



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 03:39 AM UTC

PDB ID : 9CH4 / pdb\_00009ch4  
Title : Crystal structure of shark nonclassical MHC CLASS I, UGA  
Authors : Castro, C.D.; Adams, E.J.  
Deposited on : 2024-07-01  
Resolution : 2.67 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

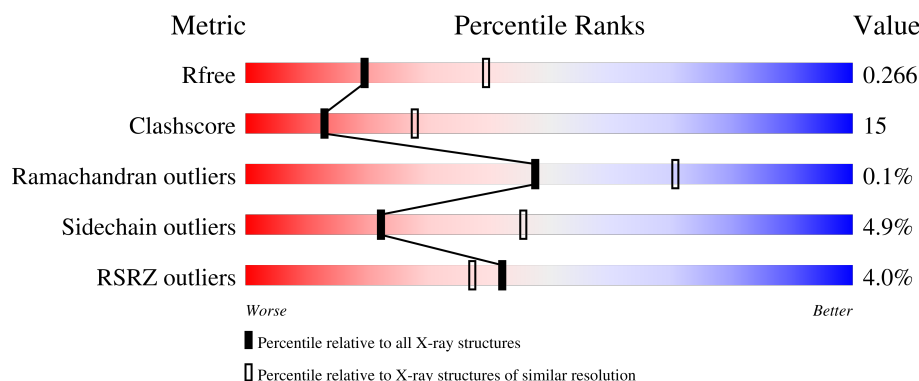
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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  $\geq 3$ , 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	268	<div> <div>4%</div> <div>66%</div> <div>33%</div> <div>.</div> </div>
1	C	268	<div> <div>4%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>
1	E	268	<div> <div>5%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>
2	B	94	<div> <div>3%</div> <div>77%</div> <div>23%</div> <div>.</div> </div>
2	D	94	<div> <div>2%</div> <div>62%</div> <div>35%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	94	<div><div></div><div>3%</div><div>70%</div><div>26%</div><div>...</div></div>
3	G	6	<div><div></div><div>33%</div><div>67%</div></div>
3	J	6	<div><div></div><div>17%</div><div>50%</div><div>33%</div></div>
4	H	2	<div><div></div><div>50%</div><div>50%</div></div>
4	I	2	<div><div></div><div>100%</div></div>
4	K	2	<div><div></div><div>100%</div></div>
4	L	2	<div><div></div><div>50%</div><div>50%</div></div>
5	M	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9578 atoms, of which 236 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.

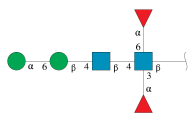
- Molecule 1 is a protein called Ig-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2178	1403	361	402	12			
1	C	268	Total	C	N	O	S	0	0	0
			2178	1403	361	402	12			
1	E	267	Total	C	N	O	S	0	0	0
			2161	1391	360	398	12			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	0	0	0
			757	481	122	151	3			
2	D	94	Total	C	N	O	S	0	0	0
			757	481	122	151	3			
2	F	93	Total	C	N	O	S	0	0	0
			744	472	121	148	3			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	6	Total	C	N	O	0	0	0
			70	40	2	28			
3	J	6	Total	C	N	O	0	0	0
			70	40	2	28			

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

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



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

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



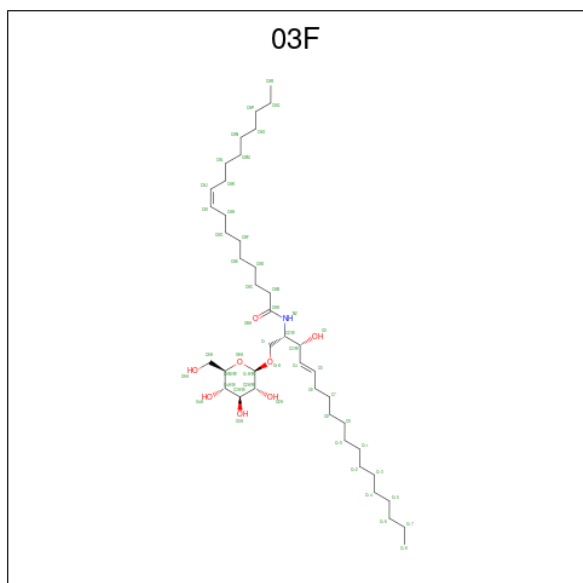
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 7 is (9Z)-N-[(2S,3R,4E)-1-(beta-D-glucopyranosyloxy)-3-hydroxyoctadec-4-en-2-yl]octadec-9-enamide (CCD ID: 03F) (formula:  $C_{42}H_{79}NO_8$ ) (labeled as "Ligand of Interest" by depositor).

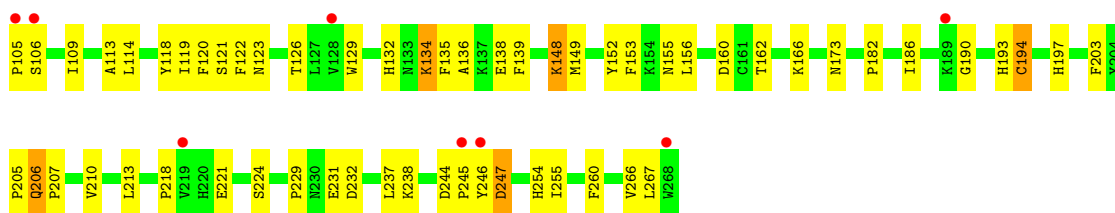


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			129	42	78	1	8		
7	C	1	Total	C	H	N	O	0	0
			130	42	79	1	8		
7	E	1	Total	C	H	N	O	0	0
			130	42	79	1	8		

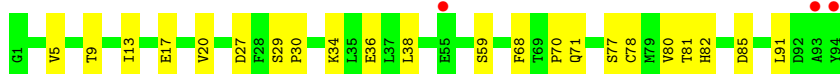
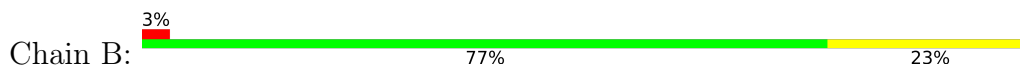
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total	O	0	0
			23	23		
8	B	8	Total	O	0	0
			8	8		
8	C	22	Total	O	0	0
			22	22		
8	D	9	Total	O	0	0
			9	9		
8	E	26	Total	O	0	0
			26	26		
8	F	8	Total	O	0	0
			8	8		





• Molecule 2: Beta-2-microglobulin



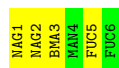
• Molecule 2: Beta-2-microglobulin



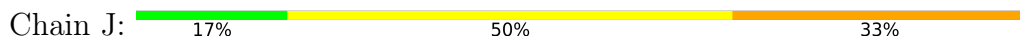
• Molecule 2: Beta-2-microglobulin



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



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



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

Chain H:  50% 50%

MAG1  
MAG2

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

Chain I:  100%


MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.77Å 95.63Å 112.37Å 90.00° 123.96° 90.00°	Depositor
Resolution (Å)	93.20 – 2.67 93.20 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.4 (93.20-2.67) 99.5 (93.20-2.67)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.239 , 0.262 0.244 , 0.266	Depositor DCC
$R_{free}$ test set	1979 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NAG, 03F, FUC, 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	0.83	0/2243	1.16	1/3039 (0.0%)
1	C	0.83	0/2243	1.18	1/3039 (0.0%)
1	E	0.84	0/2224	1.19	3/3011 (0.1%)
2	B	0.83	0/775	1.19	0/1049
2	D	0.82	0/775	1.16	0/1049
2	F	0.84	0/761	1.20	2/1031 (0.2%)
All	All	0.83	0/9021	1.18	7/12218 (0.1%)

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	C	230	ASN	N-CA-C	-7.94	98.72	110.23
1	E	229	PRO	CB-CA-C	-6.96	106.02	111.87
1	E	106	SER	N-CA-C	5.60	121.54	114.31
2	F	69	THR	CB-CA-C	5.40	115.51	110.17
2	F	54	PHE	CA-CB-CG	5.39	119.19	113.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2087	68	2
1	C	2178	0	2086	77	1
1	E	2161	0	2071	65	0
2	B	757	0	730	15	0
2	D	757	0	731	28	0
2	F	744	0	722	19	0
3	G	70	0	61	1	0
3	J	70	0	61	3	0
4	H	28	0	25	1	0
4	I	28	0	25	2	0
4	K	28	0	25	2	0
4	L	28	0	25	1	0
5	M	24	0	22	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
7	A	51	78	79	2	0
7	C	51	79	79	3	0
7	E	51	79	79	3	1
8	A	23	0	0	1	0
8	B	8	0	0	1	0
8	C	22	0	0	2	0
8	D	9	0	0	2	0
8	E	26	0	0	2	0
8	F	8	0	0	0	0
All	All	9342	236	8947	273	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 15.

