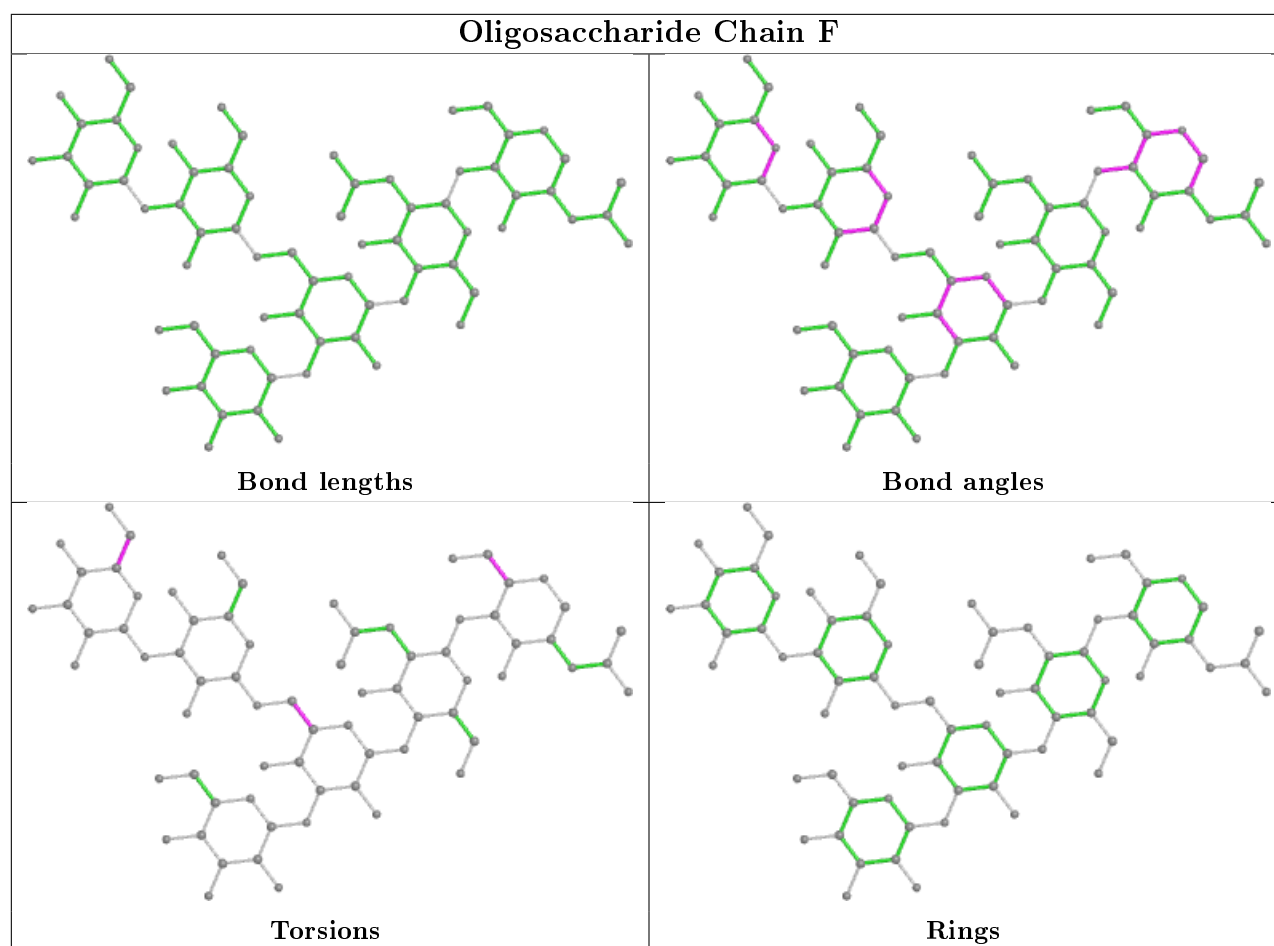












5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1319	1	14,14,15	0.28	0	17,19,21	0.61	0
7	B3P	A	1001	-	18,18,18	0.55	0	21,23,23	1.99	2 (9%)
8	NAG	A	1512	1	14,14,15	0.31	0	17,19,21	1.23	3 (17%)
8	NAG	B	1483	1	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
8	NAG	B	1357	1	14,14,15	0.35	0	17,19,21	0.93	0
8	NAG	A	1052	1	14,14,15	0.25	0	17,19,21	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	1236	1	14,14,15	0.37	0	17,19,21	0.78	0
7	B3P	B	1001	-	18,18,18	0.52	0	21,23,23	1.78	2 (9%)
8	NAG	B	1319	1	14,14,15	0.29	0	17,19,21	0.61	0
8	NAG	B	1555	1	14,14,15	0.45	0	17,19,21	0.92	1 (5%)
8	NAG	B	1644	1	14,14,15	0.39	0	17,19,21	0.82	0
8	NAG	B	1125	1	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
8	NAG	A	1125	1	14,14,15	0.48	0	17,19,21	1.13	2 (11%)
8	NAG	B	1215	1	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
8	NAG	A	1644	1	14,14,15	0.33	0	17,19,21	0.87	0
8	NAG	B	1052	1	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
8	NAG	B	1444	1	14,14,15	0.39	0	17,19,21	1.39	1 (5%)
8	NAG	A	1555	1	14,14,15	0.35	0	17,19,21	1.14	2 (11%)
8	NAG	A	1444	1	14,14,15	0.44	0	17,19,21	0.96	2 (11%)
6	FRU	B	1000	-	11,12,12	0.64	0	10,18,18	0.70	0
8	NAG	A	1483	1	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
8	NAG	A	1215	1	14,14,15	0.53	0	17,19,21	1.17	1 (5%)
6	FRU	A	1000	-	11,12,12	0.66	0	10,18,18	0.52	0
8	NAG	A	1539	1	14,14,15	0.69	0	17,19,21	1.35	2 (11%)
8	NAG	B	1539	1	14,14,15	0.49	0	17,19,21	1.55	3 (17%)
8	NAG	B	1471	1	14,14,15	0.38	0	17,19,21	0.76	0
8	NAG	A	1236	1	14,14,15	0.43	0	17,19,21	0.80	0
8	NAG	A	1357	1	14,14,15	0.39	0	17,19,21	1.32	2 (11%)
8	NAG	B	1242	1	14,14,15	0.31	0	17,19,21	1.28	3 (17%)
