



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:10 AM UTC

PDB ID : 5M8P / pdb_00005m8p
Title : Crystal structure of human tyrosinase related protein 1 in complex with tyrosine
Authors : Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on : 2016-10-29
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

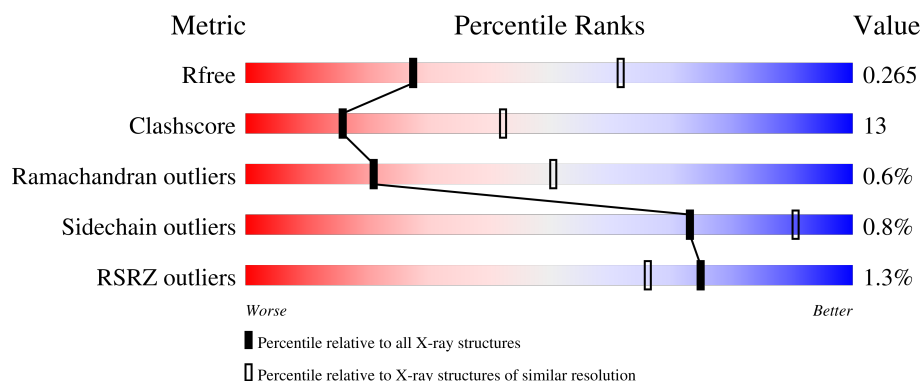
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



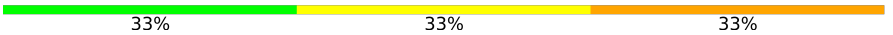
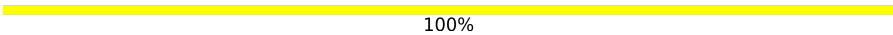
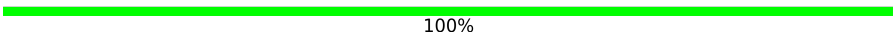
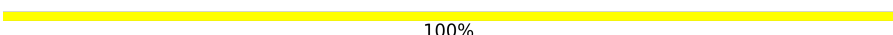
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 ≥ 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	446	% 82% 17%
1	B	446	2% 80% 19%
1	C	446	2% 70% 29%
1	D	446	% 72% 28%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	J	3	
2	O	3	
2	U	3	
3	F	2	
3	K	2	
3	Q	2	
4	G	2	
4	H	2	
4	I	2	
4	N	2	
4	P	2	
4	R	2	
4	W	2	
4	Y	2	
5	L	3	
6	M	5	
6	X	5	
7	S	2	
8	T	3	
9	V	4	

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
3	NAG	Q	1	-	-	X	-

2 Entry composition [i](#)

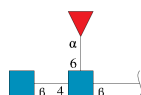
There are 14 unique types of molecules in this entry. The entry contains 15116 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	B	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	C	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			
1	D	446	Total	C	N	O	S	0	0	0
			3560	2233	632	672	23			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	O	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	U	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



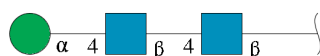
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



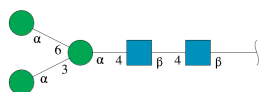
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



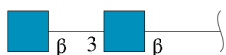
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



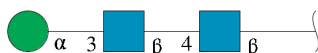
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

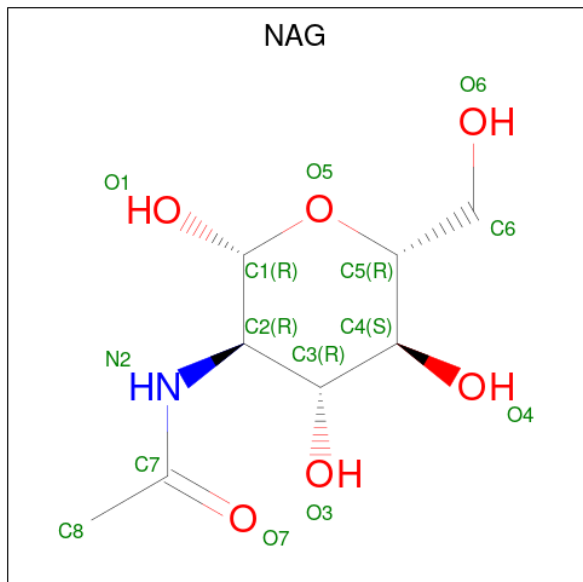


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(5-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

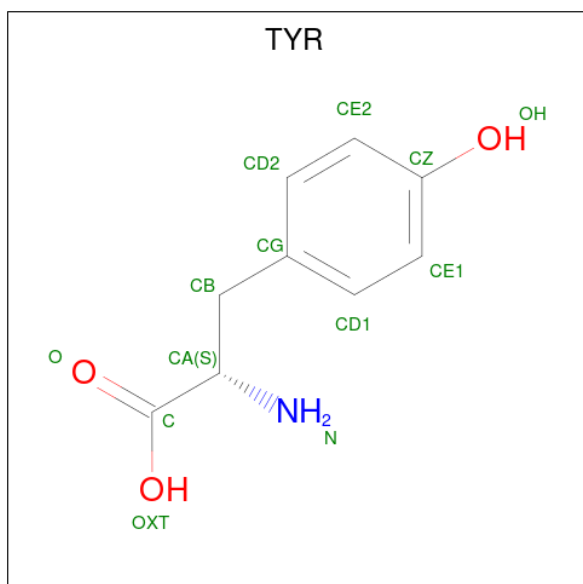
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	V	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			13	9	1	3		

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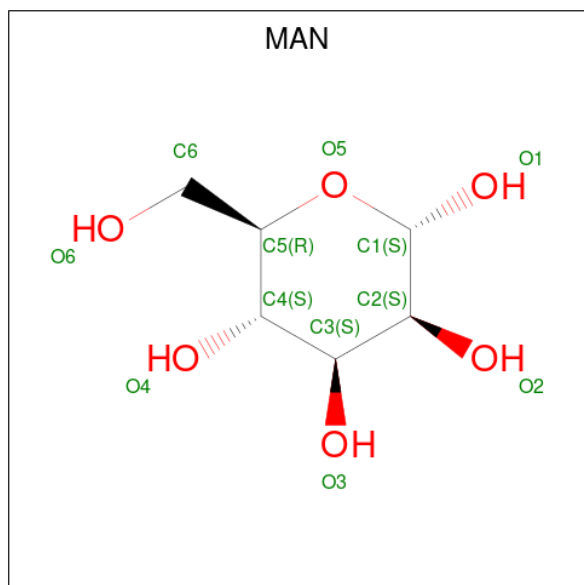
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			13	9	1	3		
11	C	1	Total	C	N	O	0	0
			13	9	1	3		
11	D	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	3	Total	Zn	0	0
			3	3		
12	B	2	Total	Zn	0	0
			2	2		
12	C	2	Total	Zn	0	0
			2	2		
12	D	2	Total	Zn	0	0
			2	2		

- Molecule 13 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			11	6	5		

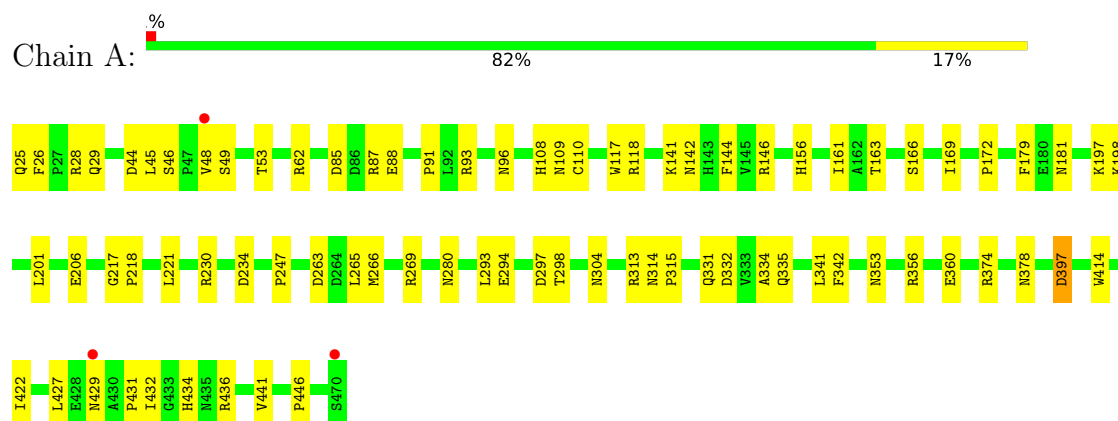
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	21	Total 21	O 21	0	0
14	B	25	Total 25	O 25	0	0
14	C	9	Total 9	O 9	0	0
14	D	10	Total 10	O 10	0	0

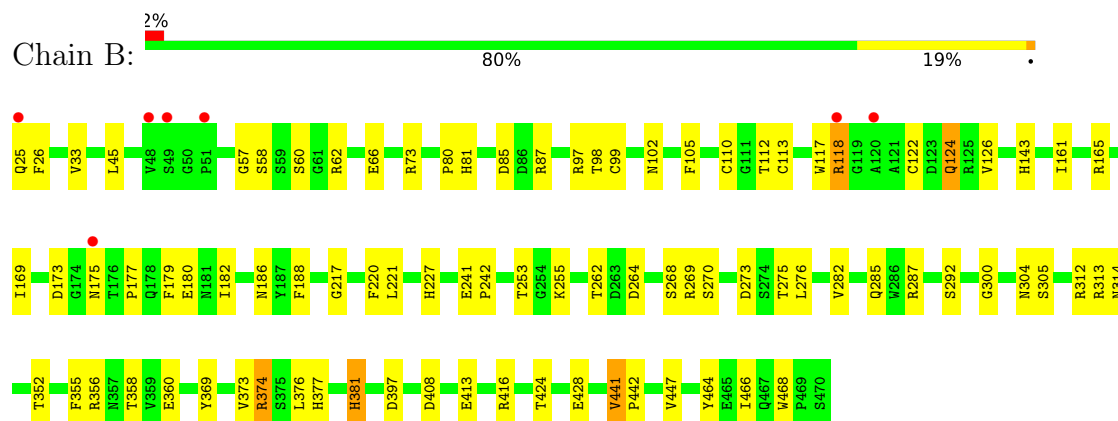
3 Residue-property plots [i](#)

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.

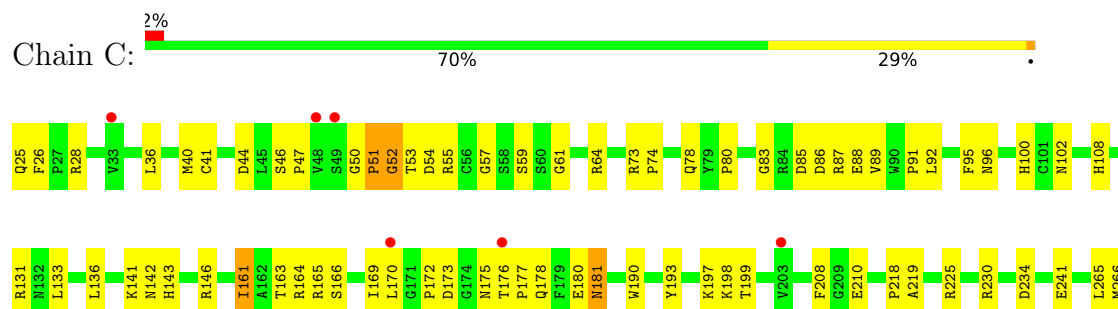
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

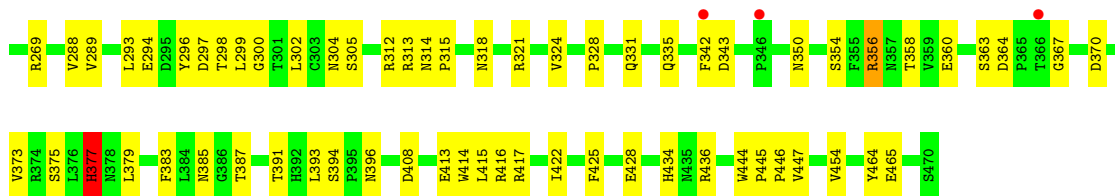


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

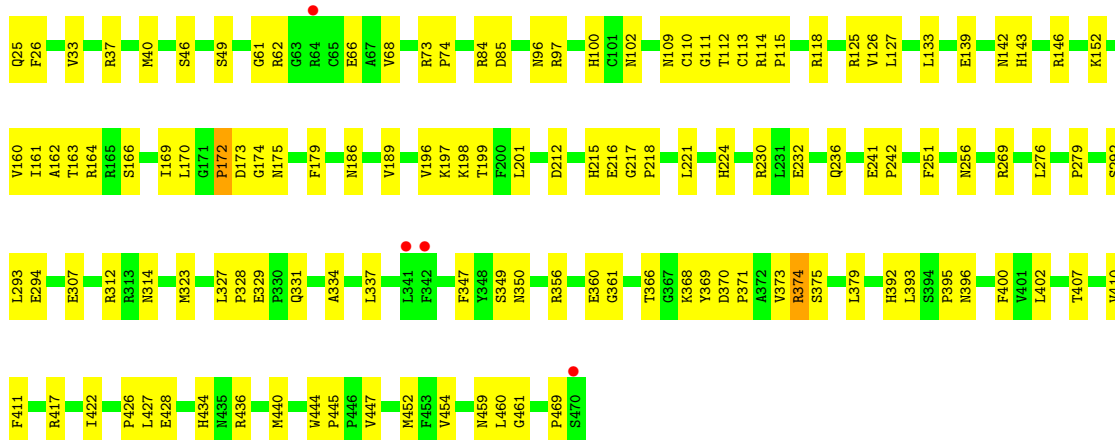


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase





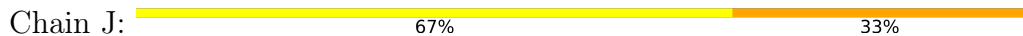
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



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



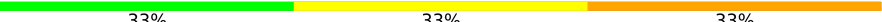
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

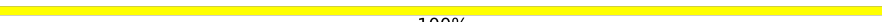


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 33% 33%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain N:  50% 50%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain W:  50% 50%

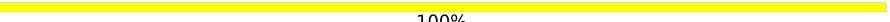
MAG1
MAG2

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

Chain Y:  50% 50%

MAG1
MAG2

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

Chain L:  100%

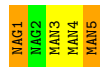
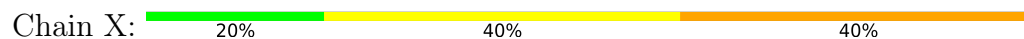
MAG1
MAG2
MAG3

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

Chain M:  80% 20%



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



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(5-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.52Å 140.32Å 191.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.80 47.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.92-2.80) 90.9 (47.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.205 , 0.262 0.209 , 0.265	Depositor DCC
R_{free} test set	2997 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15116	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: ZN, MAN, NAG, FUC

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	0.66	1/3667 (0.0%)	0.72	0/4998
1	B	0.59	0/3667	0.65	3/4998 (0.1%)
1	C	0.90	11/3667 (0.3%)	0.80	6/4998 (0.1%)
1	D	0.55	1/3667 (0.0%)	0.62	0/4998
All	All	0.69	13/14668 (0.1%)	0.70	9/19992 (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	C	0	2
1	D	0	1
All	All	0	3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	HIS	C-O	22.17	1.51	1.24
1	C	377	HIS	CB-CG	-21.01	1.20	1.50
1	C	377	HIS	C-N	-18.97	1.08	1.34
1	C	377	HIS	CA-C	-10.54	1.38	1.52
1	C	377	HIS	N-CA	9.92	1.58	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	HIS	O-C-N	-13.15	105.10	122.59
1	C	377	HIS	CA-C-O	-12.31	102.91	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	HIS	CA-C-N	11.69	137.11	120.28
1	C	377	HIS	C-N-CA	11.69	137.11	120.28
1	C	377	HIS	N-CA-C	-6.68	96.57	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	377	HIS	Peptide,Mainchain
1	D	109	ASN	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	3560	0	3325	64	0
1	B	3560	0	3325	75	0
1	C	3560	0	3326	131	1
1	D	3560	0	3326	101	0
2	E	38	0	34	2	0
2	J	38	0	34	1	0
2	O	38	0	34	2	0
2	U	38	0	34	1	0
3	F	24	0	22	0	0
3	K	24	0	22	0	0
3	Q	24	0	22	7	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0
4	I	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	3	0
4	R	28	0	25	0	0
4	W	28	0	24	0	0
4	Y	28	0	25	1	0
5	L	39	0	34	0	0
6	M	61	0	52	1	0
6	X	61	0	52	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	28	0	25	1	0
8	T	39	0	34	1	0
9	V	49	0	42	2	0
10	A	14	0	12	0	0
11	A	13	0	8	3	0
11	B	13	0	8	2	0
11	C	13	0	8	3	0
11	D	13	0	8	2	0
12	A	3	0	0	0	0
12	B	2	0	0	0	0
12	C	2	0	0	0	0
12	D	2	0	0	0	0
13	C	11	0	10	1	0
14	A	21	0	0	2	0
14	B	25	0	0	4	0
14	C	9	0	0	1	0
14	D	10	0	0	4	0
All	All	15116	0	13996	383	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 13.

