



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:38 AM BST

PDB ID : 6CRD
Title : INFLUENZA VIRUS NEURAMINIDASE SUBTYPE N9 (TERN) with tetra-brachion (TB) domain stalk
Authors : Streltsov, V.A.; Schmidt, P.; McKimm-Breschkin, J.
Deposited on : 2018-03-16
Resolution : 2.57 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

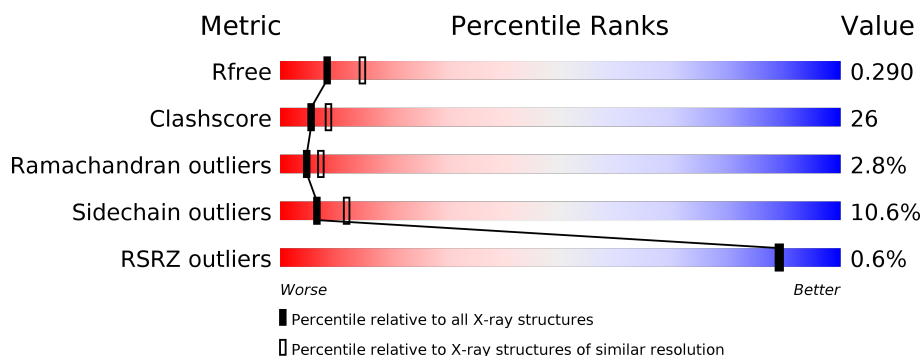
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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.




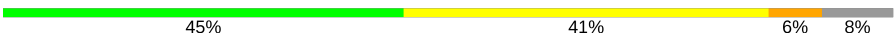
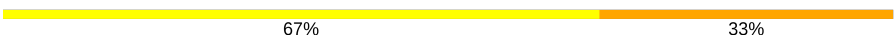


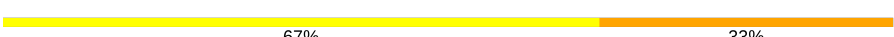
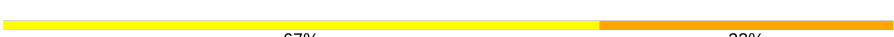

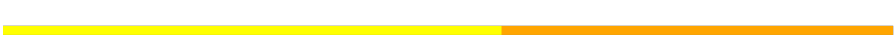

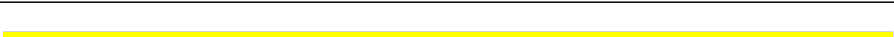


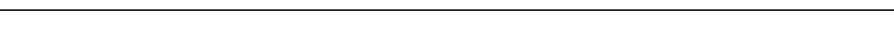


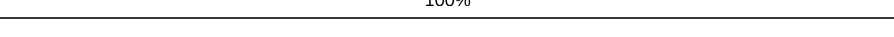


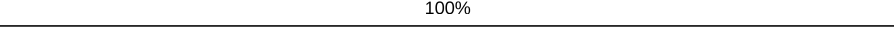
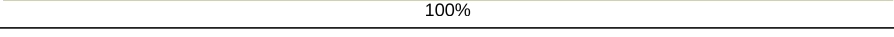
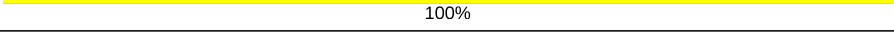
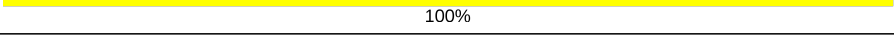
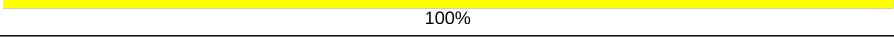
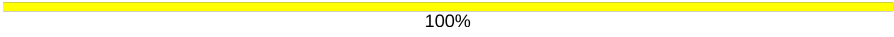
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 ≥ 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	473	
1	B	473	
1	C	473	
1	D	473	
1	E	473	
1	F	473	

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Mol	Chain	Length	Quality of chain
1	G	473	
1	H	473	
2	I	9	
2	L	9	
2	N	9	
2	Q	9	
2	T	9	
2	W	9	
2	Z	9	
2	c	9	
3	J	2	
3	M	2	
3	O	2	
3	P	2	
3	R	2	
3	S	2	
3	U	2	
3	V	2	
3	X	2	
3	Y	2	
3	a	2	
3	b	2	
3	d	2	
3	e	2	
4	K	4	

2 Entry composition [i](#)

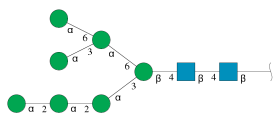
There are 6 unique types of molecules in this entry. The entry contains 29975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tetrabrachion, Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	B	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	C	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	D	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	E	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	F	438	Total	C	N	O	S	0	0	0
			3465	2163	605	673	24			
1	G	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			
1	H	435	Total	C	N	O	S	0	0	0
			3447	2152	602	669	24			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



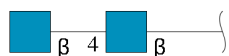
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	L	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	N	9	Total	C	N	O	0	0	0
			105	58	2	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	T	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	W	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	Z	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	c	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 3 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
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

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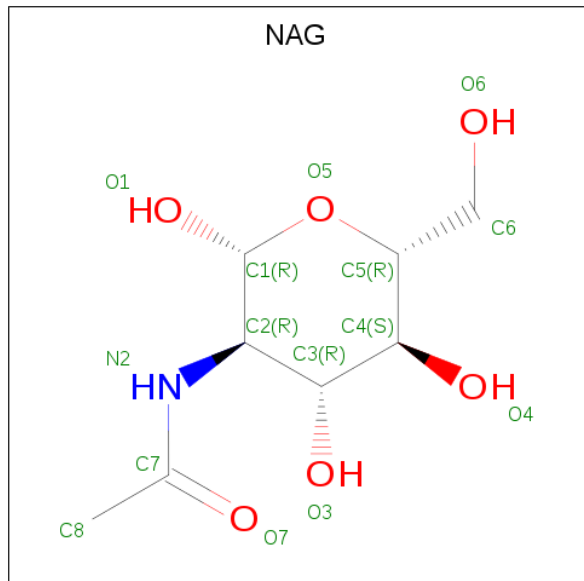
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

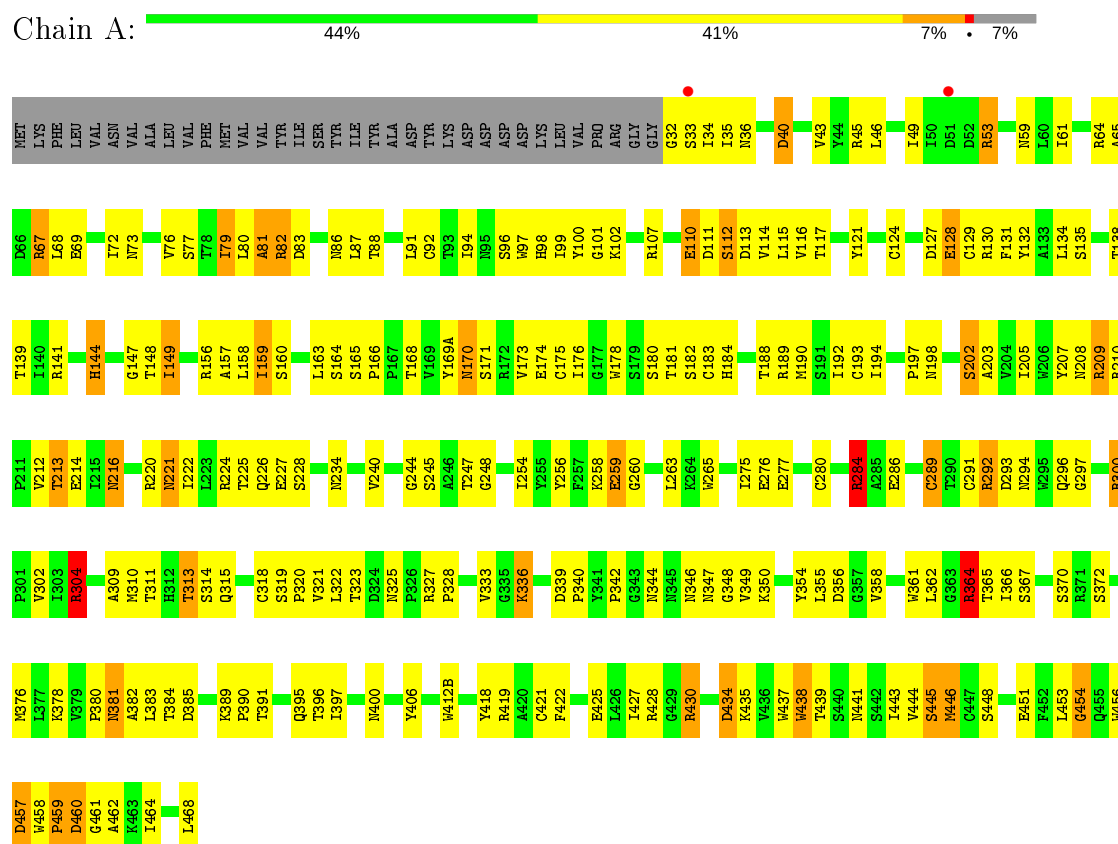
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	122	Total	O	0	0
			122	122		
6	B	111	Total	O	0	0
			111	111		
6	C	103	Total	O	0	0
			103	103		
6	D	122	Total	O	0	0
			122	122		
6	E	124	Total	O	0	0
			124	124		
6	F	111	Total	O	0	0
			111	111		
6	G	98	Total	O	0	0
			98	98		
6	H	142	Total	O	0	0
			142	142		

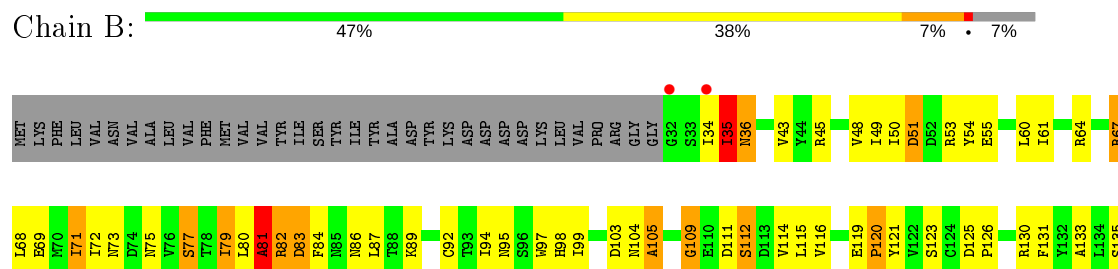
3 Residue-property plots

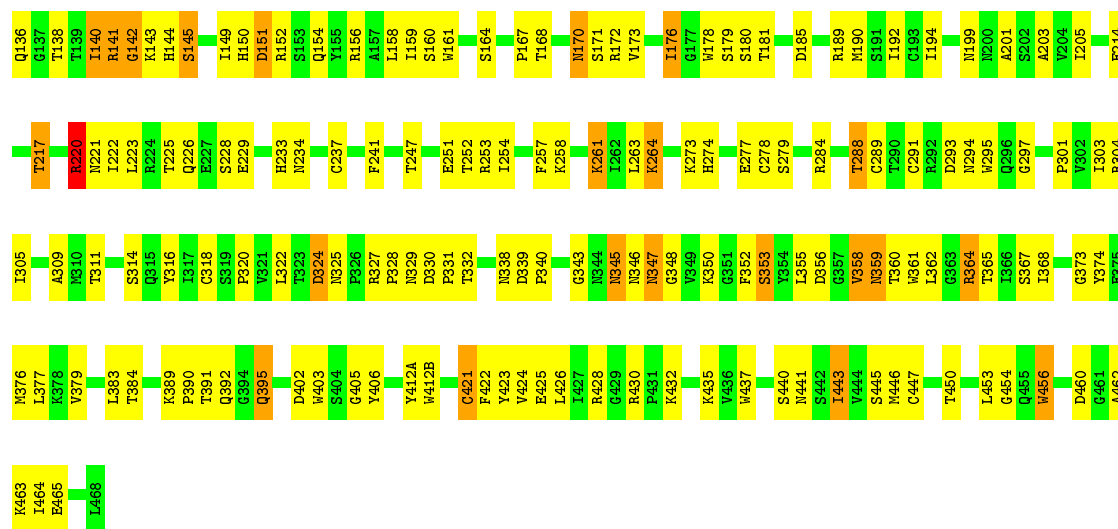
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tetrabrachion, Neuraminidase

