



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 1, 2021 – 02:07 PM EST

PDB ID : 7SN0  
Title : Crystal structure of spike protein receptor binding domain of escape mutant SARS-CoV-2 from immunocompromised patient (d146\*) in complex with human receptor ACE2  
Authors : Pan, J.; Abraham, J.; Clark, S.  
Deposited on : 2021-10-27  
Resolution : 3.08 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 : 2.24  
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) : 2.24

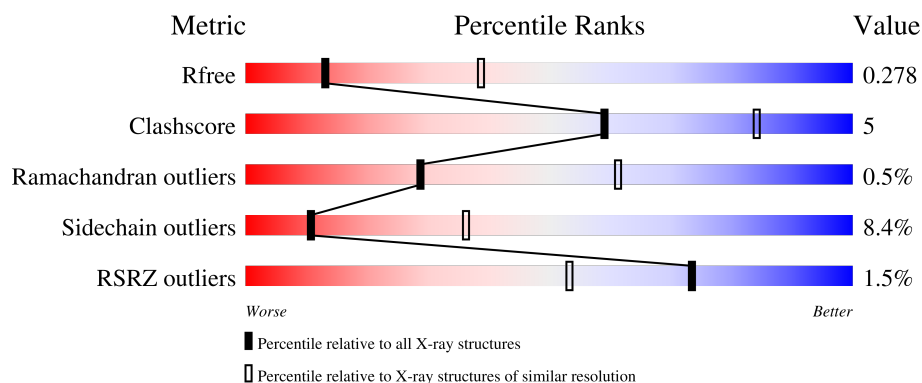
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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.




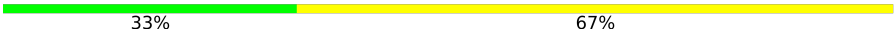

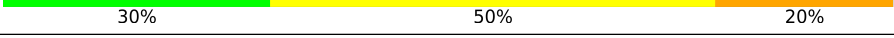

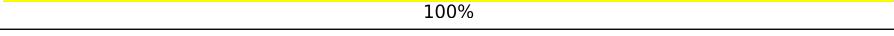
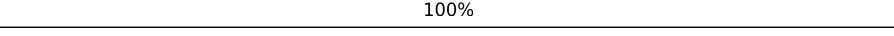
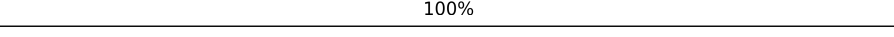
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	<div> <div>0%</div> <div> <div>76%</div> <div>19%</div> <div>5%</div> </div> </div>
1	B	621	<div> <div>0%</div> <div> <div>77%</div> <div>18%</div> <div>5%</div> </div> </div>
2	C	271	<div> <div>3%</div> <div> <div>59%</div> <div>11%</div> <div>30%</div> </div> </div>
2	D	271	<div> <div>59%</div> <div>11%</div> <div>30%</div> </div>
3	E	5	<div> <div>40%</div> <div>60%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	5	
4	F	3	
4	G	3	
4	N	3	
4	Q	3	
5	H	10	
6	I	10	
7	K	6	
8	L	2	
8	P	2	
9	M	6	
10	O	9	

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	O	5	-	-	-	X
3	MAN	E	5	-	-	-	X
4	NAG	Q	2	-	-	-	X
5	GAL	H	10	-	-	-	X
6	NAG	I	10	-	-	-	X
6	NAG	I	5	-	-	-	X
6	NAG	I	7	-	-	-	X
7	NAG	K	5	-	-	-	X
8	NAG	P	2	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13722 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	2	0
			4887	3126	811	921	29			
1	B	597	Total	C	N	O	S	0	2	0
			4887	3126	811	921	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
B	616	HIS	-	expression tag	UNP Q9BYF1
B	617	HIS	-	expression tag	UNP Q9BYF1
B	618	HIS	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	194	Total	C	N	O	S	0	0	0
			1541	991	257	285	8			
2	D	194	Total	C	N	O	S	0	0	0
			1541	991	257	285	8			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	271	MET	-	initiating methionine	UNP A0A7U0MIF7
C	272	GLY	-	expression tag	UNP A0A7U0MIF7
C	273	ILE	-	expression tag	UNP A0A7U0MIF7
C	274	LEU	-	expression tag	UNP A0A7U0MIF7
C	275	PRO	-	expression tag	UNP A0A7U0MIF7
C	276	SER	-	expression tag	UNP A0A7U0MIF7
C	277	PRO	-	expression tag	UNP A0A7U0MIF7
C	278	GLY	-	expression tag	UNP A0A7U0MIF7
C	279	MET	-	expression tag	UNP A0A7U0MIF7
C	280	PRO	-	expression tag	UNP A0A7U0MIF7
C	281	ALA	-	expression tag	UNP A0A7U0MIF7
C	282	LEU	-	expression tag	UNP A0A7U0MIF7
C	283	LEU	-	expression tag	UNP A0A7U0MIF7
C	284	SER	-	expression tag	UNP A0A7U0MIF7
C	285	LEU	-	expression tag	UNP A0A7U0MIF7
C	286	VAL	-	expression tag	UNP A0A7U0MIF7
C	287	SER	-	expression tag	UNP A0A7U0MIF7
C	288	LEU	-	expression tag	UNP A0A7U0MIF7
C	289	LEU	-	expression tag	UNP A0A7U0MIF7
C	290	SER	-	expression tag	UNP A0A7U0MIF7
C	291	VAL	-	expression tag	UNP A0A7U0MIF7
C	292	LEU	-	expression tag	UNP A0A7U0MIF7
C	293	LEU	-	expression tag	UNP A0A7U0MIF7
C	294	MET	-	expression tag	UNP A0A7U0MIF7
C	295	GLY	-	expression tag	UNP A0A7U0MIF7
C	296	CYS	-	expression tag	UNP A0A7U0MIF7
C	297	VAL	-	expression tag	UNP A0A7U0MIF7
C	298	ALA	-	expression tag	UNP A0A7U0MIF7
C	299	GLU	-	expression tag	UNP A0A7U0MIF7
C	300	THR	-	expression tag	UNP A0A7U0MIF7
C	301	GLY	-	expression tag	UNP A0A7U0MIF7
C	302	HIS	-	expression tag	UNP A0A7U0MIF7
C	303	HIS	-	expression tag	UNP A0A7U0MIF7
C	304	HIS	-	expression tag	UNP A0A7U0MIF7
C	305	HIS	-	expression tag	UNP A0A7U0MIF7
C	306	HIS	-	expression tag	UNP A0A7U0MIF7
C	307	HIS	-	expression tag	UNP A0A7U0MIF7
C	308	GLU	-	expression tag	UNP A0A7U0MIF7
C	309	ASN	-	expression tag	UNP A0A7U0MIF7
C	310	LEU	-	expression tag	UNP A0A7U0MIF7
C	311	TYR	-	expression tag	UNP A0A7U0MIF7
C	312	PHE	-	expression tag	UNP A0A7U0MIF7
C	313	GLN	-	expression tag	UNP A0A7U0MIF7

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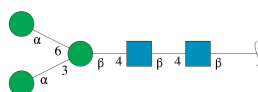
Chain	Residue	Modelled	Actual	Comment	Reference
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C	315	SER	-	expression tag	UNP A0A7U0MIF7
C	316	GLY	-	expression tag	UNP A0A7U0MIF7
C	317	SER	-	expression tag	UNP A0A7U0MIF7
C	318	GLY	-	expression tag	UNP A0A7U0MIF7
C	440	ASP	ASN	engineered mutation	UNP A0A7U0MIF7
C	478	LYS	THR	engineered mutation	UNP A0A7U0MIF7
C	489	HIS	TYR	engineered mutation	UNP A0A7U0MIF7
C	494	PRO	SER	engineered mutation	UNP A0A7U0MIF7
D	271	MET	-	initiating methionine	UNP A0A7U0MIF7
D	272	GLY	-	expression tag	UNP A0A7U0MIF7
D	273	ILE	-	expression tag	UNP A0A7U0MIF7
D	274	LEU	-	expression tag	UNP A0A7U0MIF7
D	275	PRO	-	expression tag	UNP A0A7U0MIF7
D	276	SER	-	expression tag	UNP A0A7U0MIF7
D	277	PRO	-	expression tag	UNP A0A7U0MIF7
D	278	GLY	-	expression tag	UNP A0A7U0MIF7
D	279	MET	-	expression tag	UNP A0A7U0MIF7
D	280	PRO	-	expression tag	UNP A0A7U0MIF7
D	281	ALA	-	expression tag	UNP A0A7U0MIF7
D	282	LEU	-	expression tag	UNP A0A7U0MIF7
D	283	LEU	-	expression tag	UNP A0A7U0MIF7
D	284	SER	-	expression tag	UNP A0A7U0MIF7
D	285	LEU	-	expression tag	UNP A0A7U0MIF7
D	286	VAL	-	expression tag	UNP A0A7U0MIF7
D	287	SER	-	expression tag	UNP A0A7U0MIF7
D	288	LEU	-	expression tag	UNP A0A7U0MIF7
D	289	LEU	-	expression tag	UNP A0A7U0MIF7
D	290	SER	-	expression tag	UNP A0A7U0MIF7
D	291	VAL	-	expression tag	UNP A0A7U0MIF7
D	292	LEU	-	expression tag	UNP A0A7U0MIF7
D	293	LEU	-	expression tag	UNP A0A7U0MIF7
D	294	MET	-	expression tag	UNP A0A7U0MIF7
D	295	GLY	-	expression tag	UNP A0A7U0MIF7
D	296	CYS	-	expression tag	UNP A0A7U0MIF7
D	297	VAL	-	expression tag	UNP A0A7U0MIF7
D	298	ALA	-	expression tag	UNP A0A7U0MIF7
D	299	GLU	-	expression tag	UNP A0A7U0MIF7
D	300	THR	-	expression tag	UNP A0A7U0MIF7
D	301	GLY	-	expression tag	UNP A0A7U0MIF7
D	302	HIS	-	expression tag	UNP A0A7U0MIF7
D	303	HIS	-	expression tag	UNP A0A7U0MIF7

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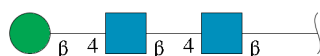
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D	304	HIS	-	expression tag	UNP A0A7U0MIF7
D	305	HIS	-	expression tag	UNP A0A7U0MIF7
D	306	HIS	-	expression tag	UNP A0A7U0MIF7
D	307	HIS	-	expression tag	UNP A0A7U0MIF7
D	308	GLU	-	expression tag	UNP A0A7U0MIF7
D	309	ASN	-	expression tag	UNP A0A7U0MIF7
D	310	LEU	-	expression tag	UNP A0A7U0MIF7
D	311	TYR	-	expression tag	UNP A0A7U0MIF7
D	312	PHE	-	expression tag	UNP A0A7U0MIF7
D	313	GLN	-	expression tag	UNP A0A7U0MIF7
D	314	GLY	-	expression tag	UNP A0A7U0MIF7
D	315	SER	-	expression tag	UNP A0A7U0MIF7
D	316	GLY	-	expression tag	UNP A0A7U0MIF7
D	317	SER	-	expression tag	UNP A0A7U0MIF7
D	318	GLY	-	expression tag	UNP A0A7U0MIF7
D	440	ASP	ASN	engineered mutation	UNP A0A7U0MIF7
D	478	LYS	THR	engineered mutation	UNP A0A7U0MIF7
D	489	HIS	TYR	engineered mutation	UNP A0A7U0MIF7
D	494	PRO	SER	engineered mutation	UNP A0A7U0MIF7

- Molecule 3 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.



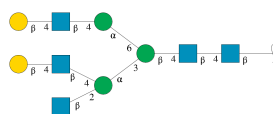
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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.



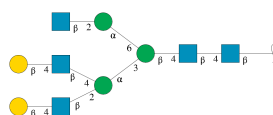
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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
5	H	10	Total	C	N	O	0	0	0
			125	70	5	50			

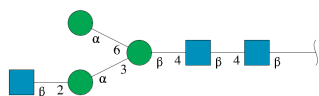
- Molecule 6 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	10	Total	C	N	O	0	0	0
			125	70	5	50			

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





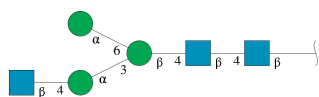
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



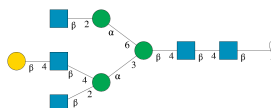
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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
9	M	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 10 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
10	O	9	Total	C	N	O	0	0	0
			114	64	5	45			

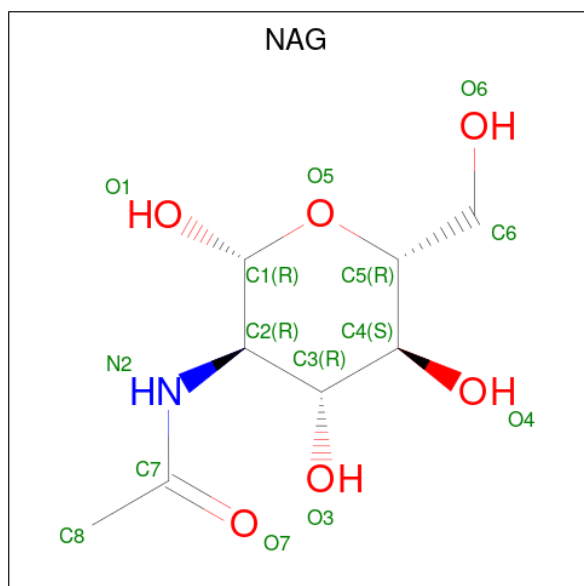
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Cl	0	0
			1	1		
12	B	1	Total	Cl	0	0
			1	1		

- 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>).

