



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2022 – 02:17 PM EDT

PDB ID : 7U0L  
Title : Crystal structure of the CCoV-HuPn-2018 RBD (domain B) in complex with canine APN  
Authors : Tortorici, M.A.; Veessler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2022-02-18  
Resolution : 3.30 Å(reported)

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

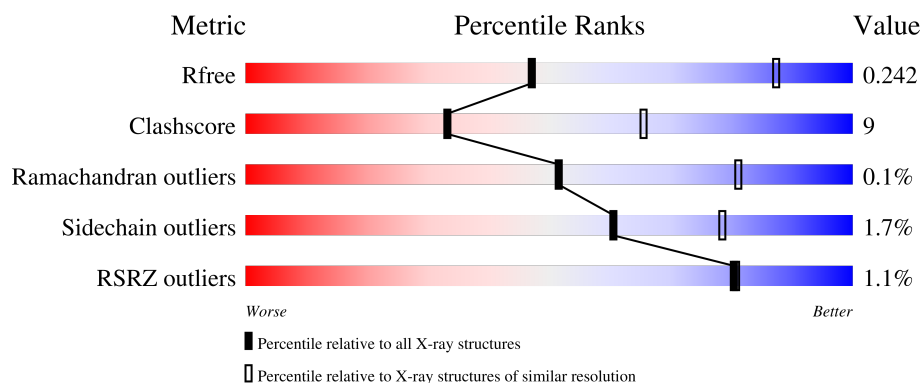
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	908	<div> <div>82%</div> <div>17%</div> </div>
2	B	182	<div> <div>6%</div> <div>66%</div> <div>13%</div> <div>•</div> <div>19%</div> </div>
3	C	4	<div> <div>75%</div> <div>25%</div> </div>
4	D	5	<div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
4	L	5	<div> <div>40%</div> <div>60%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	6	
6	F	3	
6	I	3	
7	G	2	
7	K	2	
8	H	6	
9	J	5	
9	M	5	

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
4	MAN	L	5	-	-	-	X
7	NAG	G	2	-	-	-	X
9	MAN	M	4	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8925 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7187	4603	1197	1364	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	THR	-	expression tag	UNP P79143
A	974	GLY	-	expression tag	UNP P79143
A	975	GLY	-	expression tag	UNP P79143
A	976	SER	-	expression tag	UNP P79143

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	0	0	0
			1075	676	181	210	8			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	522	THR	-	expression tag	UNP A0A8E6CMP0
B	672	GLY	-	insertion	UNP A0A8E6CMP0
B	673	SER	-	insertion	UNP A0A8E6CMP0
B	674	SER	-	insertion	UNP A0A8E6CMP0
B	675	GLY	-	insertion	UNP A0A8E6CMP0
B	676	GLY	-	insertion	UNP A0A8E6CMP0
B	680	ASN	HIS	conflict	UNP A0A8E6CMP0
B	682	ILE	LEU	conflict	UNP A0A8E6CMP0
B	683	PHE	-	expression tag	UNP A0A8E6CMP0
B	684	GLU	-	expression tag	UNP A0A8E6CMP0
B	685	ALA	-	expression tag	UNP A0A8E6CMP0
B	686	GLN	-	expression tag	UNP A0A8E6CMP0

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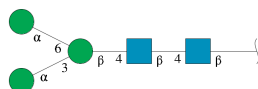
Chain	Residue	Modelled	Actual	Comment	Reference
B	687	LYS	-	expression tag	UNP A0A8E6CMP0
B	688	ILE	-	expression tag	UNP A0A8E6CMP0
B	689	GLU	-	expression tag	UNP A0A8E6CMP0
B	690	TRP	-	expression tag	UNP A0A8E6CMP0
B	691	HIS	-	expression tag	UNP A0A8E6CMP0
B	692	GLU	-	expression tag	UNP A0A8E6CMP0
B	693	GLY	-	expression tag	UNP A0A8E6CMP0
B	694	GLY	-	expression tag	UNP A0A8E6CMP0
B	695	SER	-	expression tag	UNP A0A8E6CMP0
B	696	HIS	-	expression tag	UNP A0A8E6CMP0
B	697	HIS	-	expression tag	UNP A0A8E6CMP0
B	698	HIS	-	expression tag	UNP A0A8E6CMP0
B	699	HIS	-	expression tag	UNP A0A8E6CMP0
B	700	HIS	-	expression tag	UNP A0A8E6CMP0
B	701	HIS	-	expression tag	UNP A0A8E6CMP0
B	702	HIS	-	expression tag	UNP A0A8E6CMP0
B	703	HIS	-	expression tag	UNP A0A8E6CMP0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-galactopyranose-(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	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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.



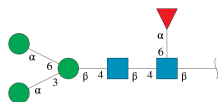
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

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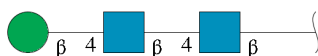
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 6 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.



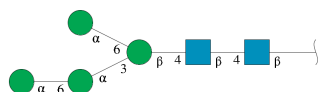
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



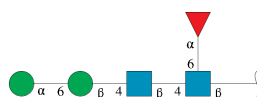
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called 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
8	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	5	Total	C	N	O	0	0	0
			60	34	2	24			
9	M	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Zn	1	0
			1	1		

- Molecule 11 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
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

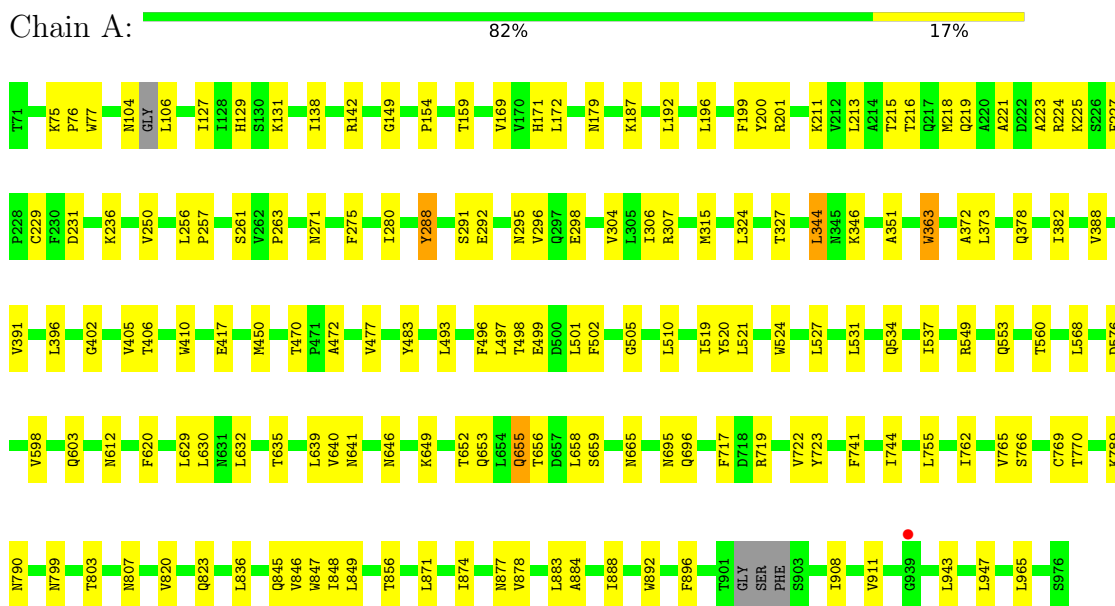
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	65	Total	O	0	0
			65	65		



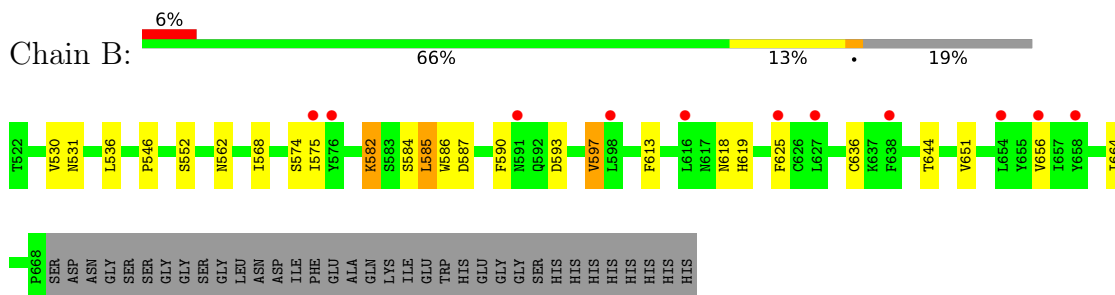
### 3 Residue-property plots

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.

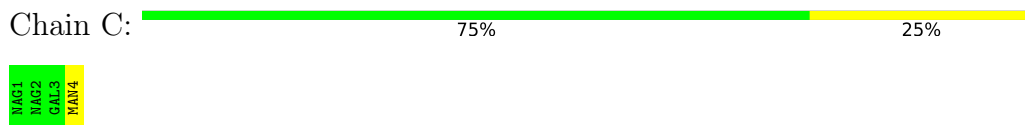
#### • Molecule 1: Aminopeptidase N



#### • Molecule 2: Spike glycoprotein

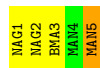


#### • Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:  20% 60% 20%



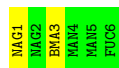
● Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  40% 60%



● Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



● Molecule 6: 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%



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

Chain I:  33% 67%



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

Chain G:  100%



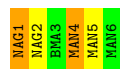
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%




- Molecule 8: 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 H:  33% 33% 33%



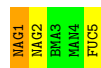
- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  80% 20%



- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  40% 40% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.43Å 107.33Å 239.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 3.30 48.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-3.30) 100.0 (48.96-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.215 , 0.240 0.216 , 0.242	Depositor DCC
$R_{free}$ test set	2198 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/7377	0.65	0/10081
2	B	0.60	0/1097	0.69	0/1503
All	All	0.54	0/8474	0.66	0/11584

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	655	GLN	Mainchain

### 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	7187	0	6884	118	1
2	B	1075	0	974	25	0
3	C	50	0	43	0	0
4	D	61	0	52	1	0
4	L	61	0	52	0	0
5	E	71	0	61	0	0
6	F	39	0	34	2	0
6	I	39	0	34	6	0
7	G	28	0	25	0	0
7	K	28	0	25	0	0
8	H	72	0	61	3	0
9	J	60	0	52	0	0
9	M	60	0	52	1	0
10	A	1	0	0	0	0
11	A	28	0	26	0	0
12	A	65	0	0	1	0
All	All	8925	0	8375	148	1

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 9.

