



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:02 AM UTC

PDB ID : 5M8L / pdb_00005m8l
Title : Crystal structure of human tyrosinase related protein 1
Authors : Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on : 2016-10-29
Resolution : 2.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

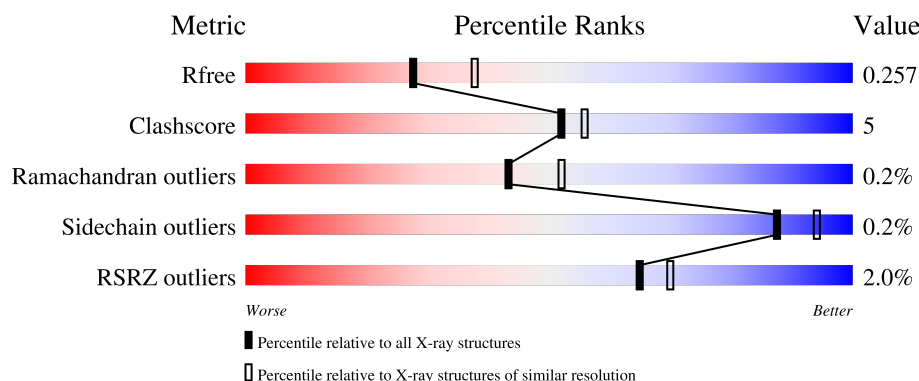
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



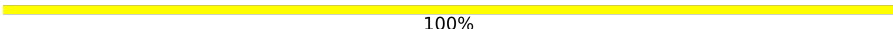
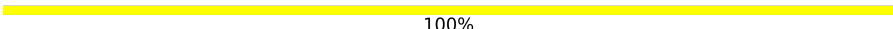
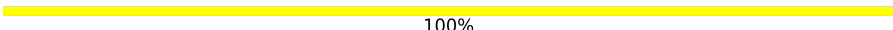
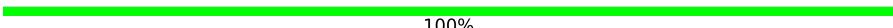
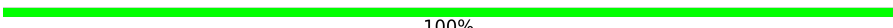
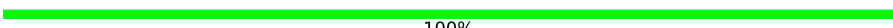
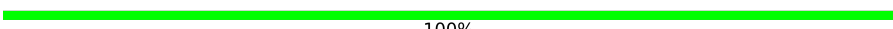
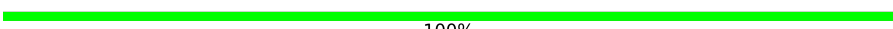
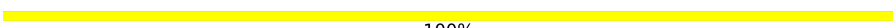
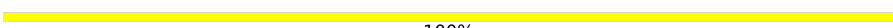
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	% 90% 10%
1	B	446	2% 92% 7%
1	C	446	4% 84% 15%
1	D	446	% 90% 10%
2	E	3	33% 33% 33%

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Mol	Chain	Length	Quality of chain
2	J	3	 33% 67%
2	O	3	 33% 67%
2	S	3	 100%
3	F	2	 100%
3	K	2	 100%
3	P	2	 50% 50%
4	G	2	 100%
4	H	2	 100%
4	I	2	 100%
4	L	2	 50% 50%
4	N	2	 50% 50%
4	Q	2	 100%
4	R	2	 50% 50%
4	U	2	 100%
4	W	2	 100%
5	M	6	 83% 17%
6	T	5	 100%
7	V	5	 100%

2 Entry composition [i](#)

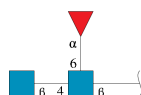
There are 10 unique types of molecules in this entry. The entry contains 15126 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	S	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.



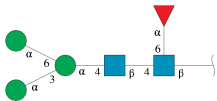
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	P	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



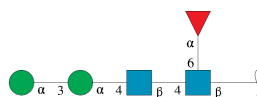
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	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			

- Molecule 5 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



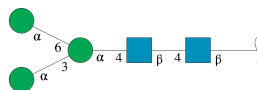
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-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
6	T	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 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
7	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

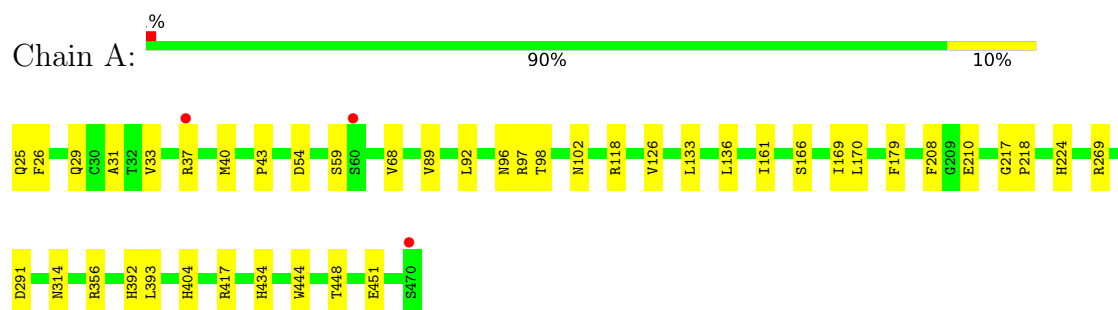
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	75	Total	O	0	0
			75	75		
10	B	57	Total	O	0	0
			57	57		
10	C	17	Total	O	0	0
			17	17		
10	D	32	Total	O	0	0
			32	32		

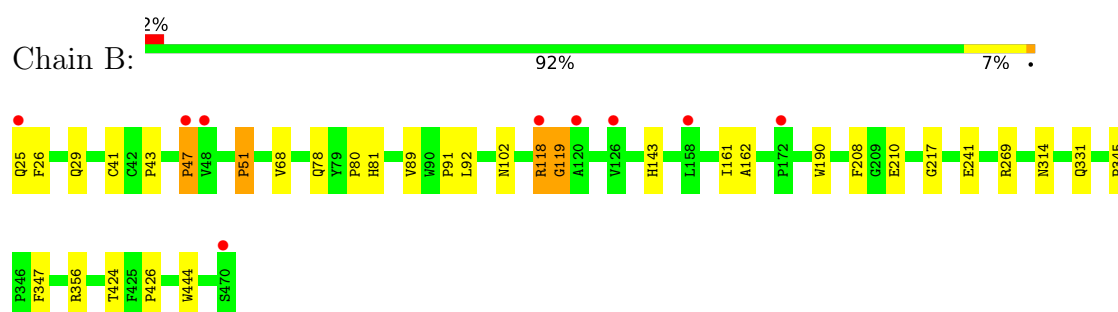
3 Residue-property plots [i](#)

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.

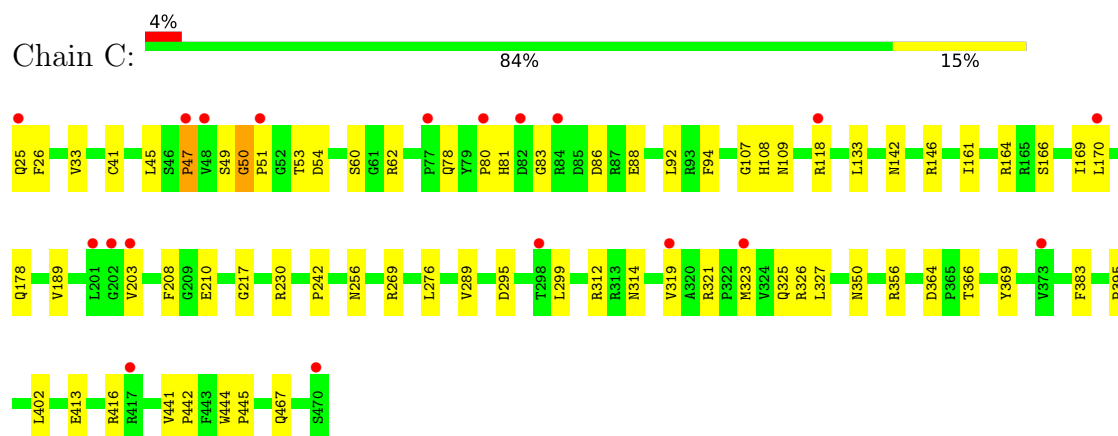
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



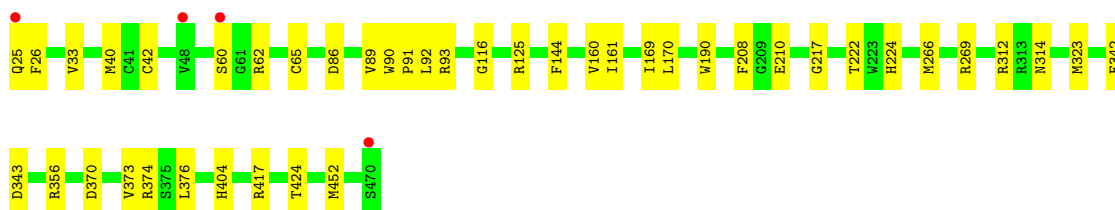
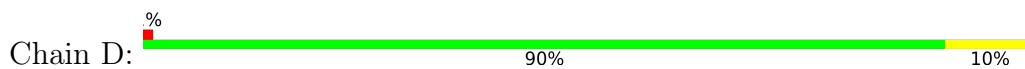
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



- 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



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



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



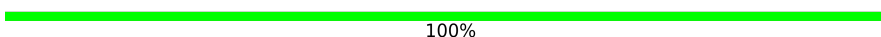


- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



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

Chain G:  100%

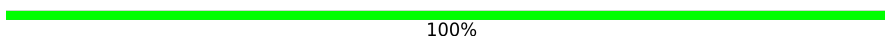


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



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

Chain I:  100%



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

Chain L:  50% 50%



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

Chain N:  50% 50%



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

Chain Q:  100%

NAG1
NAG2

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

Chain R:  50% 50%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain W:  100%

NAG1
NAG2

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

Chain M:  83% 17%

NAG1
NAG2
MAN3
MAN4
MAN5
FUC6

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

Chain T:  100%

NAG1
NAG2
MAN3
MAN4
FUC5

- Molecule 7: 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 V:  100%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.42Å 141.76Å 191.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 2.35 47.47 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.47-2.35) 92.7 (47.47-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.214 , 0.255 0.216 , 0.257	Depositor DCC
R_{free} test set	5075 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.3	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	15126	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3667	0.59	0/4998
1	B	0.54	0/3667	0.64	5/4998 (0.1%)
1	C	0.49	3/3667 (0.1%)	0.58	2/4998 (0.0%)
1	D	0.49	0/3667	0.57	0/4998
All	All	0.51	3/14668 (0.0%)	0.59	7/19992 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	GLY	C-N	5.50	1.40	1.33
1	C	51	PRO	N-CD	5.32	1.55	1.47
1	C	47	PRO	N-CD	5.29	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	PRO	CA-N-CD	-5.54	104.24	112.00
1	C	50	GLY	CA-C-N	-5.48	114.31	119.90
1	C	50	GLY	C-N-CA	-5.48	114.31	119.90
1	B	118	ARG	CA-C-N	5.34	131.88	121.41
1	B	118	ARG	C-N-CA	5.34	131.88	121.41
1	B	345	PRO	O-C-N	5.26	123.73	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	PRO	CA-N-CD	-5.21	104.70	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	GLY	Peptide

5.2 Too-close contacts [i](#)

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	3326	30	0
1	B	3560	0	3326	21	0
1	C	3560	0	3325	56	0
1	D	3560	0	3326	30	0
2	E	38	0	34	1	0
2	J	38	0	34	1	0
2	O	38	0	34	2	0
2	S	38	0	34	1	0
3	F	24	0	22	0	0
3	K	24	0	22	0	0
3	P	24	0	22	1	0
4	G	28	0	25	0	0
4	H	28	0	25	2	0
4	I	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	U	28	0	24	0	0
4	W	28	0	25	0	0
5	M	71	0	61	1	0
6	T	60	0	52	1	0
7	V	61	0	52	0	0
8	A	3	0	0	0	0
8	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	C	28	0	26	1	0
10	A	75	0	0	1	0
10	B	57	0	0	1	0
10	C	17	0	0	1	0
10	D	32	0	0	3	0
All	All	15126	0	13920	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (146) 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:118:ARG:NH1	1:C:242:PRO:HB2	1.68	1.05
1:C:118:ARG:NH1	1:C:242:PRO:CB	2.18	1.05
1:A:102:ASN:ND2	1:B:102:ASN:OD1	2.01	0.93
1:C:50:GLY:O	1:C:53:THR:OG1	1.84	0.93
1:C:118:ARG:HH12	1:C:242:PRO:HB2	1.35	0.86
2:O:1:NAG:H61	2:O:2:NAG:H82	1.61	0.83
1:C:118:ARG:HH11	1:C:242:PRO:CB	1.93	0.80
1:D:86:ASP:HA	1:D:93:ARG:HD2	1.64	0.80
1:D:116:GLY:O	1:D:125:ARG:NH1	2.15	0.79
1:C:133:LEU:HD22	1:C:402:LEU:HD21	1.66	0.77
1:D:25:GLN:HG3	1:D:161:ILE:HA	1.65	0.77
1:C:33:VAL:HG12	1:C:170:LEU:HD22	1.69	0.74
1:C:269:ARG:NH1	1:C:314:ASN:OD1	2.21	0.74
1:C:413:GLU:OE1	1:C:416:ARG:NH1	2.24	0.71
1:C:25:GLN:HG3	1:C:26:PHE:H	1.54	0.70
1:C:118:ARG:HH12	1:C:242:PRO:CB	1.95	0.68
5:M:2:NAG:O3	5:M:3:MAN:H2	1.94	0.68
1:D:269:ARG:NH1	1:D:314:ASN:OD1	2.27	0.67
1:C:118:ARG:HH11	1:C:242:PRO:HB3	1.59	0.67
1:B:269:ARG:NH1	1:B:314:ASN:OD1	2.28	0.66
1:C:81:HIS:O	1:C:83:GLY:HA2	1.96	0.66
1:C:25:GLN:HG2	1:C:161:ILE:HA	1.77	0.66
1:C:364:ASP:OD1	1:C:366:THR:OG1	2.15	0.64
1:B:29:GLN:HG3	1:B:43:PRO:HB3	1.78	0.64
1:A:96:ASN:HD22	2:E:1:NAG:H83	1.63	0.63
1:A:25:GLN:HG3	1:A:26:PHE:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:SER:HB3	1:C:53:THR:HG21	1.80	0.62
1:B:25:GLN:HG3	1:B:161:ILE:HA	1.82	0.62
1:C:118:ARG:NH1	1:C:242:PRO:CG	2.63	0.62
1:D:86:ASP:HA	1:D:93:ARG:CD	2.30	0.61
1:C:444:TRP:O	10:C:601:HOH:O	2.16	0.61
1:C:189:VAL:HG22	1:C:395:PRO:HB2	1.83	0.60
1:A:417:ARG:NH1	10:A:601:HOH:O	2.10	0.59
1:A:208:PHE:CZ	1:A:210:GLU:HB2	2.38	0.59
1:A:218:PRO:HD2	1:A:434:HIS:HB3	1.84	0.58
1:A:25:GLN:HG2	1:A:161:ILE:HA	1.84	0.58
1:A:269:ARG:NH1	1:A:314:ASN:OD1	2.36	0.58
1:A:98:THR:HG22	1:A:444:TRP:CZ2	2.39	0.57
1:A:169:ILE:HG23	1:A:170:LEU:HG	1.85	0.57
1:D:417:ARG:HD2	10:D:603:HOH:O	2.05	0.57
1:D:40:MET:HE3	1:D:65:CYS:SG	2.45	0.56
1:A:29:GLN:HG3	1:A:43:PRO:HB3	1.87	0.56
1:C:83:GLY:HA3	1:C:88:GLU:OE2	2.06	0.55
1:D:25:GLN:HG2	1:D:190:TRP:CZ3	2.42	0.55
1:C:319:VAL:HA	1:C:325:GLN:OE1	2.06	0.55
1:C:118:ARG:NH1	1:C:242:PRO:HG2	2.22	0.55
1:A:118:ARG:HD3	1:A:126:VAL:HG11	1.89	0.54
1:D:33:VAL:HG12	1:D:170:LEU:HD22	1.89	0.54
1:D:25:GLN:NE2	1:D:25:GLN:HA	2.23	0.54
1:D:370:ASP:O	1:D:373:VAL:HG12	2.07	0.54
1:C:45:LEU:HB3	1:C:54:ASP:OD2	2.08	0.54
1:A:89:VAL:HG12	1:A:92:LEU:HD12	1.90	0.54
1:B:25:GLN:NE2	1:B:25:GLN:HA	2.23	0.54
1:B:217:GLY:O	1:B:356:ARG:HD3	2.07	0.54
1:D:169:ILE:HG23	1:D:170:LEU:HG	1.90	0.54
1:A:392:HIS:CD2	1:A:393:LEU:HG	2.43	0.53
1:C:169:ILE:HG23	1:C:170:LEU:HG	1.90	0.53
1:C:208:PHE:CZ	1:C:210:GLU:HB2	2.44	0.53
1:C:256:ASN:OD1	1:C:326:ARG:NH2	2.42	0.53
1:C:118:ARG:HH12	1:C:242:PRO:CG	2.20	0.53
1:B:118:ARG:NE	1:B:119:GLY:H	2.07	0.52
1:C:217:GLY:O	1:C:356:ARG:HD3	2.10	0.52
1:C:164:ARG:HG3	1:C:178:GLN:HG3	1.90	0.52
3:P:1:NAG:H83	3:P:1:NAG:H3	1.91	0.52
1:A:40:MET:HE2	1:A:97:ARG:HE	1.74	0.52
1:C:25:GLN:HG3	1:C:26:PHE:N	2.24	0.51
1:D:222:THR:OG1	1:D:452:MET:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD12	1:A:136:LEU:HD22	1.92	0.50
1:A:217:GLY:O	1:A:356:ARG:HD3	2.12	0.50
1:B:208:PHE:CZ	1:B:210:GLU:HB2	2.47	0.50
1:C:295:ASP:O	1:C:299:LEU:HB2	2.11	0.50
1:C:467:GLN:HE21	1:C:467:GLN:HA	1.76	0.49
1:C:107:GLY:C	1:C:109:ASN:H	2.21	0.49
1:D:160:VAL:HG11	6:T:1:NAG:H82	1.94	0.49
1:D:217:GLY:O	1:D:356:ARG:HD3	2.11	0.49
1:D:342:PHE:HB3	1:D:424:THR:HG23	1.94	0.49
1:C:118:ARG:HH12	1:C:242:PRO:HG2	1.77	0.49
1:D:343:ASP:O	1:D:424:THR:OG1	2.31	0.49
4:H:2:NAG:H82	4:H:2:NAG:O3	2.12	0.49
1:A:291:ASP:OD1	1:A:393:LEU:HD11	2.13	0.49
1:D:417:ARG:NH1	10:D:603:HOH:O	2.34	0.48
4:H:1:NAG:H61	4:H:2:NAG:O5	2.14	0.48
1:B:68:VAL:HG11	1:B:91:PRO:HD2	1.96	0.47
2:J:1:NAG:H62	2:J:3:FUC:O2	2.14	0.47
1:A:25:GLN:OE1	1:A:25:GLN:HA	2.13	0.47
1:A:291:ASP:CG	1:A:393:LEU:HD11	2.39	0.47
1:B:78:GLN:NE2	10:B:610:HOH:O	2.47	0.47
1:B:80:PRO:HG2	1:B:81:HIS:CE1	2.50	0.47
1:B:78:GLN:O	1:B:80:PRO:HD3	2.15	0.47
1:C:230:ARG:O	1:C:230:ARG:HD3	2.15	0.47
1:A:166:SER:HA	1:A:169:ILE:HB	1.96	0.47
1:A:392:HIS:NE2	1:A:393:LEU:HG	2.30	0.47
9:C:504:NAG:H83	9:C:504:NAG:H3	1.96	0.46
1:D:25:GLN:HB3	1:D:26:PHE:H	1.47	0.46
1:C:327:LEU:HD21	1:C:383:PHE:CD2	2.51	0.46
1:B:331:GLN:H	1:B:331:GLN:CD	2.24	0.46
1:A:224:HIS:CD2	1:A:404:HIS:CE1	3.04	0.45
1:D:224:HIS:CD2	1:D:404:HIS:CE1	3.05	0.45
1:C:166:SER:HA	1:C:169:ILE:HB	1.99	0.45
1:A:448:THR:OG1	1:A:451:GLU:HG3	2.17	0.45
1:B:25:GLN:HG2	1:B:190:TRP:CZ3	2.52	0.45
1:B:41:CYS:HB3	1:B:444:TRP:CZ2	2.52	0.44
1:B:25:GLN:HG3	1:B:162:ALA:H	1.82	0.44
1:D:116:GLY:HA3	1:D:125:ARG:HH12	1.82	0.44
1:A:31:ALA:HB1	1:A:179:PHE:CD2	2.53	0.43
1:C:108:HIS:HA	1:C:445:PRO:HG3	1.99	0.43
1:D:312:ARG:O	10:D:601:HOH:O	2.20	0.43
2:O:2:NAG:H83	2:O:2:NAG:H3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PHE:HE2	1:D:266:MET:HE1	1.83	0.43
1:C:203:VAL:O	1:C:203:VAL:HG13	2.18	0.43
1:C:60:SER:OG	1:C:62:ARG:HG3	2.18	0.42
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.76	0.42
1:A:54:ASP:OD1	1:A:59:SER:OG	2.21	0.42
1:C:41:CYS:HB3	1:C:444:TRP:CZ2	2.54	0.42
1:D:323:MET:HE3	1:D:374:ARG:HB2	2.02	0.42
1:B:347:PHE:CG	1:B:426:PRO:HG3	2.55	0.42
1:B:143:HIS:NE2	1:B:241:GLU:OE1	2.53	0.42
1:C:321:ARG:O	1:C:323:MET:N	2.53	0.42
1:C:78:GLN:O	1:C:80:PRO:HD3	2.20	0.42
1:C:276:LEU:HD21	1:C:312:ARG:NH1	2.33	0.42
1:C:25:GLN:HA	1:C:25:GLN:OE1	2.18	0.42
1:D:60:SER:OG	1:D:62:ARG:HG3	2.20	0.42
1:C:142:ASN:O	1:C:146:ARG:HG3	2.20	0.42
1:D:25:GLN:HA	1:D:25:GLN:HE21	1.85	0.42
1:A:33:VAL:HG22	1:A:170:LEU:HD22	2.02	0.41
1:C:86:ASP:HB3	1:C:94:PHE:CE2	2.55	0.41
1:C:189:VAL:HG11	1:C:289:VAL:HG23	2.02	0.41
1:D:90:TRP:HA	1:D:91:PRO:HA	1.83	0.41
1:C:133:LEU:HD12	1:C:133:LEU:HA	1.89	0.41
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.89	0.41
1:C:276:LEU:HD21	1:C:312:ARG:CZ	2.50	0.41
1:B:89:VAL:HG12	1:B:92:LEU:HD12	2.03	0.41
1:C:364:ASP:O	1:C:366:THR:N	2.54	0.41
4:R:1:NAG:O4	4:R:2:NAG:O5	2.31	0.41
1:A:98:THR:HG22	1:A:444:TRP:CH2	2.56	0.41
1:C:80:PRO:HG2	1:C:81:HIS:CE1	2.55	0.41
1:B:25:GLN:HB3	1:B:26:PHE:H	1.58	0.41
1:C:441:VAL:HA	1:C:442:PRO:HA	1.93	0.41
1:A:33:VAL:O	1:A:37:ARG:HG3	2.20	0.41
1:C:107:GLY:C	1:C:109:ASN:N	2.79	0.41
1:B:25:GLN:HG2	1:B:190:TRP:CH2	2.56	0.40
1:D:40:MET:HE2	1:D:42:CYS:HB2	2.02	0.40
1:D:208:PHE:CZ	1:D:210:GLU:HB2	2.57	0.40
1:C:350:ASN:HA	1:C:369:TYR:CE1	2.56	0.40
1:A:68:VAL:HG22	1:A:98:THR:HG23	2.02	0.40
2:S:1:NAG:O4	2:S:2:NAG:O7	2.40	0.40

