



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 06:37 AM EDT

PDB ID : 5VTV  
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin G225M/L226T/S228A mutant in complex with 3'-SLN  
Authors : Wu, N.C.; Wilson, I.A.  
Deposited on : 2017-05-18  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

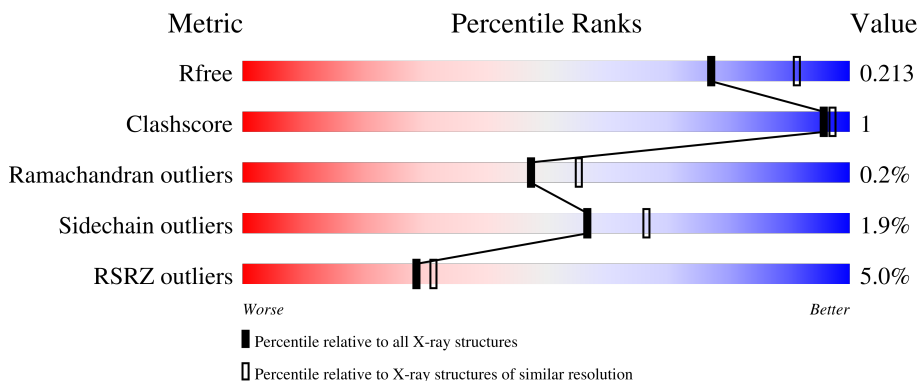
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	323	 7% 93% 6% ..
1	C	323	 2% 94% ..
1	E	323	 2% 94% ..
2	B	174	 13% 95% ..
2	D	174	 3% 95% ..

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Mol	Chain	Length	Quality of chain
2	F	174	 6% 95%
3	G	3	 33% 67%
3	H	3	 33% 67%
3	L	3	 67% 33%
4	I	2	 100%
4	K	2	 100%
4	M	2	 100%
4	P	2	 100%
5	J	2	 100%
5	N	2	 100%
5	Q	2	 50% 50%
6	O	4	 100%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12396 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2481	1553	438	476	14	0	0	0
1	C	317	2445	1532	429	470	14	0	0	0
1	E	317	2445	1532	429	470	14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q91MA7
A	8	ASP	-	expression tag	UNP Q91MA7
A	9	PRO	-	expression tag	UNP Q91MA7
A	10	GLY	-	expression tag	UNP Q91MA7
A	225	MET	GLY	engineered mutation	UNP Q91MA7
A	226	THR	LEU	engineered mutation	UNP Q91MA7
A	228	ALA	SER	engineered mutation	UNP Q91MA7
C	7	ALA	-	expression tag	UNP Q91MA7
C	8	ASP	-	expression tag	UNP Q91MA7
C	9	PRO	-	expression tag	UNP Q91MA7
C	10	GLY	-	expression tag	UNP Q91MA7
C	225	MET	GLY	engineered mutation	UNP Q91MA7
C	226	THR	LEU	engineered mutation	UNP Q91MA7
C	228	ALA	SER	engineered mutation	UNP Q91MA7
E	7	ALA	-	expression tag	UNP Q91MA7
E	8	ASP	-	expression tag	UNP Q91MA7
E	9	PRO	-	expression tag	UNP Q91MA7
E	10	GLY	-	expression tag	UNP Q91MA7
E	225	MET	GLY	engineered mutation	UNP Q91MA7
E	226	THR	LEU	engineered mutation	UNP Q91MA7
E	228	ALA	SER	engineered mutation	UNP Q91MA7

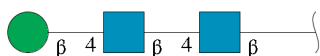
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1391	863	243	279	6	0	0	0
2	D	171	1382	858	241	277	6	0	0	0
2	F	171	1382	858	241	277	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	conflict	UNP Q91MA7
D	123	GLY	ARG	conflict	UNP Q91MA7
F	123	GLY	ARG	conflict	UNP Q91MA7

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0
3	L	3	39	22	2	15	0	0	0

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



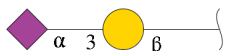
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0

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

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	2	Total	C	N	O	0	0	0
			32	17	1	14			
5	N	2	Total	C	N	O	0	0	0
			32	17	1	14			
5	Q	2	Total	C	N	O	0	0	0
			32	17	1	14			

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



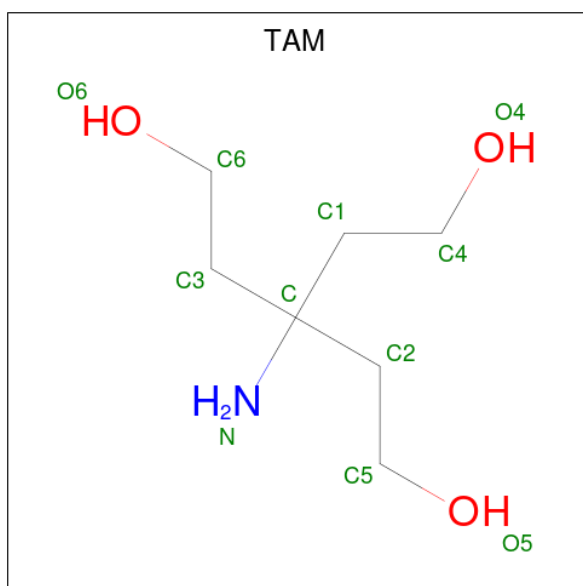
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula:  $C_7H_{17}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 9 is water.

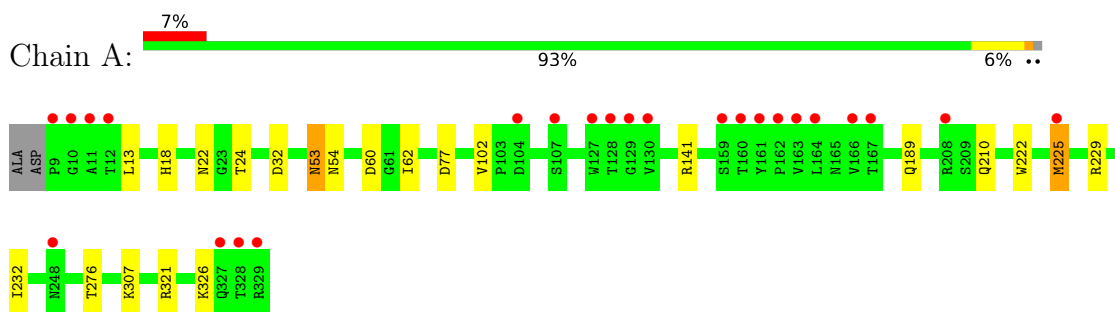
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	79	Total	O	0	0
			79	79		
9	B	54	Total	O	0	0
			54	54		
9	C	81	Total	O	0	0
			81	81		
9	D	49	Total	O	0	0
			49	49		
9	E	123	Total	O	0	0
			123	123		
9	F	56	Total	O	0	0
			56	56		



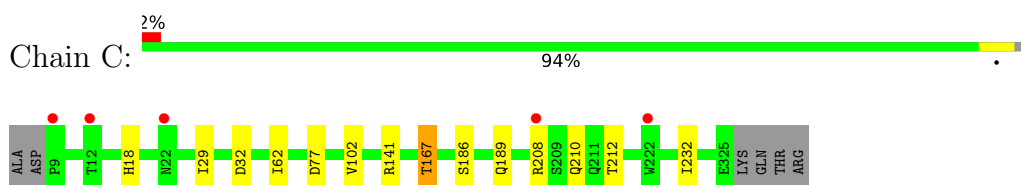
### 3 Residue-property plots

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

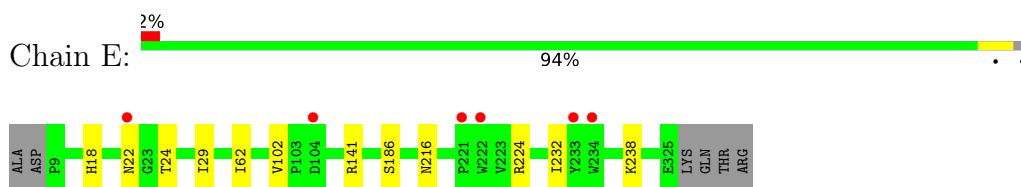
- Molecule 1: Hemagglutinin HA1 chain



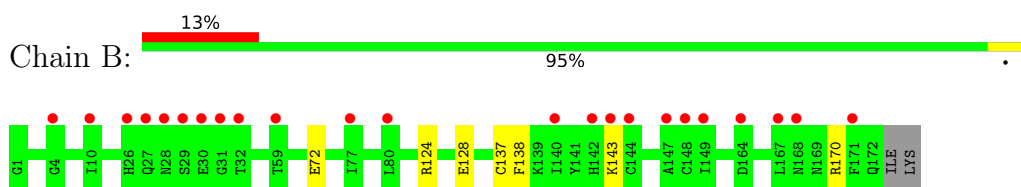
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

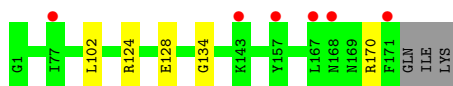


- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain





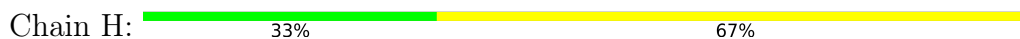
- Molecule 2: Hemagglutinin HA2 chain



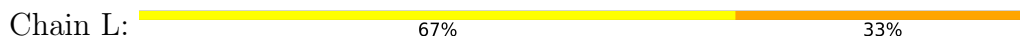
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



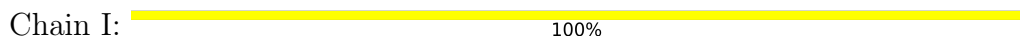
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



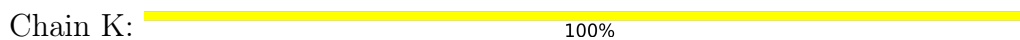
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




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



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 M:  100%

MAG1  
MAG2

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

Chain P:  100%


MAG1  
MAG2

- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain J:  100%

GAL1  
SIA2

- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain N:  100%

GAL1  
SIA2

- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain Q:  50% 50%

GAL1  
SIA2

- Molecule 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 O:  100%

MAG1  
MAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.65Å 131.35Å 72.78Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.60 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.25) 98.2 (49.60-2.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.183 , 0.212 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	4787 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: NAG, BMA, SIA, MAN, TAM, GAL

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	0.53	0/2538	0.77	5/3457 (0.1%)
1	C	0.51	0/2502	0.72	0/3410
1	E	0.55	0/2502	0.76	2/3410 (0.1%)
2	B	0.48	0/1415	0.68	0/1902
2	D	0.49	0/1406	0.68	0/1890
2	F	0.51	0/1406	0.69	0/1890
All	All	0.52	0/11769	0.73	7/15959 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	E	141	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	32	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	321	ARG	CG-CD-NE	-5.49	100.28	111.80
1	E	224	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	229	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	32	ASP	CB-CG-OD1	5.10	122.89	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	2481	0	2433	7	0
1	C	2445	0	2392	7	0
1	E	2445	0	2393	6	0
2	B	1391	0	1307	6	0
2	D	1382	0	1299	4	0
2	F	1382	0	1299	3	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0
3	L	39	0	34	1	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
5	J	32	0	28	0	0
5	N	32	0	28	0	0
5	Q	32	0	28	0	0
6	O	50	0	43	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	E	14	0	13	0	0
8	E	11	0	17	0	0
9	A	79	0	0	1	0
9	B	54	0	0	4	0
9	C	81	0	0	0	0
9	D	49	0	0	0	0
9	E	123	0	0	0	0
9	F	56	0	0	0	0
All	All	12396	0	11508	25	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.

