



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 10:12 PM EDT

PDB ID : 5UM8  
Title : Crystal structure of HIV-1 envelope trimer 16055 NFL TD CC (T569G) in complex with Fabs 35022 and PGT124  
Authors : Garces, F.; Stanfield, R.L.; Wilson, I.A.  
Deposited on : 2017-01-26  
Resolution : 3.94 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

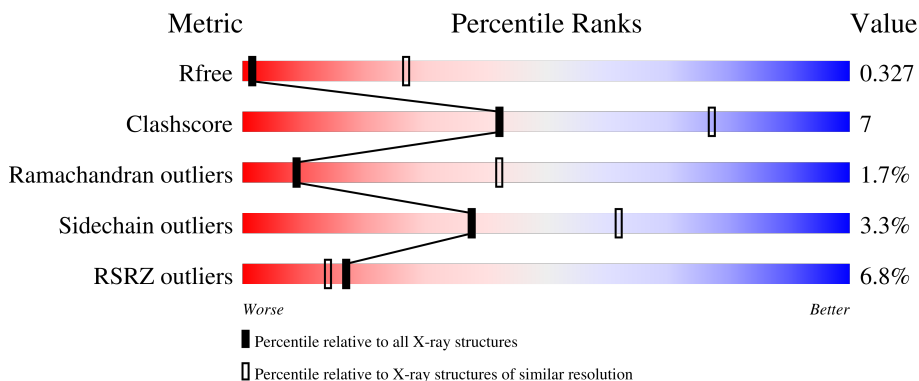
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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	G	485	 3% 72% 22% . .
2	B	153	 3% 61% 22% . 16%
3	L	214	 3% 78% 20% . .
4	H	236	 4% 77% 22% . .
5	D	240	 15% 88% 12%

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Mol	Chain	Length	Quality of chain
6	E	216	 15% 88% 10%
7	A	2	 100%
7	C	2	 100%
7	F	2	 100%
7	I	2	 100%
7	J	2	 50% 50%
7	M	2	 50% 50%
7	O	2	 50% 50%
7	S	2	 100%
8	K	5	 40% 40% 20%
9	N	3	 100%
10	P	10	 20% 80%
11	Q	7	 14% 71% 14%
12	R	6	 33% 67%

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
11	NAG	Q	2	-	-	-	X
11	BMA	Q	3	-	-	-	X
13	NAG	B	703	-	-	-	X
9	BMA	N	3	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 12221 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 glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	471	3681	2304	645	705	27	0	0	0

- Molecule 2 is a protein called glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	129	1017	641	178	193	5	0	0	0

- Molecule 3 is a protein called Fab PGT124 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	1599	1007	271	316	5	0	0	0

- Molecule 4 is a protein called Fab PGT124 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	234	1775	1123	297	349	6	0	0	0

- Molecule 5 is a protein called Fab 35022 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	240	1813	1150	303	352	8	0	0	0

- Molecule 6 is a protein called Fab 35022 light chain.

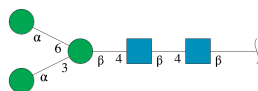
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	213	1615	1012	267	328	8	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



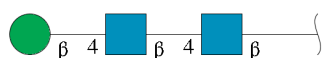
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	2	28	16	2	10	0	0	0
7	C	2	28	16	2	10	0	0	0
7	F	2	28	16	2	10	0	0	0
7	I	2	28	16	2	10	0	0	0
7	J	2	28	16	2	10	0	0	0
7	M	2	28	16	2	10	0	0	0
7	O	2	28	16	2	10	0	0	0
7	S	2	28	16	2	10	0	0	0

- 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.



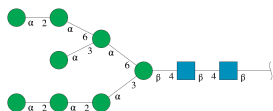
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	K	5	61	34	2	25	0	0	0

- Molecule 9 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.



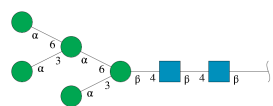
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	N	3	39	22	2	15	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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.



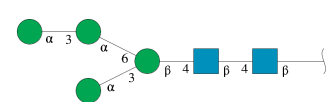
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	P	10	116	64	2	50	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 13 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>).

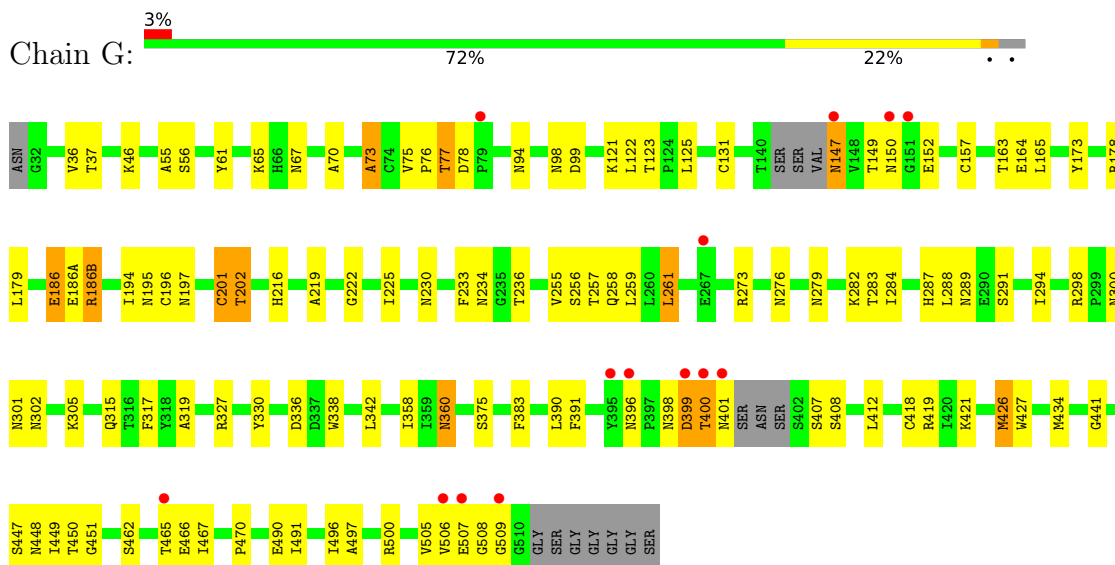


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	G	1	Total 14	C 8	N 1	O 5	0	0
13	B	1	Total 14	C 8	N 1	O 5	0	0
13	B	1	Total 14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

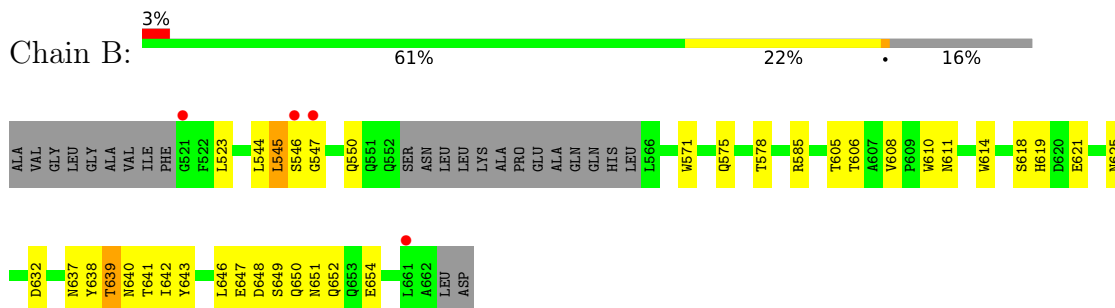
### 3 Residue-property plots

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.

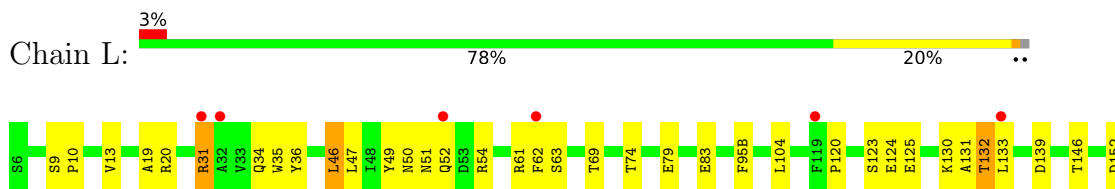
- Molecule 1: glycoprotein gp120



- Molecule 2: glycoprotein gp41



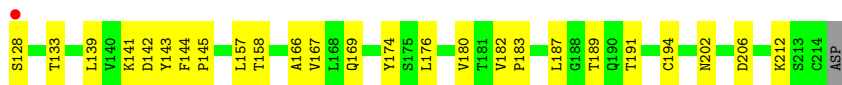
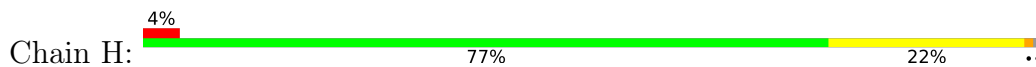
- Molecule 3: Fab PGT124 light chain



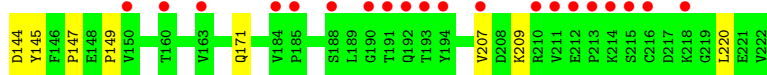
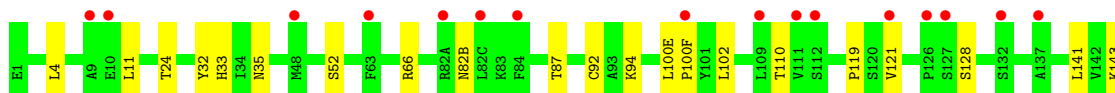
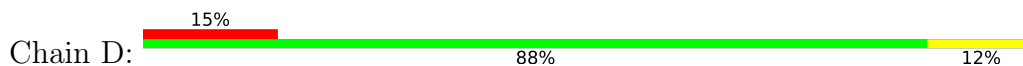




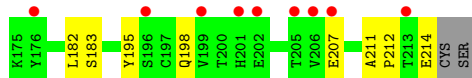
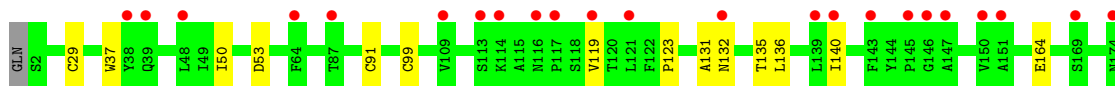
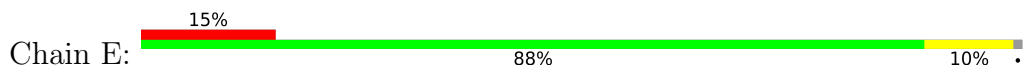
- Molecule 4: Fab PGT124 heavy chain



- Molecule 5: Fab 35022 heavy chain



- Molecule 6: Fab 35022 light chain



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



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



MAG1  
MAG2

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

Chain F:  100%MAG1  
MAG2

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

Chain I:  100%MAG1  
MAG2

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

Chain J:  50% 50%MAG1  
MAG2

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

Chain M:  50% 50%MAG1  
MAG2

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

Chain O:  50% 50%MAG1  
MAG2

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

Chain S:  100%MAG1  
MAG2

- 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 K: 



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

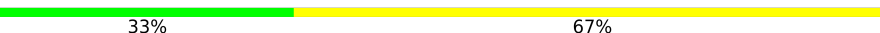


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 



- Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.46Å 126.46Å 314.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.25 – 3.94 49.25 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.25-3.94) 99.9 (49.25-3.94)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.88Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.260 , 0.329 0.261 , 0.327	Depositor DCC
$R_{free}$ test set	1259 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.1	Xtrriage
Anisotropy	0.745	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 101.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.090 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: 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	G	0.30	1/3755 (0.0%)	0.48	0/5103
2	B	0.23	0/1035	0.40	0/1403
3	L	0.24	0/1642	0.45	0/2243
4	H	0.24	0/1818	0.45	0/2480
5	D	0.24	0/1860	0.45	0/2533
6	E	0.24	0/1659	0.44	0/2269
All	All	0.26	1/11769 (0.0%)	0.45	0/16031

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186(B)	ARG	CA-C	-8.73	1.30	1.52

There are no bond angle outliers.

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	G	3681	0	3587	68	0
2	B	1017	0	992	26	0
3	L	1599	0	1542	26	0
4	H	1775	0	1742	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1813	0	1784	18	0
6	E	1615	0	1544	14	0
7	A	28	0	25	0	0
7	C	28	0	25	0	0
7	F	28	0	25	0	0
7	I	28	0	25	0	0
7	J	28	0	25	1	0
7	M	28	0	25	1	0
7	O	28	0	25	0	0
7	S	28	0	25	0	0
8	K	61	0	52	1	0
9	N	39	0	34	0	0
10	P	116	0	97	1	0
11	Q	83	0	70	2	0
12	R	72	0	61	1	0
13	B	42	0	39	1	0
13	G	84	0	78	3	0
All	All	12221	0	11822	166	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 7.