The worst 5 of 148 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:A:211:LYS:HD3	1:A:292:GLU:OE2	1.28	1.32
1:A:450:MET:HE1	1:A:639:LEU:HD12	1.42	1.02
1:A:211:LYS:CD	1:A:292:GLU:OE2	2.11	0.99
2:B:575:ILE:CG2	2:B:613:PHE:CZ	2.51	0.93
1:A:450:MET:HE1	1:A:639:LEU:CD1	2.01	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:ND2	1:A:612:ASN:ND2[3_554]	2.17	0.03

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	898/908 (99%)	866 (96%)	32 (4%)	0	100	100
2	B	145/182 (80%)	137 (94%)	7 (5%)	1 (1%)	22	54
All	All	1043/1090 (96%)	1003 (96%)	39 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	585	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	781/808 (97%)	771 (99%)	10 (1%)	69	82
2	B	114/161 (71%)	109 (96%)	5 (4%)	28	59
All	All	895/969 (92%)	880 (98%)	15 (2%)	60	78

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	896	PHE
2	B	593	ASP
1	A	943	LEU
2	B	597	VAL
2	B	582	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	823	GLN
1	A	858	ASN
2	B	562	ASN
1	A	877	ASN
1	A	297	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 ⓘ

46 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	C	1	1,3	14,14,15	0.35	0	17,19,21	0.61	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.63	0
3	GAL	C	3	3	11,11,12	0.29	0	15,15,17	0.67	0
3	MAN	C	4	3	11,11,12	0.22	0	15,15,17	0.66	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
4	BMA	D	3	4	11,11,12	0.24	0	15,15,17	0.62	0
4	MAN	D	4	4	11,11,12	0.22	0	15,15,17	0.62	0
4	MAN	D	5	4	11,11,12	0.19	0	15,15,17	1.02	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	0.72	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	E	3	5	11,11,12	0.29	0	15,15,17	1.18	2 (13%)
5	MAN	E	4	5	11,11,12	0.30	0	15,15,17	0.63	0
5	MAN	E	5	5	11,11,12	0.23	0	15,15,17	0.65	0
5	FUC	E	6	5	10,10,11	0.30	0	14,14,16	0.61	0
6	NAG	F	1	1,6	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
6	NAG	F	2	6	14,14,15	0.44	0	17,19,21	0.84	1 (5%)
6	BMA	F	3	6	11,11,12	0.24	0	15,15,17	0.57	0
7	NAG	G	1	1,7	14,14,15	0.40	0	17,19,21	0.61	0
7	NAG	G	2	7	14,14,15	0.39	0	17,19,21	0.72	0
8	NAG	H	1	1,8	14,14,15	0.44	0	17,19,21	0.96	2 (11%)
8	NAG	H	2	8	14,14,15	0.44	0	17,19,21	0.88	0
8	BMA	H	3	8	11,11,12	0.35	0	15,15,17	0.93	0
8	MAN	H	4	8	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
8	MAN	H	5	8	11,11,12	0.23	0	15,15,17	0.63	0
8	MAN	H	6	8	11,11,12	0.26	0	15,15,17	0.57	0
6	NAG	I	1	1,6	14,14,15	0.35	0	17,19,21	2.03	3 (17%)
6	NAG	I	2	6	14,14,15	0.37	0	17,19,21	1.15	1 (5%)
6	BMA	I	3	6	11,11,12	0.59	0	15,15,17	1.09	1 (6%)
9	NAG	J	1	1,9	14,14,15	0.35	0	17,19,21	0.62	0
9	NAG	J	2	9	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
9	BMA	J	3	9	11,11,12	0.27	0	15,15,17	0.65	0
9	MAN	J	4	9	11,11,12	0.21	0	15,15,17	0.64	0
9	FUC	J	5	9	10,10,11	0.28	0	14,14,16	0.56	0
7	NAG	K	1	1,7	14,14,15	0.46	0	17,19,21	1.02	2 (11%)
7	NAG	K	2	7	14,14,15	0.30	0	17,19,21	0.74	0
4	NAG	L	1	2,4	14,14,15	0.68	0	17,19,21	1.45	2 (11%)
4	NAG	L	2	4	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
4	BMA	L	3	4	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
4	MAN	L	4	4	11,11,12	0.24	0	15,15,17	0.73	0
4	MAN	L	5	4	11,11,12	0.27	0	15,15,17	0.79	0
9	NAG	M	1	2,9	14,14,15	0.84	1 (7%)	17,19,21	0.82	1 (5%)
9	NAG	M	2	9	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
9	BMA	M	3	9	11,11,12	0.29	0	15,15,17	0.54	0
9	MAN	M	4	9	11,11,12	0.22	0	15,15,17	0.66	0
9	FUC	M	5	9	10,10,11	0.66	0	14,14,16	0.88	1 (7%)

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	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	GAL	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	FUC	E	6	5	-	-	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
7	NAG	G	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
8	NAG	H	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	H	2	8	-	0/6/23/26	0/1/1/1
8	BMA	H	3	8	-	0/2/19/22	0/1/1/1
8	MAN	H	4	8	-	2/2/19/22	0/1/1/1
8	MAN	H	5	8	-	0/2/19/22	0/1/1/1
8	MAN	H	6	8	-	0/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
9	NAG	J	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	0/1/1/1
9	FUC	J	5	9	-	-	0/1/1/1
7	NAG	K	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
4	NAG	L	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	L	5	4	-	0/2/19/22	0/1/1/1
9	NAG	M	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	M	2	9	-	3/6/23/26	0/1/1/1
9	BMA	M	3	9	-	1/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	FUC	M	5	9	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1	NAG	C1-C2	2.37	1.55	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C2-N2-C7	-6.26	113.99	122.90
6	I	1	NAG	C4-C3-C2	-4.44	104.51	111.02
4	L	1	NAG	O5-C5-C4	-3.24	102.93	110.83
6	I	2	NAG	C4-C3-C2	-3.07	106.52	111.02
4	L	1	NAG	C1-O5-C5	-2.98	108.16	112.19

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 13 short contacts:

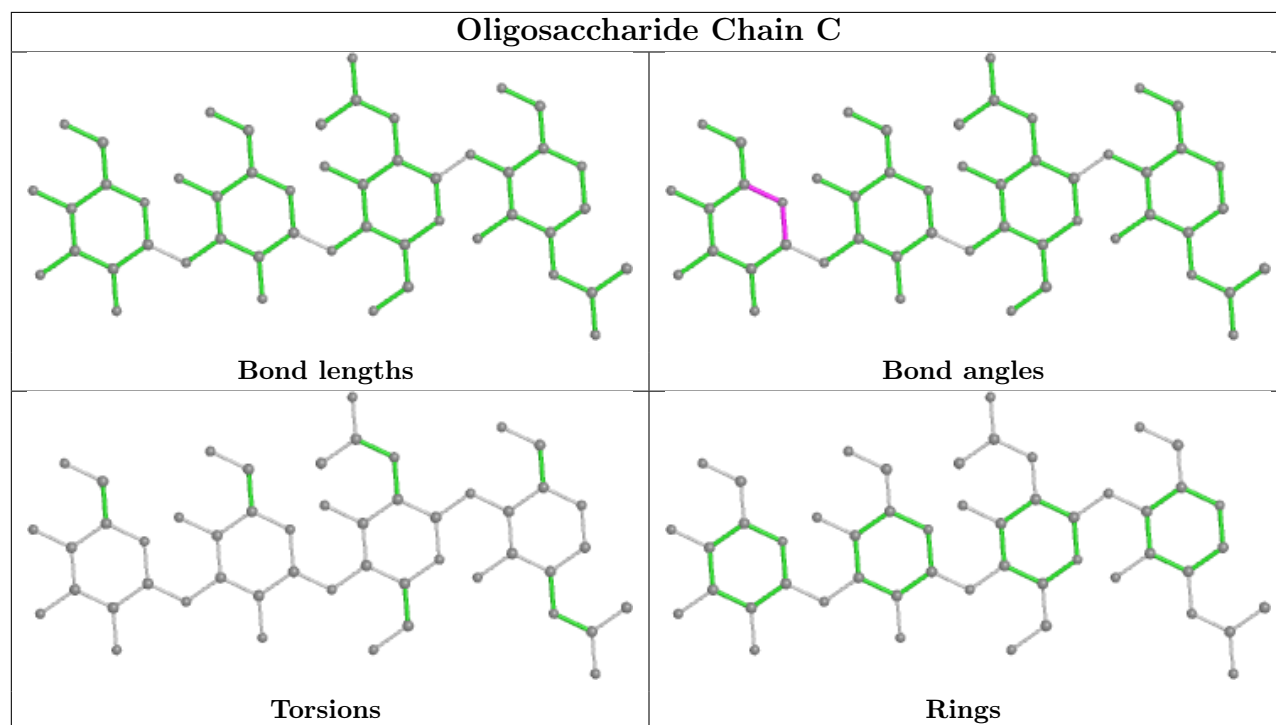
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	5	MAN	2	0
6	I	1	NAG	5	0
6	F	1	NAG	2	0
4	D	5	MAN	1	0
6	I	2	NAG	2	0

