



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2022 – 02:15 PM EDT

PDB ID : 6CK9  
Title : Crystal Structure of HIV-1 ConC\_Base0 Prefusion Env Trimer in Complex with Human Antibody Fragment 3H109L and 35O22 variants at 3.5 Angstrom  
Authors : Lai, Y.-T.; Kwong, P.D.  
Deposited on : 2018-02-27  
Resolution : 2.71 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.27  
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) : 2.27

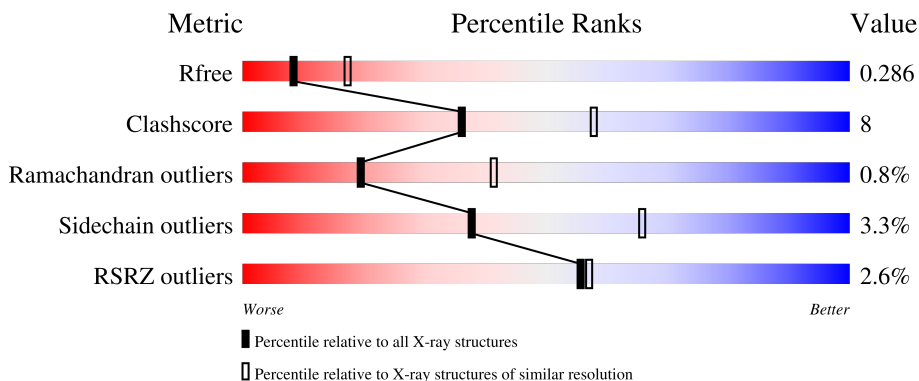
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	B	153	
2	D	134	
3	E	114	
4	G	463	
5	H	244	

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Mol	Chain	Length	Quality of chain
6	L	217	 80% 16%
7	A	5	 20% 80%
8	C	6	 17% 67% 17%
9	F	4	 50% 50%
10	I	2	 100%
10	K	2	 100%
10	M	2	 100%
10	O	2	 100%
10	P	2	 100%
11	J	2	 100%
12	N	10	 20% 70% 10%

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
10	NAG	K	2	-	-	-	X
10	NAG	O	2	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 10056 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 gp41 ectodomain of Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	129	1030	655	173	196	6	0	0	0

- Molecule 2 is a protein called 35O22 scFv heavy chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	128	994	630	168	191	5	0	0	0

- Molecule 3 is a protein called 35O22 scFv light chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	100	762	480	125	151	6	0	0	0

- Molecule 4 is a protein called gp120 of Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	430	3403	2140	597	639	27	0	0	0

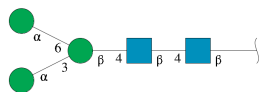
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	219	1670	1065	271	328	6	0	0	0

- Molecule 6 is a protein called 3H109L Fab light chain.

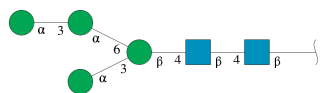
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	211	1604	1009	276	312	7	0	0	0

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



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

- Molecule 8 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			
8	C	6	72	40	2	30	0	0	0

- Molecule 9 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
			Total	C	N	O			
9	F	4	50	28	2	20	0	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



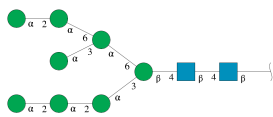
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 12 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
12	N	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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>).

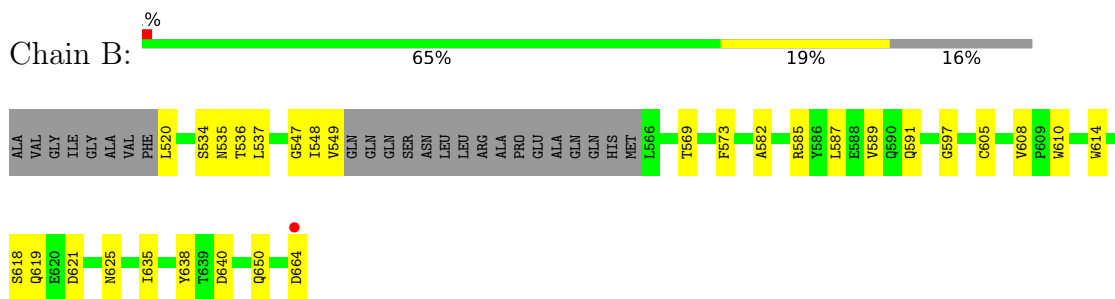


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	B	1	Total 14	8	1	5	0	0
13	B	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0

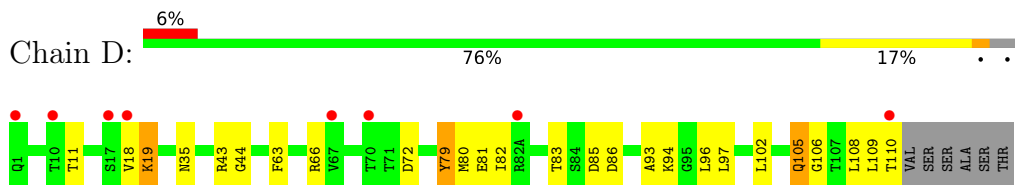
### 3 Residue-property plots

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.

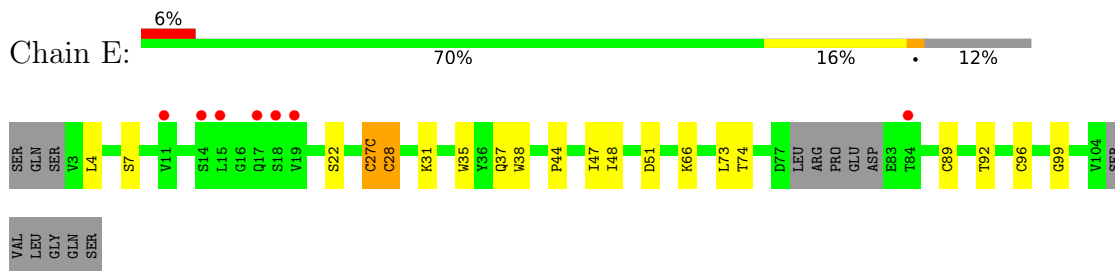
- Molecule 1: gp41 ectodomain of Envelope glycoprotein gp160



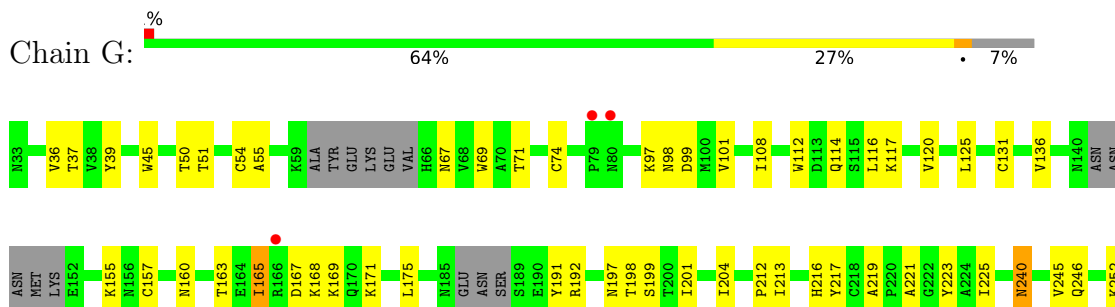
- Molecule 2: 35O22 scFv heavy chain portion



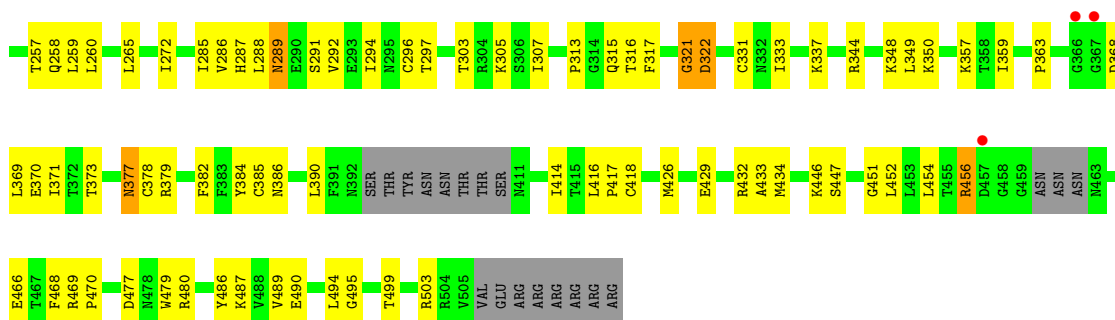
- Molecule 3: 35O22 scFv light chain portion



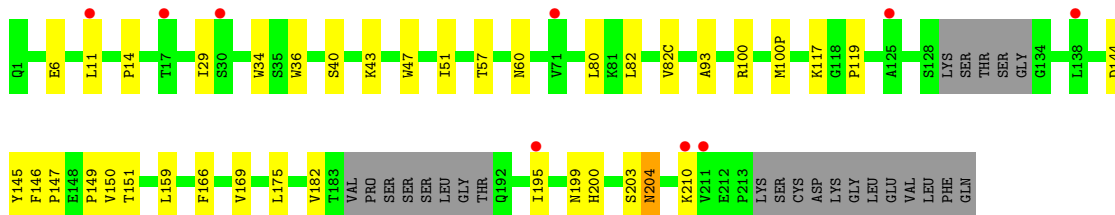
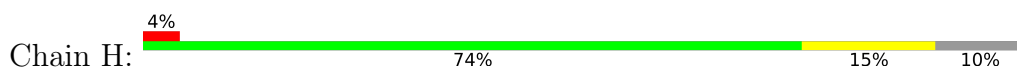
- Molecule 4: gp120 of Envelope glycoprotein gp160



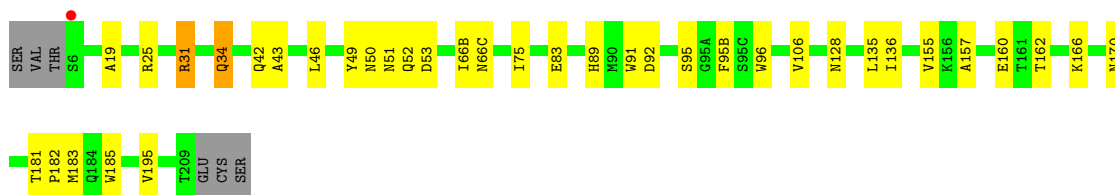
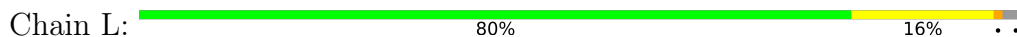




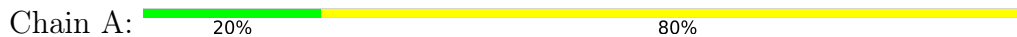
- Molecule 5: 3H109L Fab heavy chain



- Molecule 6: 3H109L Fab light chain



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



- Molecule 9: 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 F:  50% 50%

  
MAG1  
MAG2  
BMA3  
MAN4

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

  
MAG1  
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

  
MAG1  
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

  
MAG1  
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

  
MAG1  
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

  
MAG1  
MAG2

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1  
MAG2

- Molecule 12: 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 N:  20% 70% 10%MAG1  
MAG2  
MAG3  
MAG4  
MAG5  
MAG6  
MAG7  
MAG8  
MAG9  
MAG10

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.90Å 131.90Å 314.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.17 – 2.71 43.17 – 2.71	Depositor EDS
% Data completeness (in resolution range)	35.5 (43.17-2.71) 35.5 (43.17-2.71)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.248 , 0.288 0.248 , 0.286	Depositor DCC
$R_{free}$ test set	1472 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 13.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.076 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.23	0/1049	0.38	0/1423
2	D	0.24	0/1021	0.45	0/1390
3	E	0.24	0/784	0.43	0/1070
4	G	0.24	0/3471	0.44	0/4708
5	H	0.25	0/1711	0.46	0/2330
6	L	0.24	0/1647	0.44	0/2247
All	All	0.24	0/9683	0.44	0/13168

There are no bond length outliers.

