



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 11:59 AM BST

PDB ID : 6MSU  
Title : Integrin alphaV Beta3 in complex with EETI-II 2.5F  
Authors : van Agthoven, J.F.; Arnaout, M.A.  
Deposited on : 2018-10-18  
Resolution : 3.11 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 : 2.13.1  
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

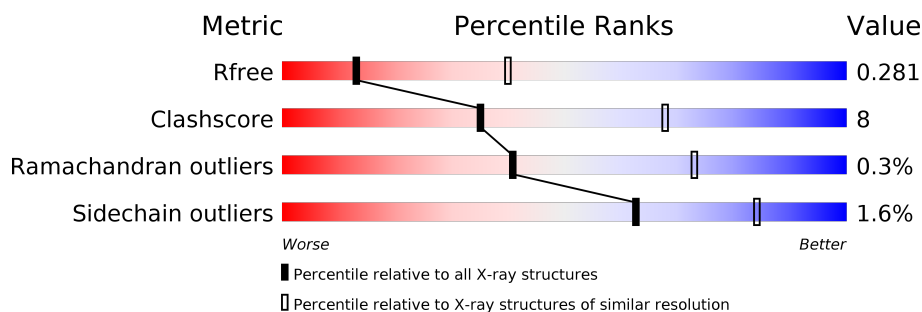
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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.







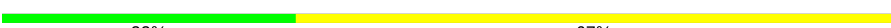
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	967	
2	B	695	
3	C	32	
4	D	4	
4	G	4	
5	E	2	
5	H	2	

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Mol	Chain	Length	Quality of chain
5	I	2	 50% 50%
5	K	2	 50% 50%
6	F	6	 33% 17% 50%
7	J	3	 33% 67%
7	L	3	 33% 67%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13158 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Engineered EETI-II 2.5F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	32	Total	C	N	O	S	0	0	0
			224	132	42	44	6			

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



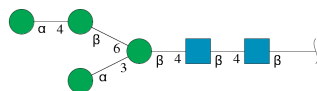
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



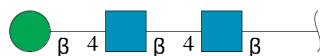
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 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
7	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Mn	0	0
			3	3		
9	A	5	Total	Mn	0	0
			5	5		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

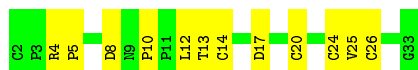
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	O 1	0	0
11	B	2	Total 2	O 2	0	0







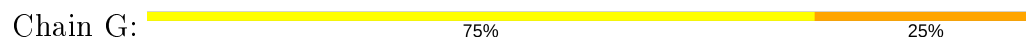
- Molecule 3: Engineered EETI-II 2.5F



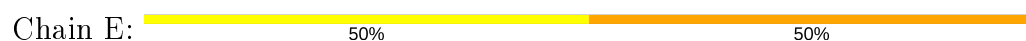
- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1  
MAG2

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

Chain F:  33% 17% 50%

MAG1  
MAG2  
EVA3  
EVA4  
MAN5  
MAN6

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

Chain J:  33% 67%

MAG1  
MAG2  
EVA3

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

Chain L:  33% 67%

MAG1  
MAG2  
EVA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.89Å 129.89Å 305.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	3.21 – 3.11 49.50 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (3.21-3.11) 91.3 (49.50-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.235 , 0.281	Depositor DCC
$R_{free}$ test set	2624 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 24.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.37	0/7352	0.67	10/9967 (0.1%)
2	B	0.34	0/5390	0.52	0/7289
3	C	0.35	0/229	0.54	0/309
All	All	0.36	0/12971	0.61	10/17565 (0.1%)

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	7
2	B	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	GLN	CG-CD-OE1	18.01	157.63	121.60
1	A	494	GLN	CG-CD-NE2	-16.36	77.43	116.70
1	A	623	ASN	CB-CG-ND2	-14.23	82.55	116.70
1	A	623	ASN	CB-CG-OD1	12.55	146.69	121.60
1	A	593	LEU	CB-CG-CD2	-8.96	95.76	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LYS	Peptide
1	A	450	TYR	Peptide
1	A	455	ASN	Sidechain
1	A	494	GLN	Sidechain
1	A	68	GLN	Sidechain

## 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	7196	0	7012	114	0
2	B	5294	0	5024	90	0
3	C	224	0	201	9	0
4	D	50	0	43	0	0
4	G	50	0	43	2	0
5	E	28	0	25	2	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	0	0
6	F	72	0	61	2	0
7	J	39	0	34	1	0
7	L	39	0	34	0	0
8	A	42	0	39	0	0
8	B	28	0	26	1	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	B	2	0	0	0	0
All	All	13158	0	12617	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 212 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:617:ILE:HB	1:A:623:ASN:ND2	1.82	0.95
2:B:443:PRO:HG2	2:B:460:CYS:HB3	1.51	0.90
1:A:914:GLN:HE22	1:A:955:ILE:HD12	1.43	0.83
1:A:455:ASN:HD22	1:A:593:LEU:HD22	1.43	0.83
3:C:4:ARG:HH21	3:C:5:PRO:HD2	1.48	0.79

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	920/967 (95%)	850 (92%)	68 (7%)	2 (0%)	47	79
2	B	688/695 (99%)	606 (88%)	79 (12%)	3 (0%)	34	68
3	C	30/32 (94%)	24 (80%)	6 (20%)	0	100	100
All	All	1638/1694 (97%)	1480 (90%)	153 (9%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	GLU
2	B	343	LEU
2	B	509	HIS
1	A	569	ALA
2	B	480	PRO

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

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	784/821 (96%)	778 (99%)	6 (1%)	81	92
2	B	612/617 (99%)	595 (97%)	17 (3%)	43	72
3	C	26/26 (100%)	26 (100%)	0	100	100
All	All	1422/1464 (97%)	1399 (98%)	23 (2%)	62	84

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	116	TYR
2	B	346	ASP
2	B	672	ASP
2	B	333	LEU
2	B	398	SER

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

Mol	Chain	Res	Type
1	A	455	ASN
1	A	494	GLN
1	A	623	ASN

### 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 ⓘ

28 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	$\# Z  > 2$
4	NAG	D	1	1,4	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	BMA	D	3	4	11,11,12	1.06	0	15,15,17	1.17	2 (13%)
4	MAN	D	4	4	11,11,12	0.90	0	15,15,17	1.17	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.46	0	17,19,21	1.32	2 (11%)
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	0.55	0
6	NAG	F	1	1,6	14,14,15	0.33	0	17,19,21	0.45	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.50	0
6	BMA	F	3	6	11,11,12	0.81	0	15,15,17	1.04	1 (6%)
6	BMA	F	4	6	11,11,12	1.82	4 (36%)	15,15,17	1.22	2 (13%)
6	MAN	F	5	6	11,11,12	1.12	2 (18%)	15,15,17	1.48	4 (26%)
6	MAN	F	6	6	11,11,12	1.08	1 (9%)	15,15,17	1.39	3 (20%)
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	G	2	4	14,14,15	0.62	1 (7%)	17,19,21	0.63	0
4	BMA	G	3	4	11,11,12	0.94	0	15,15,17	0.76	0
4	MAN	G	4	4	11,11,12	0.87	0	15,15,17	1.15	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.43	0	17,19,21	0.42	0
5	NAG	I	1	1,5	14,14,15	0.37	0	17,19,21	0.44	0
5	NAG	I	2	5	14,14,15	0.41	0	17,19,21	0.92	2 (11%)
7	NAG	J	1	1,7	14,14,15	0.54	0	17,19,21	0.59	0
7	NAG	J	2	7	14,14,15	0.41	0	17,19,21	0.43	0
7	BMA	J	3	7	11,11,12	0.83	0	15,15,17	0.82	0
5	NAG	K	1	2,5	14,14,15	0.32	0	17,19,21	0.48	0
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.85	1 (5%)
7	NAG	L	1	2,7	14,14,15	0.36	0	17,19,21	0.61	0
7	NAG	L	2	7	14,14,15	1.01	1 (7%)	17,19,21	1.45	1 (5%)
7	BMA	L	3	7	11,11,12	1.29	2 (18%)	15,15,17	1.30	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
6	BMA	F	4	6	-	2/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	4/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
7	NAG	L	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	1/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	2	NAG	O5-C1	3.62	1.49	1.43
6	F	4	BMA	C4-C5	3.23	1.59	1.53
6	F	4	BMA	C4-C3	2.64	1.59	1.52
6	F	5	MAN	C1-C2	2.57	1.58	1.52
6	F	4	BMA	O5-C5	2.55	1.48	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	L	2	NAG	C1-O5-C5	5.42	119.53	112.19
5	E	1	NAG	C2-N2-C7	4.43	129.21	122.90
7	L	3	BMA	C1-O5-C5	3.60	117.08	112.19
4	D	4	MAN	C1-O5-C5	3.12	116.42	112.19
6	F	5	MAN	C1-C2-C3	2.96	113.31	109.67

