



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 12:59 pm BST

PDB ID : 2BF1
Title : Structure of an unliganded and fully-glycosylated SIV gp120 envelope glycoprotein
Authors : Chen, B.; Vogan, E.M.; Gong, H.; Skehel, J.J.; Wiley, D.C.; Harrison, S.C.
Deposited on : 2004-12-02
Resolution : 4.00 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 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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

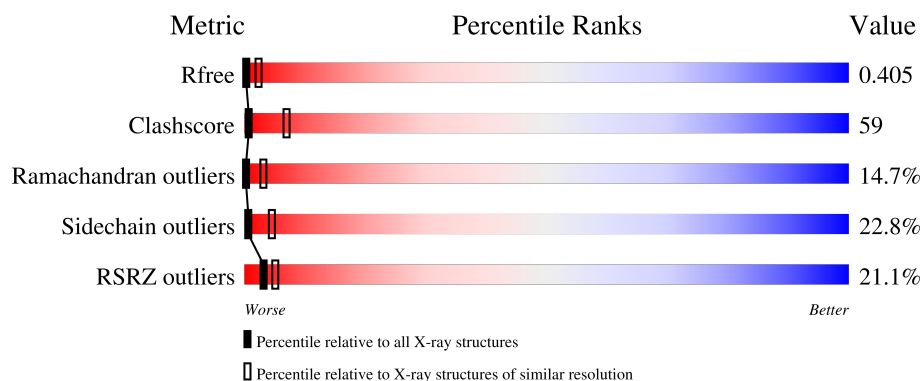
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	316	<div> <div>20%</div> <div>21%</div> <div>53%</div> <div>19%</div> <div>.</div> <div>.</div> </div>
2	B	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
2	F	4	<div> <div>25%</div> <div>75%</div> </div>
2	H	4	<div> <div>100%</div> </div>
3	C	6	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	6	
4	D	3	
4	E	3	
5	G	2	
6	I	7	
7	J	5	
8	L	4	

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	NAG	B	1	X	-	-	-
2	FUC	B	4	X	-	-	-
2	FUC	F	4	X	-	-	-
2	NAG	H	1	X	-	-	-
2	FUC	H	4	X	-	-	-
3	NAG	C	2	-	-	-	X
3	FUC	C	6	X	-	-	-
3	NAG	K	1	X	-	-	-
3	FUC	K	6	X	-	-	-
4	NAG	D	1	X	-	-	-
4	FUC	D	3	X	-	-	-
4	NAG	E	1	X	-	-	-
4	FUC	E	3	X	-	-	-
5	NAG	G	1	X	-	-	-
6	NAG	I	1	X	-	-	X
8	NAG	L	1	X	-	-	-

2 Entry composition [i](#)

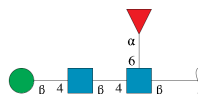
There are 9 unique types of molecules in this entry. The entry contains 3085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EXTERIOR MEMBRANE GLYCOPROTEIN GP120.

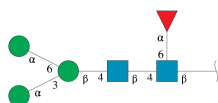
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2470	1556	436	455	23			

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



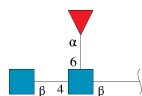
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	F	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	H	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	K	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



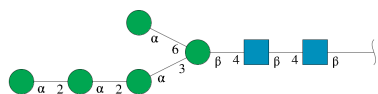
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



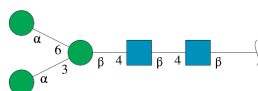
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
6	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



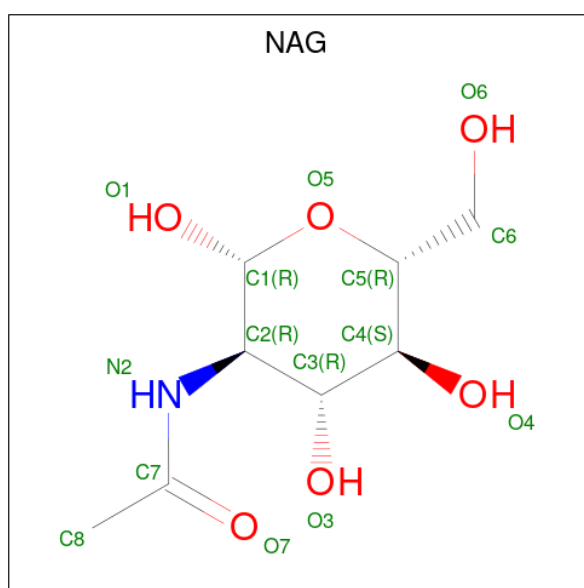
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(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
8	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

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

Chain H:  100%

MAG1
MAG2
BMA3
FUC4

- Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 33% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

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

Chain D:  100%

MAG1
MAG2
FUC3

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

Chain E:  67% 33%

MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1
MAG2

- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 I:  71% 29%

NAG1	NAG2	BNAG3	MAN4	MAN5	MAN6	MAN7
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● Molecule 7: 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 J:  100%

NAG1	NAG2	BNAG3	MAN4	MAN5
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● Molecule 8: 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 L:  100%

NAG1	NAG2	BNAG3	MAN4
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.05Å 108.05Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 4.00 26.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.00-4.00) 97.5 (26.00-4.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.385 , 0.388 0.388 , 0.405	Depositor DCC
R_{free} test set	280 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	175.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3085	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, MAN, FUC, NAG

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	0.67	0/2534	0.92	7/3441 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	244	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	240	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	414	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	293	ASP	CB-CG-OD2	5.29	123.06	118.30

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	2470	0	2350	344	0
2	B	49	0	43	1	2
2	F	49	0	43	0	0
2	H	49	0	43	0	0
3	C	71	0	61	2	0
3	K	71	0	61	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	38	0	34	4	0
4	E	38	0	34	4	0
5	G	28	0	25	1	0
6	I	83	0	70	8	0
7	J	61	0	52	0	0
8	L	50	0	43	0	0
9	A	28	0	26	0	0
All	All	3085	0	2885	354	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 59.

The worst 5 of 354 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:A:87:ILE:O	1:A:90:VAL:HG22	1.35	1.25
1:A:92:GLN:NE2	1:A:106:PRO:HG3	1.50	1.24
1:A:88:GLU:HA	1:A:91:TRP:CZ2	1.79	1.16
1:A:285:THR:HG23	1:A:302:LYS:HB2	1.23	1.15
1:A:498:LEU:O	1:A:499:VAL:HG23	1.44	1.14

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)
2:B:4:FUC:O3	2:B:4:FUC:O3[8_555]	0.65	1.55
2:B:4:FUC:C3	2:B:4:FUC:O3[8_555]	1.92	0.28

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	300/316 (95%)	191 (64%)	65 (22%)	44 (15%)	0 3

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	100	PRO
1	A	107	LEU
1	A	217	GLU
1	A	233	ALA

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	272/284 (96%)	210 (77%)	62 (23%)	0 4

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	476	GLN
1	A	377	LEU
1	A	471	TRP
1	A	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	HIS
1	A	446	ASN
1	A	468	ASN
1	A	408	ASN
1	A	92	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 ⓘ

48 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	B	1	1,2	14,14,15	0.73	0	17,19,21	0.92	0
2	NAG	B	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
2	BMA	B	3	2	11,11,12	0.81	0	15,15,17	1.12	0
2	FUC	B	4	2	10,10,11	0.79	0	14,14,16	1.42	3 (21%)
3	NAG	C	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	1.63	5 (29%)
3	NAG	C	2	3	14,14,15	1.05	2 (14%)	17,19,21	1.81	3 (17%)
3	BMA	C	3	3	11,11,12	0.96	1 (9%)	15,15,17	1.96	3 (20%)
3	MAN	C	4	3	11,11,12	0.54	0	15,15,17	1.51	2 (13%)
3	MAN	C	5	3	11,11,12	0.61	0	15,15,17	1.53	3 (20%)
3	FUC	C	6	3	10,10,11	0.75	0	14,14,16	1.08	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.68	0	17,19,21	1.72	4 (23%)
4	NAG	D	2	4	14,14,15	0.70	0	17,19,21	1.52	3 (17%)
4	FUC	D	3	4	10,10,11	0.75	0	14,14,16	1.00	1 (7%)
4	NAG	E	1	1,4	14,14,15	0.51	0	17,19,21	1.72	3 (17%)
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	1.64	3 (17%)
4	FUC	E	3	4	10,10,11	0.70	0	14,14,16	0.91	0
2	NAG	F	1	1,2	14,14,15	0.68	0	17,19,21	1.96	5 (29%)
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	1.17	1 (5%)
2	BMA	F	3	2	11,11,12	0.56	0	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	F	4	2	10,10,11	0.59	0	14,14,16	0.97	0
5	NAG	G	1	1,5	14,14,15	0.65	0	17,19,21	2.00	4 (23%)
5	NAG	G	2	5	14,14,15	0.79	0	17,19,21	1.17	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.70	0	17,19,21	1.25	3 (17%)
2	NAG	H	2	2	14,14,15	0.76	0	17,19,21	1.67	1 (5%)
2	BMA	H	3	2	11,11,12	0.86	1 (9%)	15,15,17	1.63	3 (20%)
2	FUC	H	4	2	10,10,11	0.68	0	14,14,16	1.16	1 (7%)
6	NAG	I	1	1,6	14,14,15	0.79	1 (7%)	17,19,21	1.39	3 (17%)
6	NAG	I	2	6	14,14,15	0.45	0	17,19,21	3.05	4 (23%)
6	BMA	I	3	6	11,11,12	1.00	0	15,15,17	1.93	5 (33%)
6	MAN	I	4	6	11,11,12	0.52	0	15,15,17	1.91	2 (13%)
6	MAN	I	5	6	11,11,12	0.69	0	15,15,17	1.03	1 (6%)
6	MAN	I	6	6	11,11,12	0.69	0	15,15,17	1.78	4 (26%)
6	MAN	I	7	6	11,11,12	0.58	0	15,15,17	1.87	3 (20%)
7	NAG	J	1	1,7	14,14,15	0.57	0	17,19,21	1.42	2 (11%)
7	NAG	J	2	7	14,14,15	1.00	1 (7%)	17,19,21	1.73	6 (35%)
7	BMA	J	3	7	11,11,12	0.72	0	15,15,17	1.26	2 (13%)
7	MAN	J	4	7	11,11,12	0.83	0	15,15,17	1.93	2 (13%)
7	MAN	J	5	7	11,11,12	0.59	0	15,15,17	1.25	1 (6%)
3	NAG	K	1	3,1	14,14,15	0.81	1 (7%)	17,19,21	1.81	4 (23%)
3	NAG	K	2	3	14,14,15	0.64	0	17,19,21	0.88	0
3	BMA	K	3	3	11,11,12	0.58	0	15,15,17	2.92	4 (26%)
3	MAN	K	4	3	11,11,12	0.55	0	15,15,17	1.64	3 (20%)
3	MAN	K	5	3	11,11,12	0.74	0	15,15,17	0.99	0
3	FUC	K	6	3	10,10,11	1.10	0	14,14,16	1.66	2 (14%)
8	NAG	L	1	1,8	14,14,15	0.60	0	17,19,21	1.88	3 (17%)
8	NAG	L	2	8	14,14,15	0.62	0	17,19,21	1.41	2 (11%)
8	BMA	L	3	8	11,11,12	0.75	0	15,15,17	1.32	1 (6%)
8	MAN	L	4	8	11,11,12	0.59	0	15,15,17	1.49	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	FUC	B	4	2	1/1/4/5	-	0/1/1/1
3	NAG	C	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	FUC	C	6	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	FUC	D	3	4	1/1/4/5	-	0/1/1/1
4	NAG	E	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	FUC	E	3	4	1/1/4/5	-	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
2	FUC	F	4	2	1/1/4/5	-	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	FUC	H	4	2	1/1/4/5	-	0/1/1/1
6	NAG	I	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	2/2/19/22	0/1/1/1
6	MAN	I	6	6	-	0/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	1	3,1	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	MAN	K	5	3	-	2/2/19/22	0/1/1/1
3	FUC	K	6	3	1/1/4/5	-	0/1/1/1
8	NAG	L	1	1,8	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	L	2	8	-	4/6/23/26	0/1/1/1
8	BMA	L	3	8	-	2/2/19/22	0/1/1/1
8	MAN	L	4	8	-	0/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	NAG	C1-C2	2.67	1.56	1.52
3	K	1	NAG	C1-C2	2.45	1.56	1.52
3	C	2	NAG	C1-C2	2.41	1.55	1.52
2	H	3	BMA	C2-C3	2.33	1.55	1.52
3	C	3	BMA	C2-C3	2.21	1.55	1.52