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	B	1030	0	1005	20	0
2	D	994	0	958	15	0
3	E	762	0	712	8	0
4	G	3403	0	3355	79	0
5	H	1670	0	1637	25	0
6	L	1604	0	1553	22	0
7	A	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	72	0	61	2	0
9	F	50	0	43	1	0
10	I	28	0	25	0	0
10	K	28	0	25	0	0
10	M	28	0	25	0	0
10	O	28	0	25	0	0
10	P	28	0	25	0	0
11	J	28	0	25	1	0
12	N	116	0	97	2	0
13	B	28	0	26	0	0
13	G	98	0	91	3	0
All	All	10056	0	9740	158	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 8.

The worst 5 of 158 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)
4:G:378:CYS:SG	4:G:379:ARG:N	2.52	0.83
4:G:71:THR:HG21	4:G:213:ILE:HD11	1.67	0.76
4:G:169:LYS:HB2	13:G:1601:NAG:H82	1.68	0.74
6:L:46:LEU:HD21	6:L:49:TYR:HB3	1.68	0.74
2:D:35:ASN:HB2	2:D:93:ALA:HB3	1.71	0.73

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	B	125/153 (82%)	114 (91%)	9 (7%)	2 (2%)	<b>9</b> <b>23</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	126/134 (94%)	110 (87%)	16 (13%)	0	100	100
3	E	96/114 (84%)	82 (85%)	13 (14%)	1 (1%)	15	35
4	G	418/463 (90%)	359 (86%)	57 (14%)	2 (0%)	29	53
5	H	213/244 (87%)	194 (91%)	17 (8%)	2 (1%)	17	38
6	L	209/217 (96%)	191 (91%)	16 (8%)	2 (1%)	15	35
All	All	1187/1325 (90%)	1050 (88%)	128 (11%)	9 (1%)	19	41

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	51	ASN
6	L	25	ARG
5	H	144	ASP
1	B	548	ILE
1	B	625	ASN

### 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	B	111/129 (86%)	109 (98%)	2 (2%)	59	82
2	D	107/112 (96%)	104 (97%)	3 (3%)	43	71
3	E	87/100 (87%)	81 (93%)	6 (7%)	15	34
4	G	389/421 (92%)	371 (95%)	18 (5%)	27	52
5	H	190/212 (90%)	189 (100%)	1 (0%)	88	95
6	L	175/181 (97%)	170 (97%)	5 (3%)	42	70
All	All	1059/1155 (92%)	1024 (97%)	35 (3%)	38	66

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	456	ARG

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Mol	Chain	Res	Type
5	H	204	ASN
6	L	95(B)	PHE
4	G	112	TRP
4	G	67	ASN

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

### 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](#)

37 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	4,7	14,14,15	0.98	1 (7%)	17,19,21	1.96	3 (17%)
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	0.53	0
7	BMA	A	3	7	11,11,12	0.67	0	15,15,17	0.94	0
7	MAN	A	4	7	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
7	MAN	A	5	7	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
8	NAG	C	1	4,8	14,14,15	0.32	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
8	BMA	C	3	8	11,11,12	0.59	0	15,15,17	0.75	0
8	MAN	C	4	8	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
8	MAN	C	5	8	11,11,12	0.75	0	15,15,17	1.28	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	C	6	8	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
9	NAG	F	1	4,9	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	F	2	9	14,14,15	0.26	0	17,19,21	0.41	0
9	BMA	F	3	9	11,11,12	0.62	0	15,15,17	0.88	0
9	MAN	F	4	9	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
10	NAG	I	1	4,10	14,14,15	0.36	0	17,19,21	0.54	0
10	NAG	I	2	10	14,14,15	0.29	0	17,19,21	0.35	0
11	NAG	J	1	4,11	14,14,15	0.39	0	17,19,21	0.45	0
11	NAG	J	2	11	14,14,15	0.27	0	17,19,21	0.53	0
10	NAG	K	1	4,10	14,14,15	0.23	0	17,19,21	0.41	0
10	NAG	K	2	10	14,14,15	0.29	0	17,19,21	0.47	0
10	NAG	M	1	4,10	14,14,15	0.22	0	17,19,21	0.38	0
10	NAG	M	2	10	14,14,15	0.24	0	17,19,21	0.45	0
12	NAG	N	1	4,12	14,14,15	0.30	0	17,19,21	0.59	0
12	MAN	N	10	12	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
12	NAG	N	2	12	14,14,15	0.22	0	17,19,21	0.42	0
12	BMA	N	3	12	11,11,12	0.73	0	15,15,17	1.04	0
12	MAN	N	4	12	11,11,12	0.76	1 (9%)	15,15,17	1.32	2 (13%)
12	MAN	N	5	12	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
12	MAN	N	6	12	11,11,12	1.09	2 (18%)	15,15,17	2.11	5 (33%)
12	MAN	N	7	12	11,11,12	1.13	0	15,15,17	1.33	3 (20%)
12	MAN	N	8	12	11,11,12	0.92	1 (9%)	15,15,17	1.21	2 (13%)
12	MAN	N	9	12	11,11,12	0.90	1 (9%)	15,15,17	1.42	2 (13%)
10	NAG	O	1	4,10	14,14,15	0.33	0	17,19,21	0.47	0
10	NAG	O	2	10	14,14,15	0.20	0	17,19,21	0.46	0
10	NAG	P	1	4,10	14,14,15	0.28	0	17,19,21	0.48	0
10	NAG	P	2	10	14,14,15	0.27	0	17,19,21	0.45	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	4,7	-	5/6/23/26	0/1/1/1
7	NAG	A	2	7	-	1/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
8	NAG	C	1	4,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	2	8	-	5/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	1/1/1/1
8	MAN	C	6	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	1/2/19/22	0/1/1/1
10	NAG	I	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	I	2	10	-	0/6/23/26	0/1/1/1
11	NAG	J	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
10	NAG	K	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	NAG	M	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
12	NAG	N	1	4,12	-	3/6/23/26	0/1/1/1
12	MAN	N	10	12	-	0/2/19/22	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	2/2/19/22	0/1/1/1
12	MAN	N	5	12	-	2/2/19/22	0/1/1/1
12	MAN	N	6	12	-	0/2/19/22	0/1/1/1
12	MAN	N	7	12	-	1/2/19/22	0/1/1/1
12	MAN	N	8	12	-	0/2/19/22	0/1/1/1
12	MAN	N	9	12	-	0/2/19/22	0/1/1/1
10	NAG	O	1	4,10	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	0/6/23/26	0/1/1/1
10	NAG	P	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	NAG	O5-C1	3.46	1.49	1.43
12	N	9	MAN	C1-C2	2.75	1.58	1.52
12	N	6	MAN	C1-C2	2.39	1.57	1.52
12	N	4	MAN	C1-C2	2.27	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	6	MAN	C2-C3	2.17	1.55	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1	NAG	C1-O5-C5	5.89	120.17	112.19
12	N	6	MAN	C1-C2-C3	4.53	115.24	109.67
7	A	1	NAG	C2-N2-C7	4.41	129.18	122.90
8	C	2	NAG	C2-N2-C7	4.29	129.01	122.90
12	N	6	MAN	C1-O5-C5	4.15	117.82	112.19

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	3	BMA	O5-C5-C6-O6
8	C	5	MAN	O5-C5-C6-O6
9	F	3	BMA	C4-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6

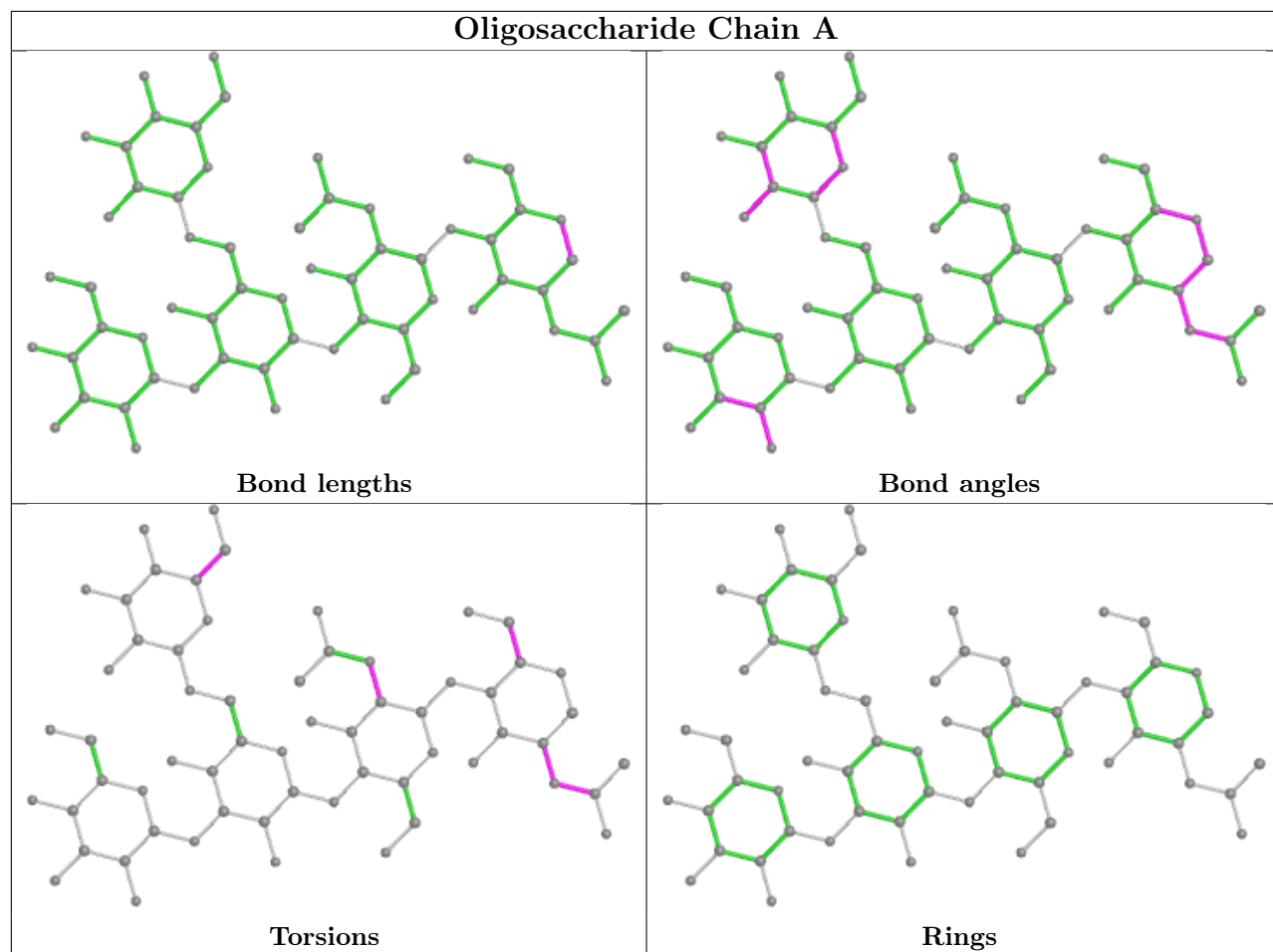
All (1) ring outliers are listed below:

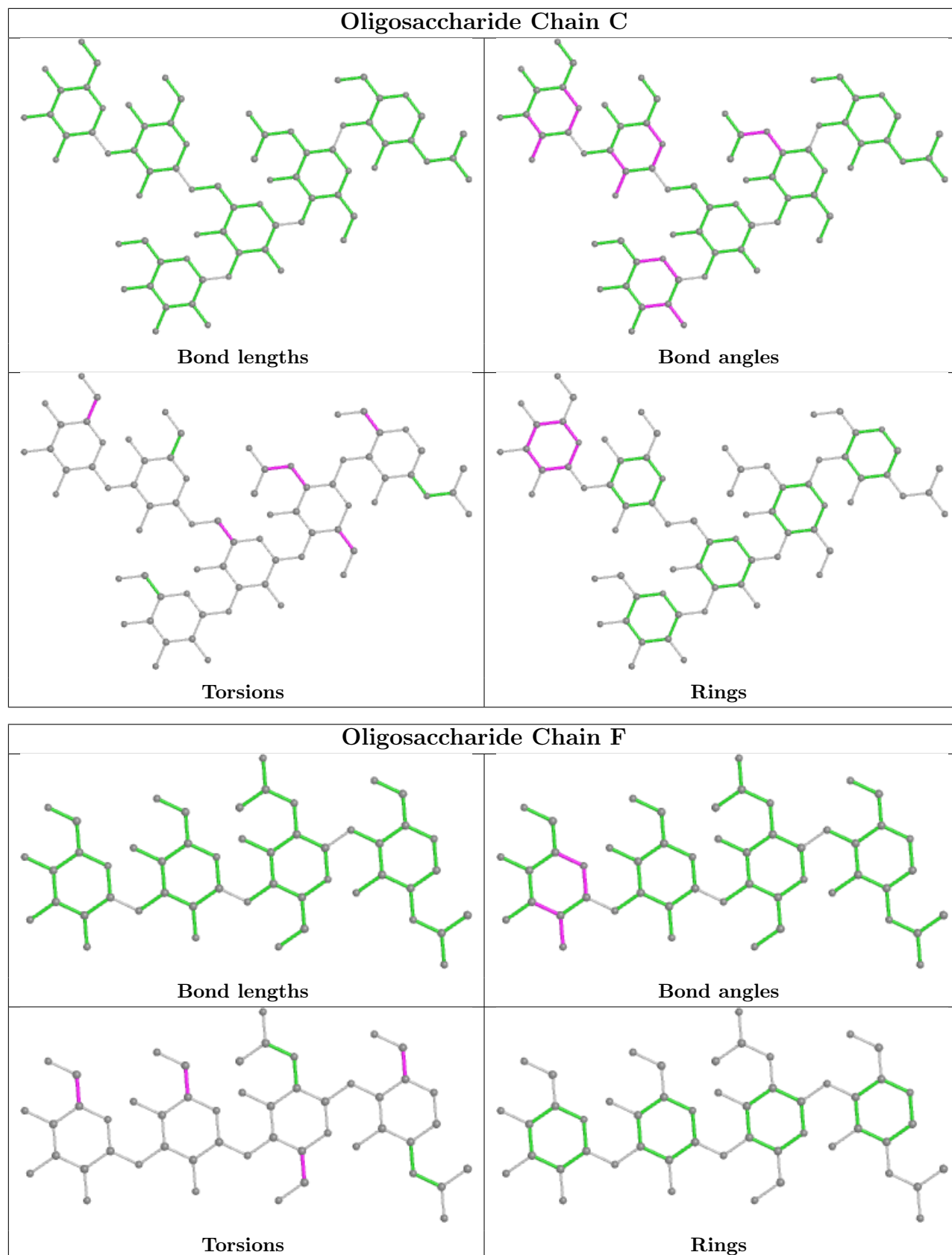
Mol	Chain	Res	Type	Atoms
8	C	5	MAN	C1-C2-C3-C4-C5-O5

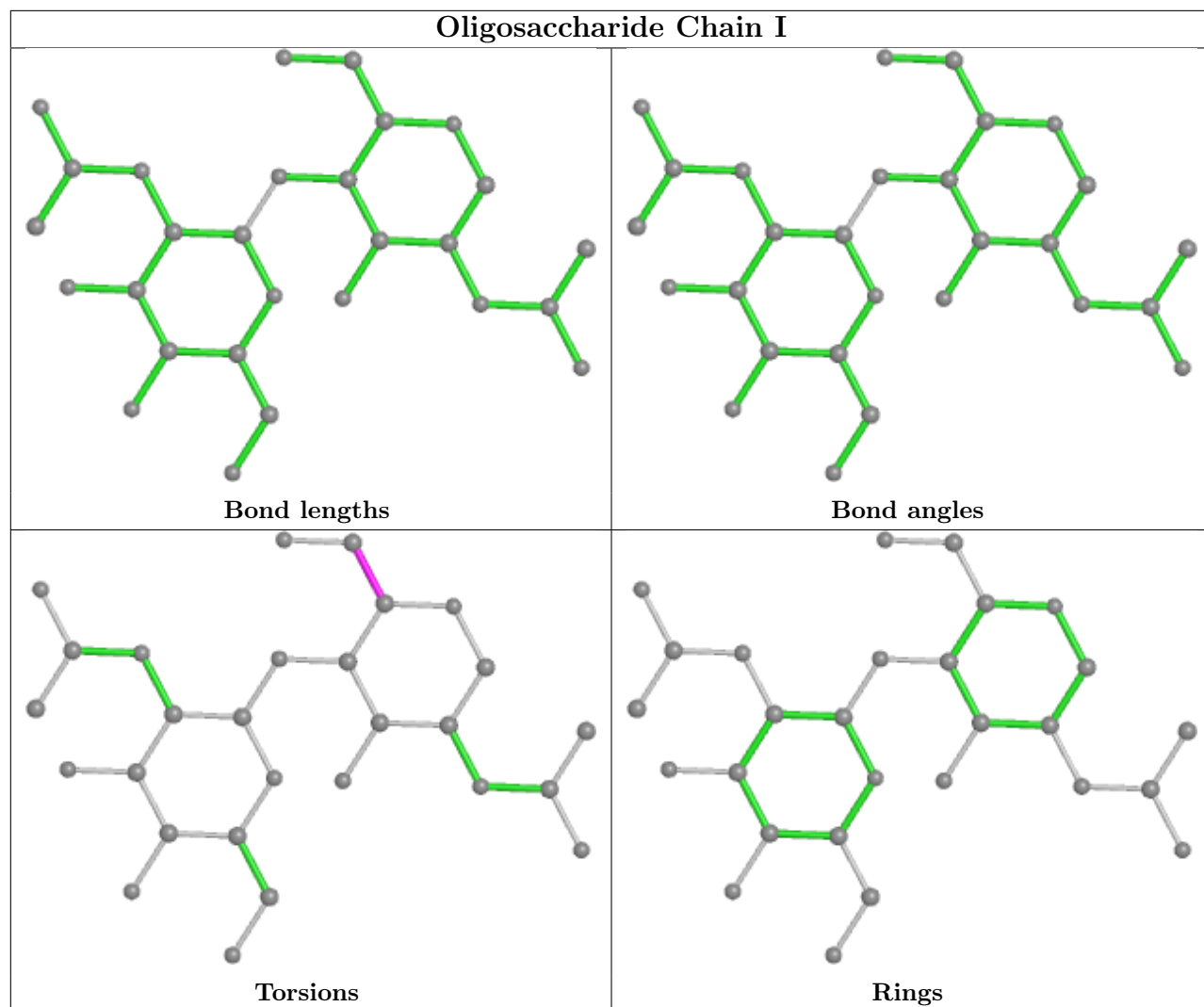
8 monomers are involved in 7 short contacts:

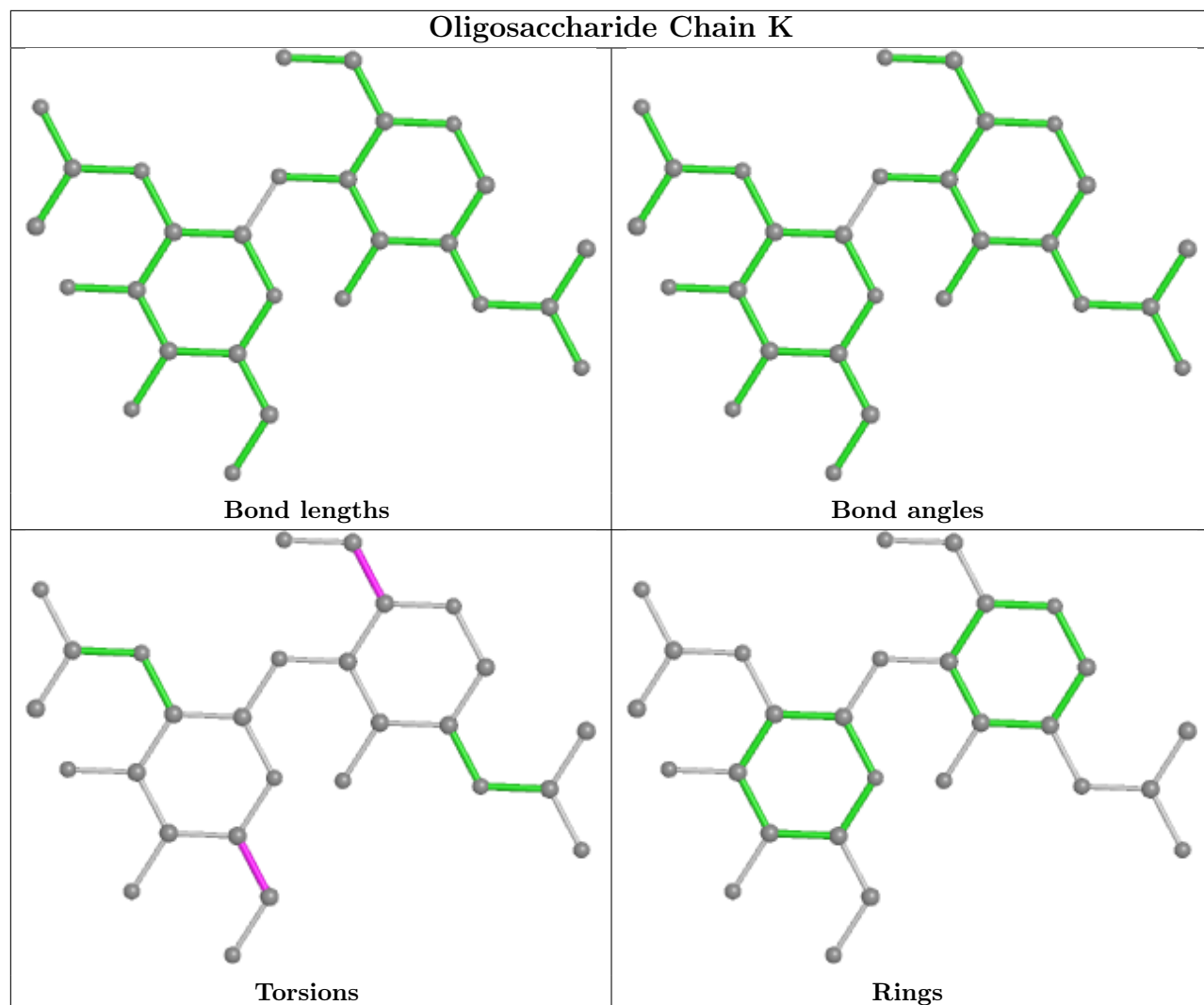
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1	NAG	1	0
12	N	1	NAG	1	0
8	C	1	NAG	1	0
11	J	1	NAG	1	0
12	N	4	MAN	1	0
8	C	2	NAG	2	0
7	A	2	NAG	1	0
11	J	2	NAG	1	0

