



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:53 PM BST

PDB ID : 6MXU  
Title : Crystal structure of hemagglutinin from influenza virus A/Texas/1/1977 (H3N2)  
Authors : Dai, Y.N.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2018-10-31  
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

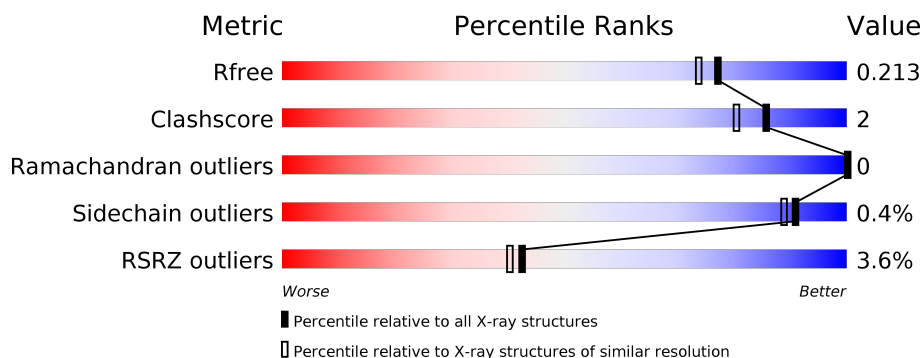
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	B	497	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	C	497	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	J	2	 50% 50%
2	K	2	 100%
2	M	2	 100%
3	G	3	 33% 67%
3	I	3	 33% 33% 33%
3	L	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	709	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13254 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3831	2392	673	748	18			
1	B	488	Total	C	N	O	S	0	0	0
			3848	2402	677	751	18			
1	C	488	Total	C	N	O	S	0	0	0
			3843	2399	677	749	18			

- Molecule 2 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
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

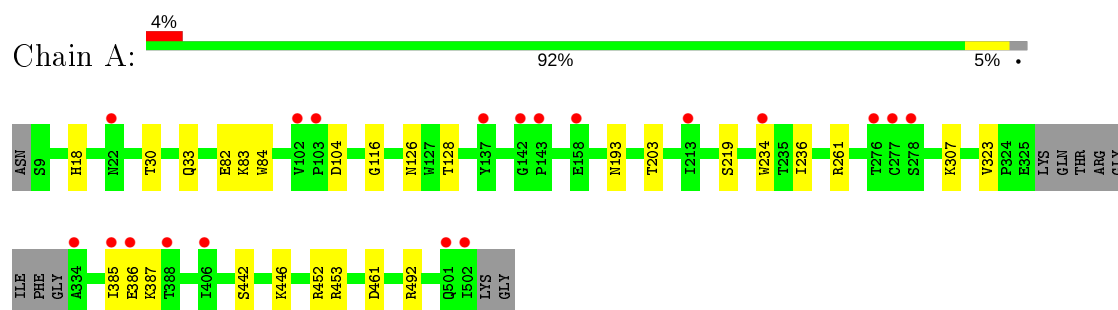
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	462	Total	O	0	0
			462	462		
5	B	466	Total	O	0	0
			466	466		
5	C	393	Total	O	0	0
			393	393		

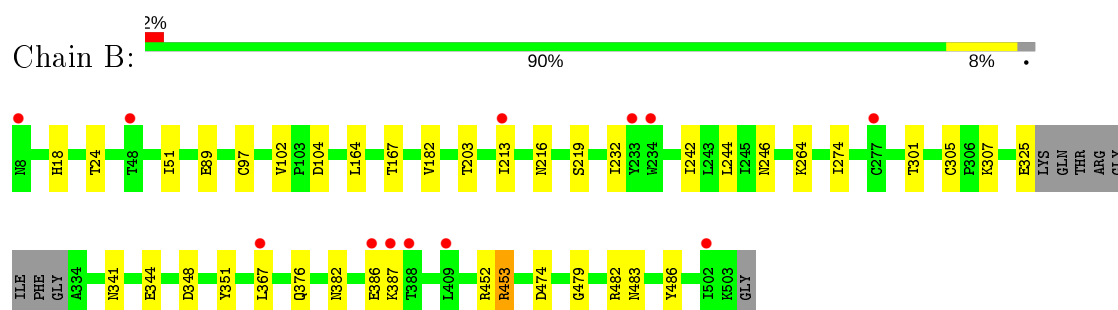
### 3 Residue-property plots [i](#)

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.

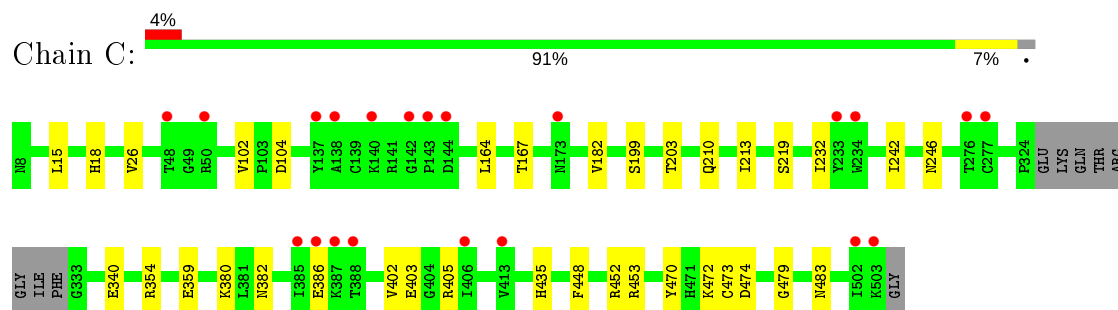
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



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



MAG1  
MAG2

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

Chain E: 

MAG1  
MAG2

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

Chain F: 

MAG1  
MAG2

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

Chain H: 

MAG1  
MAG2

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

Chain J: 

MAG1  
MAG2

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

Chain K: 

MAG1  
MAG2

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

Chain M: 

MAG1  
MAG2

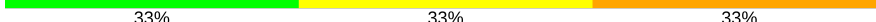


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.89Å 186.24Å 106.96Å 90.00° 110.09° 90.00°	Depositor
Resolution (Å)	46.37 – 1.85 48.55 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.37-1.85) 99.4 (48.55-1.85)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.193 , 0.212 0.194 , 0.213	Depositor DCC
$R_{free}$ test set	15275 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.92	1/3912 (0.0%)	0.88	5/5302 (0.1%)
1	B	0.91	5/3929 (0.1%)	0.88	5/5324 (0.1%)
1	C	0.80	5/3924 (0.1%)	0.82	4/5317 (0.1%)
All	All	0.88	11/11765 (0.1%)	0.86	14/15943 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	473	CYS	CB-SG	-8.94	1.67	1.82
1	B	351	TYR	CD1-CE1	7.13	1.50	1.39
1	C	403	GLU	CD-OE1	6.45	1.32	1.25
1	B	97	CYS	CB-SG	6.25	1.92	1.82
1	A	323	VAL	CB-CG1	5.65	1.64	1.52
1	C	359	GLU	CB-CG	5.50	1.62	1.52
1	B	89	GLU	CB-CG	-5.29	1.42	1.52
1	C	470	TYR	CE2-CZ	5.25	1.45	1.38
1	C	26	VAL	CB-CG2	5.16	1.63	1.52
1	B	453	ARG	CB-CG	5.13	1.66	1.52
1	B	486	TYR	CE1-CZ	5.05	1.45	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	B	104	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	104	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	C	405	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	104	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	354	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	482	ARG	NE-CZ-NH1	-5.86	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	492	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	474	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	461	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	367	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	104	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	261	ARG	NE-CZ-NH1	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3831	0	3692	18	0
1	B	3848	0	3710	21	0
1	C	3843	0	3707	19	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
3	G	39	0	34	0	0
3	I	39	0	34	1	0
3	L	39	0	34	2	0
4	B	42	0	39	1	0
4	C	56	0	52	0	0
5	A	462	0	0	3	0
5	B	466	0	0	0	0
5	C	393	0	0	3	0
All	All	13254	0	11477	51	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 2.

