



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 12:40 PM EST

PDB ID : 8D4R
Title : Crystal Structure of Mosaic HIV-1 Envelope (MosM3.2) in Complex with antibodies PGT124 and 35O22 at 3.8 Angstrom
Authors : Xian, Y.; Wilson, A.
Deposited on : 2022-06-02
Resolution : 3.81 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

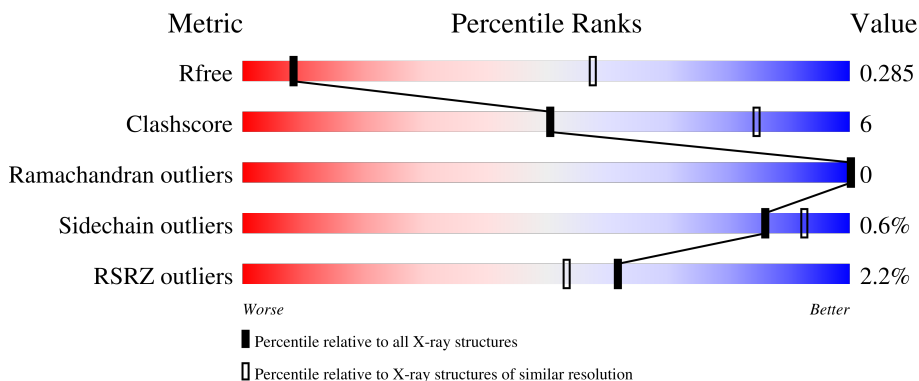
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



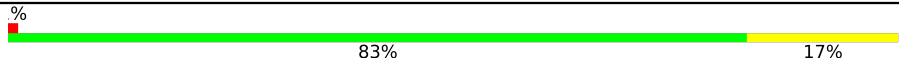
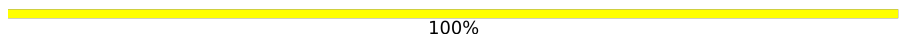

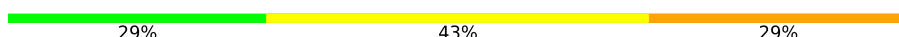
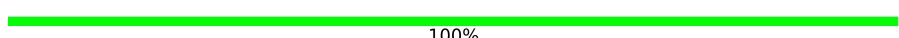
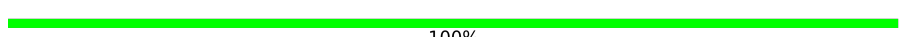
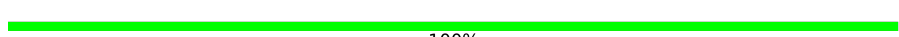



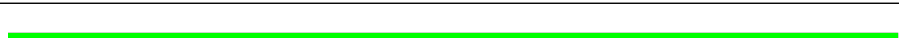

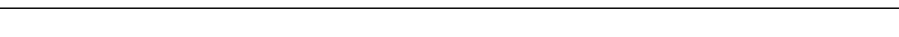
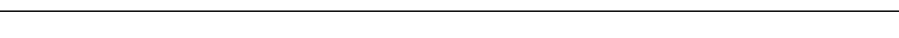
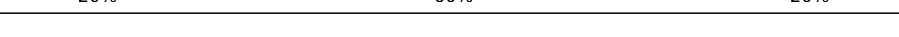
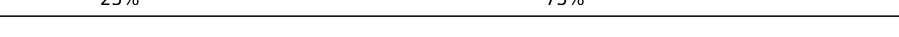
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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	G	427	 2% 81% 19%
2	B	131	 2% 87% 13%
3	D	187	 % 81% 19%
4	E	192	 6% 90% 10%
5	L	210	 2% 89% 10%

Continued on next page...

