



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:43 AM UTC

PDB ID : 5I8H / pdb_00005i8h
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer in Complex with V3 Loop-targeting Antibody PGT122 Fab and Fusion Peptide-targeting Antibody VRC34.01 Fab
Authors : Xu, K.; Zhou, T.; Kwong, P.D.
Deposited on : 2016-02-18
Resolution : 4.30 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

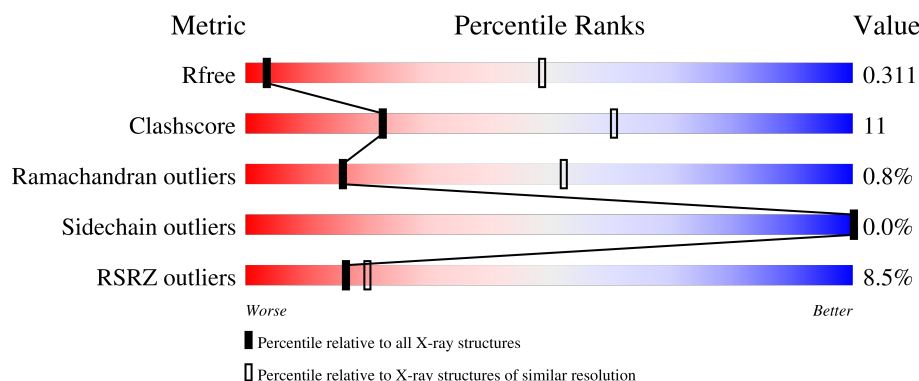
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	481	8% 71% 23% 5%
1	C	481	9% 67% 26% 6%
2	B	153	5% 58% 28% 14%
2	D	153	8% 60% 26% 14%
3	J	210	10% 71% 28% .

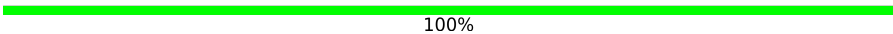
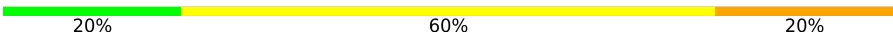
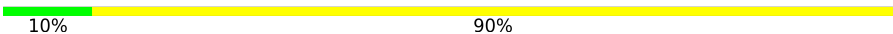
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	210	
4	E	223	
4	G	223	
5	F	212	
5	H	212	
6	I	235	
6	K	235	
7	M	7	
7	Z	7	
8	N	5	
8	a	5	
9	O	2	
9	P	2	
9	Q	2	
9	T	2	
9	V	2	
9	W	2	
9	X	2	
9	b	2	
9	c	2	
9	d	2	
9	f	2	
9	g	2	
9	i	2	
9	j	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	R	6	 50%33%17%
10	e	6	 50%33%17%
11	S	3	 33%67%
11	Y	3	 67%33%
11	k	3	 67%33%
11	l	3	 100%
12	U	10	 20%60%20%
12	h	10	 10%90%
13	m	4	 75%25%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23938 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 BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3576	2243	632	673	28			
1	C	450	Total	C	N	O	S	0	0	0
			3542	2223	625	666	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	GLU	conflict	UNP Q2N0S6
A	510	ARG	LYS	conflict	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			
2	D	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			
3	J	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 4 is a protein called VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			
4	G	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			

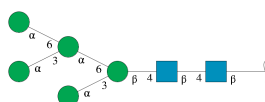
- Molecule 5 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			
5	H	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			

- Molecule 6 is a protein called PGT122 Fab heavy chain.

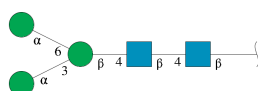
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			
6	K	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



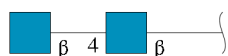
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



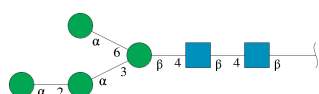
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

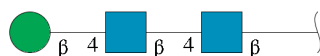
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	g	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	i	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	j	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



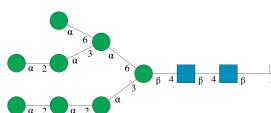
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	k	3	Total	C	N	O	0	0	0
			39	22	2	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	1	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	U	10	Total	C	N	O	0	0	0
			116	64	2	50			
12	h	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

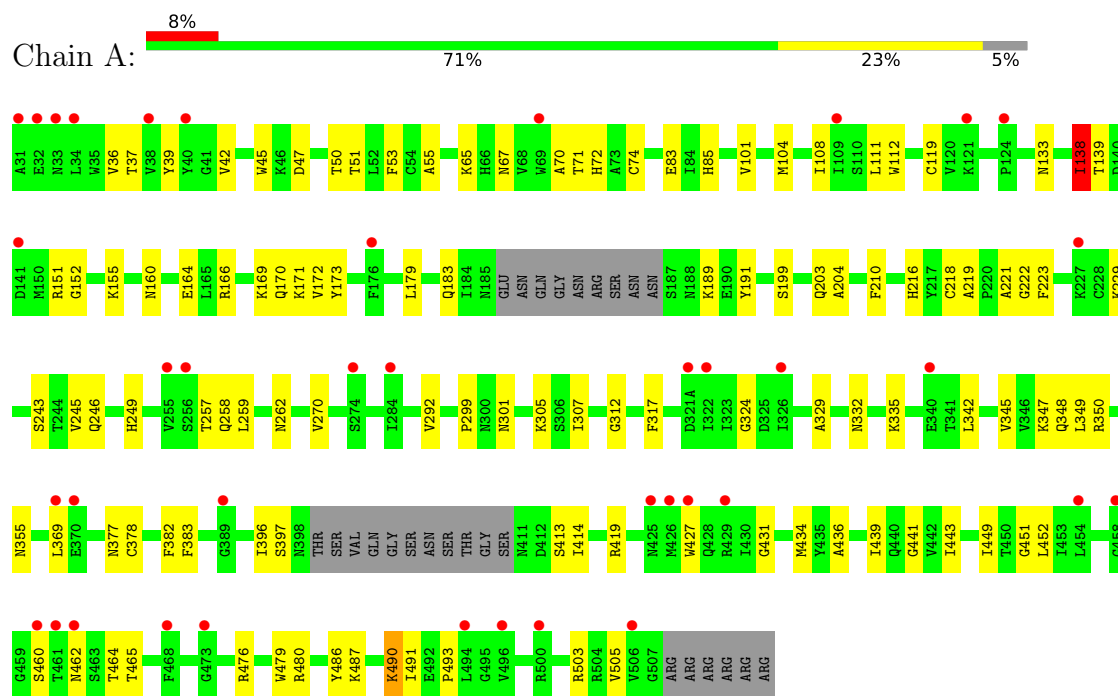
Continued from previous page...

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

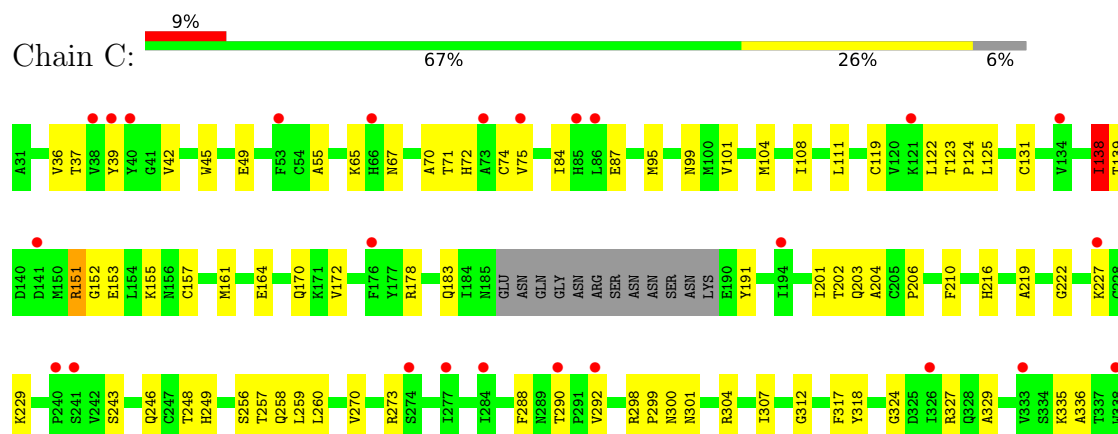
3 Residue-property plots [i](#)

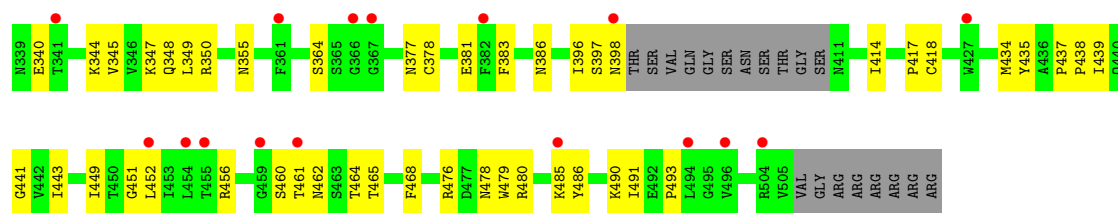
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BG505 SOSIP.664 gp120

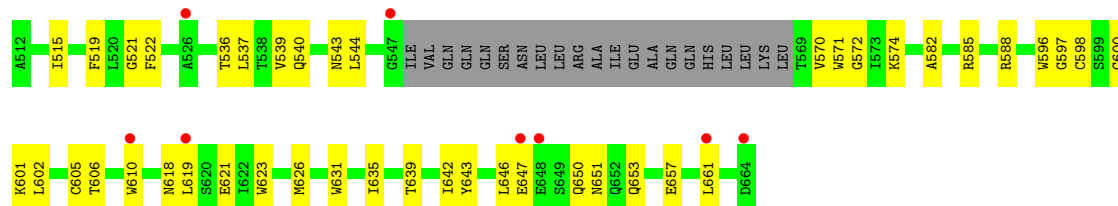


• Molecule 1: BG505 SOSIP.664 gp120

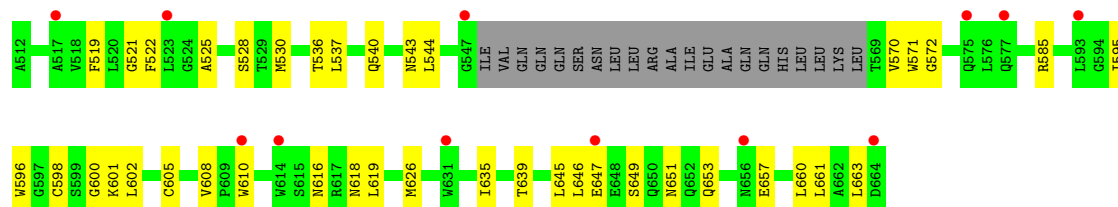




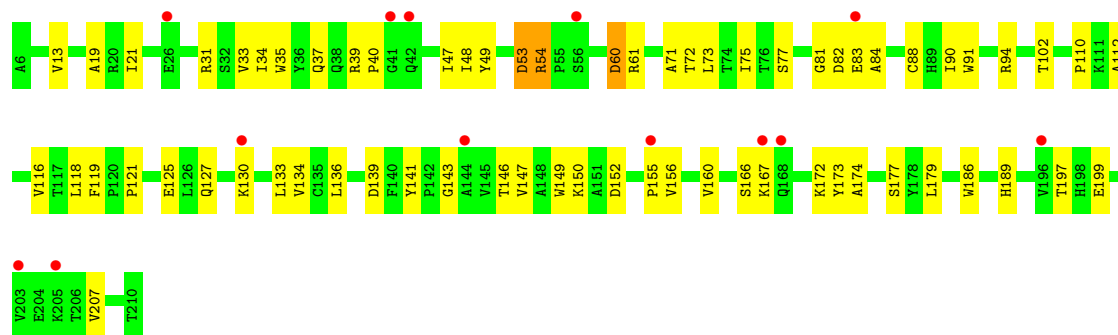
• Molecule 2: BG505 SOSIP.664 gp41



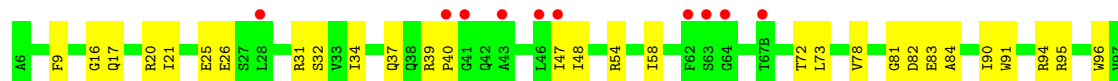
• Molecule 2: BG505 SOSIP.664 gp41

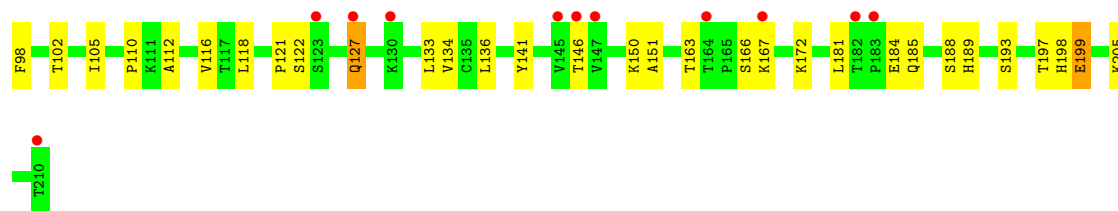


• Molecule 3: PGT122 Fab light chain

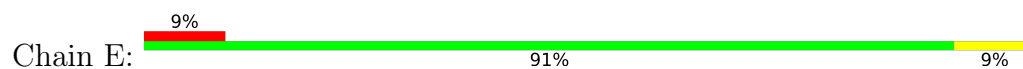


• Molecule 3: PGT122 Fab light chain

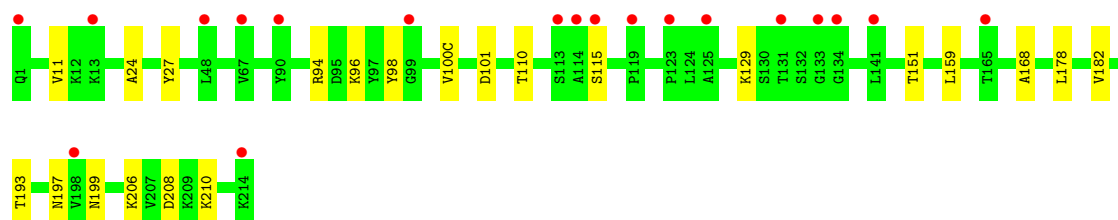
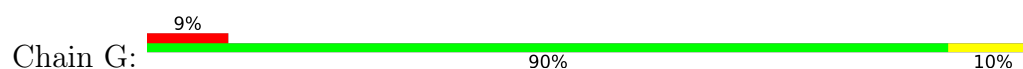




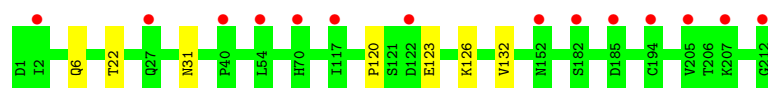
• Molecule 4: VRC34.01 Fab heavy chain



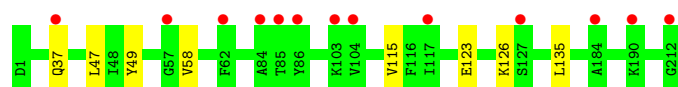
• Molecule 4: VRC34.01 Fab heavy chain



• Molecule 5: VRC34.01 Fab light chain

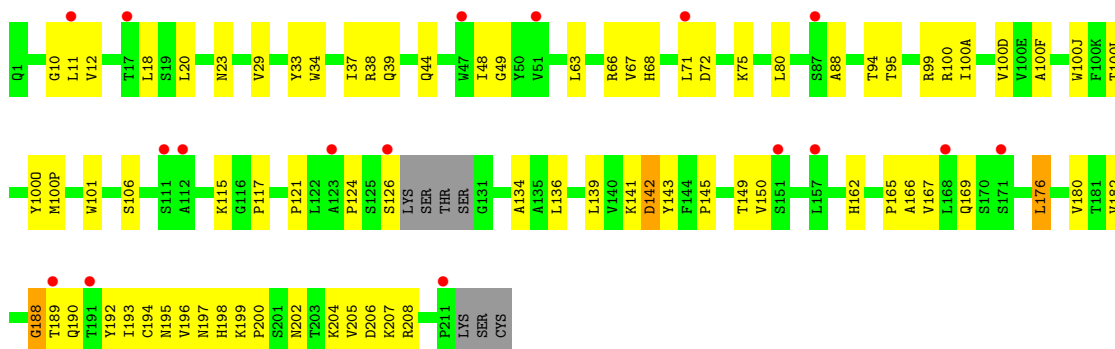


• Molecule 5: VRC34.01 Fab light chain

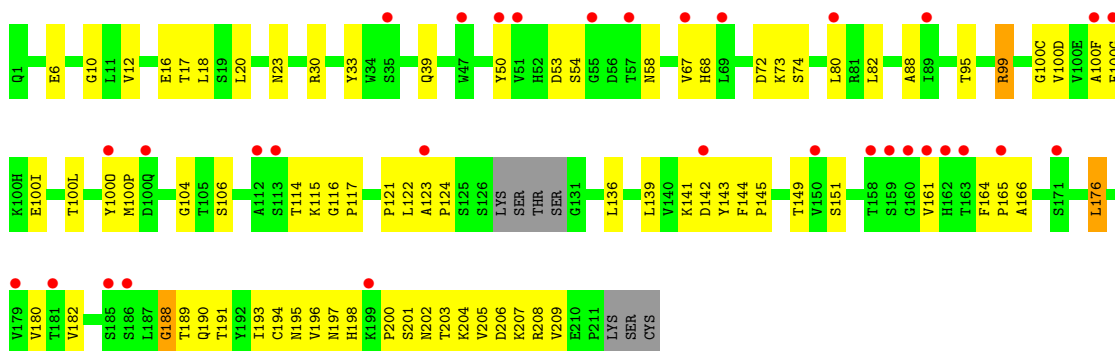


• Molecule 6: PGT122 Fab heavy chain

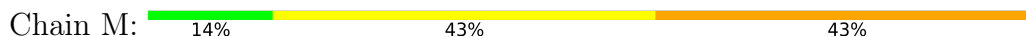




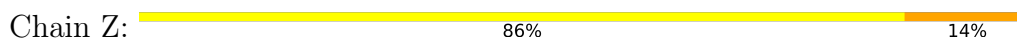
• Molecule 6: PGT122 Fab heavy chain



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  60% 40%

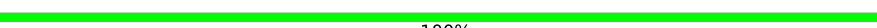


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

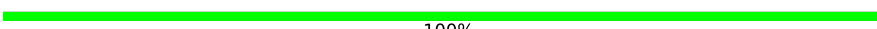


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

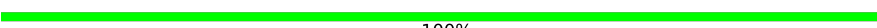


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

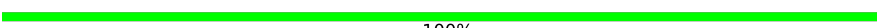


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 50% 50%



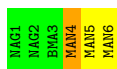
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 100%



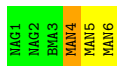
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 50% 33% 17%



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 50% 33% 17%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 33% 67%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 67% 33%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  67% 33%

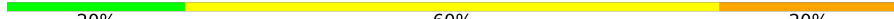
HA1
HA2
BMA3

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

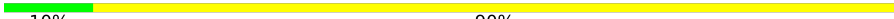
HA1
HA2
BMA3

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  20% 60% 20%

HA1
HA2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  10% 90%

HA1
HA2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 13: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  75% 25%

HA1
HA2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	252.30Å 252.30Å 561.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 4.30 48.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	54.9 (48.34-4.30) 55.0 (48.34-4.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 4.29Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.281 , 0.309 0.282 , 0.311	Depositor DCC
R_{free} test set	1319 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	127.2	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 181.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å ²)	215.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	1/3650 (0.0%)	0.76	4/4956 (0.1%)
1	C	0.29	1/3616 (0.0%)	0.72	2/4911 (0.0%)
2	B	0.26	0/1052	0.66	0/1427
2	D	0.24	0/1052	0.67	0/1427
3	J	0.32	0/1632	0.74	1/2236 (0.0%)
3	L	0.56	5/1632 (0.3%)	0.68	0/2236
4	E	0.23	0/1715	0.56	0/2337
4	G	0.17	0/1715	0.42	0/2337
5	F	0.18	0/1665	0.48	0/2262
5	H	0.15	0/1665	0.40	0/2262
6	I	0.28	0/1789	0.70	3/2443 (0.1%)
6	K	0.30	0/1789	0.73	4/2443 (0.2%)
All	All	0.29	7/22972 (0.0%)	0.65	14/31277 (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
4	E	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	54	ARG	NE-CZ	-10.72	1.21	1.33
3	L	54	ARG	CZ-NH1	-10.17	1.18	1.32
3	L	54	ARG	CD-NE	-8.41	1.34	1.46
3	L	54	ARG	CZ-NH2	-7.41	1.23	1.33
1	A	138	ILE	CA-C	5.62	1.59	1.52
1	C	138	ILE	CA-C	5.39	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	53	ASP	C-N	-5.15	1.22	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	23	ASN	CB-CA-C	7.26	121.15	110.26
1	A	490	LYS	CA-CB-CG	6.83	127.77	114.10
6	K	23	ASN	CB-CA-C	6.69	120.29	110.26
1	A	138	ILE	CG1-CB-CG2	-6.45	91.35	110.70
1	A	166	ARG	CA-CB-CG	6.28	126.66	114.10
6	K	23	ASN	N-CA-CB	-5.98	100.50	109.71
6	I	23	ASN	N-CA-CB	-5.85	100.70	109.71
6	I	176	LEU	CA-CB-CG	5.77	136.48	116.30
1	C	138	ILE	CG1-CB-CG2	-5.67	93.68	110.70
3	J	127	GLN	N-CA-CB	-5.53	101.21	110.39
1	A	138	ILE	CB-CA-C	5.37	120.10	111.29
6	K	99	ARG	CG-CD-NE	-5.31	100.32	112.00
6	K	176	LEU	CA-CB-CG	5.24	134.65	116.30
1	C	138	ILE	CB-CA-C	5.01	119.51	111.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	208	ASP	Mainchain

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	3576	0	3509	92	0
1	C	3542	0	3471	94	0
2	B	1034	0	1011	43	0
2	D	1034	0	1012	31	0
3	J	1589	0	1530	54	0
3	L	1589	0	1530	55	0
4	E	1674	0	1638	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1674	0	1638	20	0
5	F	1628	0	1588	10	0
5	H	1628	0	1588	8	0
6	I	1742	0	1713	60	0
6	K	1742	0	1715	68	0
7	M	83	0	69	4	0
7	Z	83	0	70	2	0
8	N	61	0	52	0	0
8	a	61	0	52	0	0
9	O	28	0	25	5	0
9	P	28	0	25	0	0
9	Q	28	0	25	0	0
9	T	28	0	25	0	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0
9	X	28	0	25	0	0
9	b	28	0	25	2	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	i	28	0	25	1	0
9	j	28	0	25	1	0
10	R	72	0	61	2	0
10	e	72	0	61	1	0
11	S	39	0	34	0	0
11	Y	39	0	34	1	0
11	k	39	0	34	0	0
11	l	39	0	34	0	0
12	U	116	0	97	1	0
12	h	116	0	97	1	0
13	m	50	0	42	0	0
14	A	56	0	52	3	0
14	B	42	0	39	0	0
14	C	70	0	65	1	0
14	D	28	0	26	0	0
14	I	14	0	13	0	0
14	K	14	0	13	0	0
All	All	23938	0	23238	497	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 11.