All (51) 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:219:SER:HB2	1:B:203:THR:HG21	1.74	0.69
1:A:126:ASN:OD1	1:A:128:THR:HG23	1.94	0.66
1:C:340:GLU:OE2	5:C:801:HOH:O	2.15	0.65
1:B:219:SER:HB2	1:C:203:THR:HG21	1.79	0.64
1:B:307:LYS:NZ	1:B:387:LYS:HE2	2.14	0.62
1:A:203:THR:HG21	1:C:219:SER:HB2	1.83	0.60
1:C:242:ILE:CD1	3:L:2:NAG:H81	2.33	0.59
1:B:479:GLY:O	1:B:483:ASN:HB2	2.02	0.59
1:C:15:LEU:HD22	1:C:448:PHE:HA	1.86	0.57
1:A:307:LYS:HZ3	1:A:387:LYS:HE2	1.69	0.56
1:A:128:THR:HG21	5:A:1225:HOH:O	2.05	0.55
1:A:307:LYS:NZ	1:A:387:LYS:HE2	2.22	0.55
1:C:242:ILE:HD12	3:L:2:NAG:H81	1.89	0.54
1:A:386:GLU:HG3	1:A:387:LYS:N	2.24	0.51
1:C:382:ASN:O	1:C:386:GLU:HB3	2.11	0.50
1:A:128:THR:OG1	2:F:1:NAG:H62	2.12	0.49
1:B:24:THR:OG1	4:B:608:NAG:H81	2.11	0.49
1:B:452:ARG:HD2	1:B:453:ARG:CZ	2.43	0.48
1:A:236:ILE:HD13	1:C:402:VAL:HB	1.95	0.47
1:B:348:ASP:OD1	1:B:348:ASP:N	2.45	0.47
1:C:167:THR:HB	1:C:242:ILE:HD11	1.97	0.46
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.97	0.46
1:B:382:ASN:O	1:B:386:GLU:HB2	2.15	0.46
1:B:325:GLU:HG3	1:B:344:GLU:H	1.80	0.45
1:C:164:LEU:O	1:C:246:ASN:HA	2.17	0.45
1:C:182:VAL:HG21	1:C:213:ILE:HB	1.99	0.45
1:A:30:THR:HG21	1:B:376:GLN:HG2	2.00	0.44
1:C:472:LYS:NZ	5:C:818:HOH:O	2.50	0.44
1:A:385:ILE:HG22	1:A:385:ILE:O	2.19	0.43
1:B:164:LEU:O	1:B:246:ASN:HA	2.19	0.43
1:B:242:ILE:HD12	3:I:2:NAG:H81	2.00	0.43
1:B:216:ASN:ND2	1:C:210:GLN:OE1	2.47	0.43
1:A:82:GLU:HG3	1:A:83:LYS:H	1.82	0.43
1:A:193:ASN:ND2	5:A:819:HOH:O	2.51	0.43
1:A:33:GLN:HG2	5:A:1094:HOH:O	2.18	0.43
1:C:452:ARG:HD2	1:C:453:ARG:CZ	2.48	0.43
1:B:102:VAL:HG22	1:B:232:ILE:HB	2.00	0.43
1:C:380:LYS:HZ1	1:C:435:HIS:HB3	1.84	0.43
1:B:244:LEU:C	1:B:244:LEU:HD23	2.40	0.42
1:A:442:SER:O	1:A:446:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HB	1:B:242:ILE:HD11	2.01	0.42
1:B:51:ILE:HB	1:B:274:ILE:HD13	2.02	0.41
1:B:301:THR:HB	1:B:305:CYS:SG	2.61	0.41
1:A:452:ARG:HD2	1:A:453:ARG:CZ	2.51	0.41
1:B:182:VAL:HG21	1:B:213:ILE:HB	2.02	0.41
1:A:234:TRP:HZ3	1:A:236:ILE:HD12	1.86	0.41
1:C:479:GLY:O	1:C:483:ASN:HB2	2.21	0.41
1:B:307:LYS:HZ3	1:B:387:LYS:HE2	1.83	0.40
1:C:199:SER:HA	5:C:1046:HOH:O	2.20	0.40
1:B:219:SER:CB	1:C:203:THR:HG21	2.50	0.40
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/497 (97%)	462 (96%)	20 (4%)	0	100	100
1	B	484/497 (97%)	462 (96%)	22 (4%)	0	100	100
1	C	484/497 (97%)	463 (96%)	21 (4%)	0	100	100
All	All	1450/1491 (97%)	1387 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	424/432 (98%)	423 (100%)	1 (0%)	93	92
1	B	426/432 (99%)	423 (99%)	3 (1%)	84	79
1	C	425/432 (98%)	424 (100%)	1 (0%)	93	92
All	All	1275/1296 (98%)	1270 (100%)	5 (0%)	91	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	B	18	HIS
1	B	264	LYS
1	B	341	ASN
1	C	18	HIS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

23 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
2	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
2	NAG	D	2	2	14,14,15	0.90	2 (14%)	17,19,21	1.03	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	0.43	0
2	NAG	F	1	1,2	14,14,15	2.46	1 (7%)	17,19,21	3.08	5 (29%)
2	NAG	F	2	2	14,14,15	1.08	2 (14%)	17,19,21	2.21	4 (23%)
3	NAG	G	1	1,3	14,14,15	0.34	0	17,19,21	0.93	1 (5%)
3	NAG	G	2	3	14,14,15	0.45	0	17,19,21	0.54	0
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	0.93	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.94	1 (7%)	17,19,21	0.60	0
2	NAG	H	2	2	14,14,15	0.77	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.72	0	17,19,21	0.70	0
3	NAG	I	2	3	14,14,15	0.77	1 (7%)	17,19,21	0.70	0
3	BMA	I	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.22	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.61	0	17,19,21	0.63	0
2	NAG	J	2	2	14,14,15	0.78	1 (7%)	17,19,21	0.68	0
2	NAG	K	1	1,2	14,14,15	0.43	0	17,19,21	1.84	3 (17%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	0.77	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.59	0
3	BMA	L	3	3	11,11,12	0.86	1 (9%)	15,15,17	0.95	0
2	NAG	M	1	1,2	14,14,15	0.71	1 (7%)	17,19,21	0.56	0
2	NAG	M	2	2	14,14,15	0.70	1 (7%)	17,19,21	0.67	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	8.20	1.64	1.52
2	H	1	NAG	C1-C2	3.15	1.57	1.52
2	H	2	NAG	O5-C1	-2.68	1.39	1.43
2	F	2	NAG	O5-C1	-2.53	1.39	1.43
2	D	2	NAG	C1-C2	2.49	1.56	1.52
2	J	2	NAG	O5-C1	-2.42	1.39	1.43
3	I	2	NAG	O5-C1	-2.42	1.39	1.43
2	M	2	NAG	C1-C2	2.18	1.55	1.52
3	L	3	BMA	O4-C4	-2.15	1.37	1.43
2	D	2	NAG	O5-C1	-2.11	1.40	1.43
2	F	2	NAG	C2-N2	-2.06	1.42	1.46
3	I	3	BMA	O3-C3	2.06	1.47	1.43
2	M	1	NAG	C1-C2	2.05	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-C2-N2	-10.22	93.02	110.49
2	K	1	NAG	C2-N2-C7	4.71	129.61	122.90
2	F	2	NAG	C2-N2-C7	-4.65	116.28	122.90
2	F	2	NAG	C4-C3-C2	-4.14	104.95	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C1-C2	-4.03	104.93	111.29
2	F	1	NAG	O5-C1-C2	-3.84	105.22	111.29
2	F	1	NAG	C1-O5-C5	3.71	117.21	112.19
2	H	2	NAG	C1-O5-C5	3.65	117.14	112.19
2	K	1	NAG	C1-O5-C5	3.60	117.06	112.19
2	F	1	NAG	O3-C3-C2	-3.53	102.16	109.47
2	D	2	NAG	C1-O5-C5	3.48	116.91	112.19
3	I	3	BMA	C1-O5-C5	3.23	116.57	112.19
2	F	1	NAG	O5-C5-C6	3.04	111.97	107.20
2	E	1	NAG	C1-O5-C5	3.03	116.30	112.19
3	G	1	NAG	C1-O5-C5	2.87	116.09	112.19
2	K	1	NAG	C1-C2-N2	2.84	115.34	110.49
3	G	3	BMA	C1-O5-C5	2.79	115.97	112.19
2	K	2	NAG	C1-O5-C5	2.37	115.41	112.19
3	L	1	NAG	C1-O5-C5	2.26	115.26	112.19
2	F	2	NAG	O3-C3-C4	-2.26	105.13	110.35
2	D	1	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	3	BMA	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
3	L	3	BMA	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

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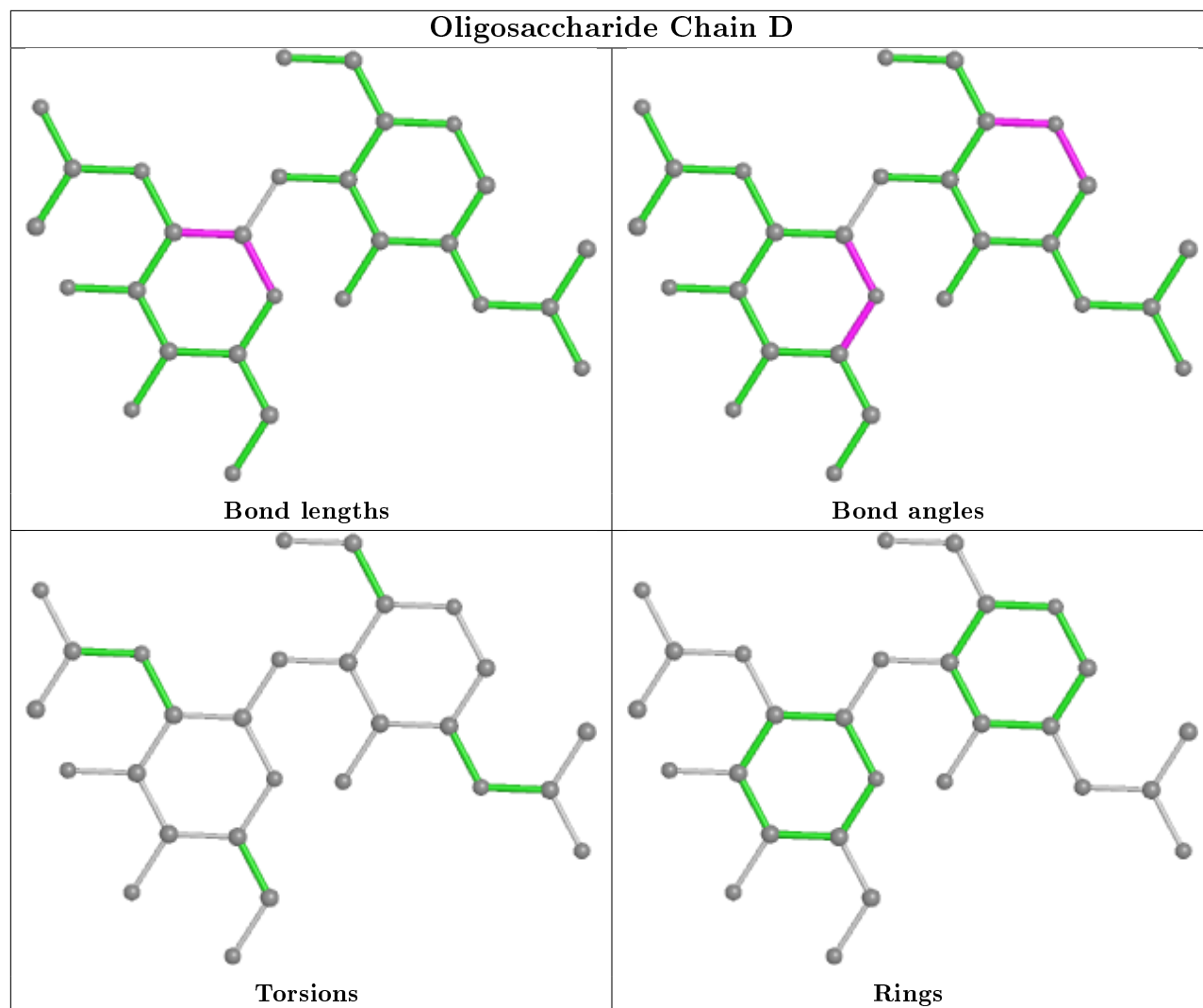
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C1-C2-N2-C7
3	G	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2

