



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:29 AM UTC

PDB ID : 6OM2 / pdb\_00006om2  
Title : Crystal structure of atypical integrin alphaV beta8 with proTGF-beta1 ligand peptide  
Authors : Wang, J.C.; Springer, T.A.  
Deposited on : 2019-04-17  
Resolution : 2.77 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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

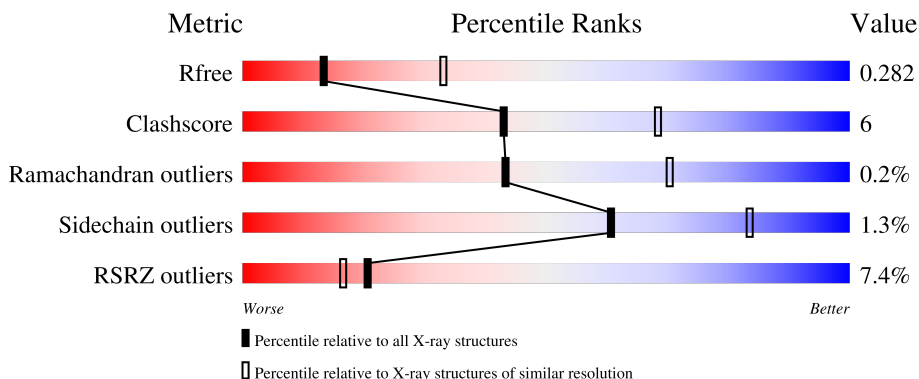
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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))
$R_{free}$	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	598	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	C	598	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
2	B	421	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div>
2	D	421	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: grey;"></div> </div>
3	E	11	<div style="display: flex; align-items: center;"> <div style="width: 45%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	F	11	 64% 9% 9% 18%
4	G	3	 100%
4	K	3	 67% 33%
4	S	3	 100%
5	H	7	 14% 86%
5	L	7	 14% 57% 29%
5	O	7	 29% 71%
6	I	5	 40% 40% 20%
7	J	4	 25% 25% 50%
8	M	2	 50% 50%
8	P	2	 100%
8	Q	2	 100%
8	R	2	 50% 50%
9	N	6	 50% 50%

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
8	NAG	M	1	-	-	X	-
8	NAG	M	2	-	-	X	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28790 atoms, of which 13455 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	
			Total	C	H	N	O				S
1	A	598	8991	2927	4371	785	887	21	0	0	0
1	C	596	8981	2923	4369	783	885	21	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	engineered mutation	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
C	400	GLY	-	insertion	UNP P06756
C	401	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	310	4747	1551	2301	419	460	16	0	0	0
2	D	330	5003	1638	2414	446	489	16	0	0	0

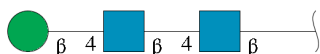
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	CYS	VAL	engineered mutation	UNP P26012
D	259	CYS	VAL	engineered mutation	UNP P26012

- Molecule 3 is a protein called proTGF-beta1 RGD peptide.

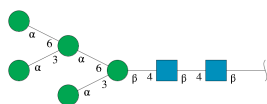
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	10	68	40	16	12	0	0	1
3	F	9	64	38	15	11	0	0	1

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



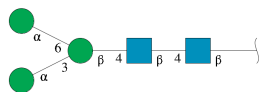
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	3	39	22	2	15	0	0	0
4	K	3	39	22	2	15	0	0	0
4	S	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	7	83	46	2	35	0	0	0
5	L	7	83	46	2	35	0	0	0
5	O	7	83	46	2	35	0	0	0

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



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

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



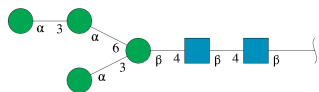
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	J	4	50	28	2	20	0	0	0

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



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

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

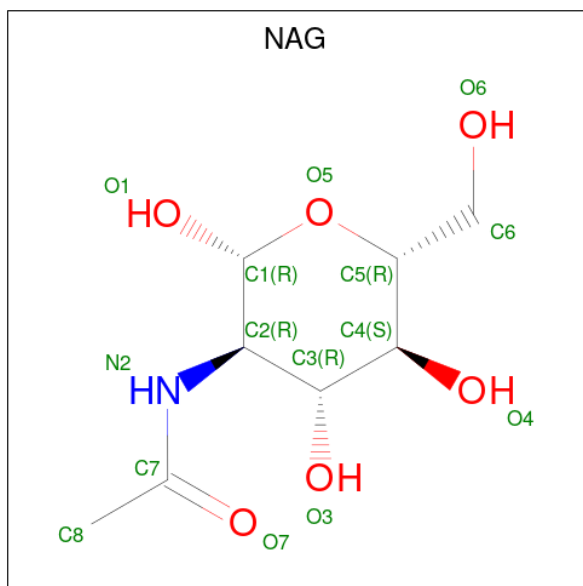


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	N	6	72	40	2	30	0	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
10	A	4	4	4	0	0
10	B	1	1	1	0	0
10	C	4	4	4	0	0
10	D	1	1	1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



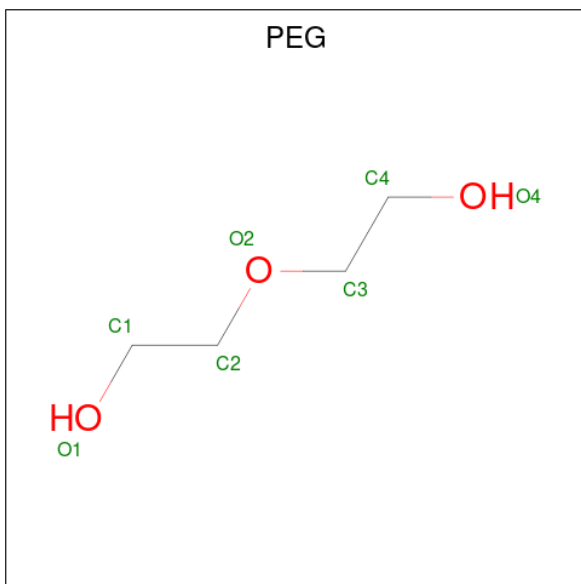
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	A	1	14	8	1	5	0	0
11	A	1	14	8	1	5	0	0

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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).

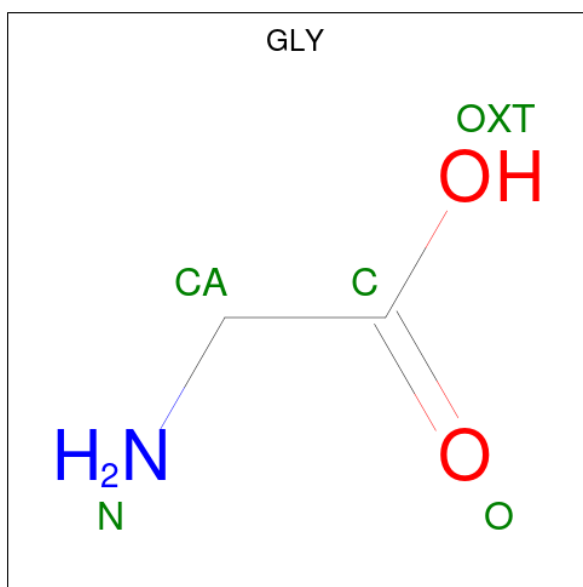


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Mg	0	0
			1	1		
13	D	1	Total	Mg	0	0
			1	1		

- Molecule 14 is GLYCINE (CCD ID: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	C	1	4	2	1	1	0	0

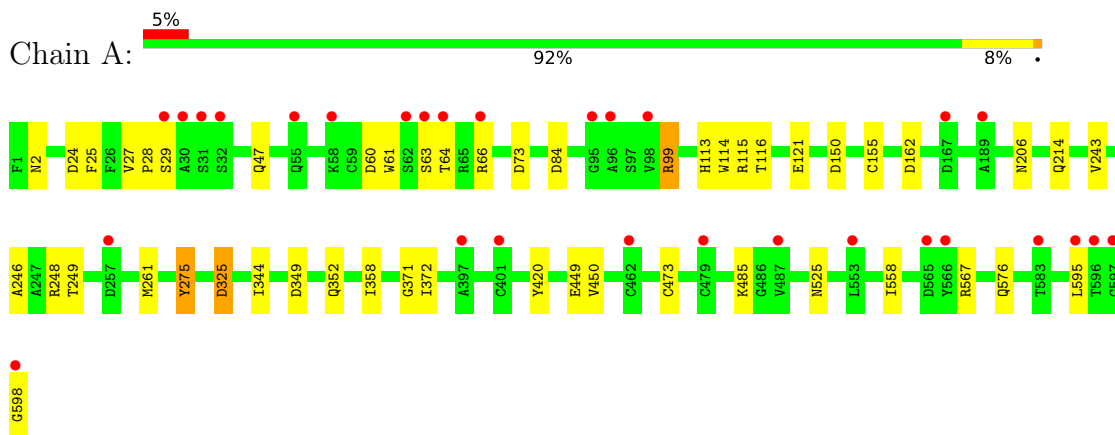
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	75	Total	O	0	0
			75	75		
15	B	11	Total	O	0	0
			11	11		
15	C	97	Total	O	0	0
			97	97		
15	D	19	Total	O	0	0
			19	19		
15	E	1	Total	O	0	0
			1	1		

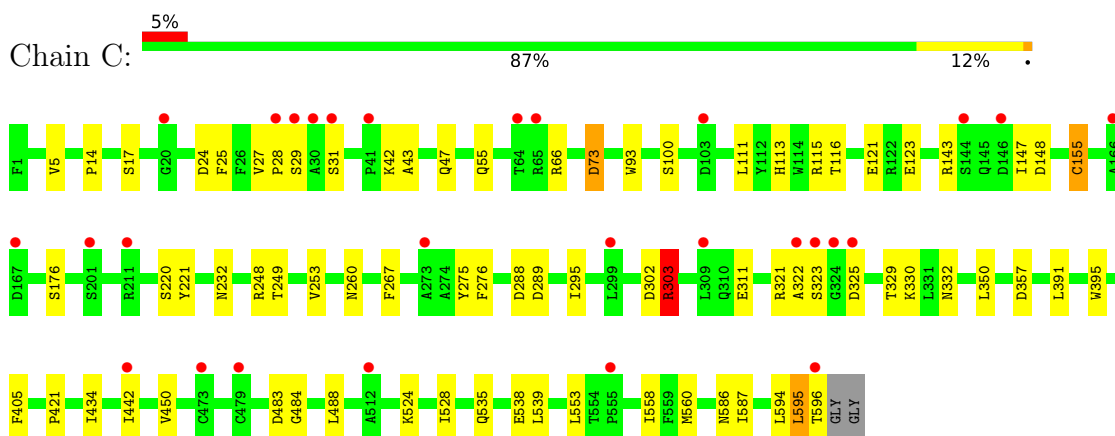
### 3 Residue-property plots [i](#)

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.