All (25) 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:THR:HG21	1:E:216:ASN:HB3	1.58	0.85
2:B:72:GLU:OE2	1:E:238:LYS:NZ	2.22	0.70
1:C:212:THR:CG2	1:E:216:ASN:HB3	2.26	0.65
1:A:222:TRP:CZ2	1:A:225:MET:HA	2.38	0.58
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.85	0.58
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.36	0.58
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:CB	1:E:216:ASN:HB3	2.36	0.54
1:A:13:LEU:N	9:B:201:HOH:O	2.41	0.54
1:A:53:ASN:HD22	1:A:54:ASN:N	2.07	0.53
1:A:53:ASN:HD22	1:A:53:ASN:C	2.15	0.50
1:A:60:ASP:OD2	9:A:501:HOH:O	2.20	0.50
1:C:167:THR:OG1	3:L:1:NAG:H62	2.15	0.47
2:B:138:PHE:O	9:B:201:HOH:O	2.20	0.46
2:B:137:CYS:HB3	9:B:201:HOH:O	2.14	0.45
2:B:124:ARG:HD3	2:D:134:GLY:HA2	1.99	0.45
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.99	0.44
2:B:128:GLU:O	2:B:170:ARG:NH1	2.49	0.44
1:E:29:ILE:HD11	2:F:102:LEU:HD23	2.00	0.43
2:D:128:GLU:O	2:D:170:ARG:NH1	2.49	0.42
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.01	0.42
1:E:102:VAL:HG22	1:E:232:ILE:HB	2.01	0.42
2:F:128:GLU:O	2:F:170:ARG:NH1	2.49	0.42
2:B:138:PHE:N	9:B:201:HOH:O	2.51	0.41
2:D:124:ARG:HD3	2:F:134:GLY:HA2	2.02	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/323 (99%)	311 (98%)	7 (2%)	1 (0%)	41	46
1	C	315/323 (98%)	308 (98%)	6 (2%)	1 (0%)	41	46
1	E	315/323 (98%)	308 (98%)	6 (2%)	1 (0%)	41	46
2	B	170/174 (98%)	162 (95%)	8 (5%)	0	100	100
2	D	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
2	F	169/174 (97%)	161 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1457/1491 (98%)	1411 (97%)	43 (3%)	3 (0%)	47 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE

### 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	282/283 (100%)	272 (96%)	10 (4%)	36 43
1	C	278/283 (98%)	271 (98%)	7 (2%)	47 56
1	E	278/283 (98%)	274 (99%)	4 (1%)	67 76
2	B	146/148 (99%)	145 (99%)	1 (1%)	84 90
2	D	145/148 (98%)	145 (100%)	0	100 100
2	F	145/148 (98%)	143 (99%)	2 (1%)	67 76
All	All	1274/1293 (98%)	1250 (98%)	24 (2%)	57 66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	22	ASN
1	A	24	THR
1	A	53	ASN
1	A	189	GLN
1	A	210	GLN
1	A	225	MET
1	A	276	THR
1	A	307	LYS

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Mol	Chain	Res	Type
1	A	326	LYS
2	B	143	LYS
1	C	18	HIS
1	C	32	ASP
1	C	167	THR
1	C	186	SER
1	C	189	GLN
1	C	208	ARG
1	C	210	GLN
1	E	18	HIS
1	E	22	ASN
1	E	24	THR
1	E	186	SER
2	F	38	LEU
2	F	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	53	ASN
2	B	125	GLN
2	D	53	ASN
2	D	125	GLN
1	E	22	ASN
2	F	53	ASN
2	F	125	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

27 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	0.42	0	17,19,21	0.98	1 (5%)
3	NAG	G	2	3	14,14,15	0.48	0	17,19,21	0.79	0
3	BMA	G	3	3	11,11,12	0.50	0	15,15,17	1.12	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.52	0	17,19,21	1.09	2 (11%)
3	NAG	H	2	3	14,14,15	0.43	0	17,19,21	0.80	0
3	BMA	H	3	3	11,11,12	0.55	0	15,15,17	1.74	4 (26%)
4	NAG	I	1	4,1	14,14,15	0.56	0	17,19,21	1.35	3 (17%)
4	NAG	I	2	4	14,14,15	0.63	0	17,19,21	1.66	4 (23%)
5	GAL	J	1	5	12,12,12	0.87	0	17,17,17	1.27	3 (17%)
5	SIA	J	2	5	20,20,21	0.79	0	24,28,31	1.17	2 (8%)
4	NAG	K	1	4,1	14,14,15	0.59	0	17,19,21	2.07	2 (11%)
4	NAG	K	2	4	14,14,15	0.48	0	17,19,21	0.96	2 (11%)
3	NAG	L	1	1,3	14,14,15	0.34	0	17,19,21	1.52	1 (5%)
3	NAG	L	2	3	14,14,15	0.46	0	17,19,21	1.18	2 (11%)
3	BMA	L	3	3	11,11,12	0.98	1 (9%)	15,15,17	2.02	3 (20%)
4	NAG	M	1	4,1	14,14,15	0.39	0	17,19,21	1.22	1 (5%)
4	NAG	M	2	4	14,14,15	0.63	0	17,19,21	2.14	2 (11%)
5	GAL	N	1	5	12,12,12	0.69	0	17,17,17	1.38	3 (17%)
5	SIA	N	2	5	20,20,21	0.75	0	24,28,31	1.15	2 (8%)
6	NAG	O	1	1,6	14,14,15	0.31	0	17,19,21	1.22	1 (5%)
6	NAG	O	2	6	14,14,15	0.41	0	17,19,21	1.26	3 (17%)
6	BMA	O	3	6	11,11,12	0.56	0	15,15,17	1.34	2 (13%)
6	MAN	O	4	6	11,11,12	0.59	0	15,15,17	1.59	4 (26%)
4	NAG	P	1	4,1	14,14,15	0.45	0	17,19,21	1.25	1 (5%)
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
5	GAL	Q	1	5	12,12,12	0.48	0	17,17,17	0.76	0
5	SIA	Q	2	5	20,20,21	0.70	0	24,28,31	1.27	3 (12%)

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	-	2/6/23/26	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
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	GAL	J	1	5	-	0/2/22/22	0/1/1/1
5	SIA	J	2	5	-	0/18/34/38	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
5	GAL	N	1	5	-	0/2/22/22	0/1/1/1
5	SIA	N	2	5	-	0/18/34/38	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
5	GAL	Q	1	5	-	0/2/22/22	0/1/1/1
5	SIA	Q	2	5	-	0/18/34/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	3	BMA	C2-C3	2.06	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	2	NAG	C1-O5-C5	7.69	122.61	112.19
4	K	1	NAG	C1-O5-C5	6.83	121.45	112.19
3	L	3	BMA	C1-C2-C3	5.05	115.87	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C1-O5-C5	5.02	118.99	112.19
3	H	3	BMA	C1-C2-C3	4.54	115.25	109.67
5	N	2	SIA	C6-O6-C2	3.89	119.65	111.34
5	Q	2	SIA	C6-O6-C2	3.75	119.36	111.34
6	O	3	BMA	C1-O5-C5	3.75	117.27	112.19
4	I	2	NAG	C4-C3-C2	3.69	116.42	111.02
4	M	1	NAG	C1-C2-N2	3.62	116.68	110.49
3	L	3	BMA	C2-C3-C4	3.54	117.02	110.89
6	O	4	MAN	C3-C4-C5	3.31	116.14	110.24
3	L	3	BMA	C3-C4-C5	3.24	116.01	110.24
5	J	2	SIA	C6-O6-C2	3.18	118.14	111.34
6	O	4	MAN	C2-C3-C4	2.95	116.00	110.89
6	O	2	NAG	C1-O5-C5	2.91	116.14	112.19
4	I	2	NAG	C1-C2-N2	-2.84	105.64	110.49
5	J	1	GAL	C3-C4-C5	2.78	115.20	110.24
6	O	1	NAG	C1-O5-C5	2.78	115.96	112.19
5	N	1	GAL	C4-C3-C2	-2.77	105.98	110.82
4	I	2	NAG	O5-C5-C4	-2.75	104.12	110.83
5	N	1	GAL	O5-C5-C4	2.75	114.68	109.69
3	H	3	BMA	C1-O5-C5	2.74	115.91	112.19
4	K	2	NAG	O5-C5-C6	2.71	111.45	107.20
6	O	2	NAG	C1-C2-N2	2.68	115.06	110.49
3	H	1	NAG	C1-O5-C5	2.67	115.81	112.19
3	H	3	BMA	O5-C1-C2	2.66	114.88	110.77
4	P	1	NAG	C1-C2-N2	2.63	114.98	110.49
5	J	1	GAL	O5-C5-C4	2.63	114.47	109.69
4	I	1	NAG	C6-C5-C4	2.62	119.14	113.00
4	P	2	NAG	C1-O5-C5	2.56	115.66	112.19
6	O	4	MAN	C1-O5-C5	2.55	115.65	112.19
6	O	2	NAG	O3-C3-C2	-2.54	104.22	109.47
5	J	1	GAL	O5-C1-C2	-2.51	105.80	110.28
6	O	3	BMA	C3-C4-C5	2.49	114.67	110.24
4	K	1	NAG	C3-C4-C5	2.47	114.64	110.24
3	H	3	BMA	O5-C5-C6	2.34	110.88	107.20
5	J	2	SIA	O1B-C1-C2	2.32	119.65	113.03
5	N	2	SIA	O1B-C1-C2	2.30	119.58	113.03
3	H	1	NAG	O5-C1-C2	-2.27	107.70	111.29
5	Q	2	SIA	O1B-C1-C2	2.25	119.44	113.03
3	L	2	NAG	O3-C3-C2	-2.23	104.85	109.47
3	G	1	NAG	C1-C2-N2	-2.18	106.76	110.49
4	M	2	NAG	O5-C5-C4	2.15	116.06	110.83
4	I	1	NAG	O5-C5-C6	-2.14	103.84	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	GAL	O3-C3-C2	2.13	115.27	110.35
4	I	1	NAG	O4-C4-C5	2.12	114.56	109.30
4	K	2	NAG	O5-C1-C2	-2.07	108.02	111.29
3	G	3	BMA	O5-C5-C6	2.03	110.39	107.20
6	O	4	MAN	O5-C1-C2	-2.03	107.64	110.77
4	I	2	NAG	O5-C5-C6	2.02	110.38	107.20
3	L	2	NAG	C1-C2-N2	2.02	113.94	110.49
5	Q	2	SIA	C3-C4-C5	-2.00	109.04	111.46

There are no chirality outliers.