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6

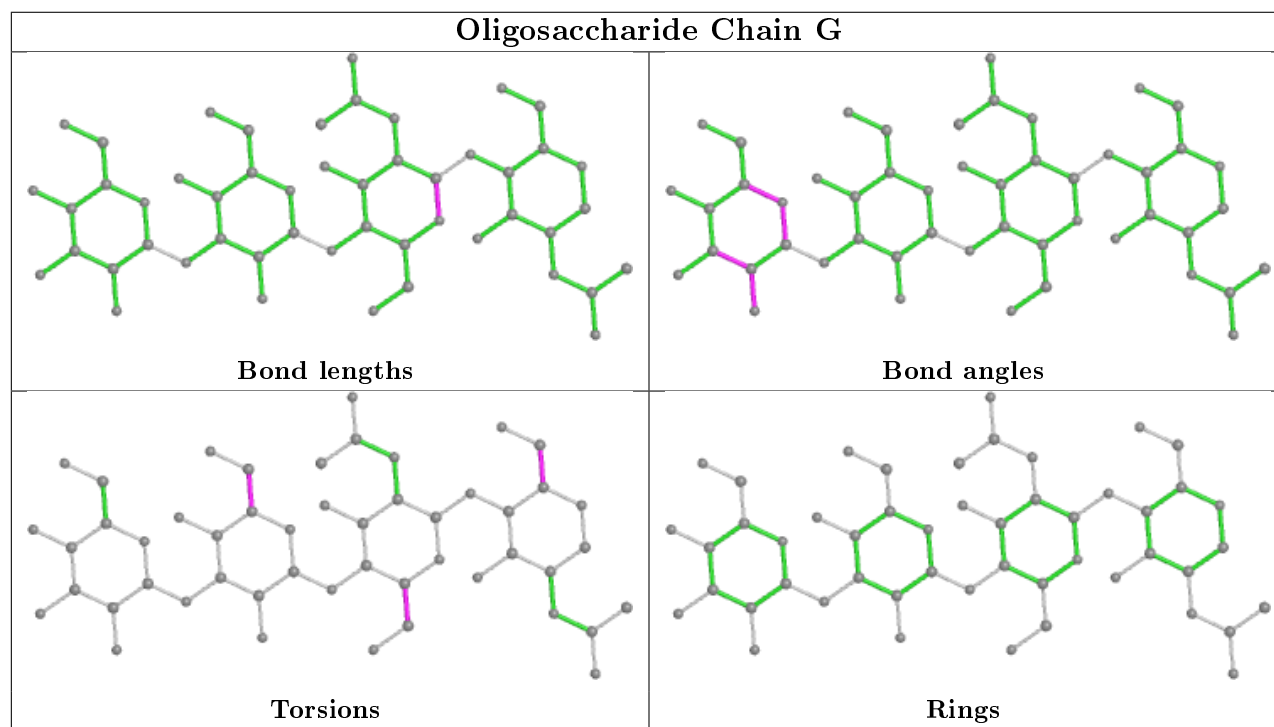
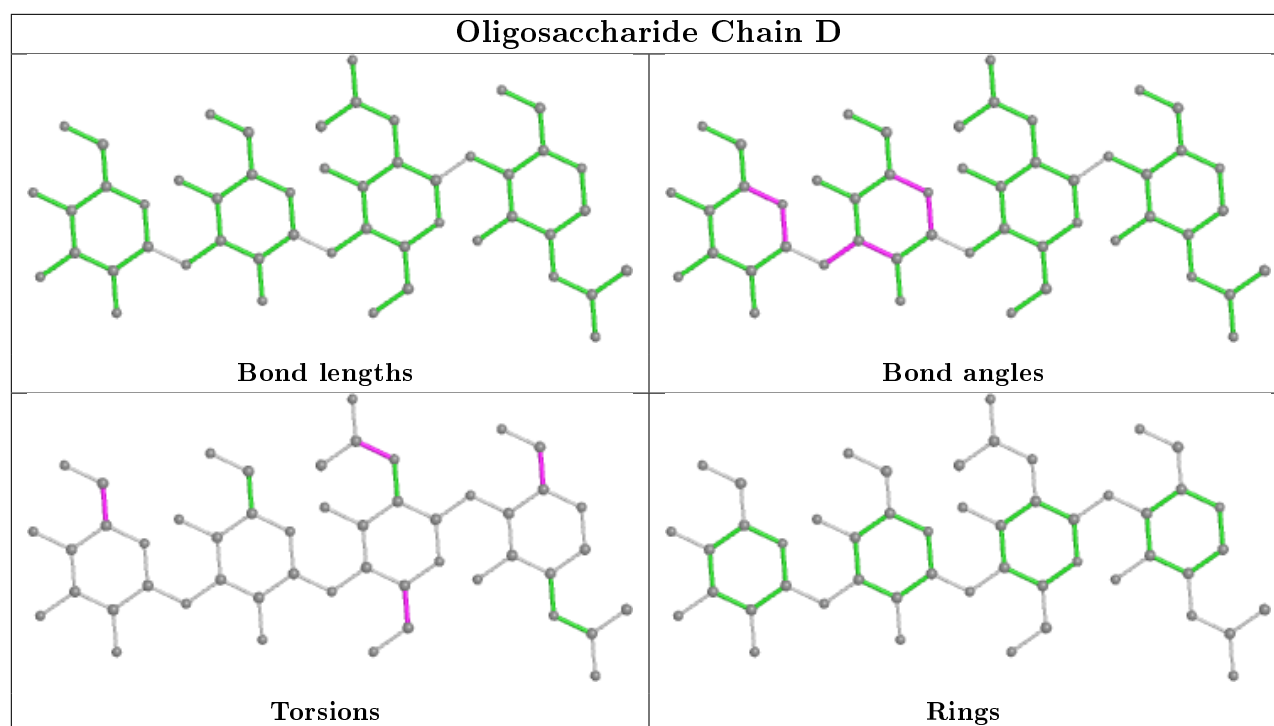
All (1) ring outliers are listed below:

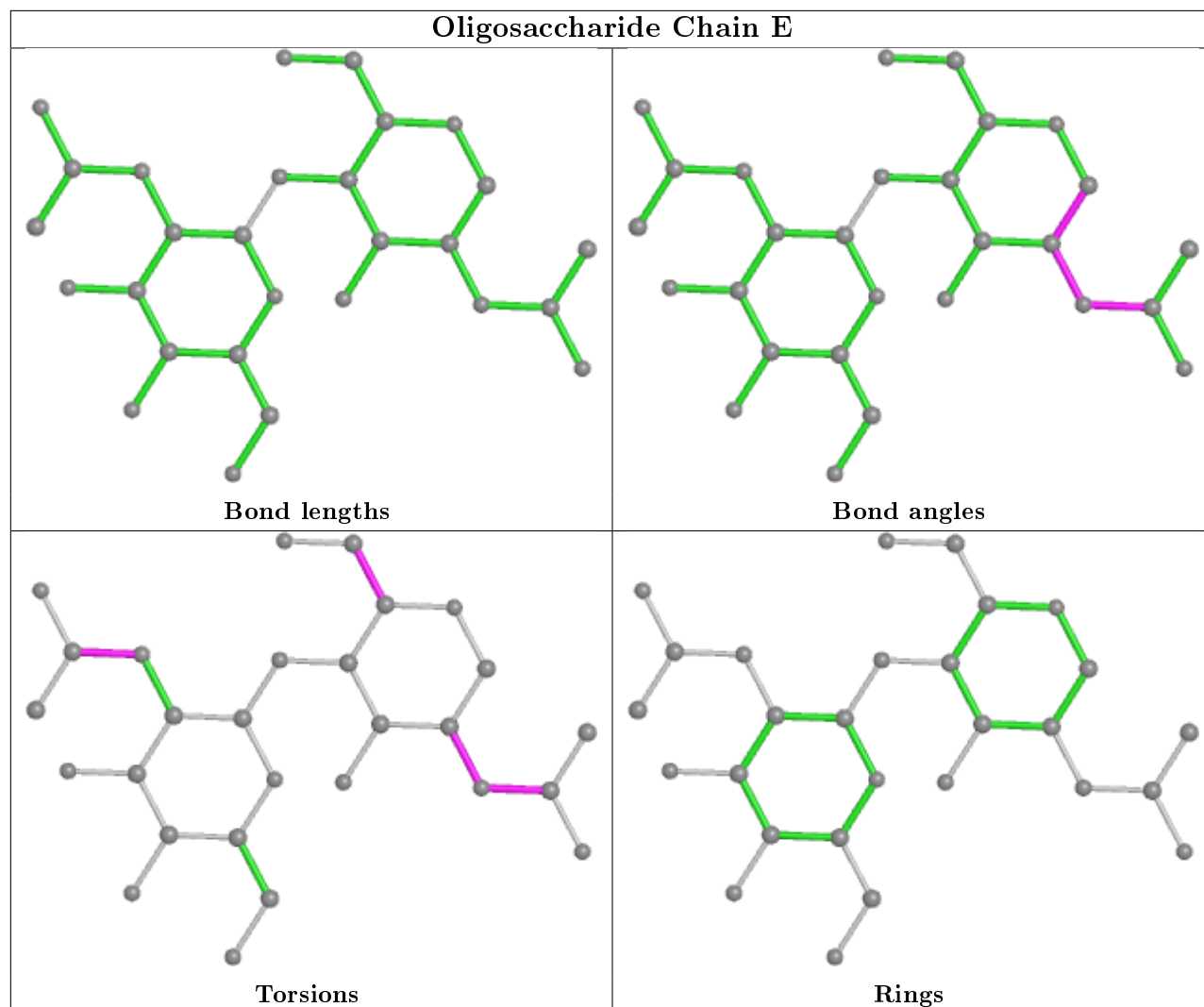
Mol	Chain	Res	Type	Atoms
7	L	3	BMA	C1-C2-C3-C4-C5-O5

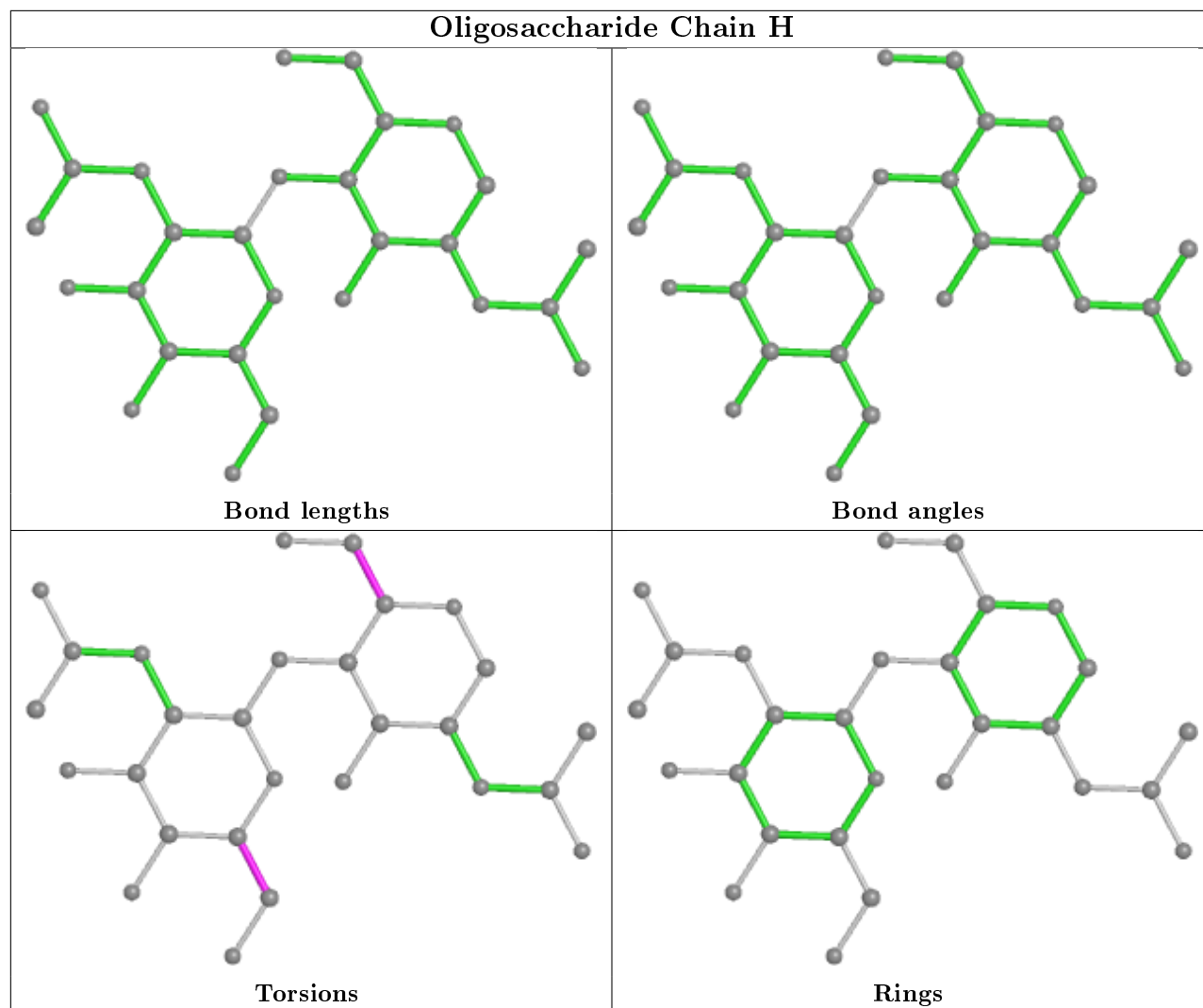
10 monomers are involved in 7 short contacts:

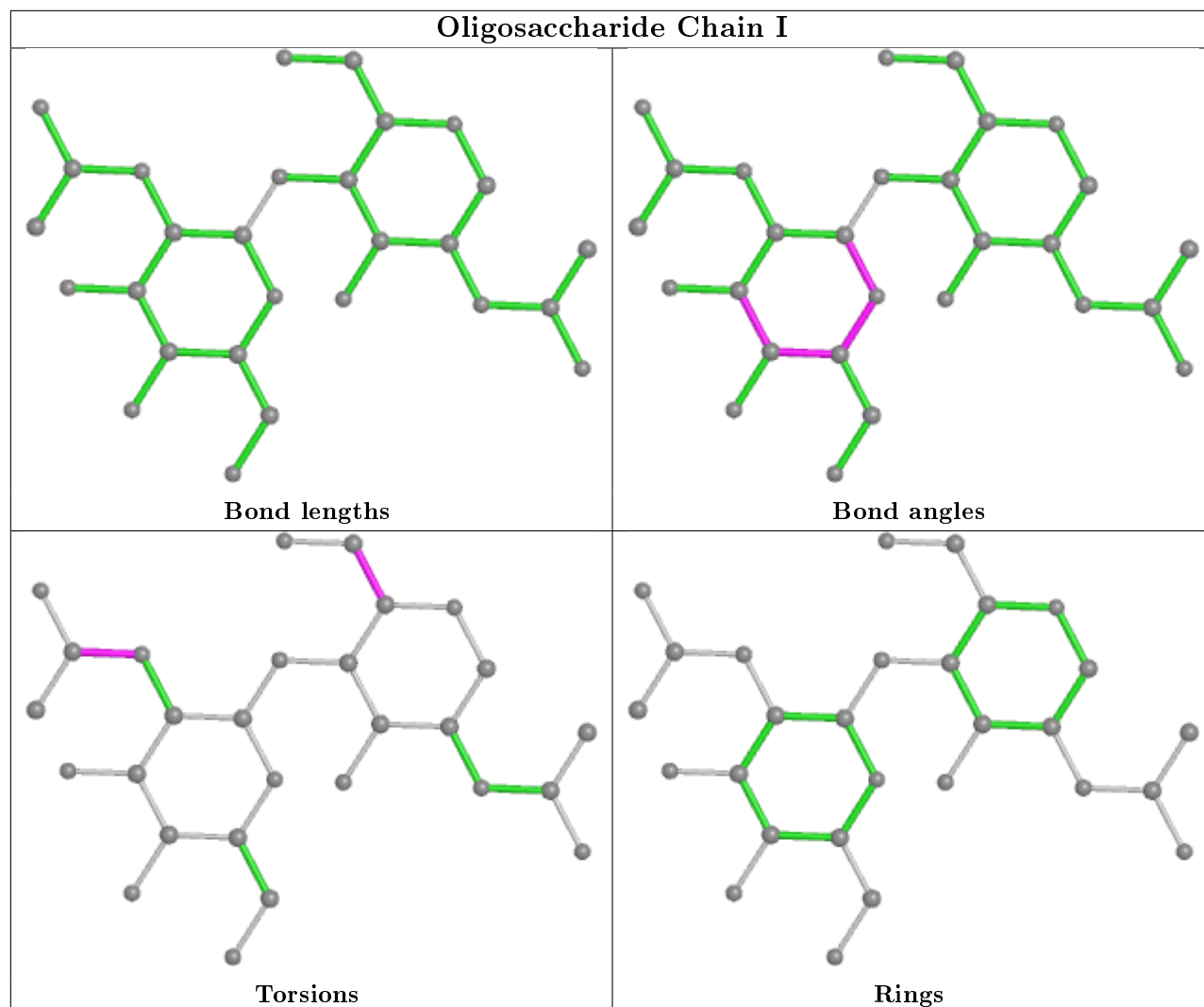
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	2	NAG	1	0
4	G	1	NAG	1	0
5	E	1	NAG	2	0
5	E	2	NAG	1	0
4	G	4	MAN	1	0
4	G	3	BMA	1	0
6	F	3	BMA	1	0
6	F	5	MAN	1	0
7	J	1	NAG	1	0
6	F	4	BMA	2	0

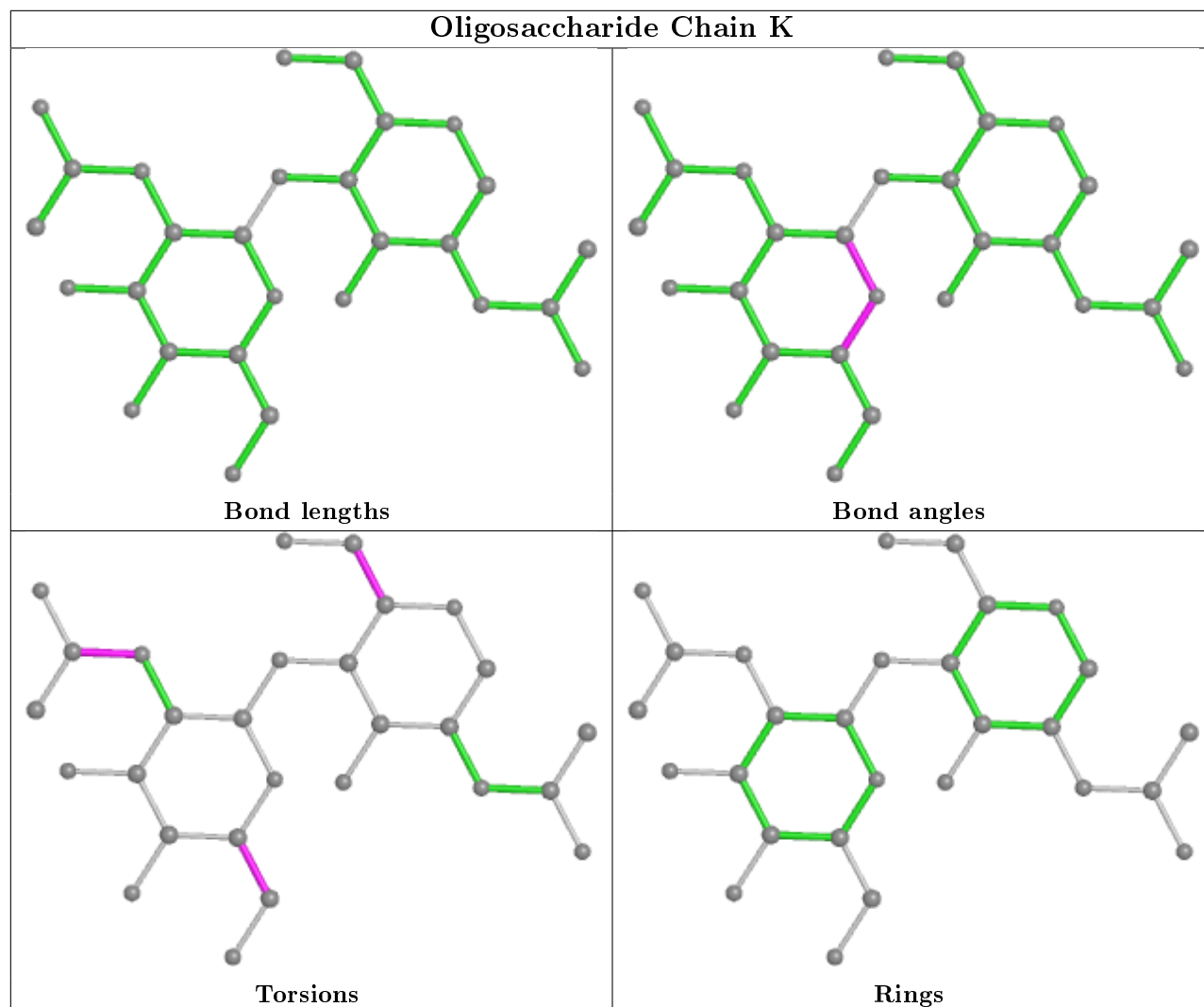
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