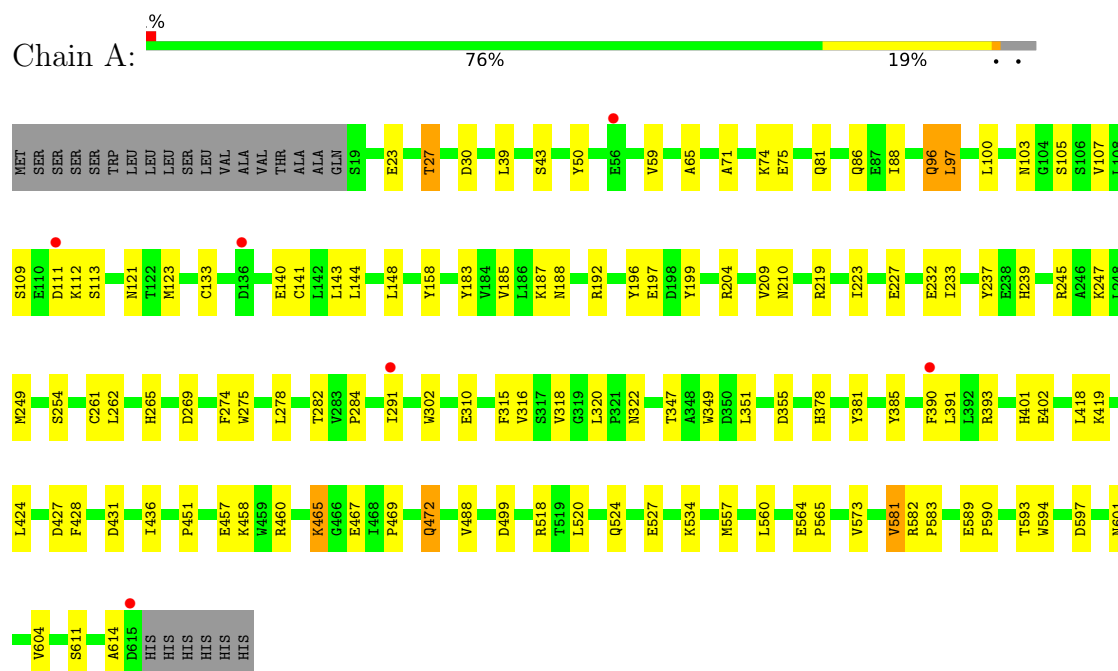


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			14	8	1	5		

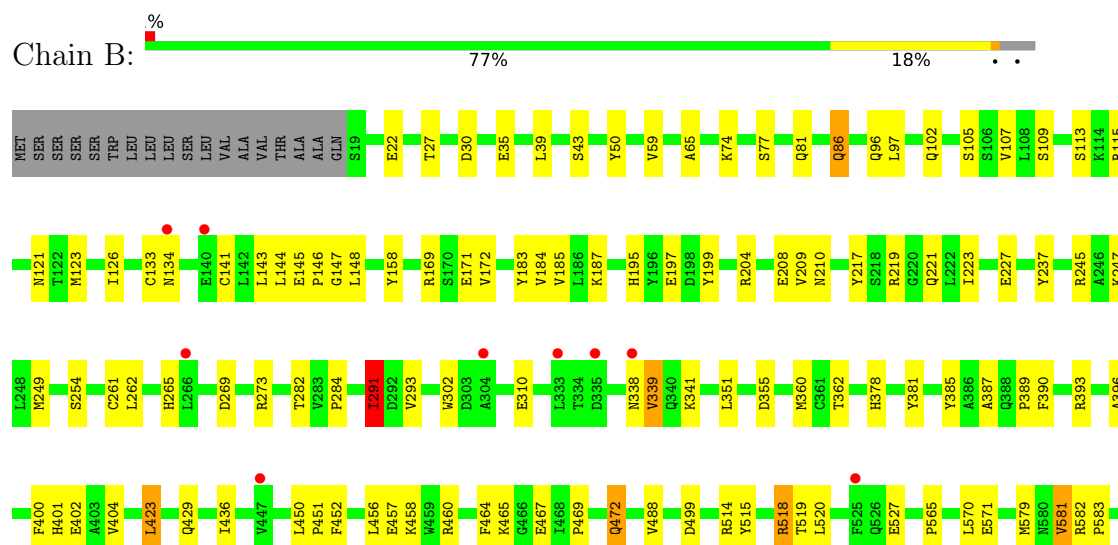
### 3 Residue-property plots [i](#)

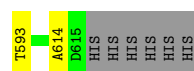
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Angiotensin-converting enzyme 2

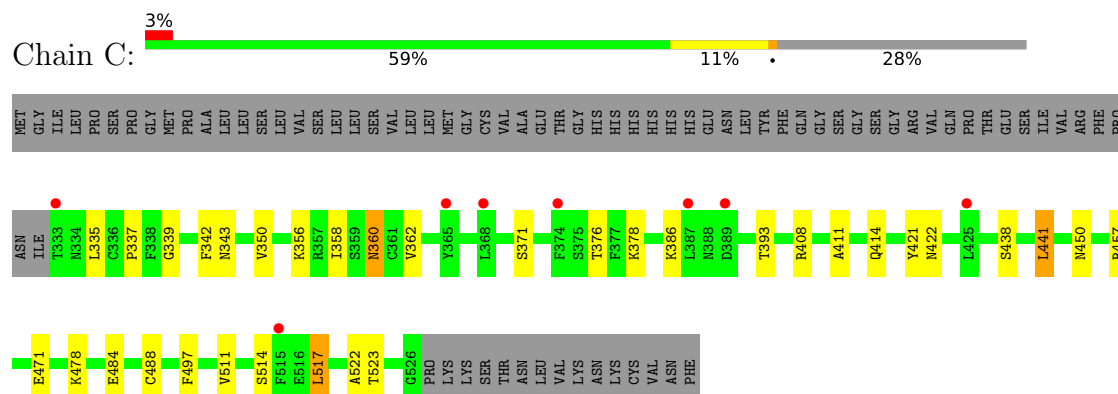


#### • Molecule 1: Angiotensin-converting enzyme 2

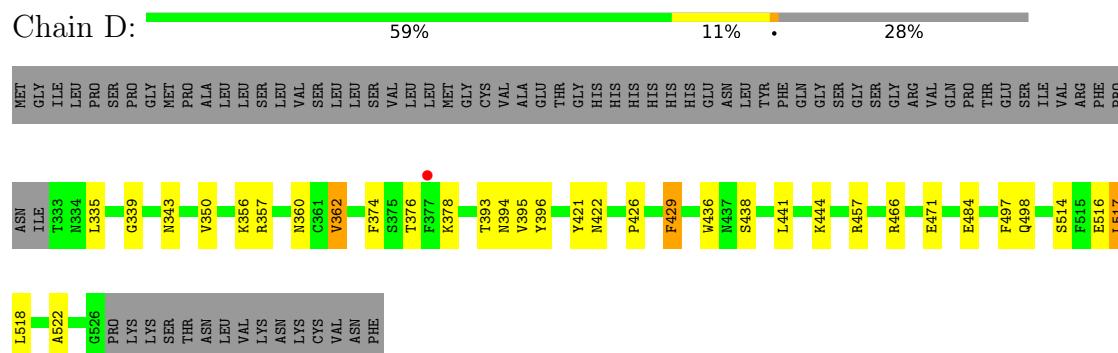




- Molecule 2: Surface glycoprotein



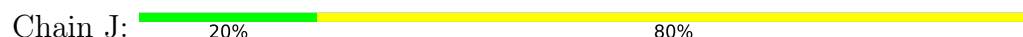
- Molecule 2: Surface glycoprotein



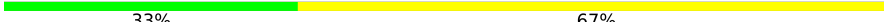
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain F:  33% 67%

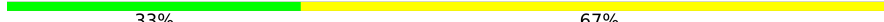
NAG1  
NAG2  
BMA3

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

Chain G:  67% 33%

NAG1  
NAG2  
BMA3

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

Chain N:  33% 67%

NAG1  
NAG2  
BMA3

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

Chain Q:  67% 33%

NAG1  
NAG2  
BMA3

- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 H:  30% 50% 20%

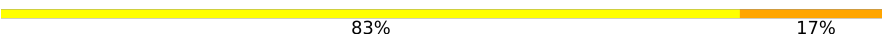
NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
GAL6  
NAG7  
MAN8  
NAG9  
GAL10

- Molecule 6: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 I:  40% 60%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
GAL6  
NAG7  
GAL8  
MAN9  
NAG10

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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:  83% 17%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
MAN6

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

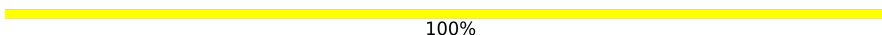
NAG1  
NAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%


NAG1  
NAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 M:  100%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
MAN6

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

Chain O:  33% 11% 56%

NAG1  
NAG2  
BMA3  
MAN4  
NAG5  
GAL6  
NAG7  
MAN8  
NAG9

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.71Å 104.02Å 223.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.96 – 3.08 111.96 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (111.96-3.08) 99.1 (111.96-3.08)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.07Å)	Xtriage
Refinement program	BUSTER 20201211	Depositor
R, $R_{free}$	0.235 , 0.286 0.230 , 0.278	Depositor DCC
$R_{free}$ test set	1846 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: CL, MAN, ZN, NAG, BMA, GAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	0/5029	0.59	0/6833
1	B	0.42	0/5029	0.58	0/6834
2	C	0.45	0/1586	0.61	0/2157
2	D	0.46	0/1586	0.63	0/2157
All	All	0.43	0/13230	0.60	0/17981

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	A	4887	0	4650	48	0
1	B	4887	0	4651	47	0
2	C	1541	0	1464	14	0
2	D	1541	0	1464	12	0
3	E	61	0	52	3	0
3	J	61	0	52	0	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
4	N	39	0	34	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	39	0	34	0	0
5	H	125	0	106	1	0
6	I	125	0	106	0	0
7	K	75	0	64	1	0
8	L	28	0	25	0	0
8	P	28	0	25	1	0
9	M	75	0	64	0	0
10	O	114	0	97	5	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	1	0	0	1	0
12	B	1	0	0	1	0
13	A	14	0	13	0	0
All	All	13722	0	12969	126	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 5.

The worst 5 of 126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PRO:HG3	10:O:2:NAG:H81	1.51	0.93
5:H:8:MAN:H3	5:H:9:NAG:H2	1.59	0.84
2:C:337:PRO:HD2	2:C:358:ILE:HD12	1.69	0.75
1:B:515:TYR:HA	1:B:518:ARG:HD3	1.70	0.72
1:A:96:GLN:HG2	1:A:391:LEU:HD12	1.72	0.71

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	597/621 (96%)	569 (95%)	28 (5%)	0	100	100
1	B	597/621 (96%)	564 (94%)	27 (4%)	6 (1%)	15	47
2	C	192/271 (71%)	180 (94%)	11 (6%)	1 (0%)	29	61
2	D	192/271 (71%)	178 (93%)	13 (7%)	1 (0%)	29	61
All	All	1578/1784 (88%)	1491 (94%)	79 (5%)	8 (0%)	29	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	497	PHE
1	B	291	ILE
1	B	338	ASN
1	B	339	VAL
2	D	497	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/548 (96%)	482 (91%)	47 (9%)	9	33
1	B	529/548 (96%)	486 (92%)	43 (8%)	11	37
2	C	167/235 (71%)	155 (93%)	12 (7%)	14	42
2	D	167/235 (71%)	153 (92%)	14 (8%)	11	36
All	All	1392/1566 (89%)	1276 (92%)	116 (8%)	11	37

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	107	VAL
2	D	466	ARG
1	B	269	ASP
2	D	444	LYS
2	C	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	601	ASN
2	D	498	GLN
2	D	481	ASN
1	B	81	GLN
1	B	472	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