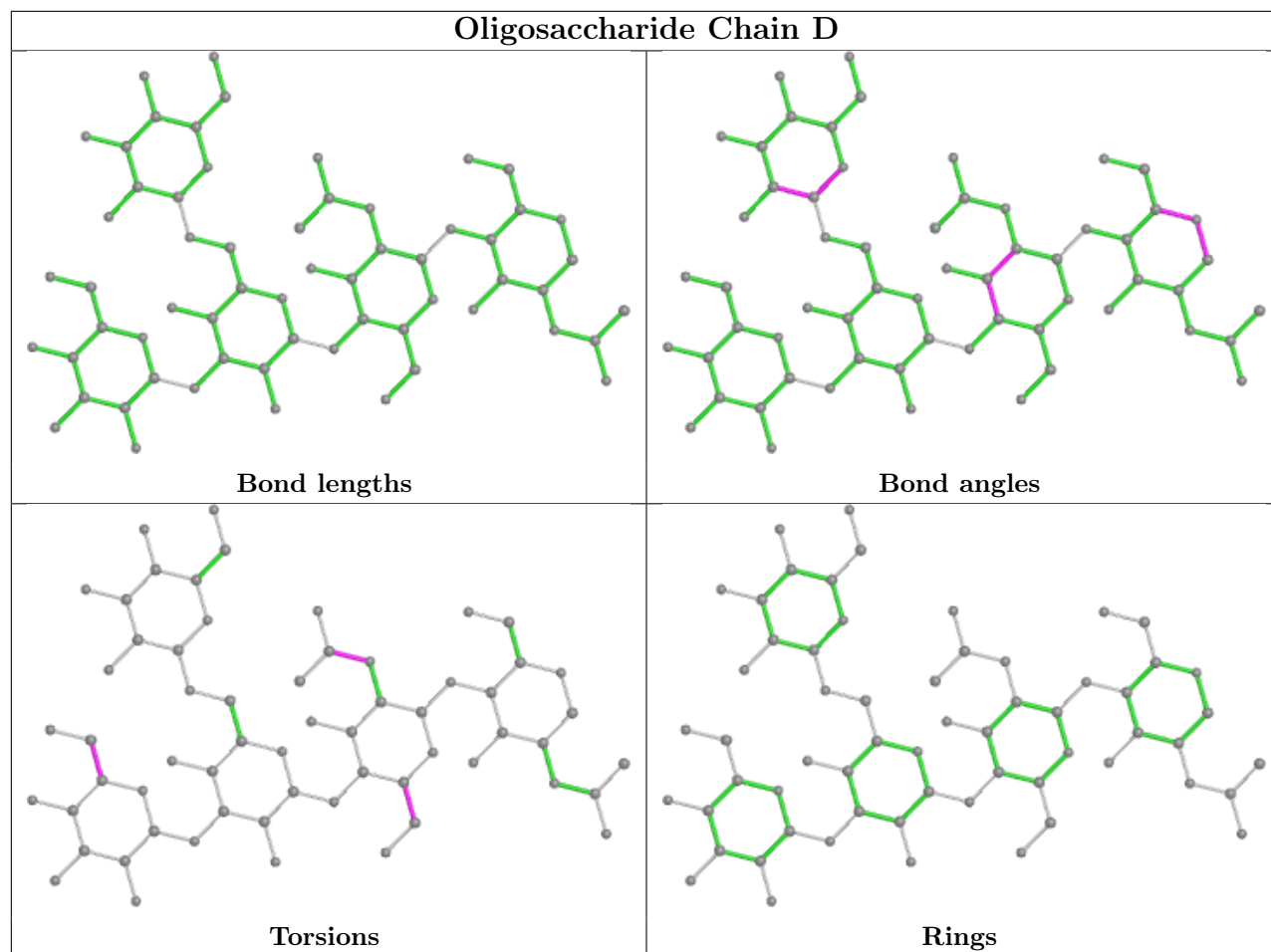
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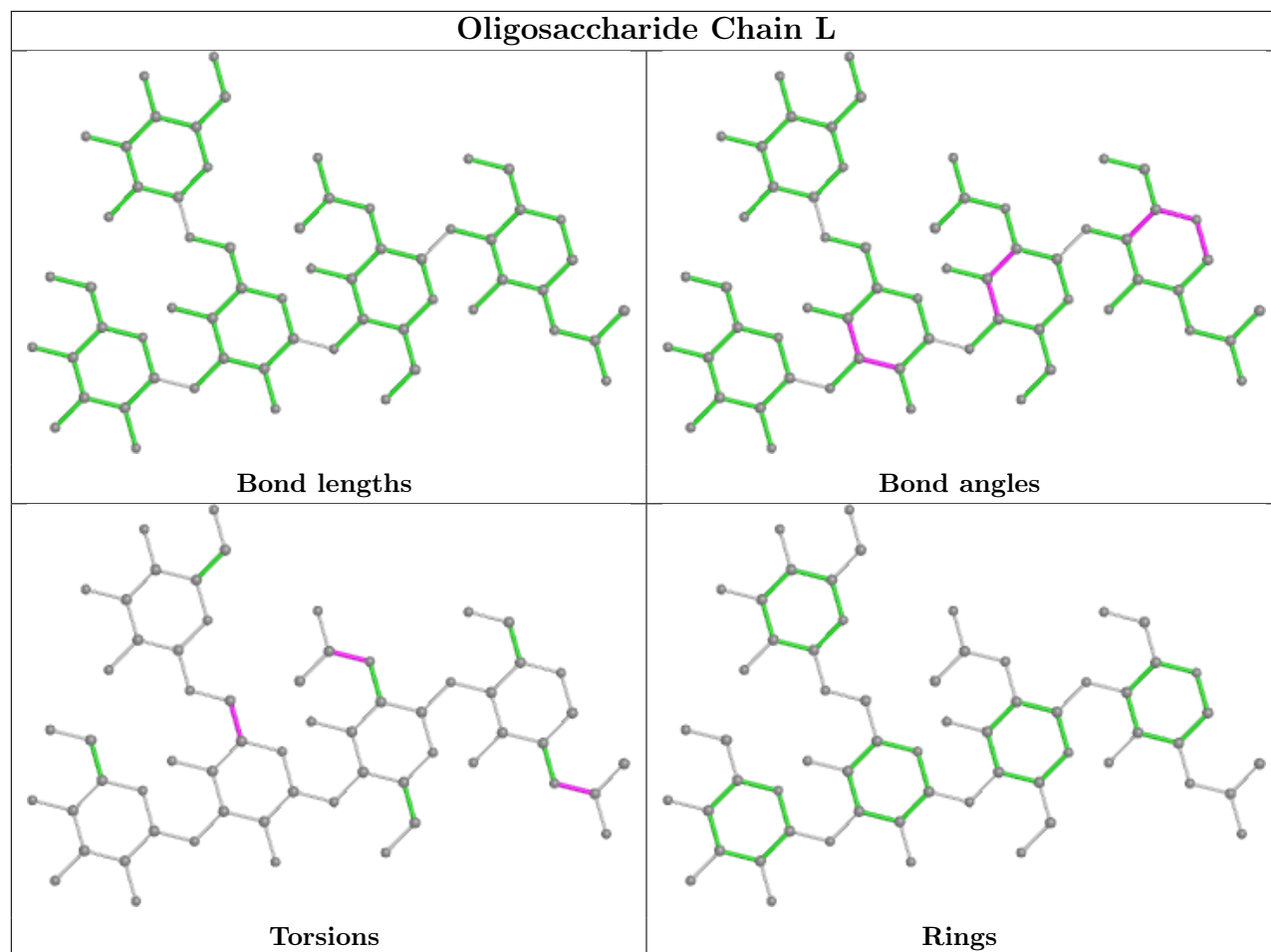
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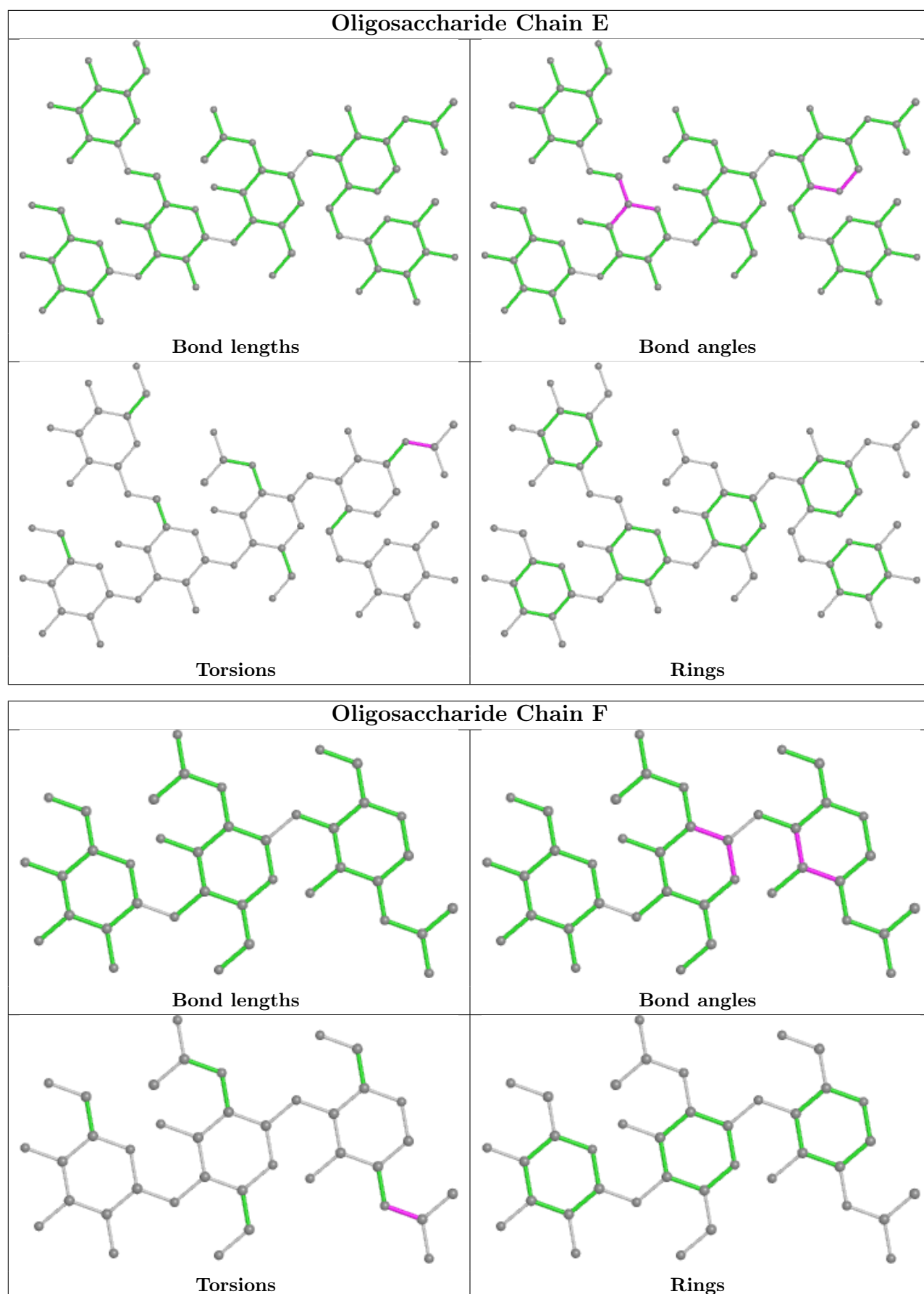
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	1	NAG	1	0
8	H	2	NAG	1	0
8	H	4	MAN	1	0
6	F	2	NAG	1	0
4	D	3	BMA	1	0
9	M	1	NAG	1	0