The worst 5 of 273 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:C:212:TRP:HD1	1:C:221:GLU:HG3	1.25	0.99
1:E:190:GLY:HA3	1:E:194:CYS:HA	1.53	0.89
1:A:27:LEU:CD1	1:A:165:LEU:CD1	2.52	0.87
1:A:27:LEU:HD11	1:A:165:LEU:CD1	2.05	0.86
1:C:6:LEU:HD23	1:C:97:GLY:HA3	1.58	0.86

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:A:148:LYS:NZ	7:E:301:03F:H6AB[2_445]	1.37	0.23
1:A:167:THR:CG2	1:C:147:THR:OG1[4_445]	2.16	0.04

## 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	266/268 (99%)	254 (96%)	12 (4%)	0	100	100
1	C	266/268 (99%)	254 (96%)	12 (4%)	0	100	100
1	E	263/268 (98%)	247 (94%)	16 (6%)	0	100	100
2	B	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
2	D	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
2	F	91/94 (97%)	86 (94%)	4 (4%)	1 (1%)	11	26
All	All	1070/1086 (98%)	1023 (96%)	46 (4%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	29	SER

### 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	237/237 (100%)	225 (95%)	12 (5%)	21	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	237/237 (100%)	221 (93%)	16 (7%)	14	32
1	E	235/237 (99%)	225 (96%)	10 (4%)	26	51
2	B	87/87 (100%)	86 (99%)	1 (1%)	65	83
2	D	87/87 (100%)	83 (95%)	4 (5%)	24	48
2	F	86/87 (99%)	82 (95%)	4 (5%)	23	47
All	All	969/972 (100%)	922 (95%)	47 (5%)	22	46

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	ASN
1	E	85	GLN
2	D	10	TYR
2	D	14	LYS
1	E	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	250	GLN
2	D	6	GLN
1	E	173	ASN
2	D	71	GLN
2	B	32	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

22 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	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
3	NAG	G	2	3	14,14,15	0.48	0	17,19,21	0.87	0
3	BMA	G	3	3	11,11,12	0.41	0	15,15,17	0.79	1 (6%)
3	MAN	G	4	3	11,11,12	0.27	0	15,15,17	0.60	0
3	FUC	G	5	3	10,10,11	0.25	0	14,14,16	0.59	0
3	FUC	G	6	3	10,10,11	0.20	0	14,14,16	0.65	0
4	NAG	H	1	1,4	14,14,15	0.42	0	17,19,21	0.72	0
4	NAG	H	2	4	14,14,15	0.36	0	17,19,21	0.90	0
4	NAG	I	1	4	14,14,15	0.85	0	17,19,21	1.19	1 (5%)
4	NAG	I	2	4	14,14,15	0.84	1 (7%)	17,19,21	2.05	4 (23%)
3	NAG	J	1	1,3	14,14,15	0.53	0	17,19,21	1.45	2 (11%)
3	NAG	J	2	3	14,14,15	0.53	0	17,19,21	0.76	0
3	BMA	J	3	3	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
3	MAN	J	4	3	11,11,12	0.40	0	15,15,17	1.56	3 (20%)
3	FUC	J	5	3	10,10,11	0.20	0	14,14,16	0.44	0
3	FUC	J	6	3	10,10,11	0.36	0	14,14,16	0.72	0
4	NAG	K	1	1,4	14,14,15	0.41	0	17,19,21	1.22	2 (11%)
4	NAG	K	2	4	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
4	NAG	L	1	4	14,14,15	0.43	0	17,19,21	1.58	4 (23%)
4	NAG	L	2	4	14,14,15	0.44	0	17,19,21	1.00	2 (11%)
5	NAG	M	1	5	14,14,15	0.47	0	17,19,21	1.40	3 (17%)
5	FUC	M	2	5	10,10,11	0.41	0	14,14,16	0.82	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	C1-C2	2.27	1.55	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C2-N2-C7	5.84	130.72	122.90
4	L	1	NAG	C4-C3-C2	-4.36	104.62	111.02
4	I	2	NAG	C4-C3-C2	4.11	117.05	111.02
3	J	4	MAN	C1-O5-C5	3.98	117.52	112.19
5	M	1	NAG	O5-C1-C2	-3.81	105.39	111.29

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C1-C2-N2-C7
4	K	1	NAG	C8-C7-N2-C2

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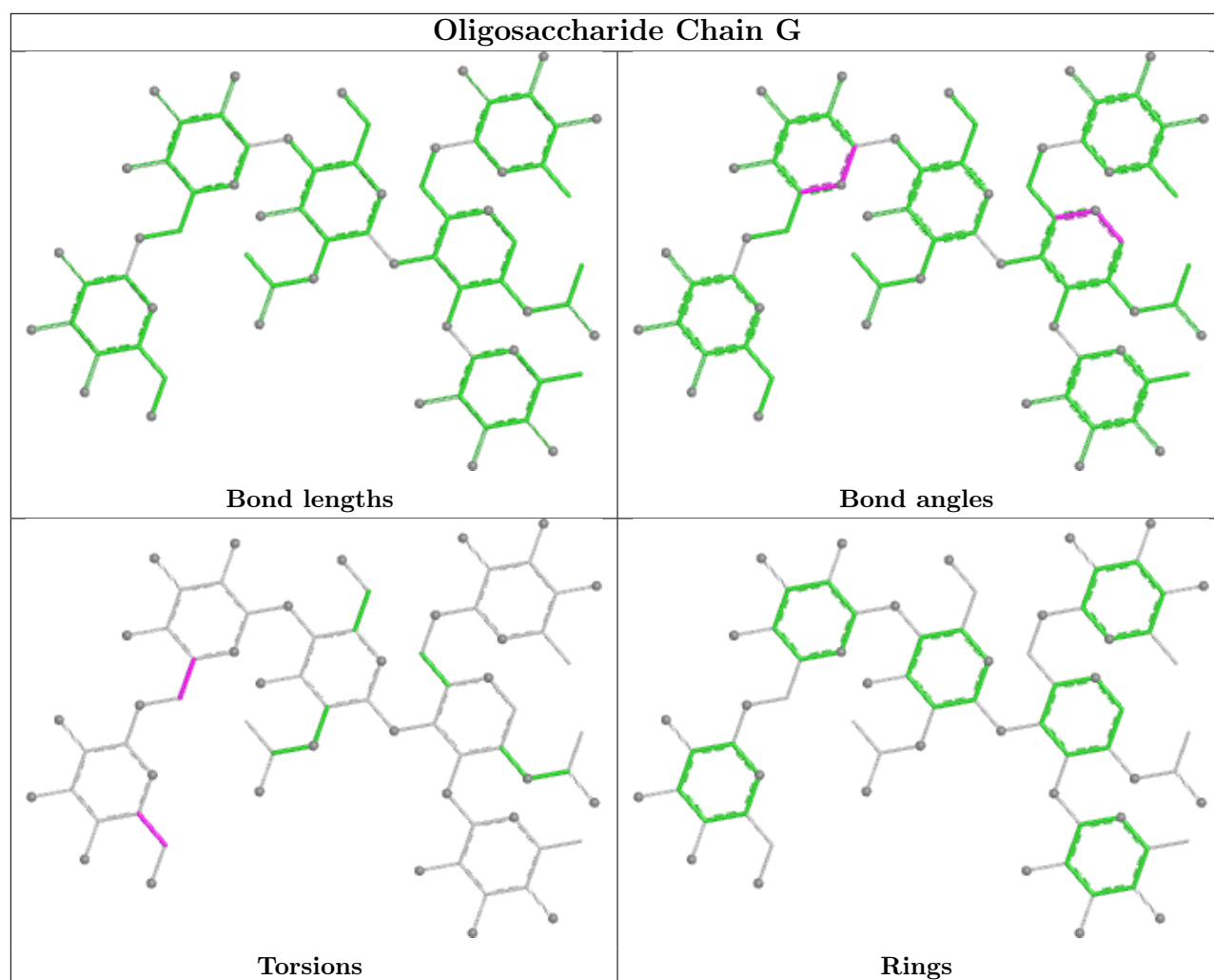
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2