All (166) 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:G:149:THR:HG22	1:G:150:ASN:H	1.13	1.11
1:G:149:THR:HG22	1:G:150:ASN:N	1.77	0.93
1:G:150:ASN:HD22	1:G:419:ARG:NH2	1.66	0.93
1:G:150:ASN:ND2	1:G:419:ARG:HH22	1.66	0.92
1:G:149:THR:CG2	1:G:150:ASN:H	1.84	0.90
1:G:121:LYS:HA	1:G:202:THR:HA	1.66	0.76
5:D:94:LYS:HB3	5:D:102:LEU:HB3	1.72	0.72
6:E:195:TYR:HD2	6:E:212:PRO:HG3	1.56	0.70
1:G:150:ASN:HD22	1:G:419:ARG:HH22	0.83	0.69
3:L:131:ALA:HB3	3:L:181:LEU:O	1.94	0.67
1:G:490:GLU:OE2	2:B:585:ARG:NH1	2.29	0.66
4:H:35:THR:HG22	4:H:50:TYR:HB3	1.78	0.66
2:B:608:VAL:HG22	2:B:649:SER:HB2	1.77	0.65
3:L:61:ARG:HH22	3:L:79:GLU:HB2	1.62	0.65
4:H:157:LEU:HD21	4:H:180:VAL:HG11	1.81	0.62
1:G:77:THR:OG1	1:G:78:ASP:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ASN:HD22	13:G:700:NAG:C7	2.13	0.61
5:D:35:ASN:O	5:D:92:CYS:HA	2.01	0.61
1:G:37:THR:HG22	2:B:605:THR:HA	1.83	0.60
1:G:55:ALA:O	1:G:216:HIS:HB2	2.01	0.60
2:B:642:ILE:O	2:B:646:LEU:HB2	2.02	0.60
4:H:100(P):MET:N	4:H:100(P):MET:SD	2.75	0.60
1:G:426:MET:HG3	1:G:427:TRP:CD1	2.37	0.59
6:E:211:ALA:HB3	6:E:214:GLU:HB3	1.82	0.59
5:D:143:LYS:HE3	6:E:135:THR:HG21	1.84	0.59
6:E:37:TRP:HB2	6:E:50:ILE:HB	1.84	0.59
13:G:704:NAG:H3	13:G:704:NAG:H83	1.84	0.58
3:L:63:SER:OG	3:L:74:THR:OG1	2.21	0.58
5:D:66:ARG:NH2	5:D:82(B):ASN:O	2.36	0.58
3:L:125:GLU:OE1	3:L:132:THR:OG1	2.21	0.58
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.85	0.58
1:G:122:LEU:HD13	1:G:125:LEU:HD22	1.85	0.57
6:E:131:ALA:N	6:E:132:ASN:HA	2.20	0.57
1:G:288:LEU:HG	1:G:451:GLY:HA2	1.86	0.57
2:B:638:TYR:O	2:B:640:ASN:N	2.36	0.57
1:G:67:ASN:HB2	1:G:70:ALA:HB3	1.87	0.57
2:B:545:LEU:O	2:B:547:GLY:N	2.38	0.56
3:L:34:GLN:HG3	3:L:49:TYR:HA	1.86	0.56
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.87	0.56
3:L:50:ASN:O	3:L:52:GLN:N	2.38	0.56
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.69	0.56
3:L:36:TYR:HA	3:L:46:LEU:HA	1.87	0.56
4:H:5:GLN:OE1	4:H:103:LYS:NZ	2.37	0.56
1:G:152:GLU:OE2	1:G:179:LEU:HG	2.05	0.56
6:E:119:VAL:HG22	6:E:140:ILE:HG23	1.88	0.55
5:D:87:THR:HG23	5:D:110:THR:HA	1.87	0.55
5:D:4:LEU:HD13	5:D:102:LEU:HD22	1.88	0.55
1:G:298:ARG:NH2	1:G:441:GLY:O	2.38	0.55
4:H:35:THR:HG23	4:H:95:ALA:HB2	1.89	0.55
4:H:2:VAL:HA	4:H:26:GLY:HA3	1.88	0.55
2:B:650:GLN:O	2:B:654:GLU:N	2.30	0.54
1:G:327:ARG:HH11	4:H:100(D):VAL:HG23	1.73	0.54
13:B:703:NAG:H3	13:B:703:NAG:H83	1.89	0.53
2:B:639:THR:O	2:B:643:TYR:N	2.38	0.53
1:G:462:SER:OG	13:G:727:NAG:O6	2.26	0.53
4:H:122:LEU:HD21	4:H:139:LEU:HD12	1.91	0.53
1:G:399:ASP:O	1:G:401:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:195:TYR:CD2	6:E:212:PRO:HG3	2.39	0.52
4:H:166:ALA:HB2	4:H:176:LEU:HB3	1.91	0.52
3:L:35:TRP:O	3:L:47:LEU:N	2.43	0.52
6:E:135:THR:HA	6:E:182:LEU:O	2.10	0.51
1:G:255:VAL:HG21	1:G:427:TRP:CZ3	2.45	0.51
6:E:198:GLN:HG2	6:E:207:GLU:HG3	1.93	0.51
1:G:173:TYR:O	1:G:305:LYS:NZ	2.44	0.51
5:D:100(E):LEU:HD12	5:D:100(F):PRO:HD2	1.92	0.51
5:D:128:SER:HA	5:D:220:LEU:HD13	1.94	0.50
1:G:163:THR:HG23	1:G:165:LEU:H	1.76	0.50
4:H:167:VAL:O	4:H:174:TYR:HA	2.12	0.50
3:L:123:SER:OG	3:L:124:GLU:OE2	2.25	0.49
1:G:358:ILE:HG23	1:G:396:ASN:HA	1.95	0.49
4:H:33:TYR:HB2	4:H:95:ALA:O	2.12	0.49
1:G:179:LEU:HB3	1:G:421:LYS:HE2	1.94	0.49
5:D:121:VAL:HA	5:D:141:LEU:O	2.12	0.49
5:D:207:VAL:HG12	5:D:209:LYS:HG2	1.94	0.49
5:D:171:GLN:HA	6:E:164:GLU:HG3	1.95	0.49
5:D:4:LEU:HG	5:D:24:THR:HG22	1.95	0.48
3:L:139:ASP:OD1	3:L:168:GLN:NE2	2.47	0.48
5:D:11:LEU:HD22	5:D:147:PRO:HD3	1.96	0.48
1:G:233:PHE:HD1	7:M:1:NAG:H81	1.79	0.48
1:G:360:ASN:OD1	1:G:467:ILE:HG23	2.12	0.48
11:Q:3:BMA:H61	11:Q:4:MAN:H3	1.96	0.47
6:E:123:PRO:HA	6:E:136:LEU:HD23	1.97	0.47
1:G:257:THR:HG22	1:G:258:GLN:HG3	1.95	0.47
1:G:56:SER:O	1:G:76:PRO:HA	2.15	0.47
1:G:98:ASN:OD1	1:G:99:ASP:N	2.48	0.47
3:L:130:LYS:HD3	4:H:141:LYS:HE2	1.97	0.46
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.98	0.46
1:G:276:ASN:ND2	1:G:279:ASN:HB2	2.30	0.46
4:H:22:CYS:HB3	4:H:78:LEU:HG	1.97	0.46
3:L:132:THR:HA	3:L:179:LEU:O	2.16	0.46
4:H:133:THR:HA	4:H:183:PRO:HA	1.97	0.46
1:G:391:PHE:CD2	1:G:470:PRO:HG3	2.50	0.46
1:G:282:LYS:HA	1:G:282:LYS:HD2	1.68	0.46
1:G:338:TRP:CZ2	1:G:390:LEU:HB3	2.50	0.46
1:G:73:ALA:HA	2:B:571:TRP:HE1	1.81	0.46
4:H:51:ILE:HD11	4:H:55:GLU:HA	1.99	0.45
6:E:135:THR:HG22	6:E:183:SER:HA	1.98	0.45
8:K:3:BMA:H62	8:K:5:MAN:H2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:ASN:HB3	2:B:614:TRP:CD2	2.51	0.45
3:L:160:VAL:HG22	3:L:179:LEU:HD13	1.99	0.45
5:D:33:HIS:CE1	5:D:52:SER:HB2	2.51	0.45
6:E:136:LEU:HD12	6:E:182:LEU:HD23	1.99	0.45
1:G:491:ILE:HD11	2:B:523:LEU:HD11	1.97	0.45
1:G:330:TYR:HE2	10:P:1:NAG:HN2	1.63	0.45
2:B:575:GLN:O	2:B:578:THR:OG1	2.26	0.45
2:B:648:ASP:O	2:B:652:GLN:HB3	2.17	0.45
4:H:34:TRP:CZ3	4:H:94:THR:HG22	2.51	0.45
1:G:195:ASN:ND2	1:G:201:CYS:HB2	2.32	0.44
4:H:29:ILE:HD11	4:H:77:GLN:N	2.32	0.44
2:B:650:GLN:HG3	2:B:651:ASN:H	1.82	0.44
3:L:83:GLU:OE1	3:L:167:LYS:NZ	2.51	0.44
3:L:156:VAL:HG11	3:L:179:LEU:HD11	2.00	0.44
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.51	0.44
1:G:505:VAL:O	1:G:507:GLU:N	2.50	0.44
2:B:625:ASN:OD1	5:D:32:TYR:OH	2.27	0.44
3:L:20:ARG:HG2	3:L:74:THR:HG22	1.99	0.44
1:G:94:ASN:HA	1:G:236:THR:HG22	1.98	0.44
1:G:147:ASN:N	1:G:147:ASN:OD1	2.51	0.44
1:G:291:SER:HB2	1:G:448:ASN:HB3	2.00	0.44
3:L:31:ARG:NH2	3:L:69:THR:O	2.44	0.44
4:H:90:TYR:O	4:H:104:GLY:HA2	2.18	0.44
3:L:120:PRO:HA	3:L:133:LEU:HD23	2.00	0.43
4:H:144:PHE:HA	4:H:145:PRO:HA	1.75	0.43
5:D:33:HIS:CD2	11:Q:2:NAG:H83	2.53	0.43
1:G:131:CYS:HA	1:G:157:CYS:HA	1.99	0.43
3:L:54:ARG:NH2	3:L:62:PHE:O	2.43	0.43
1:G:261:LEU:HA	1:G:449:ILE:HA	1.99	0.43
3:L:161:GLU:HG2	4:H:169:GLN:HG3	2.00	0.43
1:G:500:ARG:NH1	2:B:619:HIS:HB2	2.34	0.43
3:L:124:GLU:OE2	3:L:124:GLU:N	2.51	0.43
4:H:180:VAL:HG12	4:H:182:VAL:HG13	2.00	0.43
1:G:300:ASN:O	1:G:302:ASN:N	2.51	0.42
1:G:375:SER:HA	1:G:383:PHE:O	2.19	0.42
3:L:83:GLU:HG3	3:L:104:LEU:O	2.19	0.42
6:E:132:ASN:OD1	6:E:132:ASN:N	2.52	0.42
1:G:291:SER:HB3	1:G:450:THR:HG22	2.02	0.42
1:G:222:GLY:HA2	2:B:544:LEU:HD12	2.01	0.42
1:G:273:ARG:HH12	1:G:287:HIS:CD2	2.38	0.42
1:G:194:ILE:HD11	7:J:2:NAG:H82	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:638:TYR:C	2:B:639:THR:HG1	2.23	0.42
2:B:643:TYR:O	2:B:647:GLU:HG2	2.19	0.42
1:G:65:LYS:HE3	1:G:65:LYS:HB2	1.85	0.42
1:G:163:THR:OG1	1:G:164:GLU:N	2.51	0.41
2:B:606:THR:HG21	2:B:646:LEU:HD11	2.02	0.41
4:H:48:ILE:HB	4:H:63:LEU:HD12	2.02	0.41
4:H:125:SER:HB2	4:H:128:SER:HB2	2.02	0.41
1:G:46:LYS:HA	1:G:46:LYS:HD3	1.87	0.41
3:L:13:VAL:HG11	3:L:19:ALA:HB2	2.01	0.41
1:G:407:SER:OG	1:G:408:SER:N	2.52	0.41
1:G:317:PHE:CE2	1:G:319:ALA:HB2	2.56	0.41
2:B:640:ASN:OD1	2:B:641:THR:N	2.53	0.41
1:G:37:THR:OG1	1:G:497:ALA:O	2.33	0.41
1:G:256:SER:OG	1:G:259:LEU:O	2.25	0.41
2:B:618:SER:H	2:B:621:GLU:HB2	1.85	0.41
1:G:219:ALA:HB2	1:G:225:ILE:HG13	2.03	0.41
1:G:230:ASN:HB3	1:G:233:PHE:HB2	2.02	0.41
1:G:398:ASN:C	1:G:400:THR:H	2.23	0.41
2:B:614:TRP:CZ2	2:B:642:ILE:HG12	2.56	0.41
2:B:638:TYR:O	2:B:639:THR:OG1	2.34	0.41
3:L:146:THR:OG1	3:L:197:THR:HB	2.20	0.41
1:G:261:LEU:HD21	12:R:1:NAG:H82	2.02	0.41
1:G:294:ILE:HG23	1:G:447:SER:HB2	2.03	0.41
1:G:195:ASN:O	1:G:197:ASN:N	2.54	0.40
3:L:9:SER:HA	3:L:10:PRO:HD3	1.89	0.40
4:H:143:TYR:OH	4:H:176:LEU:HD23	2.22	0.40
1:G:178:ARG:O	1:G:178:ARG:HD3	2.22	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	G	465/485 (96%)	397 (85%)	55 (12%)	13 (3%)	5	33
2	B	125/153 (82%)	108 (86%)	13 (10%)	4 (3%)	4	31
3	L	209/214 (98%)	194 (93%)	13 (6%)	2 (1%)	15	52
4	H	230/236 (98%)	211 (92%)	16 (7%)	3 (1%)	12	47
5	D	238/240 (99%)	224 (94%)	12 (5%)	2 (1%)	19	57
6	E	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	29	66
All	All	1478/1544 (96%)	1335 (90%)	118 (8%)	25 (2%)	9	42

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	186(B)	ARG
1	G	400	THR
2	B	546	SER
1	G	186	GLU
1	G	301	ASN
1	G	506	VAL
2	B	550	GLN
1	G	196	CYS
1	G	412	LEU
2	B	639	THR
3	L	51	ASN
3	L	152	ASP
4	H	142	ASP
6	E	53	ASP
1	G	73	ALA
1	G	509	GLY
4	H	212	LYS
1	G	186(A)	GLU
1	G	234	ASN
1	G	426	MET
2	B	545	LEU
4	H	191	THR
5	D	144	ASP
1	G	508	GLY
5	D	149	PRO

### 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	G	416/428 (97%)	395 (95%)	21 (5%)	24	52
2	B	108/128 (84%)	106 (98%)	2 (2%)	57	75
3	L	176/180 (98%)	171 (97%)	5 (3%)	43	65
4	H	202/204 (99%)	190 (94%)	12 (6%)	19	47
5	D	203/203 (100%)	203 (100%)	0	100	100
6	E	186/189 (98%)	183 (98%)	3 (2%)	62	78
All	All	1291/1332 (97%)	1248 (97%)	43 (3%)	38	62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	61	TYR
1	G	75	VAL
1	G	77	THR
1	G	123	THR
1	G	147	ASN
1	G	186	GLU
1	G	201	CYS
1	G	202	THR
1	G	261	LEU
1	G	283	THR
1	G	284	ILE
1	G	315	GLN
1	G	336	ASP
1	G	342	LEU
1	G	360	ASN
1	G	399	ASP
1	G	418	CYS
1	G	434	MET
1	G	465	THR
1	G	466	GLU
1	G	496	ILE
2	B	632	ASP

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Mol	Chain	Res	Type
2	B	637	ASN
3	L	31	ARG
3	L	46	LEU
3	L	95(B)	PHE
3	L	132	THR
3	L	182	THR
4	H	45	LEU
4	H	78	LEU
4	H	82	LEU
4	H	100(P)	MET
4	H	105	THR
4	H	114	THR
4	H	158	THR
4	H	187	LEU
4	H	189	THR
4	H	194	CYS
4	H	202	ASN
4	H	206	ASP
6	E	29	CYS
6	E	91	CYS
6	E	99	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	147	ASN
1	G	150	ASN
6	E	201	HIS