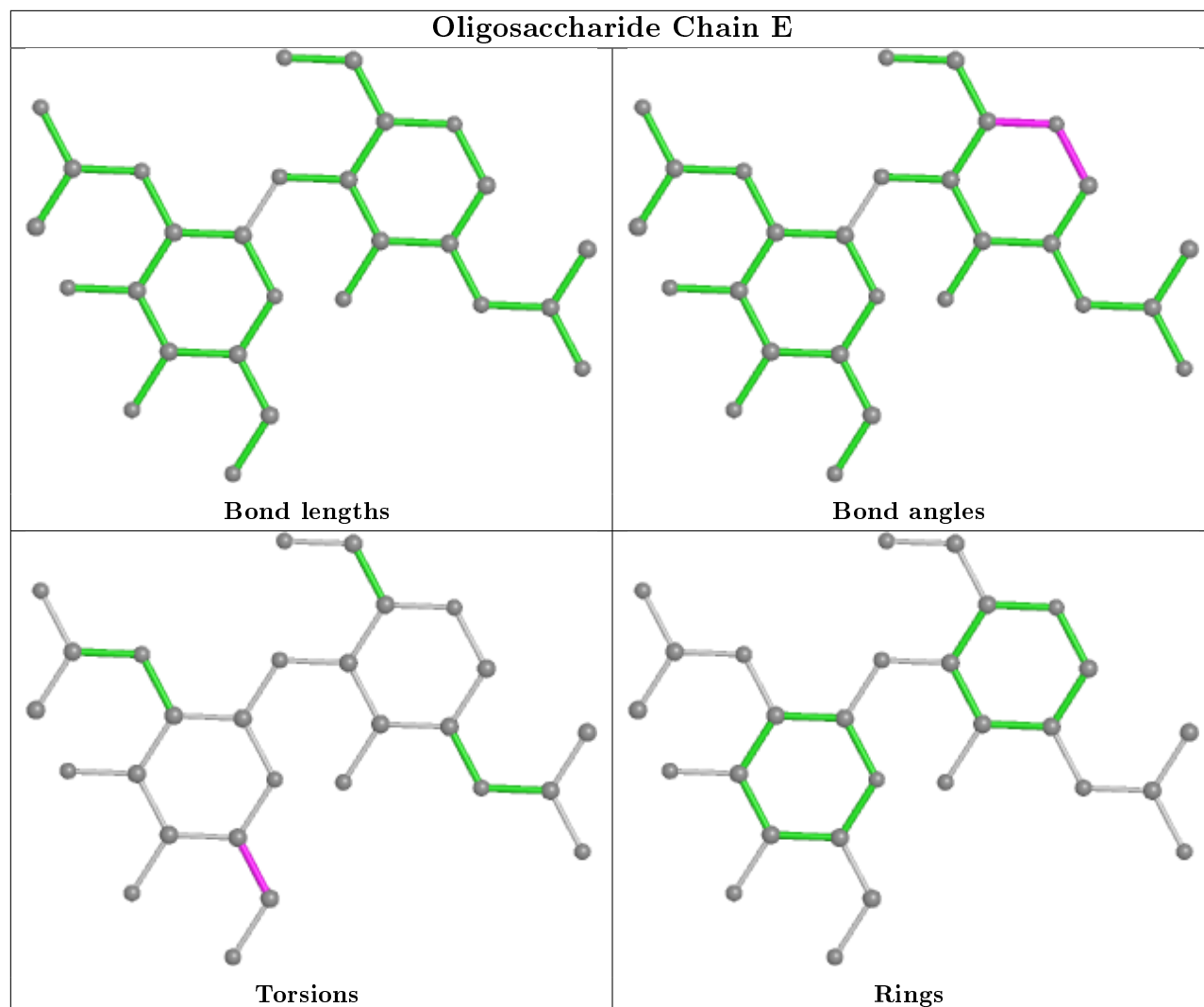
There are no ring outliers.

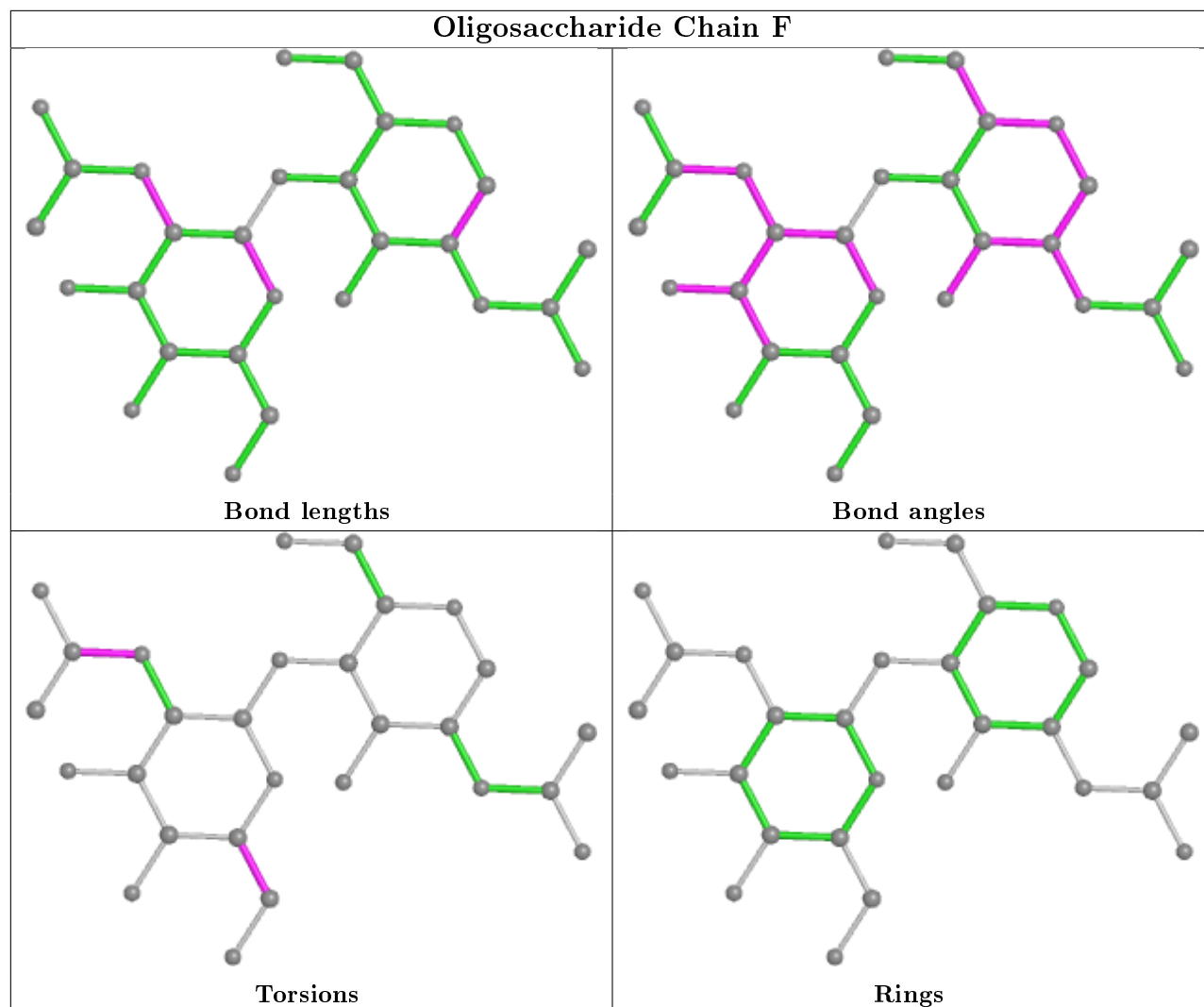
3 monomers are involved in 4 short contacts:

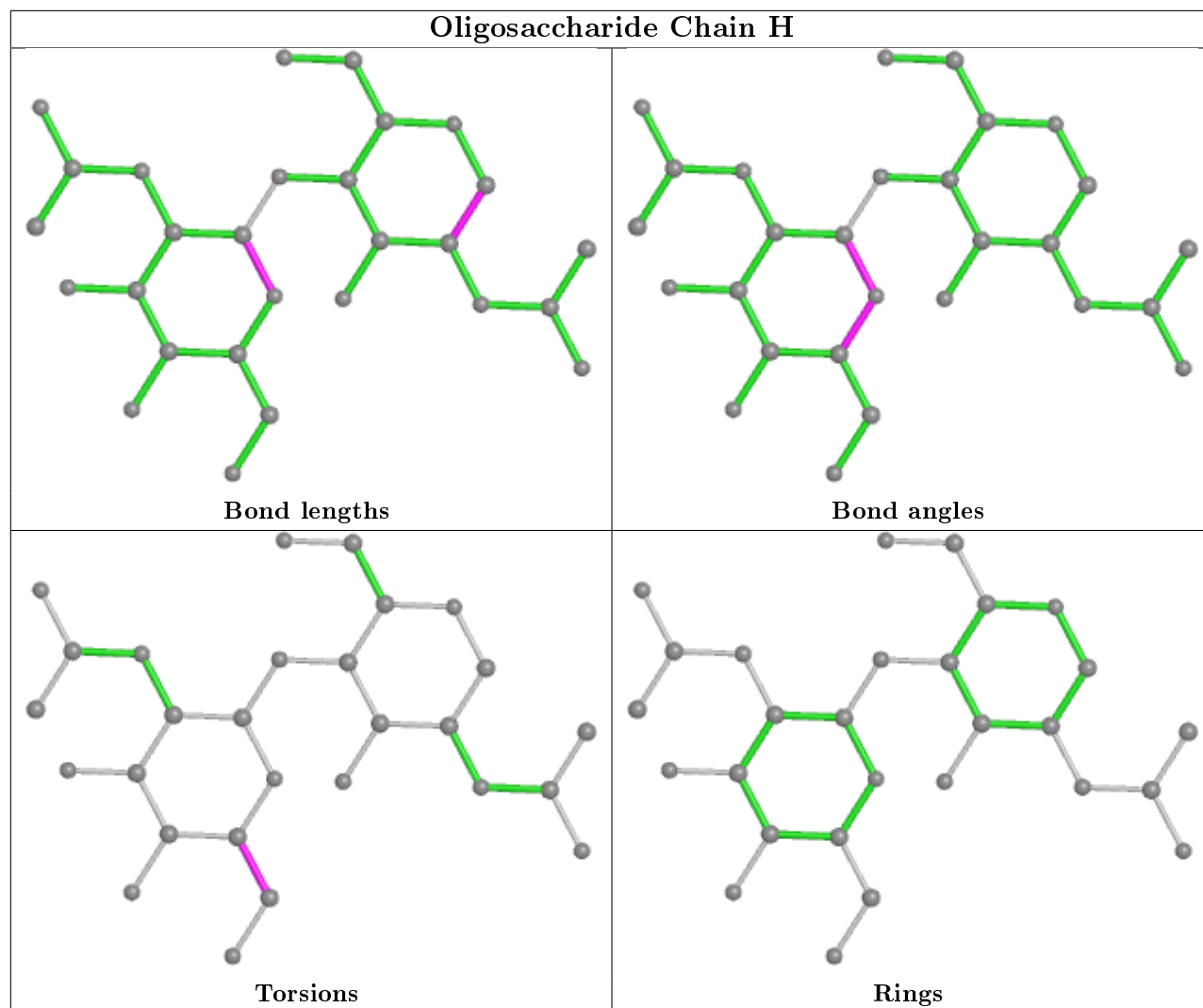
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
2	F	1	NAG	1	0
3	L	2	NAG	2	0