The worst 5 of 383 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:C:181:ASN:HD21	3:Q:1:NAG:C1	1.17	1.50
1:C:181:ASN:ND2	3:Q:1:NAG:C1	1.85	1.40
1:D:118:ARG:HH11	1:D:242:PRO:CB	1.44	1.30
1:D:118:ARG:NH1	1:D:242:PRO:CB	1.95	1.29
1:C:198:LYS:HD2	1:C:297:ASP:OD1	1.30	1.27

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:OG	6:X:5:MAN:O3[1_655]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	444/446 (100%)	413 (93%)	30 (7%)	1 (0%)	43	72
1	B	444/446 (100%)	411 (93%)	31 (7%)	2 (0%)	24	55
1	C	444/446 (100%)	413 (93%)	26 (6%)	5 (1%)	11	36
1	D	444/446 (100%)	407 (92%)	34 (8%)	3 (1%)	18	47
All	All	1776/1784 (100%)	1644 (93%)	121 (7%)	11 (1%)	21	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	GLY
1	C	51	PRO
1	C	377	HIS
1	C	172	PRO
1	D	172	PRO

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	395/395 (100%)	395 (100%)	0	100	100
1	B	395/395 (100%)	388 (98%)	7 (2%)	51	82
1	C	395/395 (100%)	393 (100%)	2 (0%)	81	93
1	D	395/395 (100%)	393 (100%)	2 (0%)	81	93
All	All	1580/1580 (100%)	1569 (99%)	11 (1%)	73	91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	VAL
1	C	447	VAL
1	D	374	ARG
1	D	292	SER
1	B	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	175	ASN
1	D	396	ASN
1	D	353	ASN
1	B	325	GLN
1	C	437	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 ⓘ

56 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	E	1	2	14,14,15	1.03	1 (7%)	17,19,21	1.13	1 (5%)
2	NAG	E	2	2	14,14,15	0.63	1 (7%)	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	E	3	2	10,10,11	0.67	0	14,14,16	2.59	6 (42%)
3	NAG	F	1	3	14,14,15	1.51	2 (14%)	17,19,21	1.33	2 (11%)
3	FUC	F	2	3	10,10,11	1.19	2 (20%)	14,14,16	1.18	2 (14%)
4	NAG	G	1	4	14,14,15	0.55	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	0.45	0
4	NAG	H	1	4	14,14,15	0.78	1 (7%)	17,19,21	0.63	0
4	NAG	H	2	4	14,14,15	1.64	1 (7%)	17,19,21	1.11	2 (11%)
4	NAG	I	1	4	14,14,15	0.72	1 (7%)	17,19,21	0.52	0
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	0.59	0
2	NAG	J	1	2	14,14,15	0.94	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.63	0
2	FUC	J	3	2	10,10,11	1.16	2 (20%)	14,14,16	0.94	0
3	NAG	K	1	3	14,14,15	0.33	0	17,19,21	0.80	0
3	FUC	K	2	3	10,10,11	1.54	2 (20%)	14,14,16	1.52	3 (21%)
5	NAG	L	1	5	14,14,15	2.08	2 (14%)	17,19,21	1.02	2 (11%)
5	NAG	L	2	5	14,14,15	1.67	1 (7%)	17,19,21	1.06	2 (11%)
5	MAN	L	3	5	11,11,12	1.14	1 (9%)	15,15,17	0.79	0
6	NAG	M	1	6	14,14,15	0.78	1 (7%)	17,19,21	0.78	0
6	NAG	M	2	6	14,14,15	0.71	0	17,19,21	0.65	0
6	MAN	M	3	6	11,11,12	1.90	2 (18%)	15,15,17	1.90	4 (26%)
6	MAN	M	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.11	0
6	MAN	M	5	6	11,11,12	1.43	1 (9%)	15,15,17	2.35	3 (20%)
4	NAG	N	1	4	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.95	1 (5%)
2	NAG	O	1	2	14,14,15	0.25	0	17,19,21	0.87	1 (5%)
2	NAG	O	2	2	14,14,15	0.33	0	17,19,21	1.49	2 (11%)
2	FUC	O	3	2	10,10,11	0.96	1 (10%)	14,14,16	1.67	4 (28%)
4	NAG	P	1	4	14,14,15	0.65	1 (7%)	17,19,21	0.89	0
4	NAG	P	2	4	14,14,15	1.24	2 (14%)	17,19,21	2.31	3 (17%)
3	NAG	Q	1	3	14,14,15	0.46	0	17,19,21	1.70	3 (17%)
3	FUC	Q	2	3	10,10,11	1.75	2 (20%)	14,14,16	1.43	4 (28%)
4	NAG	R	1	4	14,14,15	1.07	1 (7%)	17,19,21	0.65	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.62	0
7	NAG	S	1	7	14,14,15	0.26	0	17,19,21	1.27	3 (17%)
7	NAG	S	2	7	14,14,15	0.47	0	17,19,21	0.53	0
8	NAG	T	1	8	14,14,15	2.29	1 (7%)	17,19,21	2.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	T	2	8	14,14,15	0.77	1 (7%)	17,19,21	1.68	1 (5%)
8	MAN	T	3	8	11,11,12	1.29	1 (9%)	15,15,17	2.01	3 (20%)
2	NAG	U	1	2	14,14,15	0.75	1 (7%)	17,19,21	0.77	0
2	NAG	U	2	2	14,14,15	0.42	0	17,19,21	0.40	0
2	FUC	U	3	2	10,10,11	1.01	0	14,14,16	2.08	7 (50%)
9	NAG	V	1	9	14,14,15	1.07	2 (14%)	17,19,21	0.87	0
9	NAG	V	2	9	14,14,15	1.23	1 (7%)	17,19,21	0.99	1 (5%)
9	MAN	V	3	9	11,11,12	1.57	1 (9%)	15,15,17	0.96	0
9	FUC	V	4	9	10,10,11	0.55	0	14,14,16	1.35	2 (14%)
4	NAG	W	1	4	14,14,15	0.79	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	W	2	4	14,14,15	0.37	0	17,19,21	0.59	0
6	NAG	X	1	6	14,14,15	1.27	1 (7%)	17,19,21	1.33	1 (5%)
6	NAG	X	2	6	14,14,15	0.46	0	17,19,21	0.67	0
6	MAN	X	3	6	11,11,12	1.34	2 (18%)	15,15,17	1.58	2 (13%)
6	MAN	X	4	6	11,11,12	1.22	2 (18%)	15,15,17	0.97	0
6	MAN	X	5	6	11,11,12	1.00	1 (9%)	15,15,17	1.23	1 (6%)
4	NAG	Y	1	4	14,14,15	1.41	2 (14%)	17,19,21	1.65	3 (17%)
4	NAG	Y	2	4	14,14,15	0.34	0	17,19,21	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	3	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	1	6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	3/6/23/26	0/1/1/1
6	MAN	X	3	6	-	2/2/19/22	1/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	MAN	X	5	6	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	4	-	4/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	4/6/23/26	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	1	NAG	O5-C1	8.40	1.57	1.43
5	L	1	NAG	O5-C1	-7.31	1.31	1.43
5	L	2	NAG	O5-C1	-6.16	1.33	1.43
4	H	2	NAG	C1-C2	5.61	1.60	1.52
6	M	3	MAN	C2-C3	-5.28	1.44	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	1	NAG	C1-O5-C5	10.62	126.42	112.19
4	P	2	NAG	C2-N2-C7	7.86	133.44	122.90
6	M	5	MAN	C1-O5-C5	7.42	122.13	112.19
8	T	2	NAG	C1-O5-C5	6.18	120.47	112.19
2	E	3	FUC	O5-C5-C4	6.09	120.51	109.55

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C1-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
2	E	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	MAN	C1-C2-C3-C4-C5-O5

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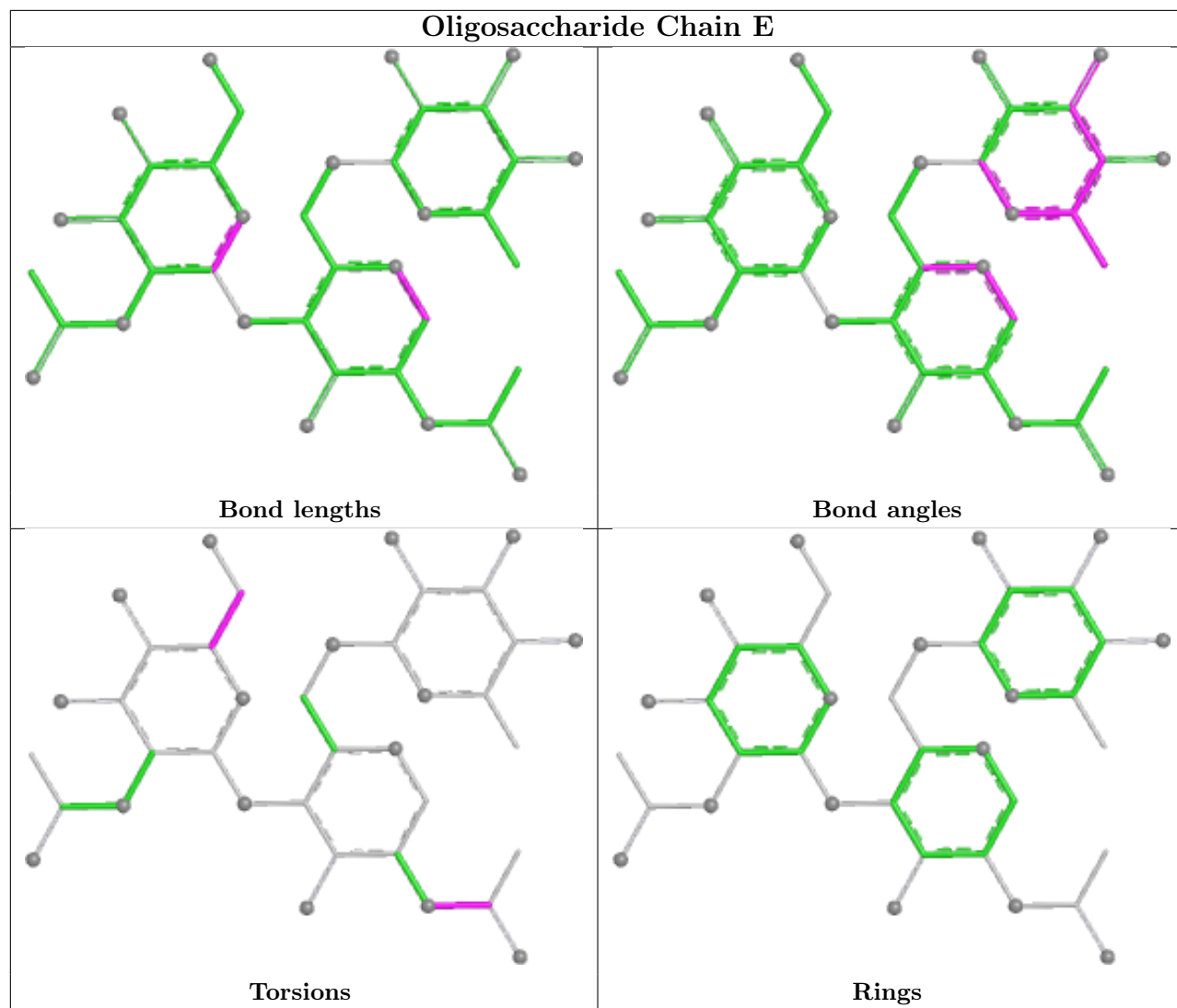
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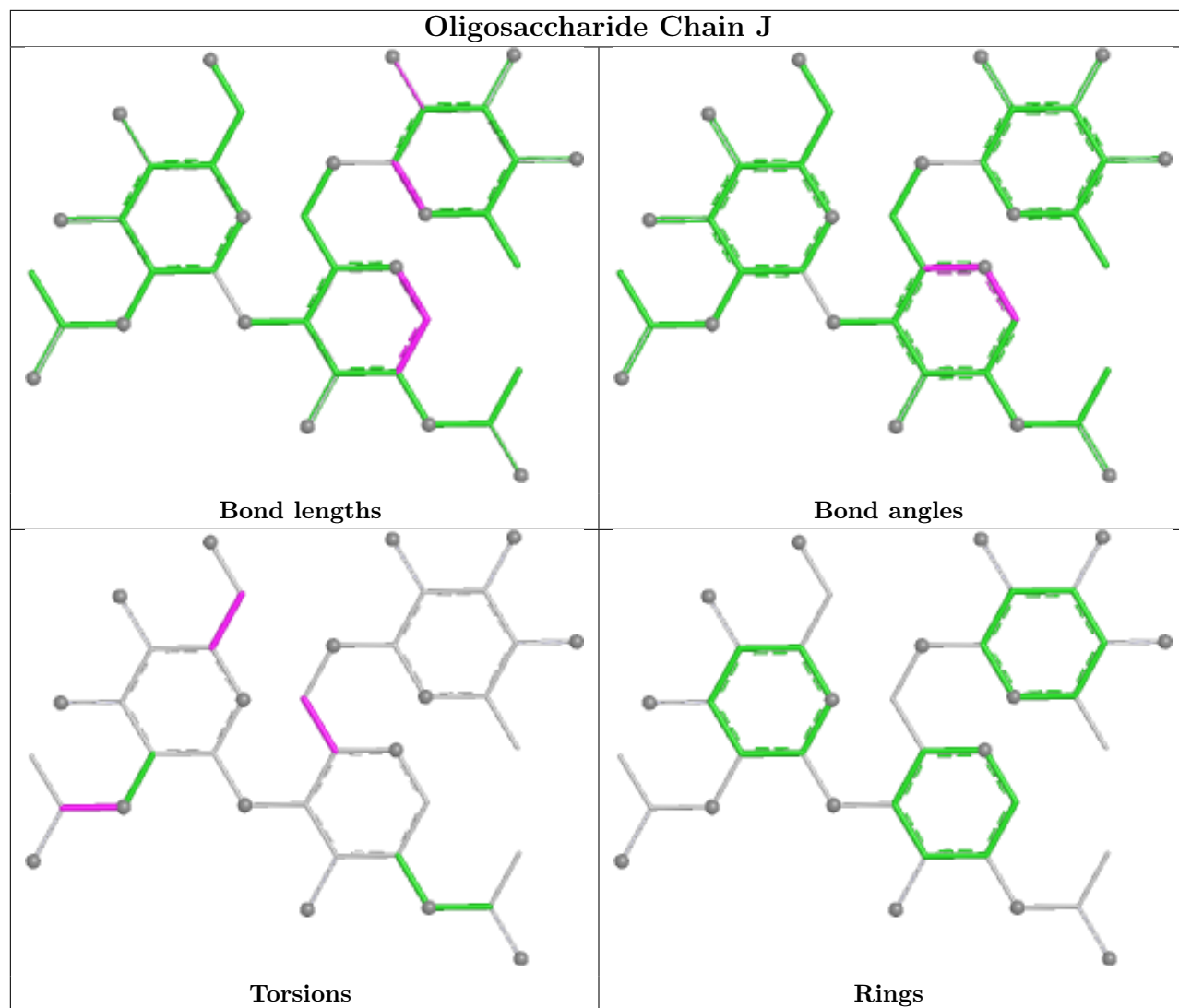
Mol	Chain	Res	Type	Atoms
6	M	3	MAN	C1-C2-C3-C4-C5-O5
6	X	3	MAN	C1-C2-C3-C4-C5-O5
9	V	3	MAN	C1-C2-C3-C4-C5-O5
6	M	4	MAN	C1-C2-C3-C4-C5-O5

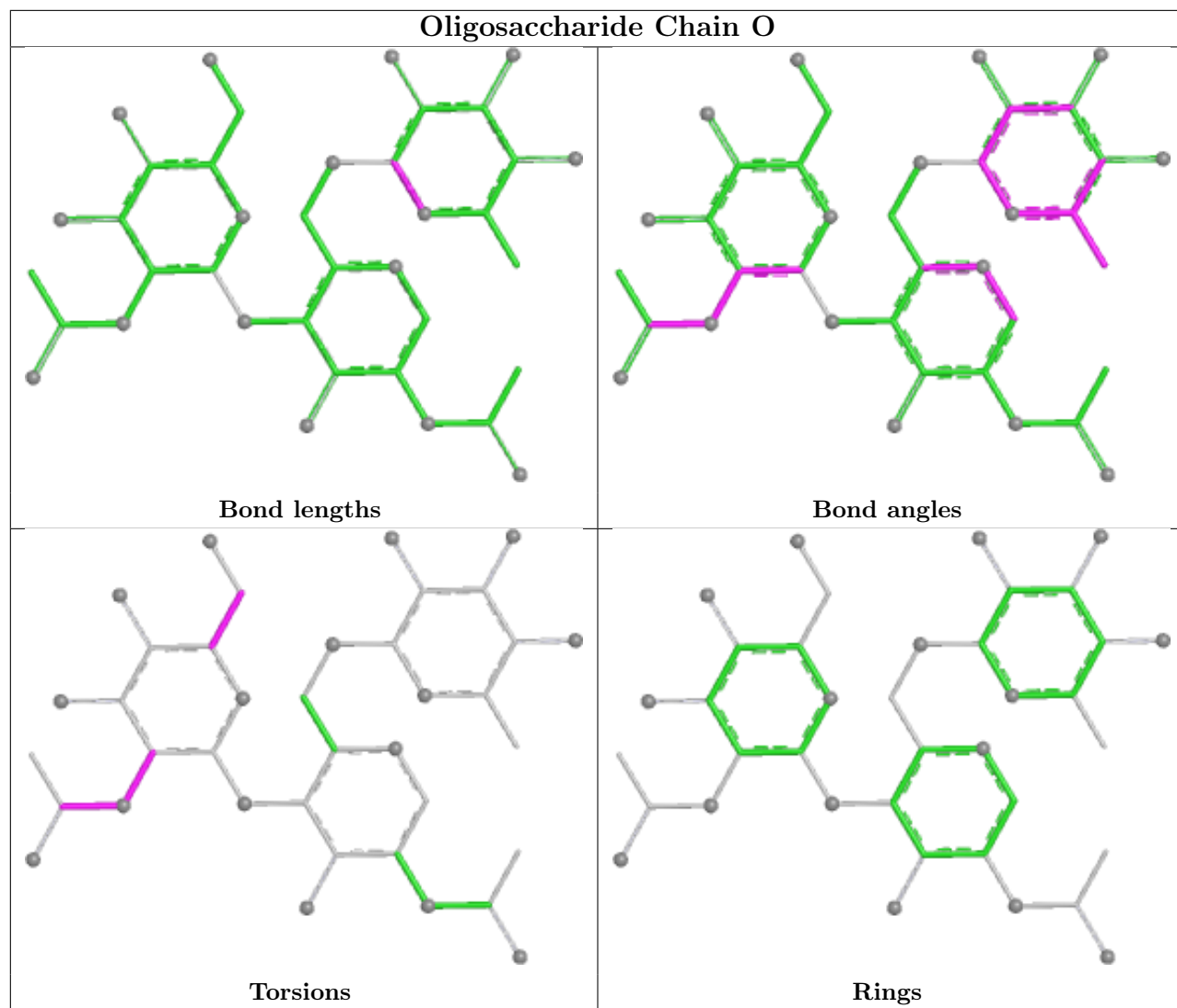
21 monomers are involved in 27 short contacts:

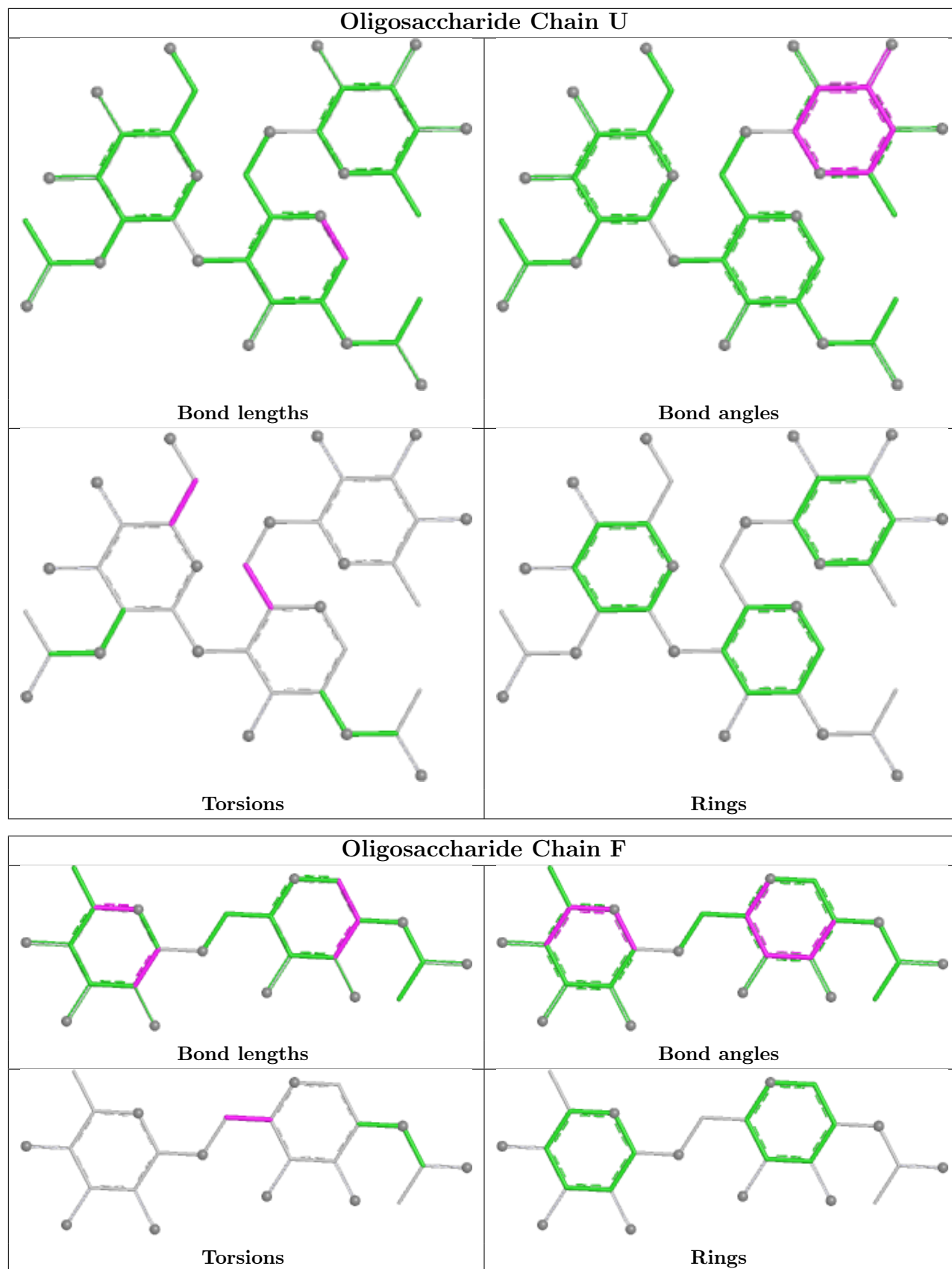
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	E	2	NAG	1	0
4	Y	1	NAG	1	0
2	J	2	NAG	1	0
2	O	1	NAG	1	0
9	V	3	MAN	1	0
2	U	1	NAG	1	0
6	M	3	MAN	1	0
6	M	2	NAG	1	0
4	H	2	NAG	1	0
6	X	1	NAG	3	0
7	S	1	NAG	1	0
6	X	5	MAN	0	1
9	V	4	FUC	1	0
4	P	2	NAG	3	0
3	Q	1	NAG	7	0
9	V	1	NAG	1	0
2	O	2	NAG	2	0
2	J	1	NAG	1	0
8	T	1	NAG	1	0
4	H	1	NAG	1	0

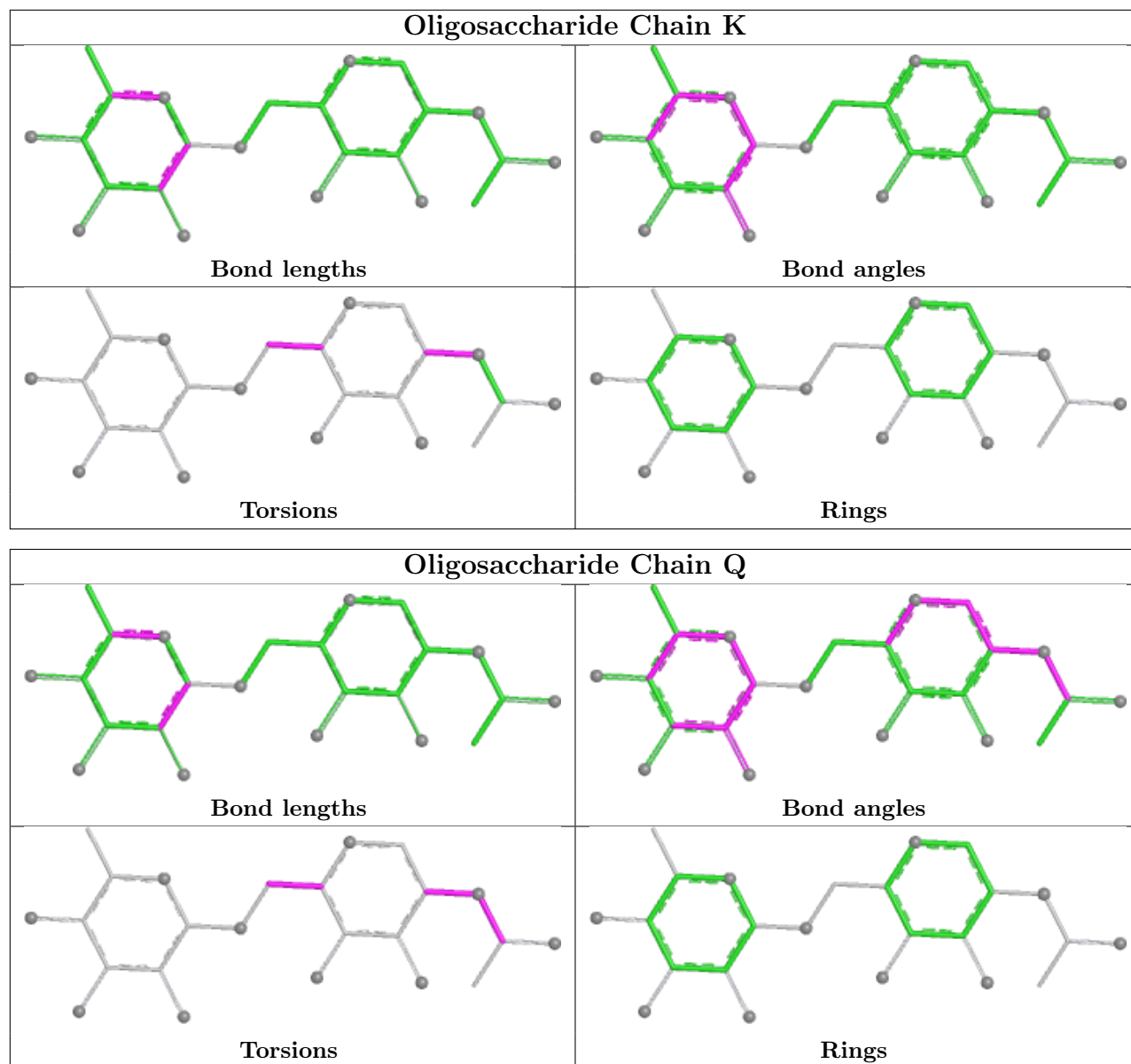
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