There are no symmetry-related clashes.

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%)	424 (96%)	20 (4%)	0	100	100
1	B	444/446 (100%)	423 (95%)	19 (4%)	2 (0%)	24	27
1	C	444/446 (100%)	417 (94%)	27 (6%)	0	100	100
1	D	444/446 (100%)	426 (96%)	17 (4%)	1 (0%)	43	52
All	All	1776/1784 (100%)	1690 (95%)	83 (5%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	PRO
1	B	51	PRO
1	D	376	LEU

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%)	394 (100%)	1 (0%)	86	92
1	C	395/395 (100%)	394 (100%)	1 (0%)	86	92
1	D	395/395 (100%)	394 (100%)	1 (0%)	86	92
All	All	1580/1580 (100%)	1577 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	THR
1	C	47	PRO
1	D	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	B	78	GLN
1	B	178	GLN
1	B	285	GLN
1	B	325	GLN
1	B	390	GLN
1	C	100	HIS
1	C	353	ASN
1	C	392	HIS
1	C	437	GLN
1	C	467	GLN
1	D	175	ASN
1	D	178	GLN
1	D	331	GLN
1	D	353	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

52 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	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.41	0
2	FUC	E	3	2	10,10,11	0.82	0	14,14,16	1.21	2 (14%)
3	NAG	F	1	1,3	14,14,15	2.25	3 (21%)	17,19,21	1.29	2 (11%)
3	FUC	F	2	3	10,10,11	1.08	1 (10%)	14,14,16	1.15	1 (7%)
4	NAG	G	1	4,1	14,14,15	0.36	0	17,19,21	0.76	0
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	H	1	4,1	14,14,15	0.43	0	17,19,21	0.72	1 (5%)
4	NAG	H	2	4	14,14,15	1.58	2 (14%)	17,19,21	1.19	2 (11%)
4	NAG	I	1	4,1	14,14,15	0.28	0	17,19,21	0.65	0
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.41	0
2	NAG	J	1	2,1	14,14,15	1.18	1 (7%)	17,19,21	0.94	1 (5%)
2	NAG	J	2	2	14,14,15	0.38	0	17,19,21	0.68	0
2	FUC	J	3	2	10,10,11	1.66	2 (20%)	14,14,16	1.33	1 (7%)
3	NAG	K	1	1,3	14,14,15	1.36	2 (14%)	17,19,21	0.89	2 (11%)
3	FUC	K	2	3	10,10,11	1.01	1 (10%)	14,14,16	1.03	2 (14%)
4	NAG	L	1	4,1	14,14,15	0.85	2 (14%)	17,19,21	1.74	1 (5%)
4	NAG	L	2	4	14,14,15	0.51	0	17,19,21	0.59	0
5	NAG	M	1	5,1	14,14,15	0.81	1 (7%)	17,19,21	0.81	0
5	NAG	M	2	5	14,14,15	0.69	0	17,19,21	0.69	0
5	MAN	M	3	5	11,11,12	1.41	1 (9%)	15,15,17	1.56	2 (13%)
5	MAN	M	4	5	11,11,12	1.27	1 (9%)	15,15,17	1.82	5 (33%)
5	MAN	M	5	5	11,11,12	1.48	2 (18%)	15,15,17	2.20	3 (20%)
5	FUC	M	6	5	10,10,11	1.07	2 (20%)	14,14,16	1.08	1 (7%)
4	NAG	N	1	4,1	14,14,15	0.53	0	17,19,21	0.53	0
4	NAG	N	2	4	14,14,15	0.52	0	17,19,21	1.11	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.26	0	17,19,21	0.96	1 (5%)
2	NAG	O	2	2	14,14,15	0.43	0	17,19,21	1.54	2 (11%)
2	FUC	O	3	2	10,10,11	1.86	3 (30%)	14,14,16	1.18	1 (7%)
3	NAG	P	1	1,3	14,14,15	0.72	0	17,19,21	1.44	2 (11%)
3	FUC	P	2	3	10,10,11	1.39	1 (10%)	14,14,16	1.22	1 (7%)
4	NAG	Q	1	4,1	14,14,15	0.55	0	17,19,21	0.48	0
4	NAG	Q	2	4	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	R	1	4,1	14,14,15	0.63	0	17,19,21	1.16	3 (17%)
4	NAG	R	2	4	14,14,15	0.59	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	S	1	2,1	14,14,15	0.47	0	17,19,21	0.94	0
2	NAG	S	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	FUC	S	3	2	10,10,11	1.17	0	14,14,16	1.62	4 (28%)
6	NAG	T	1	6,1	14,14,15	0.54	0	17,19,21	0.54	0
6	NAG	T	2	6	14,14,15	0.76	1 (7%)	17,19,21	0.67	1 (5%)
6	MAN	T	3	6	11,11,12	0.86	0	15,15,17	0.90	1 (6%)
6	MAN	T	4	6	11,11,12	0.85	0	15,15,17	1.31	1 (6%)
6	FUC	T	5	6	10,10,11	1.29	1 (10%)	14,14,16	1.85	2 (14%)
4	NAG	U	1	4,1	14,14,15	0.60	0	17,19,21	0.74	0
4	NAG	U	2	4	14,14,15	0.33	0	17,19,21	0.48	0
7	NAG	V	1	7,1	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
7	NAG	V	2	7	14,14,15	0.58	1 (7%)	17,19,21	0.71	0
7	MAN	V	3	7	11,11,12	1.29	2 (18%)	15,15,17	1.07	1 (6%)
7	MAN	V	4	7	11,11,12	1.17	1 (9%)	15,15,17	1.38	2 (13%)
7	MAN	V	5	7	11,11,12	1.34	1 (9%)	15,15,17	0.89	0
4	NAG	W	1	4,1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	W	2	4	14,14,15	0.44	0	17,19,21	0.49	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	FUC	J	3	2	-	-	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-6.74	1.32	1.43
4	H	2	NAG	C1-C2	5.04	1.59	1.52
2	J	1	NAG	O5-C1	-4.37	1.36	1.43
3	F	1	NAG	C1-C2	4.30	1.58	1.52
2	J	3	FUC	C1-C2	3.94	1.61	1.52
2	O	3	FUC	O5-C1	-3.89	1.37	1.43
5	M	5	MAN	C2-C3	-3.78	1.46	1.52
7	V	5	MAN	O5-C1	-3.71	1.37	1.43
3	K	1	NAG	O5-C1	-3.71	1.37	1.43
5	M	3	MAN	C2-C3	-3.54	1.47	1.52
3	P	2	FUC	C1-C2	3.47	1.60	1.52
2	O	3	FUC	O5-C5	-3.21	1.37	1.43
5	M	4	MAN	C1-C2	3.05	1.59	1.52
7	V	3	MAN	O5-C1	-2.90	1.38	1.43
3	K	1	NAG	C1-C2	2.88	1.56	1.52
2	E	1	NAG	O5-C1	-2.84	1.38	1.43
5	M	1	NAG	O5-C1	-2.84	1.38	1.43
6	T	5	FUC	O5-C1	-2.75	1.39	1.43
2	J	3	FUC	O2-C2	-2.67	1.37	1.43
7	V	4	MAN	C2-C3	-2.65	1.48	1.52
2	O	3	FUC	C2-C3	2.54	1.56	1.52
3	F	2	FUC	C1-C2	2.39	1.57	1.52
4	H	2	NAG	O5-C1	-2.38	1.39	1.43
3	K	2	FUC	O5-C1	-2.20	1.40	1.43
4	L	1	NAG	C1-C2	-2.18	1.49	1.52
3	F	1	NAG	C3-C2	2.17	1.57	1.52
5	M	6	FUC	C2-C3	2.14	1.55	1.52
4	L	1	NAG	O5-C1	-2.10	1.40	1.43
6	T	2	NAG	O5-C1	-2.10	1.40	1.43
7	V	3	MAN	O4-C4	-2.09	1.37	1.43
5	M	5	MAN	O5-C5	2.09	1.47	1.43
7	V	2	NAG	O5-C1	-2.03	1.40	1.43
5	M	6	FUC	C1-C2	2.02	1.57	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	5	MAN	C1-O5-C5	7.16	121.78	112.19
4	L	1	NAG	C1-O5-C5	6.26	120.58	112.19
2	O	2	NAG	C2-N2-C7	4.98	129.57	122.90
6	T	5	FUC	C1-C2-C3	4.96	116.86	109.64
3	P	1	NAG	C2-N2-C7	4.65	129.13	122.90
7	V	4	MAN	C1-O5-C5	3.91	117.42	112.19
3	F	1	NAG	C4-C3-C2	3.85	116.66	111.02
5	M	3	MAN	O2-C2-C3	-3.83	102.21	110.15
6	T	5	FUC	C2-C3-C4	3.48	116.99	110.86
6	T	4	MAN	C1-O5-C5	3.47	116.84	112.19
5	M	3	MAN	C2-C3-C4	-2.98	105.62	110.86
7	V	3	MAN	O2-C2-C3	-2.96	104.02	110.15
2	J	3	FUC	O2-C2-C1	2.94	115.95	109.22
3	P	2	FUC	O2-C2-C1	2.94	115.95	109.22
5	M	5	MAN	C1-C2-C3	-2.91	105.41	109.64
2	O	3	FUC	C1-C2-C3	2.86	113.81	109.64
3	F	1	NAG	O5-C5-C4	-2.84	103.92	110.83
5	M	4	MAN	C3-C4-C5	-2.83	105.10	110.23
7	V	4	MAN	O2-C2-C3	-2.72	104.51	110.15
4	H	2	NAG	C2-N2-C7	2.71	126.53	122.90
3	K	1	NAG	C4-C3-C2	2.70	114.97	111.02
2	S	3	FUC	O3-C3-C4	-2.68	104.05	110.38
4	H	2	NAG	C4-C3-C2	2.59	114.82	111.02
2	O	2	NAG	C1-C2-N2	2.59	114.51	110.43
5	M	4	MAN	C1-C2-C3	-2.58	105.89	109.64
2	O	1	NAG	C1-O5-C5	2.48	115.51	112.19
7	V	1	NAG	C1-O5-C5	2.47	115.50	112.19
4	R	1	NAG	O3-C3-C2	2.47	114.54	109.40
2	E	3	FUC	C1-O5-C5	2.45	118.75	112.97
5	M	4	MAN	C2-C3-C4	-2.42	106.60	110.86
4	R	1	NAG	C1-C2-N2	2.40	114.21	110.43
5	M	5	MAN	O2-C2-C3	-2.39	105.19	110.15
2	S	3	FUC	C1-C2-C3	2.37	113.09	109.64
5	M	4	MAN	O5-C1-C2	-2.35	105.18	110.79
2	S	3	FUC	C3-C4-C5	2.30	113.31	109.81
4	R	1	NAG	C2-N2-C7	2.29	125.97	122.90
5	M	6	FUC	C1-O5-C5	2.27	118.33	112.97
5	M	4	MAN	O2-C2-C1	2.27	114.42	109.22
3	P	1	NAG	C1-O5-C5	2.21	115.15	112.19
2	J	1	NAG	O4-C4-C3	-2.20	105.18	110.38
2	E	3	FUC	O5-C5-C4	2.16	113.44	109.55
3	K	2	FUC	O2-C2-C1	2.13	114.09	109.22
6	T	2	NAG	O4-C4-C5	-2.11	104.12	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	O5-C5-C4	-2.09	105.75	110.83
3	F	2	FUC	O2-C2-C1	2.08	113.99	109.22
3	K	2	FUC	O5-C5-C4	2.07	113.28	109.55
4	N	2	NAG	C2-N2-C7	2.07	125.67	122.90
4	H	1	NAG	O4-C4-C3	-2.05	105.54	110.38
2	S	3	FUC	O3-C3-C2	-2.03	105.91	110.05
6	T	3	MAN	C1-C2-C3	2.02	112.59	109.64

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	1	NAG	C3-C2-N2-C7
2	S	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	M	3	MAN	O5-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
5	M	5	MAN	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
7	V	5	MAN	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	V	5	MAN	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
6	T	2	NAG	C8-C7-N2-C2
6	T	2	NAG	O7-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
4	R	1	NAG	O5-C5-C6-O6
5	M	3	MAN	C4-C5-C6-O6
6	T	3	MAN	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
7	V	3	MAN	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
2	O	2	NAG	C1-C2-N2-C7
3	P	1	NAG	C1-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	R	2	NAG	C3-C2-N2-C7
6	T	3	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