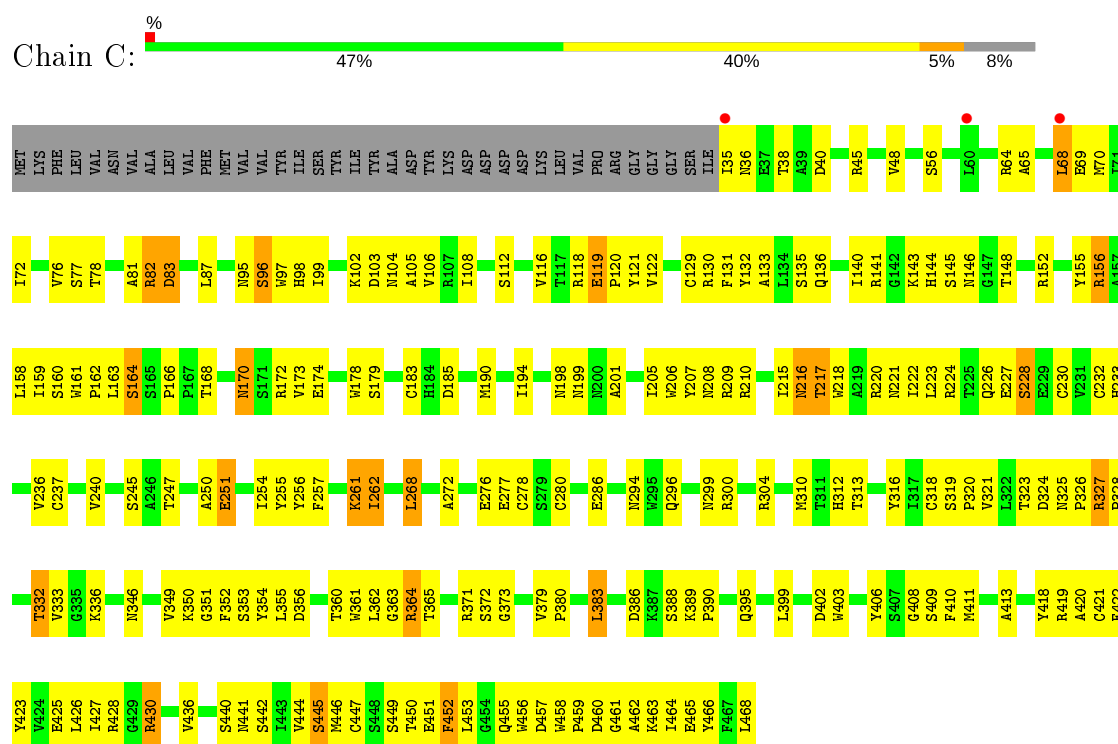


• Molecule 1: Tetrabrachion, Neuraminidase

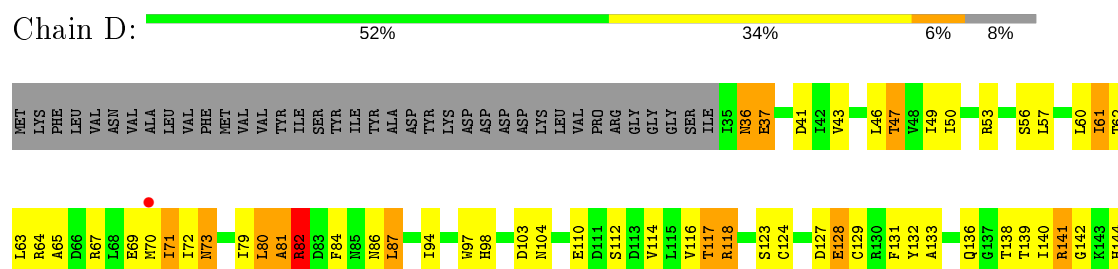


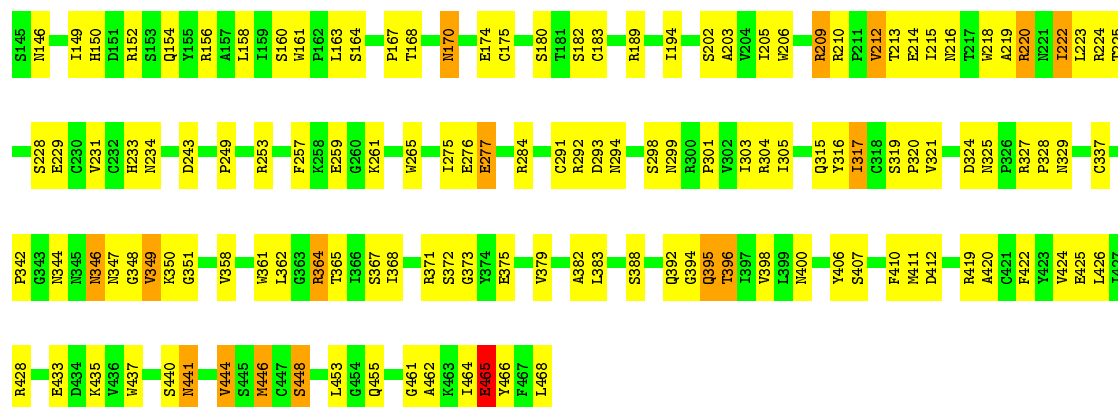


• Molecule 1: Tetrabrachion, Neuraminidase

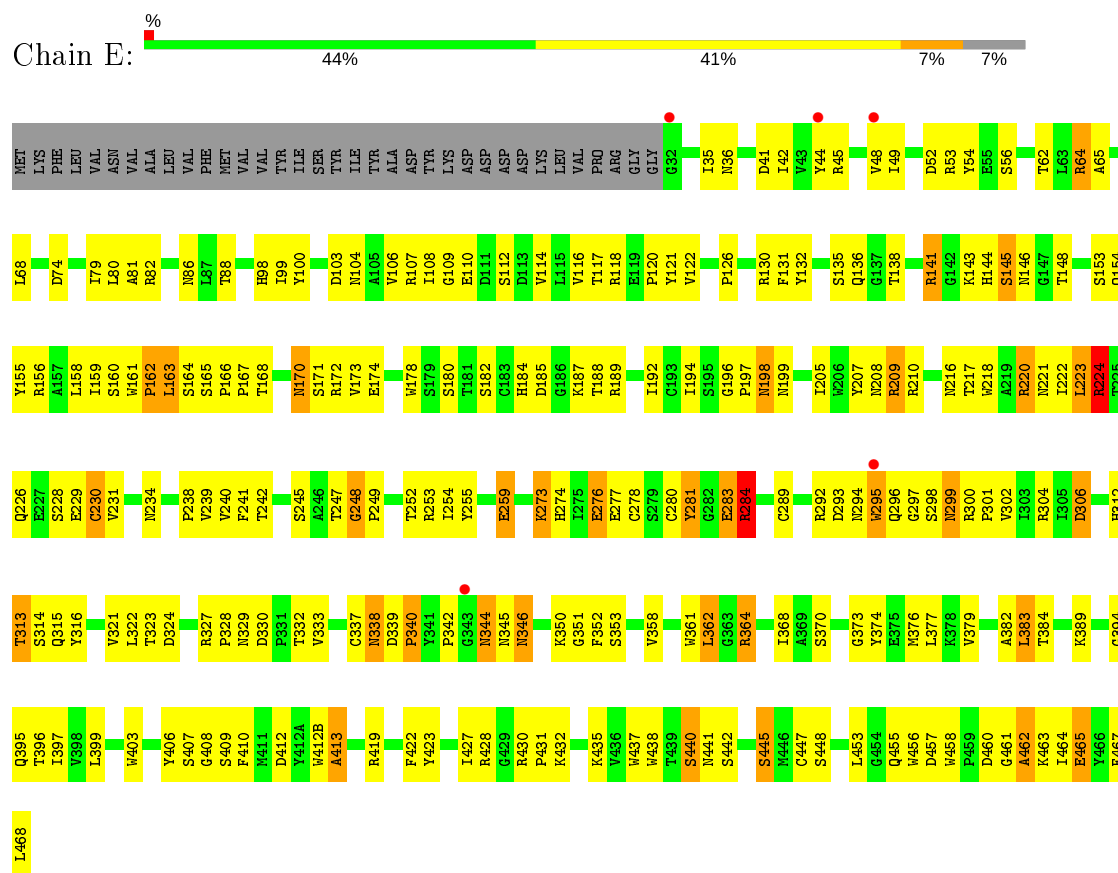


• Molecule 1: Tetrabrachion, Neuraminidase

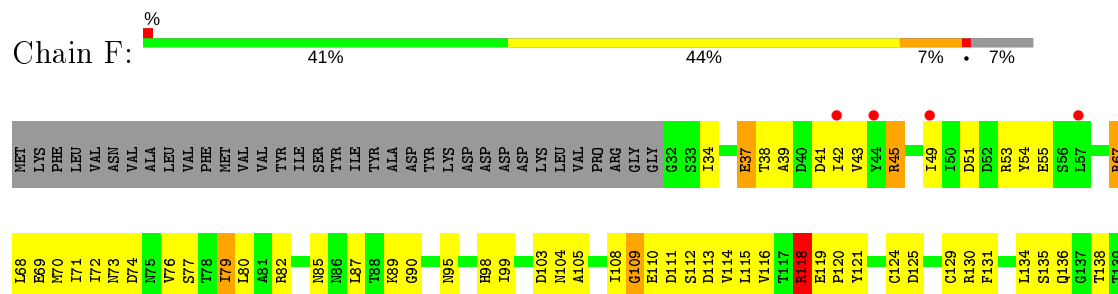


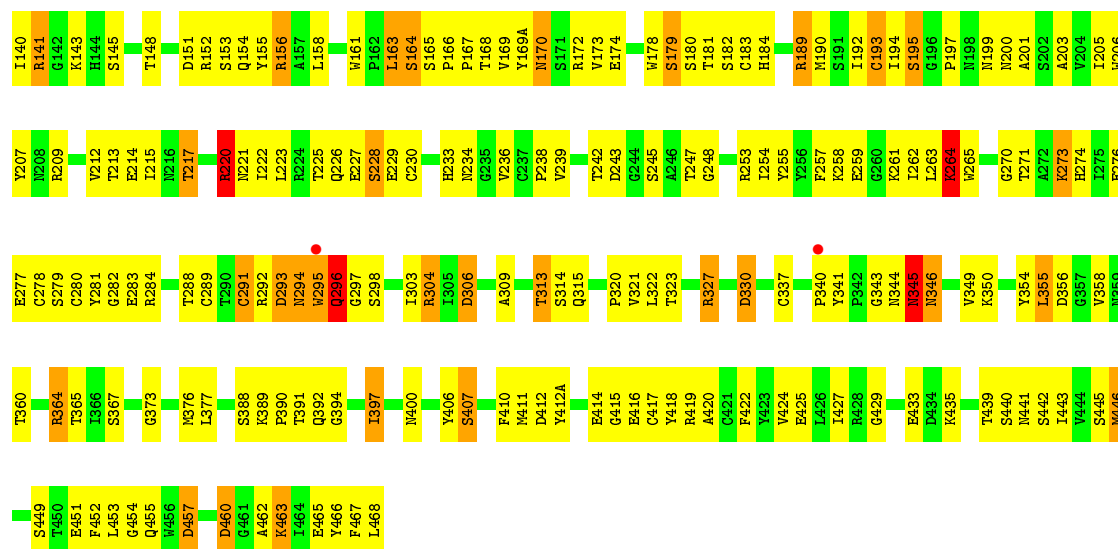


• Molecule 1: Tetrabrachion, Neuraminidase



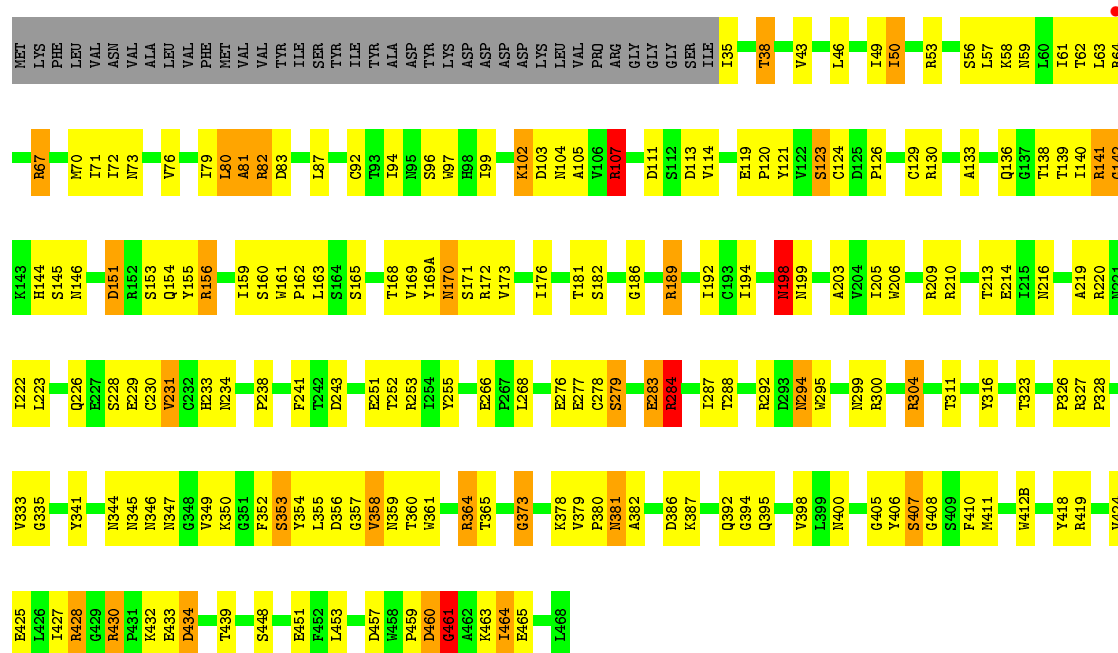
• Molecule 1: Tetrabrachion, Neuraminidase





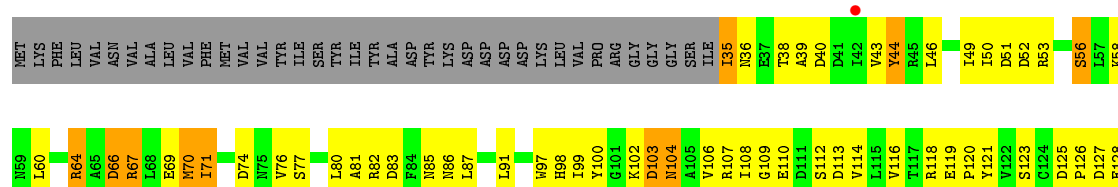
• Molecule 1: Tetrabrachion, Neuraminidase

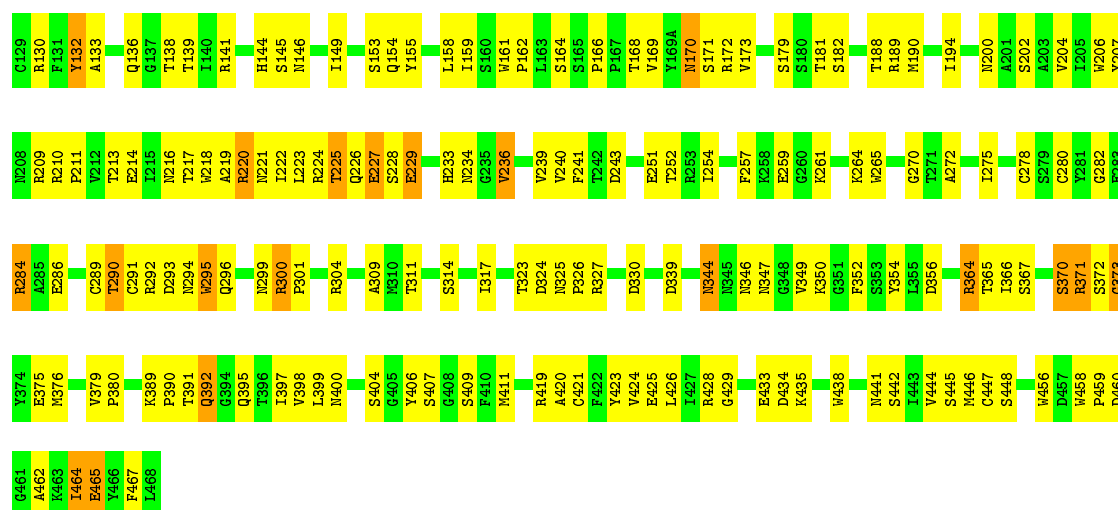
Chain G: 51% 34% 6% 8%



• Molecule 1: Tetrabrachion, Neuraminidase

Chain H: 45% 41% 6% 8%





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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: 67% 33%



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

Chain L: 67% 33%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 N: 78% 22%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 Q:  67% 33%



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

Chain T:  67% 33%



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

Chain W:  33% 67%

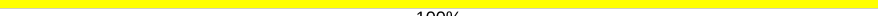


- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Z:  56% 44%



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

Chain c:  100%



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

Chain J:  100%

MAG1
MAG2

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

Chain M:  50% 50%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

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

Chain P:  100%MAG1
MAG2

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

Chain R:  50% 50%MAG1
MAG2

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

Chain S:  100%MAG1
MAG2

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

Chain U:  50% 50%MAG1
MAG2

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

Chain V:  50% 50%

NAG1
NAG2

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

Chain X:  100%

NAG1
NAG2

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

Chain Y:  100%

NAG1
NAG2

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

Chain a:  100%

NAG1
NAG2

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

Chain b:  100%

NAG1
NAG2

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

Chain d:  100%

NAG1
NAG2

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

Chain e:  100%

MAG1
MAG2

- 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

Chain K:



MAG1
MAG2
BMG3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.00Å 142.33Å 163.30Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	40.04 – 2.57 39.45 – 2.59	Depositor EDS
% Data completeness (in resolution range)	77.6 (40.04-2.57) 77.6 (39.45-2.59)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.208 , 0.306 0.210 , 0.290	Depositor DCC
R_{free} test set	5727 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 13.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtriage
Reported twinning fraction	0.854 for H, K, L 0.146 for -h,-k,l	Depositor
Outliers	1 of 114357 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29975	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/3550	0.87	3/4834 (0.1%)
1	B	0.42	0/3550	0.86	3/4834 (0.1%)
1	C	0.41	0/3532	0.87	0/4810
1	D	0.41	0/3532	0.83	0/4810
1	E	0.41	0/3550	0.87	1/4834 (0.0%)
1	F	0.39	0/3550	0.85	0/4834
1	G	0.39	0/3532	0.82	1/4810 (0.0%)
1	H	0.43	0/3532	0.87	1/4810 (0.0%)
All	All	0.41	0/28328	0.85	9/38576 (0.0%)

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	5
1	B	0	4
1	C	0	7
1	D	0	5
1	E	0	9
1	F	0	13
1	G	0	7
1	H	0	7
All	All	0	57

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	CB-CA-C	-7.21	95.99	110.40
1	A	289	CYS	CB-CA-C	-5.64	99.12	110.40
1	A	220	ARG	CG-CD-NE	-5.62	99.99	111.80
1	B	220	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	391	THR	CA-CB-OG1	-5.25	97.98	109.00

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	79	ILE	Peptide

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	3465	0	3303	212	0
1	B	3465	0	3303	201	0
1	C	3447	0	3284	181	0
1	D	3447	0	3285	170	0
1	E	3465	0	3303	215	0
1	F	3465	0	3303	216	0
1	G	3447	0	3284	176	0
1	H	3447	0	3284	195	0
2	I	105	0	88	3	0
2	L	105	0	88	5	0
2	N	105	0	88	6	0
2	Q	105	0	88	2	0
2	T	105	0	88	3	0
2	W	105	0	88	6	0
2	Z	105	0	88	4	0
2	c	105	0	88	0	0
3	J	28	0	25	0	0
3	M	28	0	25	1	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	28	0	25	2	0
3	P	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	U	28	0	25	2	0
3	V	28	0	25	4	0
3	X	28	0	25	2	0
3	Y	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
4	K	50	0	43	1	0
5	A	14	0	13	0	0
5	B	28	0	26	1	0
5	C	14	0	13	1	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	1	0
5	H	14	0	13	0	0
6	A	122	0	0	8	0
6	B	111	0	0	13	0
6	C	103	0	0	2	0
6	D	122	0	0	9	1
6	E	124	0	0	5	0
6	F	111	0	0	11	0
6	G	98	0	0	6	0
6	H	142	0	0	6	0
All	All	29975	0	27550	1455	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

The worst 5 of 1455 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:E:299:ASN:HA	6:E:612:HOH:O	1.21	1.32
1:F:169:VAL:HG23	6:F:601:HOH:O	1.26	1.27
1:B:327:ARG:HE	1:B:368:ILE:HG22	1.04	1.18
1:D:321:VAL:HG13	1:D:364:ARG:HH21	1.07	1.12
1:G:304:ARG:HG3	1:G:304:ARG:HH11	1.02	1.12

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:710:HOH:O	6:D:715:HOH:O[2_443]	2.18	0.02

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	436/473 (92%)	371 (85%)	51 (12%)	14 (3%)	4	6
1	B	436/473 (92%)	372 (85%)	52 (12%)	12 (3%)	5	7
1	C	433/473 (92%)	372 (86%)	51 (12%)	10 (2%)	6	11
1	D	433/473 (92%)	370 (86%)	52 (12%)	11 (2%)	5	9
1	E	436/473 (92%)	370 (85%)	51 (12%)	15 (3%)	3	5
1	F	436/473 (92%)	367 (84%)	55 (13%)	14 (3%)	4	6
1	G	433/473 (92%)	365 (84%)	58 (13%)	10 (2%)	6	11
1	H	433/473 (92%)	370 (86%)	52 (12%)	11 (2%)	5	9
All	All	3476/3784 (92%)	2957 (85%)	422 (12%)	97 (3%)	5	7

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	A	82	ARG
1	A	284	ARG
1	A	460	ASP
1	C	222	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/418 (93%)	341 (88%)	46 (12%)	5	9
1	B	387/418 (93%)	341 (88%)	46 (12%)	5	9
1	C	385/418 (92%)	349 (91%)	36 (9%)	8	16
1	D	385/418 (92%)	347 (90%)	38 (10%)	8	14
1	E	387/418 (93%)	353 (91%)	34 (9%)	10	18
1	F	387/418 (93%)	339 (88%)	48 (12%)	4	8
1	G	385/418 (92%)	347 (90%)	38 (10%)	8	14
1	H	385/418 (92%)	345 (90%)	40 (10%)	7	12
All	All	3088/3344 (92%)	2762 (89%)	326 (11%)	6	12

5 of 326 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	180	SER
1	E	295	TRP
1	H	149	ILE
1	D	231	VAL
1	D	465	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	216	ASN
1	E	216	ASN
1	H	216	ASN
1	D	294	ASN
1	D	395	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

104 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	I	1	1,2	14,14,15	0.72	0	17,19,21	1.27	3 (17%)
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	2.42	8 (47%)
2	BMA	I	3	2	11,11,12	0.67	0	15,15,17	2.16	4 (26%)
2	MAN	I	4	2	11,11,12	0.50	0	15,15,17	1.98	3 (20%)
2	MAN	I	5	2	11,11,12	1.10	1 (9%)	15,15,17	1.32	2 (13%)
2	MAN	I	6	2	11,11,12	0.76	0	15,15,17	2.04	6 (40%)
2	MAN	I	7	2	11,11,12	0.87	0	15,15,17	2.32	4 (26%)
2	MAN	I	8	2	11,11,12	1.13	1 (9%)	15,15,17	1.95	6 (40%)
2	MAN	I	9	2	11,11,12	0.97	0	15,15,17	1.64	3 (20%)
3	NAG	J	1	1,3	14,14,15	0.88	0	17,19,21	1.69	6 (35%)
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	1.58	4 (23%)
4	NAG	K	1	1,4	14,14,15	1.13	2 (14%)	17,19,21	2.35	9 (52%)
4	NAG	K	2	4	14,14,15	0.47	0	17,19,21	2.39	8 (47%)
4	BMA	K	3	4	11,11,12	0.86	0	15,15,17	2.82	6 (40%)
4	MAN	K	4	4	11,11,12	0.83	0	15,15,17	2.81	4 (26%)
2	NAG	L	1	1,2	14,14,15	0.47	0	17,19,21	2.15	4 (23%)
2	NAG	L	2	2	14,14,15	0.70	0	17,19,21	2.06	4 (23%)
2	BMA	L	3	2	11,11,12	0.65	0	15,15,17	1.86	5 (33%)
2	MAN	L	4	2	11,11,12	0.65	0	15,15,17	1.52	4 (26%)
2	MAN	L	5	2	11,11,12	0.69	0	15,15,17	1.79	1 (6%)
2	MAN	L	6	2	11,11,12	0.56	0	15,15,17	1.79	3 (20%)
2	MAN	L	7	2	11,11,12	0.77	0	15,15,17	2.12	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	L	8	2	11,11,12	0.79	0	15,15,17	1.16	1 (6%)
2	MAN	L	9	2	11,11,12	0.95	1 (9%)	15,15,17	2.12	4 (26%)
3	NAG	M	1	1,3	14,14,15	0.85	0	17,19,21	1.47	2 (11%)
3	NAG	M	2	3	14,14,15	0.90	0	17,19,21	1.45	2 (11%)
2	NAG	N	1	1,2	14,14,15	0.98	0	17,19,21	1.29	2 (11%)
2	NAG	N	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.71	3 (17%)
2	BMA	N	3	2	11,11,12	0.51	0	15,15,17	1.45	2 (13%)
2	MAN	N	4	2	11,11,12	0.74	0	15,15,17	2.26	6 (40%)
2	MAN	N	5	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	N	6	2	11,11,12	0.54	0	15,15,17	2.14	5 (33%)
2	MAN	N	7	2	11,11,12	0.51	0	15,15,17	1.35	1 (6%)
2	MAN	N	8	2	11,11,12	0.55	0	15,15,17	1.55	4 (26%)
2	MAN	N	9	2	11,11,12	0.75	0	15,15,17	1.88	4 (26%)
3	NAG	O	1	1,3	14,14,15	0.65	0	17,19,21	1.97	3 (17%)
3	NAG	O	2	3	14,14,15	1.15	1 (7%)	17,19,21	2.66	4 (23%)
3	NAG	P	1	1,3	14,14,15	0.57	0	17,19,21	1.25	2 (11%)
3	NAG	P	2	3	14,14,15	0.53	0	17,19,21	1.60	5 (29%)
2	NAG	Q	1	1,2	14,14,15	0.73	0	17,19,21	2.65	8 (47%)
2	NAG	Q	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.27	2 (11%)
2	BMA	Q	3	2	11,11,12	0.72	0	15,15,17	1.95	5 (33%)
2	MAN	Q	4	2	11,11,12	0.41	0	15,15,17	1.52	2 (13%)
2	MAN	Q	5	2	11,11,12	0.62	0	15,15,17	1.24	1 (6%)
2	MAN	Q	6	2	11,11,12	0.82	0	15,15,17	1.40	3 (20%)
2	MAN	Q	7	2	11,11,12	0.64	0	15,15,17	1.80	2 (13%)
2	MAN	Q	8	2	11,11,12	0.79	0	15,15,17	2.19	4 (26%)
2	MAN	Q	9	2	11,11,12	1.15	1 (9%)	15,15,17	2.74	7 (46%)
3	NAG	R	1	1,3	14,14,15	0.92	0	17,19,21	2.34	5 (29%)
3	NAG	R	2	3	14,14,15	0.68	0	17,19,21	1.90	2 (11%)
3	NAG	S	1	1,3	14,14,15	0.56	0	17,19,21	1.91	4 (23%)
3	NAG	S	2	3	14,14,15	1.11	1 (7%)	17,19,21	2.46	5 (29%)
2	NAG	T	1	1,2	14,14,15	0.96	0	17,19,21	2.45	7 (41%)
2	NAG	T	2	2	14,14,15	0.68	0	17,19,21	1.97	6 (35%)
2	BMA	T	3	2	11,11,12	0.98	1 (9%)	15,15,17	1.75	4 (26%)
2	MAN	T	4	2	11,11,12	0.42	0	15,15,17	2.16	4 (26%)
2	MAN	T	5	2	11,11,12	0.55	0	15,15,17	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	T	6	2	11,11,12	1.02	1 (9%)	15,15,17	1.45	2 (13%)
2	MAN	T	7	2	11,11,12	0.75	0	15,15,17	2.20	5 (33%)
2	MAN	T	8	2	11,11,12	0.94	0	15,15,17	1.38	4 (26%)
2	MAN	T	9	2	11,11,12	0.87	0	15,15,17	2.41	4 (26%)
3	NAG	U	1	1,3	14,14,15	0.64	0	17,19,21	1.55	2 (11%)
3	NAG	U	2	3	14,14,15	0.59	0	17,19,21	2.14	5 (29%)
3	NAG	V	1	1,3	14,14,15	0.68	0	17,19,21	1.48	3 (17%)
3	NAG	V	2	3	14,14,15	0.90	0	17,19,21	1.78	6 (35%)
2	NAG	W	1	1,2	14,14,15	0.77	0	17,19,21	1.85	6 (35%)
2	NAG	W	2	2	14,14,15	0.82	0	17,19,21	2.06	5 (29%)
2	BMA	W	3	2	11,11,12	1.02	0	15,15,17	2.10	5 (33%)
2	MAN	W	4	2	11,11,12	0.81	1 (9%)	15,15,17	2.14	3 (20%)
2	MAN	W	5	2	11,11,12	0.55	0	15,15,17	1.92	4 (26%)
2	MAN	W	6	2	11,11,12	0.67	0	15,15,17	1.47	4 (26%)
2	MAN	W	7	2	11,11,12	0.65	0	15,15,17	2.12	5 (33%)
2	MAN	W	8	2	11,11,12	0.76	0	15,15,17	1.55	2 (13%)
2	MAN	W	9	2	11,11,12	0.79	0	15,15,17	2.07	3 (20%)
3	NAG	X	1	1,3	14,14,15	0.58	0	17,19,21	1.31	1 (5%)
3	NAG	X	2	3	14,14,15	0.70	0	17,19,21	2.01	5 (29%)
3	NAG	Y	1	1,3	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
3	NAG	Y	2	3	14,14,15	1.05	1 (7%)	17,19,21	2.49	4 (23%)
2	NAG	Z	1	1,2	14,14,15	0.71	0	17,19,21	2.00	6 (35%)
2	NAG	Z	2	2	14,14,15	0.56	0	17,19,21	1.71	3 (17%)
2	BMA	Z	3	2	11,11,12	0.69	0	15,15,17	1.57	4 (26%)
2	MAN	Z	4	2	11,11,12	0.75	0	15,15,17	2.06	4 (26%)
2	MAN	Z	5	2	11,11,12	0.47	0	15,15,17	1.92	4 (26%)
2	MAN	Z	6	2	11,11,12	1.10	0	15,15,17	2.84	7 (46%)
2	MAN	Z	7	2	11,11,12	0.84	0	15,15,17	2.49	4 (26%)
2	MAN	Z	8	2	11,11,12	0.64	0	15,15,17	1.68	3 (20%)
2	MAN	Z	9	2	11,11,12	0.77	0	15,15,17	2.23	3 (20%)
3	NAG	a	1	1,3	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
3	NAG	a	2	3	14,14,15	0.66	0	17,19,21	1.42	2 (11%)
3	NAG	b	1	1,3	14,14,15	0.82	0	17,19,21	1.94	7 (41%)
3	NAG	b	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.59	3 (17%)
2	NAG	c	1	1,2	14,14,15	1.11	1 (7%)	17,19,21	2.08	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	c	2	2	14,14,15	0.72	0	17,19,21	2.20	3 (17%)
2	BMA	c	3	2	11,11,12	0.50	0	15,15,17	1.83	5 (33%)
2	MAN	c	4	2	11,11,12	0.94	0	15,15,17	1.98	5 (33%)
2	MAN	c	5	2	11,11,12	0.81	0	15,15,17	2.75	4 (26%)
2	MAN	c	6	2	11,11,12	0.65	0	15,15,17	1.28	2 (13%)
2	MAN	c	7	2	11,11,12	0.58	0	15,15,17	1.84	2 (13%)
2	MAN	c	8	2	11,11,12	0.47	0	15,15,17	1.72	1 (6%)
2	MAN	c	9	2	11,11,12	0.57	0	15,15,17	1.55	4 (26%)
3	NAG	d	1	1,3	14,14,15	1.14	2 (14%)	17,19,21	2.93	7 (41%)
3	NAG	d	2	3	14,14,15	1.13	1 (7%)	17,19,21	1.79	5 (29%)
3	NAG	e	1	1,3	14,14,15	0.54	0	17,19,21	1.79	5 (29%)
3	NAG	e	2	3	14,14,15	1.32	0	17,19,21	2.13	5 (29%)