67 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	1,3	14,14,15	0.44	0	17,19,21	1.16	1 (5%)
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	1.04	1 (5%)
3	BMA	E	3	3	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
3	MAN	E	4	3	11,11,12	0.59	0	15,15,17	1.29	2 (13%)
3	MAN	E	5	3	11,11,12	0.41	0	15,15,17	0.91	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.50	0	17,19,21	1.32	4 (23%)
4	NAG	F	2	4	14,14,15	0.33	0	17,19,21	0.96	2 (11%)
4	BMA	F	3	4	11,11,12	0.35	0	15,15,17	0.48	0
4	NAG	G	1	4,1	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	G	3	4	11,11,12	0.32	0	15,15,17	0.56	0
5	NAG	H	1	5,1	14,14,15	0.28	0	17,19,21	0.52	0
5	GAL	H	10	5	11,11,12	0.34	0	15,15,17	0.54	0
5	NAG	H	2	5	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
5	BMA	H	3	5	11,11,12	0.67	0	15,15,17	1.68	2 (13%)
5	MAN	H	4	5	11,11,12	0.60	0	15,15,17	1.86	2 (13%)
5	NAG	H	5	5	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
5	GAL	H	6	5	11,11,12	0.29	0	15,15,17	0.81	1 (6%)
5	NAG	H	7	5	14,14,15	0.32	0	17,19,21	0.69	0
5	MAN	H	8	5	11,11,12	0.38	0	15,15,17	1.37	2 (13%)
5	NAG	H	9	5	14,14,15	0.34	0	17,19,21	0.80	1 (5%)
6	NAG	I	1	1,6	14,14,15	0.29	0	17,19,21	0.65	0
6	NAG	I	10	6	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	1.13	2 (11%)
6	BMA	I	3	6	11,11,12	0.31	0	15,15,17	0.69	1 (6%)
6	MAN	I	4	6	11,11,12	0.38	0	15,15,17	0.71	0
6	NAG	I	5	6	14,14,15	0.40	0	17,19,21	1.21	1 (5%)
6	GAL	I	6	6	11,11,12	0.33	0	15,15,17	0.33	0
6	NAG	I	7	6	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
6	GAL	I	8	6	11,11,12	0.33	0	15,15,17	0.53	0
6	MAN	I	9	6	11,11,12	0.41	0	15,15,17	0.94	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.36	0	17,19,21	1.36	3 (17%)
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	1.14	1 (5%)
3	BMA	J	3	3	11,11,12	0.41	0	15,15,17	0.96	0
3	MAN	J	4	3	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
3	MAN	J	5	3	11,11,12	0.38	0	15,15,17	0.95	1 (6%)
7	NAG	K	1	1,7	14,14,15	0.39	0	17,19,21	1.74	3 (17%)
7	NAG	K	2	7	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
7	BMA	K	3	7	11,11,12	0.32	0	15,15,17	0.60	0
7	MAN	K	4	7	11,11,12	0.61	0	15,15,17	1.31	1 (6%)
7	NAG	K	5	7	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
7	MAN	K	6	7	11,11,12	0.38	0	15,15,17	0.90	1 (6%)
8	NAG	L	1	8,1	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
8	NAG	L	2	8	14,14,15	0.37	0	17,19,21	1.03	2 (11%)
9	NAG	M	1	9,1	14,14,15	0.33	0	17,19,21	1.16	1 (5%)
9	NAG	M	2	9	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
9	BMA	M	3	9	11,11,12	0.36	0	15,15,17	0.76	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	M	4	9	11,11,12	0.49	0	15,15,17	1.98	2 (13%)
9	NAG	M	5	9	14,14,15	0.32	0	17,19,21	0.84	1 (5%)
9	MAN	M	6	9	11,11,12	0.38	0	15,15,17	0.99	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	N	2	4	14,14,15	0.41	0	17,19,21	1.53	2 (11%)
4	BMA	N	3	4	11,11,12	0.48	0	15,15,17	0.97	1 (6%)
10	NAG	O	1	10,1	14,14,15	0.28	0	17,19,21	1.22	1 (5%)
10	NAG	O	2	10	14,14,15	0.36	0	17,19,21	1.13	2 (11%)
10	BMA	O	3	10	11,11,12	0.28	0	15,15,17	0.54	0
10	MAN	O	4	10	11,11,12	0.31	0	15,15,17	0.86	0
10	NAG	O	5	10	14,14,15	0.41	0	17,19,21	1.36	3 (17%)
10	GAL	O	6	10	11,11,12	0.35	0	15,15,17	1.13	1 (6%)
10	NAG	O	7	10	14,14,15	0.34	0	17,19,21	0.62	0
10	MAN	O	8	10	11,11,12	0.57	0	15,15,17	1.52	2 (13%)
10	NAG	O	9	10	14,14,15	0.53	0	17,19,21	1.75	1 (5%)
8	NAG	P	1	2,8	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
8	NAG	P	2	8	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	Q	1	2,4	14,14,15	0.35	0	17,19,21	0.65	0
4	NAG	Q	2	4	14,14,15	0.35	0	17,19,21	0.48	0
4	BMA	Q	3	4	11,11,12	0.39	0	15,15,17	0.68	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	H	10	5	-	0/2/19/22	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	1/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	NAG	H	5	5	-	1/6/23/26	0/1/1/1
5	GAL	H	6	5	-	0/2/19/22	0/1/1/1
5	NAG	H	7	5	-	0/6/23/26	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
5	NAG	H	9	5	-	0/6/23/26	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	10	6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	NAG	I	5	6	-	0/6/23/26	0/1/1/1
6	GAL	I	6	6	-	0/2/19/22	0/1/1/1
6	NAG	I	7	6	-	0/6/23/26	0/1/1/1
6	GAL	I	8	6	-	0/2/19/22	0/1/1/1
6	MAN	I	9	6	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	0/2/19/22	0/1/1/1
7	NAG	K	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	1/1/1/1
7	NAG	K	5	7	-	0/6/23/26	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
9	NAG	M	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	2/2/19/22	0/1/1/1
9	MAN	M	4	9	-	1/2/19/22	1/1/1/1
9	NAG	M	5	9	-	2/6/23/26	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	9	NAG	C1-O5-C5	6.77	121.36	112.19
9	M	4	MAN	C1-O5-C5	6.19	120.58	112.19
5	H	4	MAN	C1-O5-C5	6.18	120.57	112.19
5	H	3	BMA	C1-O5-C5	4.92	118.86	112.19
7	K	1	NAG	O5-C1-C2	-4.75	103.79	111.29

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	E	3	BMA	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
9	M	3	BMA	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	4	MAN	C1-C2-C3-C4-C5-O5
5	H	3	BMA	C1-C2-C3-C4-C5-O5
10	O	8	MAN	C1-C2-C3-C4-C5-O5

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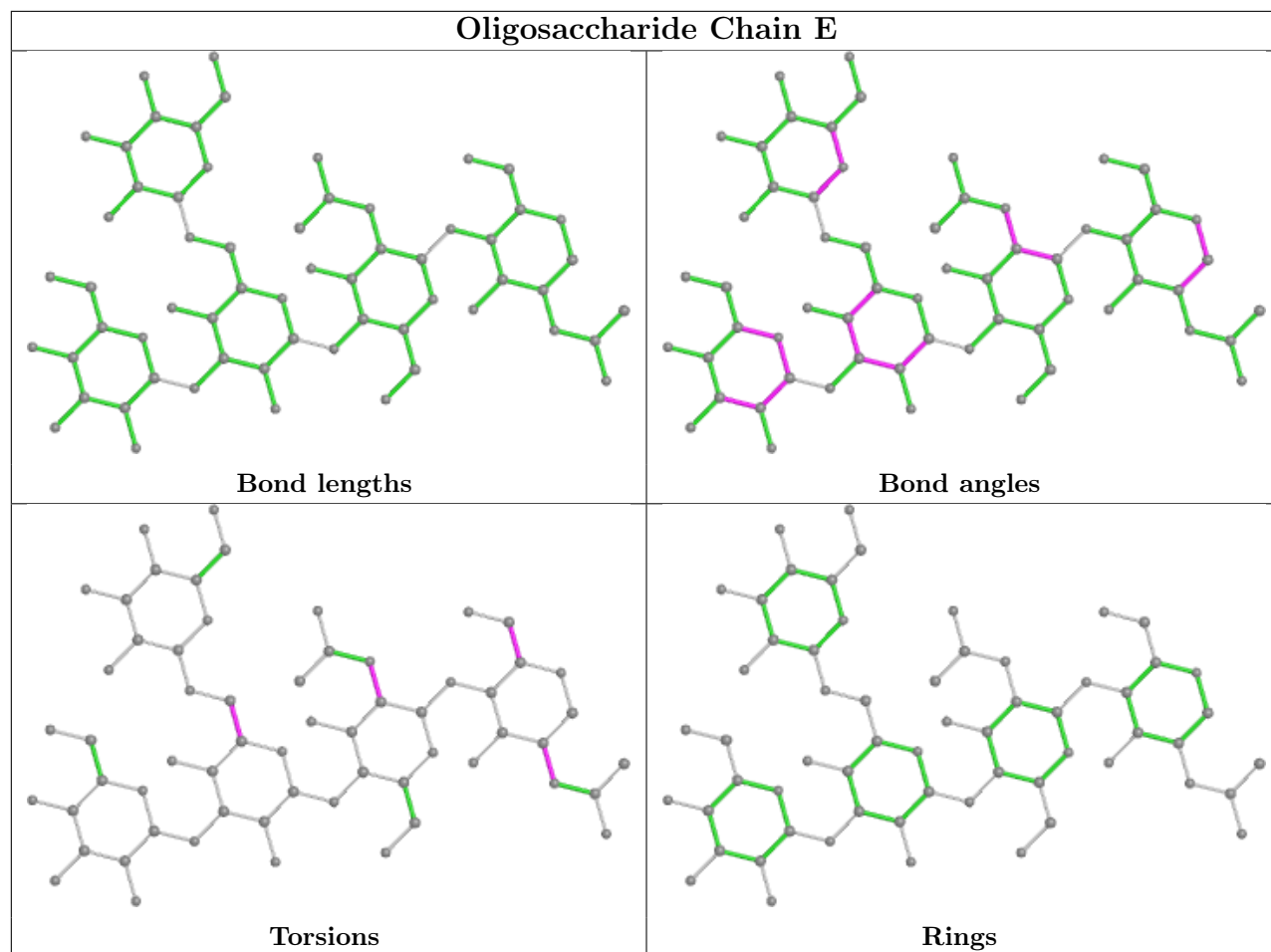
Mol	Chain	Res	Type	Atoms
7	K	4	MAN	C1-C2-C3-C4-C5-O5

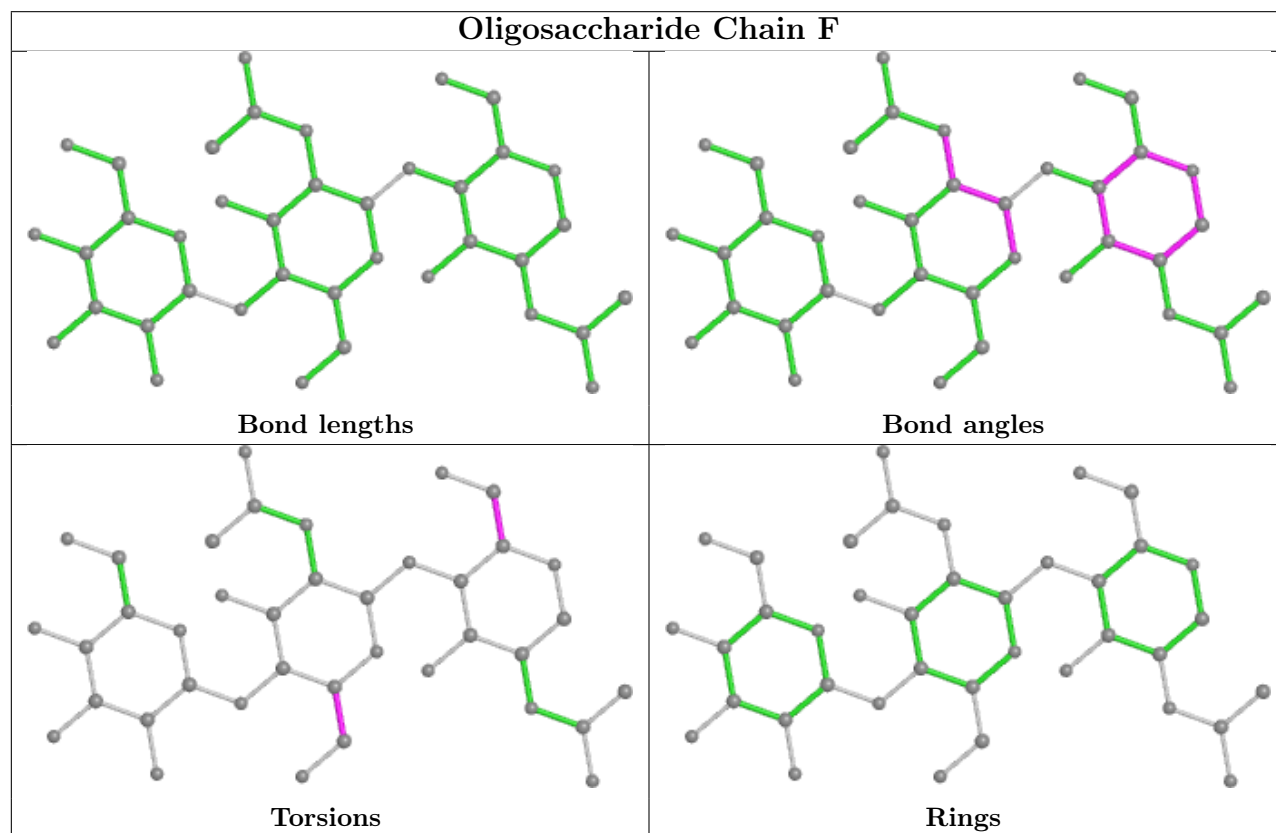
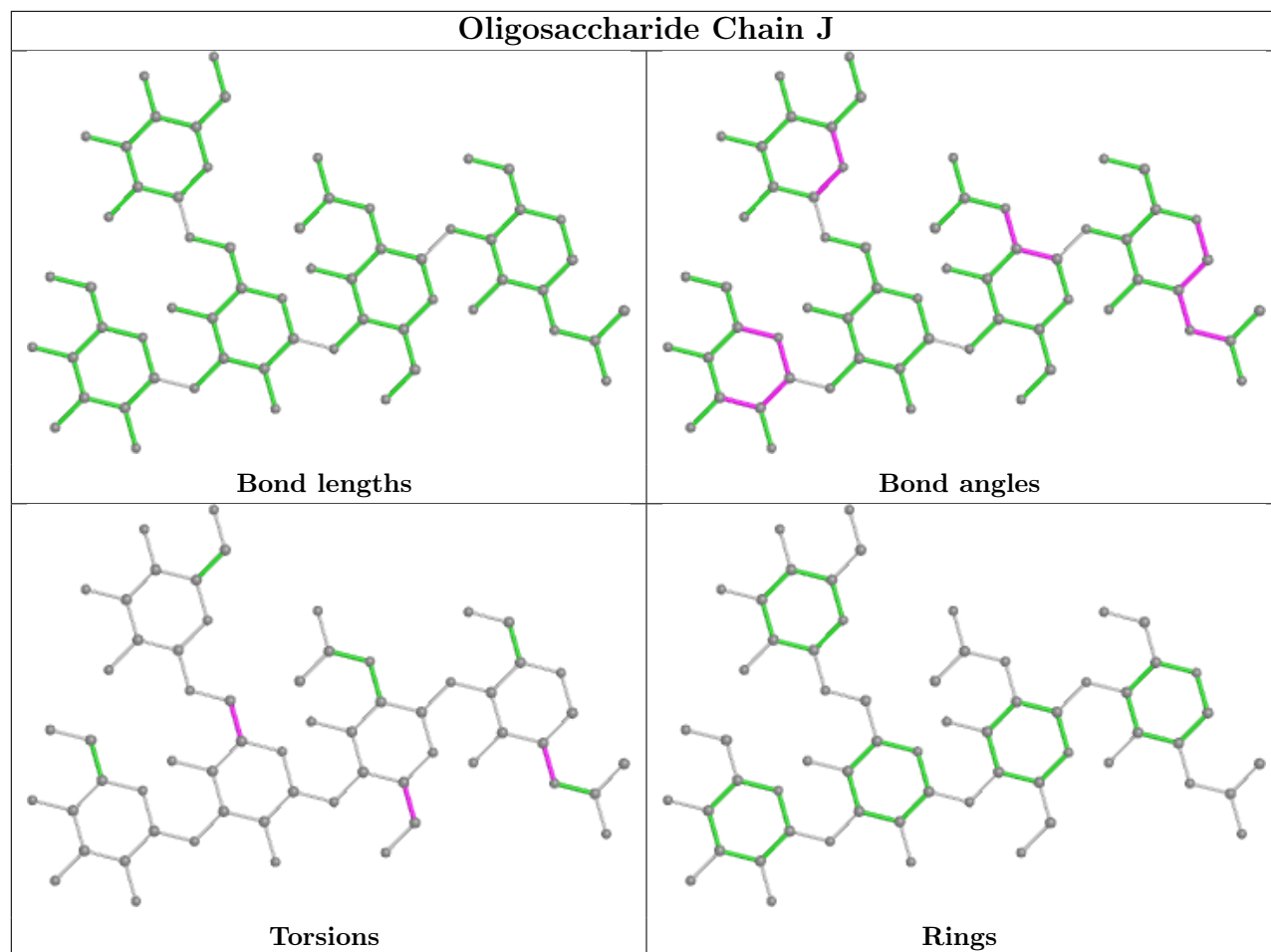
13 monomers are involved in 11 short contacts:

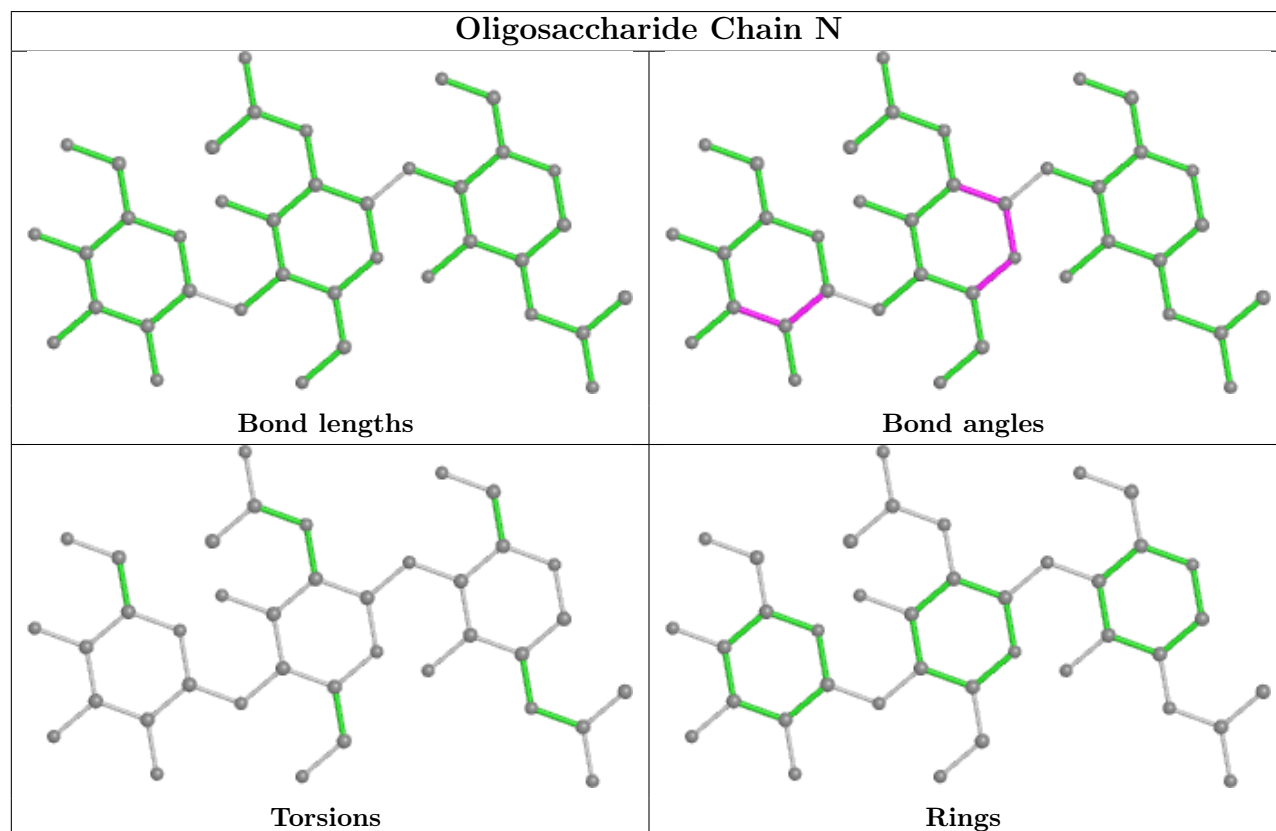
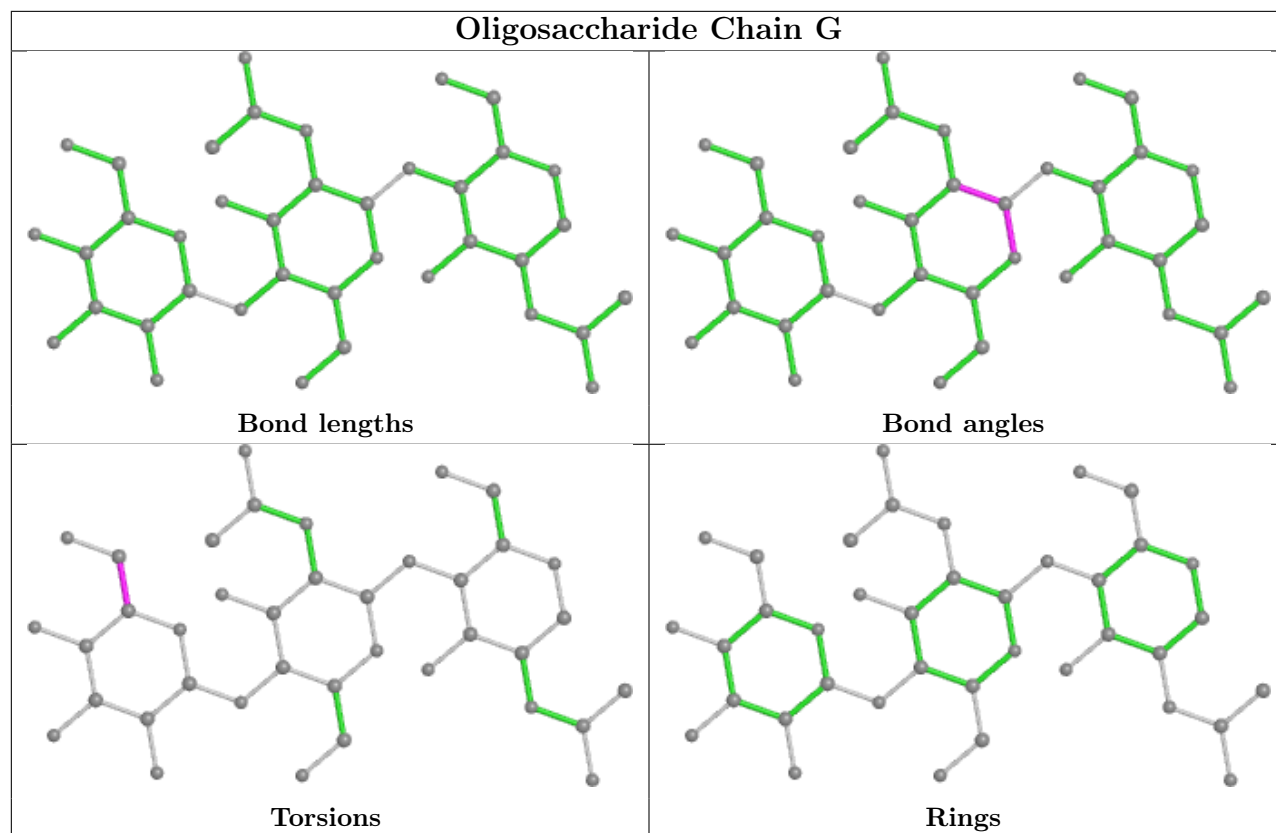
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	2	NAG	1	0
3	E	5	MAN	1	0
7	K	4	MAN	1	0
10	O	9	NAG	1	0
7	K	3	BMA	1	0
10	O	5	NAG	1	0
5	H	8	MAN	1	0
10	O	6	GAL	1	0
10	O	2	NAG	2	0
3	E	2	NAG	1	0
3	E	1	NAG	1	0
5	H	9	NAG	1	0
10	O	8	MAN	2	0

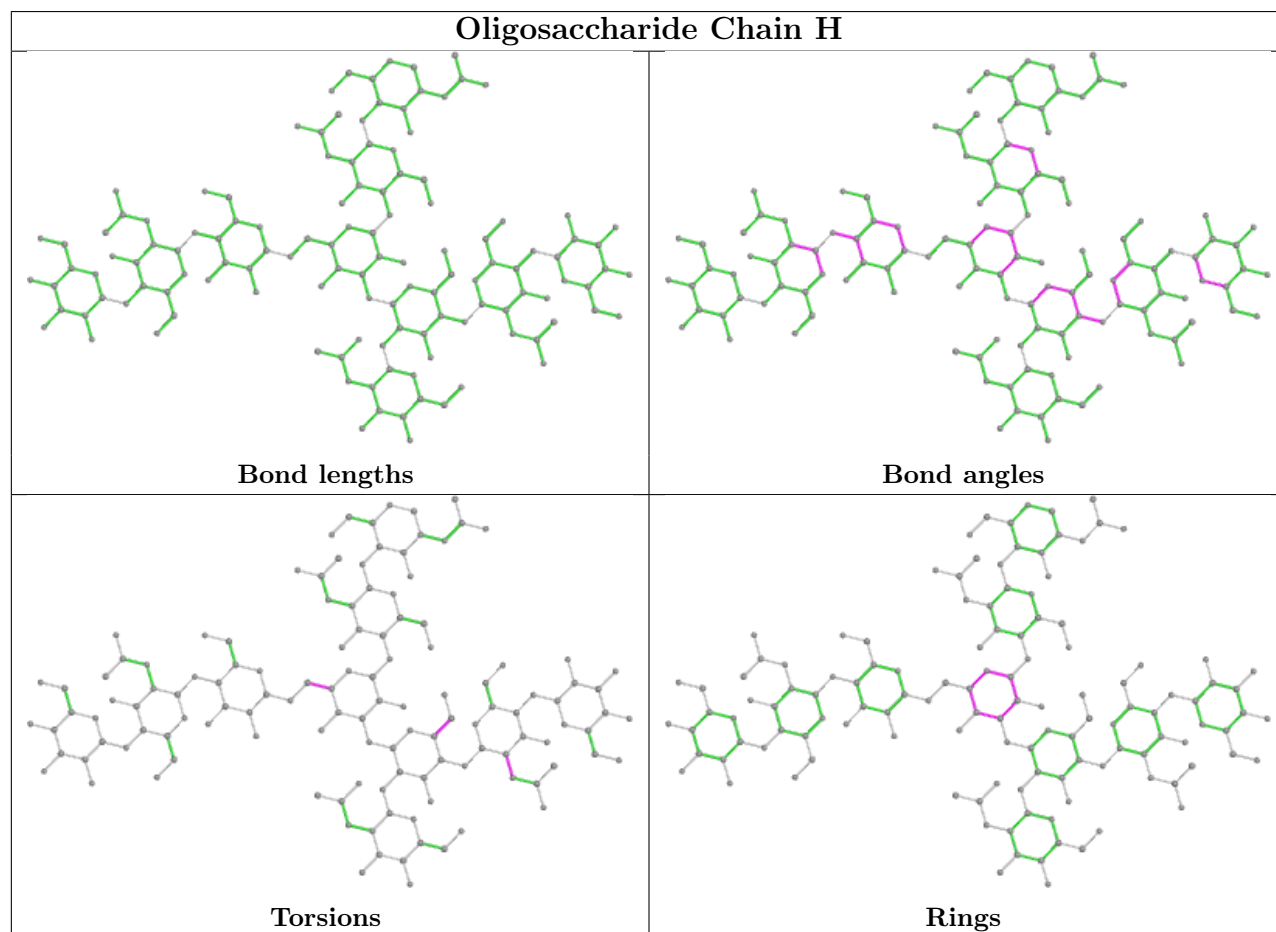
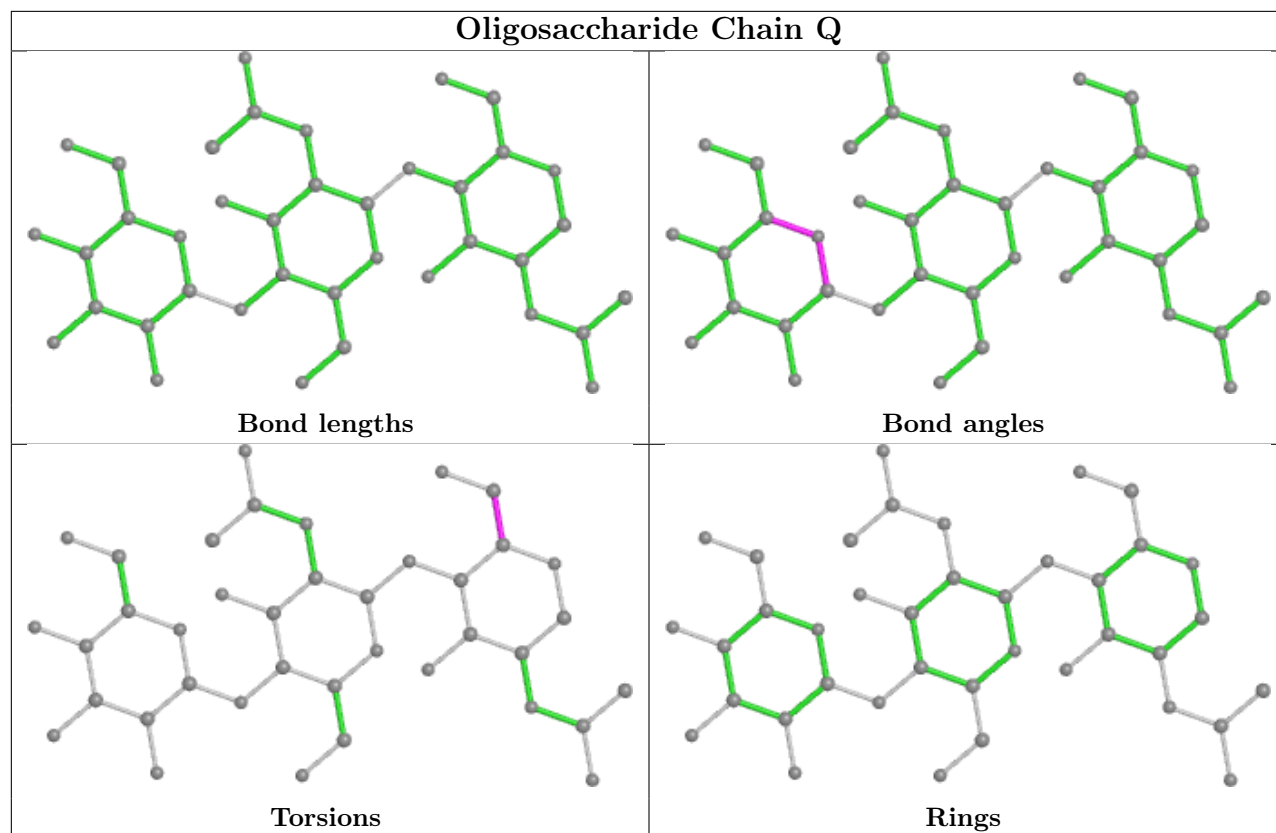
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