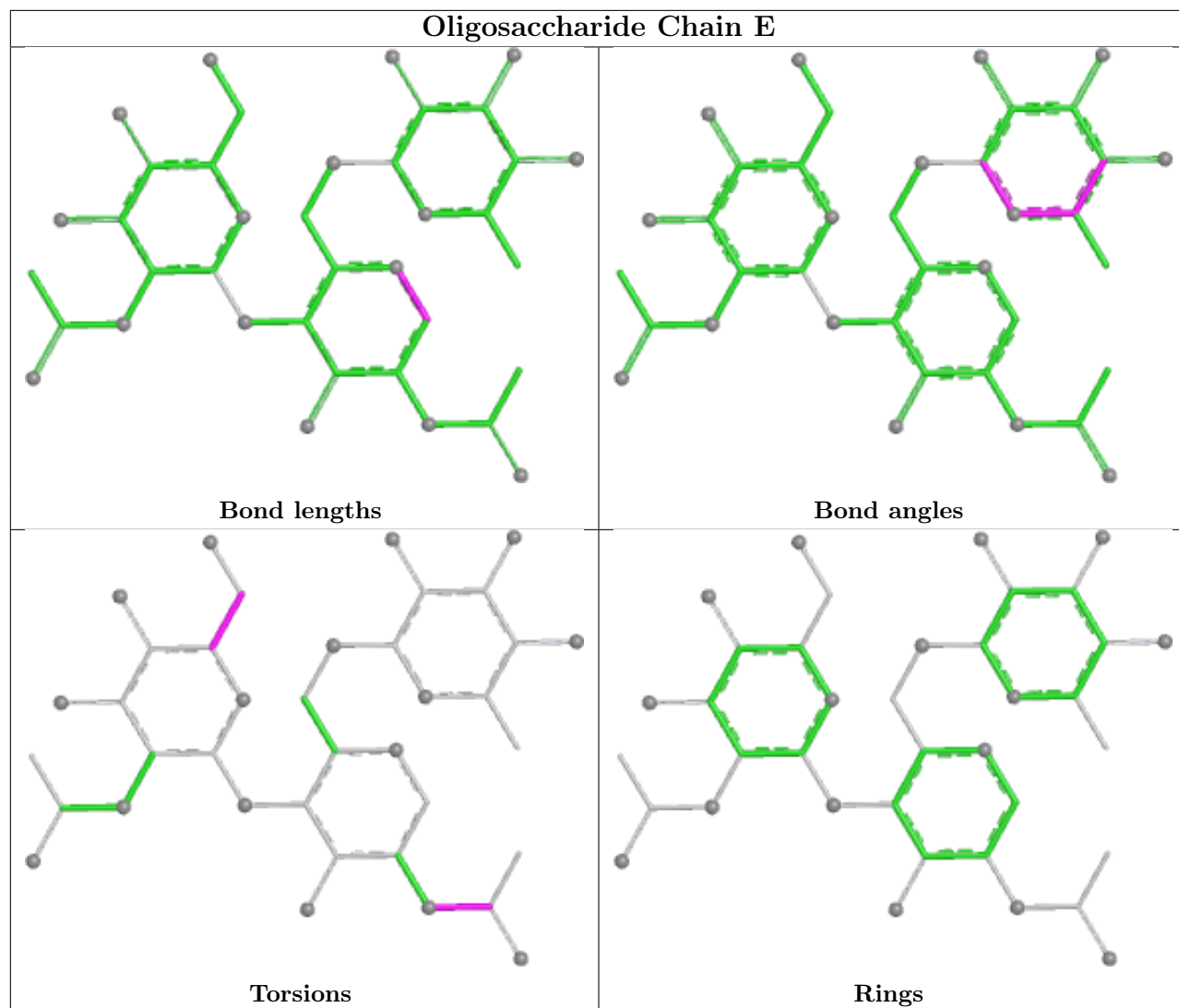
All (2) ring outliers are listed below:

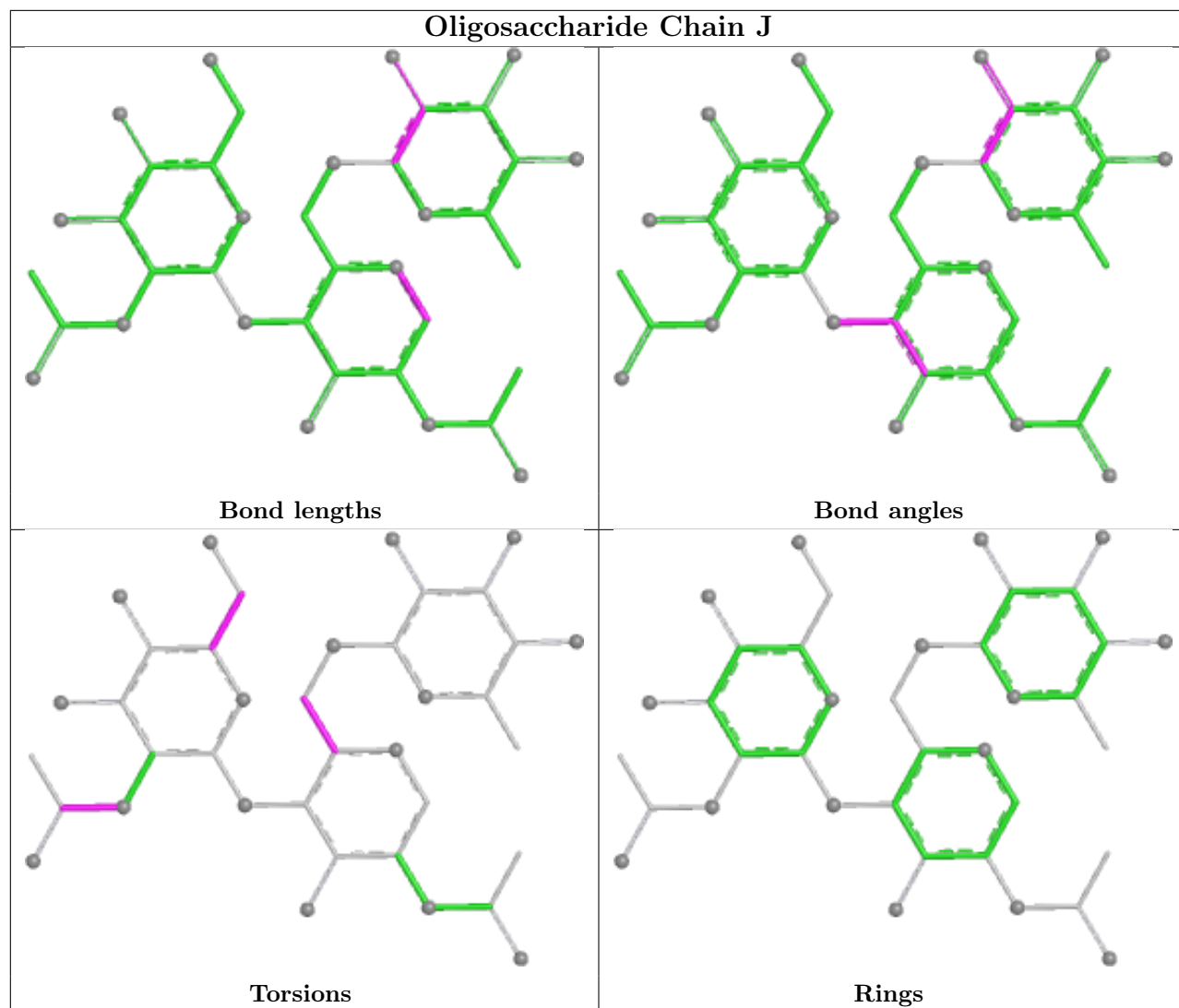
Mol	Chain	Res	Type	Atoms
5	M	3	MAN	C1-C2-C3-C4-C5-O5
5	M	4	MAN	C1-C2-C3-C4-C5-O5

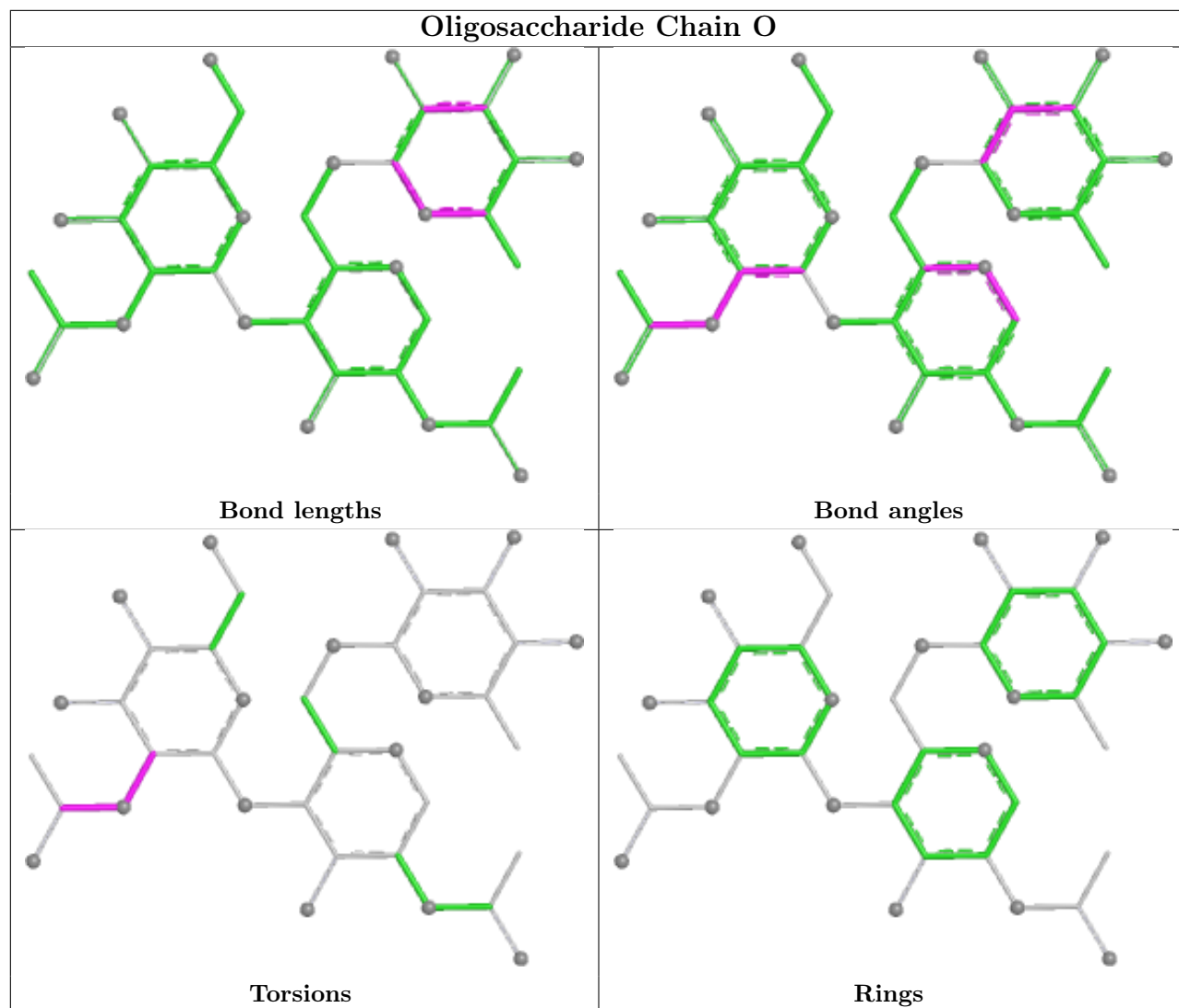
15 monomers are involved in 11 short contacts:

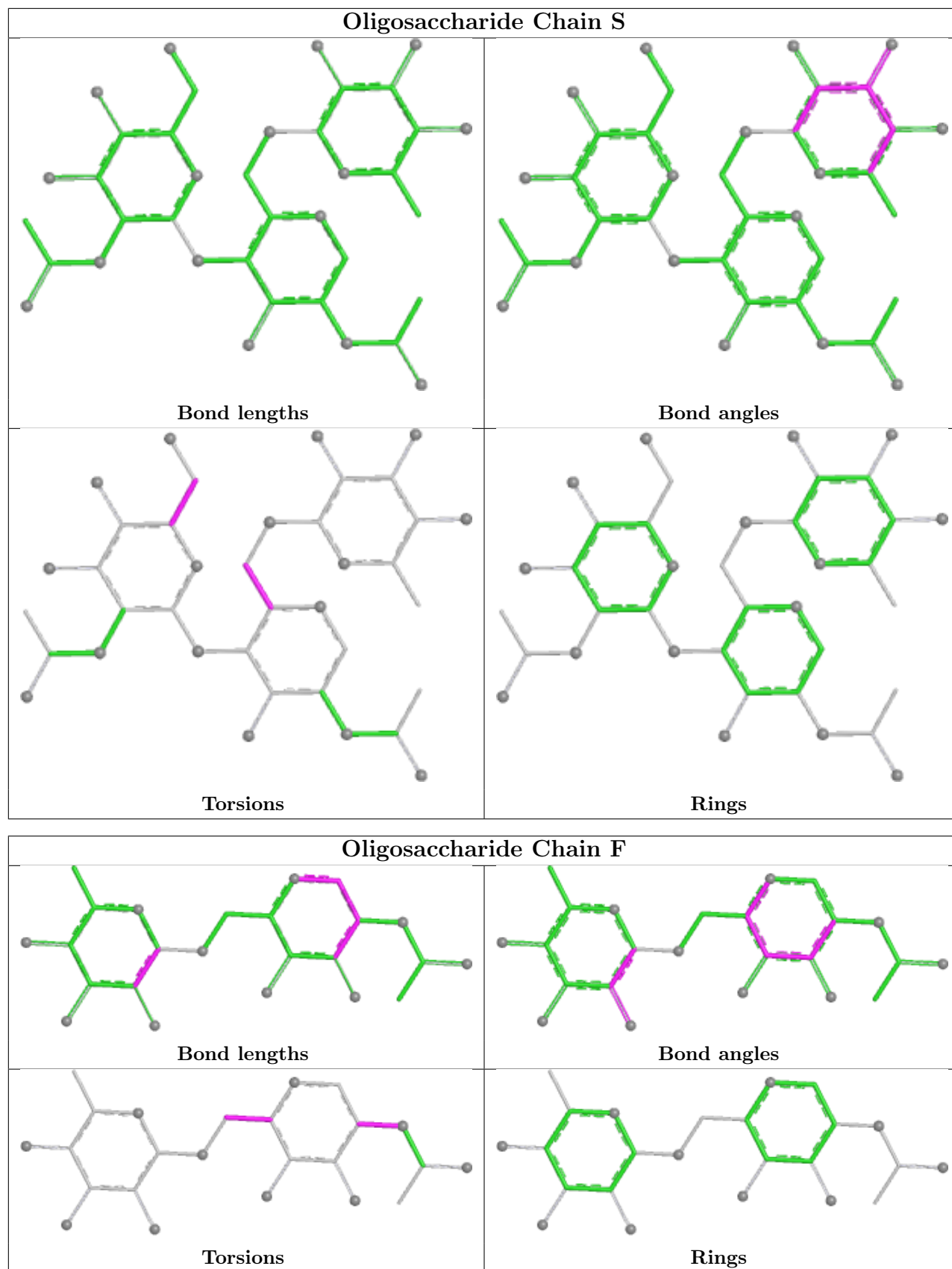
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	3	MAN	1	0
2	S	1	NAG	1	0
2	S	2	NAG	1	0
2	O	1	NAG	1	0
4	R	2	NAG	1	0
4	H	2	NAG	2	0
2	O	2	NAG	2	0
2	J	1	NAG	1	0
2	E	1	NAG	1	0
4	R	1	NAG	1	0
5	M	2	NAG	1	0
6	T	1	NAG	1	0
2	J	3	FUC	1	0
3	P	1	NAG	1	0
4	H	1	NAG	1	0