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Mol	Chain	Length	Quality of chain
6	H	226	 % 83% 17%
7	U	3	 100%
8	T	6	 33% 67%
9	A	7	 29% 43% 29%
10	C	2	 100%
10	F	2	 100%
10	K	2	 100%
10	N	2	 100%
10	O	2	 100%
10	P	2	 50% 50%
10	Q	2	 100%
10	R	2	 100%
10	S	2	 50% 50%
11	I	5	 20% 60% 20%
12	J	4	 25% 75%
13	M	4	 25% 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	C	2	-	-	-	X
10	NAG	S	1	-	-	-	X
10	NAG	S	2	-	-	-	X
11	MAN	I	4	-	-	-	X
13	BMA	M	3	-	-	-	X
14	NAG	G	604	-	-	-	X
8	MAN	T	5	-	-	-	X
8	MAN	T	6	-	-	-	X
9	MAN	A	5	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 11327 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	427	3363	2120	580	635	28	0	0	0

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	1054	665	180	202	7	0	0	0

- Molecule 3 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	187	1445	924	241	273	7	0	0	0

- Molecule 4 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	192	1465	918	241	298	8	0	0	0

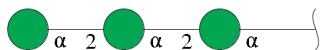
- Molecule 5 is a protein called PGT124 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	210	1595	1005	270	315	5	0	0	0

- Molecule 6 is a protein called PGT124 Fab heavy chain.

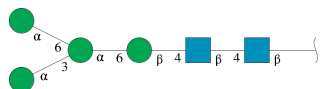
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	226	1720	1093	287	335	5	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



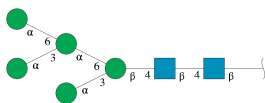
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
7	U	3	33	18	15	0	0	0

- Molecule 8 is an oligosaccharide called 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
			Total	C	N	O			
8	T	6	72	40	2	30	0	0	0

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



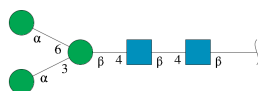
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	A	7	83	46	2	35	0	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



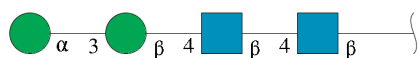
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	C	2	28	16	2	10	0	0	0
10	F	2	28	16	2	10	0	0	0
10	K	2	28	16	2	10	0	0	0
10	N	2	28	16	2	10	0	0	0
10	O	2	28	16	2	10	0	0	0
10	P	2	28	16	2	10	0	0	0
10	Q	2	28	16	2	10	0	0	0
10	R	2	28	16	2	10	0	0	0
10	S	2	28	16	2	10	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



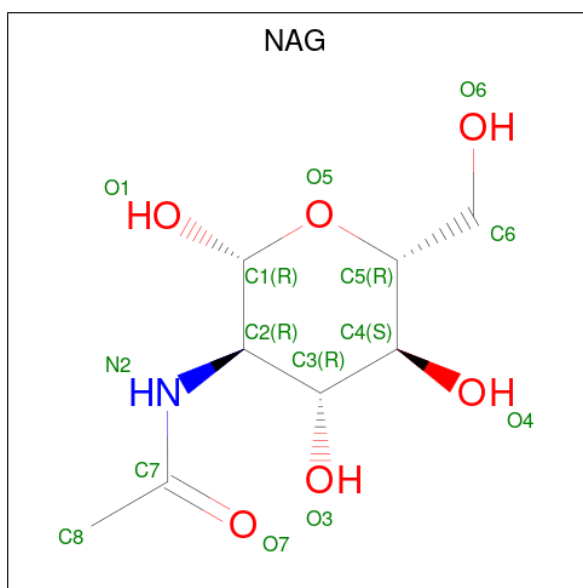
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	J	4	50	28	2	20	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

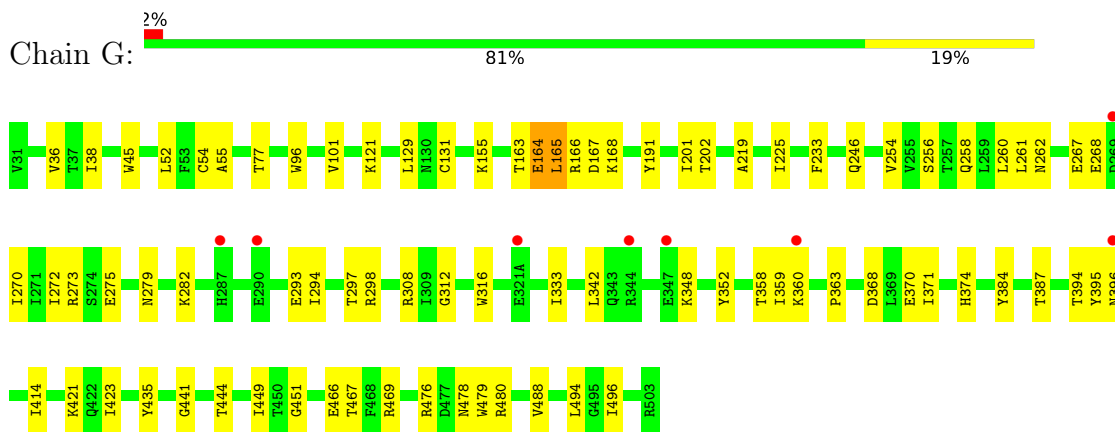


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	G	1	14	8	1	5	0	0
14	B	1	14	8	1	5	0	0