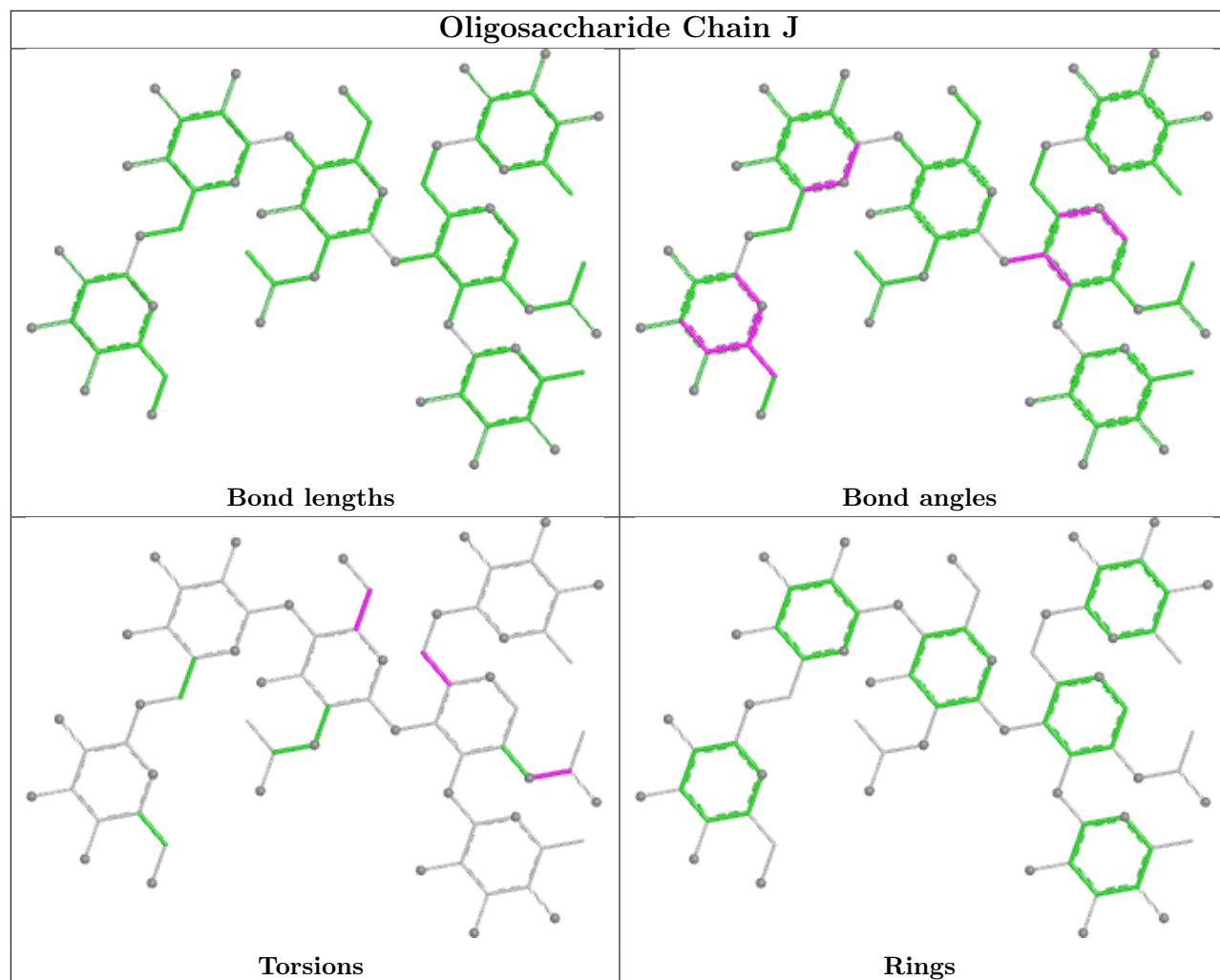
There are no ring outliers.

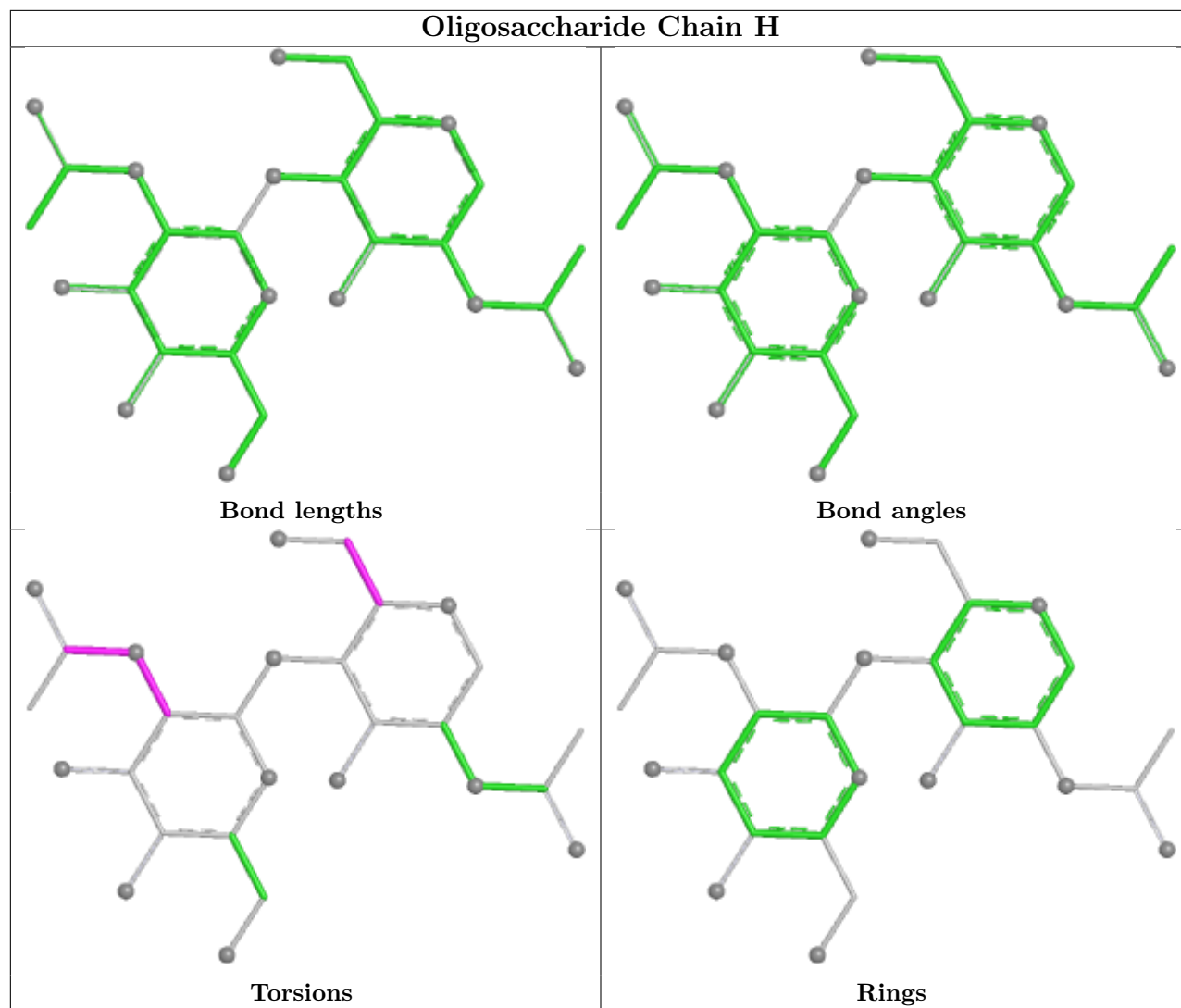
12 monomers are involved in 10 short contacts:

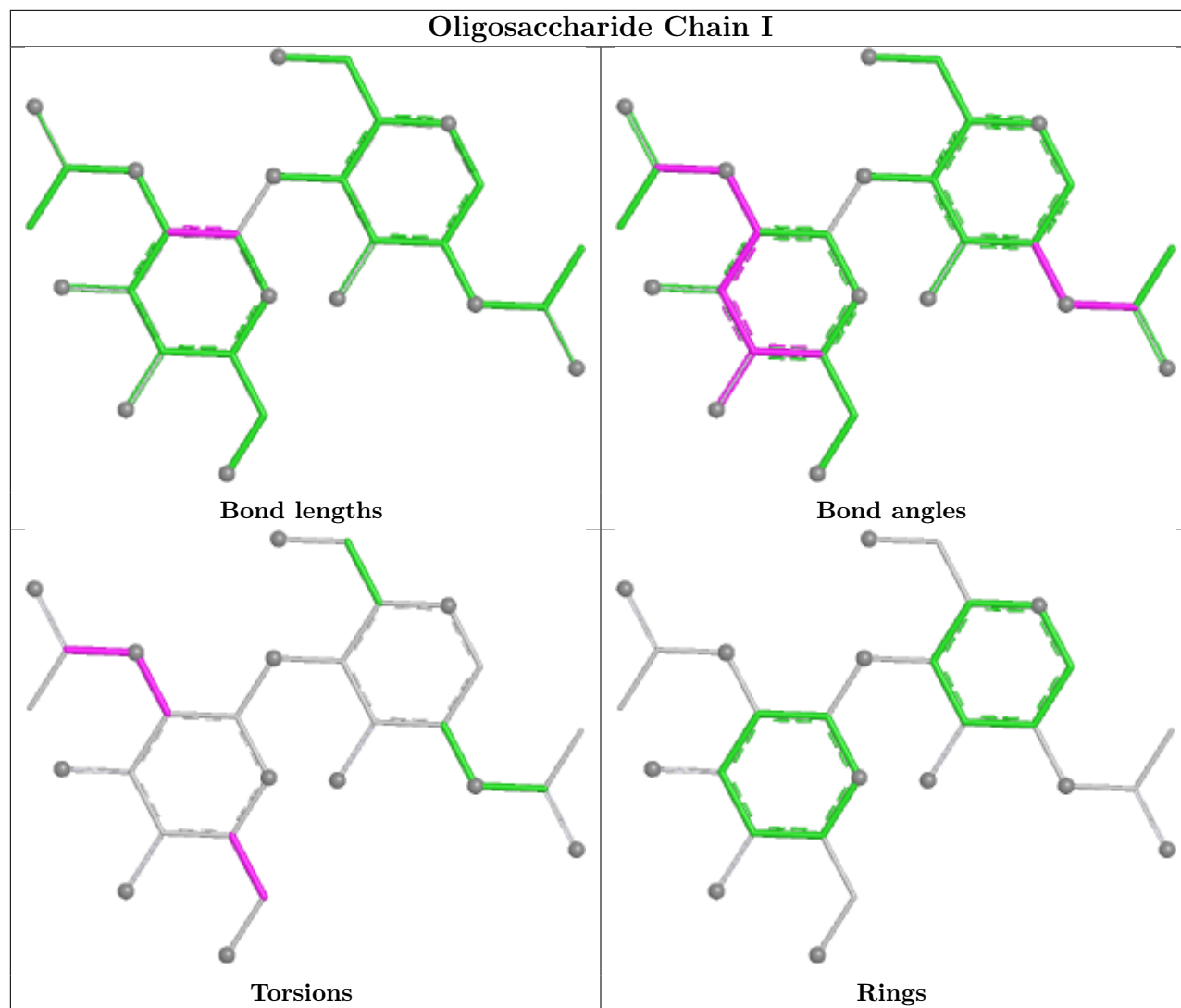
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	H	1	NAG	1	0
3	J	4	MAN	1	0
3	J	3	BMA	1	0
4	I	2	NAG	2	0
3	J	5	FUC	2	0
4	K	2	NAG	1	0
4	K	1	NAG	1	0
3	J	2	NAG	2	0
3	G	2	NAG	1	0
4	L	1	NAG	1	0
3	G	5	FUC	1	0