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	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	0/2/19/22	0/1/1/1
2	MAN	I	6	2	-	0/2/19/22	0/1/1/1
2	MAN	I	7	2	-	0/2/19/22	0/1/1/1
2	MAN	I	8	2	-	0/2/19/22	0/1/1/1
2	MAN	I	9	2	-	2/2/19/22	1/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	MAN	T	6	2	-	0/2/19/22	0/1/1/1
2	MAN	T	7	2	-	1/2/19/22	0/1/1/1
2	MAN	T	8	2	-	0/2/19/22	0/1/1/1
2	MAN	T	9	2	-	2/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	1/6/23/26	0/1/1/1
2	BMA	W	3	2	-	1/2/19/22	0/1/1/1
2	MAN	W	4	2	-	1/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	1/2/19/22	0/1/1/1
2	MAN	W	7	2	-	2/2/19/22	0/1/1/1
2	MAN	W	8	2	-	2/2/19/22	0/1/1/1
2	MAN	W	9	2	-	0/2/19/22	0/1/1/1
3	NAG	X	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	5	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	6	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	7	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	8	2	-	2/2/19/22	0/1/1/1
2	MAN	Z	9	2	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	4/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	5/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	BMA	c	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	c	4	2	-	2/2/19/22	0/1/1/1
2	MAN	c	5	2	-	0/2/19/22	0/1/1/1
2	MAN	c	6	2	-	2/2/19/22	0/1/1/1
2	MAN	c	7	2	-	0/2/19/22	0/1/1/1
2	MAN	c	8	2	-	0/2/19/22	0/1/1/1
2	MAN	c	9	2	-	1/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2	NAG	C1-C2	3.10	1.57	1.52
2	Q	9	MAN	C2-C3	2.65	1.56	1.52
2	I	8	MAN	C2-C3	2.64	1.56	1.52
3	d	2	NAG	C1-C2	2.63	1.56	1.52
2	N	2	NAG	C1-C2	2.57	1.56	1.52

The worst 5 of 413 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	5	MAN	C1-O5-C5	8.70	123.98	112.19
3	Y	2	NAG	C1-O5-C5	8.07	123.13	112.19
2	Q	1	NAG	C1-O5-C5	7.91	122.91	112.19
3	R	1	NAG	C1-O5-C5	7.64	122.55	112.19
2	I	7	MAN	C1-O5-C5	7.53	122.39	112.19

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2

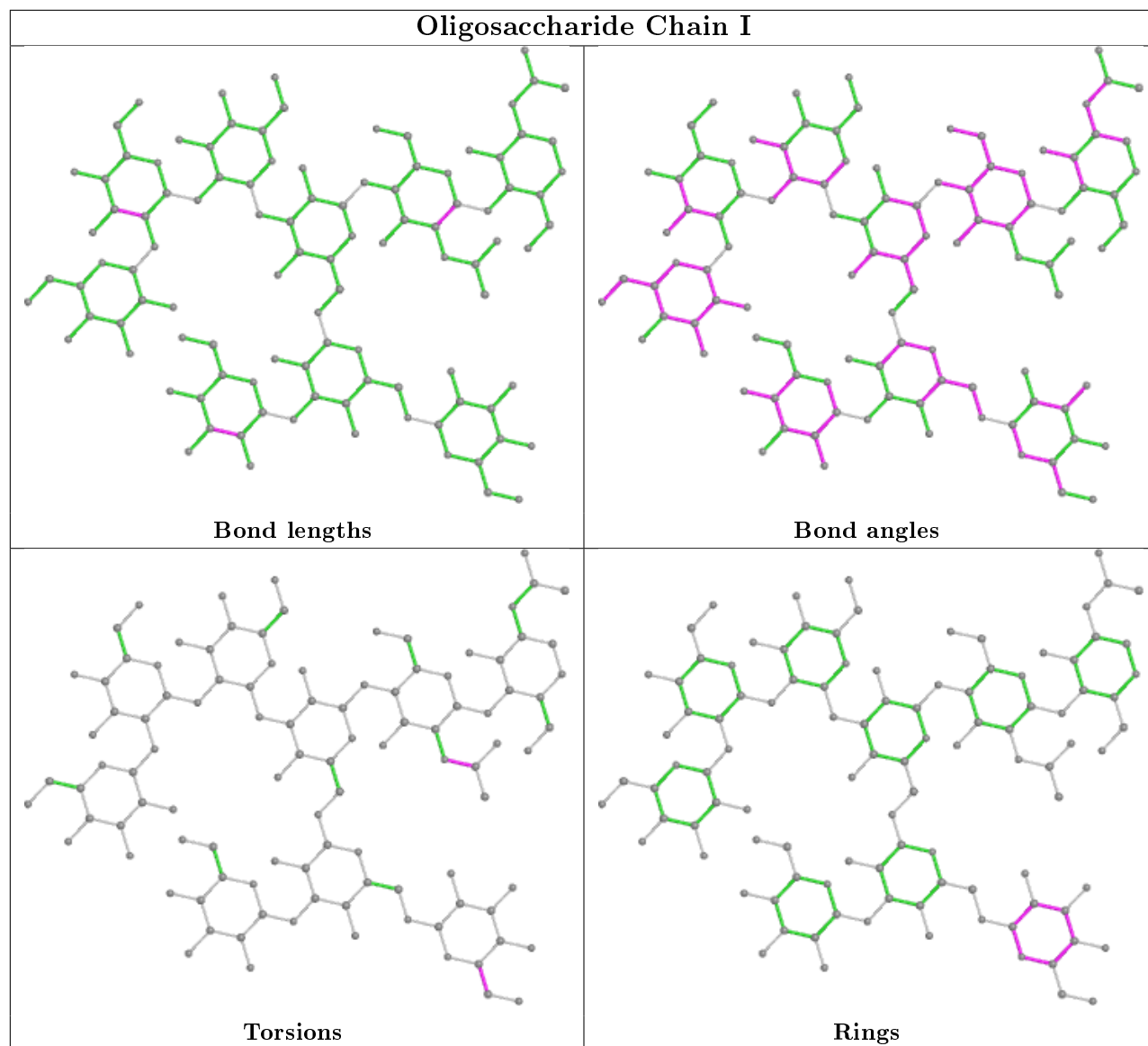
All (1) ring outliers are listed below:

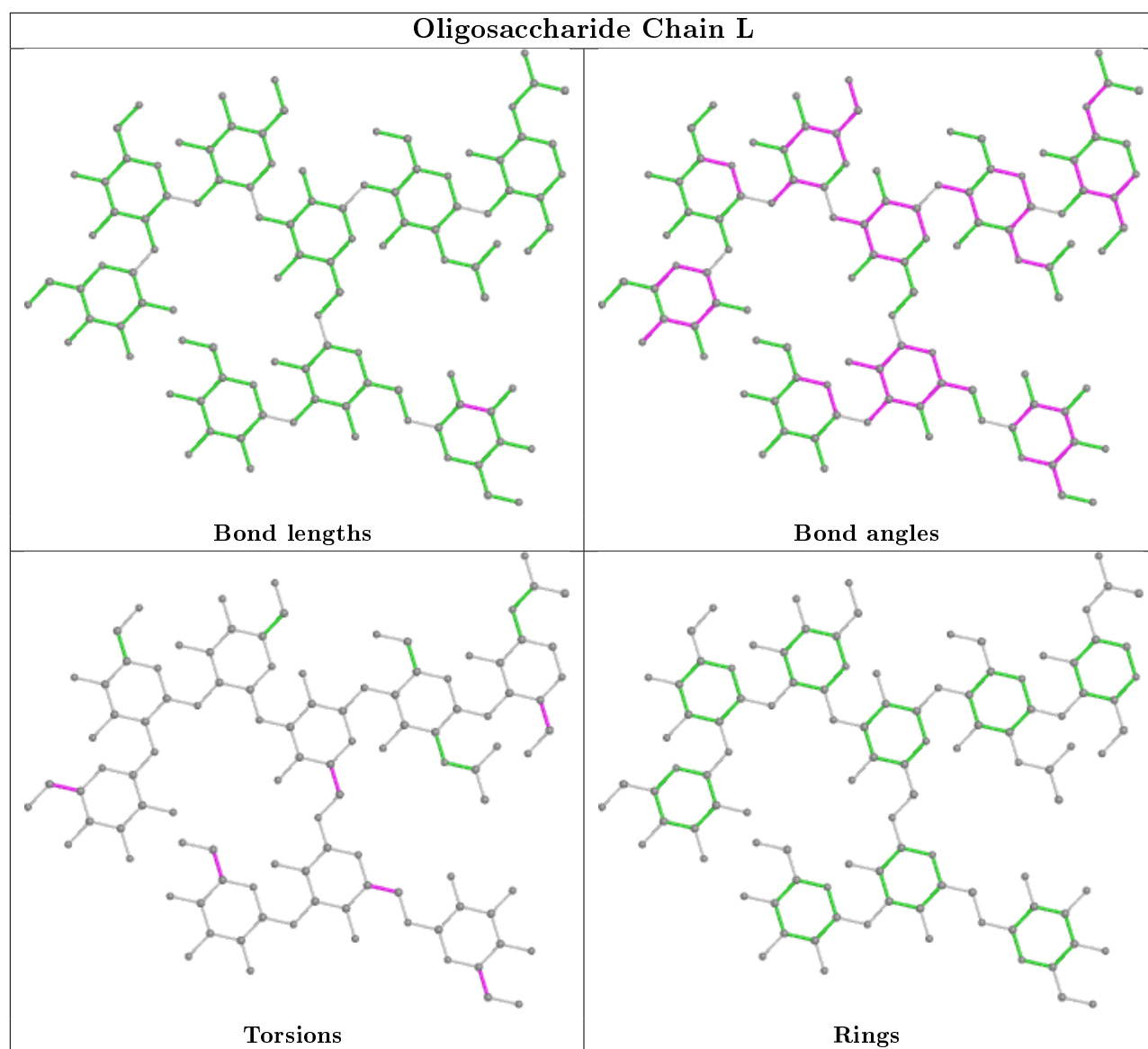
Mol	Chain	Res	Type	Atoms
2	I	9	MAN	C1-C2-C3-C4-C5-O5

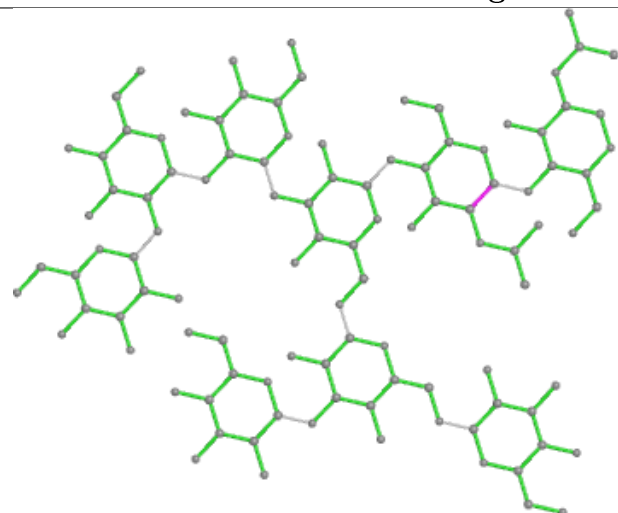
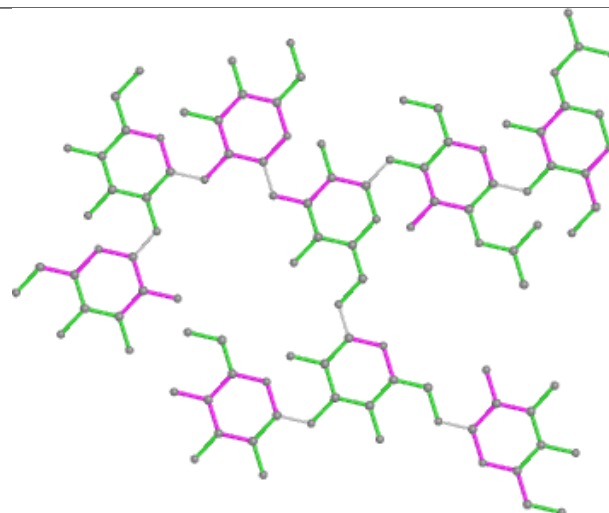
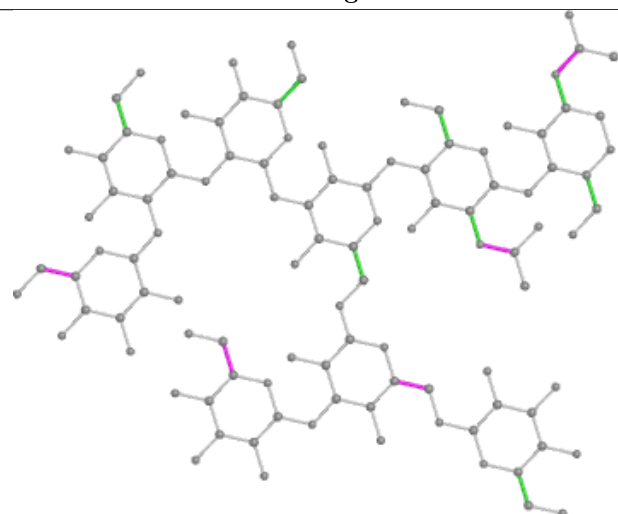
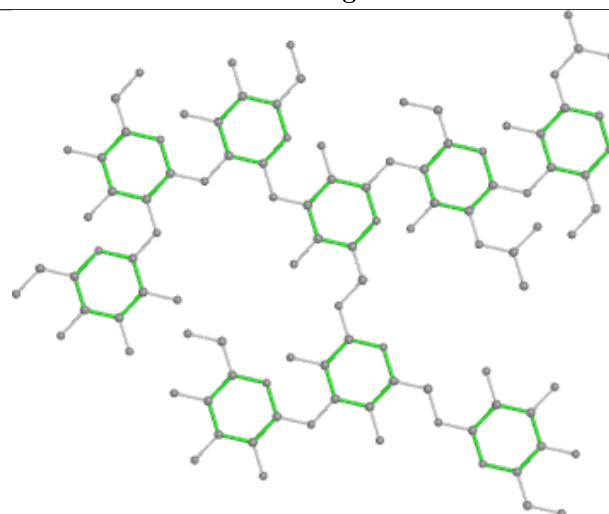
34 monomers are involved in 42 short contacts:

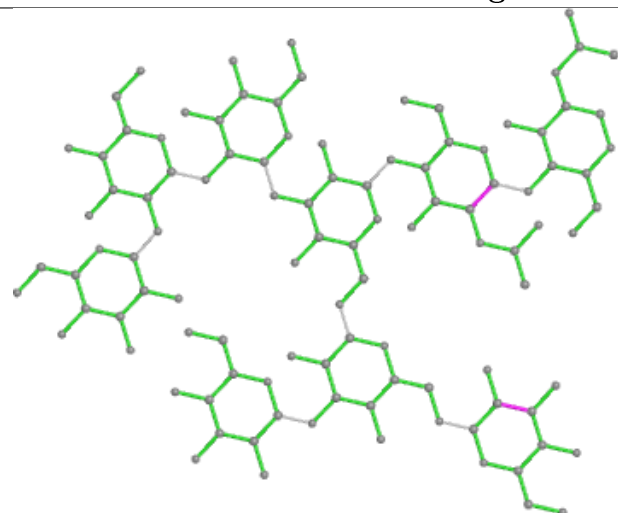
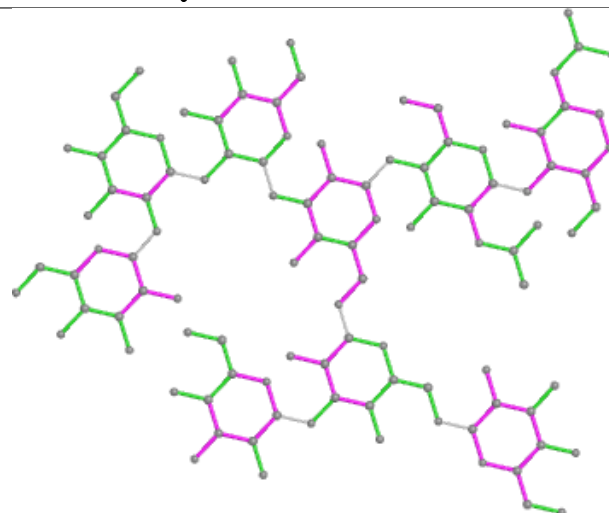
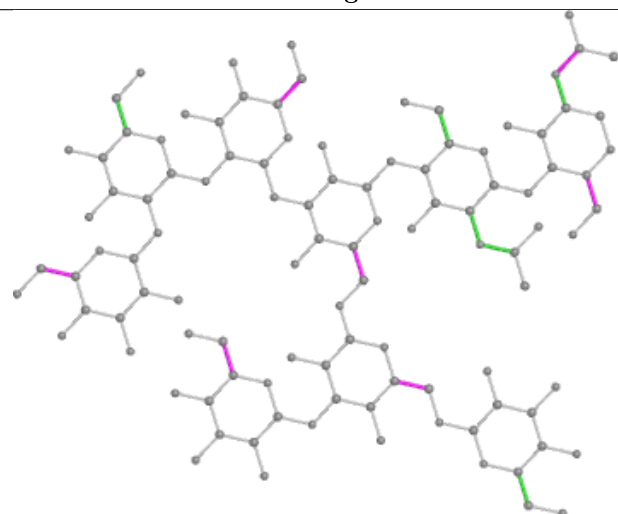
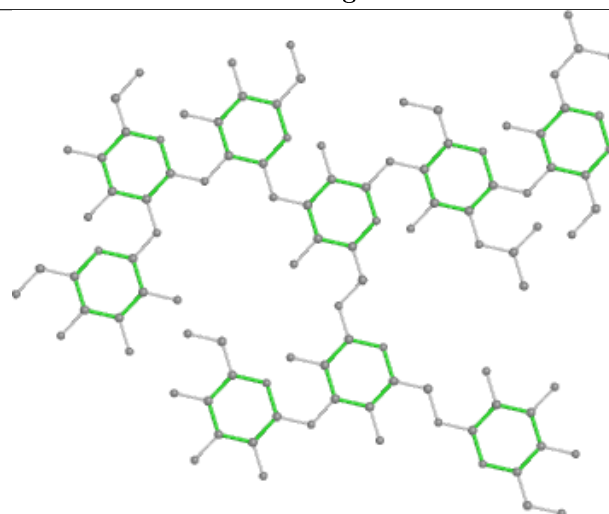
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0
2	Z	2	NAG	2	0
3	M	2	NAG	1	0
2	T	9	MAN	1	0
2	L	6	MAN	1	0
2	T	5	MAN	1	0
2	Z	6	MAN	1	0
3	O	2	NAG	1	0
3	O	1	NAG	2	0
2	I	6	MAN	2	0
3	U	1	NAG	2	0
2	L	3	BMA	1	0
2	W	1	NAG	1	0
3	V	1	NAG	4	0
4	K	1	NAG	1	0
3	R	1	NAG	1	0
2	W	7	MAN	3	0
2	W	5	MAN	2	0
2	W	3	BMA	1	0
2	I	5	MAN	1	0
2	Z	4	MAN	1	0
2	T	3	BMA	1	0
2	Q	4	MAN	1	0
2	N	6	MAN	5	0
2	Q	5	MAN	1	0
2	Q	1	NAG	1	0
2	W	9	MAN	2	0
2	I	4	MAN	1	0
2	T	7	MAN	1	0
3	X	1	NAG	2	0
2	W	4	MAN	1	0
2	Z	5	MAN	1	0
2	N	3	BMA	1	0
2	L	1	NAG	3	0