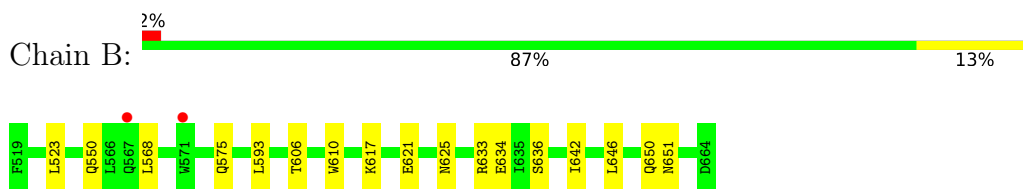
3 Residue-property plots [i](#)

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

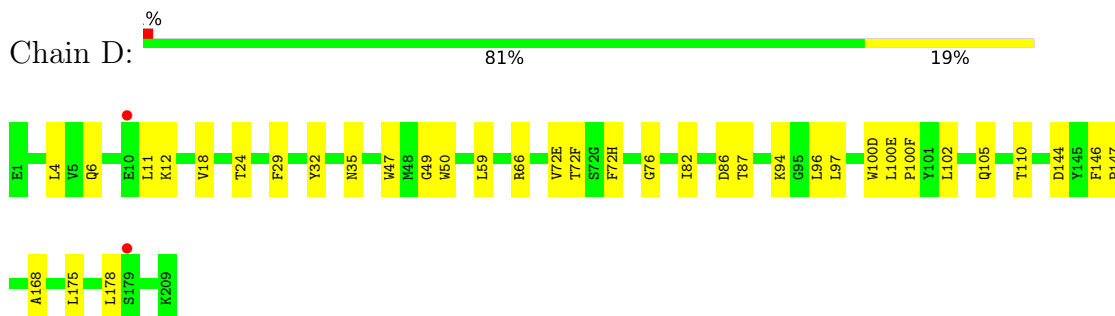
- Molecule 1: Envelope glycoprotein gp120



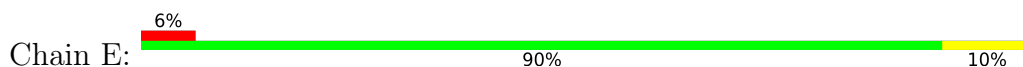
- Molecule 2: Envelope glycoprotein gp41



- Molecule 3: 35O22 Fab heavy chain

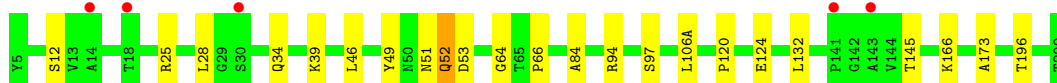
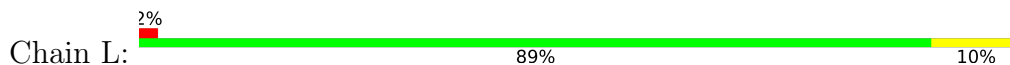


- Molecule 4: 35O22 Fab light chain

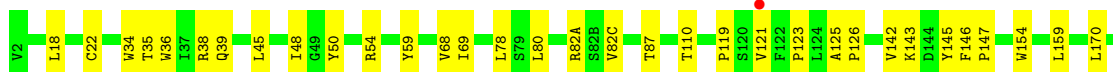
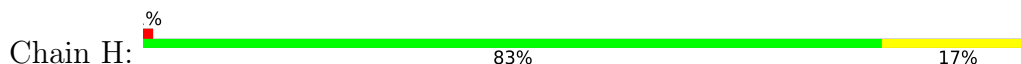