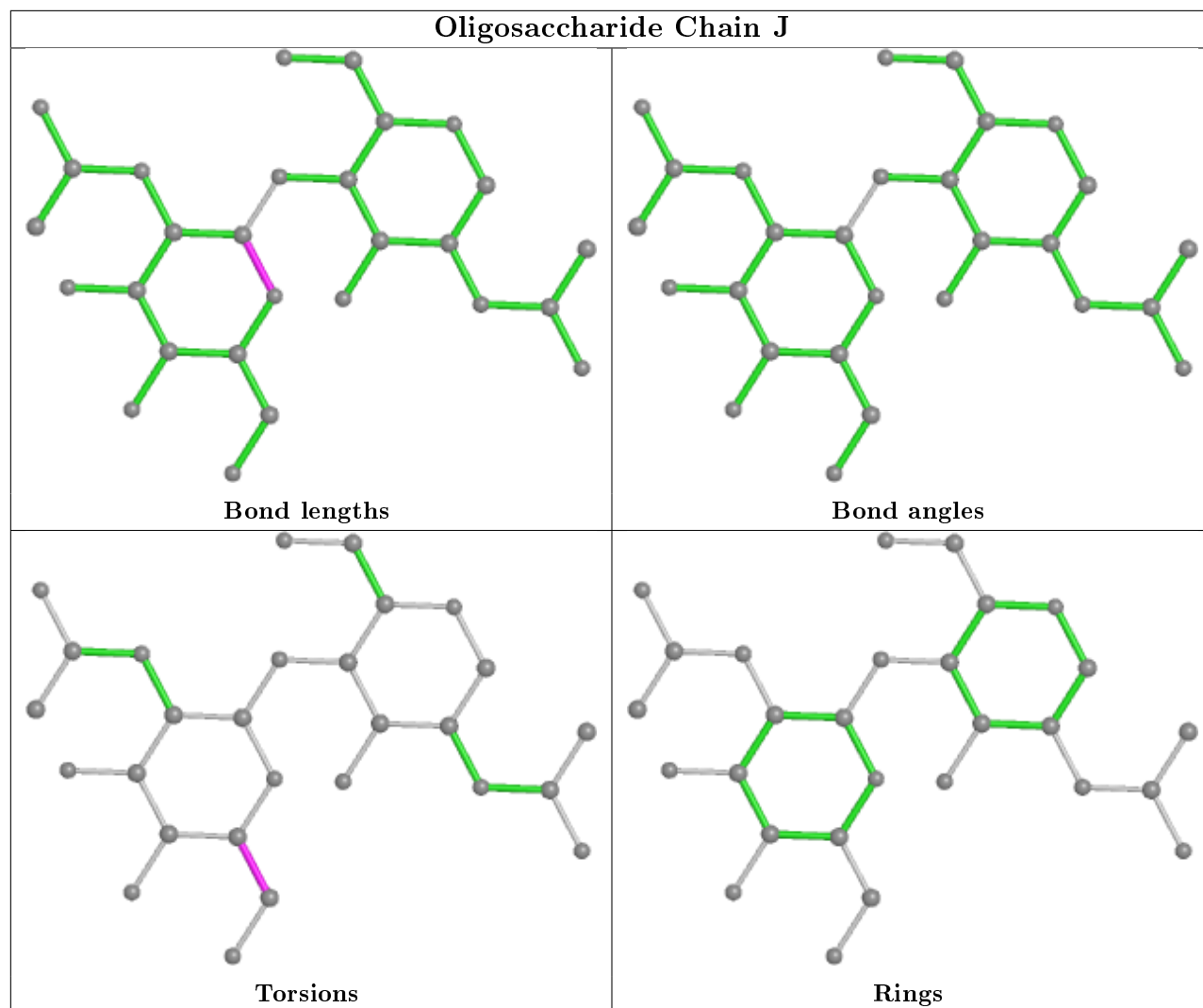
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