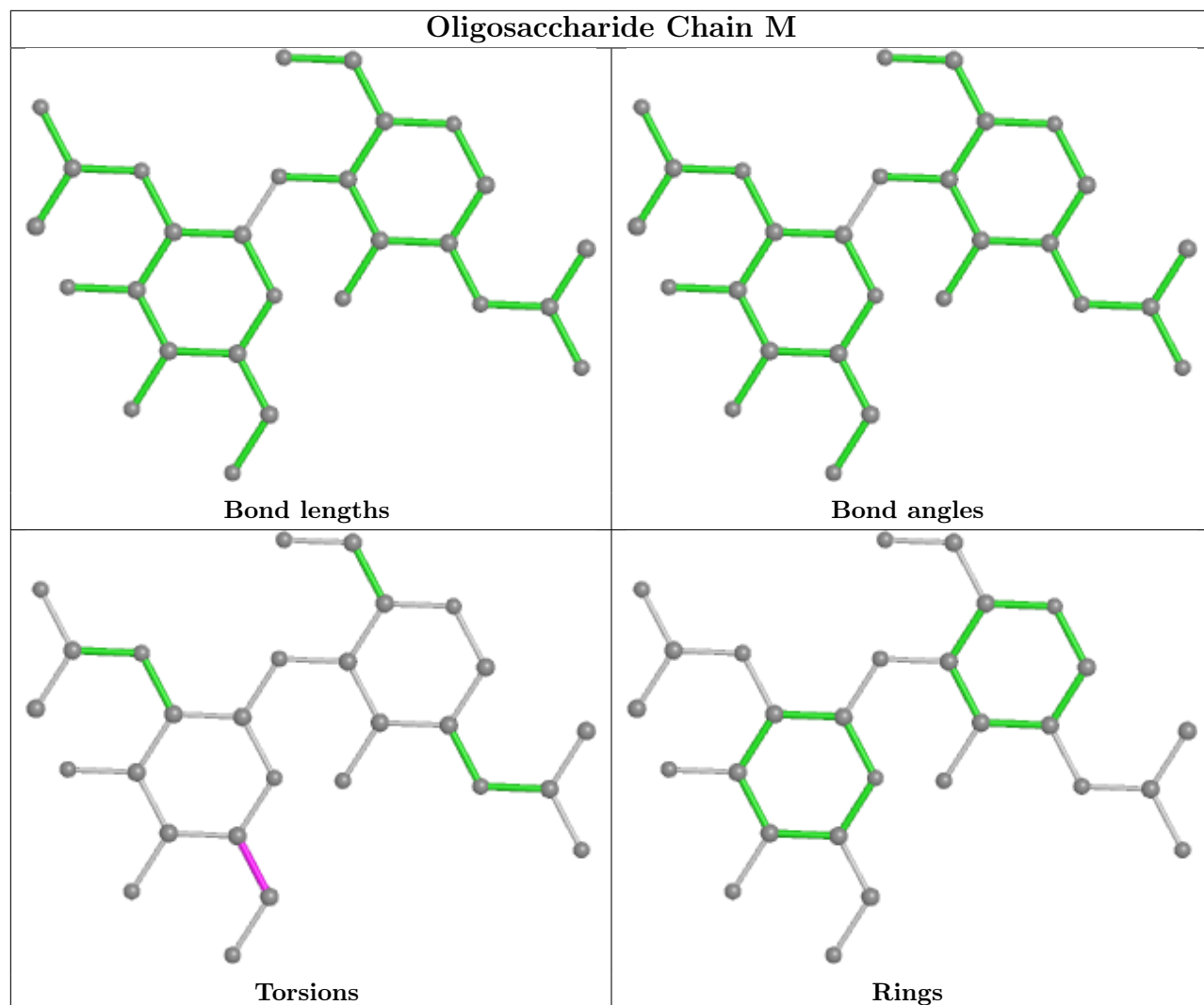
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