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2	NAG	C4-C3-C2	-9.19	97.55	111.02
3	K	3	BMA	C1-O5-C5	8.12	123.19	112.19
6	I	2	NAG	C1-O5-C5	6.53	121.04	112.19
7	J	4	MAN	C1-C2-C3	6.12	117.19	109.67
6	I	4	MAN	C1-O5-C5	6.05	120.39	112.19

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
2	B	4	FUC	C1
2	F	4	FUC	C1
2	H	1	NAG	C1
2	H	4	FUC	C1

5 of 101 torsion outliers are listed below:

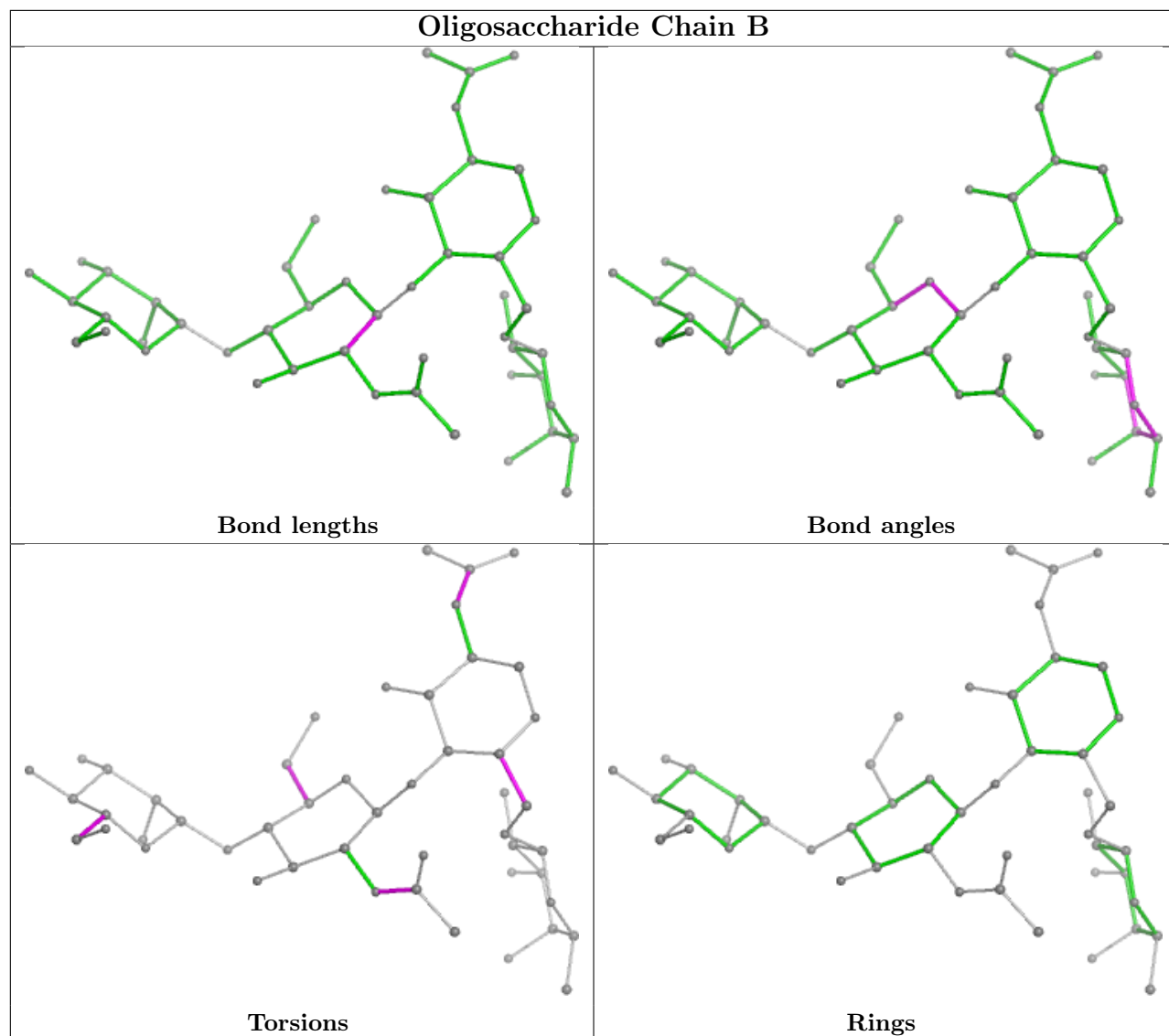
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C1-C2-N2-C7

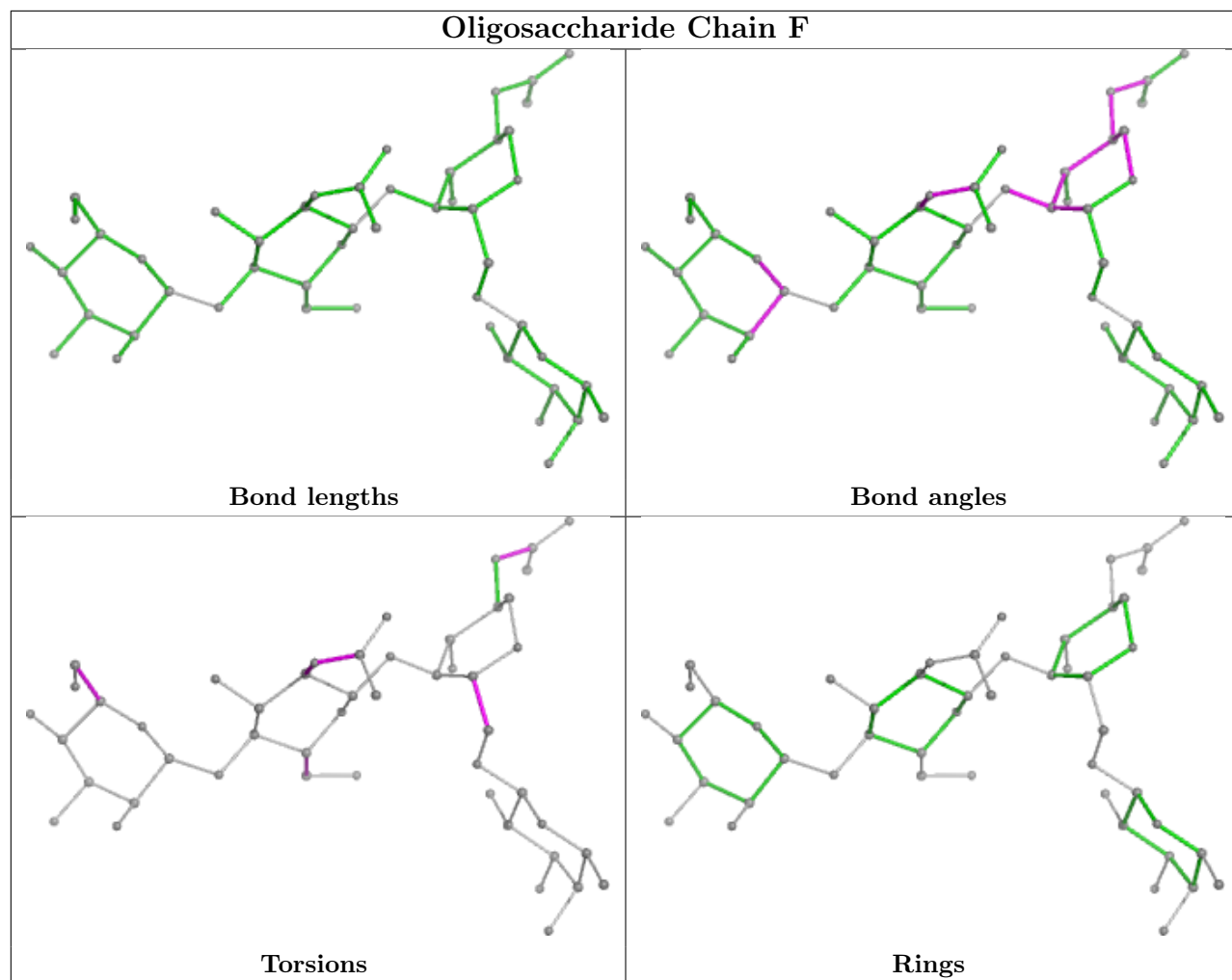
There are no ring outliers.