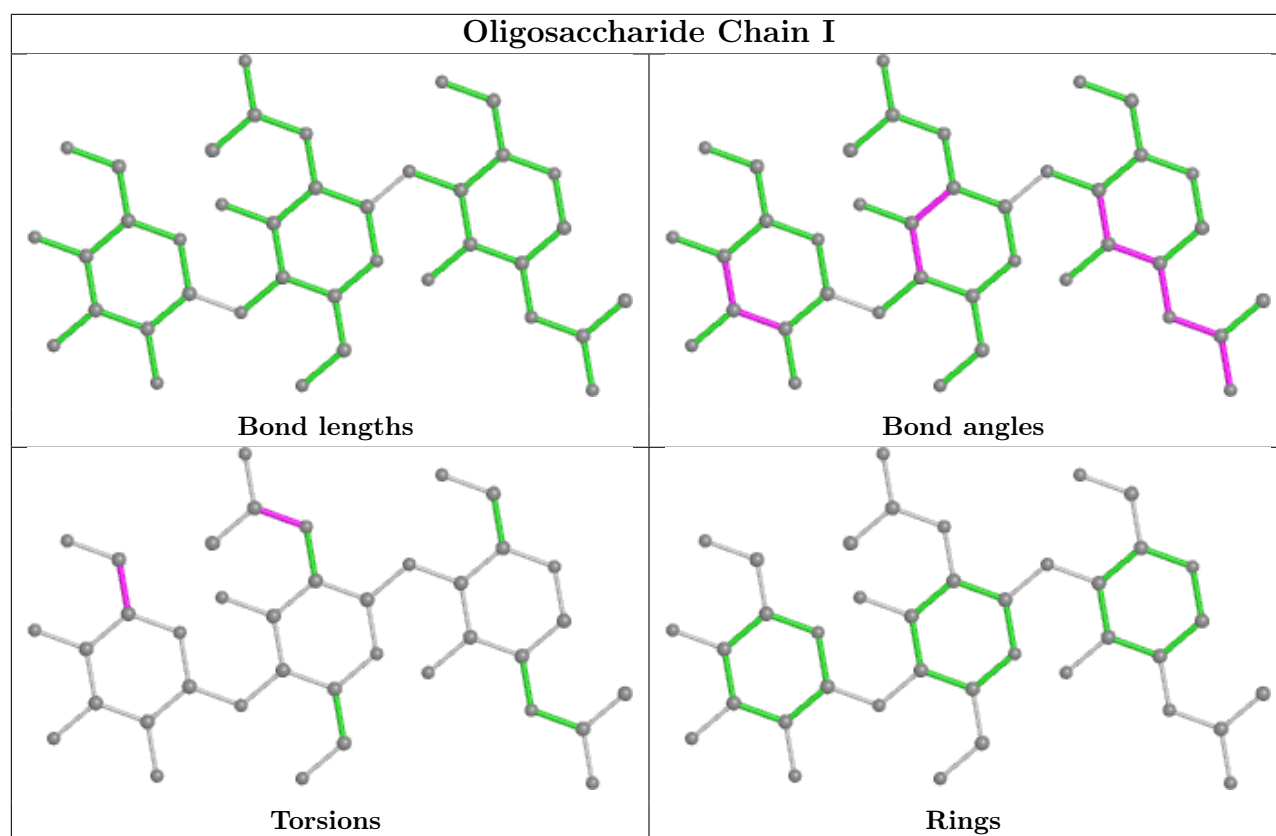
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