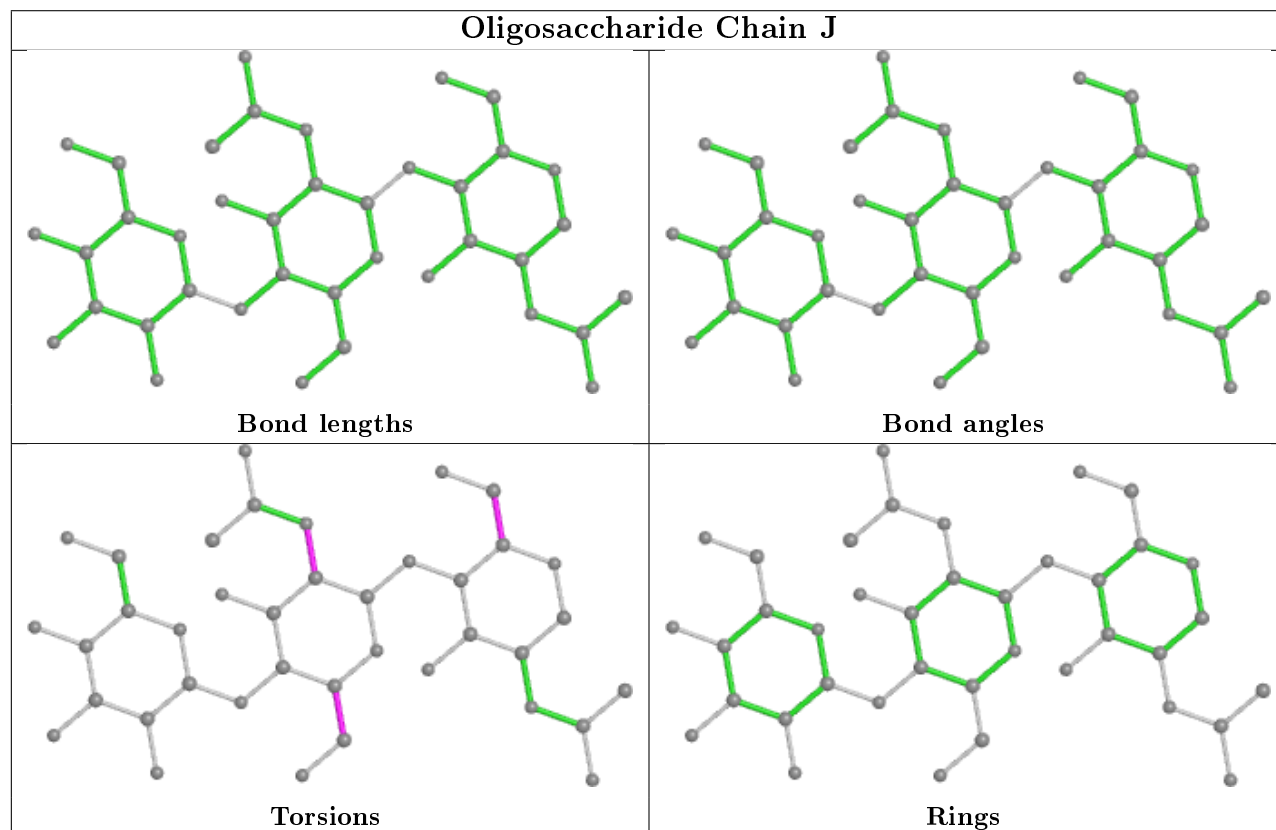
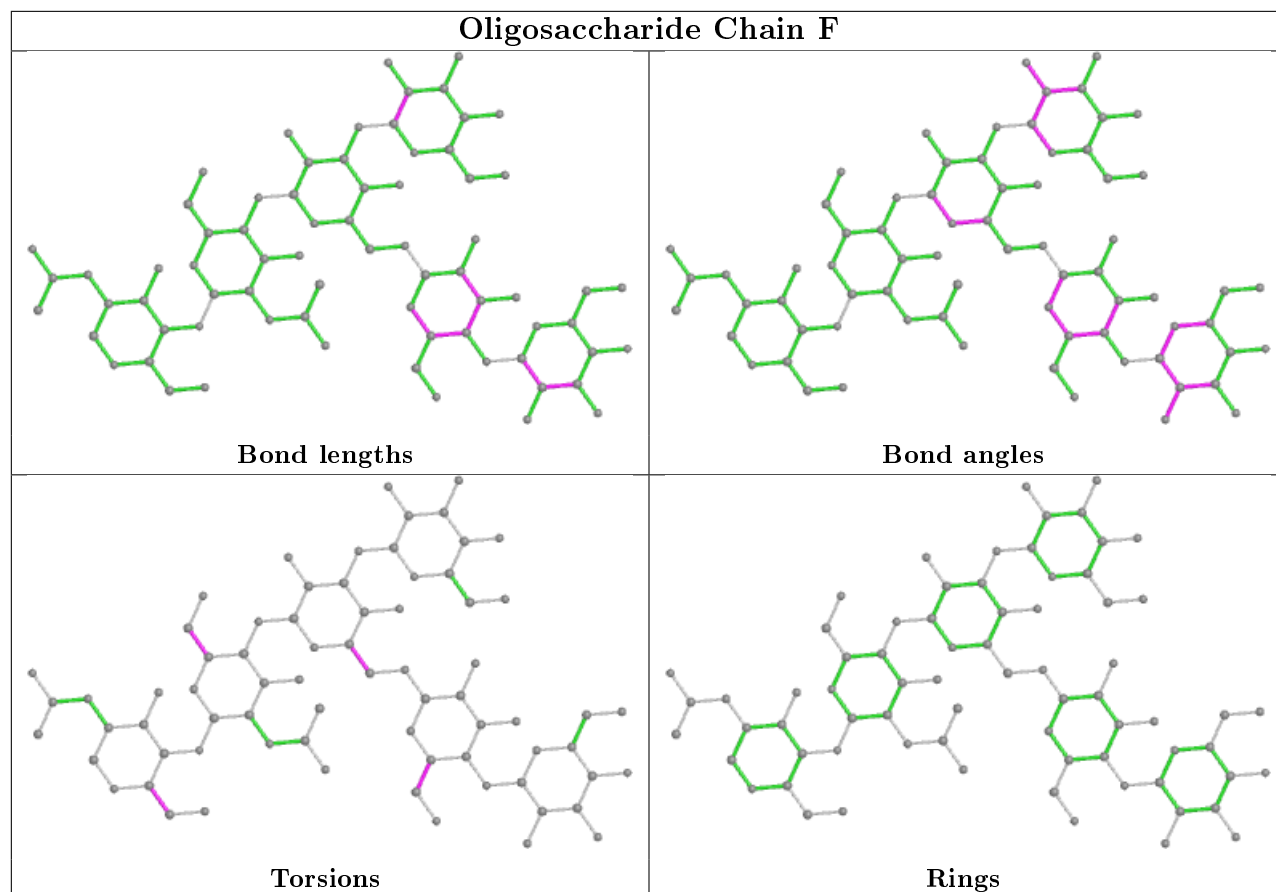