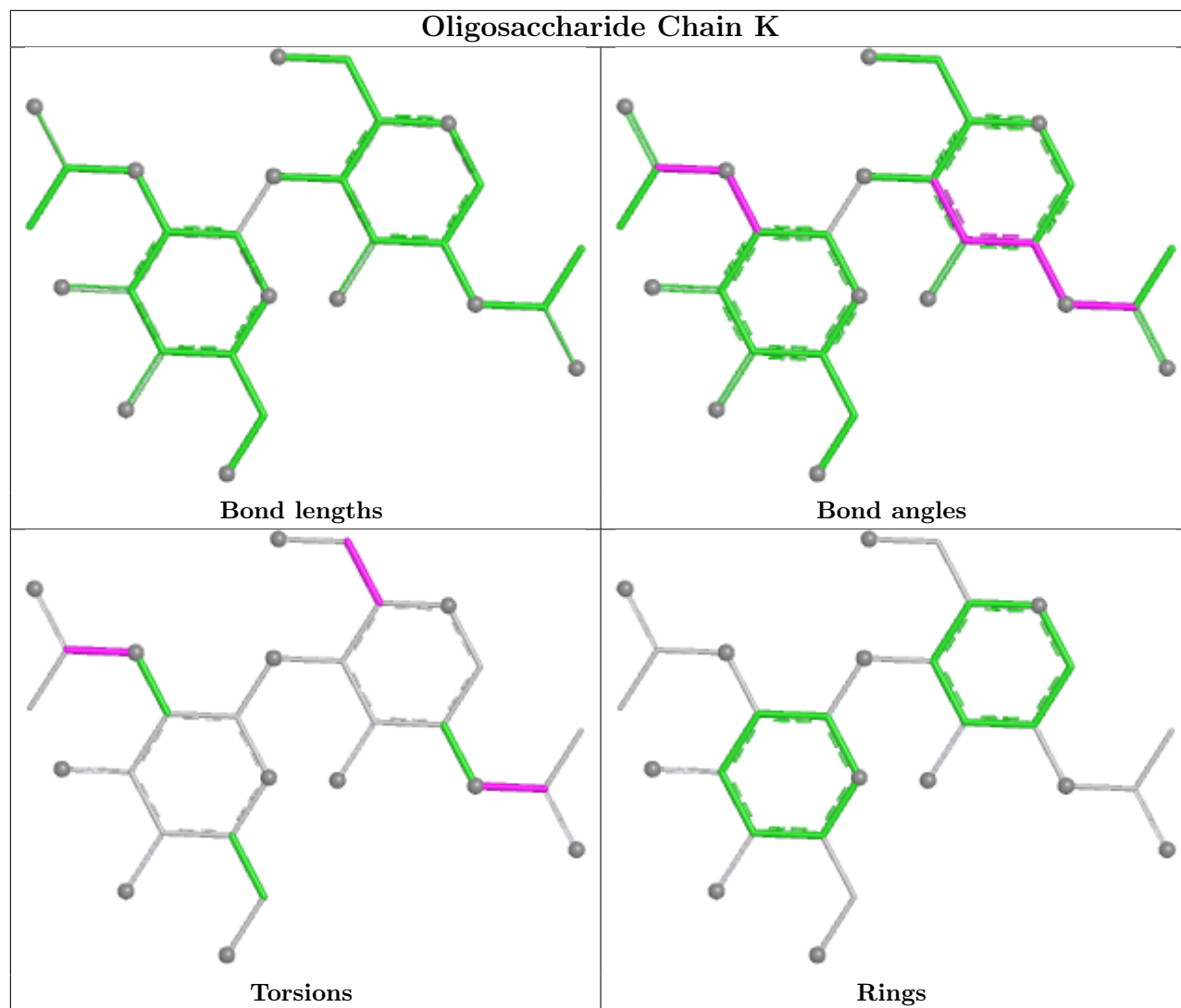
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

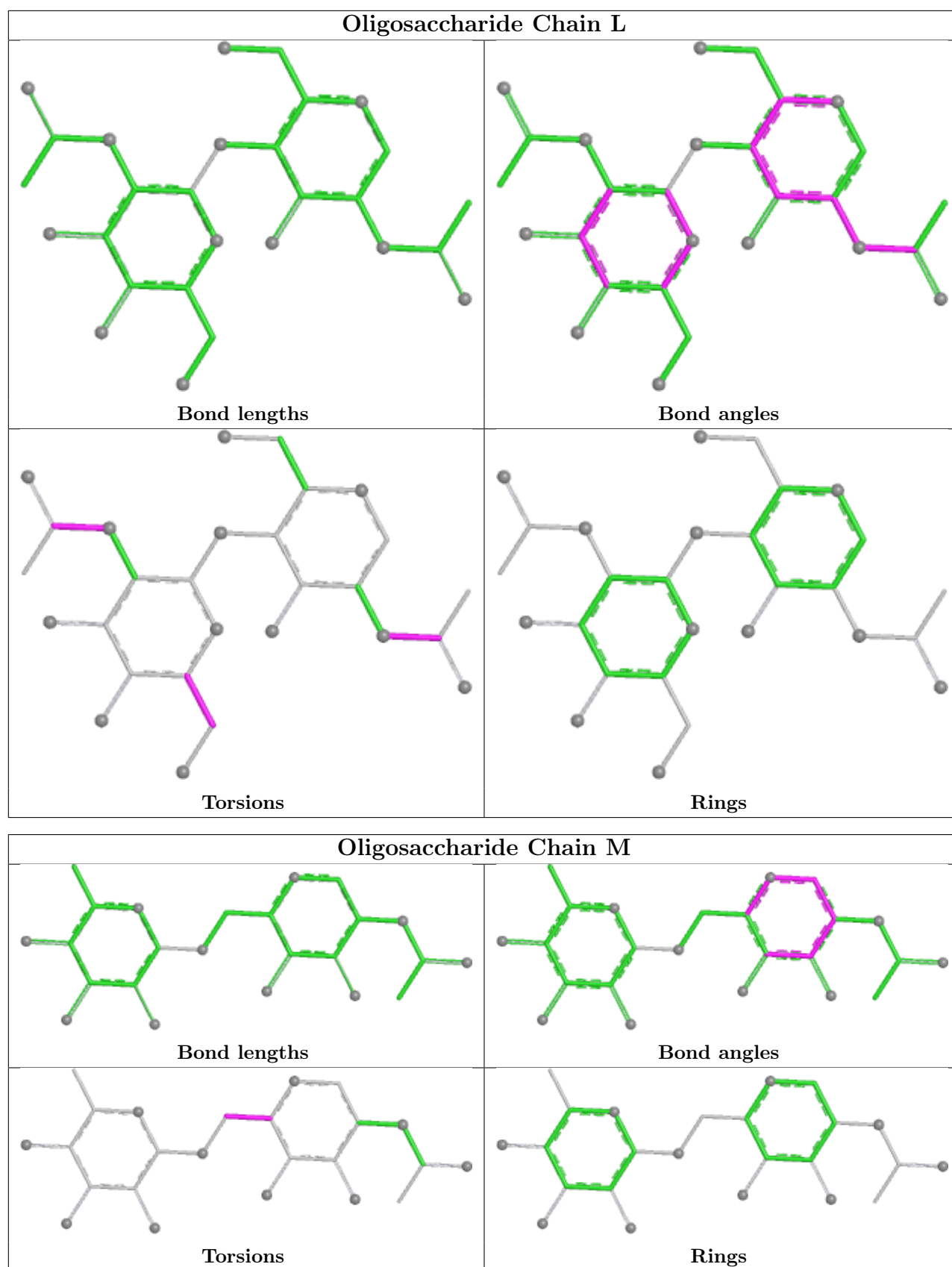












## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	03F	E	301	-	50,51,51	0.31	0	57,59,59	0.44	0
7	03F	C	302	-	50,51,51	0.30	0	57,59,59	0.30	0
6	NAG	C	301	1	14,14,15	0.80	1 (7%)	17,19,21	1.21	1 (5%)
6	NAG	A	301	1	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
6	NAG	B	101	2	14,14,15	0.42	0	17,19,21	0.84	1 (5%)
7	03F	A	302	-	50,51,51	0.32	0	57,59,59	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	03F	E	301	-	-	24/47/67/67	0/1/1/1
7	03F	C	302	-	-	19/47/67/67	0/1/1/1
6	NAG	C	301	1	-	3/6/23/26	0/1/1/1
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	101	2	-	2/6/23/26	0/1/1/1
7	03F	A	302	-	-	22/47/67/67	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	NAG	C1-C2	2.03	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	NAG	O5-C1-C2	-3.52	105.85	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	NAG	C1-O5-C5	-2.57	108.74	112.19
6	A	301	NAG	O5-C1-C2	-2.13	107.99	111.29