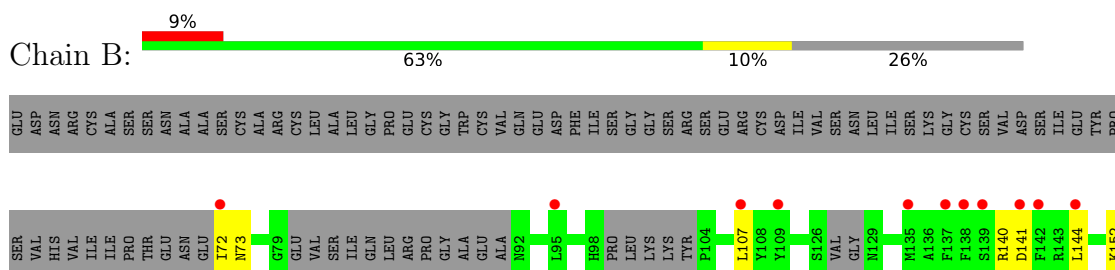
- Molecule 1: Integrin alpha-V

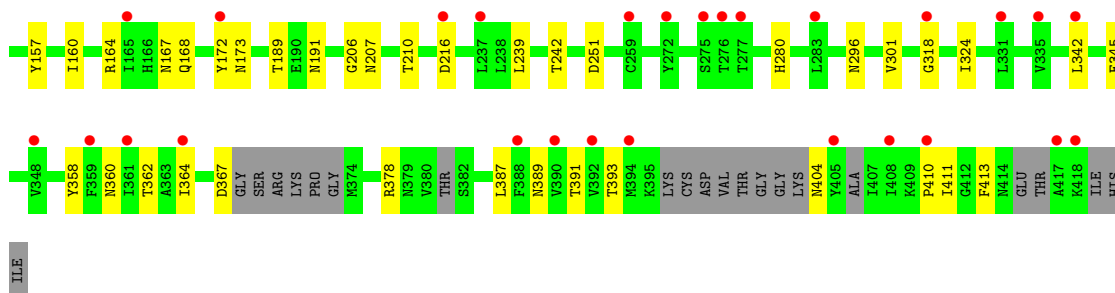


- Molecule 1: Integrin alpha-V

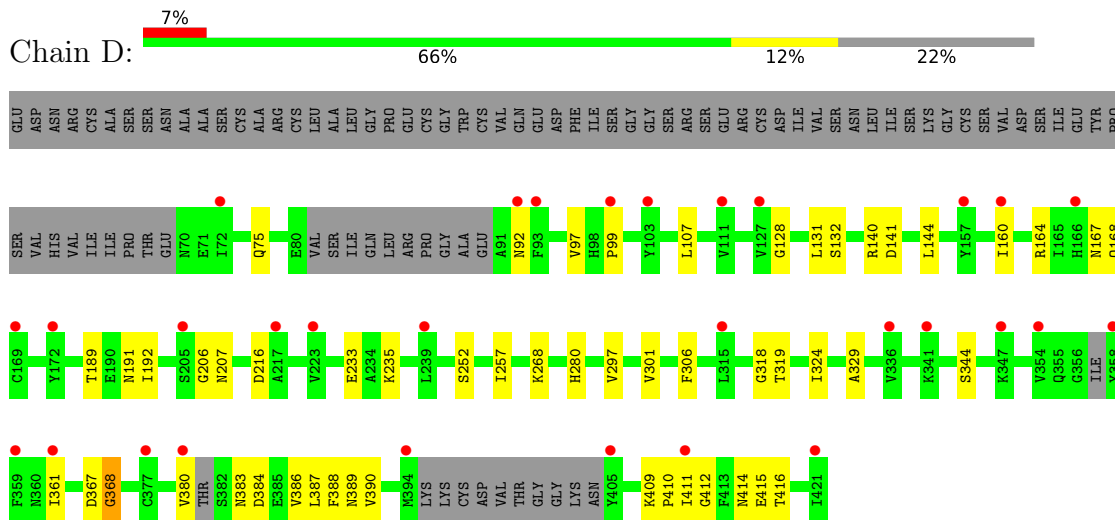


- Molecule 2: Integrin beta-8

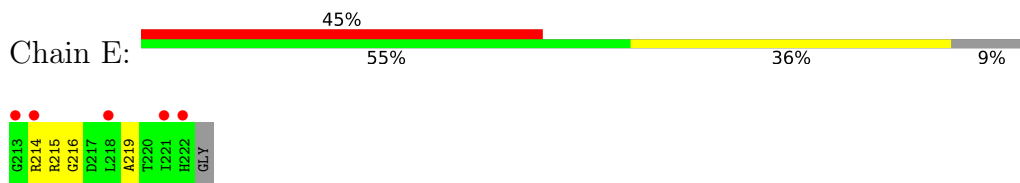




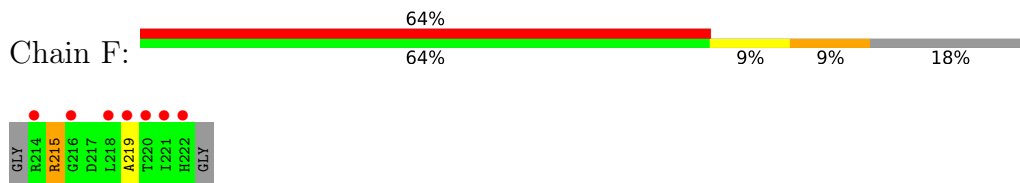
- Molecule 2: Integrin beta-8



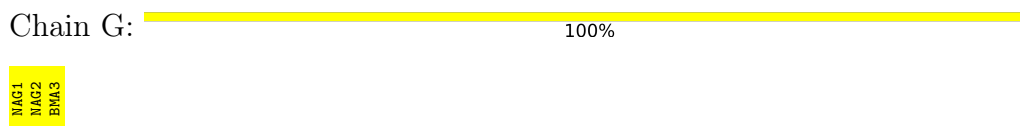
- Molecule 3: proTGF-beta1 RGD peptide



- Molecule 3: proTGF-beta1 RGD peptide



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

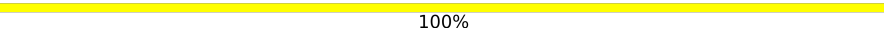


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain S:  100%

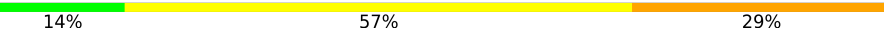
MAG1  
MAG2  
BMA3

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

Chain H:  14% 86%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

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

Chain L:  14% 57% 29%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

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

Chain O:  29% 71%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 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 I:  40% 40% 20%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 7: 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 J:  25% 25% 50%

  
MAG1  
MAG2  
BMA3  
MAN4

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

Chain M:  50% 50%

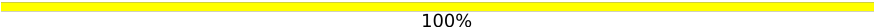
  
MAG1  
MAG2

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

Chain P:  100%

  
MAG1  
MAG2

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

Chain Q:  100%

  
MAG1  
MAG2


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

Chain R:  50% 50%

  
MAG1  
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.19Å 53.85Å 176.62Å 90.00° 111.47° 90.00°	Depositor
Resolution (Å)	47.43 – 2.77 47.43 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.43-2.77) 98.6 (47.43-2.77)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.251 , 0.282 0.253 , 0.282	Depositor DCC
$R_{free}$ test set	2000 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: NAG, BMA, MAN, PEG, CA, MG

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	0.12	0/4724	0.30	0/6395
1	C	0.14	0/4716	0.33	0/6385
2	B	0.12	0/2489	0.34	0/3361
2	D	0.12	0/2639	0.32	0/3571
3	E	0.11	0/67	0.37	0/88
3	F	0.13	0/63	0.37	0/83
All	All	0.13	0/14698	0.32	0/19883

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4620	4371	4468	35	0
1	C	4612	4369	4462	52	0
2	B	2446	2301	2412	30	0
2	D	2589	2414	2554	37	0
3	E	68	0	70	3	0
3	F	64	0	67	1	0
4	G	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	39	0	34	0	0
4	S	39	0	34	5	0
5	H	83	0	70	1	0
5	L	83	0	70	3	0
5	O	83	0	70	7	0
6	I	61	0	52	4	0
7	J	50	0	43	4	0
8	M	28	0	25	11	0
8	P	28	0	25	0	0
8	Q	28	0	25	2	0
8	R	28	0	25	5	0
9	N	72	0	61	0	0
10	A	4	0	0	0	0
10	B	1	0	0	0	0
10	C	4	0	0	0	0
10	D	1	0	0	0	0
11	A	28	0	26	0	0
11	D	14	0	13	1	0
12	A	7	0	10	0	0
12	C	7	0	10	1	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
14	C	4	0	2	1	0
15	A	75	0	0	6	0
15	B	11	0	0	0	0
15	C	97	0	0	3	0
15	D	19	0	0	2	0
15	E	1	0	0	0	0
All	All	15335	13455	14662	184	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 6.

The worst 5 of 184 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)
2:D:233:GLU:OE1	8:R:2:NAG:O4	1.88	0.89
1:A:121:GLU:OE1	2:B:164:ARG:NH2	2.12	0.82
1:C:289:ASP:OD2	5:H:2:NAG:H5	1.80	0.81
8:M:1:NAG:H62	8:M:2:NAG:N2	1.96	0.80
5:O:3:BMA:H2	5:O:7:MAN:H2	1.66	0.78

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	596/598 (100%)	551 (92%)	45 (8%)	0	100	100
1	C	594/598 (99%)	562 (95%)	31 (5%)	1 (0%)	43	70
2	B	292/421 (69%)	264 (90%)	28 (10%)	0	100	100
2	D	320/421 (76%)	295 (92%)	23 (7%)	2 (1%)	21	47
3	E	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
3	F	7/11 (64%)	7 (100%)	0	0	100	100
All	All	1817/2060 (88%)	1686 (93%)	128 (7%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	388	PHE
1	C	303	ARG
2	D	368	GLY

### 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	488/488 (100%)	482 (99%)	6 (1%)	63	84
1	C	488/488 (100%)	477 (98%)	11 (2%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	277/369 (75%)	276 (100%)	1 (0%)	84	93
2	D	291/369 (79%)	290 (100%)	1 (0%)	86	94
3	E	6/7 (86%)	6 (100%)	0	100	100
3	F	6/7 (86%)	5 (83%)	1 (17%)	2	7
All	All	1556/1728 (90%)	1536 (99%)	20 (1%)	61	83

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	323	SER
1	C	595	LEU
3	F	215	ARG
2	D	207	ASN
2	B	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	120	ASN
1	C	592	HIS
2	B	302	GLN
1	C	590	GLN
2	B	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

53 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	G	1	4,1	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	0.70	0	15,15,17	0.78	0
5	NAG	H	1	5,1	14,14,15	0.19	0	17,19,21	0.50	0
5	NAG	H	2	5	14,14,15	0.52	0	17,19,21	0.47	0
5	BMA	H	3	5	11,11,12	0.79	0	15,15,17	0.98	1 (6%)
5	MAN	H	4	5	11,11,12	1.13	1 (9%)	15,15,17	0.88	0
5	MAN	H	5	5	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
5	MAN	H	6	5	11,11,12	1.30	1 (9%)	15,15,17	1.07	1 (6%)
5	MAN	H	7	5	11,11,12	0.90	1 (9%)	15,15,17	0.82	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.45	0	17,19,21	0.51	0
6	NAG	I	2	6	14,14,15	0.18	0	17,19,21	0.51	0
6	BMA	I	3	6	11,11,12	0.71	0	15,15,17	0.81	0
6	MAN	I	4	6	11,11,12	0.68	0	15,15,17	0.94	2 (13%)
6	MAN	I	5	6	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
7	NAG	J	1	7,1	14,14,15	0.18	0	17,19,21	0.44	0
7	NAG	J	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	BMA	J	3	7	11,11,12	1.00	1 (9%)	15,15,17	1.36	1 (6%)
7	MAN	J	4	7	11,11,12	0.78	1 (9%)	15,15,17	1.27	2 (13%)
4	NAG	K	1	4,2	14,14,15	0.77	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.37	0
4	BMA	K	3	4	11,11,12	0.54	0	15,15,17	0.87	0
5	NAG	L	1	5,1	14,14,15	0.43	0	17,19,21	0.45	0
5	NAG	L	2	5	14,14,15	0.34	0	17,19,21	0.41	0
5	BMA	L	3	5	11,11,12	0.68	0	15,15,17	0.86	1 (6%)
5	MAN	L	4	5	11,11,12	0.91	1 (9%)	15,15,17	1.41	2 (13%)
5	MAN	L	5	5	11,11,12	0.86	1 (9%)	15,15,17	1.48	4 (26%)
5	MAN	L	6	5	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
5	MAN	L	7	5	11,11,12	0.61	0	15,15,17	1.06	2 (13%)
8	NAG	M	1	8,1	14,14,15	0.42	0	17,19,21	0.43	0
8	NAG	M	2	8	14,14,15	0.53	0	17,19,21	0.65	1 (5%)
9	NAG	N	1	9,1	14,14,15	0.30	0	17,19,21	0.44	0
9	NAG	N	2	9	14,14,15	0.19	0	17,19,21	0.48	0
9	BMA	N	3	9	11,11,12	0.65	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	N	4	9	11,11,12	0.83	1 (9%)	15,15,17	0.87	1 (6%)
9	MAN	N	5	9	11,11,12	0.70	0	15,15,17	1.00	2 (13%)
9	MAN	N	6	9	11,11,12	0.72	0	15,15,17	0.90	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.18	0	17,19,21	0.49	0
5	NAG	O	2	5	14,14,15	0.29	0	17,19,21	0.53	0
5	BMA	O	3	5	11,11,12	1.07	0	15,15,17	1.15	1 (6%)
5	MAN	O	4	5	11,11,12	0.86	1 (9%)	15,15,17	1.28	2 (13%)
5	MAN	O	5	5	11,11,12	0.73	0	15,15,17	1.48	2 (13%)
5	MAN	O	6	5	11,11,12	0.73	1 (9%)	15,15,17	1.34	2 (13%)
5	MAN	O	7	5	11,11,12	0.76	0	15,15,17	1.05	2 (13%)
8	NAG	P	1	8,1	14,14,15	0.40	0	17,19,21	0.53	0
8	NAG	P	2	8	14,14,15	0.36	0	17,19,21	0.53	0
8	NAG	Q	1	8,1	14,14,15	0.46	0	17,19,21	0.46	0
8	NAG	Q	2	8	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	R	1	2,8	14,14,15	0.67	0	17,19,21	0.70	1 (5%)
8	NAG	R	2	8	14,14,15	0.25	0	17,19,21	0.67	0
4	NAG	S	1	4,2	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	S	2	4	14,14,15	0.25	0	17,19,21	0.37	0
4	BMA	S	3	4	11,11,12	0.58	0	15,15,17	0.83	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
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	6	MAN	O5-C1	-3.56	1.37	1.43
5	H	4	MAN	O5-C1	-3.34	1.38	1.43
5	H	7	MAN	O5-C1	-2.47	1.39	1.43
5	L	5	MAN	C1-C2	2.34	1.57	1.52
7	J	3	BMA	O3-C3	2.31	1.48	1.43

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	5	MAN	C1-O5-C5	4.23	117.86	112.19
7	J	3	BMA	O3-C3-C2	3.72	117.64	110.05
7	J	4	MAN	C1-O5-C5	3.69	117.13	112.19
5	L	5	MAN	C1-O5-C5	3.58	116.98	112.19
5	L	4	MAN	C1-O5-C5	3.49	116.86	112.19

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	4	MAN	C4-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	C1-C2-C3-C4-C5-O5
5	O	7	MAN	C1-C2-C3-C4-C5-O5

28 monomers are involved in 44 short contacts:

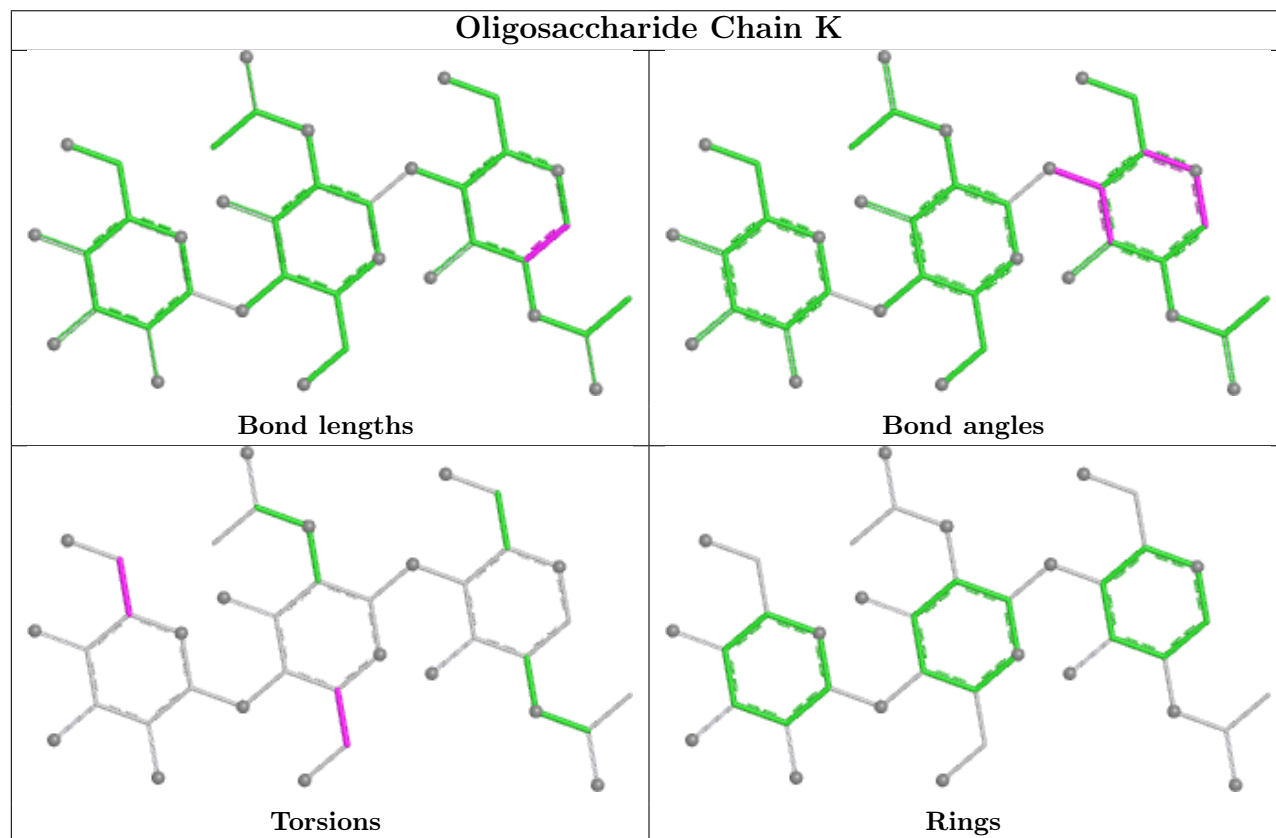
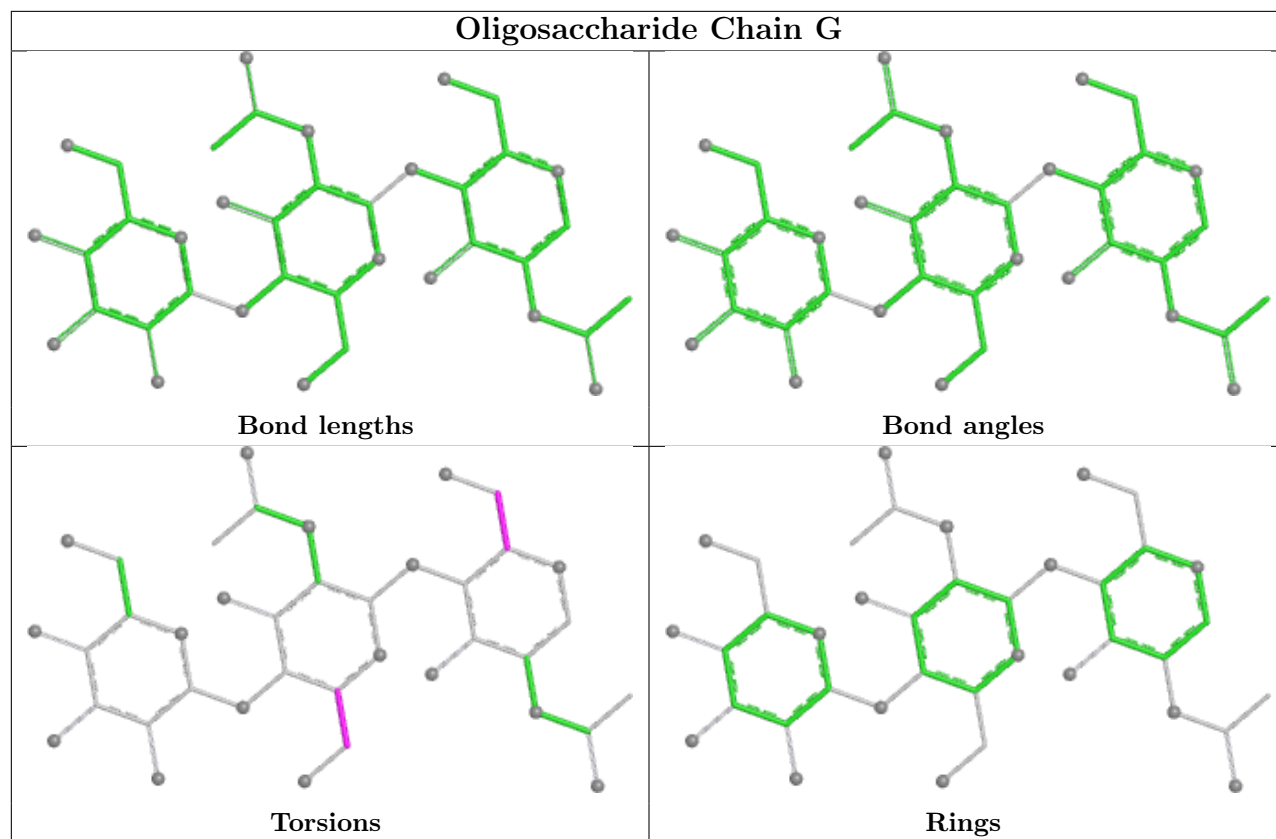
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	BMA	1	0

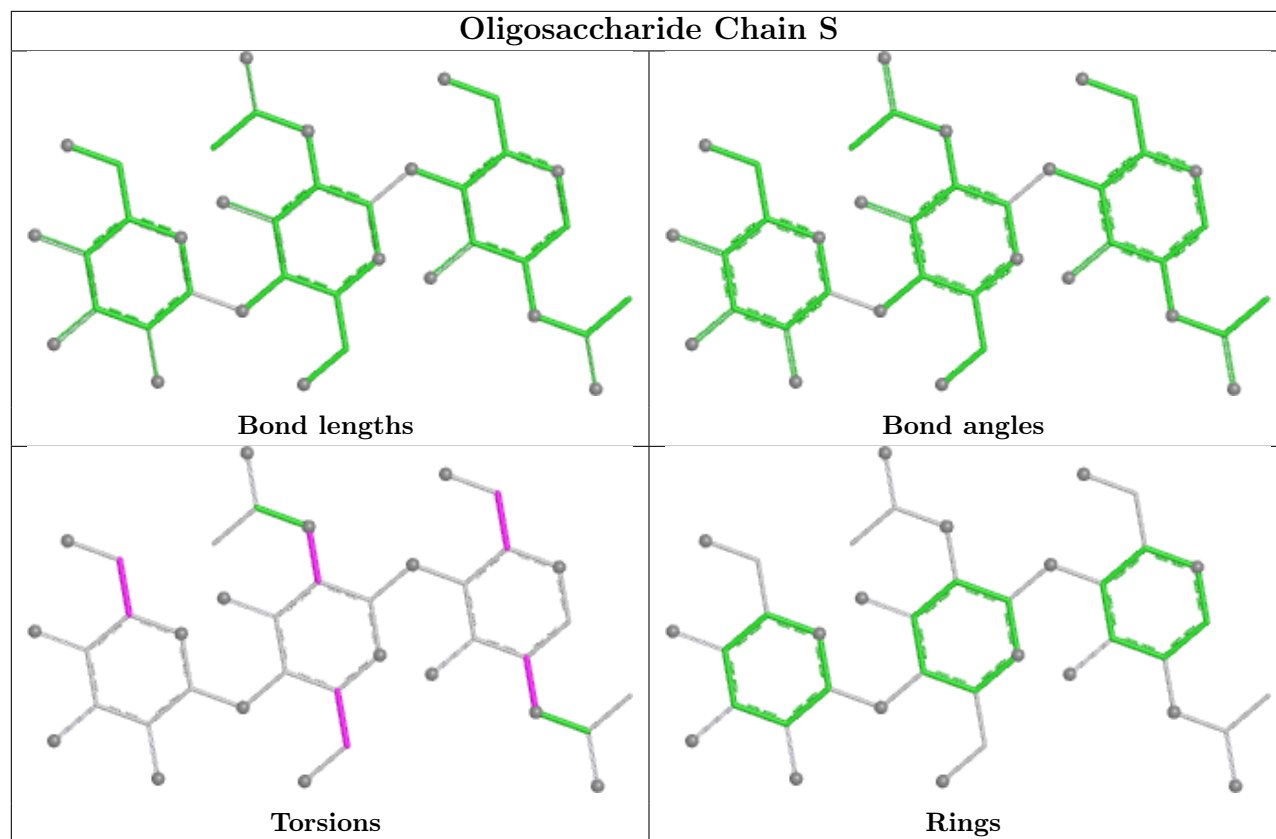
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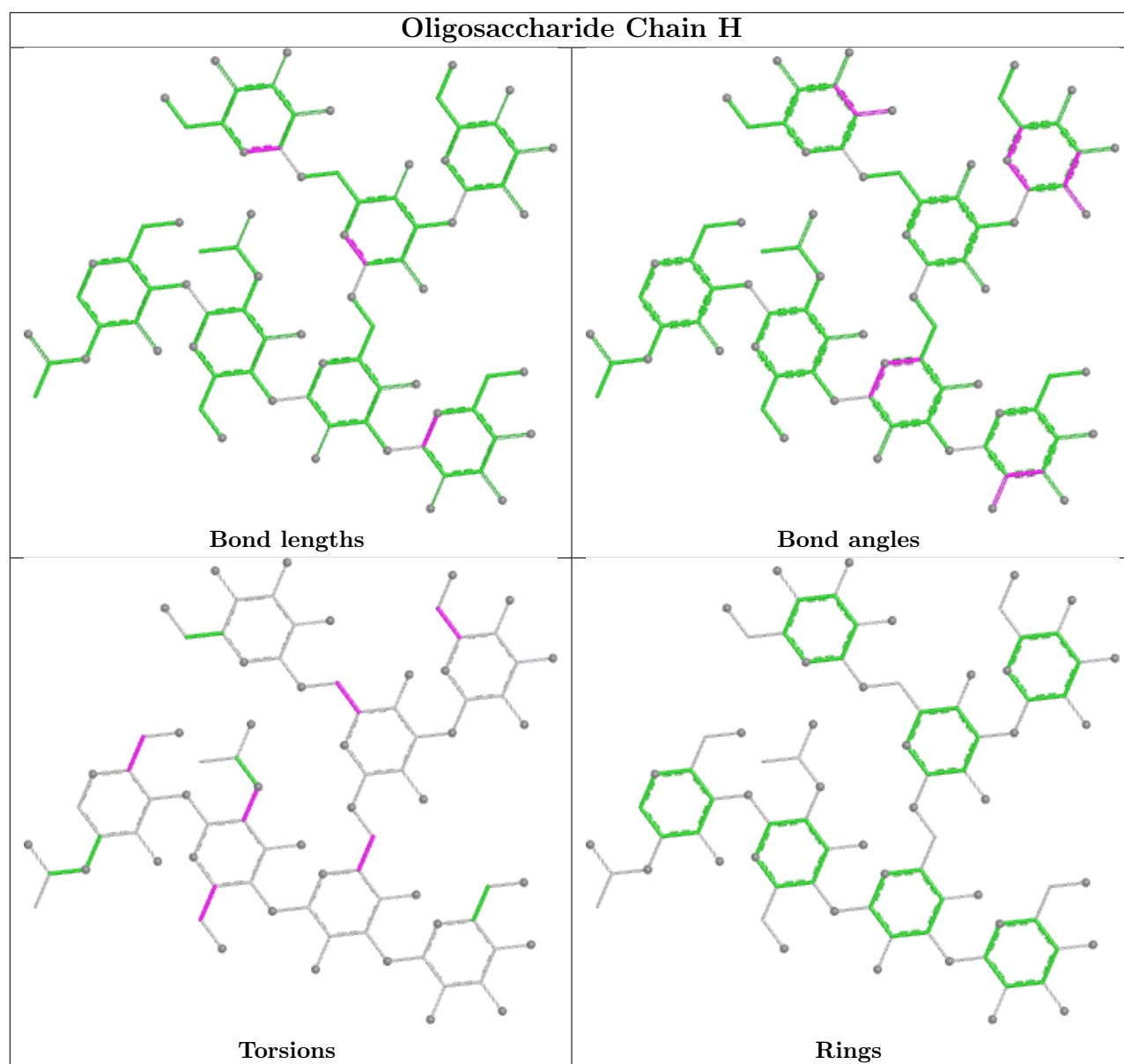
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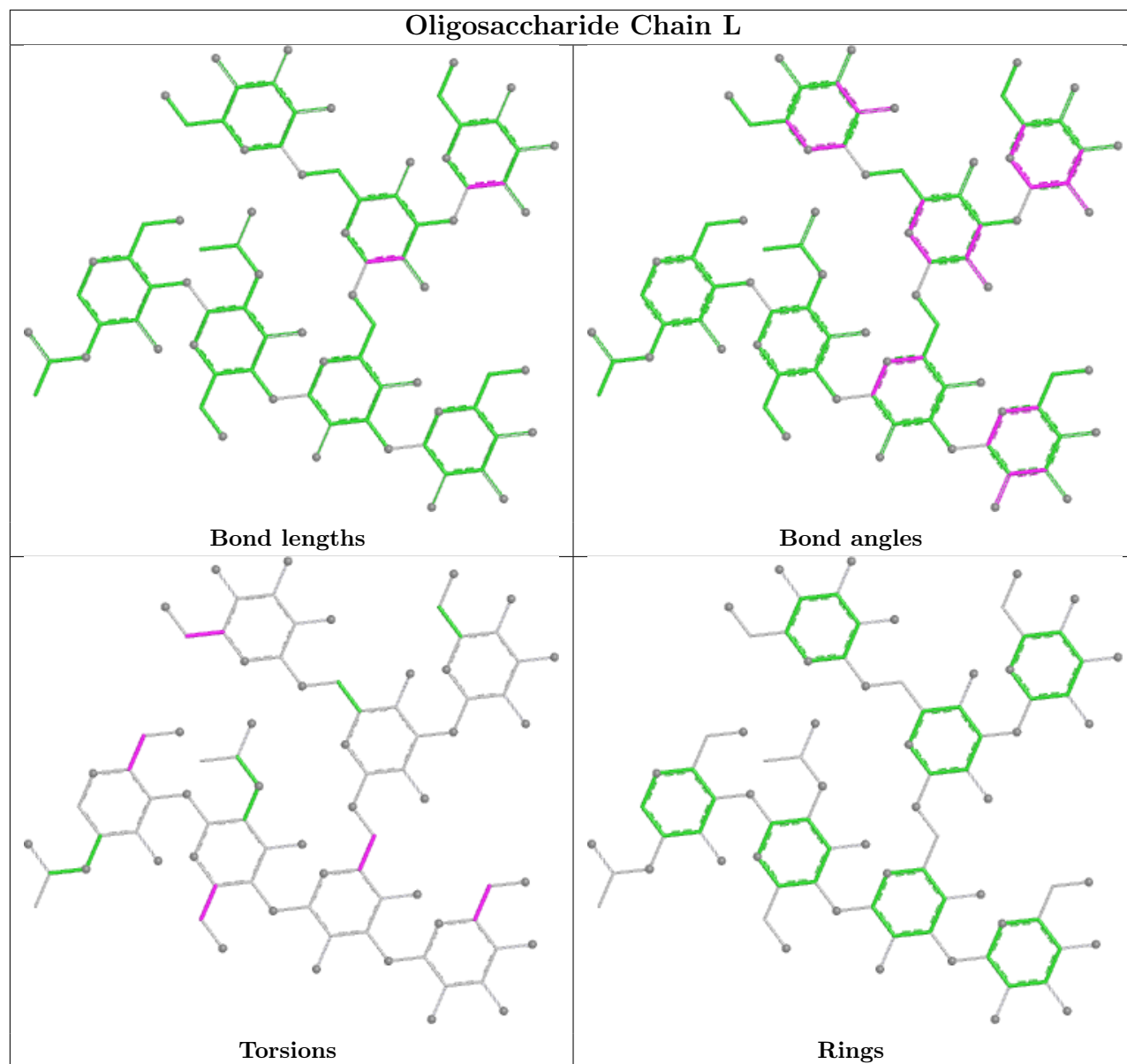
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	2	NAG	9	0
7	J	3	BMA	2	0
4	G	1	NAG	1	0
5	O	6	MAN	1	0
7	J	1	NAG	1	0
4	S	1	NAG	3	0
8	R	2	NAG	2	0
5	O	7	MAN	3	0
8	Q	2	NAG	2	0
5	O	2	NAG	1	0
5	O	5	MAN	2	0
5	L	6	MAN	2	0
4	G	2	NAG	2	0
6	I	3	BMA	2	0
5	H	2	NAG	1	0
4	S	3	BMA	2	0
5	O	4	MAN	3	0
6	I	5	MAN	2	0
7	J	4	MAN	3	0
8	M	1	NAG	7	0
5	O	3	BMA	2	0
5	O	1	NAG	1	0
4	S	2	NAG	4	0
8	Q	1	NAG	2	0
8	R	1	NAG	4	0
5	L	1	NAG	1	0
5	L	4	MAN	2	0

