



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:05 PM BST

PDB ID : 6J11  
Title : MERS-CoV spike N-terminal domain and 7D10 scFv complex  
Authors : Zhou, H.; Zhang, S.; Zhang, S.; Tang, W.; Wang, X.  
Deposited on : 2018-12-27  
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

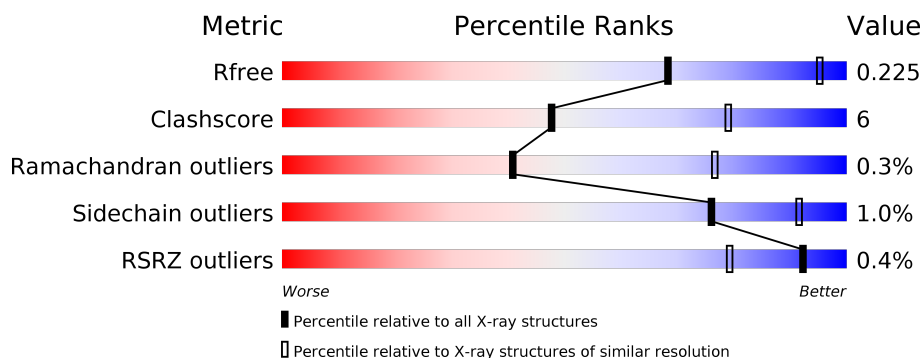
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.






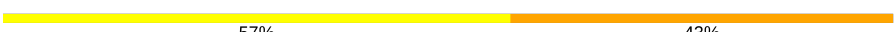










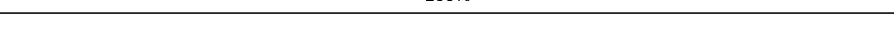

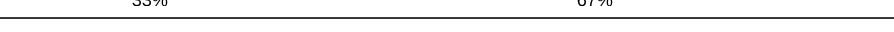
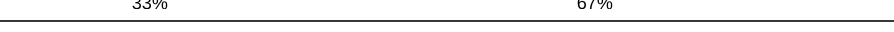
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	336	<div> <div>88%</div> <div>12%</div> </div>
1	B	336	<div> <div>89%</div> <div>11%</div> </div>
1	C	336	<div> <div>83%</div> <div>16%</div> </div>
2	D	132	<div> <div>3%</div> <div>67%</div> <div>23%</div> <div>9%</div> </div>
2	F	132	<div> <div>2%</div> <div>76%</div> <div>15%</div> <div>9%</div> </div>
2	H	132	<div> <div>85%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	111	 83% 16%
3	G	111	 80% 19%
3	L	111	 80% 19%
4	I	7	 57% 43%
4	O	7	 29% 71%
4	X	7	 14% 86%
5	J	4	 50% 50%
6	K	2	 100%
6	M	2	 50% 50%
6	P	2	 100%
6	R	2	 50% 50%
6	S	2	 50% 50%
6	T	2	 100%
6	U	2	 100%
6	V	2	 50% 50%
7	N	3	 33% 67%
7	W	3	 33% 67%
8	Q	5	 100%

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
6	NAG	S	2	-	-	-	X
9	NAG	A	409	-	-	-	X
9	NAG	B	409	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14135 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 N-terminal domain of Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			
1	B	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			
1	C	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			

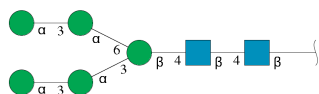
- Molecule 2 is a protein called VH of 7D10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	128	Total	C	N	O	S	0	0	0
			952	599	153	195	5			
2	D	120	Total	C	N	O	S	0	0	0
			916	581	145	185	5			
2	F	120	Total	C	N	O	S	0	0	0
			916	581	145	185	5			

- Molecule 3 is a protein called VL of 7D10.

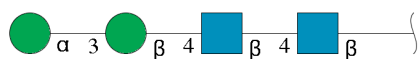
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			
3	E	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			
3	G	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			

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



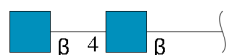
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	O	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	X	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 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
5	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

*Continued on next page...*

Continued from previous page...

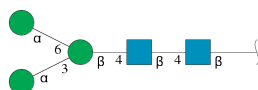
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 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
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 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
8	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 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>).

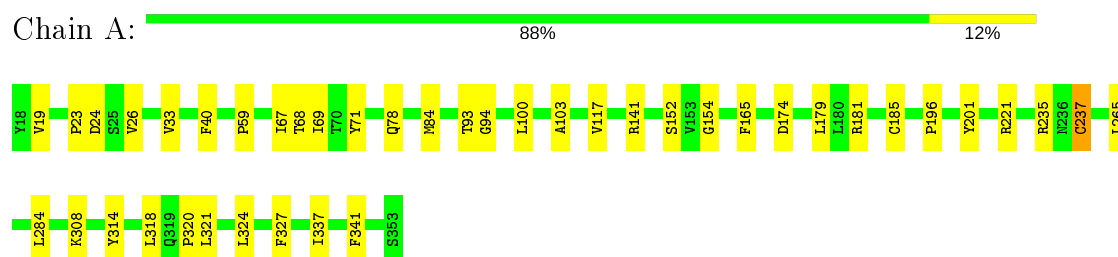


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1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

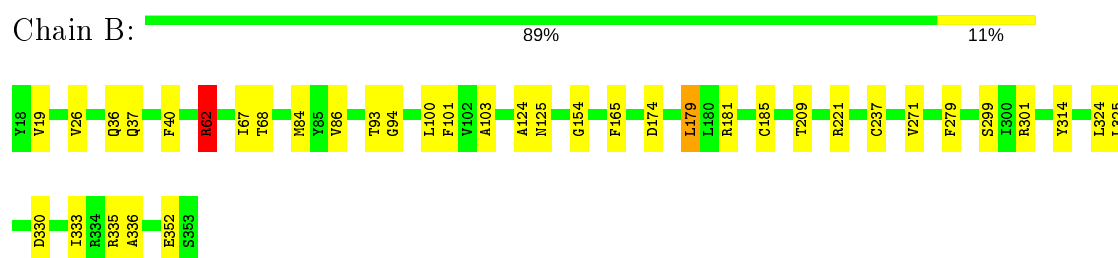
### 3 Residue-property plots

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.

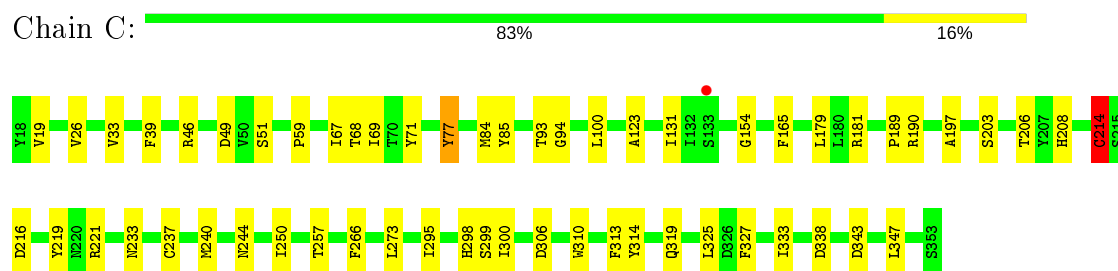
- Molecule 1: N-terminal domain of Spike glycoprotein



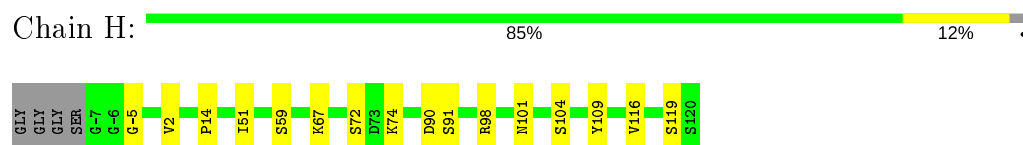
- Molecule 1: N-terminal domain of Spike glycoprotein



- Molecule 1: N-terminal domain of Spike glycoprotein

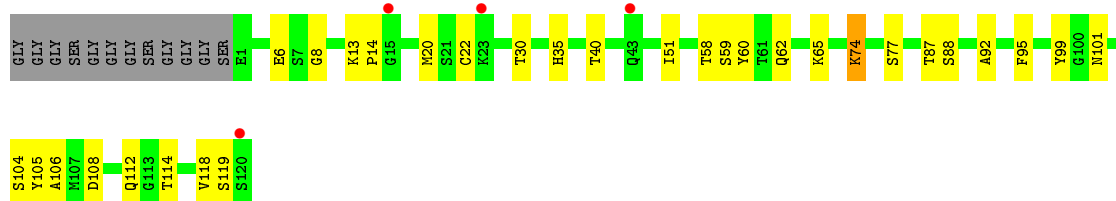


- Molecule 2: VH of 7D10

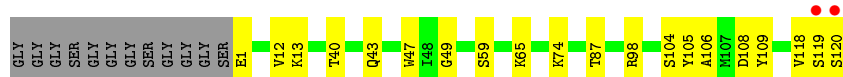
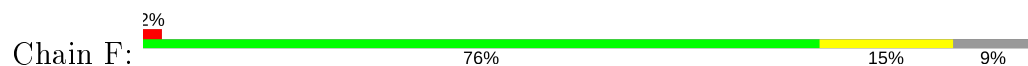


- Molecule 2: VH of 7D10

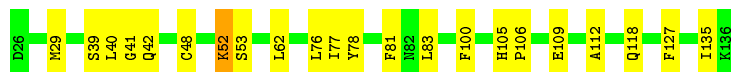
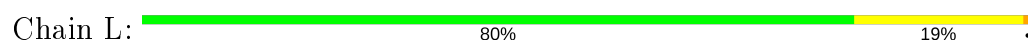




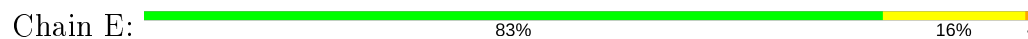
- Molecule 2: VH of 7D10



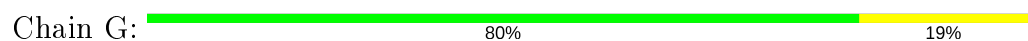
- Molecule 3: VL of 7D10



- Molecule 3: VL of 7D10



- Molecule 3: VL of 7D10



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



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

Chain O:  29% 71%



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

Chain X:  14% 86%



- Molecule 5: 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 J:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%




- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



- Molecule 8:  $\alpha$ -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 Q:

100%

MAG1  
MAG2  
EMAG  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.57Å 180.35Å 245.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 3.00 49.25 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.31-3.00) 98.9 (49.25-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155: ???	Depositor
R, $R_{free}$	0.188 , 0.225 0.188 , 0.225	Depositor DCC
$R_{free}$ test set	4781 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	1/2738 (0.0%)	0.73	0/3725
1	B	0.49	0/2738	0.68	2/3725 (0.1%)
1	C	0.51	2/2738 (0.1%)	0.70	4/3725 (0.1%)
2	D	0.57	0/940	0.72	0/1277
2	F	0.58	0/940	0.72	0/1277
2	H	0.65	0/976	0.78	1/1323 (0.1%)
3	E	0.51	0/881	0.67	0/1197
3	G	0.53	0/881	0.72	1/1197 (0.1%)
3	L	0.58	0/881	0.79	1/1197 (0.1%)
All	All	0.54	3/13713 (0.0%)	0.72	9/18643 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	CYS	CB-SG	-5.81	1.72	1.81
1	C	77	TYR	CE1-CZ	-5.80	1.31	1.38
1	C	237	CYS	CB-SG	-5.18	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	CYS	CA-CB-SG	7.05	126.69	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	C	338	ASP	CB-CG-OD1	6.09	123.78	118.30
3	L	76	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	214	CYS	CA-CB-SG	5.81	124.47	114.00
1	B	179	LEU	CA-CB-CG	5.81	128.66	115.30
2	H	98	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	77	TYR	CB-CG-CD2	5.40	124.24	121.00
3	G	62	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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	2662	0	2519	26	0
1	B	2662	0	2517	24	0
1	C	2662	0	2517	30	0
2	D	916	0	871	25	0
2	F	916	0	873	14	0
2	H	952	0	901	9	0
3	E	859	0	828	12	0
3	G	859	0	828	15	0
3	L	859	0	828	14	0
4	I	83	0	69	2	0
4	O	83	0	70	6	0
4	X	83	0	69	4	0
5	J	50	0	43	0	0
6	K	28	0	25	2	0
6	M	28	0	25	0	0
6	P	28	0	25	0	0
6	R	28	0	25	2	0
6	S	28	0	25	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	28	0	25	0	0
6	U	28	0	25	2	0
6	V	28	0	25	0	0
7	N	39	0	34	0	0
7	W	39	0	34	0	0
8	Q	61	0	52	0	0
9	A	42	0	39	0	0
9	B	42	0	39	0	0
9	C	42	0	39	0	0
All	All	14135	0	13370	167	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 6.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:NH2	1:B:221:ARG:O	2.07	0.88
2:F:104:SER:O	2:F:106:ALA:N	2.15	0.79
3:G:84:GLU:O	3:G:87:VAL:HG12	1.91	0.70
1:A:93:THR:HG23	1:A:94:GLY:H	1.56	0.70
2:D:6:GLU:O	2:D:112:GLN:NE2	2.25	0.69
2:D:104:SER:O	2:D:106:ALA:N	2.24	0.68
2:F:13:LYS:NZ	2:F:120:SER:O	2.19	0.68
1:C:257:THR:HG22	1:C:266:PHE:HE1	1.58	0.67
1:C:26:VAL:O	2:D:59:SER:HB2	1.94	0.67
1:C:19:VAL:HG11	4:X:7:MAN:H61	1.76	0.67
2:F:40:THR:HG23	2:F:43:GLN:HB2	1.77	0.67
3:E:81:PHE:HZ	6:U:2:NAG:H82	1.59	0.67
1:A:181:ARG:NH2	1:A:221:ARG:O	2.28	0.67
1:B:19:VAL:HG21	4:O:7:MAN:H61	1.77	0.67
3:E:68:ARG:NH1	3:E:110:GLU:O	2.26	0.66
1:B:174:ASP:HB3	1:B:179:LEU:HD22	1.76	0.66
2:D:20:MET:SD	2:D:114:THR:OG1	2.53	0.66
3:L:81:PHE:HZ	6:K:2:NAG:H82	1.59	0.66
3:G:81:PHE:HZ	6:R:2:NAG:H82	1.61	0.65
1:A:196:PRO:HA	1:A:201:TYR:CD1	2.33	0.64
1:A:26:VAL:O	2:H:59:SER:HB2	1.96	0.64
1:A:84:MET:HG3	1:A:314:TYR:CE2	2.33	0.64
1:A:19:VAL:HG21	4:I:7:MAN:H61	1.80	0.63
2:F:108:ASP:HB3	2:F:109:TYR:CD2	2.35	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ARG:NH2	4:O:4:MAN:O6	2.33	0.61
4:O:4:MAN:H4	4:O:5:MAN:H2	1.81	0.61
1:C:33:VAL:HG11	1:C:203:SER:O	2.00	0.61
2:F:87:THR:O	2:F:118:VAL:HG21	2.01	0.61
1:A:24:ASP:OD2	1:A:235:ARG:NH2	2.34	0.61
1:C:93:THR:OG1	1:C:94:GLY:N	2.35	0.60
4:X:4:MAN:H4	4:X:5:MAN:H2	1.82	0.60
1:B:179:LEU:HD12	1:B:221:ARG:CZ	2.32	0.59
3:G:118:GLN:HB2	3:G:127:PHE:CD2	2.37	0.59
2:D:62:GLN:HG3	2:D:65:LYS:NZ	2.17	0.59
2:F:104:SER:OG	2:F:104:SER:O	2.16	0.59
3:E:118:GLN:HB2	3:E:127:PHE:CD2	2.37	0.59
3:L:52:LYS:HD3	3:L:53:SER:N	2.17	0.59
2:D:74:LYS:HD2	2:D:74:LYS:H	1.66	0.59
3:L:40:LEU:HD11	3:L:109:GLU:HG2	1.85	0.59
1:C:33:VAL:HG23	1:C:100:LEU:HB2	1.85	0.58
3:L:81:PHE:CZ	6:K:2:NAG:H82	2.37	0.58
2:H:104:SER:HA	3:L:78:TYR:CD1	2.39	0.57
2:D:87:THR:O	2:D:118:VAL:HG21	2.03	0.57
1:A:185:CYS:HB3	1:A:237:CYS:SG	2.45	0.56
1:B:84:MET:HG3	1:B:314:TYR:CE2	2.40	0.56
2:F:1:GLU:OE1	4:O:5:MAN:O3	2.20	0.56
2:D:13:LYS:HG3	2:D:14:PRO:HD2	1.88	0.56
3:E:81:PHE:CZ	6:U:2:NAG:H82	2.40	0.55
3:E:49:ARG:NH1	3:E:99:ASP:OD1	2.37	0.55
2:F:12:VAL:O	2:F:118:VAL:HA	2.07	0.55
1:C:214:CYS:HB3	1:C:219:TYR:HD1	1.71	0.55
1:B:179:LEU:HD12	1:B:221:ARG:NH2	2.22	0.55
1:C:84:MET:HG3	1:C:314:TYR:CE2	2.42	0.55
3:L:77:ILE:HG12	3:L:83:LEU:HD23	1.89	0.54
3:G:81:PHE:CZ	6:R:2:NAG:H82	2.42	0.54
1:A:174:ASP:HB3	1:A:179:LEU:HD22	1.89	0.54
3:L:29:MET:HE2	3:L:48:CYS:SG	2.48	0.53
3:G:29:MET:HE1	3:G:50:ALA:HB2	1.90	0.53
3:L:62:LEU:HD22	3:L:100:PHE:CG	2.44	0.53
1:A:179:LEU:HD12	1:A:221:ARG:CZ	2.38	0.52
1:C:181:ARG:HD3	1:C:240:MET:SD	2.50	0.52
2:D:14:PRO:HD3	2:D:119:SER:O	2.10	0.52
1:C:85:TYR:HB2	1:C:313:PHE:CE1	2.45	0.52
3:L:118:GLN:HB2	3:L:127:PHE:CD2	2.45	0.52
3:G:66:GLN:HB2	3:G:76:LEU:HD22	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:52:LYS:HD3	3:L:53:SER:H	1.74	0.51
1:A:154:GLY:HA3	1:A:165:PHE:HE2	1.75	0.51
1:A:93:THR:HG23	1:A:94:GLY:N	2.24	0.51
1:B:154:GLY:HA3	1:B:165:PHE:HE2	1.76	0.51
2:D:60:TYR:HB2	2:D:65:LYS:HG3	1.93	0.51
1:C:46:ARG:HH12	1:C:123:ALA:CA	2.24	0.51
1:A:320:PRO:O	1:A:321:LEU:HD23	2.11	0.50
2:D:87:THR:HG22	2:D:88:SER:H	1.76	0.50
1:C:206:THR:HG23	1:C:298:HIS:ND1	2.26	0.50
3:E:42:GLN:O	3:E:107:VAL:HG23	2.10	0.50
1:A:23:PRO:HA	2:H:101:ASN:OD1	2.11	0.50
1:A:324:LEU:HD12	1:A:337:ILE:HD12	1.93	0.50
1:A:141:ARG:HE	1:A:308:LYS:HD3	1.77	0.50
1:B:93:THR:OG1	1:B:94:GLY:N	2.45	0.49
1:A:265:LEU:HD11	1:A:284:LEU:HD11	1.94	0.49
2:F:104:SER:C	2:F:106:ALA:H	2.11	0.49
3:G:29:MET:HE2	3:G:48:CYS:SG	2.52	0.49
1:C:85:TYR:CZ	1:C:295:ILE:HG13	2.47	0.49
1:C:257:THR:HG22	1:C:266:PHE:CE1	2.44	0.49
1:C:100:LEU:HD22	1:C:299:SER:HB3	1.94	0.49
1:C:59:PRO:HB3	1:C:71:TYR:CZ	2.47	0.48
3:E:40:LEU:N	3:E:135:ILE:HD11	2.29	0.48
1:C:46:ARG:HH12	1:C:123:ALA:HA	1.79	0.48
2:F:104:SER:HB2	3:G:78:TYR:CG	2.49	0.48
1:A:69:ILE:HG12	1:A:327:PHE:HE1	1.79	0.48
1:C:49:ASP:OD1	1:C:51:SER:OG	2.30	0.48
2:D:104:SER:OG	2:D:104:SER:O	2.25	0.48
2:F:119:SER:OG	2:F:120:SER:N	2.46	0.48
1:A:40:PHE:CG	1:A:103:ALA:HB2	2.49	0.47
2:D:30:THR:HG23	4:X:1:NAG:H83	1.96	0.47
1:B:100:LEU:HD22	1:B:299:SER:HB3	1.96	0.47
1:B:325:LEU:HD22	1:B:333:ILE:HD13	1.97	0.47
2:D:104:SER:C	2:D:106:ALA:H	2.14	0.46
2:H:14:PRO:HD3	2:H:119:SER:O	2.16	0.46
1:B:181:ARG:NH1	4:O:1:NAG:O6	2.48	0.46
2:D:74:LYS:CD	2:D:74:LYS:H	2.25	0.46
3:L:41:GLY:HA2	3:L:106:PRO:HB2	1.97	0.46
3:E:55:SER:HB3	3:E:60:ASN:OD1	2.16	0.46
3:G:38:VAL:HG13	3:G:42:GLN:HG3	1.98	0.46
4:X:3:BMA:H61	4:X:6:MAN:O2	2.16	0.46
1:A:33:VAL:HG22	1:A:100:LEU:HD12	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG13	1:A:318:LEU:HD21	1.98	0.45
1:B:335:ARG:NH2	1:B:352:GLU:OE2	2.42	0.45
3:G:62:LEU:HD22	3:G:100:PHE:CG	2.51	0.45
1:C:250:ILE:HD12	1:C:273:LEU:HD21	1.98	0.45
2:D:95:PHE:HE2	3:E:72:PRO:HB3	1.80	0.45
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.51	0.45
1:B:209:THR:HG22	1:B:301:ARG:HB2	1.99	0.45
1:C:325:LEU:HD22	1:C:333:ILE:HD13	1.98	0.45
3:E:46:ILE:HG12	3:E:131:THR:HG21	1.99	0.45
1:B:36:GLN:HG3	1:B:101:PHE:HE1	1.82	0.44
1:C:221:ARG:NH2	1:C:244:ASN:OD1	2.50	0.44
1:C:300:ILE:HD13	1:C:310:TRP:NE1	2.33	0.44
2:D:62:GLN:HG3	2:D:65:LYS:HZ2	1.81	0.44
3:G:83:LEU:HB3	3:G:87:VAL:CG1	2.47	0.44
1:B:62:ARG:N	1:B:62:ARG:HD3	2.32	0.44
3:G:46:ILE:HG12	3:G:131:THR:HG21	2.00	0.44
2:H:51:ILE:HD13	2:H:72:SER:HB3	1.99	0.44
1:C:343:ASP:O	1:C:347:LEU:HD22	2.17	0.44
2:H:74:LYS:HE3	2:H:74:LYS:HB2	1.69	0.44
1:C:154:GLY:HA3	1:C:165:PHE:HE2	1.83	0.44
1:B:271:VAL:HB	1:B:279:PHE:CD1	2.52	0.43
3:E:62:LEU:HD13	3:E:100:PHE:CD1	2.53	0.43
2:D:51:ILE:HD12	2:D:58:THR:HG22	2.00	0.43
3:E:49:ARG:HA	3:E:98:THR:O	2.18	0.43
3:L:112:ALA:HB2	3:L:135:ILE:HD13	2.00	0.43
1:B:40:PHE:HD2	1:B:86:VAL:HG13	1.83	0.43
1:B:67:ILE:HG13	1:B:68:THR:N	2.34	0.43
4:I:3:BMA:H61	4:I:6:MAN:O2	2.19	0.43
2:D:87:THR:HG22	2:D:88:SER:N	2.33	0.43
3:G:40:LEU:HD23	3:G:40:LEU:HA	1.69	0.43
2:D:40:THR:HG22	2:D:92:ALA:HB2	2.01	0.43
1:A:152:SER:HB2	1:A:165:PHE:HB2	2.01	0.42
2:D:65:LYS:HB2	2:D:65:LYS:HE2	1.63	0.42
1:B:62:ARG:HD3	1:B:62:ARG:H	1.83	0.42
1:C:69:ILE:HG12	1:C:327:PHE:HE1	1.84	0.42
4:O:3:BMA:H61	4:O:6:MAN:O2	2.19	0.42
1:B:330:ASP:N	1:B:330:ASP:OD1	2.52	0.42
1:C:189:PRO:HB2	1:C:197:ALA:HB2	2.02	0.42
1:C:190:ARG:NH1	1:C:233:ASN:OD1	2.51	0.42
1:C:67:ILE:HG13	1:C:68:THR:N	2.35	0.42
2:H:67:LYS:NZ	2:H:90:ASP:OD2	2.40	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:OE1	1:B:103:ALA:HB1	2.21	0.41
2:D:35:HIS:CD2	2:D:99:TYR:HB2	2.55	0.41
1:B:124:ALA:O	1:B:125:ASN:HB2	2.20	0.41
2:D:6:GLU:HA	2:D:22:CYS:HA	2.01	0.41
3:L:105:HIS:HA	3:L:106:PRO:HA	1.77	0.41
1:A:67:ILE:HG12	1:A:68:THR:N	2.36	0.41
1:A:59:PRO:HB3	1:A:71:TYR:CZ	2.55	0.41
2:D:77:SER:OG	2:D:77:SER:O	2.37	0.41
1:B:26:VAL:O	2:F:59:SER:HB2	2.21	0.41
1:A:78:GLN:HG2	1:A:341:PHE:CD2	2.56	0.41
1:C:59:PRO:HB3	1:C:71:TYR:CE1	2.56	0.41
3:G:68:ARG:HH11	3:G:68:ARG:HD3	1.75	0.41
3:L:39:SER:HB2	3:L:42:GLN:HG3	2.03	0.41
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.89	0.40
3:G:134:GLU:C	3:G:135:ILE:HD13	2.42	0.40
1:B:324:LEU:O	1:B:336:ALA:HA	2.21	0.40
1:C:39:PHE:O	1:C:131:ILE:HG23	2.21	0.40
2:H:91:SER:HA	2:H:116:VAL:O	2.22	0.40
2:D:8:GLY:O	2:D:114:THR:HB	2.22	0.40
2:H:2:VAL:HB	2:H:109:TYR:CE2	2.56	0.40

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	334/336 (99%)	317 (95%)	17 (5%)	0	100	100
1	B	334/336 (99%)	316 (95%)	18 (5%)	0	100	100
1	C	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	41	76
2	D	118/132 (89%)	109 (92%)	7 (6%)	2 (2%)	9	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	118/132 (89%)	108 (92%)	9 (8%)	1 (1%)	19	57
2	H	126/132 (96%)	117 (93%)	8 (6%)	1 (1%)	19	57
3	E	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	G	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	L	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
All	All	1691/1737 (97%)	1596 (94%)	90 (5%)	5 (0%)	41	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	-5	GLY
2	D	105	TYR
2	F	105	TYR
2	D	101	ASN
1	C	216	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/288 (100%)	288 (100%)	0	100	100
1	B	288/288 (100%)	286 (99%)	2 (1%)	84	94
1	C	288/288 (100%)	282 (98%)	6 (2%)	53	82
2	D	100/103 (97%)	98 (98%)	2 (2%)	55	83
2	F	100/103 (97%)	98 (98%)	2 (2%)	55	83
2	H	102/103 (99%)	102 (100%)	0	100	100
3	E	94/94 (100%)	93 (99%)	1 (1%)	73	90
3	G	94/94 (100%)	94 (100%)	0	100	100
3	L	94/94 (100%)	93 (99%)	1 (1%)	73	90
All	All	1448/1455 (100%)	1434 (99%)	14 (1%)	76	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	ARG
1	B	237	CYS
1	C	77	TYR
1	C	179	LEU
1	C	208	HIS
1	C	214	CYS
1	C	306	ASP
1	C	319	GLN
3	L	52	LYS
2	D	74	LYS
2	D	108	ASP
3	E	62	LEU
2	F	65	LYS
2	F	74	LYS

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

### 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 ⓘ

52 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	$\# Z  > 2$
4	NAG	I	1	1,4	14,14,15	0.92	1 (7%)	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	I	2	4	14,14,15	1.16	1 (7%)	17,19,21	2.00	2 (11%)
4	BMA	I	3	4	11,11,12	2.05	6 (54%)	15,15,17	1.70	3 (20%)
4	MAN	I	4	4	11,11,12	1.60	3 (27%)	15,15,17	1.57	2 (13%)
4	MAN	I	5	4	11,11,12	1.87	4 (36%)	15,15,17	1.45	3 (20%)
4	MAN	I	6	4	11,11,12	2.78	8 (72%)	15,15,17	2.12	5 (33%)
4	MAN	I	7	4	11,11,12	2.25	4 (36%)	15,15,17	1.77	4 (26%)
5	NAG	J	1	1,5	14,14,15	0.54	0	17,19,21	0.87	0
5	NAG	J	2	5	14,14,15	0.25	0	17,19,21	0.50	0
5	BMA	J	3	5	11,11,12	1.79	4 (36%)	15,15,17	1.59	4 (26%)
5	MAN	J	4	5	11,11,12	1.00	2 (18%)	15,15,17	1.64	3 (20%)
6	NAG	K	1	1,6	14,14,15	0.65	0	17,19,21	1.62	2 (11%)
6	NAG	K	2	6	14,14,15	0.33	0	17,19,21	0.50	0
6	NAG	M	1	1,6	14,14,15	1.50	1 (7%)	17,19,21	2.57	3 (17%)
6	NAG	M	2	6	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	N	1	1,7	14,14,15	0.26	0	17,19,21	0.72	0
7	NAG	N	2	7	14,14,15	1.07	1 (7%)	17,19,21	0.66	0
7	BMA	N	3	7	11,11,12	1.92	4 (36%)	15,15,17	2.09	7 (46%)
4	NAG	O	1	1,4	14,14,15	0.48	0	17,19,21	0.60	0
4	NAG	O	2	4	14,14,15	0.68	0	17,19,21	1.67	1 (5%)
4	BMA	O	3	4	11,11,12	1.00	1 (9%)	15,15,17	1.49	2 (13%)
4	MAN	O	4	4	11,11,12	1.58	2 (18%)	15,15,17	1.46	2 (13%)
4	MAN	O	5	4	11,11,12	1.51	3 (27%)	15,15,17	1.35	1 (6%)
4	MAN	O	6	4	11,11,12	2.72	7 (63%)	15,15,17	1.88	3 (20%)
4	MAN	O	7	4	11,11,12	2.23	5 (45%)	15,15,17	1.89	3 (20%)
6	NAG	P	1	1,6	14,14,15	0.47	0	17,19,21	0.45	0
6	NAG	P	2	6	14,14,15	0.60	0	17,19,21	0.65	0
8	NAG	Q	1	1,8	14,14,15	0.45	0	17,19,21	1.00	2 (11%)
8	NAG	Q	2	8	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
8	BMA	Q	3	8	11,11,12	2.41	4 (36%)	15,15,17	2.26	6 (40%)
8	MAN	Q	4	8	11,11,12	1.78	3 (27%)	15,15,17	2.30	2 (13%)
8	MAN	Q	5	8	11,11,12	2.13	5 (45%)	15,15,17	1.30	2 (13%)
6	NAG	R	1	1,6	14,14,15	0.45	0	17,19,21	1.84	2 (11%)
6	NAG	R	2	6	14,14,15	0.26	0	17,19,21	1.05	1 (5%)
6	NAG	S	1	1,6	14,14,15	0.65	0	17,19,21	1.86	2 (11%)
6	NAG	S	2	6	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	T	1	1,6	14,14,15	0.51	0	17,19,21	0.51	0
6	NAG	T	2	6	14,14,15	0.19	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	U	1	1,6	14,14,15	0.56	0	17,19,21	1.79	2 (11%)
6	NAG	U	2	6	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	V	1	1,6	14,14,15	0.86	1 (7%)	17,19,21	2.02	2 (11%)
6	NAG	V	2	6	14,14,15	0.45	0	17,19,21	0.49	0
7	NAG	W	1	1,7	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
7	NAG	W	2	7	14,14,15	0.52	0	17,19,21	0.59	0
7	BMA	W	3	7	11,11,12	2.10	4 (36%)	15,15,17	1.79	6 (40%)
4	NAG	X	1	1,4	14,14,15	0.60	0	17,19,21	1.10	2 (11%)
4	NAG	X	2	4	14,14,15	0.54	0	17,19,21	1.51	1 (5%)
4	BMA	X	3	4	11,11,12	1.15	1 (9%)	15,15,17	1.35	1 (6%)
4	MAN	X	4	4	11,11,12	1.38	1 (9%)	15,15,17	1.66	3 (20%)
4	MAN	X	5	4	11,11,12	1.17	1 (9%)	15,15,17	1.19	1 (6%)
4	MAN	X	6	4	11,11,12	2.68	6 (54%)	15,15,17	2.09	3 (20%)
4	MAN	X	7	4	11,11,12	1.55	2 (18%)	15,15,17	1.82	3 (20%)