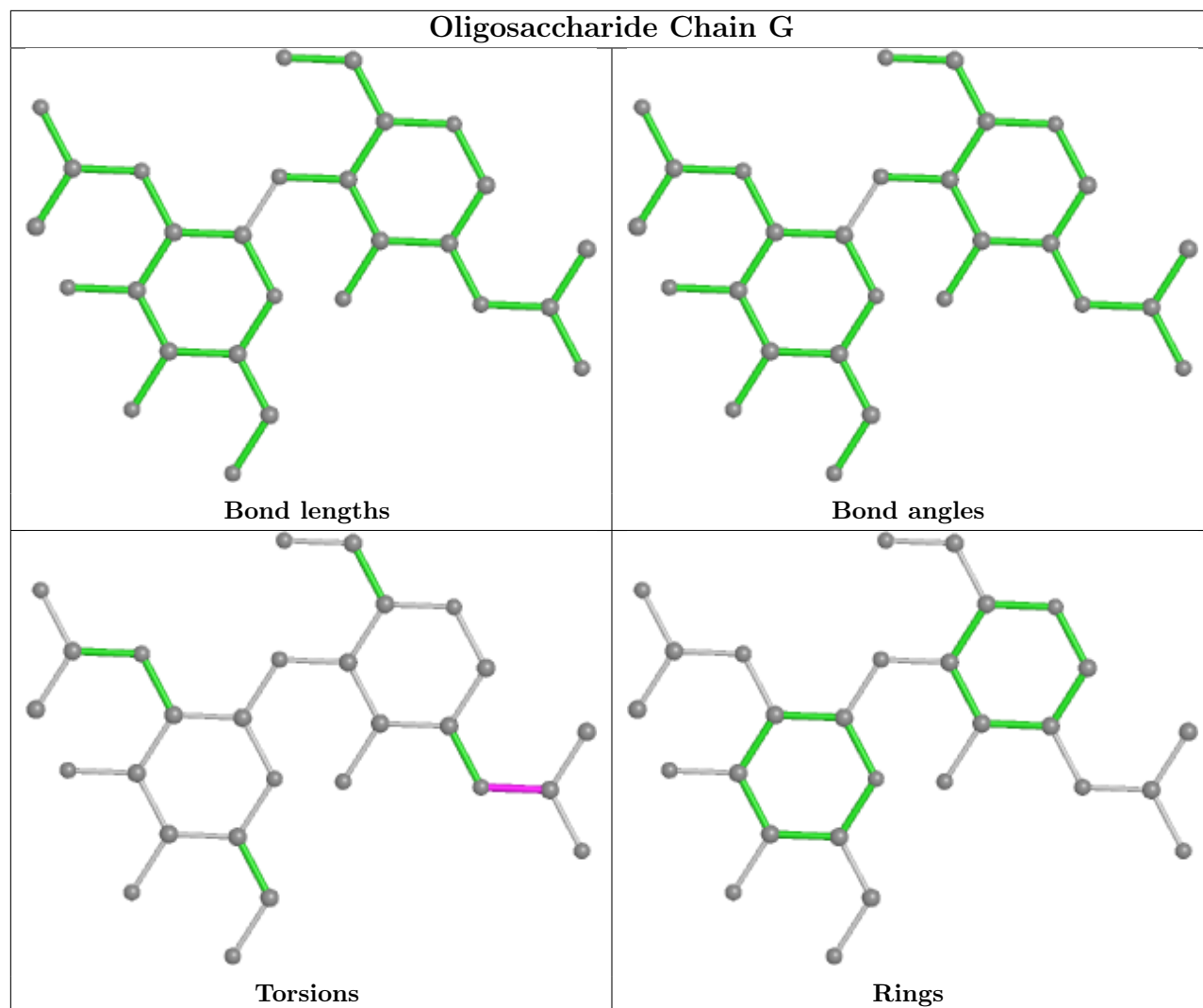


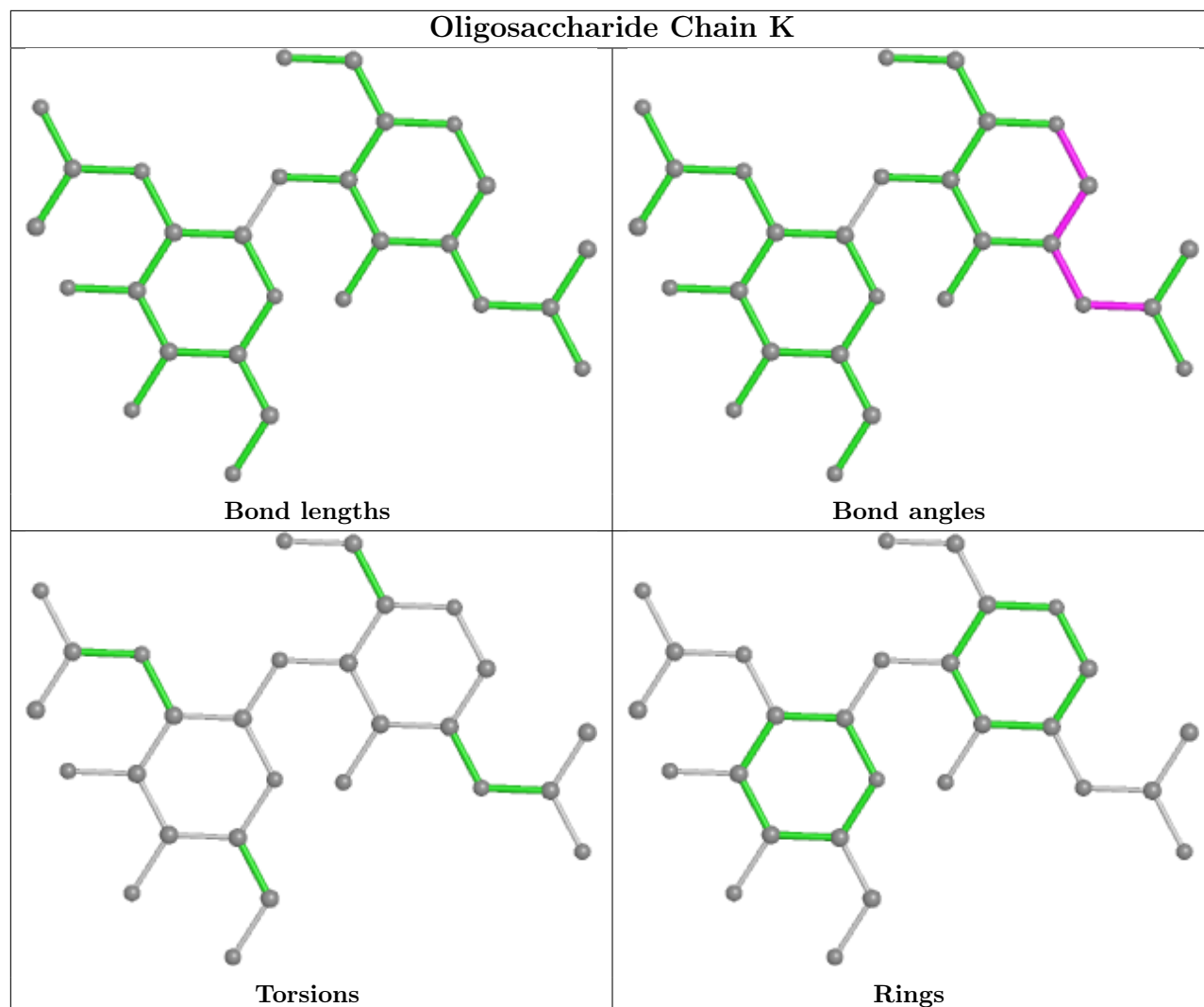




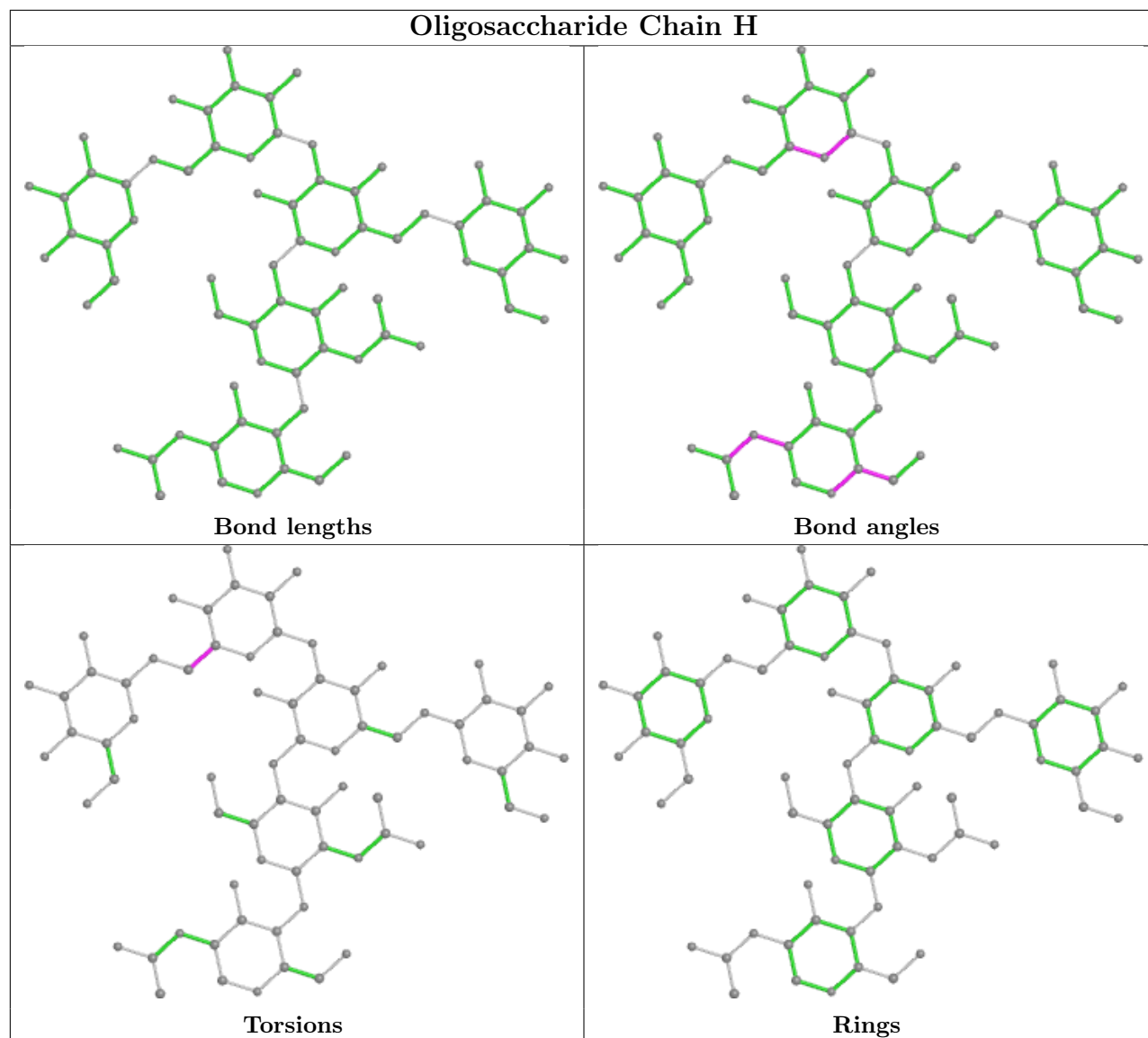


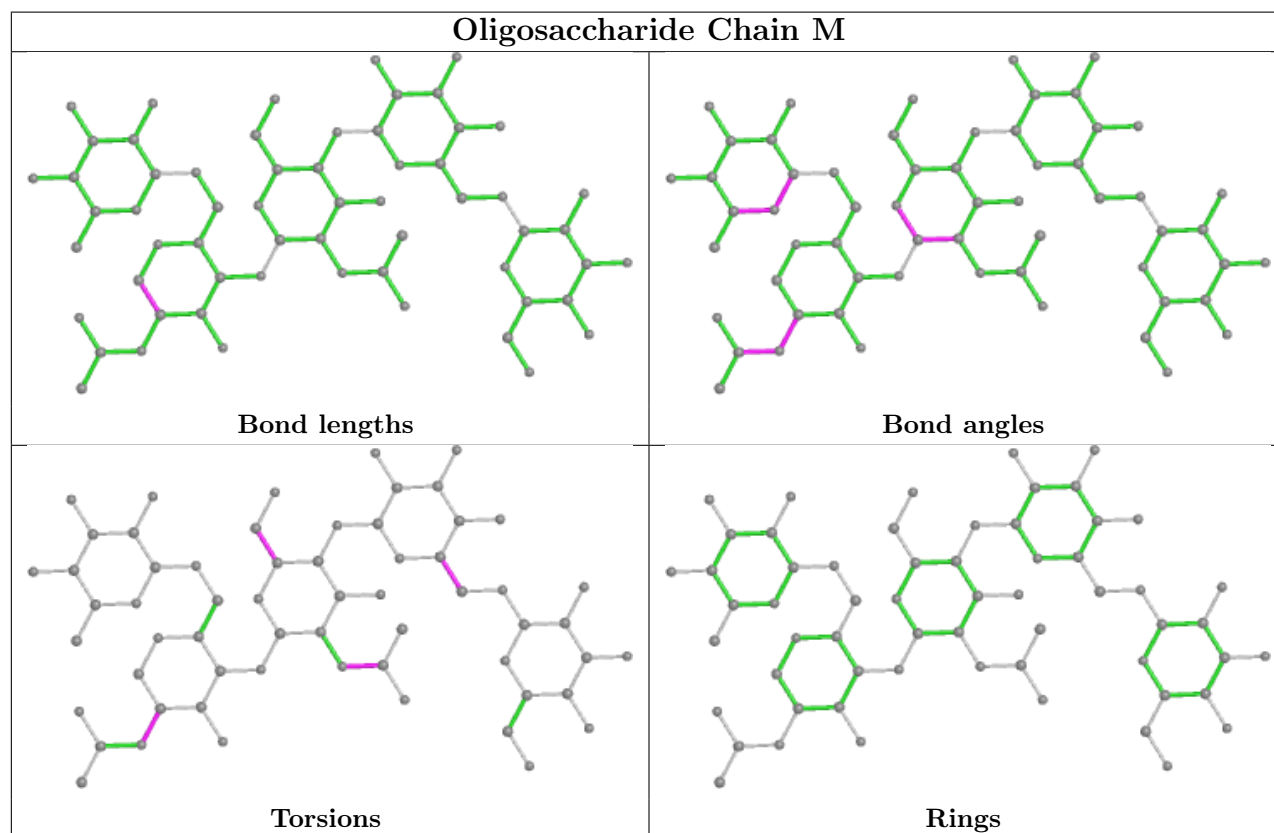
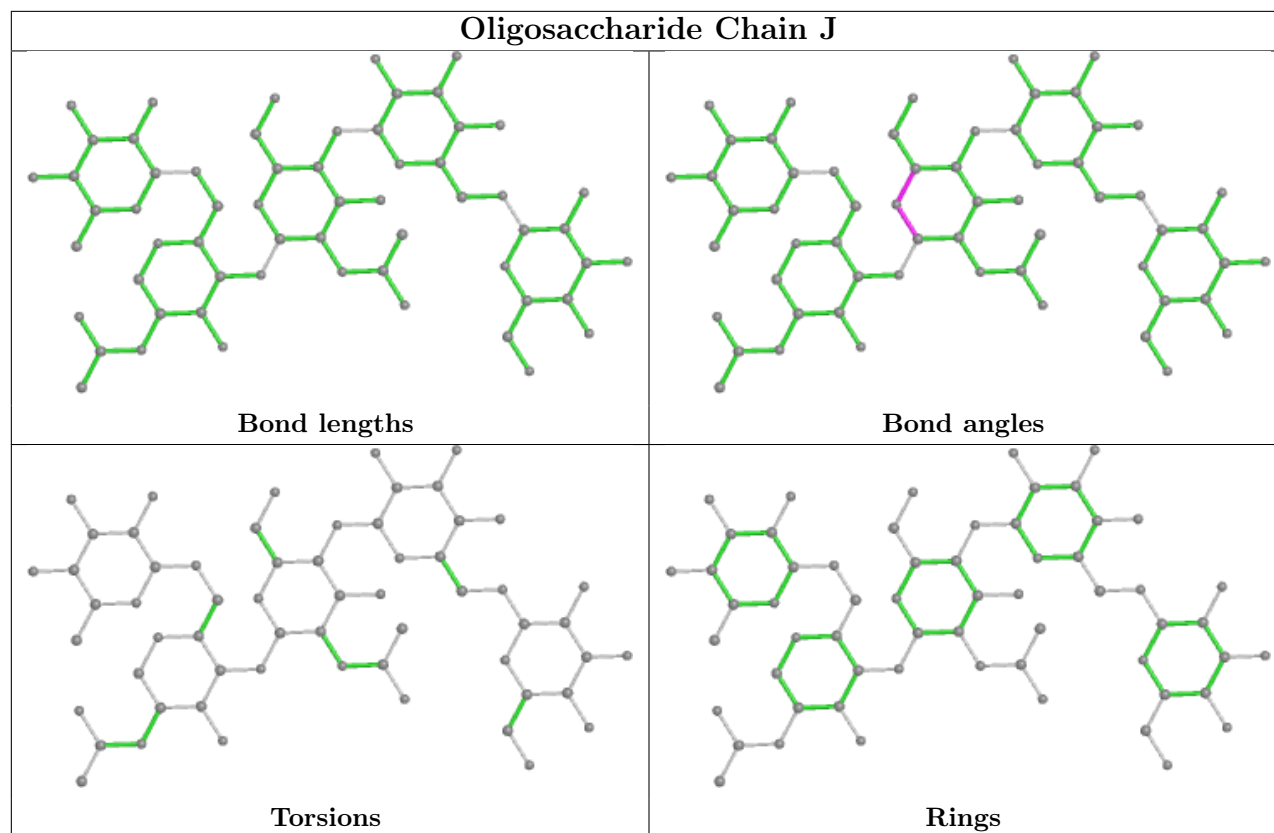