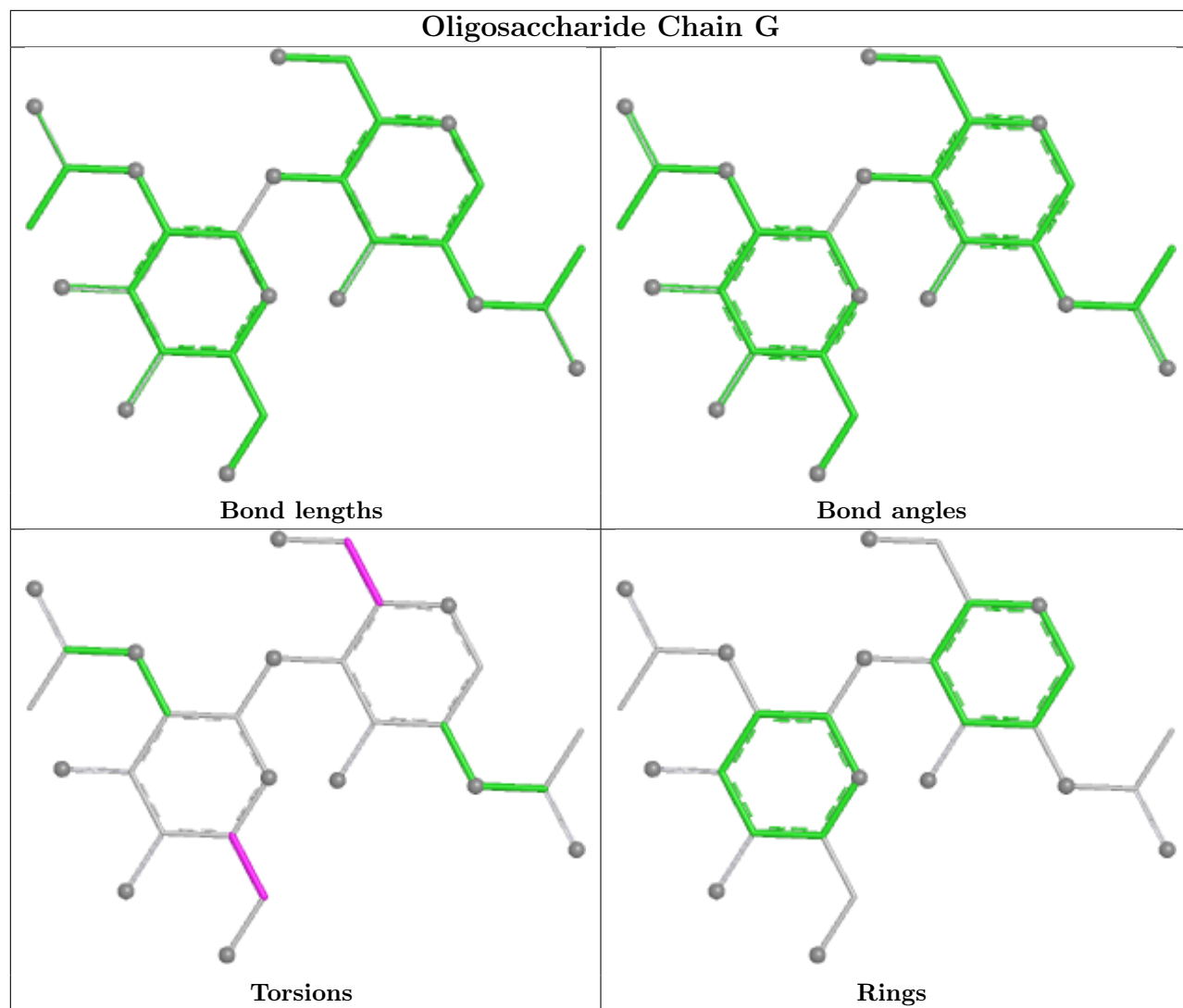




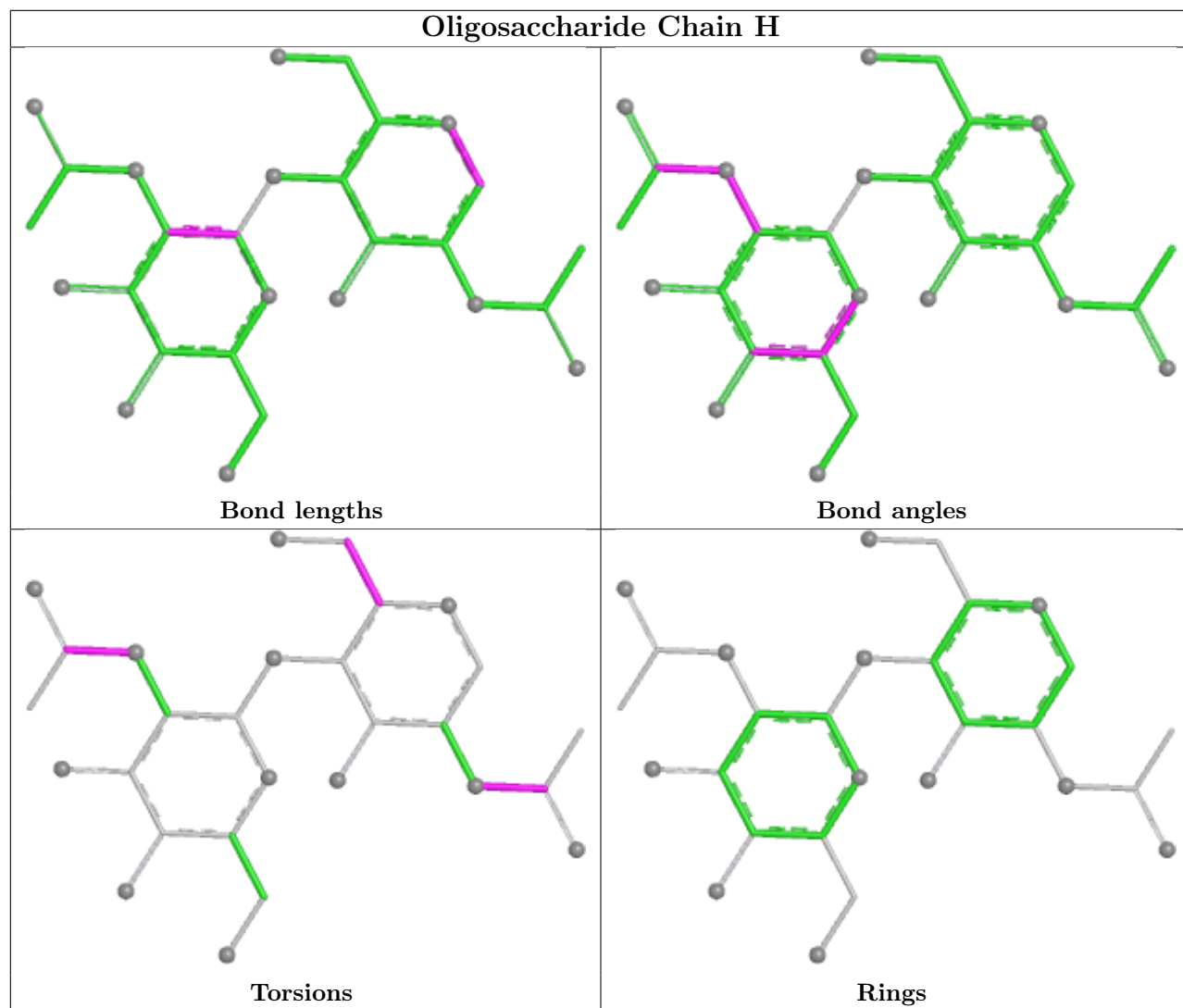


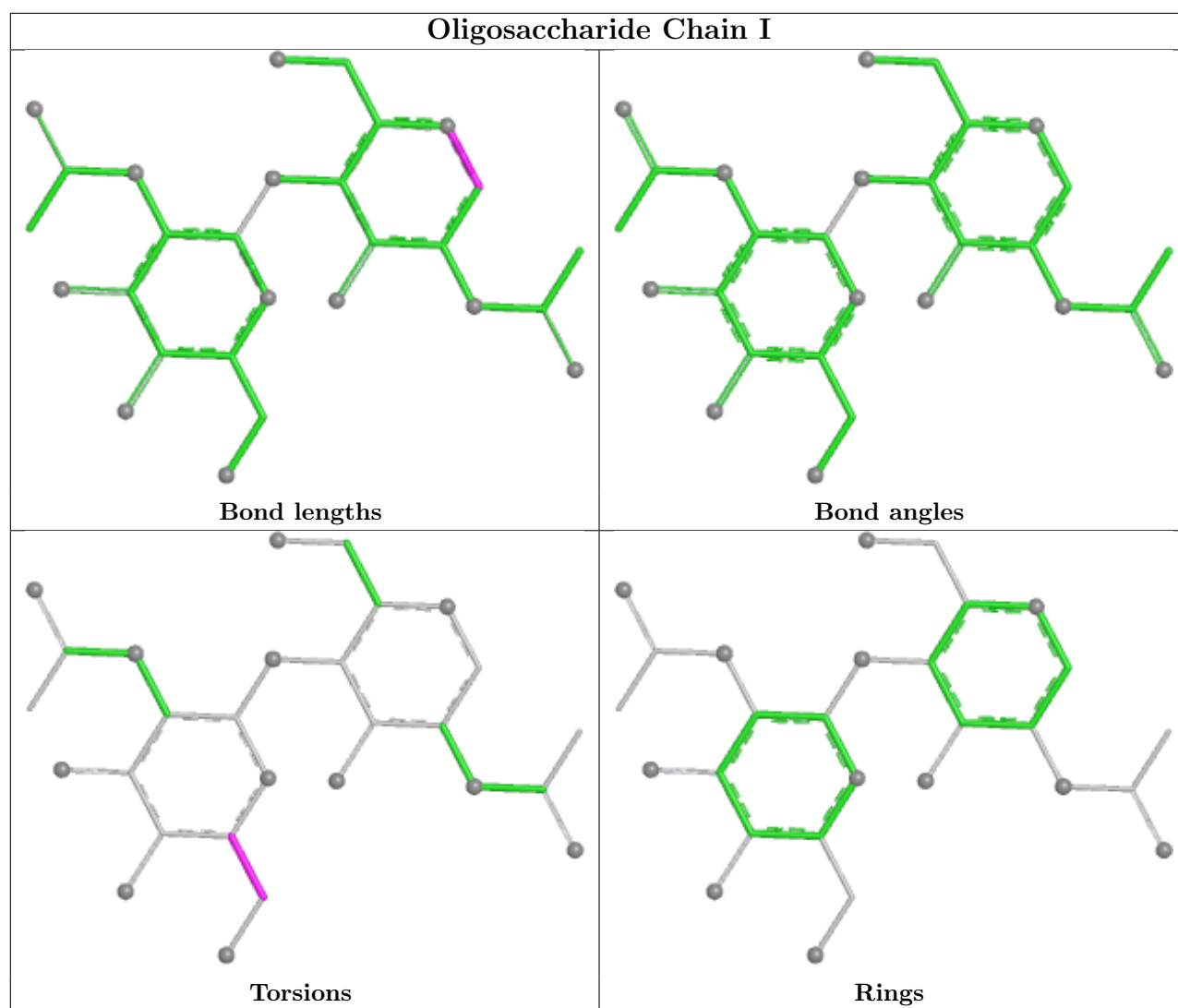


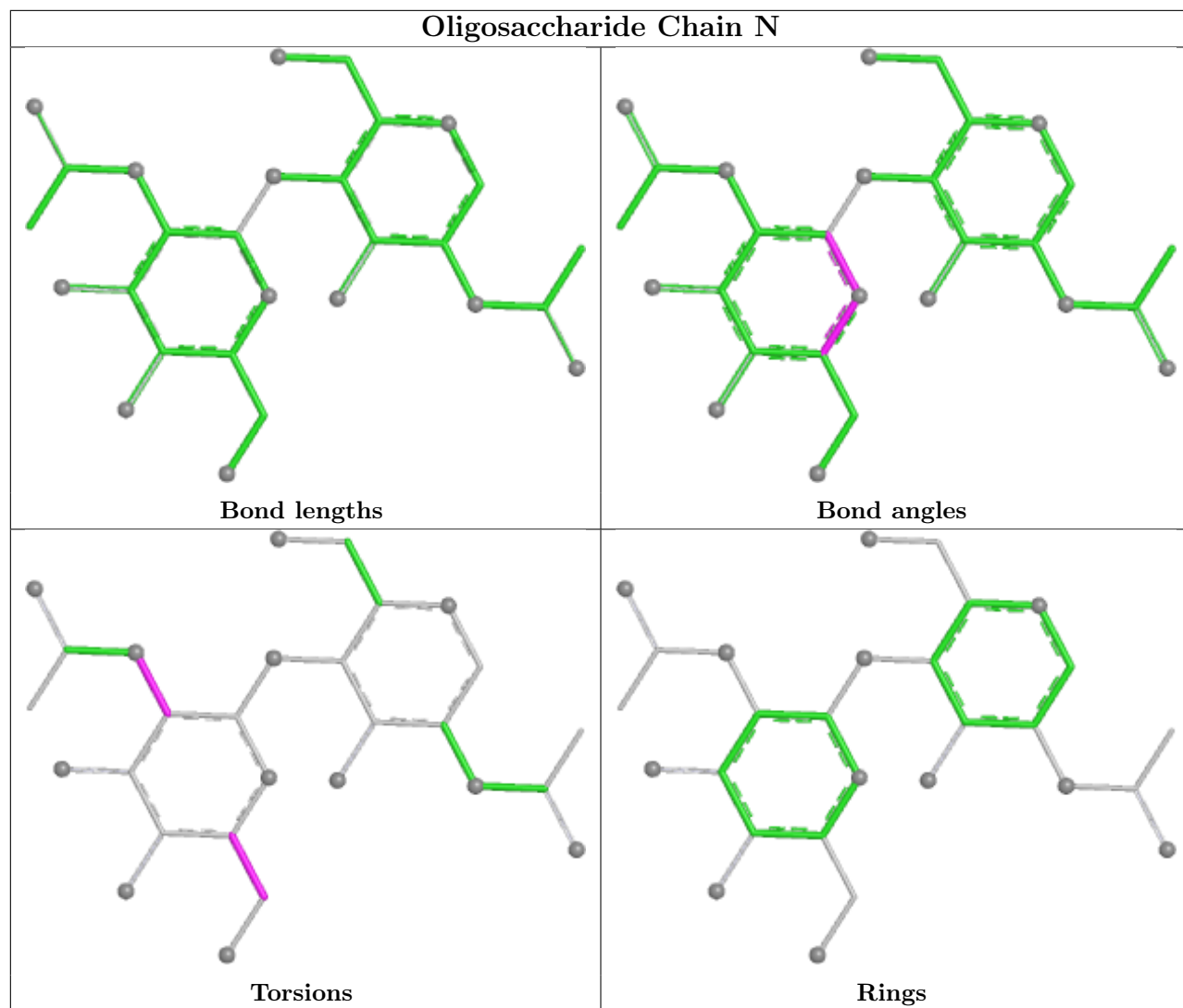


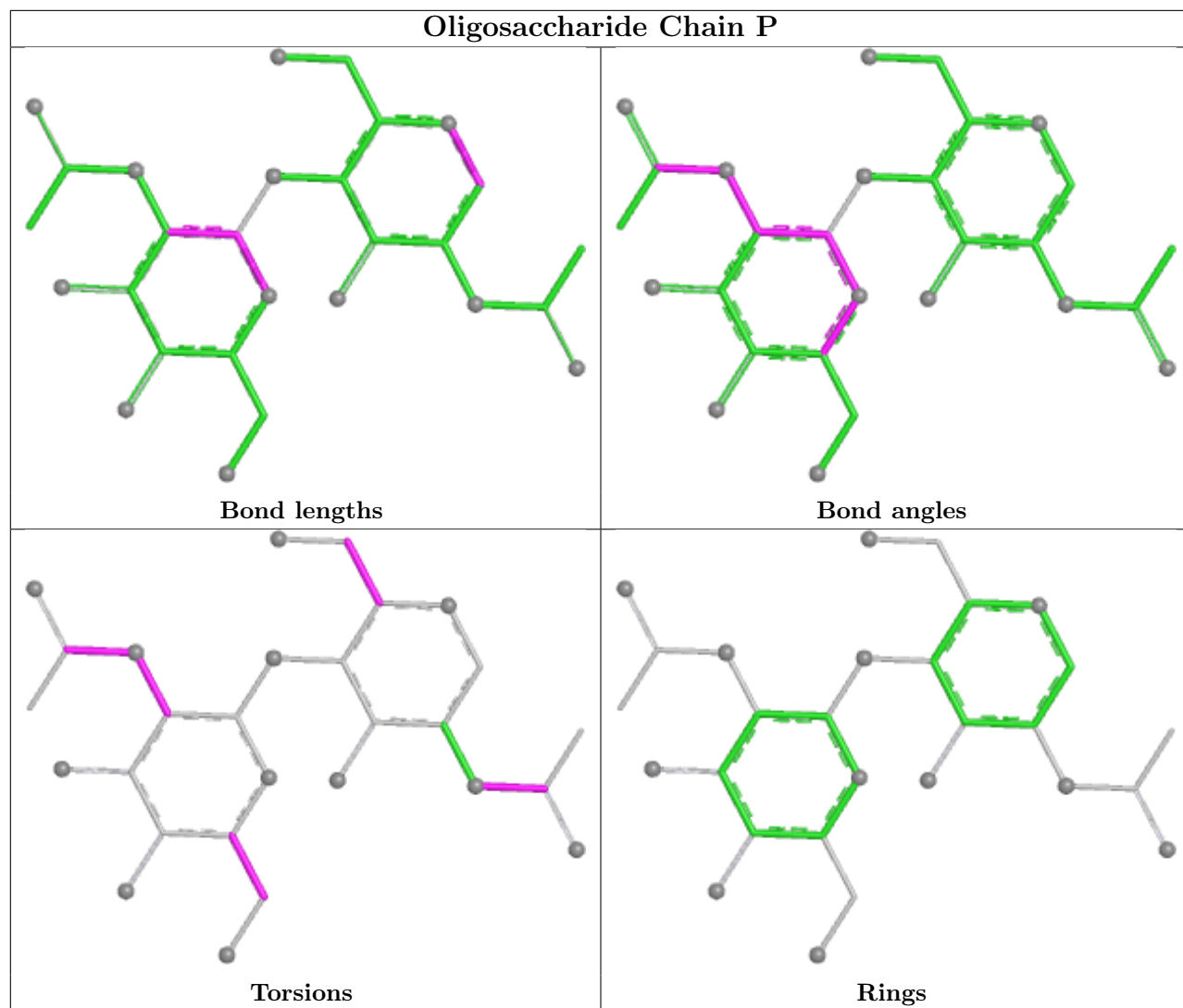