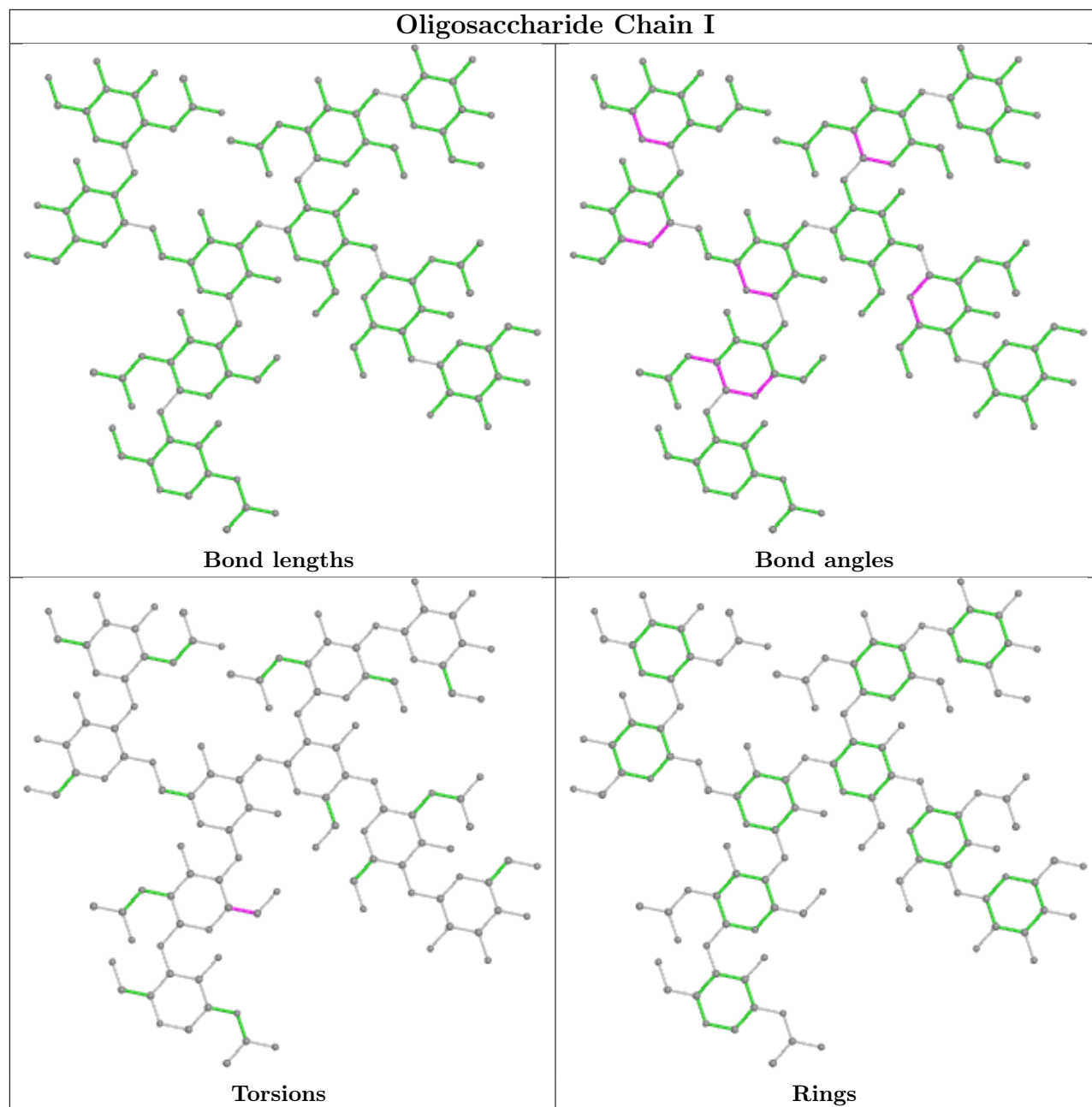


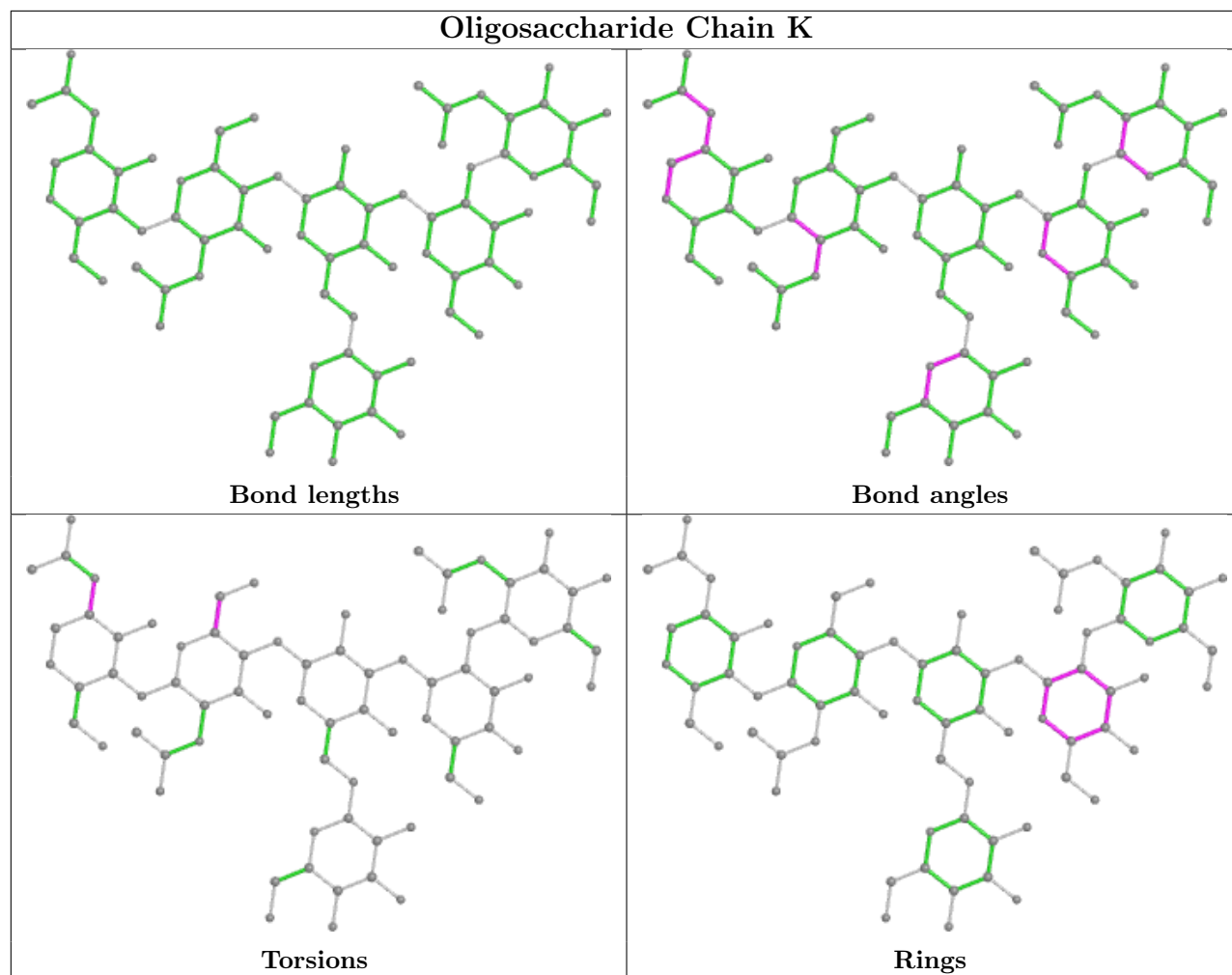


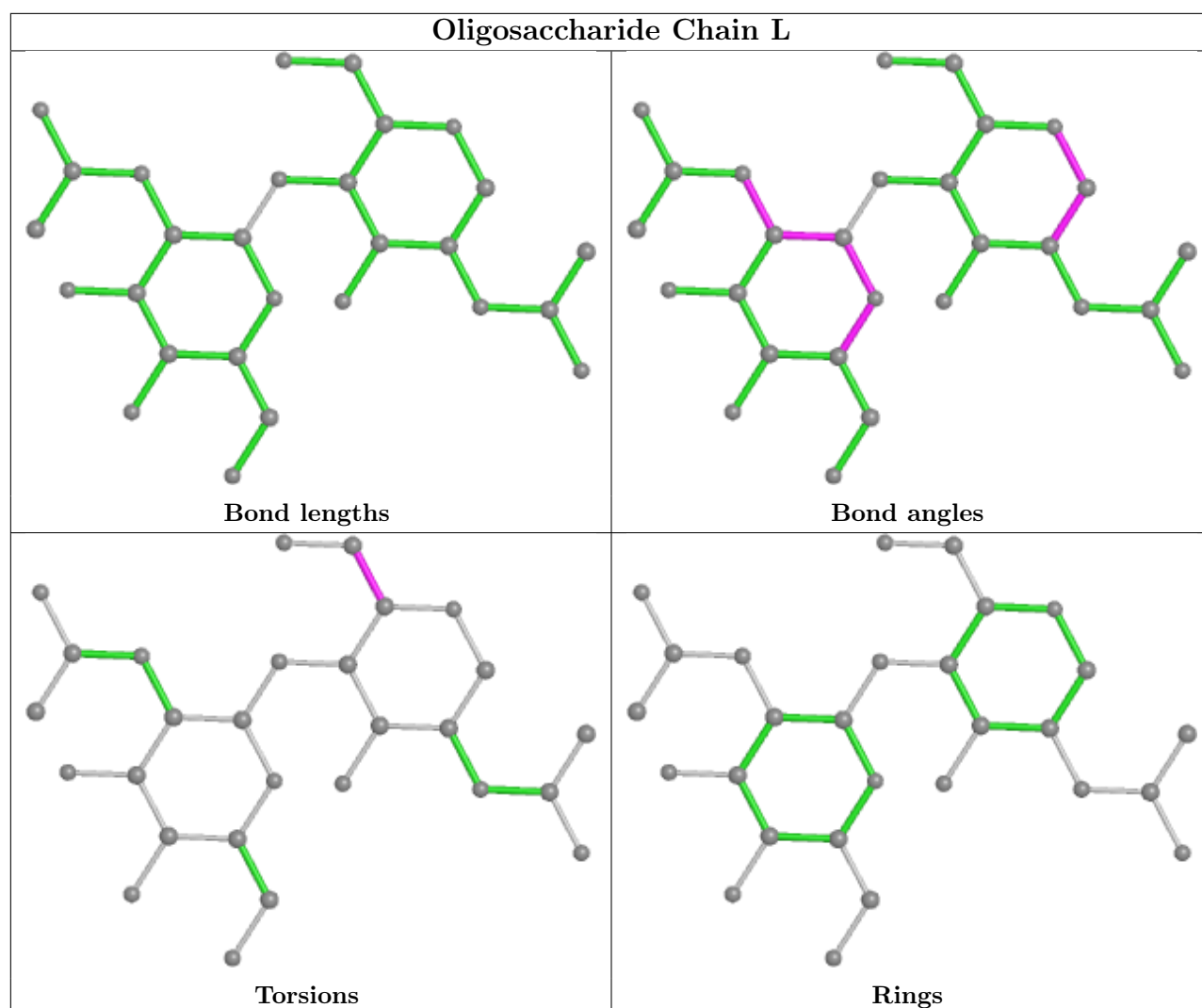


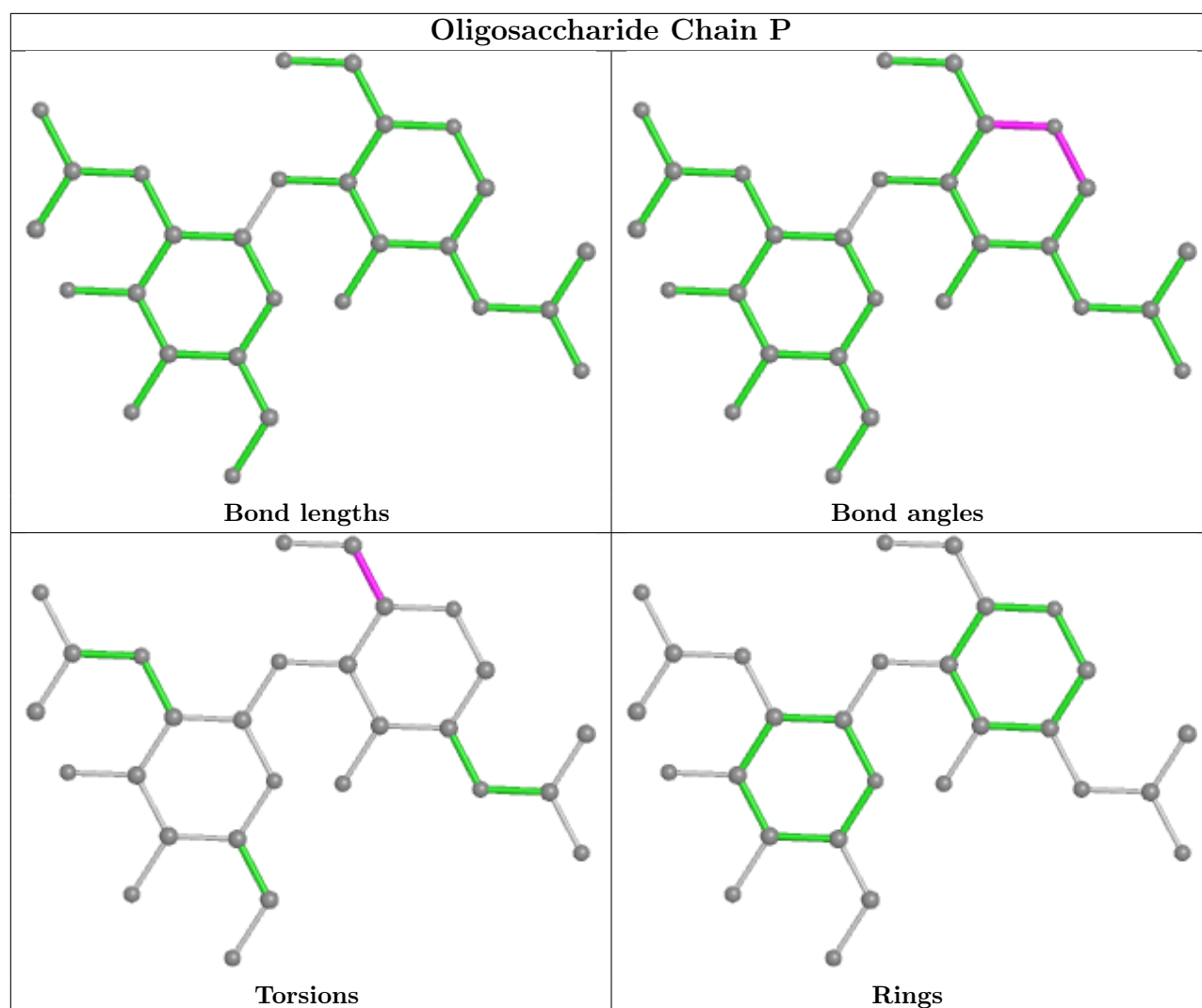




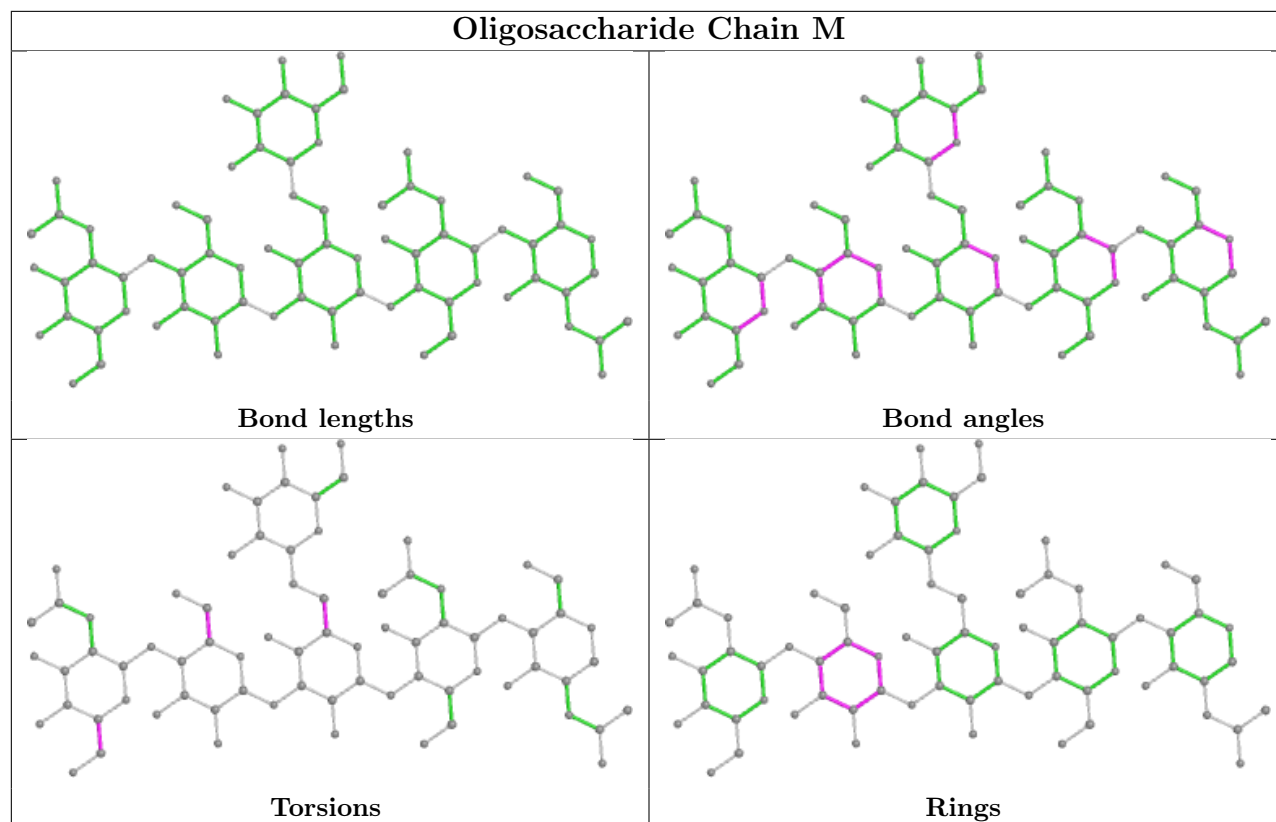


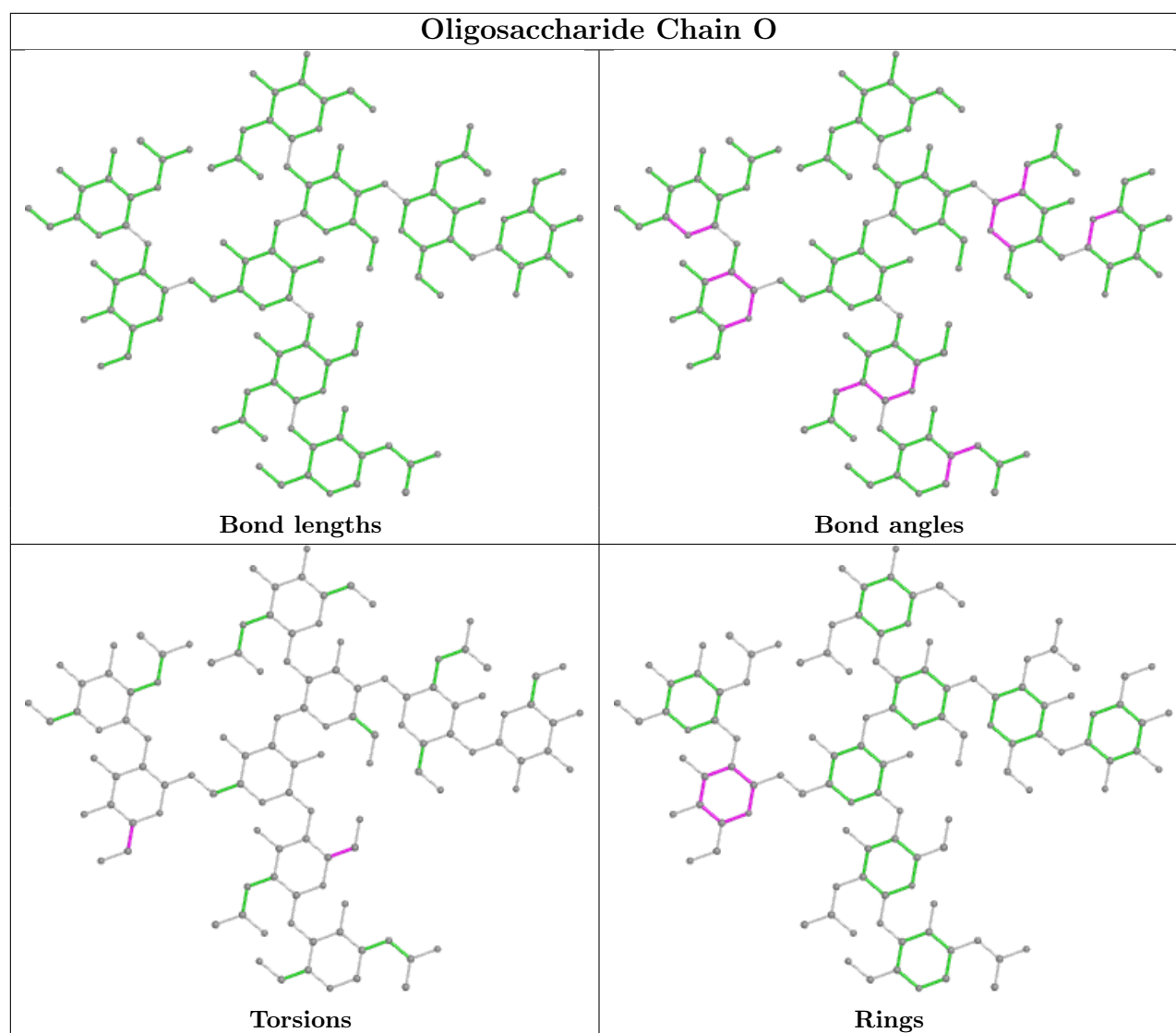












## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	A	903	1	14,14,15	0.35	0	17,19,21	1.36	3 (17%)

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	A	903	1	-	3/6/23/26	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	A	903	NAG	C1-O5-C5	3.82	117.37	112.19
13	A	903	NAG	C1-C2-N2	2.91	115.45	110.49
13	A	903	NAG	C2-N2-C7	2.28	126.14	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	903	NAG	O5-C5-C6-O6
13	A	903	NAG	C1-C2-N2-C7
13	A	903	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	597/621 (96%)	0.11	6 (1%) 82 66	66, 92, 119, 140	0
1	B	597/621 (96%)	0.15	9 (1%) 73 53	71, 93, 121, 128	0
2	C	194/271 (71%)	0.29	8 (4%) 37 18	72, 91, 123, 144	0
2	D	194/271 (71%)	0.03	1 (0%) 91 80	71, 91, 124, 143	0
All	All	1582/1784 (88%)	0.13	24 (1%) 73 53	66, 92, 121, 144	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	333	THR	3.6
1	A	136	ASP	3.2
2	C	389	ASP	2.9
2	C	368	LEU	2.9
2	D	377	PHE	2.7

### 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
7	MAN	K	6	11/12	0.40	0.34	155,156,156,156	0
5	NAG	H	9	14/15	0.44	0.36	168,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GAL	H	10	11/12	0.47	0.51	169,170,170,170	0
5	BMA	H	3	11/12	0.51	0.25	161,163,164,165	0
6	NAG	I	5	14/15	0.53	0.42	159,160,160,161	0
3	BMA	J	3	11/12	0.57	0.29	148,150,152,152	0
3	MAN	J	4	11/12	0.59	0.30	149,150,150,150	0
10	NAG	O	5	14/15	0.59	0.58	159,160,160,160	0