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
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	1/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	1/1/1/1
4	MAN	I	7	4	-	2/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	3/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	0/6/23/26	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	2/2/19/22	1/1/1/1
4	MAN	O	5	4	-	1/2/19/22	1/1/1/1
4	MAN	O	6	4	-	0/2/19/22	1/1/1/1
4	MAN	O	7	4	-	2/2/19/22	0/1/1/1
6	NAG	P	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	1/2/19/22	1/1/1/1
6	NAG	R	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	4/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	BMA	X	3	4	-	2/2/19/22	0/1/1/1
4	MAN	X	4	4	-	2/2/19/22	1/1/1/1
4	MAN	X	5	4	-	0/2/19/22	1/1/1/1
4	MAN	X	6	4	-	0/2/19/22	1/1/1/1
4	MAN	X	7	4	-	2/2/19/22	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1	NAG	O5-C1	5.33	1.52	1.43
4	I	7	MAN	O5-C1	-5.13	1.35	1.43
4	X	6	MAN	O5-C1	5.06	1.51	1.43
8	Q	3	BMA	C4-C5	4.92	1.63	1.53
4	I	6	MAN	O5-C5	4.51	1.52	1.43
8	Q	4	MAN	O5-C1	4.04	1.50	1.43
8	Q	3	BMA	C6-C5	4.02	1.65	1.51
4	O	7	MAN	O5-C1	-3.99	1.37	1.43
4	I	2	NAG	O5-C1	-3.98	1.37	1.43
4	I	6	MAN	O5-C1	3.91	1.50	1.43
7	W	3	BMA	C2-C3	3.89	1.58	1.52
8	Q	5	MAN	O5-C5	3.85	1.51	1.43
7	W	3	BMA	C1-C2	3.81	1.60	1.52
4	I	5	MAN	C4-C5	3.79	1.61	1.53
4	O	7	MAN	O2-C2	3.77	1.51	1.43
7	N	2	NAG	O5-C1	-3.75	1.37	1.43
7	N	3	BMA	C4-C3	3.68	1.61	1.52
4	X	4	MAN	O3-C3	3.63	1.51	1.43
4	I	6	MAN	C6-C5	3.63	1.64	1.51
4	O	6	MAN	C4-C3	3.62	1.61	1.52
4	X	6	MAN	O5-C5	3.60	1.50	1.43
8	Q	5	MAN	O5-C1	3.56	1.49	1.43
4	O	6	MAN	O5-C1	3.54	1.49	1.43
4	O	6	MAN	O3-C3	3.54	1.51	1.43
4	O	4	MAN	O3-C3	3.46	1.51	1.43
4	X	6	MAN	C1-C2	3.41	1.60	1.52
4	I	7	MAN	C4-C5	3.29	1.60	1.53
4	I	1	NAG	O5-C1	-3.29	1.38	1.43
4	I	3	BMA	O6-C6	3.27	1.56	1.42
4	O	6	MAN	C2-C3	-3.25	1.47	1.52
5	J	3	BMA	C2-C3	-3.23	1.47	1.52
4	O	6	MAN	C1-C2	3.22	1.59	1.52
4	I	3	BMA	C6-C5	3.22	1.62	1.51
4	X	6	MAN	C6-C5	3.13	1.62	1.51
4	I	5	MAN	C1-C2	3.07	1.59	1.52
4	O	6	MAN	C6-C5	3.02	1.62	1.51
4	I	4	MAN	O3-C3	3.00	1.50	1.43
4	X	7	MAN	O5-C1	-2.98	1.39	1.43
4	I	6	MAN	O2-C2	-2.97	1.37	1.43
7	W	3	BMA	C4-C3	2.94	1.59	1.52
4	I	7	MAN	O5-C5	2.89	1.49	1.43
4	O	7	MAN	O5-C5	2.85	1.49	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	4	MAN	C1-C2	2.84	1.58	1.52
8	Q	3	BMA	C2-C3	2.83	1.56	1.52
4	X	5	MAN	C1-C2	2.82	1.58	1.52
8	Q	4	MAN	O5-C5	2.78	1.49	1.43
4	X	6	MAN	C4-C3	2.75	1.59	1.52
5	J	3	BMA	C4-C3	2.73	1.59	1.52
4	I	3	BMA	O5-C5	2.71	1.48	1.43
8	Q	5	MAN	C1-C2	2.63	1.58	1.52
4	O	7	MAN	C4-C5	2.63	1.58	1.53
7	N	3	BMA	C2-C3	2.62	1.56	1.52
5	J	3	BMA	C1-C2	-2.60	1.46	1.52
4	O	5	MAN	C1-C2	2.60	1.58	1.52
7	N	3	BMA	C6-C5	2.56	1.60	1.51
4	I	6	MAN	C4-C3	2.52	1.58	1.52
4	O	5	MAN	O5-C1	2.51	1.47	1.43
4	O	7	MAN	C1-C2	2.51	1.57	1.52
6	V	1	NAG	O5-C1	2.49	1.47	1.43
7	N	3	BMA	C1-C2	2.49	1.57	1.52
4	X	7	MAN	O5-C5	2.48	1.48	1.43
4	O	6	MAN	O2-C2	-2.43	1.38	1.43
4	I	7	MAN	O2-C2	2.42	1.48	1.43
4	I	6	MAN	C2-C3	-2.41	1.49	1.52
4	I	5	MAN	O5-C5	2.39	1.48	1.43
4	I	6	MAN	O3-C3	2.39	1.48	1.43
8	Q	5	MAN	C4-C5	2.38	1.58	1.53
8	Q	5	MAN	C4-C3	2.30	1.58	1.52
4	X	6	MAN	O3-C3	2.29	1.48	1.43
4	O	4	MAN	C1-C2	-2.23	1.47	1.52
4	I	5	MAN	C2-C3	2.17	1.55	1.52
8	Q	3	BMA	O3-C3	2.17	1.48	1.43
7	W	3	BMA	C6-C5	2.16	1.59	1.51
4	O	3	BMA	C2-C3	-2.16	1.49	1.52
4	I	3	BMA	O2-C2	-2.15	1.38	1.43
4	I	4	MAN	C2-C3	2.11	1.55	1.52
4	O	5	MAN	O5-C5	2.11	1.47	1.43
4	I	6	MAN	C1-C2	2.07	1.56	1.52
4	I	3	BMA	O5-C1	2.07	1.47	1.43
5	J	3	BMA	O5-C1	-2.04	1.40	1.43
4	X	3	BMA	C2-C3	-2.03	1.49	1.52
5	J	4	MAN	O5-C5	2.03	1.47	1.43
5	J	4	MAN	C4-C3	2.03	1.57	1.52
4	I	3	BMA	O3-C3	-2.02	1.38	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	4	MAN	C1-C2	-2.02	1.47	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	8.39	123.56	112.19
8	Q	4	MAN	C1-O5-C5	7.67	122.59	112.19
6	V	1	NAG	C1-O5-C5	7.34	122.13	112.19
4	I	2	NAG	C1-O5-C5	7.10	121.81	112.19
6	R	1	NAG	C1-O5-C5	6.78	121.37	112.19
6	U	1	NAG	C1-O5-C5	6.21	120.61	112.19
4	O	2	NAG	C1-O5-C5	6.20	120.60	112.19
4	I	6	MAN	O5-C5-C6	5.88	116.43	107.20
6	K	1	NAG	C1-O5-C5	5.68	119.88	112.19
6	S	1	NAG	C1-O5-C5	5.62	119.81	112.19
4	O	7	MAN	O5-C1-C2	-5.41	102.42	110.77
4	X	2	NAG	C1-O5-C5	5.32	119.40	112.19
4	X	6	MAN	O5-C5-C6	5.25	115.43	107.20
4	X	7	MAN	O5-C1-C2	-5.01	103.03	110.77
8	Q	3	BMA	C6-C5-C4	4.69	123.98	113.00
6	M	1	NAG	C3-C4-C5	4.48	118.24	110.24
4	O	5	MAN	C1-O5-C5	4.44	118.21	112.19
4	I	7	MAN	O5-C1-C2	-4.40	103.97	110.77
4	X	4	MAN	C1-O5-C5	4.09	117.73	112.19
7	N	3	BMA	O5-C5-C6	4.08	113.60	107.20
4	I	3	BMA	C1-O5-C5	4.05	117.68	112.19
4	O	6	MAN	O5-C5-C6	4.02	113.51	107.20
4	O	6	MAN	O2-C2-C3	-3.98	102.17	110.14
5	J	4	MAN	C1-O5-C5	3.91	117.49	112.19
4	O	4	MAN	C1-O5-C5	3.90	117.48	112.19
4	O	3	BMA	C1-O5-C5	3.82	117.37	112.19
4	X	6	MAN	C1-O5-C5	3.76	117.29	112.19
6	S	1	NAG	C3-C4-C5	3.73	116.89	110.24
4	I	4	MAN	C1-O5-C5	3.69	117.19	112.19
4	X	5	MAN	C1-O5-C5	3.63	117.11	112.19
8	Q	3	BMA	O3-C3-C2	3.62	116.94	109.99
6	R	2	NAG	C1-O5-C5	3.61	117.08	112.19
8	Q	3	BMA	C1-O5-C5	3.56	117.02	112.19
5	J	3	BMA	O3-C3-C2	-3.55	103.19	109.99
7	N	3	BMA	C1-C2-C3	3.48	113.94	109.67
4	X	1	NAG	C2-N2-C7	3.39	127.74	122.90
4	I	6	MAN	O2-C2-C3	-3.36	103.42	110.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	3	BMA	C1-O5-C5	3.34	116.72	112.19
7	W	3	BMA	O5-C5-C6	3.25	112.30	107.20
4	I	4	MAN	O3-C3-C2	3.15	116.02	109.99
4	X	4	MAN	O3-C3-C2	3.13	115.99	109.99
4	I	3	BMA	O5-C5-C6	2.96	111.84	107.20
7	W	3	BMA	C1-C2-C3	2.93	113.27	109.67
4	I	2	NAG	O5-C5-C6	-2.90	102.66	107.20
8	Q	3	BMA	O6-C6-C5	2.89	121.20	111.29
4	X	7	MAN	O2-C2-C3	-2.88	104.37	110.14
4	X	6	MAN	O2-C2-C3	-2.85	104.43	110.14
5	J	4	MAN	O5-C1-C2	2.84	115.16	110.77
4	I	7	MAN	O2-C2-C3	-2.81	104.51	110.14
7	W	3	BMA	O2-C2-C1	2.76	114.81	109.15
4	O	3	BMA	O2-C2-C3	-2.70	104.72	110.14
6	V	1	NAG	C3-C4-C5	2.69	115.04	110.24
4	O	6	MAN	C1-O5-C5	2.66	115.80	112.19
4	I	3	BMA	C3-C4-C5	2.65	114.97	110.24
7	N	3	BMA	C6-C5-C4	2.65	119.21	113.00
4	O	4	MAN	O3-C3-C2	2.64	115.06	109.99
8	Q	4	MAN	O5-C1-C2	2.62	114.82	110.77
7	N	3	BMA	O5-C5-C4	-2.61	104.48	110.83
8	Q	1	NAG	C1-O5-C5	2.60	115.72	112.19
4	I	5	MAN	C1-O5-C5	-2.58	108.70	112.19
8	Q	5	MAN	C1-C2-C3	-2.58	106.50	109.67
7	W	3	BMA	C2-C3-C4	2.53	115.28	110.89
4	O	7	MAN	O2-C2-C3	-2.53	105.07	110.14
6	M	1	NAG	O6-C6-C5	2.53	119.96	111.29
5	J	3	BMA	O2-C2-C3	-2.49	105.16	110.14
7	N	3	BMA	C2-C3-C4	2.47	115.17	110.89
4	I	7	MAN	O2-C2-C1	2.47	114.21	109.15
4	I	6	MAN	C1-O5-C5	2.46	115.52	112.19
6	U	1	NAG	C3-C4-C5	2.46	114.62	110.24
5	J	3	BMA	C3-C4-C5	2.43	114.57	110.24
5	J	3	BMA	C1-O5-C5	2.40	115.45	112.19
7	N	3	BMA	C1-O5-C5	-2.37	108.98	112.19
4	O	7	MAN	C3-C4-C5	2.26	114.27	110.24
4	I	6	MAN	O5-C5-C4	-2.26	105.34	110.83
7	N	3	BMA	O3-C3-C4	2.26	115.56	110.35
8	Q	3	BMA	C3-C4-C5	2.25	114.25	110.24
4	X	7	MAN	C3-C4-C5	2.23	114.22	110.24
4	I	6	MAN	O3-C3-C2	2.22	114.25	109.99
4	I	5	MAN	C1-C2-C3	-2.21	106.95	109.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	5	MAN	O5-C1-C2	-2.21	107.36	110.77
4	I	7	MAN	O6-C6-C5	-2.20	103.73	111.29
5	J	4	MAN	O2-C2-C1	2.19	113.64	109.15
8	Q	5	MAN	O5-C5-C6	2.17	110.61	107.20
8	Q	3	BMA	O5-C5-C6	-2.17	103.80	107.20
7	W	1	NAG	C1-O5-C5	2.13	115.07	112.19
7	W	3	BMA	O5-C1-C2	2.11	114.03	110.77
7	W	3	BMA	O5-C5-C4	-2.11	105.70	110.83
8	Q	1	NAG	O6-C6-C5	2.09	118.47	111.29
4	X	4	MAN	O5-C5-C4	-2.07	105.79	110.83
4	X	1	NAG	O4-C4-C5	-2.06	104.19	109.30
8	Q	2	NAG	O4-C4-C5	-2.05	104.21	109.30
6	R	1	NAG	C3-C4-C5	2.04	113.88	110.24
6	K	1	NAG	C3-C4-C5	2.03	113.86	110.24

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	W	2	NAG	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
4	X	4	MAN	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	O	7	MAN	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
4	O	4	MAN	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
4	I	4	MAN	C4-C5-C6-O6
4	X	7	MAN	O5-C5-C6-O6
4	O	4	MAN	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	X	2	NAG	O5-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	I	7	MAN	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
6	K	1	NAG	C4-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
4	I	7	MAN	C4-C5-C6-O6
4	X	7	MAN	C4-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
4	O	7	MAN	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
7	N	3	BMA	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
8	Q	5	MAN	C4-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
4	O	5	MAN	O5-C5-C6-O6

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Q	5	MAN	C1-C2-C3-C4-C5-O5
4	O	5	MAN	C1-C2-C3-C4-C5-O5
4	O	4	MAN	C1-C2-C3-C4-C5-O5
4	X	4	MAN	C1-C2-C3-C4-C5-O5
4	O	6	MAN	C1-C2-C3-C4-C5-O5
4	X	5	MAN	C1-C2-C3-C4-C5-O5
4	X	6	MAN	C1-C2-C3-C4-C5-O5
4	I	4	MAN	C1-C2-C3-C4-C5-O5
4	I	6	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	1	NAG	1	0
4	I	6	MAN	1	0
6	R	2	NAG	2	0