8	NAG	A	1606	1	14,14,15	0.75	0	17,19,21	2.10	6 (35%)
8	NAG	A	1242	1	14,14,15	0.23	0	17,19,21	0.95	0
8	NAG	A	1471	1	14,14,15	0.37	0	17,19,21	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1319	1	-	4/6/23/26	0/1/1/1
7	B3P	A	1001	-	-	6/28/28/28	-
8	NAG	A	1512	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1357	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1052	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1236	1	-	0/6/23/26	0/1/1/1
7	B3P	B	1001	-	-	1/28/28/28	-
8	NAG	B	1319	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1644	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1125	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1125	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1052	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1444	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1555	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1444	1	-	2/6/23/26	0/1/1/1
6	FRU	B	1000	-	-	1/5/24/24	0/1/1/1
8	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1215	1	-	2/6/23/26	0/1/1/1
6	FRU	A	1000	-	-	1/5/24/24	0/1/1/1
8	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1539	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1357	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1242	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1606	1	-	5/6/23/26	0/1/1/1
8	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1471	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	B3P	C2-N2-C8	6.18	124.85	116.08
7	A	1001	B3P	C3-N1-C4	5.59	124.01	116.08
7	B	1001	B3P	C2-N2-C8	5.35	123.68	116.08
8	B	1444	NAG	C1-O5-C5	5.01	118.99	112.19
7	B	1001	B3P	C3-N1-C4	4.79	122.88	116.08