10	NAG	O	7	14/15	0.59	0.28	155,157,157,157	0
9	NAG	M	5	14/15	0.60	0.22	166,166,166,167	0
4	BMA	N	3	11/12	0.62	0.23	121,121,122,122	0
9	MAN	M	4	11/12	0.63	0.18	163,164,165,165	0
6	NAG	I	10	14/15	0.64	0.42	149,149,150,150	0
3	MAN	J	5	11/12	0.64	0.27	153,154,154,154	0
8	NAG	L	2	14/15	0.64	0.27	137,138,139,139	0
9	BMA	M	3	11/12	0.64	0.24	159,160,161,162	0
6	BMA	I	3	11/12	0.65	0.20	149,150,152,154	0
3	MAN	E	5	11/12	0.65	0.50	145,145,145,146	0
7	MAN	K	4	11/12	0.66	0.33	152,153,153,153	0
4	BMA	Q	3	11/12	0.67	0.28	136,137,137,137	0
7	NAG	K	5	14/15	0.68	0.61	152,153,153,153	0
9	MAN	M	6	11/12	0.69	0.38	162,162,162,162	0
6	NAG	I	7	14/15	0.70	0.40	162,162,164,164	0
6	GAL	I	6	11/12	0.71	0.33	161,161,162,162	0
10	NAG	O	9	14/15	0.71	0.27	155,156,156,156	0
5	MAN	H	4	11/12	0.72	0.14	165,165,166,167	0
4	NAG	Q	2	14/15	0.72	0.43	133,135,135,136	0
6	MAN	I	4	11/12	0.72	0.17	156,158,159,160	0
8	NAG	P	1	14/15	0.73	0.38	129,130,132,134	0
3	NAG	E	2	14/15	0.73	0.34	131,133,134,137	0
9	NAG	M	2	14/15	0.74	0.25	150,151,154,156	0
3	MAN	E	4	11/12	0.75	0.28	141,142,142,142	0
8	NAG	P	2	14/15	0.75	0.58	136,137,137,137	0
6	NAG	I	2	14/15	0.77	0.27	140,141,144,146	0
7	BMA	K	3	11/12	0.77	0.28	151,153,154,155	0
5	GAL	H	6	11/12	0.77	0.24	169,170,170,170	0
5	MAN	H	8	11/12	0.77	0.27	166,166,167,168	0
4	NAG	N	2	14/15	0.78	0.31	116,117,119,120	0
4	BMA	F	3	11/12	0.79	0.21	128,129,129,129	0
10	NAG	O	2	14/15	0.80	0.25	147,149,150,151	0
5	NAG	H	2	14/15	0.80	0.21	152,155,157,159	0
3	BMA	E	3	11/12	0.81	0.16	140,141,143,144	0
10	GAL	O	6	11/12	0.81	0.72	160,161,161,161	0
6	MAN	I	9	11/12	0.82	0.16	148,148,149,149	0