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

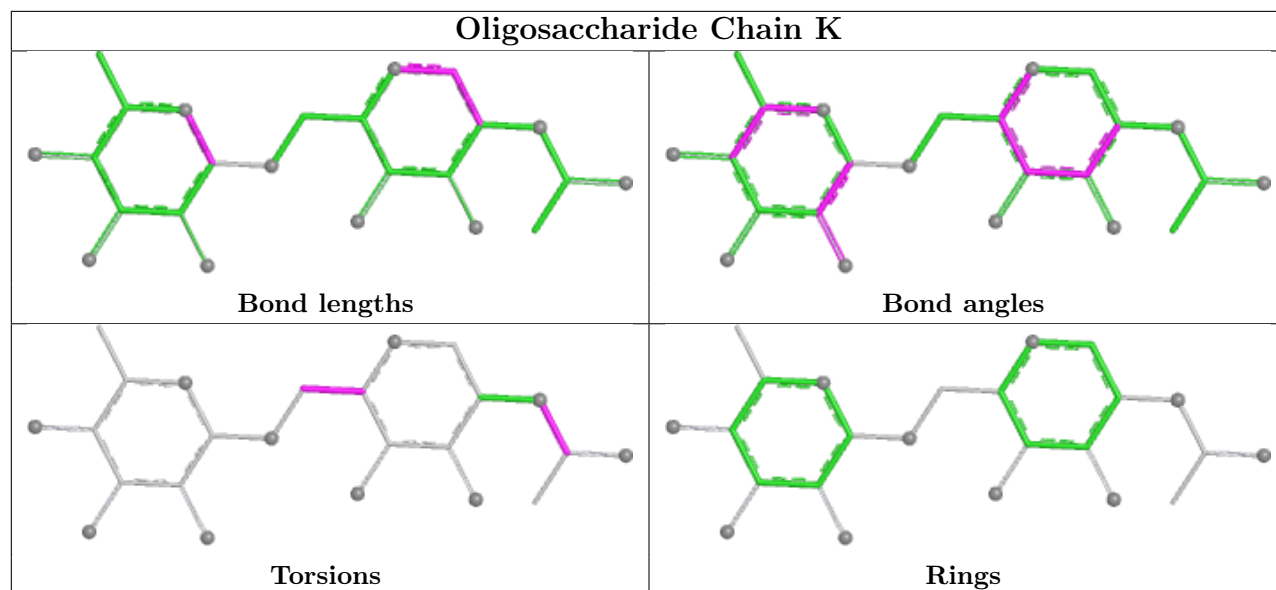




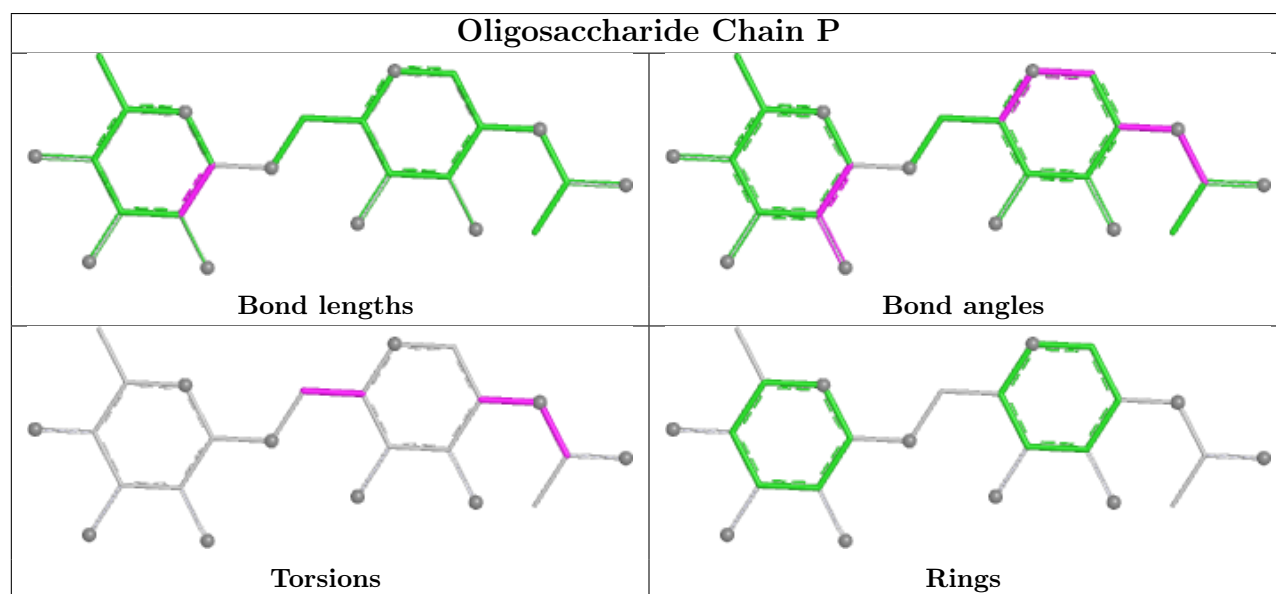


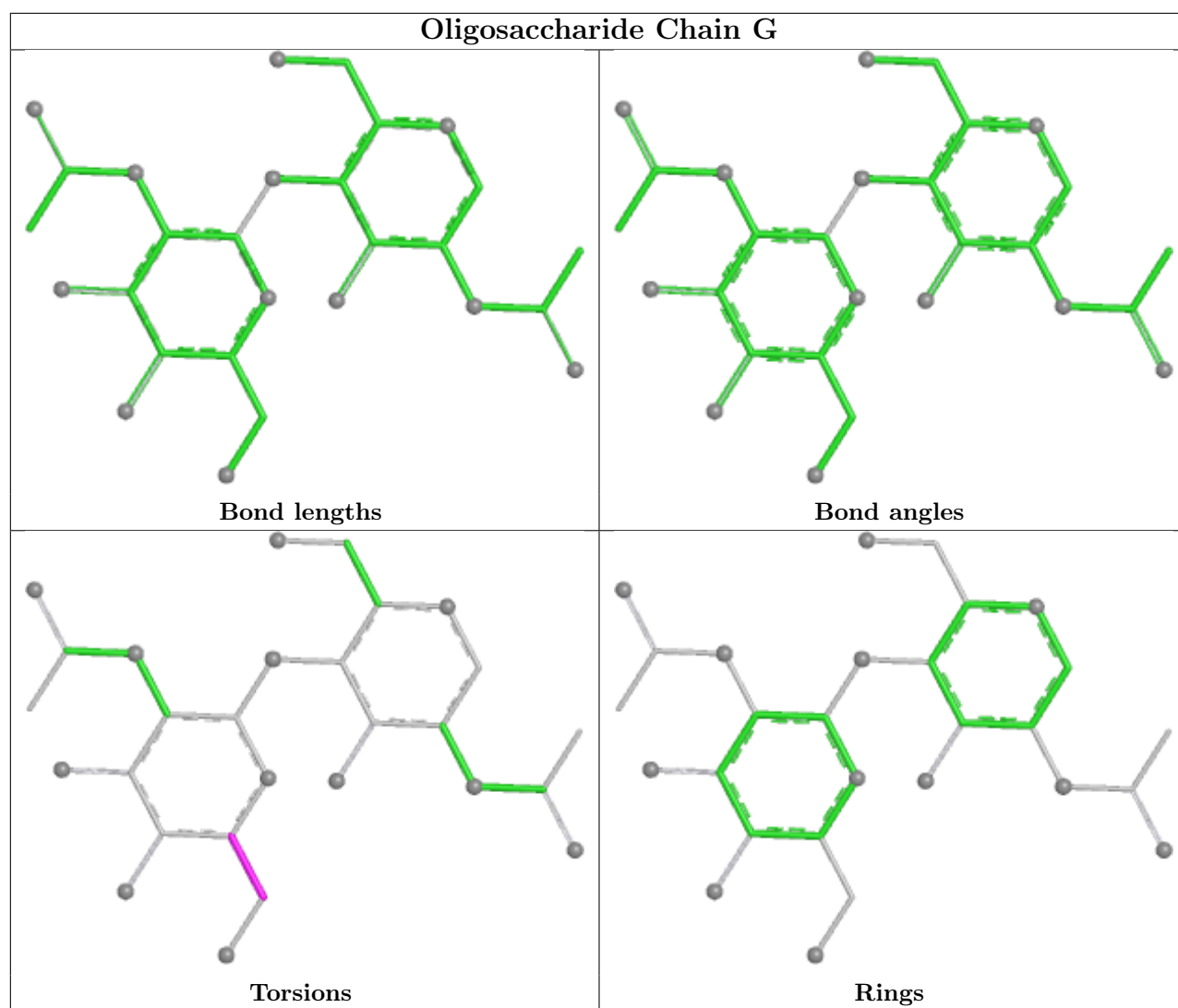


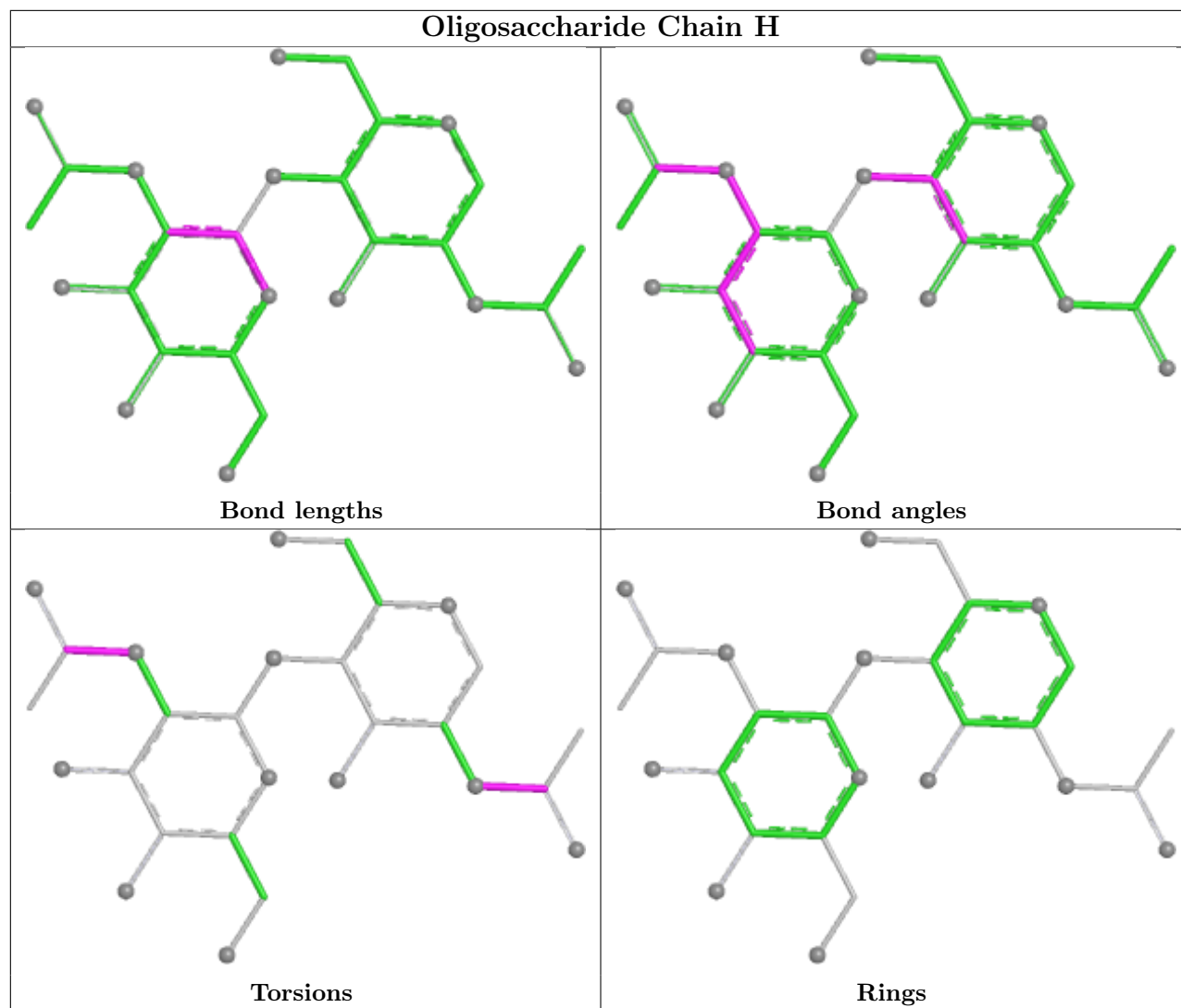
Oligosaccharide Chain K

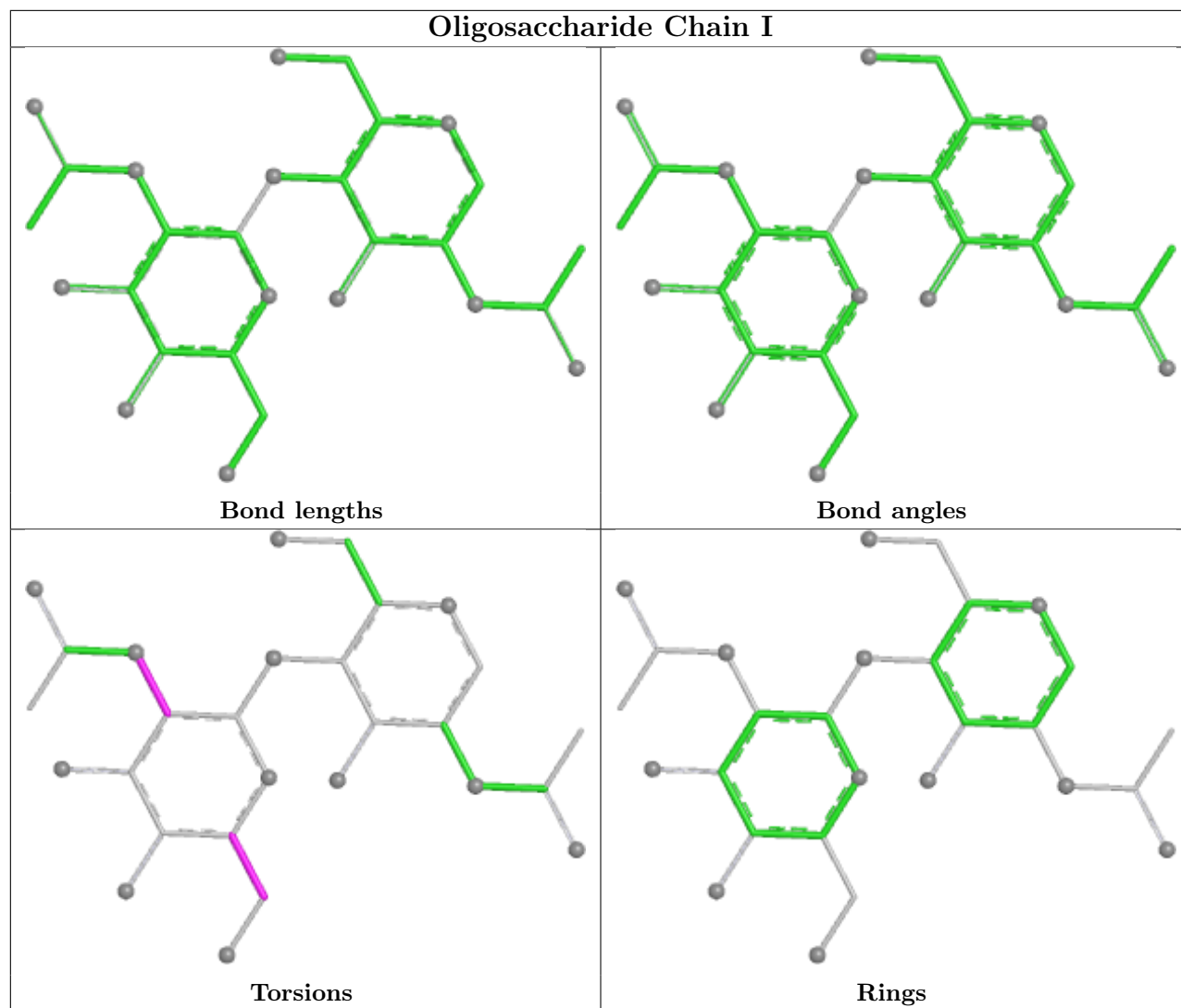


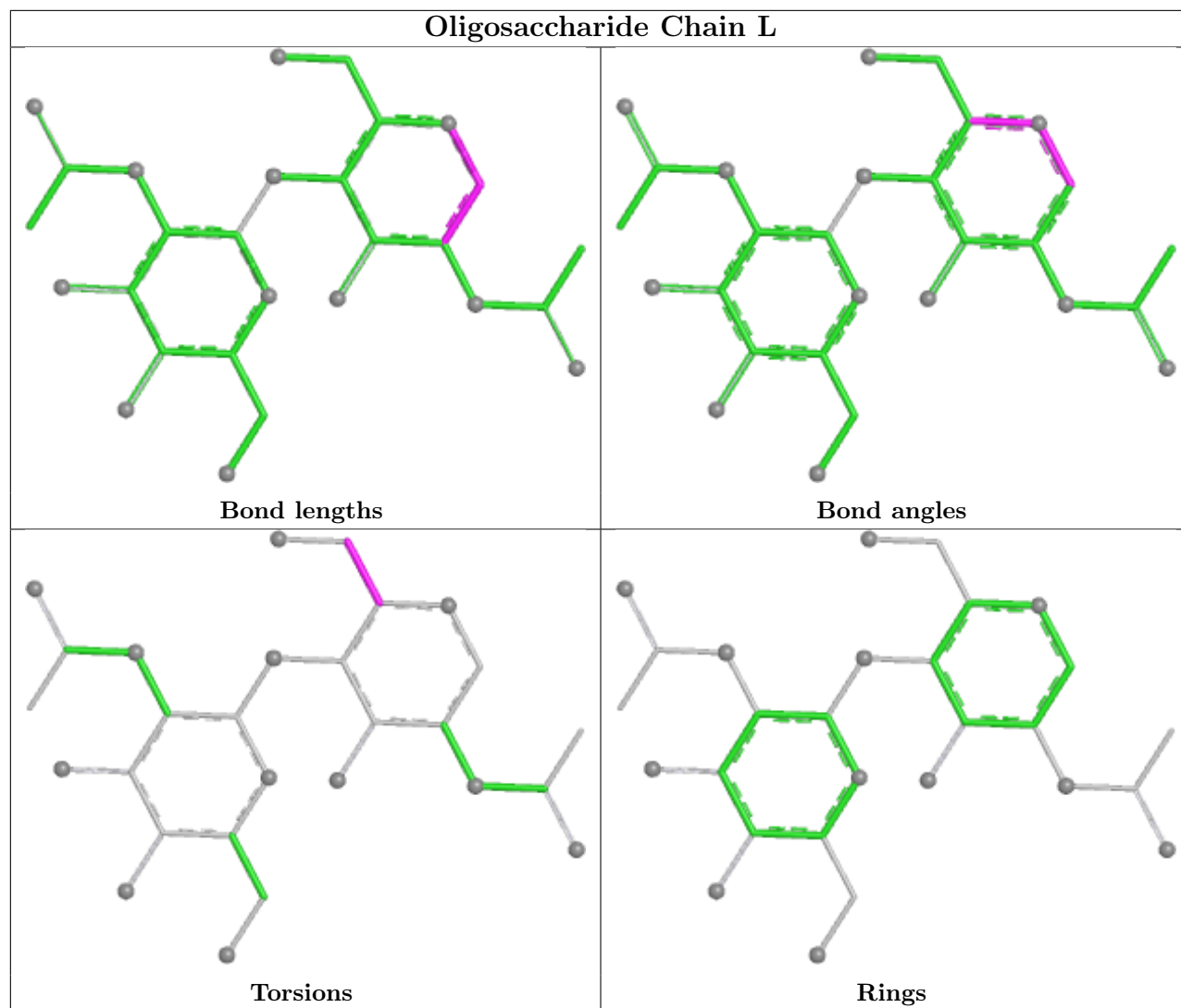
Oligosaccharide Chain P

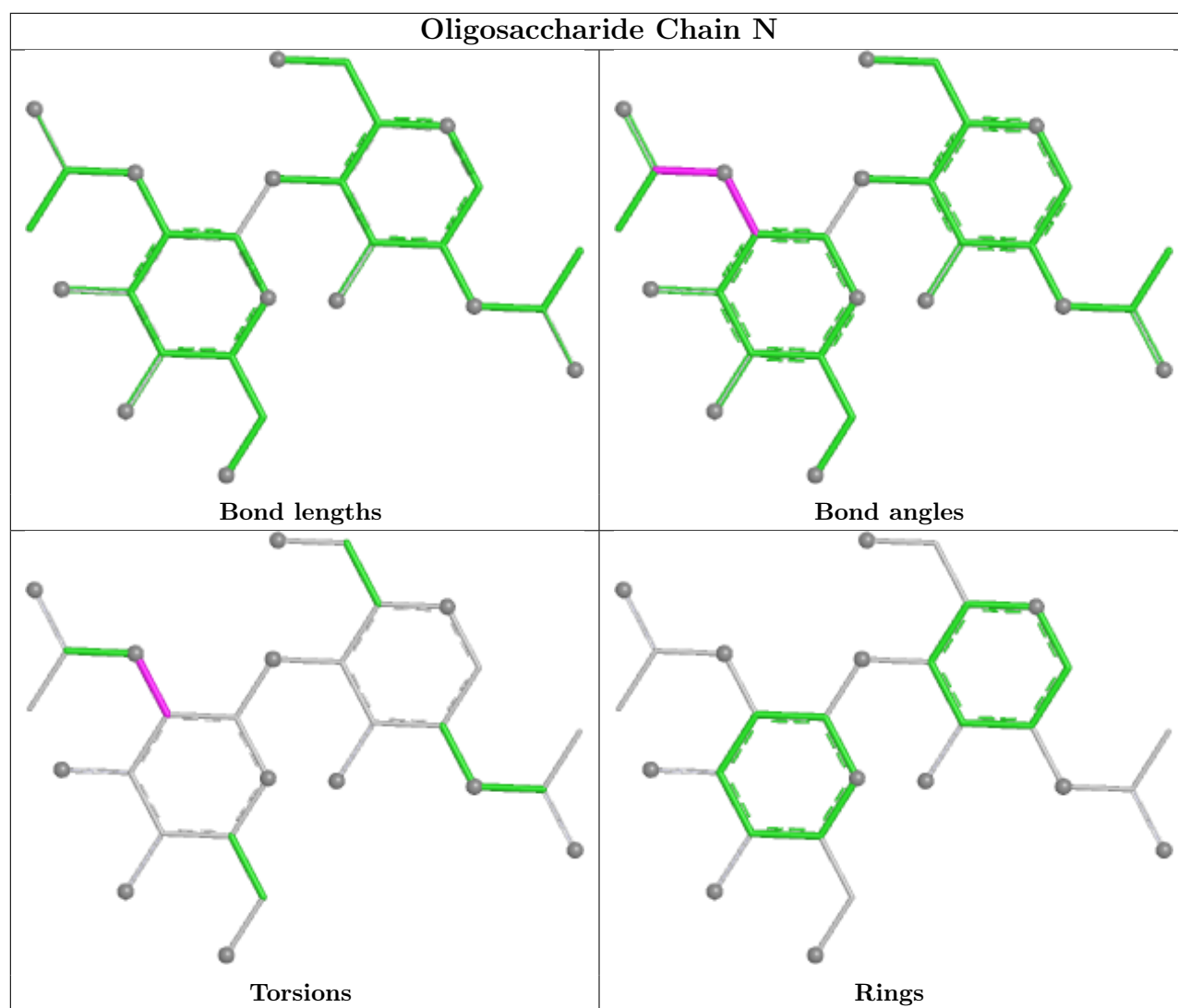


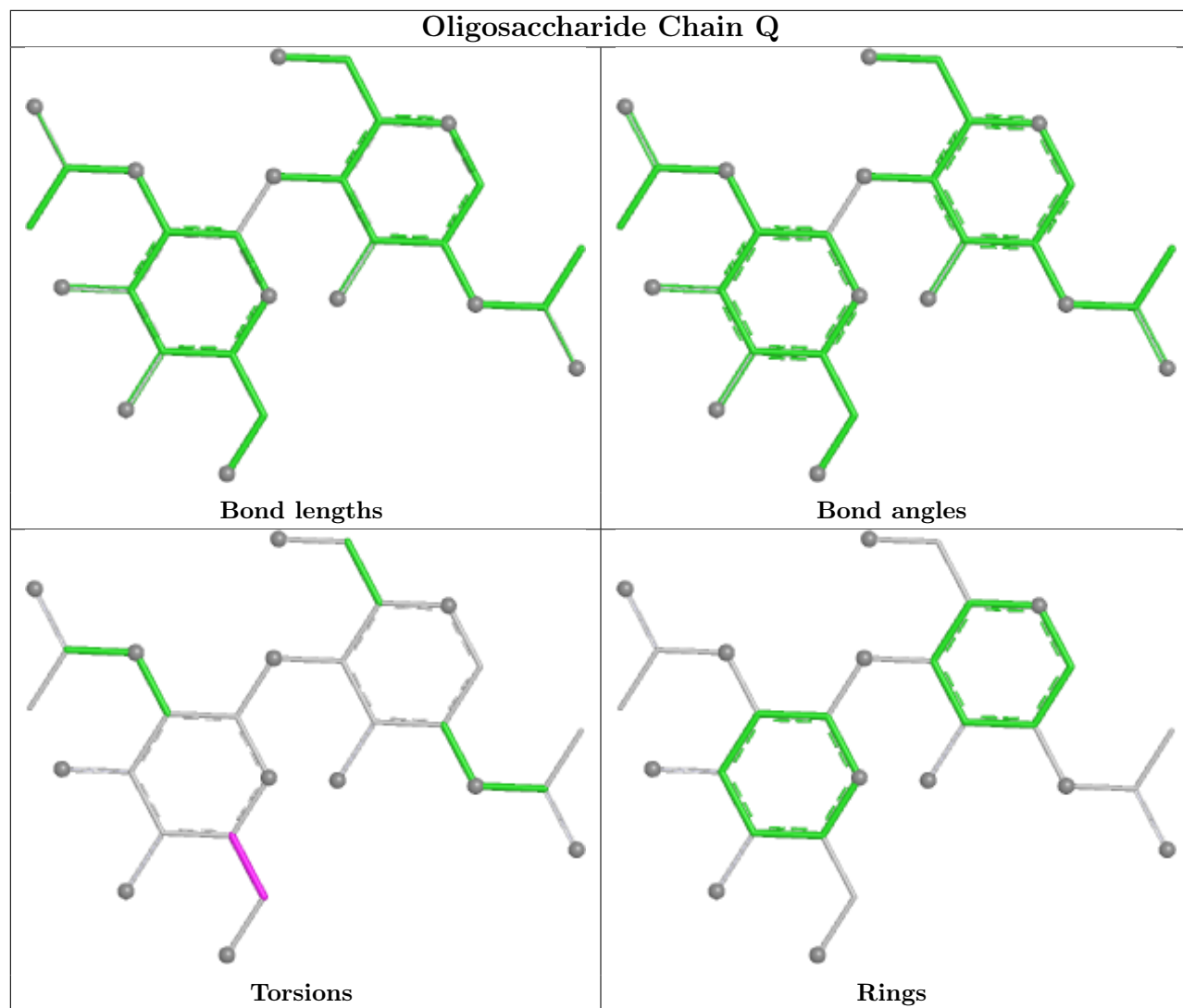


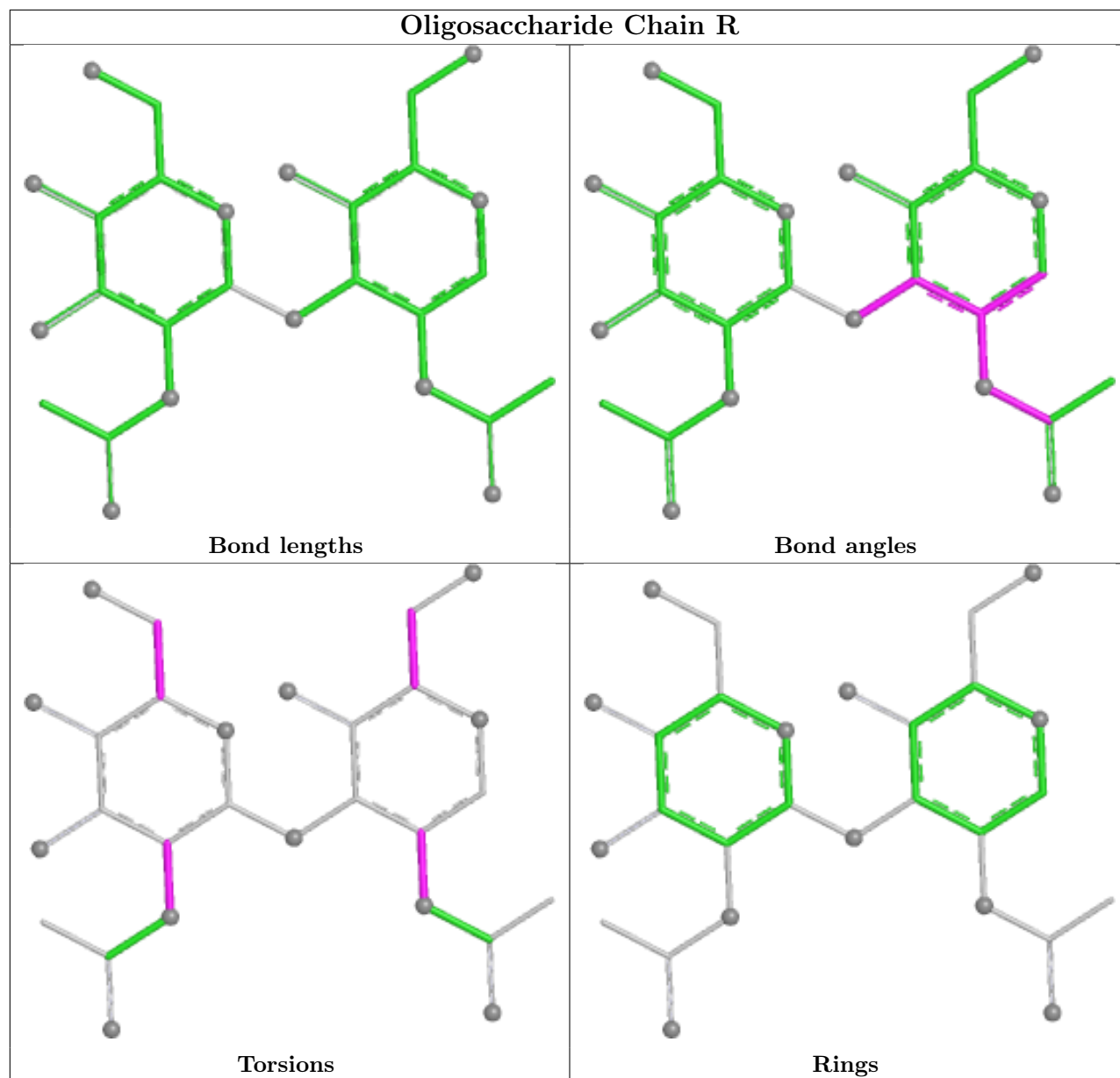


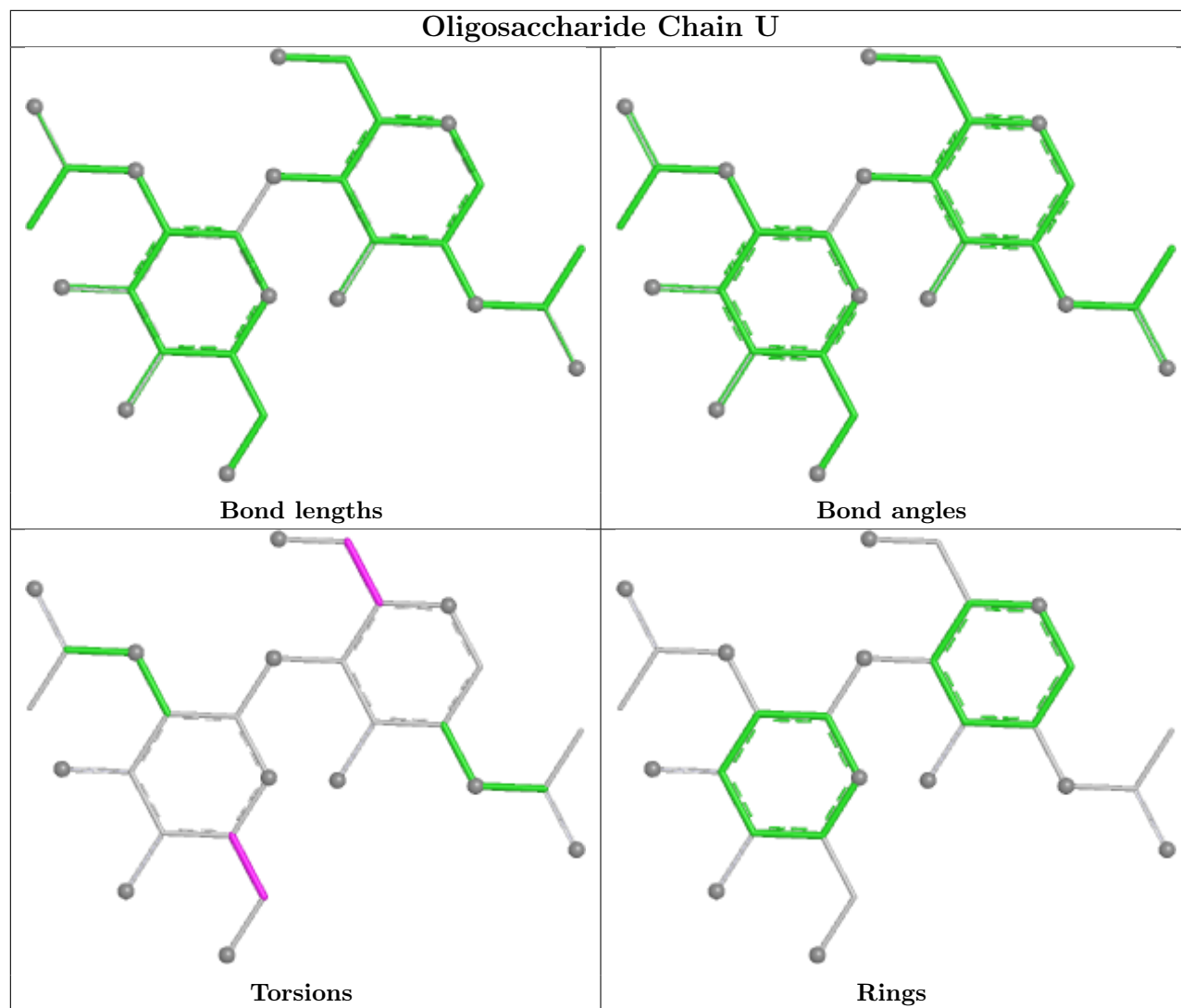


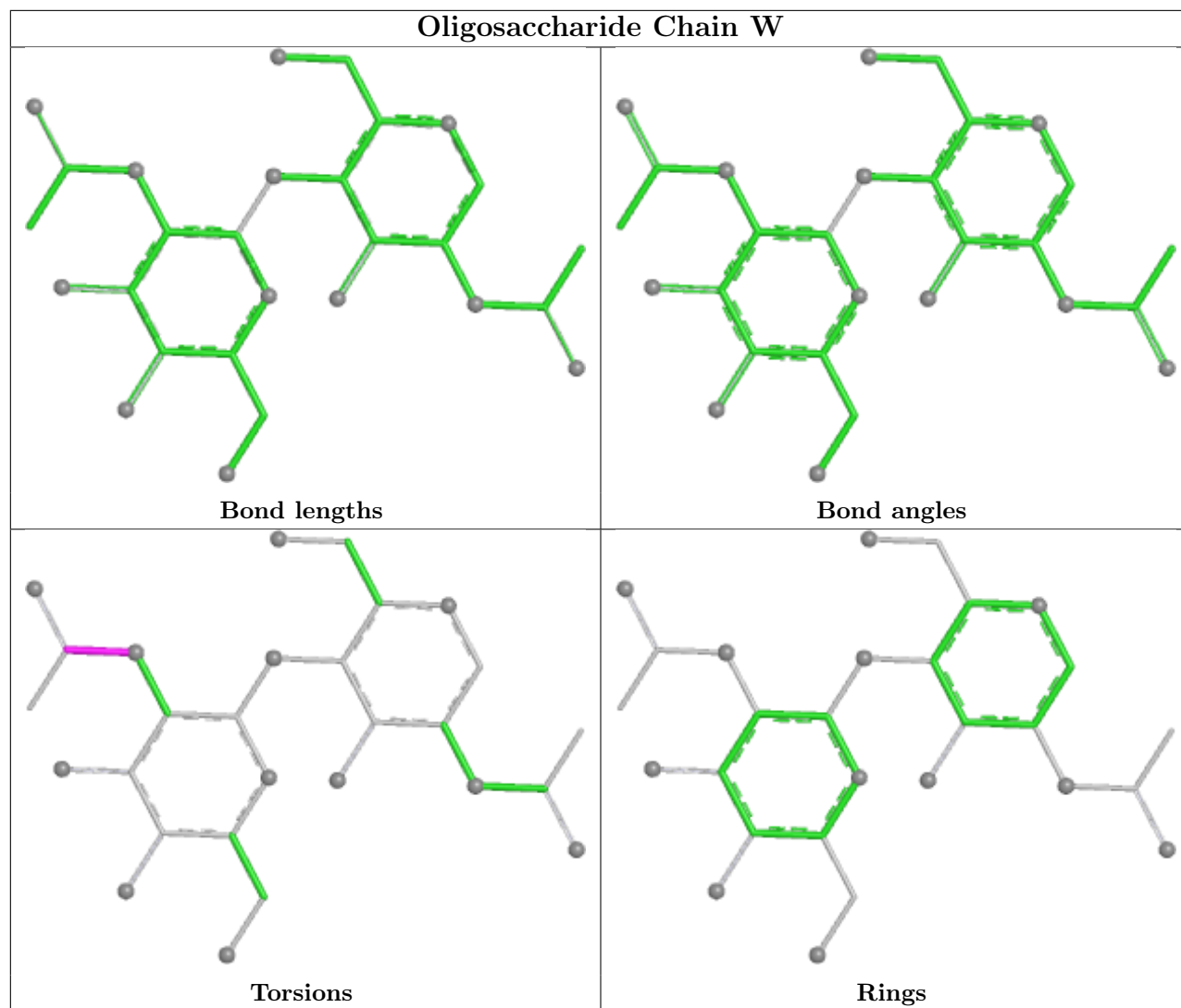


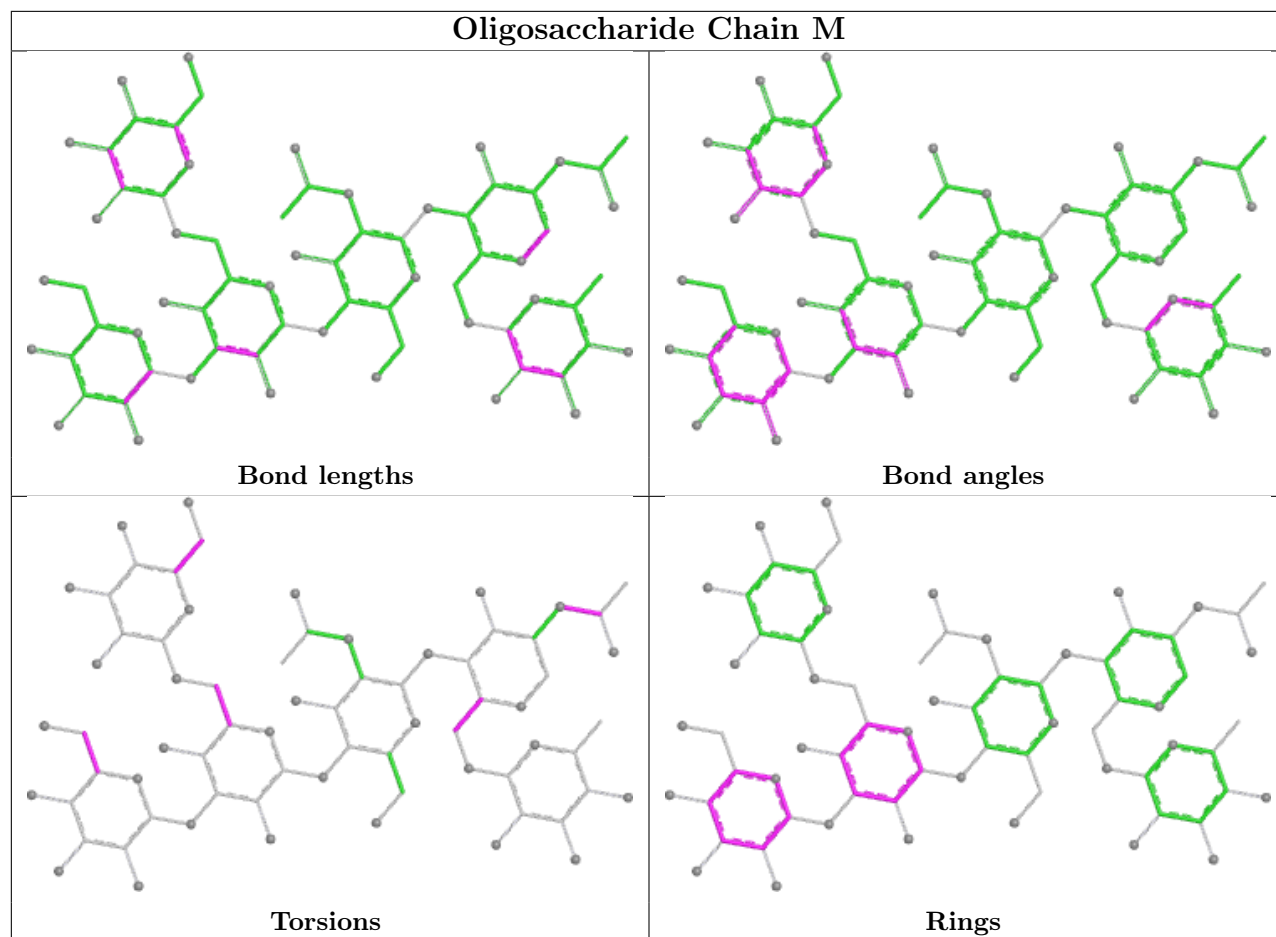


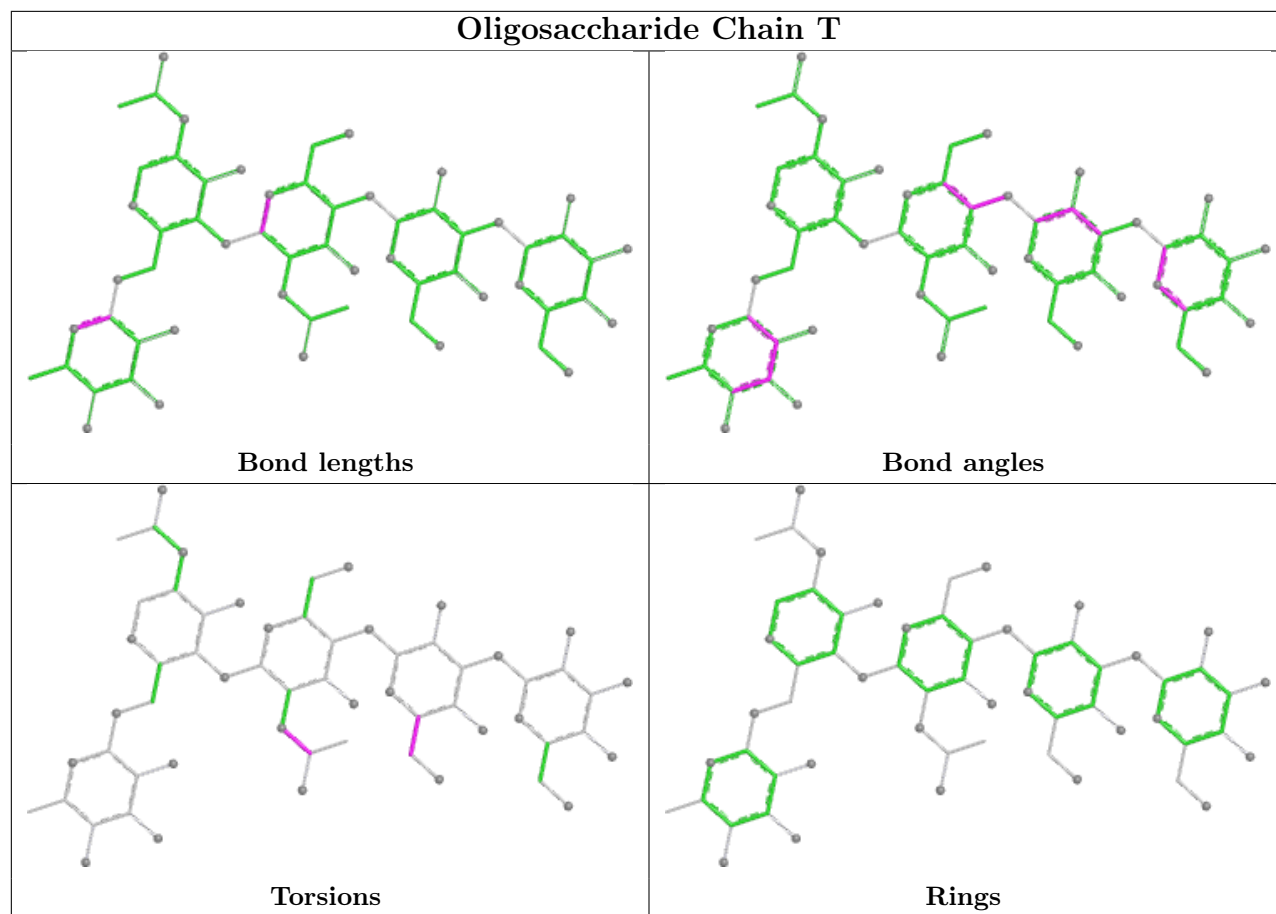


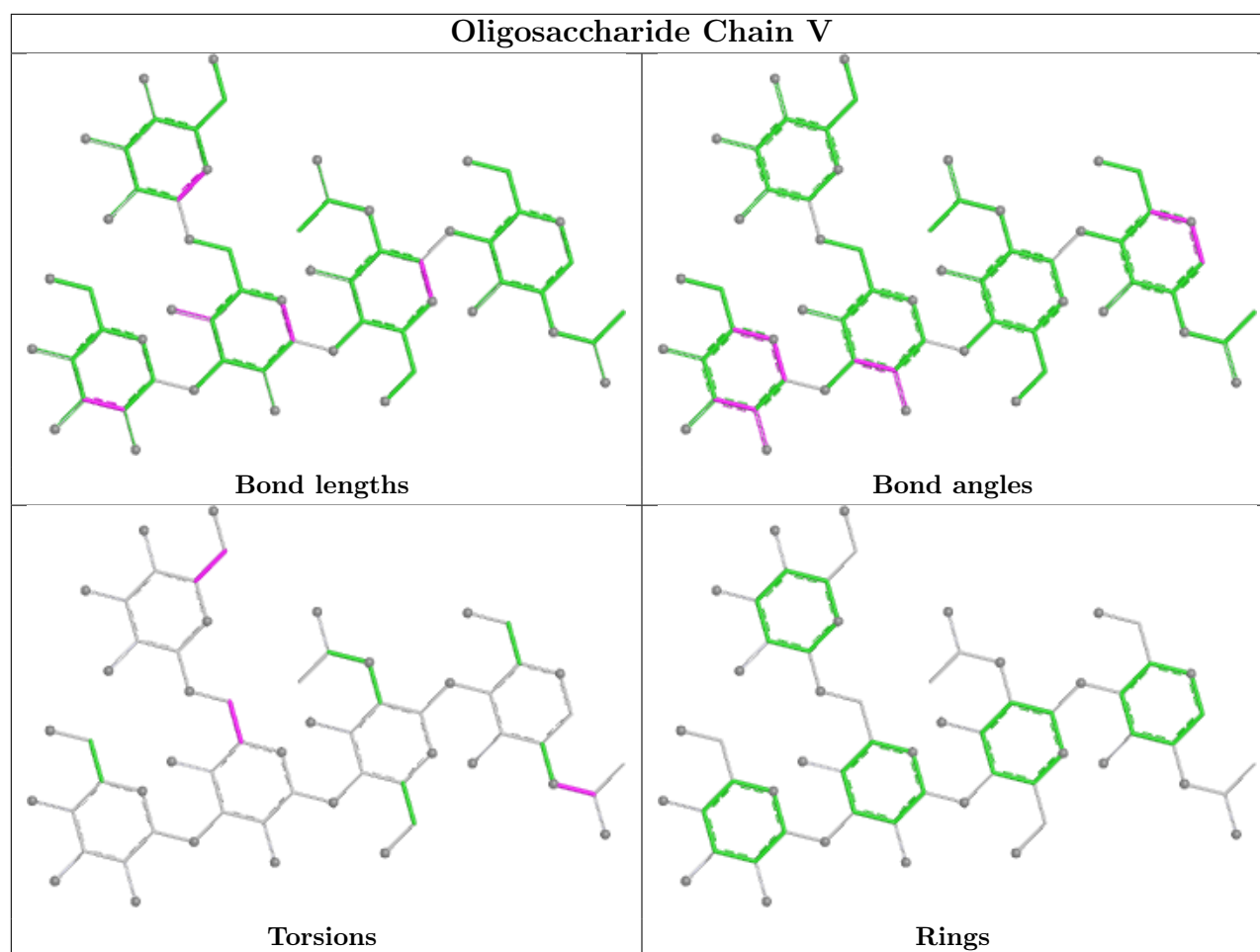












5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z > 2$
9	NAG	C	504	1	14,14,15	0.57	0	17,19,21	1.45	2 (11%)
9	NAG	C	511	1	14,14,15	0.47	0	17,19,21	0.81	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	504	1	-	6/6/23/26	0/1/1/1
9	NAG	C	511	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	504	NAG	C2-N2-C7	4.63	129.10	122.90
9	C	504	NAG	C1-C2-N2	2.52	114.41	110.43
9	C	511	NAG	C1-O5-C5	2.42	115.43	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	504	NAG	O5-C5-C6-O6
9	C	504	NAG	C4-C5-C6-O6
9	C	504	NAG	C8-C7-N2-C2
9	C	504	NAG	O7-C7-N2-C2
9	C	504	NAG	C1-C2-N2-C7
9	C	504	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	504	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.15	3 (0%) 84 87	20, 32, 47, 70	0
1	B	446/446 (100%)	0.08	9 (2%) 65 70	23, 36, 58, 77	0
1	C	446/446 (100%)	0.50	19 (4%) 40 45	28, 45, 68, 81	0