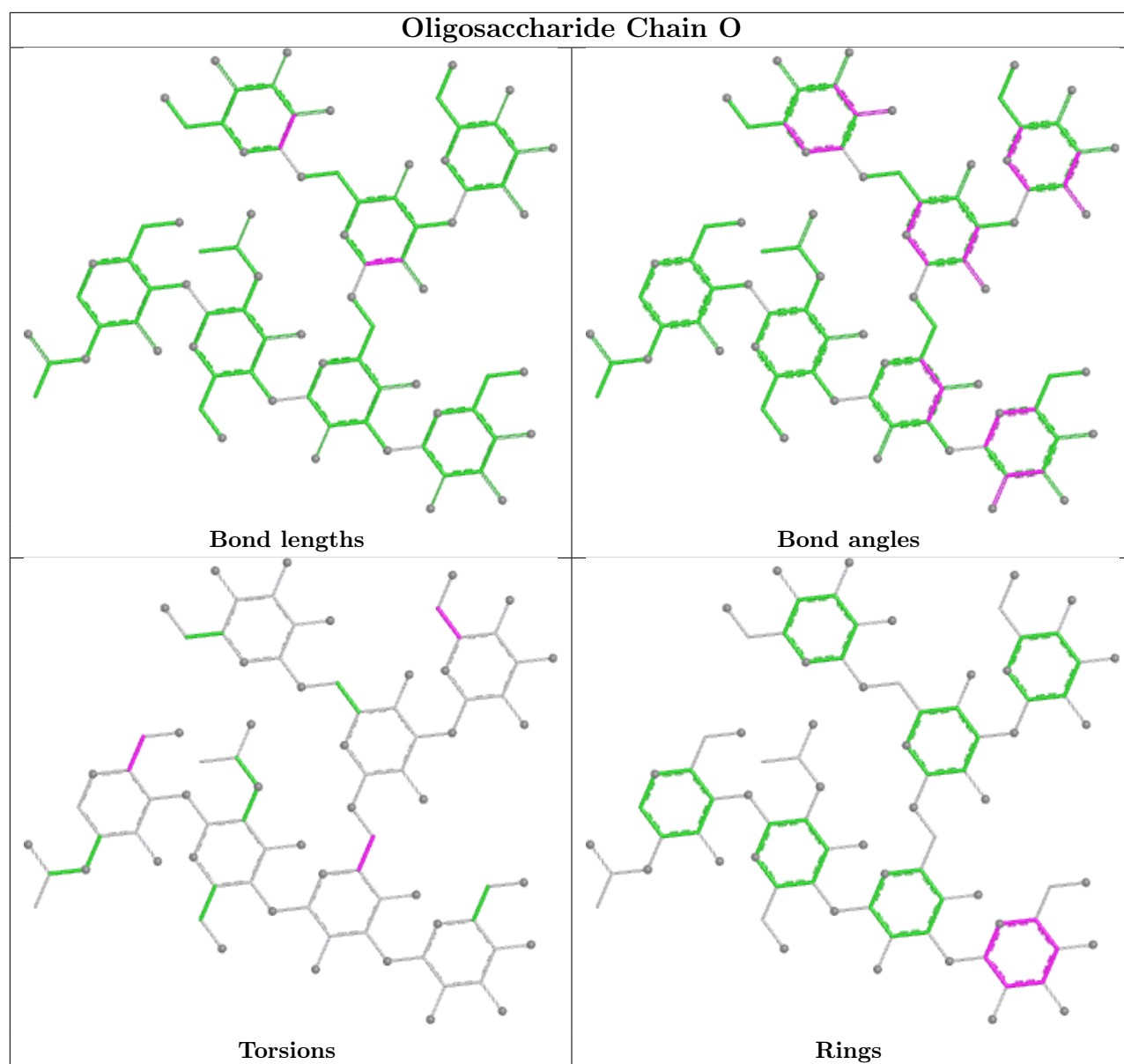
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