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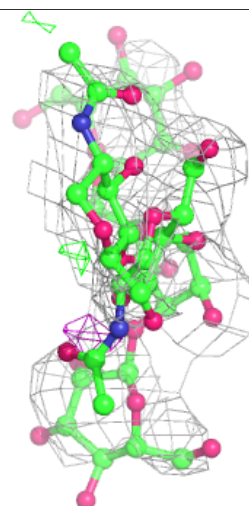
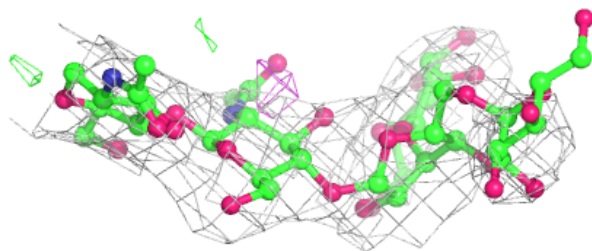
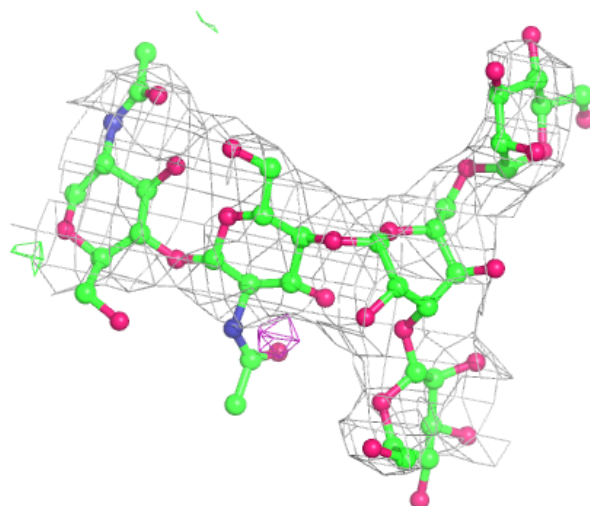
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	M	1	14/15	0.82	0.23	139,140,144,147	0
7	NAG	K	2	14/15	0.82	0.27	145,147,148,150	0
3	NAG	J	2	14/15	0.83	0.17	141,142,144,146	0
5	NAG	H	5	14/15	0.84	0.27	168,169,169,170	0
5	NAG	H	7	14/15	0.84	0.17	164,165,165,165	0
7	NAG	K	1	14/15	0.85	0.28	135,137,140,143	0
10	BMA	O	3	11/12	0.85	0.12	153,154,155,155	0
5	NAG	H	1	14/15	0.85	0.21	141,143,146,149	0
6	GAL	I	8	11/12	0.85	0.39	165,165,165,166	0
4	NAG	F	1	14/15	0.85	0.32	120,122,122,124	0
3	NAG	E	1	14/15	0.85	0.26	122,123,126,128	0
4	NAG	F	2	14/15	0.86	0.18	125,125,126,127	0
4	BMA	G	3	11/12	0.86	0.20	121,122,122,122	0
8	NAG	L	1	14/15	0.87	0.13	133,134,136,137	0
6	NAG	I	1	14/15	0.87	0.25	130,131,134,137	0
10	NAG	O	1	14/15	0.87	0.20	140,141,143,145	0
4	NAG	G	2	14/15	0.88	0.20	118,119,119,120	0
10	MAN	O	4	11/12	0.88	0.23	156,157,158,158	0
10	MAN	O	8	11/12	0.88	0.14	155,155,156,156	0
4	NAG	Q	1	14/15	0.88	0.25	125,126,128,131	0
3	NAG	J	1	14/15	0.90	0.21	133,134,136,138	0
4	NAG	N	1	14/15	0.90	0.14	106,109,111,114	0
4	NAG	G	1	14/15	0.95	0.14	112,113,114,116	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.

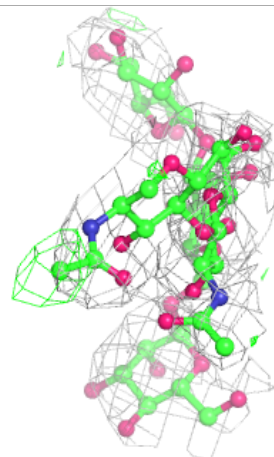
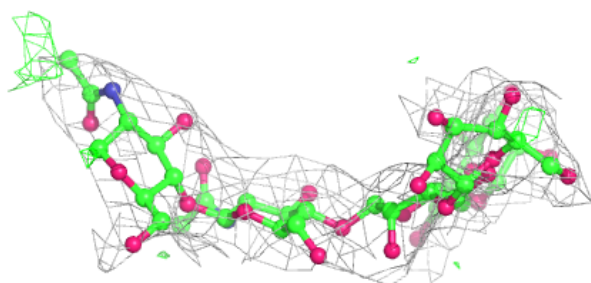
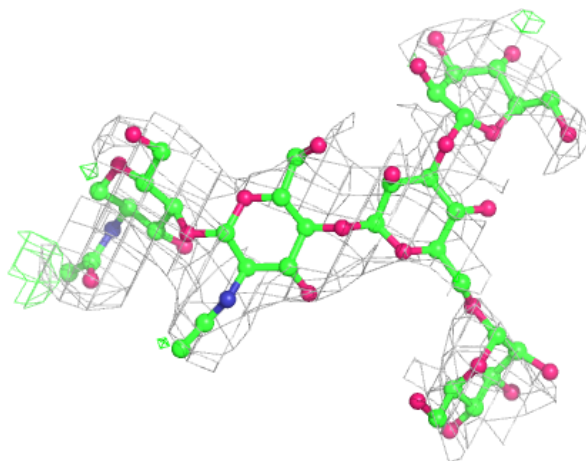
**Electron density around Chain E:**

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



**Electron density around Chain J:**

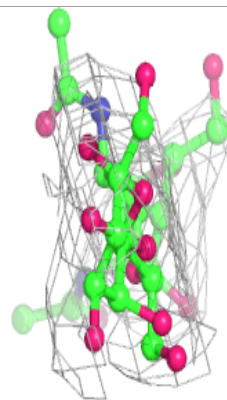
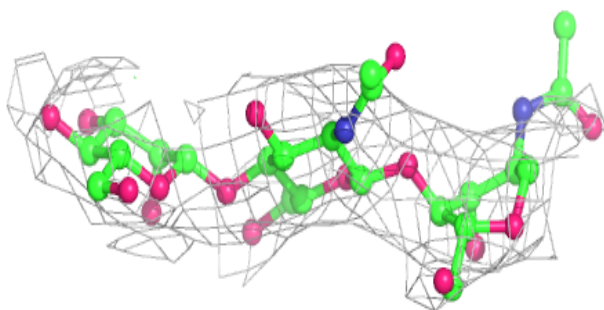
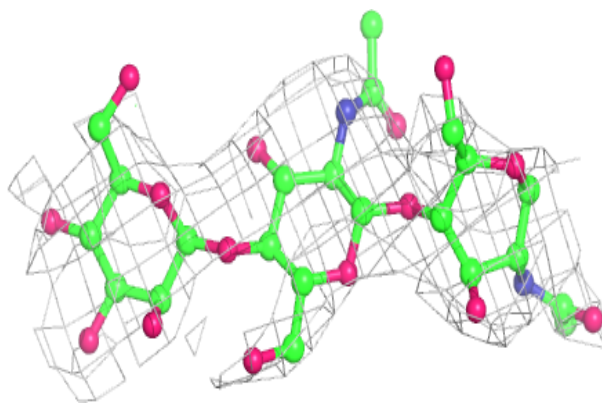
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



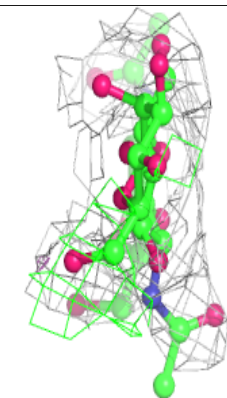
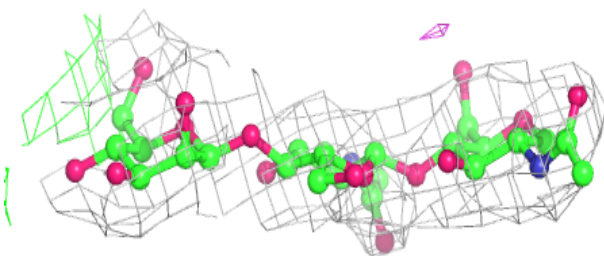
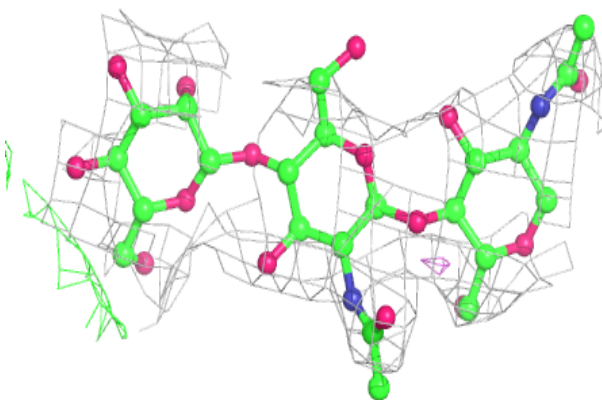


**Electron density around Chain F:**

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

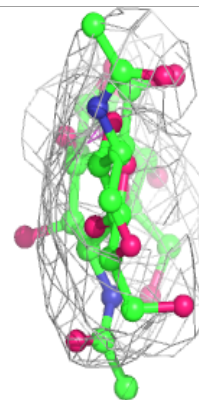
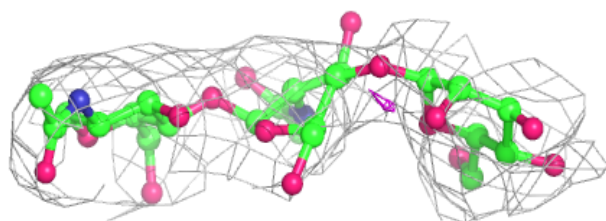
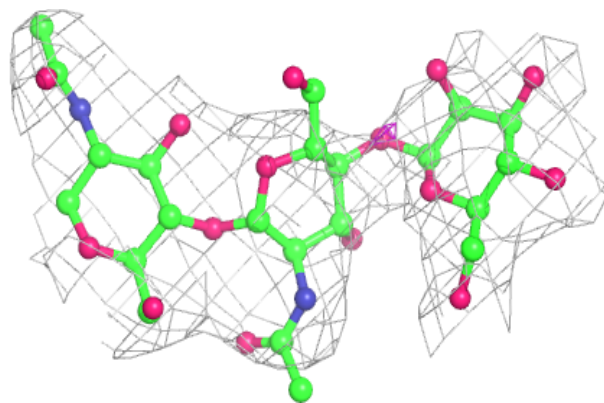
**Electron density around Chain G:**

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

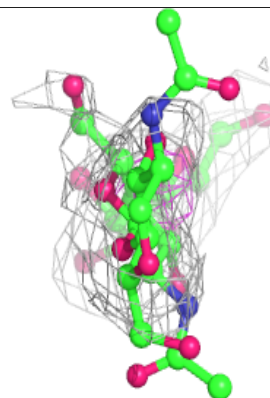
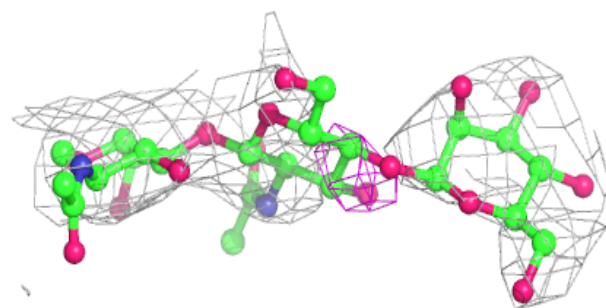
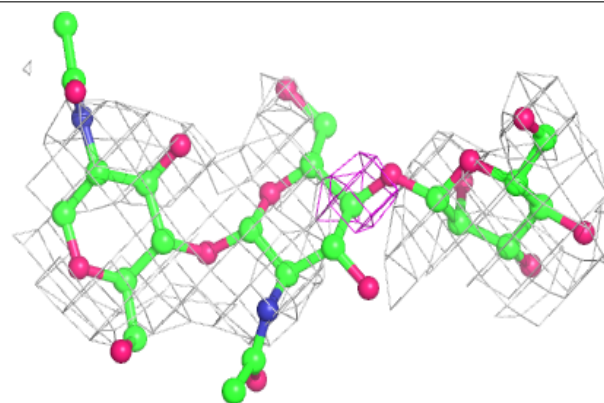


**Electron density around Chain N:**

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

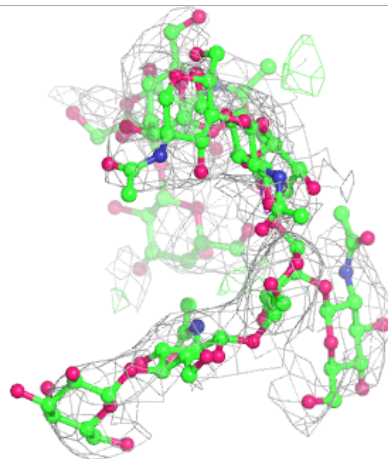
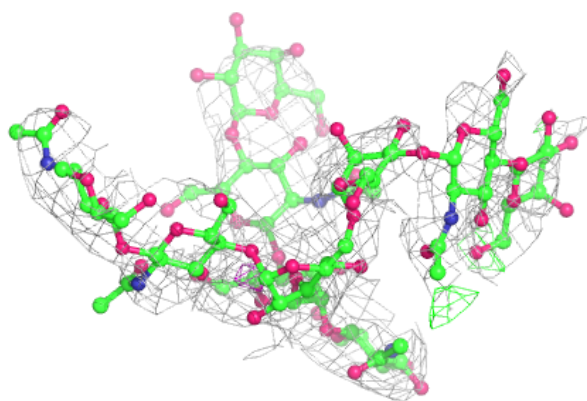
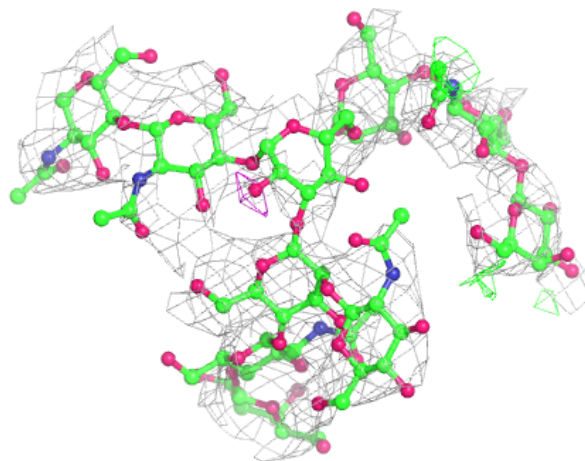
**Electron density around Chain Q:**