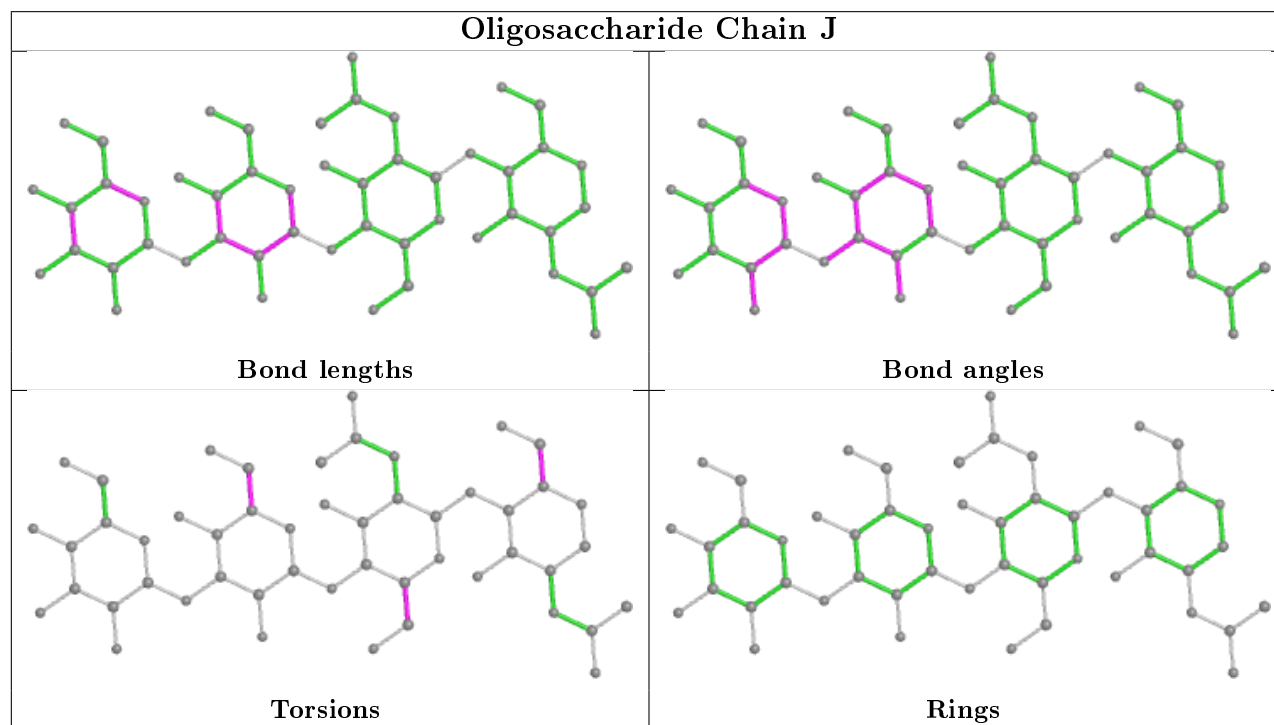
*Continued on next page...*

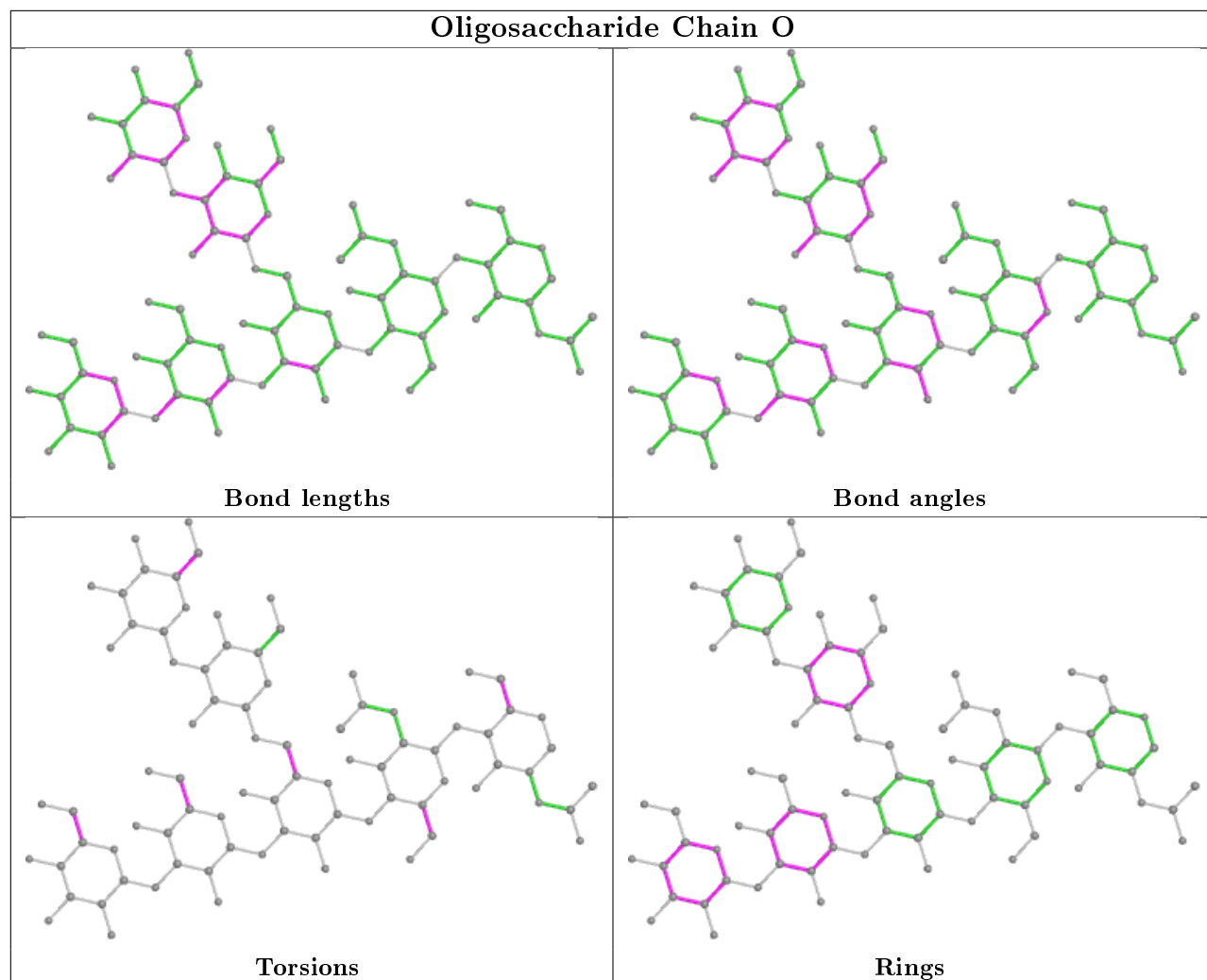


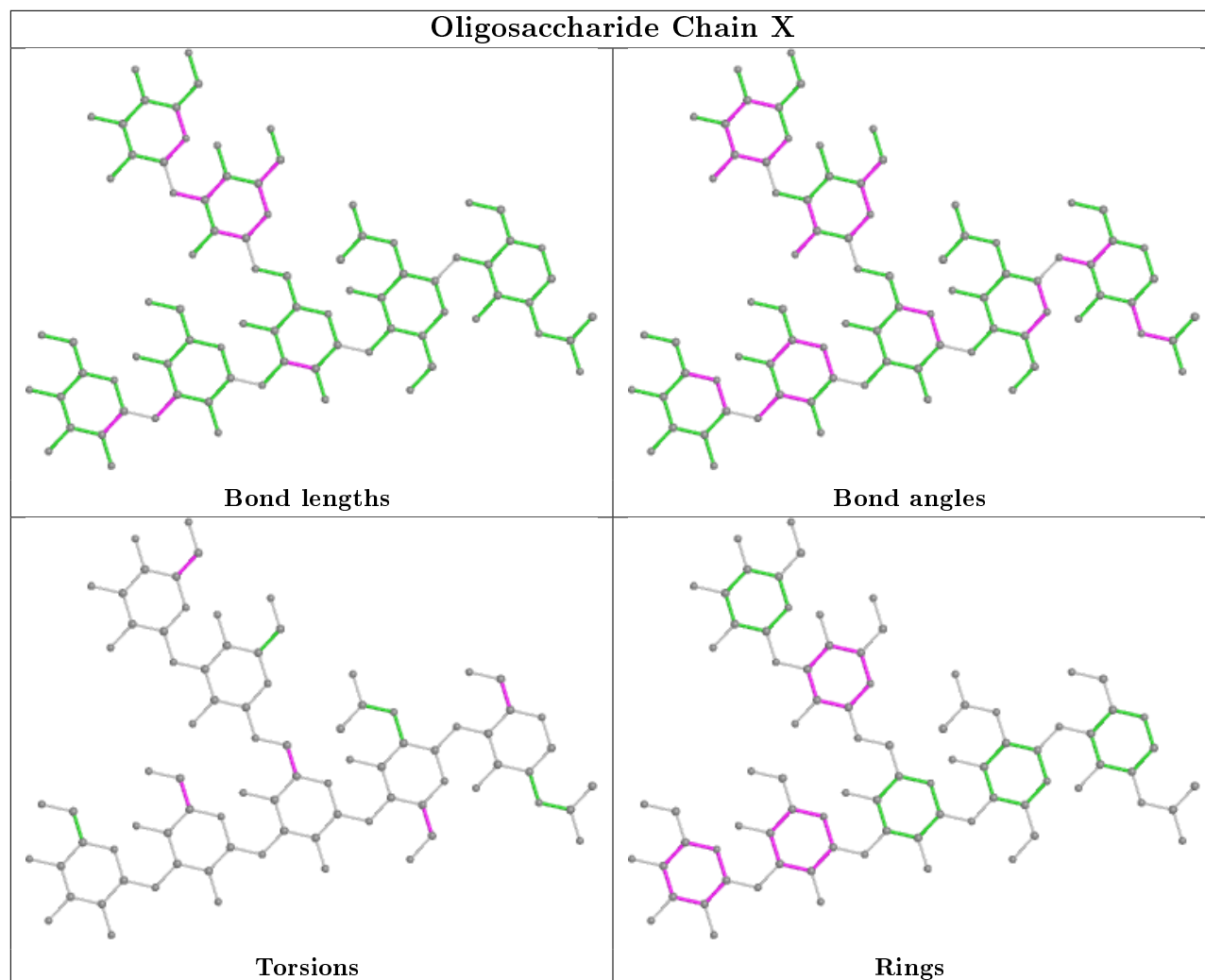
*Continued from previous page...*

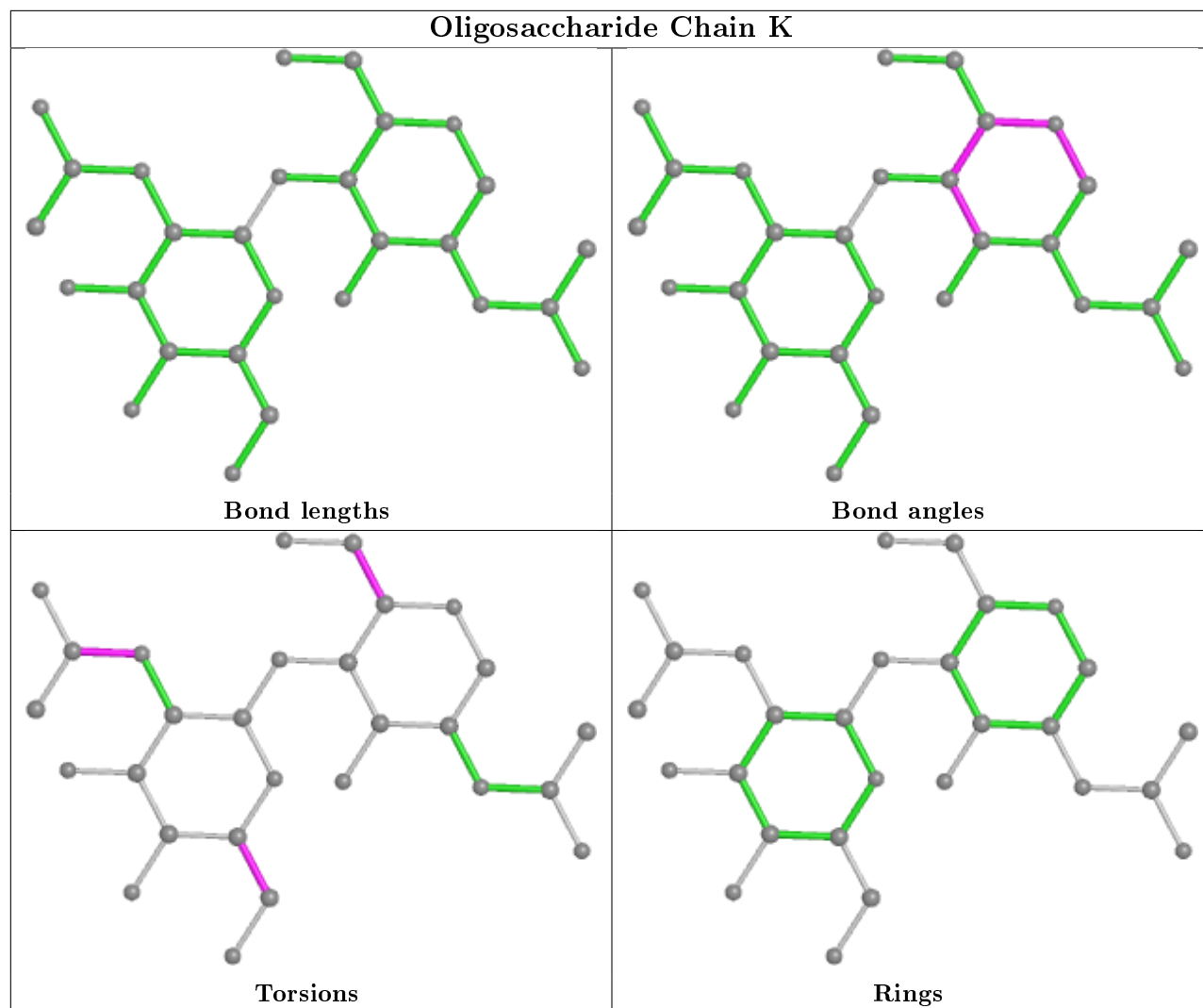
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	2	0
4	O	6	MAN	1	0
4	X	4	MAN	1	0
4	X	3	BMA	1	0
4	I	7	MAN	1	0
4	X	7	MAN	1	0
4	O	4	MAN	2	0
4	X	6	MAN	1	0
4	X	5	MAN	1	0
4	O	7	MAN	1	0
6	U	2	NAG	2	0
4	O	5	MAN	2	0
4	O	1	NAG	1	0
4	I	3	BMA	1	0
4	O	3	BMA	1	0

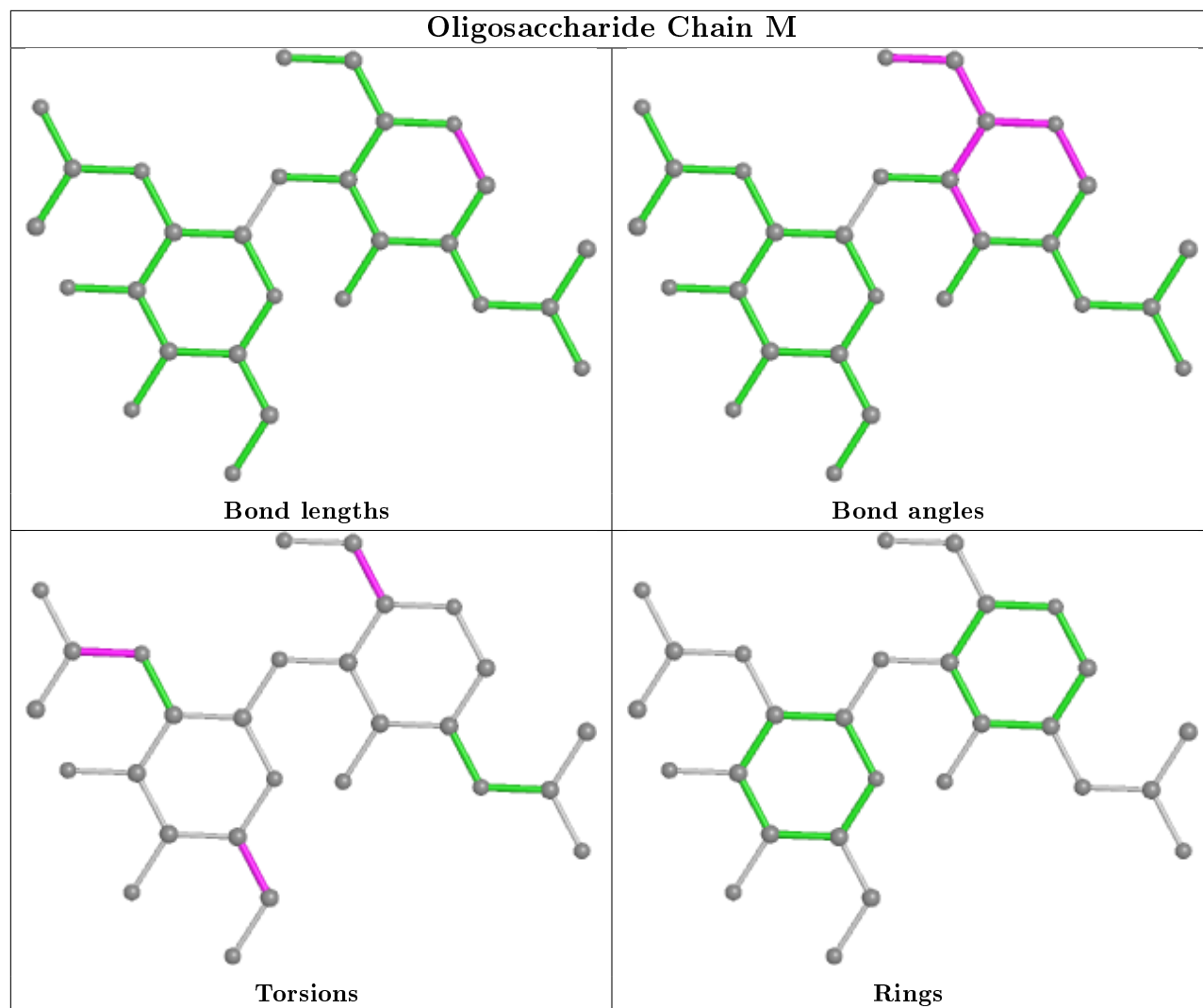
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