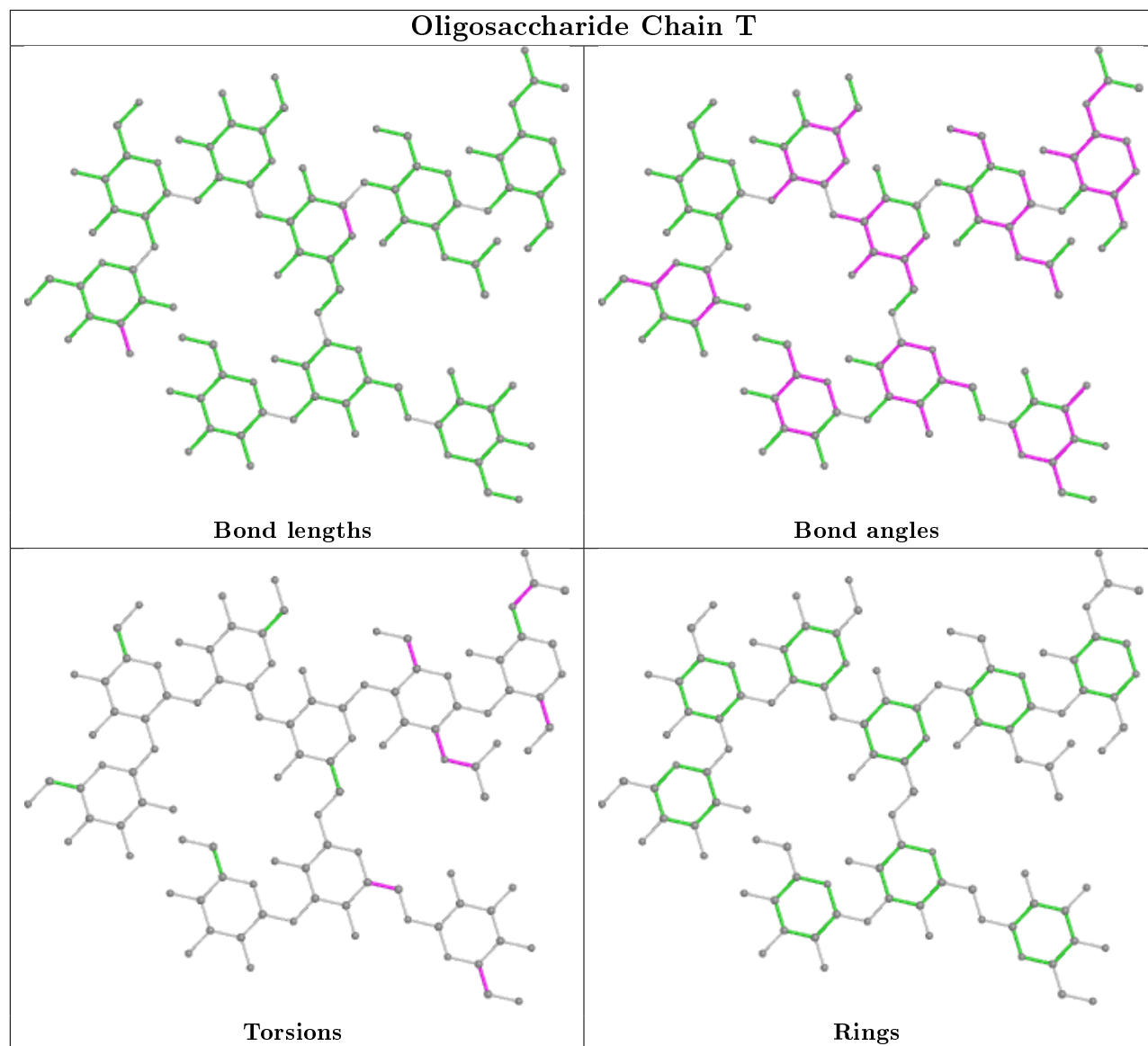
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

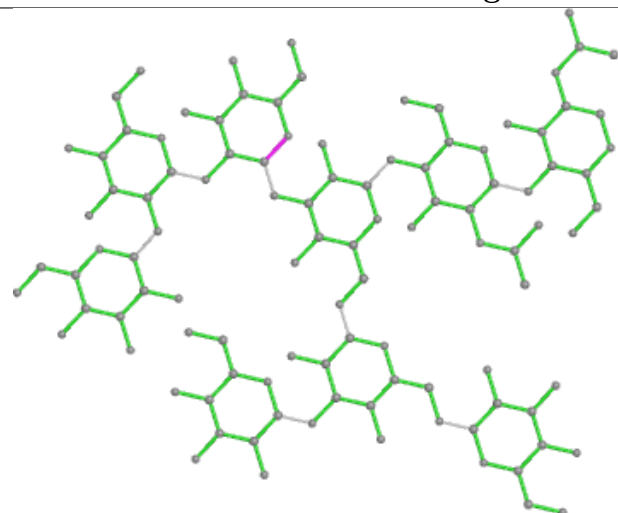
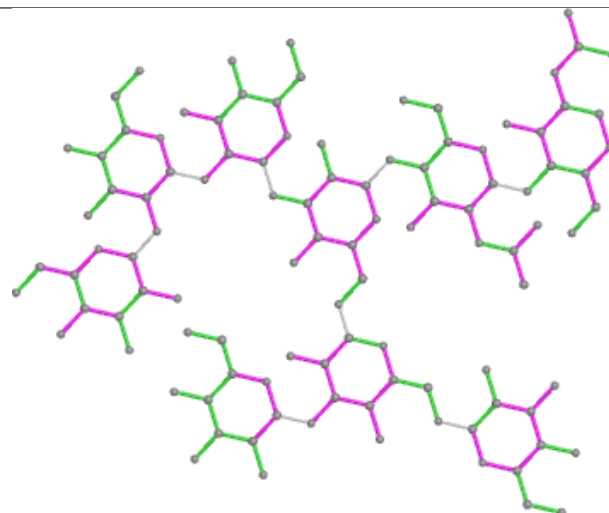
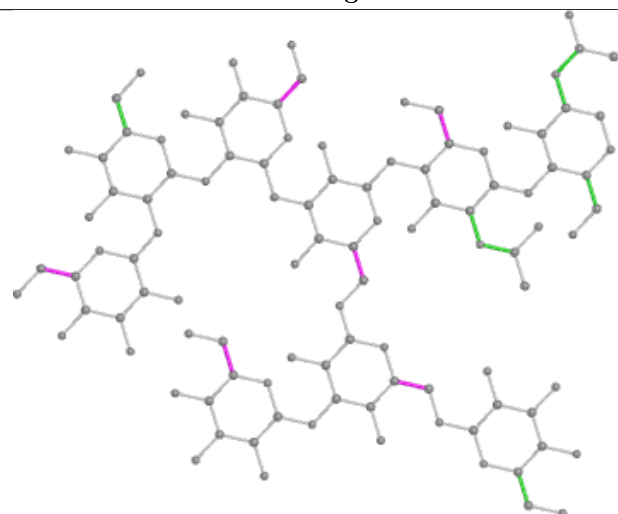
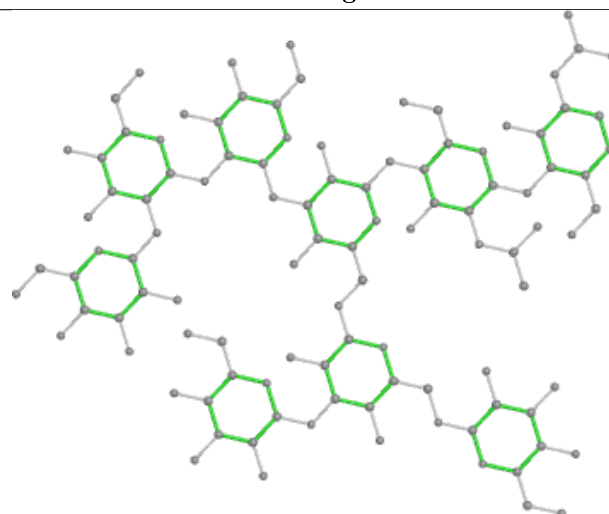


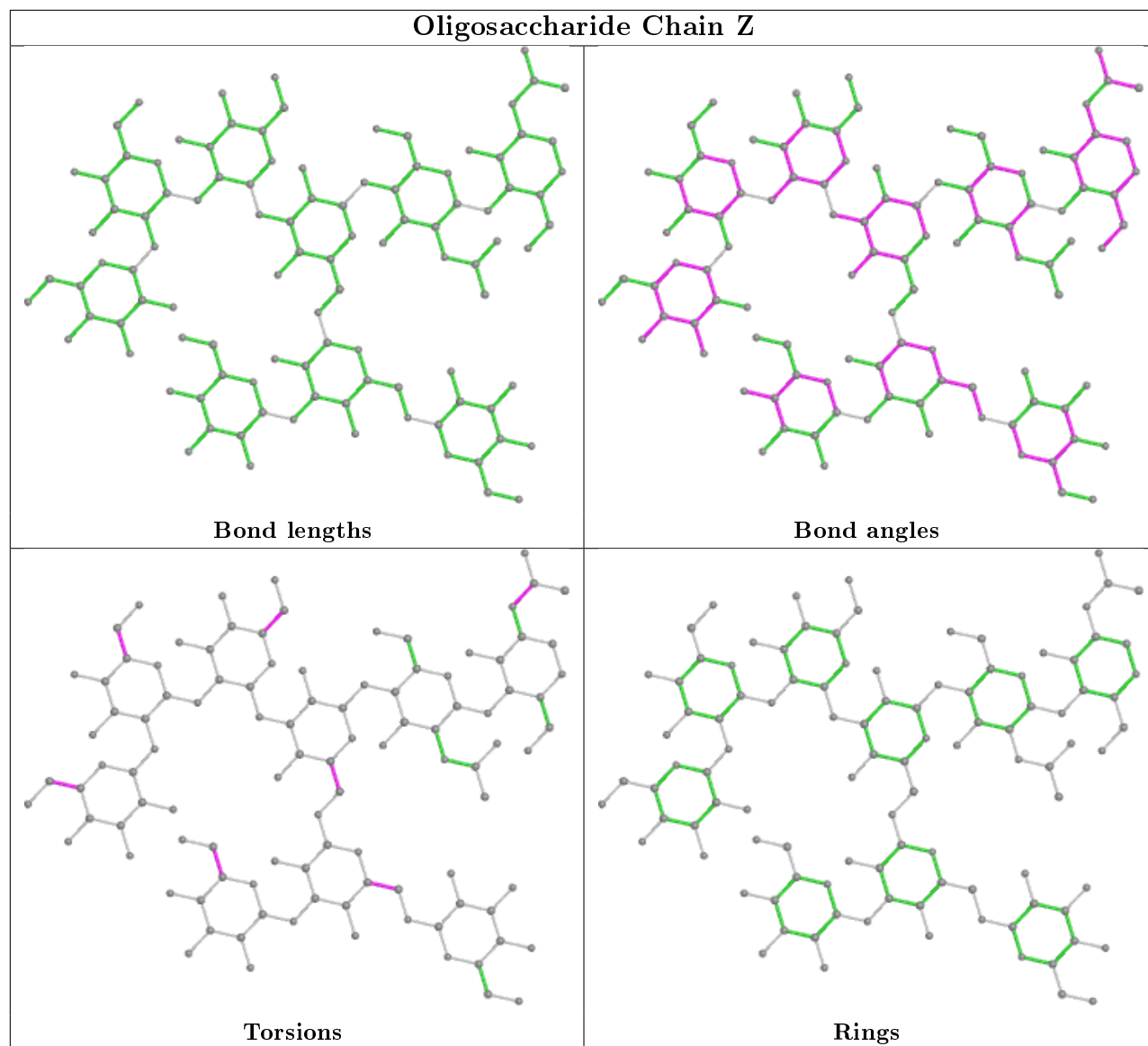


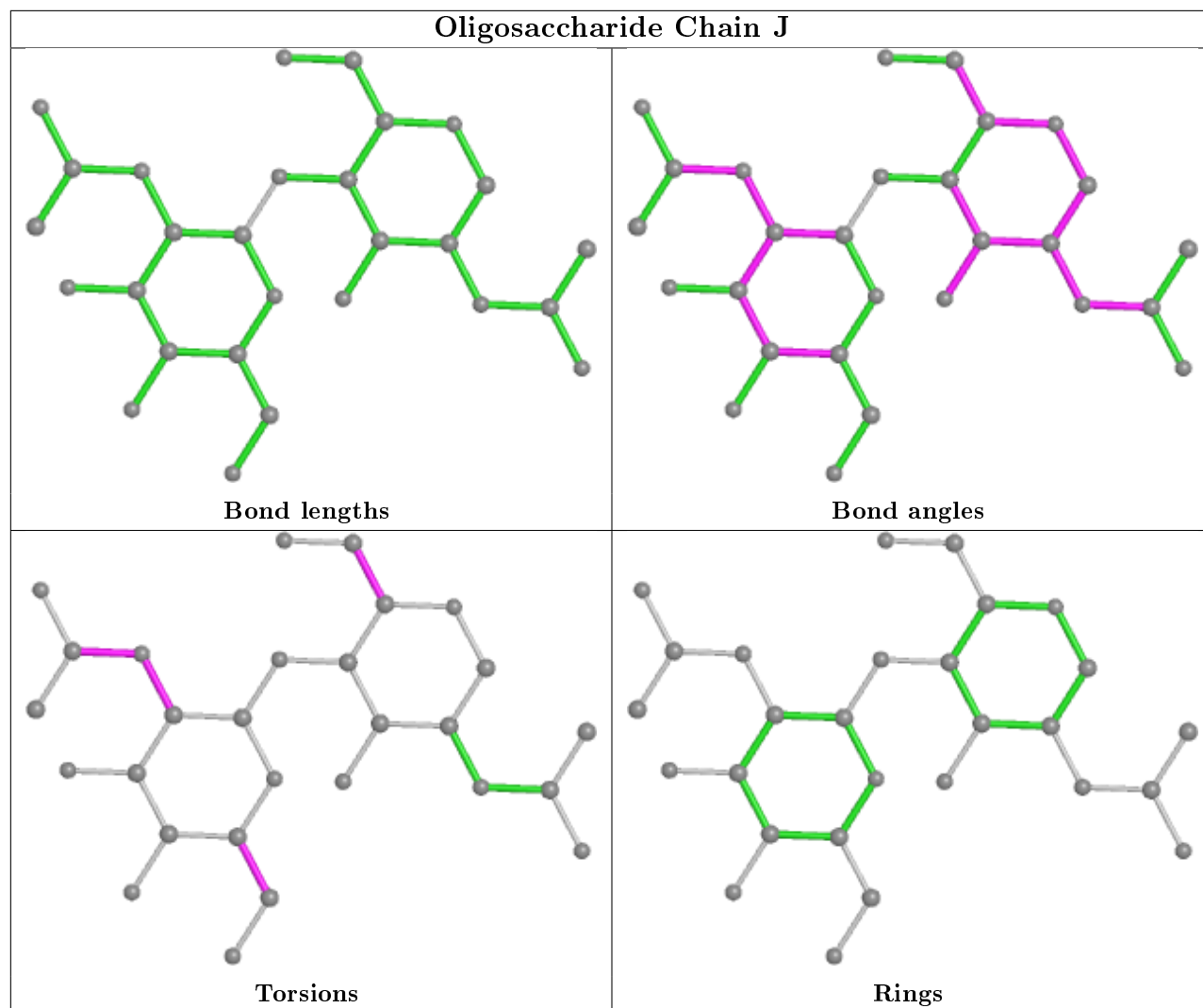
Oligosaccharide Chain N**Bond lengths****Bond angles****Torsions****Rings**

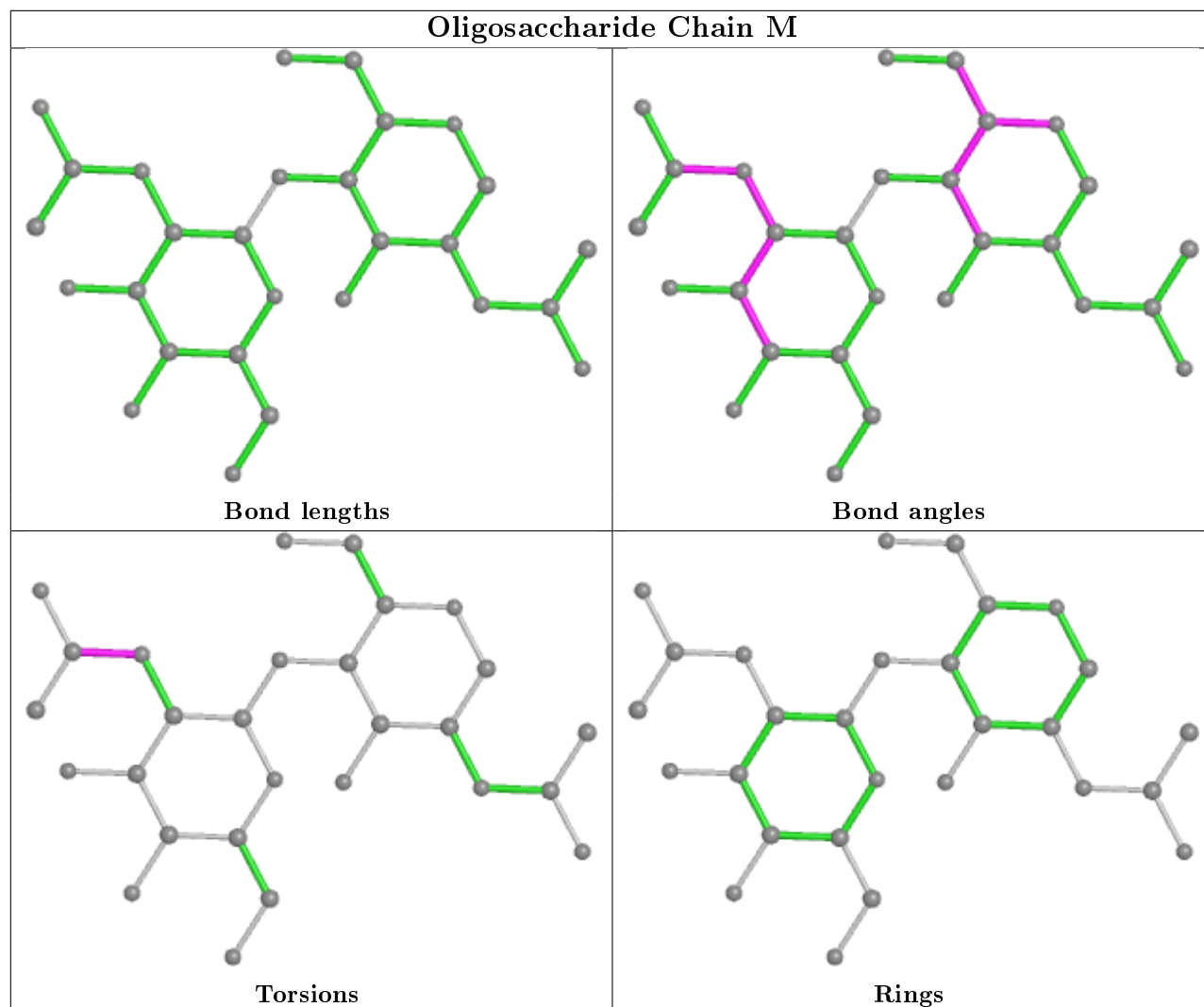
Oligosaccharide Chain Q**Bond lengths****Bond angles****Torsions****Rings**