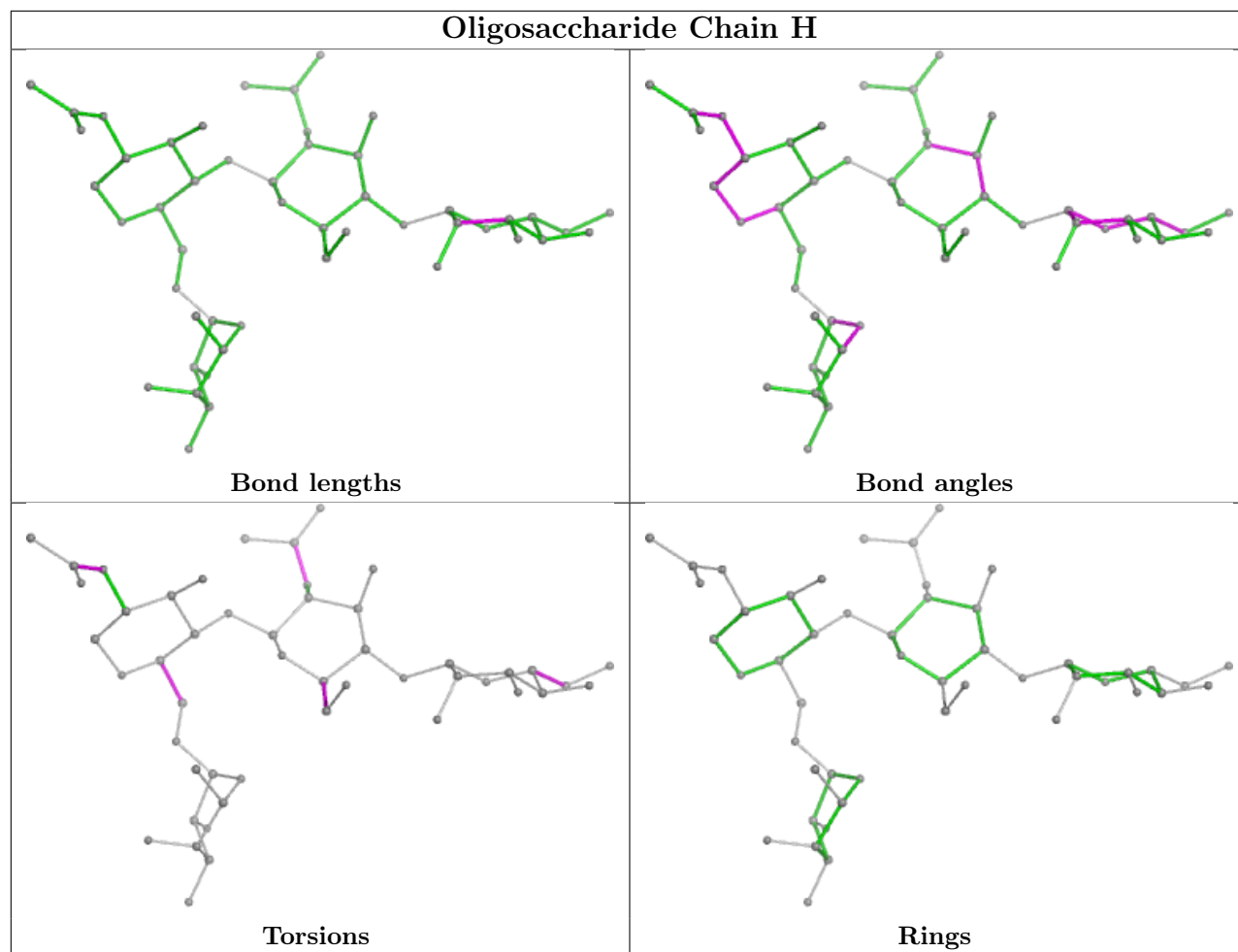
16 monomers are involved in 25 short contacts:

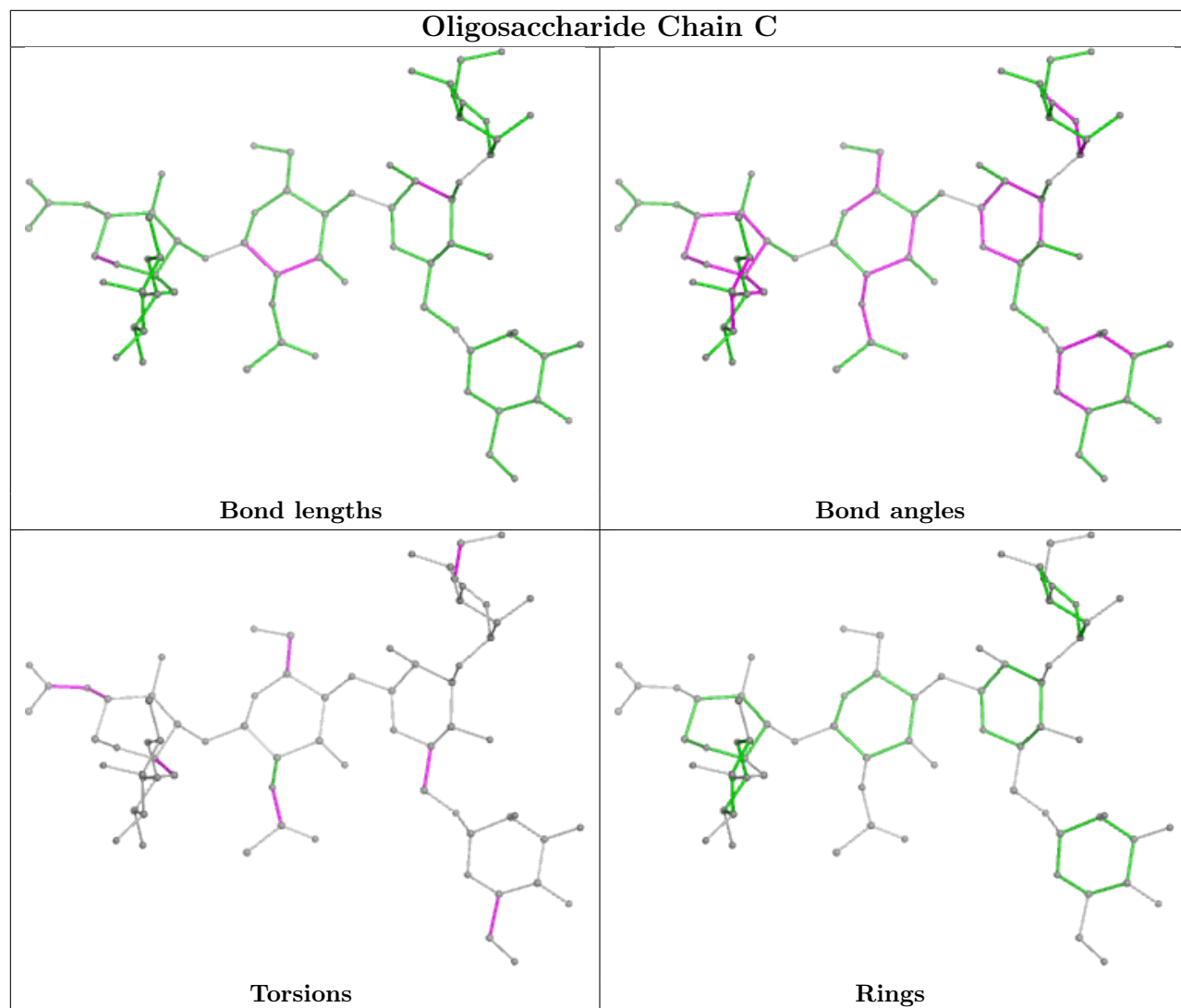
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	3	0
2	B	4	FUC	0	2
4	D	2	NAG	2	0
3	C	5	MAN	1	0
4	D	3	FUC	2	0
3	K	6	FUC	2	0
3	C	1	NAG	1	0
4	D	1	NAG	3	0
2	B	3	BMA	1	0
6	I	2	NAG	6	0
4	E	1	NAG	4	0
4	E	3	FUC	2	0
5	G	1	NAG	1	0
3	C	3	BMA	1	0
3	K	1	NAG	3	0
2	B	2	NAG	1	0