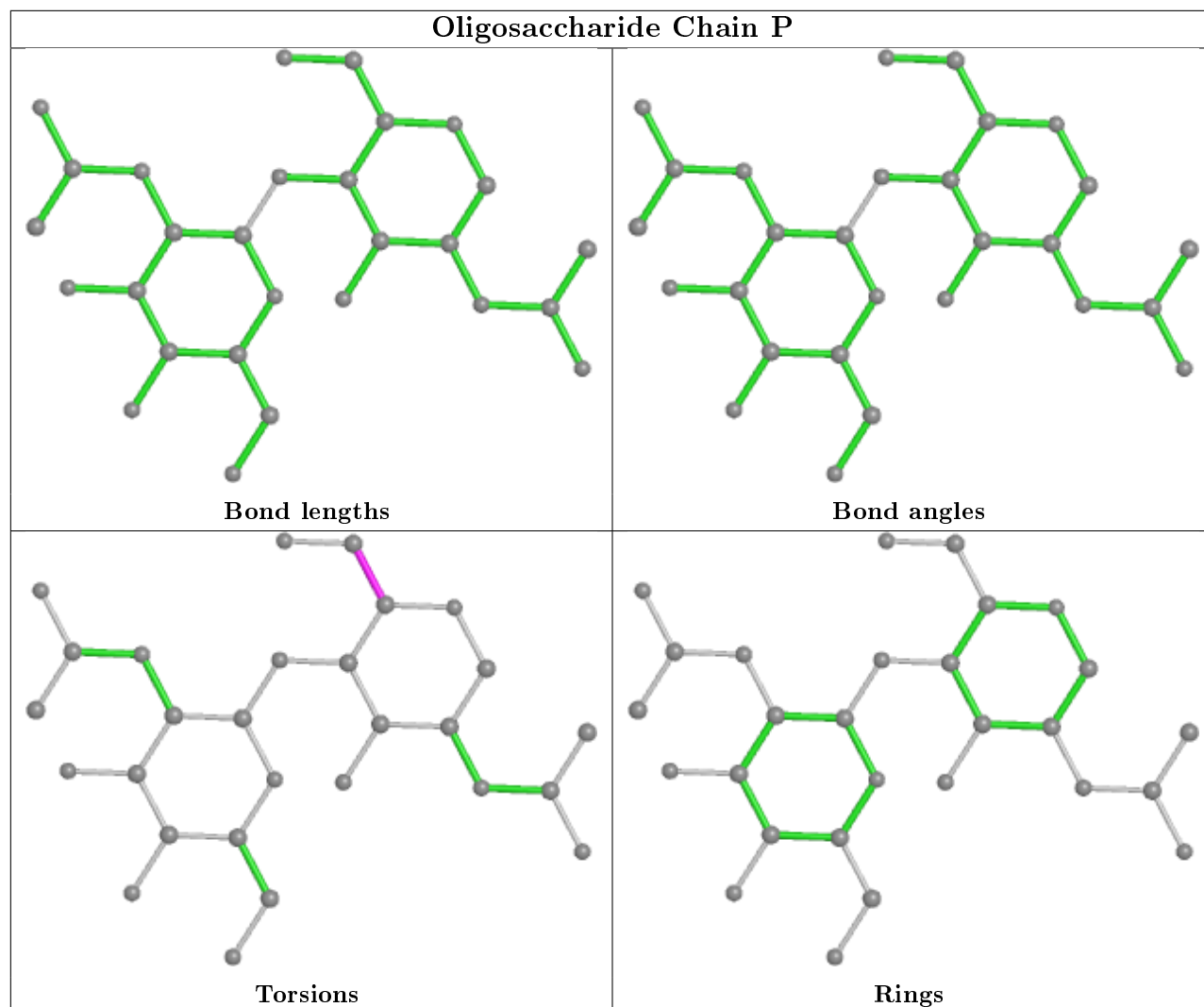


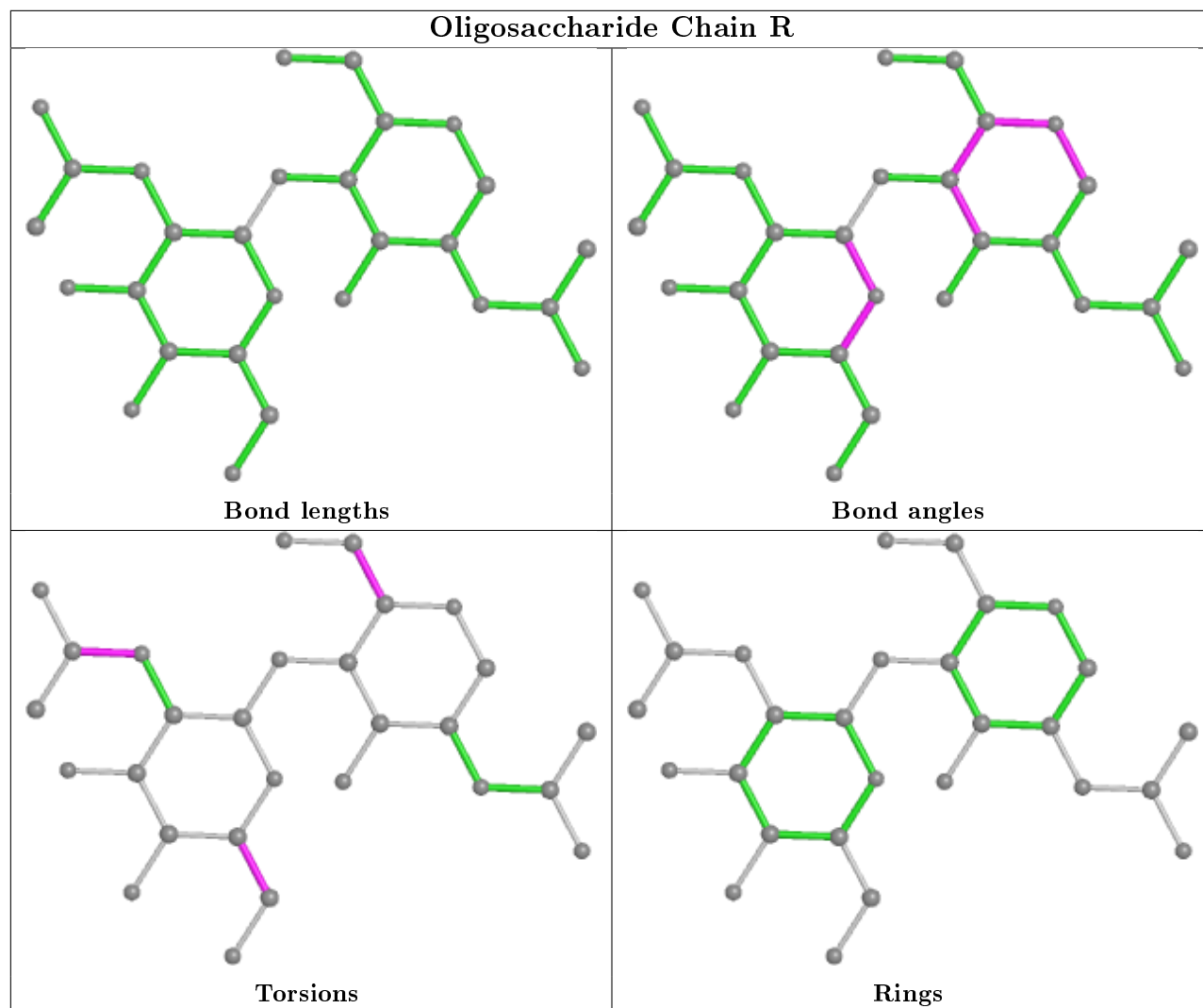


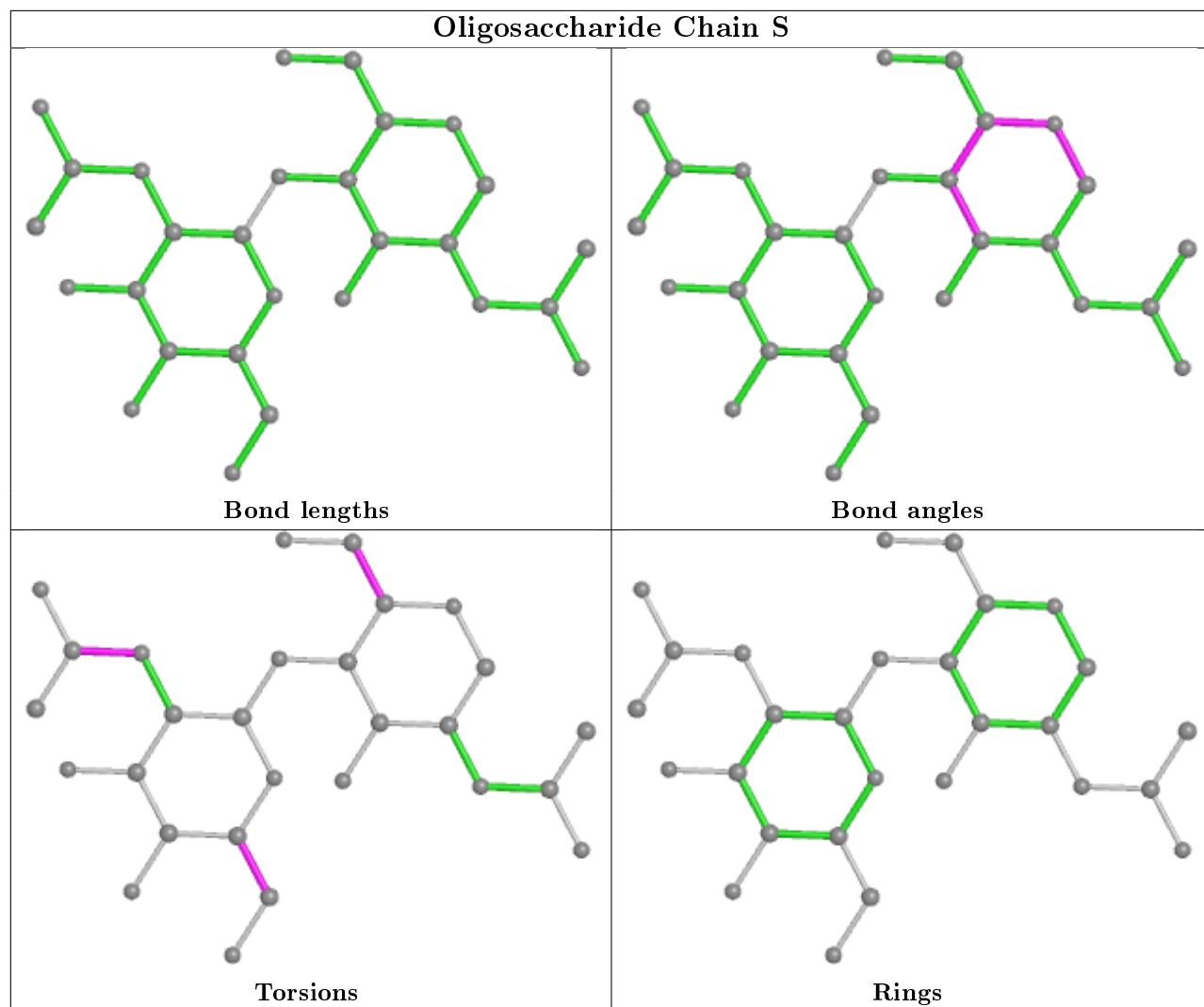




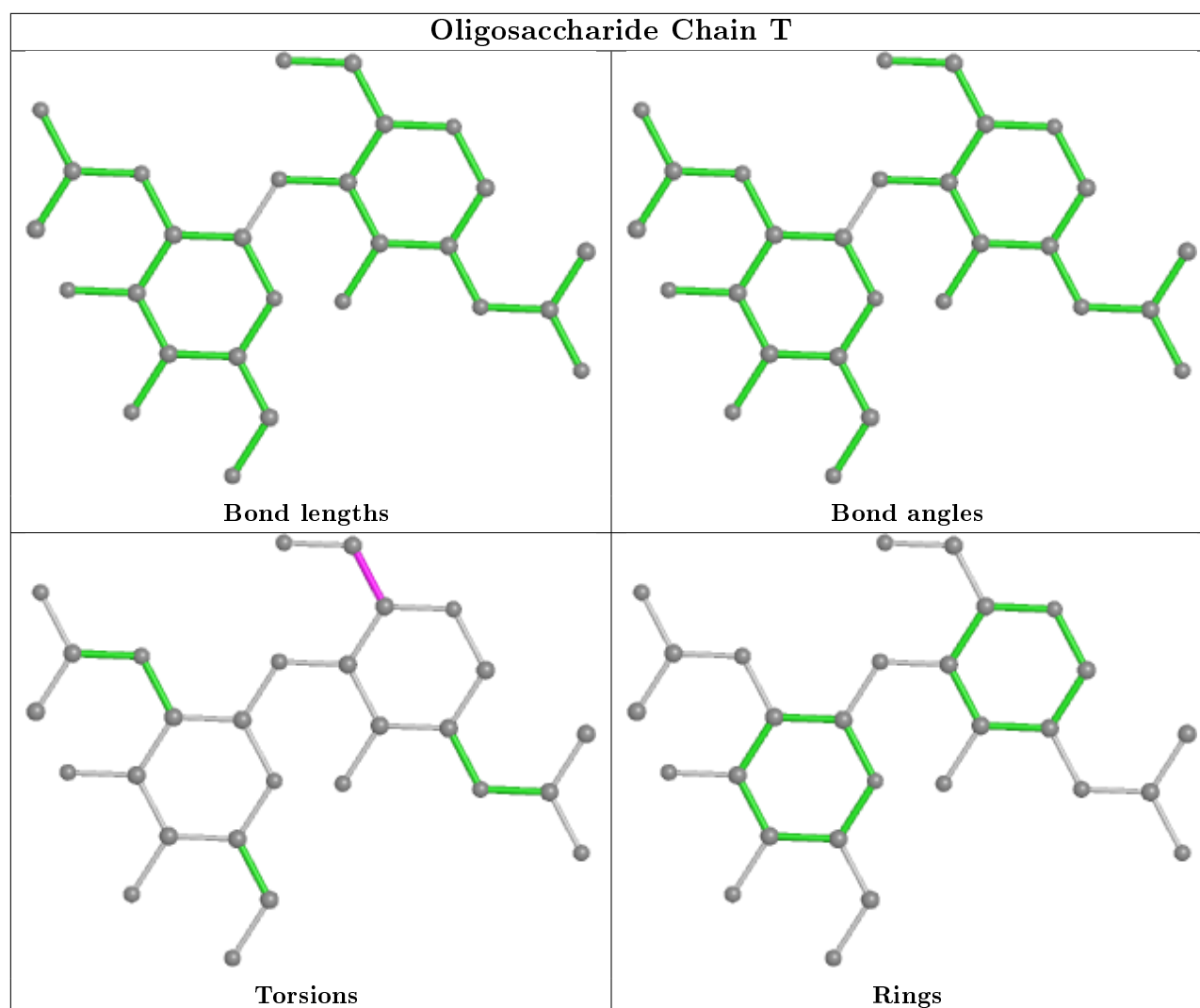


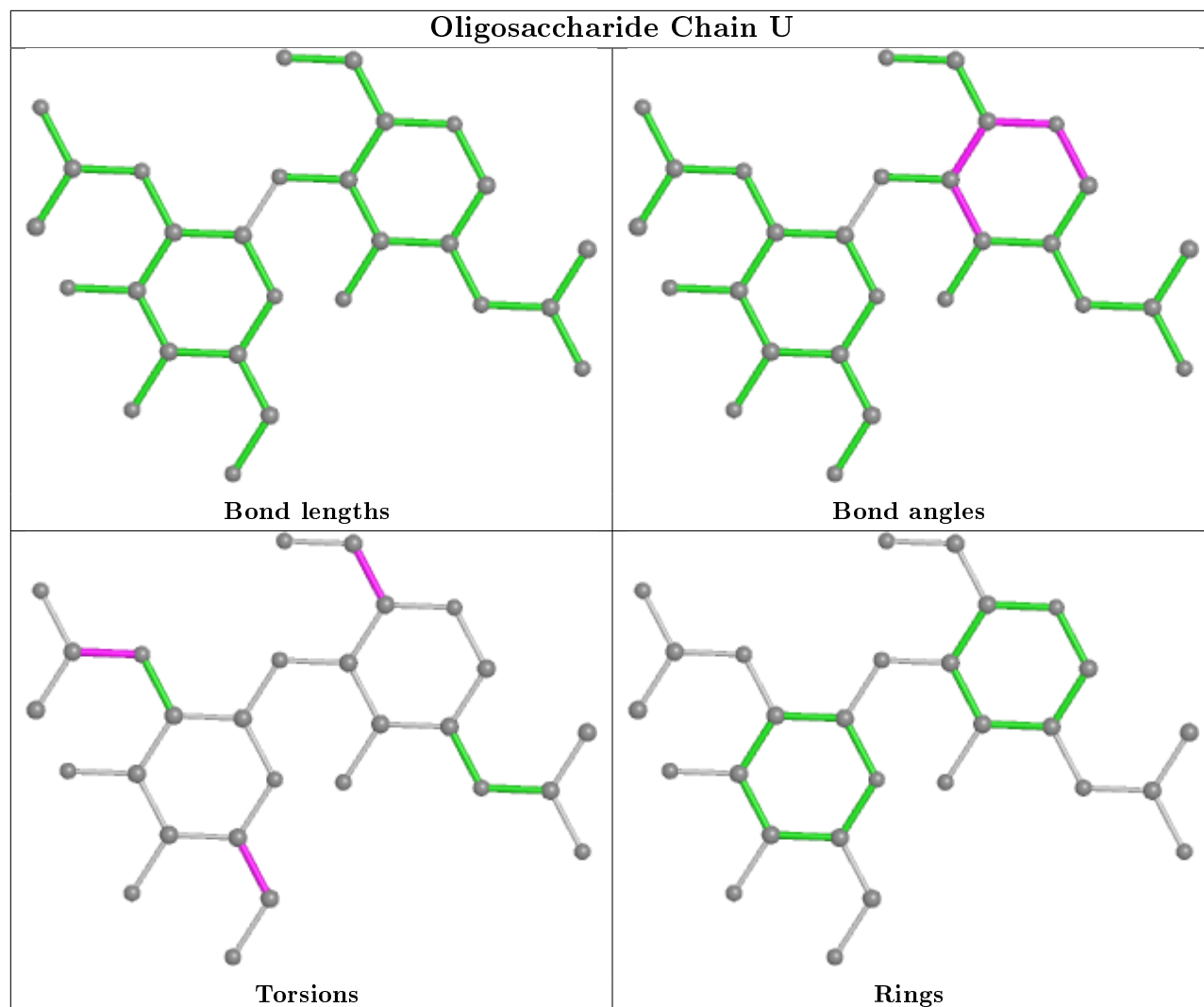


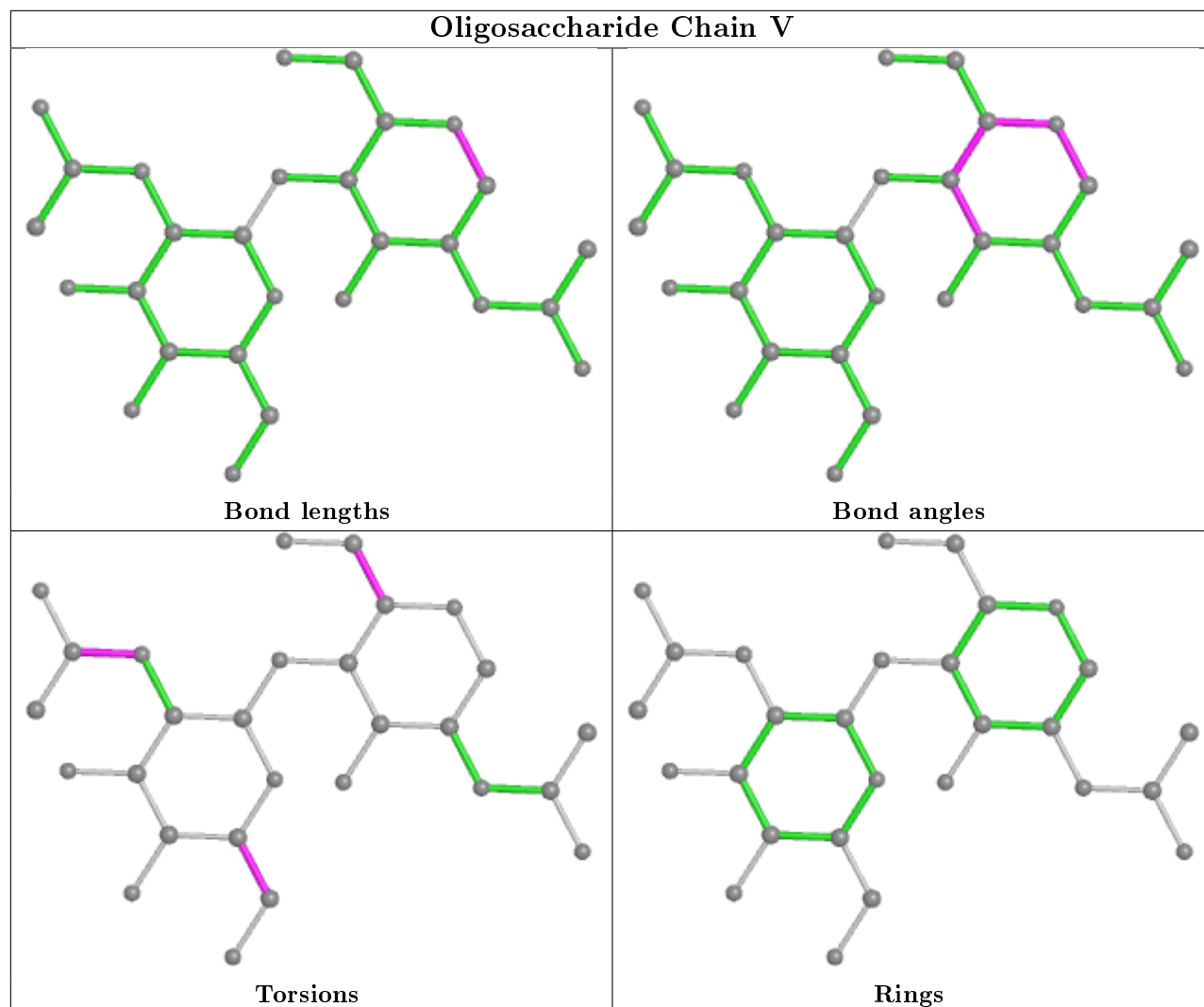


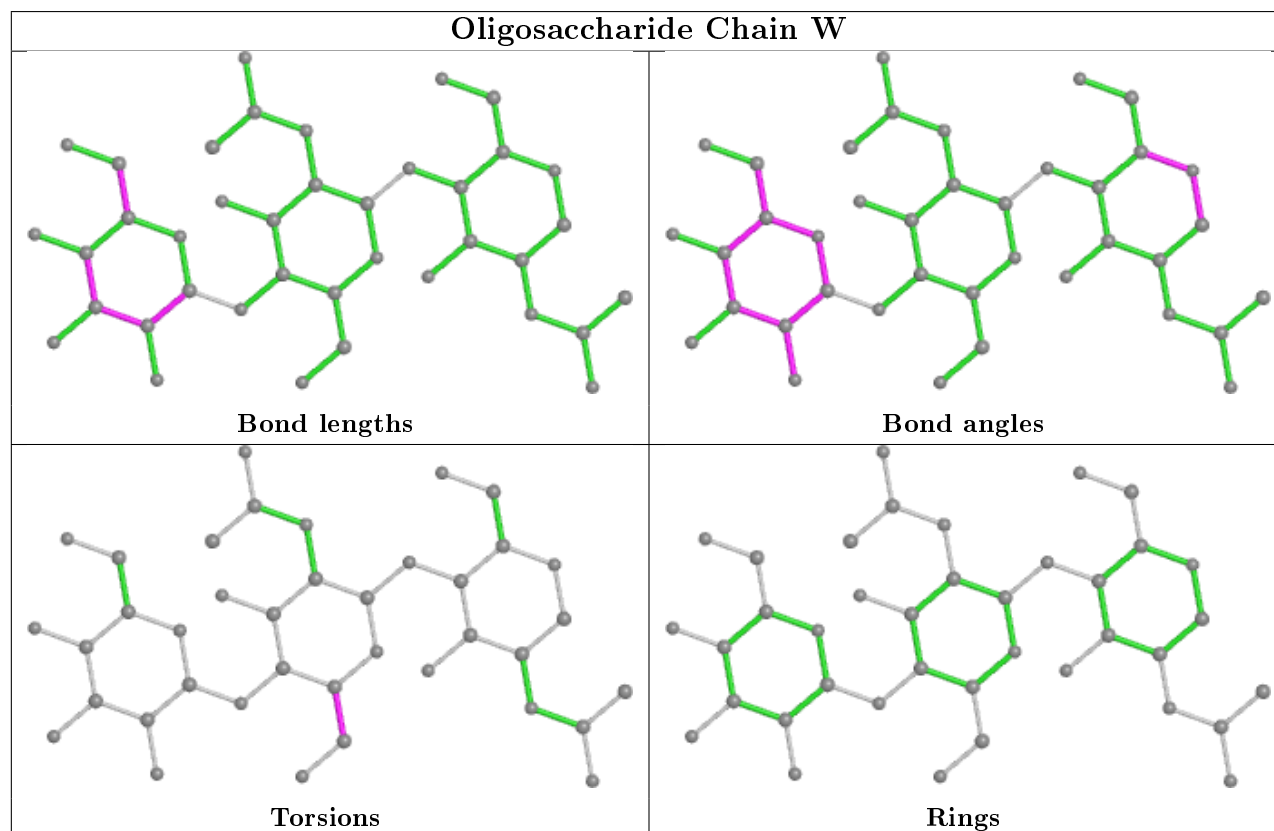
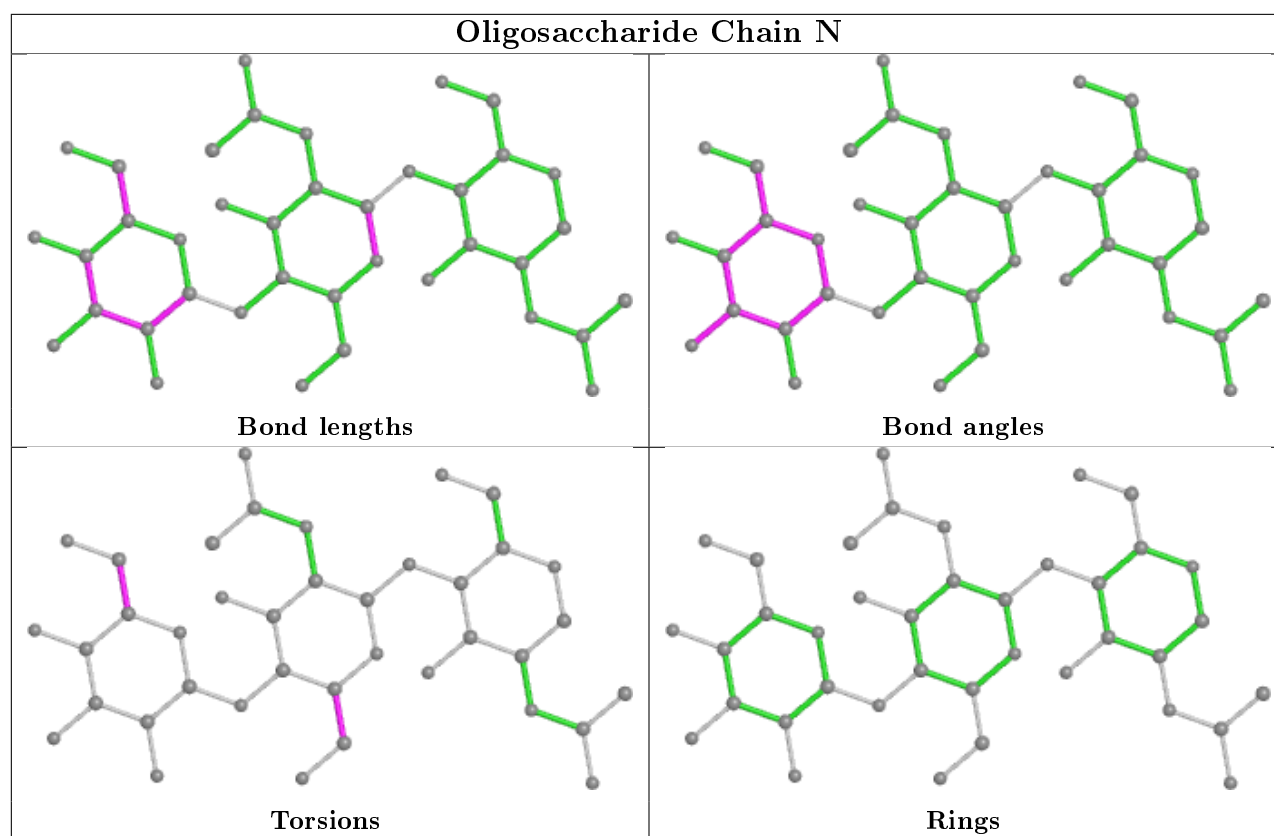


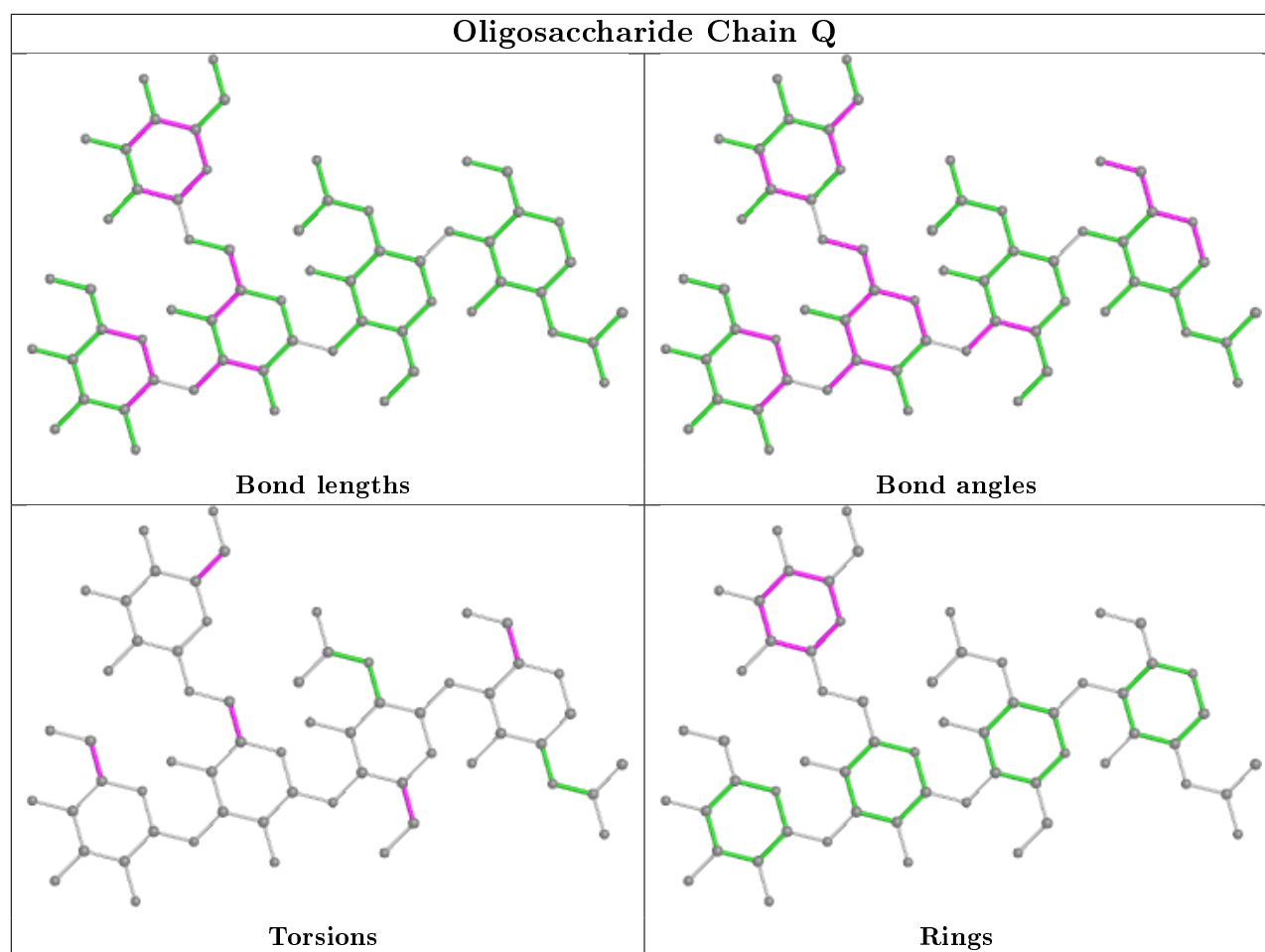












## 5.6 Ligand geometry [i](#)

9 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	408	1	14,14,15	0.29	0	17,19,21	0.44	0
9	NAG	C	501	1	14,14,15	0.29	0	17,19,21	0.45	0
9	NAG	A	409	1	14,14,15	1.35	2 (14%)	17,19,21	0.88	1 (5%)
9	NAG	C	503	1	14,14,15	1.26	1 (7%)	17,19,21	1.11	2 (11%)
9	NAG	B	410	1	14,14,15	1.25	1 (7%)	17,19,21	1.16	2 (11%)
9	NAG	A	410	1	14,14,15	1.43	1 (7%)	17,19,21	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	B	409	1	14,14,15	0.30	0	17,19,21	0.58	0
9	NAG	C	502	1	14,14,15	0.94	1 (7%)	17,19,21	0.74	1 (5%)
9	NAG	B	408	1	14,14,15	0.47	0	17,19,21	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	408	1	-	2/6/23/26	0/1/1/1
9	NAG	C	501	1	-	0/6/23/26	0/1/1/1
9	NAG	A	409	1	-	4/6/23/26	0/1/1/1
9	NAG	C	503	1	-	4/6/23/26	0/1/1/1
9	NAG	B	410	1	-	4/6/23/26	0/1/1/1
9	NAG	A	410	1	-	4/6/23/26	0/1/1/1
9	NAG	B	409	1	-	0/6/23/26	0/1/1/1
9	NAG	C	502	1	-	2/6/23/26	0/1/1/1
9	NAG	B	408	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	410	NAG	O5-C1	-5.19	1.35	1.43
9	B	410	NAG	O5-C1	-4.47	1.36	1.43
9	C	503	NAG	O5-C1	-4.32	1.36	1.43
9	A	409	NAG	O5-C1	4.31	1.50	1.43
9	C	502	NAG	O5-C1	2.90	1.48	1.43
9	A	409	NAG	C1-C2	2.33	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	410	NAG	C1-O5-C5	-2.95	108.20	112.19
9	C	503	NAG	C1-O5-C5	-2.76	108.45	112.19
9	B	410	NAG	C3-C4-C5	2.75	115.14	110.24