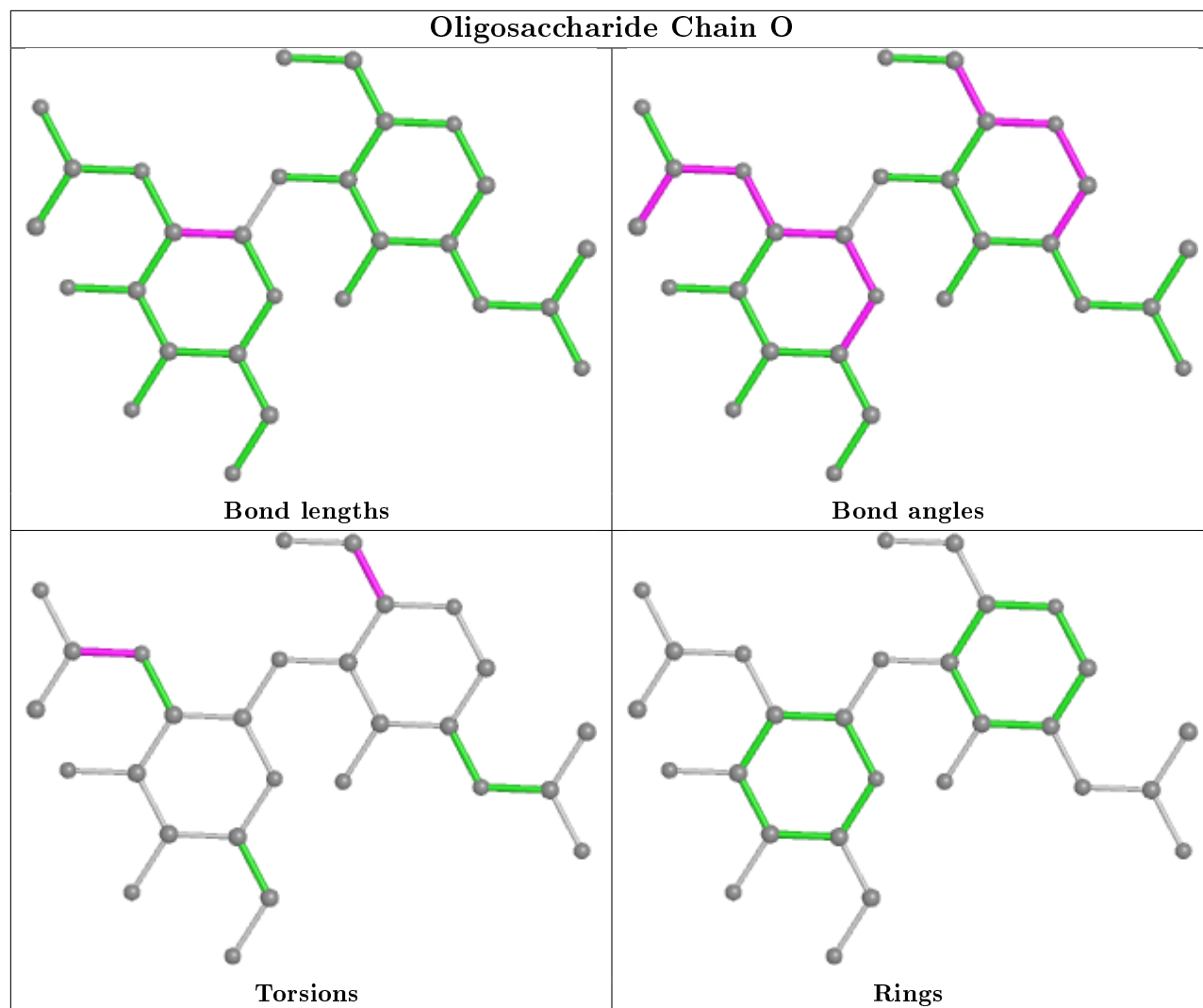


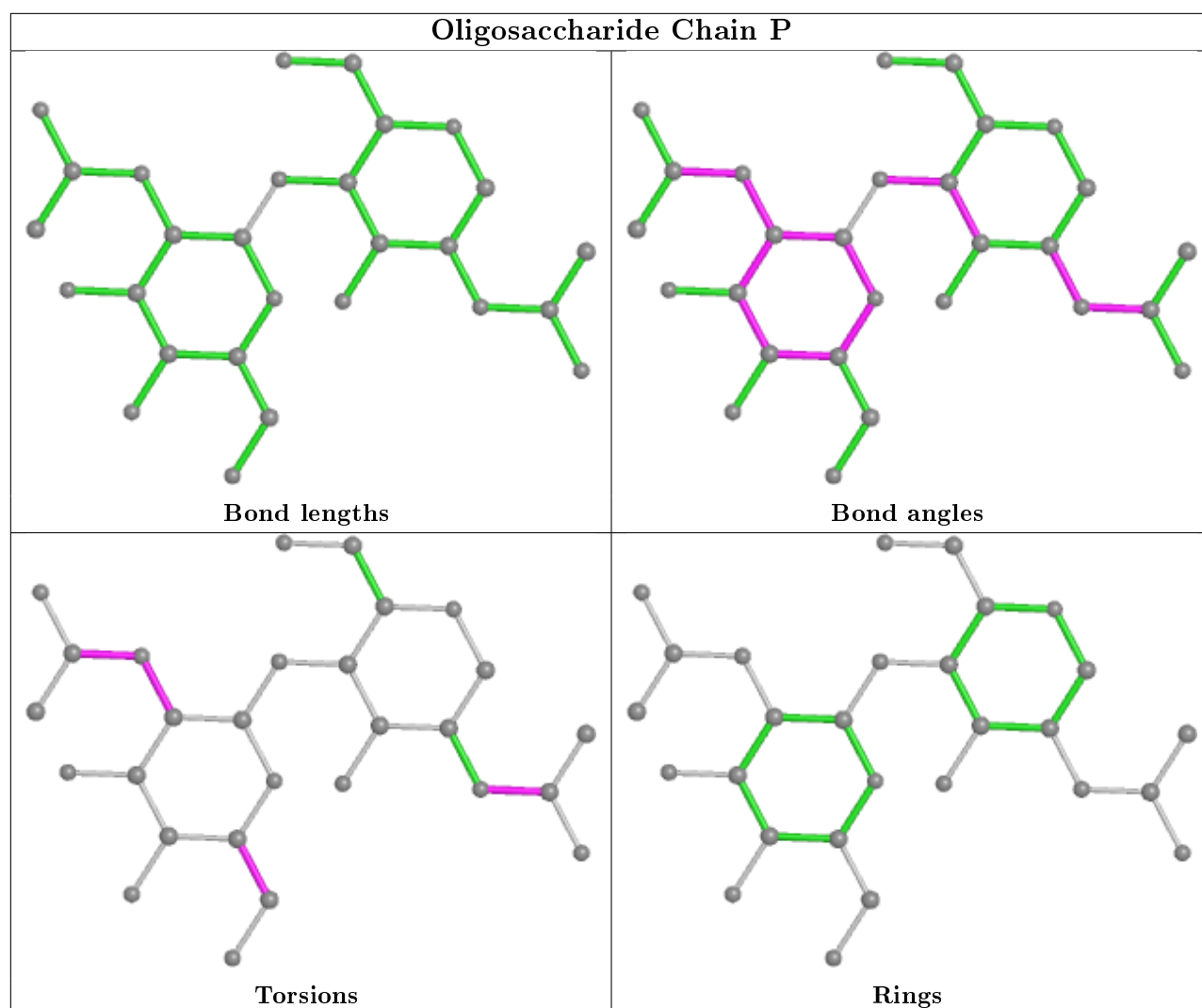
Oligosaccharide Chain W**Bond lengths****Bond angles****Torsions****Rings**