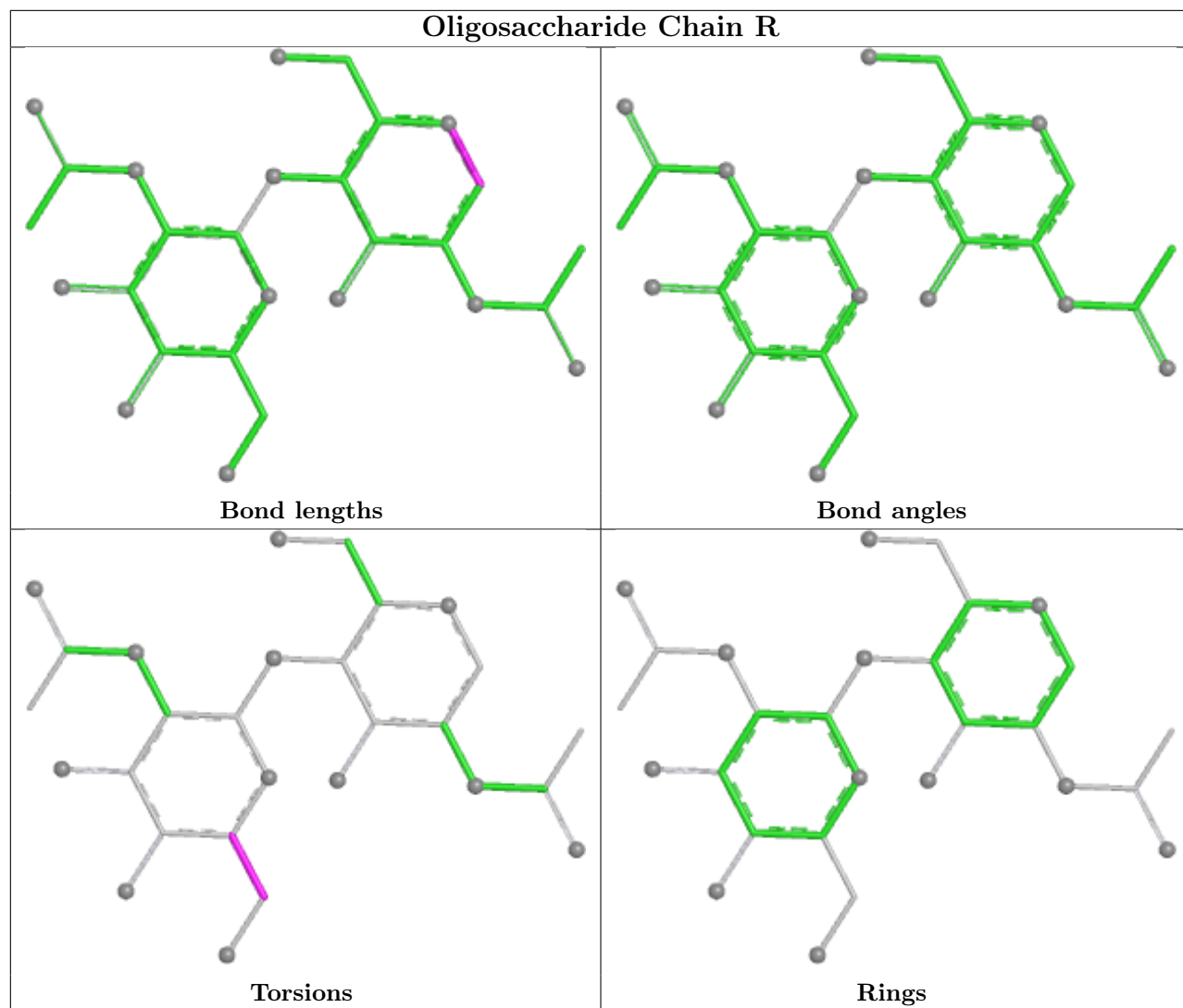
Oligosaccharide Chain H



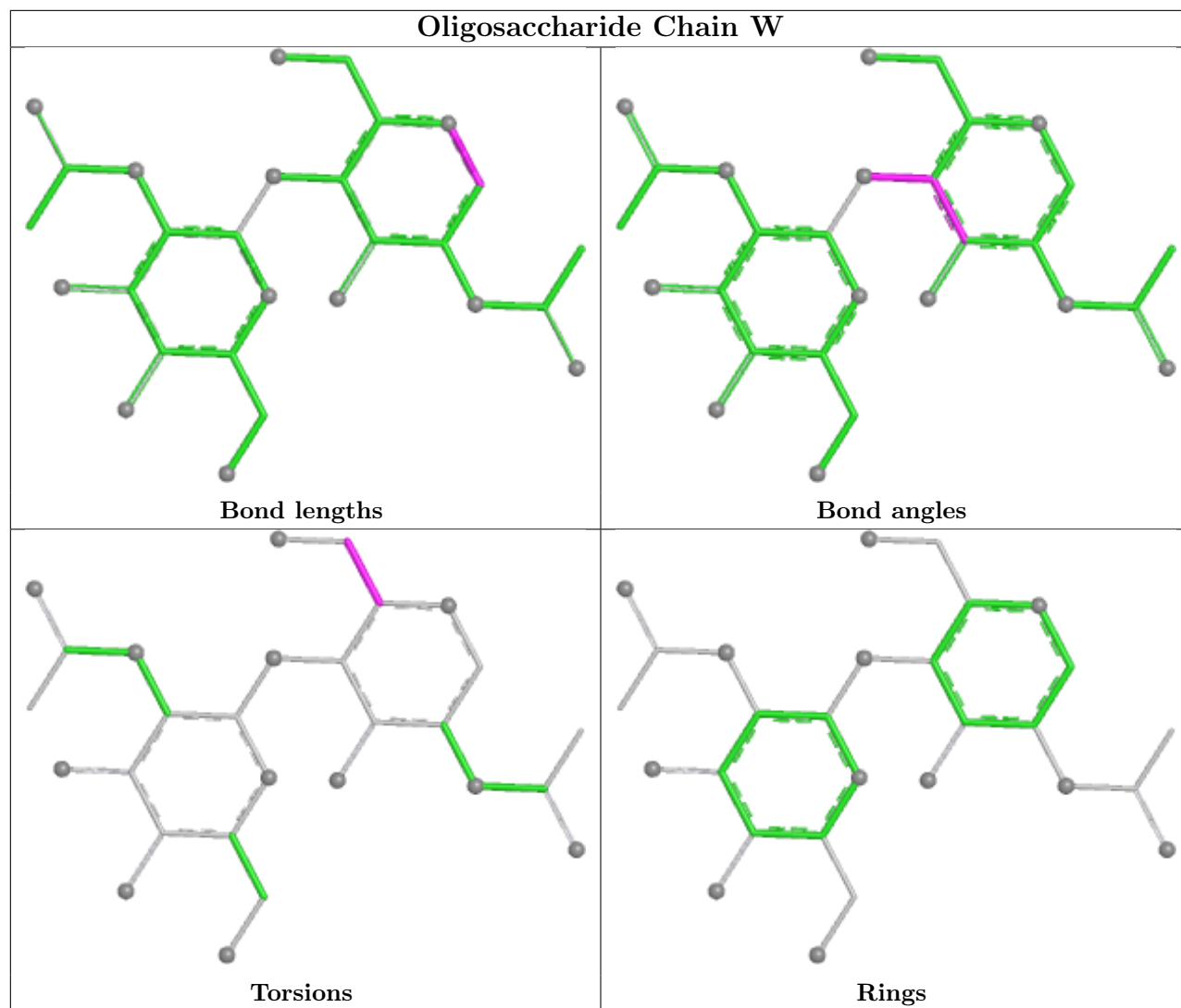


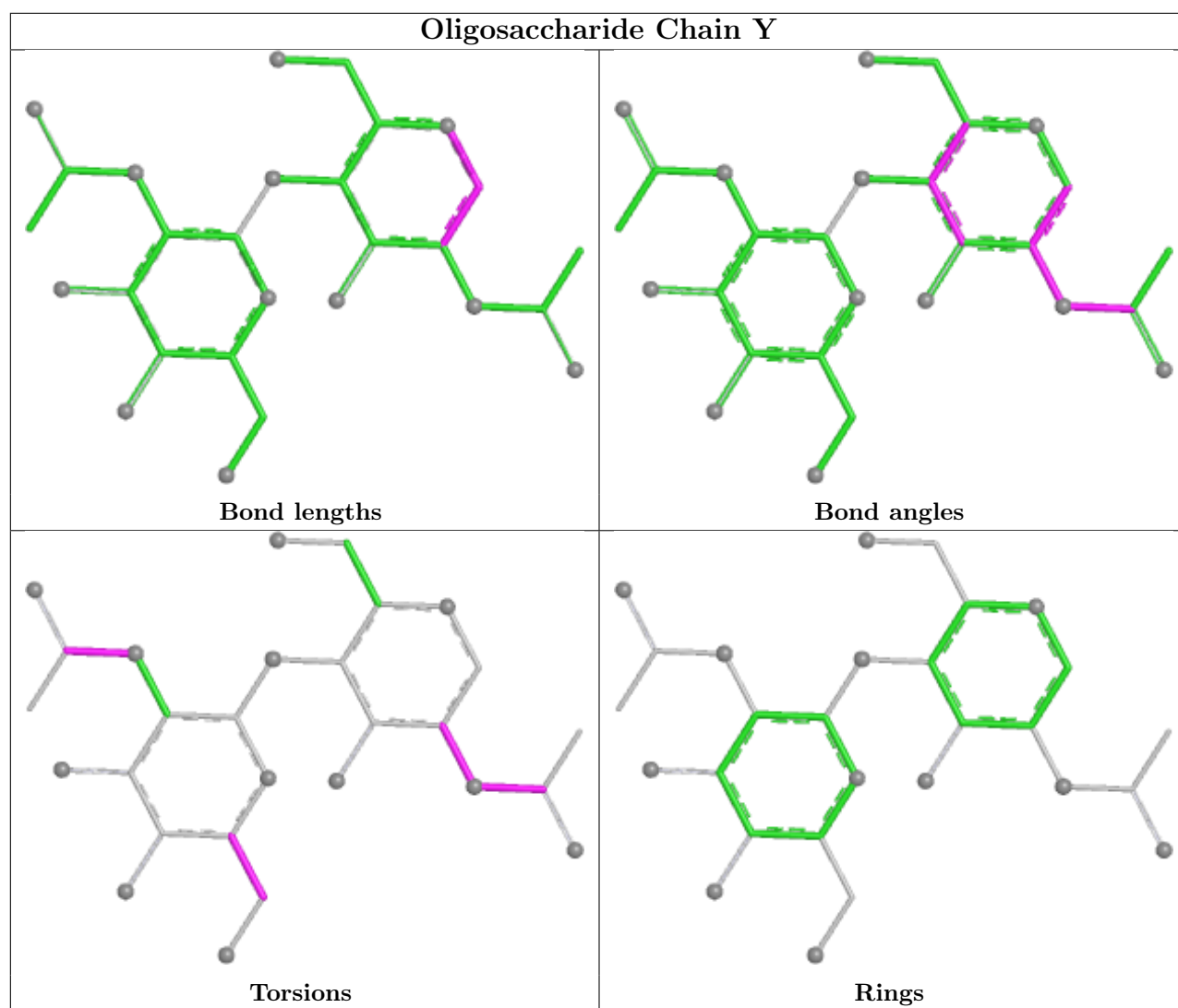


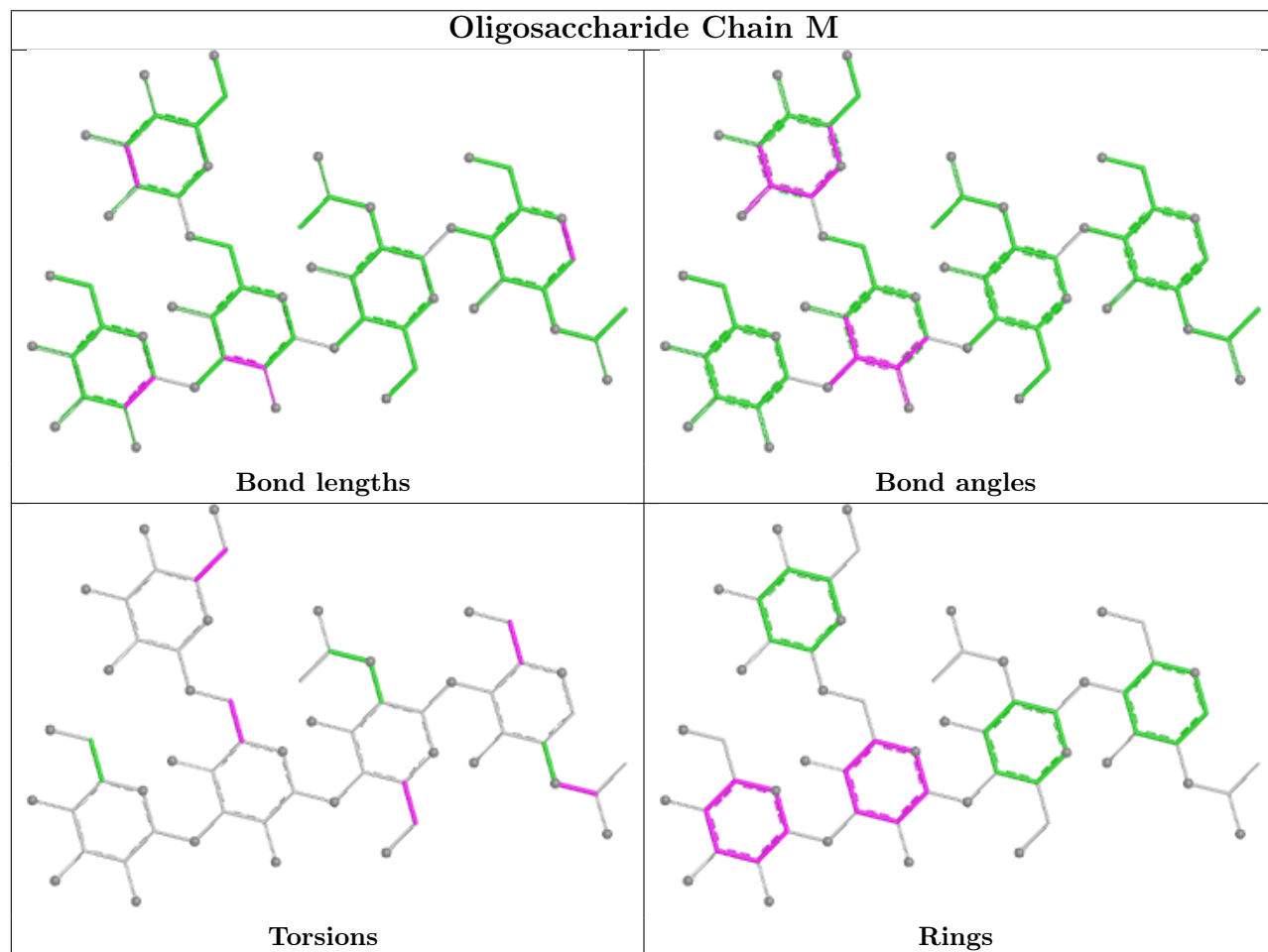
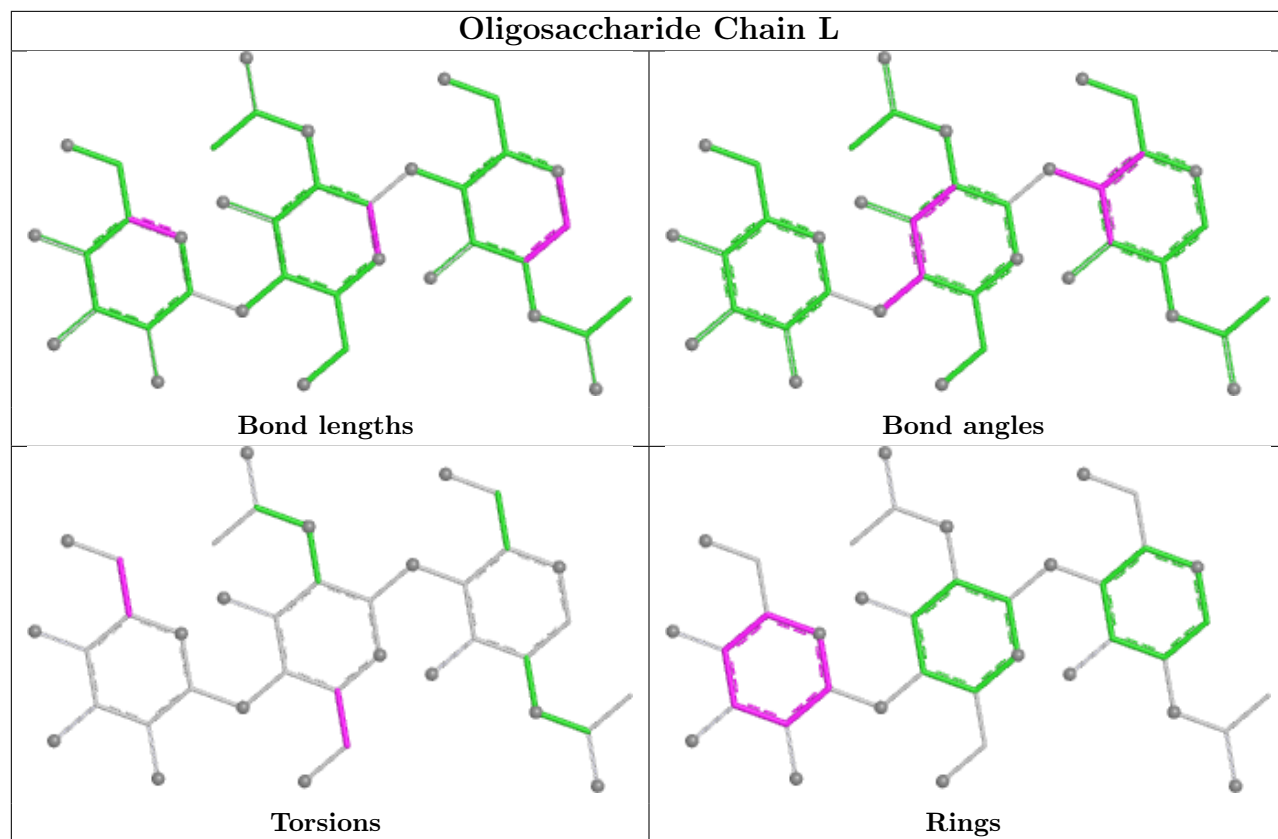