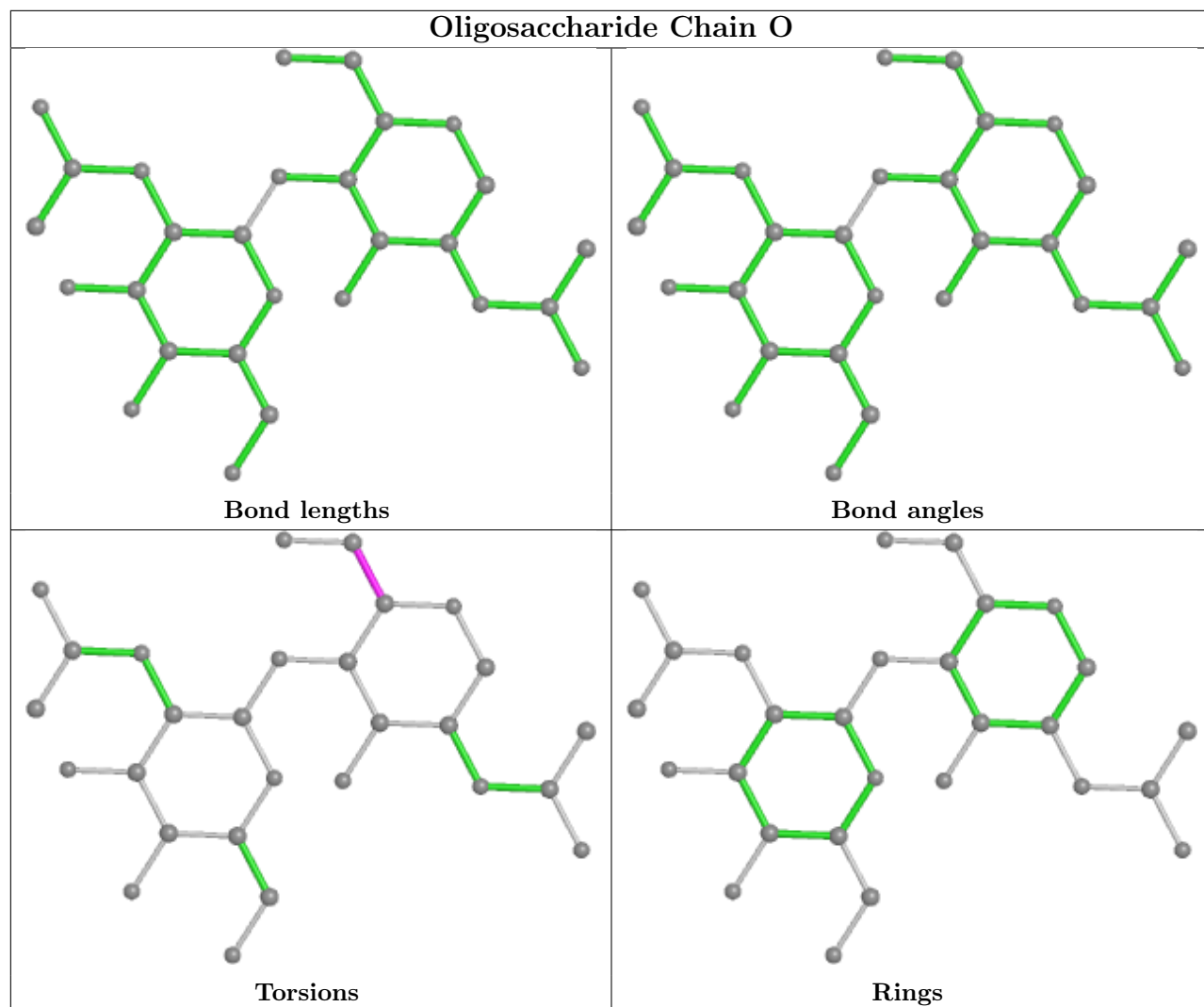


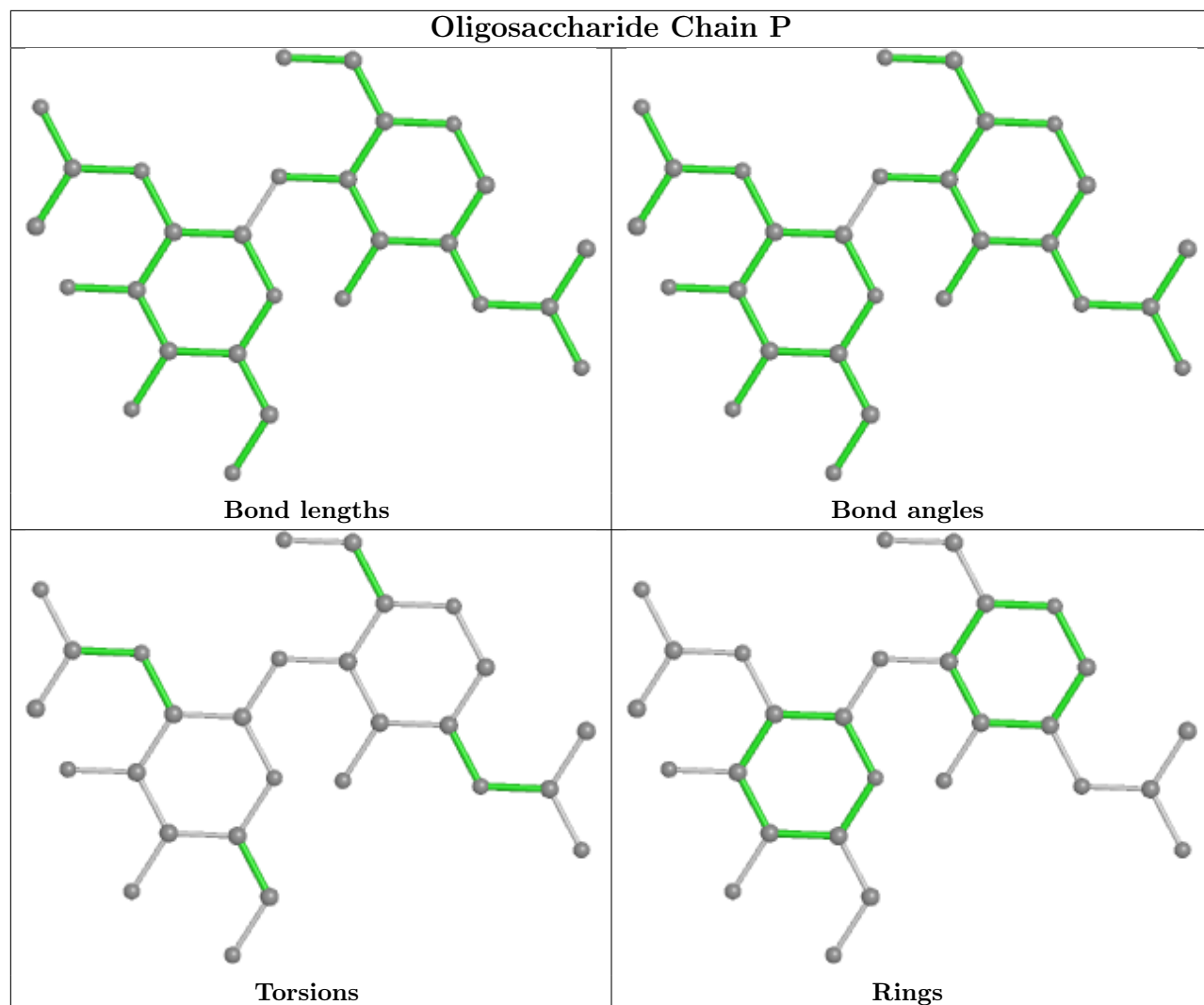


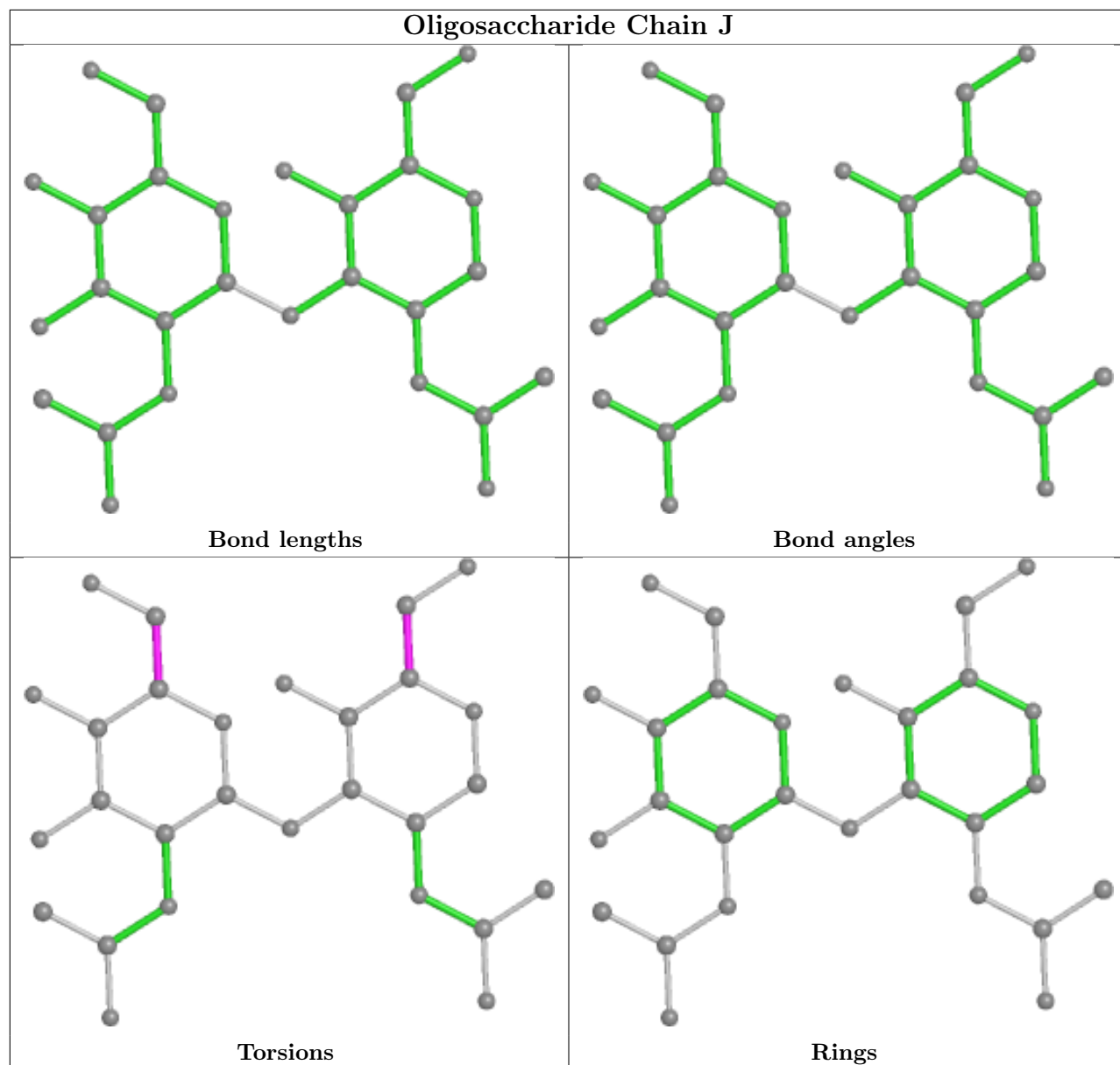


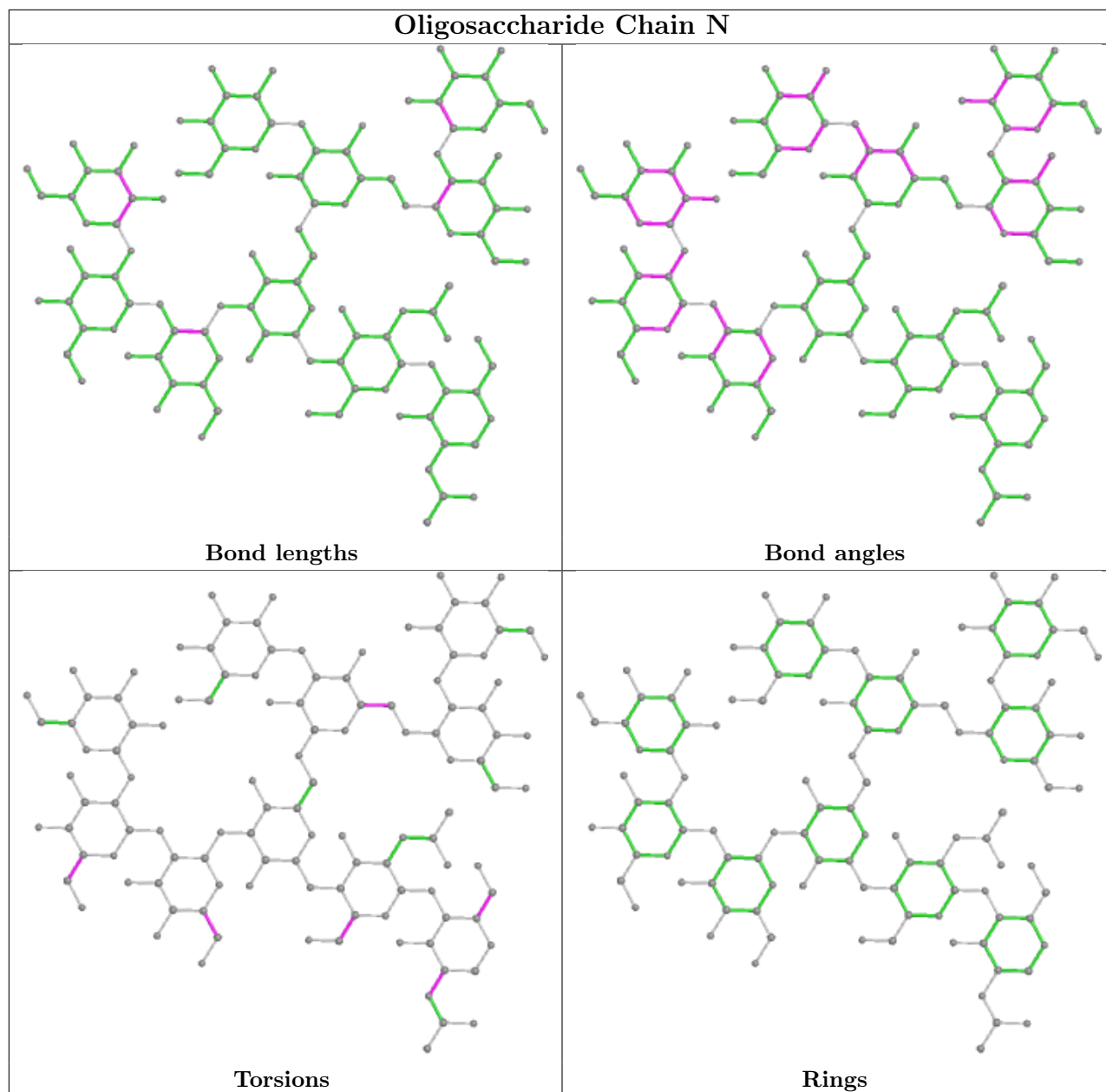












## 5.6 Ligand geometry [i](#)

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	G	1601	4	14,14,15	0.31	0	17,19,21	0.37	0
13	NAG	G	617	4	14,14,15	0.27	0	17,19,21	0.41	0
13	NAG	G	4421	4	14,14,15	0.20	0	17,19,21	0.41	0
13	NAG	G	2761	4	14,14,15	0.26	0	17,19,21	0.44	0
13	NAG	G	2891	4	14,14,15	0.45	0	17,19,21	0.58	0
13	NAG	G	2411	4	14,14,15	0.23	0	17,19,21	0.37	0
13	NAG	B	6371	1	14,14,15	0.25	0	17,19,21	0.46	0
13	NAG	B	6111	1	14,14,15	0.27	0	17,19,21	0.47	0
13	NAG	G	1301	4	14,14,15	0.28	0	17,19,21	0.45	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	G	1601	4	-	2/6/23/26	0/1/1/1
13	NAG	G	617	4	-	1/6/23/26	0/1/1/1
13	NAG	G	4421	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2761	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2891	4	-	2/6/23/26	0/1/1/1
13	NAG	G	2411	4	-	1/6/23/26	0/1/1/1
13	NAG	B	6371	1	-	0/6/23/26	0/1/1/1
13	NAG	B	6111	1	-	2/6/23/26	0/1/1/1
13	NAG	G	1301	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	1601	NAG	O5-C5-C6-O6
13	B	6111	NAG	O5-C5-C6-O6
13	G	1601	NAG	C4-C5-C6-O6
13	B	6111	NAG	C4-C5-C6-O6
13	G	2761	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	1601	NAG	1	0
13	G	2891	NAG	2	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	B	129/153 (84%)	-0.36	1 (0%) 86 87	14, 32, 63, 100	0
2	D	128/134 (95%)	0.23	8 (6%) 20 19	47, 82, 122, 136	0
3	E	100/114 (87%)	0.27	7 (7%) 16 15	64, 79, 107, 116	0
4	G	430/463 (92%)	-0.37	6 (1%) 75 77	21, 42, 87, 113	0
5	H	219/244 (89%)	0.12	9 (4%) 37 36	48, 68, 98, 111	0
6	L	211/217 (97%)	-0.43	1 (0%) 91 92	36, 50, 69, 95	0
All	All	1217/1325 (91%)	-0.17	32 (2%) 56 57	14, 55, 101, 136	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	VAL	4.9
4	G	367	GLY	4.5
5	H	30	SER	4.0
3	E	15	LEU	3.8
2	D	82(A)	ARG	3.6