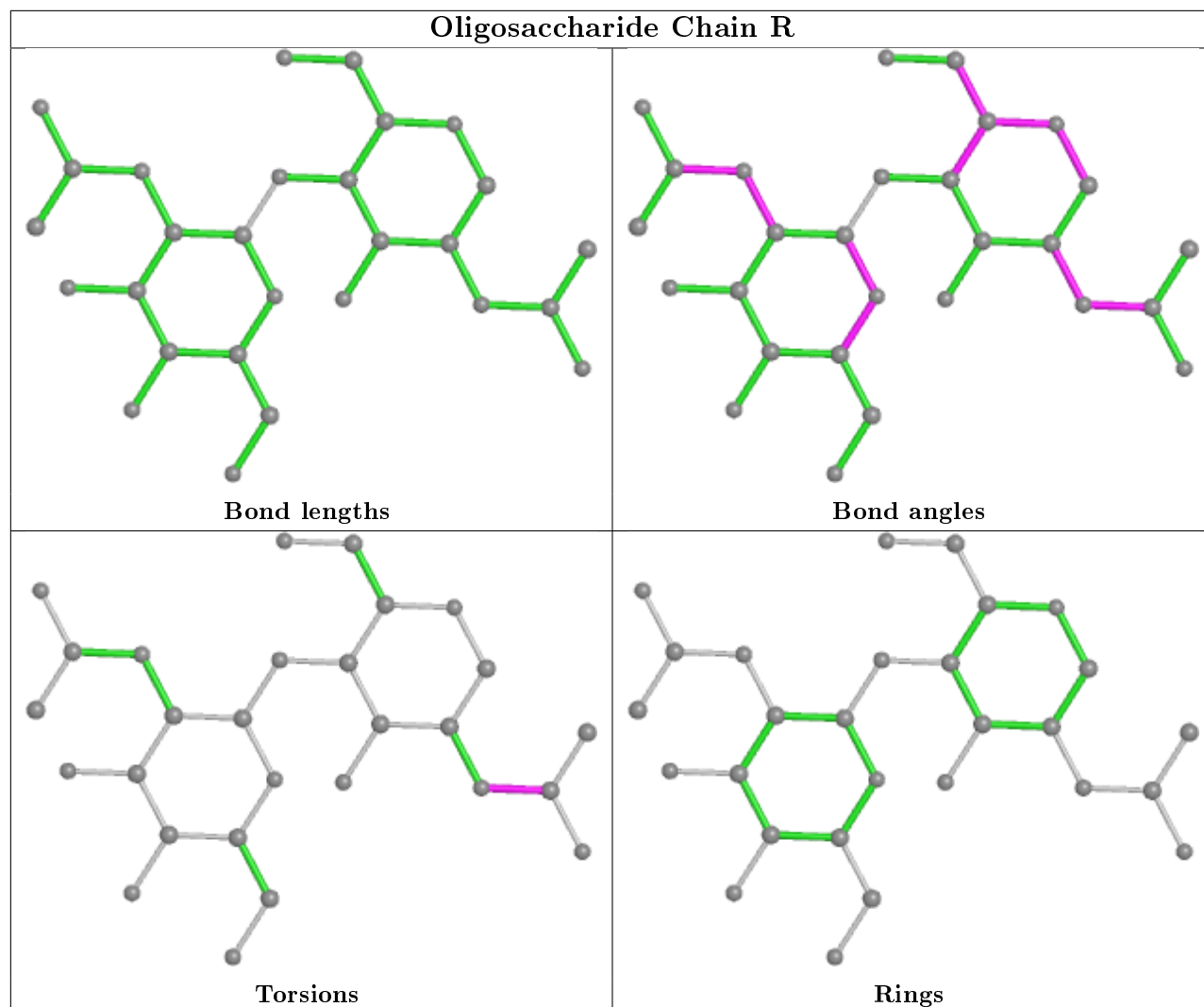


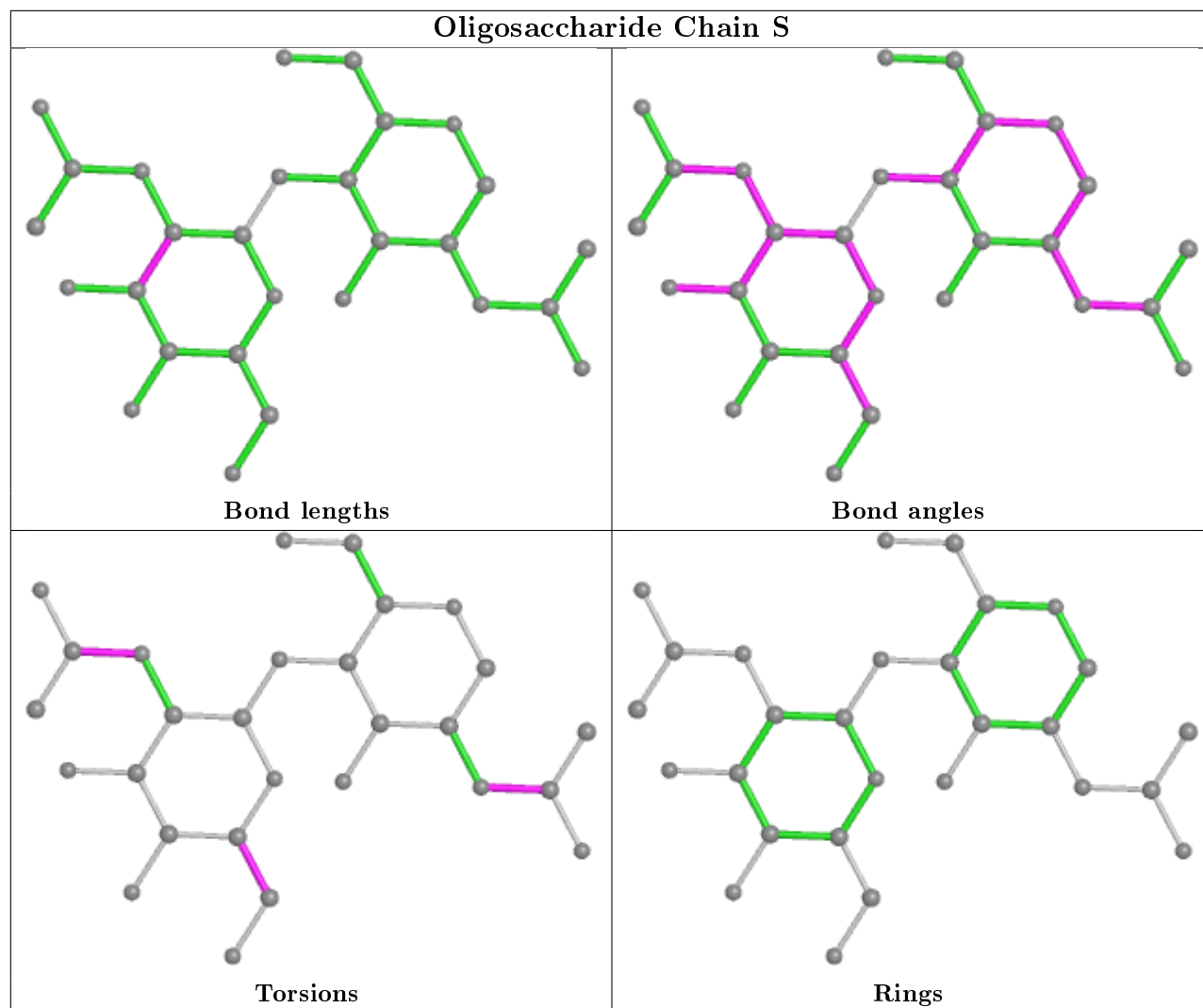


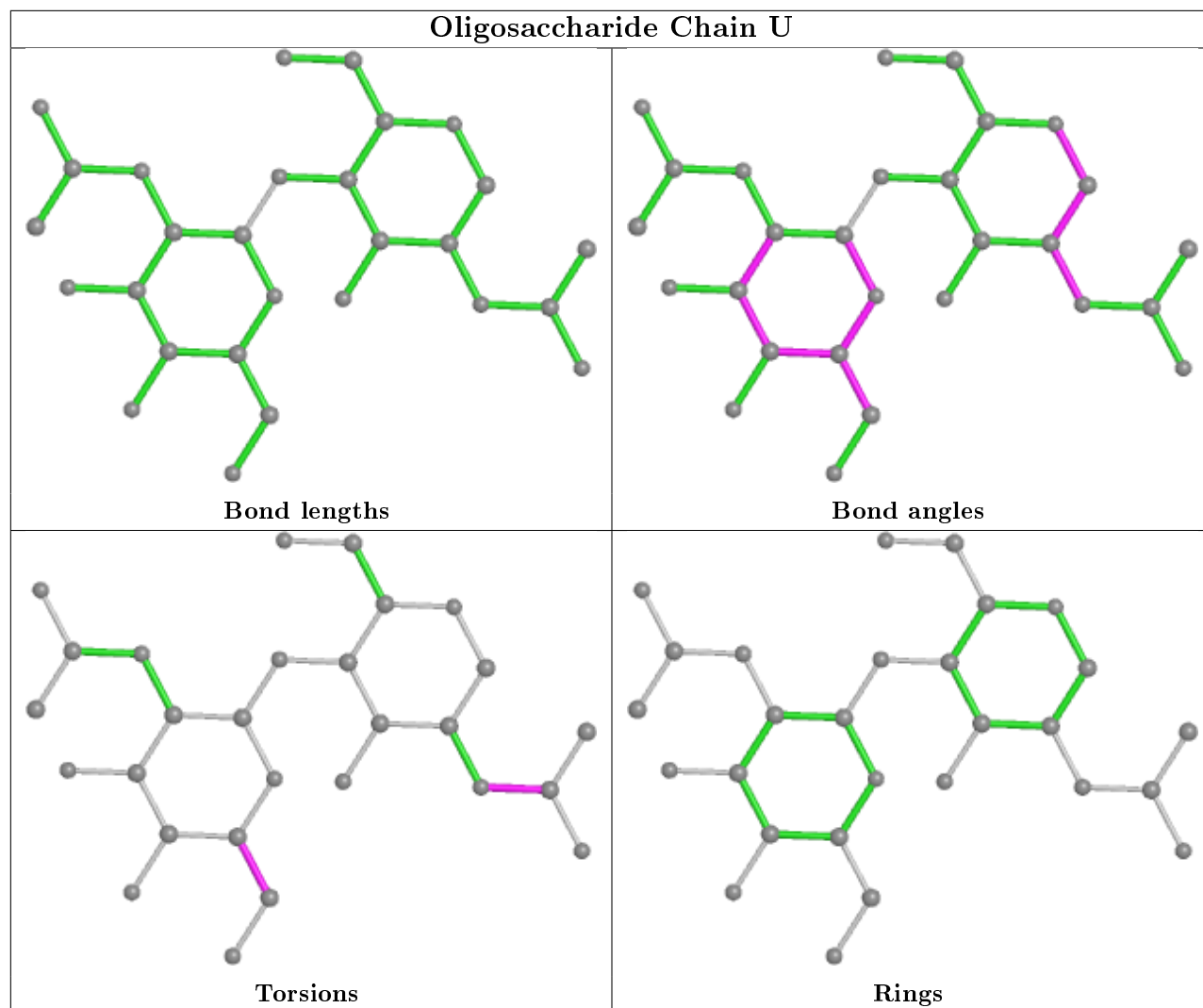


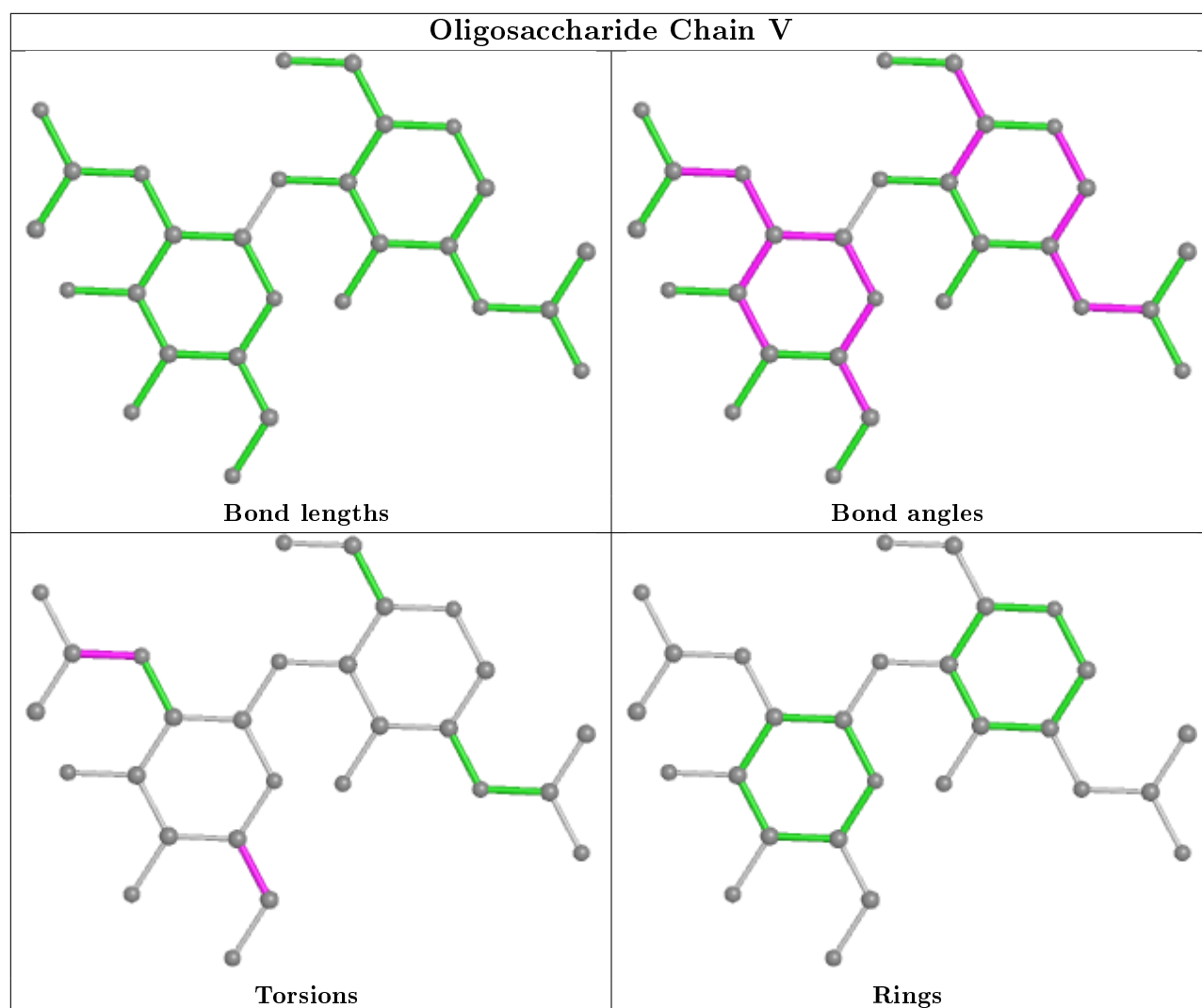


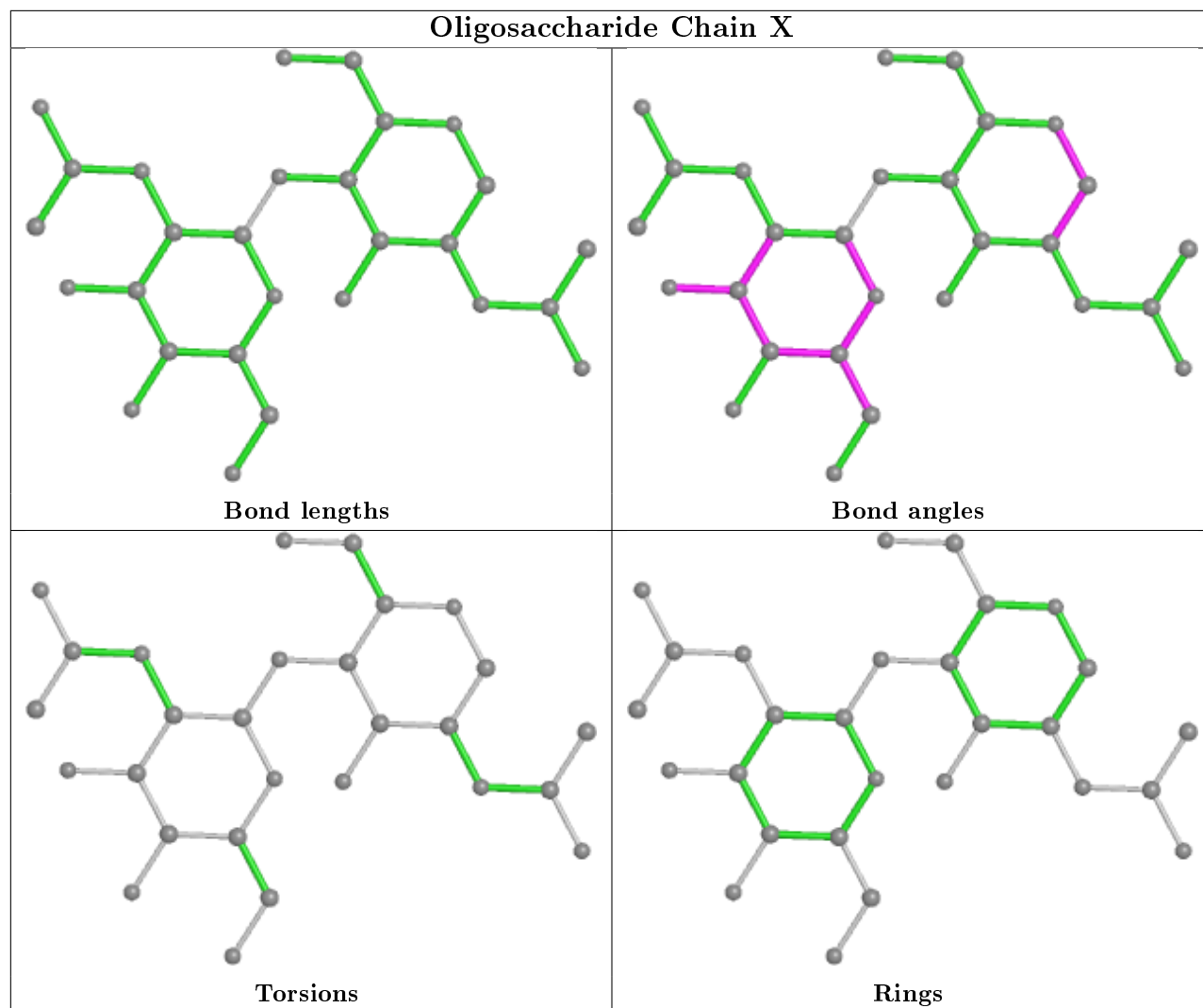


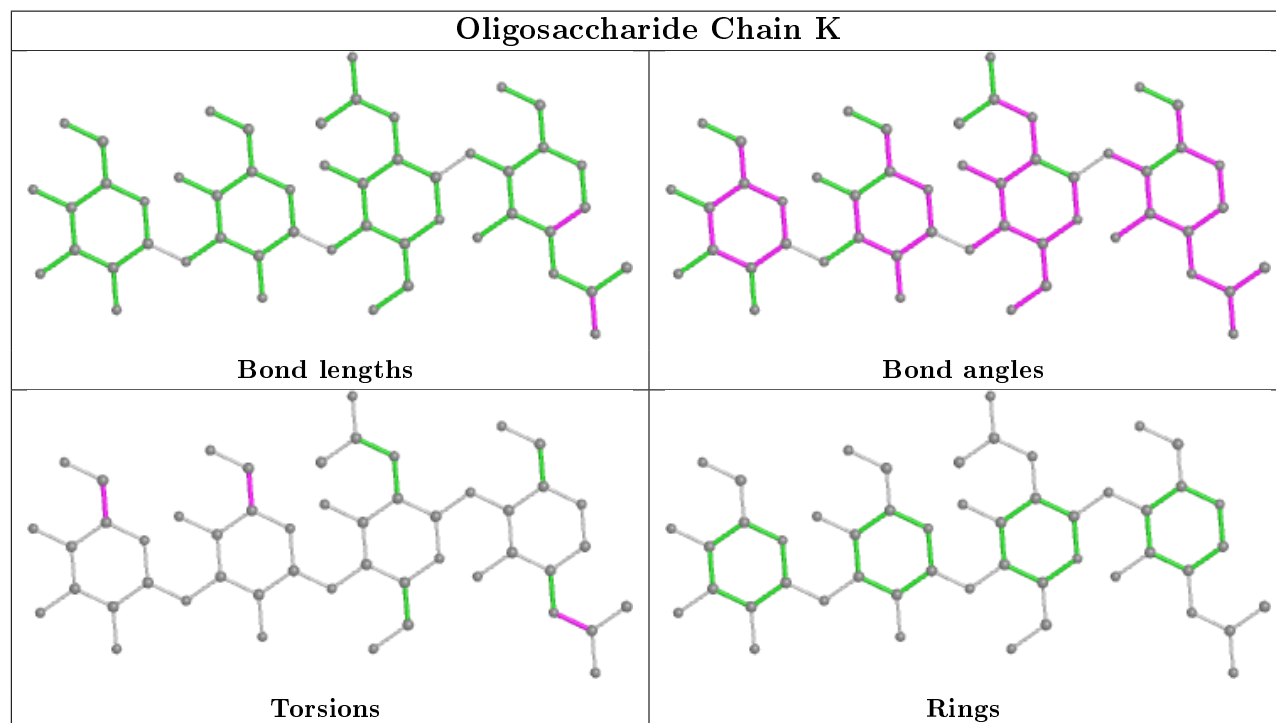
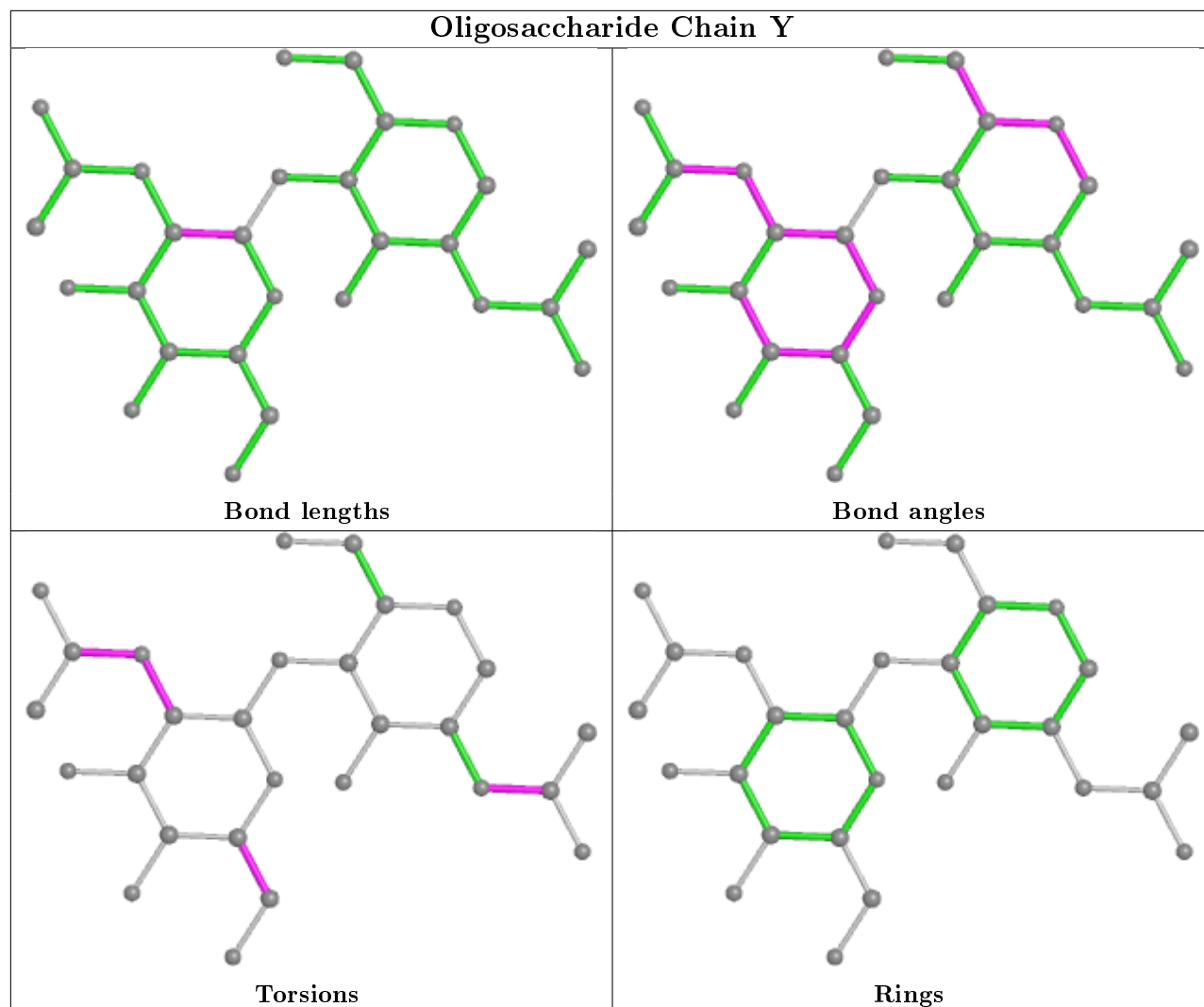












5.6 Ligand geometry

8 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
5	NAG	E	514	1	14,14,15	0.74	1 (7%)	17,19,21	1.68	2 (11%)
5	NAG	B	512	1	14,14,15	1.04	1 (7%)	17,19,21	2.28	4 (23%)
5	NAG	A	516	1	14,14,15	0.73	0	17,19,21	1.53	3 (17%)
5	NAG	H	514	1	14,14,15	0.86	1 (7%)	17,19,21	1.73	3 (17%)
5	NAG	F	514	1	14,14,15	0.91	1 (7%)	17,19,21	1.50	4 (23%)
5	NAG	G	514	1	14,14,15	0.91	1 (7%)	17,19,21	1.84	2 (11%)
5	NAG	B	513	1	14,14,15	0.71	0	17,19,21	1.66	3 (17%)
5	NAG	C	514	1	14,14,15	0.76	0	17,19,21	2.76	5 (29%)

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
5	NAG	E	514	1	-	2/6/23/26	0/1/1/1
5	NAG	B	512	1	-	3/6/23/26	0/1/1/1
5	NAG	A	516	1	-	1/6/23/26	0/1/1/1
5	NAG	H	514	1	-	6/6/23/26	0/1/1/1
5	NAG	F	514	1	-	3/6/23/26	0/1/1/1
5	NAG	G	514	1	-	4/6/23/26	0/1/1/1
5	NAG	B	513	1	-	4/6/23/26	0/1/1/1
5	NAG	C	514	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	512	NAG	C1-C2	2.69	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	514	NAG	C1-C2	2.46	1.56	1.52
5	F	514	NAG	C1-C2	2.32	1.55	1.52
5	H	514	NAG	C3-C2	2.17	1.57	1.52
5	E	514	NAG	C1-C2	2.12	1.55	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	512	NAG	C1-O5-C5	7.68	122.60	112.19
5	C	514	NAG	C2-N2-C7	6.84	132.65	122.90
5	C	514	NAG	C1-O5-C5	6.22	120.61	112.19
5	E	514	NAG	C1-O5-C5	5.45	119.58	112.19
5	A	516	NAG	C4-C3-C2	4.71	117.92	111.02

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	514	NAG	C1-C2-N2-C7
5	G	514	NAG	C8-C7-N2-C2
5	G	514	NAG	O7-C7-N2-C2
5	B	513	NAG	C8-C7-N2-C2
5	B	513	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	514	NAG	1	0
5	B	513	NAG	1	0
5	C	514	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 [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, 95th 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 ²)	Q<0.9
1	A	438/473 (92%)	-0.43	2 (0%) 91 90	8, 18, 40, 69	0
1	B	438/473 (92%)	-0.47	2 (0%) 91 90	9, 18, 36, 68	0
1	C	435/473 (91%)	-0.44	3 (0%) 87 86	10, 20, 42, 71	0
1	D	435/473 (91%)	-0.38	1 (0%) 95 95	8, 20, 40, 63	0
1	E	438/473 (92%)	-0.42	5 (1%) 80 79	6, 19, 45, 79	0
1	F	438/473 (92%)	-0.29	6 (1%) 75 73	11, 23, 50, 78	0
1	G	435/473 (91%)	-0.37	1 (0%) 95 95	13, 24, 43, 74	0
1	H	435/473 (91%)	-0.51	1 (0%) 95 95	9, 16, 36, 57	0
All	All	3492/3784 (92%)	-0.41	21 (0%) 89 89	6, 20, 43, 79	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	TRP	5.1
1	B	34	ILE	4.2
1	E	295	TRP	3.5
1	F	340	PRO	3.5
1	F	44	TYR	3.3

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, 95th 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 ²)	Q<0.9
2	MAN	L	9	11/12	0.77	0.23	72,75,77,78	0
2	MAN	Q	9	11/12	0.79	0.22	42,55,57,57	0
3	NAG	Y	2	14/15	0.80	0.25	45,57,59,63	0
3	NAG	J	2	14/15	0.81	0.22	54,69,77,80	0
3	NAG	O	2	14/15	0.82	0.27	58,62,66,66	0
3	NAG	V	2	14/15	0.83	0.20	45,52,58,59	0
3	NAG	P	2	14/15	0.84	0.21	58,64,71,72	0
2	MAN	I	9	11/12	0.84	0.16	37,39,43,44	0
3	NAG	R	2	14/15	0.84	0.23	40,58,61,64	0
3	NAG	b	2	14/15	0.84	0.31	75,81,83,86	0
3	NAG	J	1	14/15	0.85	0.23	53,57,65,71	0
3	NAG	a	2	14/15	0.86	0.30	45,55,64,71	0
3	NAG	b	1	14/15	0.86	0.20	41,52,61,73	0
2	MAN	c	9	11/12	0.87	0.15	33,37,39,39	0
3	NAG	e	2	14/15	0.87	0.21	29,34,35,35	0
3	NAG	d	2	14/15	0.87	0.24	37,45,47,50	0
2	MAN	N	9	11/12	0.88	0.13	36,50,53,58	0
2	MAN	N	4	11/12	0.88	0.17	25,29,32,32	0
3	NAG	X	2	14/15	0.89	0.26	47,63,71,71	0
4	MAN	K	4	11/12	0.89	0.16	41,44,52,52	0
3	NAG	M	1	14/15	0.89	0.20	40,46,50,57	0
3	NAG	O	1	14/15	0.90	0.17	36,45,51,60	0
2	MAN	W	8	11/12	0.90	0.19	42,44,46,49	0
3	NAG	X	1	14/15	0.91	0.15	33,44,53,55	0
3	NAG	M	2	14/15	0.91	0.33	49,57,61,61	0
2	MAN	Z	9	11/12	0.91	0.13	43,51,51,57	0
3	NAG	V	1	14/15	0.91	0.15	31,42,48,52	0
2	MAN	T	9	11/12	0.92	0.18	32,37,45,45	0
3	NAG	P	1	14/15	0.92	0.13	35,41,49,57	0
3	NAG	S	2	14/15	0.92	0.12	27,31,35,36	0
2	MAN	Q	8	11/12	0.92	0.15	36,41,44,45	0
3	NAG	U	2	14/15	0.92	0.20	43,48,52,54	0
2	MAN	c	8	11/12	0.93	0.11	29,37,38,41	0
4	BMA	K	3	11/12	0.93	0.13	37,42,46,47	0
2	MAN	N	8	11/12	0.93	0.16	39,43,45,45	0
3	NAG	R	1	14/15	0.93	0.21	42,46,52,61	0
2	MAN	Q	7	11/12	0.93	0.11	38,43,46,51	0
2	BMA	L	3	11/12	0.93	0.14	28,31,37,39	0
2	MAN	W	9	11/12	0.93	0.15	42,46,50,55	0
2	MAN	I	8	11/12	0.93	0.14	23,26,28,29	0
3	NAG	d	1	14/15	0.94	0.14	25,31,34,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	L	7	11/12	0.94	0.11	35,38,47,60	0
2	MAN	L	8	11/12	0.94	0.11	28,33,40,41	0
3	NAG	Y	1	14/15	0.94	0.12	37,41,45,51	0
2	MAN	Z	6	11/12	0.94	0.12	22,25,28,29	0
2	MAN	N	5	11/12	0.94	0.15	25,27,29,32	0
2	MAN	I	5	11/12	0.94	0.15	20,23,26,26	0
2	NAG	L	2	14/15	0.94	0.12	23,25,27,31	0
2	BMA	Q	3	11/12	0.94	0.16	26,29,36,40	0
3	NAG	a	1	14/15	0.94	0.20	44,52,56,57	0
2	MAN	T	8	11/12	0.94	0.12	30,34,37,37	0
2	MAN	T	6	11/12	0.95	0.12	23,26,28,32	0
2	BMA	W	3	11/12	0.95	0.10	26,28,31,31	0
4	NAG	K	2	14/15	0.95	0.12	29,32,40,45	0
3	NAG	U	1	14/15	0.95	0.14	23,29,34,36	0
2	MAN	W	7	11/12	0.95	0.13	30,33,39,45	0
2	MAN	I	6	11/12	0.95	0.11	13,16,17,17	0
2	MAN	Z	5	11/12	0.95	0.13	25,27,29,29	0
2	NAG	N	1	14/15	0.95	0.13	25,29,36,37	0
2	MAN	Z	8	11/12	0.95	0.10	37,41,44,45	0
2	MAN	I	7	11/12	0.95	0.11	25,30,36,39	0
2	NAG	Q	1	14/15	0.95	0.12	18,19,21,21	0
2	MAN	Z	4	11/12	0.95	0.13	29,31,34,36	0
2	BMA	T	3	11/12	0.95	0.11	21,22,24,25	0
2	MAN	T	7	11/12	0.96	0.11	24,27,31,33	0
2	NAG	T	2	14/15	0.96	0.12	15,19,21,23	0
2	BMA	Z	3	11/12	0.96	0.09	23,25,30,34	0
2	NAG	I	1	14/15	0.96	0.11	14,17,18,18	0
2	MAN	N	6	11/12	0.96	0.09	19,23,24,24	0
4	NAG	K	1	14/15	0.96	0.11	15,20,22,28	0
2	MAN	W	4	11/12	0.96	0.13	25,26,28,29	0
2	MAN	c	7	11/12	0.96	0.12	29,34,38,39	0
2	MAN	Q	6	11/12	0.96	0.10	27,31,32,33	0
3	NAG	e	1	14/15	0.96	0.12	20,25,31,35	0
2	MAN	c	4	11/12	0.96	0.15	20,22,24,24	0
2	MAN	L	6	11/12	0.96	0.16	25,26,28,29	0
2	BMA	N	3	11/12	0.96	0.11	27,28,30,37	0
2	MAN	Z	7	11/12	0.96	0.10	37,40,49,50	0
2	NAG	Z	1	14/15	0.96	0.12	23,24,27,29	0
2	MAN	L	5	11/12	0.96	0.13	26,26,29,29	0
2	MAN	W	6	11/12	0.96	0.12	17,20,24,27	0
2	NAG	I	2	14/15	0.96	0.14	18,19,22,23	0
3	NAG	S	1	14/15	0.97	0.11	26,28,30,30	0