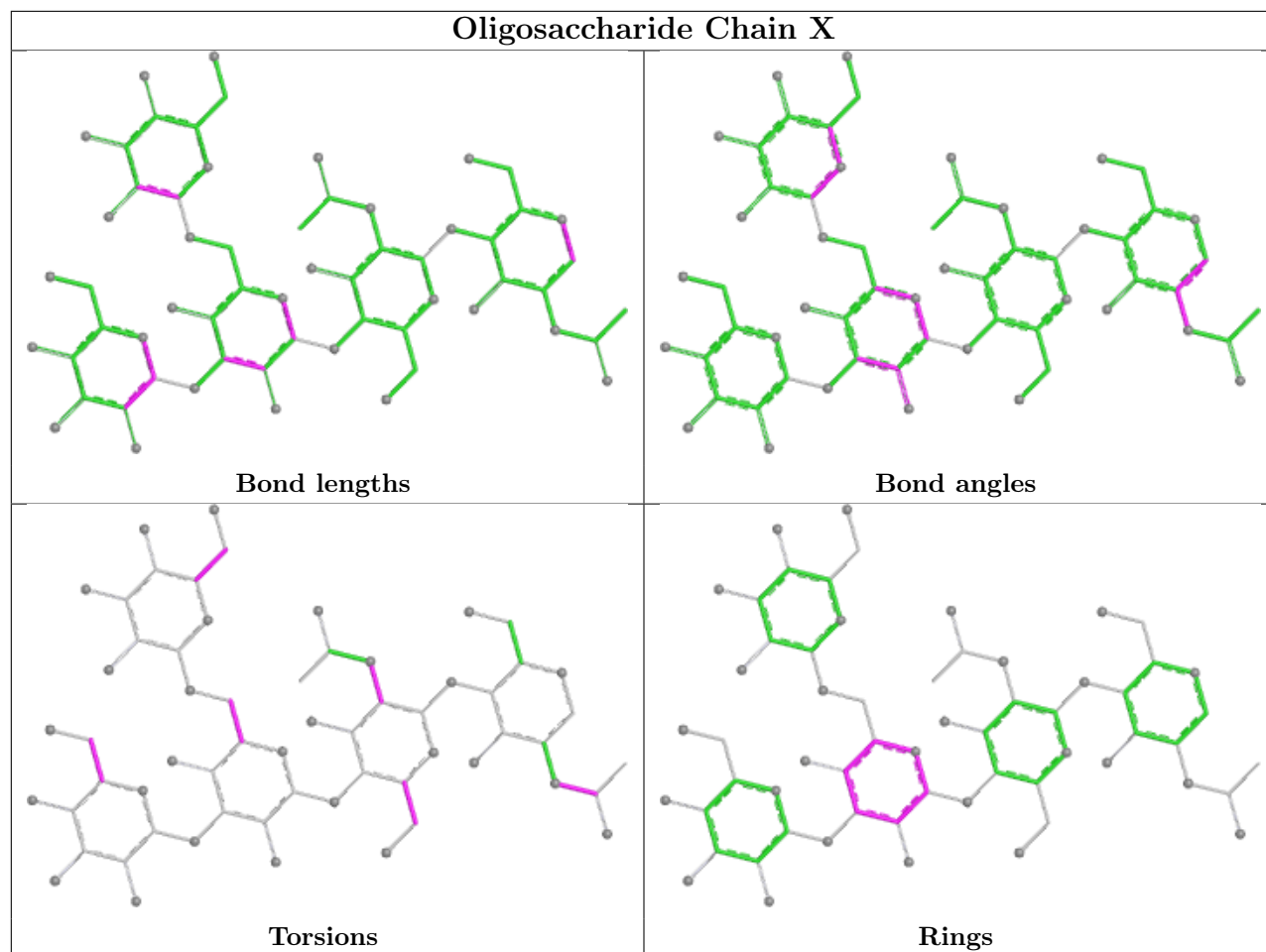


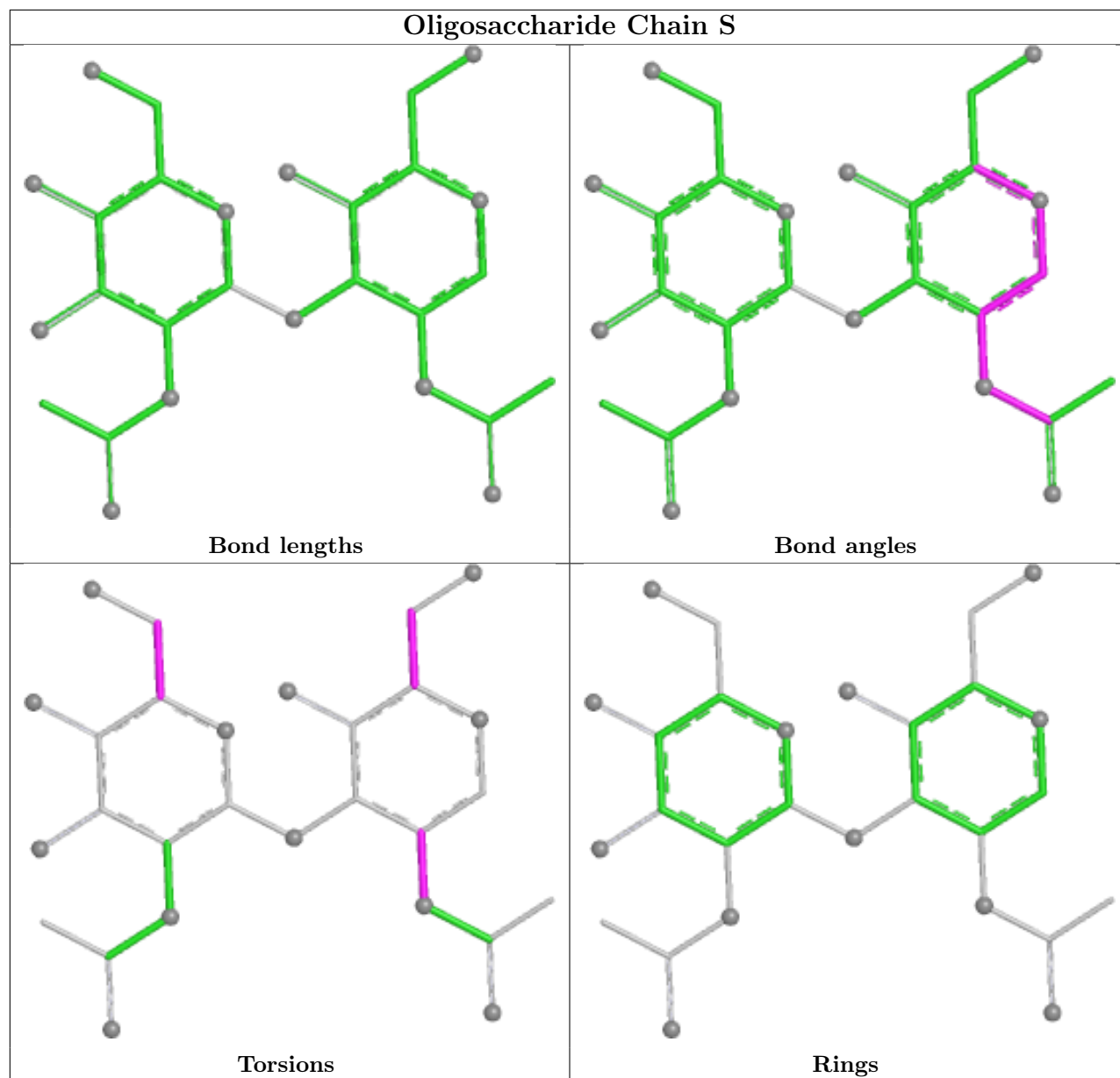
Oligosaccharide Chain W



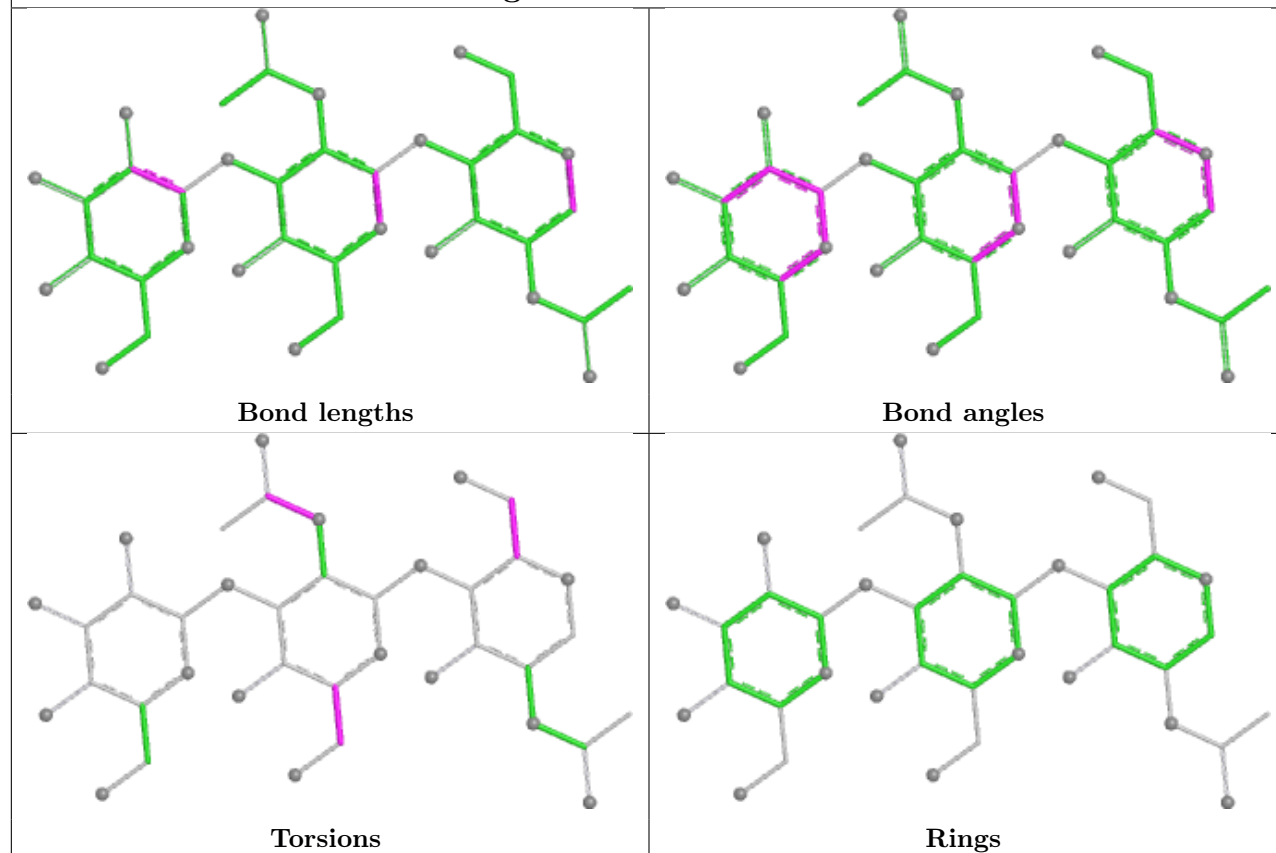




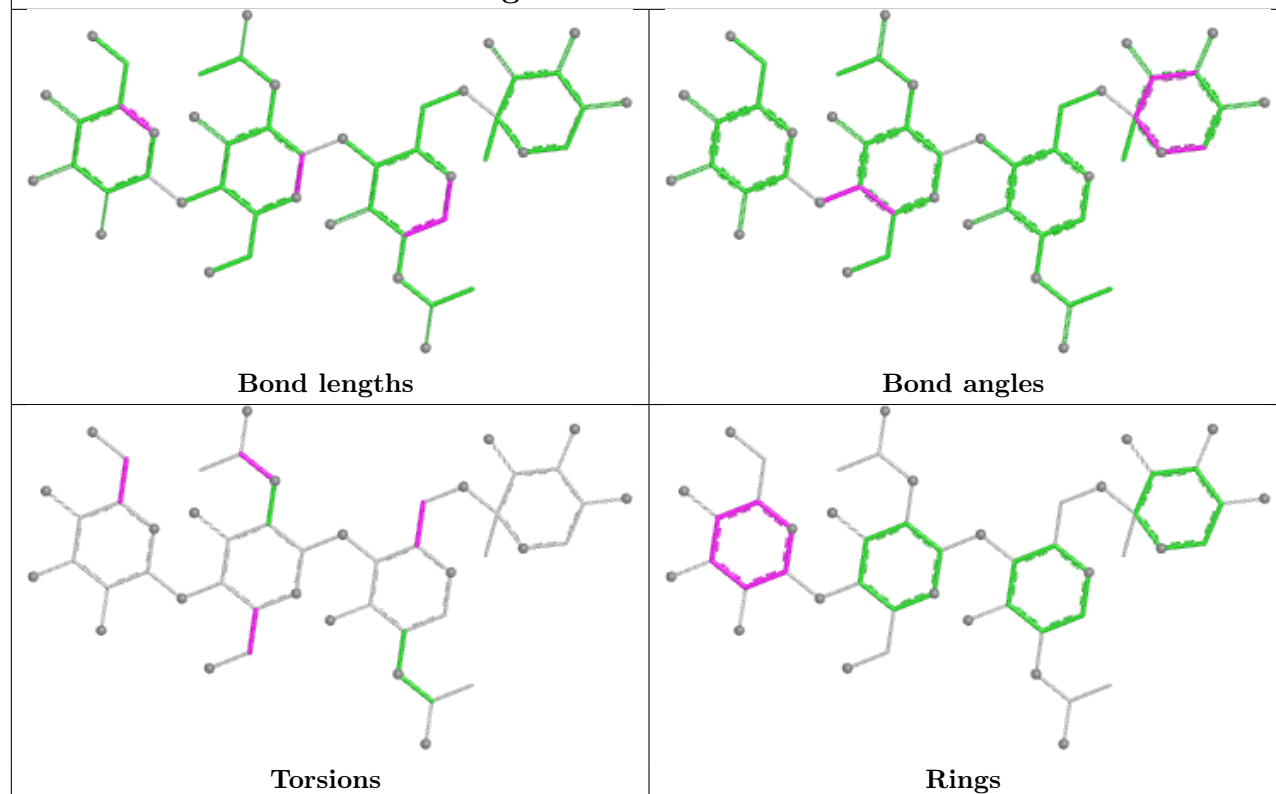




Oligosaccharide Chain T



Oligosaccharide Chain V



5.6 Ligand geometry

Of 15 ligands modelled in this entry, 9 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	TYR	A	513	-	12,13,13	1.36	2 (16%)	13,17,17	0.60	0
13	MAN	C	515	-	11,11,12	2.34	4 (36%)	15,15,17	1.57	3 (20%)
11	TYR	B	516	-	12,13,13	1.21	1 (8%)	13,17,17	0.76	0
11	TYR	D	517	-	12,13,13	1.20	1 (8%)	13,17,17	0.70	0
10	NAG	A	504	-	14,14,15	0.53	0	17,19,21	0.73	1 (5%)
11	TYR	C	516	-	12,13,13	1.19	1 (8%)	13,17,17	1.13	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	TYR	A	513	-	-	2/8/8/8	0/1/1/1
13	MAN	C	515	-	-	2/2/19/22	0/1/1/1
11	TYR	B	516	-	-	3/8/8/8	0/1/1/1
11	TYR	D	517	-	-	3/8/8/8	0/1/1/1
10	NAG	A	504	-	-	2/6/23/26	0/1/1/1
11	TYR	C	516	-	-	3/8/8/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	515	MAN	O5-C1	-5.32	1.34	1.43
13	C	515	MAN	C2-C3	-3.46	1.47	1.52
13	C	515	MAN	C4-C5	3.05	1.59	1.53
11	B	516	TYR	CE1-CZ	-2.33	1.34	1.39
11	A	513	TYR	CE1-CZ	-2.28	1.34	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	515	MAN	C3-C4-C5	3.68	116.90	110.23
11	C	516	TYR	CB-CA-N	3.50	124.81	111.40
13	C	515	MAN	O2-C2-C3	-3.24	103.45	110.15
10	A	504	NAG	C1-O5-C5	2.39	115.39	112.19
13	C	515	MAN	O4-C4-C3	-2.06	105.51	110.38

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	516	TYR	N-CA-CB-CG
13	C	515	MAN	O5-C5-C6-O6
10	A	504	NAG	O5-C5-C6-O6
13	C	515	MAN	C4-C5-C6-O6
10	A	504	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	513	TYR	3	0
13	C	515	MAN	1	0
11	B	516	TYR	2	0
11	D	517	TYR	2	0
11	C	516	TYR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	46:SER	C	47:PRO	N	1.14
1	C	377:HIS	C	378:ASN	N	1.08

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	446/446 (100%)	-0.30	3 (0%) 84 77	24, 43, 64, 103	0
1	B	446/446 (100%)	-0.22	7 (1%) 70 61	30, 47, 76, 106	0
1	C	446/446 (100%)	0.21	9 (2%) 65 56	36, 61, 93, 115	0
1	D	446/446 (100%)	-0.02	4 (0%) 81 74	31, 57, 82, 111	0
All	All	1784/1784 (100%)	-0.08	23 (1%) 75 66	24, 50, 84, 115	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	470	SER	3.8
1	A	429	ASN	3.1
1	B	48	VAL	3.0
1	B	49	SER	2.9
1	A	48	VAL	2.8

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
8	MAN	T	3	11/12	0.43	0.13	89,110,115,115	0
4	NAG	Y	2	14/15	0.44	0.17	90,96,104,105	0

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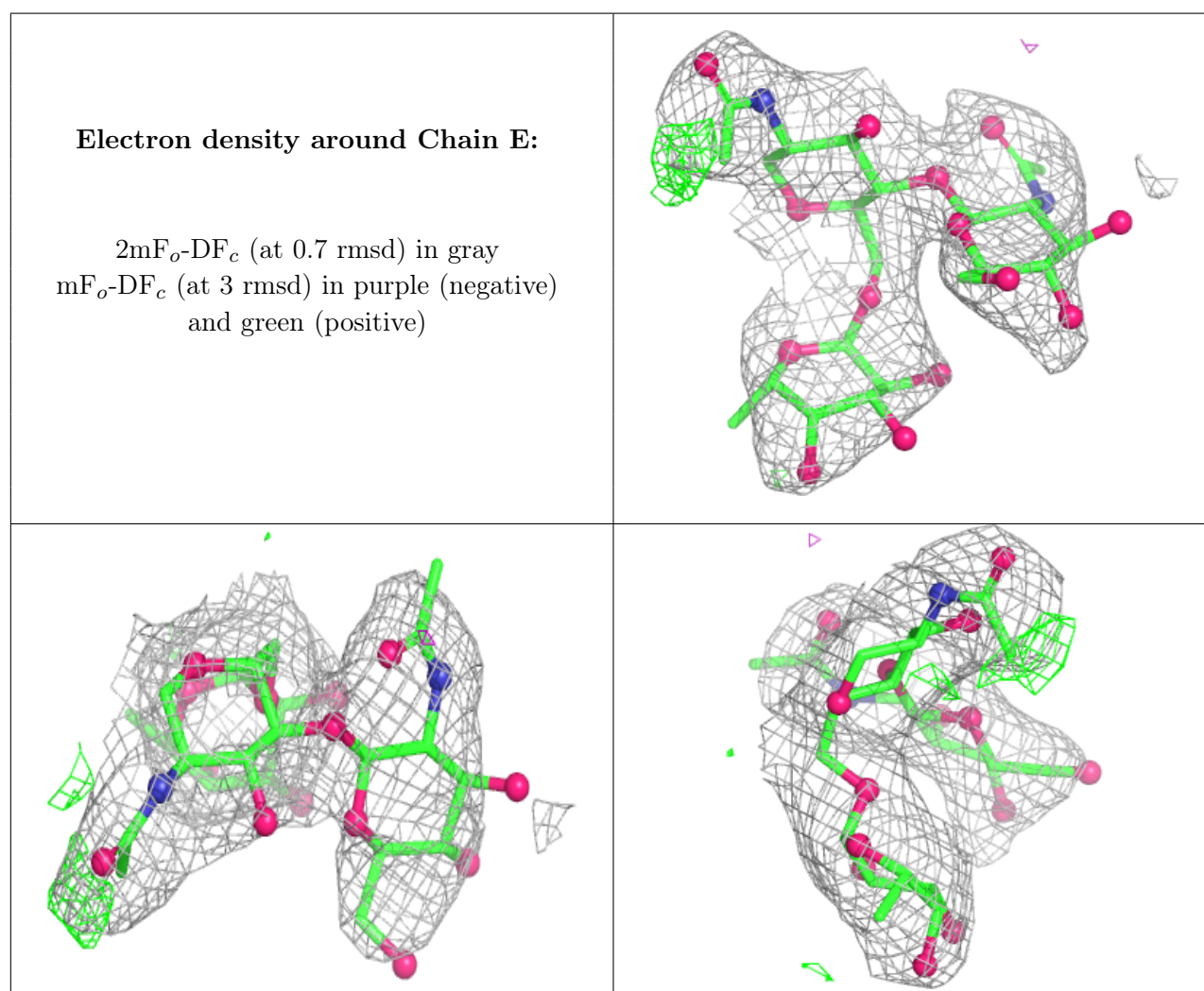
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	T	2	14/15	0.47	0.15	95,106,111,116	0
7	NAG	S	2	14/15	0.57	0.17	111,116,118,119	0
4	NAG	H	2	14/15	0.59	0.15	71,89,100,107	0
7	NAG	S	1	14/15	0.65	0.16	82,95,105,109	0
3	NAG	F	1	14/15	0.65	0.14	57,73,81,82	0
4	NAG	P	2	14/15	0.66	0.17	69,83,89,89	0
5	MAN	L	3	11/12	0.66	0.14	73,79,86,89	0
4	NAG	R	2	14/15	0.67	0.13	90,95,97,102	0
6	MAN	X	5	11/12	0.67	0.13	54,72,78,85	0
3	NAG	Q	1	14/15	0.68	0.13	72,79,83,85	0
3	NAG	K	1	14/15	0.68	0.13	66,73,77,81	0
4	NAG	I	2	14/15	0.68	0.14	65,72,84,84	0
2	NAG	J	2	14/15	0.69	0.14	71,84,89,91	0
9	MAN	V	3	11/12	0.69	0.14	80,89,94,102	0
4	NAG	H	1	14/15	0.70	0.13	64,68,92,94	0
2	NAG	E	1	14/15	0.71	0.13	69,75,83,92	0
2	NAG	O	2	14/15	0.71	0.12	81,92,98,98	0
2	NAG	U	2	14/15	0.75	0.13	86,90,94,98	0
6	NAG	X	1	14/15	0.75	0.16	62,79,88,89	0
9	FUC	V	4	10/11	0.77	0.14	61,72,76,85	0
2	FUC	O	3	10/11	0.78	0.12	71,81,90,93	0
2	NAG	E	2	14/15	0.79	0.13	78,88,97,104	0
4	NAG	N	2	14/15	0.79	0.11	60,67,73,77	0
3	FUC	F	2	10/11	0.79	0.11	70,80,86,92	0
6	MAN	M	4	11/12	0.79	0.15	60,69,75,78	0
2	FUC	E	3	10/11	0.80	0.14	66,72,80,89	0
2	NAG	U	1	14/15	0.80	0.11	74,78,92,94	0
4	NAG	Y	1	14/15	0.81	0.13	72,86,94,103	0
9	NAG	V	2	14/15	0.81	0.12	62,75,83,85	0
4	NAG	W	2	14/15	0.82	0.13	71,75,82,88	0
2	NAG	O	1	14/15	0.82	0.10	68,76,85,86	0
6	MAN	M	5	11/12	0.82	0.14	65,72,81,87	0
2	FUC	U	3	10/11	0.82	0.14	67,75,83,86	0
3	FUC	Q	2	10/11	0.83	0.10	77,86,92,93	0
4	NAG	R	1	14/15	0.83	0.10	63,74,82,91	0
2	FUC	J	3	10/11	0.85	0.12	53,66,70,70	0
4	NAG	P	1	14/15	0.86	0.13	58,67,77,83	0
4	NAG	G	2	14/15	0.86	0.10	63,72,83,85	0
6	MAN	M	3	11/12	0.86	0.11	55,58,61,61	0
6	NAG	X	2	14/15	0.86	0.12	61,69,74,75	0
3	FUC	K	2	10/11	0.87	0.09	70,79,82,82	0
6	MAN	X	4	11/12	0.87	0.10	63,67,74,79	0

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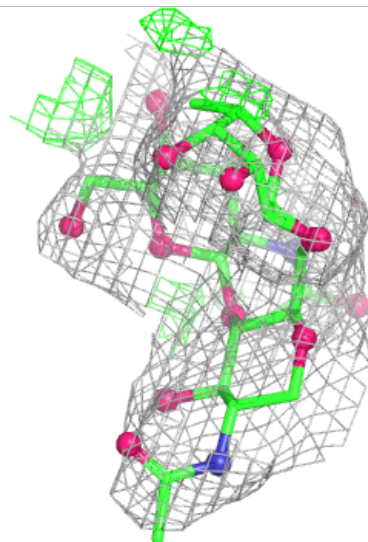
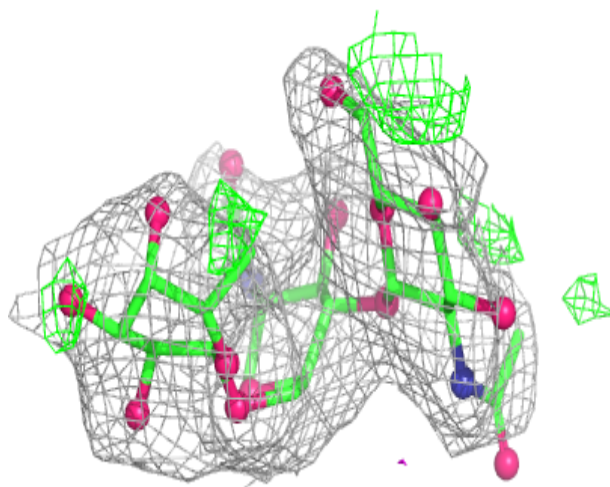
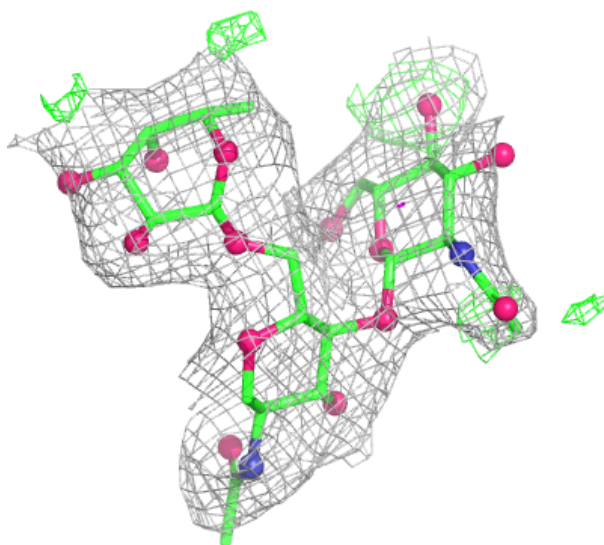
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	L	2	14/15	0.88	0.09	61,69,75,75	0
4	NAG	W	1	14/15	0.88	0.11	57,60,74,75	0
2	NAG	J	1	14/15	0.88	0.10	61,67,75,83	0
5	NAG	L	1	14/15	0.88	0.10	47,54,59,64	0
6	MAN	X	3	11/12	0.90	0.08	58,67,73,73	0
6	NAG	M	2	14/15	0.91	0.09	45,49,55,60	0
6	NAG	M	1	14/15	0.91	0.11	43,50,62,68	0
8	NAG	T	1	14/15	0.92	0.10	83,94,98,106	0
4	NAG	I	1	14/15	0.93	0.07	43,53,57,64	0
4	NAG	N	1	14/15	0.93	0.08	48,56,62,68	0
4	NAG	G	1	14/15	0.94	0.09	48,58,67,69	0
9	NAG	V	1	14/15	0.95	0.06	46,58,73,79	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.