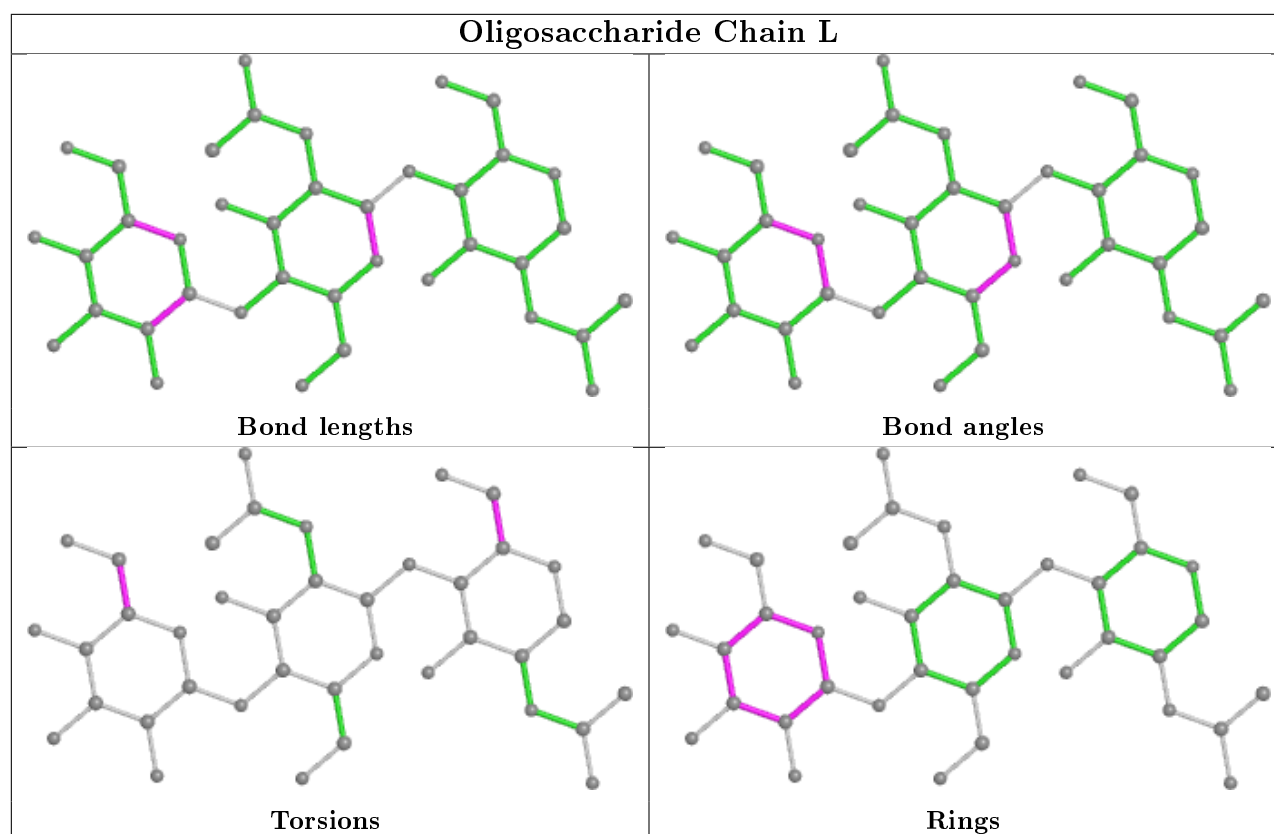












## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	$\# Z  > 2$
8	NAG	A	1017	1	14,14,15	0.33	0	17,19,21	0.50	0
8	NAG	B	701	2	14,14,15	0.85	1 (7%)	17,19,21	0.92	1 (5%)
8	NAG	A	1020	1	14,14,15	0.65	0	17,19,21	0.61	0
8	NAG	A	1021	1	14,14,15	0.46	0	17,19,21	0.58	0
8	NAG	B	702	2	14,14,15	0.47	0	17,19,21	0.78	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
8	NAG	A	1017	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	A	1020	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1021	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	NAG	O5-C1	2.52	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	NAG	C1-O5-C5	3.52	116.96	112.19
8	B	702	NAG	C1-O5-C5	2.69	115.84	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1017	NAG	C4-C5-C6-O6
8	A	1017	NAG	O5-C5-C6-O6
8	A	1020	NAG	O5-C5-C6-O6
8	A	1020	NAG	C4-C5-C6-O6
8	B	701	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
8	B	701	NAG	1	0

## 5.7 Other polymers

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

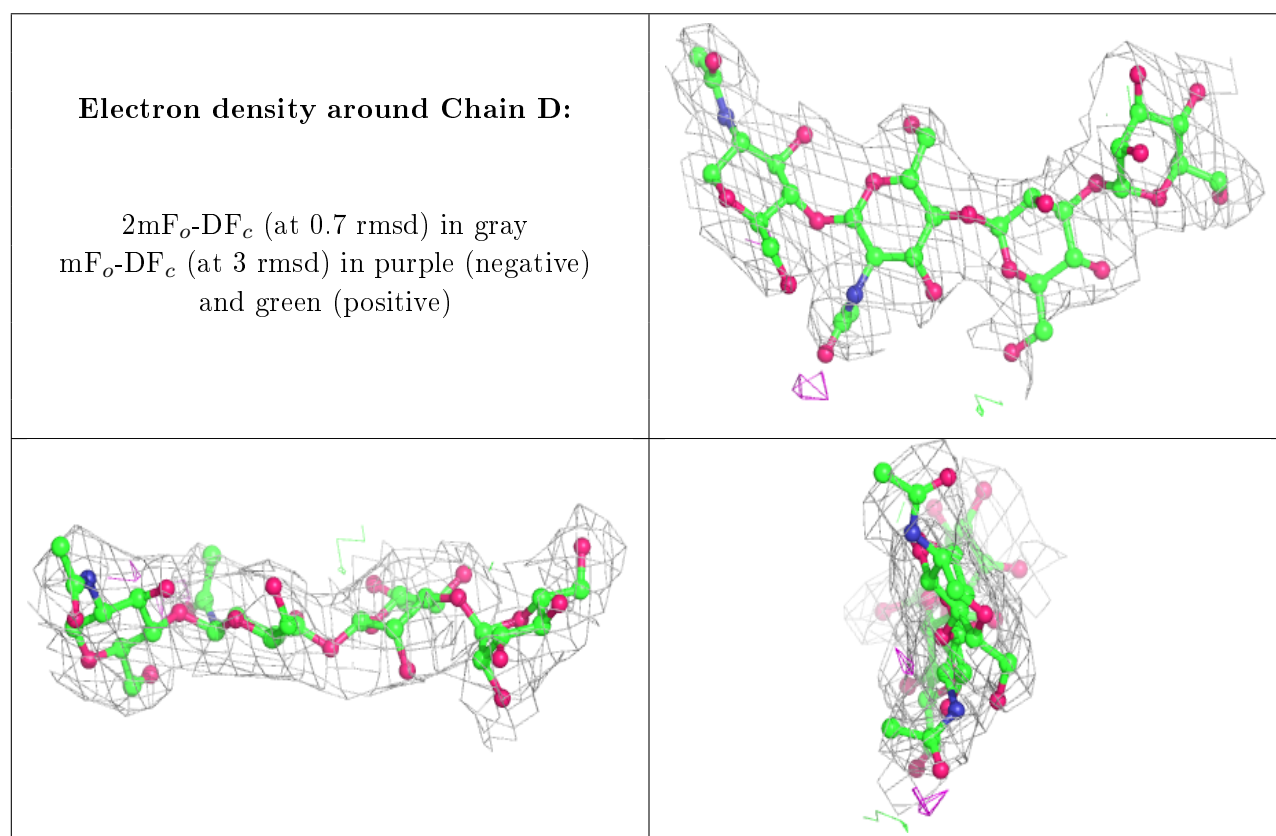
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

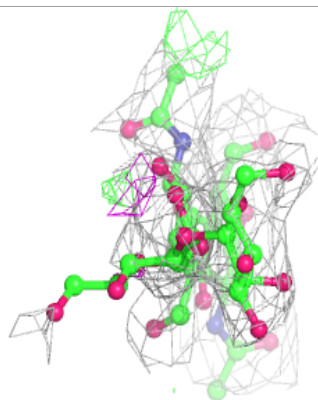
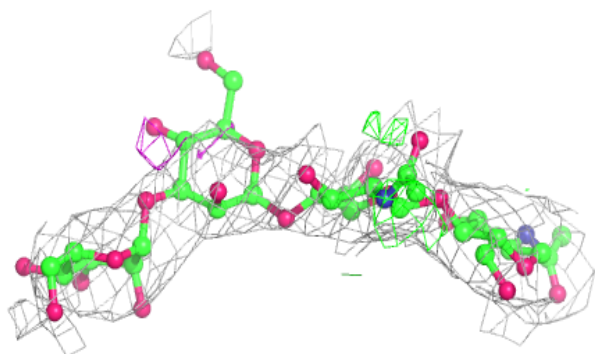
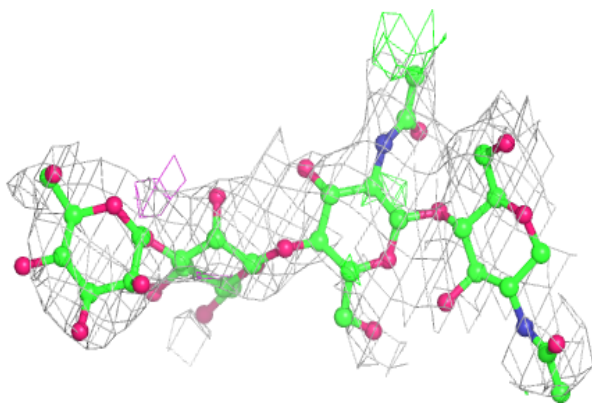
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