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

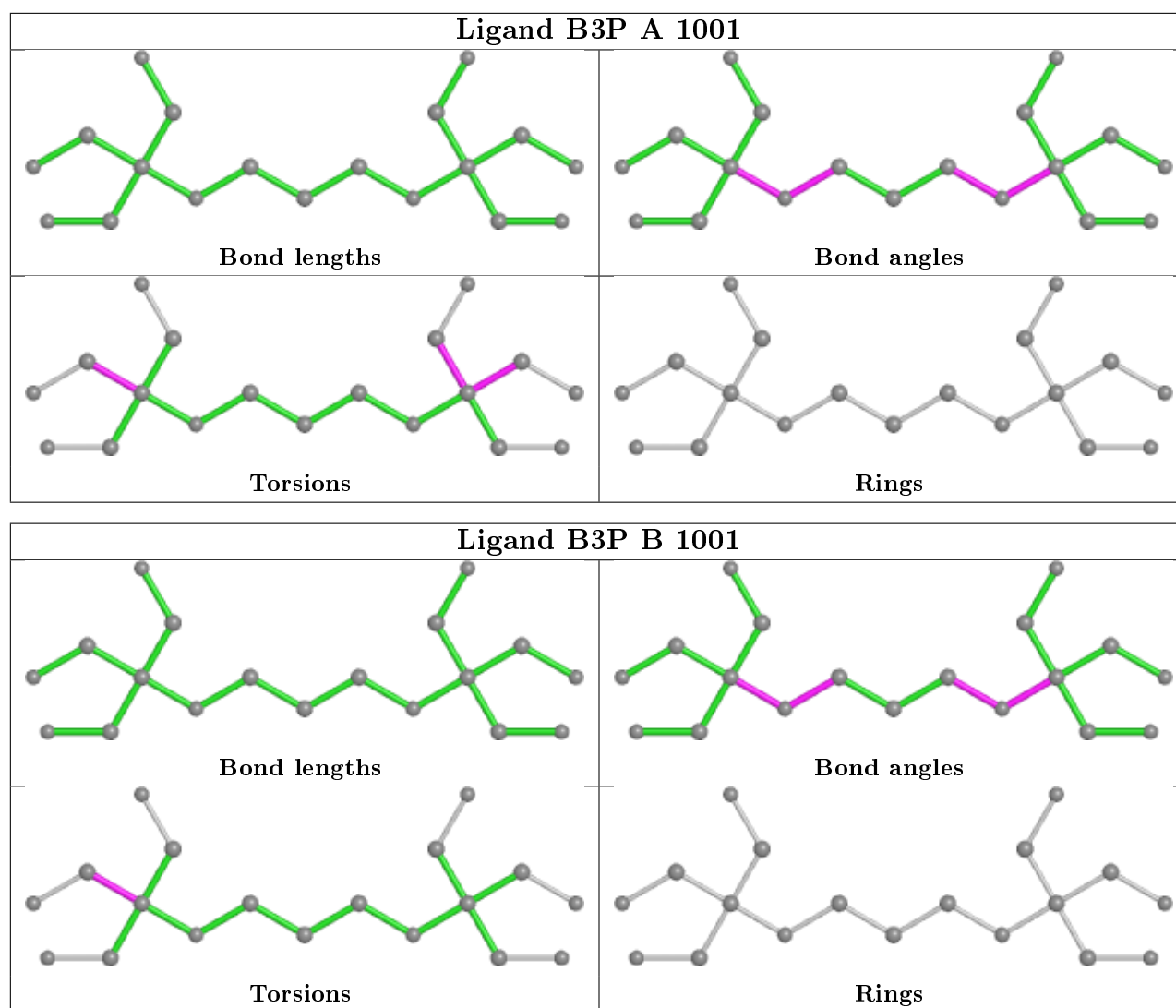
Mol	Chain	Res	Type	Atoms
8	A	1319	NAG	C8-C7-N2-C2
8	A	1319	NAG	O7-C7-N2-C2
7	A	1001	B3P	C7-C4-C6-O5
8	B	1319	NAG	C8-C7-N2-C2
8	A	1319	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1319	NAG	3	0
7	A	1001	B3P	1	0
7	B	1001	B3P	1	0
8	B	1319	NAG	1	0
8	A	1606	NAG	3	0
8	A	1471	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	590:ALA	C	591:ASN	N	1.01
1	B	590:ALA	C	591:ASN	N	0.88

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	624/663 (94%)	-0.29	4 (0%) 89 89	12, 19, 30, 51	0
1	B	624/663 (94%)	-0.08	9 (1%) 75 75	15, 26, 41, 50	0
All	All	1248/1326 (94%)	-0.19	13 (1%) 82 82	12, 22, 38, 51	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	CYS	4.1
1	B	240	ILE	3.7
1	A	42	CYS	3.5
1	B	569	GLY	2.9
1	B	571	GLU	2.8

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	C	5	11/12	0.48	0.43	81,85,90,94	0
4	NAG	E	2	14/15	0.64	0.37	69,74,80,80	0
5	MAN	F	6	11/12	0.64	0.38	61,67,71,71	0
3	MAN	D	6	11/12	0.67	0.53	79,84,90,91	0
3	MAN	G	9	11/12	0.72	0.20	52,56,58,60	0