## Oligosaccharide Chain H





## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
11	NAG	A	1003	1	14,14,15	0.28	0	17,19,21	0.63	0
11	NAG	A	1002	1	14,14,15	0.27	0	17,19,21	0.69	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
11	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
11	NAG	A	1002	1	-	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.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1002	NAG	C8-C7-N2-C2
11	A	1002	NAG	O7-C7-N2-C2

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 ⓘ

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	904/908 (99%)	-0.24	1 (0%) 95 97	38, 60, 104, 153	0
2	B	147/182 (80%)	0.54	11 (7%) 14 13	64, 97, 127, 159	0
All	All	1051/1090 (96%)	-0.13	12 (1%) 80 81	38, 63, 114, 159	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	939	GLY	3.1
2	B	654	LEU	2.8
2	B	576	TYR	2.8
2	B	616	LEU	2.6
2	B	591	ASN	2.4

### 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
4	MAN	D	5	11/12	0.52	0.32	130,147,165,166	0
9	BMA	M	3	11/12	0.54	0.35	125,155,178,180	0
6	BMA	I	3	11/12	0.55	0.30	95,153,160,164	0
3	GAL	C	3	11/12	0.63	0.26	133,143,163,169	0
5	BMA	E	3	11/12	0.64	0.25	108,139,152,159	0

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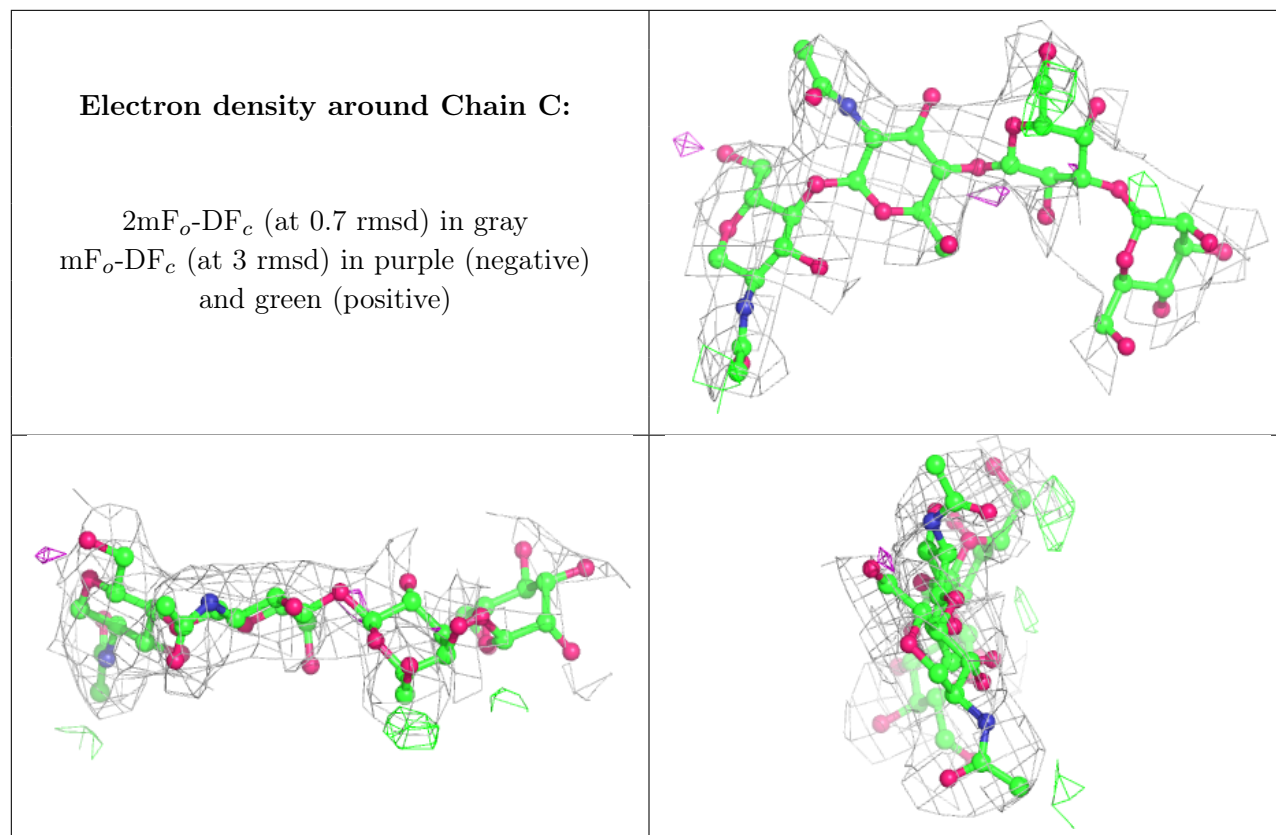
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	D	3	11/12	0.65	0.28	153,161,168,180	0
5	MAN	E	4	11/12	0.66	0.35	99,157,170,170	0
9	MAN	J	4	11/12	0.68	0.36	95,127,138,140	0
5	MAN	E	5	11/12	0.68	0.26	90,126,143,145	0
9	MAN	M	4	11/12	0.68	0.42	135,152,175,179	0
4	MAN	D	4	11/12	0.69	0.34	133,163,171,173	0
4	BMA	L	3	11/12	0.69	0.30	152,158,166,166	0
8	MAN	H	6	11/12	0.69	0.22	94,135,149,154	0
7	NAG	G	2	14/15	0.70	0.45	126,146,158,161	0
3	MAN	C	4	11/12	0.71	0.17	110,142,159,165	0
8	MAN	H	4	11/12	0.73	0.26	135,149,162,162	0
9	BMA	J	3	11/12	0.75	0.20	87,109,119,127	0
8	MAN	H	5	11/12	0.75	0.31	76,130,140,146	0
4	NAG	L	1	14/15	0.76	0.24	79,104,126,144	0
4	MAN	L	4	11/12	0.76	0.25	94,139,153,161	0
4	MAN	L	5	11/12	0.76	0.62	151,181,190,198	0
4	NAG	L	2	14/15	0.78	0.34	119,136,149,158	0
6	BMA	F	3	11/12	0.79	0.39	120,148,157,159	0
7	NAG	K	2	14/15	0.80	0.35	108,145,153,157	0
6	NAG	I	2	14/15	0.80	0.32	126,143,153,153	0
9	FUC	M	5	10/11	0.81	0.77	137,153,157,160	0
6	NAG	F	2	14/15	0.84	0.35	110,142,154,164	0
7	NAG	G	1	14/15	0.84	0.31	86,115,145,147	0
9	NAG	M	1	14/15	0.85	0.34	117,137,142,144	0
6	NAG	I	1	14/15	0.85	0.21	63,93,118,131	0
4	NAG	D	2	14/15	0.86	0.20	91,112,152,159	0
8	BMA	H	3	11/12	0.86	0.18	126,130,137,142	0
9	NAG	M	2	14/15	0.86	0.32	107,138,157,175	0
5	FUC	E	6	10/11	0.88	0.27	75,88,95,97	0
8	NAG	H	2	14/15	0.89	0.18	69,84,116,139	0
5	NAG	E	2	14/15	0.89	0.21	86,107,123,139	0
7	NAG	K	1	14/15	0.89	0.20	67,98,119,130	0
6	NAG	F	1	14/15	0.89	0.26	102,122,135,145	0
3	NAG	C	2	14/15	0.90	0.25	84,102,133,148	0
9	NAG	J	2	14/15	0.91	0.20	64,78,97,101	0
5	NAG	E	1	14/15	0.92	0.21	71,79,89,102	0
9	FUC	J	5	10/11	0.93	0.42	87,97,104,113	0
3	NAG	C	1	14/15	0.93	0.17	46,68,85,87	0
9	NAG	J	1	14/15	0.94	0.17	57,64,73,91	0
4	NAG	D	1	14/15	0.95	0.16	56,65,90,94	0
8	NAG	H	1	14/15	0.97	0.12	43,50,66,68	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

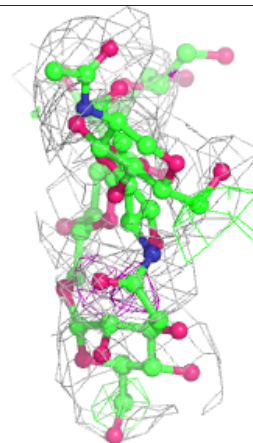
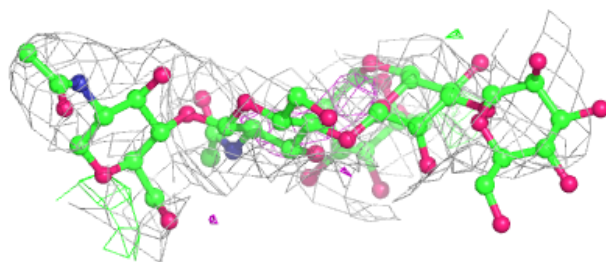
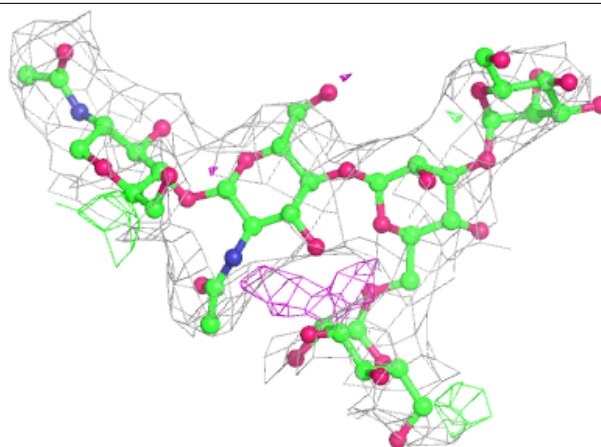


charide. Each fit is shown from different orientation to approximate a three-dimensional view.