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

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

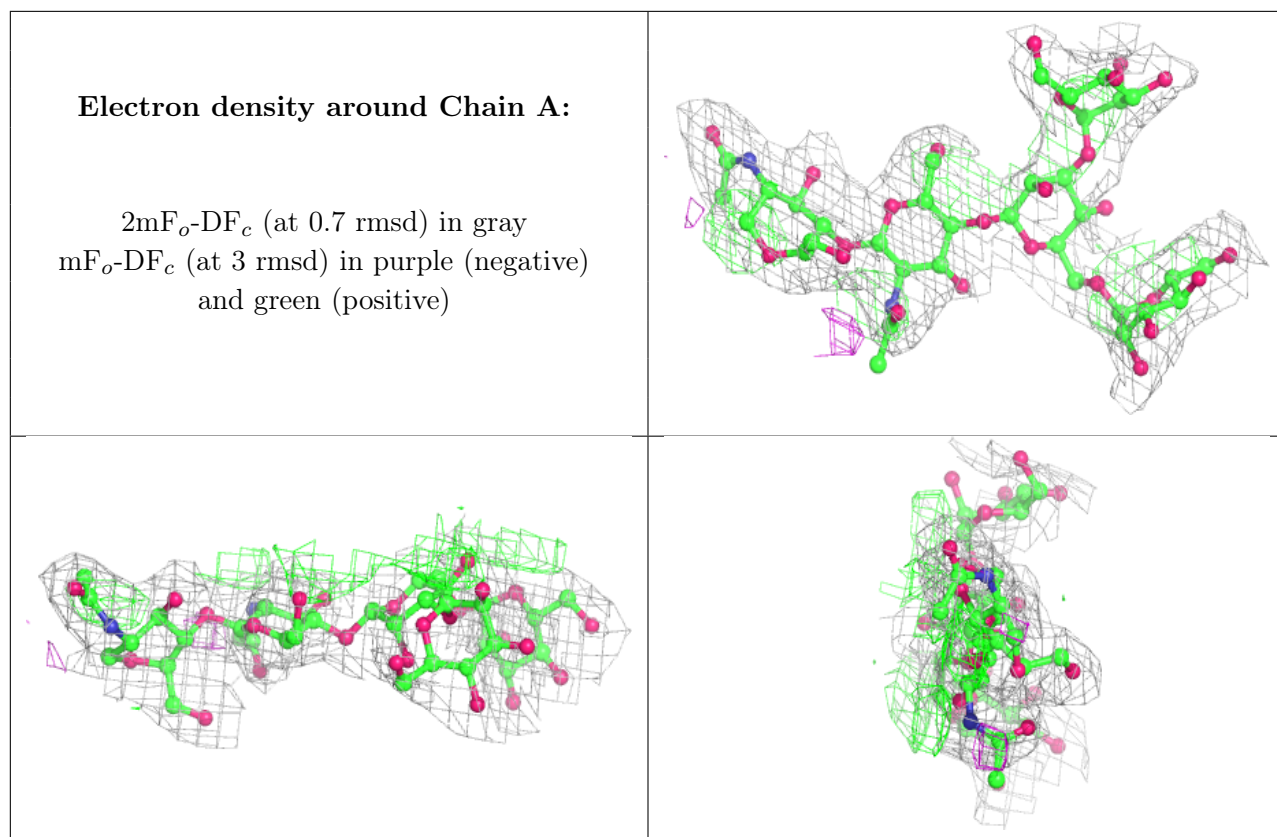
### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	F	4	11/12	0.72	0.31	116,125,135,136	0
7	MAN	A	4	11/12	0.73	0.21	95,102,107,111	0
8	MAN	C	5	11/12	0.76	0.33	107,116,122,127	0
9	BMA	F	3	11/12	0.77	0.28	106,115,129,131	0
10	NAG	K	2	14/15	0.78	0.42	117,136,159,162	0
10	NAG	O	2	14/15	0.78	0.40	108,121,130,132	0
7	BMA	A	3	11/12	0.79	0.17	103,115,125,127	0
7	MAN	A	5	11/12	0.81	0.23	69,88,102,108	0
10	NAG	M	2	14/15	0.82	0.34	93,112,125,127	0
8	MAN	C	4	11/12	0.85	0.17	86,98,107,109	0
10	NAG	I	2	14/15	0.86	0.27	82,102,110,111	0
11	NAG	J	2	14/15	0.88	0.26	102,107,115,115	0
11	NAG	J	1	14/15	0.90	0.19	38,89,105,106	0
10	NAG	I	1	14/15	0.90	0.17	44,69,92,102	0
12	MAN	N	9	11/12	0.90	0.29	86,98,106,108	0
12	MAN	N	8	11/12	0.91	0.15	58,68,78,90	0
7	NAG	A	2	14/15	0.92	0.17	50,63,93,93	0
10	NAG	P	2	14/15	0.92	0.22	53,101,112,112	0
12	MAN	N	10	11/12	0.92	0.13	71,84,99,108	0
12	MAN	N	6	11/12	0.93	0.17	41,60,67,76	0
10	NAG	O	1	14/15	0.93	0.15	63,71,92,104	0
8	NAG	C	1	14/15	0.94	0.16	30,35,63,75	0
12	MAN	N	7	11/12	0.95	0.11	78,87,97,105	0
9	NAG	F	2	14/15	0.95	0.14	57,73,93,97	0
12	NAG	N	1	14/15	0.95	0.10	37,51,67,68	0
10	NAG	P	1	14/15	0.95	0.11	54,63,88,101	0
12	NAG	N	2	14/15	0.96	0.14	41,47,61,71	0
8	BMA	C	3	11/12	0.96	0.10	32,34,48,69	0
10	NAG	M	1	14/15	0.96	0.11	32,72,86,92	0
8	MAN	C	6	11/12	0.96	0.10	30,39,59,62	0
9	NAG	F	1	14/15	0.96	0.13	39,51,57,65	0
8	NAG	C	2	14/15	0.96	0.15	32,40,63,70	0
12	BMA	N	3	11/12	0.97	0.11	40,41,60,73	0
10	NAG	K	1	14/15	0.97	0.08	38,50,69,91	0
7	NAG	A	1	14/15	0.97	0.12	30,36,55,56	0
12	MAN	N	5	11/12	0.98	0.10	39,40,51,62	0
12	MAN	N	4	11/12	0.98	0.09	38,43,49,65	0

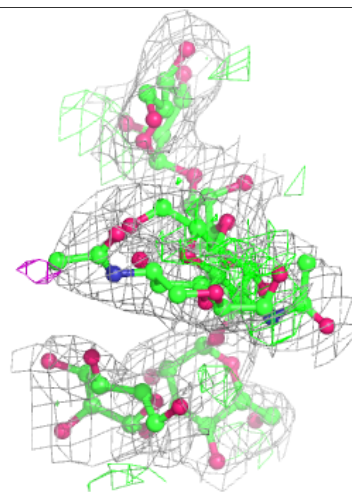
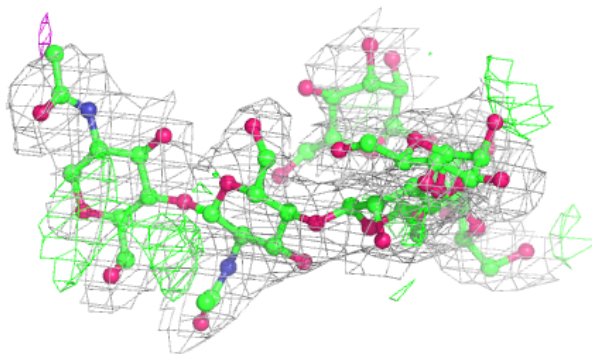
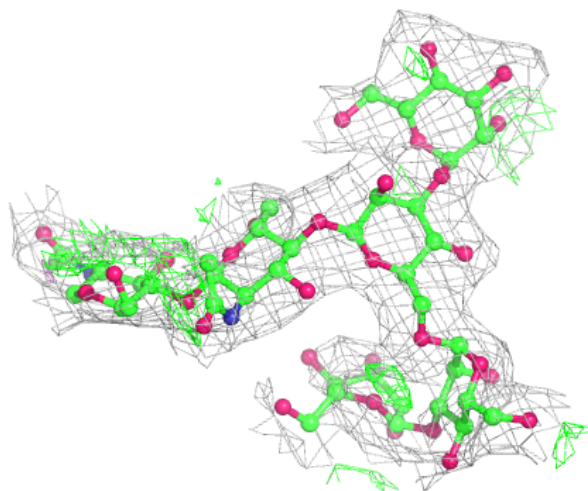
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





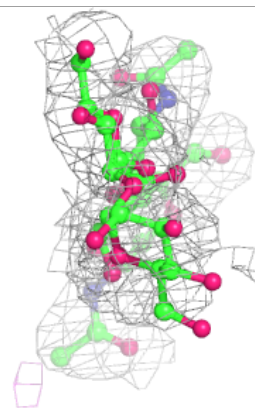
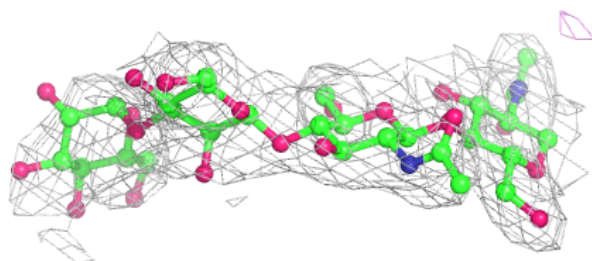
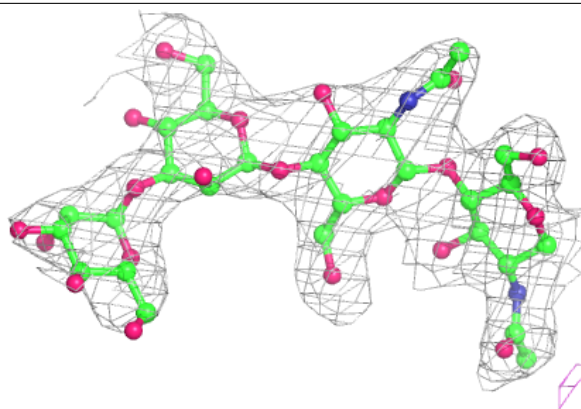
**Electron density around Chain C:**