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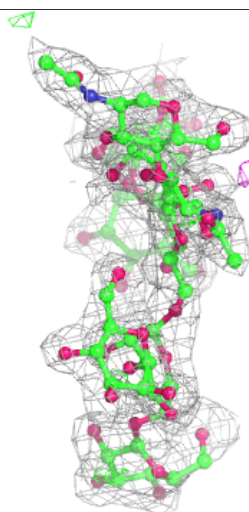
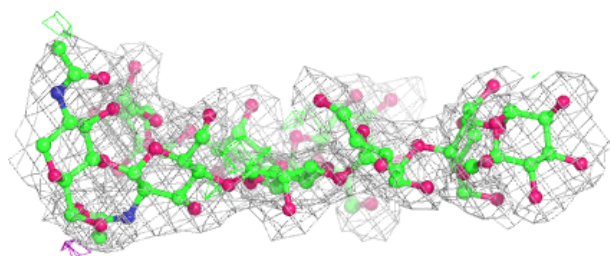
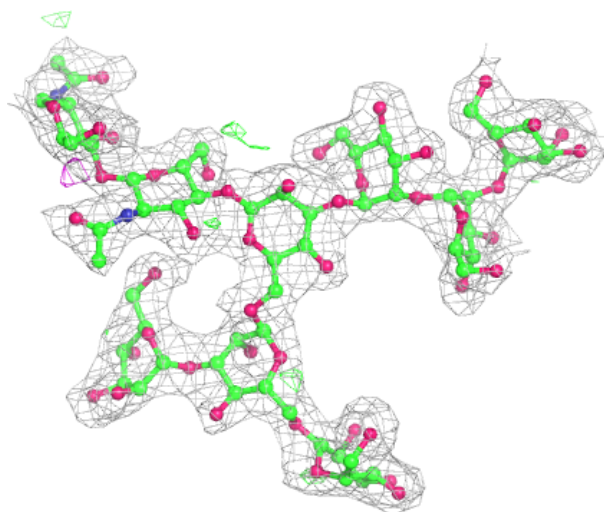
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	Q	5	11/12	0.97	0.13	28,32,35,36	0
2	NAG	W	2	14/15	0.97	0.10	20,26,30,32	0
2	NAG	T	1	14/15	0.97	0.14	17,18,19,19	0
2	MAN	T	5	11/12	0.97	0.10	27,28,31,36	0
2	MAN	Q	4	11/12	0.97	0.13	28,30,32,34	0
2	NAG	N	2	14/15	0.97	0.10	24,27,30,31	0
2	NAG	Z	2	14/15	0.97	0.13	19,21,24,24	0
2	MAN	I	4	11/12	0.97	0.10	19,20,20,23	0
2	NAG	Q	2	14/15	0.97	0.11	15,18,19,23	0
2	NAG	c	1	14/15	0.97	0.10	15,17,21,21	0
2	MAN	L	4	11/12	0.97	0.12	22,26,28,28	0
2	BMA	I	3	11/12	0.97	0.10	17,19,23,26	0
2	NAG	W	1	14/15	0.97	0.11	23,25,26,26	0
2	MAN	N	7	11/12	0.97	0.08	35,38,42,49	0
2	MAN	c	5	11/12	0.98	0.09	17,19,20,22	0
2	MAN	c	6	11/12	0.98	0.12	13,15,15,17	0
2	MAN	W	5	11/12	0.98	0.09	21,24,26,26	0
2	NAG	L	1	14/15	0.98	0.10	17,21,22,24	0
2	BMA	c	3	11/12	0.98	0.10	18,20,22,26	0
2	MAN	T	4	11/12	0.98	0.09	24,26,28,29	0
2	NAG	c	2	14/15	0.98	0.09	14,17,19,19	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.

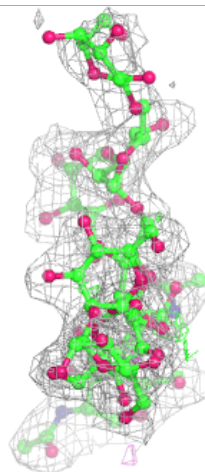
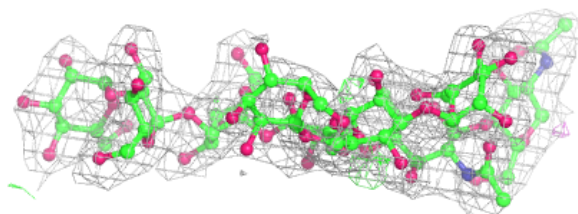
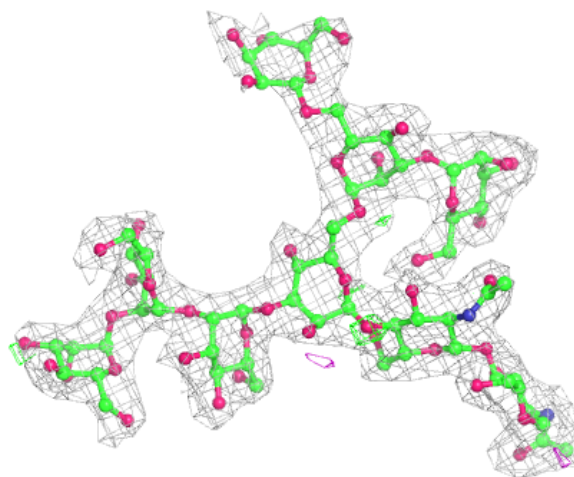
Electron density around Chain I:

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



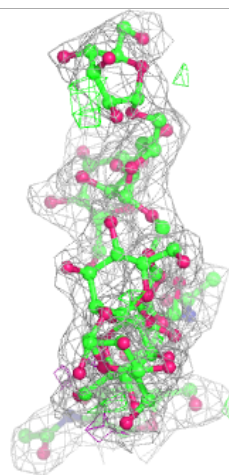
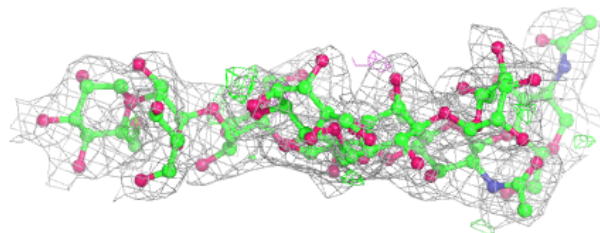
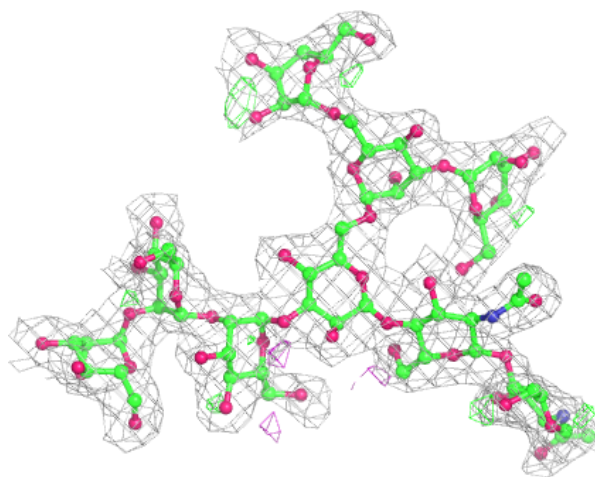
Electron density around Chain L:

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and green (positive)



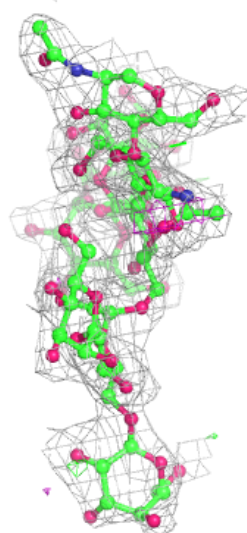
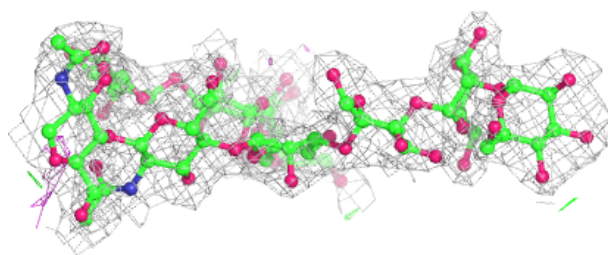
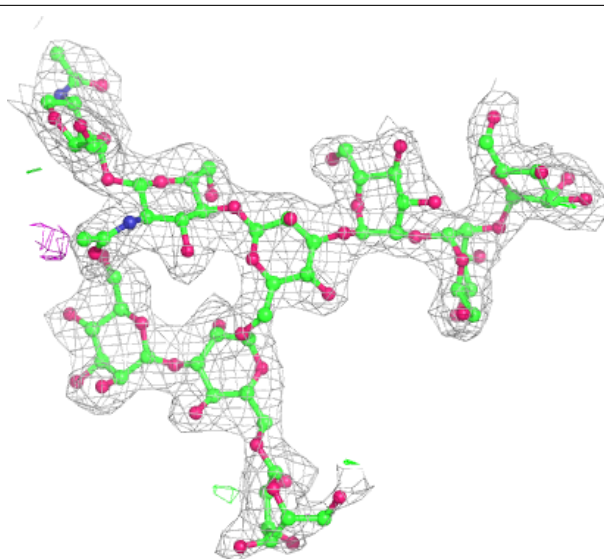
Electron density around Chain N:

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and green (positive)



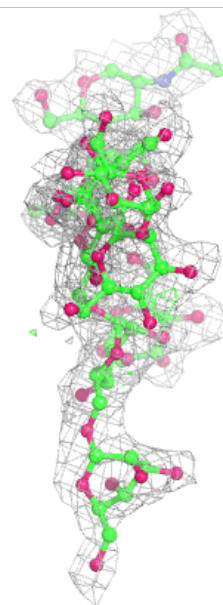
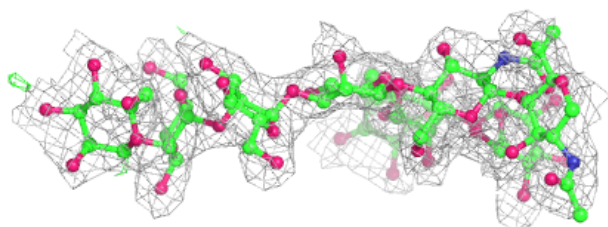
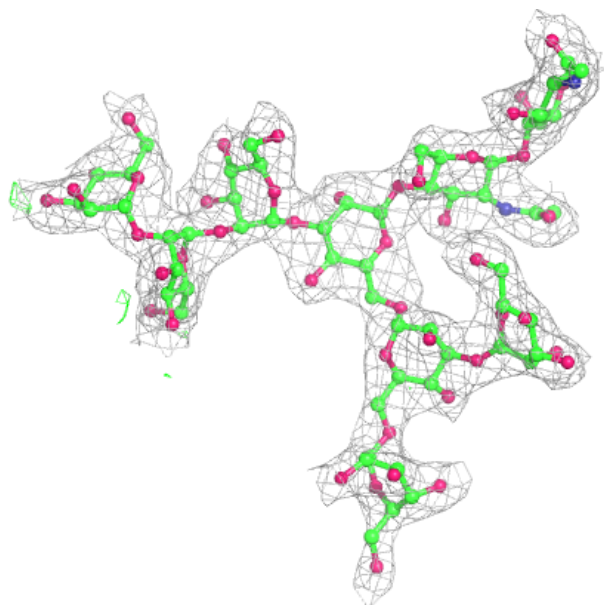
Electron density around Chain Q:

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



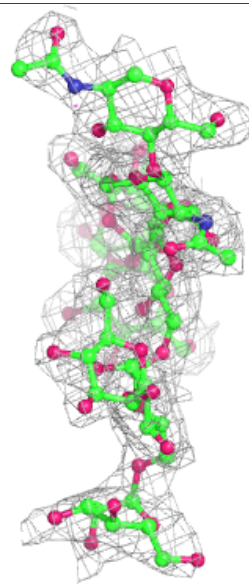
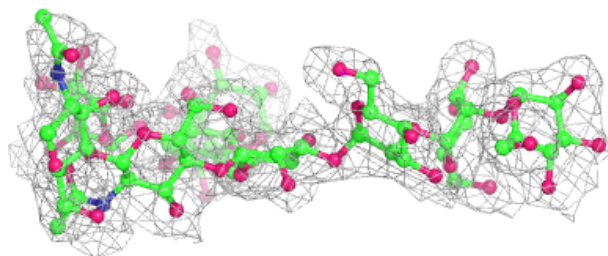
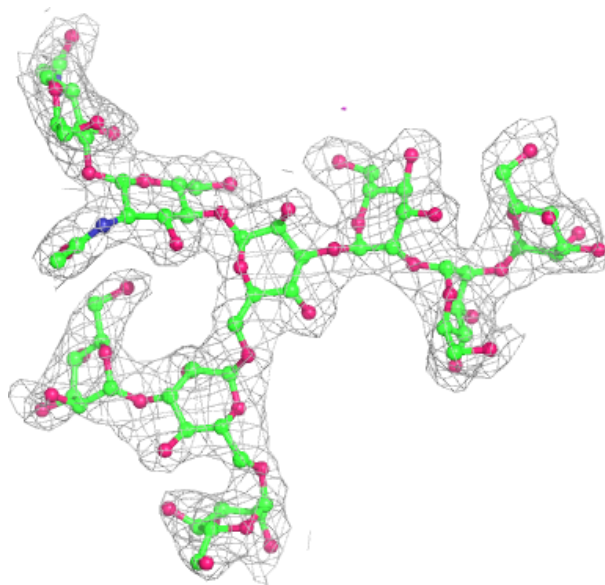
Electron density around Chain T:

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and green (positive)



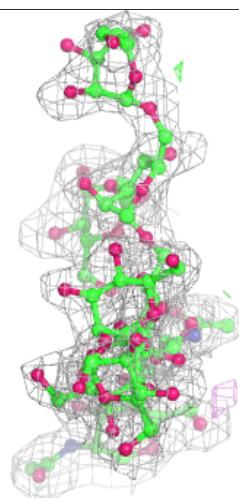
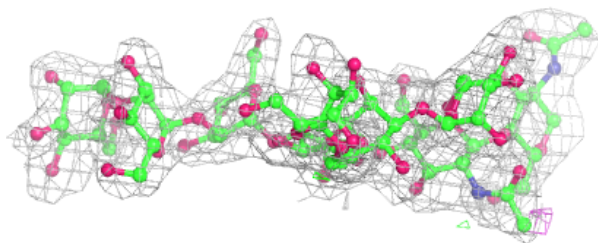
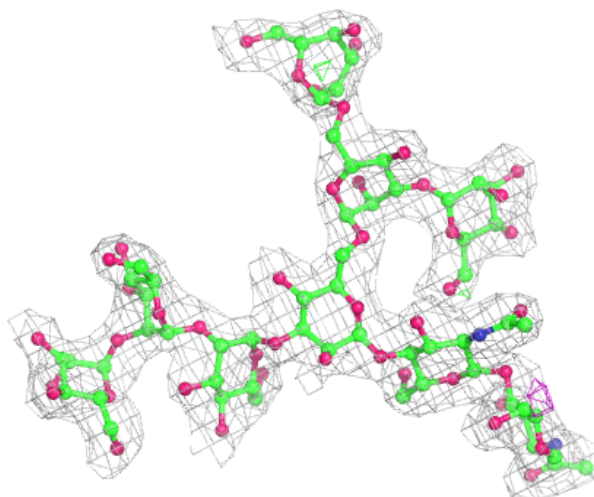
Electron density around Chain W:

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and green (positive)



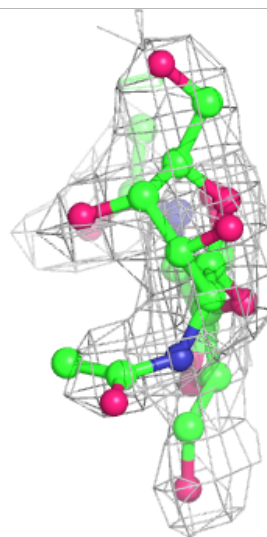
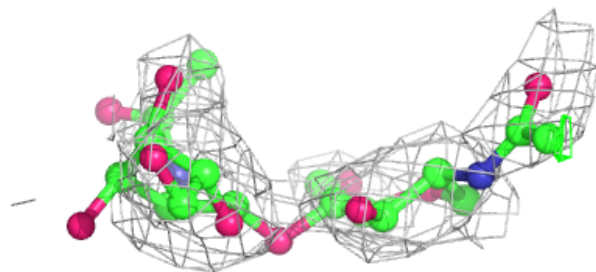
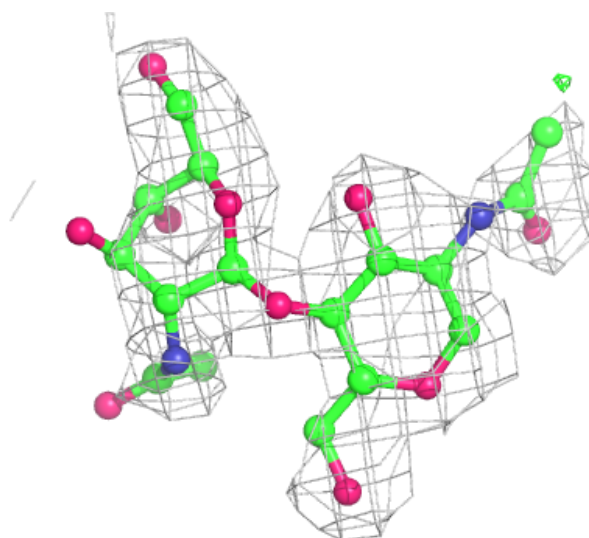
Electron density around Chain Z:

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and green (positive)



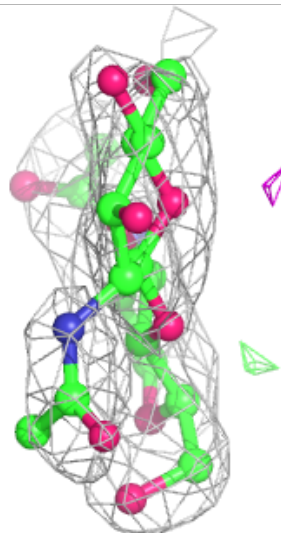
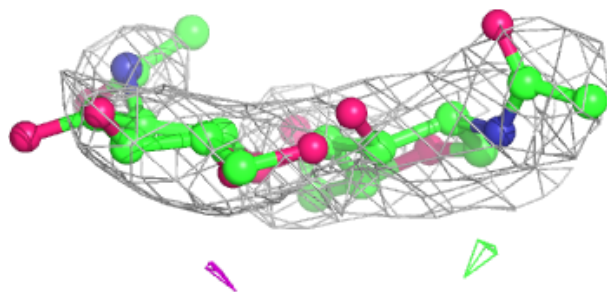
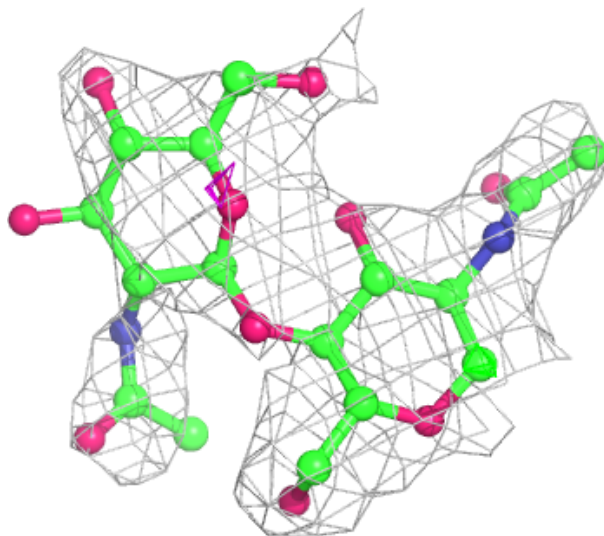
Electron density around Chain J:

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



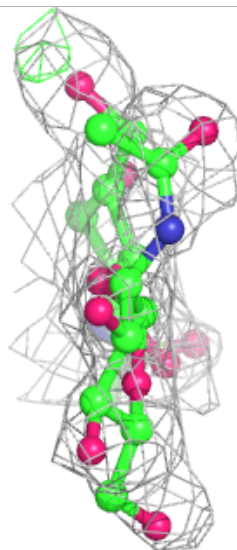
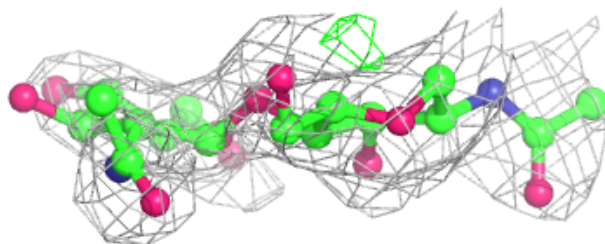
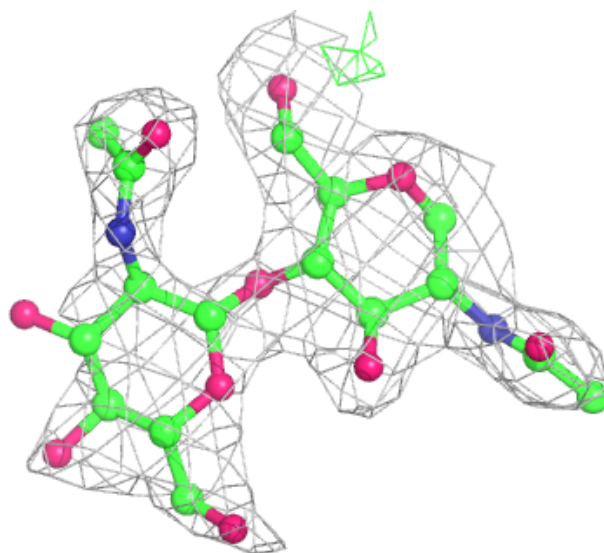
Electron density around Chain M:

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



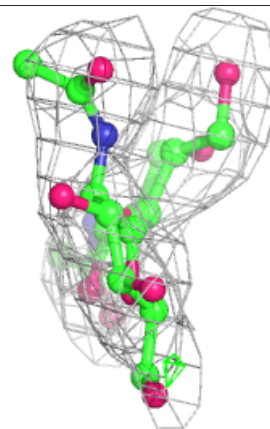
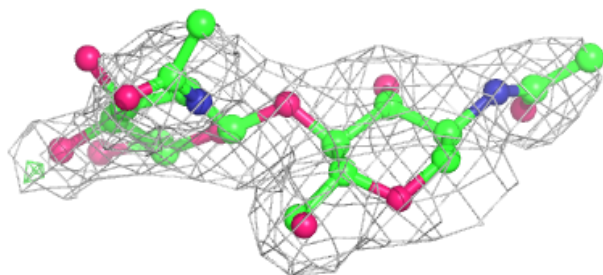
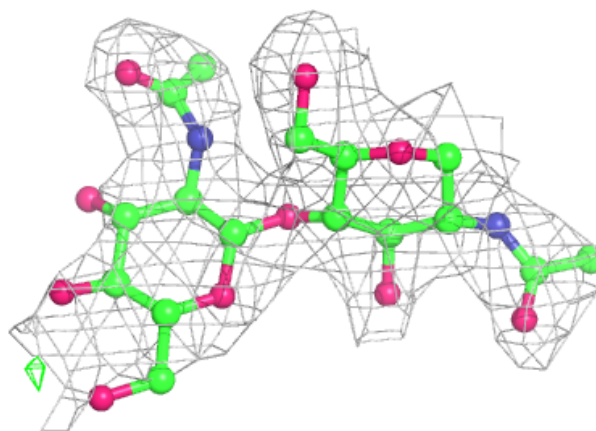
Electron density around Chain O:

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and green (positive)



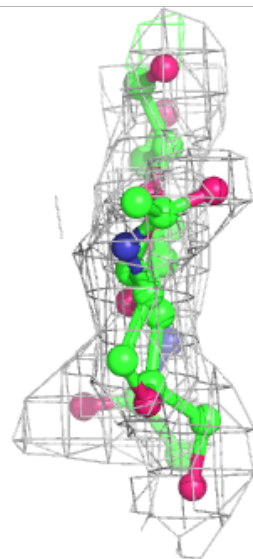
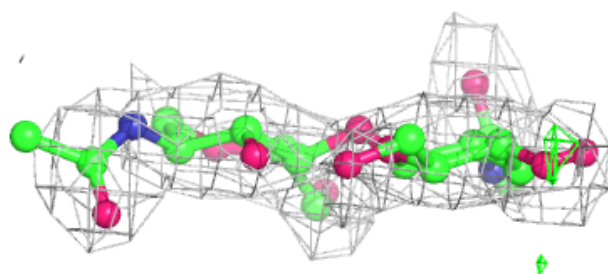
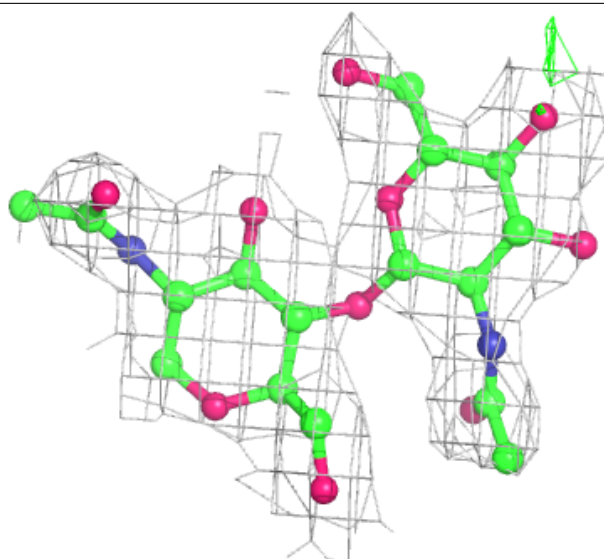
Electron density around Chain P:

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



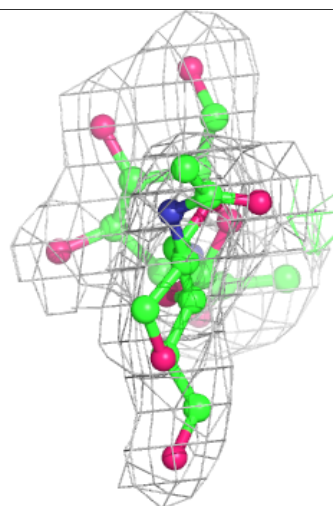
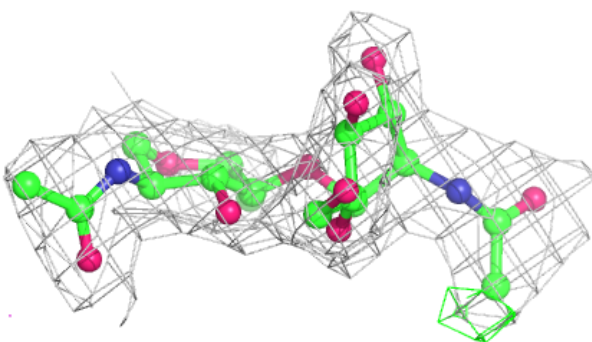
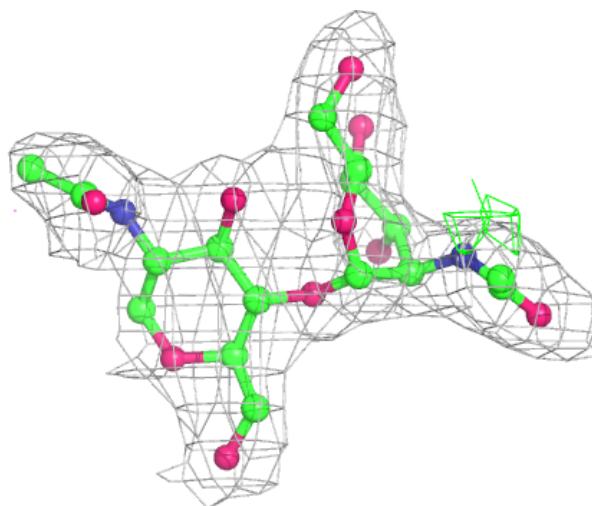
Electron density around Chain R:

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



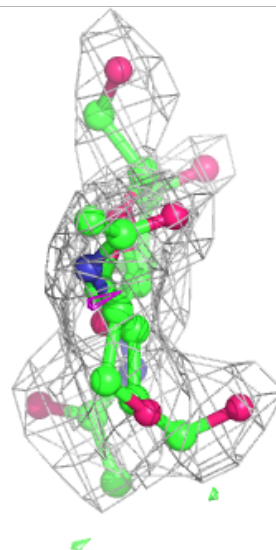
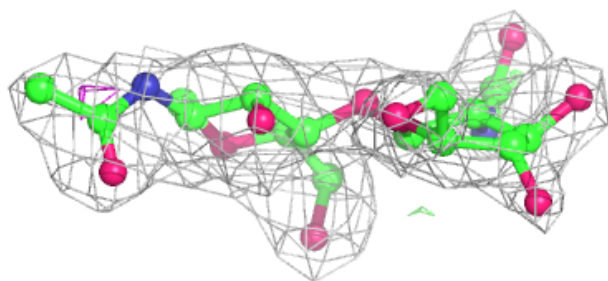
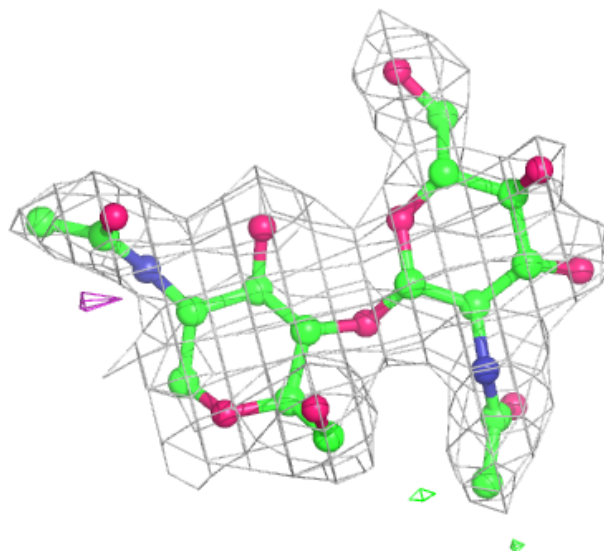
Electron density around Chain S:

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



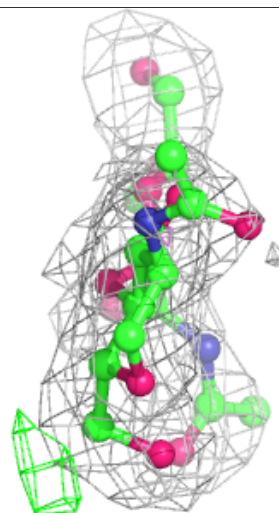
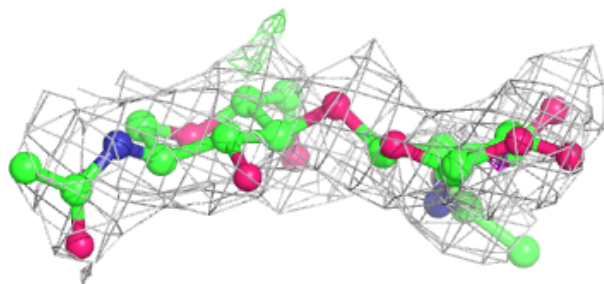
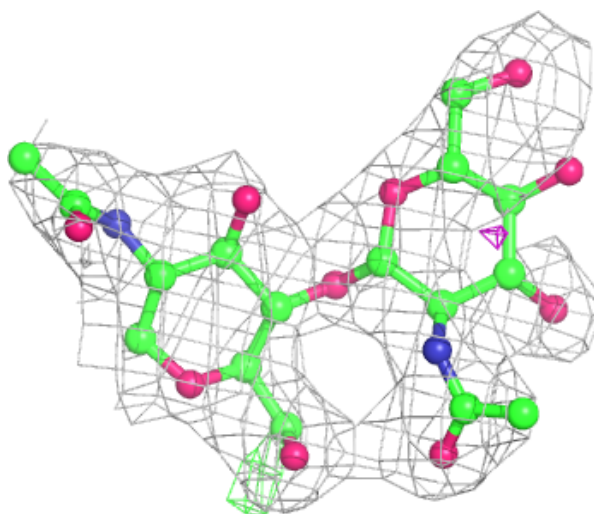
Electron density around Chain U:

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



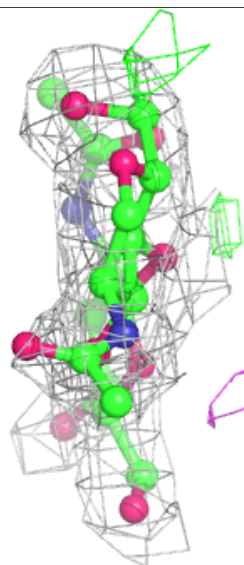
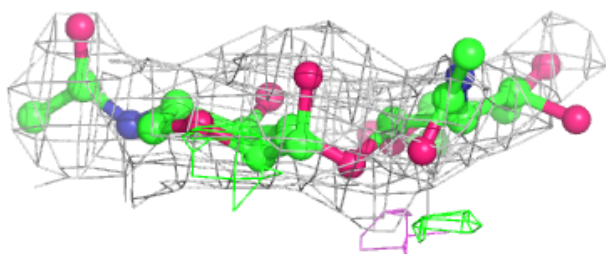
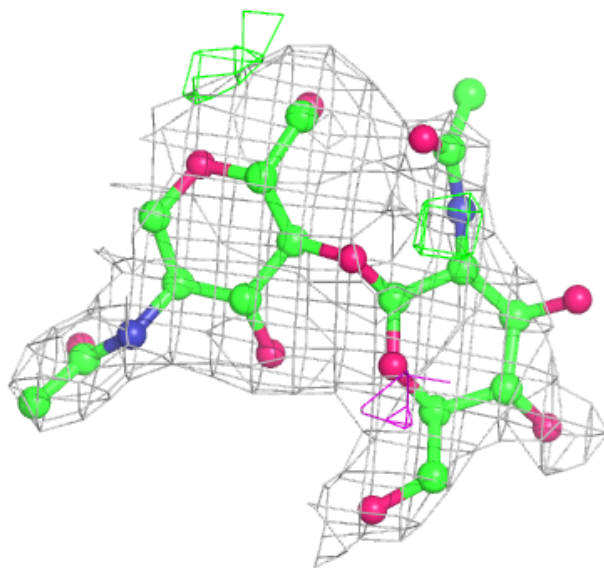
Electron density around Chain V:

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



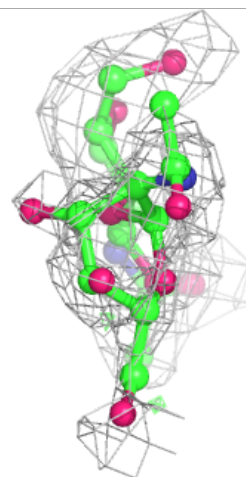
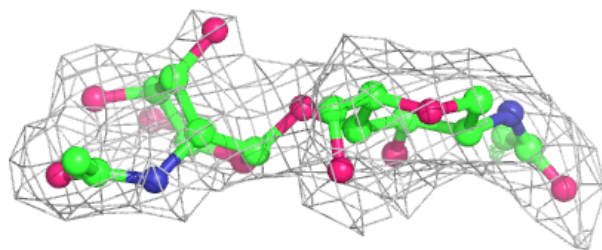
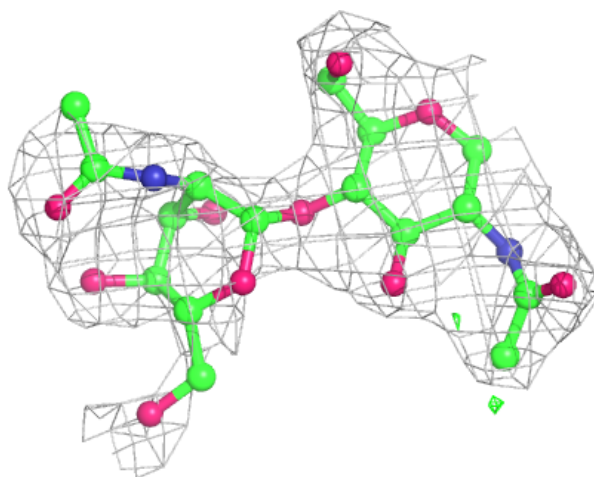
Electron density around Chain X:

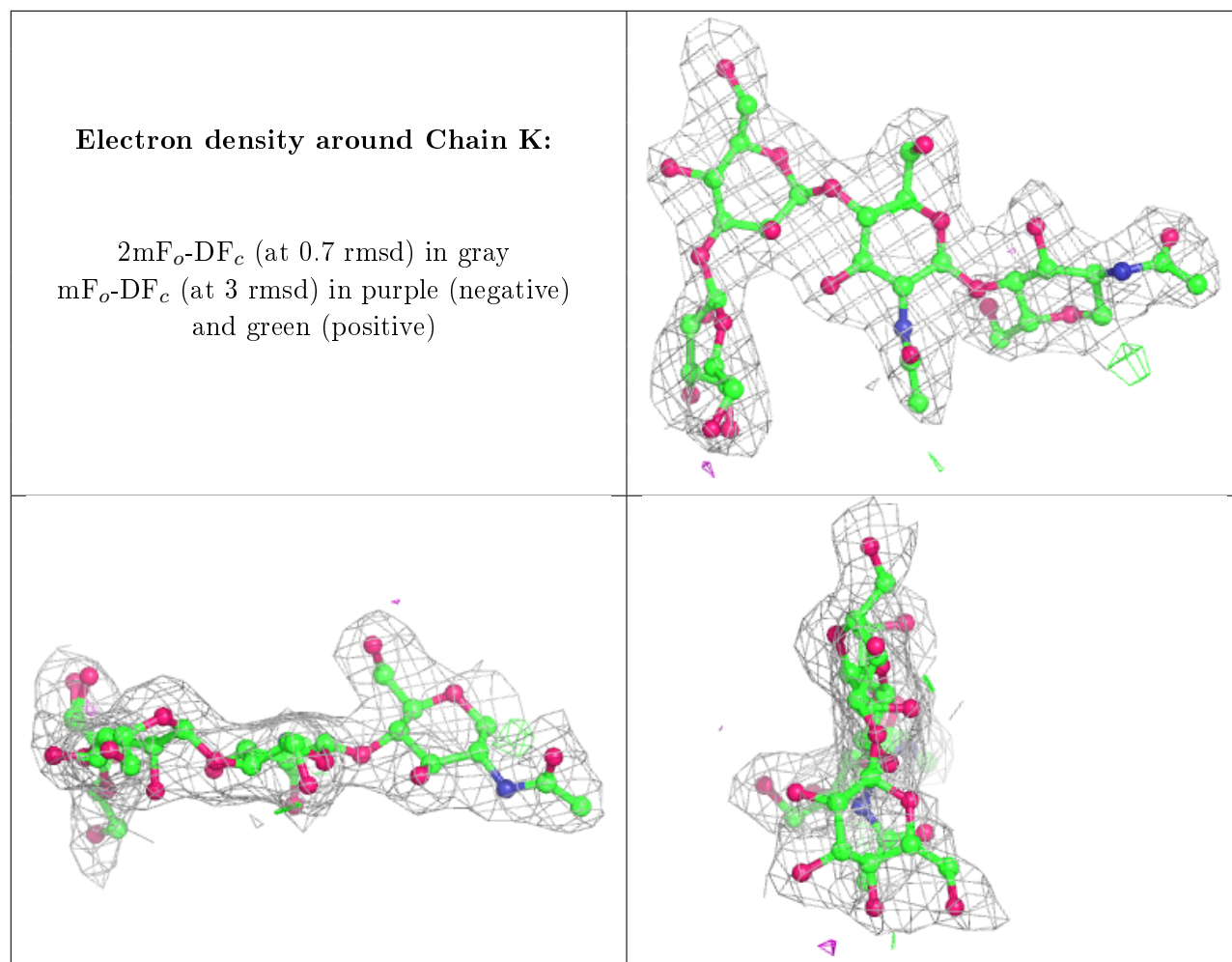
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Y:

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





6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
5	NAG	F	514	14/15	0.86	0.16	42,48,55,58	0
5	NAG	H	514	14/15	0.89	0.16	33,36,39,42	0
5	NAG	G	514	14/15	0.89	0.13	36,42,45,45	0
5	NAG	B	513	14/15	0.90	0.15	37,42,44,44	0
5	NAG	E	514	14/15	0.91	0.15	31,35,39,42	0
5	NAG	B	512	14/15	0.93	0.15	39,47,51,51	0
5	NAG	A	516	14/15	0.94	0.11	39,42,47,48	0
5	NAG	C	514	14/15	0.94	0.12	32,37,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.