1	D	446/446 (100%)	0.08	4 (0%) 81 84	22, 37, 53, 76	0
All	All	1784/1784 (100%)	0.13	35 (1%) 65 70	20, 37, 61, 81	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	VAL	4.1
1	C	470	SER	4.0
1	D	470	SER	4.0
1	C	319	VAL	3.5
1	B	48	VAL	3.4
1	B	172	PRO	3.4
1	C	203	VAL	3.3
1	B	120	ALA	3.2
1	D	48	VAL	3.1
1	C	47	PRO	3.1
1	C	118	ARG	3.0
1	B	47	PRO	3.0
1	A	470	SER	3.0
1	C	202	GLY	2.8
1	C	323	MET	2.7
1	B	470	SER	2.7
1	B	118	ARG	2.7
1	A	60	SER	2.6
1	C	201	LEU	2.5
1	C	25	GLN	2.5
1	C	51	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	82	ASP	2.4
1	D	60	SER	2.4
1	C	417	ARG	2.4
1	C	373	VAL	2.4
1	B	158	LEU	2.3
1	C	84	ARG	2.3
1	C	298	THR	2.2
1	C	80	PRO	2.2
1	B	25	GLN	2.2
1	B	126	VAL	2.1
1	D	25	GLN	2.1
1	C	170	LEU	2.1
1	A	37	ARG	2.1
1	C	77	PRO	2.0

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
4	NAG	R	2	14/15	0.54	0.22	102,106,112,113	0
4	NAG	H	2	14/15	0.55	0.21	77,87,96,98	0
3	NAG	P	1	14/15	0.59	0.16	62,66,71,71	0
2	NAG	E	2	14/15	0.62	0.18	69,71,76,78	0
6	MAN	T	3	11/12	0.66	0.16	67,69,73,77	0
2	NAG	J	2	14/15	0.67	0.18	61,77,81,90	0
3	NAG	K	1	14/15	0.67	0.14	44,61,65,67	0
3	NAG	F	1	14/15	0.69	0.14	44,55,62,63	0
4	NAG	H	1	14/15	0.70	0.17	55,62,78,85	0
3	FUC	P	2	10/11	0.70	0.18	70,77,79,79	0
5	MAN	M	4	11/12	0.71	0.18	46,51,61,62	0
4	NAG	Q	2	14/15	0.71	0.16	74,79,85,85	0
4	NAG	R	1	14/15	0.72	0.17	71,87,97,97	0
6	FUC	T	5	10/11	0.73	0.15	49,57,66,70	0

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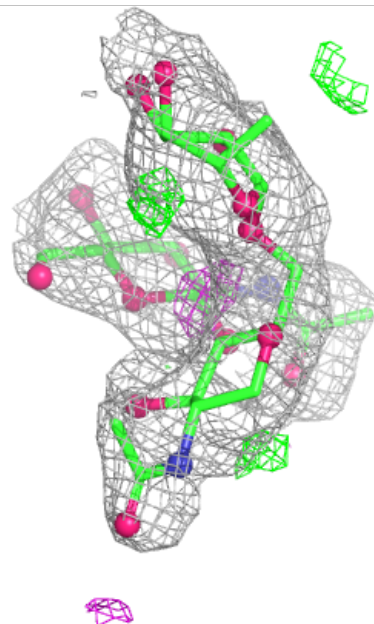
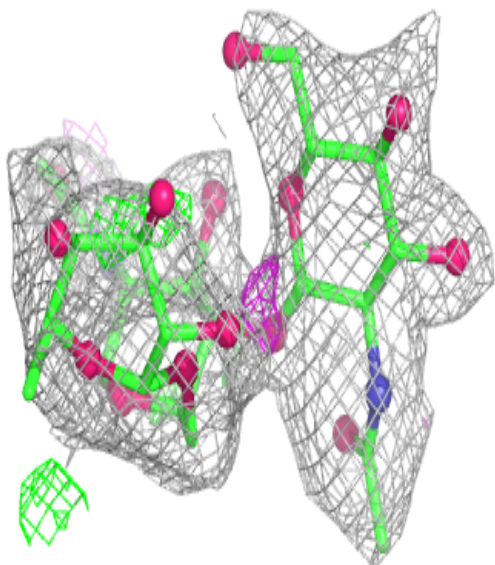
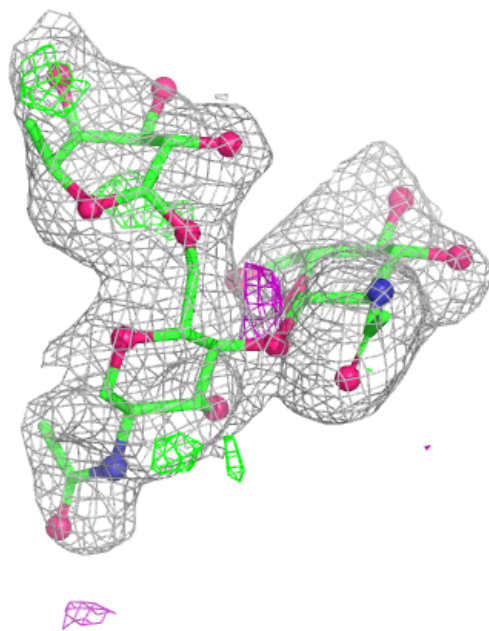
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	W	2	14/15	0.74	0.15	58,63,67,71	0