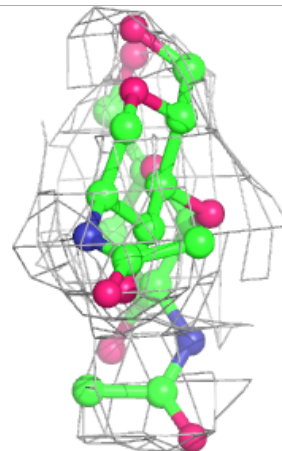
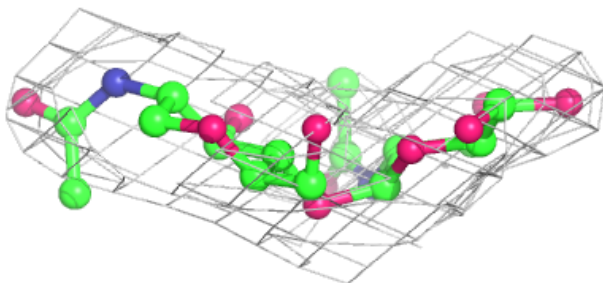
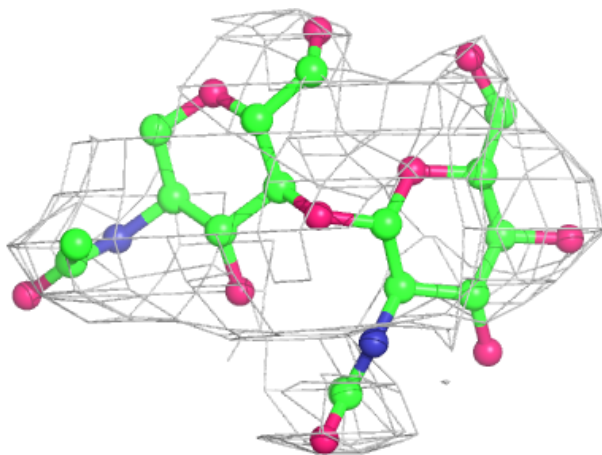
**Electron density around Chain G:**

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



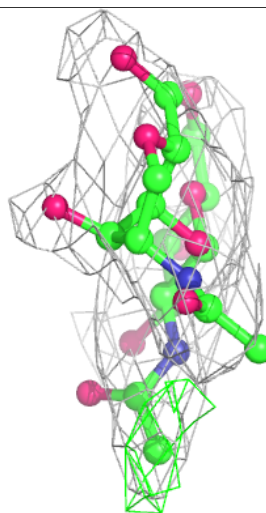
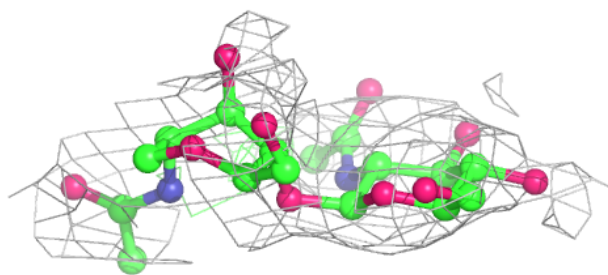
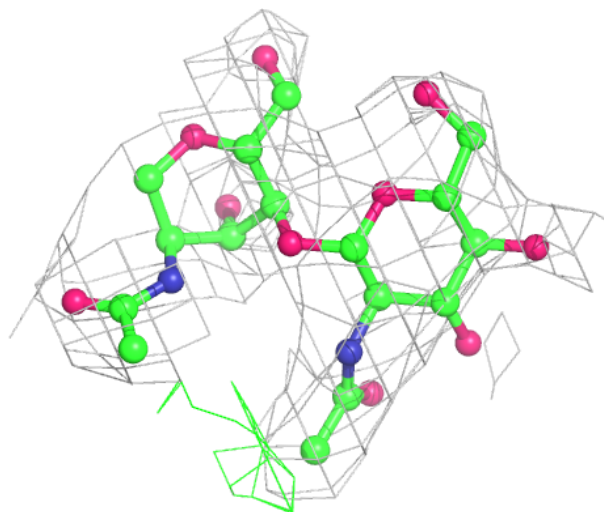
**Electron density around Chain E:**

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



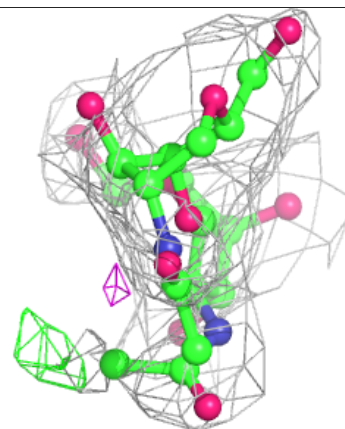
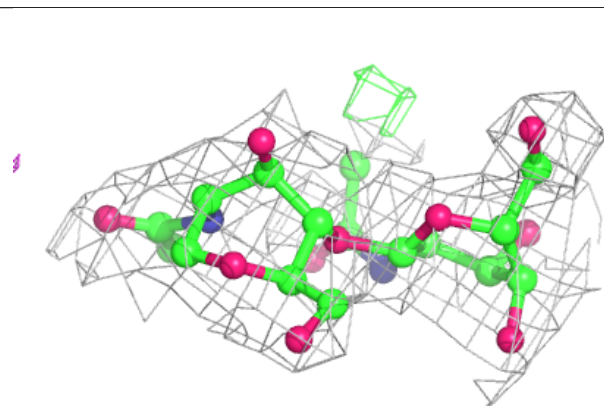
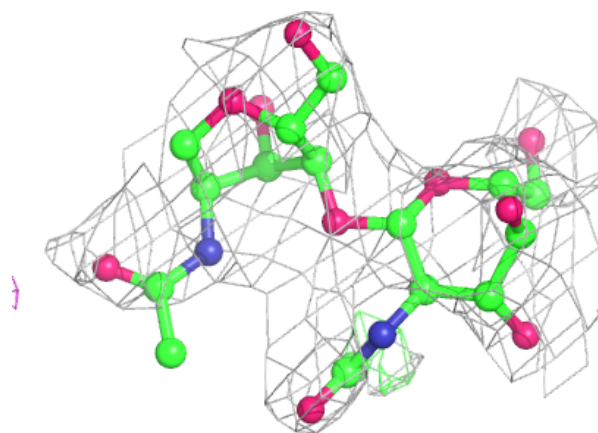
**Electron density around Chain H:**

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



**Electron density around Chain I:**

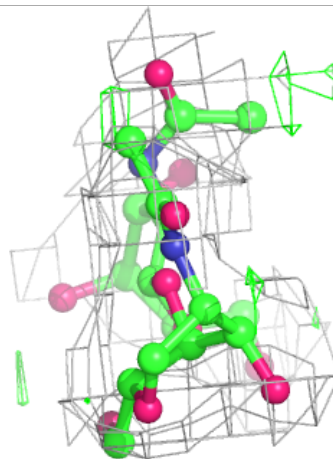
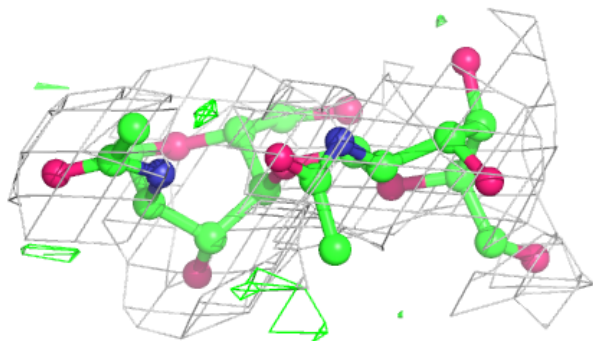
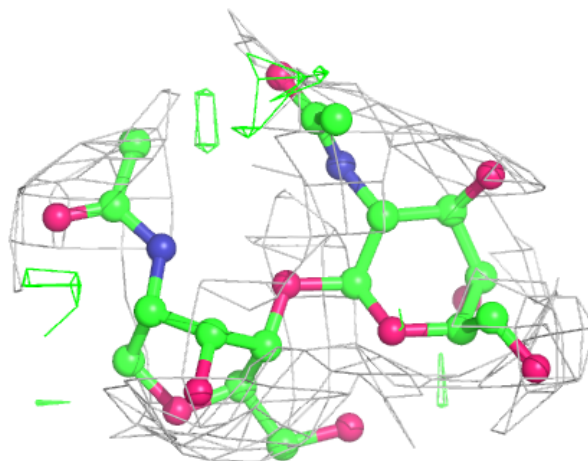
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