9	C	503	NAG	C3-C4-C5	2.72	115.09	110.24
9	A	410	NAG	C3-C4-C5	2.60	114.88	110.24
9	C	502	NAG	C1-O5-C5	2.50	115.57	112.19
9	A	410	NAG	C1-O5-C5	-2.43	108.90	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	409	NAG	C1-O5-C5	2.32	115.34	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	410	NAG	C1-C2-N2-C7
9	A	409	NAG	C4-C5-C6-O6
9	B	410	NAG	O5-C5-C6-O6
9	C	502	NAG	C4-C5-C6-O6
9	A	408	NAG	O5-C5-C6-O6
9	A	409	NAG	O5-C5-C6-O6
9	C	503	NAG	C1-C2-N2-C7
9	C	502	NAG	O5-C5-C6-O6
9	C	503	NAG	O5-C5-C6-O6
9	A	410	NAG	O5-C5-C6-O6
9	B	410	NAG	C4-C5-C6-O6
9	A	408	NAG	C4-C5-C6-O6
9	C	503	NAG	C4-C5-C6-O6
9	B	410	NAG	C1-C2-N2-C7
9	A	410	NAG	C4-C5-C6-O6
9	A	409	NAG	C1-C2-N2-C7
9	C	503	NAG	C3-C2-N2-C7
9	A	410	NAG	C3-C2-N2-C7
9	A	409	NAG	C3-C2-N2-C7
9	B	410	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	336/336 (100%)	-0.50	0 100 100	30, 47, 76, 97	0
1	B	336/336 (100%)	-0.41	0 100 100	38, 62, 96, 133	0
1	C	336/336 (100%)	-0.22	1 (0%) 94 84	43, 74, 117, 143	0
2	D	120/132 (90%)	0.31	4 (3%) 46 20	49, 92, 129, 157	0
2	F	120/132 (90%)	0.14	2 (1%) 70 41	43, 71, 107, 153	0
2	H	128/132 (96%)	-0.49	0 100 100	32, 44, 90, 147	0
3	E	111/111 (100%)	-0.23	0 100 100	45, 64, 95, 126	0
3	G	111/111 (100%)	-0.34	0 100 100	43, 57, 85, 103	0
3	L	111/111 (100%)	-0.51	0 100 100	33, 47, 72, 86	0
All	All	1709/1737 (98%)	-0.30	7 (0%) 92 79	30, 61, 106, 157	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	GLN	3.9
2	F	119	SER	3.5
2	F	120	SER	2.8
2	D	120	SER	2.7
2	D	23	LYS	2.1
1	C	133	SER	2.0
2	D	15	GLY	2.0

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

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



## 6.3 Carbohydrates

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.