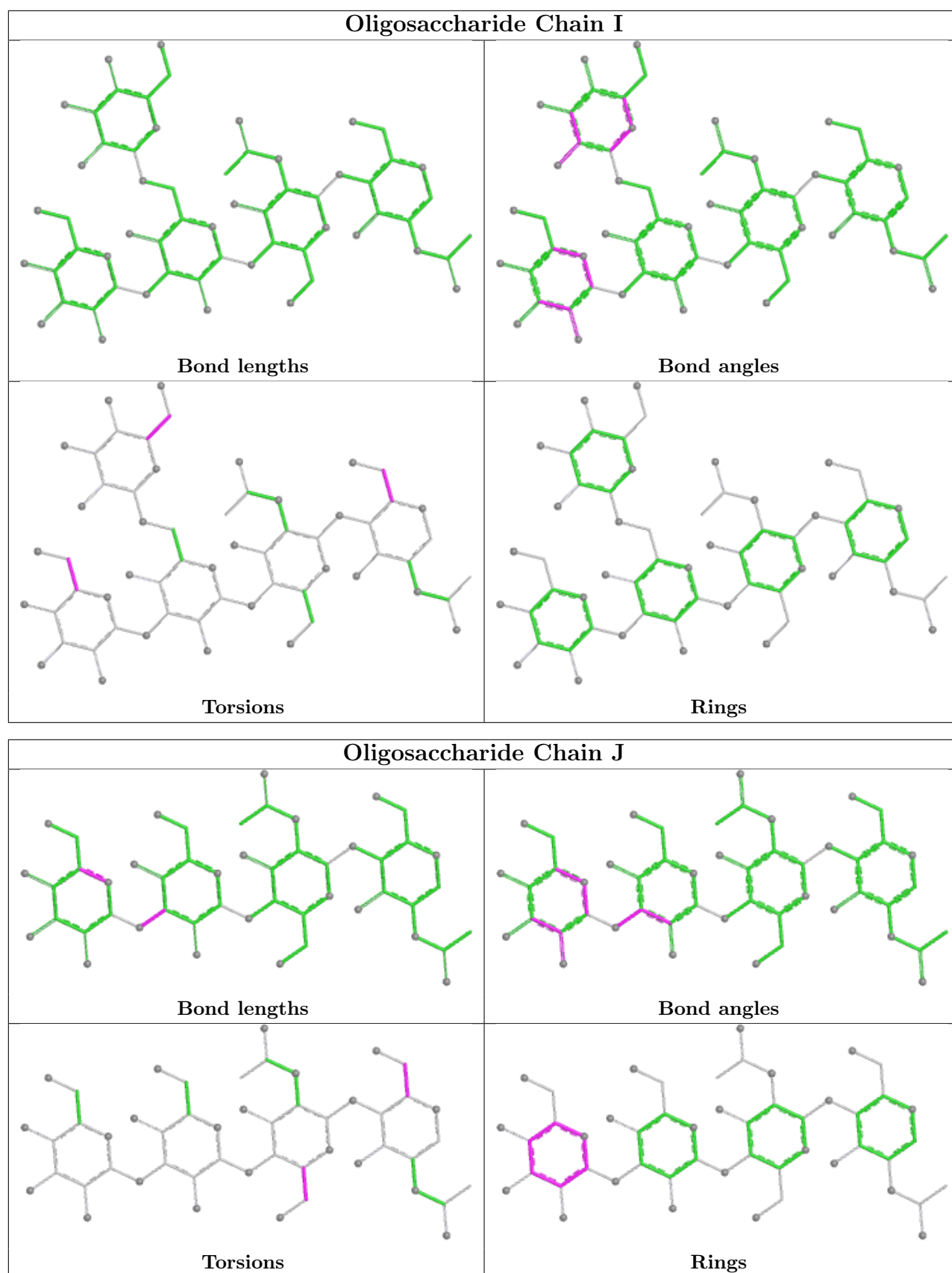


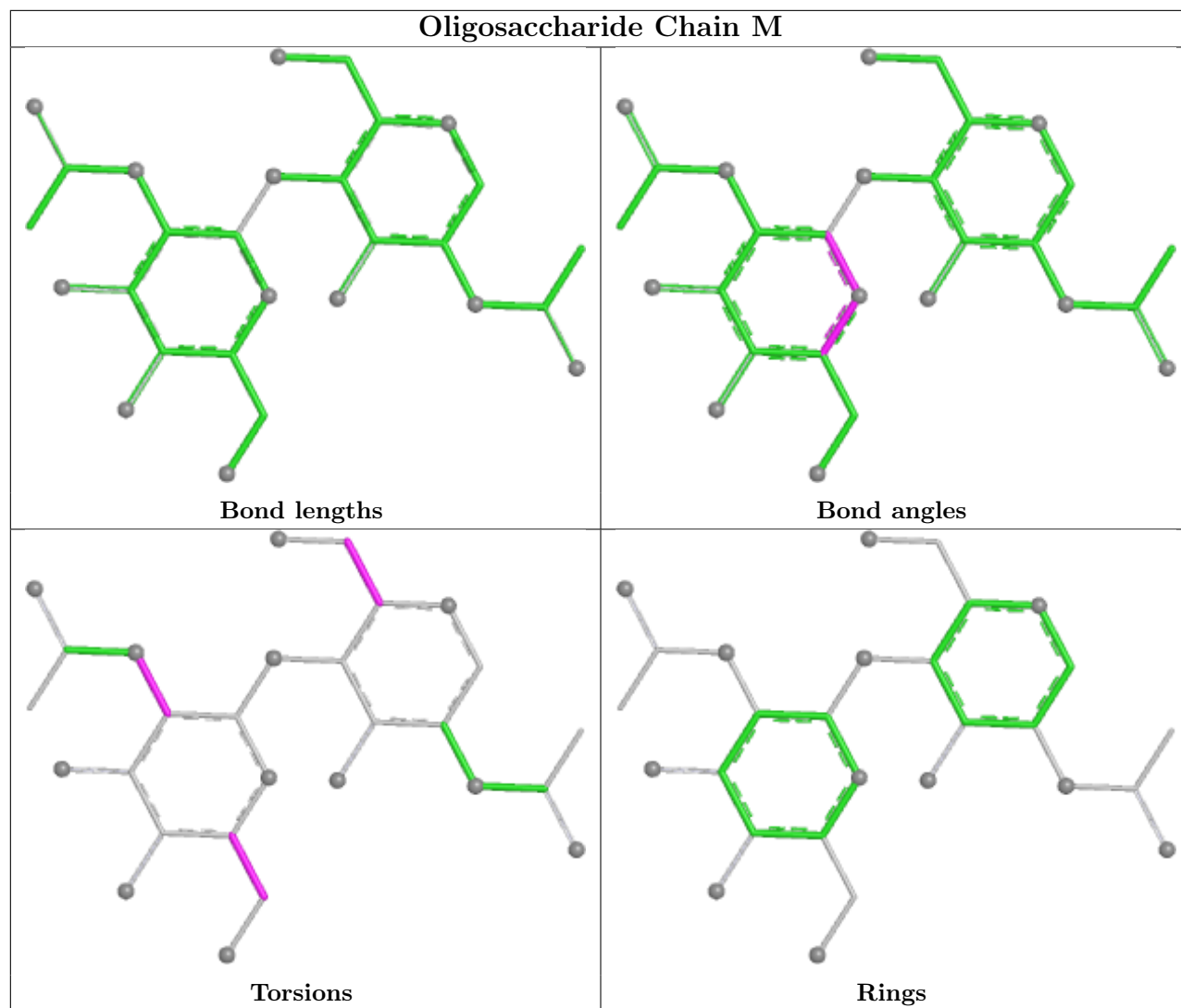


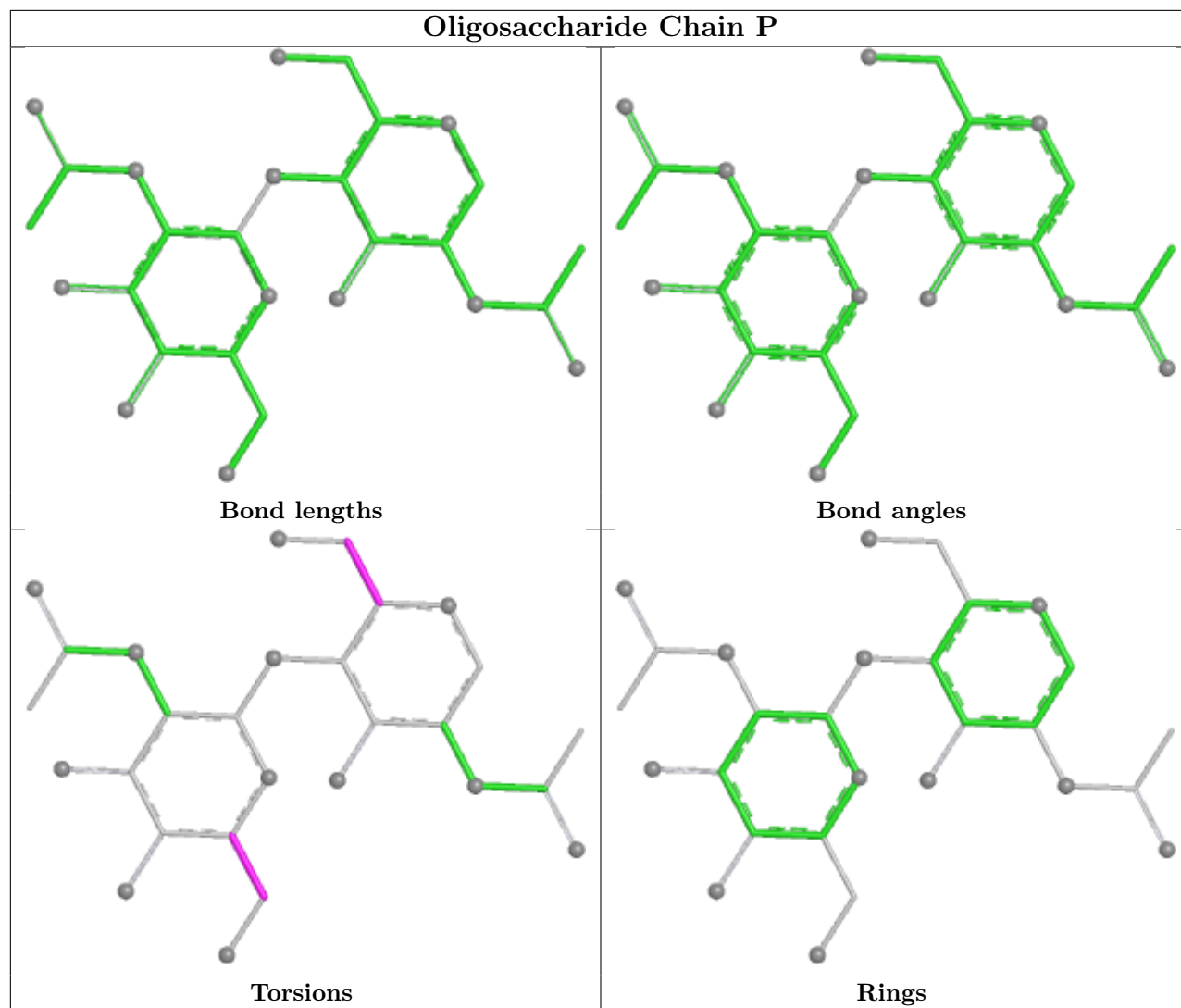


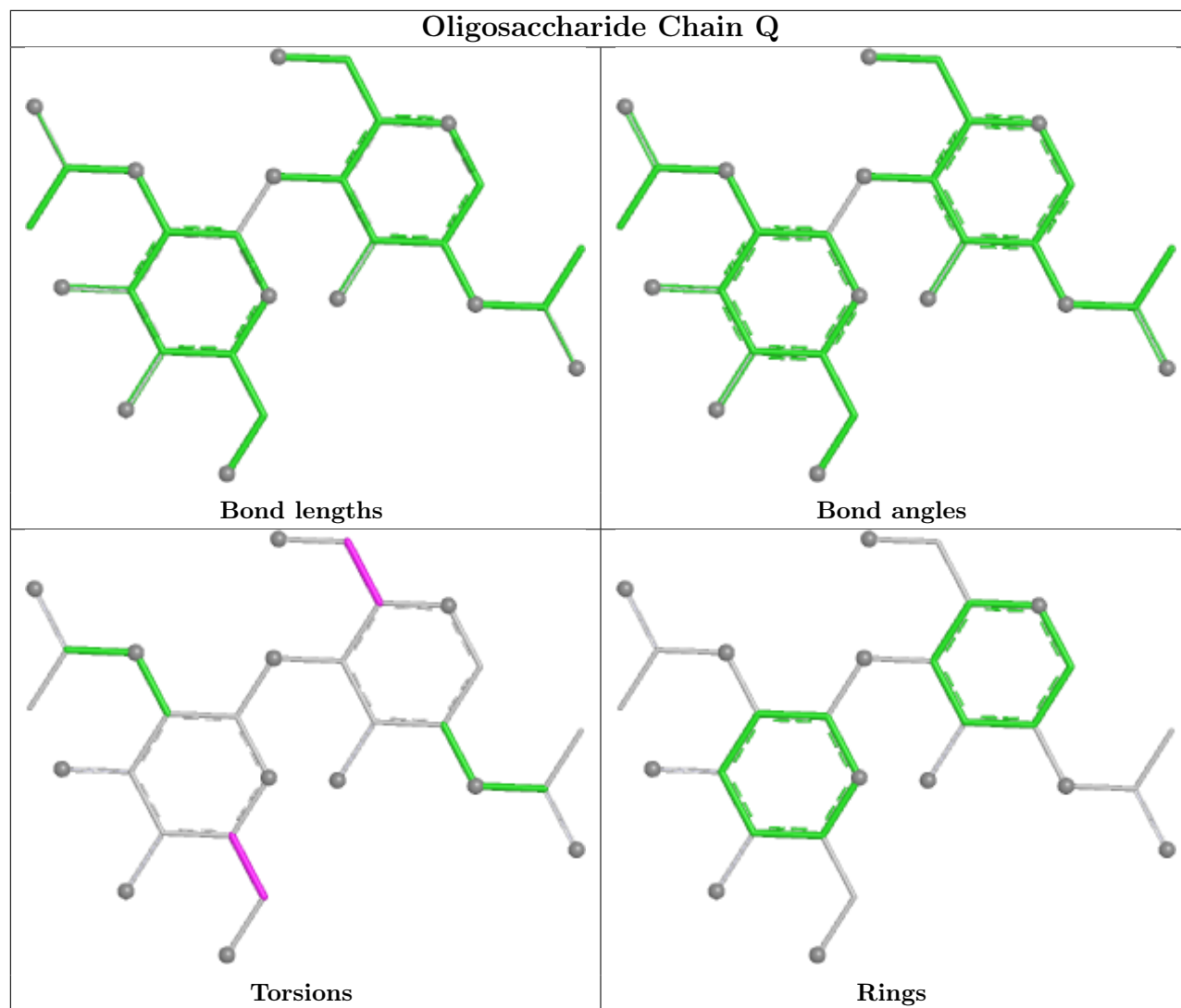


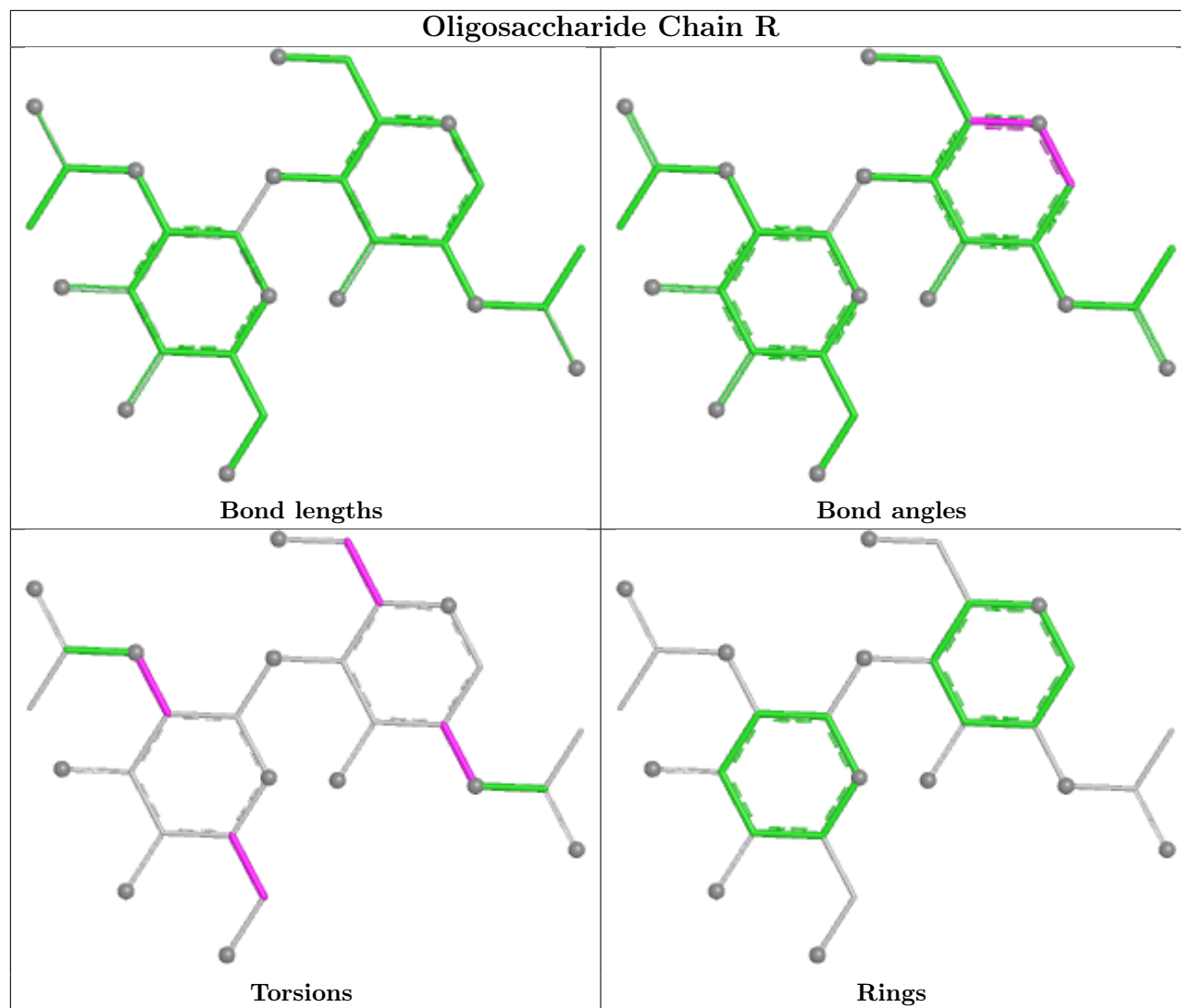


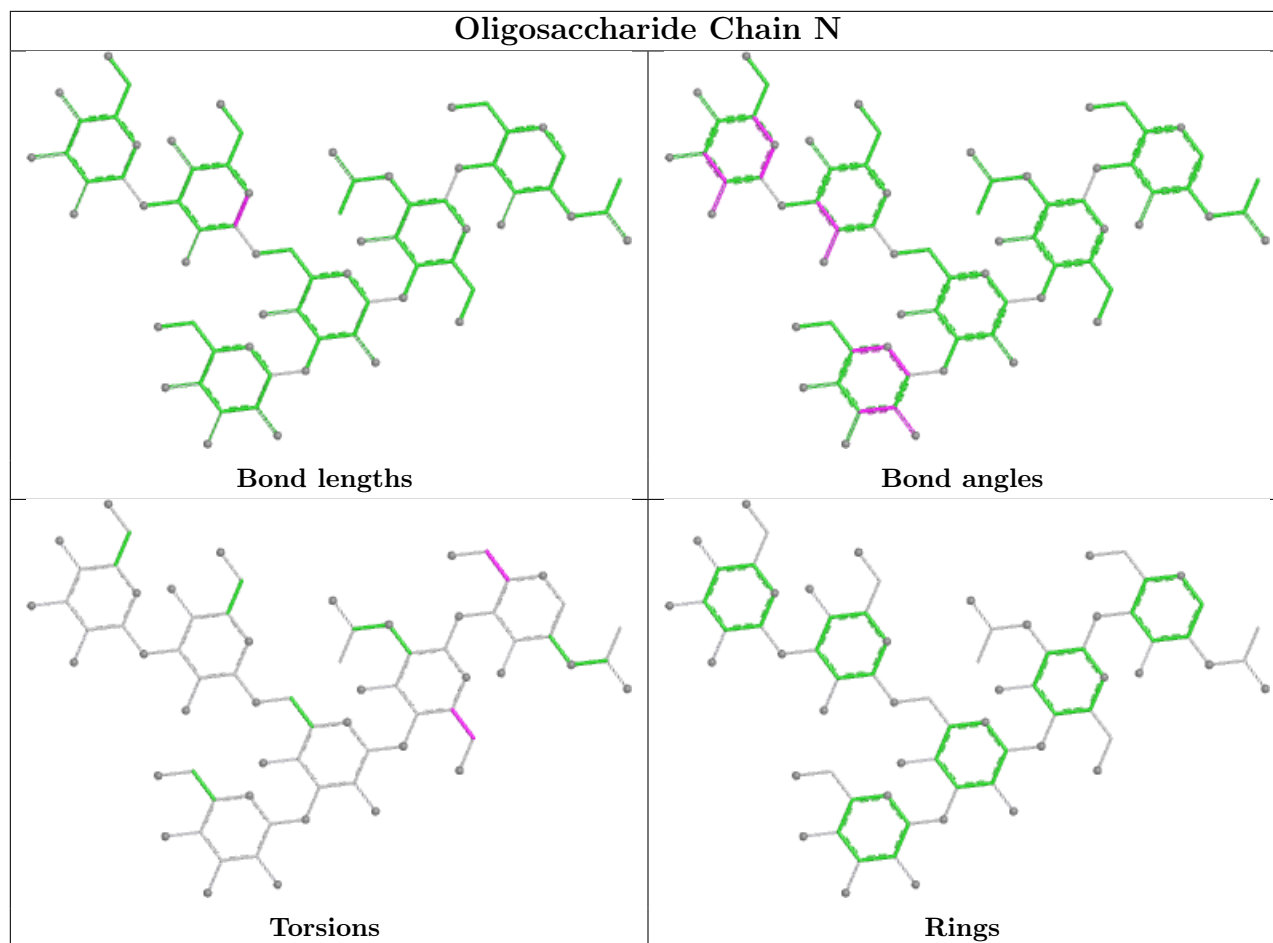












## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	2024	1	14,14,15	0.27	0	17,19,21	0.46	0
12	PEG	C	632	-	6,6,6	0.51	0	5,5,5	0.32	0
11	NAG	D	3201	2	14,14,15	0.24	0	17,19,21	0.34	0
12	PEG	A	2026	-	6,6,6	0.50	0	5,5,5	0.24	0
11	NAG	A	2025	1	14,14,15	0.25	0	17,19,21	0.45	0
14	GLY	C	601	-	3,3,4	0.60	0	1,2,4	0.33	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	2024	1	-	2/6/23/26	0/1/1/1
12	PEG	C	632	-	-	1/4/4/4	-
11	NAG	D	3201	2	-	4/6/23/26	0/1/1/1
12	PEG	A	2026	-	-	1/4/4/4	-
11	NAG	A	2025	1	-	2/6/23/26	0/1/1/1
14	GLY	C	601	-	-	0/0/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2024	NAG	O5-C5-C6-O6
11	A	2024	NAG	C4-C5-C6-O6
11	A	2025	NAG	C4-C5-C6-O6
11	A	2025	NAG	O5-C5-C6-O6
11	D	3201	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	632	PEG	1	0
11	D	3201	NAG	1	0
14	C	601	GLY	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 [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	598/598 (100%)	0.56	29 (4%) 35 30	64, 102, 170, 252	0
1	C	596/598 (99%)	0.55	28 (4%) 36 31	63, 96, 144, 244	0
2	B	310/421 (73%)	1.10	38 (12%) 8 6	76, 173, 241, 303	0
2	D	330/421 (78%)	0.99	30 (9%) 15 12	75, 150, 220, 288	0
3	E	10/11 (90%)	2.30	5 (50%) 0 0	102, 118, 135, 135	0
3	F	9/11 (81%)	3.15	7 (77%) 0 0	102, 114, 151, 153	0
All	All	1853/2060 (89%)	0.74	137 (7%) 20 16	63, 112, 214, 303	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	222	HIS	6.5
3	E	222	HIS	5.7
2	B	95	LEU	5.5
1	A	487	VAL	5.2
1	C	596	THR	5.1

### 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.

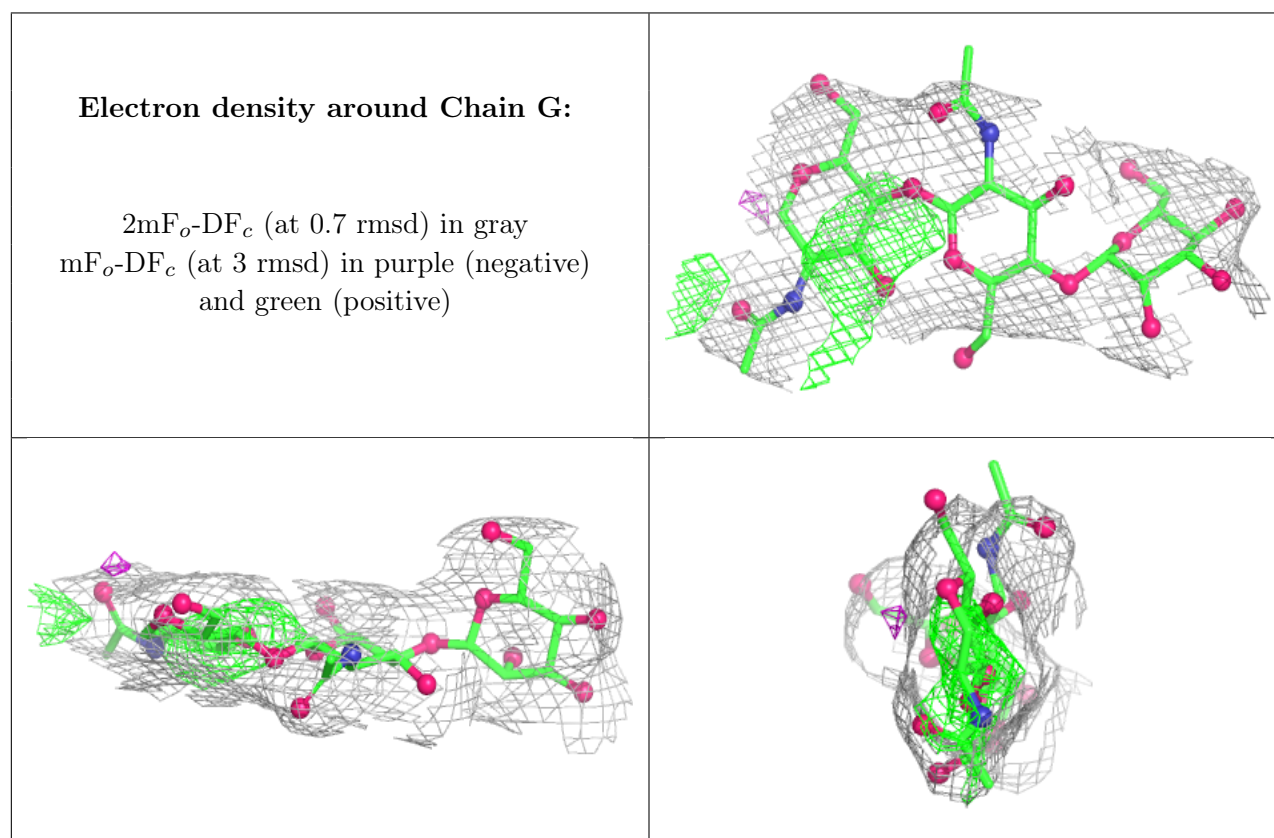
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	K	3	11/12	0.11	0.12	207,209,211,211	0