All (13) torsion outliers are listed below:

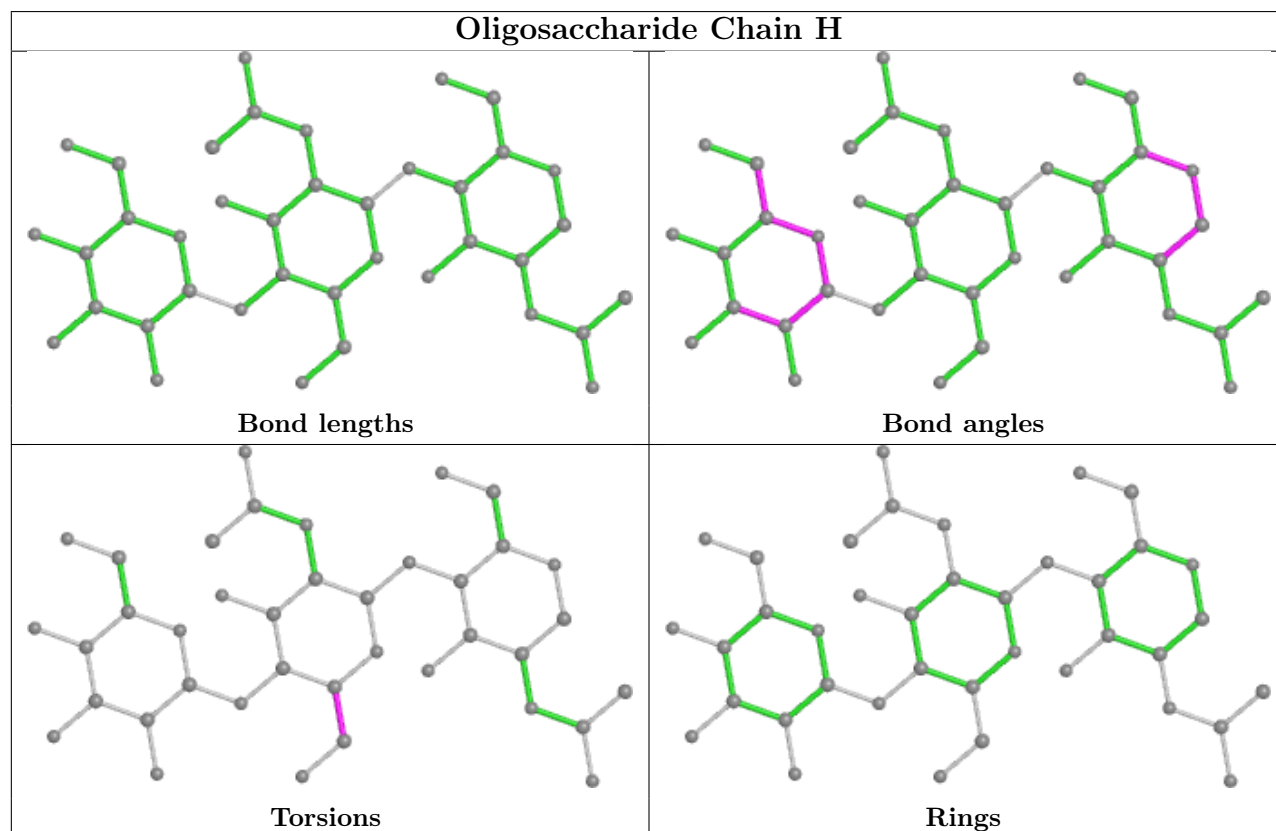
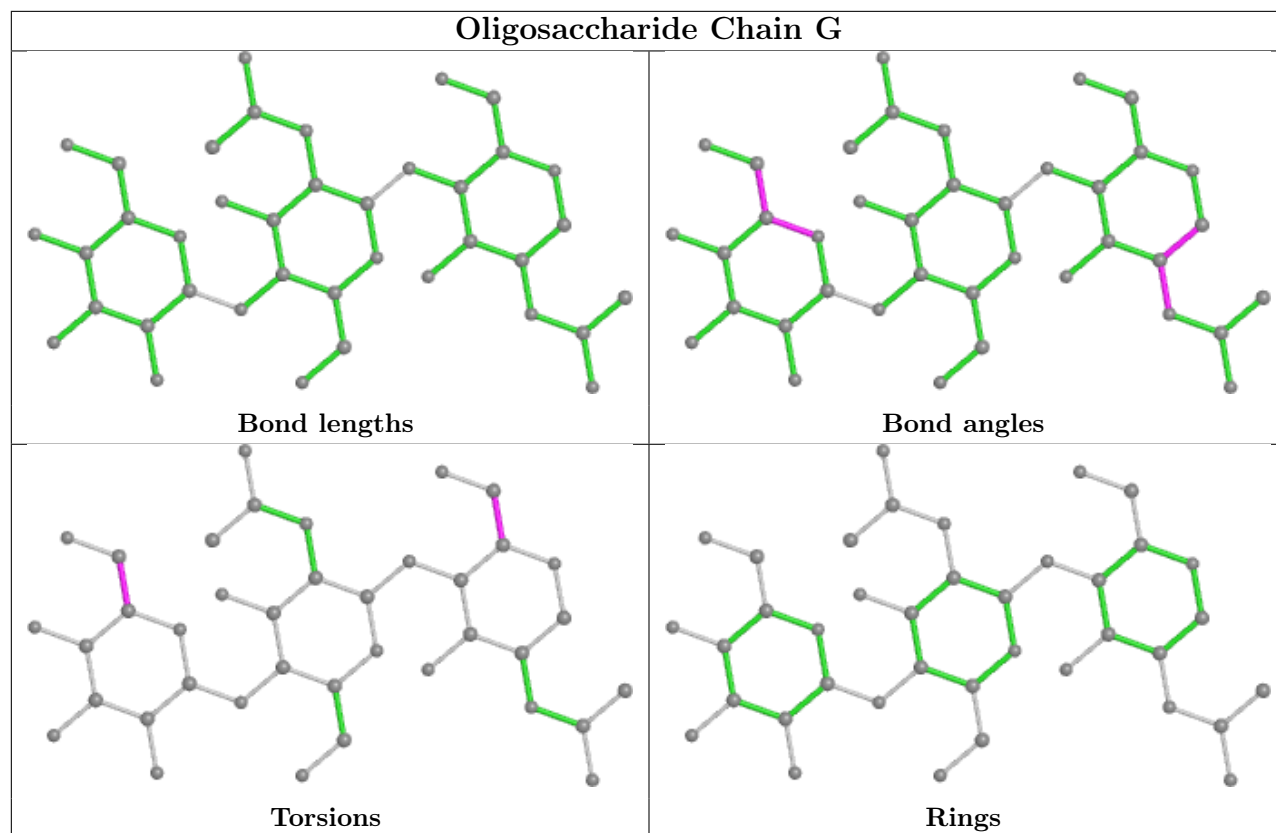
Mol	Chain	Res	Type	Atoms
3	L	3	BMA	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

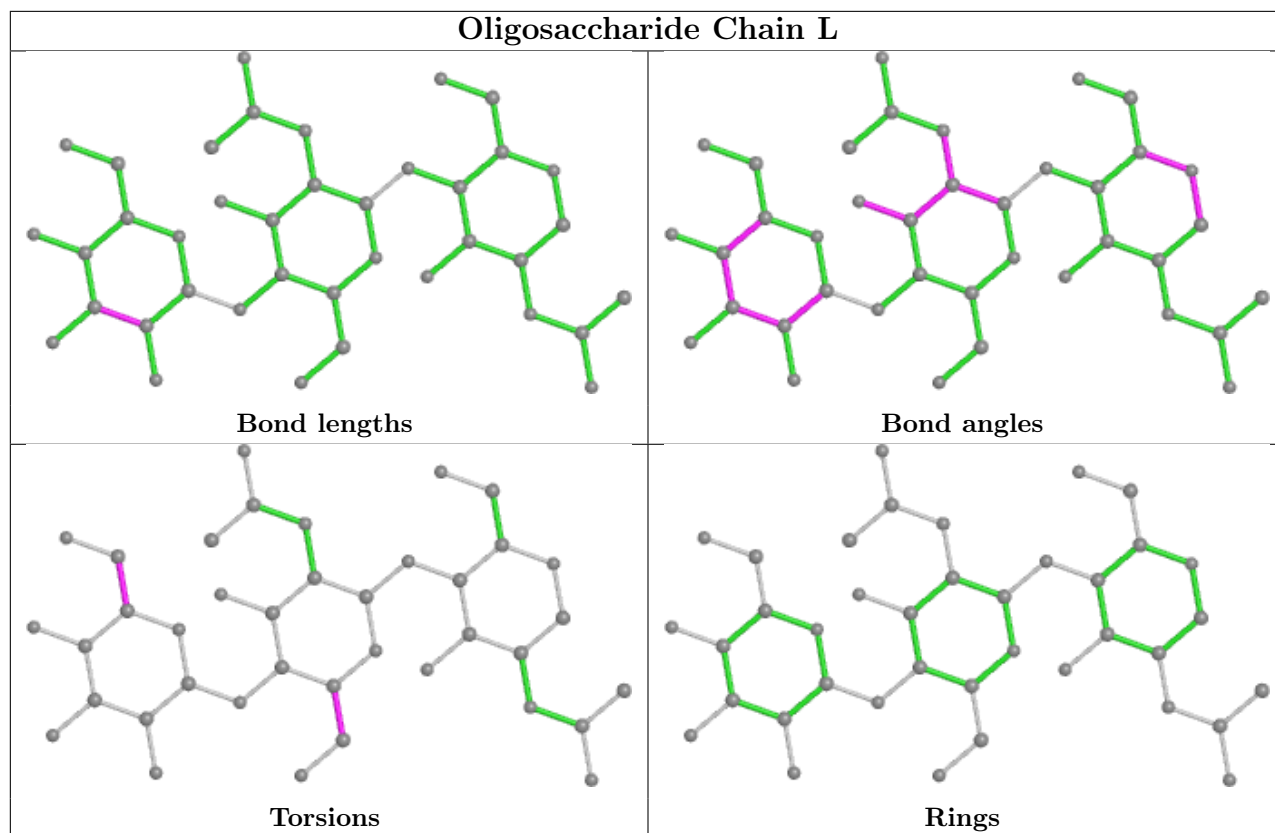
There are no ring outliers.

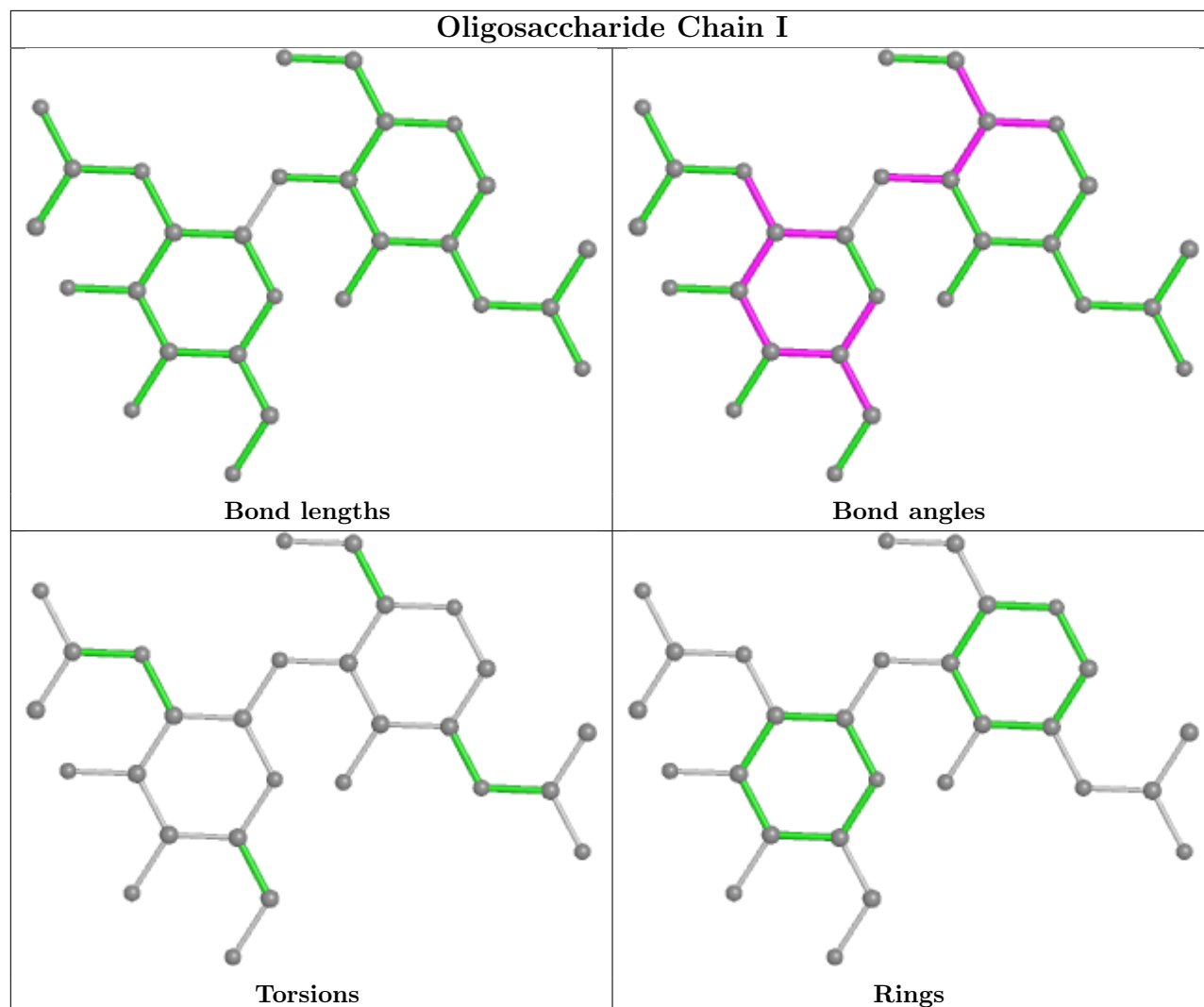
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0