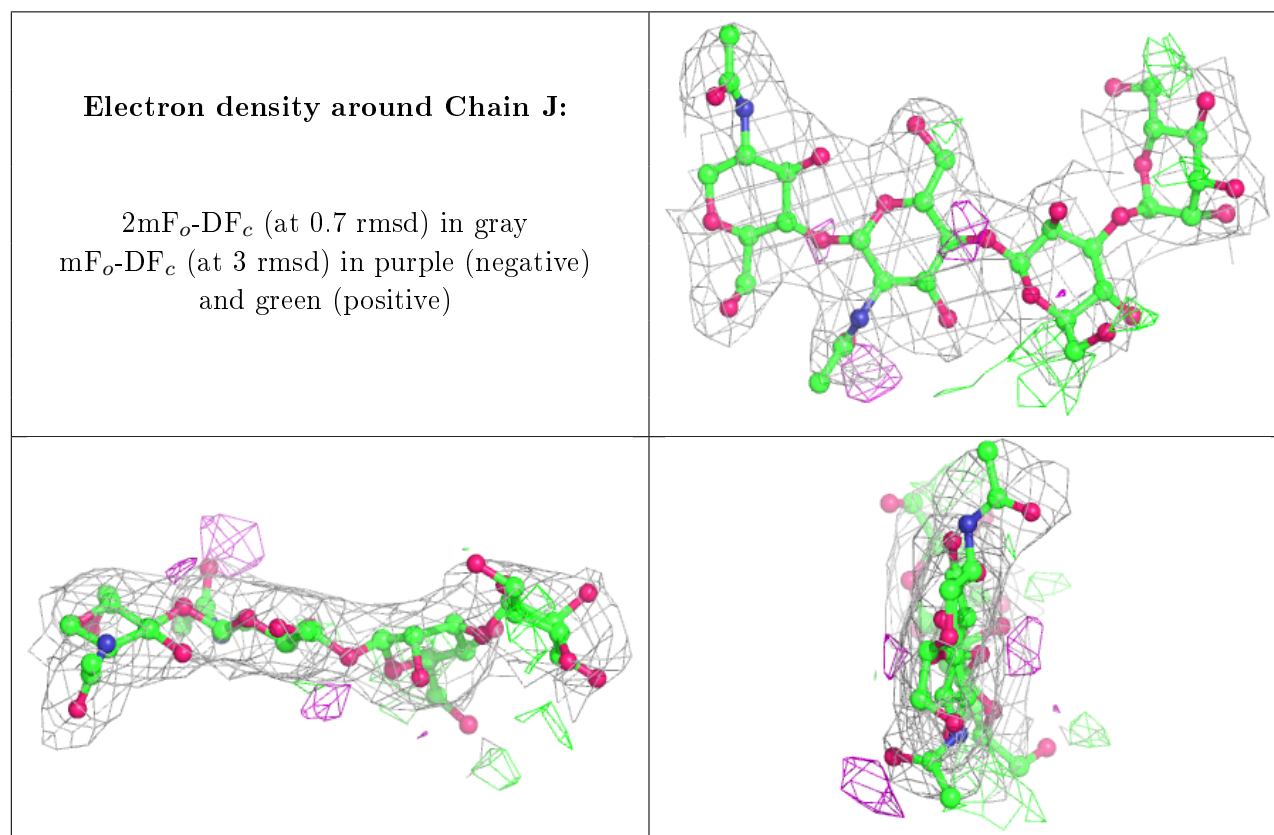
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	MAN	Q	4	11/12	0.66	0.33	137,146,156,159	0
4	MAN	X	6	11/12	0.76	0.18	60,86,96,103	0
6	NAG	S	2	14/15	0.76	0.49	131,163,173,176	0
4	MAN	X	5	11/12	0.77	0.27	131,145,152,154	0
6	NAG	P	1	14/15	0.77	0.29	122,143,148,149	0
6	NAG	P	2	14/15	0.79	0.37	126,147,152,152	0
4	MAN	I	5	11/12	0.80	0.29	82,113,122,123	0
4	MAN	O	5	11/12	0.81	0.28	114,126,140,140	0
8	MAN	Q	5	11/12	0.81	0.21	103,121,125,127	0
7	BMA	N	3	11/12	0.81	0.22	71,91,105,109	0
4	MAN	I	6	11/12	0.82	0.20	46,64,87,93	0
4	MAN	X	4	11/12	0.83	0.20	107,115,126,135	0
6	NAG	V	2	14/15	0.83	0.23	131,160,174,179	0
7	BMA	W	3	11/12	0.84	0.21	78,104,116,117	0
8	BMA	Q	3	11/12	0.85	0.17	89,96,115,123	0
5	MAN	J	4	11/12	0.85	0.19	118,128,135,137	0
4	MAN	X	7	11/12	0.85	0.19	70,97,106,107	0
4	MAN	O	7	11/12	0.86	0.20	69,86,96,96	0
6	NAG	S	1	14/15	0.86	0.22	76,87,107,138	0
6	NAG	V	1	14/15	0.87	0.14	56,91,109,130	0
6	NAG	R	2	14/15	0.88	0.24	63,95,121,124	0
6	NAG	M	2	14/15	0.88	0.33	107,117,129,143	0
4	MAN	O	6	11/12	0.88	0.16	62,88,104,113	0
4	MAN	I	4	11/12	0.88	0.22	64,81,93,112	0
6	NAG	R	1	14/15	0.89	0.18	58,66,81,86	0
6	NAG	U	2	14/15	0.89	0.23	71,89,103,115	0
4	MAN	I	7	11/12	0.90	0.19	52,69,75,78	0
6	NAG	M	1	14/15	0.90	0.15	43,66,84,104	0
6	NAG	U	1	14/15	0.90	0.15	53,74,87,90	0
6	NAG	K	2	14/15	0.91	0.24	64,86,91,92	0
5	BMA	J	3	11/12	0.91	0.20	88,108,124,130	0
4	MAN	O	4	11/12	0.91	0.17	71,89,110,119	0
6	NAG	T	2	14/15	0.91	0.34	128,143,157,162	0
8	NAG	Q	1	14/15	0.92	0.19	40,51,77,87	0
7	NAG	W	2	14/15	0.95	0.20	97,104,120,123	0
8	NAG	Q	2	14/15	0.95	0.17	44,69,79,81	0
6	NAG	T	1	14/15	0.95	0.24	78,96,115,116	0

*Continued on next page...*

*Continued from previous page...*

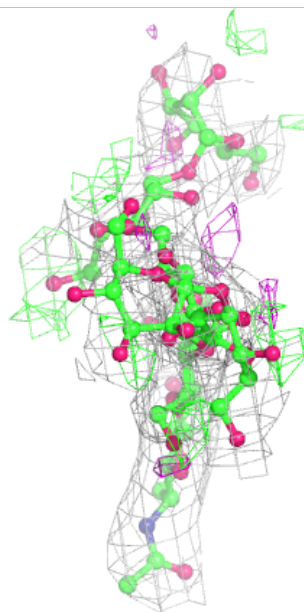
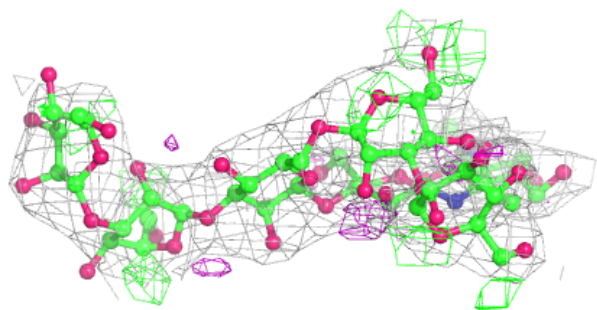
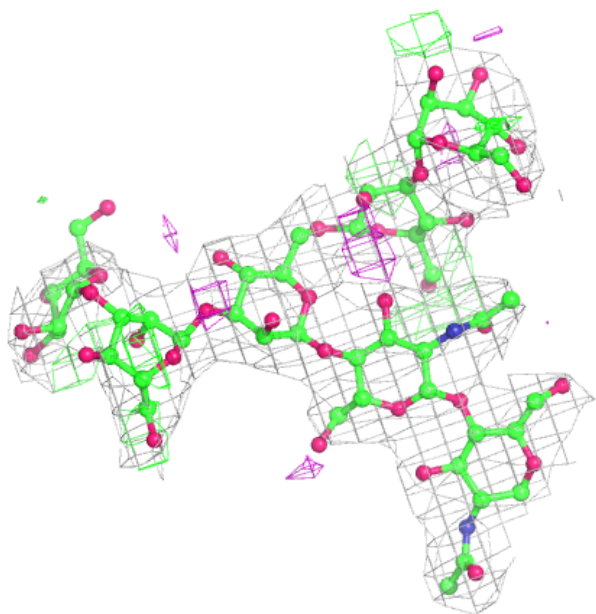
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	X	1	14/15	0.95	0.15	57,63,89,96	0
4	NAG	X	2	14/15	0.95	0.20	55,65,100,106	0
4	BMA	X	3	11/12	0.96	0.09	81,89,95,105	0
5	NAG	J	2	14/15	0.96	0.17	40,55,69,71	0
6	NAG	K	1	14/15	0.96	0.14	36,51,68,69	0
7	NAG	W	1	14/15	0.96	0.17	76,84,110,117	0
5	NAG	J	1	14/15	0.97	0.16	35,37,50,55	0
7	NAG	N	2	14/15	0.97	0.24	54,70,82,87	0
7	NAG	N	1	14/15	0.97	0.17	50,56,66,70	0
4	BMA	O	3	11/12	0.97	0.10	56,66,75,78	0
4	NAG	O	2	14/15	0.98	0.15	36,50,63,85	0
4	NAG	I	2	14/15	0.98	0.17	27,34,52,64	0
4	BMA	I	3	11/12	0.98	0.13	27,39,47,51	0
4	NAG	I	1	14/15	0.98	0.17	27,33,43,52	0
4	NAG	O	1	14/15	0.99	0.16	36,41,54,62	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.



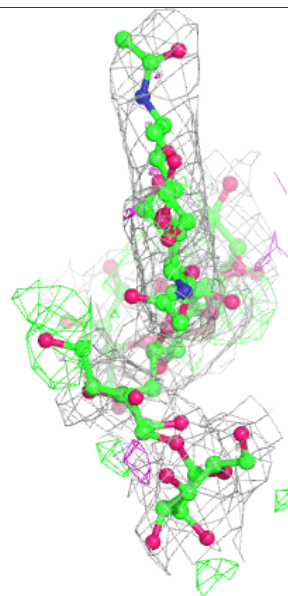
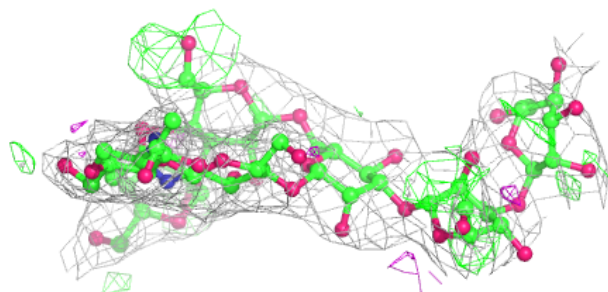
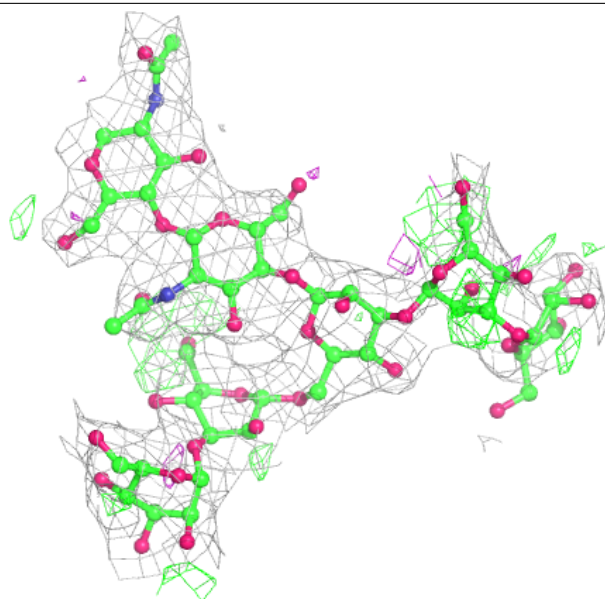
**Electron density around Chain O:**

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



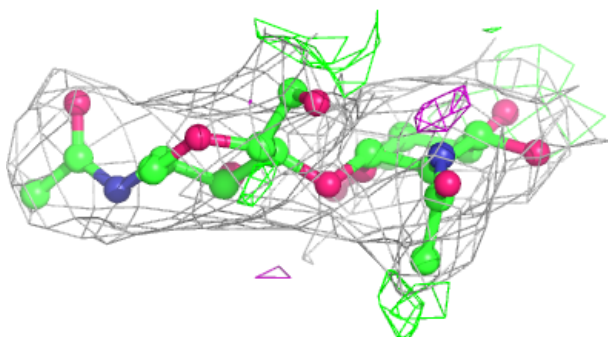
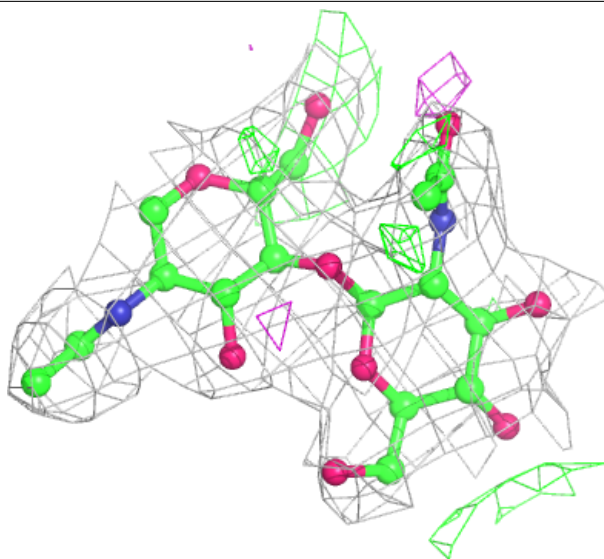
**Electron density around Chain X:**

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



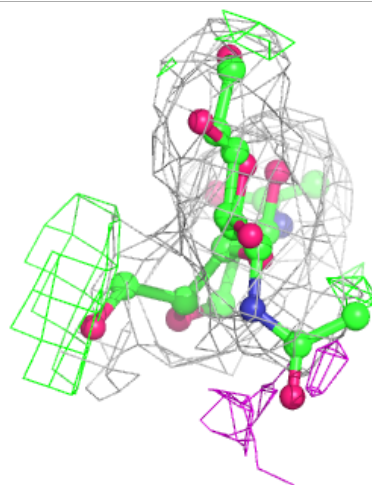
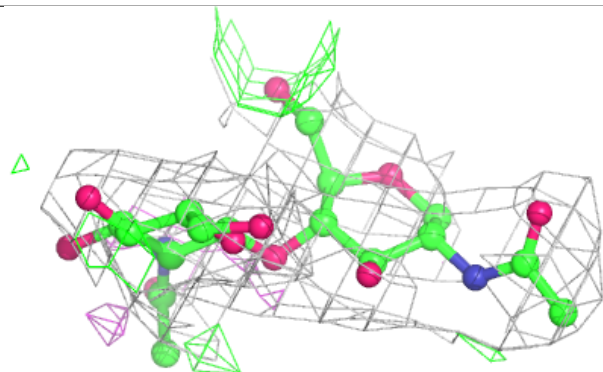
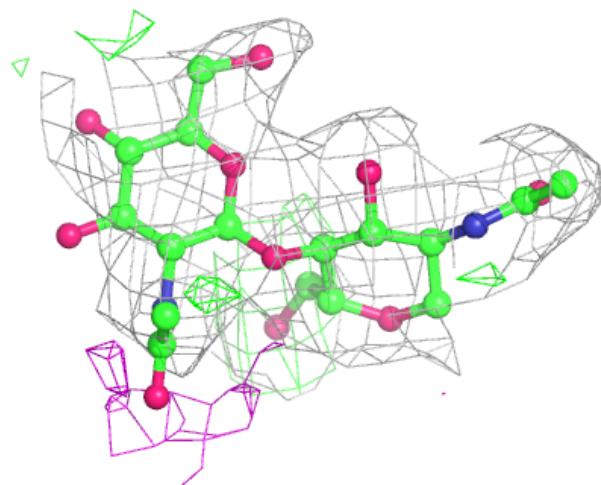
**Electron density around Chain K:**

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



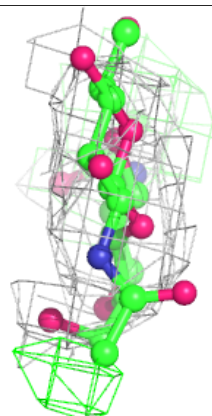
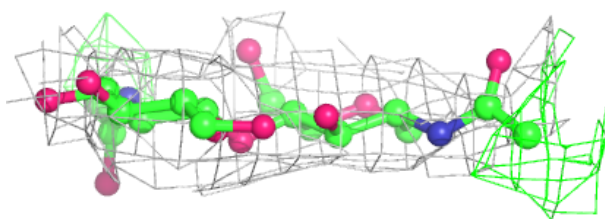
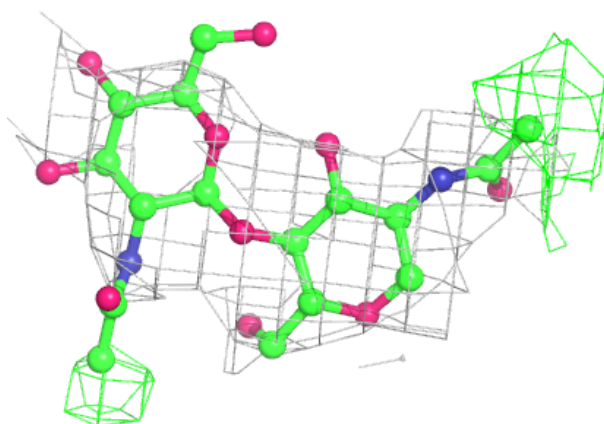
**Electron density around Chain M:**