### 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](#)

47 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	$\# Z  > 2$
7	NAG	A	1	1,7	14,14,15	0.50	0	17,19,21	0.57	0
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	0.65	0
7	NAG	C	1	1,7	14,14,15	0.28	0	17,19,21	0.54	0
7	NAG	C	2	7	14,14,15	0.24	0	17,19,21	0.41	0
7	NAG	F	1	1,7	14,14,15	0.32	0	17,19,21	0.42	0
7	NAG	F	2	7	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	I	1	1,7	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	I	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	NAG	J	1	1,7	14,14,15	0.30	0	17,19,21	0.37	0
7	NAG	J	2	7	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	K	1	1,8	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	K	2	8	14,14,15	0.21	0	17,19,21	0.40	0
8	BMA	K	3	8	11,11,12	0.58	0	15,15,17	0.77	0
8	MAN	K	4	8	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
8	MAN	K	5	8	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
7	NAG	M	1	1,7	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	M	2	7	14,14,15	0.24	0	17,19,21	0.45	0
9	NAG	N	1	1,9	14,14,15	0.24	0	17,19,21	0.39	0
9	NAG	N	2	9	14,14,15	0.22	0	17,19,21	0.41	0
9	BMA	N	3	9	11,11,12	0.58	0	15,15,17	0.75	0
7	NAG	O	1	1,7	14,14,15	0.25	0	17,19,21	0.64	1 (5%)
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.42	0
10	NAG	P	1	10,1	14,14,15	0.21	0	17,19,21	0.40	0
10	MAN	P	10	10	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
10	NAG	P	2	10	14,14,15	0.19	0	17,19,21	0.41	0
10	BMA	P	3	10	11,11,12	0.66	0	15,15,17	0.94	0
10	MAN	P	4	10	11,11,12	0.81	1 (9%)	15,15,17	1.32	2 (13%)
10	MAN	P	5	10	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
10	MAN	P	6	10	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
10	MAN	P	7	10	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
10	MAN	P	8	10	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
10	MAN	P	9	10	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
11	NAG	Q	1	1,11	14,14,15	0.26	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	Q	2	11	14,14,15	0.37	0	17,19,21	0.46	0
11	BMA	Q	3	11	11,11,12	0.61	0	15,15,17	0.70	0
11	MAN	Q	4	11	11,11,12	1.52	2 (18%)	15,15,17	2.10	3 (20%)
11	MAN	Q	5	11	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
11	MAN	Q	6	11	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
11	MAN	Q	7	11	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
12	NAG	R	1	12,1	14,14,15	0.35	0	17,19,21	0.52	0
12	NAG	R	2	12	14,14,15	0.24	0	17,19,21	0.38	0
12	BMA	R	3	12	11,11,12	0.89	0	15,15,17	0.85	0
12	MAN	R	4	12	11,11,12	1.24	1 (9%)	15,15,17	1.29	2 (13%)
12	MAN	R	5	12	11,11,12	0.74	0	15,15,17	0.86	1 (6%)
12	MAN	R	6	12	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
7	NAG	S	1	1,7	14,14,15	0.50	0	17,19,21	0.51	0
7	NAG	S	2	7	14,14,15	0.26	0	17,19,21	0.52	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	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	NAG	C	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	2/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
8	NAG	K	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	2/2/19/22	0/1/1/1
8	MAN	K	4	8	-	1/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	N	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	BMA	N	3	9	-	0/2/19/22	0/1/1/1
7	NAG	O	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
10	NAG	P	1	10,1	-	4/6/23/26	0/1/1/1
10	MAN	P	10	10	-	0/2/19/22	0/1/1/1
10	NAG	P	2	10	-	1/6/23/26	0/1/1/1
10	BMA	P	3	10	-	0/2/19/22	0/1/1/1
10	MAN	P	4	10	-	0/2/19/22	0/1/1/1
10	MAN	P	5	10	-	1/2/19/22	0/1/1/1
10	MAN	P	6	10	-	0/2/19/22	0/1/1/1
10	MAN	P	7	10	-	0/2/19/22	0/1/1/1
10	MAN	P	8	10	-	0/2/19/22	0/1/1/1
10	MAN	P	9	10	-	0/2/19/22	0/1/1/1
11	NAG	Q	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Q	2	11	-	0/6/23/26	0/1/1/1
11	BMA	Q	3	11	-	1/2/19/22	0/1/1/1
11	MAN	Q	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	6	11	-	2/2/19/22	0/1/1/1
11	MAN	Q	7	11	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	R	2	12	-	0/6/23/26	0/1/1/1
12	BMA	R	3	12	-	2/2/19/22	0/1/1/1
12	MAN	R	4	12	-	0/2/19/22	0/1/1/1
12	MAN	R	5	12	-	0/2/19/22	0/1/1/1
12	MAN	R	6	12	-	1/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	4	MAN	C1-C2	4.02	1.61	1.52
11	Q	4	MAN	O5-C1	2.42	1.47	1.43
10	P	4	MAN	C1-C2	2.36	1.57	1.52
12	R	4	MAN	C2-C3	2.33	1.55	1.52

All (33) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	4	MAN	C1-O5-C5	5.87	120.14	112.19
11	Q	4	MAN	C1-C2-C3	4.44	115.13	109.67
10	P	4	MAN	C1-O5-C5	3.14	116.45	112.19
12	R	4	MAN	C1-O5-C5	2.88	116.09	112.19
10	P	8	MAN	C1-O5-C5	2.56	115.66	112.19
11	Q	6	MAN	C1-O5-C5	2.48	115.56	112.19
10	P	5	MAN	C1-O5-C5	2.42	115.47	112.19
10	P	9	MAN	C1-O5-C5	2.41	115.46	112.19
11	Q	4	MAN	O2-C2-C3	-2.40	105.33	110.14
8	K	4	MAN	C1-O5-C5	2.38	115.42	112.19
8	K	5	MAN	C1-O5-C5	2.36	115.39	112.19
12	R	4	MAN	C1-C2-C3	2.35	112.56	109.67
11	Q	6	MAN	O2-C2-C3	-2.29	105.55	110.14
10	P	6	MAN	C1-O5-C5	2.29	115.29	112.19
10	P	7	MAN	C1-O5-C5	2.26	115.26	112.19
12	R	6	MAN	O2-C2-C3	-2.26	105.61	110.14
8	K	4	MAN	O2-C2-C3	-2.23	105.67	110.14
11	Q	5	MAN	O2-C2-C3	-2.22	105.69	110.14
11	Q	7	MAN	O2-C2-C3	-2.22	105.69	110.14
12	R	5	MAN	O2-C2-C3	-2.22	105.70	110.14
10	P	10	MAN	O2-C2-C3	-2.22	105.70	110.14
10	P	10	MAN	C1-O5-C5	2.21	115.19	112.19
10	P	9	MAN	O2-C2-C3	-2.21	105.71	110.14
12	R	6	MAN	C1-O5-C5	2.20	115.17	112.19
10	P	6	MAN	O2-C2-C3	-2.20	105.74	110.14
10	P	8	MAN	O2-C2-C3	-2.19	105.74	110.14
7	O	1	NAG	C1-O5-C5	2.18	115.14	112.19
10	P	7	MAN	O2-C2-C3	-2.18	105.78	110.14
8	K	5	MAN	O2-C2-C3	-2.17	105.79	110.14
11	Q	5	MAN	C1-O5-C5	2.12	115.06	112.19
10	P	5	MAN	O2-C2-C3	-2.07	105.99	110.14
10	P	4	MAN	C1-C2-C3	2.05	112.19	109.67
11	Q	7	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1	NAG	O5-C5-C6-O6
8	K	3	BMA	C4-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
7	F	2	NAG	O5-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6

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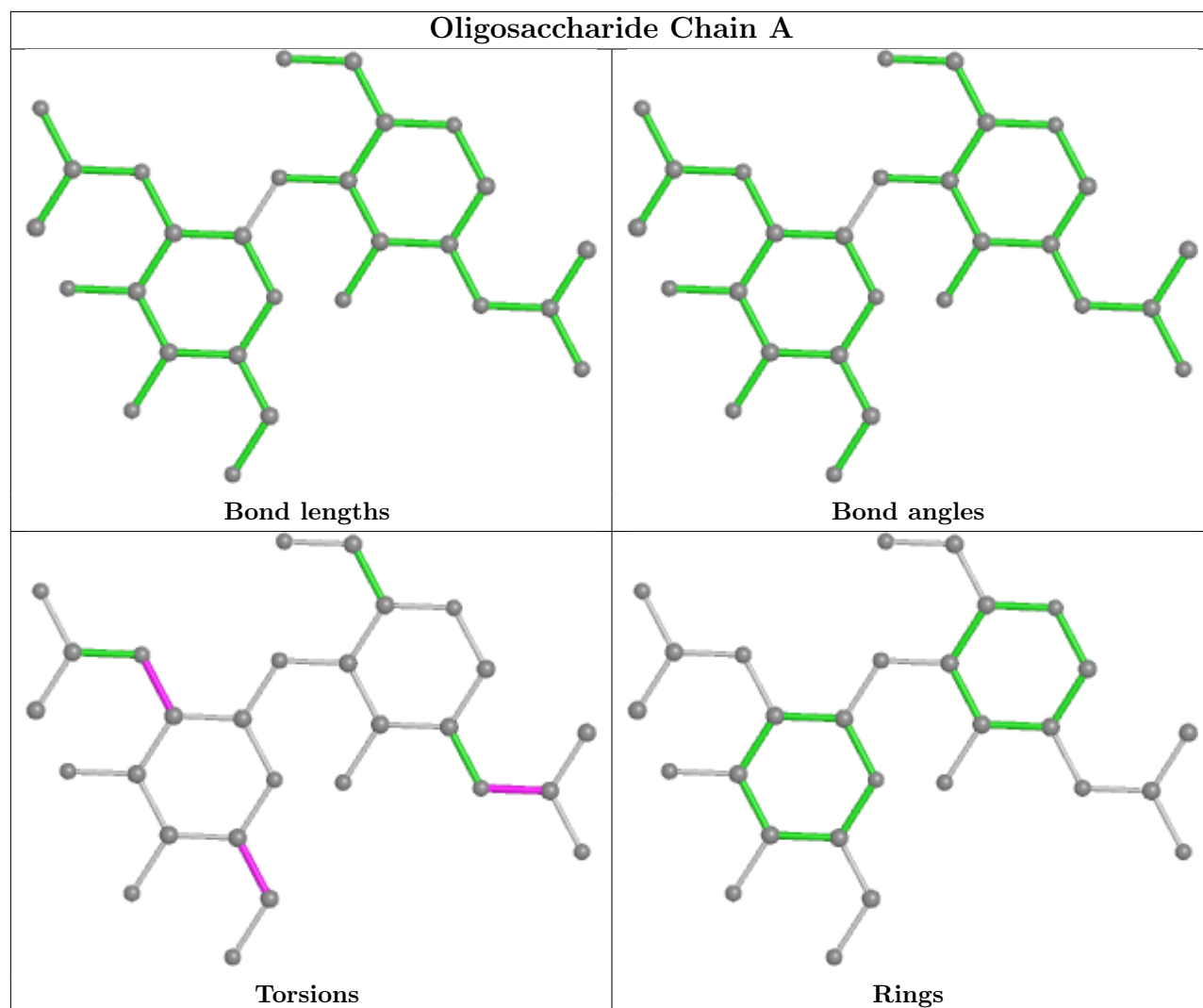
Mol	Chain	Res	Type	Atoms
7	F	1	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	C	1	NAG	C4-C5-C6-O6
8	K	3	BMA	O5-C5-C6-O6
8	K	1	NAG	O5-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
11	Q	6	MAN	O5-C5-C6-O6
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
7	C	1	NAG	C8-C7-N2-C2
7	C	1	NAG	O7-C7-N2-C2
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
10	P	1	NAG	C8-C7-N2-C2
10	P	1	NAG	O7-C7-N2-C2
10	P	1	NAG	O5-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
7	F	2	NAG	C4-C5-C6-O6
8	K	2	NAG	C4-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
11	Q	3	BMA	O5-C5-C6-O6
11	Q	6	MAN	C4-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
8	K	2	NAG	O5-C5-C6-O6
12	R	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
12	R	3	BMA	O5-C5-C6-O6
12	R	6	MAN	O5-C5-C6-O6
7	C	2	NAG	C4-C5-C6-O6
8	K	4	MAN	O5-C5-C6-O6
11	Q	1	NAG	C4-C5-C6-O6
7	C	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
11	Q	1	NAG	O5-C5-C6-O6
10	P	5	MAN	O5-C5-C6-O6

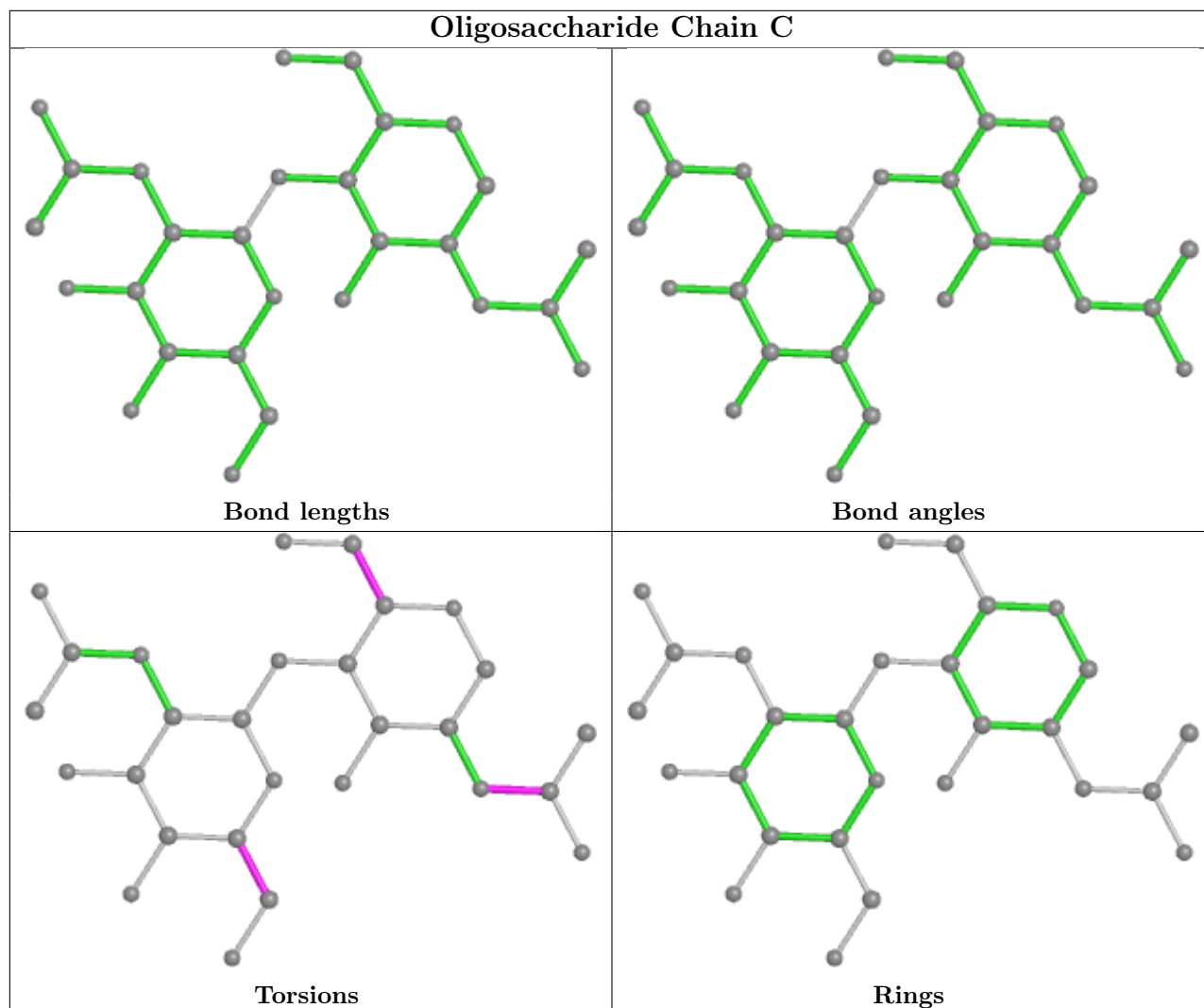
There are no ring outliers.