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

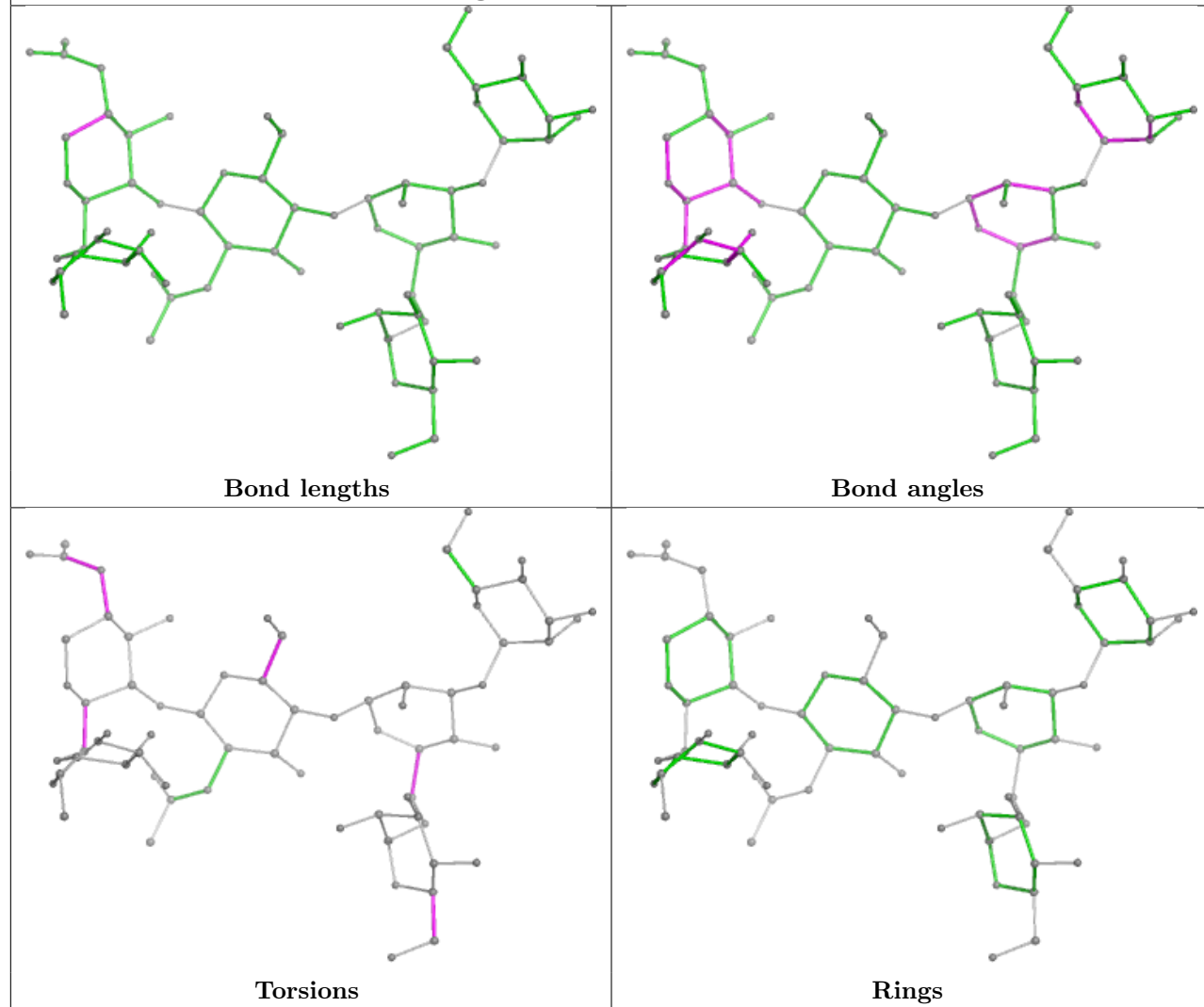


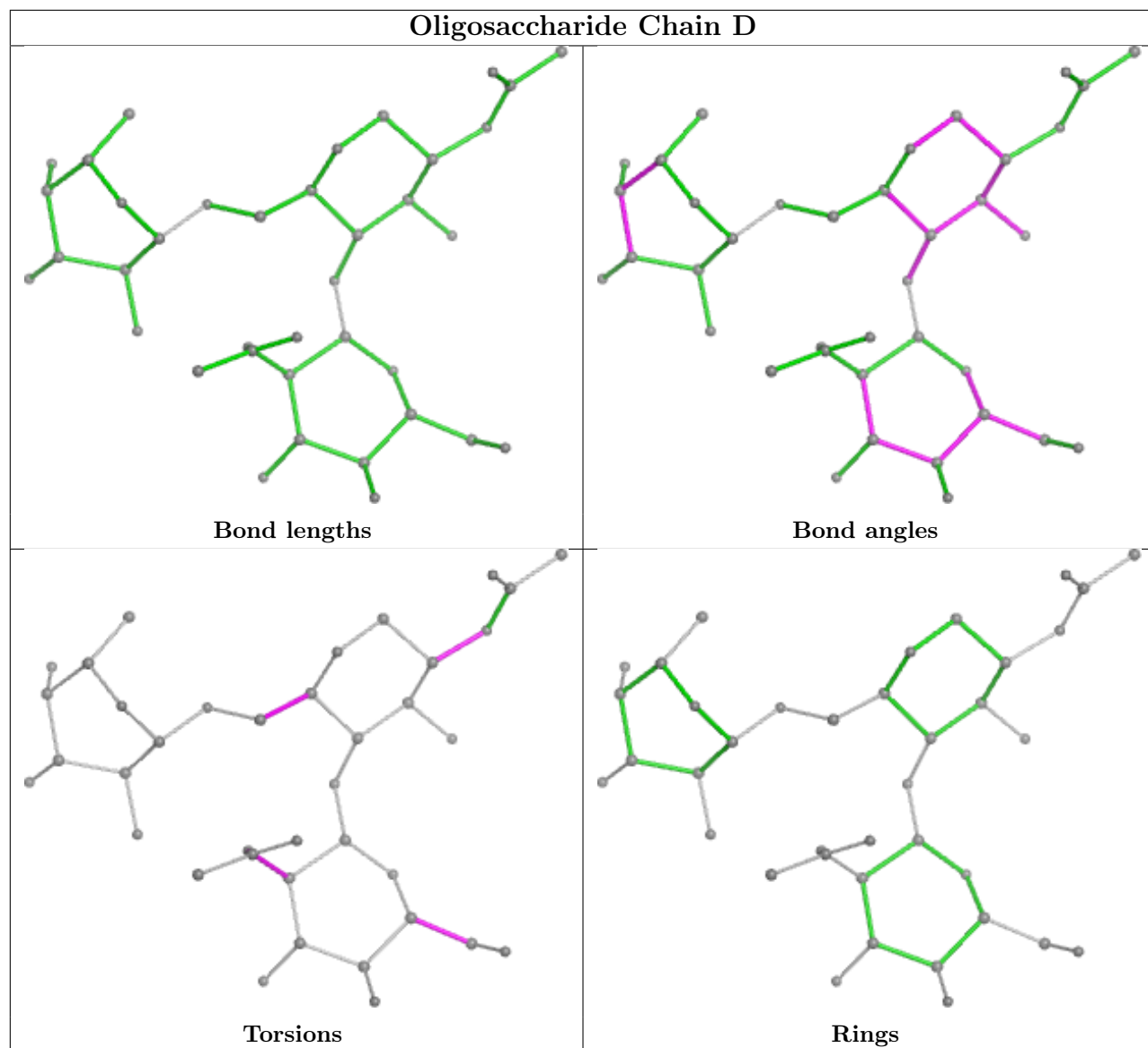




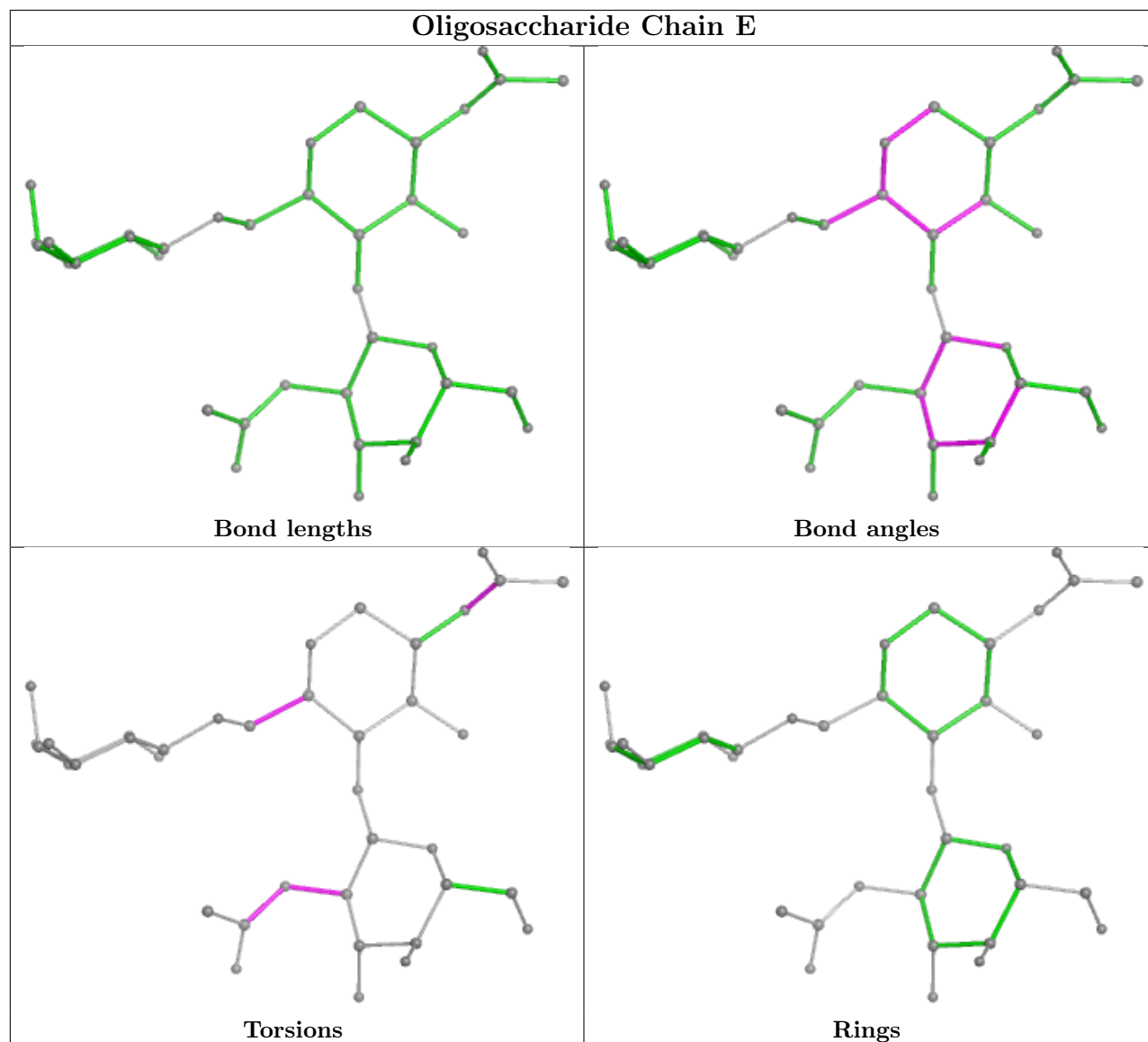


Oligosaccharide Chain K

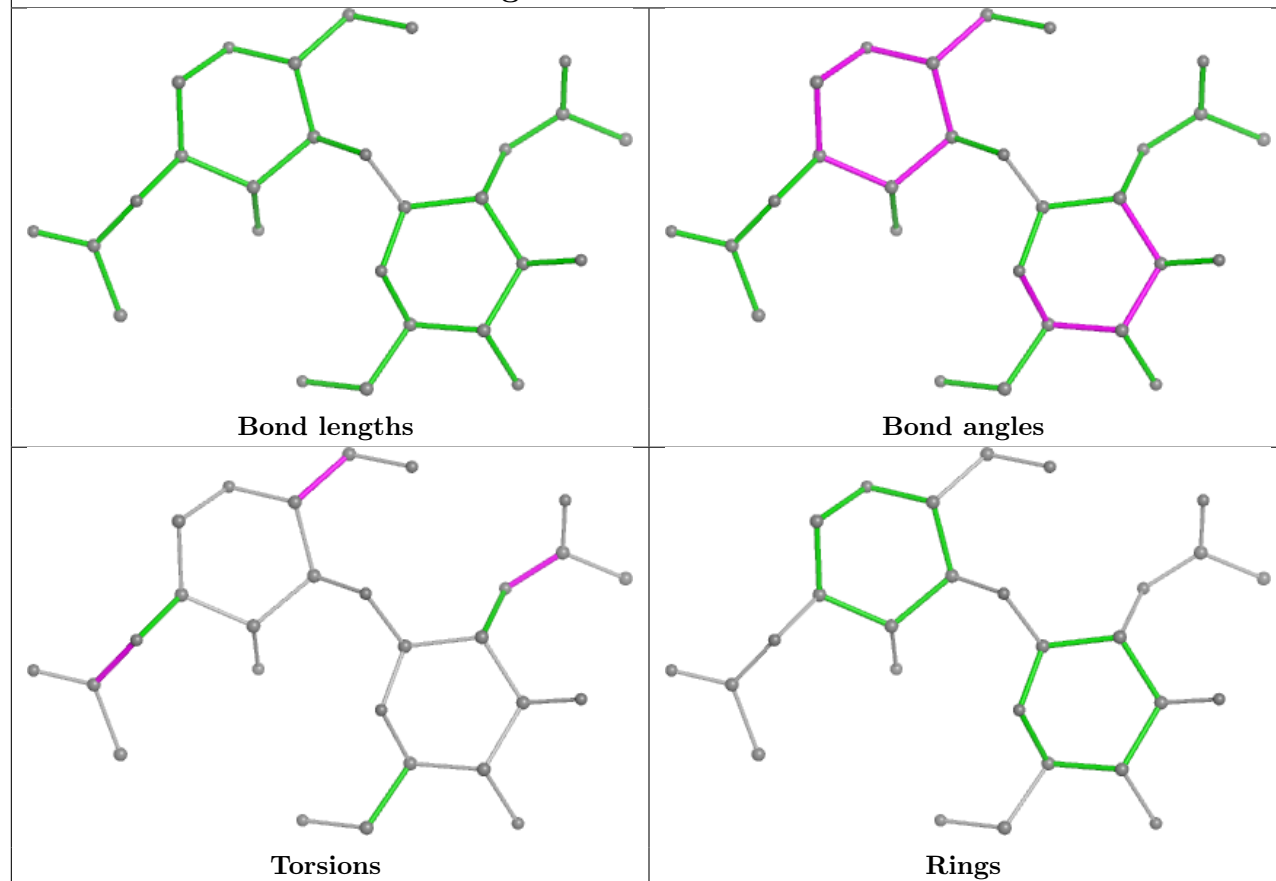




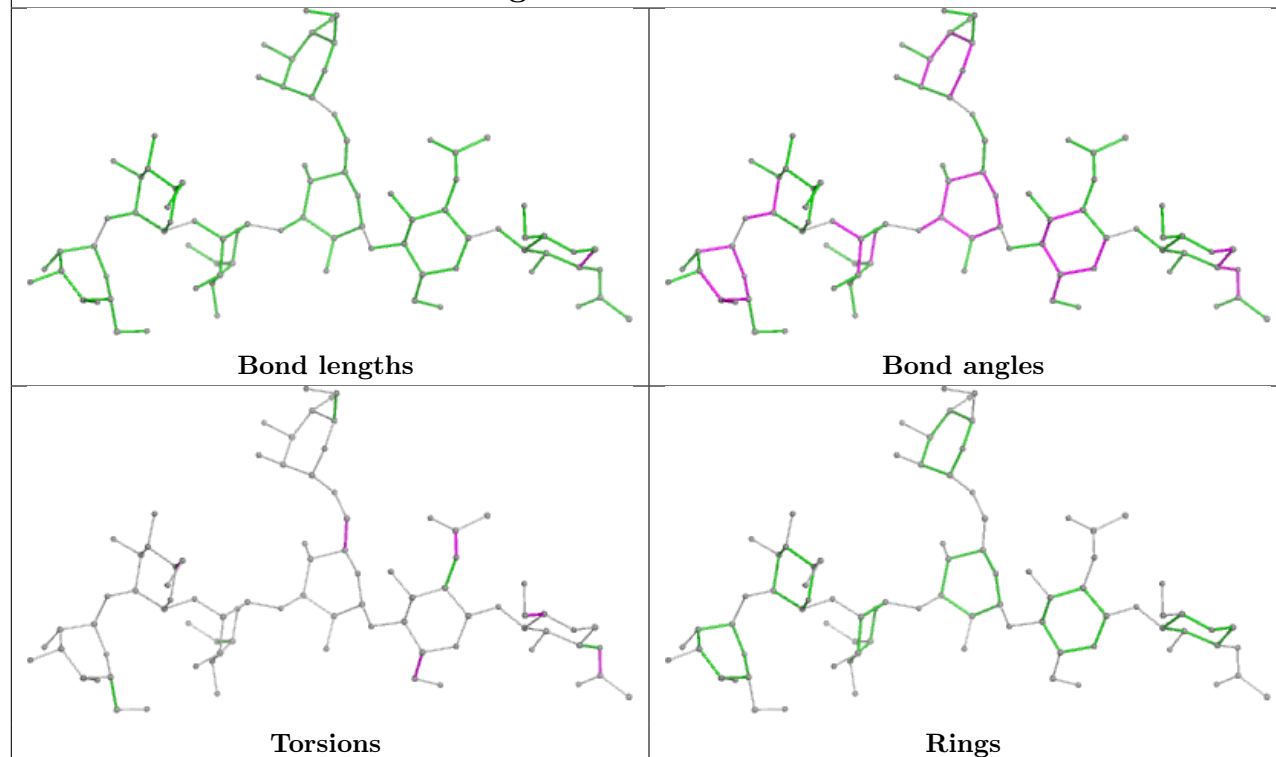
Oligosaccharide Chain E



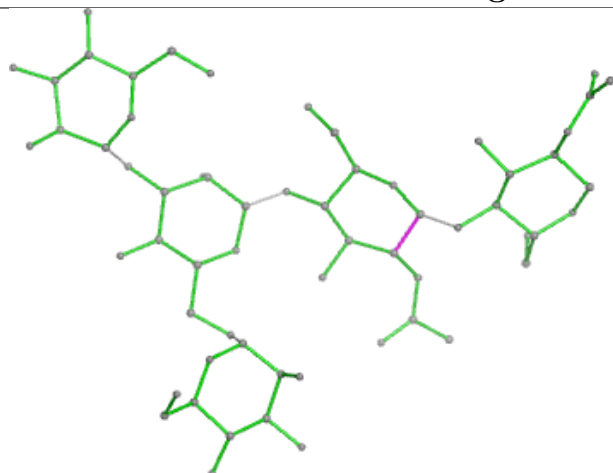
Oligosaccharide Chain G



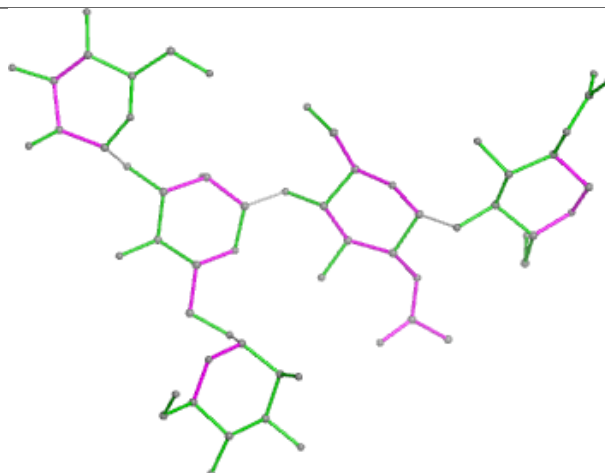