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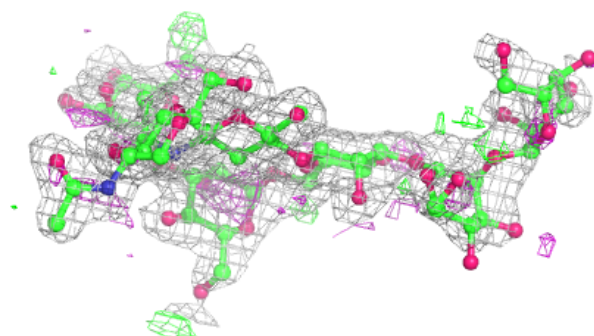
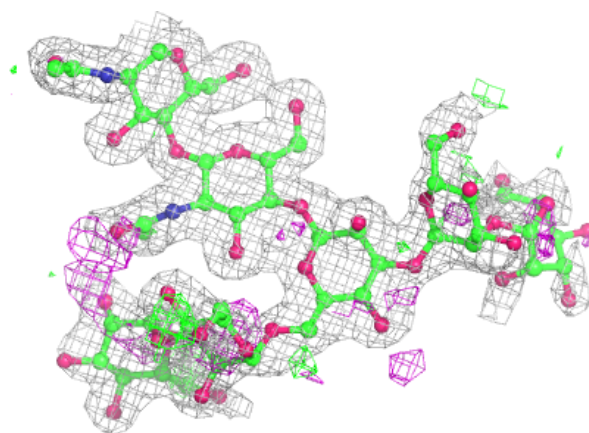
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	H	2	14/15	0.73	0.37	70,81,86,87	0
3	MAN	G	6	11/12	0.76	0.57	79,84,87,90	0
2	MAN	C	4	11/12	0.79	0.30	54,62,69,70	0
3	MAN	D	5	11/12	0.81	0.25	53,57,60,69	0
2	MAN	C	7	11/12	0.82	0.34	46,48,51,52	0
5	MAN	F	5	11/12	0.82	0.39	60,61,63,63	0
5	MAN	F	4	11/12	0.82	0.38	56,59,61,61	0
3	MAN	G	5	11/12	0.82	0.25	57,61,65,70	0
3	MAN	D	9	11/12	0.83	0.17	53,56,61,62	0
2	MAN	C	6	11/12	0.83	0.36	46,48,52,57	0
3	MAN	G	8	11/12	0.84	0.12	37,39,41,46	0
3	MAN	D	4	11/12	0.88	0.15	36,43,47,52	0
4	NAG	H	1	14/15	0.88	0.17	46,51,58,68	0
5	BMA	F	3	11/12	0.91	0.15	36,43,51,52	0
4	NAG	E	1	14/15	0.91	0.14	37,41,48,59	0
2	BMA	C	3	11/12	0.91	0.12	28,32,41,43	0
3	MAN	G	4	11/12	0.91	0.16	38,42,48,49	0
3	MAN	D	8	11/12	0.91	0.11	33,36,39,45	0
2	NAG	C	1	14/15	0.94	0.10	17,19,24,24	0
3	MAN	G	7	11/12	0.94	0.09	19,21,27,33	0
3	BMA	D	3	11/12	0.95	0.08	20,21,23,29	0
5	NAG	F	2	14/15	0.95	0.13	25,26,27,31	0
3	NAG	D	2	14/15	0.96	0.08	16,17,18,19	0
3	BMA	G	3	11/12	0.96	0.07	22,23,26,31	0
2	NAG	C	2	14/15	0.96	0.09	19,21,24,31	0
3	MAN	D	7	11/12	0.96	0.08	16,19,25,29	0
3	NAG	G	1	14/15	0.97	0.08	17,18,20,20	0
3	NAG	D	1	14/15	0.97	0.07	14,15,16,16	0
3	NAG	G	2	14/15	0.97	0.07	19,19,22,22	0
5	NAG	F	1	14/15	0.97	0.08	22,25,29,30	0
3	MAN	D	10	11/12	0.98	0.08	14,15,15,16	0
3	MAN	G	10	11/12	0.98	0.09	16,18,18,18	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.

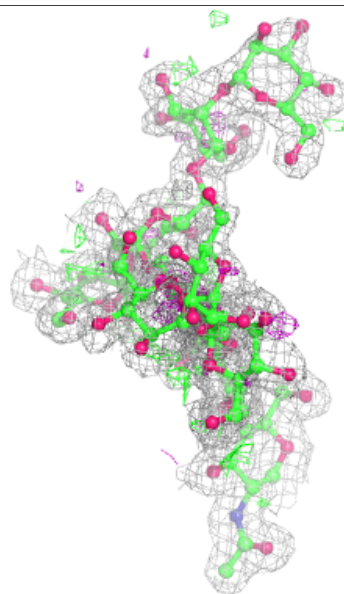
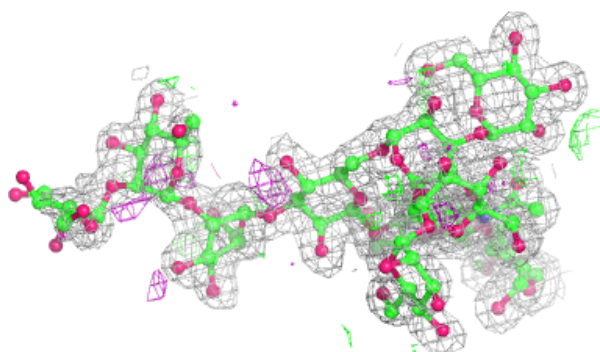
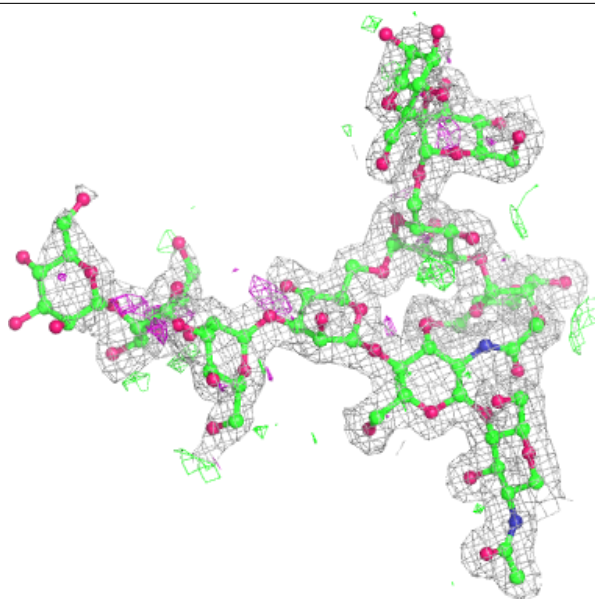
Electron density around Chain C:

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



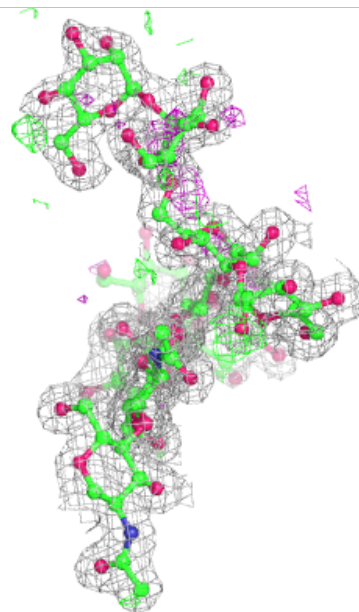
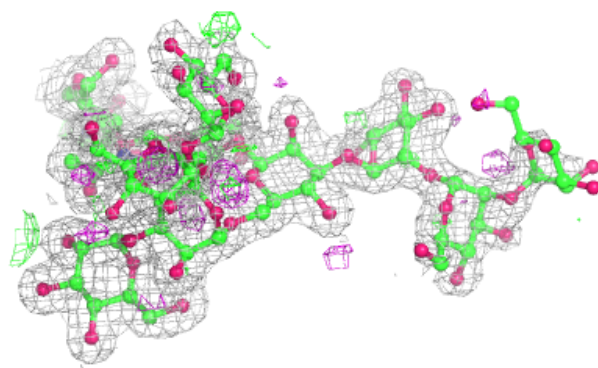
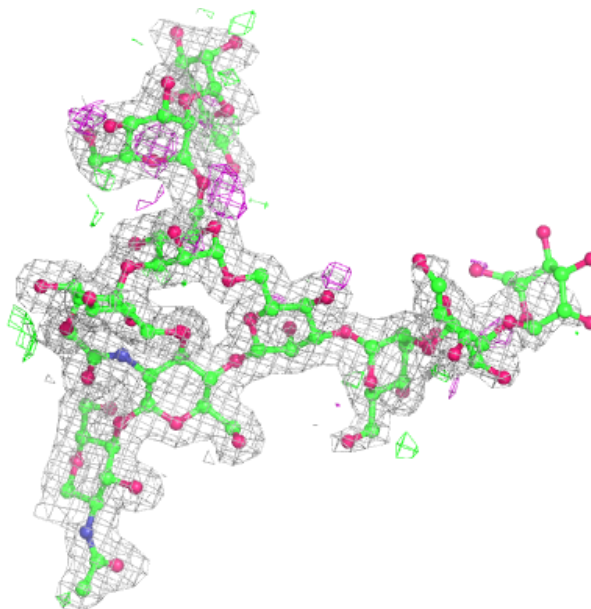
Electron density around Chain D:

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



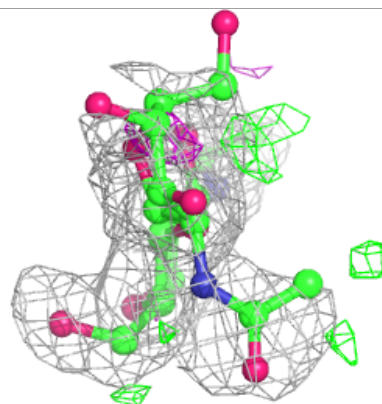
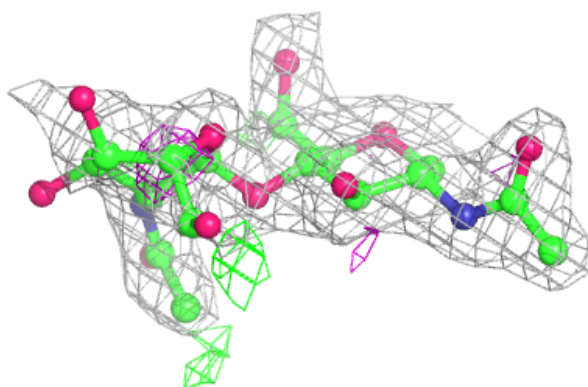
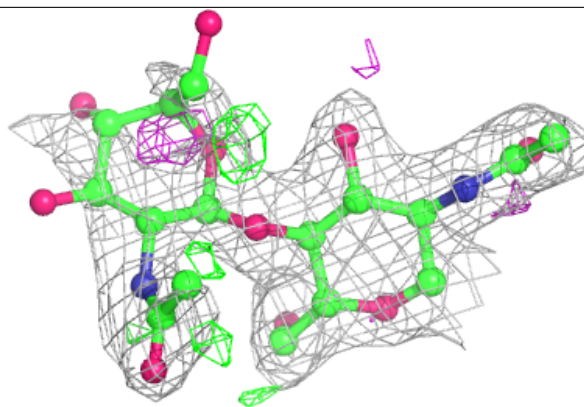
Electron density around Chain G:

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



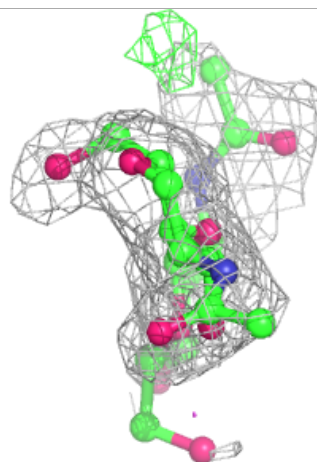
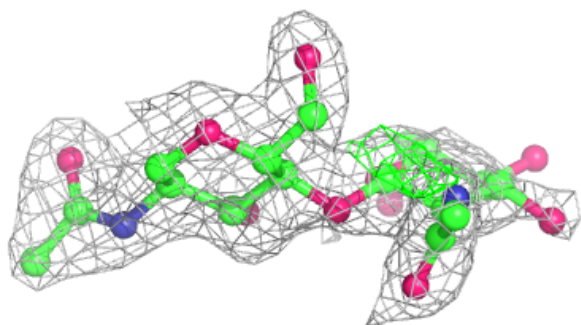
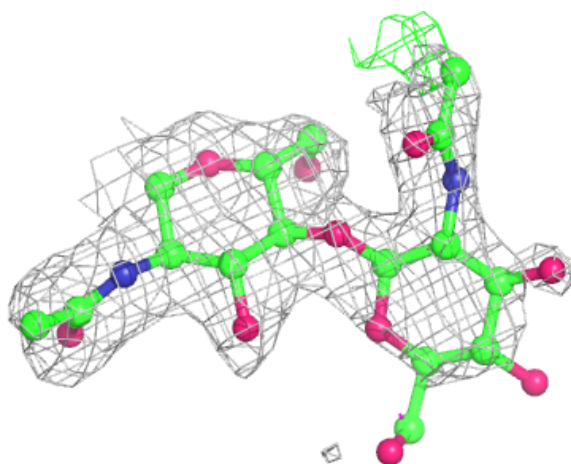
Electron density around Chain E:

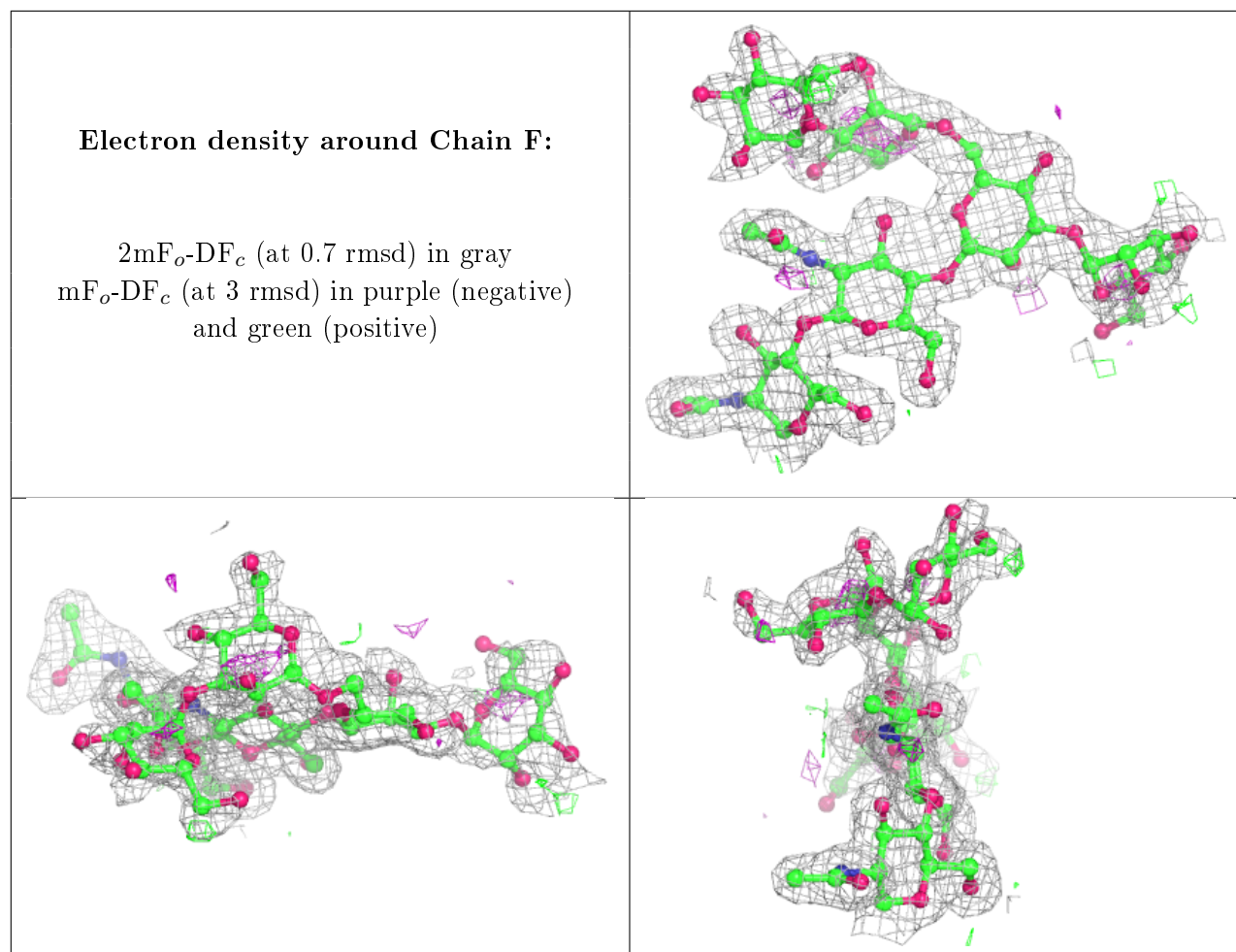
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\AA^2)	Q<0.9
8	NAG	B	1125	14/15	0.51	0.32	56,63,65,66	0
8	NAG	B	1215	14/15	0.62	0.52	74,83,86,89	0
8	NAG	A	1125	14/15	0.70	0.29	54,62,66,66	0
8	NAG	A	1606	14/15	0.70	0.31	50,56,57,60	0
8	NAG	B	1539	14/15	0.73	0.29	55,61,65,69	0
8	NAG	A	1555	14/15	0.74	0.26	55,63,68,69	0
8	NAG	B	1052	14/15	0.76	0.35	64,71,76,76	0
8	NAG	A	1215	14/15	0.77	0.43	62,74,75,79	0
8	NAG	B	1319	14/15	0.77	0.43	72,79,81,82	0
8	NAG	B	1242	14/15	0.77	0.44	67,70,74,76	0