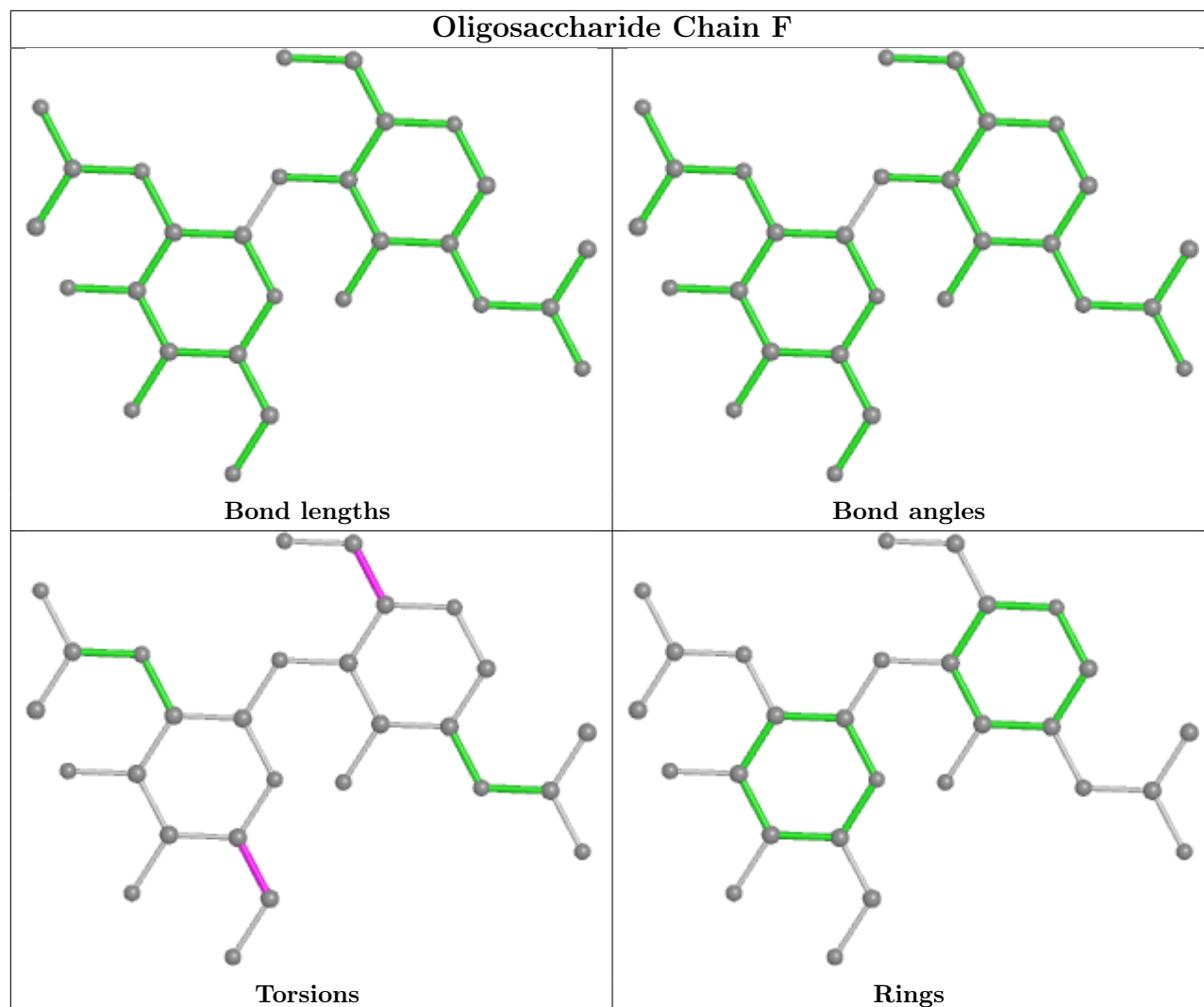
9 monomers are involved in 7 short contacts:

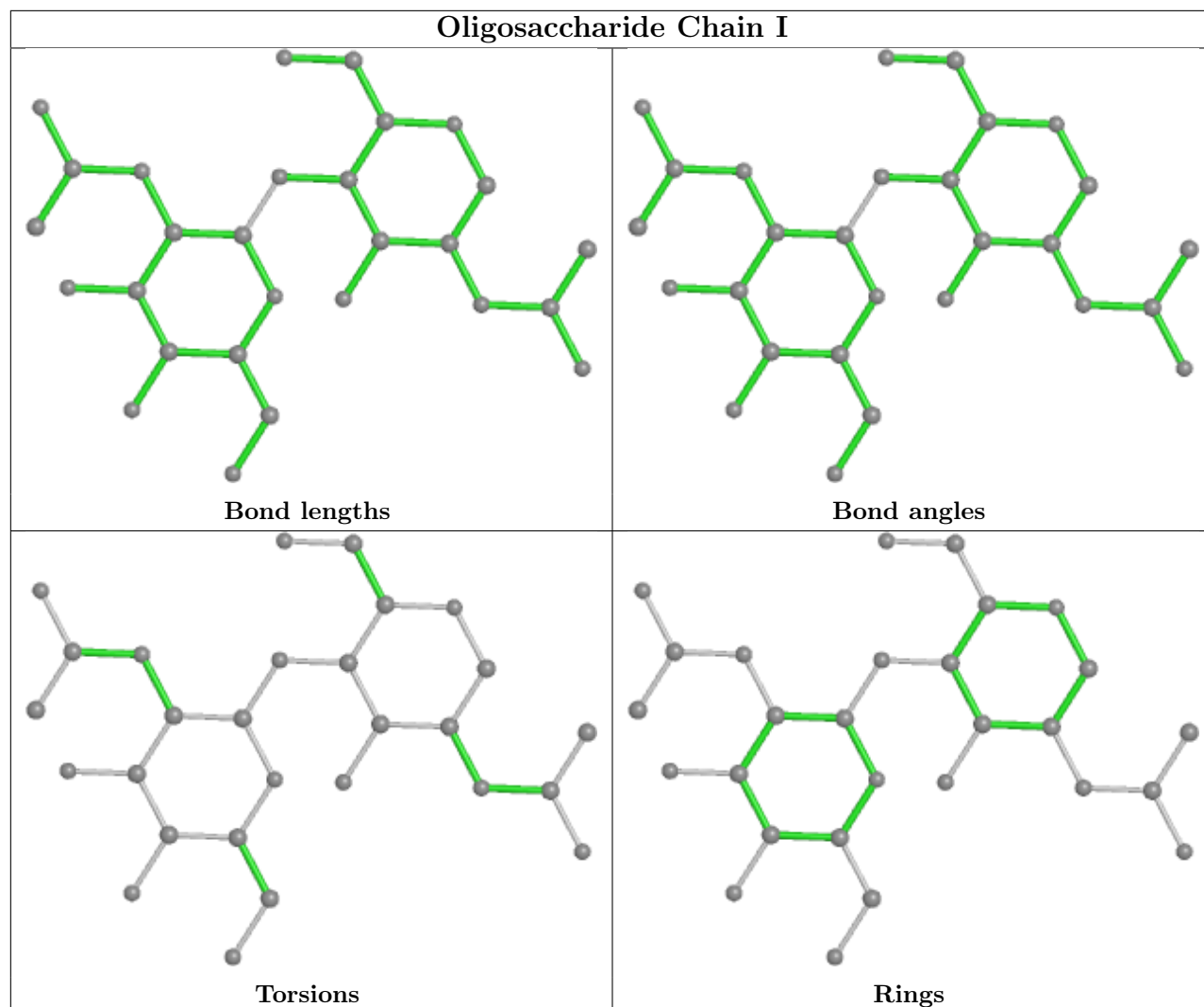
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	1	NAG	1	0
11	Q	3	BMA	1	0
7	J	2	NAG	1	0
8	K	5	MAN	1	0
11	Q	2	NAG	1	0
11	Q	4	MAN	1	0
12	R	1	NAG	1	0
8	K	3	BMA	1	0
7	M	1	NAG	1	0

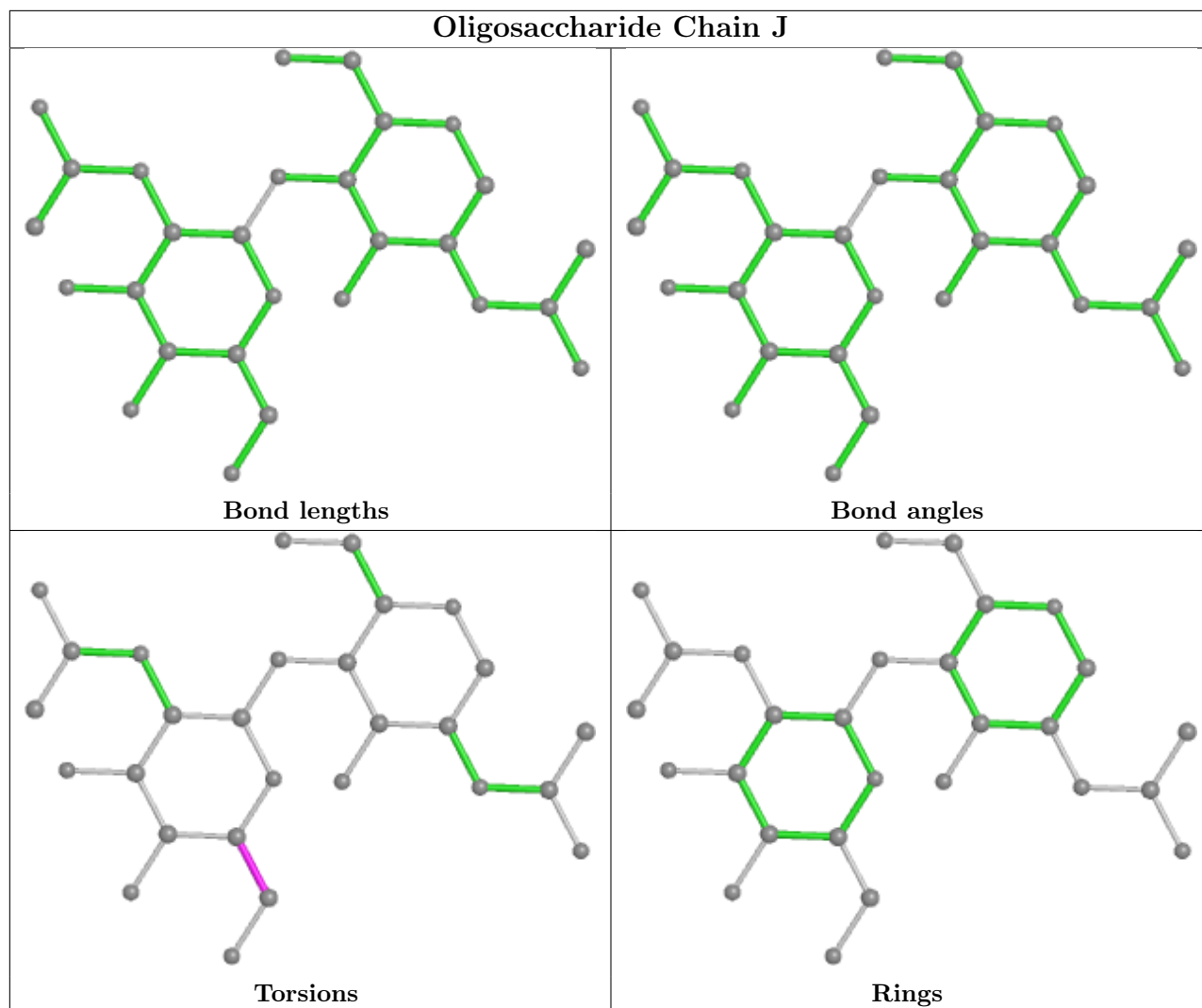
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