4	BMA	S	3	11/12	0.24	0.13	182,186,187,188	0
4	NAG	K	2	14/15	0.31	0.17	215,219,221,223	0
8	NAG	M	1	14/15	0.45	0.18	122,133,145,152	0
8	NAG	M	2	14/15	0.48	0.19	155,156,158,159	0
4	NAG	S	2	14/15	0.51	0.14	192,197,201,203	0
5	MAN	L	4	11/12	0.52	0.13	151,152,153,154	0
5	MAN	L	7	11/12	0.52	0.13	152,153,154,154	0
8	NAG	Q	1	14/15	0.54	0.19	136,157,164,171	0
5	MAN	L	5	11/12	0.55	0.13	143,151,154,154	0
8	NAG	R	2	14/15	0.55	0.17	199,201,204,206	0
4	NAG	K	1	14/15	0.62	0.16	215,227,231,231	0
5	MAN	O	5	11/12	0.62	0.17	123,124,125,125	0
4	NAG	S	1	14/15	0.63	0.15	184,201,212,214	0
5	MAN	O	7	11/12	0.63	0.20	117,123,125,126	0
8	NAG	Q	2	14/15	0.66	0.13	175,178,180,180	0
4	BMA	G	3	11/12	0.66	0.10	135,136,138,139	0
8	NAG	R	1	14/15	0.68	0.19	206,211,213,214	0
9	MAN	N	5	11/12	0.71	0.15	121,124,126,127	0
7	BMA	J	3	11/12	0.72	0.14	115,116,118,118	0
5	MAN	L	6	11/12	0.75	0.19	151,152,153,155	0
7	MAN	J	4	11/12	0.75	0.17	113,116,120,120	0
5	MAN	H	6	11/12	0.75	0.18	83,90,94,95	0
5	MAN	O	6	11/12	0.76	0.23	132,138,140,141	0
9	MAN	N	6	11/12	0.76	0.12	108,109,111,111	0
8	NAG	P	1	14/15	0.77	0.18	99,105,110,111	0
4	NAG	G	2	14/15	0.78	0.14	133,135,137,137	0
8	NAG	P	2	14/15	0.79	0.16	109,110,111,113	0
5	BMA	L	3	11/12	0.81	0.08	143,145,150,151	0
5	BMA	O	3	11/12	0.81	0.14	109,112,120,120	0
5	MAN	O	4	11/12	0.81	0.15	121,122,124,127	0
6	MAN	I	4	11/12	0.81	0.22	112,114,115,117	0
5	NAG	O	2	14/15	0.82	0.17	109,114,117,118	0
9	NAG	N	2	14/15	0.82	0.16	82,90,94,95	0
5	NAG	L	2	14/15	0.83	0.16	126,129,135,139	0
5	MAN	H	5	11/12	0.83	0.17	88,90,94,96	0
6	BMA	I	3	11/12	0.84	0.11	100,102,105,109	0
9	MAN	N	4	11/12	0.84	0.11	107,111,115,118	0
5	BMA	H	3	11/12	0.85	0.10	85,87,91,93	0
7	NAG	J	1	14/15	0.85	0.15	101,111,115,119	0
5	MAN	H	7	11/12	0.85	0.14	95,96,97,97	0
4	NAG	G	1	14/15	0.85	0.18	122,127,127,132	0
6	MAN	I	5	11/12	0.87	0.12	94,97,100,100	0