All (497) 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)
3:L:39:ARG:HD3	3:L:84:ALA:HB2	1.35	1.09
1:C:138:ILE:HG22	1:C:139:THR:HA	1.40	1.04
1:A:490:LYS:HG2	2:B:585:ARG:HH12	1.25	0.95
1:A:138:ILE:HG22	1:A:139:THR:HA	1.48	0.94
1:A:350:ARG:NH2	1:A:396:ILE:O	2.04	0.90
1:A:70:ALA:HB2	1:A:111:LEU:HD11	1.53	0.90
1:C:249:HIS:HD1	1:C:486:TYR:HH	1.19	0.89
3:L:39:ARG:HH12	3:L:82:ASP:C	1.81	0.89
3:L:34:ILE:HD13	6:K:100(O):TYR:HB3	1.56	0.87
1:A:249:HIS:HD1	1:A:486:TYR:HH	0.87	0.86
1:C:350:ARG:NH2	1:C:396:ILE:O	2.09	0.85
6:I:99:ARG:HG2	6:I:100(L):THR:HG22	1.59	0.84
6:K:121:PRO:HD3	6:K:207:LYS:HE3	1.59	0.84
1:A:292:VAL:HB	1:A:449:ILE:HB	1.60	0.83
3:L:127:GLN:NE2	4:E:117:LYS:HB2	1.93	0.83
3:J:39:ARG:HD3	3:J:84:ALA:HB2	1.60	0.82
5:F:126:LYS:NZ	6:K:115:LYS:HB2	1.95	0.81
4:G:210:LYS:HB3	6:I:202:ASN:HD22	1.47	0.79
6:K:30:ARG:HD3	6:K:73:LYS:HD2	1.64	0.79
3:J:54:ARG:NE	3:J:58:ILE:O	2.18	0.76
1:C:70:ALA:HB2	1:C:111:LEU:HD11	1.66	0.76
3:L:54:ARG:NH1	3:L:60:ASP:HA	1.99	0.76
1:A:219:ALA:O	1:A:246:GLN:NE2	2.19	0.76
2:D:570:VAL:HG12	2:D:571:TRP:H	1.50	0.75
3:J:83:GLU:HG2	3:J:167:LYS:HZ1	1.51	0.75
2:B:570:VAL:HG12	2:B:571:TRP:H	1.50	0.75
1:A:490:LYS:CG	2:B:585:ARG:HH12	2.00	0.75
1:A:490:LYS:HG2	2:B:585:ARG:NH1	2.00	0.75
1:C:292:VAL:HB	1:C:449:ILE:HB	1.68	0.74
2:B:653:GLN:O	2:B:657:GLU:HG2	1.87	0.73
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.73
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.71	0.73
2:B:596:TRP:HE1	2:B:647:GLU:HG2	1.54	0.72
3:J:9:PHE:HD2	3:J:105:ILE:HD11	1.54	0.72
6:I:162:HIS:CE1	3:J:172:LYS:HZ2	2.07	0.71
2:B:536:THR:O	2:B:540:GLN:NE2	2.23	0.71
6:I:100:ARG:NH2	6:I:100(A):ILE:O	2.23	0.71
3:L:37:GLN:OE1	3:L:39:ARG:NH2	2.23	0.71
1:C:206:PRO:HG3	1:C:318:TYR:HE2	1.55	0.71
1:C:219:ALA:O	1:C:246:GLN:NE2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.72	0.70
3:J:39:ARG:HG3	3:J:40:PRO:HD2	1.72	0.70
3:L:127:GLN:HE22	4:E:117:LYS:HB2	1.57	0.70
5:F:126:LYS:HZ2	6:K:115:LYS:HB2	1.53	0.70
2:D:657:GLU:O	2:D:661:LEU:HG	1.91	0.70
3:L:39:ARG:NH1	3:L:82:ASP:C	2.49	0.69
2:D:653:GLN:O	2:D:657:GLU:HG2	1.93	0.69
3:J:16:GLY:N	3:J:78:VAL:O	2.24	0.69
2:B:597:GLY:HA2	2:B:651:ASN:HD21	1.59	0.68
3:J:83:GLU:OE2	3:J:167:LYS:NZ	2.22	0.68
1:C:101:VAL:HG13	1:C:479:TRP:HB2	1.75	0.68
6:I:142:ASP:OD1	6:I:169:GLN:NE2	2.26	0.68
1:A:47:ASP:OD2	1:A:487:LYS:NZ	2.22	0.67
6:I:193:ILE:HG12	6:I:208:ARG:HB2	1.76	0.67
6:K:161:VAL:HG12	6:K:180:VAL:HG22	1.74	0.67
6:I:198:HIS:CD2	6:I:200:PRO:HD2	2.28	0.67
3:J:25:GLU:OE2	3:J:95:ARG:NH1	2.27	0.67
6:K:196:VAL:O	6:K:205:VAL:N	2.27	0.66
1:C:155:LYS:NZ	1:C:191:TYR:OH	2.19	0.66
3:L:39:ARG:CD	3:L:84:ALA:HB2	2.22	0.66
3:J:198:HIS:CE1	3:J:199:GLU:HG2	2.31	0.66
1:A:179:LEU:HD11	1:A:419:ARG:HG2	1.77	0.66
4:E:206:LYS:O	6:K:205:VAL:HA	1.95	0.65
1:C:123:THR:HG23	1:C:124:PRO:HD3	1.79	0.65
6:K:99:ARG:HG3	6:K:100(L):THR:HG22	1.76	0.65
3:L:150:LYS:HD3	3:L:155:PRO:HA	1.78	0.64
3:J:83:GLU:HG2	3:J:167:LYS:NZ	2.12	0.64
4:G:206:LYS:HD2	6:I:206:ASP:OD2	1.98	0.63
1:C:299:PRO:O	1:C:300:ASN:ND2	2.32	0.63
4:G:206:LYS:O	6:I:205:VAL:HA	1.99	0.63
5:H:126:LYS:HZ2	6:I:115:LYS:HB2	1.63	0.63
1:C:87:GLU:HG2	7:Z:1:NAG:H82	1.80	0.63
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.81	0.62
2:D:660:LEU:HA	2:D:663:LEU:HD23	1.81	0.62
1:C:299:PRO:C	1:C:300:ASN:HD22	2.07	0.62
1:C:417:PRO:HG3	6:K:100(G):PHE:HZ	1.64	0.62
6:I:121:PRO:HD3	6:I:207:LYS:HZ3	1.65	0.62
4:G:98:TYR:HB2	4:G:100(C):VAL:HG21	1.81	0.62
4:G:210:LYS:HB3	6:I:202:ASN:ND2	2.15	0.61
6:K:198:HIS:N	6:K:203:THR:O	2.33	0.61
2:D:645:LEU:O	2:D:649:SER:OG	2.17	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASN:ND2	11:Y:1:NAG:O7	2.33	0.61
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.81	0.61
3:J:25:GLU:CD	3:J:95:ARG:HH11	2.09	0.60
1:A:503:ARG:NH2	2:B:597:GLY:HA3	2.16	0.60
3:L:166:SER:OG	6:K:165:PRO:HG3	2.01	0.60
3:J:39:ARG:HH12	3:J:82:ASP:C	2.10	0.60
3:L:139:ASP:H	3:L:172:LYS:HG3	1.65	0.60
2:B:618:ASN:HB3	2:B:621:GLU:HB2	1.84	0.59
1:A:503:ARG:HH22	2:B:597:GLY:HA3	1.67	0.59
2:D:536:THR:O	2:D:540:GLN:NE2	2.35	0.59
3:L:167:LYS:HG3	3:L:173:TYR:CE2	2.38	0.59
2:B:606:THR:HG22	2:B:650:GLN:HE21	1.68	0.59
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.85	0.59
6:K:188:GLY:HA3	6:K:190:GLN:N	2.17	0.59
1:C:229:LYS:HE3	1:C:243:SER:HB3	1.83	0.59
1:A:67:ASN:HD21	1:A:72:HIS:HB2	1.68	0.59
6:I:188:GLY:HA3	6:I:190:GLN:N	2.17	0.59
2:B:596:TRP:NE1	2:B:647:GLU:HG2	2.18	0.58
1:C:206:PRO:HG3	1:C:318:TYR:CE2	2.38	0.58
6:I:149:THR:OG1	6:I:197:ASN:HB3	2.03	0.58
1:A:39:TYR:HD2	2:B:537:LEU:HD11	1.68	0.58
6:K:53:ASP:OD2	6:K:73:LYS:HD3	2.03	0.58
6:K:139:LEU:HD21	6:K:141:LYS:HB2	1.85	0.58
6:K:6:GLU:OE2	6:K:104:GLY:N	2.36	0.58
1:A:138:ILE:HG22	1:A:139:THR:CA	2.29	0.58
3:L:31:ARG:NH1	3:L:90:ILE:HD12	2.19	0.58
3:L:167:LYS:HG3	3:L:173:TYR:CZ	2.38	0.58
3:L:54:ARG:HH11	3:L:60:ASP:HA	1.67	0.57
4:E:206:LYS:HD2	6:K:206:ASP:OD2	2.04	0.57
4:E:208:ASP:OD2	6:K:204:LYS:HB2	2.04	0.57
6:I:167:VAL:HB	3:J:163:THR:HG22	1.85	0.57
3:L:112:ALA:HB3	3:L:141:TYR:N	2.20	0.57
3:J:184:GLU:O	3:J:188:SER:OG	2.18	0.57
6:K:117:PRO:HB3	6:K:143:TYR:HB3	1.86	0.57
3:J:112:ALA:HB3	3:J:141:TYR:N	2.20	0.57
2:B:585:ARG:HG3	2:B:588:ARG:HH21	1.69	0.56
1:A:464:THR:OG1	1:A:465:THR:N	2.33	0.56
1:C:476:ARG:O	1:C:480:ARG:HG3	2.04	0.56
1:A:138:ILE:CG2	1:A:139:THR:HA	2.29	0.56
1:C:491:ILE:O	2:D:585:ARG:NH2	2.39	0.56
1:C:210:PHE:HD2	1:C:377:ASN:HD21	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:190:GLN:HG3	6:I:192:TYR:CE1	2.41	0.56
3:J:31:ARG:NH1	3:J:90:ILE:HD12	2.21	0.56
3:L:48:ILE:HG12	3:L:54:ARG:HG2	1.86	0.56
1:A:133:ASN:CG	1:A:155:LYS:HZ3	2.13	0.55
1:C:151:ARG:O	1:C:153:GLU:N	2.39	0.55
1:C:300:ASN:ND2	1:C:327:ARG:O	2.35	0.55
3:J:47:ILE:HG22	3:J:48:ILE:HG13	1.89	0.55
2:B:570:VAL:C	2:B:572:GLY:H	2.14	0.55
6:I:115:LYS:HZ2	6:I:142:ASP:HB3	1.70	0.55
9:b:2:NAG:H83	9:b:2:NAG:H3	1.88	0.55
1:C:227:LYS:HA	1:C:485:LYS:O	2.07	0.55
7:Z:2:NAG:H3	7:Z:2:NAG:H83	1.88	0.55
1:C:336:ALA:O	1:C:340:GLU:HG2	2.06	0.55
4:G:208:ASP:OD2	6:I:204:LYS:HB3	2.06	0.55
2:B:570:VAL:HG12	2:B:571:TRP:N	2.21	0.55
1:C:67:ASN:HD21	1:C:72:HIS:HB2	1.71	0.55
1:C:151:ARG:HH21	1:C:178:ARG:HD2	1.72	0.55
2:D:618:ASN:OD1	2:D:619:LEU:N	2.39	0.55
1:C:45:TRP:HB3	1:C:491:ILE:HD13	1.88	0.54
1:A:204:ALA:HB2	1:A:434:MET:HE3	1.89	0.54
14:C:927:NAG:H3	14:C:927:NAG:H83	1.89	0.54
6:K:194:CYS:O	6:K:206:ASP:HA	2.07	0.54
1:A:36:VAL:HG12	2:B:610:TRP:HE3	1.71	0.54
4:E:168:ALA:HA	4:E:178:LEU:HB3	1.90	0.54
6:I:115:LYS:NZ	6:I:142:ASP:HB3	2.21	0.54
7:M:2:NAG:H3	7:M:2:NAG:H83	1.89	0.54
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.90	0.54
3:J:118:LEU:HD12	3:J:134:VAL:O	2.07	0.54
1:C:70:ALA:CB	1:C:111:LEU:HD11	2.35	0.54
1:C:138:ILE:HG22	1:C:139:THR:CA	2.25	0.54
1:C:138:ILE:CG2	1:C:139:THR:HA	2.26	0.54
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.90	0.54
6:I:99:ARG:HD3	6:I:100(J):TRP:CZ3	2.43	0.54
6:I:100(O):TYR:HB3	3:J:34:ILE:HD13	1.90	0.54
3:J:146:THR:OG1	3:J:197:THR:HB	2.08	0.54
1:A:183:GLN:HA	1:A:191:TYR:HA	1.89	0.53
1:A:307:ILE:HD11	1:A:317:PHE:HD2	1.74	0.53
1:A:37:THR:HG22	2:B:605:CYS:HA	1.90	0.53
2:D:570:VAL:HG12	2:D:571:TRP:N	2.21	0.53
1:A:491:ILE:O	2:B:585:ARG:NH2	2.42	0.53
4:E:204:ASN:O	6:K:206:ASP:O	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:38:ARG:HB2	6:I:48:ILE:HD11	1.90	0.53
14:A:926:NAG:H83	14:A:926:NAG:H3	1.89	0.53
1:C:464:THR:OG1	1:C:465:THR:N	2.42	0.53
6:I:67:VAL:O	6:I:68:HIS:ND1	2.42	0.53
6:I:100(D):VAL:O	6:I:100(F):ALA:N	2.35	0.53
6:K:6:GLU:CD	6:K:104:GLY:H	2.16	0.53
6:K:196:VAL:O	6:K:204:LYS:HA	2.09	0.53
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.44	0.53
3:J:21:ILE:HG23	3:J:102:THR:HB	1.90	0.53
1:A:270:VAL:HG23	1:A:348:GLN:HG3	1.90	0.53
6:K:20:LEU:HD12	6:K:80:LEU:HD22	1.90	0.53
3:J:112:ALA:HB3	3:J:141:TYR:H	1.74	0.53
2:B:515:ILE:HG23	4:E:52:ASN:HB2	1.91	0.52
1:C:36:VAL:HG21	2:D:646:LEU:HD21	1.91	0.52
1:C:364:SER:O	9:i:1:NAG:H82	2.10	0.52
6:I:121:PRO:HD3	6:I:207:LYS:NZ	2.25	0.52
2:D:530:MET:HG3	2:D:626:MET:O	2.09	0.52
6:I:34:TRP:CZ3	6:I:94:THR:HG22	2.44	0.52
9:O:2:NAG:H83	9:O:2:NAG:H3	1.89	0.52
4:E:1:GLN:CD	4:E:1:GLN:N	2.68	0.52
2:B:618:ASN:OD1	2:B:619:LEU:N	2.43	0.52
3:L:47:ILE:HD12	3:L:47:ILE:N	2.25	0.52
3:L:118:LEU:HD12	3:L:134:VAL:O	2.10	0.52
6:K:100(D):VAL:O	6:K:100(F):ALA:N	2.36	0.52
1:A:67:ASN:ND2	1:A:72:HIS:HB2	2.25	0.51
1:A:347:LYS:HD2	1:A:350:ARG:HH12	1.74	0.51
2:D:596:TRP:CD1	2:D:647:GLU:HB3	2.45	0.51
3:L:143:GLY:HA3	3:L:173:TYR:CD2	2.46	0.51
9:O:1:NAG:H62	9:O:2:NAG:H82	1.91	0.51
1:A:85:HIS:HB3	4:E:27:TYR:HA	1.93	0.51
6:I:166:ALA:N	6:I:176:LEU:HD23	2.26	0.51
6:K:198:HIS:ND1	6:K:200:PRO:HD2	2.26	0.51
3:L:39:ARG:HH11	3:L:83:GLU:C	2.19	0.51
6:I:44:GLN:HG3	3:J:98:PHE:O	2.11	0.51
2:D:598:CYS:O	2:D:600:GLY:N	2.43	0.51
3:J:83:GLU:CD	3:J:167:LYS:HZ2	2.15	0.50
6:K:149:THR:OG1	6:K:197:ASN:HB3	2.11	0.50
1:A:210:PHE:HD2	1:A:377:ASN:HD21	1.57	0.50
1:C:386:ASN:HB3	1:C:417:PRO:HD2	1.93	0.50
1:C:396:ILE:HG22	1:C:398:ASN:H	1.76	0.50
5:H:126:LYS:NZ	6:I:115:LYS:HB2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HD11	1:C:435:TYR:HB2	1.94	0.50
1:A:332:ASN:HB3	1:A:413:SER:OG	2.11	0.50
1:A:45:TRP:HA	1:A:490:LYS:O	2.12	0.50
1:C:439:ILE:HB	1:C:443:ILE:HD11	1.93	0.50
2:D:570:VAL:C	2:D:572:GLY:H	2.20	0.50
1:A:179:LEU:CD1	1:A:419:ARG:HG2	2.40	0.50
2:D:608:VAL:HG21	2:D:646:LEU:HD23	1.93	0.50
6:I:180:VAL:HG12	6:I:182:VAL:HG13	1.93	0.50
6:I:199:LYS:HB2	6:I:200:PRO:HD3	1.93	0.50
6:K:194:CYS:SG	6:K:207:LYS:HB3	2.52	0.50
6:I:117:PRO:HB3	6:I:143:TYR:HB3	1.94	0.50
1:A:171:LYS:NZ	9:O:1:NAG:HN2	2.10	0.49
1:A:345:VAL:O	1:A:349:LEU:HG	2.12	0.49
2:B:598:CYS:O	2:B:600:GLY:N	2.44	0.49
1:C:298:ARG:NH2	1:C:439:ILE:O	2.45	0.49
1:C:476:ARG:HA	1:C:479:TRP:CD1	2.47	0.49
3:L:13:VAL:HG21	3:L:19:ALA:HA	1.94	0.49
5:F:123:GLU:HG3	6:K:115:LYS:HA	1.93	0.49
6:K:10:GLY:HA2	6:K:106:SER:O	2.11	0.49
2:B:626:MET:HE2	2:B:631:TRP:HA	1.94	0.49
1:C:350:ARG:HD3	1:C:355:ASN:O	2.11	0.49
1:C:67:ASN:ND2	1:C:72:HIS:HB2	2.27	0.49
1:C:183:GLN:HA	1:C:191:TYR:HA	1.95	0.49
3:L:61:ARG:HD2	3:L:77:SER:HB3	1.95	0.49
1:C:260:LEU:HD12	1:C:451:GLY:HA3	1.94	0.49
3:L:37:GLN:HB3	3:L:47:ILE:HD11	1.95	0.49
4:E:208:ASP:OD2	6:K:204:LYS:HD2	2.13	0.49
4:G:197:ASN:ND2	4:G:208:ASP:OD1	2.30	0.49
2:B:619:LEU:HD12	2:B:623:TRP:CD1	2.48	0.49
1:A:382:PHE:HE2	1:A:436:ALA:HB2	1.78	0.49
1:A:36:VAL:HG12	2:B:610:TRP:CE3	2.47	0.48
1:A:42:VAL:HG22	1:A:493:PRO:O	2.13	0.48
1:A:133:ASN:HD22	14:A:908:NAG:C7	2.25	0.48
1:C:460:SER:HA	1:C:461:THR:CG2	2.42	0.48
4:G:129:LYS:HD2	4:G:129:LYS:N	2.28	0.48
1:C:288:PHE:HE2	1:C:449:ILE:HG22	1.78	0.48
3:J:116:VAL:HG23	3:J:205:LYS:HE2	1.94	0.48
6:K:100(C):GLY:O	12:h:2:NAG:H2	2.13	0.48
1:A:85:HIS:CB	4:E:27:TYR:HA	2.43	0.48
4:E:1:GLN:CD	4:E:1:GLN:H3	2.20	0.48
6:I:63:LEU:HD22	6:I:66:ARG:HH21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ILE:O	2:B:646:LEU:HG	2.12	0.48
1:C:39:TYR:HD2	2:D:537:LEU:HD11	1.79	0.48
1:C:324:GLY:O	3:L:94:ARG:HD2	2.13	0.48
1:C:460:SER:HB2	1:C:462:ASN:HB2	1.95	0.48
3:L:121:PRO:HD3	3:L:133:LEU:HD23	1.94	0.48
6:K:6:GLU:N	6:K:6:GLU:OE1	2.46	0.48
1:A:173:TYR:CZ	1:A:305:LYS:NZ	2.82	0.48
1:C:164:GLU:HG3	1:C:312:GLY:HA3	1.96	0.48
4:E:98:TYR:HB2	4:E:100(C):VAL:HG21	1.94	0.48
1:C:490:LYS:HB2	2:D:585:ARG:HH12	1.79	0.48
6:I:162:HIS:CG	3:J:172:LYS:HZ2	2.31	0.48
1:C:122:LEU:HD13	1:C:125:LEU:HD11	1.96	0.48
9:j:1:NAG:H61	9:j:2:NAG:N2	2.28	0.48
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.48	0.48
5:F:31:ASN:HD21	7:M:4:MAN:H2	1.79	0.48
1:C:460:SER:HA	1:C:461:THR:HG22	1.96	0.48
3:L:21:ILE:O	3:L:72:THR:HA	2.14	0.48
1:C:122:LEU:HB3	1:C:125:LEU:CD1	2.44	0.47
1:C:204:ALA:HB2	1:C:434:MET:SD	2.53	0.47
6:K:188:GLY:HA3	6:K:189:THR:C	2.38	0.47
1:A:65:LYS:HG3	10:R:4:MAN:O4	2.14	0.47
1:A:171:LYS:HZ2	9:O:1:NAG:HN2	1.61	0.47
3:L:156:VAL:HG11	3:L:179:LEU:HD11	1.96	0.47
6:K:166:ALA:N	6:K:176:LEU:HD23	2.29	0.47
1:A:50:THR:HB	1:A:223:PHE:CE2	2.49	0.47
1:A:164:GLU:HG3	1:A:312:GLY:HA3	1.96	0.47
1:C:304:ARG:NH2	1:C:437:PRO:HB2	2.29	0.47
4:E:129:LYS:HE3	4:E:129:LYS:HA	1.96	0.47
2:B:519:PHE:CE2	2:B:521:GLY:HA2	2.50	0.47
3:L:34:ILE:HG23	3:L:49:TYR:HA	1.96	0.47
5:H:37:GLN:HB2	5:H:47:LEU:HD11	1.96	0.47
3:J:37:GLN:OE1	3:J:39:ARG:NH2	2.47	0.47
1:A:439:ILE:HB	1:A:443:ILE:HD11	1.96	0.47
1:A:104:MET:HE2	1:A:108:ILE:HD11	1.97	0.47
1:C:151:ARG:O	1:C:178:ARG:NH2	2.48	0.47
1:C:456:ARG:HD3	1:C:468:PHE:HE1	1.80	0.47
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.96	0.47
1:A:301:ASN:OD1	1:A:441:GLY:HA2	2.14	0.47
1:C:347:LYS:HD3	1:C:350:ARG:NH1	2.29	0.47
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.97	0.47
1:C:256:SER:O	1:C:478:ASN:ND2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:115:SER:HB2	3:J:127:GLN:HG2	1.96	0.46
6:I:11:LEU:HD12	6:I:145:PRO:HD3	1.97	0.46
6:I:12:VAL:HG21	6:I:18:LEU:HD13	1.96	0.46
6:K:180:VAL:HG12	6:K:182:VAL:HG13	1.97	0.46
1:A:396:ILE:HG22	1:A:397:SER:H	1.80	0.46
1:C:36:VAL:HG12	2:D:610:TRP:HE3	1.81	0.46
6:I:196:VAL:O	6:I:205:VAL:N	2.40	0.46
3:J:21:ILE:O	3:J:72:THR:HA	2.14	0.46
1:A:257:THR:O	1:A:259:LEU:N	2.47	0.46
7:M:3:BMA:O6	7:M:3:BMA:O4	2.30	0.46
6:K:121:PRO:HD3	6:K:207:LYS:CE	2.39	0.46
1:A:222:GLY:HA2	2:B:544:LEU:HD12	1.97	0.46
6:I:72:ASP:OD2	6:I:75:LYS:HD2	2.16	0.46
6:I:139:LEU:HD21	6:I:141:LYS:HB2	1.98	0.46
6:I:196:VAL:O	6:I:204:LYS:HA	2.15	0.46
1:A:170:GLN:HG2	1:A:172:VAL:HG13	1.97	0.45
5:F:123:GLU:OE2	6:K:116:GLY:N	2.46	0.45
5:F:126:LYS:HZ1	6:K:115:LYS:HB2	1.80	0.45
4:G:24:ALA:HB1	4:G:27:TYR:CE1	2.51	0.45
6:I:39:GLN:C	6:I:88:ALA:HB1	2.40	0.45
1:A:189:LYS:HE3	14:A:908:NAG:H82	1.97	0.45
1:A:490:LYS:HG2	2:B:585:ARG:HH22	1.82	0.45
1:C:65:LYS:HG3	10:e:4:MAN:O4	2.16	0.45
1:A:222:GLY:C	1:A:223:PHE:HD1	2.24	0.45
1:C:335:LYS:HA	1:C:414:ILE:HD11	1.98	0.45
2:D:519:PHE:CE2	2:D:521:GLY:HA2	2.51	0.45
2:D:522:PHE:CD1	2:D:543:ASN:HB2	2.52	0.45
6:K:196:VAL:N	6:K:205:VAL:O	2.37	0.45
1:A:299:PRO:HD2	1:A:329:ALA:HA	1.97	0.45
4:G:115:SER:HB3	3:J:127:GLN:CD	2.42	0.45
3:L:54:ARG:H	3:L:54:ARG:HG3	1.63	0.45
3:L:127:GLN:OE1	4:E:115:SER:O	2.35	0.45
4:E:197:ASN:ND2	4:E:208:ASP:OD1	2.35	0.45
6:K:144:PHE:HA	6:K:145:PRO:HA	1.77	0.45
2:B:635:ILE:O	2:B:639:THR:HG23	2.16	0.45
6:K:16:GLU:HG2	6:K:17:THR:H	1.82	0.45
6:I:33:TYR:HB2	6:I:95:THR:O	2.16	0.45
5:F:123:GLU:HA	5:F:126:LYS:HE2	1.98	0.45
1:A:179:LEU:HD22	1:A:369:LEU:HD22	1.99	0.45
1:C:95:MET:SD	1:C:273:ARG:HD3	2.57	0.45
6:K:18:LEU:HB3	6:K:82:LEU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:67:VAL:O	6:K:68:HIS:ND1	2.50	0.45
1:A:83:GLU:HG2	1:A:245:VAL:CG1	2.48	0.44
1:C:301:ASN:OD1	1:C:441:GLY:HA2	2.16	0.44
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.52	0.44
6:I:188:GLY:HA3	6:I:189:THR:C	2.40	0.44
3:J:181:LEU:HD22	3:J:185:GLN:HG2	1.99	0.44
6:K:191:THR:HG22	6:K:193:ILE:HG13	1.98	0.44
1:C:49:GLU:OE2	1:C:99:ASN:HB2	2.17	0.44
1:C:257:THR:O	1:C:259:LEU:N	2.48	0.44
3:L:49:TYR:O	3:L:53:ASP:HB2	2.17	0.44
4:E:208:ASP:O	6:K:202:ASN:O	2.36	0.44
2:B:631:TRP:O	2:B:635:ILE:HG12	2.17	0.44
1:C:37:THR:HG22	2:D:605:CYS:HA	1.99	0.44
1:C:202:THR:O	1:C:434:MET:HA	2.18	0.44
3:L:116:VAL:HA	3:L:136:LEU:O	2.18	0.44
3:J:116:VAL:HA	3:J:136:LEU:O	2.18	0.44
2:B:522:PHE:CE1	2:B:543:ASN:HB2	2.53	0.44
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.52	0.44
5:F:31:ASN:ND2	7:M:4:MAN:H2	2.32	0.44
4:G:96:LYS:HE2	5:H:49:TYR:CE2	2.53	0.44
4:G:151:THR:OG1	4:G:199:ASN:HB2	2.18	0.44
6:K:100(D):VAL:HG22	6:K:100(I):GLU:OE1	2.18	0.44
1:C:42:VAL:HG22	1:C:493:PRO:O	2.18	0.44
3:L:119:PHE:HB3	6:K:122:LEU:HD22	2.00	0.44
2:D:651:ASN:N	2:D:651:ASN:HD22	2.15	0.44
3:J:150:LYS:HB2	3:J:193:SER:OG	2.18	0.44
1:C:222:GLY:HA2	2:D:544:LEU:HD12	1.99	0.44
3:J:151:ALA:HB1	3:J:189:HIS:CD2	2.51	0.44
1:A:221:ALA:HB3	2:B:582:ALA:HB1	2.00	0.44
2:B:574:LYS:HD2	2:B:574:LYS:HA	1.83	0.44
2:B:619:LEU:HD12	2:B:623:TRP:HD1	1.82	0.44
5:H:123:GLU:HA	5:H:126:LYS:HE2	1.99	0.44
4:E:129:LYS:HD2	4:E:129:LYS:N	2.33	0.43
6:I:100(P):MET:SD	6:I:100(P):MET:N	2.91	0.43
3:J:20:ARG:HA	3:J:73:LEU:O	2.18	0.43
3:J:32:SER:HB3	3:J:91:TRP:HB2	2.00	0.43
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.85	0.43
2:B:536:THR:HG22	2:B:539:VAL:HB	2.01	0.43
4:E:24:ALA:HB1	4:E:27:TYR:CE1	2.54	0.43
6:I:49:GLY:HA2	3:J:96:TRP:CZ3	2.53	0.43
6:I:49:GLY:HA2	3:J:96:TRP:HZ3	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:136:LEU:HG	6:K:209:VAL:HG11	2.00	0.43
9:b:1:NAG:H62	9:b:2:NAG:H82	2.00	0.43
3:L:31:ARG:HA	3:L:91:TRP:O	2.17	0.43
4:E:94:ARG:NH2	4:E:101:ASP:OD2	2.28	0.43
4:G:94:ARG:NH2	4:G:101:ASP:OD2	2.38	0.43
6:K:50:TYR:CE1	6:K:58:ASN:HB3	2.54	0.43
1:C:270:VAL:HG23	1:C:348:GLN:HG3	2.00	0.43
4:E:204:ASN:HB3	6:K:208:ARG:H	1.83	0.43
4:G:168:ALA:HA	4:G:178:LEU:HB3	2.00	0.43
6:I:20:LEU:HD12	6:I:80:LEU:HD22	2.01	0.43
6:I:145:PRO:HD2	6:I:200:PRO:CB	2.48	0.43
6:I:165:PRO:HG3	3:J:166:SER:OG	2.18	0.43
6:I:194:CYS:O	6:I:206:ASP:HA	2.19	0.43
6:K:33:TYR:HB2	6:K:95:THR:O	2.17	0.43
1:A:324:GLY:O	3:J:94:ARG:HD2	2.19	0.43
3:L:149:TRP:CD1	3:L:160:VAL:HG12	2.53	0.43
1:A:65:LYS:HE3	10:R:4:MAN:O3	2.19	0.43
3:L:54:ARG:HH12	3:L:60:ASP:HA	1.80	0.43
4:G:11:VAL:HG22	4:G:110:THR:HB	1.99	0.43
3:J:17:GLN:O	3:J:78:VAL:HG23	2.18	0.43
1:A:451:GLY:O	1:A:452:LEU:HD23	2.18	0.43
3:L:119:PHE:CD1	6:K:122:LEU:HB3	2.54	0.43
6:K:114:THR:HG22	6:K:201:SER:OG	2.18	0.43
1:C:119:CYS:HB3	1:C:203:GLN:O	2.19	0.43
3:L:174:ALA:HB1	6:K:164:PHE:CD2	2.54	0.43
3:J:105:ILE:HD12	3:J:105:ILE:N	2.33	0.43
1:A:50:THR:OG1	1:A:51:THR:N	2.52	0.43
1:C:170:GLN:HG2	1:C:172:VAL:HG13	2.00	0.43
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.54	0.43
5:F:120:PRO:HD3	5:F:132:VAL:HG22	2.01	0.43
6:I:126:SER:C	6:I:134:ALA:HA	2.43	0.43
6:K:151:SER:OG	6:K:195:ASN:HB2	2.19	0.43
1:A:169:LYS:HB2	1:A:169:LYS:HE2	1.82	0.42
3:J:54:ARG:CZ	3:J:58:ILE:O	2.66	0.42
3:J:121:PRO:HD3	3:J:133:LEU:CD2	2.49	0.42
3:L:21:ILE:HG23	3:L:102:THR:HB	2.00	0.42
3:L:39:ARG:CZ	3:L:81:GLY:O	2.67	0.42
2:D:635:ILE:O	2:D:639:THR:HG23	2.19	0.42
1:A:223:PHE:HD1	1:A:223:PHE:N	2.18	0.42
1:A:223:PHE:CD1	1:A:223:PHE:N	2.87	0.42
1:A:350:ARG:HD3	1:A:355:ASN:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:31:ARG:HA	3:J:91:TRP:O	2.19	0.42
3:J:54:ARG:NH2	3:J:58:ILE:O	2.53	0.42
2:D:525:ALA:HB1	2:D:528:SER:HB2	2.01	0.42
6:I:37:ILE:HD13	6:I:101:TRP:CZ3	2.54	0.42
3:L:147:VAL:HG11	3:L:177:SER:OG	2.19	0.42
1:A:476:ARG:O	1:A:480:ARG:HG3	2.19	0.42
1:C:437:PRO:HA	1:C:438:PRO:HD3	1.96	0.42
3:L:112:ALA:HB3	3:L:141:TYR:H	1.83	0.42
3:L:125:GLU:HG3	3:L:130:LYS:O	2.20	0.42
3:L:146:THR:OG1	3:L:197:THR:HB	2.19	0.42
3:L:186:TRP:HH2	3:L:207:VAL:HG22	1.84	0.42
1:A:169:LYS:H	1:A:169:LYS:HD3	1.85	0.42
1:A:229:LYS:O	4:E:1:GLN:HG2	2.20	0.42
2:B:522:PHE:CD1	2:B:543:ASN:HB2	2.55	0.42
3:L:152:ASP:OD1	3:L:189:HIS:HB3	2.20	0.42
6:I:162:HIS:CG	3:J:172:LYS:NZ	2.88	0.42
1:A:160:ASN:HD22	9:O:1:NAG:H83	1.85	0.42
1:A:229:LYS:HE3	1:A:243:SER:OG	2.18	0.42
1:C:67:ASN:OD1	1:C:72:HIS:HB2	2.19	0.42
5:H:47:LEU:HA	5:H:58:VAL:HG21	2.02	0.42
1:A:347:LYS:HD2	1:A:350:ARG:NH1	2.35	0.41
1:C:349:LEU:HD13	1:C:468:PHE:CE2	2.55	0.41
4:E:207:VAL:HG13	6:K:203:THR:HG23	2.01	0.41
2:D:522:PHE:CE1	2:D:543:ASN:HB2	2.55	0.41
6:K:198:HIS:O	6:K:202:ASN:N	2.53	0.41
1:C:206:PRO:CG	1:C:318:TYR:HE2	2.30	0.41
1:C:307:ILE:HD11	1:C:317:PHE:HD2	1.85	0.41
6:K:12:VAL:HG21	6:K:18:LEU:HD13	2.02	0.41
4:G:159:LEU:HD21	4:G:182:VAL:HG21	2.01	0.41
1:A:335:LYS:HG2	1:A:414:ILE:CG1	2.50	0.41
1:C:124:PRO:O	1:C:161:MET:HE1	2.21	0.41
1:C:216:HIS:ND1	1:C:248:THR:O	2.40	0.41
6:I:10:GLY:HA2	6:I:106:SER:O	2.20	0.41
3:J:39:ARG:CZ	3:J:81:GLY:O	2.69	0.41
1:C:55:ALA:HA	1:C:75:VAL:O	2.20	0.41
1:C:104:MET:O	1:C:108:ILE:HG12	2.21	0.41
1:C:451:GLY:O	1:C:452:LEU:HD23	2.21	0.41
6:K:100(P):MET:SD	6:K:100(P):MET:N	2.94	0.41
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.56	0.41
1:A:199:SER:HB2	1:A:431:GLY:HA2	2.03	0.41
1:C:131:CYS:HA	1:C:157:CYS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:96:LYS:HE2	5:H:49:TYR:CZ	2.55	0.41
6:K:39:GLN:C	6:K:88:ALA:HB1	2.46	0.41
6:K:197:ASN:OD1	6:K:198:HIS:N	2.53	0.41
1:A:53:PHE:CE2	1:A:218:CYS:HB2	2.56	0.41
1:C:329:ALA:C	1:C:418:CYS:HB2	2.46	0.41
1:C:345:VAL:O	1:C:349:LEU:HG	2.21	0.41
5:F:6:GLN:HA	5:F:22:THR:O	2.20	0.41
6:I:188:GLY:HA3	6:I:190:GLN:H	1.84	0.41
3:J:39:ARG:NH1	3:J:81:GLY:O	2.54	0.41
1:A:307:ILE:HD11	1:A:317:PHE:CD2	2.54	0.41
1:A:382:PHE:CE2	1:A:436:ALA:HB2	2.56	0.41
1:A:460:SER:HB3	1:A:462:ASN:CA	2.51	0.41
1:C:101:VAL:HG21	1:C:480:ARG:HG2	2.01	0.41
1:C:298:ARG:NH1	1:C:381:GLU:OE2	2.49	0.41
4:E:35:HIS:CG	4:E:100(E):MET:HE2	2.55	0.41
4:G:115:SER:CB	3:J:127:GLN:HG2	2.51	0.41
2:D:595:ILE:HD12	2:D:647:GLU:OE2	2.21	0.41
6:I:29:VAL:CG1	6:I:71:LEU:HD22	2.50	0.41
3:J:25:GLU:CG	3:J:26:GLU:N	2.84	0.41
6:K:67:VAL:C	6:K:68:HIS:ND1	2.79	0.41
6:K:72:ASP:OD1	6:K:74:SER:OG	2.31	0.41
12:U:8:MAN:H2	12:U:9:MAN:H2	1.81	0.41
1:C:74:CYS:HB2	2:D:571:TRP:CH2	2.55	0.41
2:B:657:GLU:O	2:B:661:LEU:HG	2.20	0.40
1:C:84:ILE:HD13	2:D:522:PHE:N	2.36	0.40
6:K:123:ALA:HA	6:K:124:PRO:HD3	1.97	0.40
1:A:112:TRP:CD2	1:A:427:TRP:HZ3	2.39	0.40
1:C:290:THR:OG1	1:C:344:LYS:NZ	2.54	0.40
1:C:490:LYS:HB2	2:D:585:ARG:NH1	2.36	0.40
4:E:208:ASP:O	6:K:203:THR:HA	2.22	0.40
6:I:150:VAL:HA	6:I:195:ASN:O	2.21	0.40
2:B:643:TYR:O	2:B:647:GLU:HG3	2.21	0.40
4:G:193:THR:HG23	4:G:210:LYS:HE3	2.03	0.40
6:I:121:PRO:O	3:J:122:SER:HB3	2.21	0.40
6:I:124:PRO:HG3	6:I:136:LEU:HD12	2.04	0.40
6:I:162:HIS:ND1	3:J:172:LYS:NZ	2.70	0.40
6:K:151:SER:O	6:K:195:ASN:N	2.34	0.40
1:A:74:CYS:HB2	2:B:571:TRP:CH2	2.56	0.40
1:A:112:TRP:CG	1:A:427:TRP:HZ3	2.39	0.40
1:A:119:CYS:HB3	1:A:203:GLN:O	2.22	0.40
1:A:155:LYS:HD3	1:A:155:LYS:HA	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:THR:O	2:B:536:THR:HG22	2.21	0.40
4:E:94:ARG:O	4:E:100(E):MET:HA	2.21	0.40
2:D:616:ASN:OD1	2:D:616:ASN:N	2.54	0.40
5:H:115:VAL:HA	5:H:135:LEU:O	2.21	0.40
6:K:53:ASP:OD1	6:K:54:SER:N	2.44	0.40
1:C:396:ILE:CG2	1:C:397:SER:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/481 (93%)	405 (90%)	38 (8%)	6 (1%)	9	41
1	C	444/481 (92%)	402 (90%)	37 (8%)	5 (1%)	11	45
2	B	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	7	37
2	D	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	7	37
3	J	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	12	47
3	L	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	12	47
4	E	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
4	G	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
5	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
5	H	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
6	I	224/235 (95%)	213 (95%)	9 (4%)	2 (1%)	14	49
6	K	224/235 (95%)	212 (95%)	10 (4%)	2 (1%)	14	49
All	All	2875/3028 (95%)	2691 (94%)	161 (6%)	23 (1%)	16	52

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	C	138	ILE
3	L	110	PRO
3	J	110	PRO
1	A	71	THR
1	C	71	THR
1	A	151	ARG
1	A	152	GLY
2	B	602	LEU
1	C	152	GLY
2	D	602	LEU
1	A	258	GLN
1	C	151	ARG
1	C	258	GLN
3	L	199	GLU
6	K	142	ASP
2	B	601	LYS
2	D	601	LYS
6	I	142	ASP
3	J	199	GLU
1	A	505	VAL
6	K	188	GLY
6	I	188	GLY

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	405/428 (95%)	405 (100%)	0	100	100
1	C	401/428 (94%)	401 (100%)	0	100	100
2	B	110/129 (85%)	110 (100%)	0	100	100
2	D	110/129 (85%)	110 (100%)	0	100	100
3	J	178/178 (100%)	178 (100%)	0	100	100
3	L	178/178 (100%)	177 (99%)	1 (1%)	78	80
4	E	187/187 (100%)	187 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	187/187 (100%)	187 (100%)	0	100	100
5	F	185/185 (100%)	185 (100%)	0	100	100
5	H	185/185 (100%)	185 (100%)	0	100	100
6	I	198/205 (97%)	198 (100%)	0	100	100
6	K	198/205 (97%)	198 (100%)	0	100	100
All	All	2522/2624 (96%)	2521 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	60	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	188	ASN
2	B	543	ASN
2	B	650	GLN
2	B	651	ASN
1	C	67	ASN
4	G	100	ASN
2	D	540	GLN
2	D	543	ASN
6	I	190	GLN
6	I	202	ASN
3	J	189	HIS
6	K	44	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