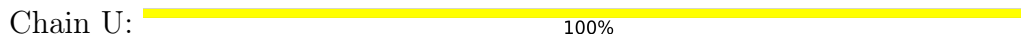
- Molecule 5: PGT124 Fab light chain



- Molecule 6: PGT124 Fab heavy chain



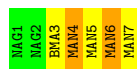
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose



- Molecule 8: 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



- Molecule 9: 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 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%


MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

MAG1
MAG2

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  20% 60% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain J:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 13: 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 M:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	125.47Å 125.47Å 315.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.19 – 3.81 41.19 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.19-3.81) 99.4 (41.19-3.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.76Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.277 , 0.296 0.278 , 0.285	Depositor DCC
R_{free} test set	1395 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	126.1	Xtrriage
Anisotropy	0.612	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 98.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.115 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	G	0.24	0/3433	0.47	0/4662
2	B	0.25	0/1073	0.50	0/1454
3	D	0.25	0/1483	0.48	0/2013
4	E	0.24	0/1502	0.46	0/2050
5	L	0.24	0/1638	0.46	0/2238
6	H	0.24	0/1763	0.49	0/2407
All	All	0.24	0/10892	0.48	0/14824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3363	0	3279	50	0
2	B	1054	0	1025	13	0
3	D	1445	0	1410	22	0
4	E	1465	0	1399	11	0
5	L	1595	0	1541	13	0
6	H	1720	0	1686	23	0
7	U	33	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	72	0	61	0	0
9	A	83	0	70	2	0
10	C	28	0	25	0	0
10	F	28	0	25	0	0
10	K	28	0	25	0	0
10	N	28	0	25	0	0
10	O	28	0	25	0	0
10	P	28	0	25	1	0
10	Q	28	0	25	0	0
10	R	28	0	25	0	0
10	S	28	0	25	0	0
11	I	61	0	52	1	0
12	J	50	0	43	0	0
13	M	50	0	43	0	0
14	B	14	0	13	1	0
14	G	70	0	65	1	0
All	All	11327	0	10940	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (127) 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)
5:L:52:GLN:NE2	5:L:64:GLY:O	2.20	0.74
1:G:38:ILE:HD11	2:B:646:LEU:HD21	1.71	0.72
6:H:119:PRO:HB3	6:H:145:TYR:HB3	1.72	0.71
4:E:26:ASN:HA	4:E:29:CYS:HB2	1.73	0.70
5:L:145:THR:HB	5:L:196:THR:HB	1.76	0.67
5:L:51:ASN:HB3	5:L:66:PRO:HA	1.77	0.67
4:E:91:CYS:SG	4:E:100:VAL:N	2.69	0.65
1:G:298:ARG:NH2	1:G:441:GLY:O	2.30	0.64
1:G:297:THR:HG22	1:G:444:THR:HG22	1.80	0.63
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.80	0.62
4:E:37:TRP:HB2	4:E:50:ILE:HB	1.79	0.62
5:L:25:ARG:HH22	5:L:97:SER:HB3	1.65	0.61
6:H:125:ALA:HB1	6:H:213:PRO:HA	1.84	0.60
1:G:256:SER:O	1:G:478:ASN:ND2	2.32	0.60
6:H:159:LEU:HD21	6:H:182:VAL:HG11	1.83	0.60
6:H:22:CYS:HB3	6:H:78:LEU:HB3	1.84	0.60