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



**Electron density around Chain P:**

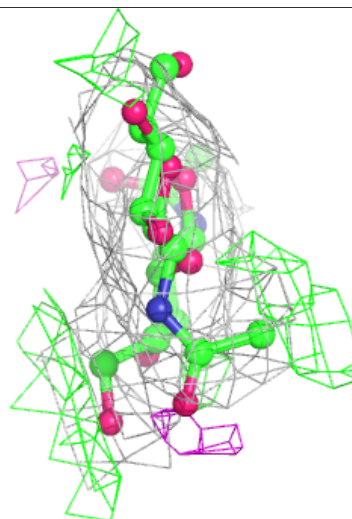
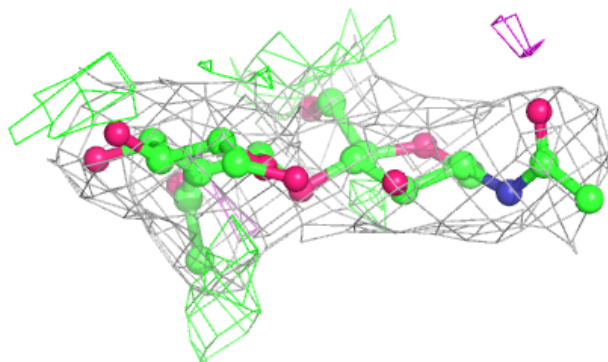
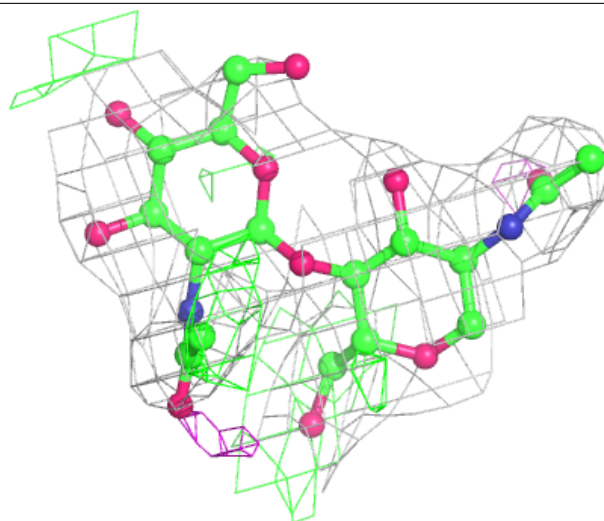
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain R:**

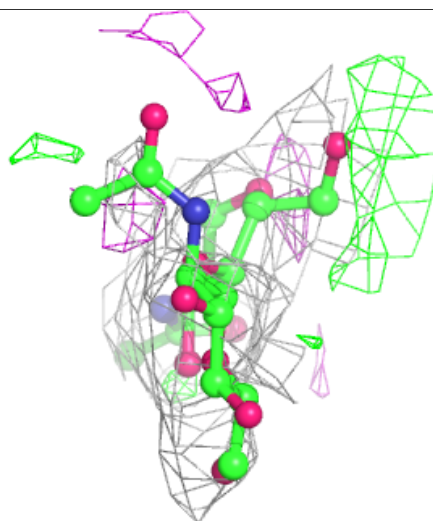
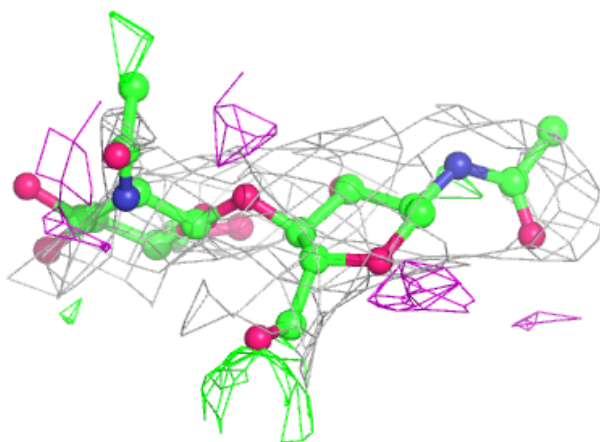
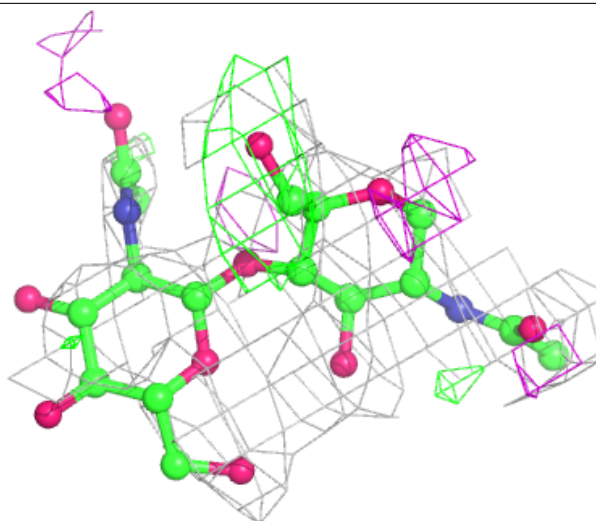
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





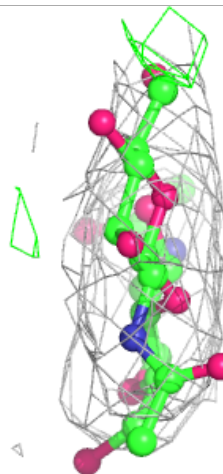
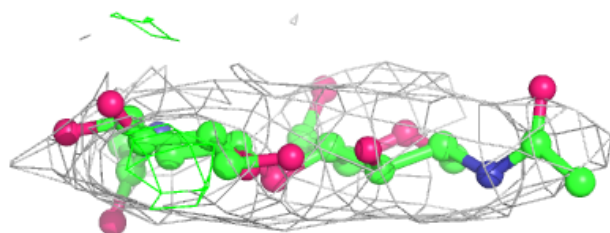
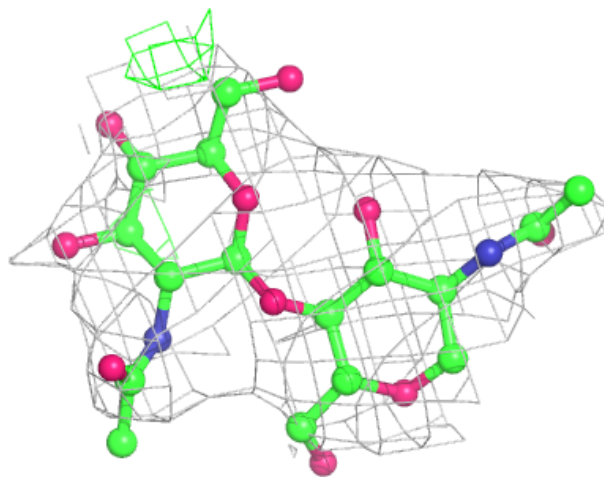
**Electron density around Chain S:**

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



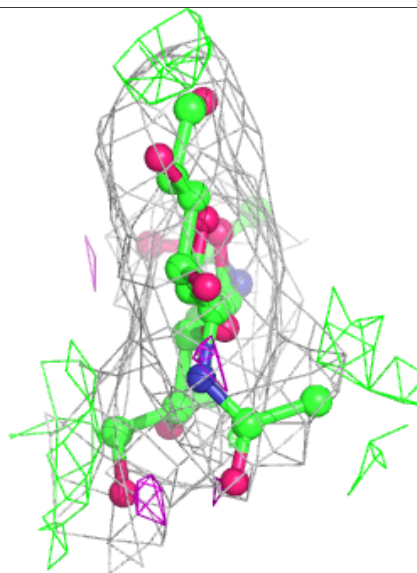
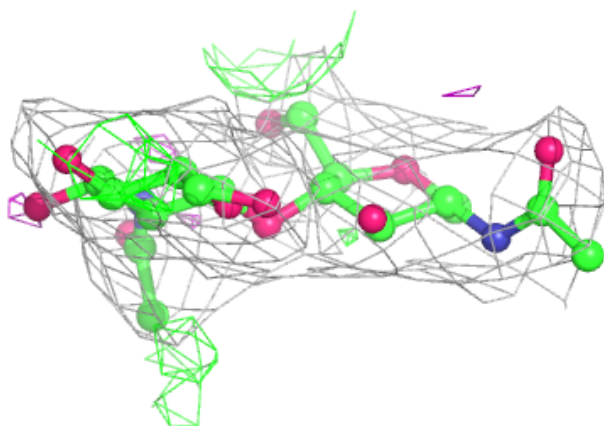
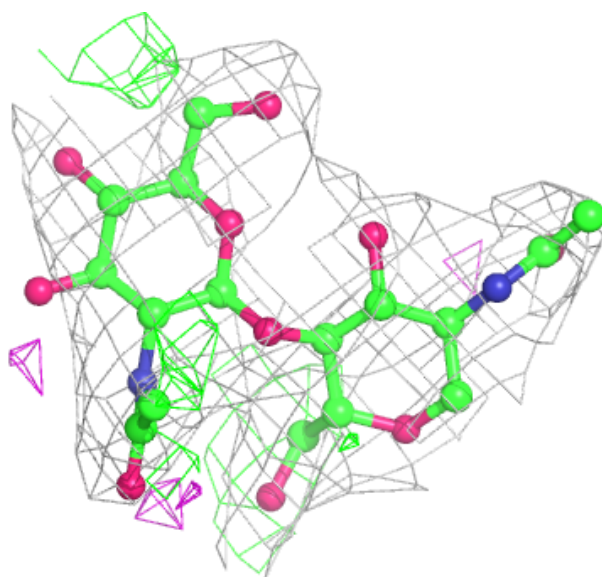
**Electron density around Chain T:**

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



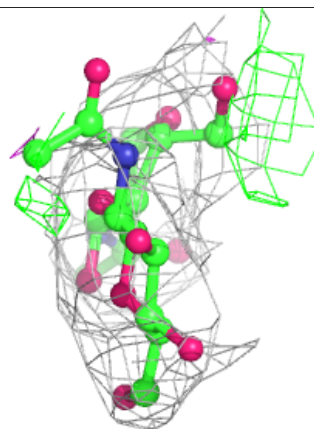
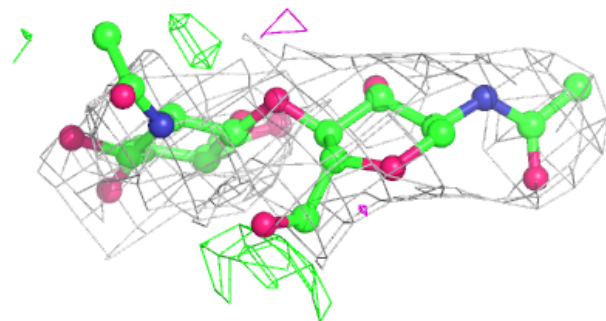
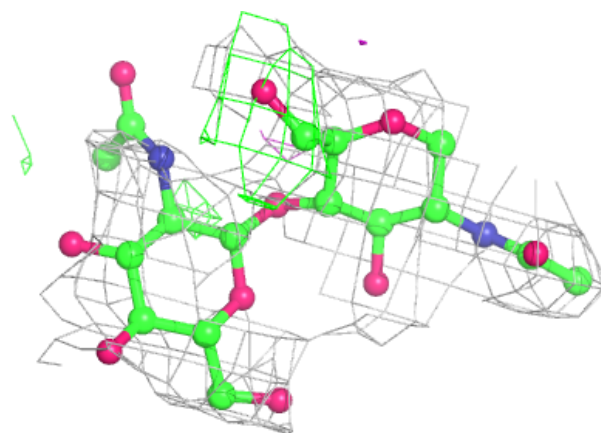
**Electron density around Chain U:**

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

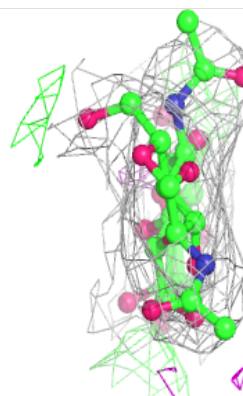
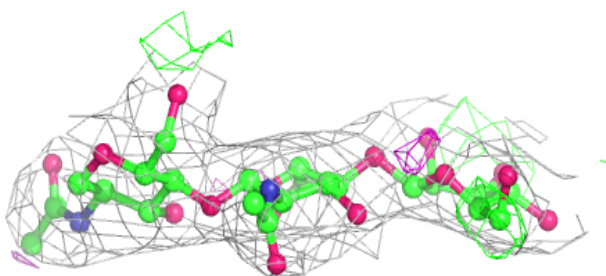
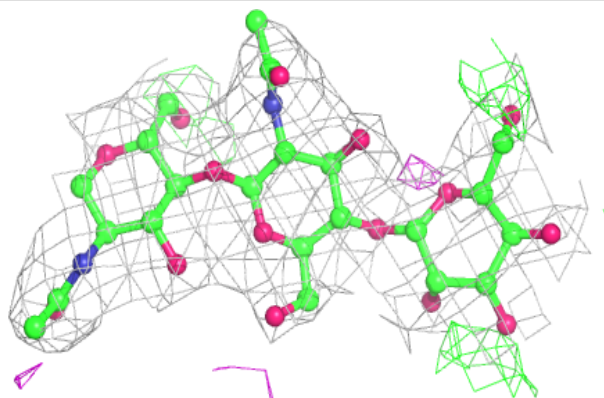


**Electron density around Chain V:**

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

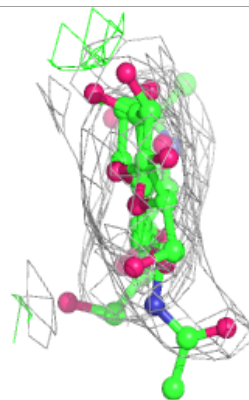
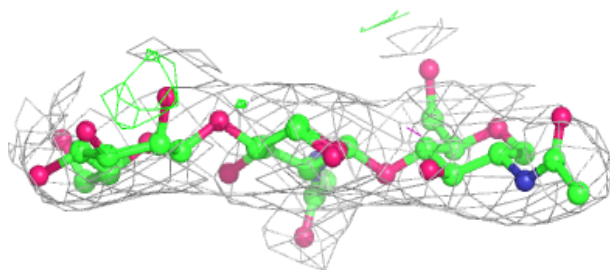
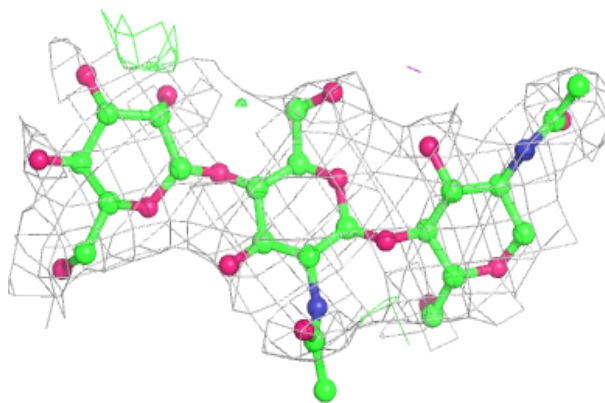
**Electron density around Chain N:**

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

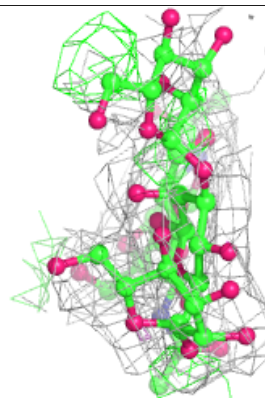
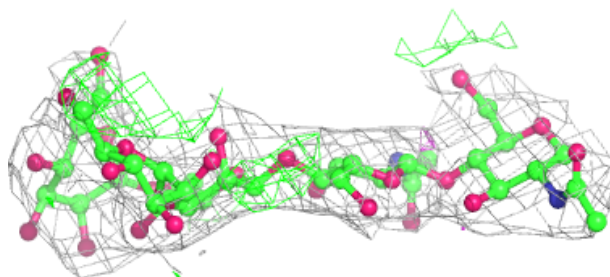
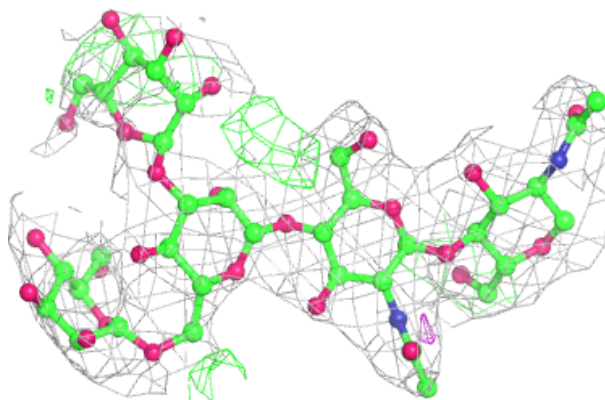


**Electron density around Chain W:**

$2mF_o-DF_c$  (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
9	NAG	A	409	14/15	0.73	0.41	81,108,114,118	0
9	NAG	C	503	14/15	0.75	0.33	112,128,139,140	0
9	NAG	C	501	14/15	0.79	0.39	106,132,142,144	0
9	NAG	A	408	14/15	0.80	0.29	95,119,132,136	0
9	NAG	B	409	14/15	0.80	0.48	126,140,146,152	0
9	NAG	B	408	14/15	0.82	0.23	75,97,109,120	0
9	NAG	C	502	14/15	0.84	0.49	115,151,154,156	0
9	NAG	A	410	14/15	0.87	0.36	106,122,129,135	0
9	NAG	B	410	14/15	0.90	0.18	112,124,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.