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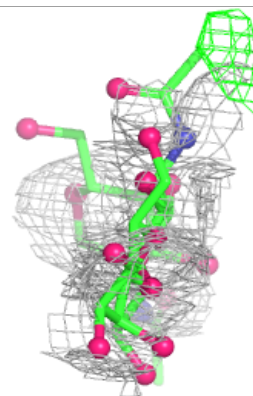
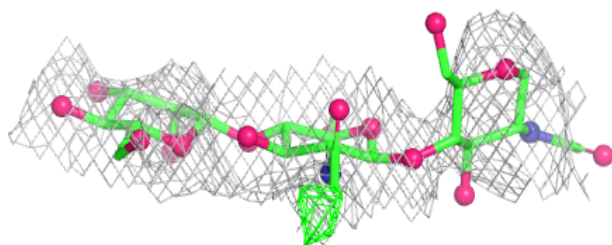
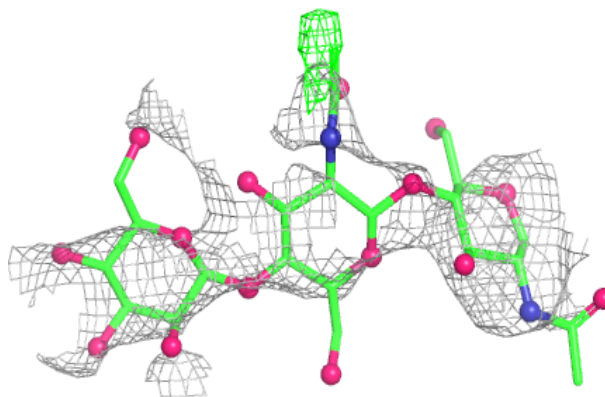
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	O	1	14/15	0.88	0.15	83,99,107,108	0
5	MAN	H	4	11/12	0.89	0.15	80,84,87,88	0
5	NAG	H	2	14/15	0.90	0.11	85,88,90,91	0
9	BMA	N	3	11/12	0.90	0.09	97,103,107,108	0
6	NAG	I	2	14/15	0.90	0.14	91,95,97,99	0
5	NAG	H	1	14/15	0.90	0.12	82,91,96,99	0
5	NAG	L	1	14/15	0.90	0.14	110,116,119,122	0
7	NAG	J	2	14/15	0.91	0.12	111,113,114,115	0
6	NAG	I	1	14/15	0.92	0.16	76,84,90,97	0
9	NAG	N	1	14/15	0.93	0.11	75,80,83,88	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.

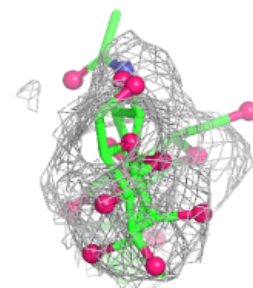
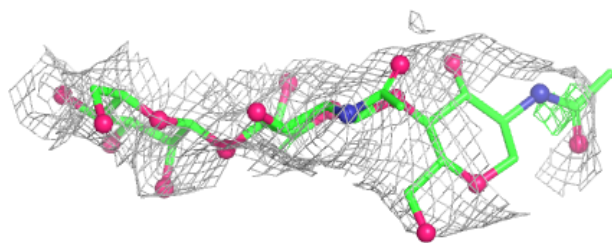
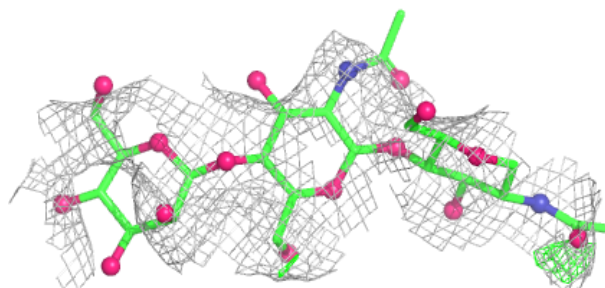


**Electron density around Chain K:**

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

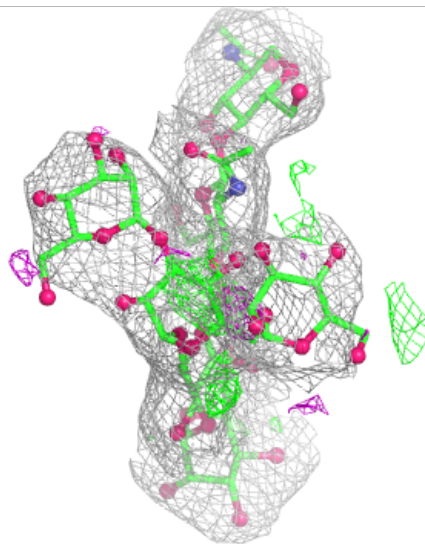
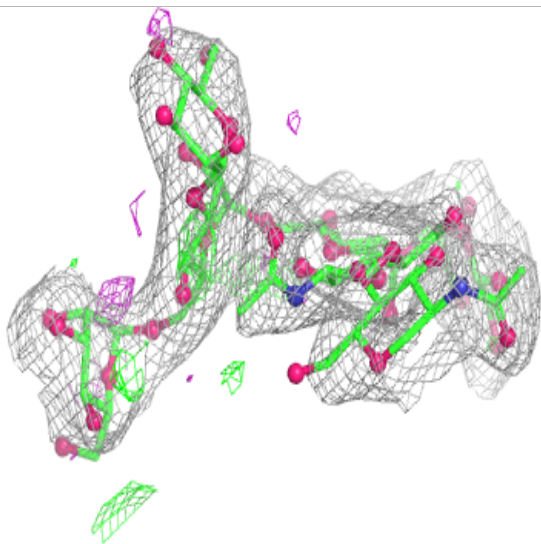
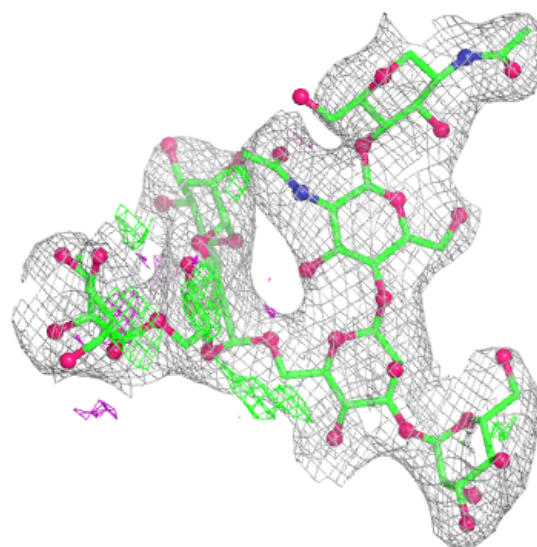
**Electron density around Chain S:**

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



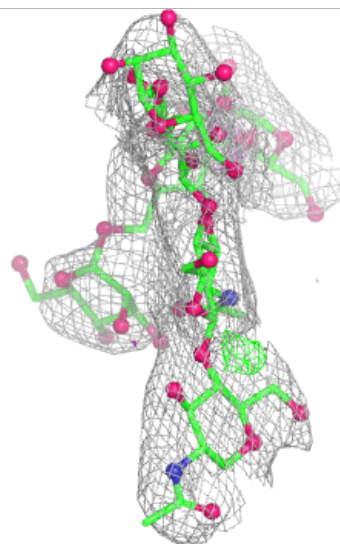
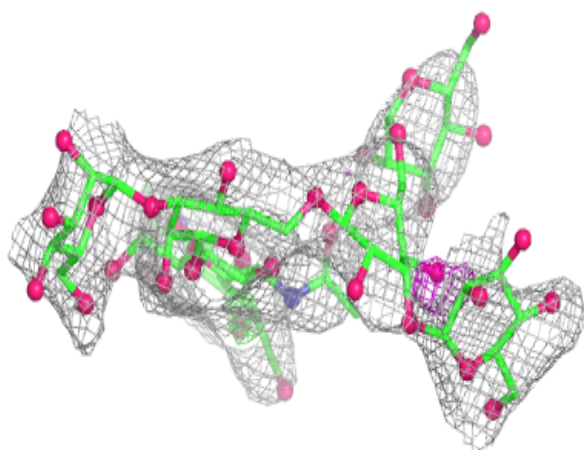
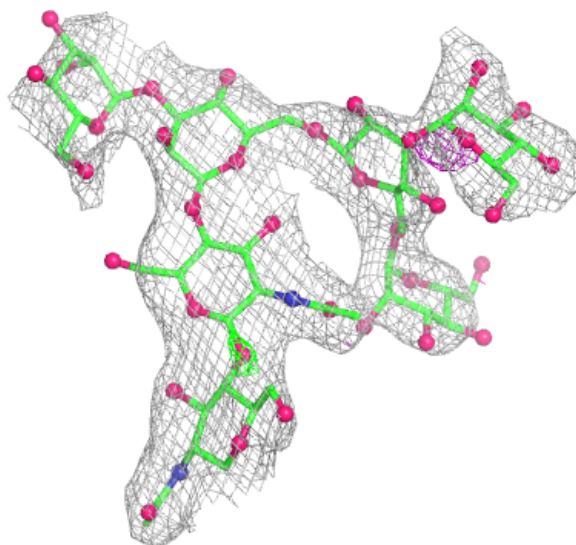
**Electron density around Chain H:**

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



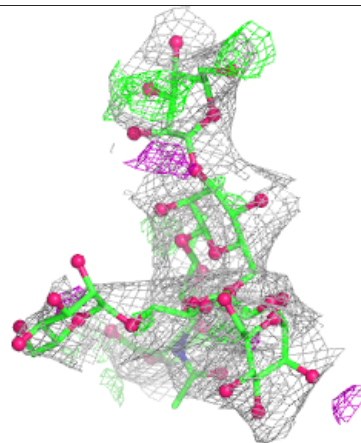
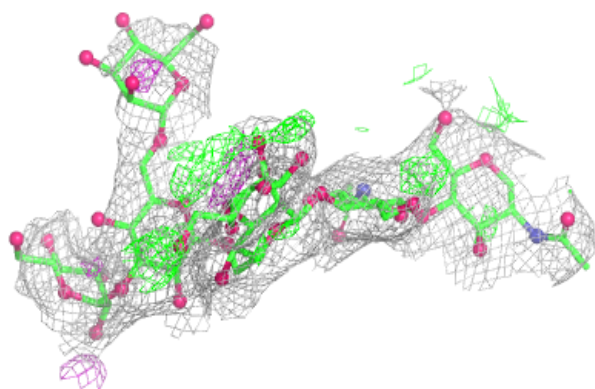
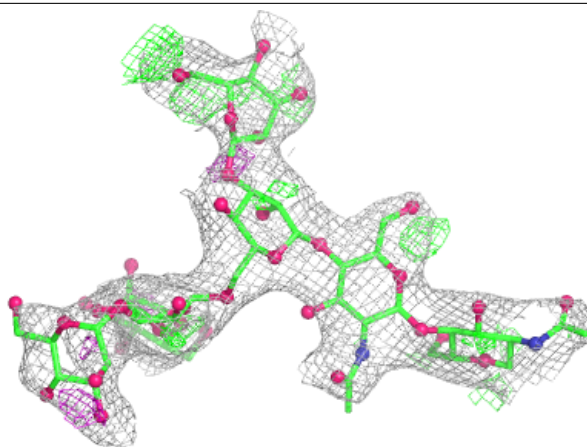
**Electron density around Chain L:**