1:G:101:VAL:HG11	1:G:480:ARG:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:ARG:NH2	3:D:86:ASP:OD2	2.35	0.59
1:G:36:VAL:HG22	2:B:610:TRP:HE3	1.68	0.57
4:E:18:VAL:HB	4:E:80:LEU:HD11	1.87	0.56
1:G:294:ILE:HG13	1:G:449:ILE:HG13	1.87	0.56
1:G:233:PHE:O	1:G:273:ARG:NH1	2.38	0.56
1:G:260:LEU:HD12	1:G:451:GLY:HA3	1.87	0.56
1:G:360:LYS:HB3	1:G:467:THR:HG22	1.86	0.56
5:L:124:GLU:OE2	6:H:143:LYS:NZ	2.39	0.55
3:D:94:LYS:HB3	3:D:102:LEU:HB2	1.88	0.55
5:L:12:SER:HB2	5:L:106(A):LEU:HD11	1.88	0.55
1:G:131:CYS:HB3	1:G:155:LYS:HD2	1.87	0.55
3:D:87:THR:HG23	3:D:110:THR:HA	1.89	0.55
1:G:496:ILE:HD12	2:B:642:ILE:HG21	1.88	0.55
1:G:54:CYS:SG	1:G:55:ALA:N	2.80	0.54
6:H:18:LEU:HB2	6:H:82(C):VAL:HG11	1.90	0.54
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.90	0.54
4:E:96:ASN:HB2	9:A:4:MAN:H62	1.90	0.54
5:L:34:GLN:HG3	5:L:49:TYR:HA	1.88	0.54
1:G:254:VAL:HG21	1:G:262:ASN:HB2	1.88	0.53
5:L:46:LEU:HD21	5:L:49:TYR:HB3	1.90	0.53
1:G:363:PRO:O	1:G:469:ARG:NH1	2.41	0.53
5:L:34:GLN:NE2	5:L:49:TYR:O	2.35	0.52
1:G:167:ASP:OD1	1:G:168:LYS:N	2.42	0.52
1:G:368:ASP:HB3	1:G:371:ILE:HG12	1.91	0.52
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.45	0.52
6:H:39:GLN:HB2	6:H:45:LEU:HD23	1.90	0.52
14:G:601:NAG:H82	14:G:603:NAG:H81	1.91	0.52
1:G:270:ILE:O	1:G:348:LYS:NZ	2.40	0.51
6:H:38:ARG:HB3	6:H:48:ILE:HD11	1.93	0.51
6:H:123:PRO:HB3	6:H:211:VAL:HG22	1.93	0.51
1:G:360:LYS:HA	1:G:394:THR:HG22	1.92	0.51
1:G:358:THR:O	1:G:466:GLU:N	2.43	0.51
1:G:267:GLU:HG3	1:G:268:GLU:HG2	1.93	0.51
6:H:87:THR:HG23	6:H:110:THR:HA	1.92	0.50
3:D:49:GLY:HA3	3:D:59:LEU:HD23	1.94	0.50
1:G:421:LYS:NZ	1:G:423:ILE:O	2.32	0.50
5:L:166:LYS:HB3	5:L:173:ALA:HB3	1.93	0.49
6:H:68:VAL:HG23	6:H:82(A):ARG:HH12	1.78	0.49
6:H:121:VAL:HG22	6:H:142:VAL:HG22	1.95	0.48
6:H:194:TYR:H	6:H:210:LYS:HZ3	1.60	0.48
1:G:494:LEU:HD21	2:B:593:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:96:LEU:HG	3:D:97:LEU:HG	1.95	0.48
1:G:52:LEU:HD11	1:G:488:VAL:HG21	1.96	0.48
2:B:606:THR:HB	2:B:650:GLN:OE1	2.14	0.47
1:G:294:ILE:HD12	1:G:333:ILE:HG22	1.96	0.47
1:G:272:ILE:HB	1:G:352:TYR:HE2	1.79	0.47
2:B:617:LYS:NZ	2:B:634:GLU:OE2	2.43	0.47
4:E:63:ARG:HD2	4:E:79:ASP:HB3	1.95	0.47
2:B:650:GLN:HG3	2:B:651:ASN:N	2.29	0.47
6:H:34:TRP:HB3	6:H:78:LEU:HD22	1.96	0.47
2:B:625:ASN:HB2	3:D:97:LEU:HD22	1.96	0.46
9:A:4:MAN:H61	9:A:6:MAN:H2	1.67	0.46
6:H:146:PHE:HA	6:H:147:PRO:HA	1.72	0.46
1:G:55:ALA:HB1	1:G:77:THR:HB	1.98	0.46
3:D:4:LEU:HG	3:D:24:THR:HG22	1.97	0.46
3:D:144:ASP:HB3	3:D:175:LEU:HD13	1.98	0.46
1:G:121:LYS:HD3	1:G:202:THR:HB	1.97	0.46
5:L:120:PRO:HD3	5:L:132:LEU:HG	1.98	0.45
3:D:12:LYS:HG3	3:D:18:VAL:HB	1.99	0.45
4:E:16:GLN:HG2	4:E:17:SER:H	1.82	0.45
1:G:494:LEU:HD23	1:G:494:LEU:HA	1.75	0.45
1:G:272:ILE:HG12	1:G:348:LYS:HZ3	1.82	0.45
6:H:194:TYR:H	6:H:210:LYS:NZ	2.15	0.45
1:G:96:TRP:CD2	1:G:275:GLU:HG3	2.52	0.44
1:G:165:LEU:HD22	1:G:167:ASP:OD1	2.17	0.44
2:B:621:GLU:O	2:B:625:ASN:HB3	2.17	0.44