6	NAG	T	2	14/15	0.75	0.14	57,61,65,70	0
4	NAG	G	2	14/15	0.77	0.13	42,50,54,56	0
4	NAG	N	2	14/15	0.77	0.14	50,56,64,68	0
2	FUC	O	3	10/11	0.78	0.13	50,62,70,72	0
5	MAN	M	5	11/12	0.78	0.19	61,76,82,84	0
5	FUC	M	6	10/11	0.78	0.19	50,58,64,66	0
2	NAG	S	2	14/15	0.80	0.15	67,77,79,80	0
2	NAG	E	1	14/15	0.80	0.14	49,57,66,73	0
2	NAG	O	2	14/15	0.80	0.12	55,64,68,70	0
3	FUC	K	2	10/11	0.80	0.13	53,66,69,72	0
2	FUC	E	3	10/11	0.80	0.14	47,54,59,69	0
2	FUC	J	3	10/11	0.81	0.16	46,63,68,76	0
2	NAG	S	1	14/15	0.81	0.14	54,61,67,70	0
4	NAG	L	2	14/15	0.82	0.12	43,47,54,59	0
2	NAG	O	1	14/15	0.82	0.13	43,56,62,63	0
4	NAG	I	2	14/15	0.82	0.13	48,55,63,63	0
3	FUC	F	2	10/11	0.83	0.11	53,57,67,74	0
6	MAN	T	4	11/12	0.84	0.12	59,62,71,71	0
7	MAN	V	5	11/12	0.84	0.10	50,55,60,60	0
4	NAG	U	2	14/15	0.85	0.13	48,55,62,64	0
2	FUC	S	3	10/11	0.85	0.13	45,55,62,64	0
2	NAG	J	1	14/15	0.87	0.12	51,59,64,74	0
4	NAG	U	1	14/15	0.87	0.12	40,42,51,55	0
4	NAG	L	1	14/15	0.87	0.10	33,39,42,43	0
7	MAN	V	4	11/12	0.88	0.10	41,47,50,55	0
4	NAG	I	1	14/15	0.88	0.10	28,43,49,51	0
5	MAN	M	3	11/12	0.89	0.09	36,38,48,51	0
7	NAG	V	1	14/15	0.89	0.09	35,40,43,43	0
4	NAG	Q	1	14/15	0.89	0.10	48,56,62,70	0
6	NAG	T	1	14/15	0.89	0.09	38,51,57,60	0
7	NAG	V	2	14/15	0.91	0.09	39,42,49,49	0
4	NAG	W	1	14/15	0.91	0.08	29,49,53,57	0
5	NAG	M	1	14/15	0.91	0.10	31,34,41,45	0
4	NAG	N	1	14/15	0.92	0.08	34,41,48,53	0
7	MAN	V	3	11/12	0.92	0.08	40,45,51,52	0
5	NAG	M	2	14/15	0.92	0.08	29,36,39,41	0
4	NAG	G	1	14/15	0.92	0.09	37,39,46,48	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.