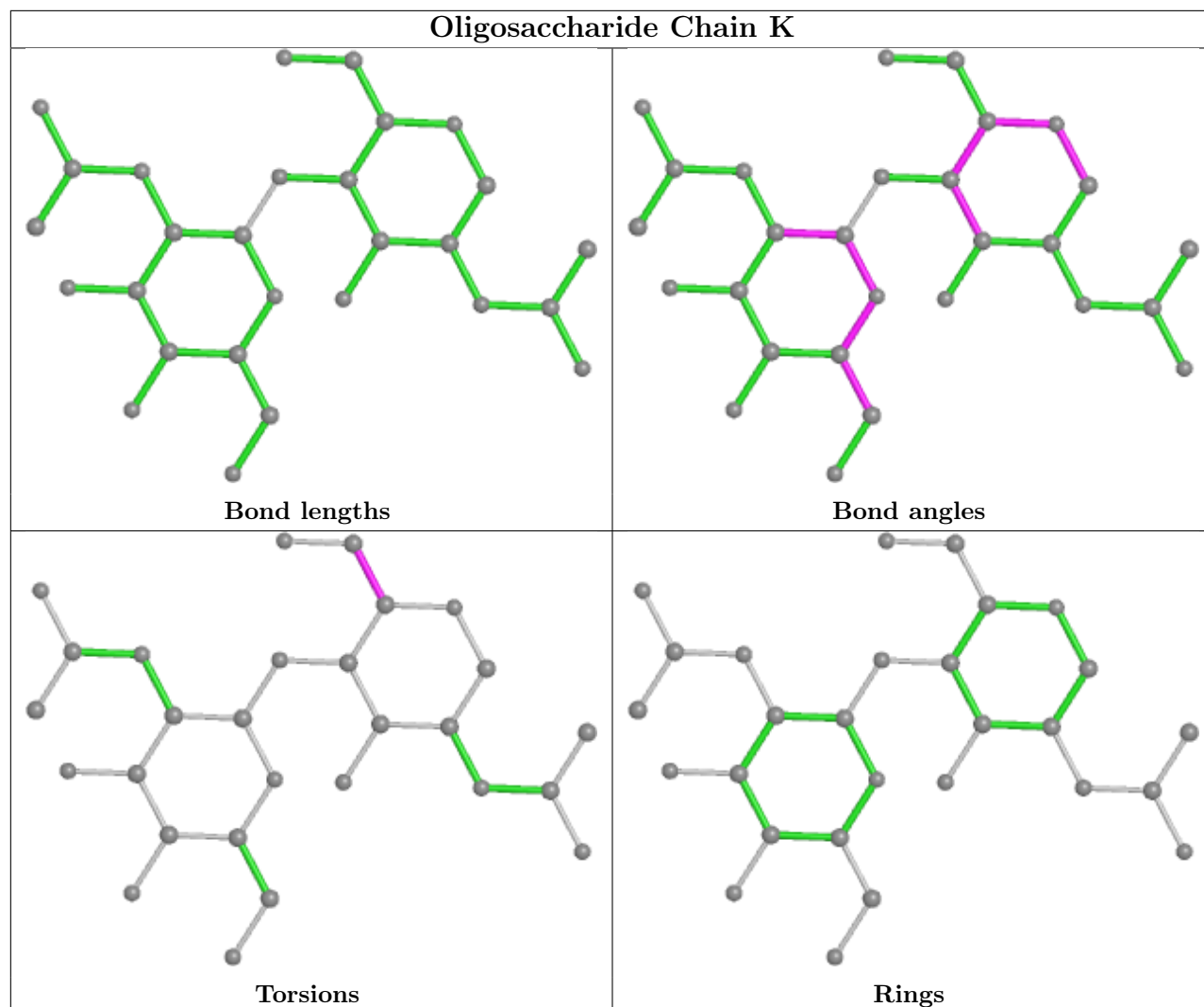
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