100 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	$\# Z > 2$
7	NAG	M	1	1,7	14,14,15	0.35	0	17,19,21	0.48	0
7	NAG	M	2	7	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
7	BMA	M	3	7	11,11,12	0.64	0	15,15,17	0.86	1 (6%)
7	MAN	M	4	7	11,11,12	0.83	0	15,15,17	1.41	2 (13%)
7	MAN	M	5	7	11,11,12	1.22	1 (9%)	15,15,17	1.02	1 (6%)
7	MAN	M	6	7	11,11,12	4.17	8 (72%)	15,15,17	2.66	5 (33%)
7	MAN	M	7	7	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
8	NAG	N	1	8,1	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	N	2	8	14,14,15	0.25	0	17,19,21	0.42	0
8	BMA	N	3	8	11,11,12	0.68	0	15,15,17	0.72	0
8	MAN	N	4	8	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
8	MAN	N	5	8	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
9	NAG	O	1	9,1	14,14,15	0.24	0	17,19,21	0.48	0
9	NAG	O	2	9	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
9	NAG	P	1	9,1	14,14,15	0.20	0	17,19,21	0.44	0
9	NAG	P	2	9	14,14,15	0.32	0	17,19,21	0.44	0
9	NAG	Q	1	9,1	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	Q	2	9	14,14,15	0.29	0	17,19,21	0.40	0
10	NAG	R	1	10	14,14,15	0.19	0	17,19,21	0.55	0
10	NAG	R	2	10	14,14,15	0.30	0	17,19,21	0.54	0
10	BMA	R	3	10	11,11,12	0.56	0	15,15,17	0.64	0
10	MAN	R	4	10	11,11,12	0.52	0	15,15,17	1.03	2 (13%)
10	MAN	R	5	10	11,11,12	0.85	0	15,15,17	1.17	2 (13%)
10	MAN	R	6	10	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
11	NAG	S	1	1,11	14,14,15	0.44	0	17,19,21	0.55	0
11	NAG	S	2	11	14,14,15	0.44	0	17,19,21	0.67	1 (5%)
11	BMA	S	3	11	11,11,12	1.23	1 (9%)	15,15,17	0.97	1 (6%)
9	NAG	T	1	9,1	14,14,15	0.26	0	17,19,21	0.40	0
9	NAG	T	2	9	14,14,15	0.31	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	U	1	1,12	14,14,15	0.17	0	17,19,21	0.46	0
12	MAN	U	10	12	11,11,12	0.68	0	15,15,17	0.94	2 (13%)
12	NAG	U	2	12	14,14,15	0.22	0	17,19,21	0.55	0
12	BMA	U	3	12	11,11,12	0.78	0	15,15,17	1.20	1 (6%)
12	MAN	U	4	12	11,11,12	0.60	0	15,15,17	1.04	1 (6%)
12	MAN	U	5	12	11,11,12	0.77	0	15,15,17	0.96	1 (6%)
12	MAN	U	6	12	11,11,12	0.77	1 (9%)	15,15,17	1.32	1 (6%)
12	MAN	U	7	12	11,11,12	0.57	0	15,15,17	0.89	1 (6%)
12	MAN	U	8	12	11,11,12	0.72	0	15,15,17	0.97	2 (13%)
12	MAN	U	9	12	11,11,12	0.87	1 (9%)	15,15,17	1.13	1 (6%)
9	NAG	V	1	9	14,14,15	0.28	0	17,19,21	0.39	0
9	NAG	V	2	9	14,14,15	0.25	0	17,19,21	0.43	0
9	NAG	W	1	9,1	14,14,15	0.27	0	17,19,21	0.65	0
9	NAG	W	2	9	14,14,15	0.30	0	17,19,21	0.45	0
9	NAG	X	1	9,1	14,14,15	0.20	0	17,19,21	0.45	0
9	NAG	X	2	9	14,14,15	0.27	0	17,19,21	0.45	0
11	NAG	Y	1	1,11	14,14,15	0.74	1 (7%)	17,19,21	0.56	0
11	NAG	Y	2	11	14,14,15	0.27	0	17,19,21	0.44	0
11	BMA	Y	3	11	11,11,12	0.61	0	15,15,17	0.75	0
7	NAG	Z	1	1,7	14,14,15	0.42	0	17,19,21	0.58	0
7	NAG	Z	2	7	14,14,15	0.65	0	17,19,21	1.65	3 (17%)
7	BMA	Z	3	7	11,11,12	1.46	1 (9%)	15,15,17	1.54	2 (13%)
7	MAN	Z	4	7	11,11,12	1.63	2 (18%)	15,15,17	1.15	1 (6%)
7	MAN	Z	5	7	11,11,12	2.47	4 (36%)	15,15,17	2.46	8 (53%)
7	MAN	Z	6	7	11,11,12	1.70	1 (9%)	15,15,17	1.23	1 (6%)
7	MAN	Z	7	7	11,11,12	1.16	2 (18%)	15,15,17	1.22	2 (13%)
8	NAG	a	1	8,1	14,14,15	0.32	0	17,19,21	0.42	0
8	NAG	a	2	8	14,14,15	0.24	0	17,19,21	0.41	0
8	BMA	a	3	8	11,11,12	0.77	0	15,15,17	0.71	0
8	MAN	a	4	8	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
8	MAN	a	5	8	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
9	NAG	b	1	9,1	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	b	2	9	14,14,15	0.57	0	17,19,21	1.36	2 (11%)
9	NAG	c	1	9,1	14,14,15	0.22	0	17,19,21	0.45	0
9	NAG	c	2	9	14,14,15	0.31	0	17,19,21	0.44	0
9	NAG	d	1	9,1	14,14,15	0.27	0	17,19,21	0.42	0
9	NAG	d	2	9	14,14,15	0.31	0	17,19,21	0.41	0
10	NAG	e	1	1,10	14,14,15	0.45	0	17,19,21	0.58	0
10	NAG	e	2	10	14,14,15	0.26	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	e	3	10	11,11,12	0.67	0	15,15,17	0.73	0
10	MAN	e	4	10	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
10	MAN	e	5	10	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
10	MAN	e	6	10	11,11,12	0.57	0	15,15,17	1.00	2 (13%)
9	NAG	f	1	9,1	14,14,15	0.53	0	17,19,21	0.54	0
9	NAG	f	2	9	14,14,15	0.33	0	17,19,21	0.39	0
9	NAG	g	1	9,1	14,14,15	0.23	0	17,19,21	0.39	0
9	NAG	g	2	9	14,14,15	0.30	0	17,19,21	0.46	0
12	NAG	h	1	1,12	14,14,15	0.20	0	17,19,21	0.48	0
12	MAN	h	10	12	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
12	NAG	h	2	12	14,14,15	0.22	0	17,19,21	0.58	0
12	BMA	h	3	12	11,11,12	0.65	0	15,15,17	1.18	1 (6%)
12	MAN	h	4	12	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
12	MAN	h	5	12	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
12	MAN	h	6	12	11,11,12	0.86	1 (9%)	15,15,17	1.32	1 (6%)
12	MAN	h	7	12	11,11,12	0.65	0	15,15,17	0.89	2 (13%)
12	MAN	h	8	12	11,11,12	0.68	0	15,15,17	0.95	1 (6%)
12	MAN	h	9	12	11,11,12	0.85	0	15,15,17	1.23	2 (13%)
9	NAG	i	1	9,1	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	i	2	9	14,14,15	0.27	0	17,19,21	0.48	0
9	NAG	j	1	9,1	14,14,15	0.44	0	17,19,21	0.69	0
9	NAG	j	2	9	14,14,15	0.35	0	17,19,21	0.45	0
11	NAG	k	1	1,11	14,14,15	0.40	0	17,19,21	0.58	0
11	NAG	k	2	11	14,14,15	0.37	0	17,19,21	0.75	0
11	BMA	k	3	11	11,11,12	0.72	0	15,15,17	0.86	1 (6%)
11	NAG	l	1	1,11	14,14,15	0.36	0	17,19,21	0.62	0
11	NAG	l	2	11	14,14,15	0.31	0	17,19,21	0.37	0
11	BMA	l	3	11	11,11,12	0.55	0	15,15,17	0.78	0
13	NAG	m	1	13,1	14,14,15	0.42	0	17,19,21	0.55	0
13	NAG	m	2	13	14,14,15	0.37	0	17,19,21	0.39	0
13	BMA	m	3	13	11,11,12	0.59	0	15,15,17	0.73	0
13	MAN	m	4	13,6	11,11,12	0.93	1 (9%)	15,15,17	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	4/6/23/26	0/1/1/1
7	BMA	M	3	7	-	2/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	1/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
7	MAN	M	6	7	-	0/2/19/22	1/1/1/1
7	MAN	M	7	7	-	0/2/19/22	0/1/1/1
8	NAG	N	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	2/6/23/26	0/1/1/1
8	BMA	N	3	8	-	2/2/19/22	0/1/1/1
8	MAN	N	4	8	-	1/2/19/22	0/1/1/1
8	MAN	N	5	8	-	0/2/19/22	0/1/1/1
9	NAG	O	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	O	2	9	-	5/6/23/26	0/1/1/1
9	NAG	P	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	P	2	9	-	2/6/23/26	0/1/1/1
9	NAG	Q	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	1/6/23/26	0/1/1/1
10	NAG	R	1	10	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	0/2/19/22	0/1/1/1
10	MAN	R	4	10	-	2/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	1/1/1/1
10	MAN	R	6	10	-	0/2/19/22	0/1/1/1
11	NAG	S	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	S	2	11	-	1/6/23/26	0/1/1/1
11	BMA	S	3	11	-	2/2/19/22	0/1/1/1
9	NAG	T	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
12	NAG	U	1	1,12	-	2/6/23/26	0/1/1/1
12	MAN	U	10	12	-	0/2/19/22	0/1/1/1
12	NAG	U	2	12	-	4/6/23/26	0/1/1/1
12	BMA	U	3	12	-	0/2/19/22	0/1/1/1
12	MAN	U	4	12	-	0/2/19/22	0/1/1/1
12	MAN	U	5	12	-	0/2/19/22	0/1/1/1
12	MAN	U	6	12	-	1/2/19/22	0/1/1/1
12	MAN	U	7	12	-	2/2/19/22	0/1/1/1
12	MAN	U	8	12	-	0/2/19/22	0/1/1/1
12	MAN	U	9	12	-	0/2/19/22	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	V	1	9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	NAG	W	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	NAG	X	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
11	NAG	Y	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	1/2/19/22	0/1/1/1
7	NAG	Z	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	4/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	1/1/1/1
7	MAN	Z	5	7	-	1/2/19/22	1/1/1/1
7	MAN	Z	6	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	7	7	-	0/2/19/22	0/1/1/1
8	NAG	a	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	1/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1
9	NAG	b	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	b	2	9	-	6/6/23/26	0/1/1/1
9	NAG	c	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	1/6/23/26	0/1/1/1
10	NAG	e	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	0/2/19/22	0/1/1/1
10	MAN	e	4	10	-	2/2/19/22	0/1/1/1
10	MAN	e	5	10	-	0/2/19/22	1/1/1/1
10	MAN	e	6	10	-	0/2/19/22	0/1/1/1
9	NAG	f	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	1/6/23/26	0/1/1/1
9	NAG	g	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
12	NAG	h	1	1,12	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	h	10	12	-	0/2/19/22	0/1/1/1
12	NAG	h	2	12	-	4/6/23/26	0/1/1/1
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	MAN	h	4	12	-	0/2/19/22	0/1/1/1
12	MAN	h	5	12	-	0/2/19/22	0/1/1/1
12	MAN	h	6	12	-	1/2/19/22	0/1/1/1
12	MAN	h	7	12	-	2/2/19/22	0/1/1/1
12	MAN	h	8	12	-	0/2/19/22	0/1/1/1
12	MAN	h	9	12	-	0/2/19/22	1/1/1/1
9	NAG	i	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
9	NAG	j	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
11	NAG	k	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	k	2	11	-	1/6/23/26	0/1/1/1
11	BMA	k	3	11	-	0/2/19/22	0/1/1/1
11	NAG	l	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	l	2	11	-	0/6/23/26	0/1/1/1
11	BMA	l	3	11	-	2/2/19/22	0/1/1/1
13	NAG	m	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	m	2	13	-	1/6/23/26	0/1/1/1
13	BMA	m	3	13	-	0/2/19/22	0/1/1/1
13	MAN	m	4	13,6	-	1/2/19/22	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	6	MAN	O5-C5	7.43	1.57	1.43
7	M	6	MAN	O2-C2	5.61	1.55	1.43
7	M	6	MAN	C4-C5	5.37	1.64	1.53
7	M	6	MAN	C2-C3	5.20	1.60	1.52
7	Z	5	MAN	C1-C2	4.55	1.63	1.52
7	Z	6	MAN	C1-C2	4.51	1.63	1.52
7	Z	4	MAN	C1-C2	4.29	1.62	1.52
7	Z	3	BMA	O5-C1	-4.14	1.36	1.43
7	Z	5	MAN	O5-C5	3.87	1.51	1.43
7	Z	5	MAN	C4-C5	3.64	1.60	1.53
7	M	6	MAN	C4-C3	3.57	1.61	1.52
7	M	6	MAN	O4-C4	-3.55	1.34	1.43
7	M	6	MAN	O3-C3	3.47	1.51	1.43
7	Z	5	MAN	C2-C3	3.44	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	5	MAN	O5-C1	-3.25	1.38	1.43
7	M	6	MAN	O5-C1	-2.63	1.39	1.43
7	Z	7	MAN	O5-C1	-2.52	1.39	1.43
7	Z	7	MAN	O5-C5	2.39	1.48	1.43
13	m	4	MAN	C1-C2	2.38	1.57	1.52
11	Y	1	NAG	O5-C1	2.30	1.47	1.43
12	h	6	MAN	C1-C2	2.28	1.57	1.52
11	S	3	BMA	O5-C5	2.20	1.47	1.43
7	Z	4	MAN	C4-C5	2.10	1.57	1.53
12	U	6	MAN	C1-C2	2.06	1.57	1.52
12	U	9	MAN	C1-C2	2.01	1.57	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	6	MAN	O3-C3-C2	6.02	122.33	110.05
7	Z	5	MAN	C1-C2-C3	5.10	117.07	109.64
7	M	6	MAN	C3-C4-C5	-5.07	101.05	110.23
7	Z	2	NAG	C2-N2-C7	4.83	129.37	122.90
9	O	2	NAG	C2-N2-C7	4.72	129.22	122.90
7	M	2	NAG	C2-N2-C7	4.70	129.20	122.90
9	b	2	NAG	C2-N2-C7	4.70	129.20	122.90
7	Z	3	BMA	O6-C6-C5	-4.44	96.22	111.33
12	h	6	MAN	C1-O5-C5	4.28	117.92	112.19
7	Z	5	MAN	O5-C5-C6	4.23	115.90	107.66
12	U	6	MAN	C1-O5-C5	4.16	117.76	112.19
7	M	4	MAN	C1-O5-C5	3.94	117.47	112.19
7	Z	6	MAN	C1-O5-C5	3.89	117.39	112.19
12	h	9	MAN	C1-O5-C5	3.78	117.25	112.19
7	Z	5	MAN	O5-C5-C4	3.59	119.56	110.83
10	R	5	MAN	C1-O5-C5	3.54	116.93	112.19
7	M	6	MAN	O5-C5-C6	3.53	114.53	107.66
10	e	5	MAN	C1-O5-C5	3.52	116.90	112.19
7	Z	2	NAG	O4-C4-C5	-3.42	100.89	109.32
12	U	9	MAN	C1-O5-C5	3.42	116.77	112.19
12	h	5	MAN	C1-O5-C5	3.17	116.44	112.19
12	U	4	MAN	C1-O5-C5	3.09	116.33	112.19
12	h	4	MAN	C1-O5-C5	2.97	116.17	112.19
12	U	5	MAN	C1-O5-C5	2.97	116.17	112.19
7	M	6	MAN	O2-C2-C1	2.95	115.97	109.22
7	Z	4	MAN	O5-C5-C6	-2.82	102.17	107.66
12	U	3	BMA	C1-O5-C5	2.82	115.96	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	e	4	MAN	C1-O5-C5	2.80	115.94	112.19
12	h	3	BMA	C1-O5-C5	2.76	115.89	112.19
7	Z	7	MAN	O2-C2-C3	-2.74	104.47	110.15
10	R	4	MAN	C1-O5-C5	2.74	115.85	112.19
12	h	8	MAN	C1-O5-C5	2.71	115.82	112.19
10	R	6	MAN	C1-O5-C5	2.71	115.81	112.19
12	U	8	MAN	C1-O5-C5	2.64	115.72	112.19
7	M	7	MAN	C1-O5-C5	2.64	115.72	112.19
7	M	6	MAN	C6-C5-C4	2.62	119.46	113.02
8	a	4	MAN	C1-O5-C5	2.57	115.63	112.19
10	e	6	MAN	C1-O5-C5	2.57	115.63	112.19
7	Z	5	MAN	C6-C5-C4	2.48	119.12	113.02
8	a	5	MAN	C1-O5-C5	2.47	115.50	112.19
7	M	5	MAN	O2-C2-C3	-2.47	105.04	110.15
8	N	4	MAN	C1-O5-C5	2.46	115.49	112.19
7	Z	7	MAN	C1-O5-C5	2.44	115.46	112.19
10	R	4	MAN	O2-C2-C3	-2.43	105.12	110.15
7	Z	5	MAN	C1-O5-C5	2.42	115.43	112.19
7	Z	3	BMA	O2-C2-C3	-2.41	105.16	110.15
7	Z	2	NAG	C1-C2-N2	2.40	114.22	110.43
7	M	2	NAG	C1-C2-N2	2.38	114.18	110.43
8	N	5	MAN	C1-O5-C5	2.37	115.36	112.19
12	h	10	MAN	C1-O5-C5	2.36	115.35	112.19
13	m	4	MAN	C1-O5-C5	2.34	115.32	112.19
9	b	2	NAG	C1-C2-N2	2.27	114.01	110.43
12	U	10	MAN	C1-O5-C5	2.26	115.22	112.19
12	h	10	MAN	O2-C2-C3	-2.21	105.58	110.15
7	M	4	MAN	O2-C2-C3	-2.19	105.62	110.15
7	Z	5	MAN	O3-C3-C2	2.18	114.50	110.05
10	e	4	MAN	O2-C2-C3	-2.17	105.65	110.15
8	N	5	MAN	O2-C2-C3	-2.17	105.66	110.15
7	Z	5	MAN	C3-C4-C5	-2.13	106.37	110.23
7	Z	5	MAN	O2-C2-C3	-2.11	105.77	110.15
7	M	3	BMA	O6-C6-C5	-2.11	104.15	111.33
11	S	3	BMA	O2-C2-C3	-2.09	105.83	110.15
10	R	5	MAN	O2-C2-C3	-2.08	105.84	110.15
10	e	5	MAN	O2-C2-C3	-2.07	105.86	110.15
11	S	2	NAG	O4-C4-C5	-2.07	104.23	109.32
12	h	9	MAN	O2-C2-C3	-2.06	105.89	110.15
11	k	3	BMA	C1-O5-C5	2.06	114.94	112.19
7	M	7	MAN	O2-C2-C3	-2.05	105.90	110.15
9	O	2	NAG	C1-C2-N2	2.05	113.66	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	10	MAN	O2-C2-C3	-2.04	105.92	110.15
12	U	7	MAN	C1-O5-C5	2.04	114.92	112.19
12	h	7	MAN	C1-O5-C5	2.03	114.90	112.19
12	U	8	MAN	O2-C2-C3	-2.02	105.96	110.15
12	h	7	MAN	O2-C2-C3	-2.02	105.96	110.15
8	N	4	MAN	O2-C2-C3	-2.02	105.97	110.15
8	a	5	MAN	O2-C2-C3	-2.01	105.98	110.15
10	e	6	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	3	BMA	C4-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
12	U	2	NAG	O5-C5-C6-O6
7	Z	3	BMA	C4-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
7	M	3	BMA	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
11	S	1	NAG	O5-C5-C6-O6
12	h	2	NAG	O5-C5-C6-O6
9	g	2	NAG	O5-C5-C6-O6
10	R	4	MAN	O5-C5-C6-O6
10	e	4	MAN	O5-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
11	l	3	BMA	O5-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6
9	g	2	NAG	C4-C5-C6-O6
12	U	2	NAG	C4-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
13	m	1	NAG	O5-C5-C6-O6
7	M	3	BMA	C4-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
11	S	1	NAG	C4-C5-C6-O6
7	Z	3	BMA	O5-C5-C6-O6
10	R	4	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	T	2	NAG	C4-C5-C6-O6
9	d	1	NAG	C4-C5-C6-O6
10	e	4	MAN	C4-C5-C6-O6
13	m	1	NAG	C4-C5-C6-O6
8	N	1	NAG	C4-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
12	h	2	NAG	C4-C5-C6-O6
8	N	2	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	j	1	NAG	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2
9	O	1	NAG	C8-C7-N2-C2
9	O	1	NAG	O7-C7-N2-C2
9	O	2	NAG	C8-C7-N2-C2
9	O	2	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	b	1	NAG	C8-C7-N2-C2
9	b	1	NAG	O7-C7-N2-C2
9	b	2	NAG	C8-C7-N2-C2
9	b	2	NAG	O7-C7-N2-C2
9	c	1	NAG	C8-C7-N2-C2
9	c	1	NAG	O7-C7-N2-C2
11	Y	1	NAG	C8-C7-N2-C2
11	Y	1	NAG	O7-C7-N2-C2
11	l	1	NAG	C8-C7-N2-C2
11	l	1	NAG	O7-C7-N2-C2
9	W	1	NAG	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
9	d	1	NAG	O5-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
9	f	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	Y	3	BMA	O5-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
12	U	7	MAN	O5-C5-C6-O6
12	h	7	MAN	O5-C5-C6-O6
11	S	3	BMA	C4-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
12	U	7	MAN	C4-C5-C6-O6
12	h	7	MAN	C4-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
12	U	6	MAN	O5-C5-C6-O6
12	h	6	MAN	O5-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
7	Z	5	MAN	O5-C5-C6-O6
8	N	4	MAN	O5-C5-C6-O6
8	a	4	MAN	O5-C5-C6-O6
13	m	4	MAN	O5-C5-C6-O6
13	m	2	NAG	O5-C5-C6-O6
11	l	3	BMA	C4-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
9	P	2	NAG	C4-C5-C6-O6
11	S	3	BMA	O5-C5-C6-O6
9	W	1	NAG	C1-C2-N2-C7
9	j	1	NAG	C1-C2-N2-C7
12	U	2	NAG	C1-C2-N2-C7
9	i	1	NAG	C4-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
12	U	1	NAG	C4-C5-C6-O6
11	k	2	NAG	O5-C5-C6-O6
9	j	1	NAG	C3-C2-N2-C7
12	h	2	NAG	C3-C2-N2-C7
9	b	2	NAG	C4-C5-C6-O6
12	U	1	NAG	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
11	S	2	NAG	C4-C5-C6-O6
7	M	2	NAG	C1-C2-N2-C7
7	Z	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	O	2	NAG	C1-C2-N2-C7
9	b	2	NAG	C1-C2-N2-C7
12	h	2	NAG	C1-C2-N2-C7
7	M	2	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7
9	O	2	NAG	C3-C2-N2-C7
9	W	1	NAG	C3-C2-N2-C7
9	b	2	NAG	C3-C2-N2-C7
12	U	2	NAG	C3-C2-N2-C7
9	f	2	NAG	C4-C5-C6-O6
12	h	1	NAG	C4-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6
12	h	1	NAG	O5-C5-C6-O6

All (8) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	4	MAN	C1-C2-C3-C4-C5-O5
7	Z	5	MAN	C1-C2-C3-C4-C5-O5
7	Z	4	MAN	C1-C2-C3-C4-C5-O5
12	U	9	MAN	C1-C2-C3-C4-C5-O5
12	h	9	MAN	C1-C2-C3-C4-C5-O5
7	M	6	MAN	C1-C2-C3-C4-C5-O5
10	R	5	MAN	C1-C2-C3-C4-C5-O5
10	e	5	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 21 short contacts:

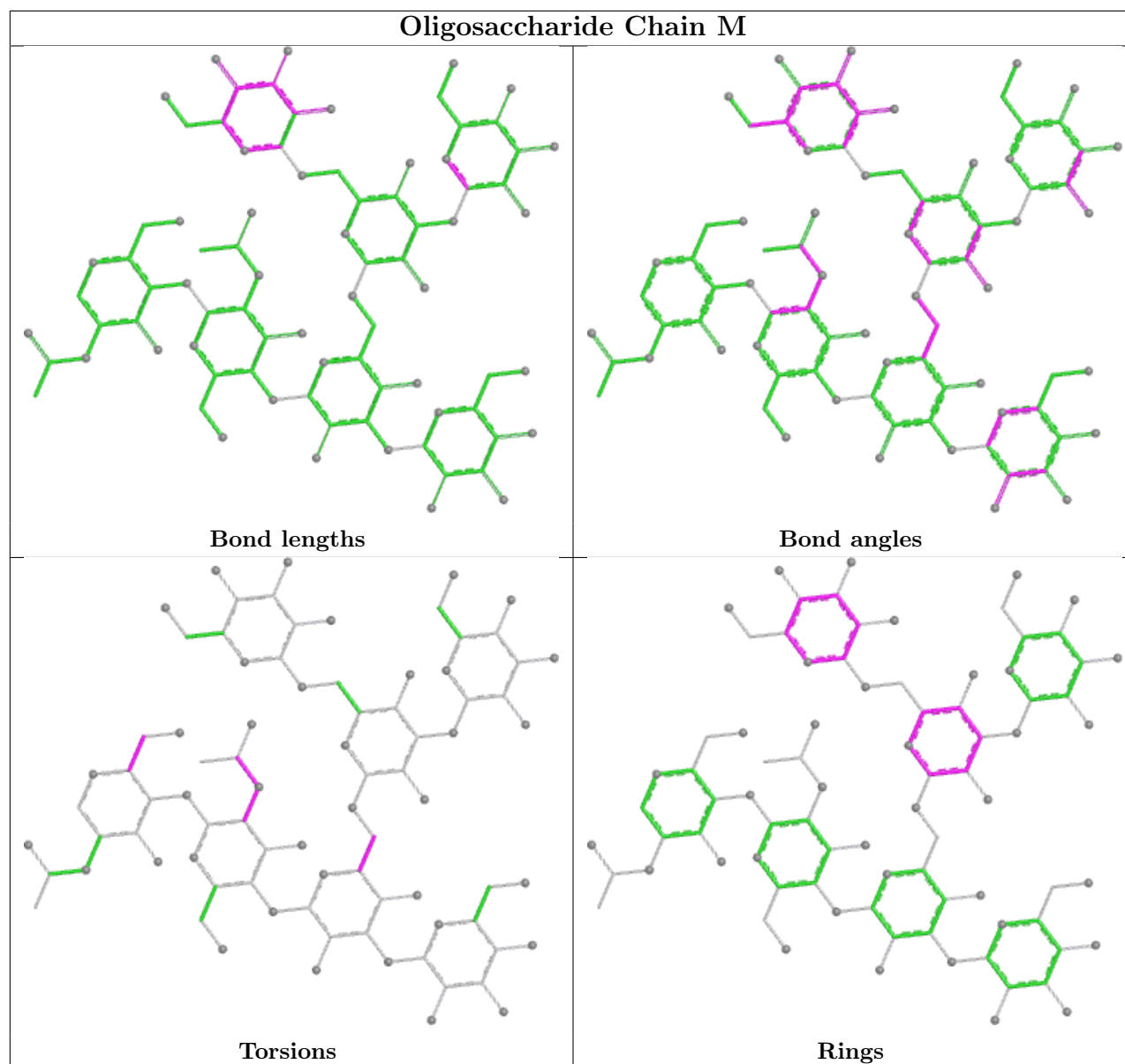
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	j	2	NAG	1	0
9	b	1	NAG	1	0
12	U	8	MAN	1	0
7	M	2	NAG	1	0
7	Z	1	NAG	1	0
12	h	2	NAG	1	0
7	Z	2	NAG	1	0
12	U	9	MAN	1	0
7	M	3	BMA	1	0
9	b	2	NAG	2	0
9	O	2	NAG	2	0
7	M	4	MAN	2	0

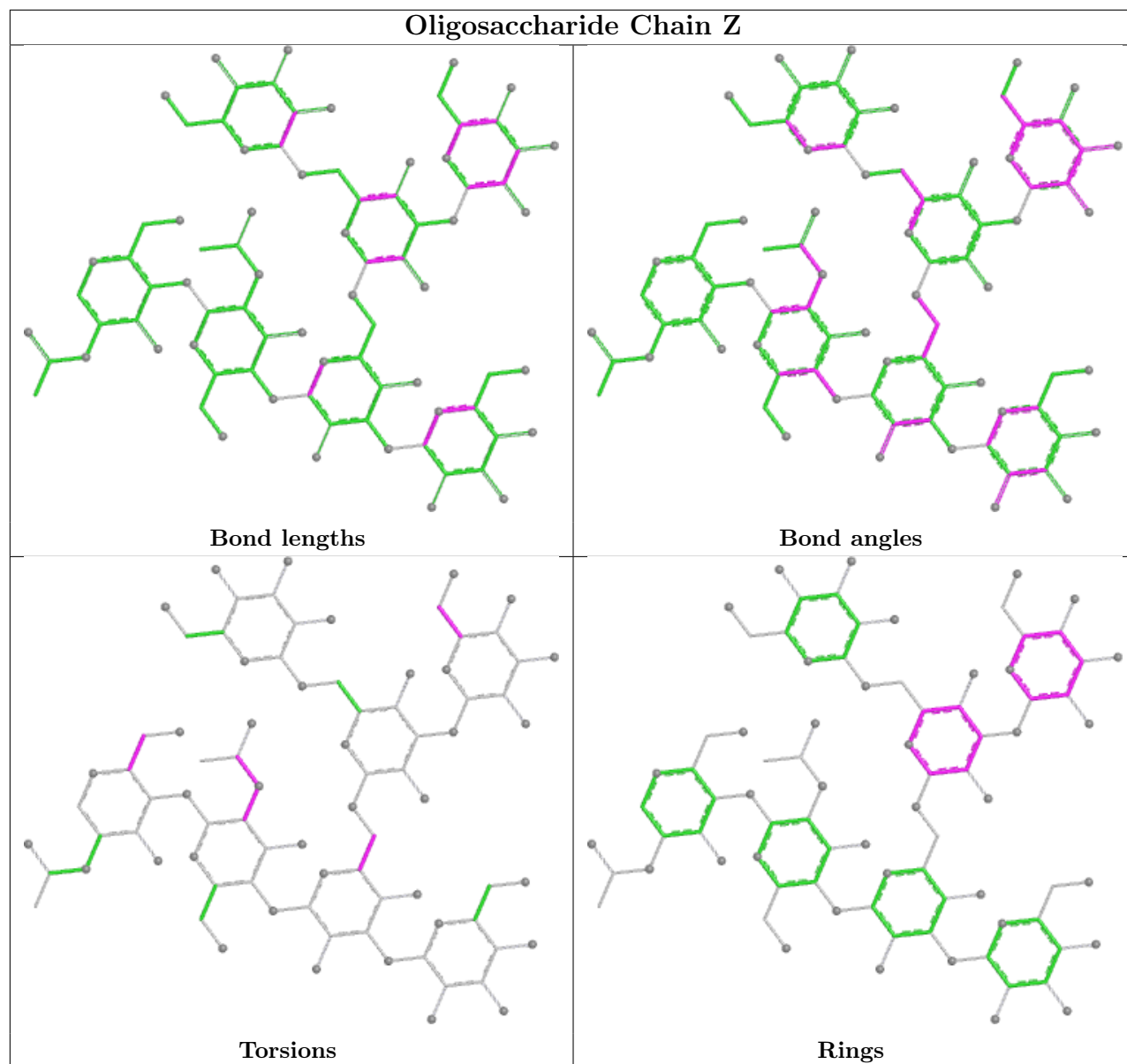
Continued on next page...