Oligosaccharide Chain I



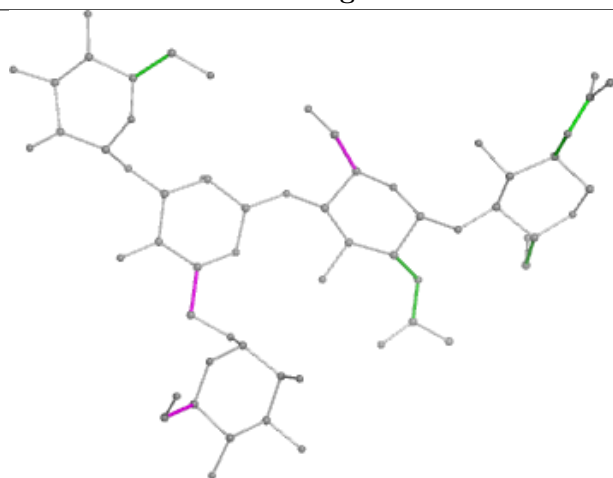
Oligosaccharide Chain J



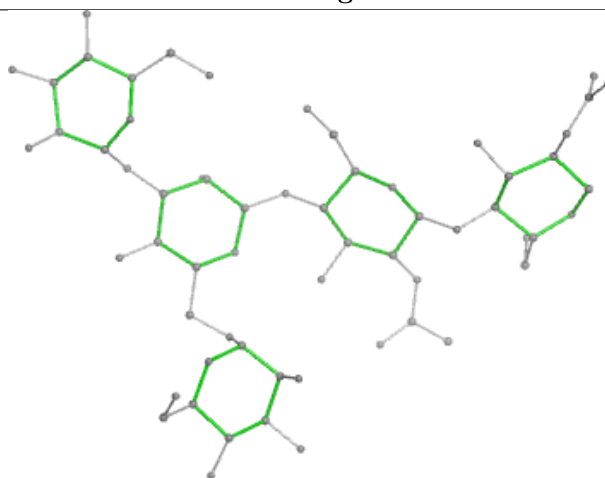
Bond lengths



Bond angles

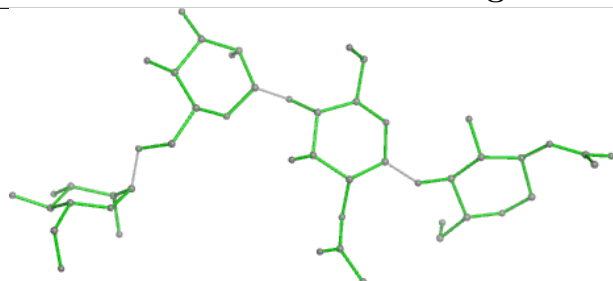


Torsions

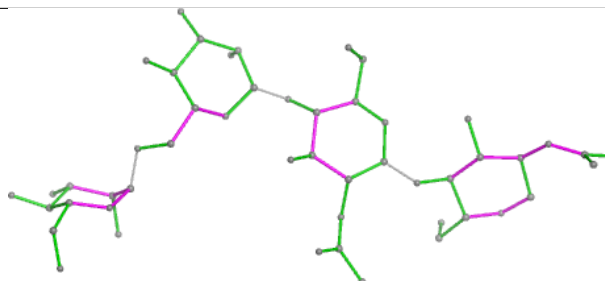


Rings

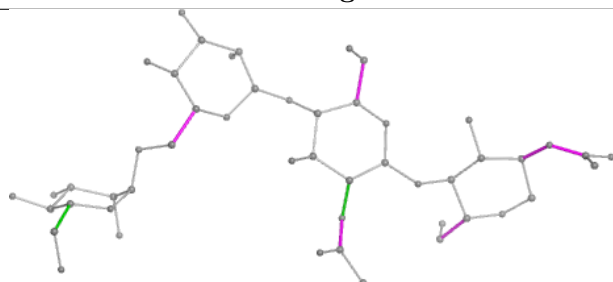
Oligosaccharide Chain L



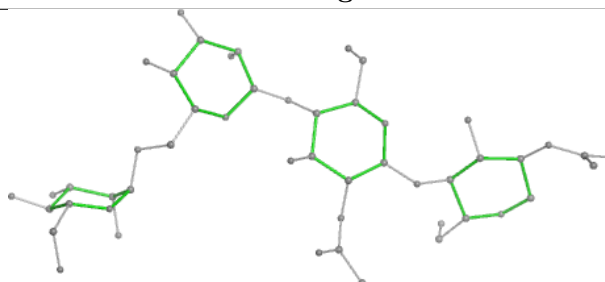
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