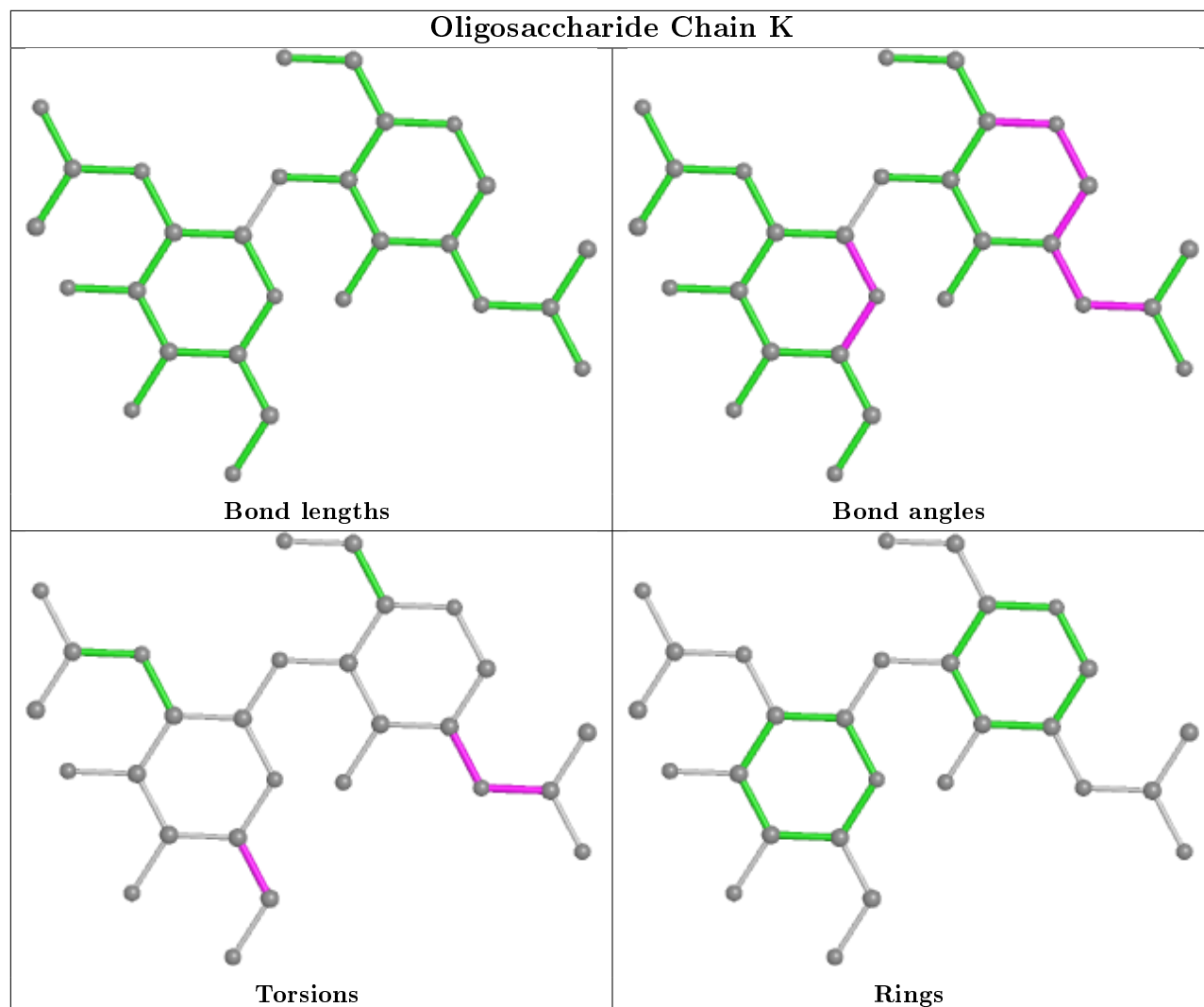


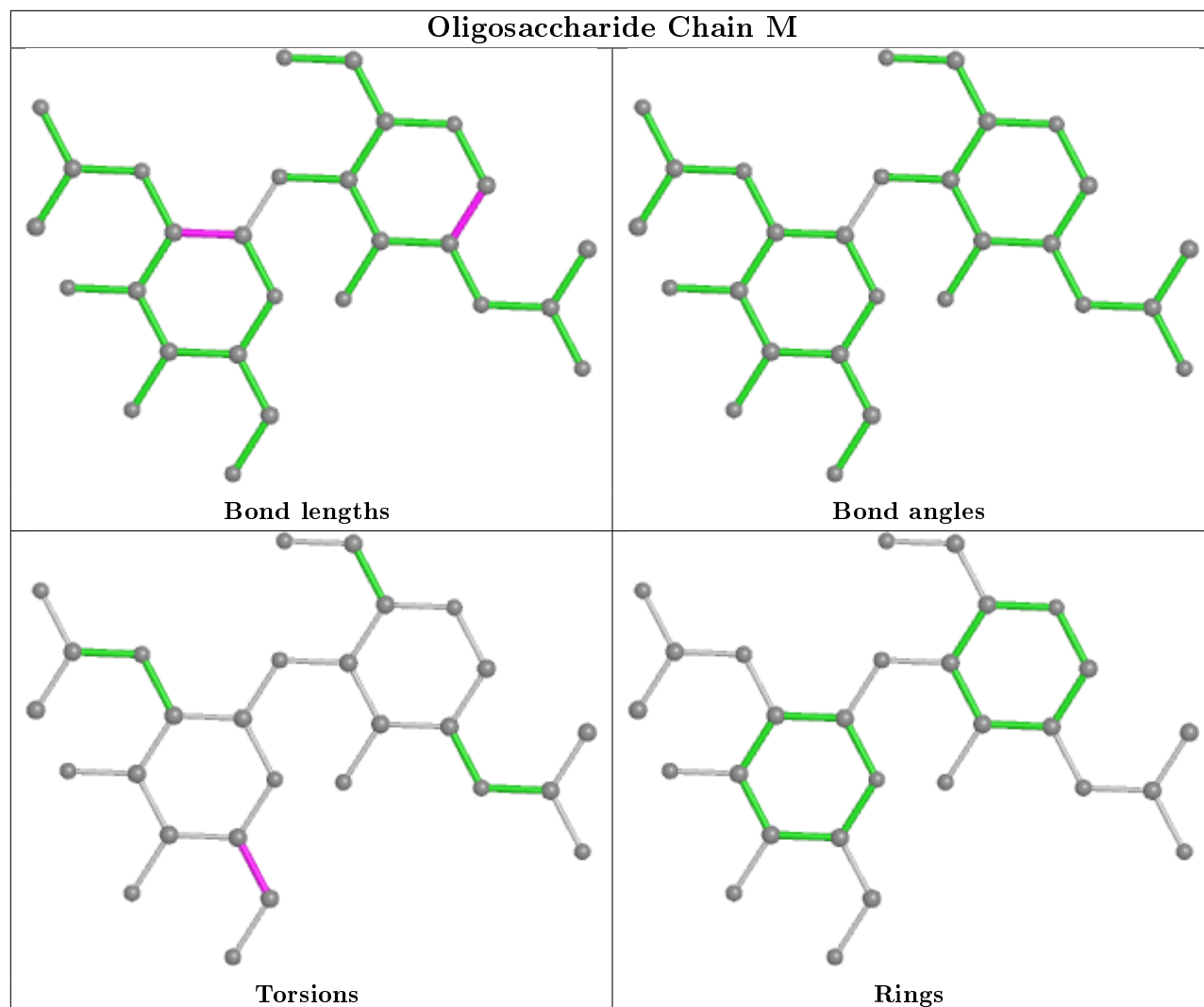


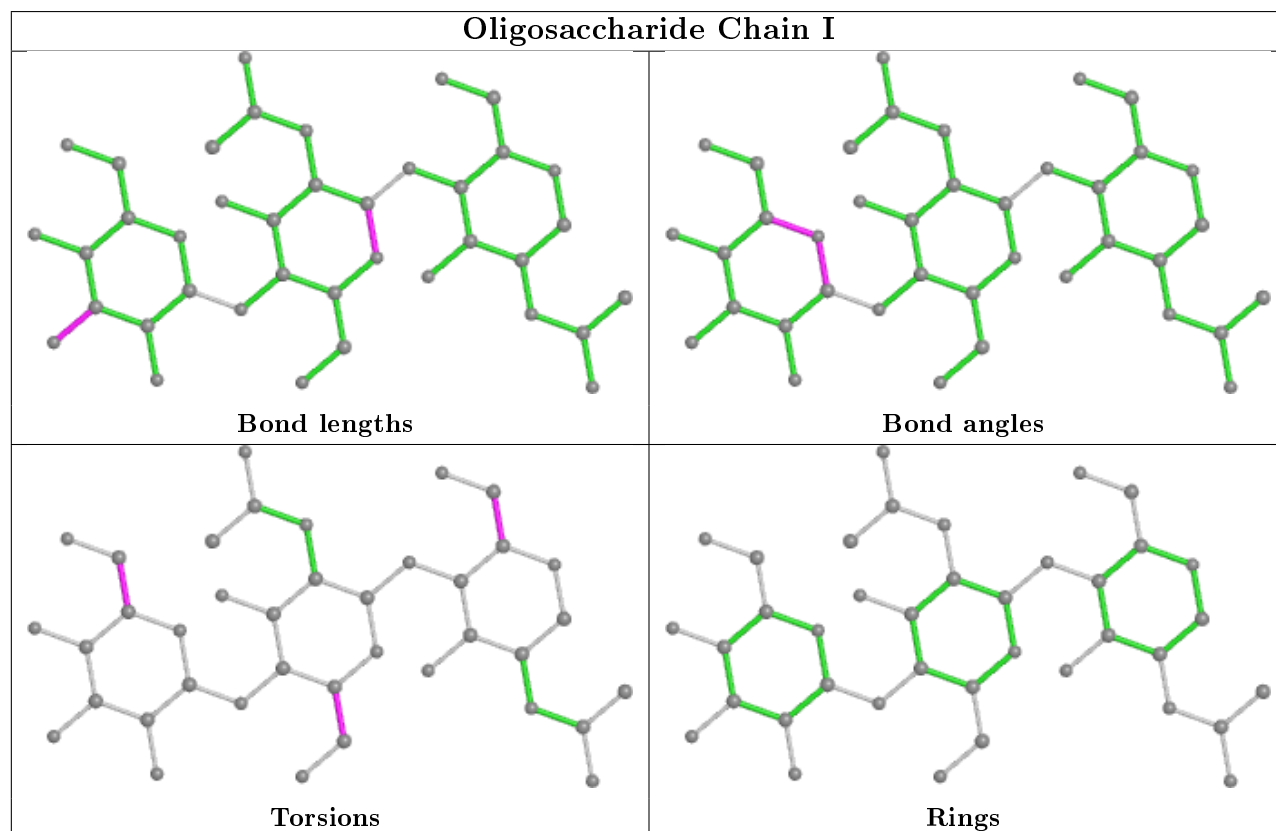
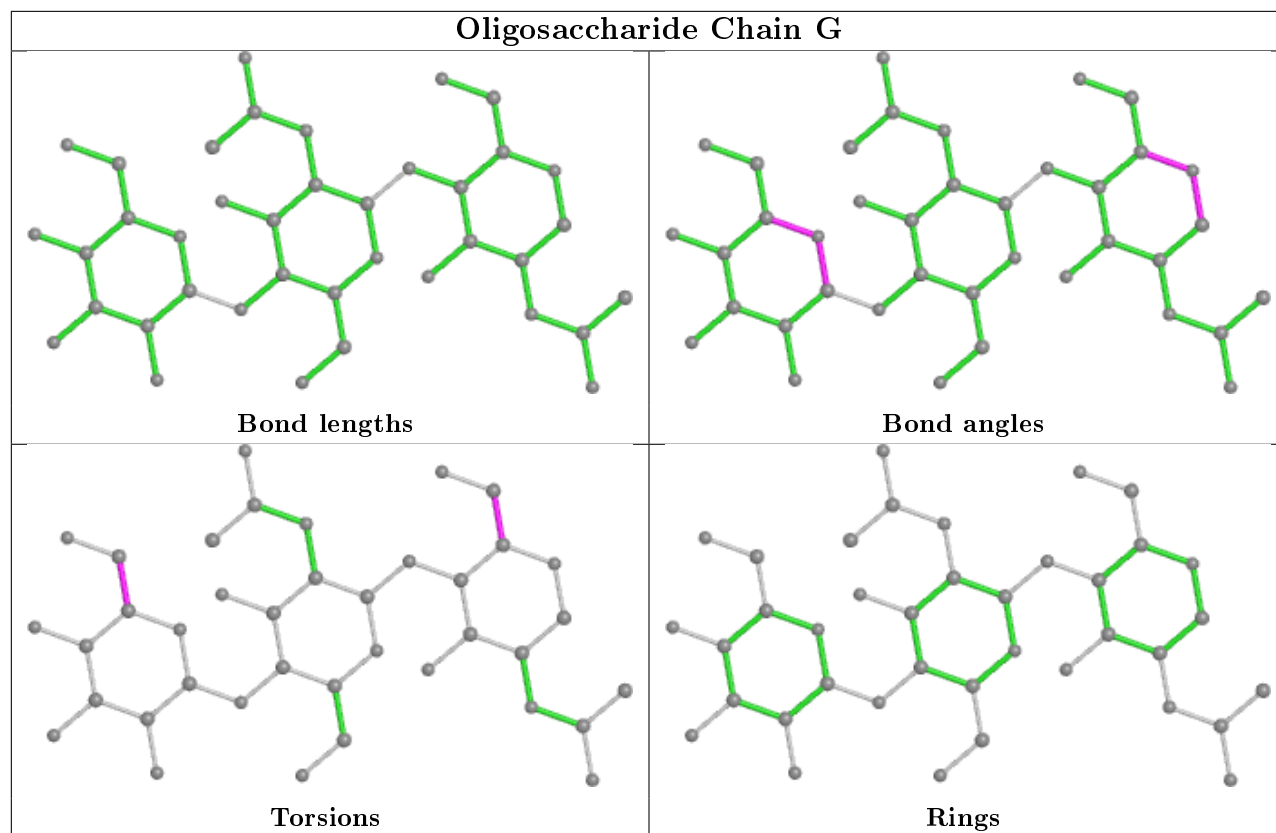