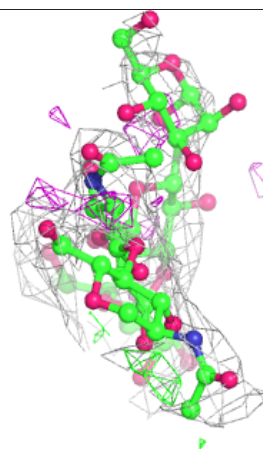
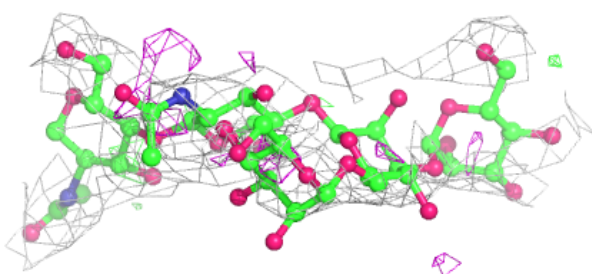
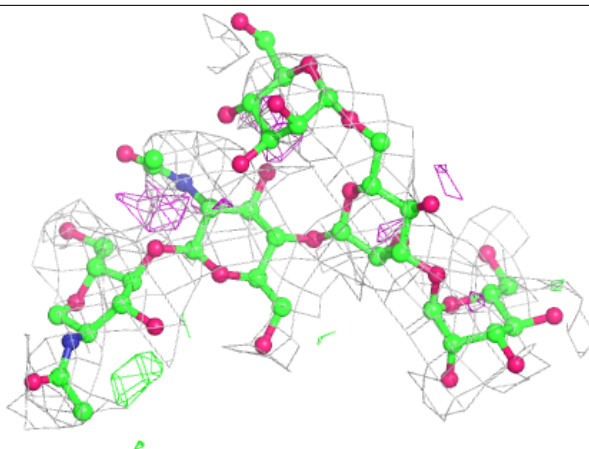
**Electron density around Chain D:**

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



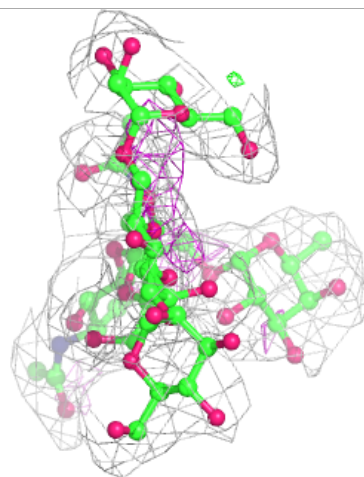
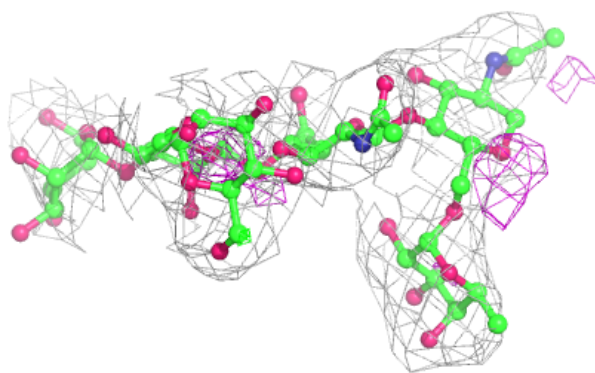
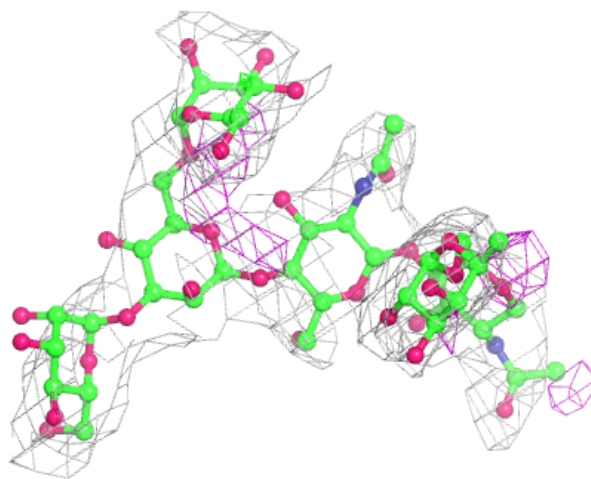
**Electron density around Chain L:**

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



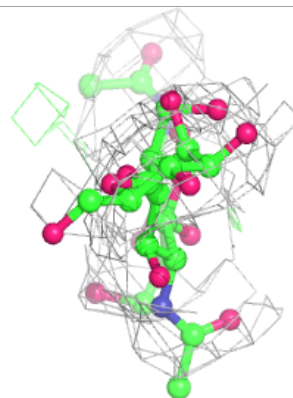
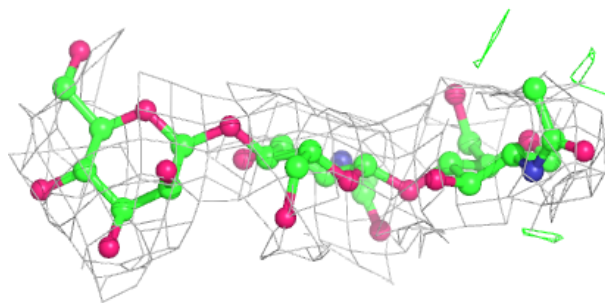
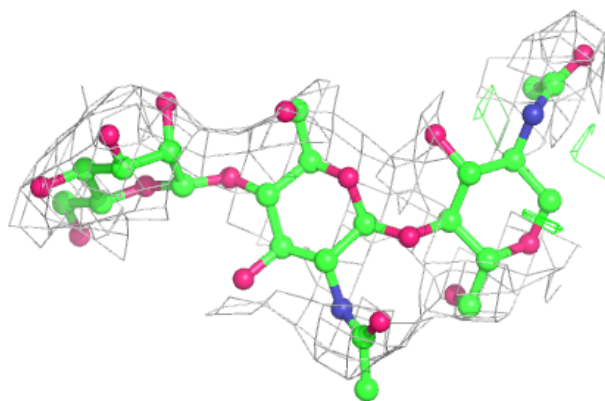
**Electron density around Chain E:**

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

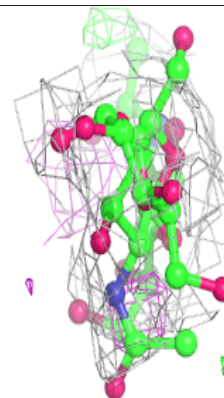
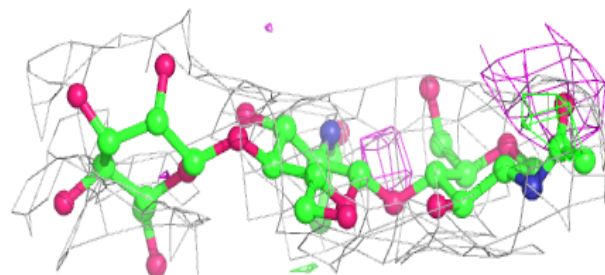
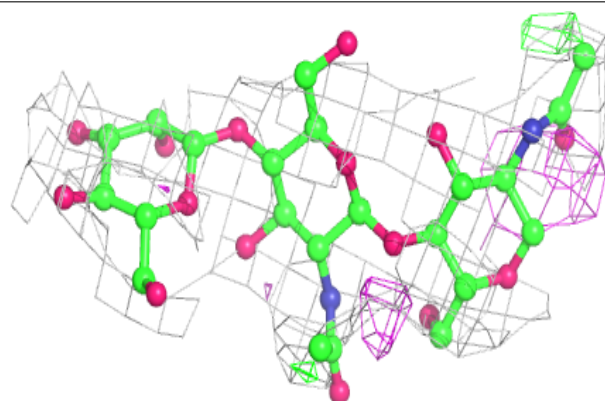


**Electron density around Chain F:**

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

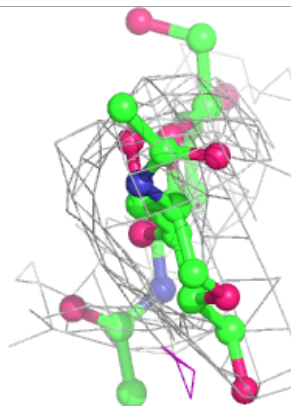
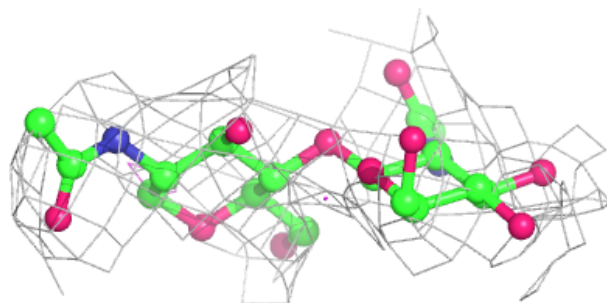
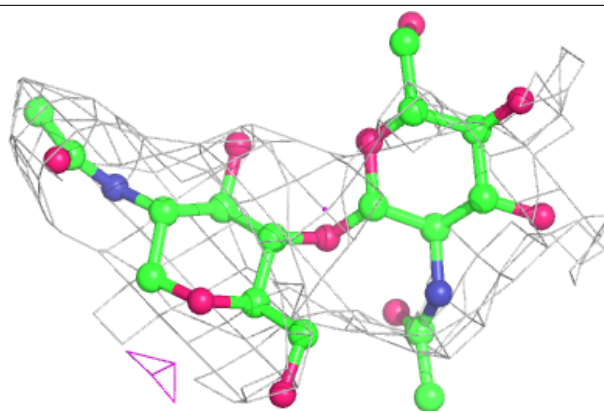
**Electron density around Chain I:**