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

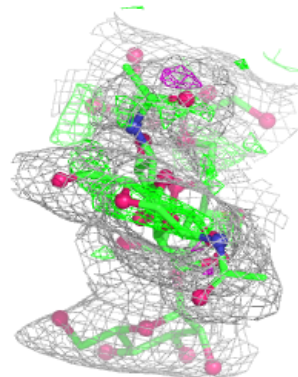
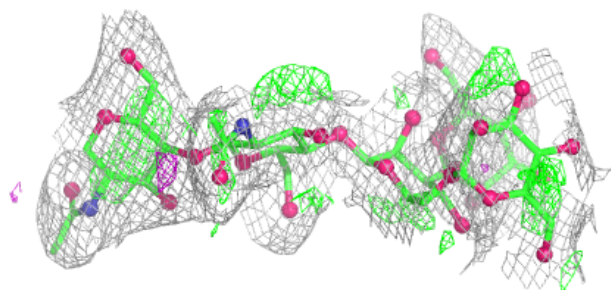
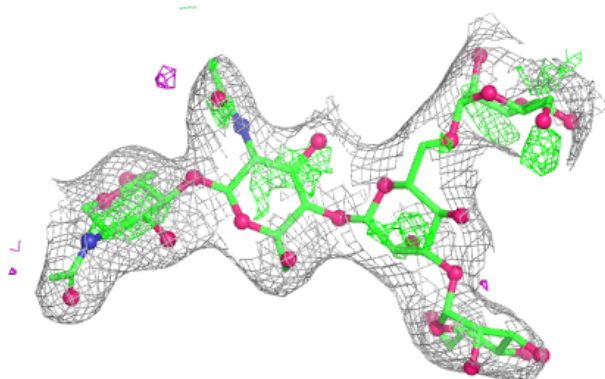


**Electron density around Chain O:**

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

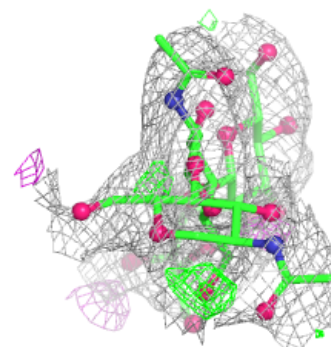
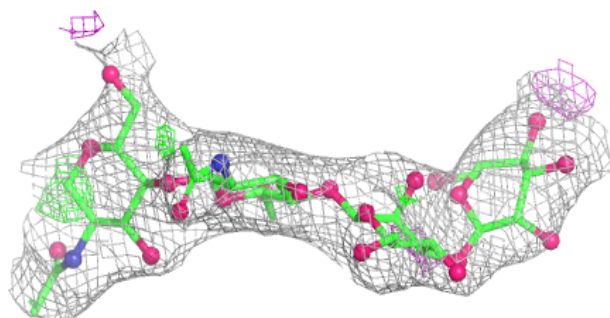
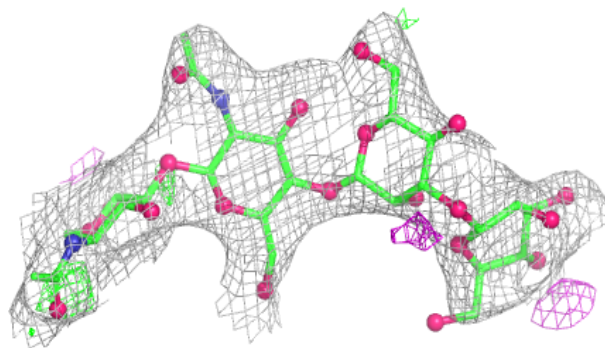
**Electron density around Chain I:**

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

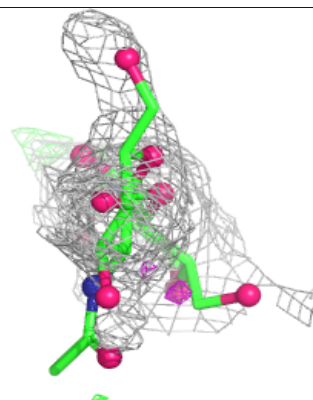
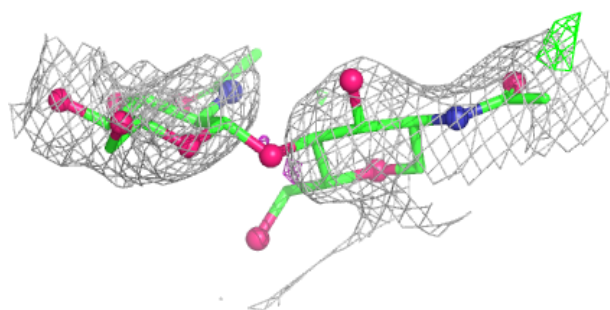
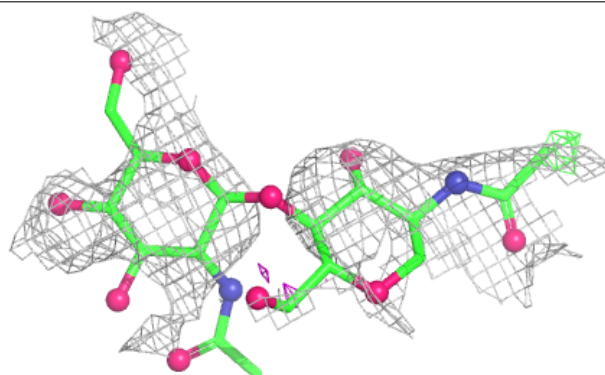


**Electron density around Chain J:**

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

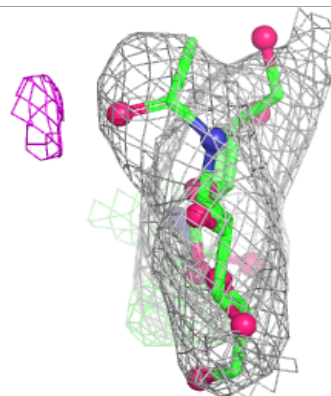
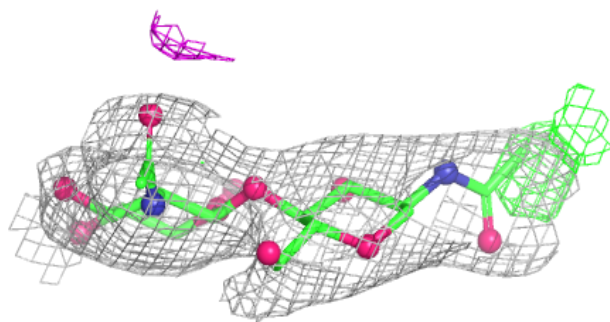
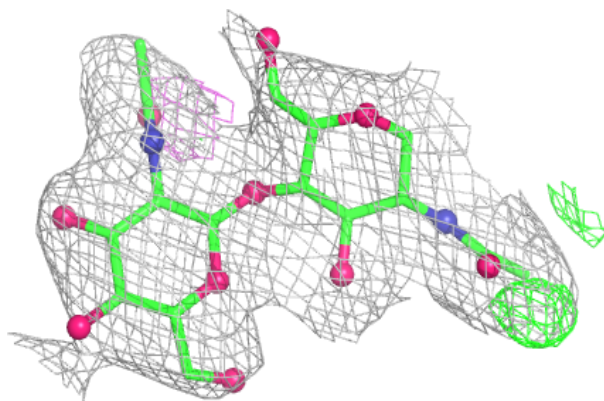
**Electron density around Chain M:**

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and green (positive)

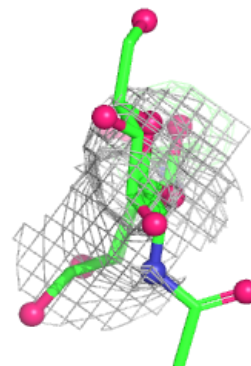
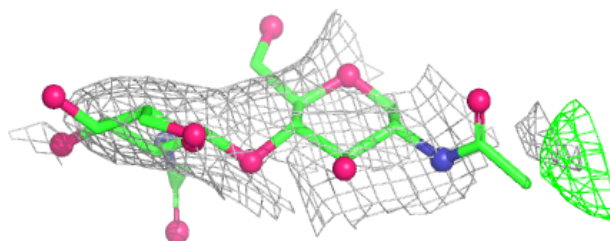
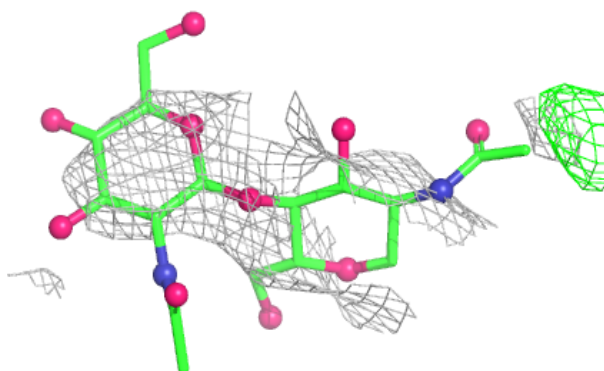


**Electron density around Chain P:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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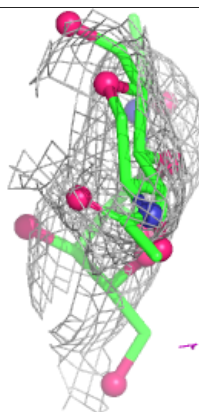
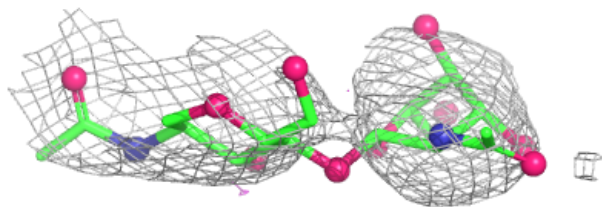
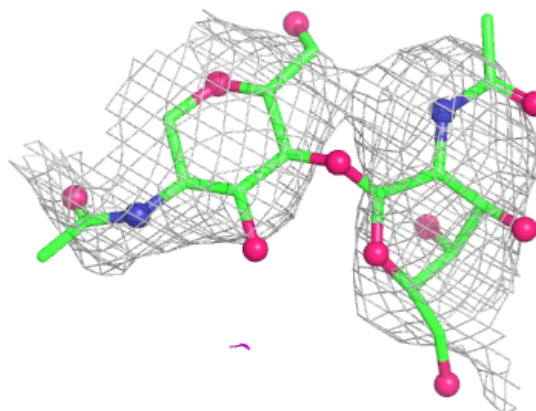
**Electron density around Chain Q:**

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and green (positive)

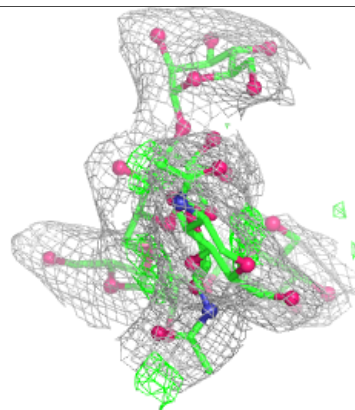
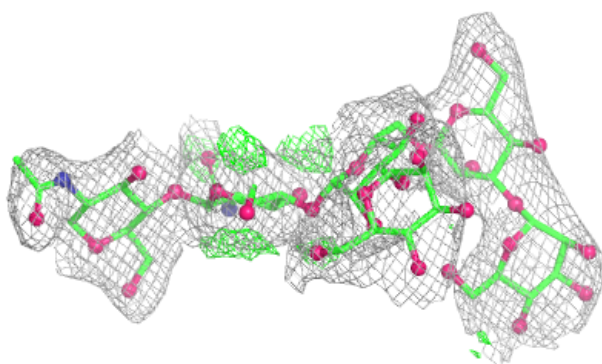
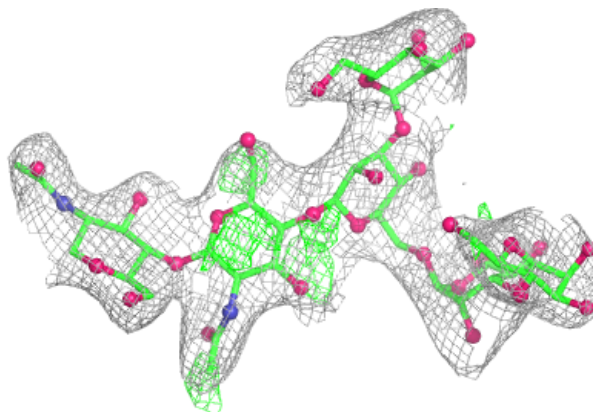


**Electron density around Chain R:**

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

**Electron density around Chain N:**

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



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	NAG	D	3201	14/15	0.46	0.16	189,202,212,212	0
14	GLY	C	601	4/5	0.58	0.29	102,102,103,104	0
11	NAG	A	2024	14/15	0.64	0.20	125,132,136,137	0
11	NAG	A	2025	14/15	0.70	0.14	104,122,126,128	0
12	PEG	C	632	7/7	0.82	0.24	75,77,78,79	0
12	PEG	A	2026	7/7	0.86	0.19	84,87,87,88	0
13	MG	D	3208	1/1	0.95	0.07	106,106,106,106	0
10	CA	B	2002	1/1	0.96	0.05	94,94,94,94	0
10	CA	D	3204	1/1	0.97	0.05	92,92,92,92	0
13	MG	B	2001	1/1	0.98	0.04	103,103,103,103	0
10	CA	A	2004	1/1	0.98	0.05	78,78,78,78	0
10	CA	C	604	1/1	0.98	0.04	66,66,66,66	0
10	CA	C	603	1/1	0.99	0.04	61,61,61,61	0
10	CA	A	2003	1/1	0.99	0.05	73,73,73,73	0
10	CA	C	605	1/1	0.99	0.06	82,82,82,82	0
10	CA	A	2001	1/1	0.99	0.02	69,69,69,69	0
10	CA	A	2002	1/1	0.99	0.04	70,70,70,70	0
10	CA	C	602	1/1	0.99	0.03	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.