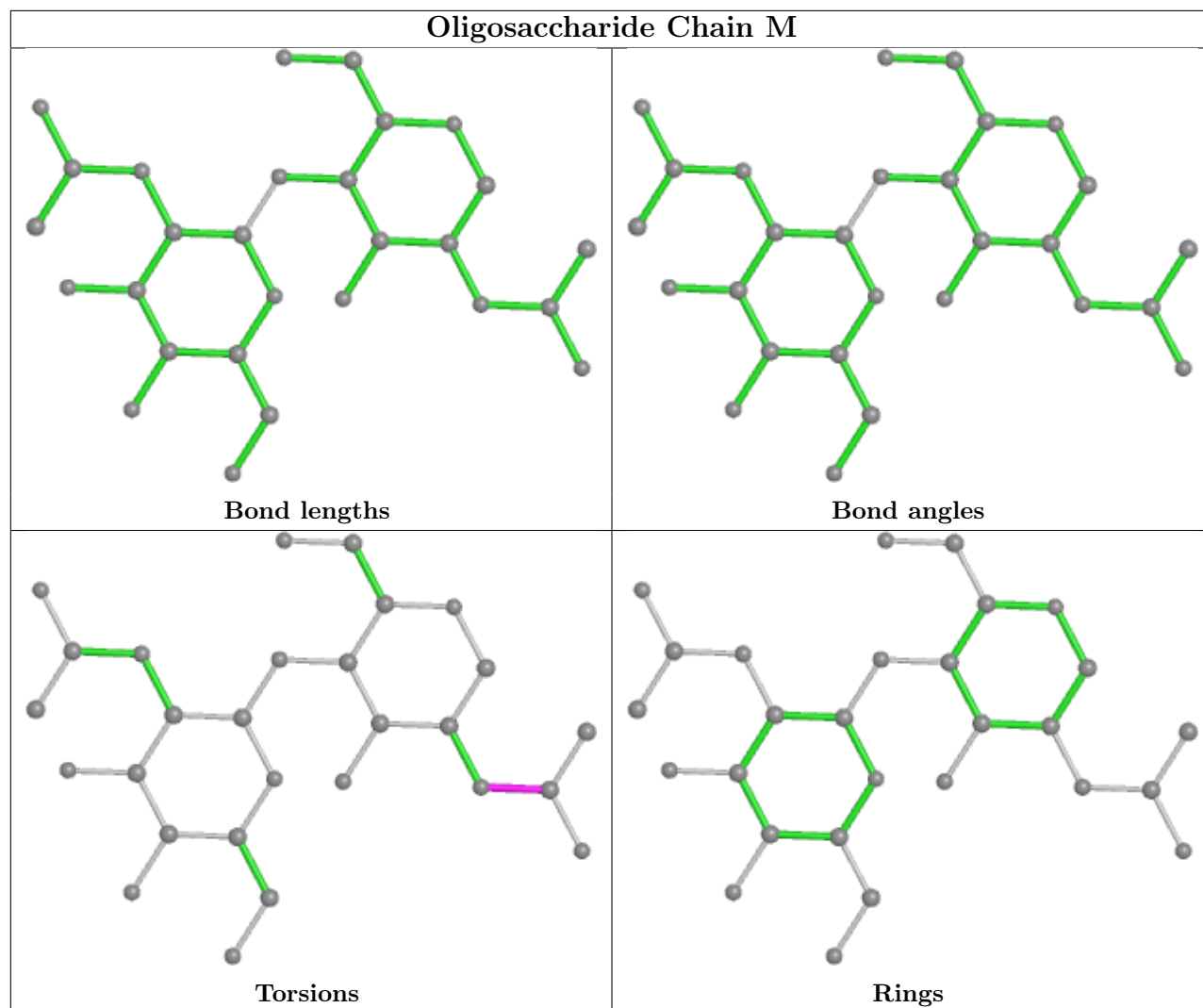




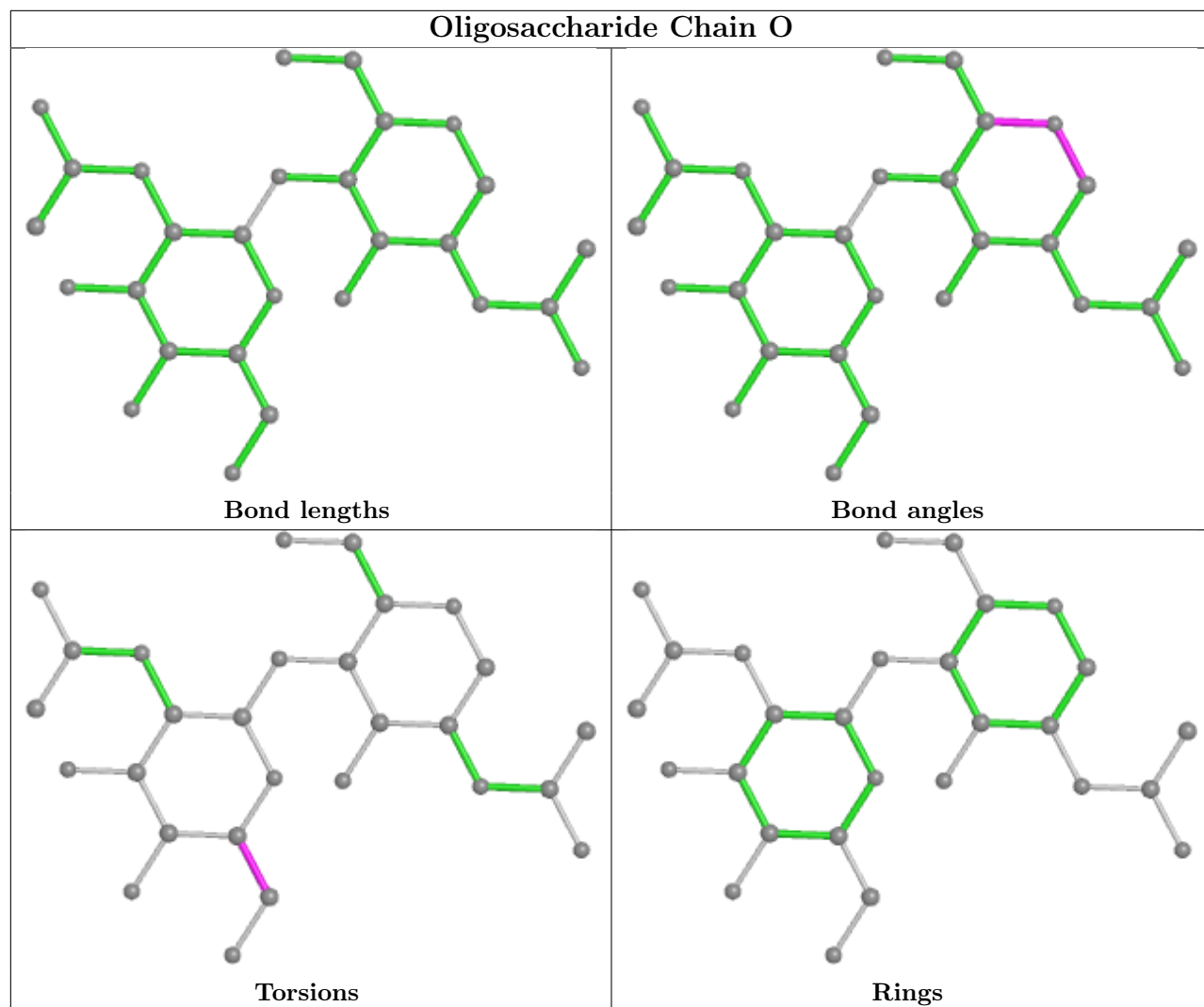


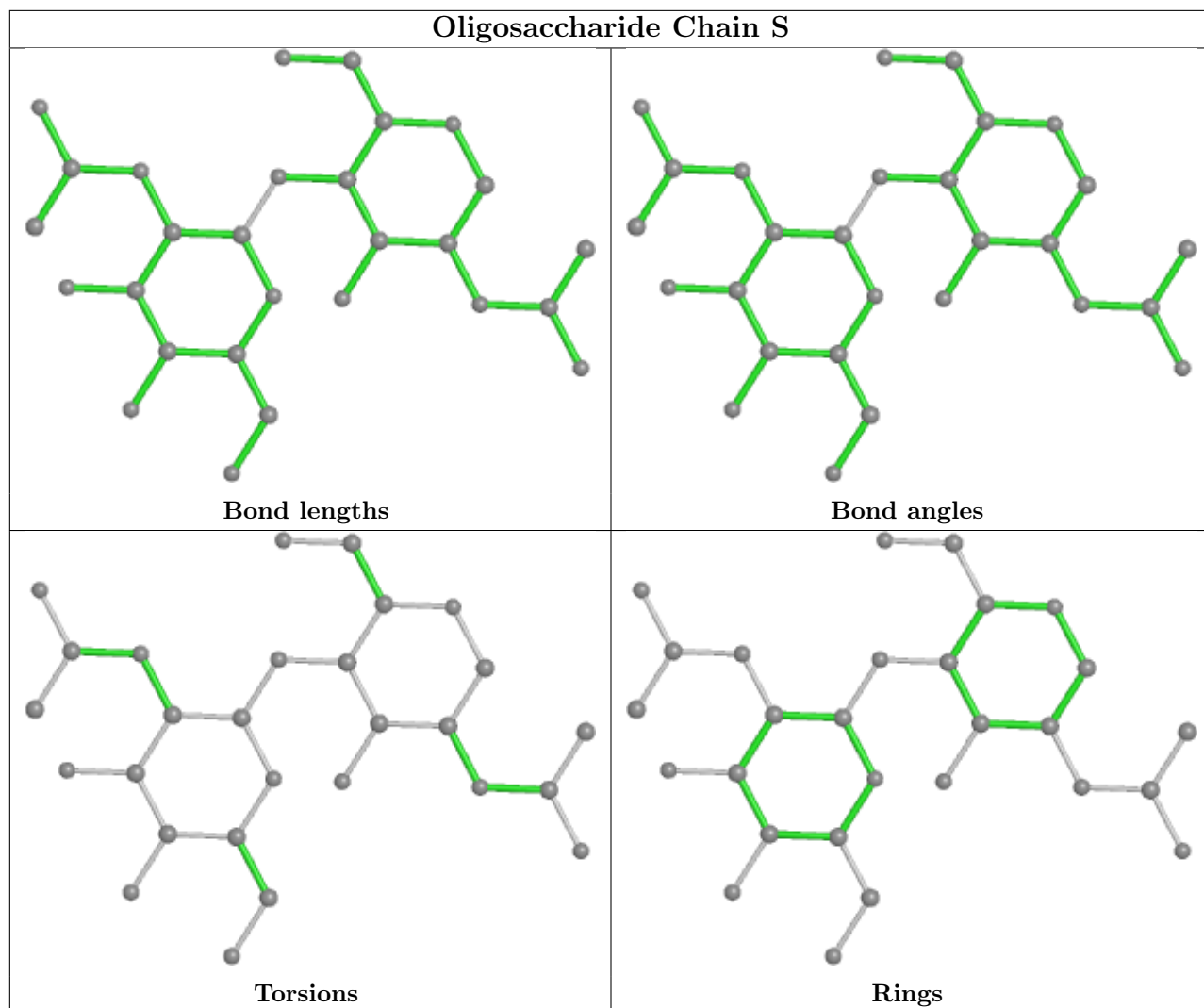


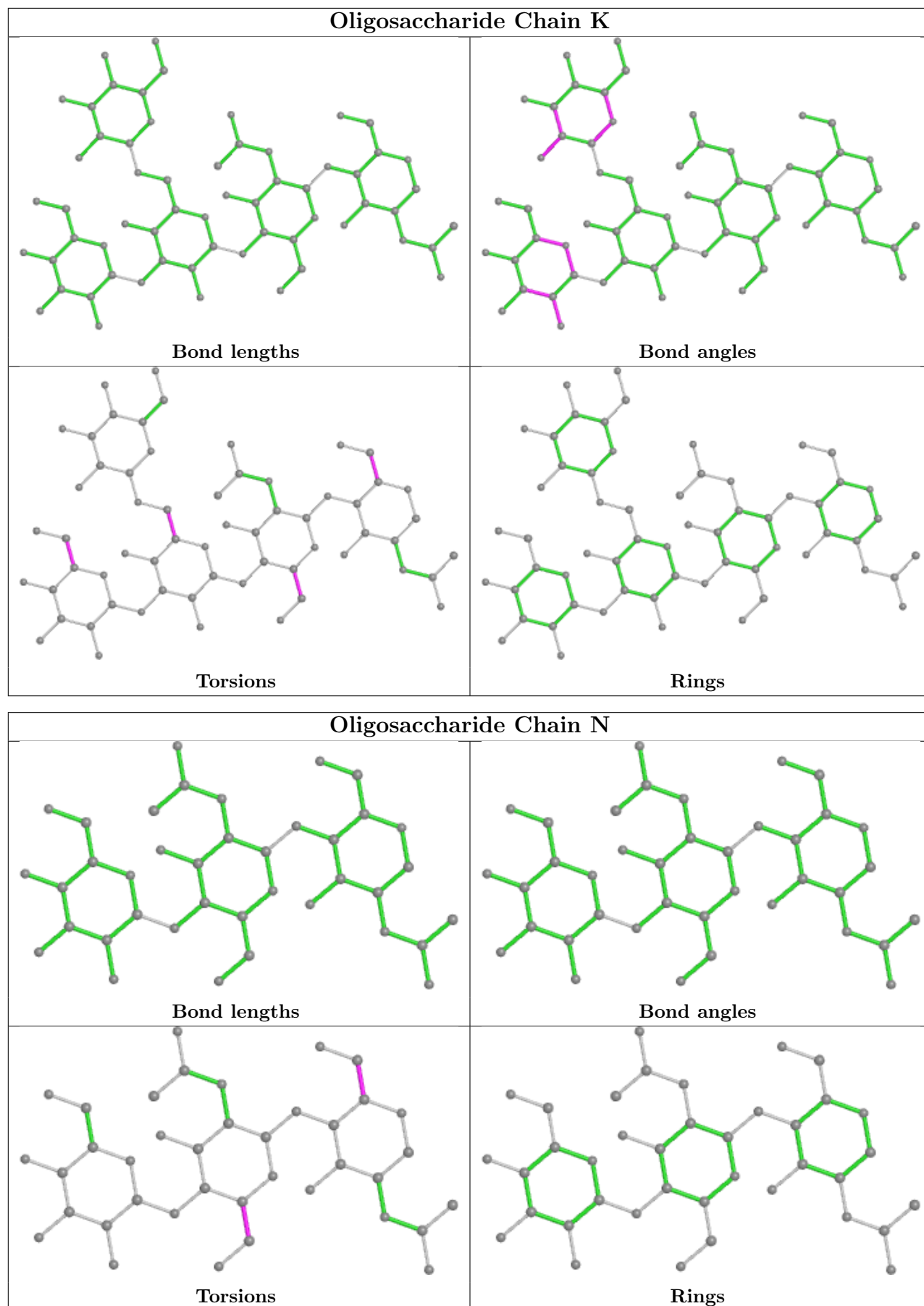


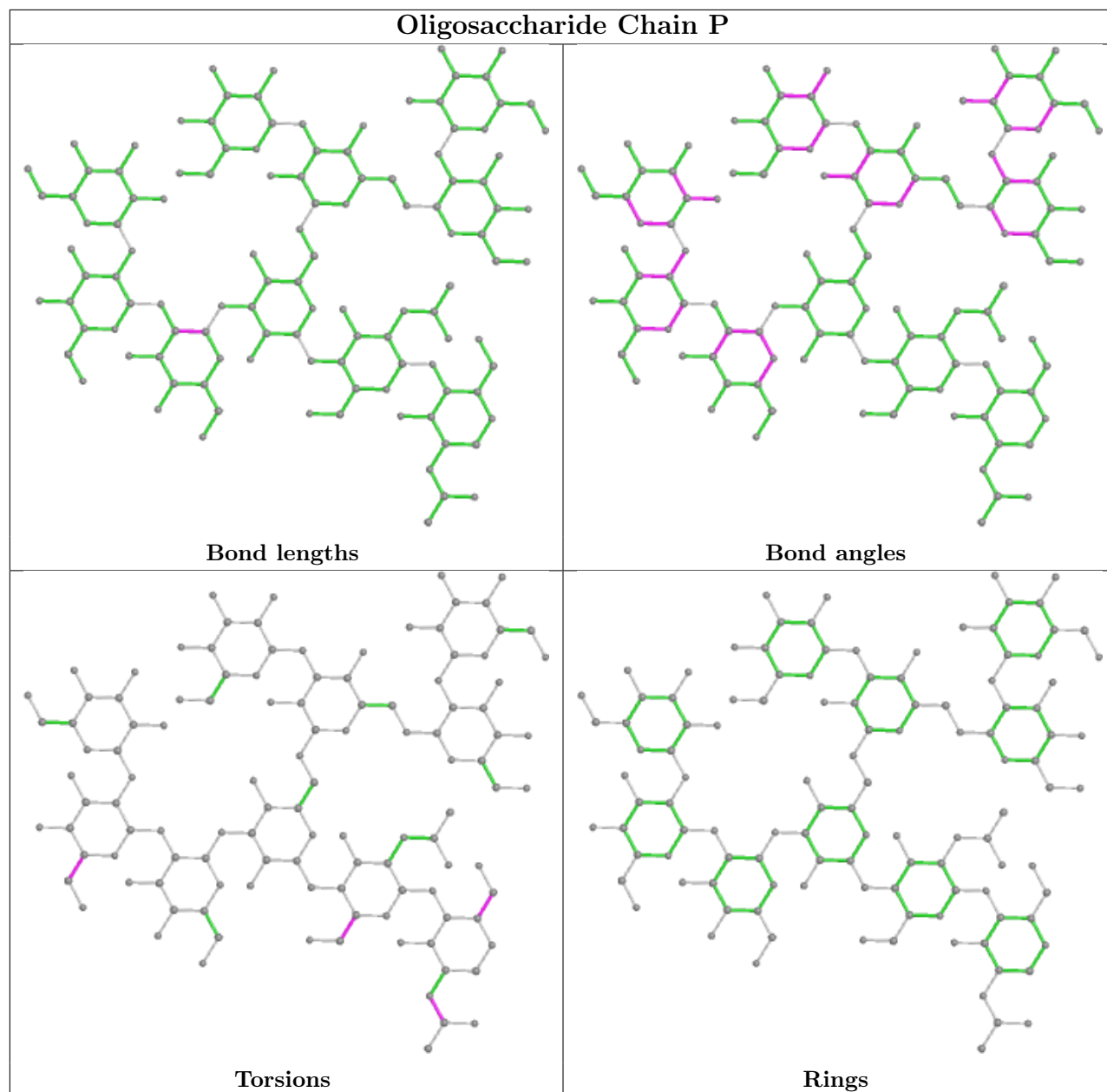


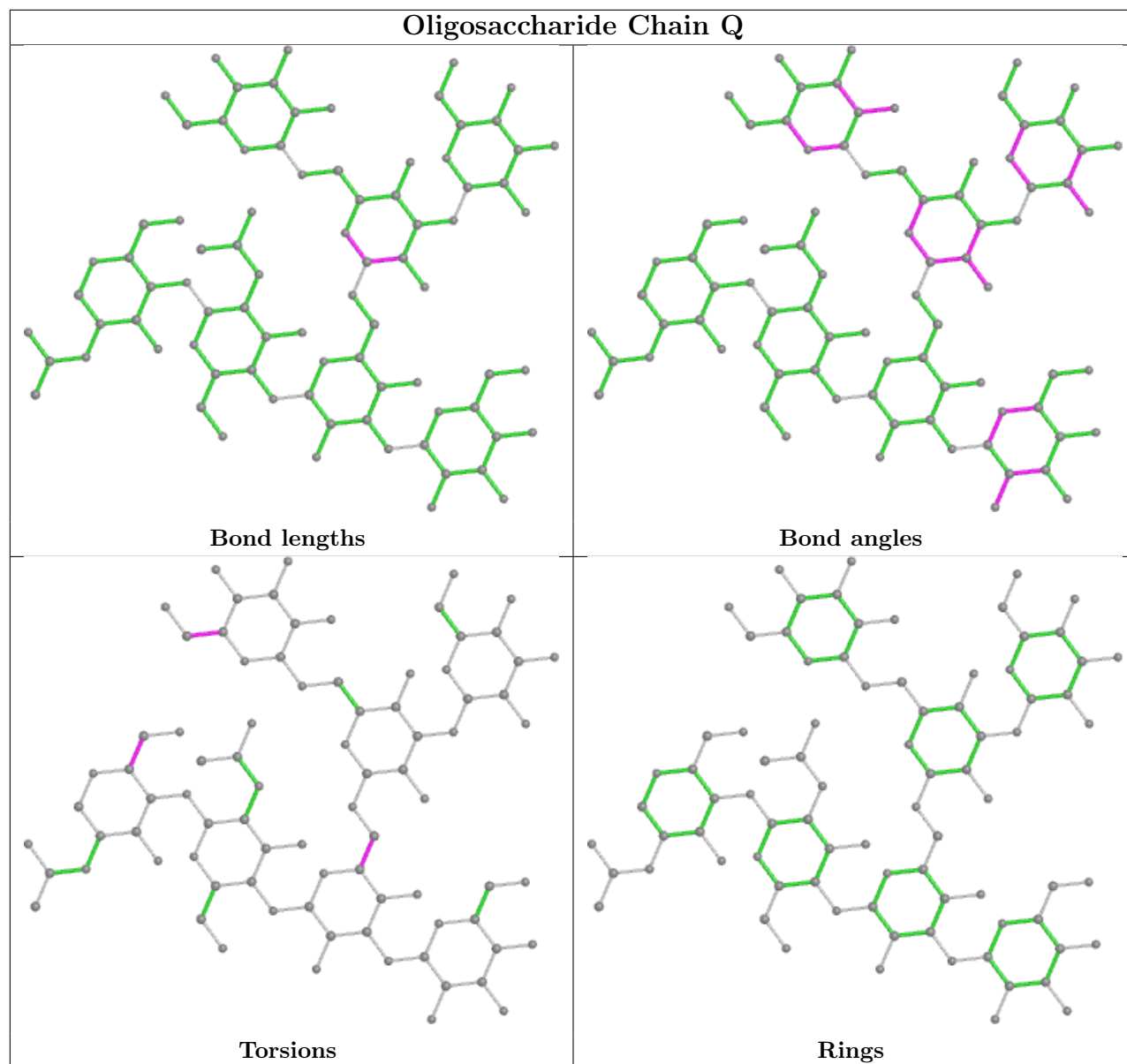


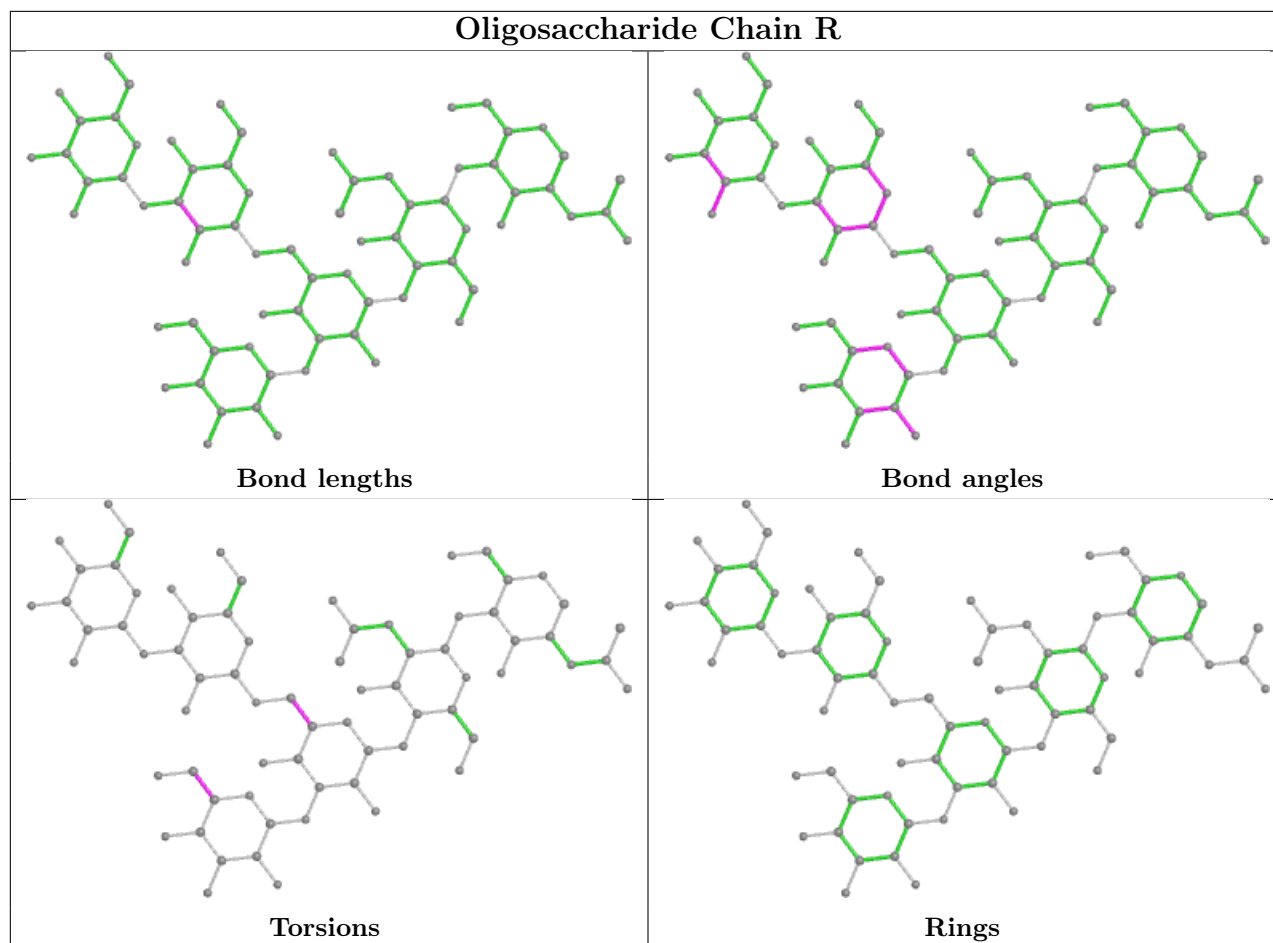












## 5.6 Ligand geometry [i](#)

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
13	NAG	B	701	2	14,14,15	0.17	0	17,19,21	0.35	0
13	NAG	B	703	2	14,14,15	0.40	0	17,19,21	1.25	2 (11%)
13	NAG	G	703	1	14,14,15	0.18	0	17,19,21	0.36	0
13	NAG	G	707	1	14,14,15	0.20	0	17,19,21	0.42	0
13	NAG	G	700	1	14,14,15	0.44	0	17,19,21	0.40	0
13	NAG	G	704	1	14,14,15	0.49	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	G	708	1	14,14,15	0.19	0	17,19,21	0.42	0
13	NAG	G	727	1	14,14,15	0.22	0	17,19,21	0.42	0
13	NAG	B	702	2	14,14,15	0.22	0	17,19,21	0.39	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
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
13	NAG	B	703	2	-	3/6/23/26	0/1/1/1
13	NAG	G	703	1	-	0/6/23/26	0/1/1/1
13	NAG	G	707	1	-	2/6/23/26	0/1/1/1
13	NAG	G	700	1	-	2/6/23/26	0/1/1/1
13	NAG	G	704	1	-	5/6/23/26	0/1/1/1
13	NAG	G	708	1	-	2/6/23/26	0/1/1/1
13	NAG	G	727	1	-	4/6/23/26	0/1/1/1
13	NAG	B	702	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	703	NAG	C2-N2-C7	4.35	129.09	122.90
13	G	704	NAG	C2-N2-C7	4.29	129.01	122.90
13	B	703	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	727	NAG	O5-C5-C6-O6
13	G	707	NAG	O5-C5-C6-O6
13	G	708	NAG	O5-C5-C6-O6
13	G	727	NAG	C4-C5-C6-O6
13	G	704	NAG	C8-C7-N2-C2
13	G	704	NAG	O7-C7-N2-C2
13	G	727	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
13	G	727	NAG	O7-C7-N2-C2
13	B	703	NAG	C8-C7-N2-C2
13	B	703	NAG	O7-C7-N2-C2
13	G	707	NAG	C4-C5-C6-O6
13	G	708	NAG	C4-C5-C6-O6
13	G	704	NAG	O5-C5-C6-O6
13	G	704	NAG	C4-C5-C6-O6
13	B	702	NAG	C4-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	G	700	NAG	C4-C5-C6-O6
13	G	700	NAG	O5-C5-C6-O6
13	G	704	NAG	C3-C2-N2-C7
13	B	703	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	703	NAG	1	0
13	G	700	NAG	1	0
13	G	704	NAG	1	0
13	G	727	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	G	471/485 (97%)	0.28	14 (2%) 50 39	86, 136, 248, 325	0