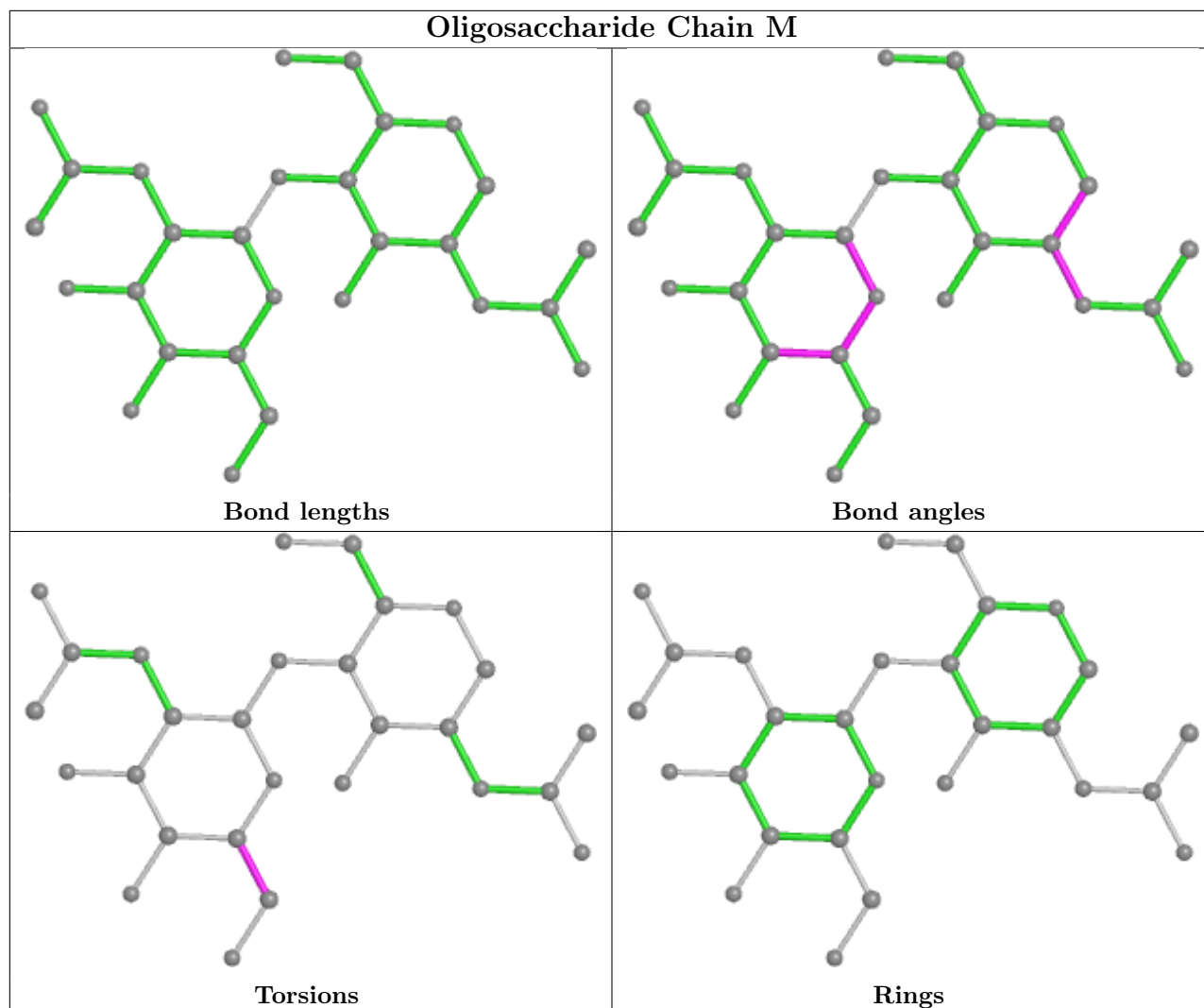


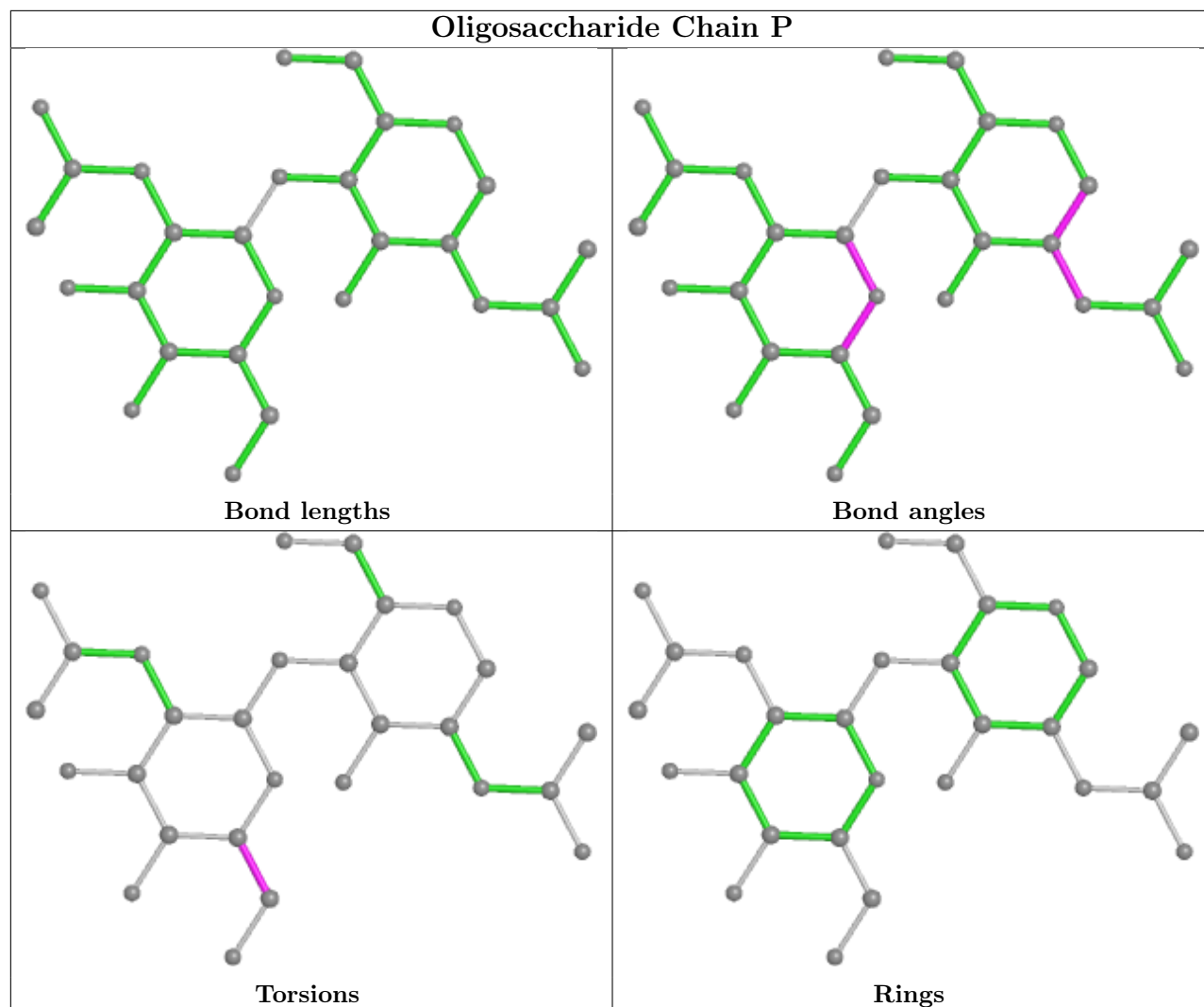


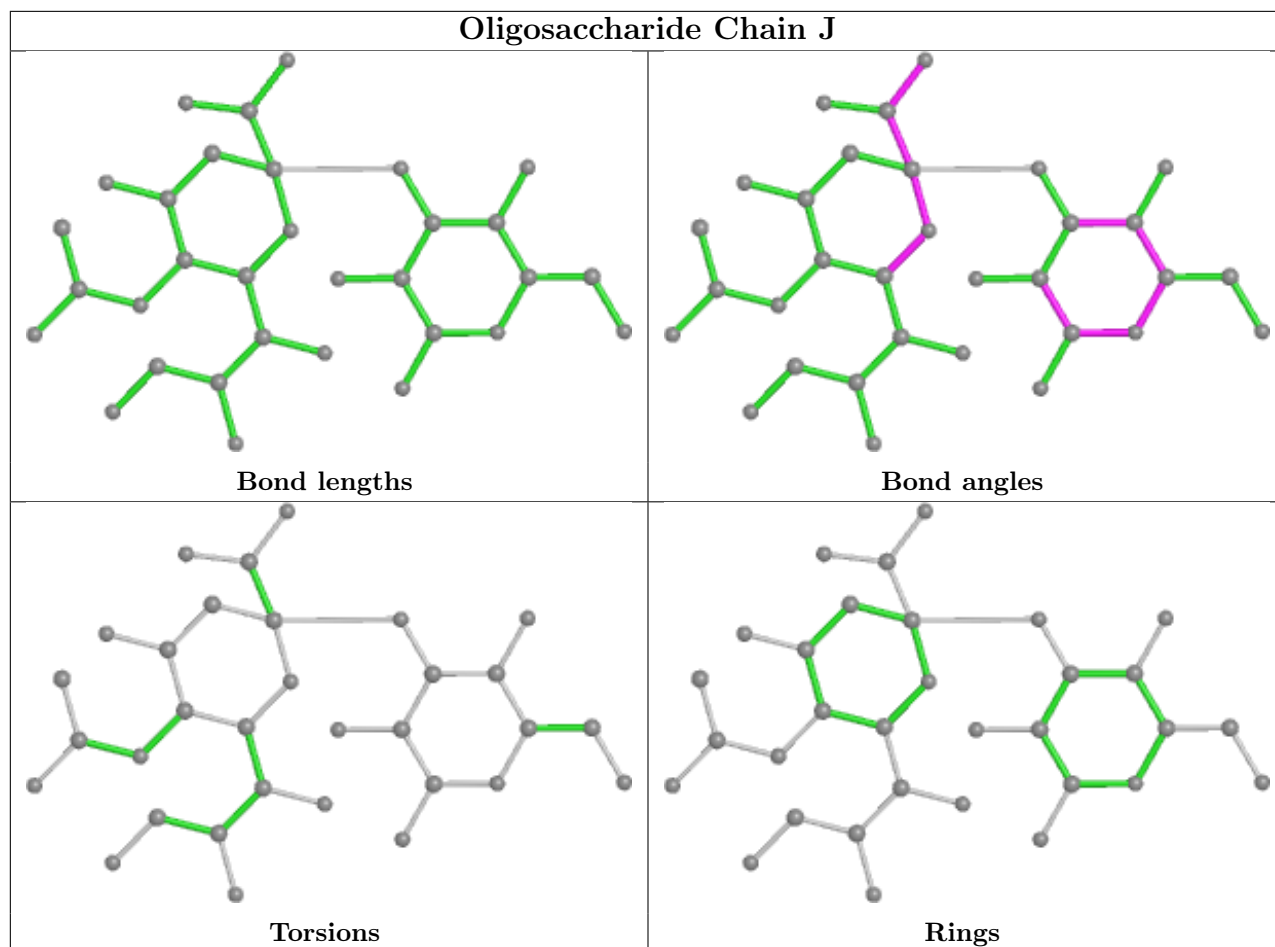


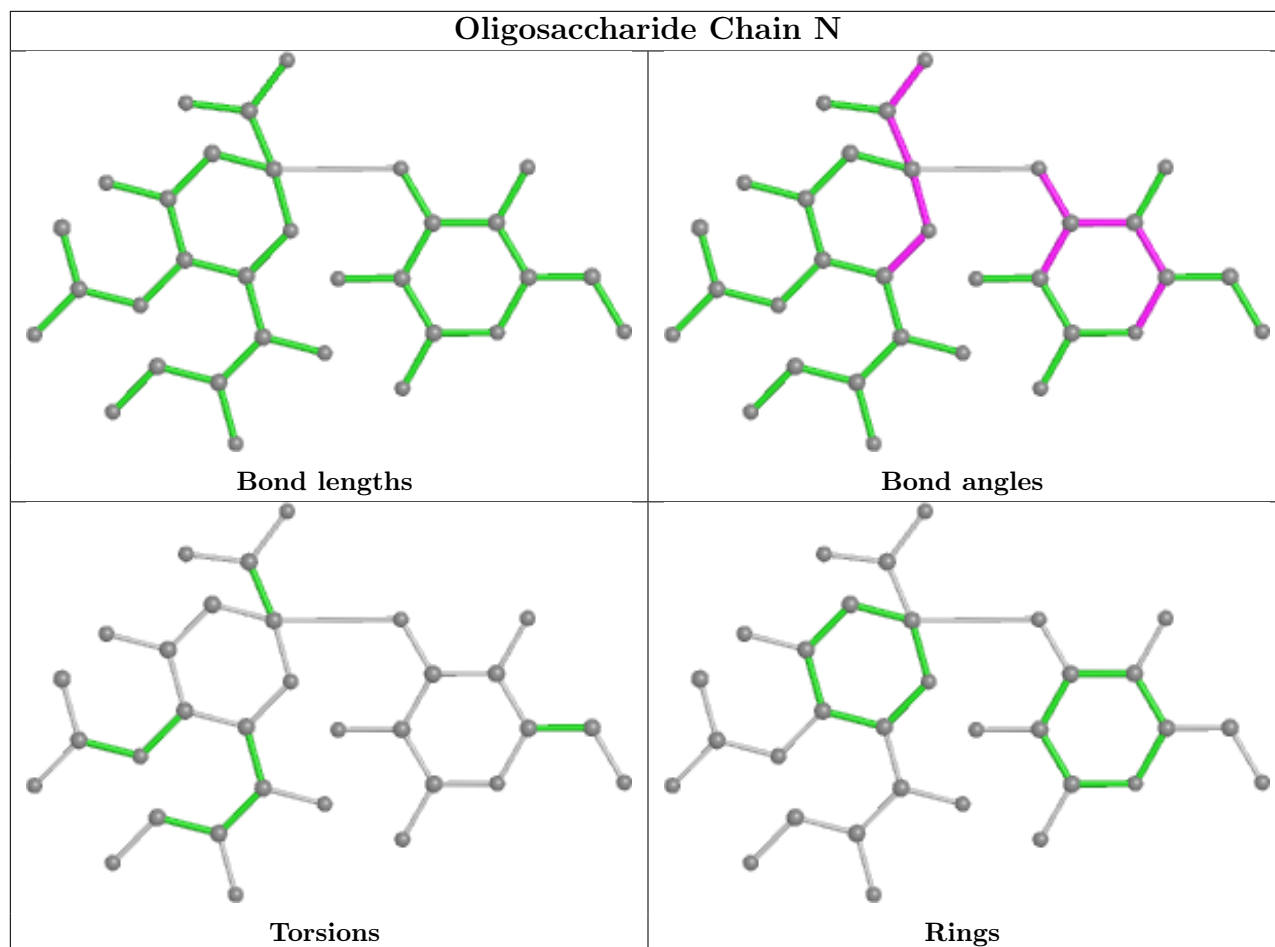


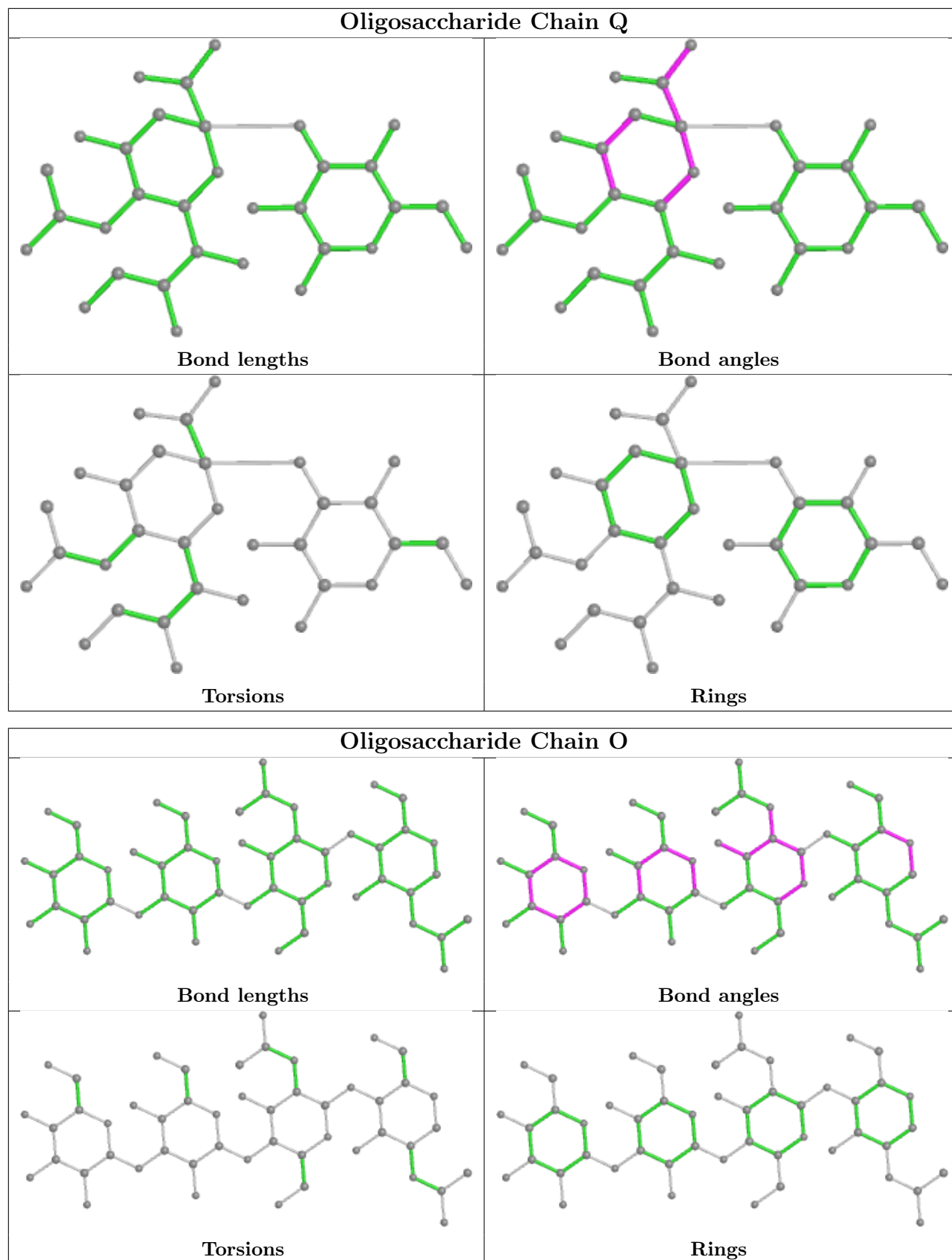












## 5.6 Ligand geometry

4 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	NAG	E	501	1	14,14,15	0.58	0	17,19,21	1.34	1 (5%)
7	NAG	C	503	1	14,14,15	0.77	0	17,19,21	2.00	2 (11%)
7	NAG	A	404	1	14,14,15	0.56	0	17,19,21	1.29	3 (17%)
8	TAM	E	508	-	7,10,10	0.65	0	9,12,12	0.90	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	NAG	E	501	1	-	0/6/23/26	0/1/1/1
7	NAG	C	503	1	-	0/6/23/26	0/1/1/1
7	NAG	A	404	1	-	1/6/23/26	0/1/1/1
8	TAM	E	508	-	-	3/12/12/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	NAG	C1-O5-C5	6.37	120.83	112.19
7	E	501	NAG	C1-O5-C5	4.86	118.78	112.19
7	A	404	NAG	O5-C1-C2	-3.10	106.40	111.29
7	C	503	NAG	C3-C4-C5	3.09	115.75	110.24
7	A	404	NAG	O5-C5-C6	2.27	110.76	107.20
7	A	404	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	508	TAM	C-C3-C6-O6
8	E	508	TAM	C-C2-C5-O5
8	E	508	TAM	C2-C-C1-C4
7	A	404	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/323 (99%)	0.26	24 (7%) 14 15	36, 55, 93, 122	0
1	C	317/323 (98%)	-0.09	5 (1%) 72 74	40, 55, 75, 115	0
1	E	317/323 (98%)	0.01	6 (1%) 66 69	33, 46, 70, 111	0
2	B	172/174 (98%)	0.67	23 (13%) 3 2	33, 67, 99, 125	0
2	D	171/174 (98%)	0.29	6 (3%) 44 46	37, 63, 93, 112	0
2	F	171/174 (98%)	0.36	10 (5%) 23 25	35, 68, 100, 122	0
All	All	1469/1491 (98%)	0.19	74 (5%) 28 31	33, 55, 93, 125	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	171	PHE	8.1
1	A	128	THR	5.4
1	A	164	LEU	5.1
1	A	11	ALA	5.1
2	B	147	ALA	4.7
1	A	9	PRO	4.7
2	B	31	GLY	4.6
2	B	29	SER	4.5
1	A	10	GLY	4.5
2	B	143	LYS	4.4
2	B	27	GLN	4.2
1	C	9	PRO	4.1
1	A	12	THR	4.0
1	A	127	TRP	3.7
2	F	164	ASP	3.7
2	B	144	CYS	3.7
1	A	161	TYR	3.6
2	F	167	LEU	3.4
1	C	22	ASN	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	32	THR	3.3
2	B	28	ASN	3.2
2	B	59	THR	3.2
1	A	129	GLY	3.1
1	A	160	THR	3.1
2	F	168	ASN	3.1
2	D	171	PHE	3.1
1	A	327	GLN	3.0
2	D	77	ILE	3.0
2	F	77	ILE	2.9
2	B	77	ILE	2.9
2	B	26	HIS	2.9
1	A	167	THR	2.8
1	C	12	THR	2.8
1	A	162	PRO	2.8
2	B	140	ILE	2.8
2	B	30	GLU	2.8
2	D	167	LEU	2.7