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

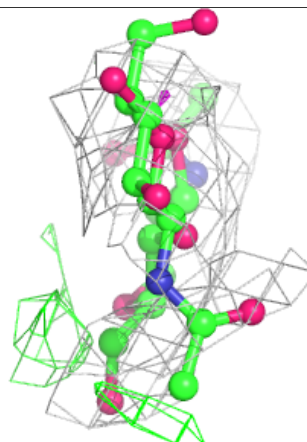
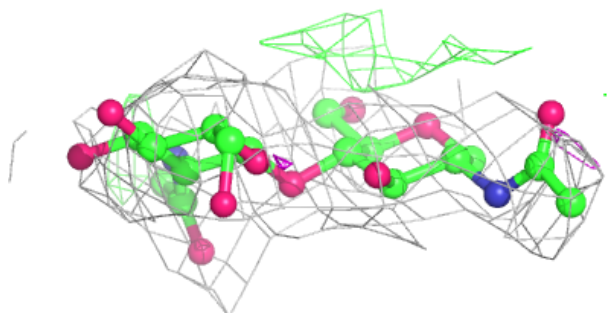
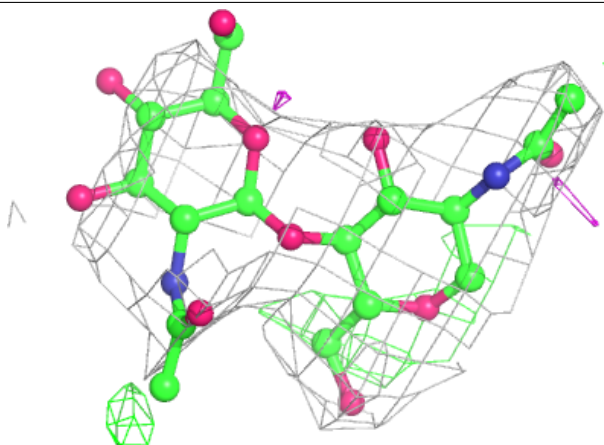


**Electron density around Chain G:**

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

**Electron density around Chain K:**

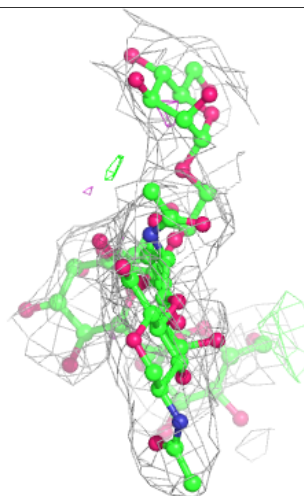
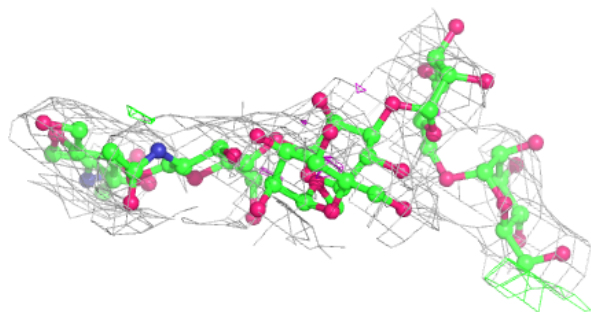
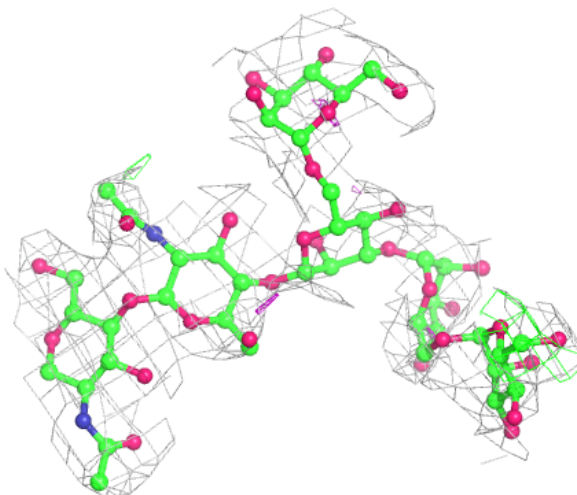
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





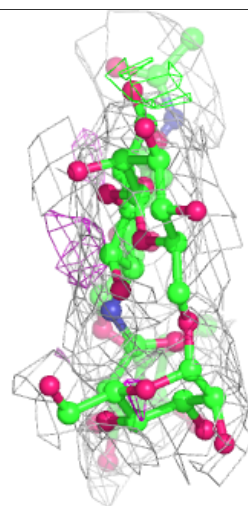
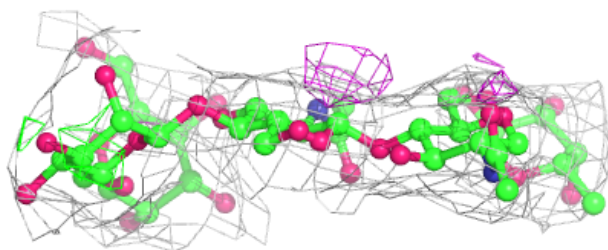
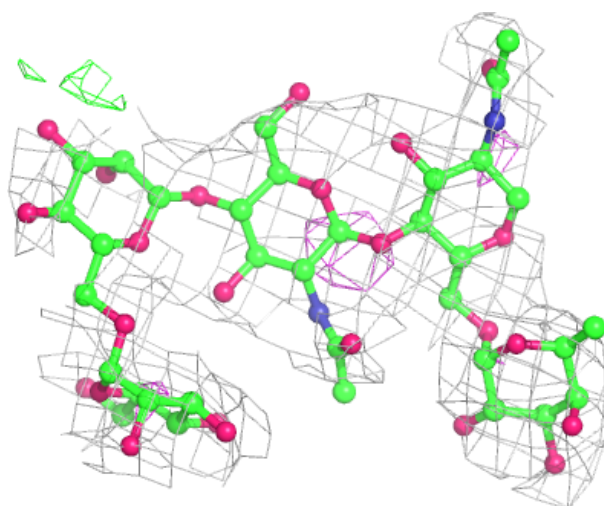
**Electron density around Chain H:**

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

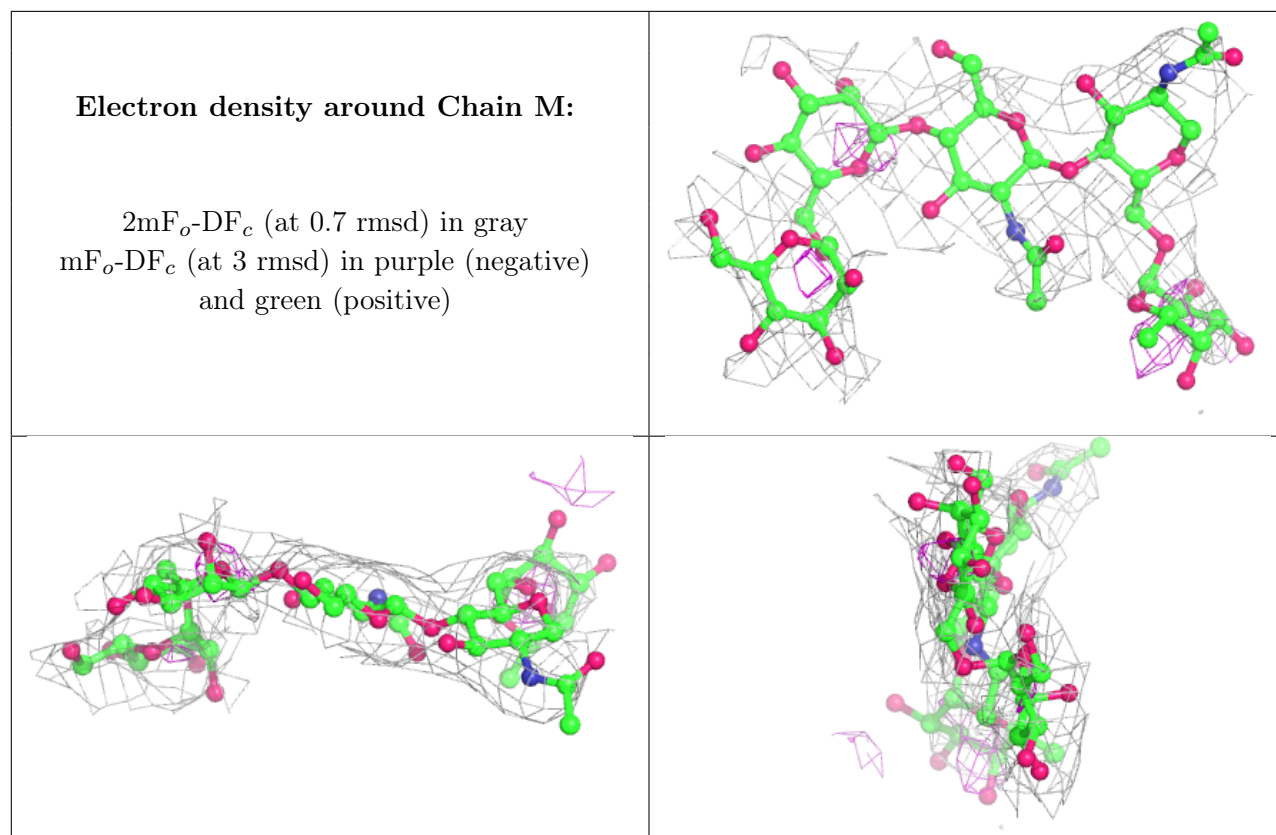


**Electron density around Chain J:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
11	NAG	A	1002	14/15	0.71	0.28	111,145,151,157	0
11	NAG	A	1003	14/15	0.75	0.28	81,125,137,143	0
10	ZN	A	1001	1/1	-	-	47,47,47,47	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.