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

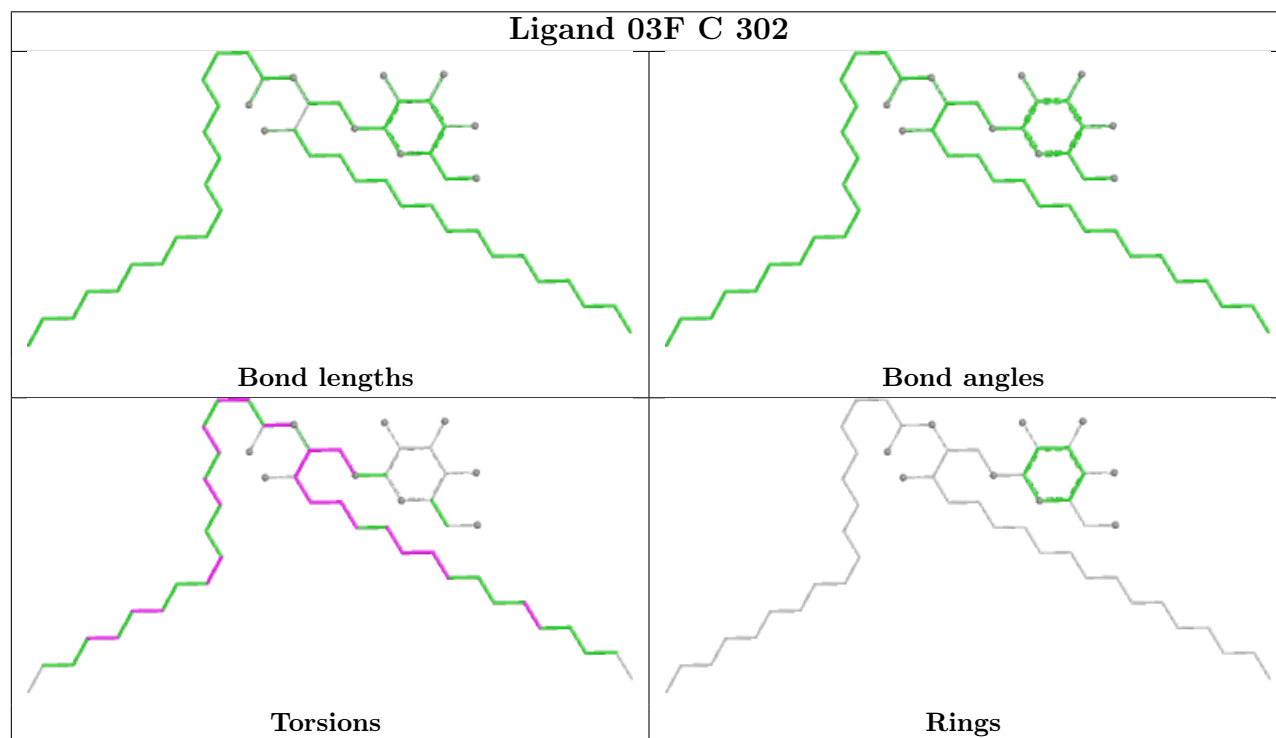
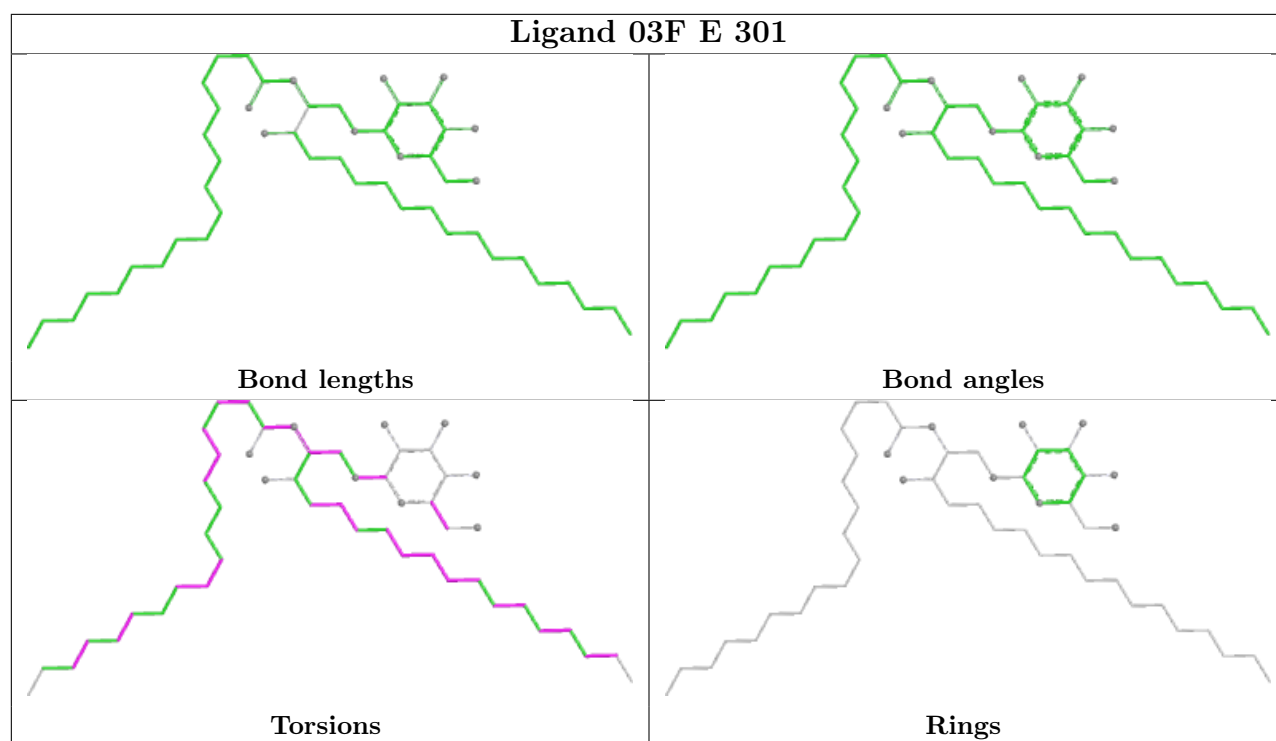
Mol	Chain	Res	Type	Atoms
6	B	101	NAG	C8-C7-N2-C2
6	B	101	NAG	O7-C7-N2-C2
7	A	302	03F	O1A-C1-C2-N2
7	A	302	03F	O1A-C1-C2-C3
7	A	302	03F	OAA-CAA-N2-C2