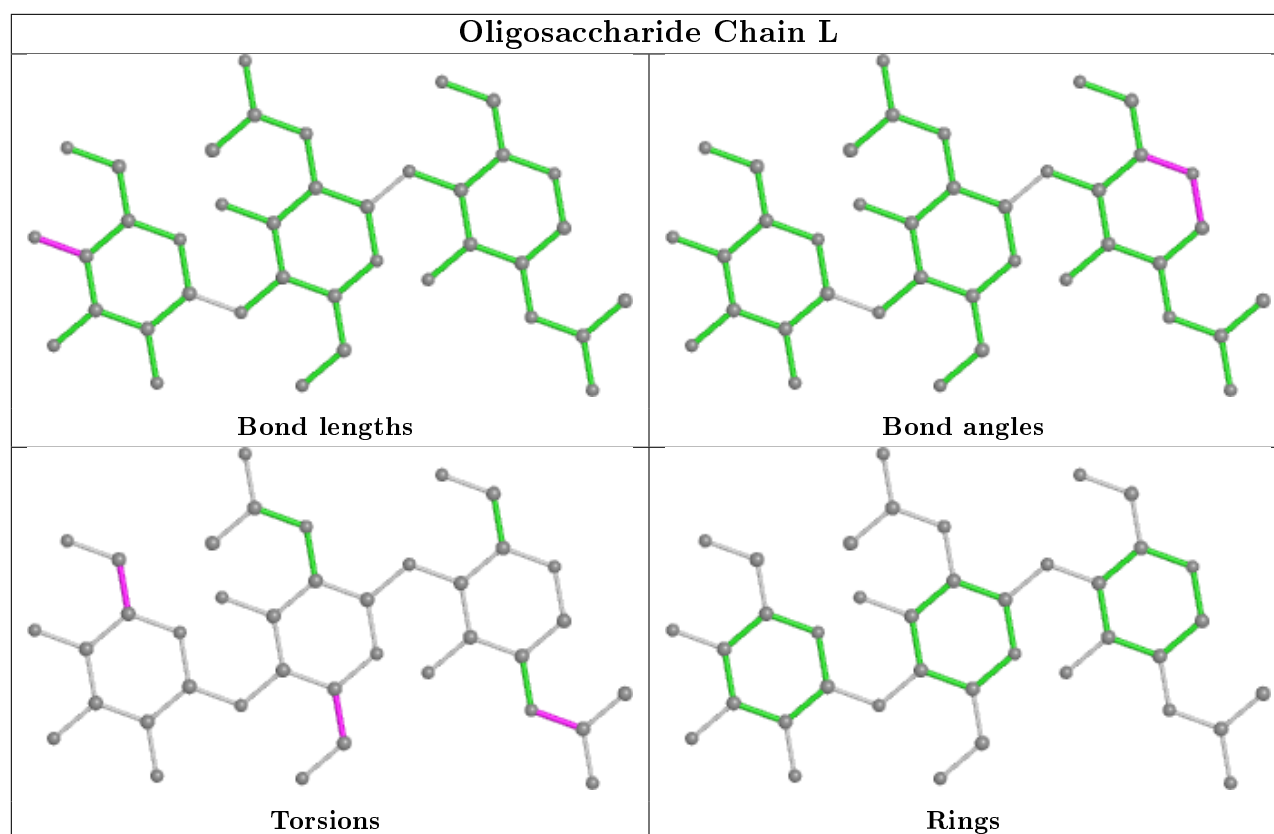












## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	701	1	14,14,15	0.97	1 (7%)	17,19,21	0.69	1 (5%)
4	NAG	B	608	1	14,14,15	1.25	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	B	602	1	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
4	NAG	C	709	1	14,14,15	0.98	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	B	601	1	14,14,15	0.75	1 (7%)	17,19,21	1.15	1 (5%)
4	NAG	C	703	1	14,14,15	0.52	0	17,19,21	0.55	0
4	NAG	C	702	1	14,14,15	0.32	0	17,19,21	0.96	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	608	1	-	0/6/23/26	0/1/1/1
4	NAG	B	602	1	-	2/6/23/26	0/1/1/1
4	NAG	C	709	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	703	1	-	2/6/23/26	0/1/1/1
4	NAG	C	702	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	NAG	C1-C2	3.50	1.57	1.52
4	C	701	NAG	O5-C1	3.29	1.49	1.43
4	C	709	NAG	O5-C1	3.11	1.48	1.43
4	B	608	NAG	O5-C1	2.88	1.48	1.43
4	B	601	NAG	O5-C1	-2.57	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	NAG	C1-O5-C5	3.44	116.86	112.19
4	C	709	NAG	C1-O5-C5	3.13	116.43	112.19
4	C	702	NAG	C1-O5-C5	3.07	116.35	112.19
4	B	602	NAG	C1-O5-C5	2.95	116.19	112.19
4	B	608	NAG	C2-N2-C7	2.45	126.39	122.90
4	C	701	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	703	NAG	C4-C5-C6-O6
4	C	709	NAG	O5-C5-C6-O6
4	C	703	NAG	O5-C5-C6-O6
4	C	709	NAG	C4-C5-C6-O6
4	B	602	NAG	C4-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	608	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	486/497 (97%)	-0.15	19 (3%)	39 38	20, 35, 59, 82	0
1	B	488/497 (98%)	-0.11	12 (2%)	57 56	21, 36, 60, 82	0
1	C	488/497 (98%)	-0.01	21 (4%)	35 33	22, 41, 66, 84	0
All	All	1462/1491 (98%)	-0.09	52 (3%)	42 40	20, 38, 63, 84	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	CYS	5.4
1	C	388	THR	5.4
1	C	386	GLU	4.9
1	C	277	CYS	4.8
1	C	137	TYR	4.3
1	A	277	CYS	4.2
1	C	142	GLY	4.2
1	C	385	ILE	4.1
1	C	387	LYS	4.1
1	B	8	ASN	4.1
1	C	143	PRO	3.9
1	C	173	ASN	3.8
1	A	502	ILE	3.8
1	B	48	THR	3.7
1	C	276	THR	3.7
1	C	503	LYS	3.6
1	A	388	THR	3.3
1	A	385	ILE	3.2
1	A	137	TYR	3.0
1	A	143	PRO	3.0
1	B	502	ILE	2.8
1	A	234	TRP	2.7
1	C	502	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	367	LEU	2.7
1	C	140	LYS	2.6
1	B	409	LEU	2.5
1	B	233	TYR	2.5
1	B	387	LYS	2.4
1	A	102	VAL	2.4
1	C	144	ASP	2.4
1	A	103	PRO	2.4
1	A	22	ASN	2.4
1	B	234	TRP	2.3
1	C	48	THR	2.3
1	B	213	ILE	2.3
1	B	388	THR	2.3
1	C	234	TRP	2.3
1	C	406	ILE	2.3
1	A	406	ILE	2.2
1	A	386	GLU	2.2
1	A	501	GLN	2.2
1	A	142	GLY	2.2
1	A	213	ILE	2.2
1	A	276	THR	2.2
1	C	50	ARG	2.1
1	A	278	SER	2.1
1	A	158	GLU	2.1
1	C	138	ALA	2.1
1	C	413	VAL	2.1
1	A	334	ALA	2.0
1	C	233	TYR	2.0
1	B	386	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

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

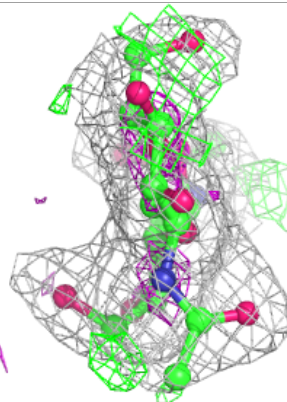
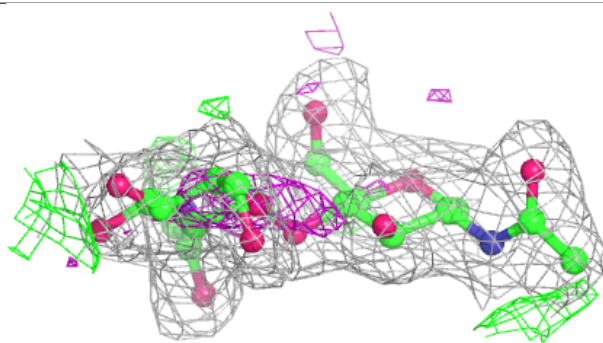
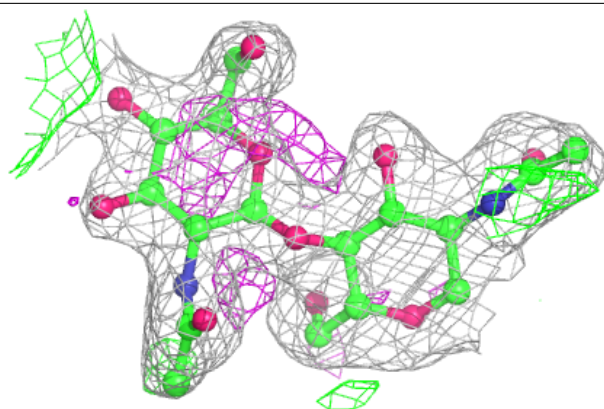


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	H	2	14/15	0.79	0.26	70,77,82,82	0
2	NAG	J	2	14/15	0.80	0.30	72,77,84,85	0
2	NAG	M	2	14/15	0.82	0.29	73,77,83,84	0
2	NAG	E	2	14/15	0.82	0.41	86,96,101,102	0
2	NAG	F	2	14/15	0.83	0.36	59,76,94,95	0
2	NAG	K	2	14/15	0.84	0.33	57,64,71,73	0
2	NAG	D	2	14/15	0.86	0.32	61,67,74,77	0
2	NAG	K	1	14/15	0.89	0.20	41,51,63,64	0
2	NAG	F	1	14/15	0.90	0.18	38,48,59,62	0
3	NAG	L	1	14/15	0.91	0.16	49,60,78,86	0
3	BMA	L	3	11/12	0.91	0.23	78,82,86,87	0
3	BMA	G	3	11/12	0.91	0.26	73,75,77,79	0
3	BMA	I	3	11/12	0.91	0.25	71,77,83,87	0
2	NAG	E	1	14/15	0.93	0.20	46,59,67,79	0
3	NAG	G	2	14/15	0.94	0.22	55,60,65,67	0
2	NAG	J	1	14/15	0.94	0.17	40,46,56,62	0
2	NAG	D	1	14/15	0.94	0.14	42,50,55,58	0
3	NAG	I	2	14/15	0.94	0.14	47,51,55,63	0
2	NAG	H	1	14/15	0.94	0.19	38,45,52,62	0
3	NAG	I	1	14/15	0.95	0.18	38,51,63,65	0
3	NAG	G	1	14/15	0.95	0.14	42,55,70,70	0
3	NAG	L	2	14/15	0.95	0.16	65,68,71,77	0
2	NAG	M	1	14/15	0.96	0.16	43,50,54,64	0