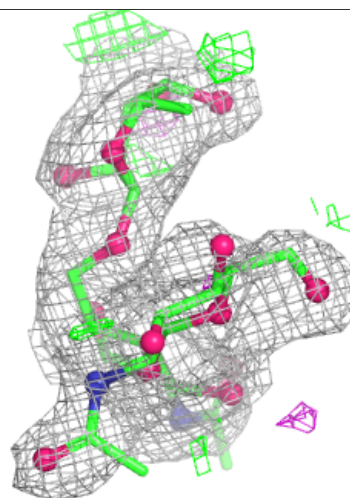
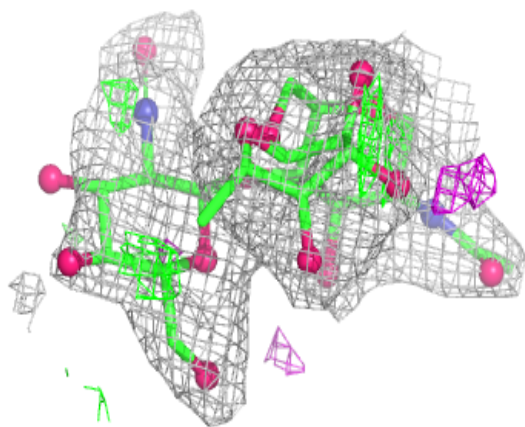
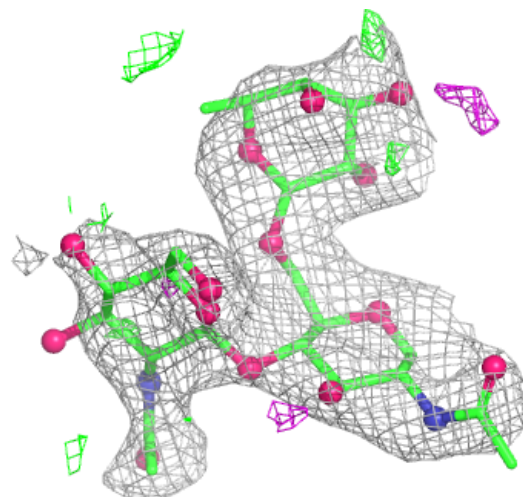
Electron density around Chain E:

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



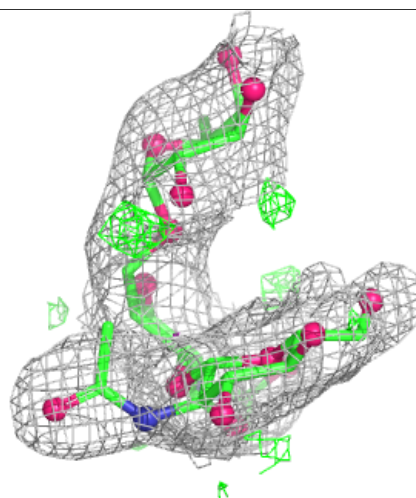
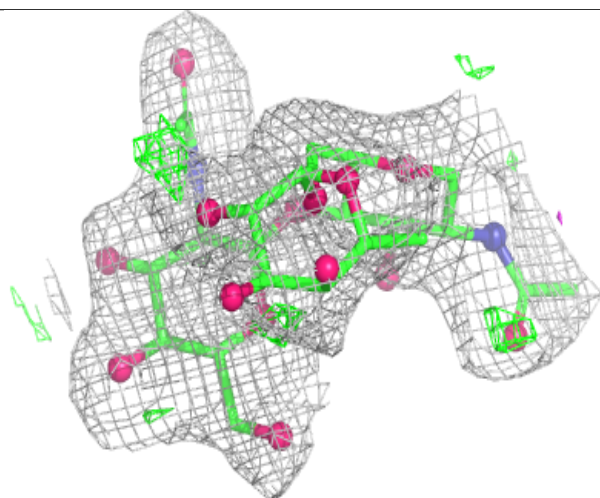
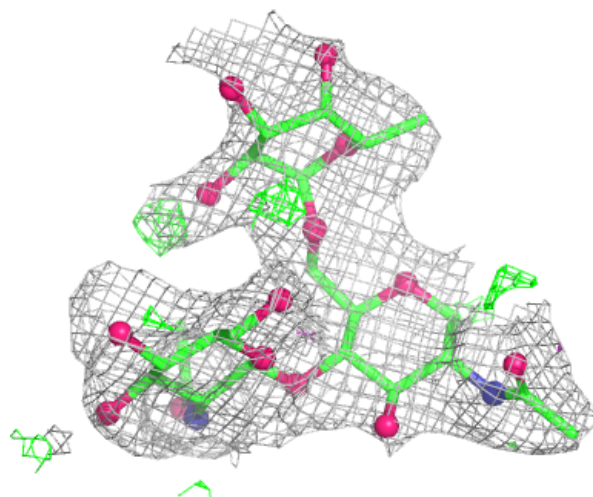
Electron density around Chain J:

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



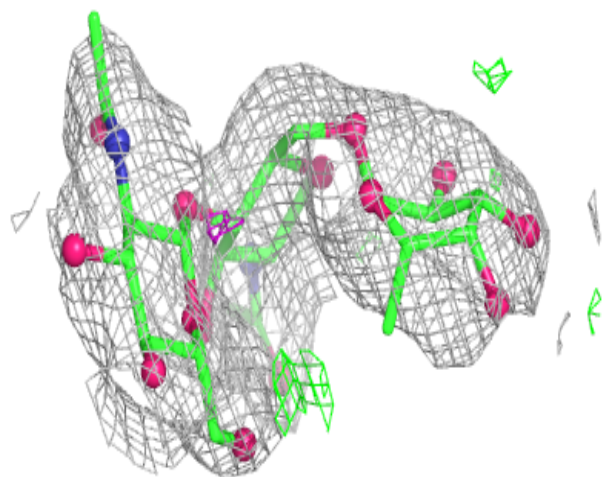
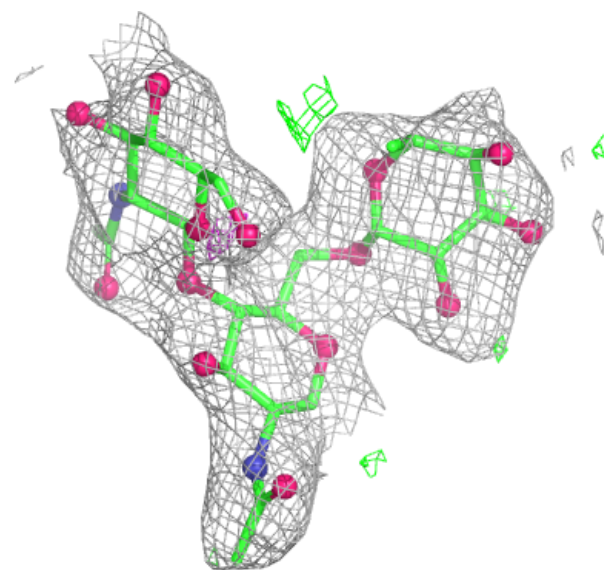
Electron density around Chain O:

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and green (positive)



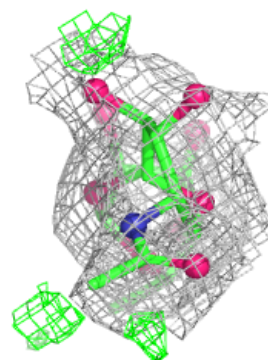
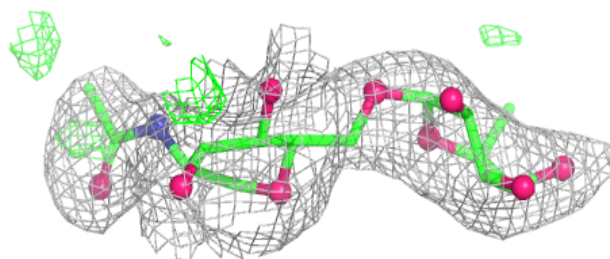
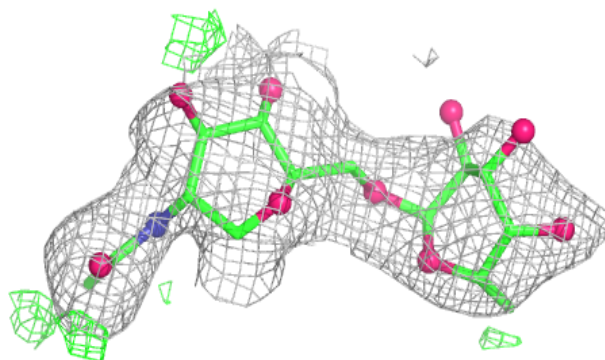
Electron density around Chain S:

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and green (positive)

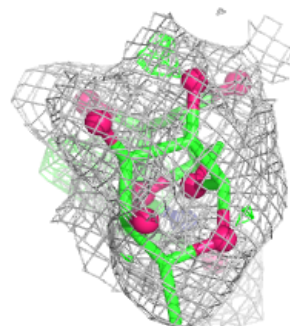
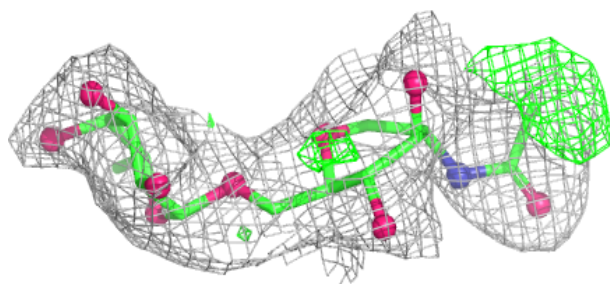
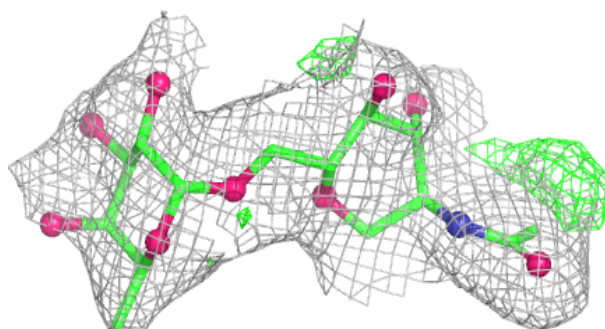


Electron density around Chain F:

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and green (positive)

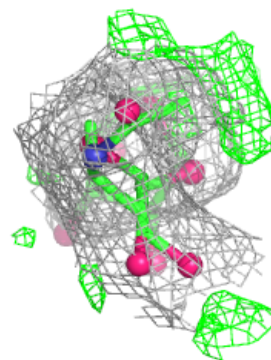
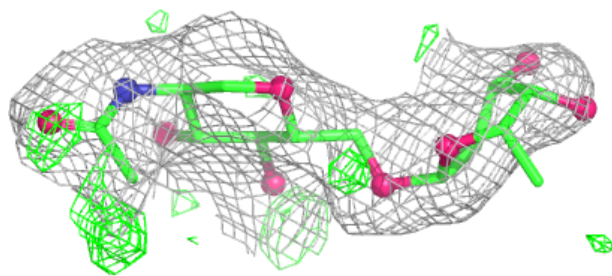
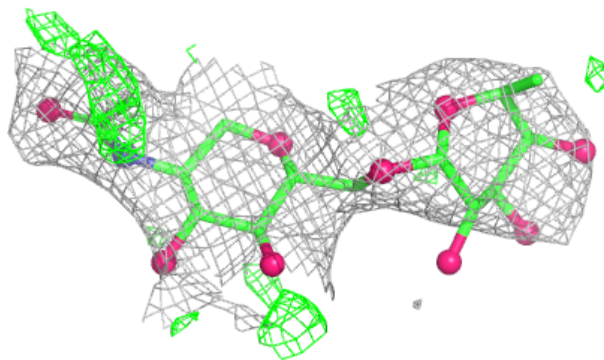
**Electron density around Chain K:**

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and green (positive)



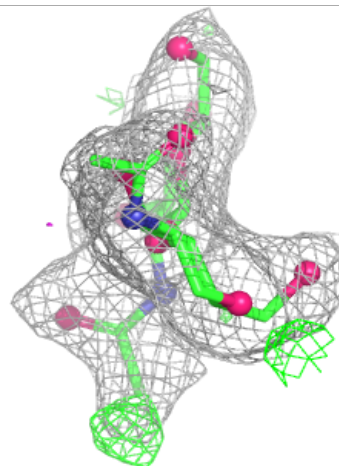
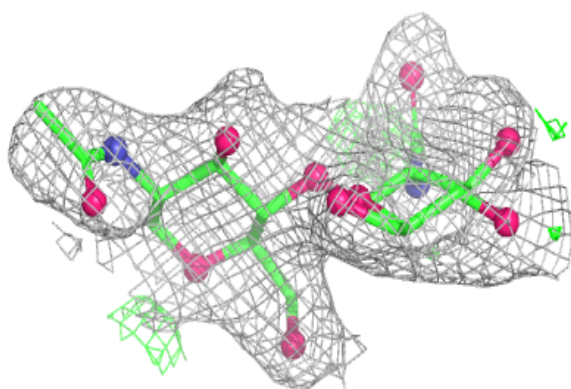
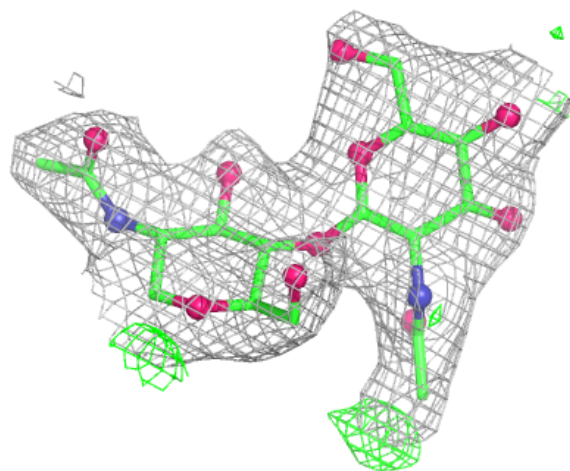
Electron density around Chain P:

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and green (positive)



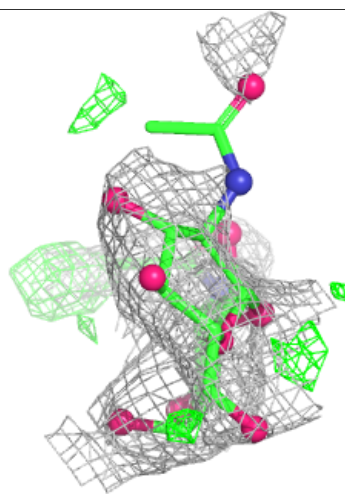
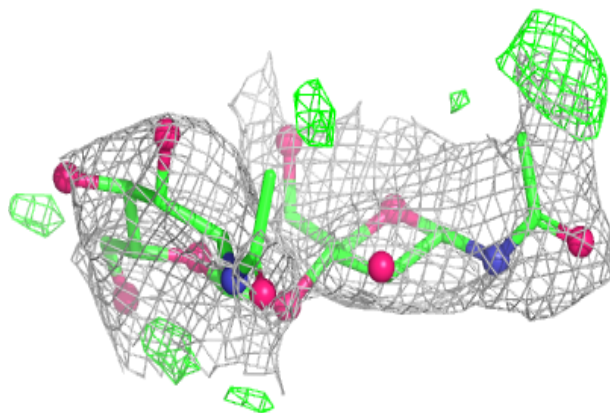
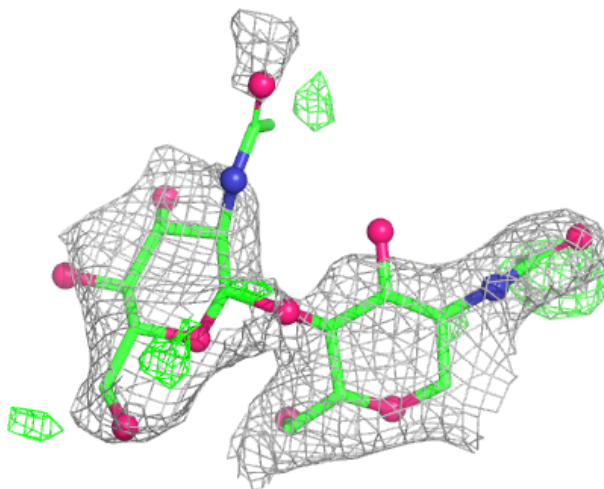
Electron density around Chain G:

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and green (positive)



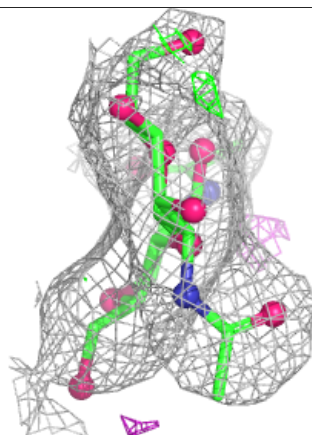
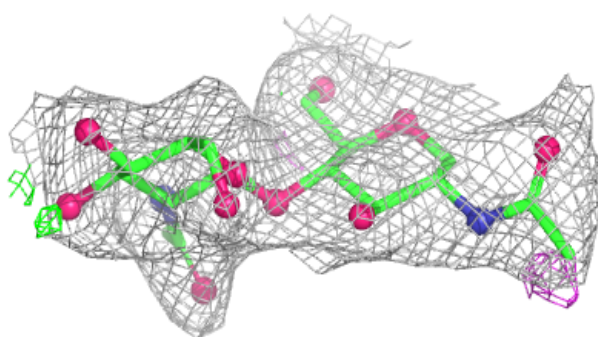
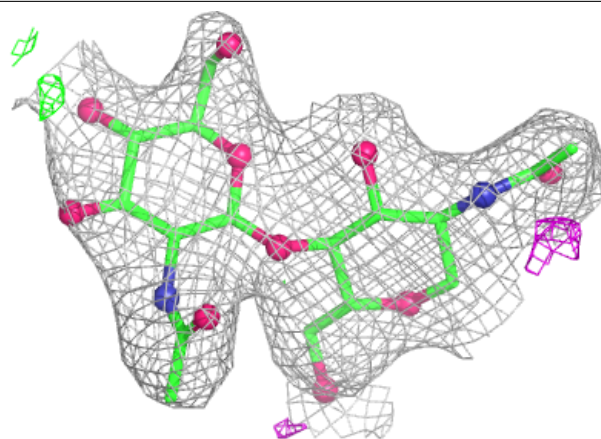
Electron density around Chain H:

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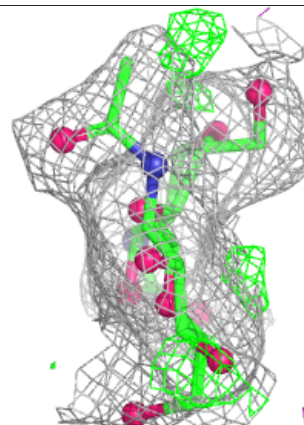
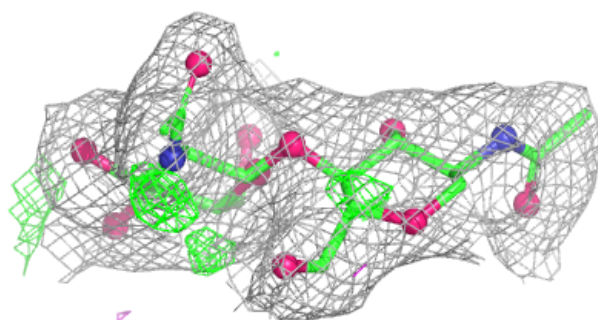
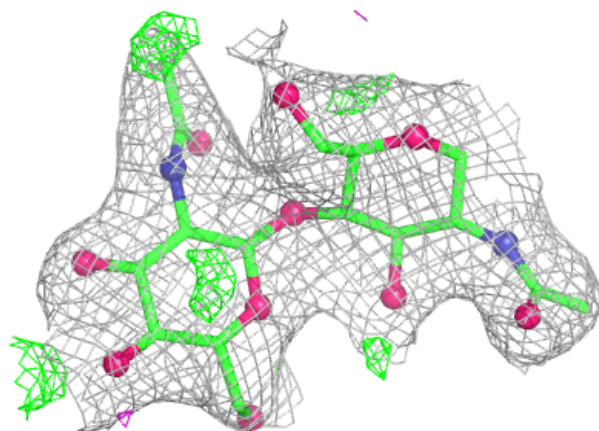
Electron density around Chain I:

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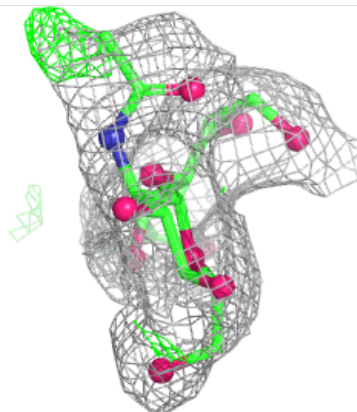
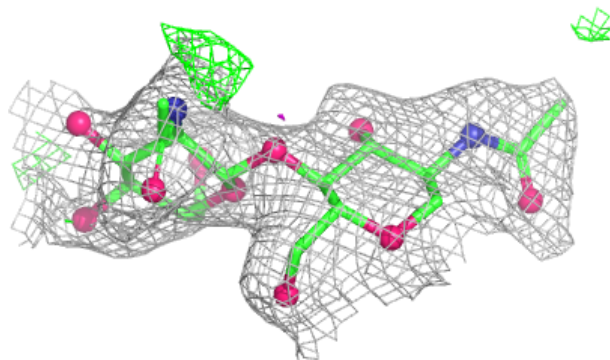
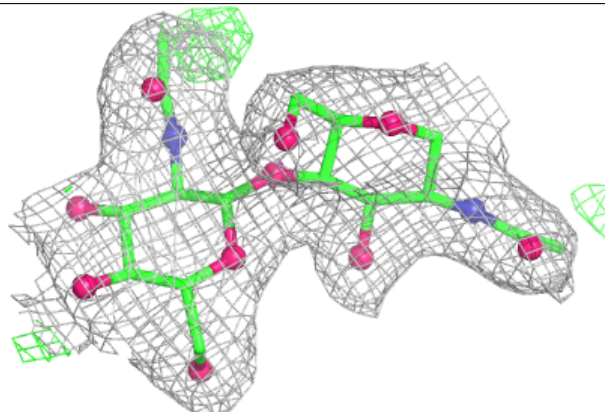


Electron density around Chain L:

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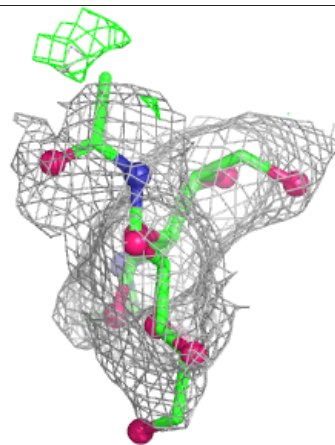
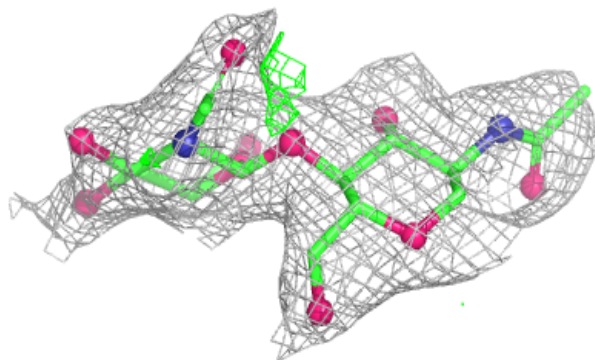
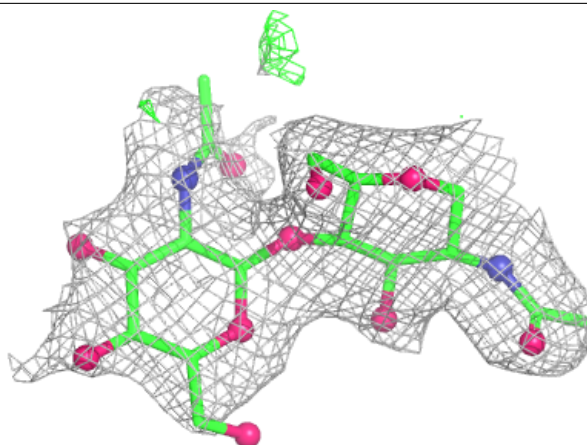
**Electron density around Chain N:**

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



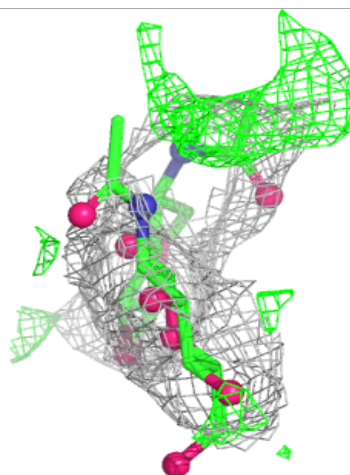
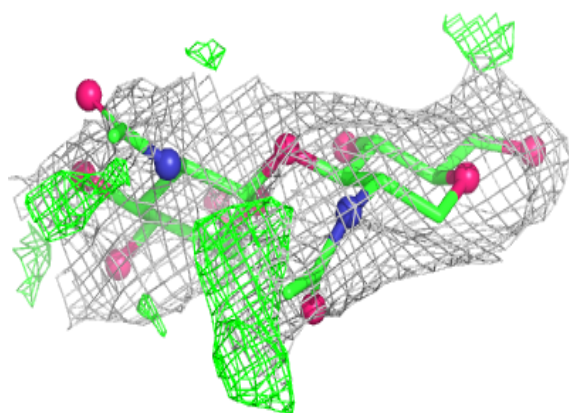
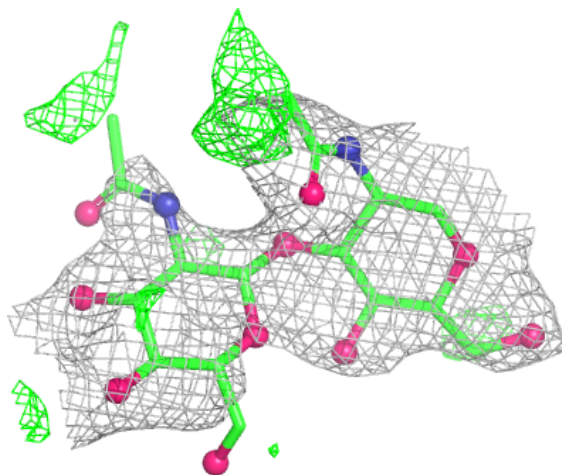
Electron density around Chain Q:

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



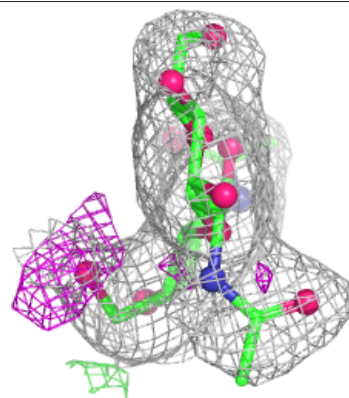
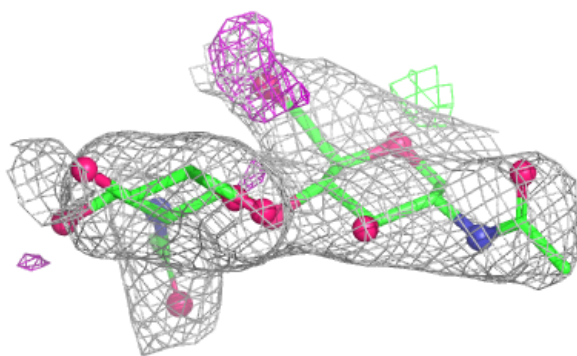
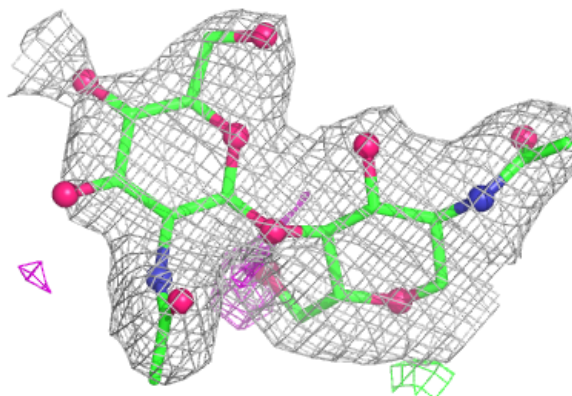
Electron density around Chain R:

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

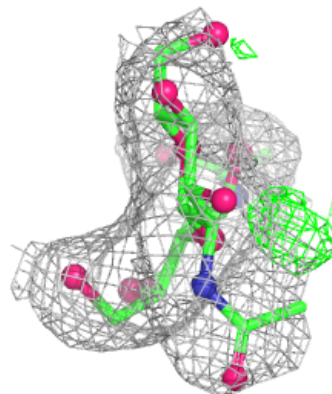
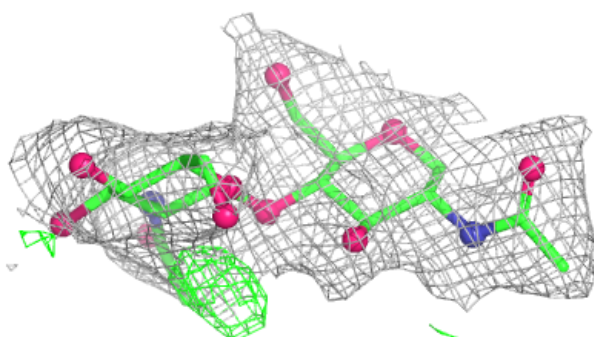
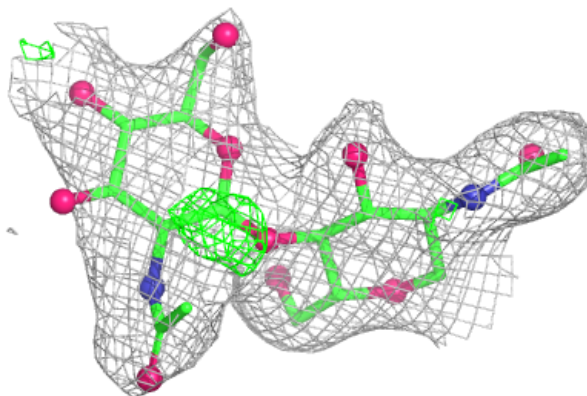


Electron density around Chain U:

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

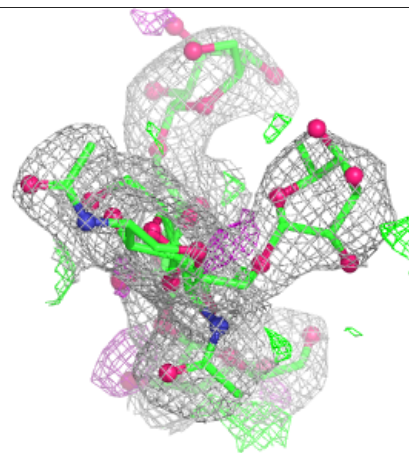
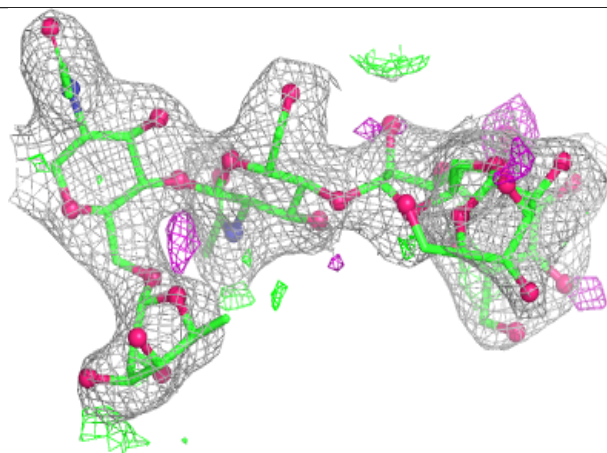
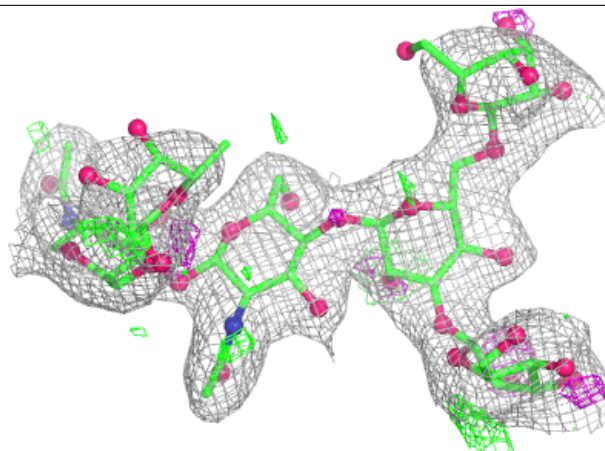
**Electron density around Chain W:**

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

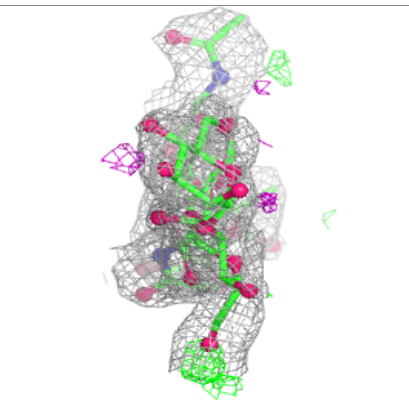
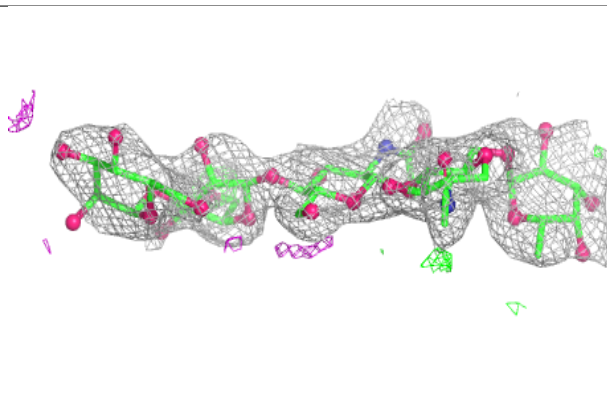
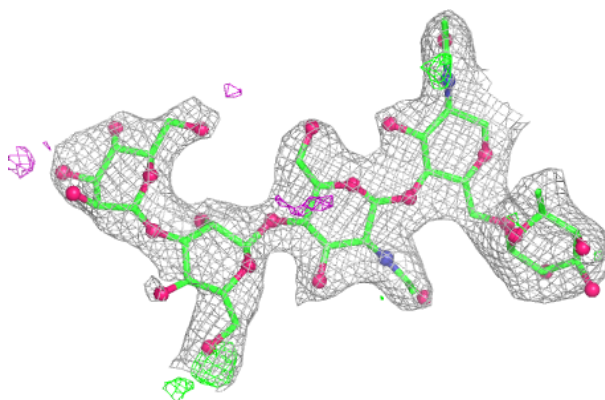


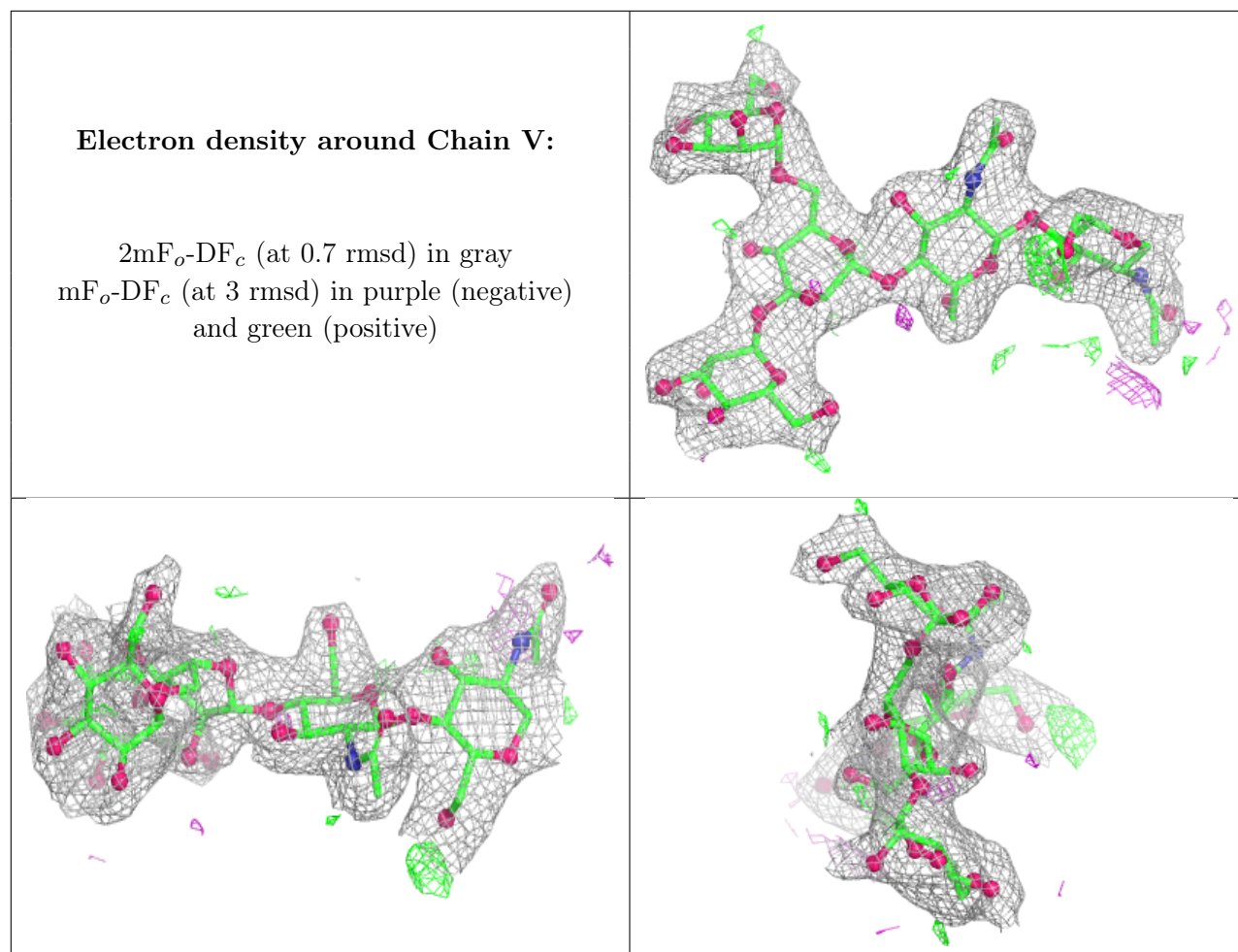
Electron density around Chain M:

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

**Electron density around Chain T:**

$2mF_o-DF_c$ (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
9	NAG	C	504	14/15	0.69	0.17	52,64,68,72	0
9	NAG	C	511	14/15	0.80	0.15	59,76,81,86	0
8	ZN	A	513	1/1	0.98	0.03	28,28,28,28	0
8	ZN	D	518	1/1	0.98	0.05	31,31,31,31	0
8	ZN	B	517	1/1	0.99	0.03	27,27,27,27	0
8	ZN	C	512	1/1	0.99	0.02	44,44,44,44	0
8	ZN	C	513	1/1	0.99	0.02	44,44,44,44	0
8	ZN	A	512	1/1	0.99	0.04	30,30,30,30	0
8	ZN	D	519	1/1	0.99	0.08	42,42,42,42	0
8	ZN	A	514	1/1	0.99	0.14	83,83,83,83	0
8	ZN	B	516	1/1	0.99	0.18	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.