2	B	142	HIS	2.7
2	F	143	LYS	2.7
1	E	22	ASN	2.6
1	A	130	VAL	2.6
2	D	168	ASN	2.6
1	A	208	ARG	2.5
1	E	222	TRP	2.5
1	A	163	VAL	2.5
2	F	141	TYR	2.5
1	A	225	MET	2.5
1	E	234	TRP	2.5
2	B	149	ILE	2.5
1	A	159	SER	2.4
2	B	148	CYS	2.4
1	C	208	ARG	2.4
1	E	104	ASP	2.3
1	A	166	VAL	2.3
2	B	80	LEU	2.3
1	A	328	THR	2.3
1	A	107	SER	2.2
2	D	157	TYR	2.2
2	D	143	LYS	2.2
1	E	221	PRO	2.2
2	B	171	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	4	GLY	2.2
2	F	18	ILE	2.1
2	B	168	ASN	2.1
1	E	233	TYR	2.1
2	B	164	ASP	2.1
1	A	248	ASN	2.1
1	A	104	ASP	2.1
1	C	222	TRP	2.1
1	A	329	ARG	2.0
2	B	10	ILE	2.0
2	F	80	LEU	2.0
2	F	118	LEU	2.0
2	B	167	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

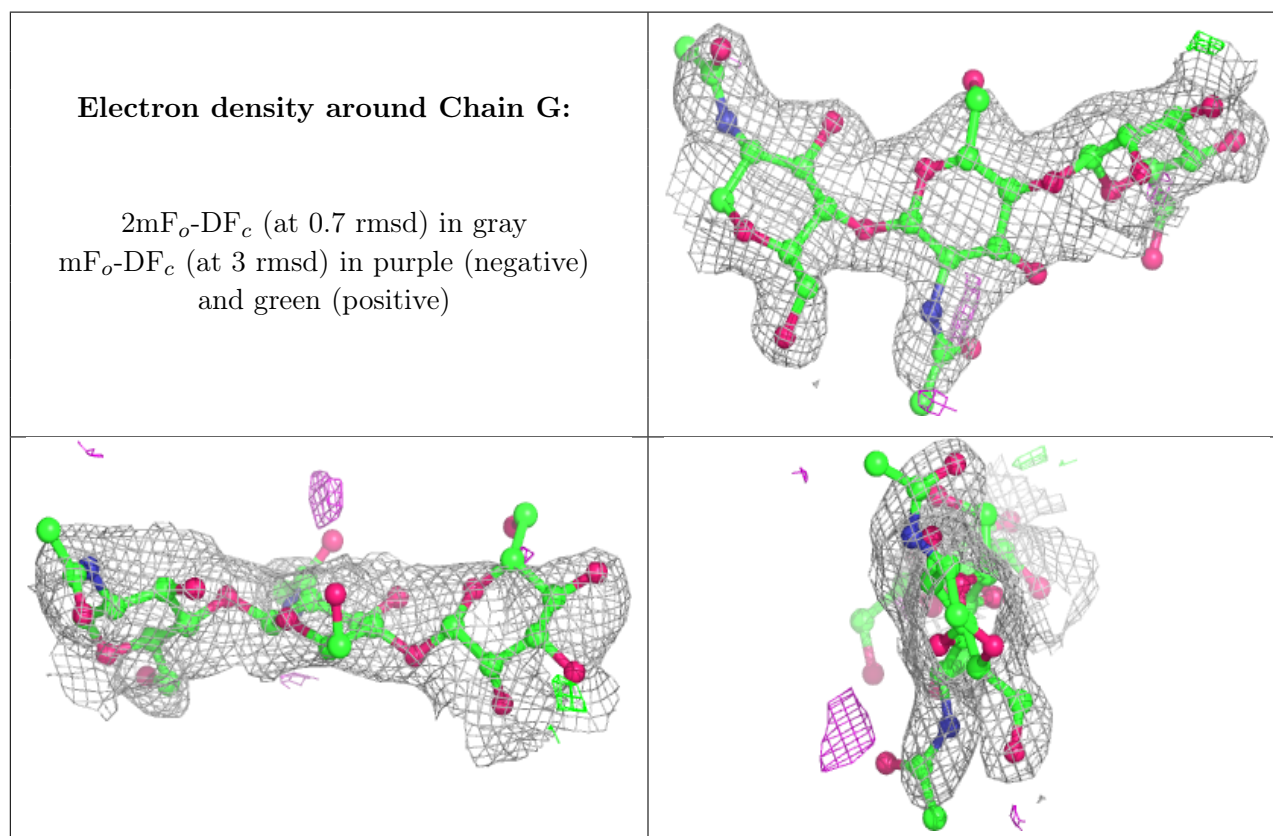
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	L	3	11/12	0.56	0.31	100,106,109,109	0
5	GAL	J	1	12/12	0.64	0.38	122,129,135,136	0
3	BMA	G	3	11/12	0.71	0.26	110,117,119,120	0
5	GAL	N	1	12/12	0.74	0.30	102,113,122,123	0
6	BMA	O	3	11/12	0.74	0.24	86,90,96,100	0
6	MAN	O	4	11/12	0.78	0.37	100,105,107,107	0
3	BMA	H	3	11/12	0.84	0.23	96,101,103,104	0
4	NAG	I	2	14/15	0.84	0.21	83,95,107,112	0
4	NAG	M	2	14/15	0.87	0.20	83,90,97,99	0
5	SIA	J	2	20/21	0.88	0.21	80,94,111,111	0
4	NAG	K	2	14/15	0.88	0.21	99,102,105,105	0
4	NAG	P	2	14/15	0.89	0.26	84,91,99,99	0
3	NAG	G	2	14/15	0.89	0.35	101,108,114,117	0
4	NAG	K	1	14/15	0.89	0.16	73,85,94,101	0
5	SIA	N	2	20/21	0.91	0.11	60,70,86,86	0

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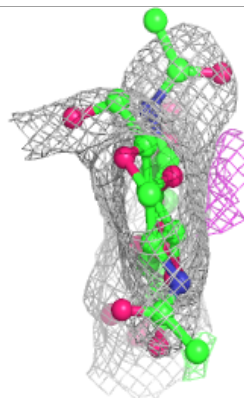
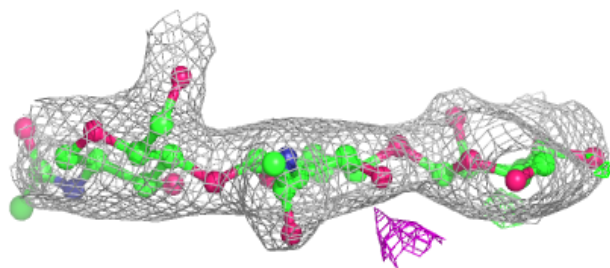
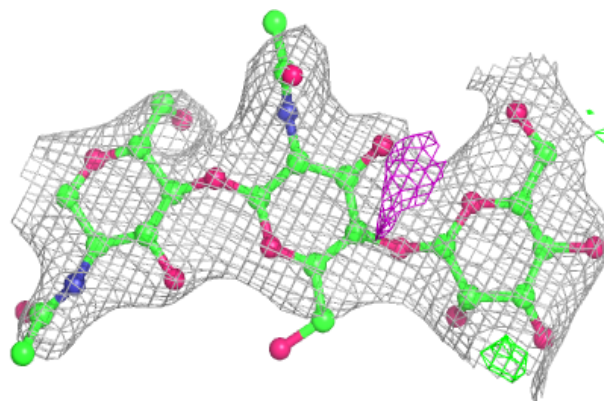
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	1	14/15	0.92	0.26	69,78,83,92	0
5	GAL	Q	1	12/12	0.92	0.24	75,88,92,92	0
3	NAG	L	2	14/15	0.94	0.16	65,73,85,95	0
3	NAG	H	2	14/15	0.94	0.28	79,87,96,97	0
6	NAG	O	2	14/15	0.94	0.16	52,64,72,75	0
3	NAG	H	1	14/15	0.94	0.25	68,75,89,93	0
4	NAG	P	1	14/15	0.94	0.12	47,55,65,72	0
6	NAG	O	1	14/15	0.95	0.12	56,60,69,73	0
4	NAG	I	1	14/15	0.95	0.19	54,61,66,79	0
4	NAG	M	1	14/15	0.95	0.11	54,62,65,76	0
5	SIA	Q	2	20/21	0.95	0.16	53,57,64,65	0
3	NAG	L	1	14/15	0.96	0.09	50,60,66,66	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.