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

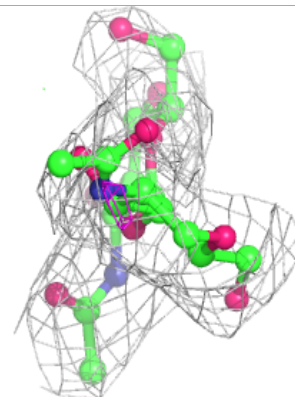
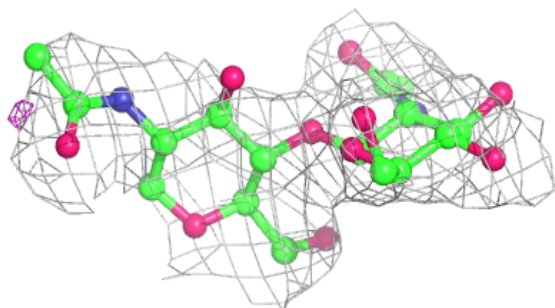
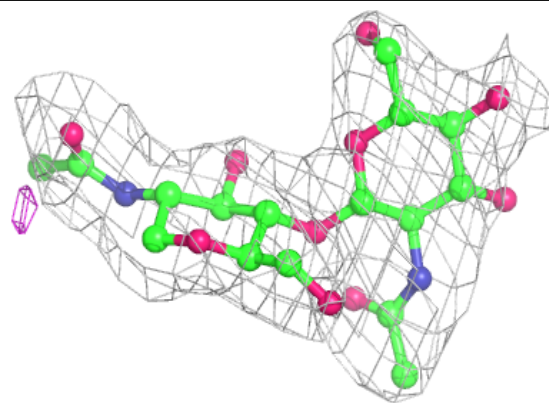


**Electron density around Chain F:**

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

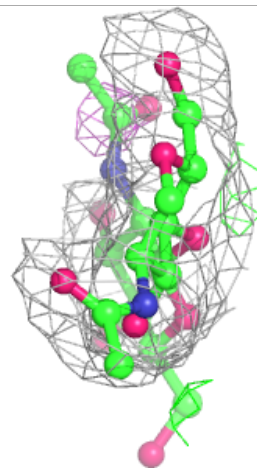
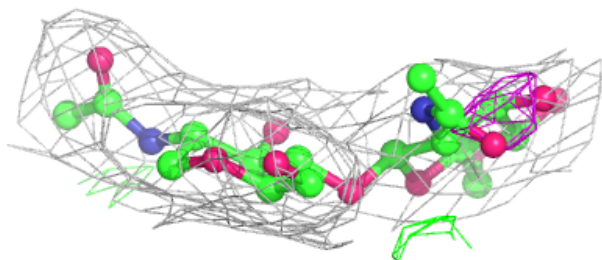
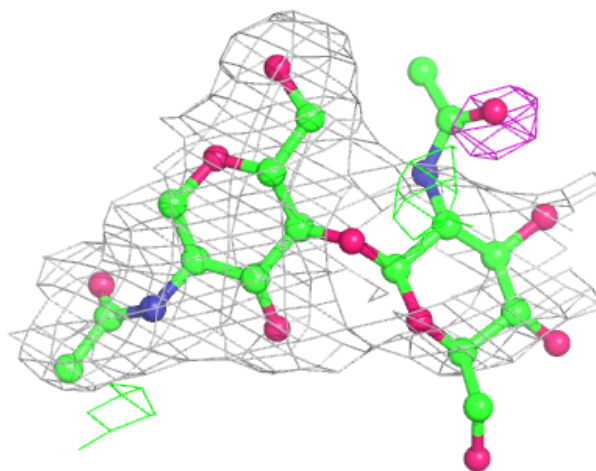
**Electron density around Chain I:**

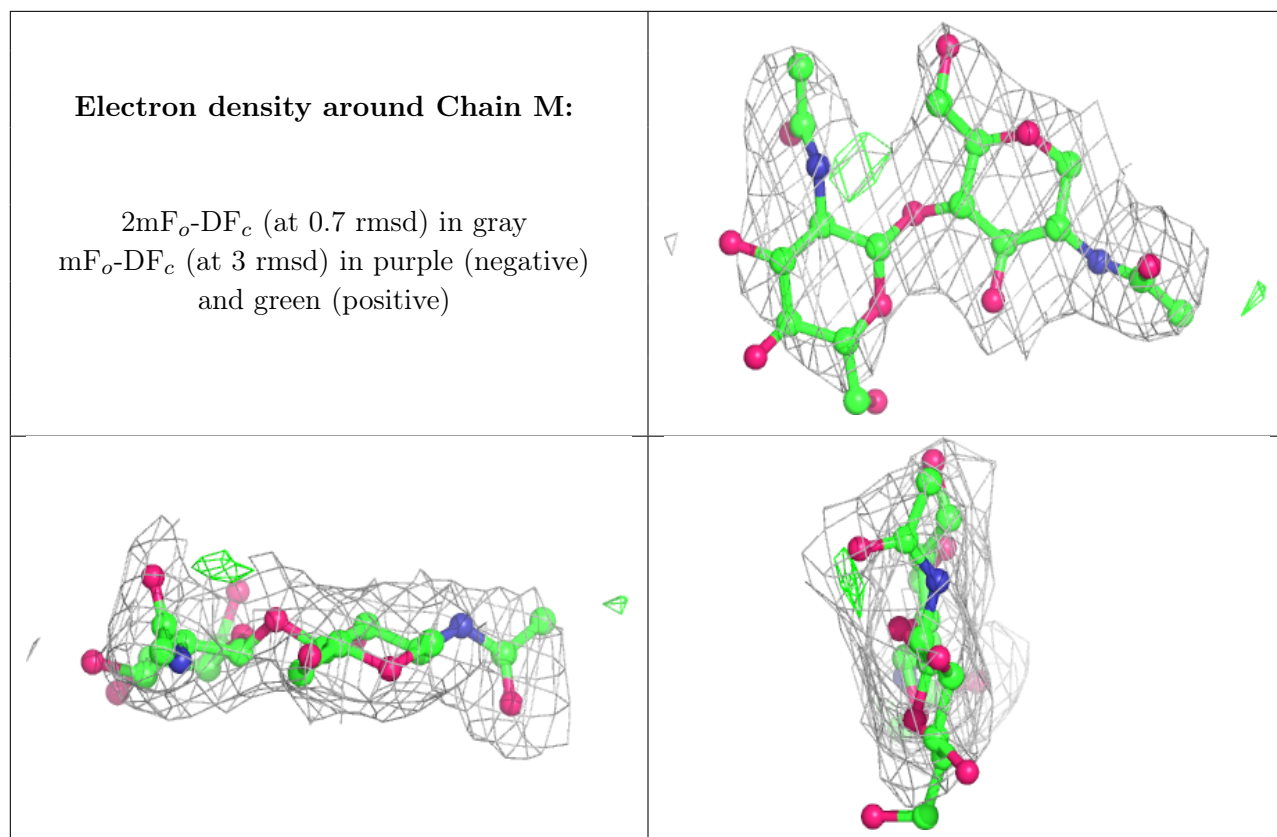
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain K:**

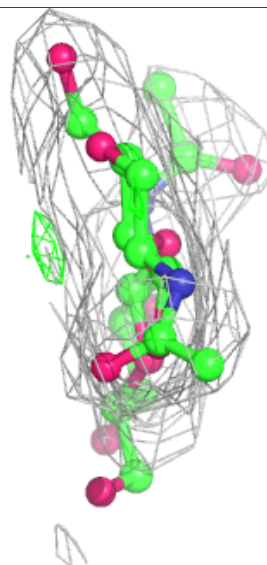
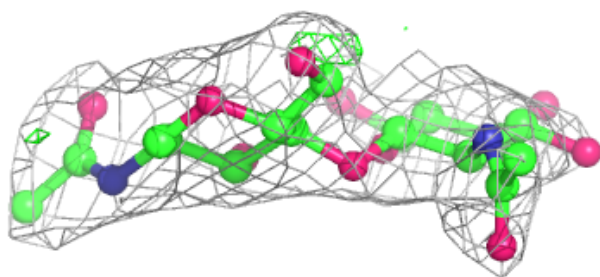
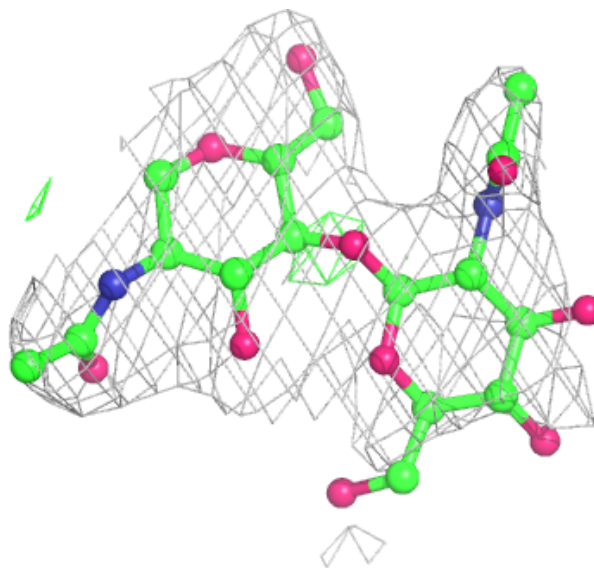
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