4:E:136:LEU:HD12	4:E:182:LEU:HD23	1.98	0.44
3:D:146:PHE:HB2	3:D:175:LEU:HA	1.99	0.44
1:G:219:ALA:HB2	1:G:225:ILE:HG13	2.00	0.44
6:H:170:LEU:HD13	6:H:176:TYR:CZ	2.53	0.44
4:E:124:PRO:HB3	4:E:135:THR:H	1.83	0.44
1:G:294:ILE:HG23	1:G:333:ILE:HG22	1.99	0.43
6:H:154:TRP:HB3	6:H:159:LEU:HD23	2.00	0.43
1:G:219:ALA:O	1:G:246:GLN:NE2	2.52	0.43
3:D:168:ALA:HB2	3:D:178:LEU:HB3	2.00	0.43
1:G:308:ARG:HG2	1:G:316:TRP:CE2	2.54	0.43
5:L:39:LYS:HG2	5:L:84:ALA:HB2	2.00	0.43
1:G:164:GLU:HA	1:G:312:GLY:HA2	2.00	0.43
1:G:370:GLU:HG3	1:G:384:TYR:HE2	1.83	0.43
1:G:333:ILE:HD11	1:G:414:ILE:HD12	2.01	0.43
1:G:45:TRP:CE3	2:B:523:LEU:HD13	2.53	0.43
1:G:293:GLU:HG2	10:P:1:NAG:H3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:38:TYR:CZ	4:E:48:LEU:HD13	2.54	0.43
1:G:258:GLN:NE2	1:G:387:THR:OG1	2.45	0.42
2:B:633:ARG:HD2	3:D:72(H):PHE:HE2	1.83	0.42
6:H:36:TRP:CD1	6:H:80:LEU:HB2	2.54	0.42
1:G:279:ASN:HB2	1:G:282:LYS:HG2	2.02	0.42
4:E:135:THR:HG22	4:E:183:SER:HA	2.01	0.42
3:D:66:ARG:HE	3:D:82:ILE:HD11	1.83	0.42
5:L:28:LEU:HB3	5:L:94:ARG:HD3	2.02	0.42
2:B:636:SER:OG	14:B:701:NAG:H82	2.20	0.42
3:D:29:PHE:CG	3:D:76:GLY:HA3	2.55	0.42
3:D:100(E):LEU:HD12	3:D:100(F):PRO:HD2	2.02	0.42
6:H:35:THR:HA	6:H:50:TYR:HA	2.01	0.42
1:G:342:LEU:HD23	1:G:395:TYR:CG	2.54	0.42
1:G:359:ILE:HB	1:G:396:ASN:HD21	1.85	0.42
3:D:11:LEU:HD22	3:D:147:PRO:HG3	2.01	0.42
2:B:550:GLN:NE2	2:B:575:GLN:OE1	2.53	0.41
3:D:6:GLN:H	3:D:105:GLN:HE22	1.68	0.41
6:H:126:PRO:HG2	6:H:213:PRO:HB3	2.03	0.41
3:D:47:TRP:HZ2	3:D:50:TRP:CD1	2.38	0.41
6:H:59:TYR:HE1	6:H:69:ILE:HG13	1.85	0.41
11:I:1:NAG:H62	11:I:2:NAG:N2	2.35	0.41
3:D:32:TYR:CD2	3:D:94:LYS:HE3	2.56	0.41
1:G:129:LEU:O	1:G:191:TYR:N	2.55	0.40
1:G:261:LEU:HD21	1:G:374:HIS:CE1	2.56	0.40
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.56	0.40
3:D:72(E):VAL:HG12	3:D:72(F):THR:HG23	2.03	0.40
6:H:54:ARG:HA	6:H:54:ARG:HD2	1.86	0.40
3:D:35:ASN:ND2	3:D:100(D):TRP:O	2.53	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	G	413/427 (97%)	390 (94%)	23 (6%)	0	100	100
2	B	127/131 (97%)	121 (95%)	6 (5%)	0	100	100
3	D	179/187 (96%)	170 (95%)	9 (5%)	0	100	100
4	E	186/192 (97%)	173 (93%)	13 (7%)	0	100	100
5	L	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
6	H	222/226 (98%)	215 (97%)	7 (3%)	0	100	100
All	All	1335/1373 (97%)	1268 (95%)	67 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	381/381 (100%)	377 (99%)	4 (1%)	76	86
2	B	115/115 (100%)	114 (99%)	1 (1%)	78	88
3	D	160/160 (100%)	160 (100%)	0	100	100
4	E	171/171 (100%)	171 (100%)	0	100	100
5	L	176/176 (100%)	174 (99%)	2 (1%)	73	85
6	H	194/194 (100%)	194 (100%)	0	100	100
All	All	1197/1197 (100%)	1190 (99%)	7 (1%)	86	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	163	THR
1	G	164	GLU
1	G	165	LEU
1	G	166	ARG
2	B	568	LEU
5	L	52	GLN
5	L	53	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	276	ASN
5	L	52	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