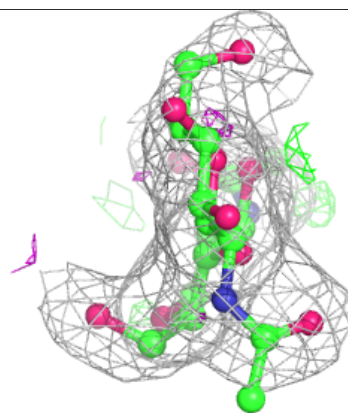
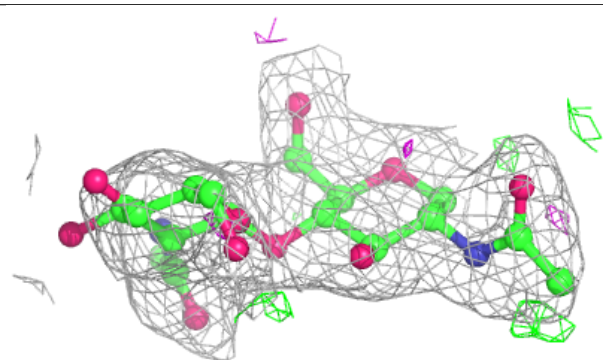
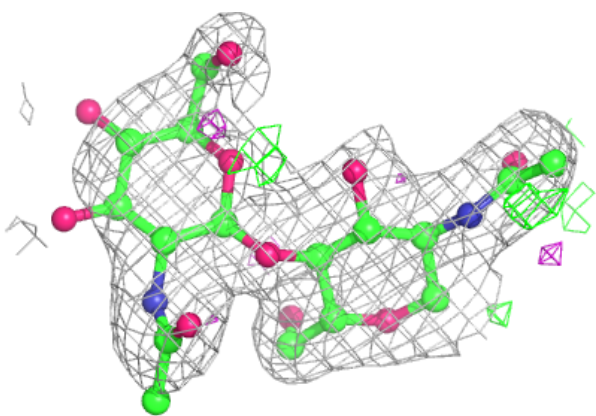
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain D:**

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

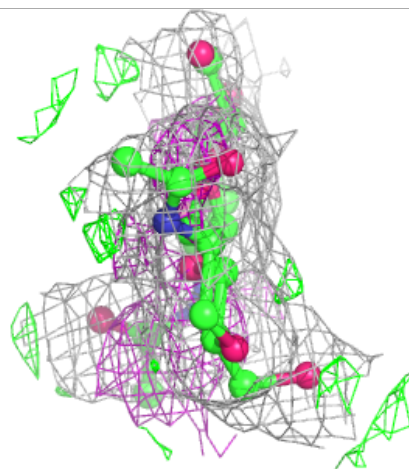
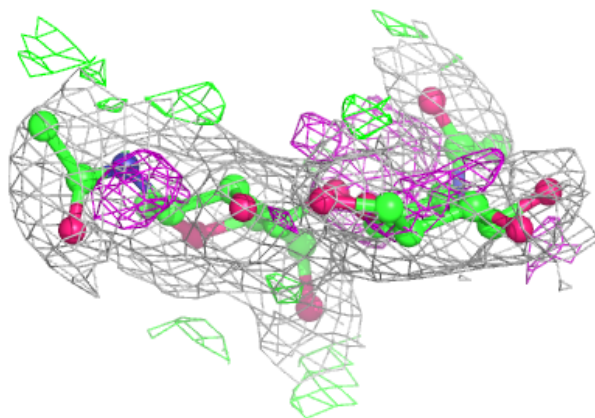
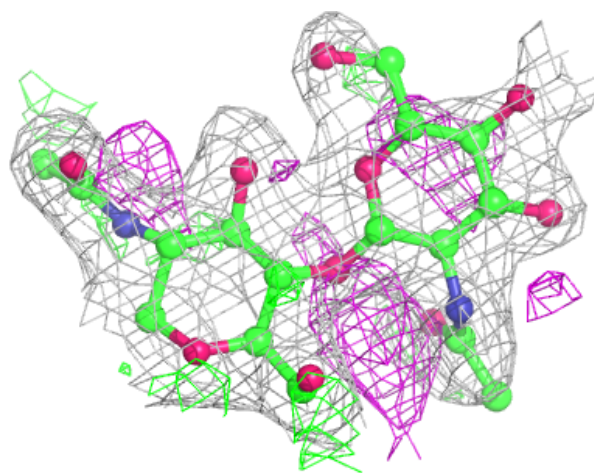
**Electron density around Chain E:**

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



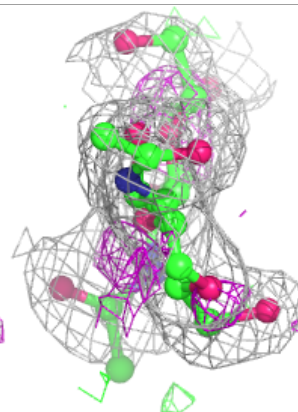
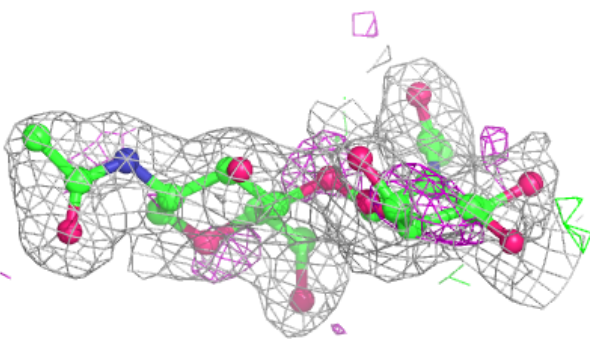
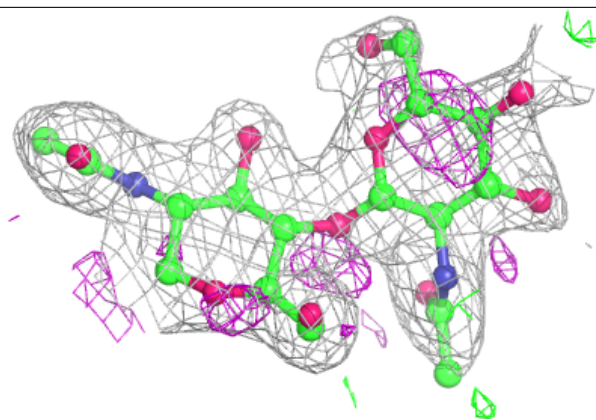
**Electron density around Chain F:**

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

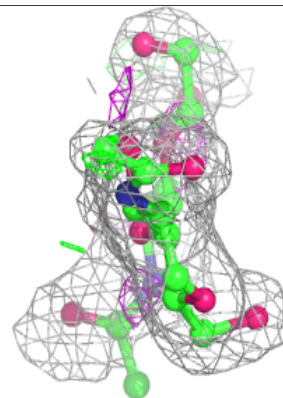
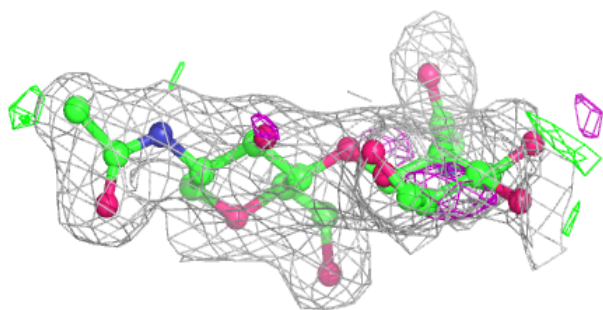
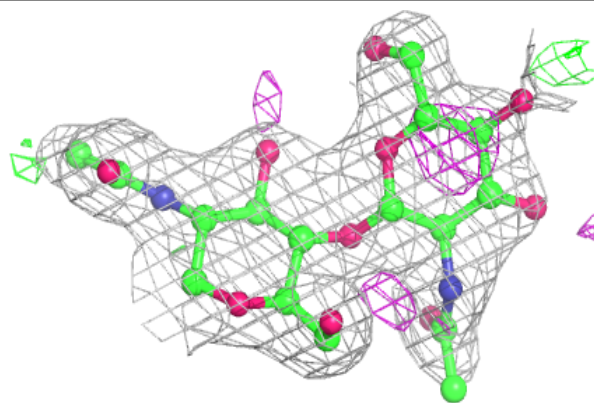


**Electron density around Chain H:**

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

**Electron density around Chain J:**

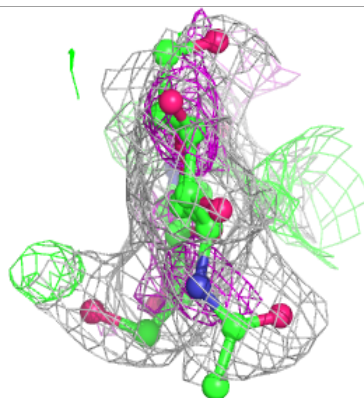
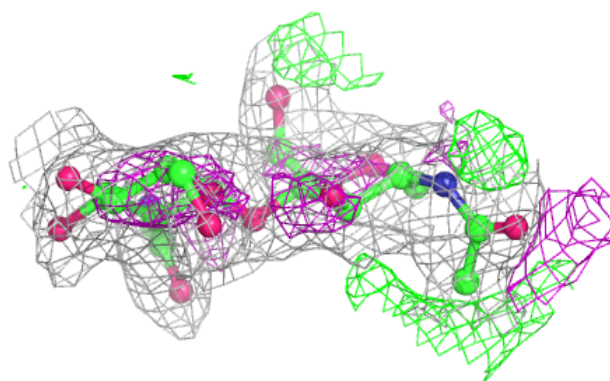
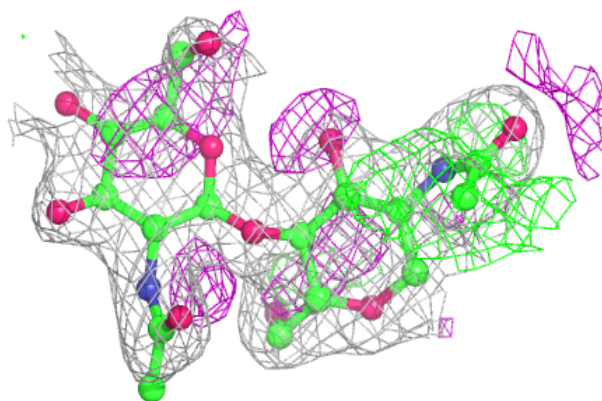
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