2	B	129/153 (84%)	0.18	4 (3%) 49 38	93, 165, 267, 311	0
3	L	211/214 (98%)	0.13	6 (2%) 53 42	97, 150, 215, 274	0
4	H	234/236 (99%)	0.27	10 (4%) 35 29	91, 174, 255, 308	0
5	D	240/240 (100%)	0.89	36 (15%) 2 2	112, 202, 342, 382	0
6	E	213/216 (98%)	0.79	32 (15%) 2 2	124, 219, 333, 413	0
All	All	1498/1544 (97%)	0.42	102 (6%) 17 14	86, 165, 294, 413	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	213	PRO	11.7
5	D	191	THR	7.7
6	E	146	GLY	6.4
5	D	211	VAL	6.2
5	D	215	SER	6.0
1	G	147	ASN	5.4
5	D	212	GLU	5.3
5	D	192	GLN	5.3
5	D	126	PRO	4.6
6	E	207	GLU	4.5
5	D	214	LYS	4.3
6	E	176	TYR	4.3
6	E	206	VAL	4.2
6	E	117	PRO	4.2
6	E	147	ALA	4.1
5	D	10	GLU	4.1
1	G	400	THR	4.0
1	G	79	PRO	4.0
1	G	507	GLU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	D	216	CYS	3.9
1	G	151	GLY	3.9
5	D	163	VAL	3.8
1	G	401	ASN	3.8
6	E	145	PRO	3.8
5	D	188	SER	3.7
5	D	190	GLY	3.7
5	D	193	THR	3.7
6	E	143	PHE	3.7
5	D	218	LYS	3.5
5	D	132	SER	3.4
5	D	185	PRO	3.2
2	B	546	SER	3.2
5	D	127	SER	3.2
5	D	210	ARG	3.2
5	D	109	LEU	3.1
6	E	121	LEU	3.1
4	H	24	VAL	3.1
5	D	194	TYR	3.1
6	E	114	LYS	3.1
2	B	547	GLY	3.0
6	E	140	ILE	3.0
1	G	395	TYR	2.9
5	D	184	VAL	2.9
1	G	150	ASN	2.9
2	B	661	LEU	2.9
4	H	27	GLY	2.8
6	E	39	GLN	2.8
3	L	32	ALA	2.8
4	H	4	LEU	2.8
6	E	109	VAL	2.7
6	E	64	PHE	2.7
5	D	111	VAL	2.7
6	E	169	SER	2.7
6	E	202	GLU	2.7
4	H	2	VAL	2.7
6	E	38	TYR	2.6
5	D	137	ALA	2.6
5	D	150	VAL	2.6
6	E	213	THR	2.6
6	E	132	ASN	2.6
6	E	199	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	D	82(C)	LEU	2.6
1	G	396	ASN	2.6
6	E	196	SER	2.6
3	L	133	LEU	2.5
6	E	174	ASN	2.4
5	D	112	SER	2.4
6	E	201	HIS	2.4
5	D	121	VAL	2.4
4	H	35	THR	2.4
2	B	521	GLY	2.4
1	G	267	GLU	2.4
4	H	70	SER	2.4
5	D	84	PHE	2.4
6	E	119	VAL	2.3
6	E	151	ALA	2.3
6	E	205	THR	2.3
1	G	506	VAL	2.3
6	E	48	LEU	2.3
3	L	52	GLN	2.3
5	D	82(A)	ARG	2.3
4	H	128	SER	2.2
5	D	9	ALA	2.2
6	E	150	VAL	2.2
1	G	399	ASP	2.2
3	L	31	ARG	2.2
6	E	139	LEU	2.2
1	G	509	GLY	2.1
4	H	1	GLN	2.1
3	L	62	PHE	2.1
4	H	36	TRP	2.1
5	D	100(F)	PRO	2.1
1	G	465	THR	2.1
4	H	100	ARG	2.1
6	E	113	SER	2.1
6	E	116	ASN	2.1
3	L	119	PHE	2.1
5	D	207	VAL	2.1
5	D	160	THR	2.0
5	D	63	PHE	2.0
6	E	87	THR	2.0
5	D	48	MET	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.