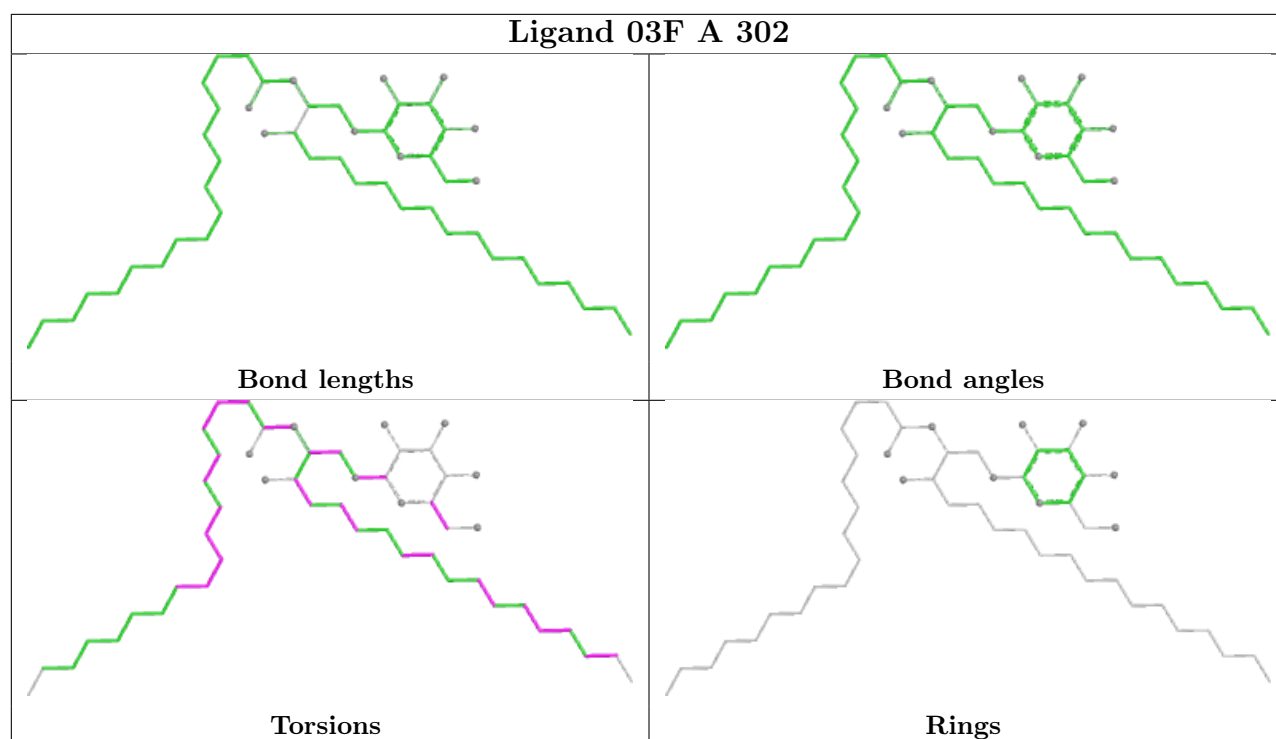
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	301	03F	3	1
7	C	302	03F	3	0
7	A	302	03F	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	268/268 (100%)	0.65	11 (4%) 41 36	36, 52, 88, 102	0
1	C	268/268 (100%)	0.69	11 (4%) 41 36	37, 54, 96, 117	0
1	E	267/268 (99%)	0.73	13 (4%) 35 30	30, 56, 94, 111	0
2	B	94/94 (100%)	0.35	3 (3%) 50 45	35, 53, 73, 85	0
2	D	94/94 (100%)	0.51	2 (2%) 63 60	38, 56, 81, 89	0
2	F	93/94 (98%)	0.53	3 (3%) 50 45	40, 54, 75, 91	0
All	All	1084/1086 (99%)	0.63	43 (3%) 42 37	30, 55, 89, 117	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	93	ALA	6.2
1	E	246	TYR	4.6
1	C	246	TYR	4.1
1	A	135	PHE	3.8
1	C	248	GLY	3.6

### 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](#)

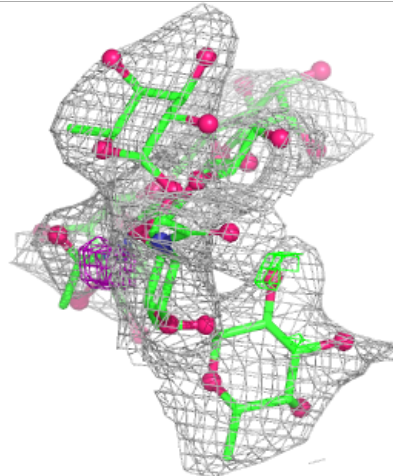
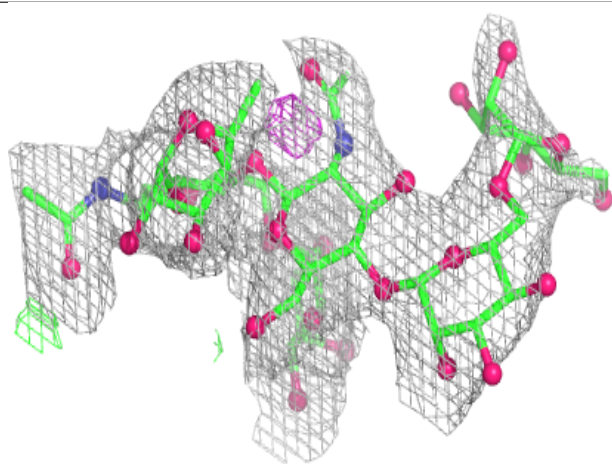
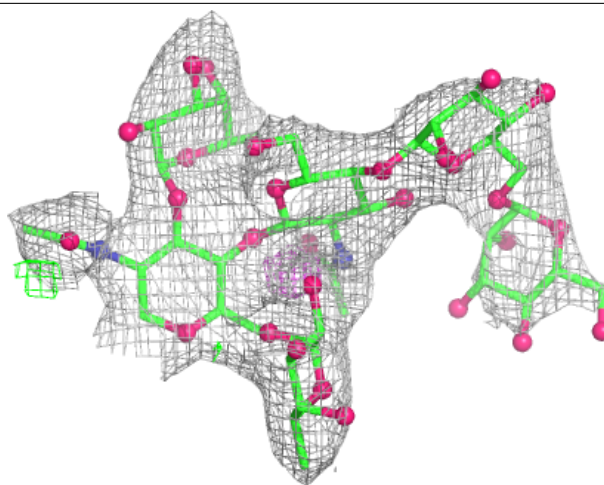
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	L	2	14/15	0.34	0.21	106,112,121,122	0
3	MAN	J	4	11/12	0.36	0.17	93,99,104,104	0
3	MAN	G	4	11/12	0.45	0.16	98,104,110,112	0
4	NAG	I	2	14/15	0.51	0.16	94,108,118,119	0
4	NAG	K	1	14/15	0.55	0.20	93,115,120,120	0
4	NAG	H	2	14/15	0.56	0.16	102,108,113,116	0
4	NAG	K	2	14/15	0.57	0.15	107,121,126,126	0
4	NAG	L	1	14/15	0.59	0.16	101,109,117,122	0
5	NAG	M	1	14/15	0.60	0.18	68,76,87,96	0
3	NAG	J	1	14/15	0.61	0.15	62,71,81,81	0
4	NAG	H	1	14/15	0.66	0.15	93,99,104,105	0
4	NAG	I	1	14/15	0.66	0.13	92,108,116,118	0
3	BMA	G	3	11/12	0.71	0.13	84,88,97,100	0
3	BMA	J	3	11/12	0.71	0.11	82,89,95,95	0
3	FUC	G	6	10/11	0.72	0.13	57,74,80,84	0
3	FUC	J	5	10/11	0.73	0.14	69,76,82,86	0
3	FUC	G	5	10/11	0.73	0.12	82,86,90,95	0
3	FUC	J	6	10/11	0.76	0.14	64,73,82,83	0
3	NAG	G	1	14/15	0.79	0.11	55,71,79,79	0
3	NAG	J	2	14/15	0.80	0.11	69,78,92,99	0
3	NAG	G	2	14/15	0.80	0.12	68,81,84,86	0
5	FUC	M	2	10/11	0.83	0.14	69,83,91,91	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.

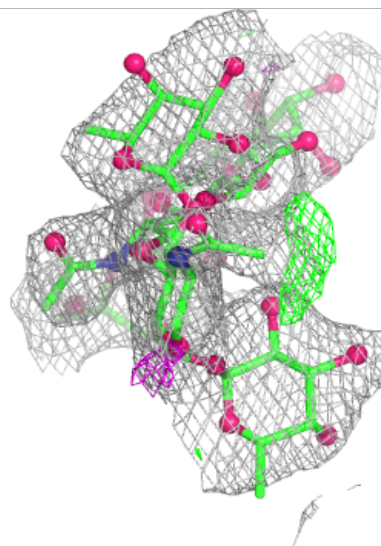
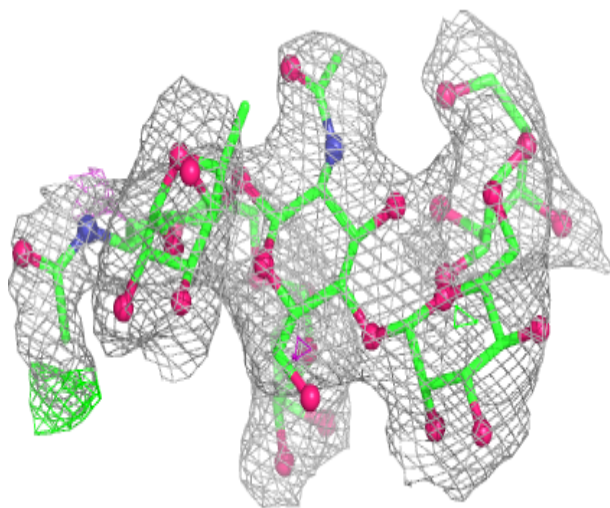
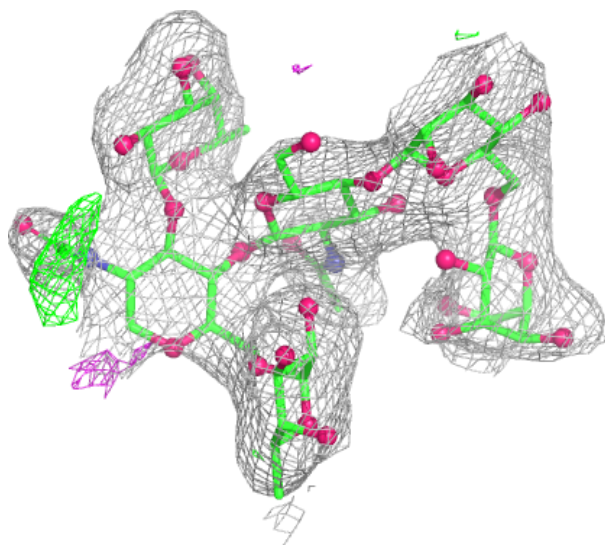
**Electron density around Chain G:**