2 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	1501	1	14,14,15	0.91	1 (7%)	17,19,21	0.99	0
9	NAG	A	1500	1	14,14,15	0.70	0	17,19,21	1.32	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
9	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
9	NAG	A	1500	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1501	NAG	O6-C6	2.47	1.52	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1500	NAG	C2-N2-C7	-3.40	118.07	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1500	NAG	C8-C7-N2-C2
9	A	1500	NAG	O7-C7-N2-C2
9	A	1501	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	A	1501	NAG	O7-C7-N2-C2
9	A	1501	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	304/316 (96%)	1.35	64 (21%) 3 5	96, 124, 157, 183	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	GLU	10.6
1	A	210	CYS	7.7
1	A	255	SER	7.3
1	A	459	ASN	7.2
1	A	311	ARG	7.1

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	NAG	H	2	14/15	0.20	0.25	151,156,162,163	0
2	NAG	B	2	14/15	0.24	0.20	114,121,126,130	0
7	NAG	J	2	14/15	0.34	0.21	168,172,184,186	0
2	BMA	H	3	11/12	0.36	0.26	165,174,183,185	0
3	MAN	C	5	11/12	0.46	0.17	132,137,143,145	0
7	MAN	J	5	11/12	0.49	0.16	164,169,173,173	0
2	BMA	B	3	11/12	0.50	0.15	132,135,141,141	0

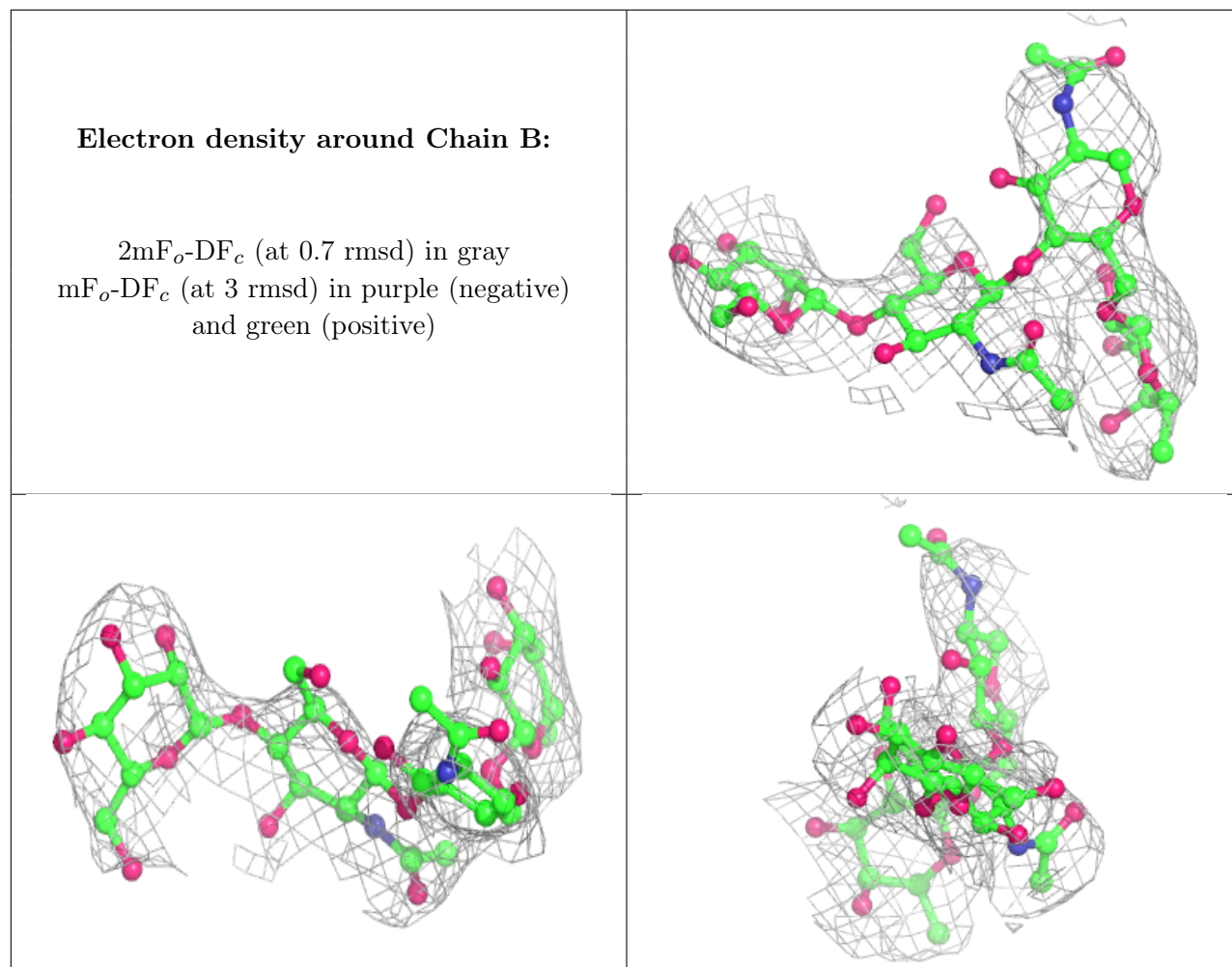
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	2	14/15	0.52	0.13	125,135,142,145	0
6	MAN	I	4	11/12	0.52	0.15	143,149,156,158	0
8	MAN	L	4	11/12	0.52	0.14	176,184,190,194	0
2	FUC	F	4	10/11	0.54	0.13	121,126,130,132	0
5	NAG	G	2	14/15	0.54	0.20	185,198,212,214	0
3	NAG	C	2	14/15	0.54	0.43	112,115,119,123	0
7	BMA	J	3	11/12	0.56	0.12	177,185,195,199	0
3	MAN	K	5	11/12	0.57	0.14	117,121,125,126	0
3	FUC	K	6	10/11	0.57	0.16	112,117,121,122	0
8	BMA	L	3	11/12	0.58	0.13	163,171,177,180	0
6	MAN	I	6	11/12	0.61	0.19	160,163,168,170	0
7	MAN	J	4	11/12	0.63	0.16	195,203,214,216	0
5	NAG	G	1	14/15	0.66	0.21	182,192,205,210	0
4	NAG	D	1	14/15	0.67	0.16	122,125,128,129	0
4	NAG	D	2	14/15	0.68	0.15	133,138,145,146	0
4	FUC	E	3	10/11	0.69	0.28	154,158,162,163	0
8	NAG	L	2	14/15	0.70	0.15	145,149,157,158	0
3	BMA	C	3	11/12	0.71	0.11	125,129,136,136	0
2	NAG	B	1	14/15	0.72	0.13	110,113,117,117	0
4	NAG	E	2	14/15	0.72	0.14	162,170,178,178	0
3	FUC	C	6	10/11	0.73	0.13	109,111,113,114	0
6	MAN	I	5	11/12	0.73	0.33	140,146,153,155	0
8	NAG	L	1	14/15	0.74	0.12	123,131,138,141	0
7	NAG	J	1	14/15	0.74	0.29	159,163,167,168	0
2	BMA	F	3	11/12	0.75	0.09	149,153,162,164	0
6	MAN	I	7	11/12	0.76	0.17	123,129,133,136	0
2	NAG	H	1	14/15	0.76	0.20	136,140,147,148	0
6	NAG	I	1	14/15	0.77	0.55	114,122,128,131	0
3	MAN	K	4	11/12	0.77	0.07	117,119,124,126	0
6	BMA	I	3	11/12	0.79	0.14	129,133,140,141	0
4	FUC	D	3	10/11	0.79	0.13	121,127,129,132	0
4	NAG	E	1	14/15	0.81	0.17	137,146,154,159	0
3	NAG	C	1	14/15	0.81	0.12	101,106,109,110	0
3	BMA	K	3	11/12	0.82	0.08	111,114,117,118	0
2	FUC	B	4	10/11	0.83	0.10	114,117,121,121	0
2	FUC	H	4	10/11	0.83	0.14	136,141,143,145	0
3	MAN	C	4	11/12	0.84	0.09	136,140,144,147	0
2	NAG	F	1	14/15	0.86	0.15	120,123,128,130	0
6	NAG	I	2	14/15	0.87	0.12	118,125,134,134	0
3	NAG	K	2	14/15	0.87	0.12	107,110,112,112	0
3	NAG	K	1	14/15	0.87	0.16	105,108,110,112	0

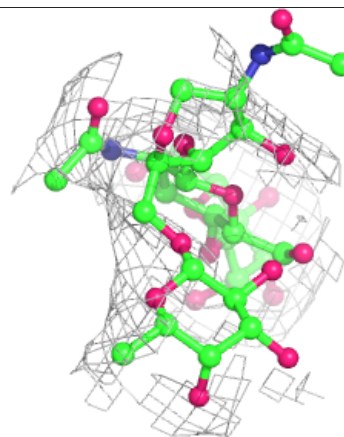
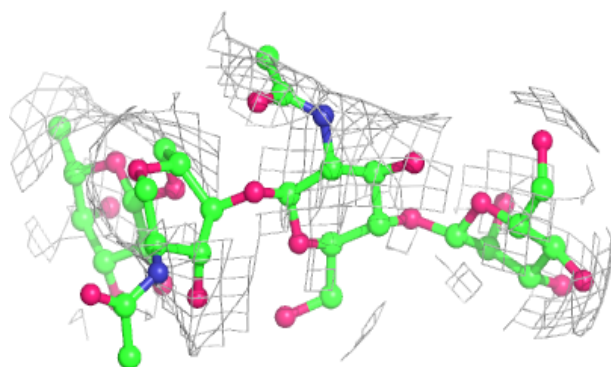
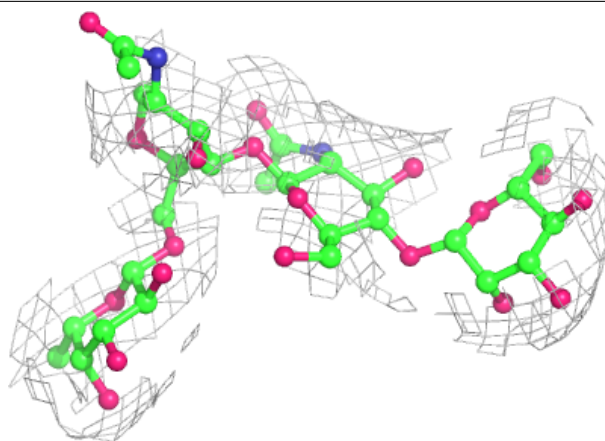
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