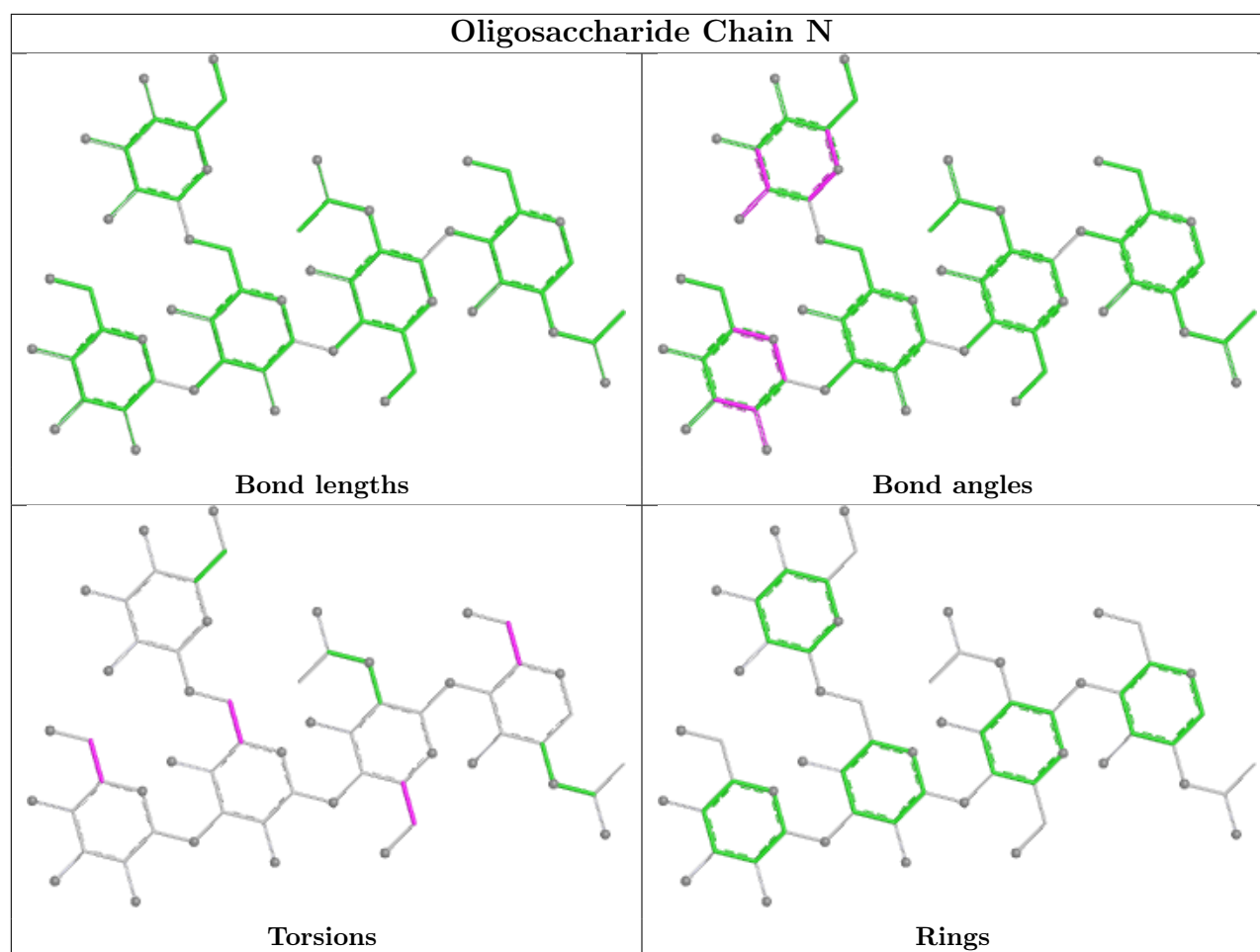
Continued from previous page...

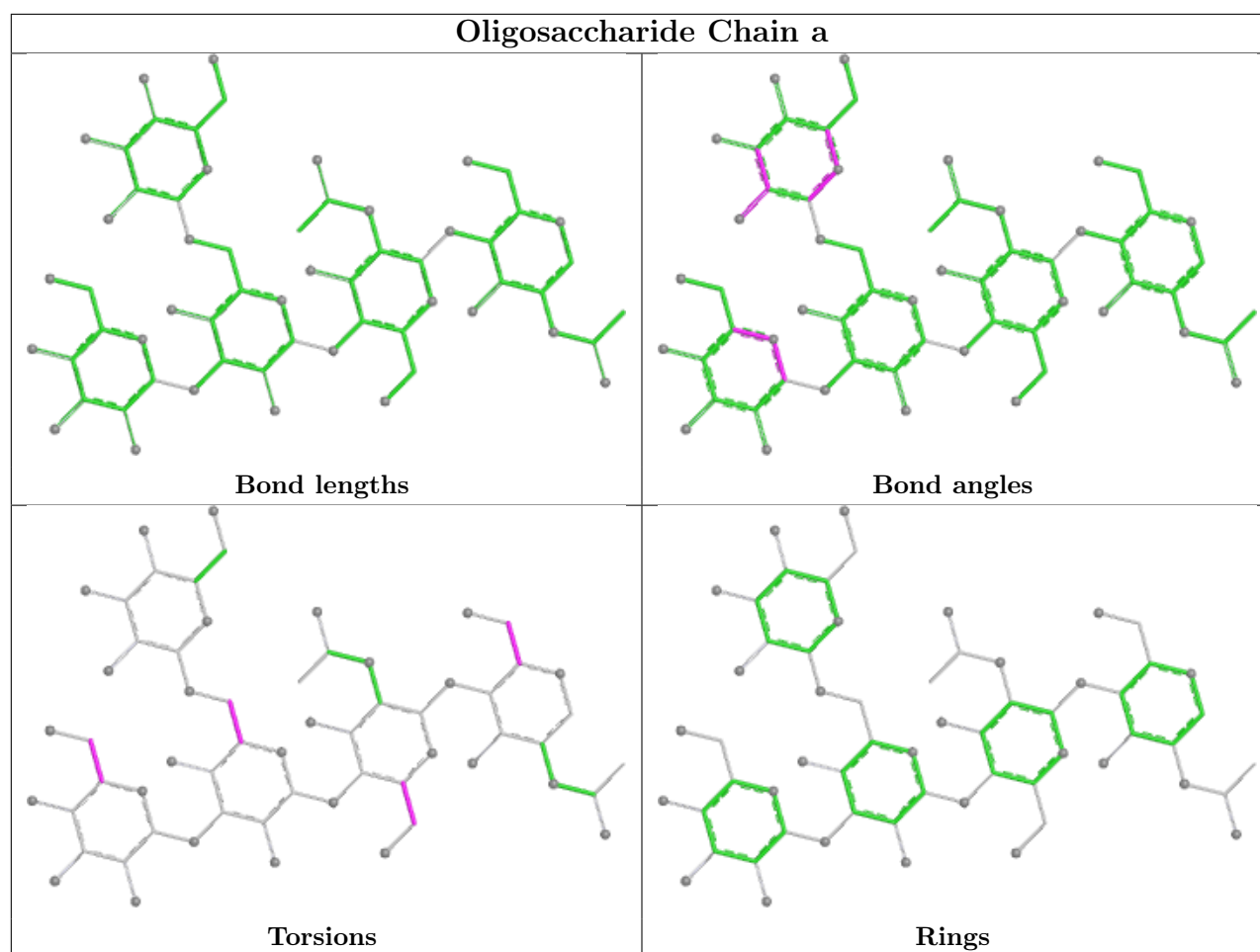
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	i	1	NAG	1	0
9	j	1	NAG	1	0
10	R	4	MAN	2	0
10	e	4	MAN	1	0
9	O	1	NAG	4	0
11	Y	1	NAG	1	0

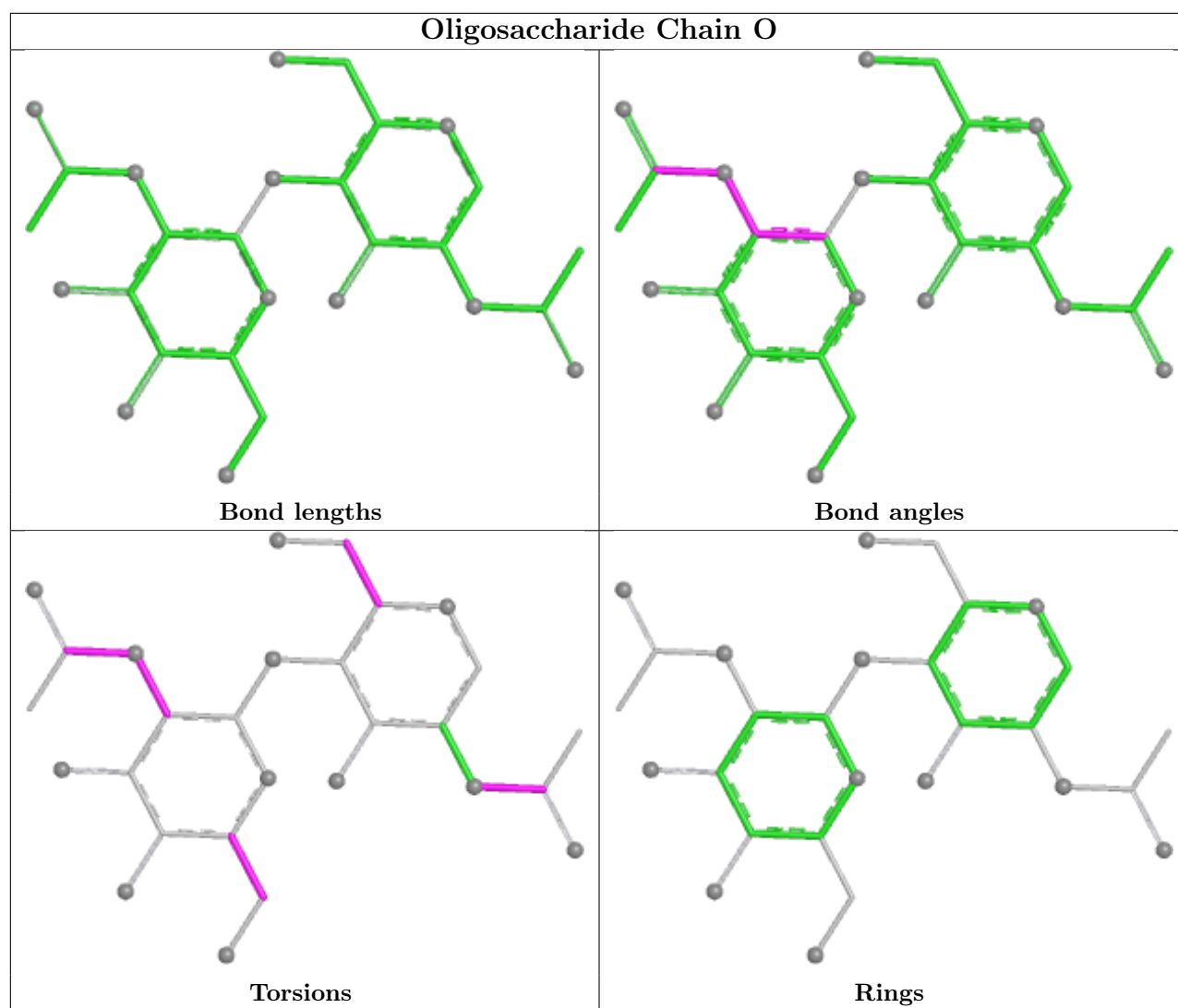
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