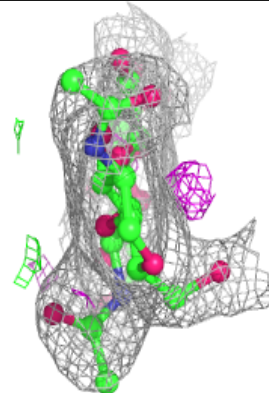
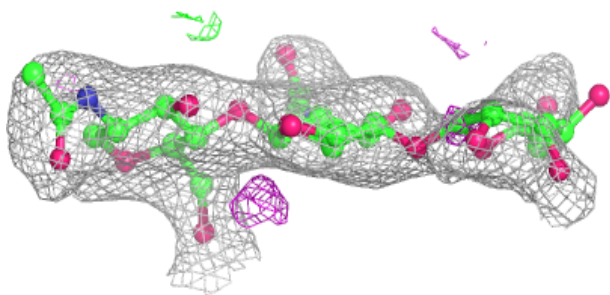
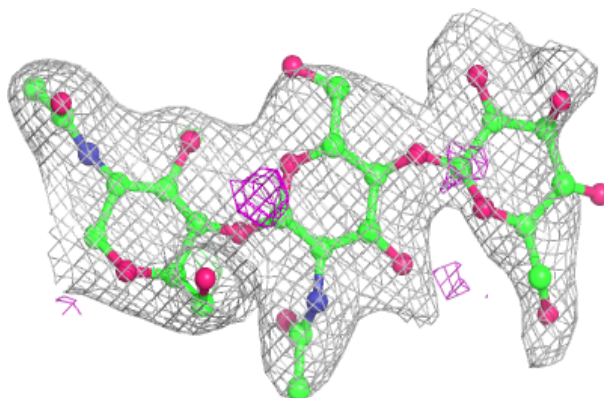


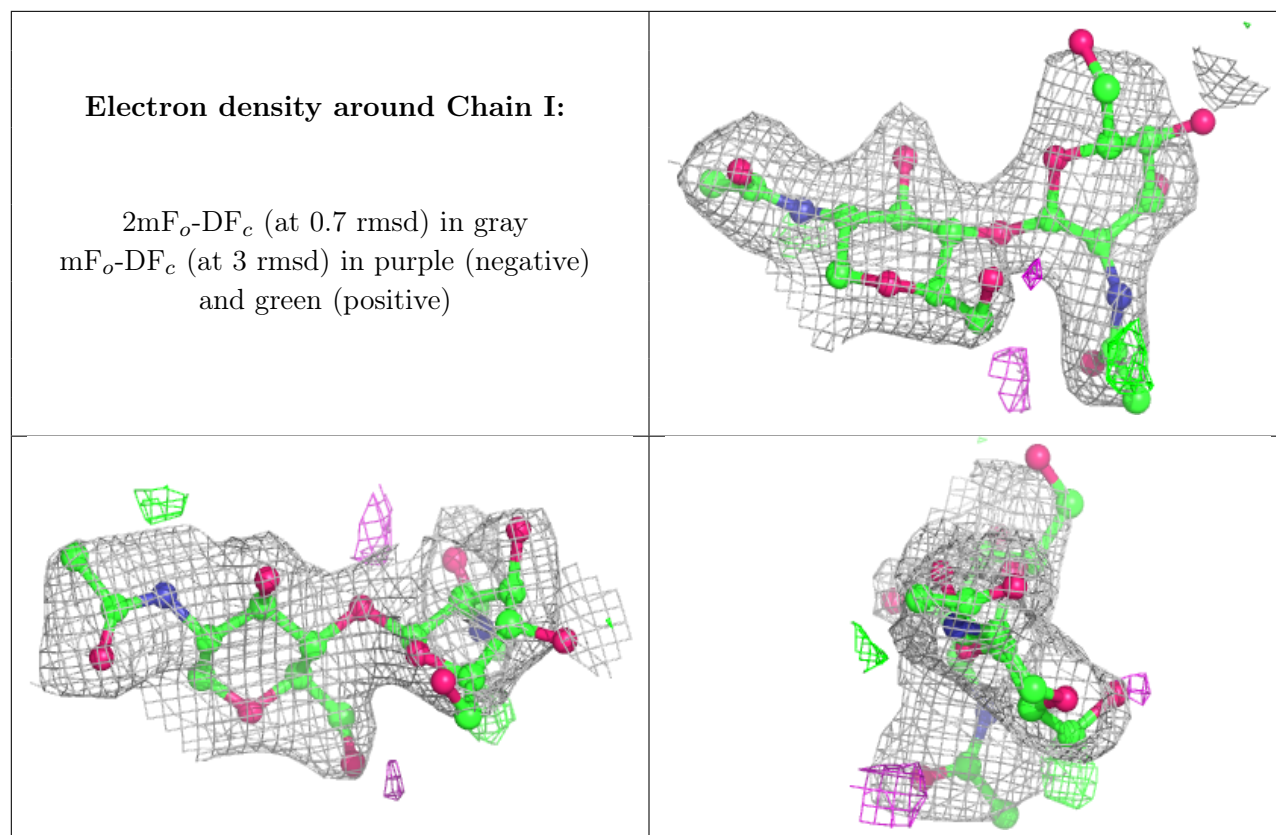
**Electron density around Chain H:**

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

**Electron density around Chain L:**

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

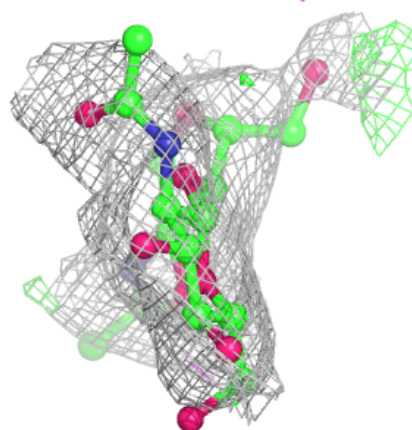
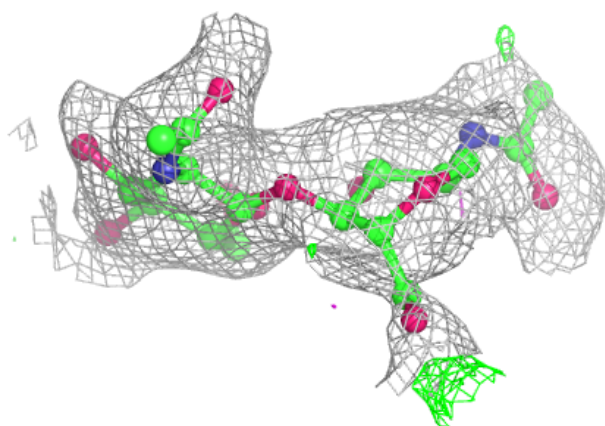
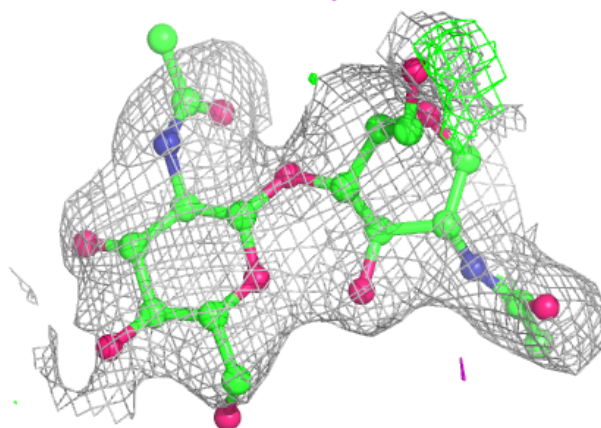






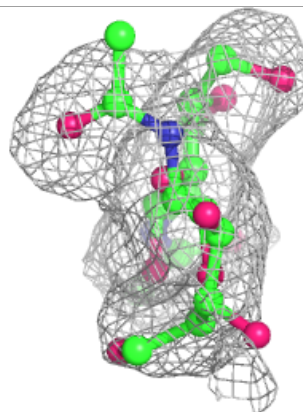
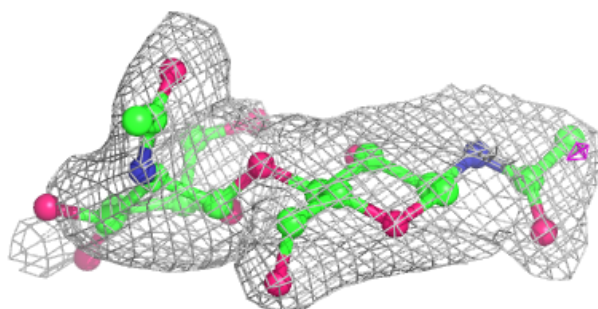
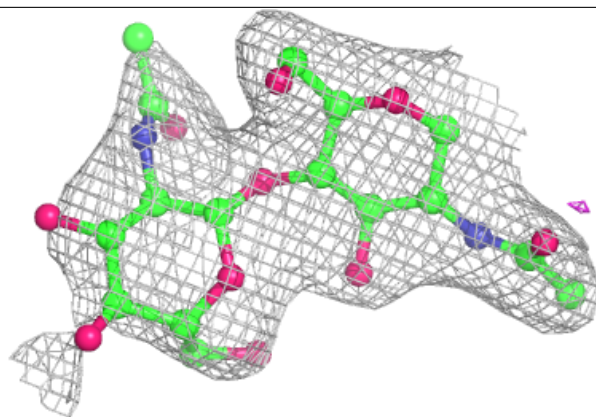
**Electron density around Chain K:**