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



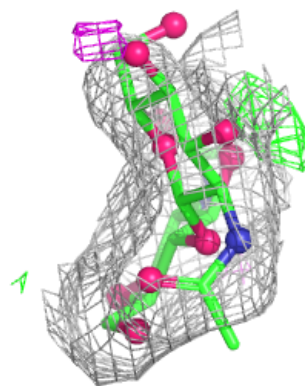
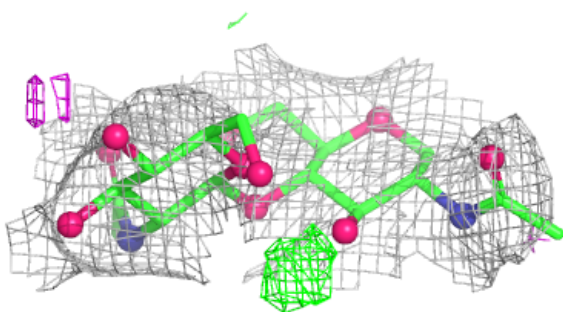
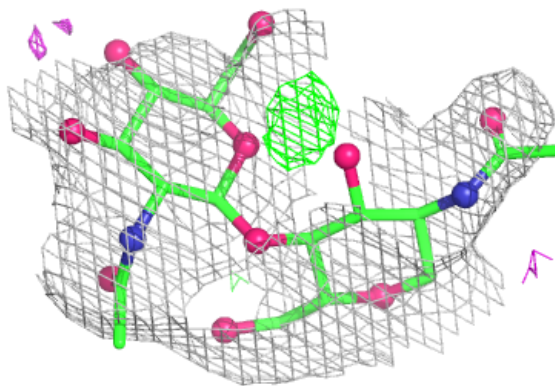
**Electron density around Chain J:**

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



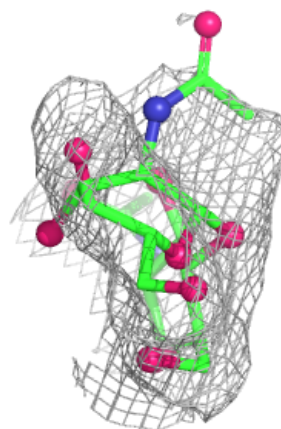
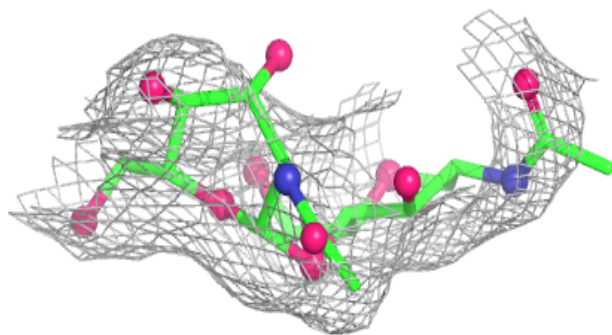
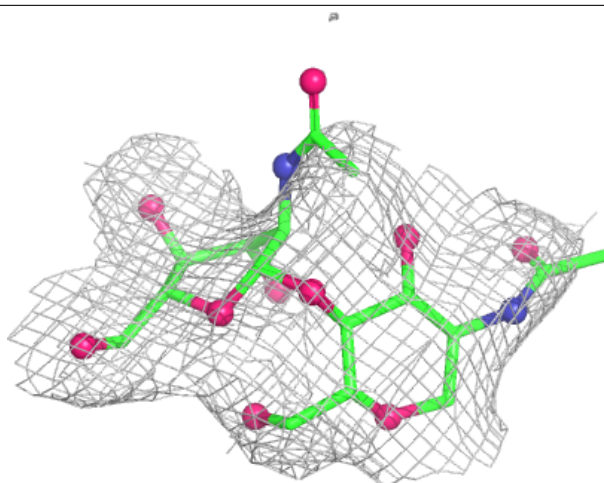
**Electron density around Chain H:**

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



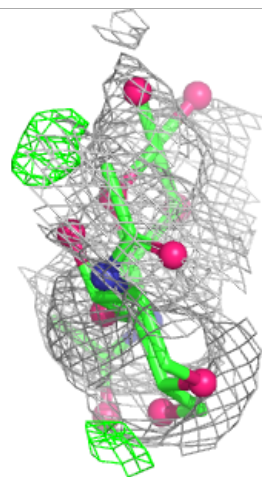
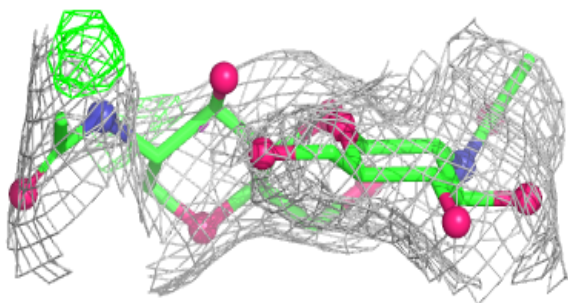
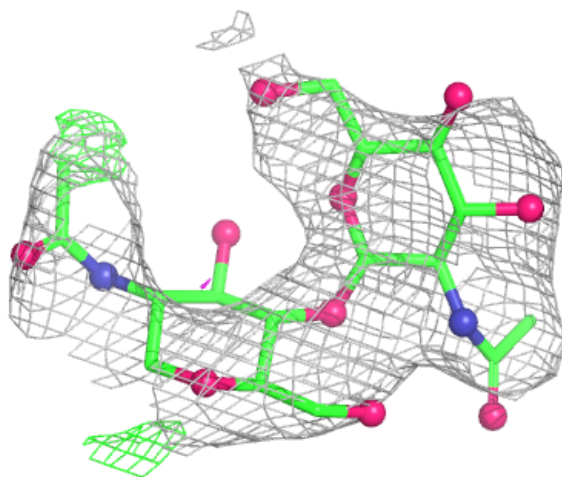
**Electron density around Chain I:**

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



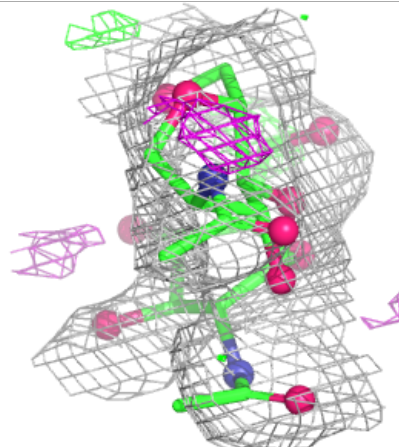
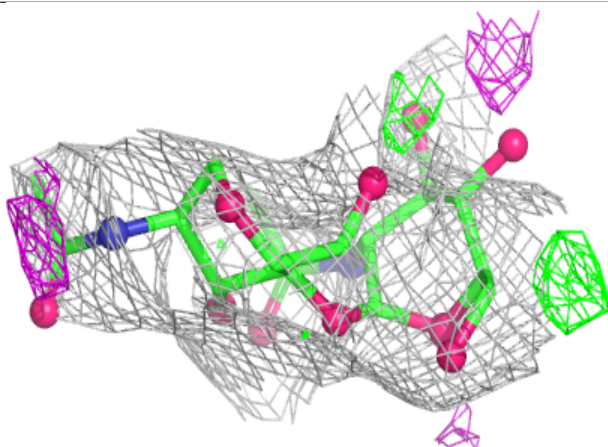
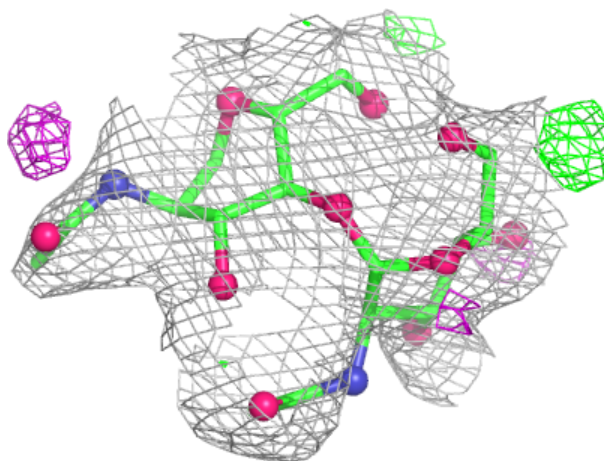
**Electron density around Chain K:**