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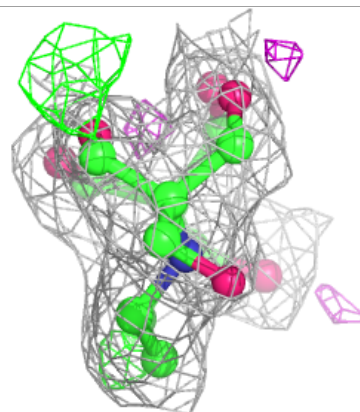
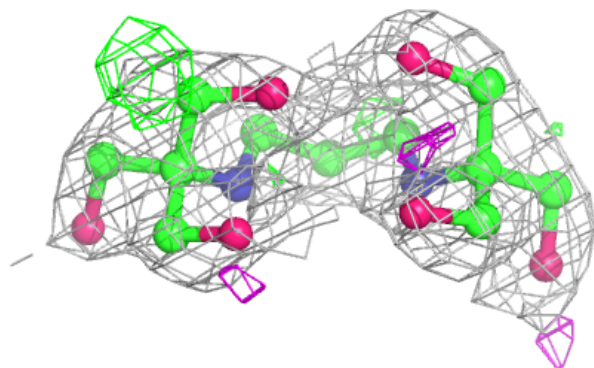
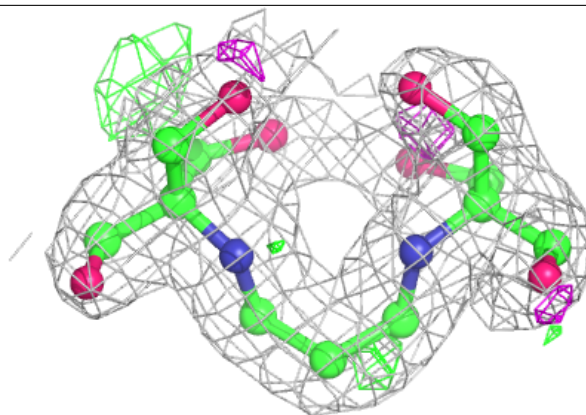
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	A	1319	14/15	0.79	0.44	55,62,68,68	0
8	NAG	B	1236	14/15	0.79	0.40	76,82,88,89	0
8	NAG	A	1242	14/15	0.79	0.33	50,56,59,59	0
8	NAG	A	1539	14/15	0.80	0.24	39,46,49,52	0
8	NAG	A	1512	14/15	0.81	0.23	47,54,67,68	0
8	NAG	B	1483	14/15	0.84	0.21	53,57,61,63	0
8	NAG	B	1555	14/15	0.85	0.19	39,40,43,44	0
8	NAG	A	1236	14/15	0.85	0.15	28,33,36,36	0
7	B3P	B	1001	19/19	0.86	0.13	39,41,46,47	0
8	NAG	A	1052	14/15	0.87	0.26	45,50,54,54	0
7	B3P	A	1001	19/19	0.87	0.12	32,36,39,40	0
8	NAG	B	1471	14/15	0.90	0.15	31,35,38,38	0
8	NAG	A	1471	14/15	0.91	0.12	29,31,37,40	0
8	NAG	A	1483	14/15	0.92	0.15	35,39,42,45	0
8	NAG	B	1644	14/15	0.93	0.14	26,28,34,39	0
8	NAG	B	1444	14/15	0.93	0.10	32,35,37,37	0
8	NAG	B	1357	14/15	0.94	0.15	39,42,46,48	0
8	NAG	A	1644	14/15	0.94	0.12	22,24,33,35	0
8	NAG	A	1357	14/15	0.95	0.09	31,33,36,38	0
8	NAG	A	1444	14/15	0.95	0.08	23,24,28,32	0
6	FRU	B	1000	12/12	0.98	0.09	18,18,19,20	0
6	FRU	A	1000	12/12	0.99	0.10	13,13,15,15	0

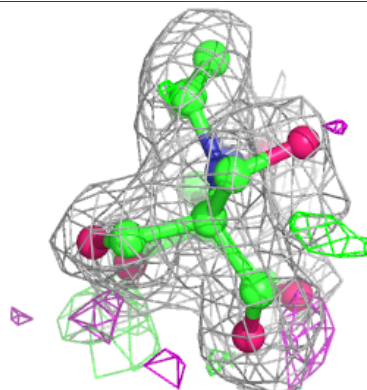
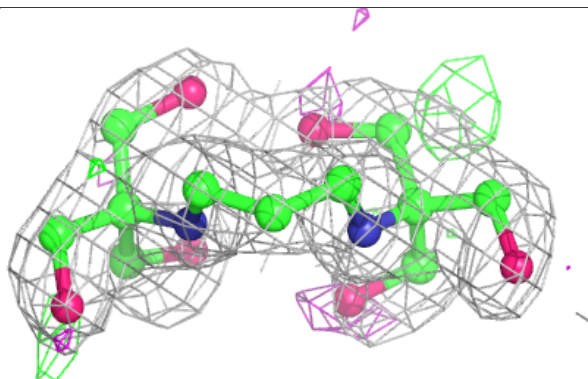
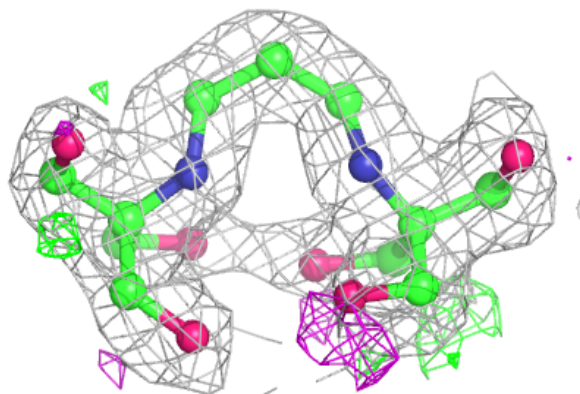
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P B 1001:

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

**Electron density around B3P A 1001:**

$2mF_o-DF_c$ (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.