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

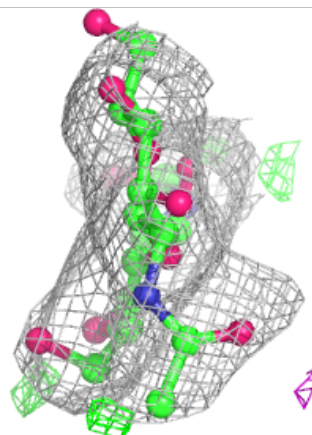
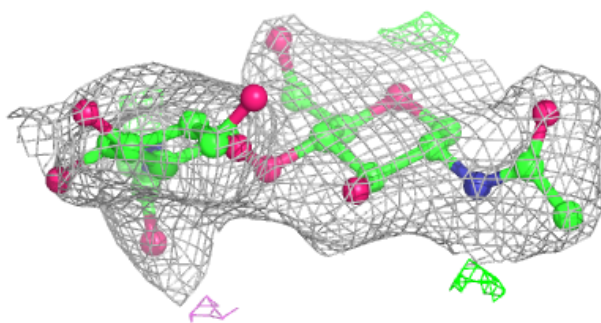
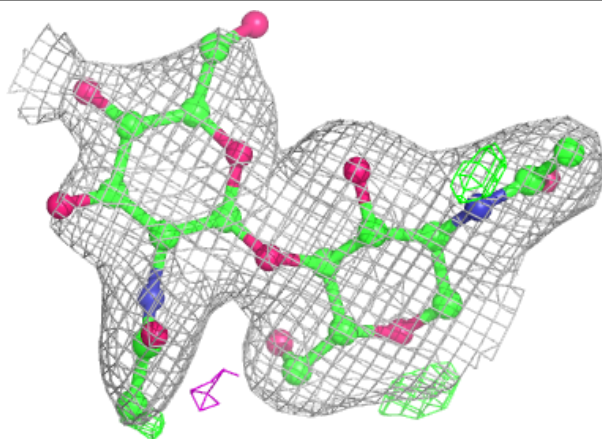


**Electron density around Chain M:**

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

**Electron density around Chain P:**

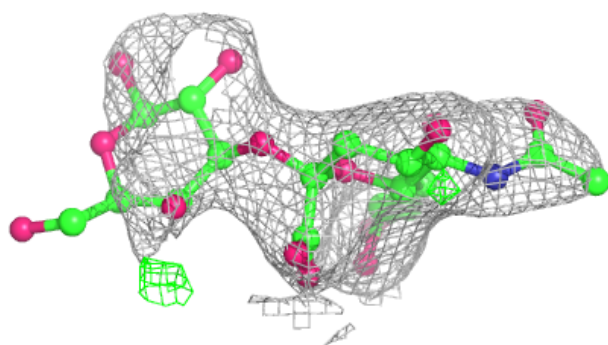
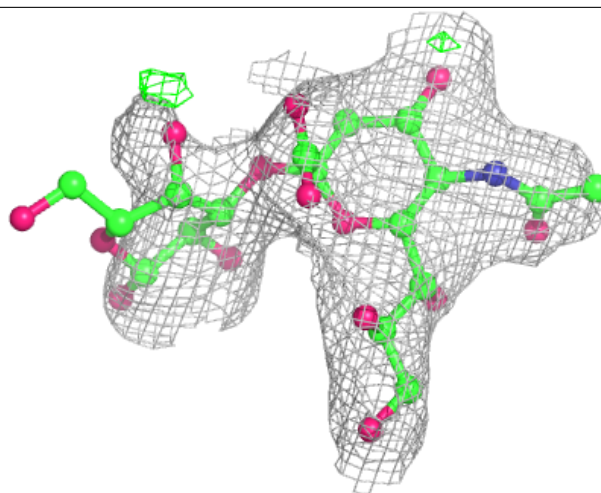
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





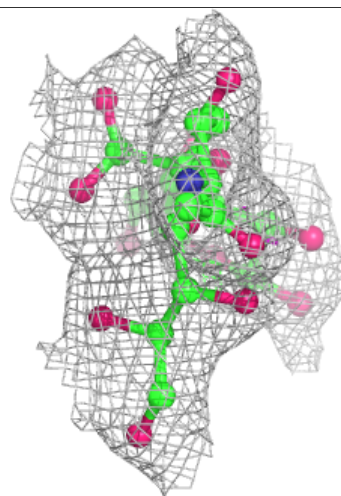
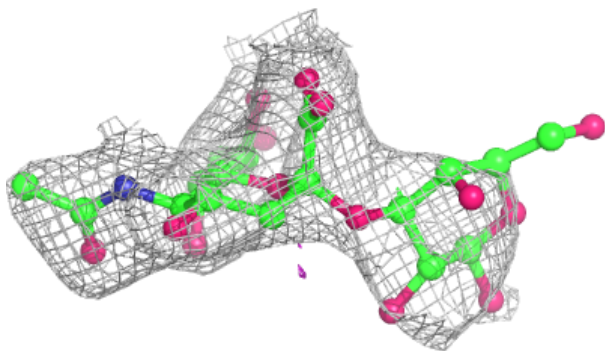
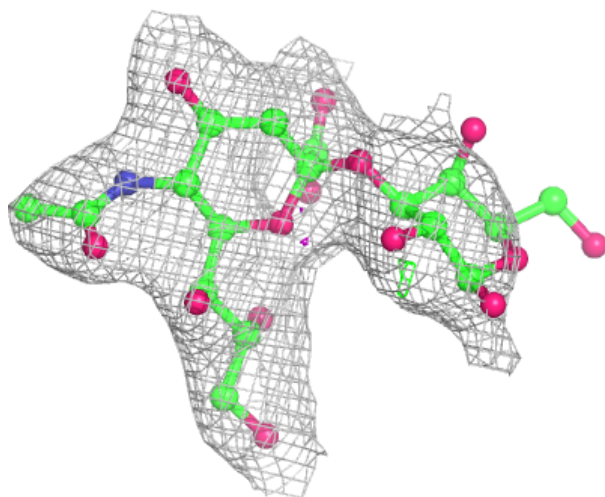
**Electron density around Chain J:**

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



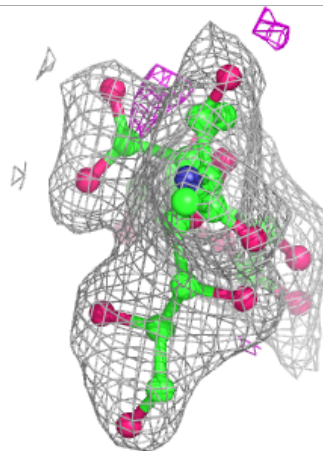
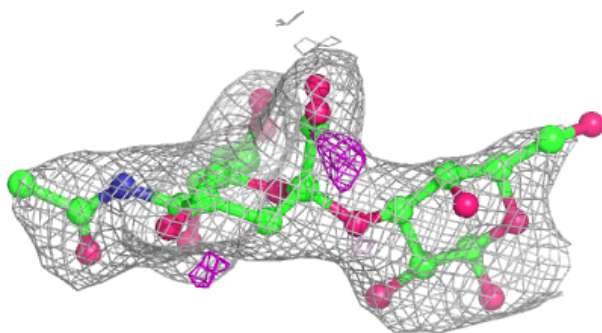
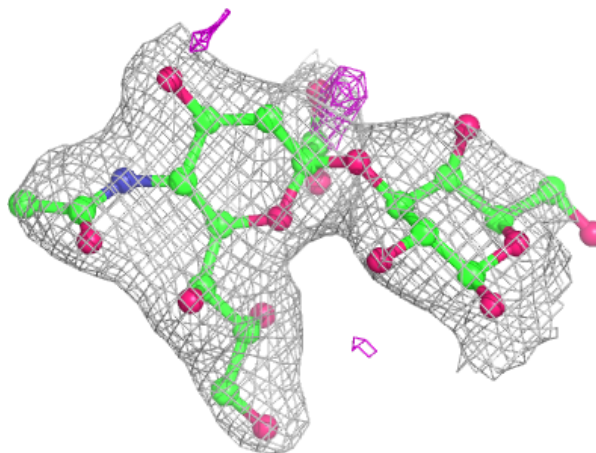
**Electron density around Chain N:**

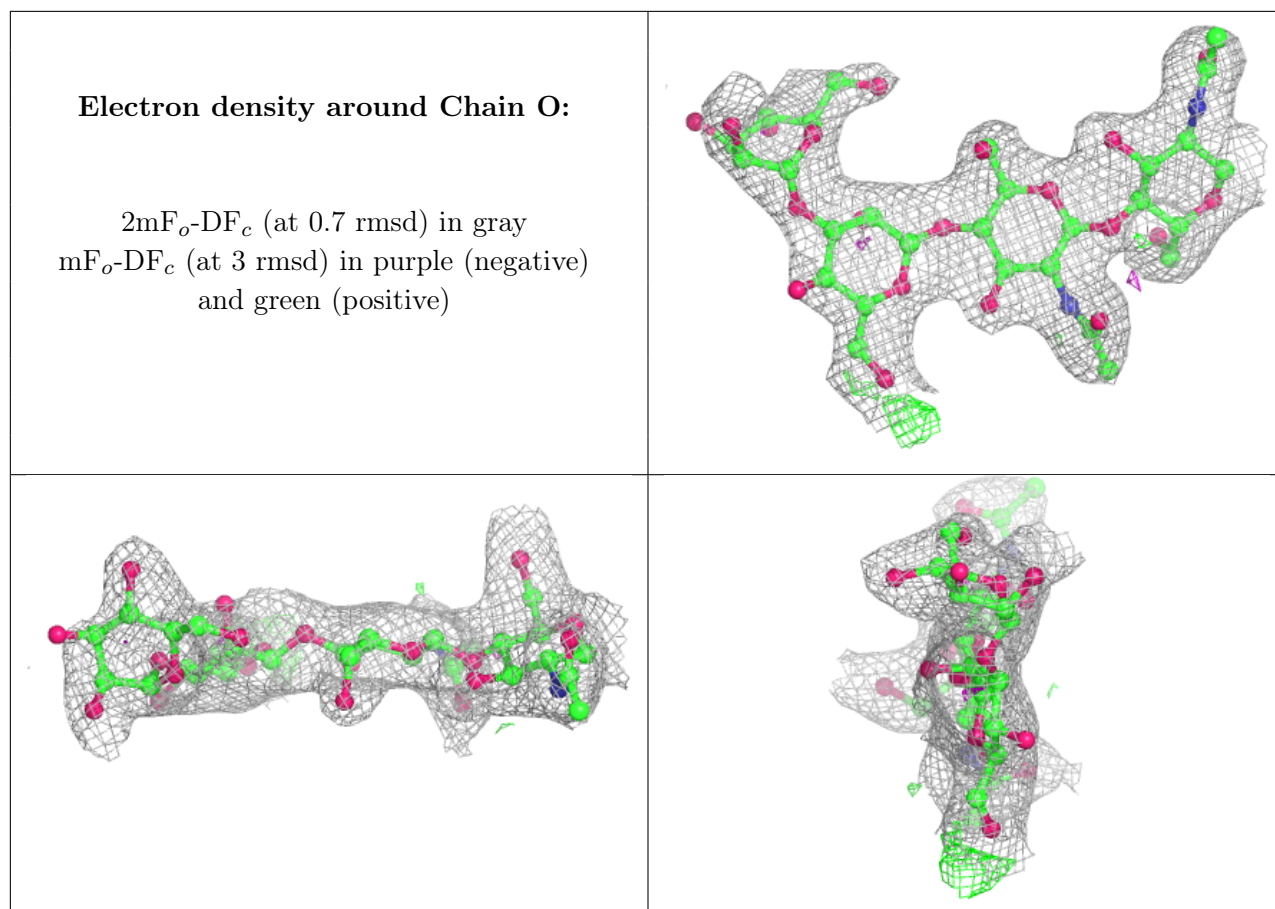
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain Q:**

$2mF_o-DF_c$  (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
7	NAG	C	503	14/15	0.68	0.38	88,97,104,104	0
8	TAM	E	508	11/11	0.83	0.18	70,81,83,84	0
7	NAG	A	404	14/15	0.85	0.27	73,82,86,90	0
7	NAG	E	501	14/15	0.90	0.14	69,78,81,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.