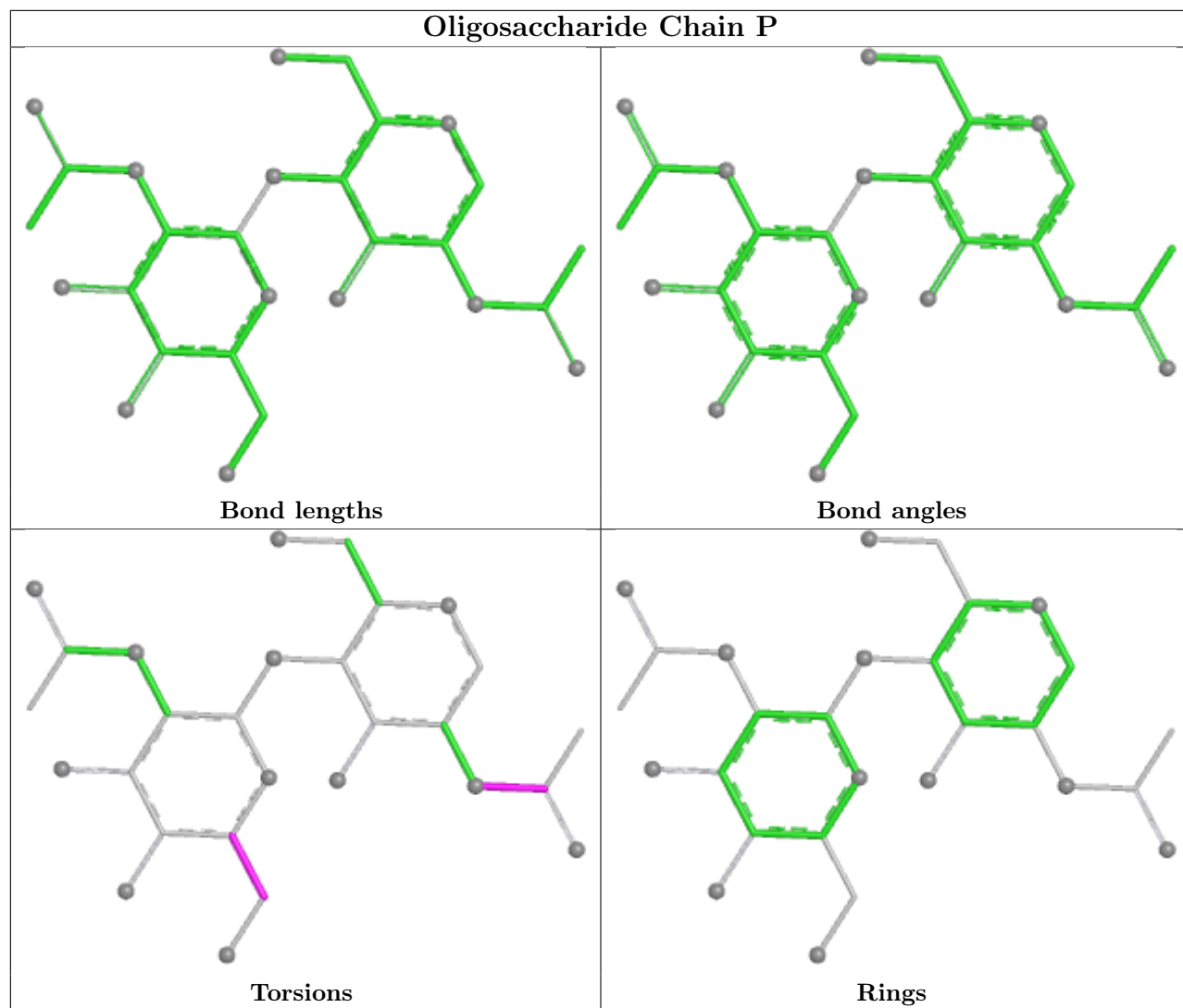


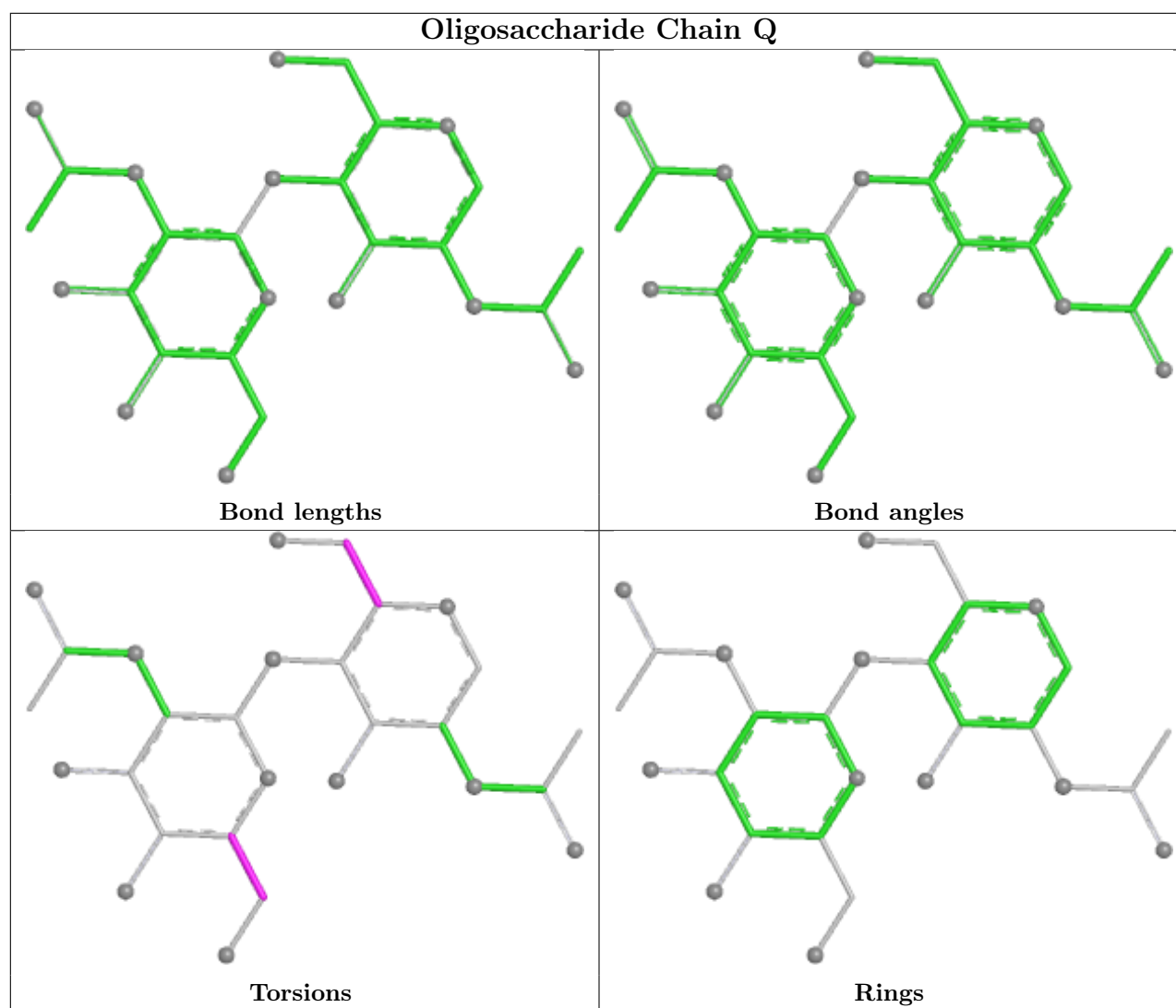


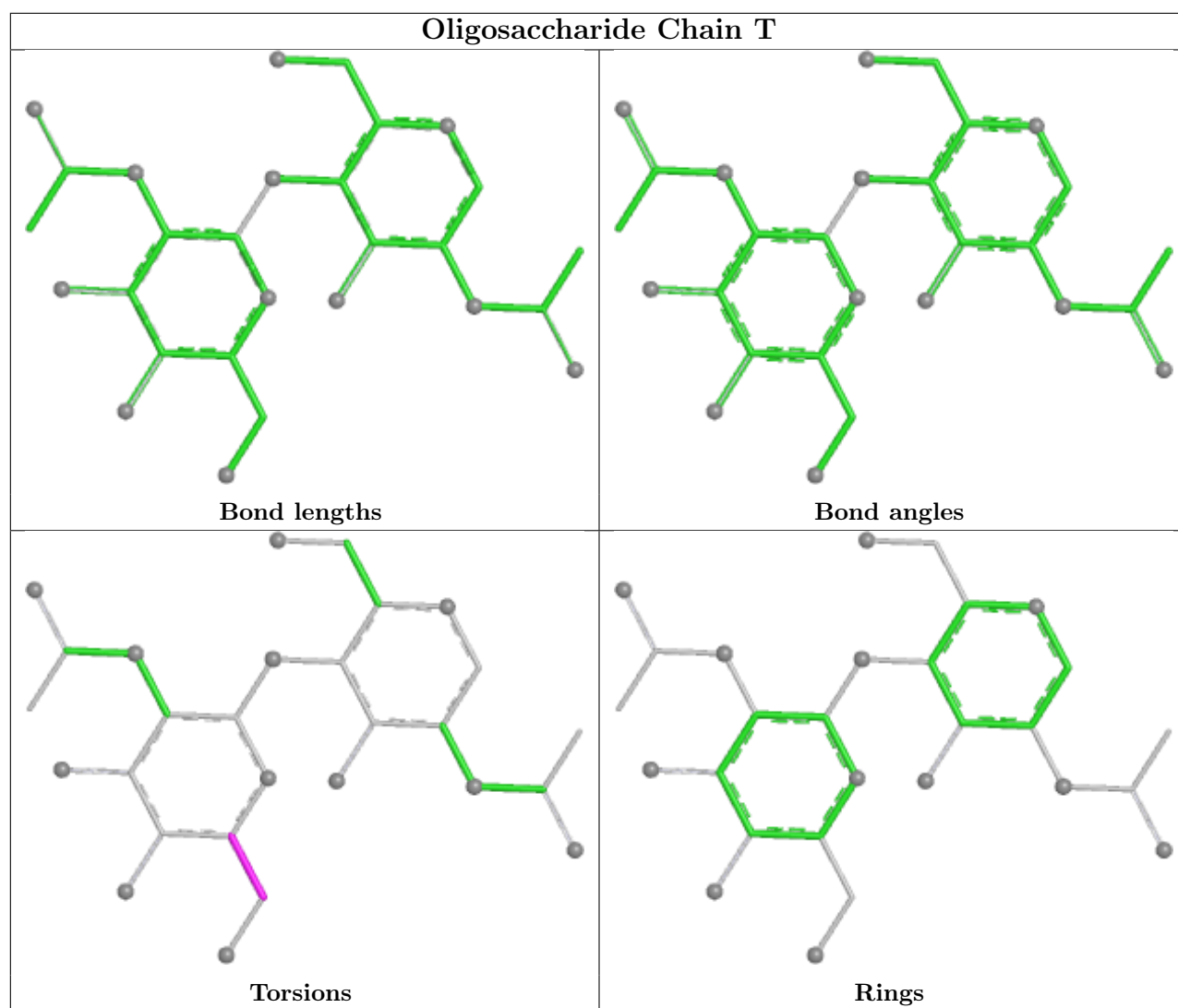


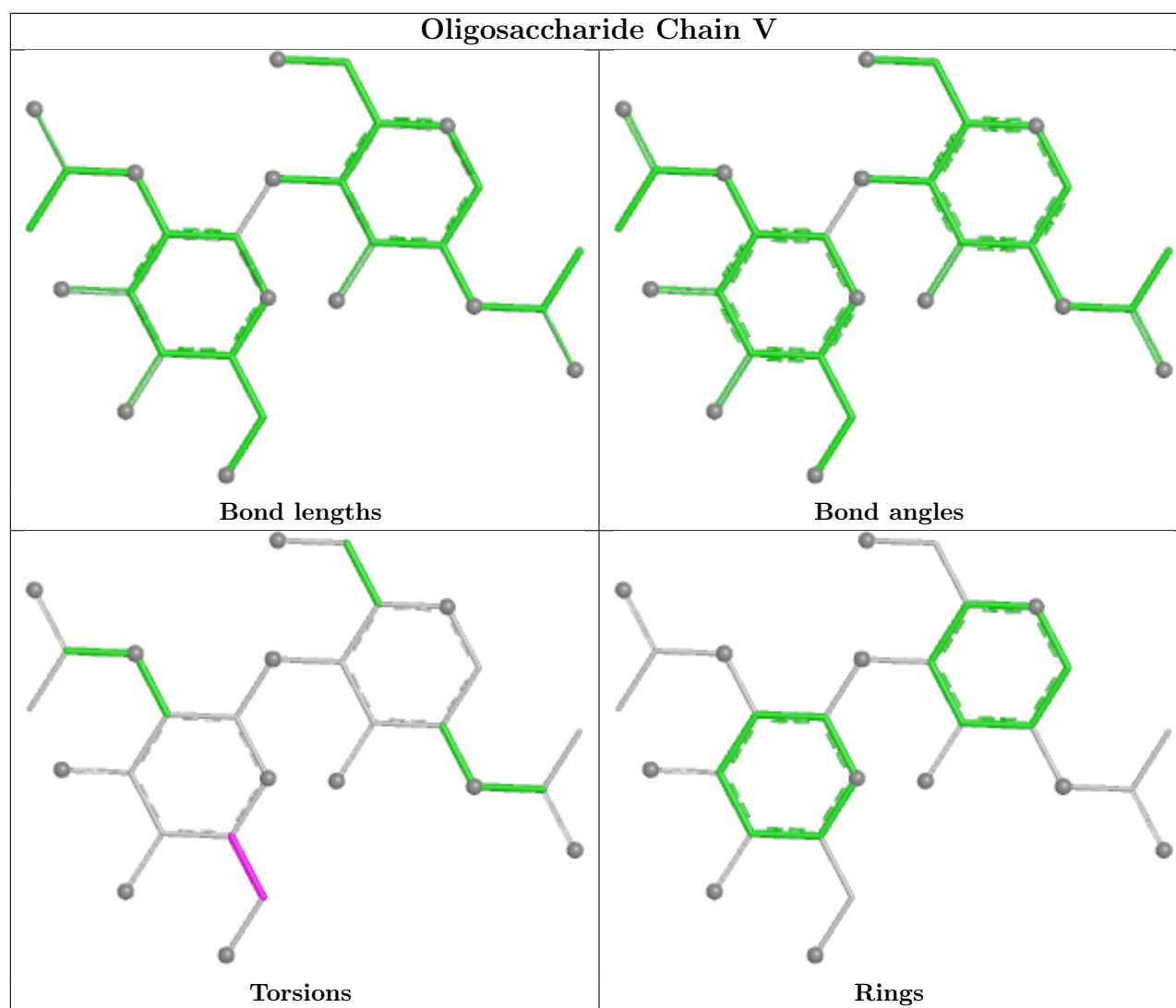


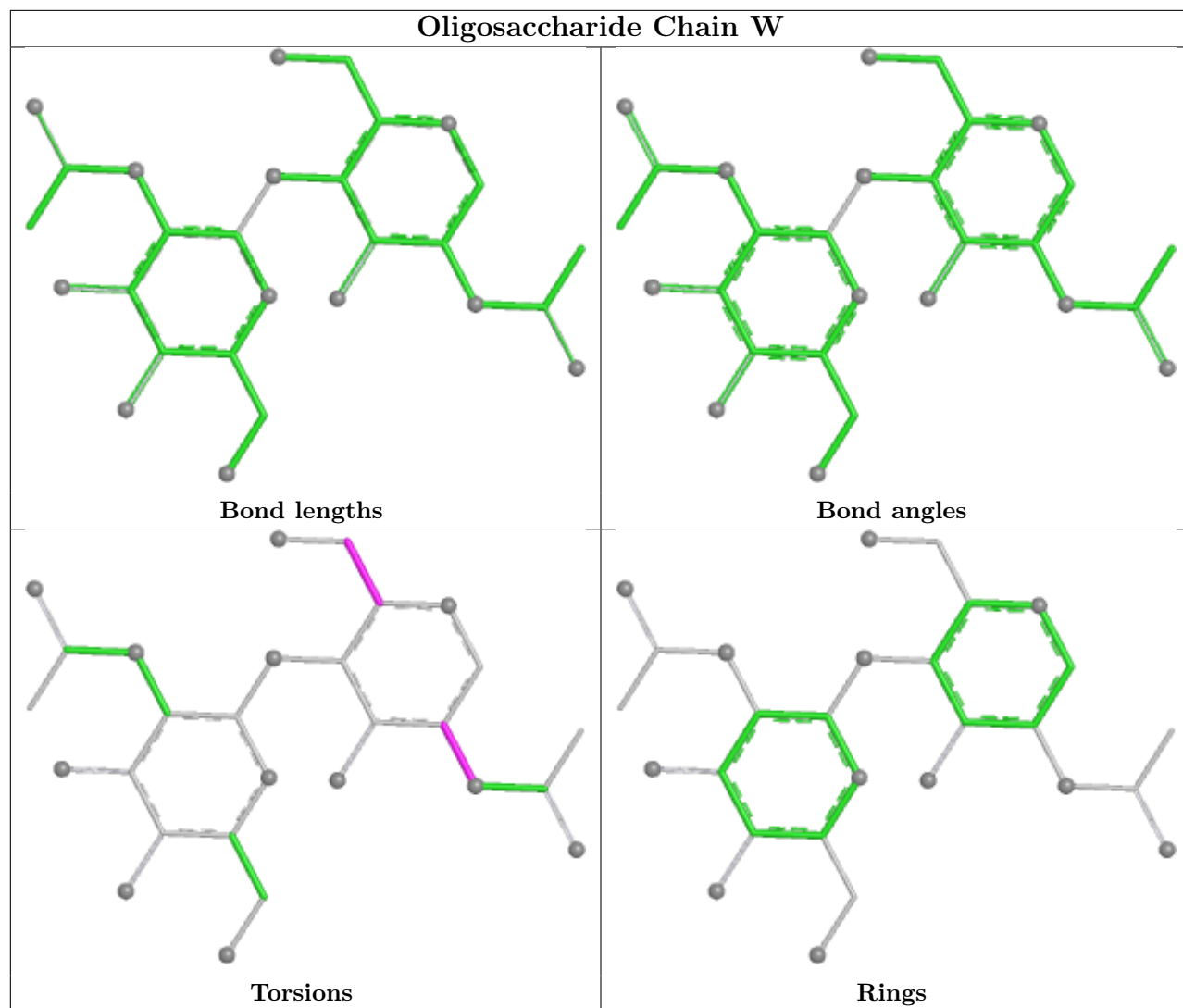


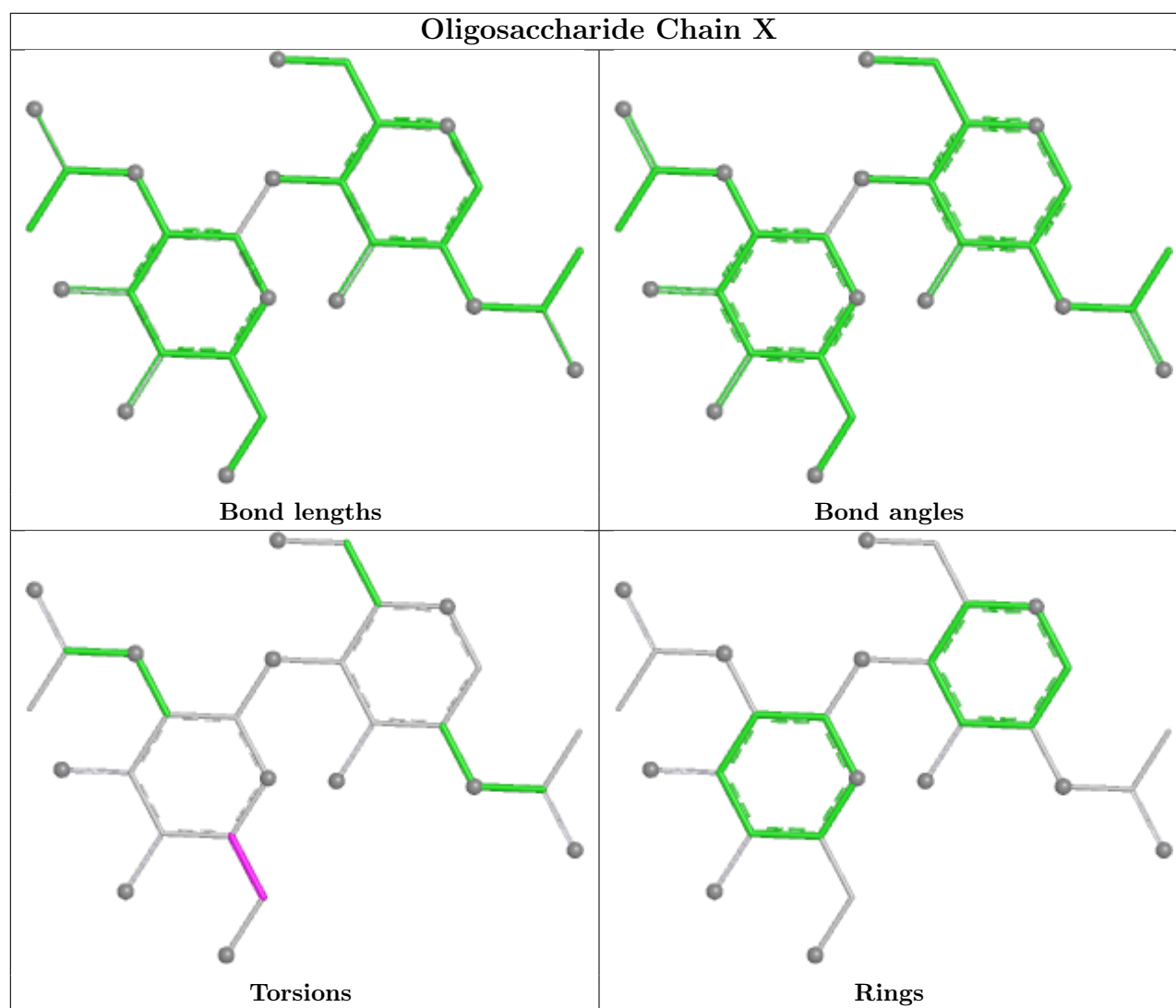


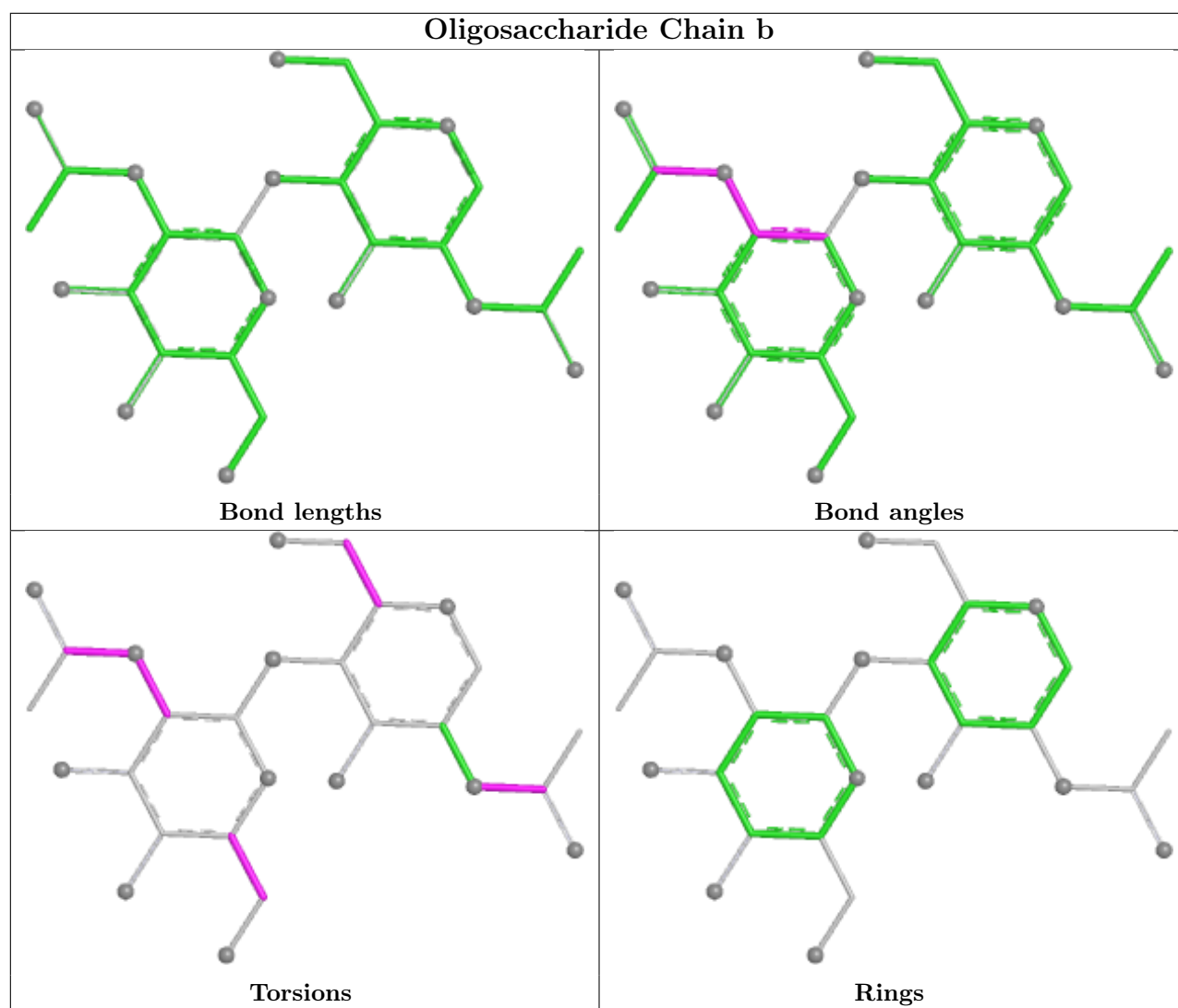


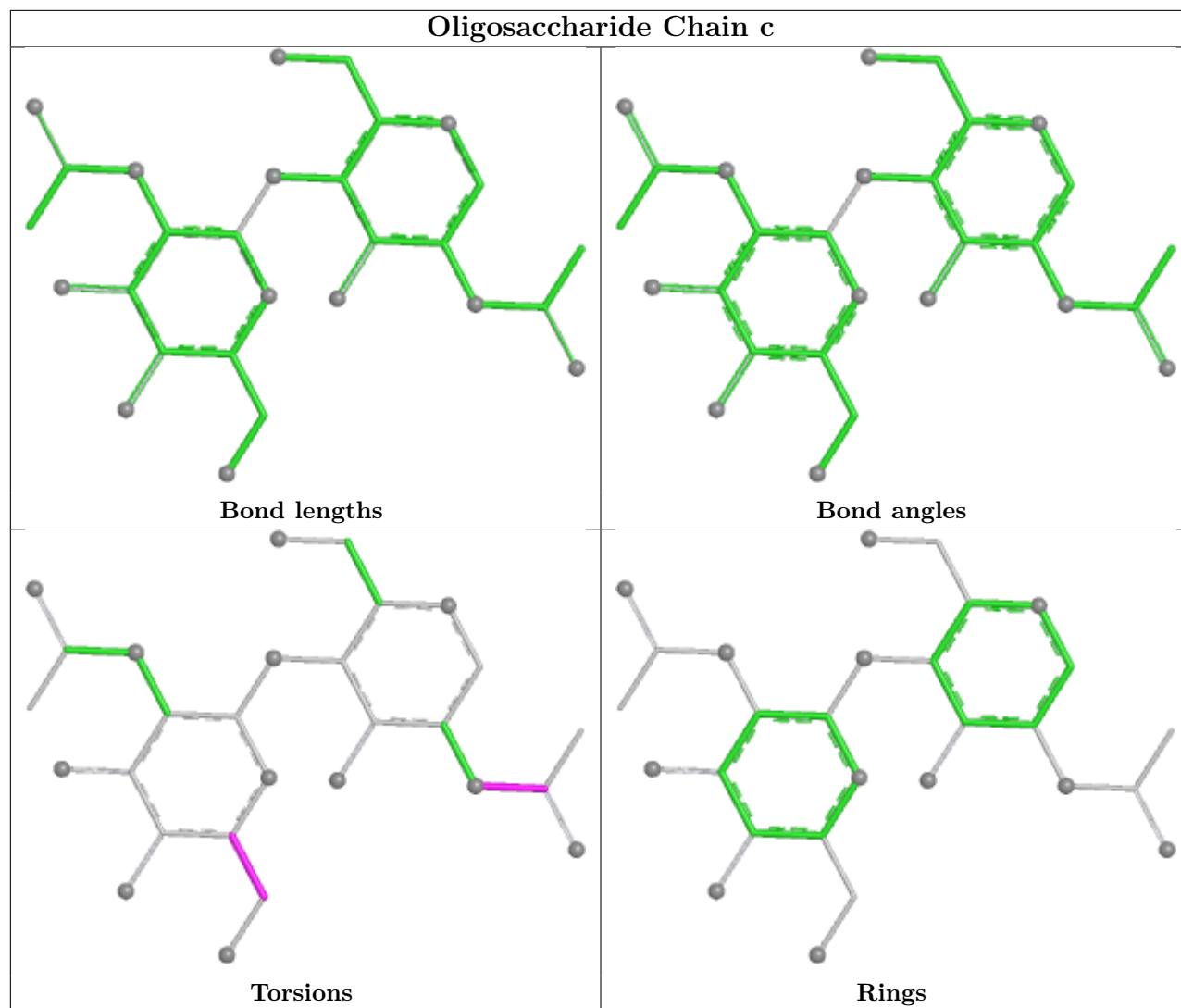


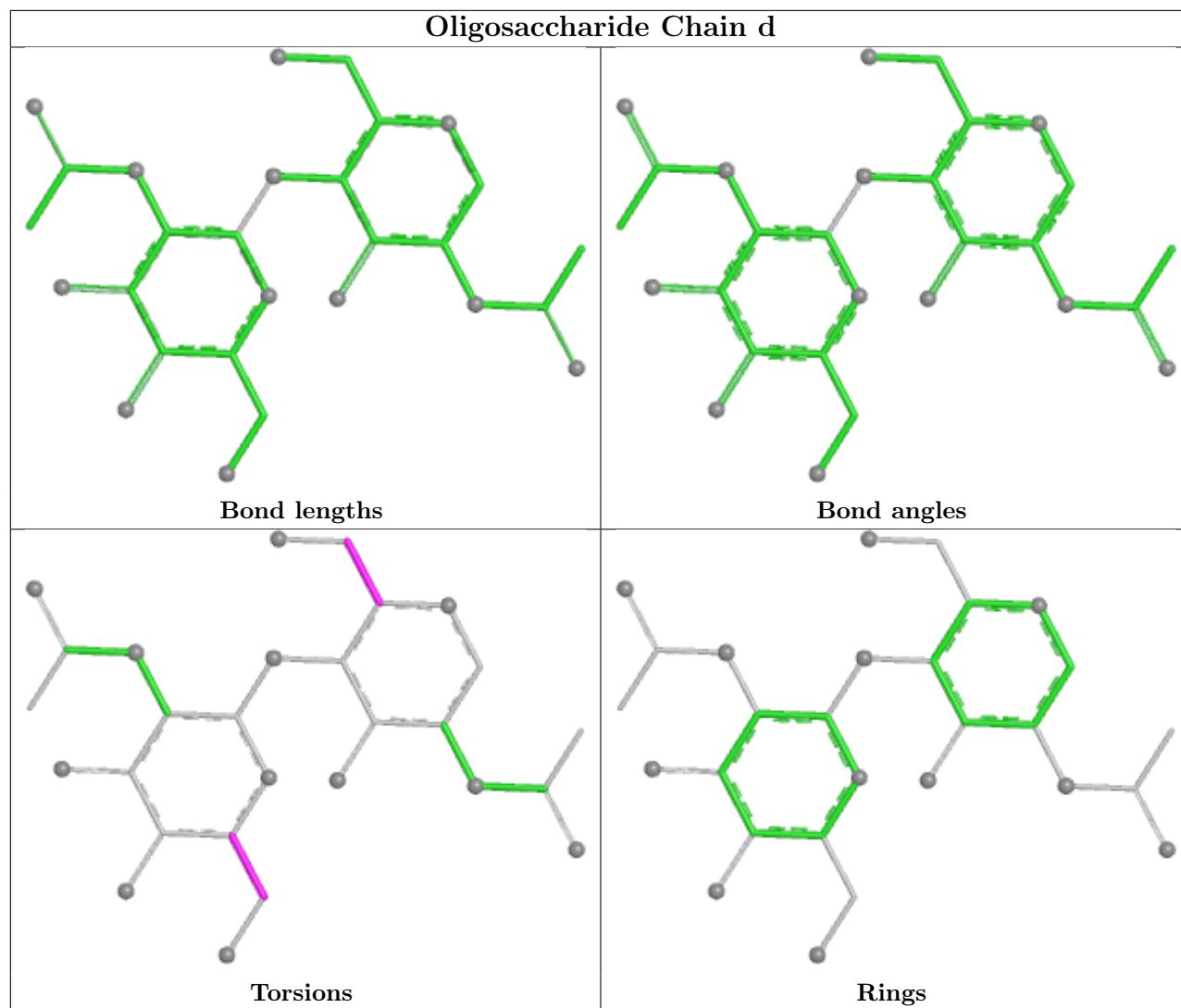


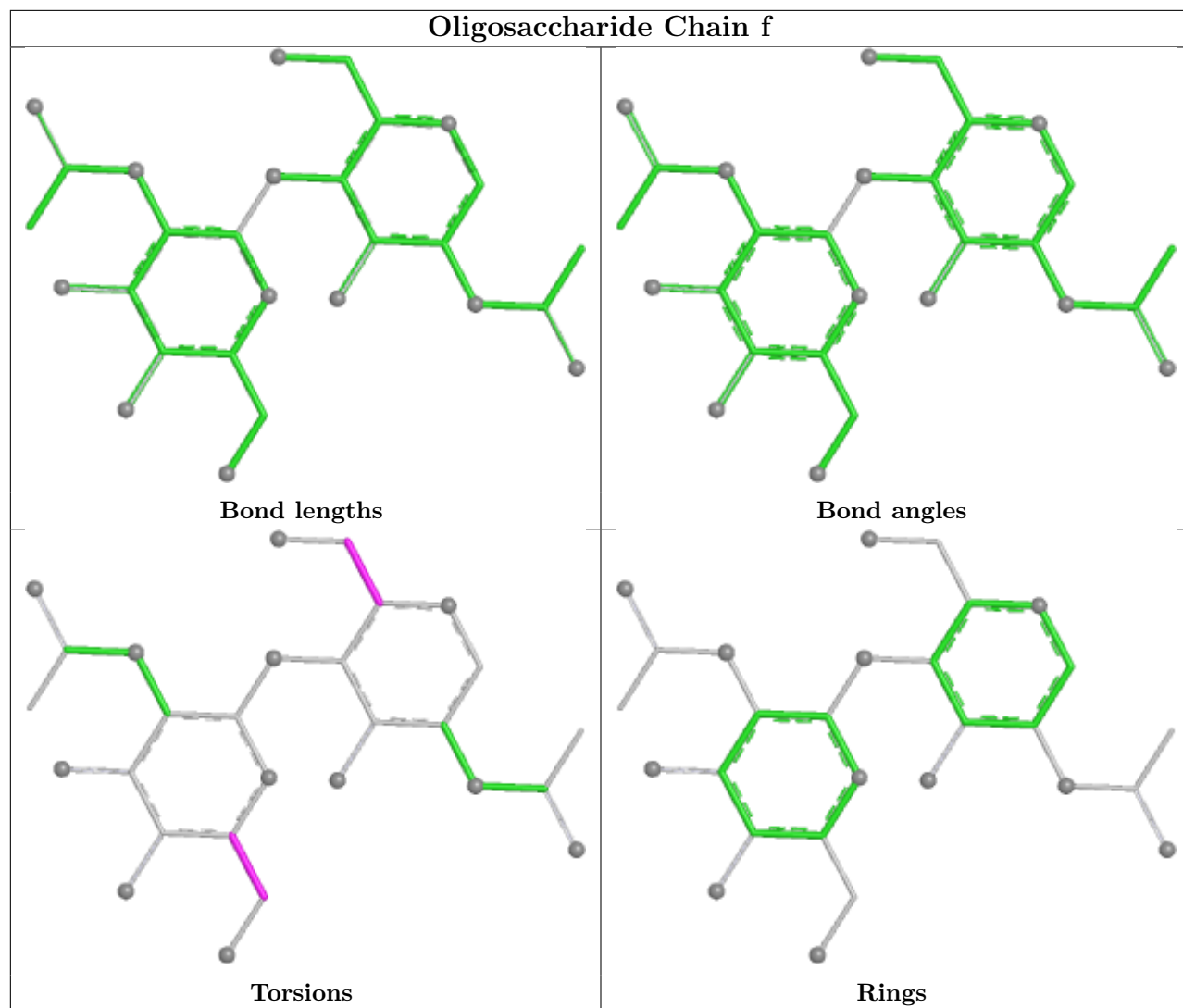


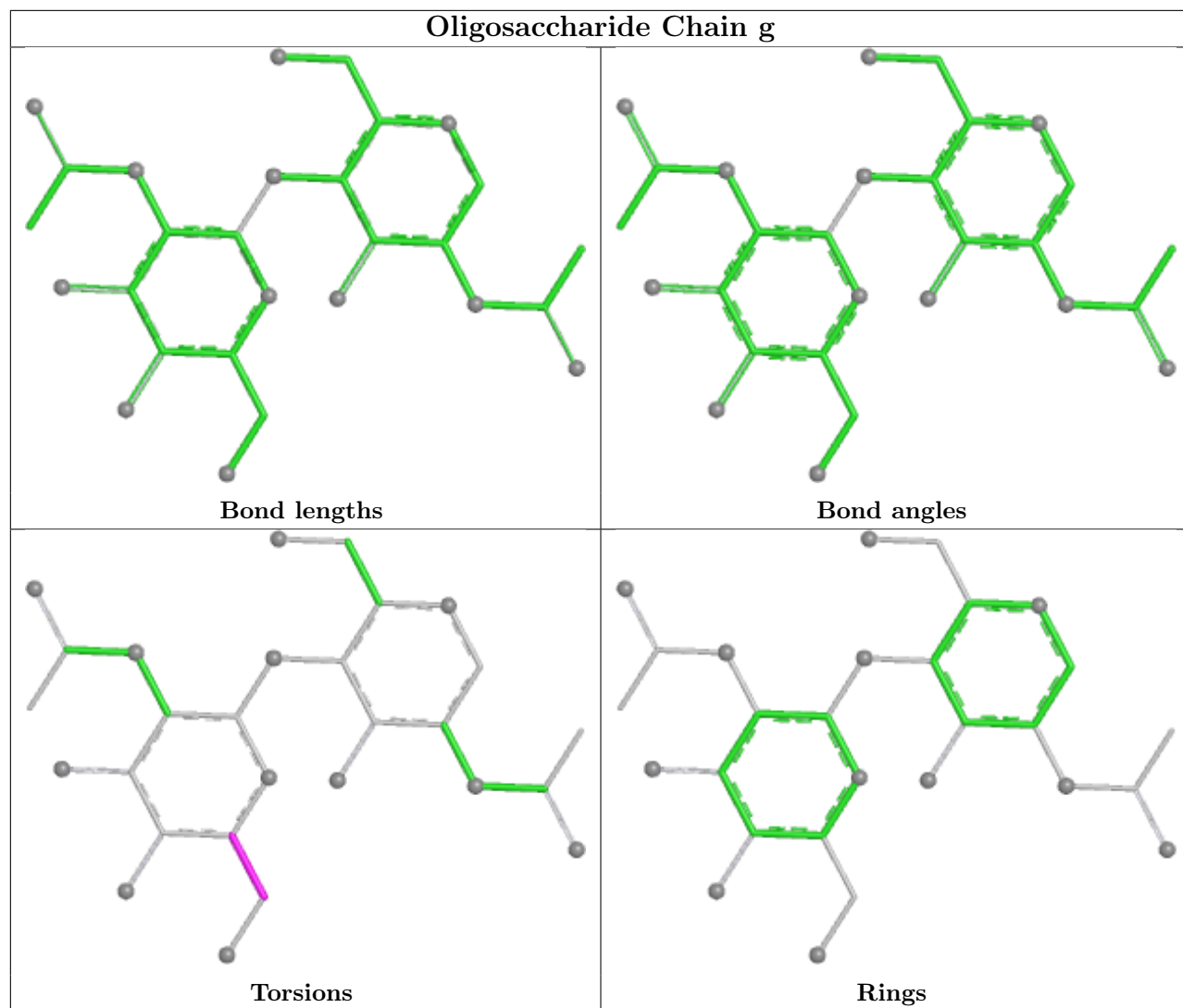


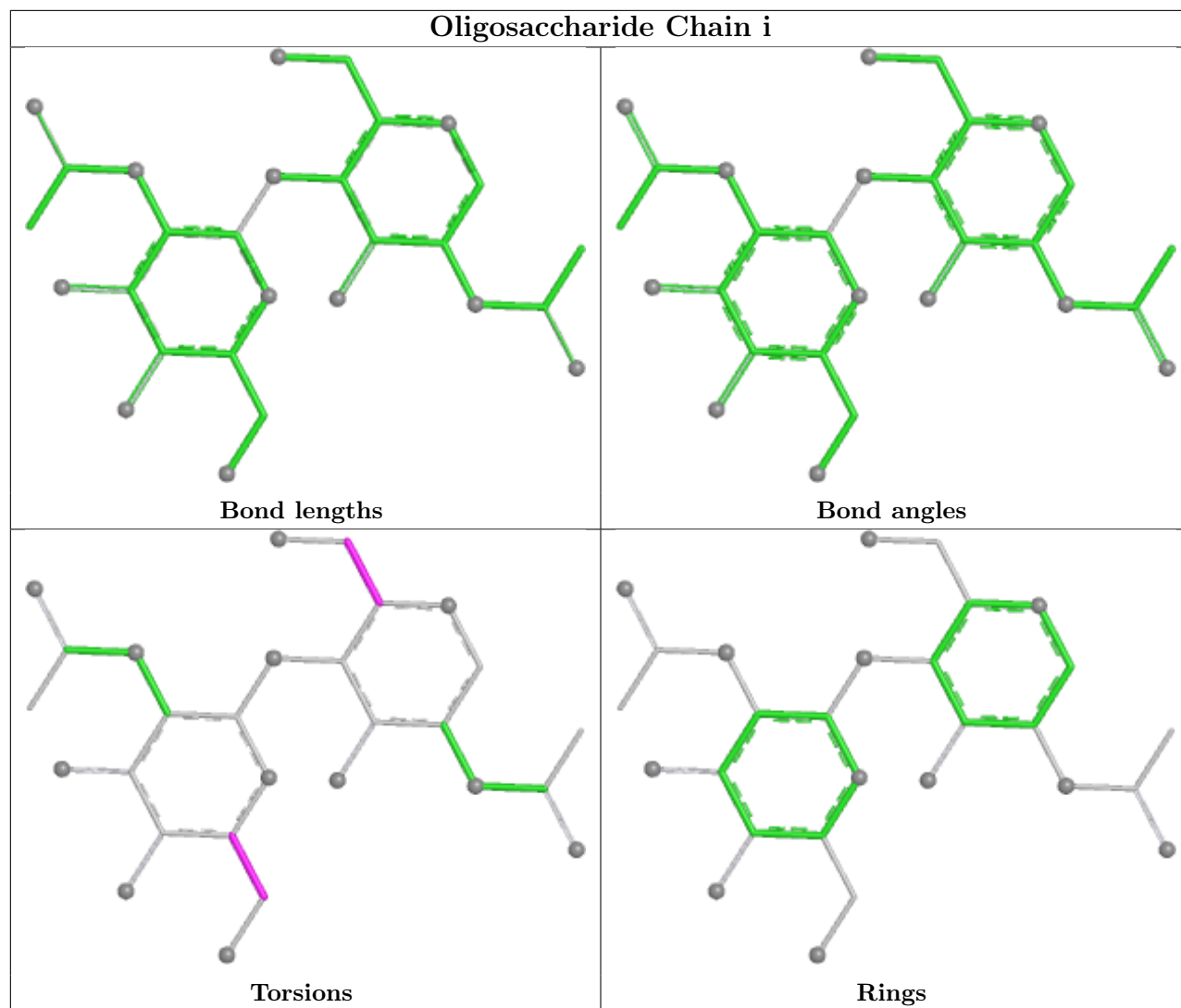


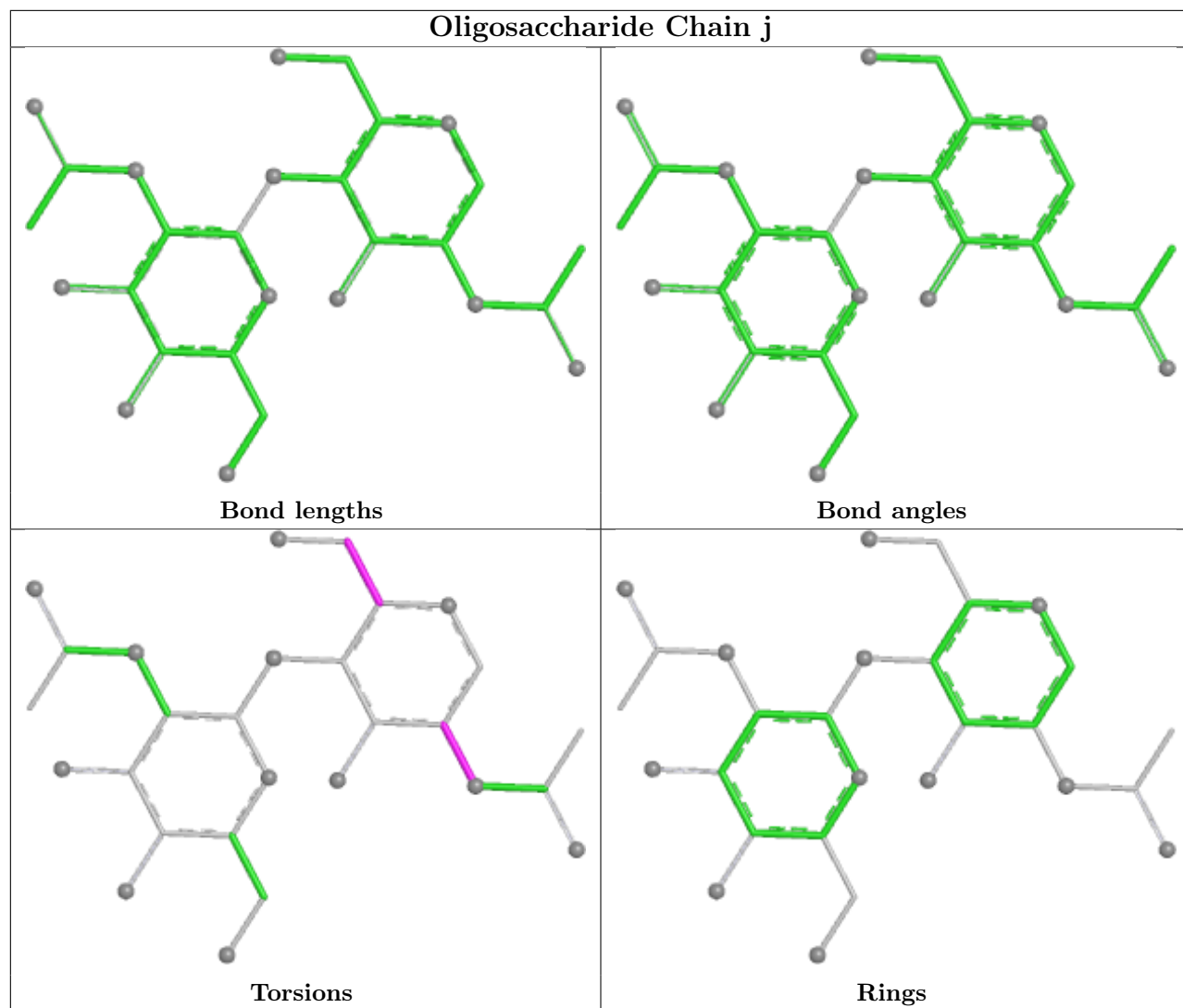


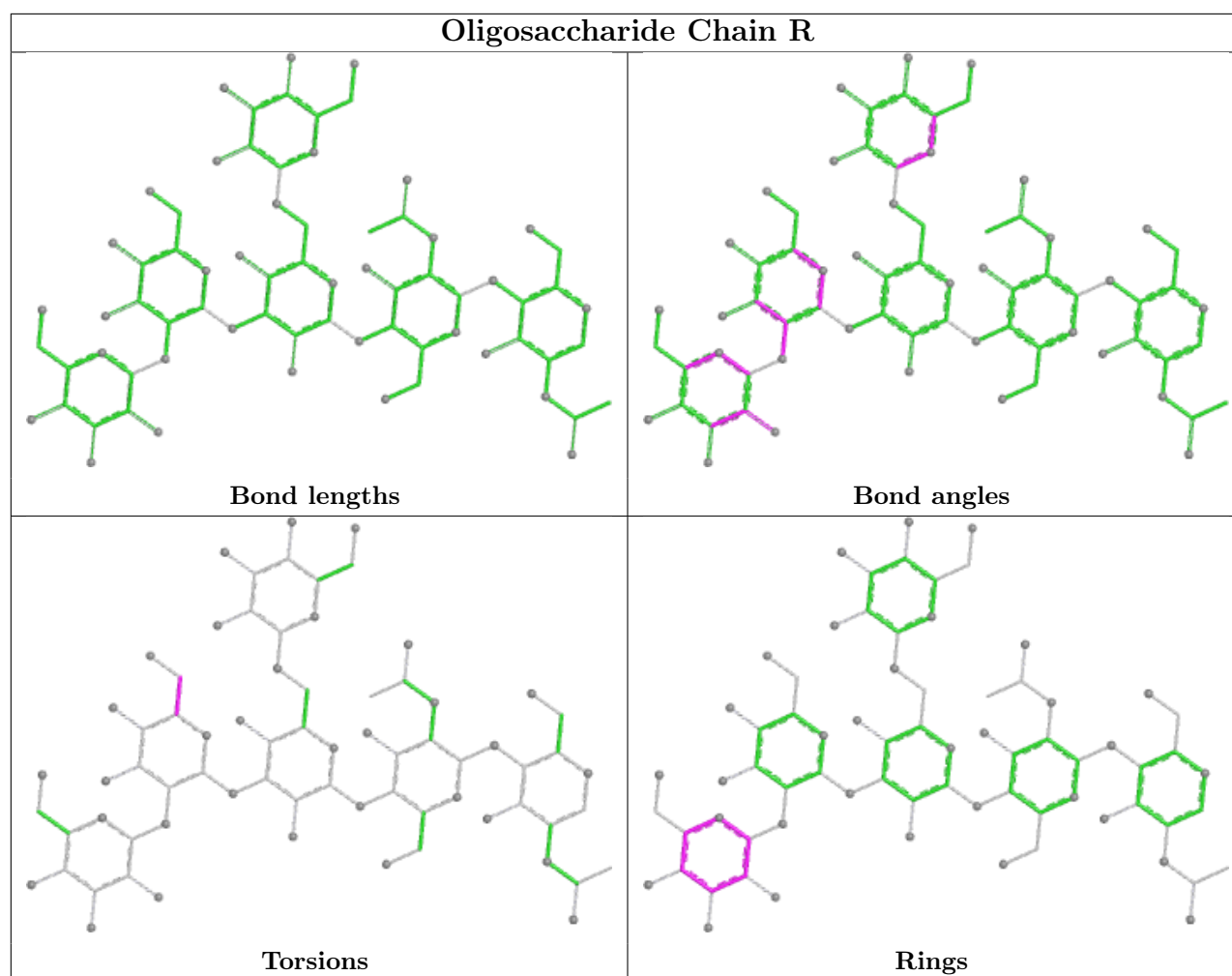


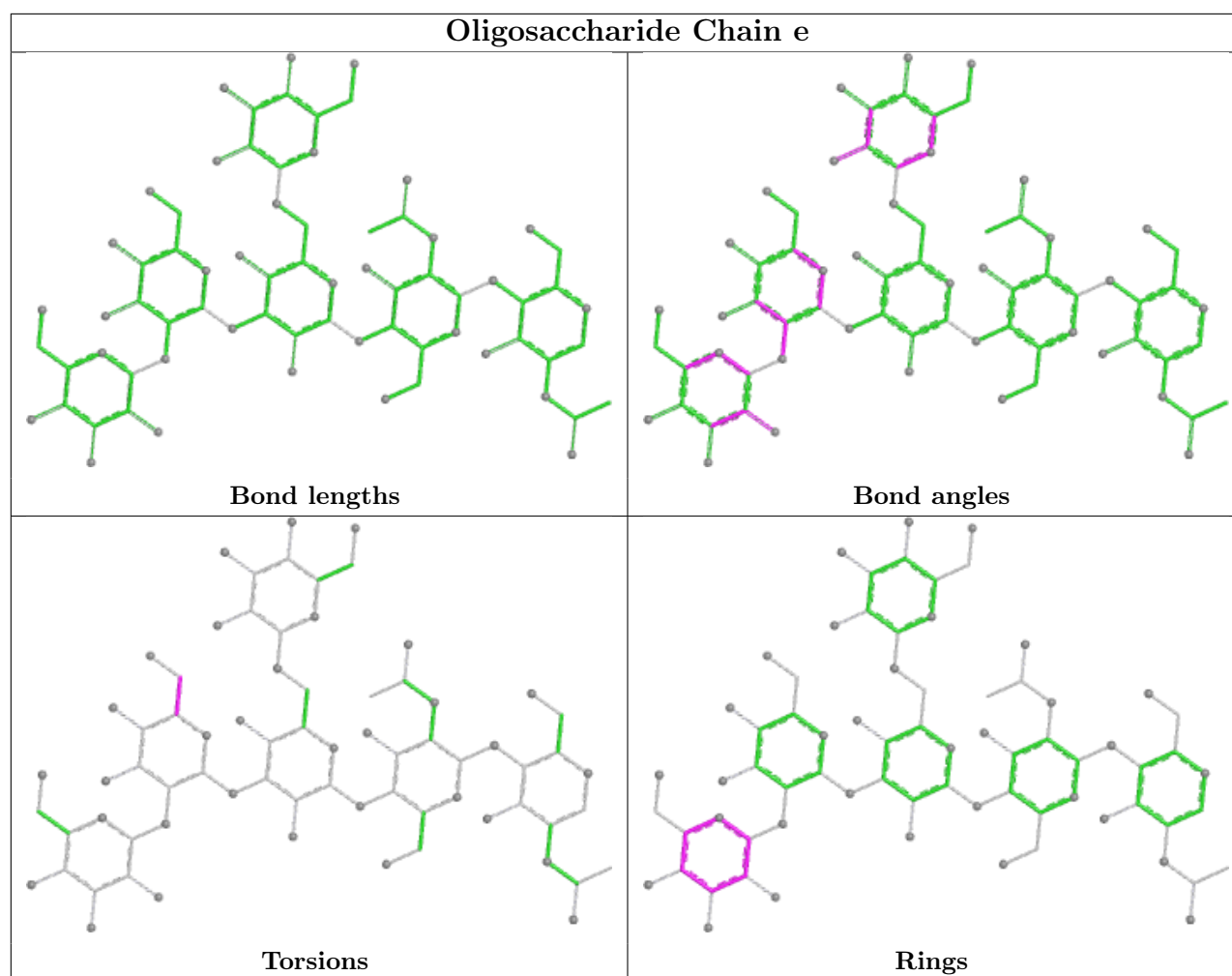


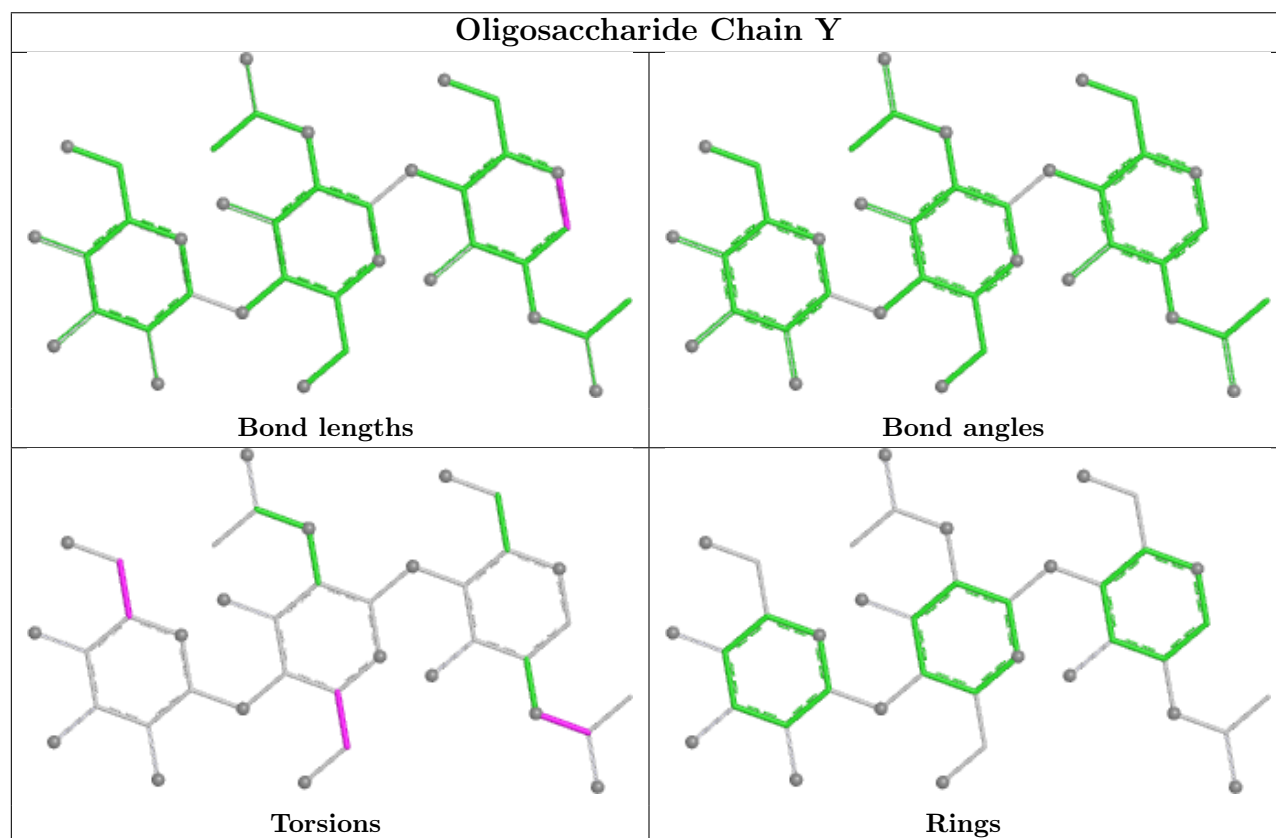
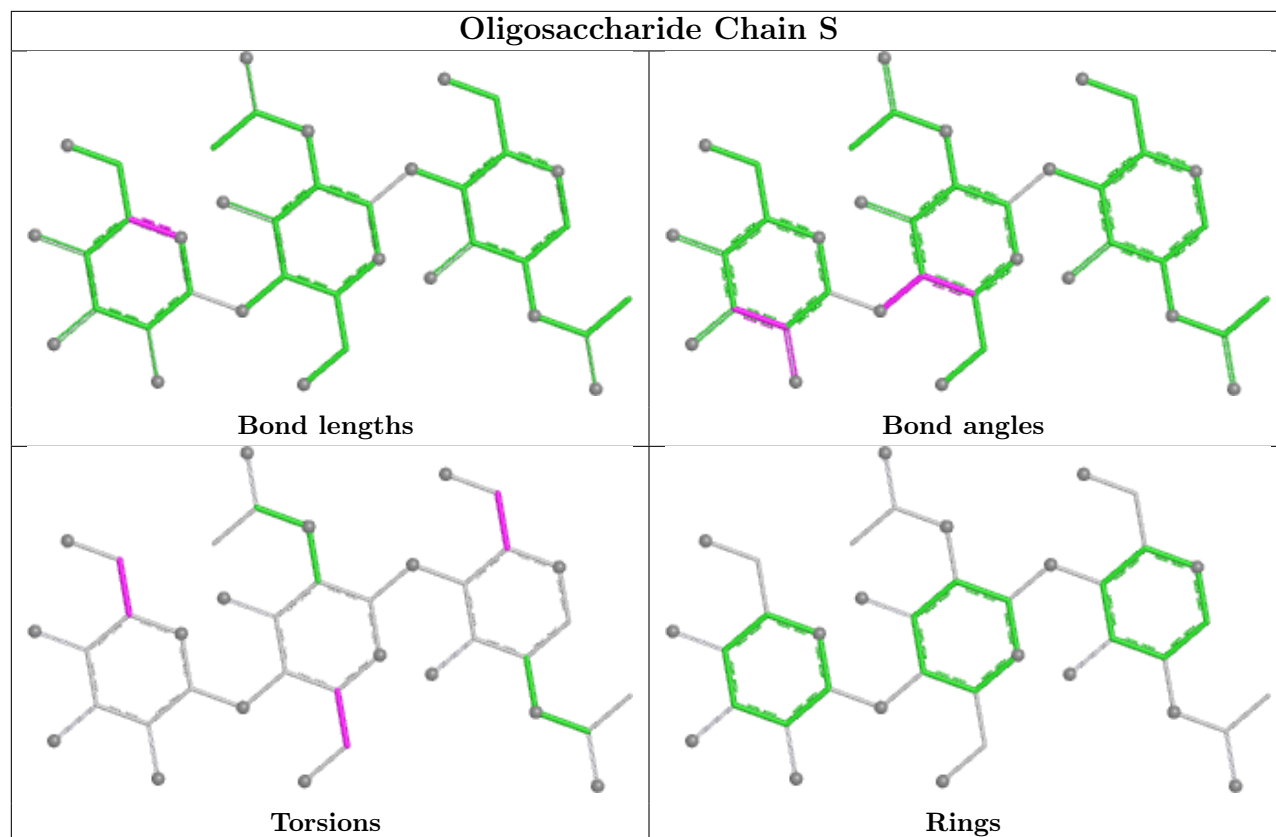


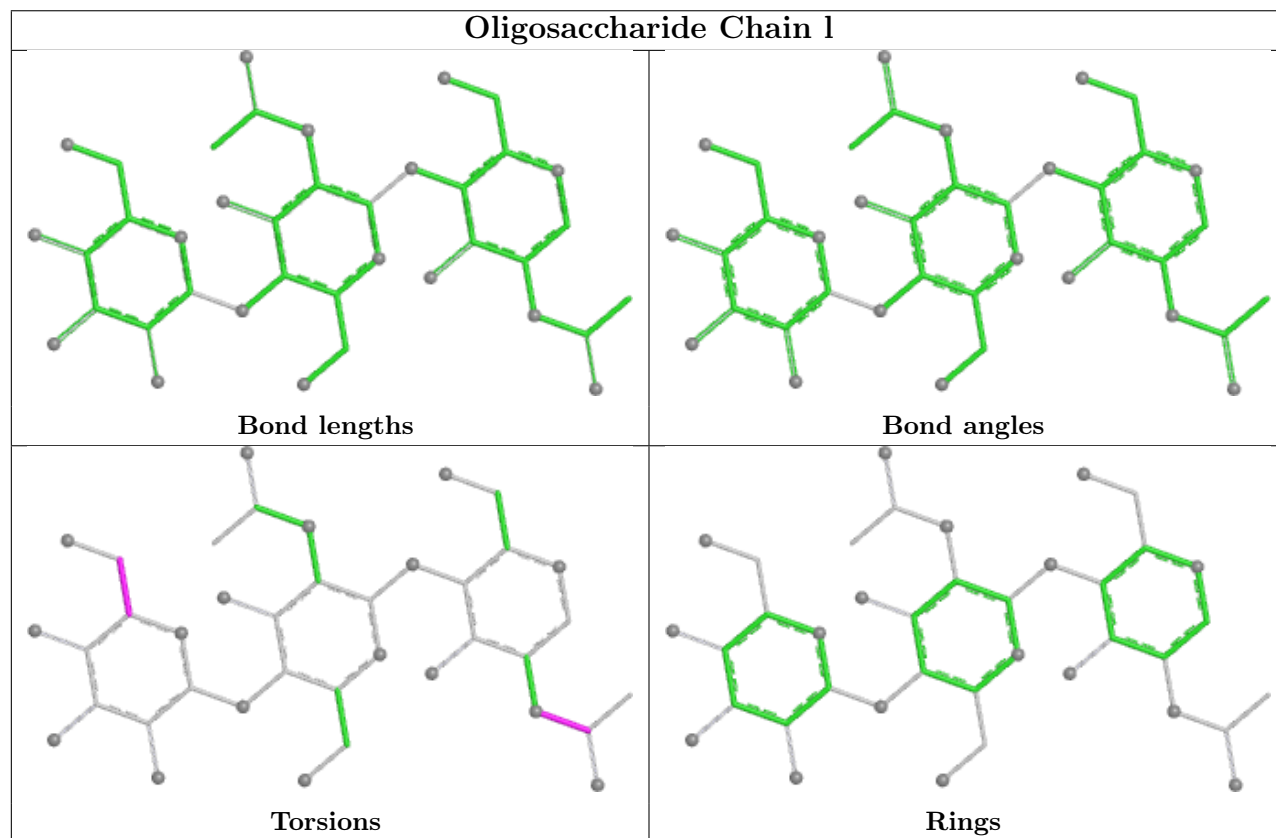
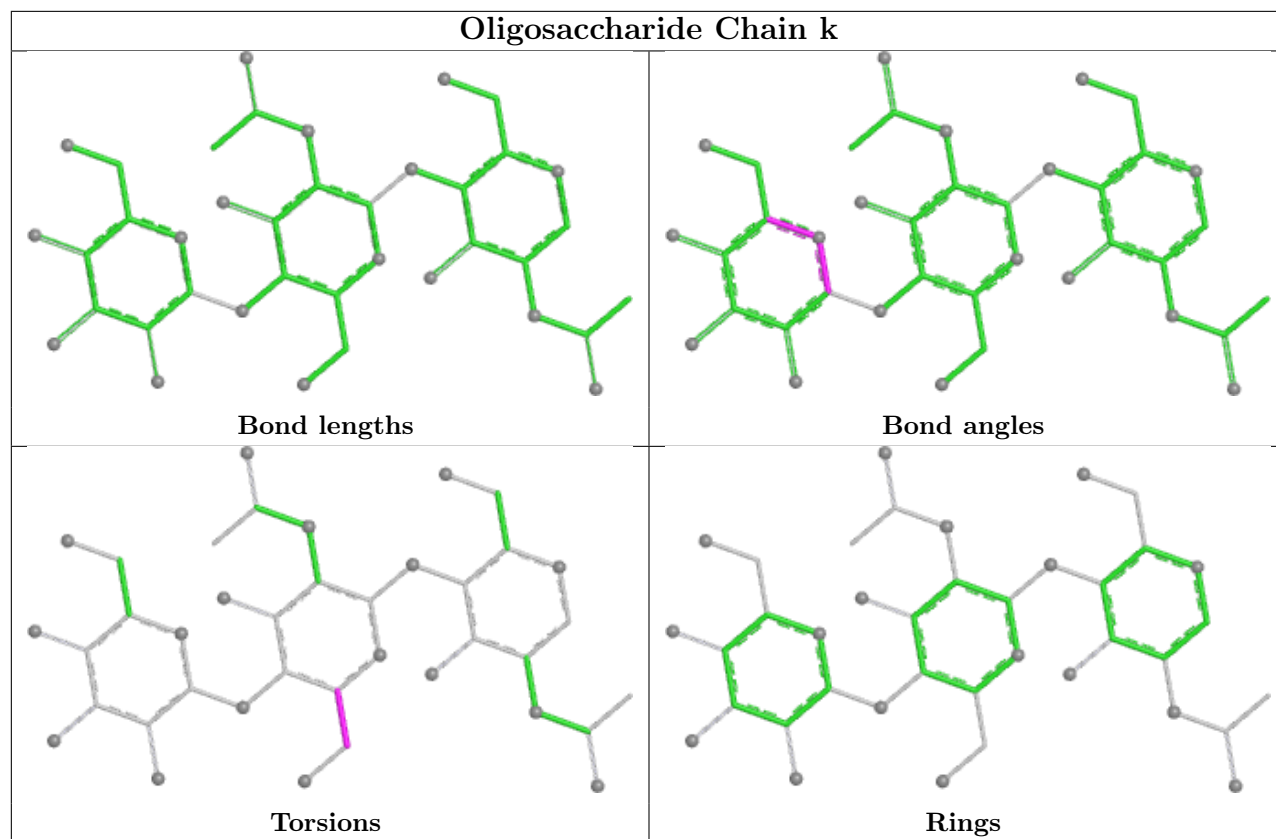


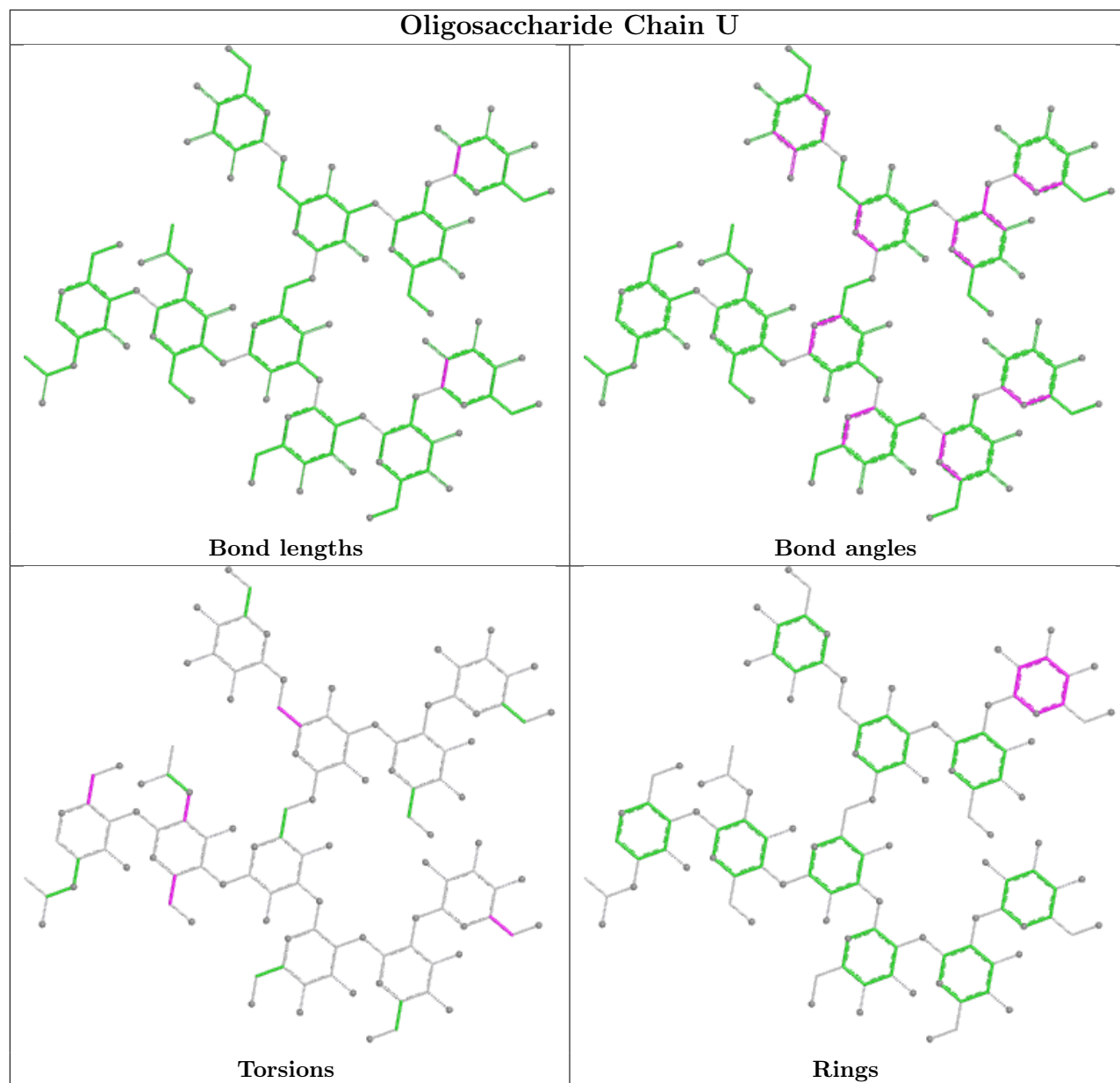


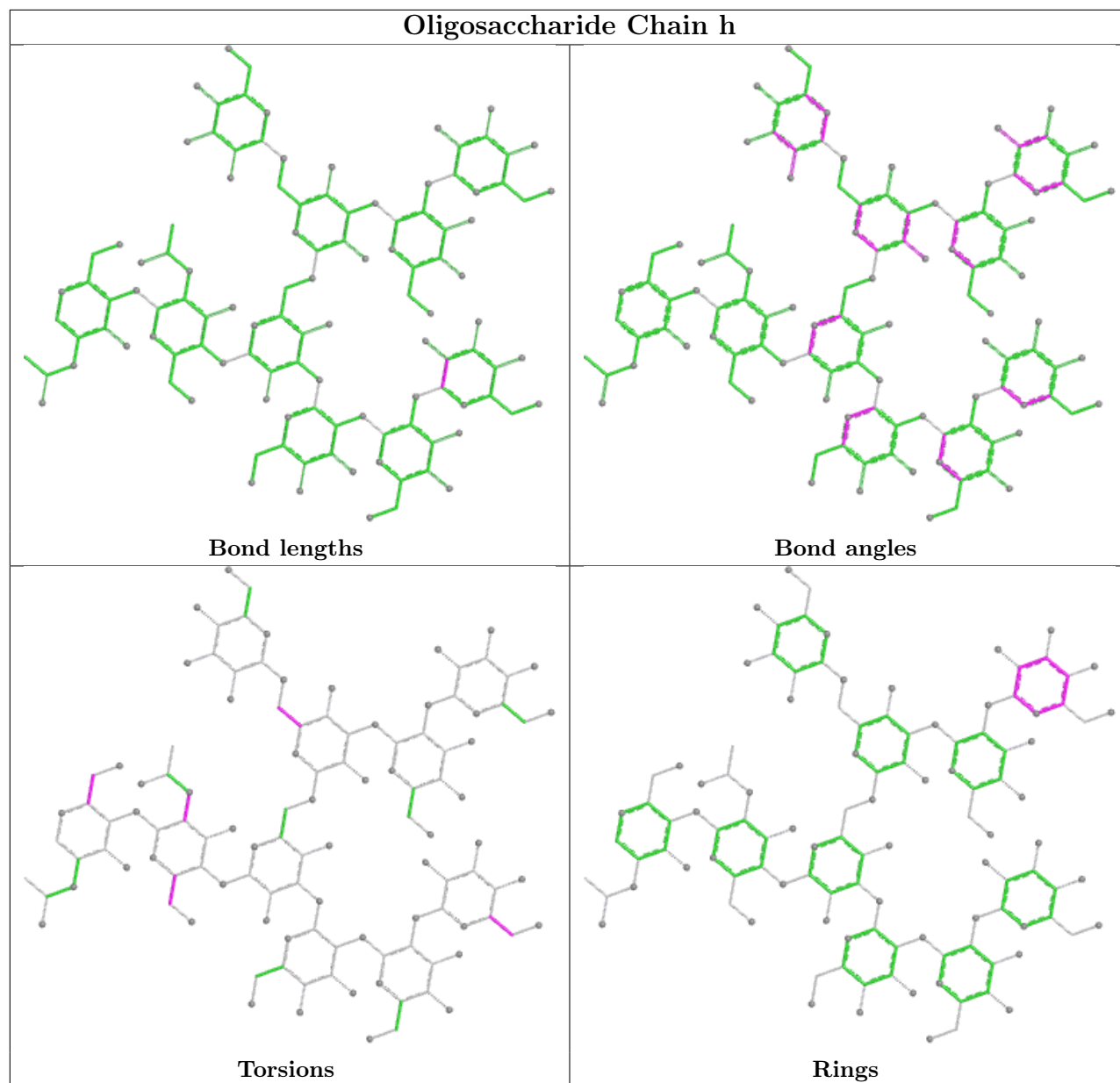


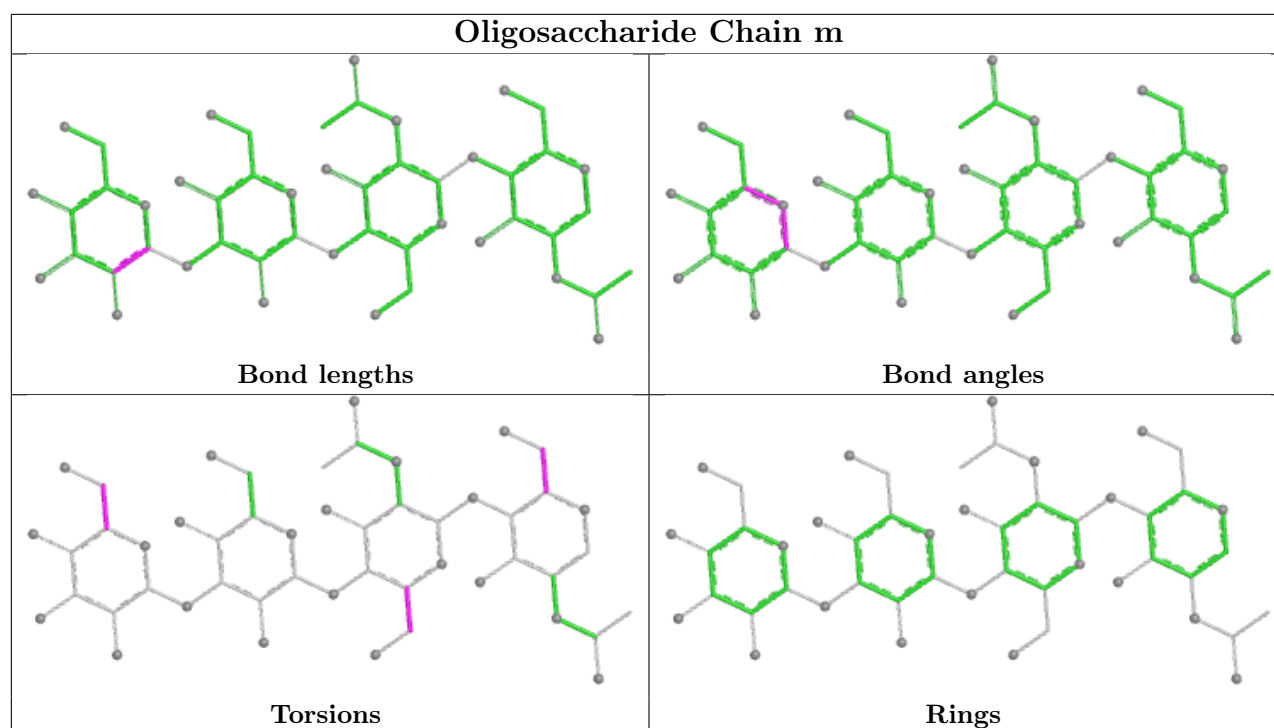












5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	C	942	1	14,14,15	0.29	0	17,19,21	0.76	0
14	NAG	K	301	6	14,14,15	1.98	2 (14%)	17,19,21	0.91	0
14	NAG	A	926	1	14,14,15	0.47	0	17,19,21	1.34	2 (11%)
14	NAG	I	305	6	14,14,15	2.07	2 (14%)	17,19,21	0.89	0
14	NAG	A	908	1	14,14,15	0.20	0	17,19,21	0.46	0
14	NAG	C	953	1	14,14,15	0.27	0	17,19,21	0.45	0
14	NAG	B	901	2	14,14,15	0.33	0	17,19,21	0.59	0
14	NAG	D	901	2	14,14,15	0.41	0	17,19,21	0.61	0
14	NAG	C	909	1	14,14,15	0.33	0	17,19,21	0.52	0
14	NAG	B	902	2	14,14,15	0.16	0	17,19,21	0.49	0
14	NAG	C	927	1	14,14,15	0.48	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	A	942	1	14,14,15	0.19	0	17,19,21	0.37	0
14	NAG	C	908	1	14,14,15	0.29	0	17,19,21	0.43	0
14	NAG	B	903	2	14,14,15	0.34	0	17,19,21	0.41	0
14	NAG	A	952	1	14,14,15	0.67	1 (7%)	17,19,21	0.49	0
14	NAG	D	902	2	14,14,15	0.34	0	17,19,21	0.40	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
14	NAG	C	942	1	-	4/6/23/26	0/1/1/1
14	NAG	K	301	6	-	2/6/23/26	0/1/1/1
14	NAG	A	926	1	-	6/6/23/26	0/1/1/1
14	NAG	I	305	6	-	1/6/23/26	0/1/1/1
14	NAG	A	908	1	-	1/6/23/26	0/1/1/1
14	NAG	C	953	1	-	2/6/23/26	0/1/1/1
14	NAG	B	901	2	-	1/6/23/26	0/1/1/1
14	NAG	D	901	2	-	2/6/23/26	0/1/1/1
14	NAG	C	909	1	-	2/6/23/26	0/1/1/1
14	NAG	B	902	2	-	2/6/23/26	0/1/1/1
14	NAG	C	927	1	-	6/6/23/26	0/1/1/1
14	NAG	A	942	1	-	2/6/23/26	0/1/1/1
14	NAG	C	908	1	-	1/6/23/26	0/1/1/1
14	NAG	B	903	2	-	2/6/23/26	0/1/1/1
14	NAG	A	952	1	-	0/6/23/26	0/1/1/1
14	NAG	D	902	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	I	305	NAG	O5-C1	7.06	1.55	1.43
14	K	301	NAG	O5-C1	6.81	1.55	1.43
14	I	305	NAG	C1-C2	-2.77	1.48	1.52
14	K	301	NAG	C1-C2	-2.52	1.48	1.52
14	A	952	NAG	O5-C1	-2.31	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	926	NAG	C2-N2-C7	4.61	129.07	122.90
14	C	927	NAG	C2-N2-C7	4.60	129.06	122.90
14	A	926	NAG	C1-C2-N2	2.16	113.84	110.43
14	C	927	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	926	NAG	O5-C5-C6-O6
14	C	927	NAG	O5-C5-C6-O6
14	C	942	NAG	O5-C5-C6-O6
14	B	902	NAG	O5-C5-C6-O6
14	C	927	NAG	C4-C5-C6-O6
14	C	909	NAG	O5-C5-C6-O6
14	A	926	NAG	C4-C5-C6-O6
14	B	902	NAG	C4-C5-C6-O6
14	B	903	NAG	O5-C5-C6-O6
14	C	942	NAG	C4-C5-C6-O6
14	C	909	NAG	C4-C5-C6-O6
14	B	903	NAG	C4-C5-C6-O6
14	D	902	NAG	O5-C5-C6-O6
14	A	926	NAG	C8-C7-N2-C2
14	A	926	NAG	O7-C7-N2-C2
14	A	942	NAG	C8-C7-N2-C2
14	A	942	NAG	O7-C7-N2-C2
14	C	927	NAG	C8-C7-N2-C2
14	C	927	NAG	O7-C7-N2-C2
14	C	942	NAG	C8-C7-N2-C2
14	C	942	NAG	O7-C7-N2-C2
14	C	953	NAG	O5-C5-C6-O6
14	D	902	NAG	C4-C5-C6-O6
14	D	901	NAG	C4-C5-C6-O6
14	A	908	NAG	O5-C5-C6-O6
14	K	301	NAG	O5-C5-C6-O6
14	C	908	NAG	O5-C5-C6-O6
14	D	901	NAG	O5-C5-C6-O6
14	I	305	NAG	O5-C5-C6-O6
14	C	953	NAG	C4-C5-C6-O6
14	B	901	NAG	C4-C5-C6-O6
14	K	301	NAG	C4-C5-C6-O6
14	A	926	NAG	C1-C2-N2-C7
14	C	927	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	926	NAG	C3-C2-N2-C7
14	C	927	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	926	NAG	1	0
14	A	908	NAG	2	0
14	C	927	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	455/481 (94%)	0.64	39 (8%)	16 19	118, 169, 241, 272	0
1	C	450/481 (93%)	0.64	41 (9%)	15 18	125, 167, 239, 284	0
2	B	132/153 (86%)	0.66	8 (6%)	27 27	115, 171, 238, 256	0
2	D	132/153 (86%)	0.81	12 (9%)	15 18	122, 177, 233, 246	0
3	J	210/210 (100%)	0.68	21 (10%)	12 16	190, 267, 327, 375	0
3	L	210/210 (100%)	0.74	13 (6%)	26 27	188, 278, 318, 331	0
4	E	223/223 (100%)	0.57	20 (8%)	15 18	136, 205, 293, 332	0
4	G	223/223 (100%)	0.51	19 (8%)	16 20	141, 192, 284, 320	0
5	F	212/212 (100%)	0.61	14 (6%)	24 25	171, 266, 317, 340	0
5	H	212/212 (100%)	0.55	13 (6%)	27 27	157, 244, 296, 314	0
6	I	228/235 (97%)	0.46	17 (7%)	20 23	187, 251, 285, 313	0
6	K	228/235 (97%)	0.75	32 (14%)	6 10	188, 249, 281, 302	0
All	All	2915/3028 (96%)	0.63	249 (8%)	16 20	115, 214, 301, 375	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	ALA	11.5
5	F	2	ILE	6.2
1	C	454	LEU	5.8
4	G	114	ALA	5.7
4	E	67	VAL	5.6
6	K	51	VAL	5.4
2	B	647	GLU	5.4
5	H	85	THR	5.3
3	J	64	GLY	4.8
6	K	162	HIS	4.6
4	G	214	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	K	161	VAL	4.6
4	E	198	VAL	4.5
5	H	84	ALA	4.5
4	E	82	VAL	4.4
1	A	454	LEU	4.4
1	C	326	ILE	4.4
5	H	212	GLY	4.4
1	A	427	TRP	4.3
1	A	227	LYS	4.3
3	J	67(B)	THR	4.2
1	C	227	LYS	4.1
6	K	160	GLY	4.1
2	D	547	GLY	4.1
4	E	48	LEU	4.0
6	K	159	SER	4.0
1	C	38	VAL	3.9
1	C	496	VAL	3.9
3	J	127	GLN	3.9
6	K	67	VAL	3.8
1	C	241	SER	3.7
4	G	119	PRO	3.7
4	G	1	GLN	3.7
1	C	427	TRP	3.7
1	A	34	LEU	3.7
6	K	123	ALA	3.6
3	J	145	VAL	3.6
6	K	163	THR	3.6
6	K	181	THR	3.6
1	C	284	ILE	3.6
5	F	194	CYS	3.6