47 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
9	NAG	A	1	9,1	14,14,15	0.26	0	17,19,21	0.53	0
9	NAG	A	2	9	14,14,15	0.26	0	17,19,21	0.43	0
9	BMA	A	3	9	11,11,12	1.12	1 (9%)	15,15,17	1.41	2 (13%)
9	MAN	A	4	9	11,11,12	1.01	0	15,15,17	1.42	3 (20%)
9	MAN	A	5	9	11,11,12	0.87	0	15,15,17	1.30	2 (13%)
9	MAN	A	6	9	11,11,12	0.88	0	15,15,17	1.41	2 (13%)
9	MAN	A	7	9	11,11,12	1.01	1 (9%)	15,15,17	0.91	2 (13%)
10	NAG	C	1	1,10	14,14,15	0.47	0	17,19,21	0.52	0
10	NAG	C	2	10	14,14,15	0.19	0	17,19,21	0.44	0
10	NAG	F	1	1,10	14,14,15	0.27	0	17,19,21	0.39	0
10	NAG	F	2	10	14,14,15	0.26	0	17,19,21	0.52	0
11	NAG	I	1	11,1	14,14,15	0.62	1 (7%)	17,19,21	0.57	0
11	NAG	I	2	11	14,14,15	0.19	0	17,19,21	0.48	0
11	BMA	I	3	11	11,11,12	0.59	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	I	4	11	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
11	MAN	I	5	11	11,11,12	0.86	0	15,15,17	1.23	2 (13%)
12	NAG	J	1	1,12	14,14,15	0.22	0	17,19,21	0.42	0
12	NAG	J	2	12	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
12	BMA	J	3	12	11,11,12	1.23	2 (18%)	15,15,17	1.20	2 (13%)
12	MAN	J	4	12	11,11,12	0.98	1 (9%)	15,15,17	1.48	3 (20%)
10	NAG	K	1	1,10	14,14,15	0.44	0	17,19,21	0.48	0
10	NAG	K	2	10	14,14,15	0.21	0	17,19,21	0.43	0
13	NAG	M	1	13,1	14,14,15	0.70	1 (7%)	17,19,21	0.79	0
13	NAG	M	2	13	14,14,15	0.23	0	17,19,21	0.50	0
13	BMA	M	3	13	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
13	MAN	M	4	13	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
10	NAG	N	1	1,10	14,14,15	0.24	0	17,19,21	0.50	0
10	NAG	N	2	10	14,14,15	0.26	0	17,19,21	0.46	0
10	NAG	O	1	1,10	14,14,15	0.18	0	17,19,21	0.44	0
10	NAG	O	2	10	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	P	1	1,10	14,14,15	0.25	0	17,19,21	0.39	0
10	NAG	P	2	10	14,14,15	0.25	0	17,19,21	0.39	0
10	NAG	Q	1	10	14,14,15	0.17	0	17,19,21	0.48	0
10	NAG	Q	2	10	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	R	1	1,10	14,14,15	0.23	0	17,19,21	0.54	0
10	NAG	R	2	10	14,14,15	0.26	0	17,19,21	0.42	0
10	NAG	S	1	10	14,14,15	1.42	1 (7%)	17,19,21	1.07	2 (11%)
10	NAG	S	2	10	14,14,15	0.24	0	17,19,21	0.50	0
8	NAG	T	1	1,8	14,14,15	0.27	0	17,19,21	0.41	0
8	NAG	T	2	8	14,14,15	0.24	0	17,19,21	0.59	0
8	BMA	T	3	8	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
8	MAN	T	4	8	11,11,12	0.59	0	15,15,17	1.13	2 (13%)
8	MAN	T	5	8	11,11,12	0.84	1 (9%)	15,15,17	0.83	1 (6%)
8	MAN	T	6	8	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
7	MAN	U	1	7	11,11,12	1.17	2 (18%)	15,15,17	1.32	3 (20%)