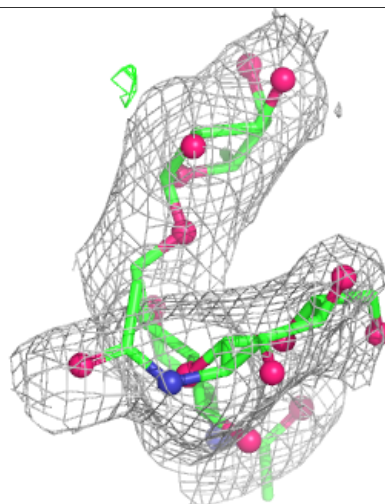
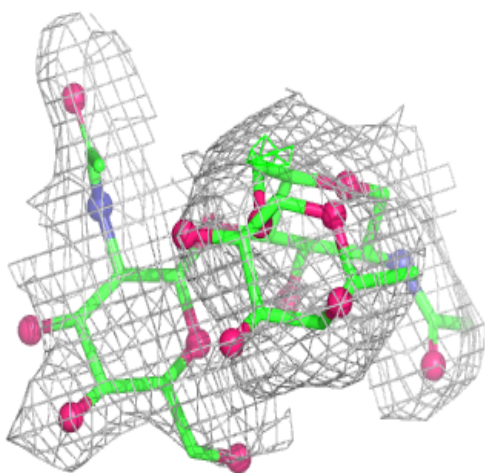
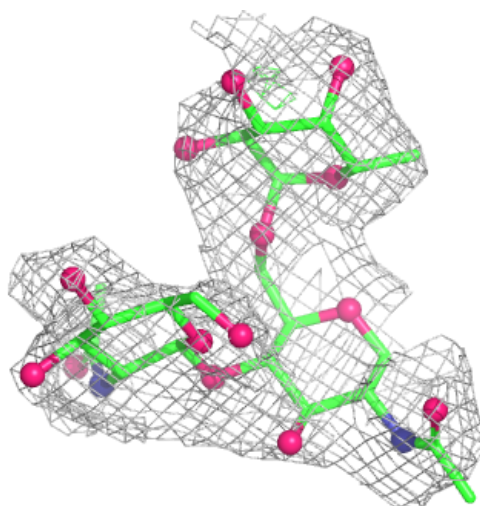
Electron density around Chain J:

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



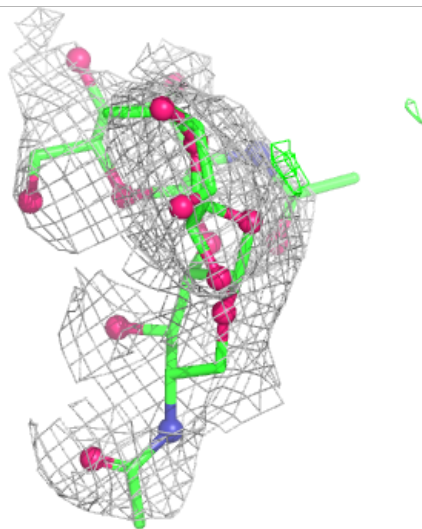
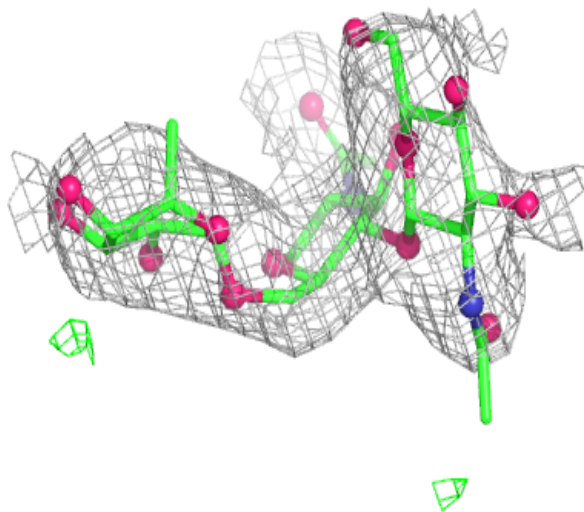
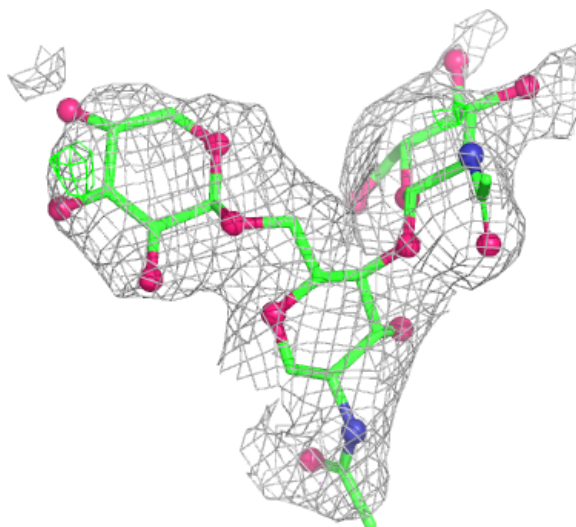
Electron density around Chain O:

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



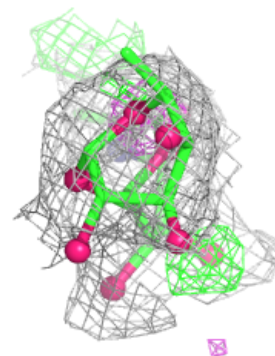
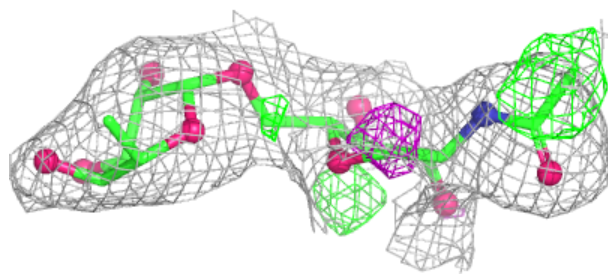
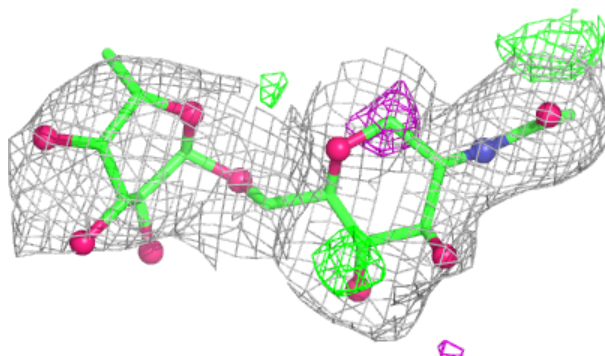
Electron density around Chain U:

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and green (positive)

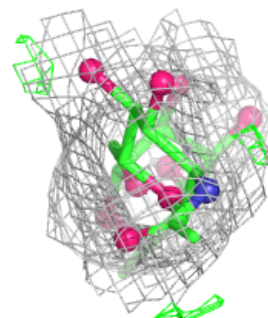
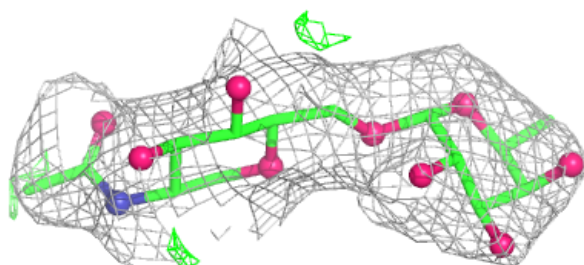
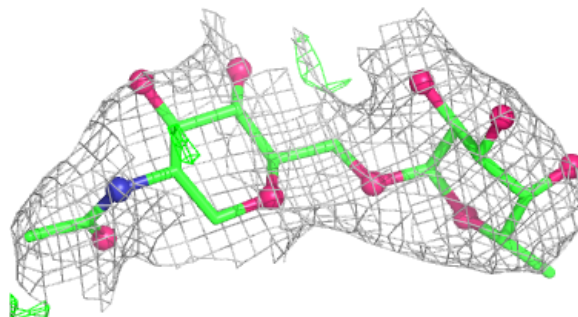


Electron density around Chain F:

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and green (positive)

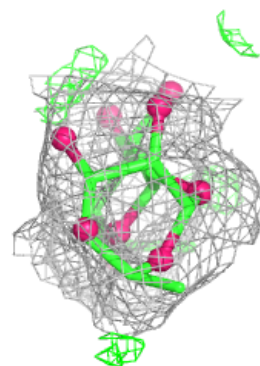
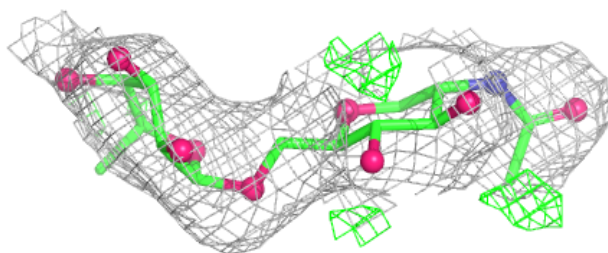
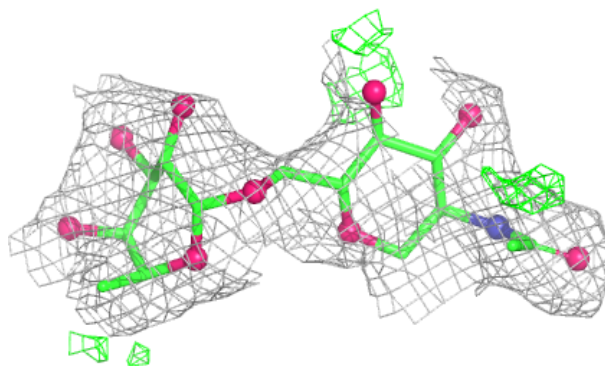
**Electron density around Chain K:**

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

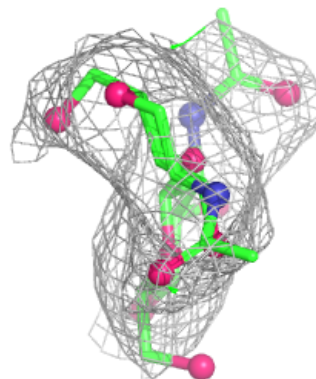
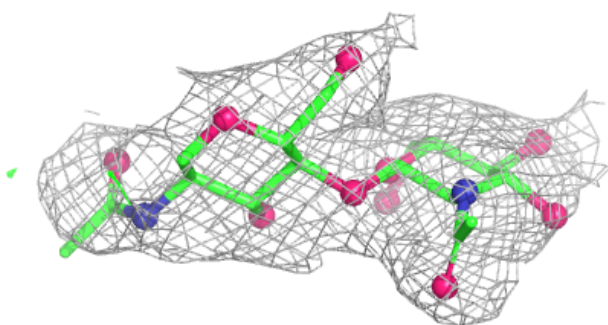
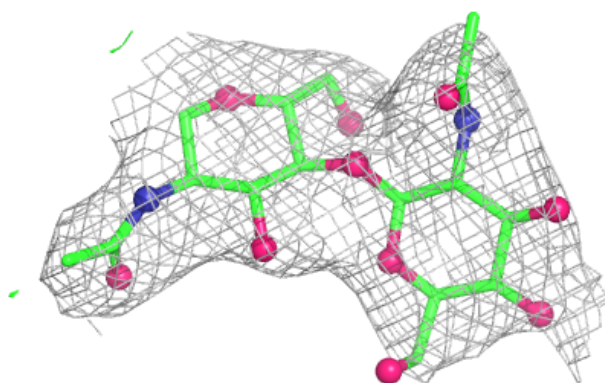


Electron density around Chain Q:

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and green (positive)

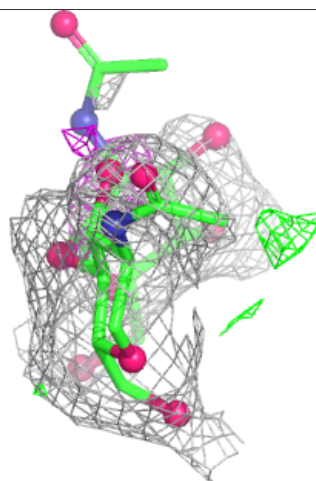
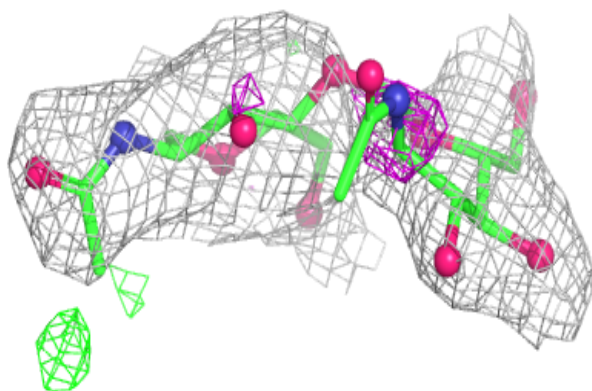
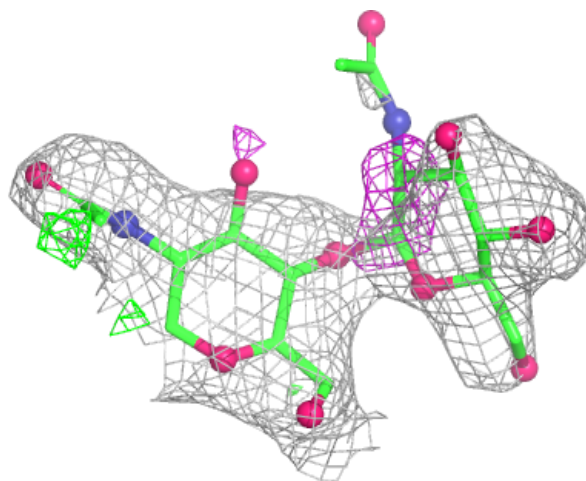
**Electron density around Chain G:**

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



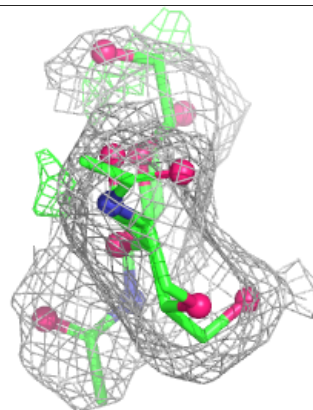
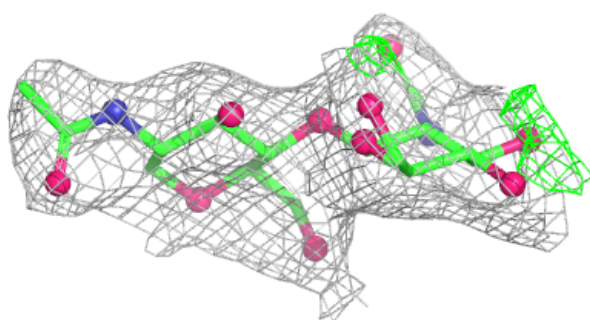
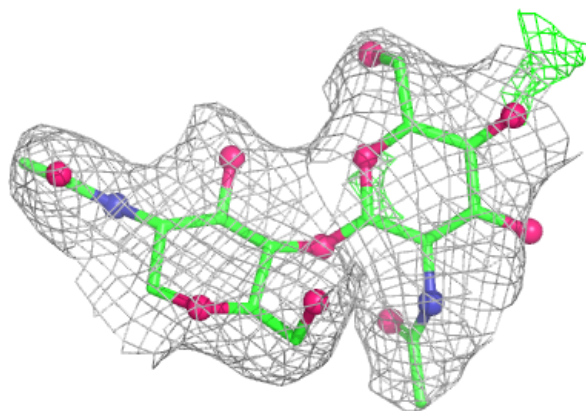
Electron density around Chain H:

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

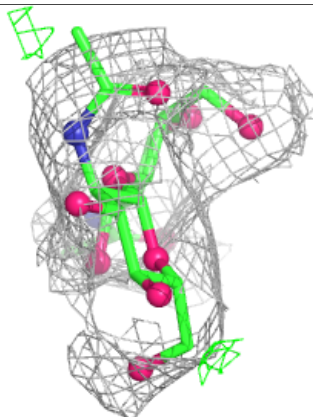
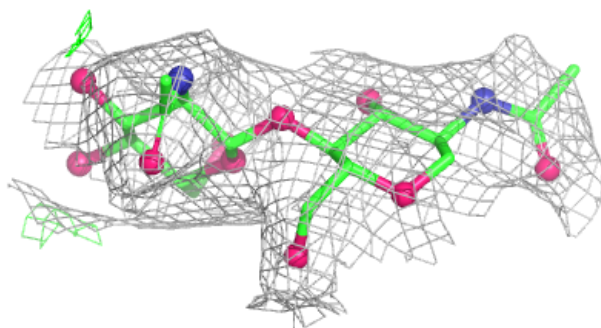
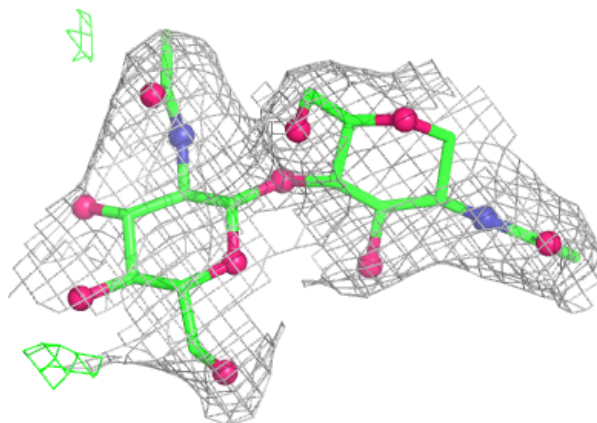


Electron density around Chain I:

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

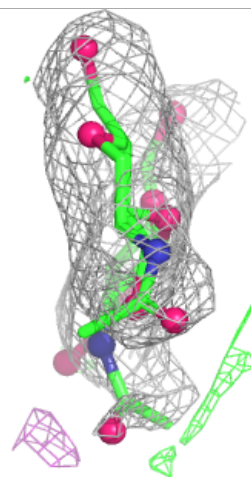
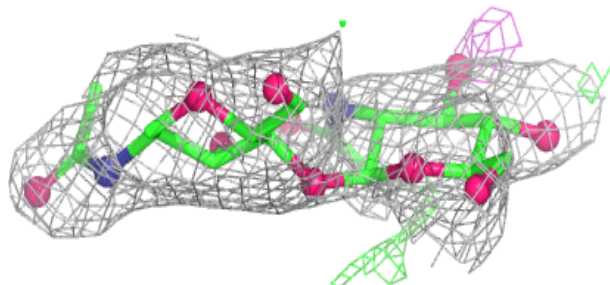
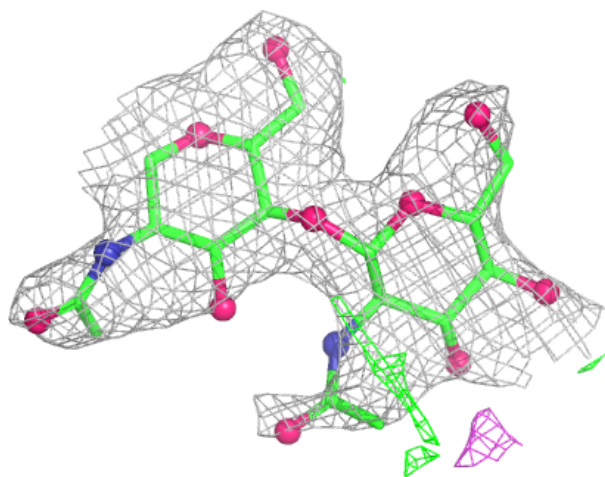
**Electron density around Chain N:**