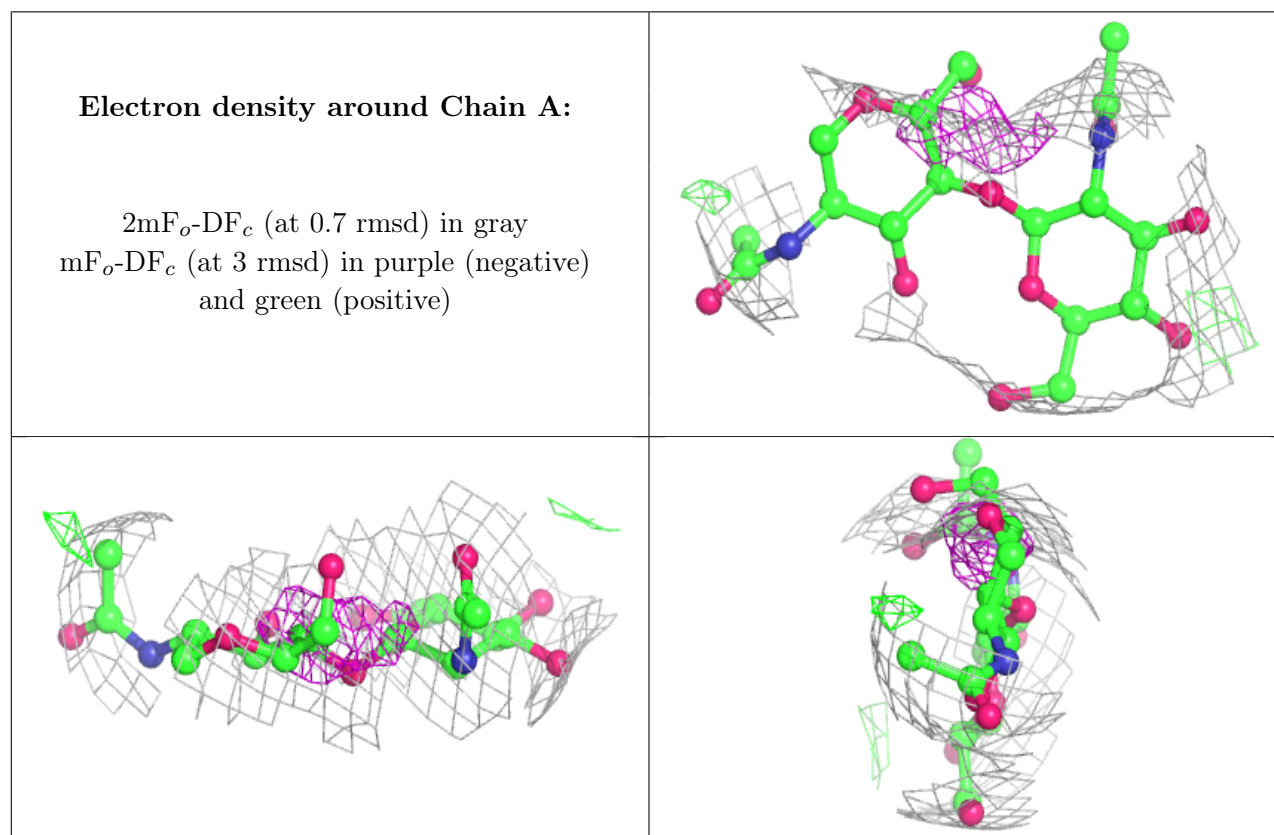
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	MAN	R	5	11/12	0.56	0.20	211,219,221,221	0
11	MAN	Q	4	11/12	0.71	0.39	148,166,174,175	0
7	NAG	M	2	14/15	0.73	0.32	161,187,210,240	0
9	BMA	N	3	11/12	0.75	0.64	190,202,208,209	0
8	BMA	K	3	11/12	0.76	0.19	172,190,202,220	0
7	NAG	A	2	14/15	0.76	0.24	180,181,183,184	0
11	NAG	Q	2	14/15	0.76	0.40	132,133,134,134	0
7	NAG	F	2	14/15	0.76	0.29	140,168,176,184	0
7	NAG	A	1	14/15	0.76	0.29	168,171,172,174	0
10	MAN	P	10	11/12	0.77	0.27	166,176,184,191	0
11	BMA	Q	3	11/12	0.79	0.43	139,141,153,157	0
7	NAG	C	2	14/15	0.81	0.42	152,173,190,207	0
8	MAN	K	4	11/12	0.81	0.25	161,190,203,205	0
7	NAG	I	1	14/15	0.82	0.26	145,159,192,208	0
7	NAG	I	2	14/15	0.82	0.24	146,183,218,219	0
7	NAG	F	1	14/15	0.82	0.28	137,142,155,156	0
11	MAN	Q	6	11/12	0.82	0.32	159,169,189,200	0
7	NAG	S	1	14/15	0.82	0.28	129,144,154,159	0
8	MAN	K	5	11/12	0.83	0.22	172,190,210,211	0
11	MAN	Q	5	11/12	0.83	0.31	171,175,184,187	0
7	NAG	C	1	14/15	0.84	0.26	134,150,160,162	0
7	NAG	O	2	14/15	0.84	0.38	172,215,223,231	0
12	MAN	R	4	11/12	0.85	0.13	196,200,216,218	0
7	NAG	M	1	14/15	0.85	0.28	143,155,164,187	0
12	MAN	R	6	11/12	0.85	0.17	170,181,196,202	0
9	NAG	N	2	14/15	0.86	0.39	147,165,202,209	0
10	BMA	P	3	11/12	0.86	0.23	137,137,140,153	0
10	MAN	P	8	11/12	0.86	0.21	185,189,202,203	0
7	NAG	S	2	14/15	0.87	0.30	150,167,176,177	0
10	MAN	P	7	11/12	0.87	0.18	160,167,182,184	0
7	NAG	J	2	14/15	0.87	0.23	129,151,181,185	0
12	BMA	R	3	11/12	0.88	0.14	160,171,187,194	0

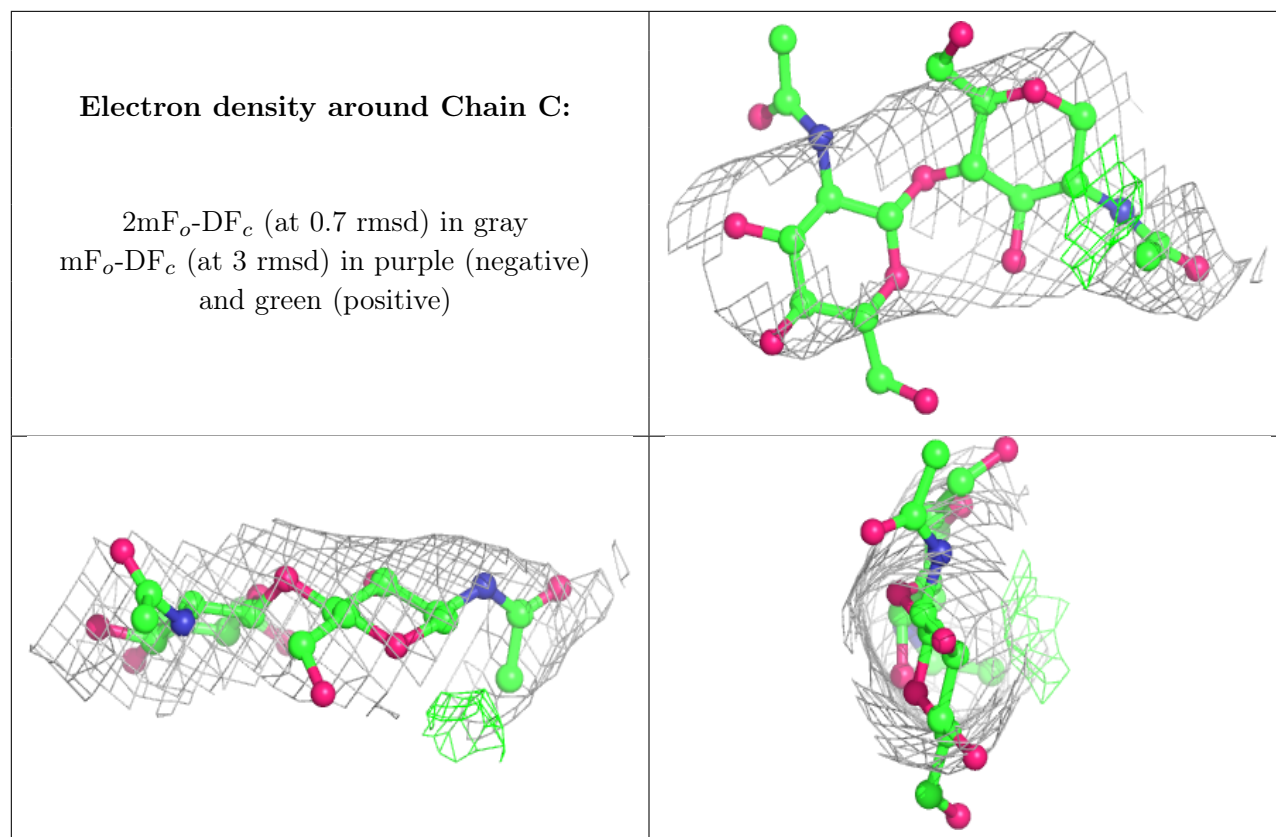
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	K	2	14/15	0.88	0.25	147,169,195,195	0
10	MAN	P	9	11/12	0.89	0.37	181,189,200,206	0
12	NAG	R	2	14/15	0.89	0.20	125,134,158,174	0
11	NAG	Q	1	14/15	0.89	0.32	120,123,125,125	0
11	MAN	Q	7	11/12	0.90	0.49	143,147,153,153	0
7	NAG	O	1	14/15	0.90	0.36	168,191,208,215	0
10	NAG	P	1	14/15	0.91	0.33	126,128,134,139	0
7	NAG	J	1	14/15	0.91	0.18	131,134,144,148	0
9	NAG	N	1	14/15	0.91	0.22	137,140,162,165	0
10	MAN	P	6	11/12	0.92	0.23	143,144,151,152	0
10	NAG	P	2	14/15	0.92	0.24	130,135,145,146	0
8	NAG	K	1	14/15	0.92	0.24	127,130,154,155	0
10	MAN	P	5	11/12	0.92	0.26	138,139,141,160	0
12	NAG	R	1	14/15	0.92	0.23	118,119,133,134	0
10	MAN	P	4	11/12	0.95	0.17	136,137,140,153	0

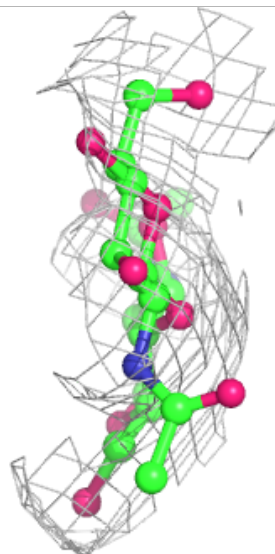
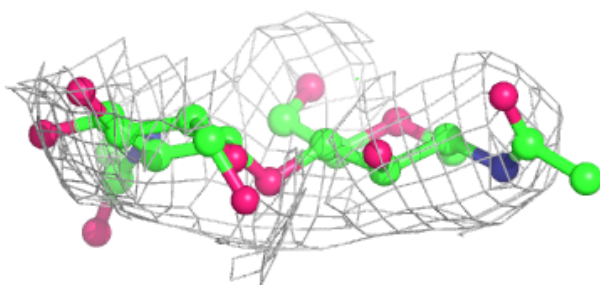
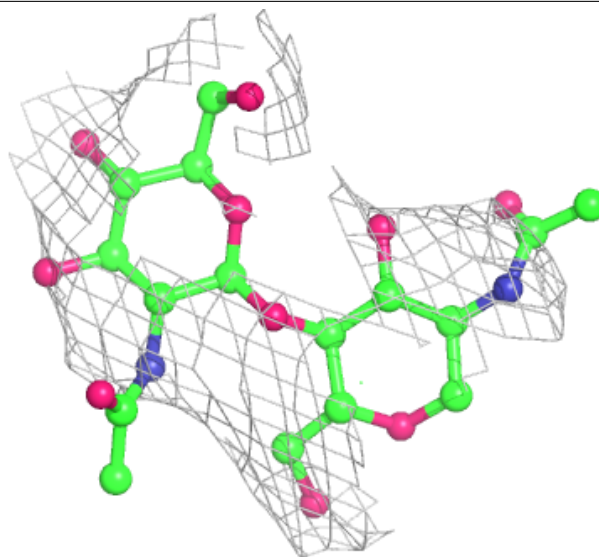
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





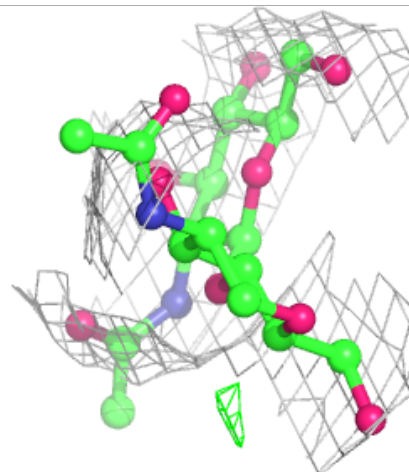
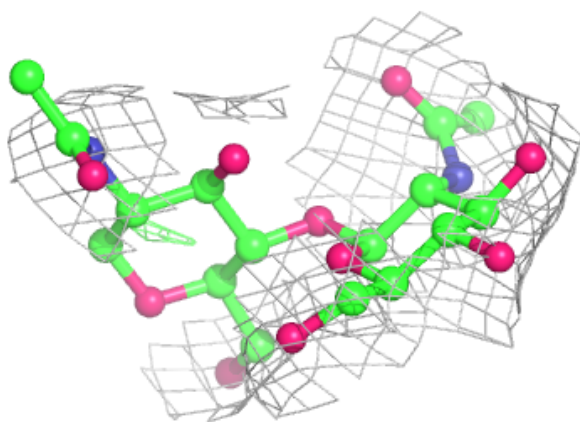
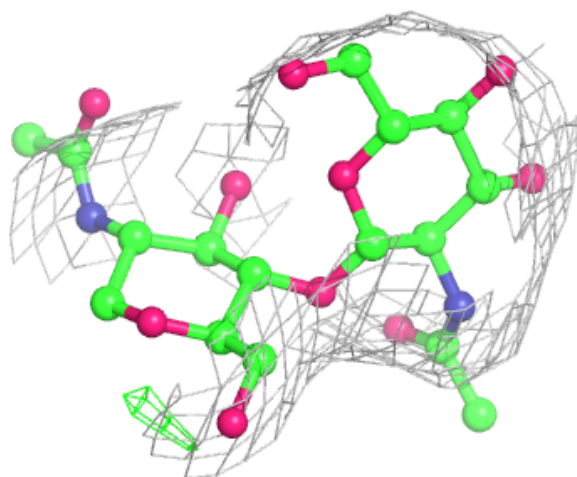
**Electron density around Chain F:**

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



**Electron density around Chain I:**

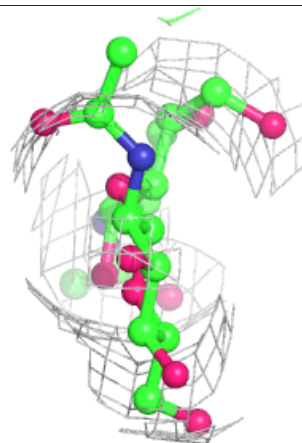
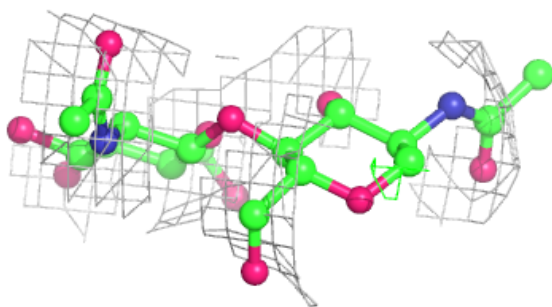
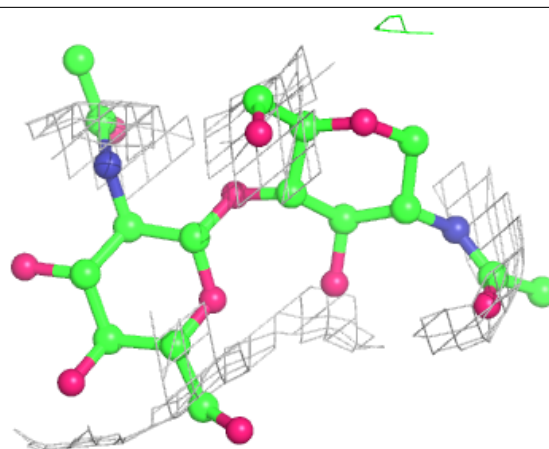
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