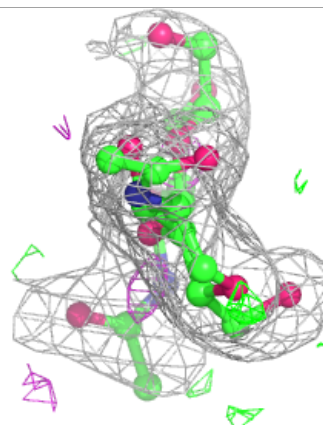
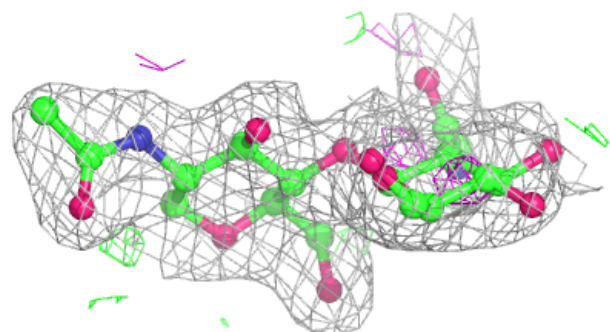
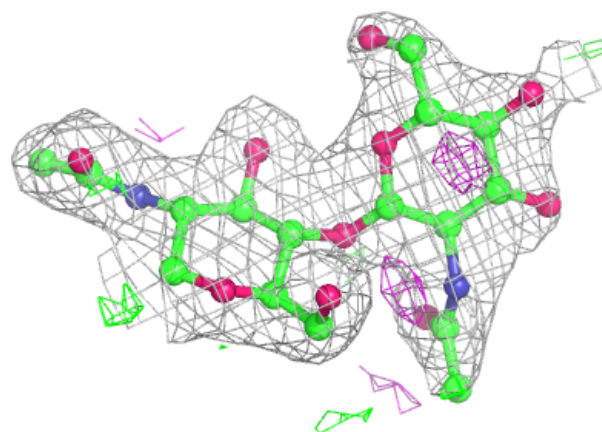


**Electron density around Chain K:**

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

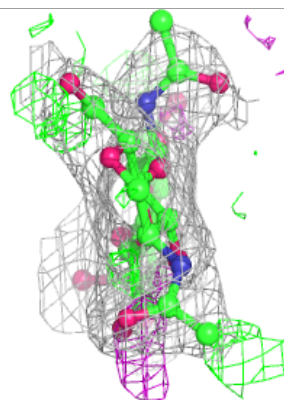
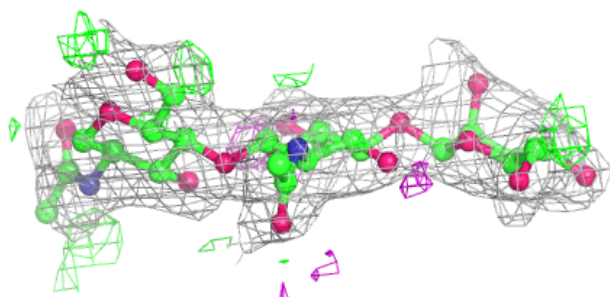
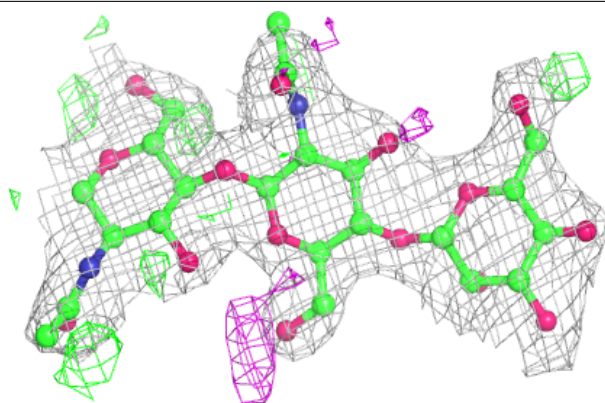
**Electron density around Chain M:**

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

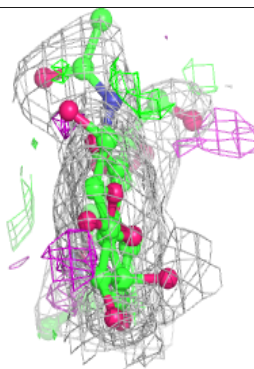
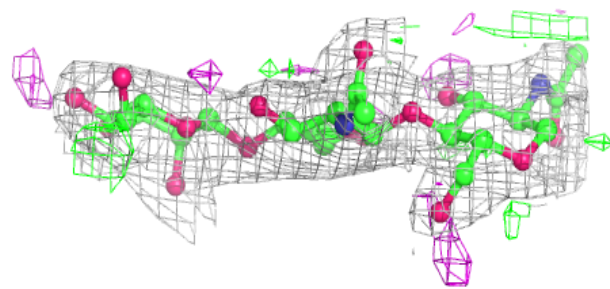
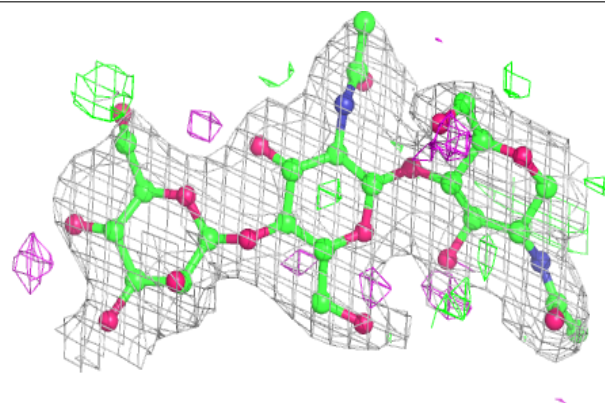


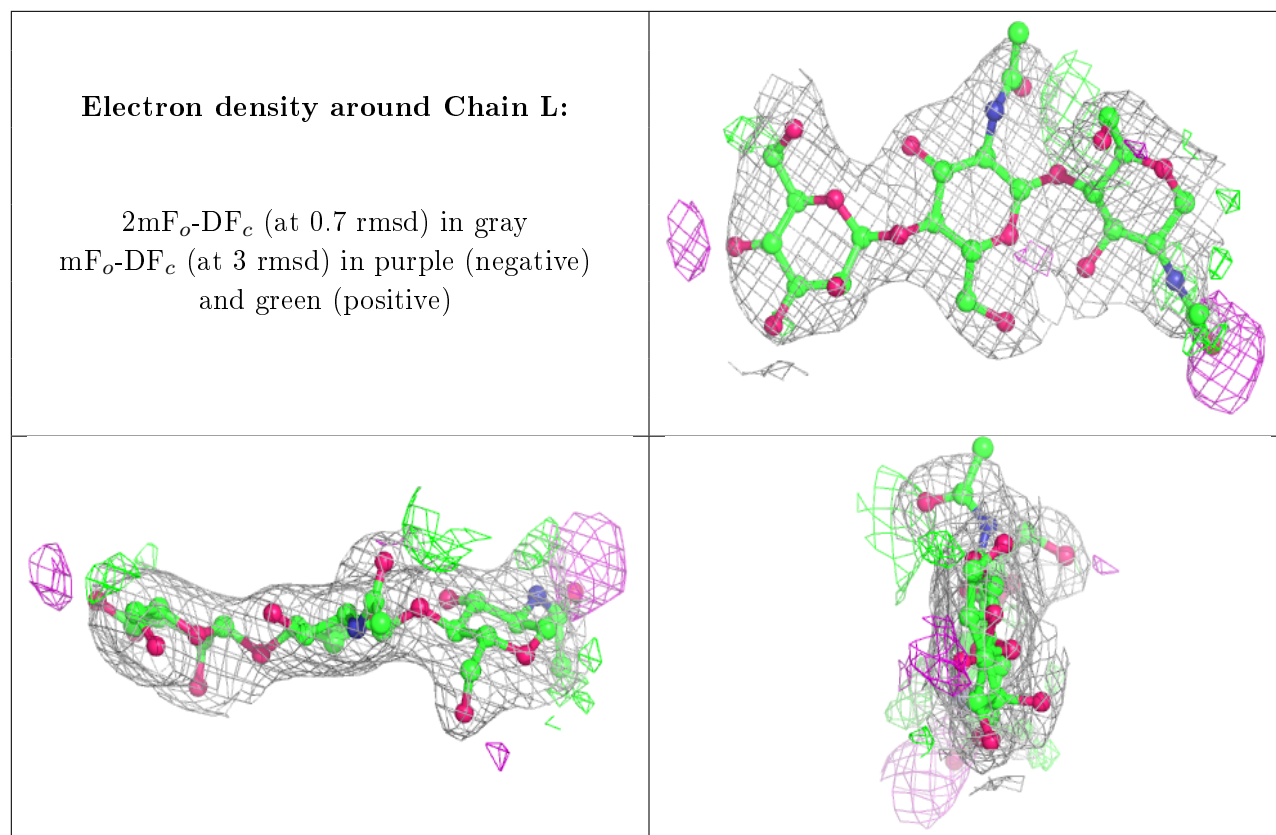
**Electron density around Chain G:**

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

**Electron density around Chain I:**

$2mF_o-DF_c$  (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
4	NAG	C	709	14/15	0.58	0.45	74,91,95,96	0
4	NAG	C	703	14/15	0.83	0.36	67,84,90,93	0
4	NAG	B	608	14/15	0.84	0.35	53,61,66,66	0
4	NAG	B	602	14/15	0.85	0.33	58,74,79,80	0
4	NAG	C	702	14/15	0.85	0.25	49,59,66,68	0
4	NAG	C	701	14/15	0.89	0.24	53,62,63,63	0
4	NAG	B	601	14/15	0.94	0.16	39,51,60,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.