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



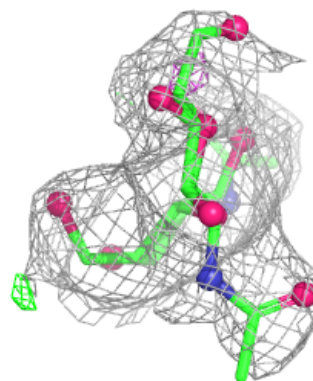
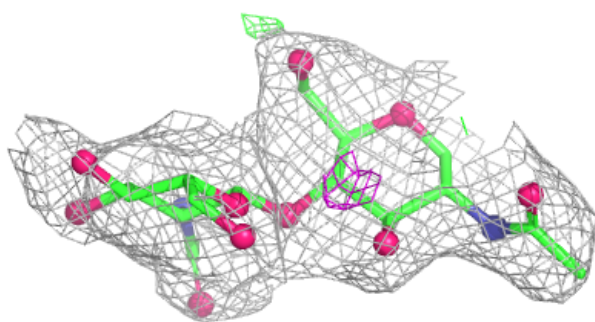
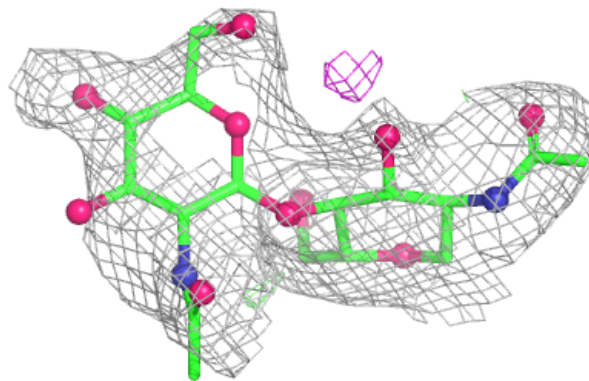
Electron density around Chain P:

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



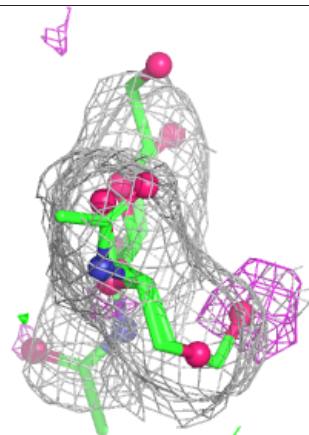
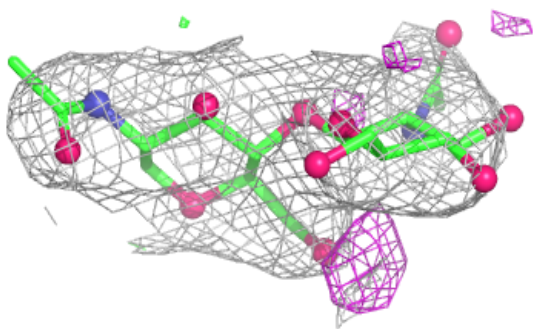
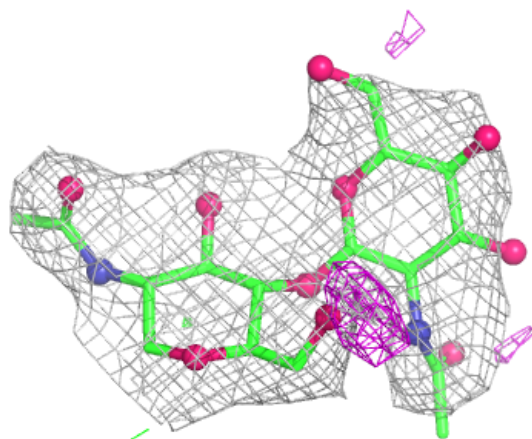
Electron density around Chain R:

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



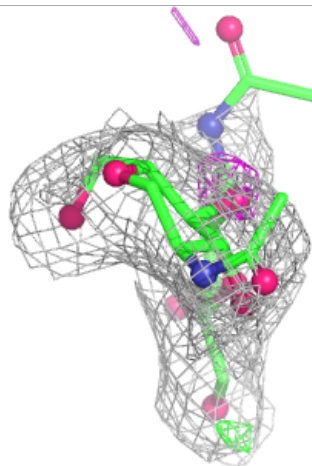
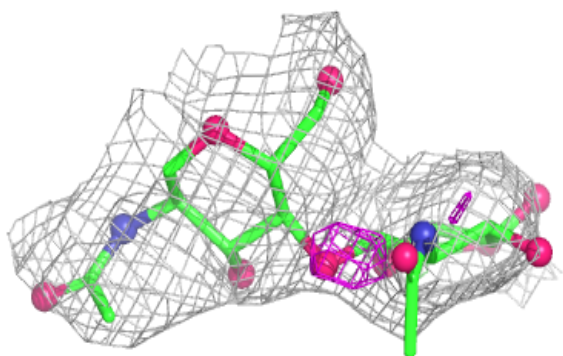
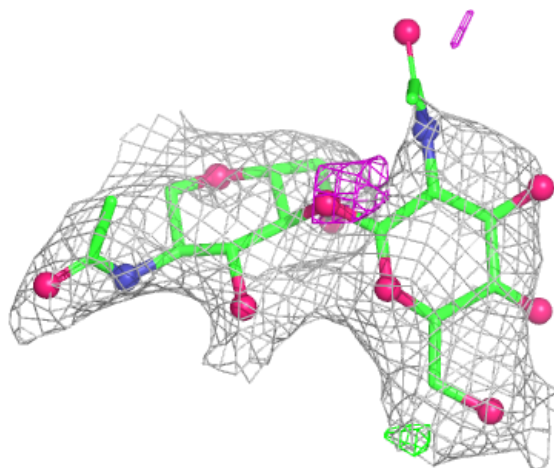
Electron density around Chain W:

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



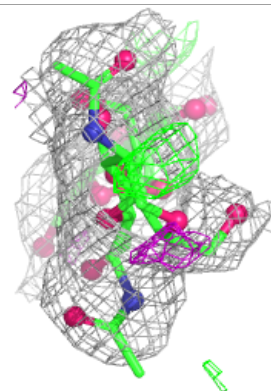
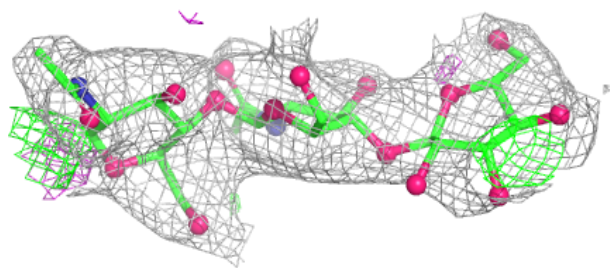
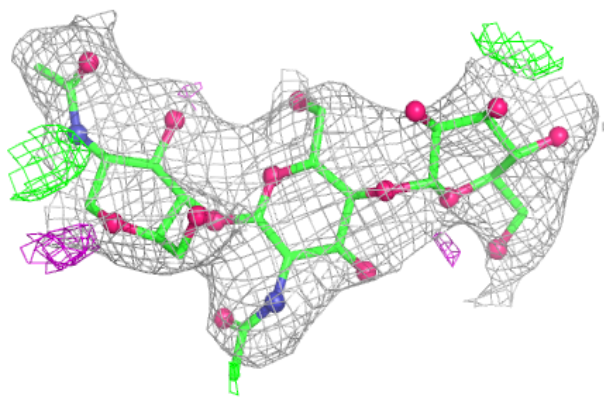
Electron density around Chain Y:

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

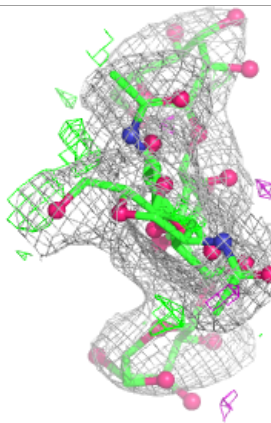
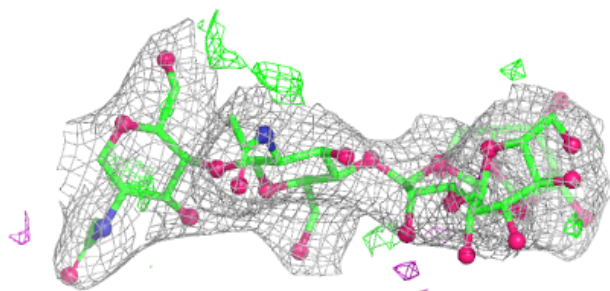
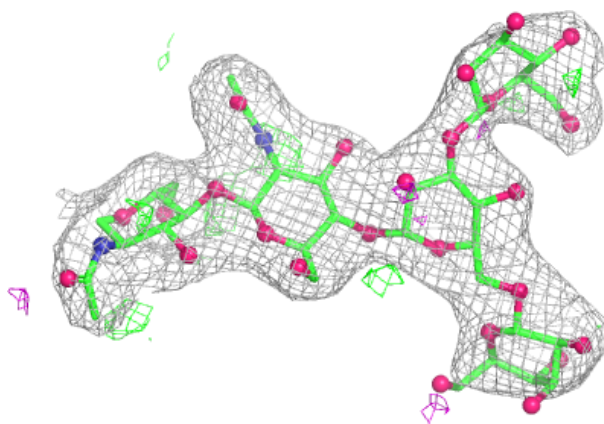


Electron density around Chain L:

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

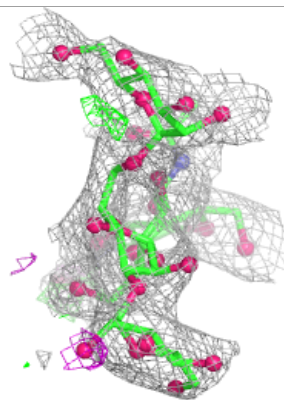
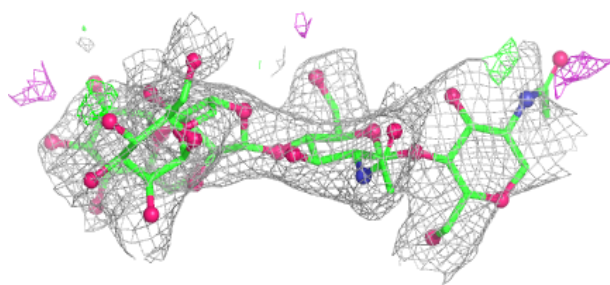
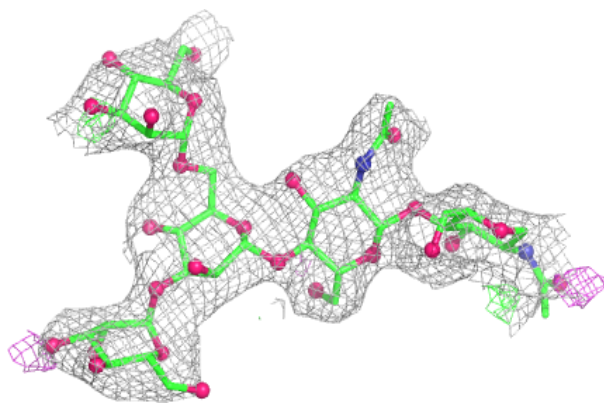
**Electron density around Chain M:**

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



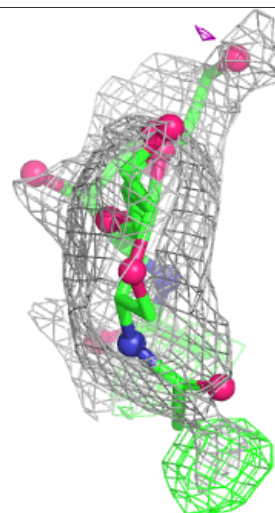
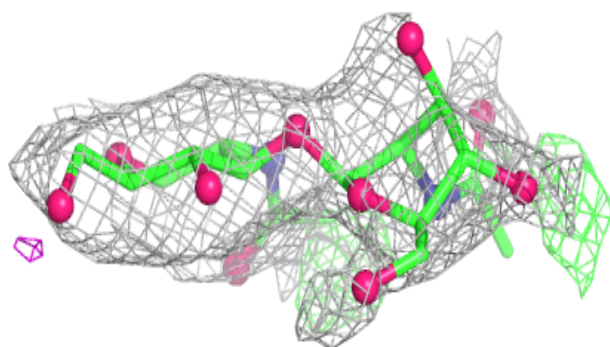
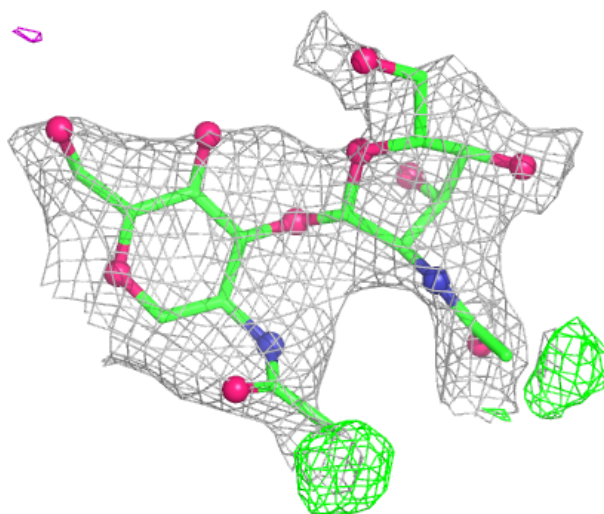
Electron density around Chain X:

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



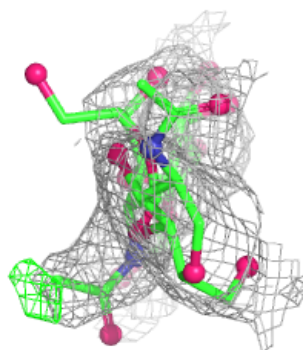
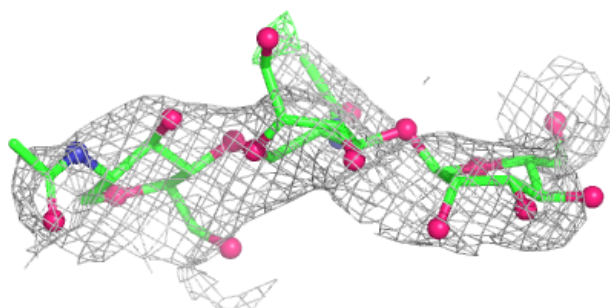
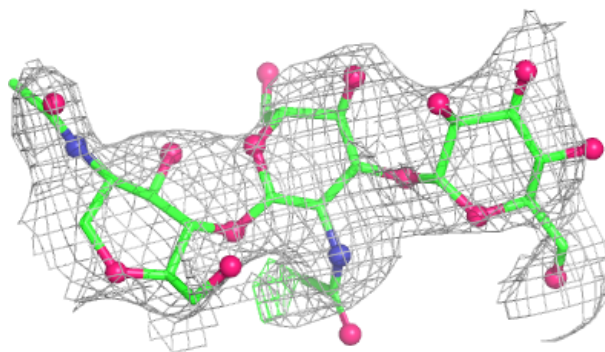
Electron density around Chain S:

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

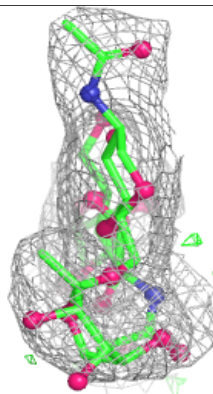
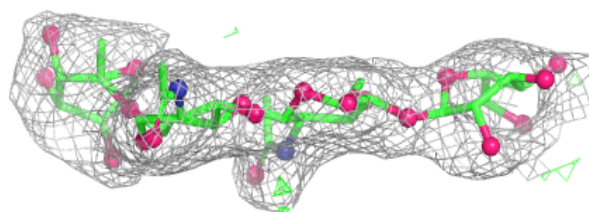
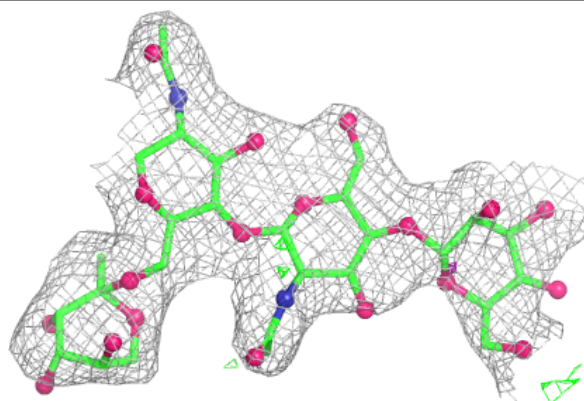


Electron density around Chain T:

$2mF_o-DF_c$ (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)



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, 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
10	NAG	A	504	14/15	0.55	0.20	86,94,106,107	0
11	TYR	C	516	13/13	0.70	0.19	75,87,96,97	0
11	TYR	D	517	13/13	0.71	0.18	57,67,75,84	0
13	MAN	C	515	11/12	0.81	0.12	84,88,93,93	0
11	TYR	A	513	13/13	0.86	0.12	38,43,56,59	0
11	TYR	B	516	13/13	0.90	0.11	37,47,54,61	0
12	ZN	B	518	1/1	0.98	0.03	47,47,47,47	0
12	ZN	B	517	1/1	0.98	0.06	46,46,46,46	0
12	ZN	A	514	1/1	0.99	0.05	38,38,38,38	0
12	ZN	A	515	1/1	0.99	0.03	36,36,36,36	0
12	ZN	C	517	1/1	0.99	0.03	50,50,50,50	0
12	ZN	C	518	1/1	0.99	0.03	63,63,63,63	0
12	ZN	D	518	1/1	0.99	0.03	48,48,48,48	0
12	ZN	D	519	1/1	0.99	0.04	58,58,58,58	0
12	ZN	A	516	1/1	0.99	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.