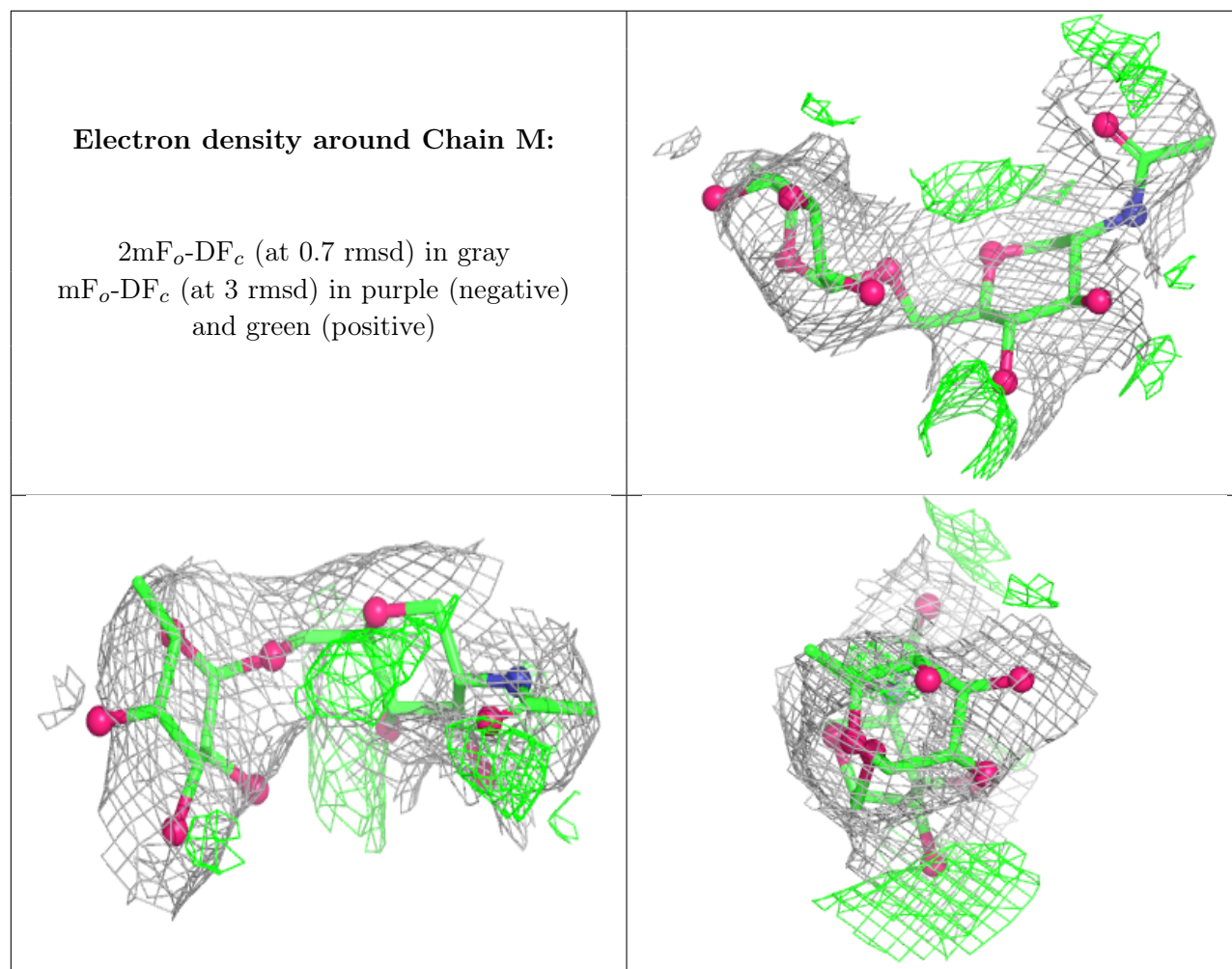
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

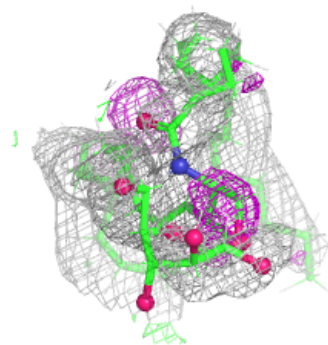
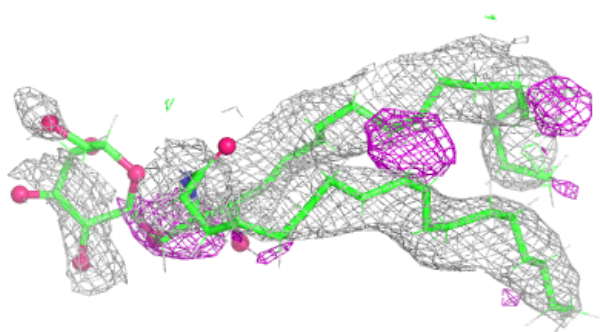
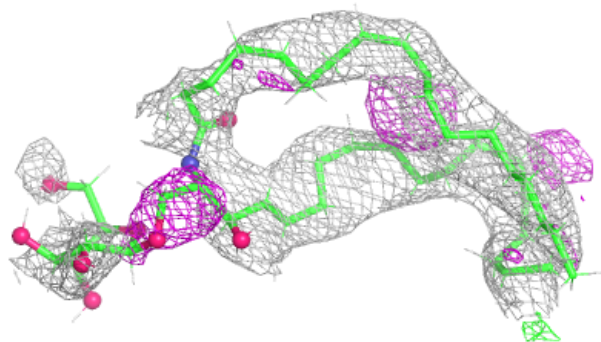
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	B	101	14/15	0.43	0.14	93,109,116,123	0
6	NAG	C	301	14/15	0.50	0.20	86,105,115,121	0
7	03F	A	302	51/51	0.63	0.18	51,77,162,191	0
7	03F	C	302	51/51	0.64	0.19	57,93,206,213	0
7	03F	E	301	51/51	0.70	0.20	43,90,151,169	0
6	NAG	A	301	14/15	0.71	0.14	85,96,106,109	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.

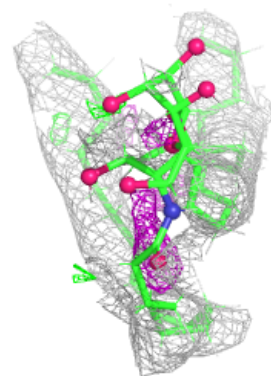
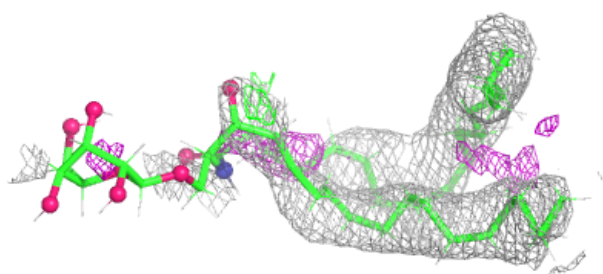
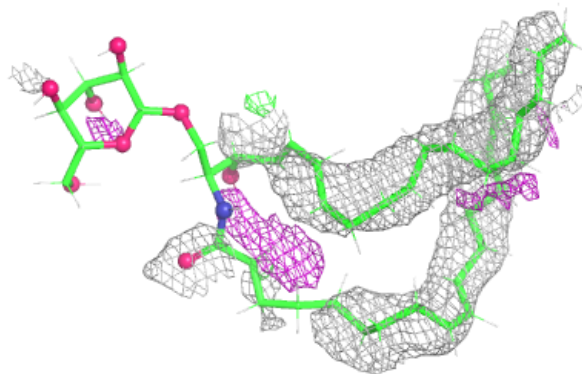
**Electron density around 03F A 302:**

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

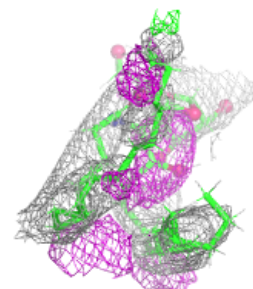
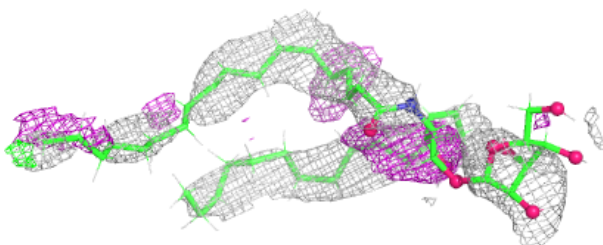
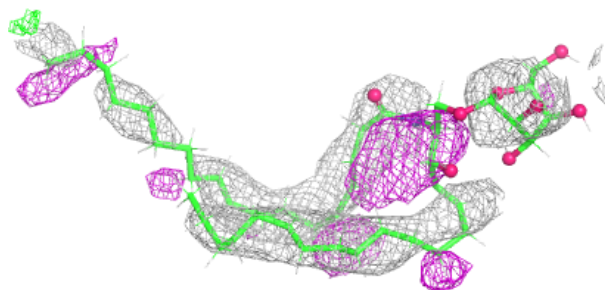


**Electron density around 03F C 302:**

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

**Electron density around 03F E 301:**

$2mF_o-DF_c$  (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.