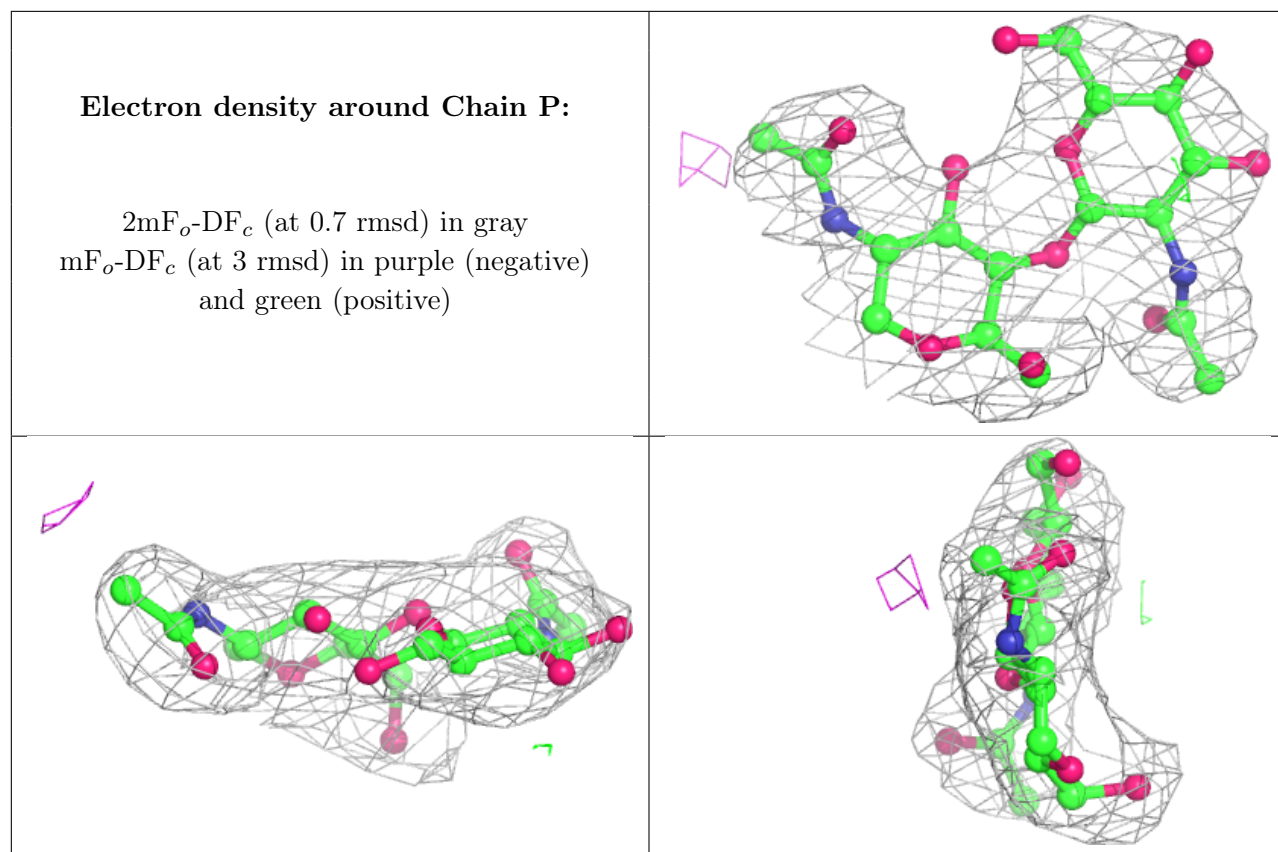


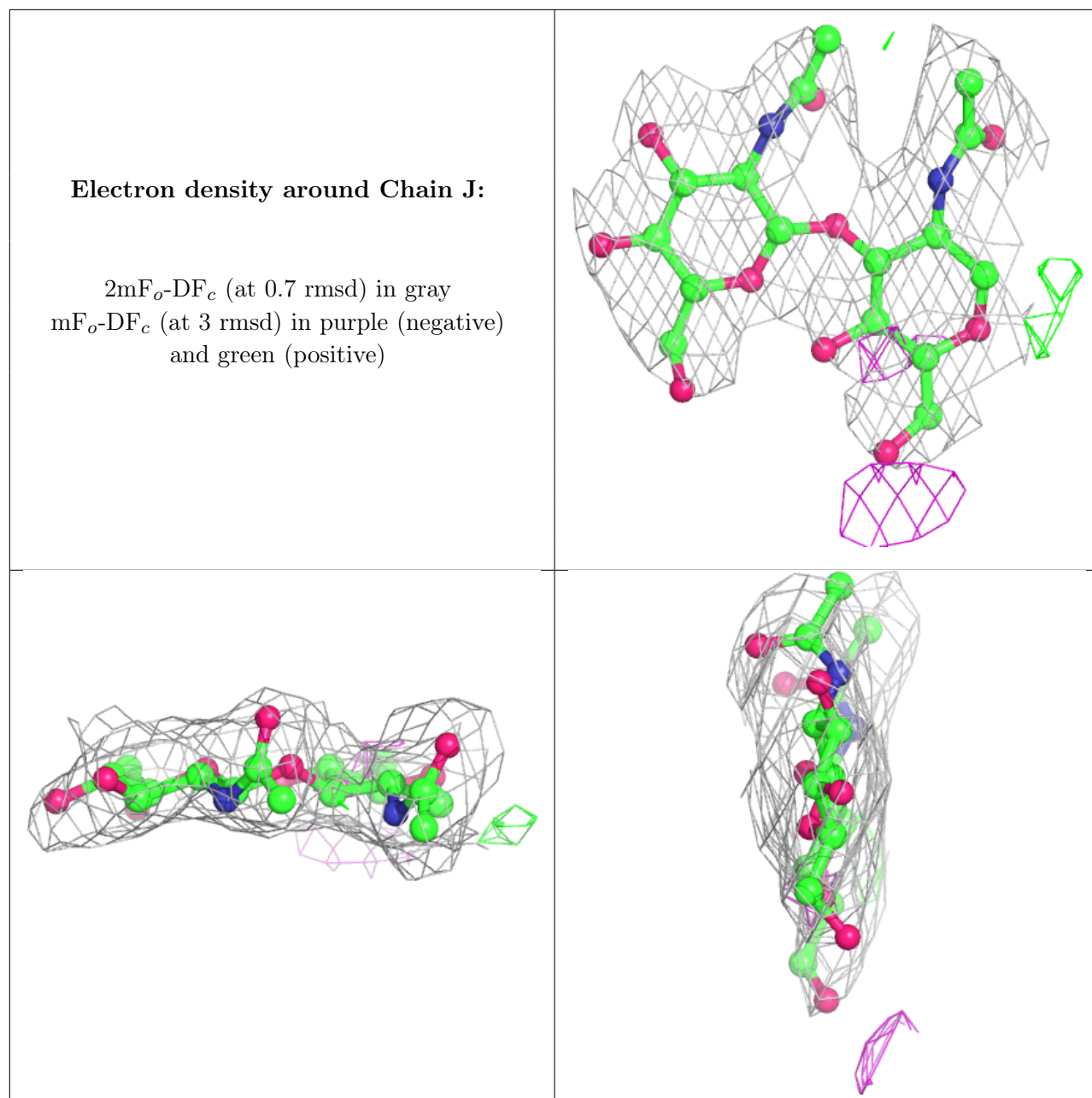


**Electron density around Chain O:**

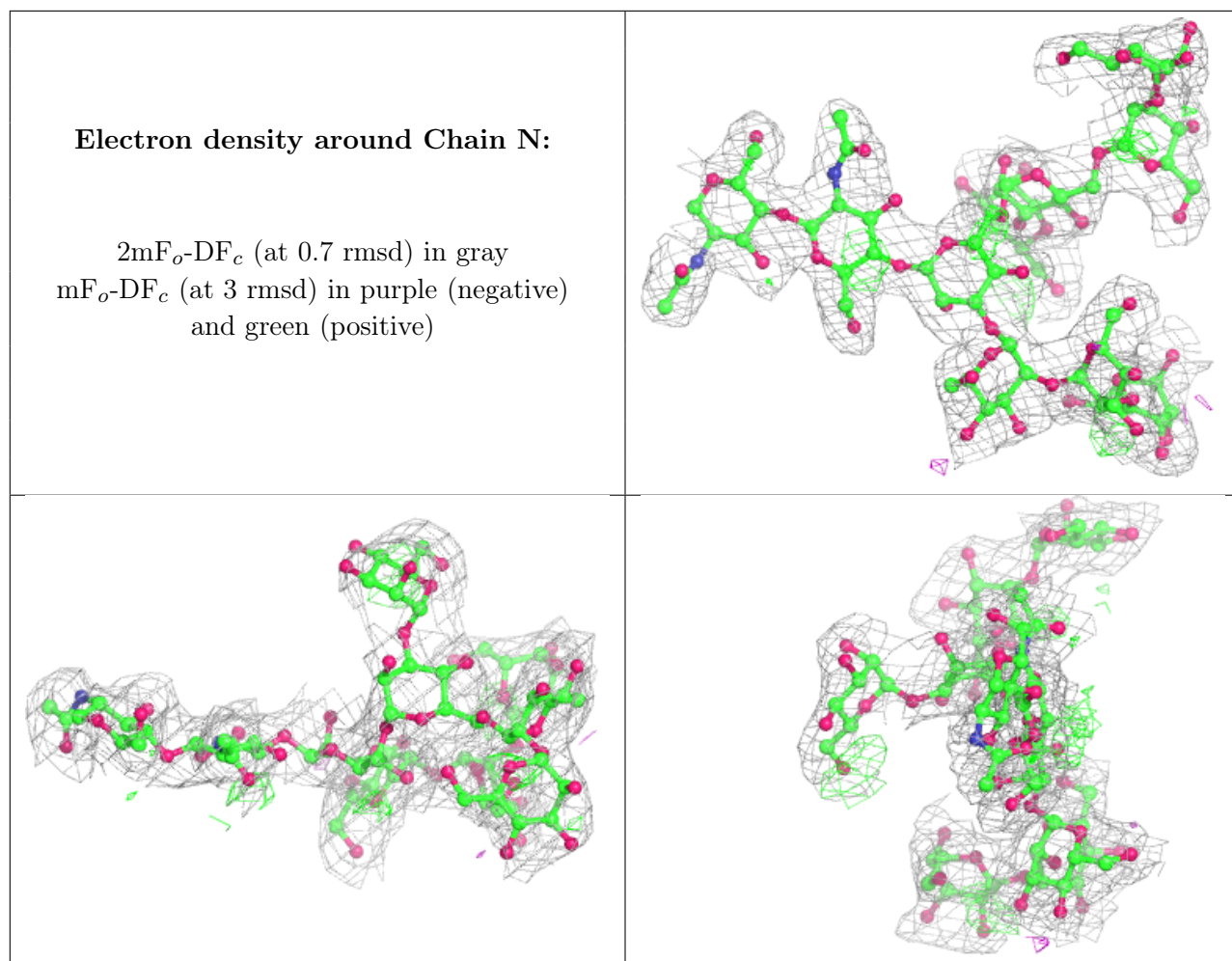
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)











## 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	G	4421	14/15	0.83	0.46	105,117,125,130	0
13	NAG	G	1601	14/15	0.86	0.19	72,91,97,97	0
13	NAG	B	6111	14/15	0.87	0.28	48,72,85,96	0
13	NAG	G	2411	14/15	0.91	0.19	56,74,97,103	0
13	NAG	G	1301	14/15	0.91	0.19	86,89,96,98	0
13	NAG	G	2761	14/15	0.92	0.34	86,101,118,118	0
13	NAG	G	617	14/15	0.94	0.14	56,68,72,80	0
13	NAG	B	6371	14/15	0.94	0.28	79,91,98,106	0
13	NAG	G	2891	14/15	0.95	0.14	41,45,75,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.