2	B	661	LEU	3.6
1	A	256	SER	3.5
2	D	647	GLU	3.5
3	J	147	VAL	3.4
4	G	48	LEU	3.4
3	J	46	LEU	3.4
1	C	461	THR	3.4
1	A	326	ILE	3.4
6	K	113	SER	3.4
4	G	198	VAL	3.3
4	E	214	LYS	3.3
1	C	455	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	124	PRO	3.3
5	F	182	SER	3.3
5	H	62	PHE	3.2
5	F	207	LYS	3.2
1	A	284	ILE	3.2
3	J	146	THR	3.2
2	D	656	ASN	3.2
1	A	496	VAL	3.2
1	C	485	LYS	3.2
2	B	610	TRP	3.2
2	B	619	LEU	3.2
6	I	11	LEU	3.2
1	C	40	TYR	3.1
1	A	461	THR	3.1
2	D	593	LEU	3.1
6	K	100(F)	ALA	3.1
4	E	90	TYR	3.1
1	C	277	ILE	3.1
6	K	158	THR	3.0
3	J	28	LEU	3.0
1	C	121	LYS	3.0
2	D	577	GLN	3.0
3	L	205	LYS	3.0
5	F	185	ASP	3.0
1	A	33	ASN	3.0
3	J	40	PRO	3.0
6	K	100(G)	PHE	3.0
6	K	47	TRP	2.9
1	C	240	PRO	2.9
6	I	123	ALA	2.9
1	A	109	ILE	2.9
3	J	130	LYS	2.9
1	C	452	LEU	2.9
5	F	212	GLY	2.9
5	F	205	VAL	2.9
4	E	119	PRO	2.9
1	A	176	PHE	2.9
1	C	398	ASN	2.9
1	A	473	GLY	2.8
5	H	86	TYR	2.8
6	K	100(O)	TYR	2.8
3	J	43	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	H	103	LYS	2.8
3	L	42	GLN	2.8
4	G	125	ALA	2.8
1	A	500	ARG	2.8
1	A	458	GLY	2.8
4	E	126	PRO	2.8
6	K	50	TYR	2.7
4	G	67	VAL	2.7
3	J	183	PRO	2.7
4	E	37	VAL	2.7
5	H	117	ILE	2.7
1	C	141	ASP	2.7
4	G	133	GLY	2.7
1	C	504	ARG	2.6
4	G	13	LYS	2.6
1	A	38	VAL	2.6
1	A	32	GLU	2.6
5	H	37	GLN	2.6
1	A	426	MET	2.6
1	A	494	LEU	2.6
6	K	55	GLY	2.6
1	C	290	THR	2.6
5	H	127	SER	2.6
1	C	53	PHE	2.6
1	C	73	ALA	2.6
1	A	121	LYS	2.5
6	K	186	SER	2.5
1	C	85	HIS	2.5
5	F	117	ILE	2.5
3	L	130	LYS	2.5
1	C	338	TRP	2.5
6	K	35	SER	2.5
1	A	389	GLY	2.5
3	J	123	SER	2.5
3	L	26	GLU	2.5
1	A	255	VAL	2.5
3	J	182	THR	2.5
4	E	207	VAL	2.5
3	L	167	LYS	2.5
6	K	199	LYS	2.5
1	A	322	ILE	2.5
6	K	179	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	460	SER	2.5
6	I	111	SER	2.5
2	D	664	ASP	2.5
4	G	123	PRO	2.5
6	I	171	SER	2.4
6	K	185	SER	2.4
2	B	664	ASP	2.4
1	C	341	THR	2.4
4	G	90	TYR	2.4
3	L	41	GLY	2.4
4	G	165	THR	2.4
6	K	165	PRO	2.4
1	A	274	SER	2.4
1	C	459	GLY	2.4
4	E	157	GLY	2.4
3	J	47	ILE	2.4
1	A	506	VAL	2.4
3	L	168	GLN	2.4
4	G	131	THR	2.4
5	H	190	LYS	2.4
1	A	370	GLU	2.4
1	C	494	LEU	2.4
2	D	523	LEU	2.4
5	H	57	GLY	2.4
6	I	191	THR	2.4
6	K	57	THR	2.4
6	I	151	SER	2.4
1	C	75	VAL	2.4
1	C	134	VAL	2.4
4	E	18	VAL	2.3
6	K	150	VAL	2.3
2	D	575	GLN	2.3
6	I	112	ALA	2.3
4	E	205	THR	2.3
1	C	292	VAL	2.3
4	G	141	LEU	2.3
6	K	80	LEU	2.3
3	L	155	PRO	2.3
5	H	104	VAL	2.3
1	A	141	ASP	2.3
1	C	367	GLY	2.3
4	E	125	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	I	157	LEU	2.3
6	K	69	LEU	2.3
2	D	614	TRP	2.3
4	E	46	GLU	2.3
2	D	610	TRP	2.3
4	G	113	SER	2.3
5	H	184	ALA	2.3
1	C	194	ILE	2.2
3	L	196	VAL	2.2
4	E	40	ALA	2.2
6	I	51	VAL	2.2
1	C	86	LEU	2.2
2	B	547	GLY	2.2
3	J	41	GLY	2.2
1	A	321(A)	ASP	2.2
1	C	361	PHE	2.2
2	D	517	ALA	2.2
4	E	99	GLY	2.2
5	F	152	ASN	2.2
3	L	56	SER	2.2
3	L	144	ALA	2.2
3	J	63	SER	2.2
2	B	526	ALA	2.1
1	A	69	TRP	2.1
1	C	66	HIS	2.1
4	E	194	TYR	2.1
1	A	340	GLU	2.1
4	G	134	GLY	2.1
6	I	71	LEU	2.1
1	A	425	ASN	2.1
1	C	333	VAL	2.1
1	A	429	ARG	2.1
3	J	164	THR	2.1
6	I	189	THR	2.1
2	B	648	GLU	2.1
1	C	176	PHE	2.1
3	J	167	LYS	2.1
5	F	54	LEU	2.1
5	F	122	ASP	2.1
6	I	47	TRP	2.1
1	A	462	ASN	2.1
3	L	83	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	40	PRO	2.1
6	K	171	SER	2.1
6	I	168	LEU	2.1
1	C	382	PHE	2.1
1	C	274	SER	2.1
4	E	161	SER	2.1
1	A	369	LEU	2.0
1	A	40	TYR	2.0
1	A	468	PHE	2.0
1	C	366	GLY	2.0
3	J	210	THR	2.0
6	I	211	PRO	2.0
1	C	39	TYR	2.0
6	K	89	ILE	2.0
6	K	112	ALA	2.0
6	K	142	ASP	2.0
6	I	17	THR	2.0
6	I	87	SER	2.0
4	G	99	GLY	2.0
5	F	70	HIS	2.0
6	K	100(Q)	ASP	2.0
2	D	631	TRP	2.0
3	L	203	VAL	2.0
4	E	38	ARG	2.0
5	F	27	GLN	2.0
4	G	115	SER	2.0
6	I	126	SER	2.0
3	J	62	PHE	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($\text{\AA}^2$)	Q<0.9
8	MAN	N	5	11/12	-0.17	0.21	288,291,294,297	0
10	MAN	R	6	11/12	0.10	0.16	232,250,257,258	0
8	MAN	N	4	11/12	0.34	0.16	241,253,257,259	0
11	BMA	S	3	11/12	0.35	0.17	238,239,241,241	0
7	MAN	Z	4	11/12	0.49	0.18	199,208,215,215	0
9	NAG	X	2	14/15	0.50	0.12	243,268,273,274	0
9	NAG	T	2	14/15	0.57	0.14	222,235,246,253	0
9	NAG	O	1	14/15	0.58	0.15	180,203,213,224	0
10	BMA	R	3	11/12	0.66	0.14	225,231,246,253	0
11	BMA	Y	3	11/12	0.66	0.13	209,244,274,327	0
9	NAG	W	2	14/15	0.68	0.14	226,244,249,249	0
7	MAN	Z	7	11/12	0.68	0.18	196,199,218,231	0
8	BMA	N	3	11/12	0.68	0.12	256,265,276,285	0
9	NAG	O	2	14/15	0.70	0.14	224,236,248,255	0
7	BMA	Z	3	11/12	0.70	0.15	192,205,231,233	0
9	NAG	V	2	14/15	0.70	0.16	252,267,276,276	0
7	MAN	Z	5	11/12	0.71	0.26	193,214,225,236	0
11	NAG	Y	1	14/15	0.72	0.26	189,207,219,223	0
7	MAN	M	4	11/12	0.72	0.19	221,227,234,235	0
8	NAG	a	1	14/15	-	-	152,193,211,215	0
8	NAG	a	2	14/15	-	-	206,220,230,238	0
8	BMA	a	3	11/12	-	-	245,253,263,273	0
8	MAN	a	4	11/12	-	-	229,240,246,246	0
8	MAN	a	5	11/12	-	-	291,294,295,297	0
7	BMA	M	3	11/12	0.73	0.15	192,202,224,227	0
12	MAN	U	9	11/12	0.75	0.11	237,244,248,248	0
7	MAN	Z	6	11/12	0.76	0.14	220,225,239,240	0
12	MAN	U	6	11/12	0.76	0.14	233,240,243,244	0
11	NAG	S	2	14/15	0.76	0.15	212,223,235,244	0
11	NAG	Y	2	14/15	0.77	0.19	199,221,246,273	0
7	MAN	M	5	11/12	0.77	0.24	189,208,218,228	0
7	MAN	M	7	11/12	0.78	0.18	207,216,231,247	0
7	NAG	Z	2	14/15	0.80	0.24	173,188,199,202	0
9	NAG	Q	2	14/15	0.81	0.13	241,246,251,252	0
11	NAG	S	1	14/15	0.81	0.11	177,194,220,229	0
9	NAG	P	1	14/15	0.81	0.13	167,198,218,233	0
7	NAG	M	2	14/15	0.82	0.24	171,183,199,203	0
9	NAG	P	2	14/15	0.82	0.13	235,250,266,269	0
9	NAG	b	1	14/15	-	-	174,198,206,219	0
9	NAG	b	2	14/15	-	-	224,237,247,255	0
9	NAG	c	1	14/15	-	-	160,193,213,228	0
9	NAG	c	2	14/15	-	-	224,242,261,263	0
9	NAG	d	1	14/15	-	-	216,233,245,258	0