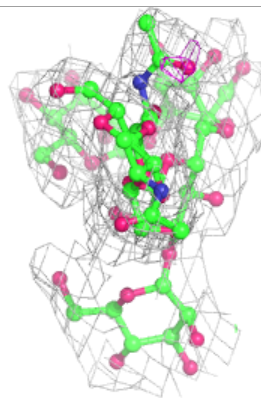
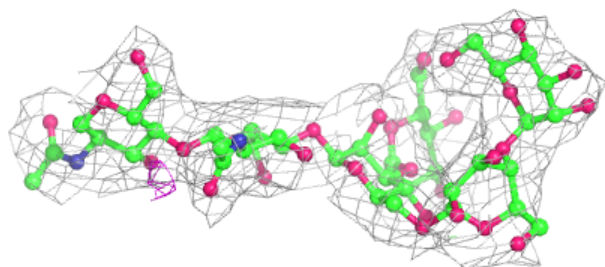
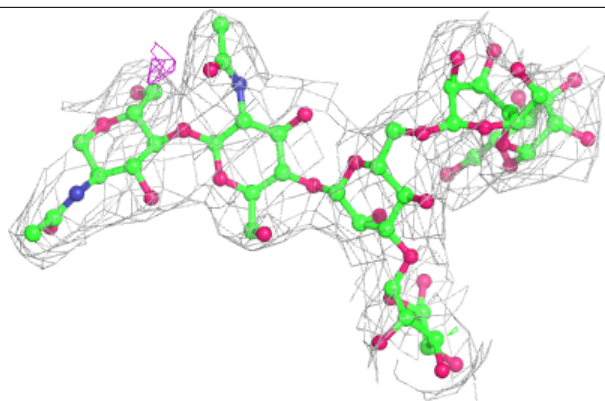
**Electron density around Chain K:**

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

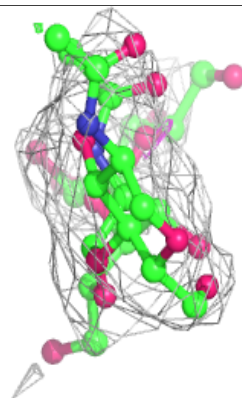
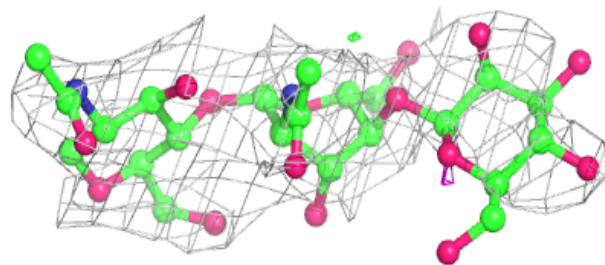
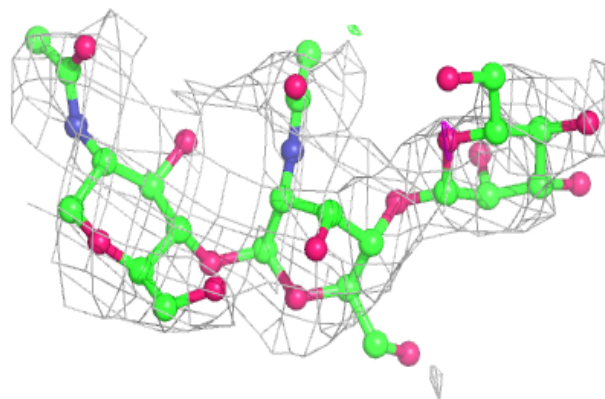


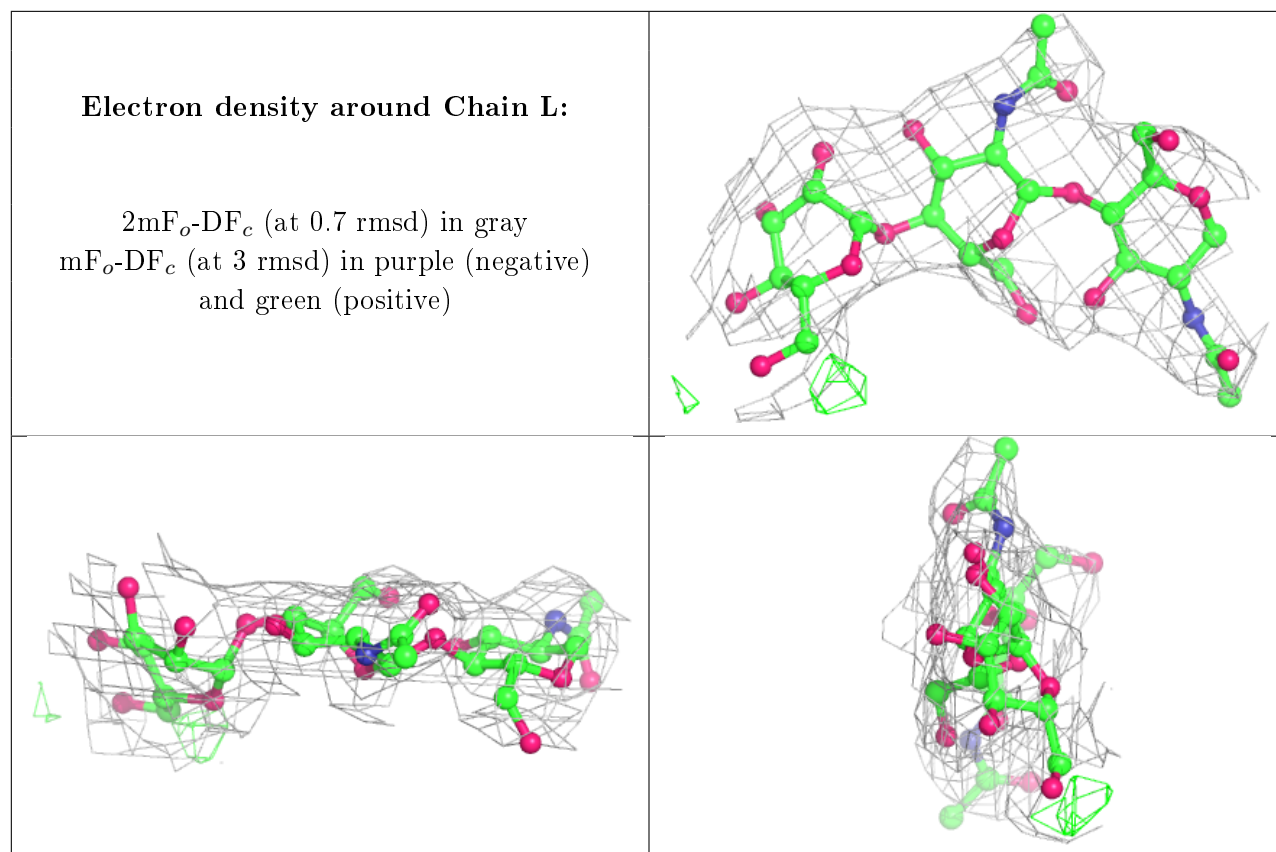
**Electron density around Chain F:**

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

**Electron density around Chain 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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.