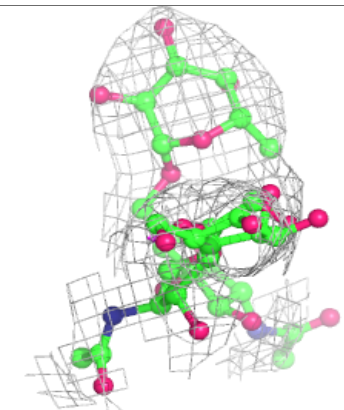
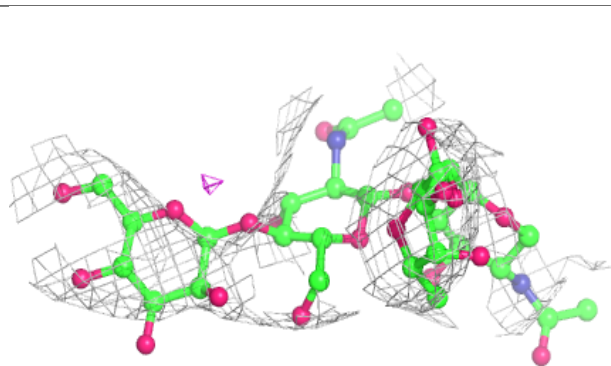
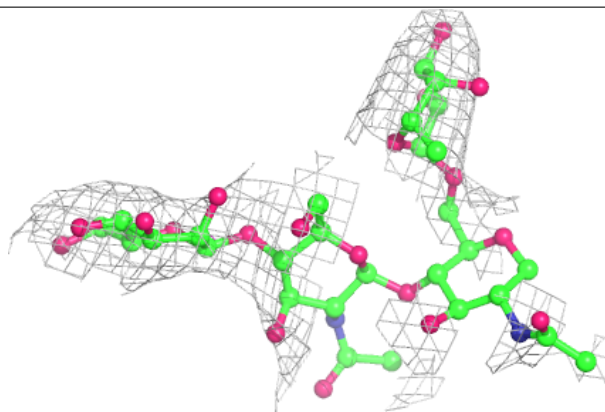


Electron density around Chain F:

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

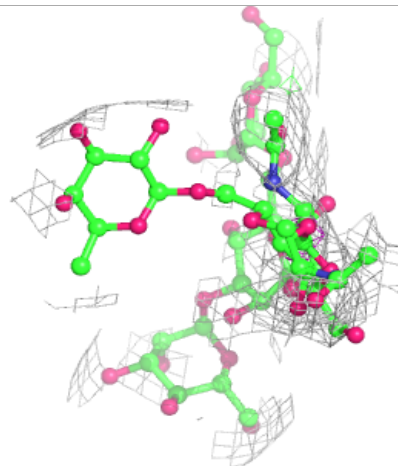
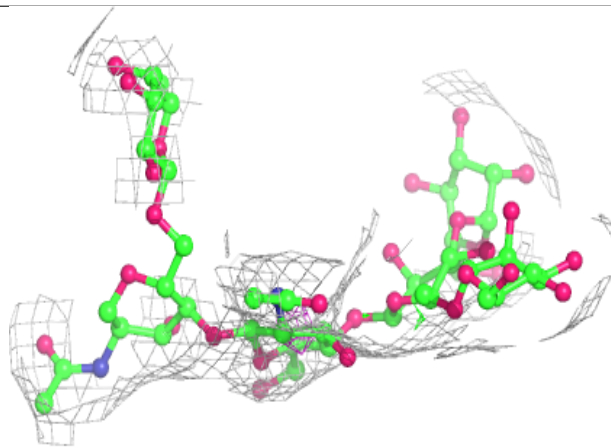
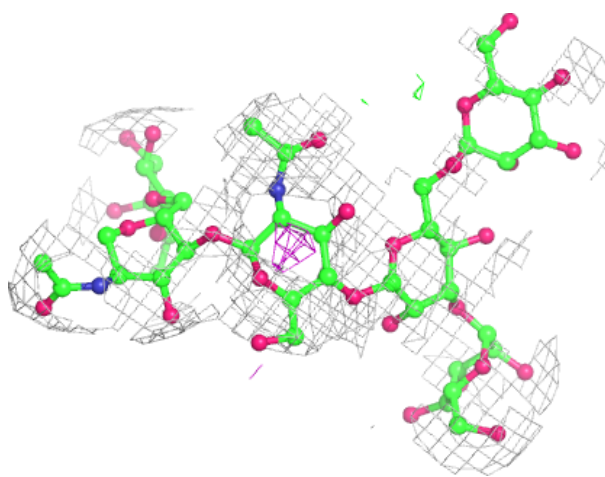
**Electron density around Chain H:**

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



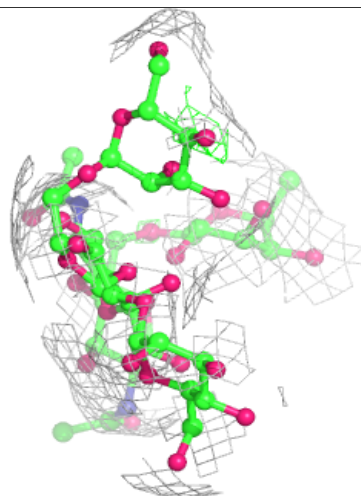
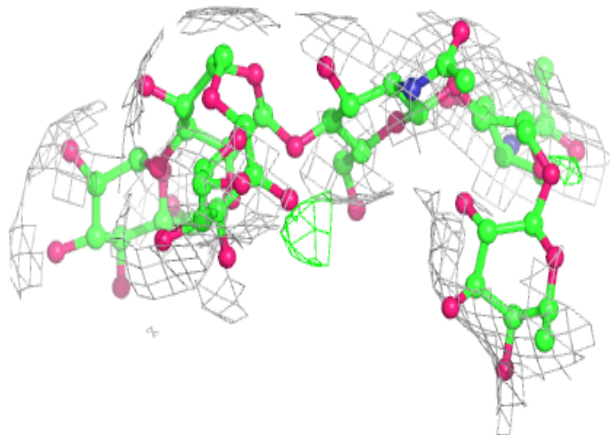
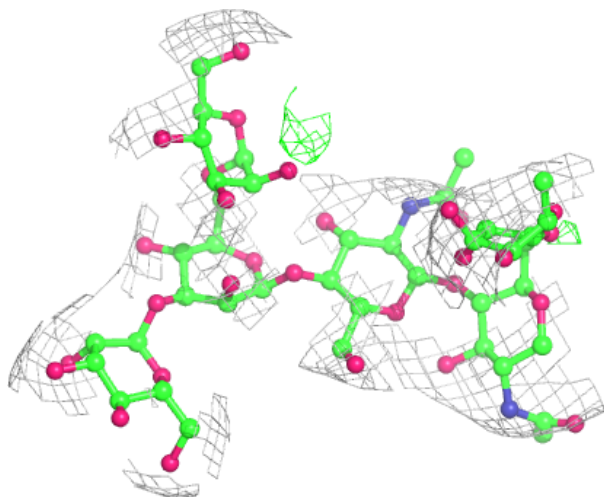
Electron density around Chain C:

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



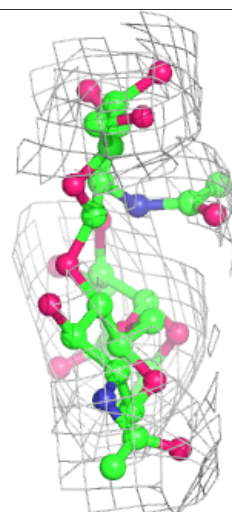
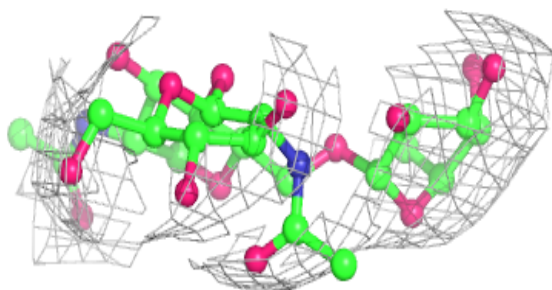
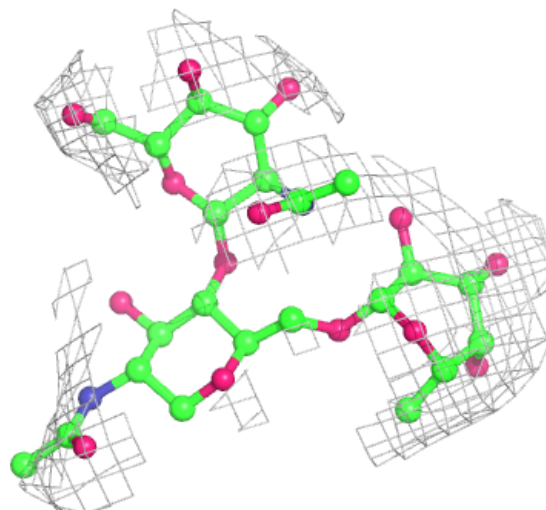
Electron density around Chain K:

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



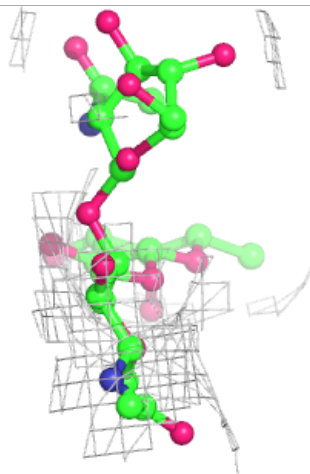
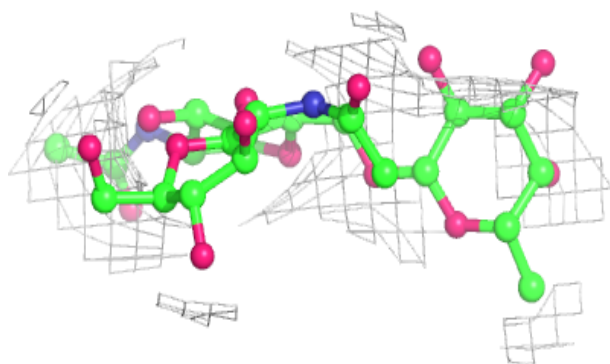
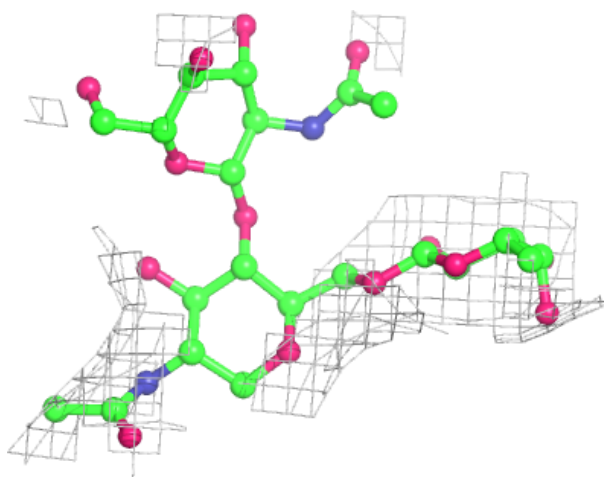
Electron density around Chain D:

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



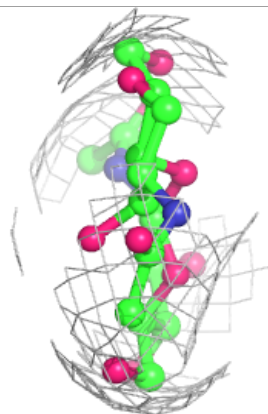
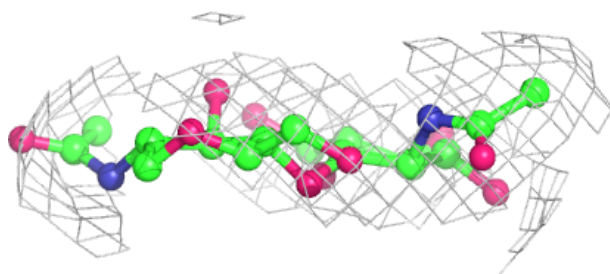
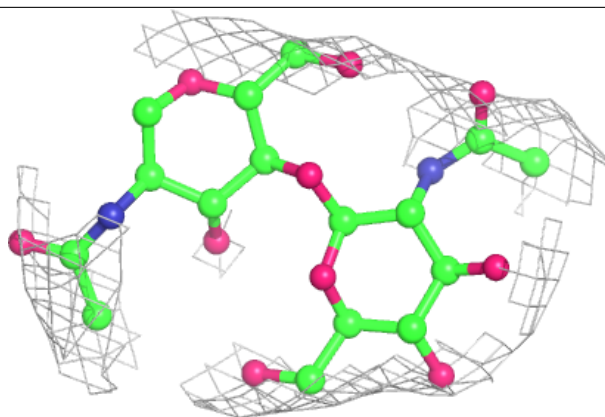
Electron density around Chain E:

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

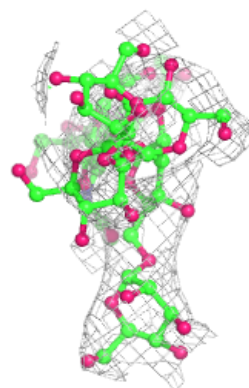
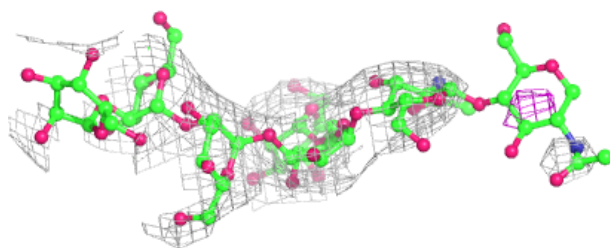
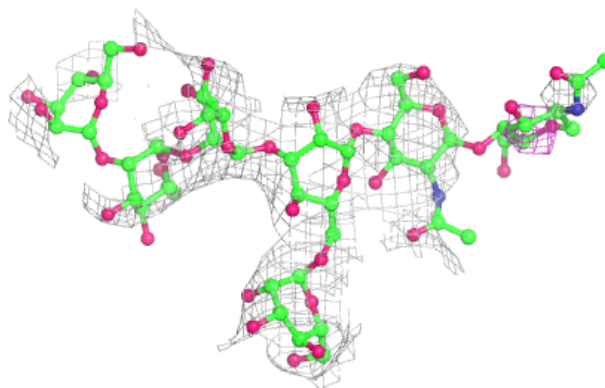


Electron density around Chain G:

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

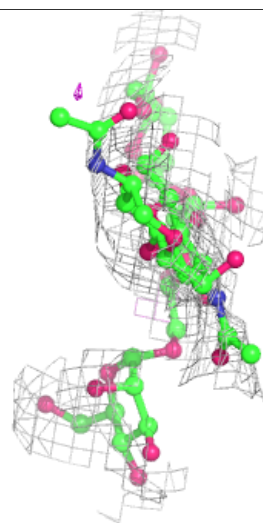
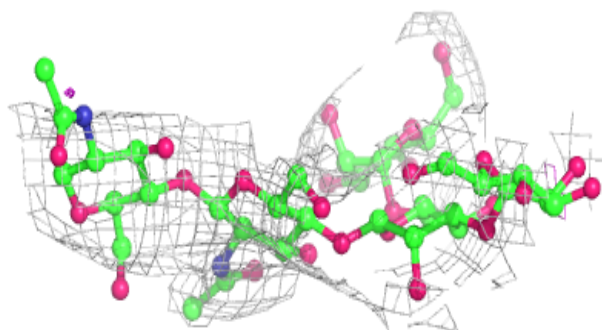
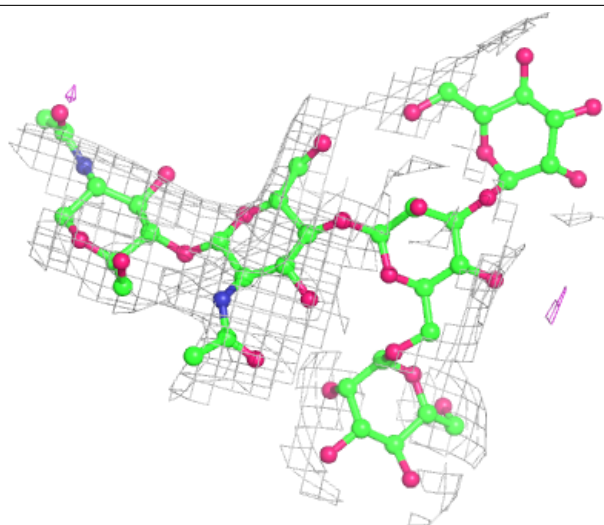
**Electron density around Chain I:**

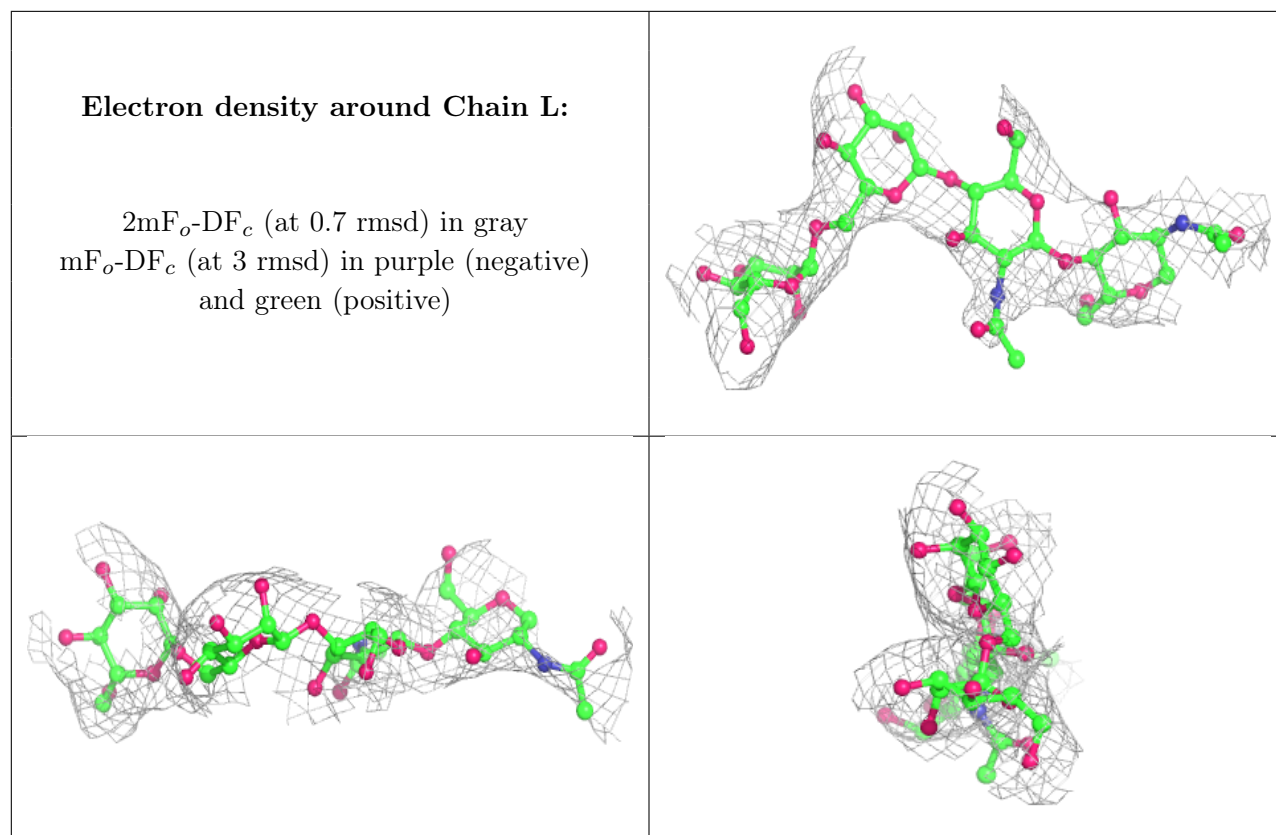
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
9	NAG	A	1500	14/15	0.71	0.12	147,151,157,160	0
9	NAG	A	1501	14/15	0.84	0.12	140,145,150,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.