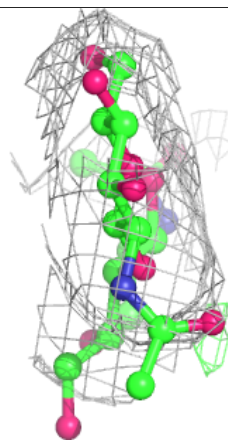
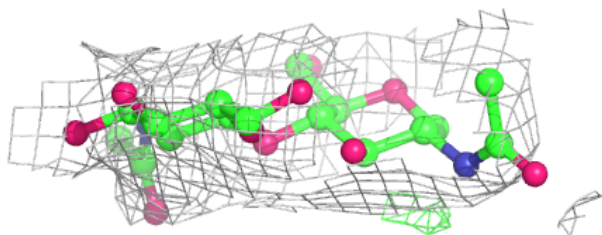
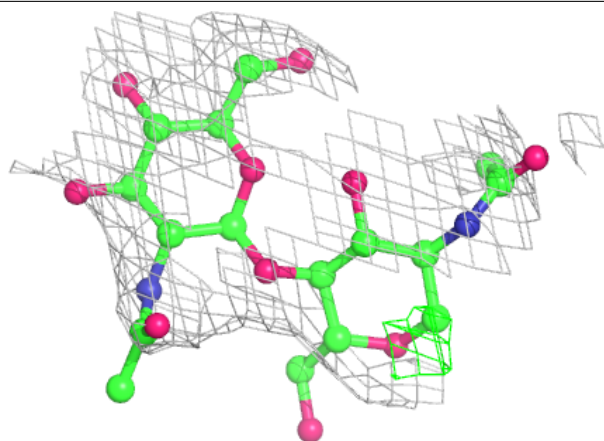
**Electron density around Chain J:**

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



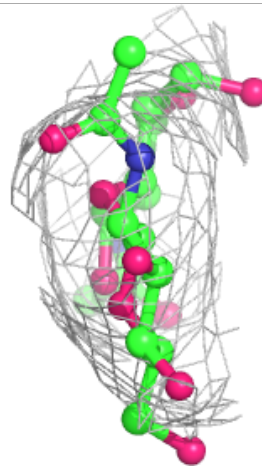
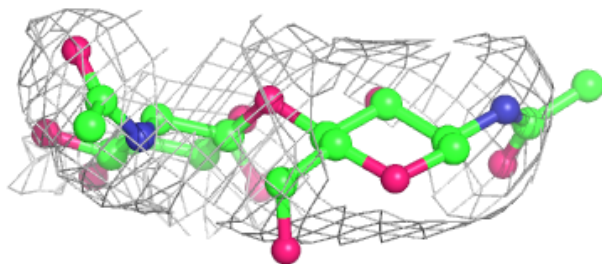
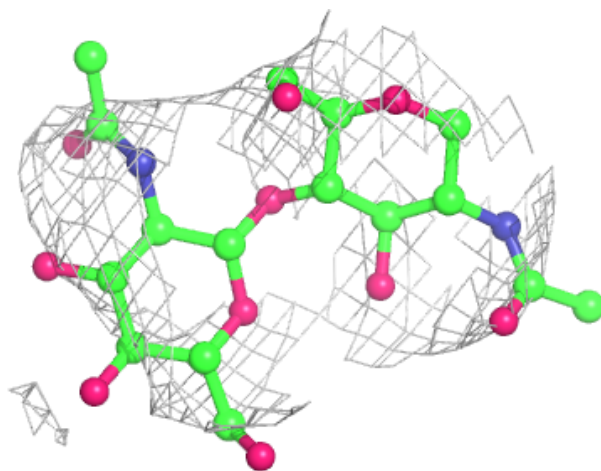
**Electron density around Chain M:**

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



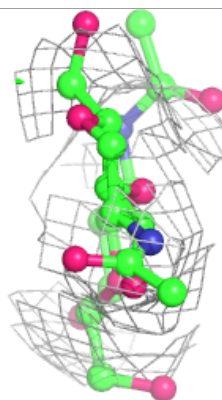
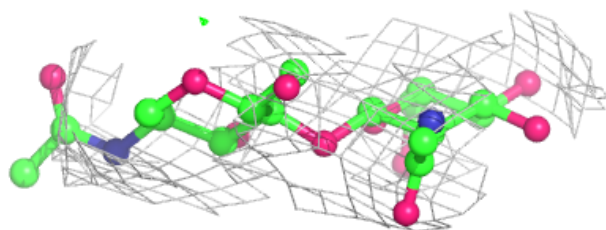
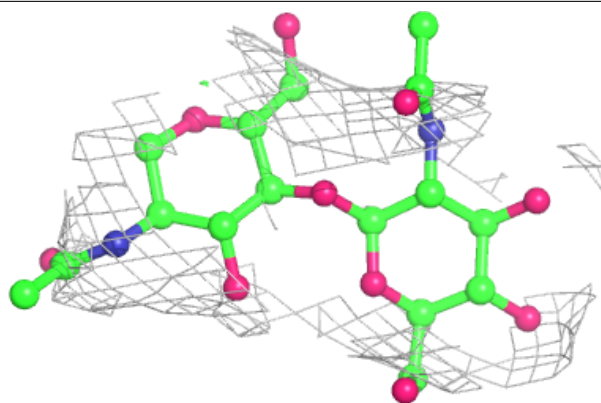
**Electron density around Chain O:**

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

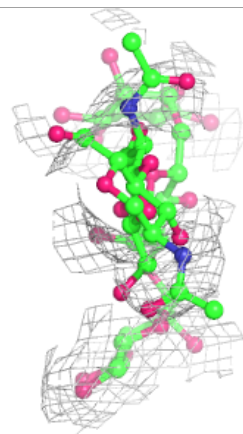
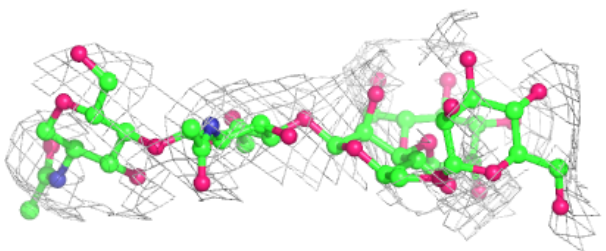
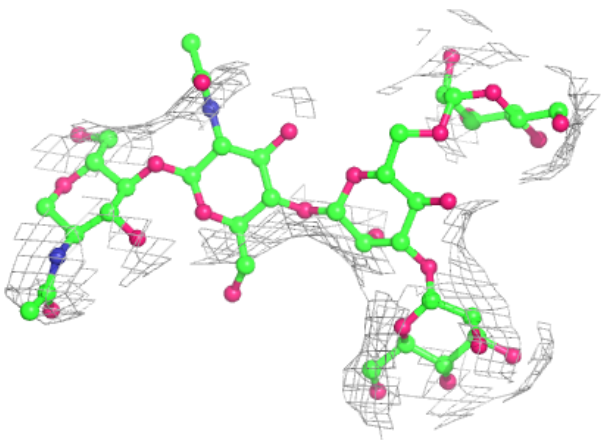


**Electron density around Chain S:**

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

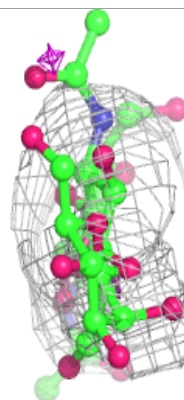
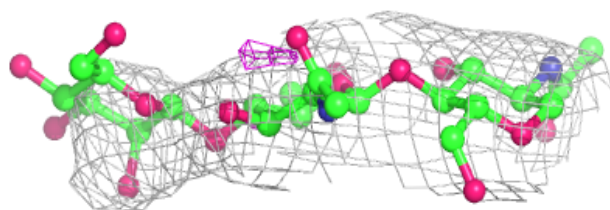
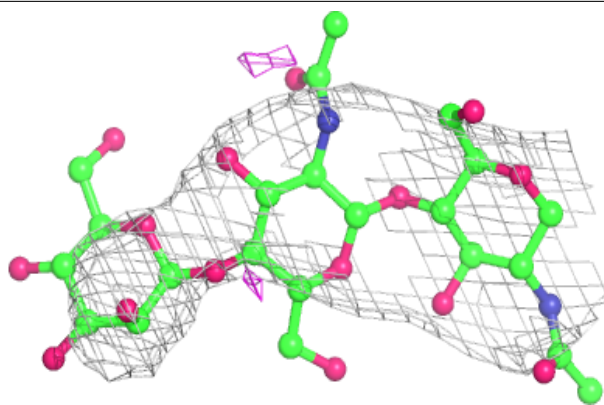
**Electron density around Chain K:**

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

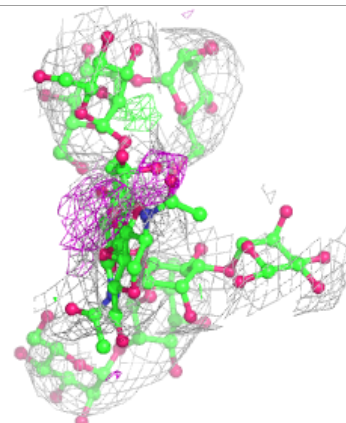
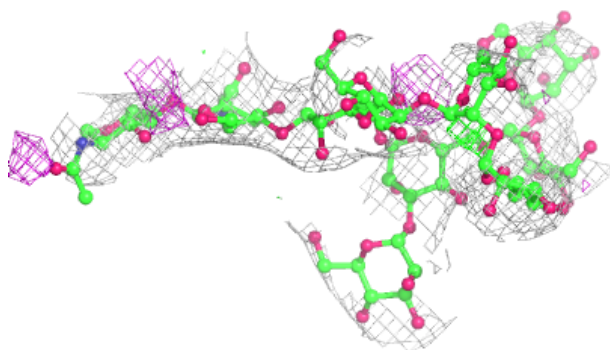
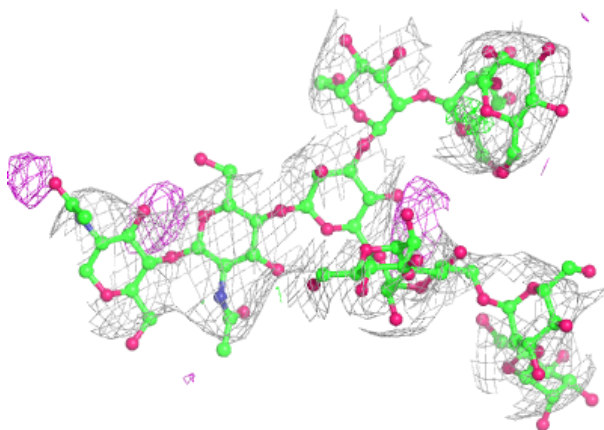


**Electron density around Chain N:**

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

**Electron density around Chain P:**

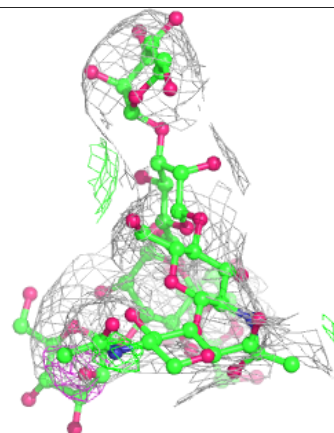
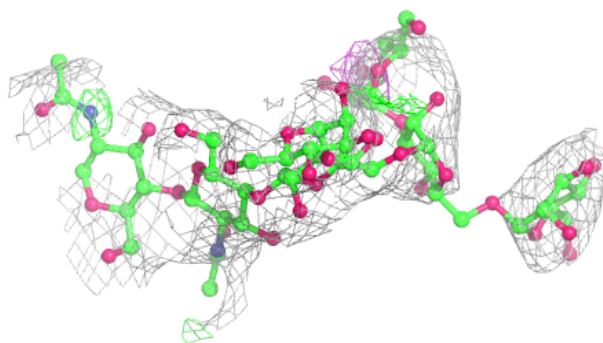
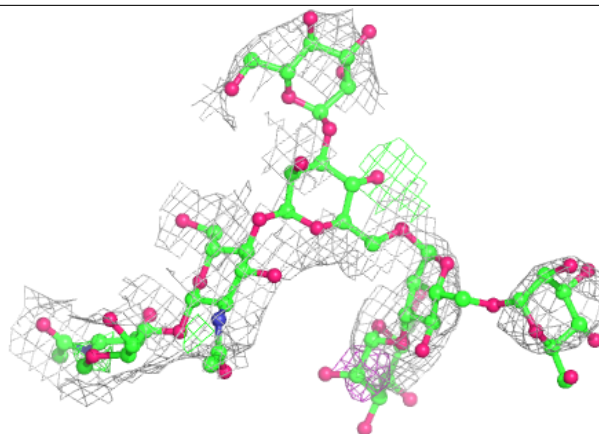
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



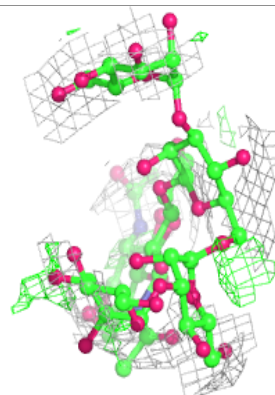
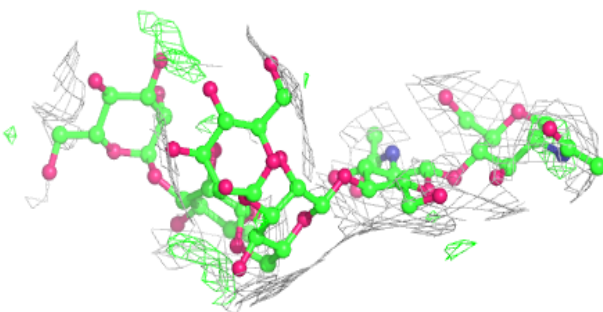
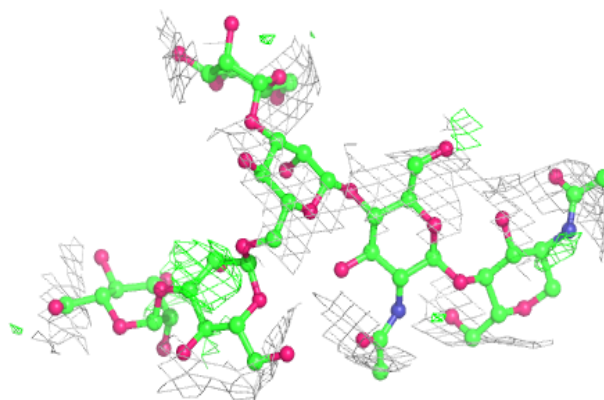


**Electron density around Chain Q:**

$2mF_o-DF_c$  (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)



## 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
13	NAG	B	702	14/15	0.57	0.33	190,222,235,237	0
13	NAG	G	700	14/15	0.78	0.28	142,143,144,145	0
13	NAG	B	703	14/15	0.78	0.43	139,143,173,175	0
13	NAG	B	701	14/15	0.79	0.31	181,190,203,206	0
13	NAG	G	704	14/15	0.79	0.29	197,215,223,230	0
13	NAG	G	727	14/15	0.79	0.18	164,201,239,247	0
13	NAG	G	708	14/15	0.80	0.33	155,162,169,182	0
13	NAG	G	707	14/15	0.82	0.25	127,149,181,198	0
13	NAG	G	703	14/15	0.83	0.31	136,138,138,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.