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



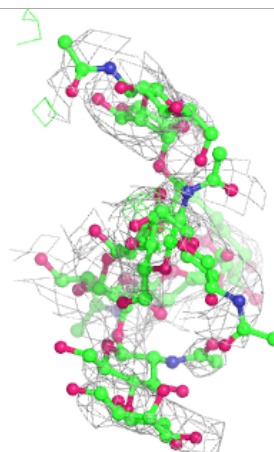
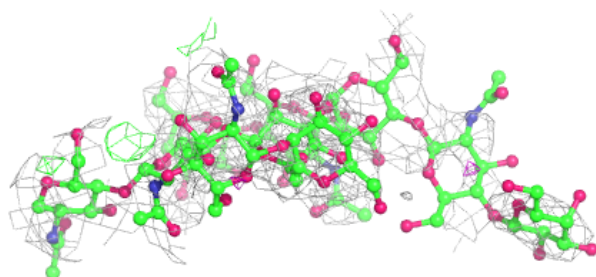
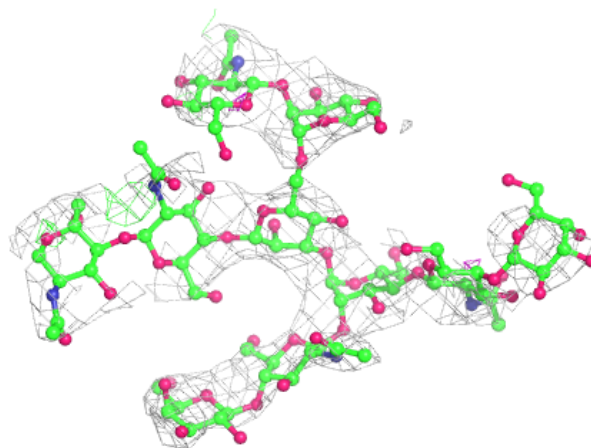
**Electron density around Chain H:**

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



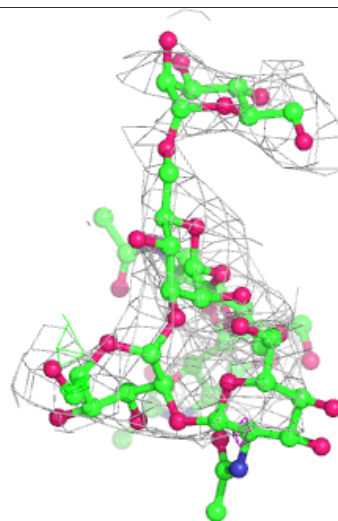
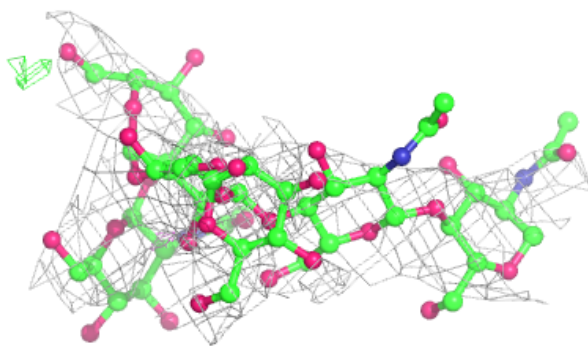
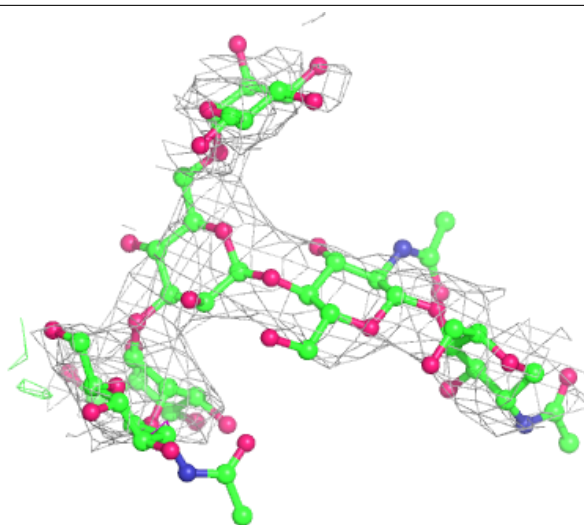
**Electron density around Chain I:**

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



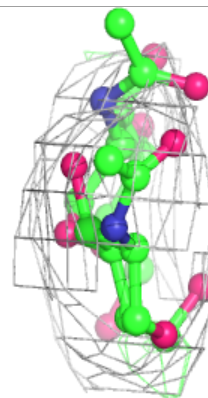
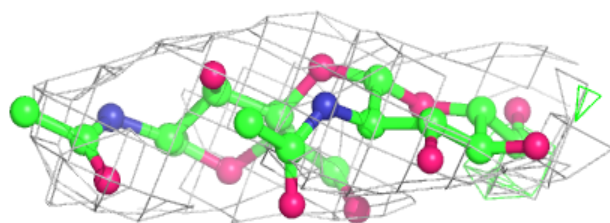
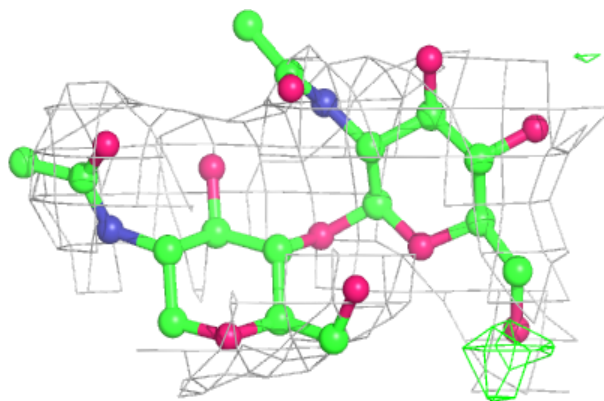
**Electron density around Chain K:**

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



**Electron density around Chain L:**

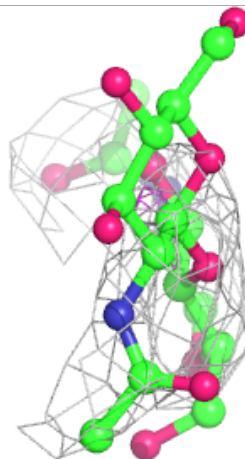
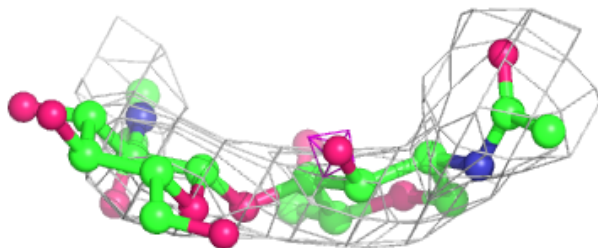
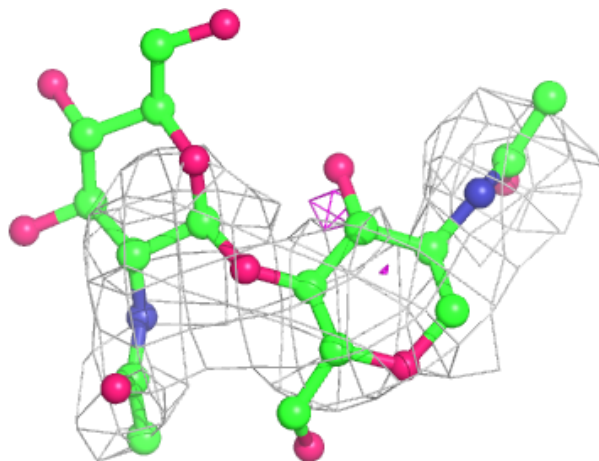
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





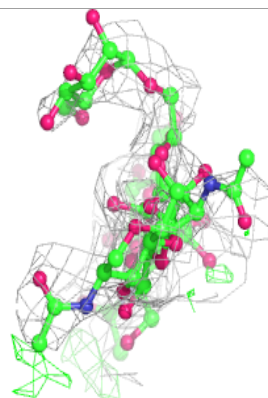
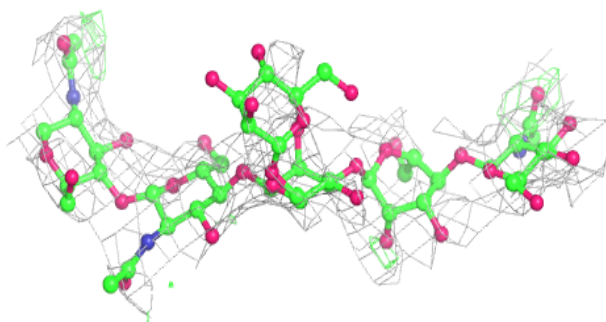
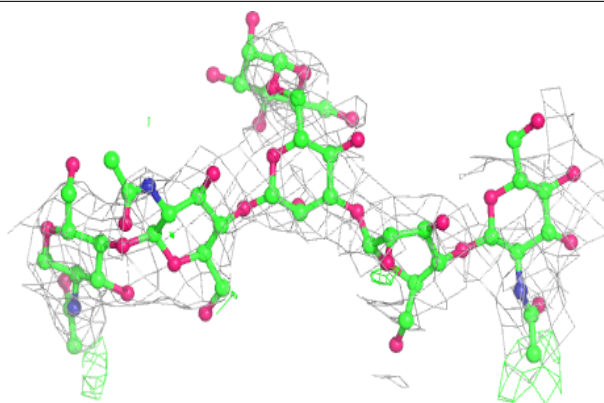
**Electron density around Chain P:**

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

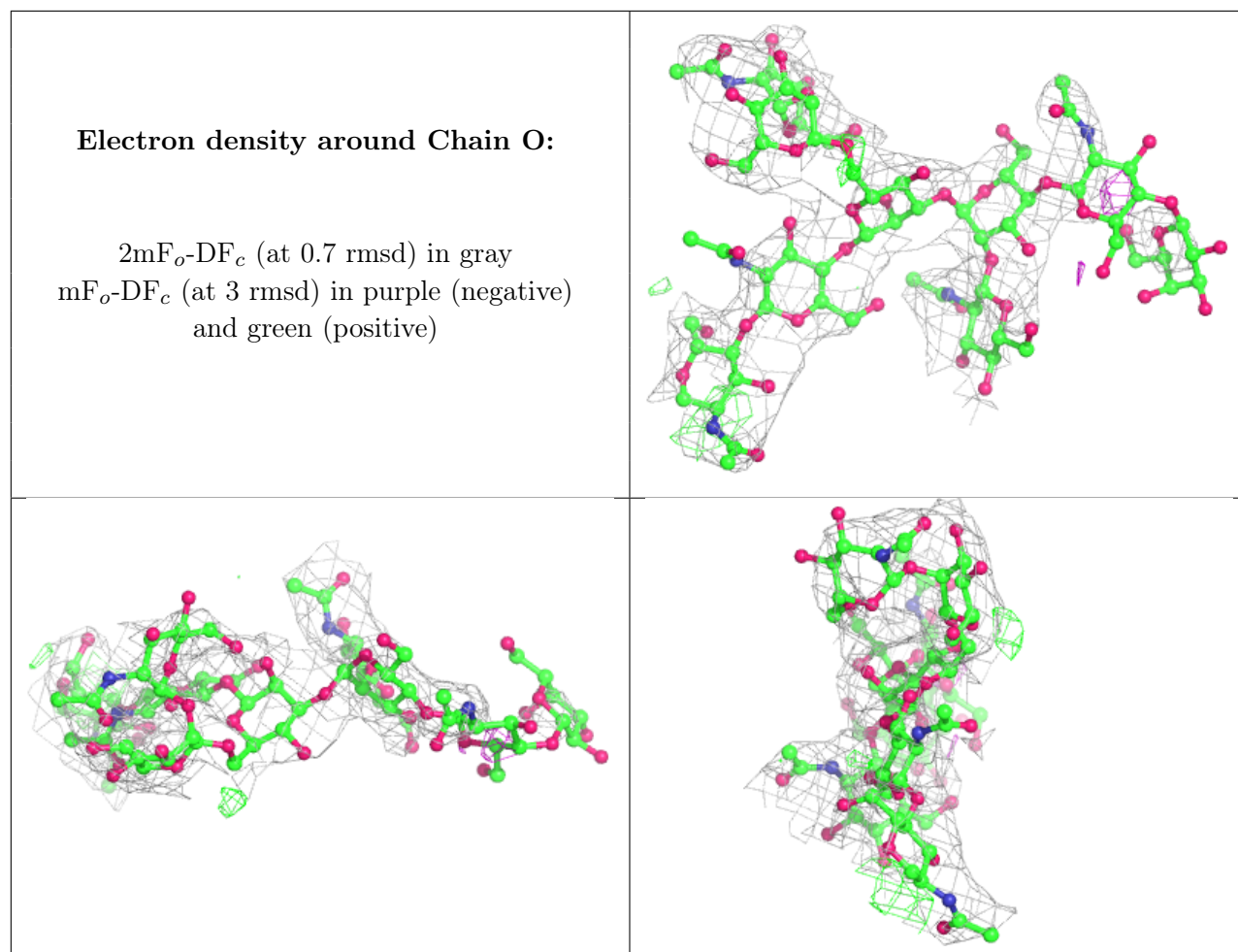


**Electron density around Chain M:**

$2mF_o-DF_c$  (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
12	CL	A	902	1/1	0.86	0.22	96,96,96,96	0
13	NAG	A	903	14/15	0.86	0.17	129,130,130,130	0
12	CL	B	902	1/1	0.93	0.85	110,110,110,110	0
11	ZN	B	901	1/1	0.93	0.21	108,108,108,108	0
11	ZN	A	901	1/1	0.95	0.17	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.