Continued on next page...

Continued from previous page...

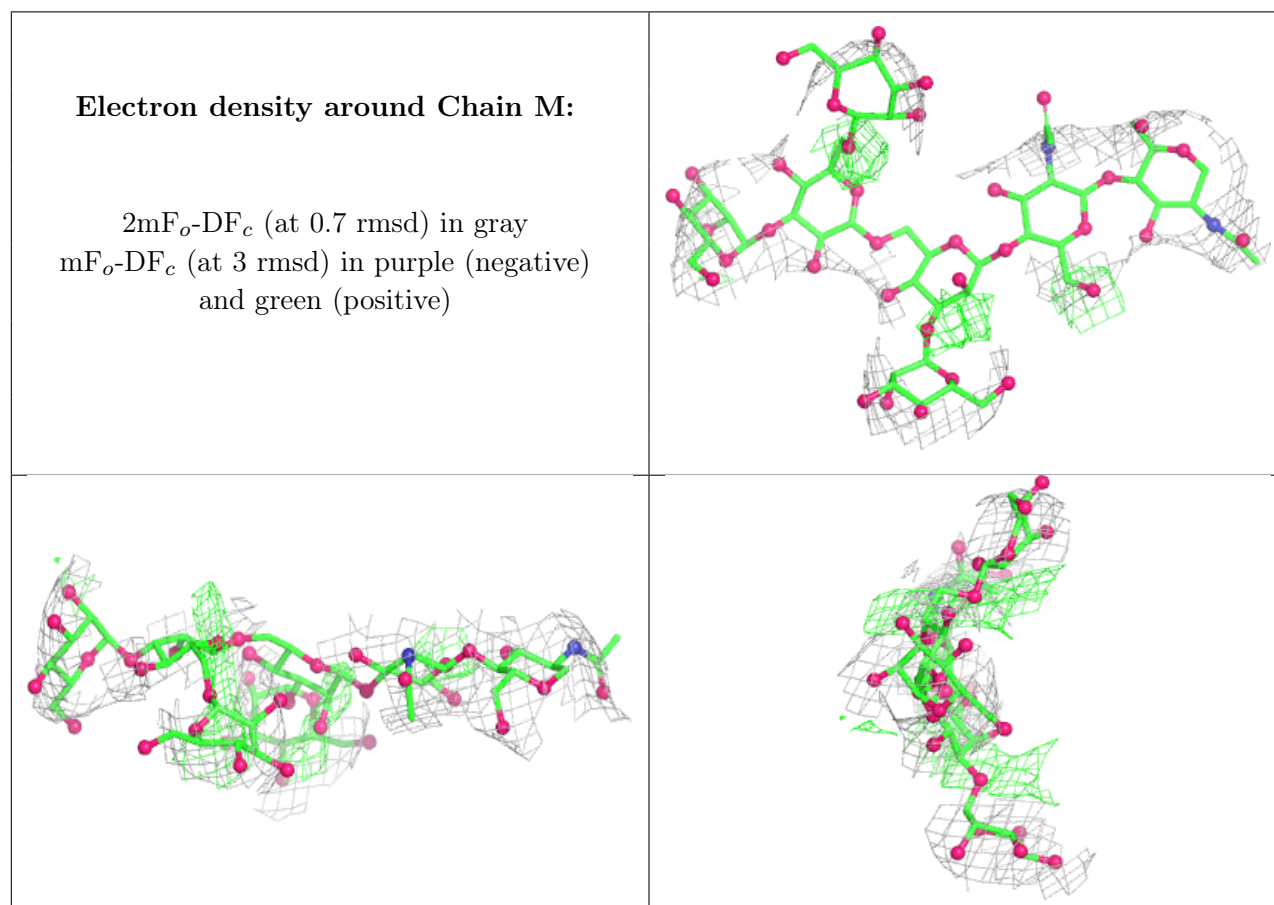
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	d	2	14/15	-	-	262,273,276,279	0
9	NAG	f	1	14/15	-	-	175,193,219,228	0
9	NAG	f	2	14/15	-	-	204,213,227,236	0
9	NAG	g	1	14/15	-	-	182,197,215,223	0
9	NAG	g	2	14/15	-	-	219,230,241,248	0
9	NAG	i	1	14/15	-	-	229,247,272,295	0
9	NAG	i	2	14/15	-	-	276,295,304,306	0
9	NAG	j	1	14/15	-	-	178,218,237,249	0
9	NAG	j	2	14/15	-	-	224,246,254,254	0
9	NAG	Q	1	14/15	0.82	0.12	193,211,222,236	0
9	NAG	V	1	14/15	0.84	0.13	219,234,259,280	0
10	MAN	R	4	11/12	0.84	0.23	235,244,255,261	0
12	MAN	U	7	11/12	0.84	0.08	189,208,215,222	0
10	MAN	R	5	11/12	0.84	0.20	226,232,234,235	0
12	MAN	U	10	11/12	0.84	0.09	200,214,222,222	0
10	NAG	e	1	14/15	-	-	150,168,186,195	0
10	NAG	e	2	14/15	-	-	197,210,221,229	0
10	BMA	e	3	11/12	-	-	238,243,259,266	0
10	MAN	e	4	11/12	-	-	248,257,269,274	0
10	MAN	e	5	11/12	-	-	254,262,264,266	0
10	MAN	e	6	11/12	-	-	246,266,272,274	0
9	NAG	X	1	14/15	0.85	0.09	231,245,265,272	0
12	MAN	U	5	11/12	0.85	0.12	220,225,240,246	0
12	NAG	U	1	14/15	0.86	0.10	171,178,197,199	0
12	MAN	U	8	11/12	0.87	0.05	235,238,245,250	0
10	NAG	R	2	14/15	0.88	0.12	182,197,208,218	0
8	NAG	N	2	14/15	0.88	0.24	219,233,244,254	0
11	NAG	k	1	14/15	-	-	233,245,258,269	0
11	NAG	k	2	14/15	-	-	241,271,282,284	0
11	BMA	k	3	11/12	-	-	273,279,285,287	0
11	NAG	l	1	14/15	-	-	196,212,229,234	0
11	NAG	l	2	14/15	-	-	226,247,272,300	0
11	BMA	l	3	11/12	-	-	268,300,328,382	0
7	MAN	M	6	11/12	0.89	0.23	219,226,240,243	0
8	NAG	N	1	14/15	0.90	0.12	154,199,216,219	0
7	NAG	M	1	14/15	0.91	0.17	163,173,183,185	0
9	NAG	W	1	14/15	0.92	0.15	184,222,240,252	0
9	NAG	T	1	14/15	0.92	0.15	179,194,209,223	0
7	NAG	Z	1	14/15	0.93	0.26	177,185,200,200	0
10	NAG	R	1	14/15	0.94	0.20	134,153,170,180	0
12	NAG	U	2	14/15	0.94	0.09	173,191,216,220	0
12	MAN	U	4	11/12	0.94	0.10	193,197,218,238	0

Continued on next page...

Continued from previous page...

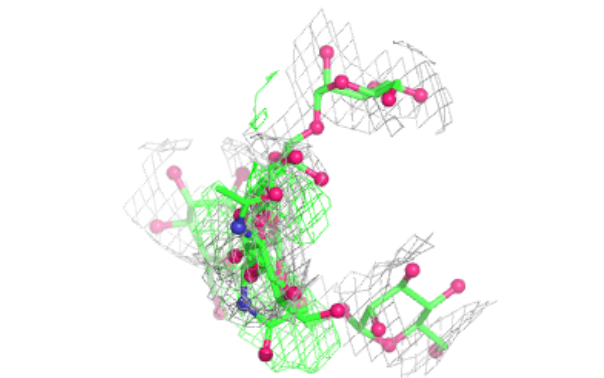
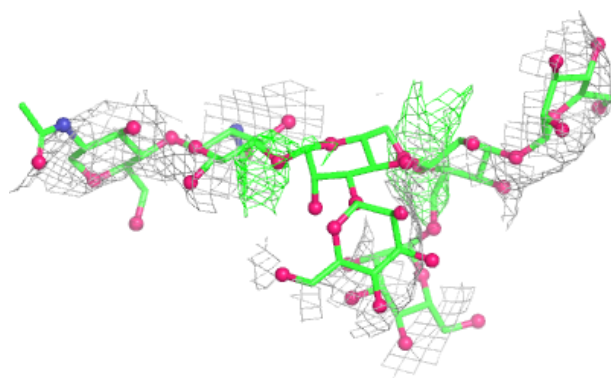
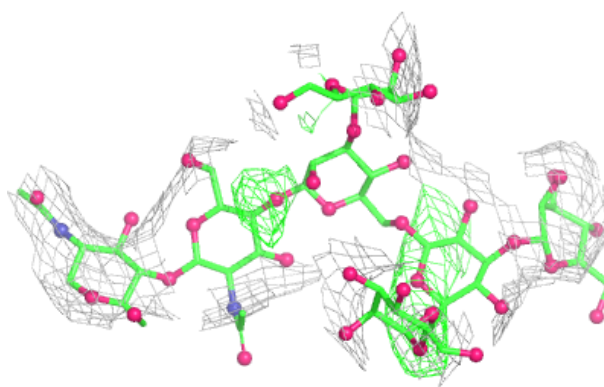
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	BMA	U	3	11/12	0.95	0.06	178,197,213,217	0
12	NAG	h	1	14/15	-	-	173,180,196,200	0
12	NAG	h	2	14/15	-	-	182,200,232,234	0
12	BMA	h	3	11/12	-	-	178,200,214,222	0
12	MAN	h	4	11/12	-	-	194,198,219,238	0
12	MAN	h	5	11/12	-	-	214,223,238,241	0
12	MAN	h	6	11/12	-	-	229,236,242,244	0
12	MAN	h	7	11/12	-	-	201,219,226,237	0
12	MAN	h	8	11/12	-	-	236,237,242,246	0
12	MAN	h	9	11/12	-	-	227,237,242,243	0
12	MAN	h	10	11/12	-	-	207,223,229,232	0
13	NAG	m	1	14/15	-	-	213,241,264,267	0
13	NAG	m	2	14/15	-	-	242,251,265,266	0
13	BMA	m	3	11/12	-	-	259,268,274,282	0
13	MAN	m	4	11/12	-	-	245,269,280,281	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.

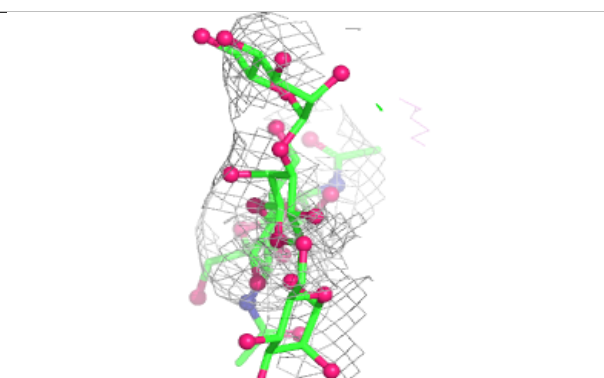
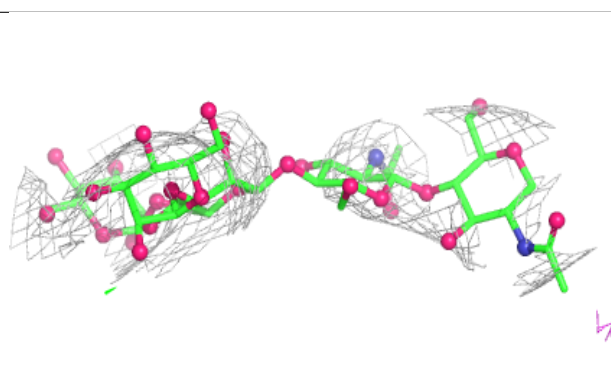
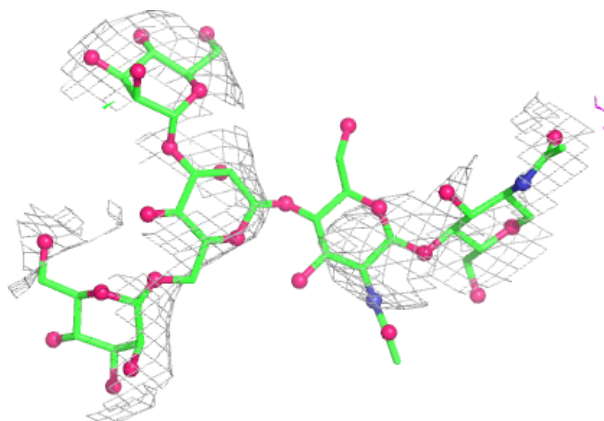


Electron density around Chain Z:

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

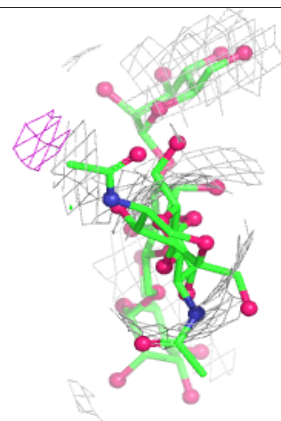
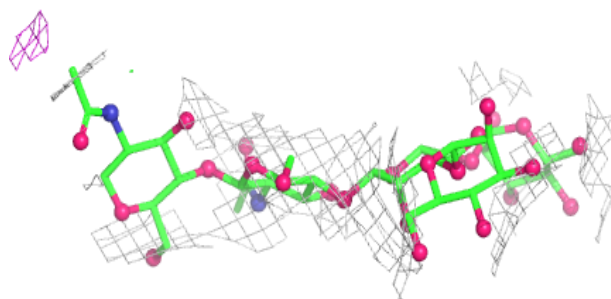
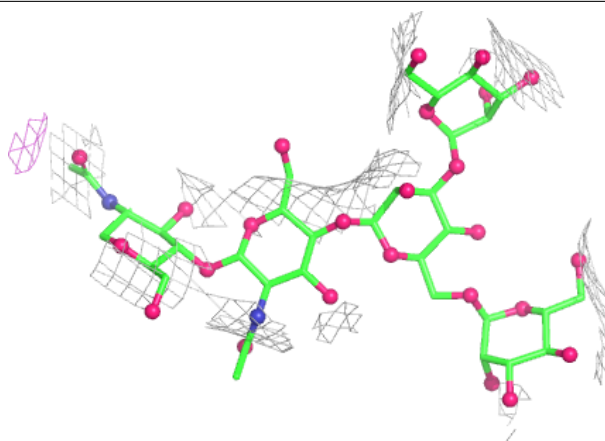
**Electron density around Chain N:**

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



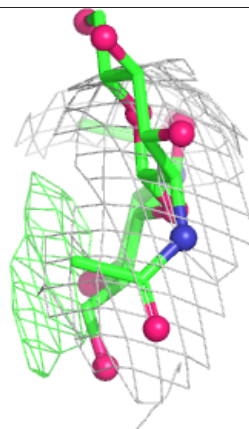
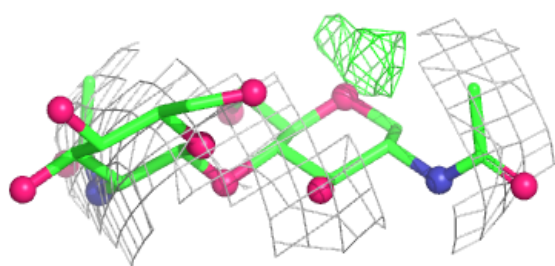
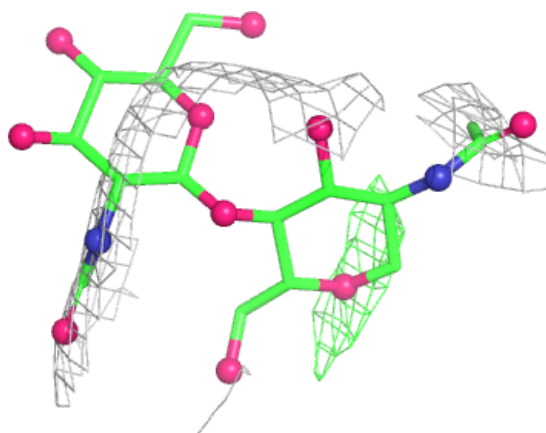
Electron density around Chain a:

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



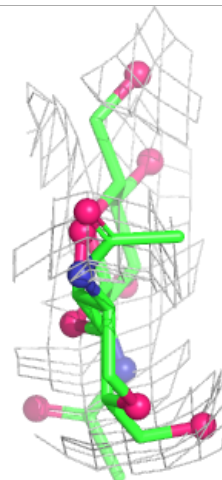
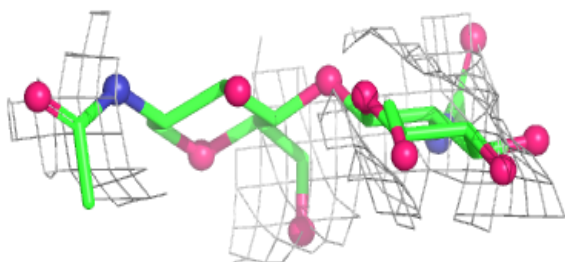
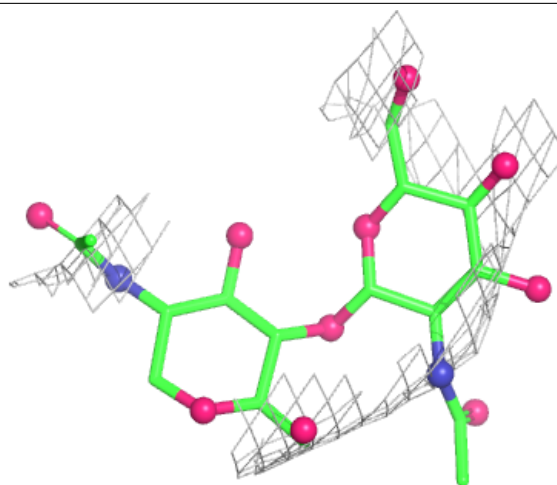
Electron density around Chain O:

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



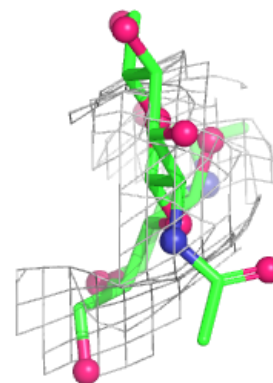
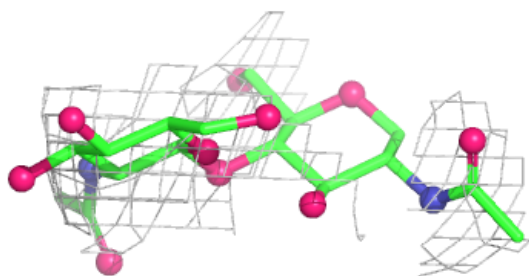
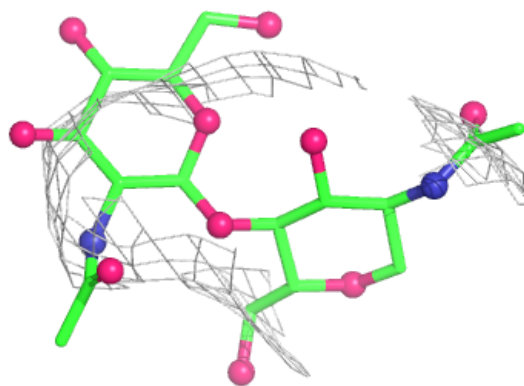
Electron density around Chain P:

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



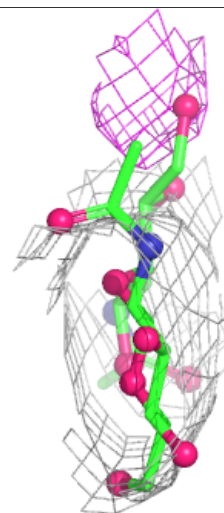
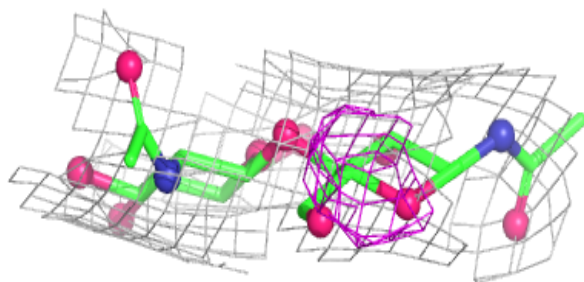
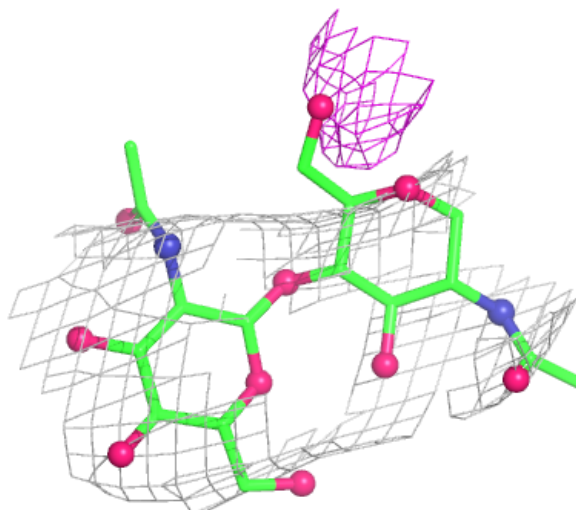
Electron density around Chain Q:

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



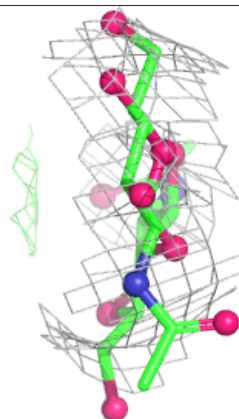
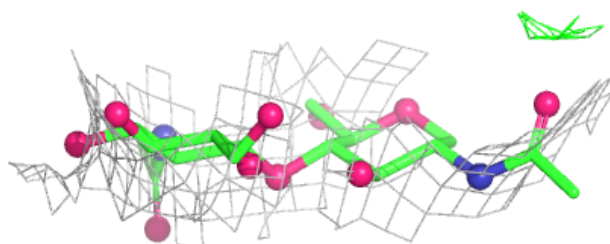
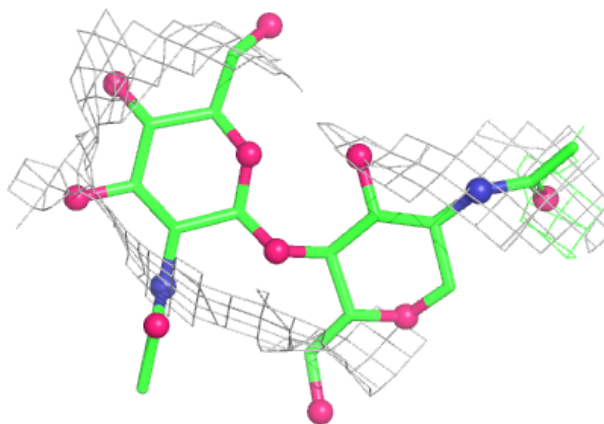
Electron density around Chain T:

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



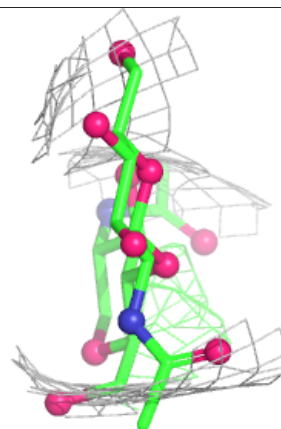
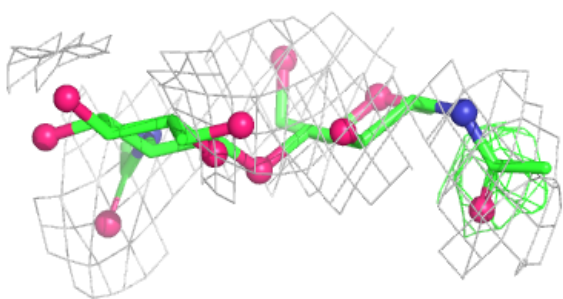
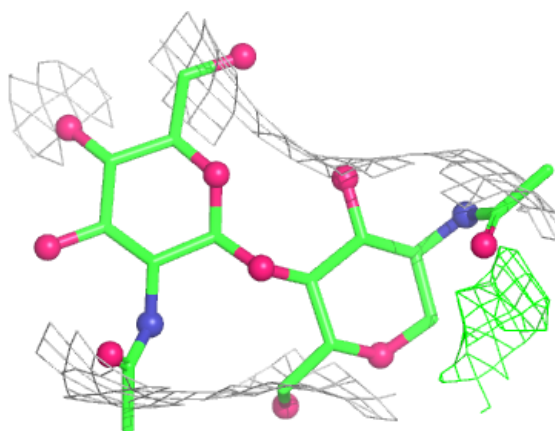
Electron density around Chain V:

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

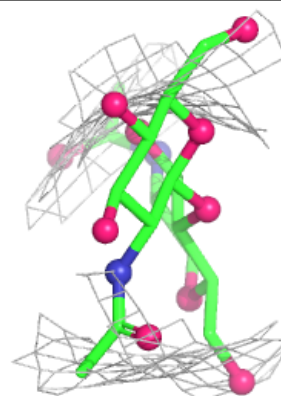
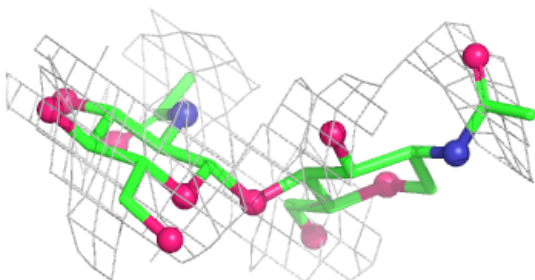
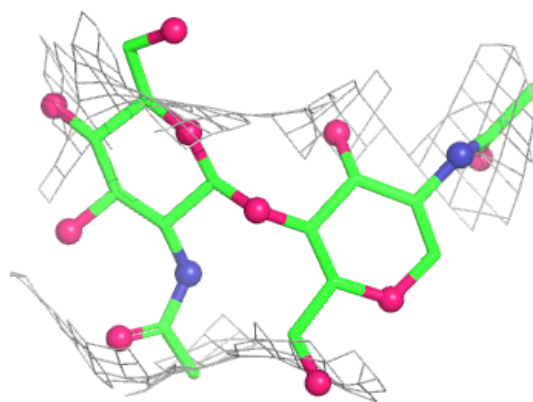


Electron density around Chain W:

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

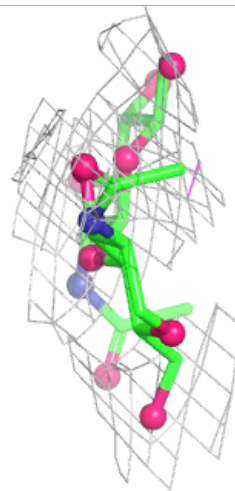
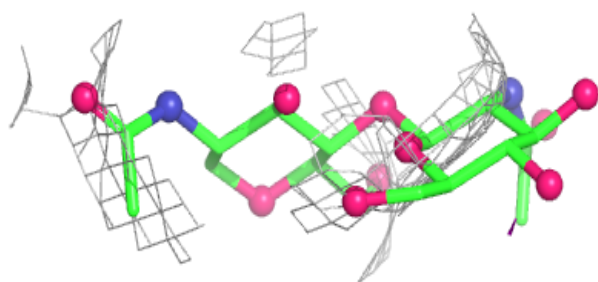
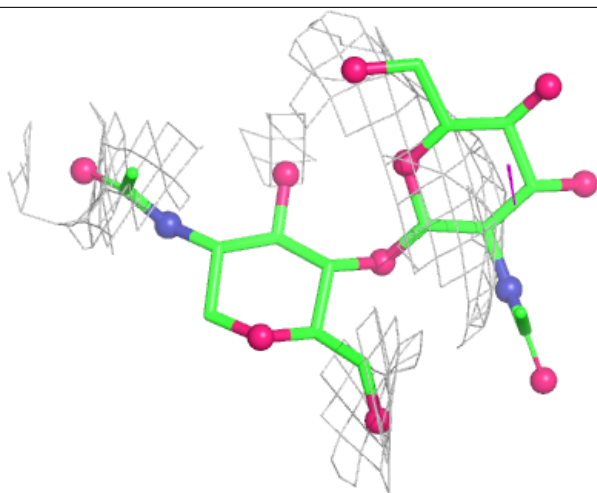
**Electron density around Chain X:**

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



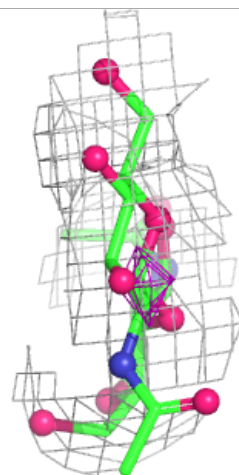
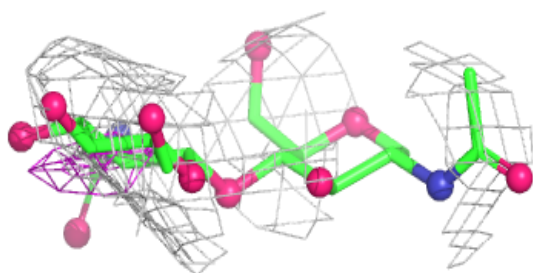
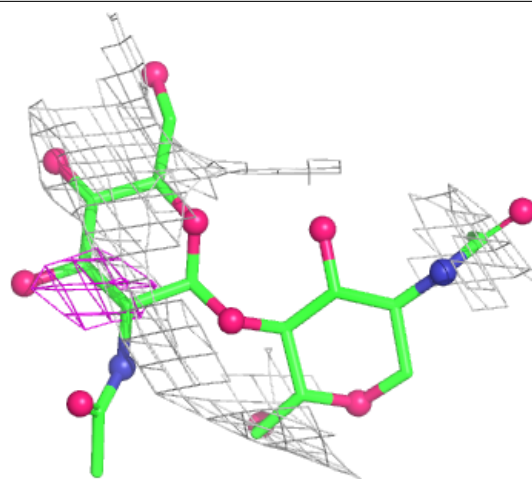
Electron density around Chain b:

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



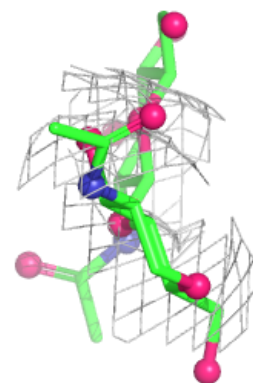
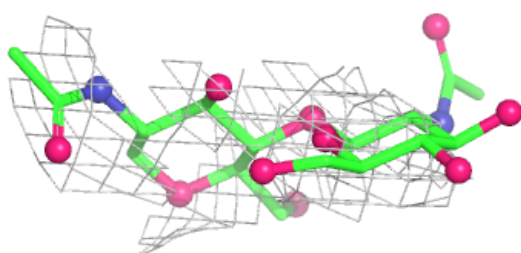
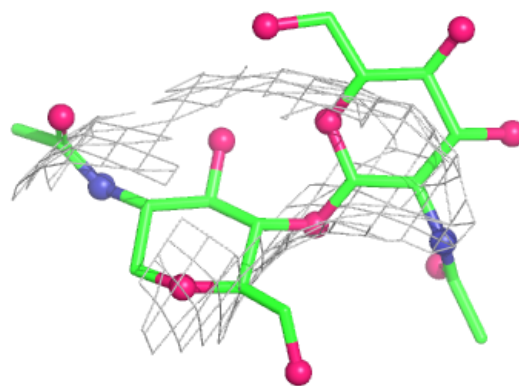
Electron density around Chain c:

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

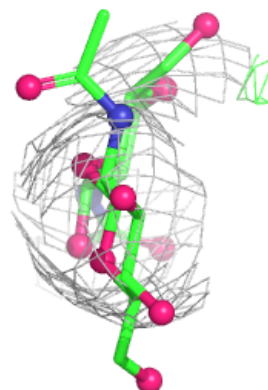
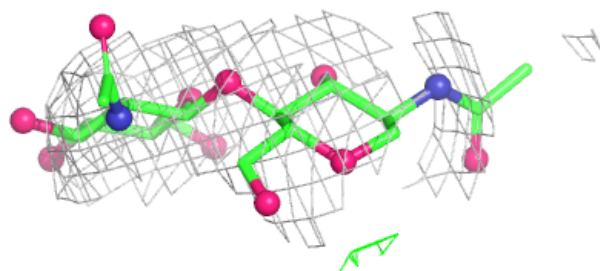
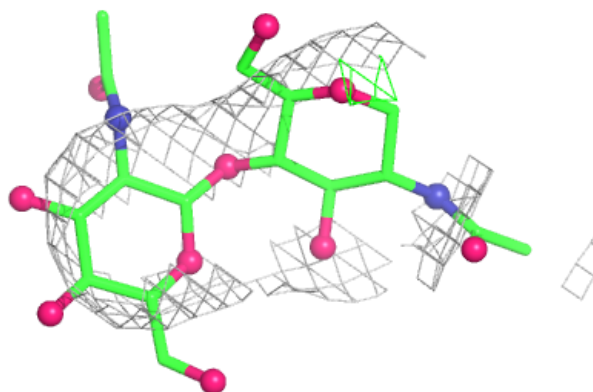


Electron density around Chain d:

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

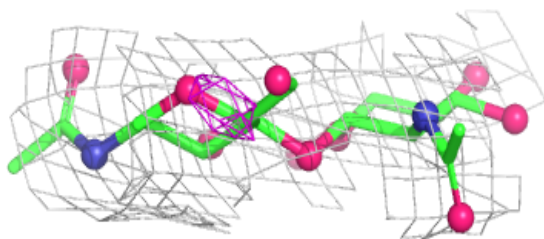
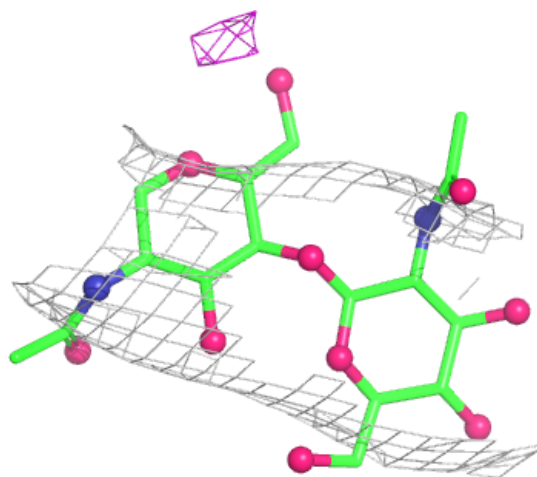
**Electron density around Chain f:**

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



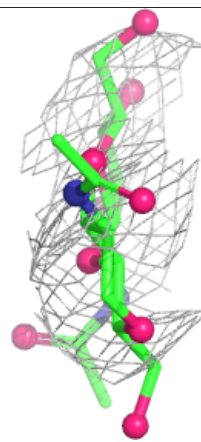
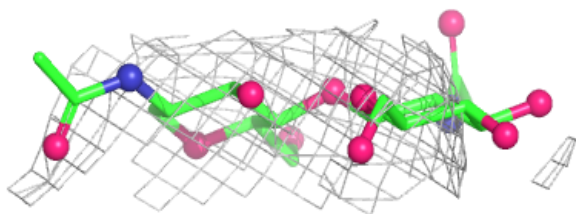
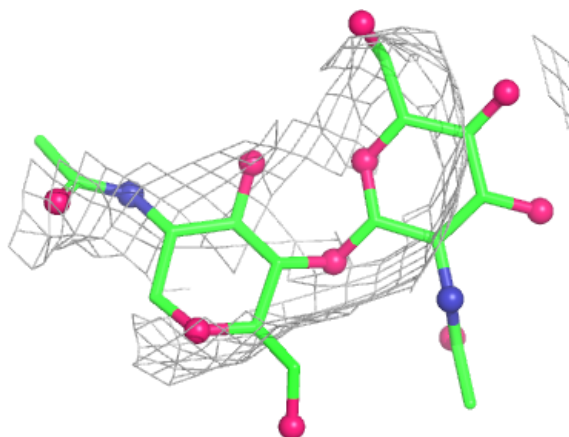
Electron density around Chain g:

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



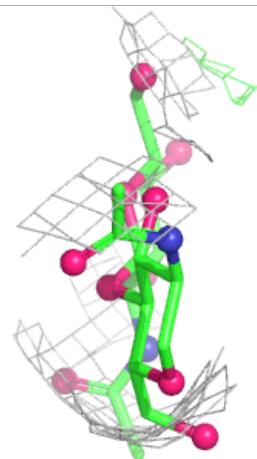
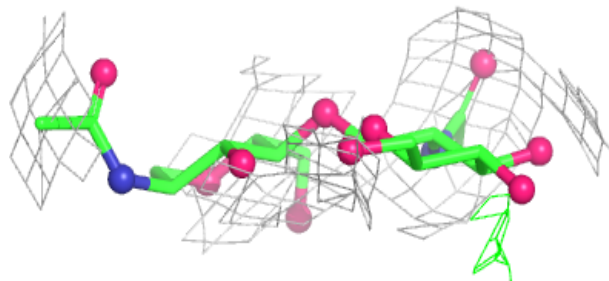
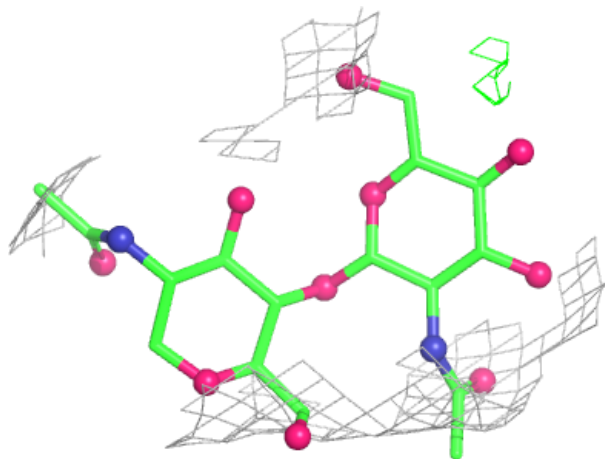
Electron density around Chain i:

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



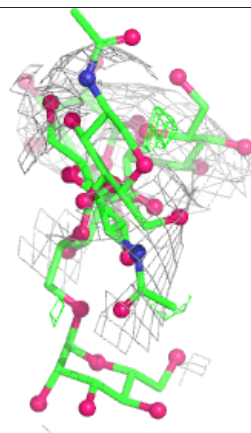
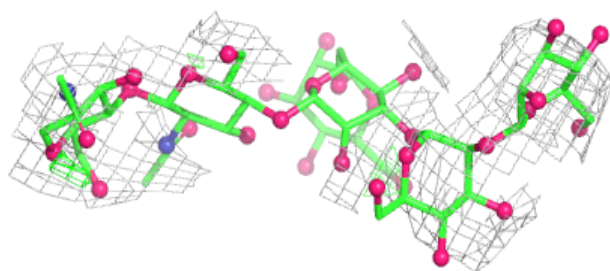
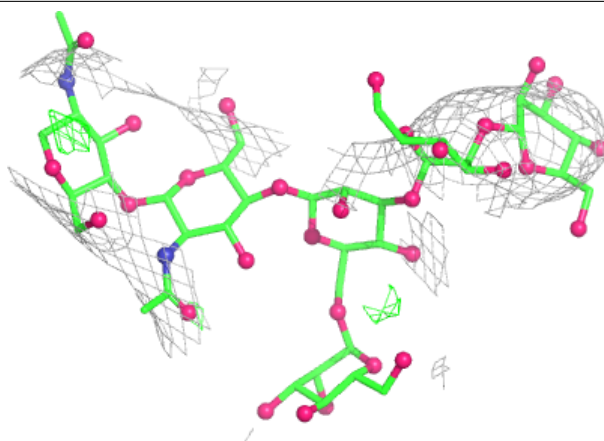
Electron density around Chain j:

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



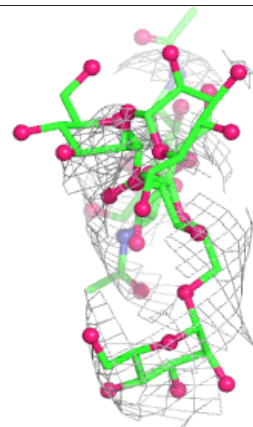
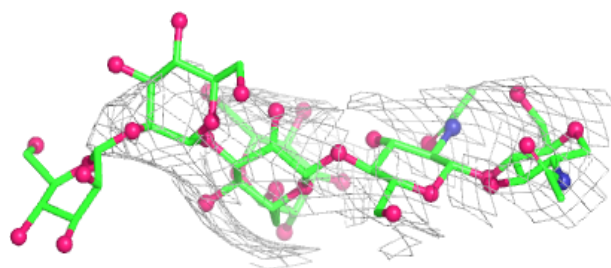
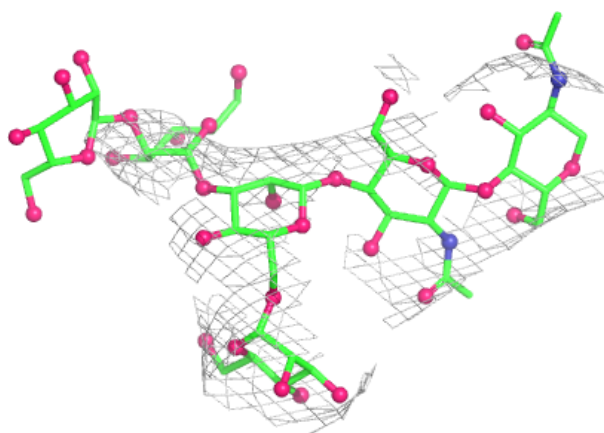
Electron density around Chain R:

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

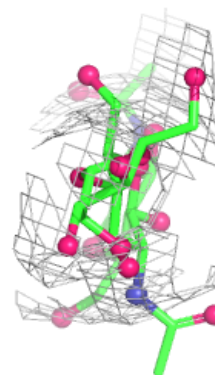
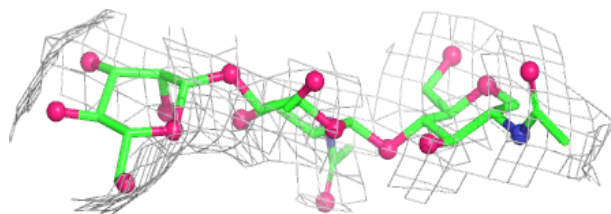
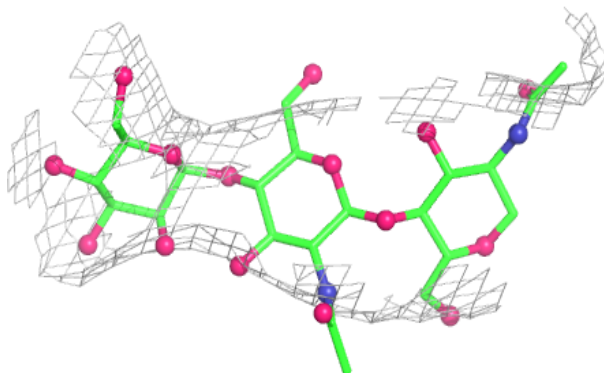


Electron density around Chain e:

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

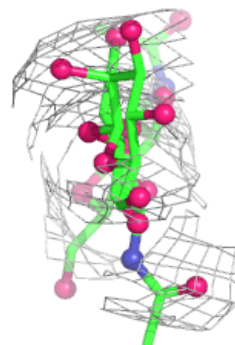
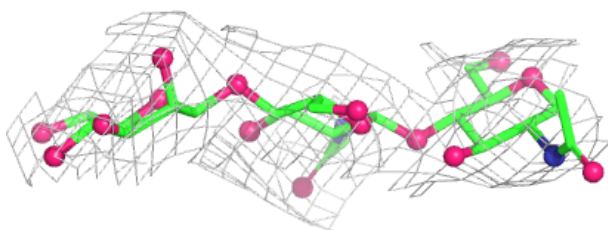
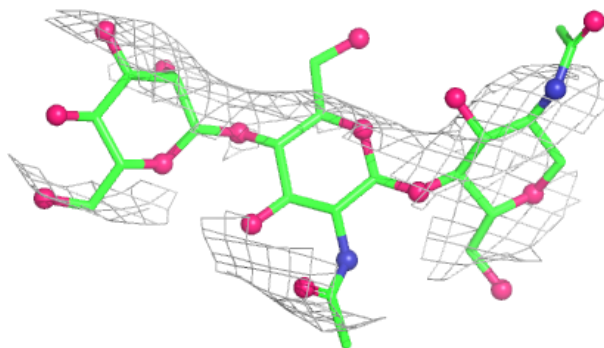
**Electron density around Chain S:**

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

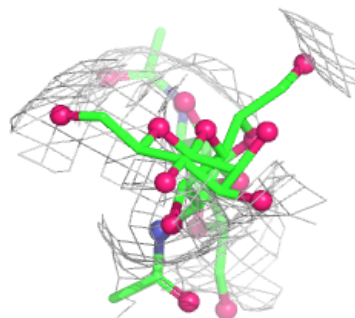
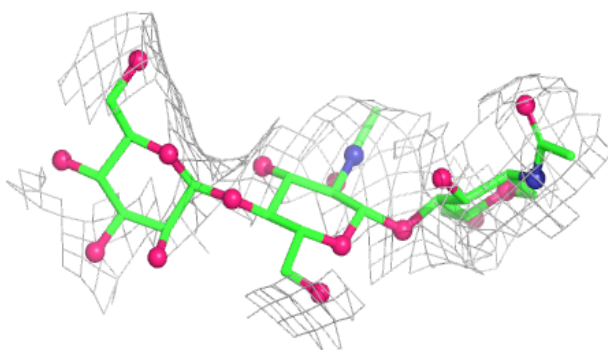
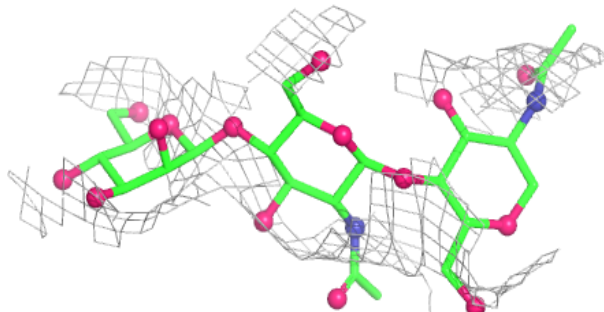


Electron density around Chain Y:

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

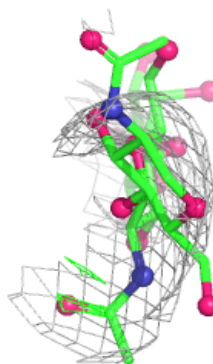
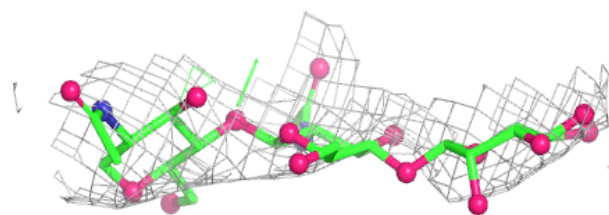
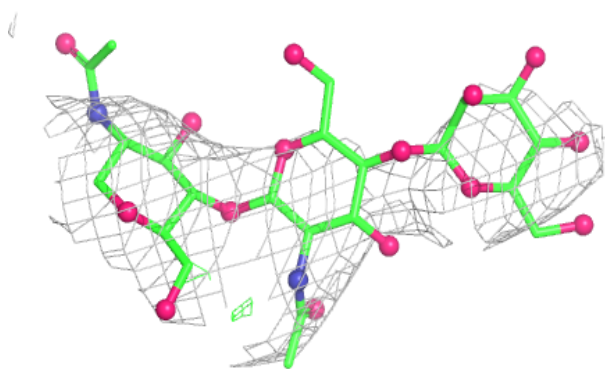
**Electron density around Chain k:**

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



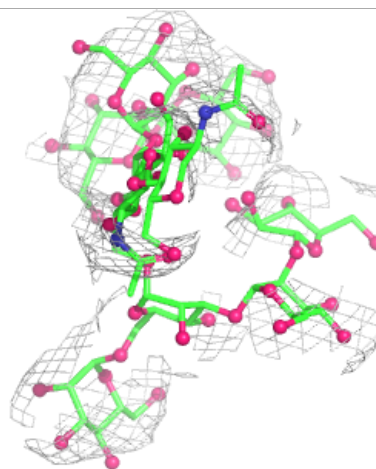
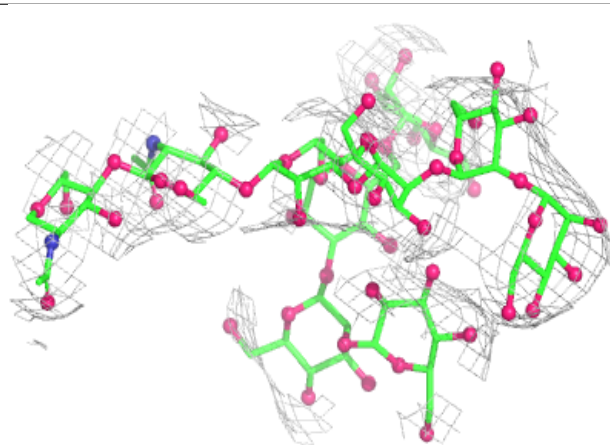
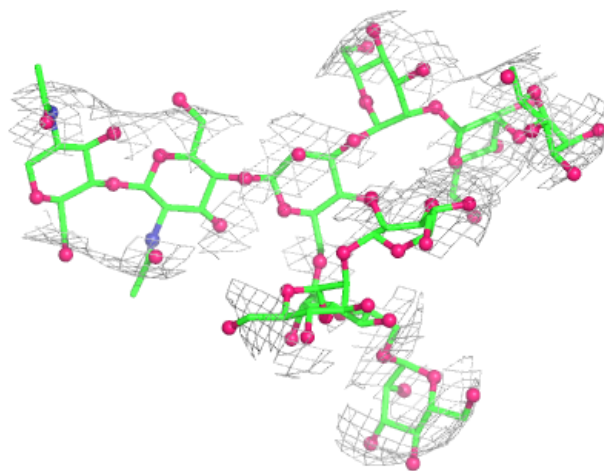
Electron density around Chain 1:

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



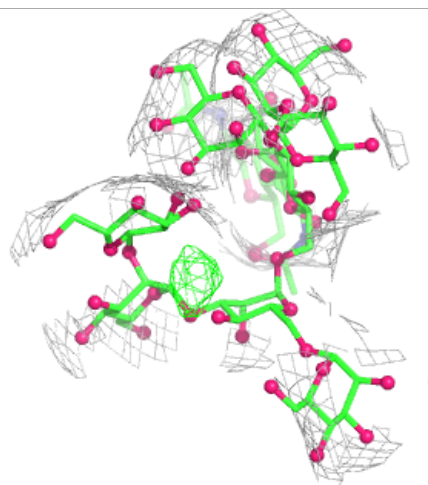
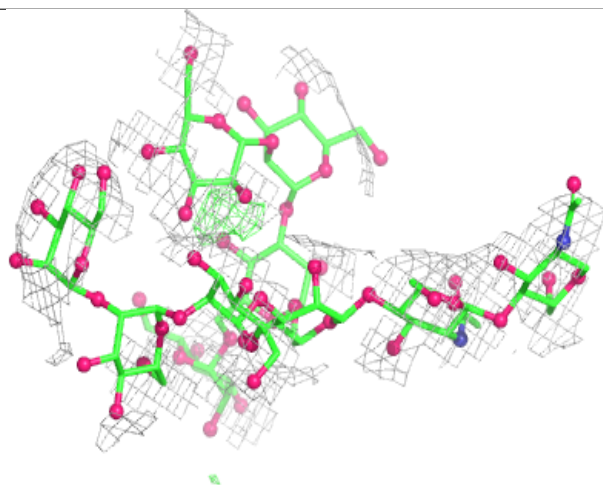
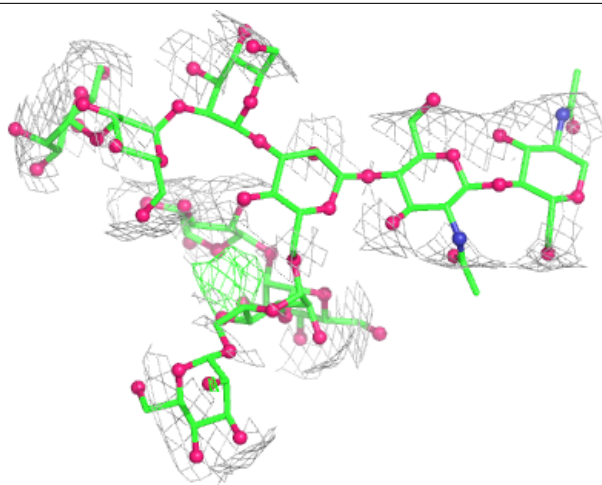
Electron density around Chain U:

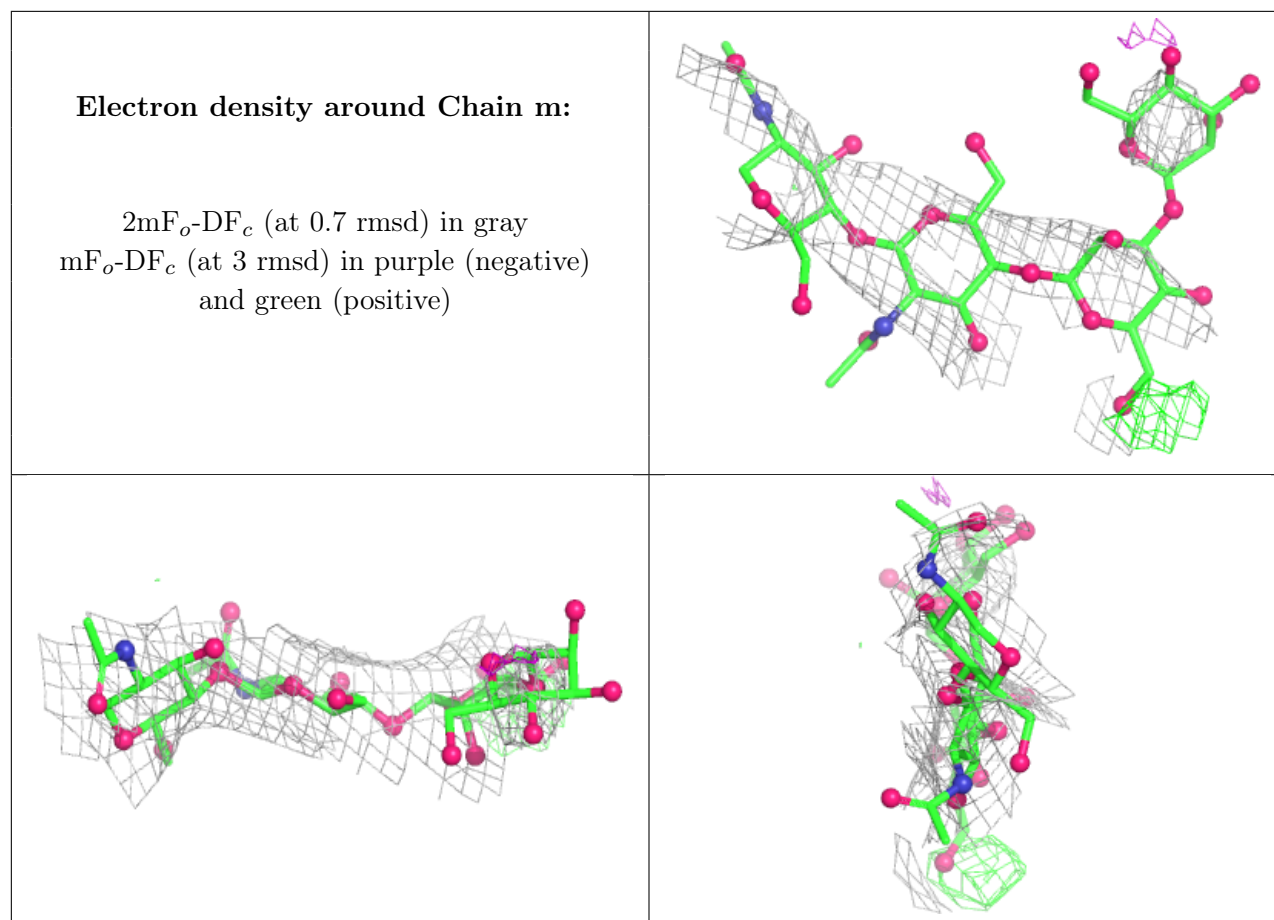
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain h:

$2mF_o-DF_c$ (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
14	NAG	A	942	14/15	0.15	0.18	246,259,268,272	0
14	NAG	K	301	14/15	0.28	0.19	255,274,293,293	0
14	NAG	I	305	14/15	0.29	0.15	262,282,291,294	0
14	NAG	B	902	14/15	0.44	0.16	260,274,299,300	0
14	NAG	A	926	14/15	0.54	0.17	210,217,221,223	0
14	NAG	C	908	14/15	0.56	0.21	232,249,265,272	0
14	NAG	C	942	14/15	0.58	0.13	230,246,255,260	0
14	NAG	D	902	14/15	0.60	0.13	225,248,271,272	0
14	NAG	C	953	14/15	0.62	0.17	212,234,244,246	0
14	NAG	B	903	14/15	0.66	0.12	230,262,292,295	0
14	NAG	A	908	14/15	0.72	0.19	217,234,248,253	0
14	NAG	A	952	14/15	0.72	0.15	233,255,262,265	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	NAG	C	927	14/15	0.74	0.13	218,225,232,234	0
14	NAG	C	909	14/15	0.74	0.26	197,225,250,254	0
14	NAG	D	901	14/15	0.77	0.14	265,277,303,319	0
14	NAG	B	901	14/15	0.84	0.10	239,260,288,303	0

6.5 Other polymers [i](#)

There are no such residues in this entry.