7	MAN	U	2	7	11,11,12	0.84	1 (9%)	15,15,17	1.54	2 (13%)
7	MAN	U	3	7	11,11,12	0.93	1 (9%)	15,15,17	0.85	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
9	NAG	A	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	A	2	9	-	2/6/23/26	0/1/1/1
9	BMA	A	3	9	-	2/2/19/22	0/1/1/1
9	MAN	A	4	9	-	0/2/19/22	0/1/1/1
9	MAN	A	5	9	-	1/2/19/22	1/1/1/1
9	MAN	A	6	9	-	0/2/19/22	0/1/1/1
9	MAN	A	7	9	-	1/2/19/22	1/1/1/1
10	NAG	C	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	2	10	-	4/6/23/26	0/1/1/1
10	NAG	F	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	3/6/23/26	0/1/1/1
11	NAG	I	1	11,1	-	1/6/23/26	0/1/1/1
11	NAG	I	2	11	-	0/6/23/26	0/1/1/1
11	BMA	I	3	11	-	2/2/19/22	0/1/1/1
11	MAN	I	4	11	-	1/2/19/22	0/1/1/1
11	MAN	I	5	11	-	1/2/19/22	1/1/1/1
12	NAG	J	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
12	BMA	J	3	12	-	1/2/19/22	0/1/1/1
12	MAN	J	4	12	-	0/2/19/22	0/1/1/1
10	NAG	K	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	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	-	2/2/19/22	0/1/1/1
13	MAN	M	4	13	-	0/2/19/22	0/1/1/1
10	NAG	N	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	NAG	O	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	O	2	10	-	0/6/23/26	0/1/1/1
10	NAG	P	1	1,10	-	4/6/23/26	0/1/1/1
10	NAG	P	2	10	-	1/6/23/26	0/1/1/1
10	NAG	Q	1	10	-	4/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	0/6/23/26	0/1/1/1
10	NAG	R	1	1,10	-	3/6/23/26	0/1/1/1
10	NAG	R	2	10	-	1/6/23/26	0/1/1/1
10	NAG	S	1	10	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	1/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	T	2	8	-	3/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	2/2/19/22	0/1/1/1
8	MAN	T	5	8	-	1/2/19/22	0/1/1/1
8	MAN	T	6	8	-	0/2/19/22	0/1/1/1
7	MAN	U	1	7	-	0/2/19/22	0/1/1/1
7	MAN	U	2	7	-	1/2/19/22	0/1/1/1
7	MAN	U	3	7	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	S	1	NAG	O5-C1	-4.87	1.35	1.43
12	J	4	MAN	C1-C2	2.98	1.59	1.52
7	U	1	MAN	C2-C3	2.69	1.56	1.52
12	J	3	BMA	O5-C1	2.66	1.48	1.43
7	U	3	MAN	O5-C1	-2.64	1.39	1.43
9	A	7	MAN	C1-C2	2.59	1.58	1.52
12	J	3	BMA	C1-C2	2.53	1.58	1.52
13	M	1	NAG	O5-C1	-2.41	1.39	1.43
9	A	3	BMA	O3-C3	2.21	1.48	1.43
11	I	1	NAG	O5-C1	-2.20	1.40	1.43
8	T	5	MAN	O5-C1	-2.20	1.40	1.43
7	U	2	MAN	C1-C2	2.12	1.57	1.52
7	U	1	MAN	C1-C2	2.00	1.56	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	2	MAN	O2-C2-C3	-4.01	102.10	110.14
12	J	4	MAN	C1-O5-C5	3.96	117.56	112.19
9	A	6	MAN	C1-O5-C5	3.93	117.52	112.19
7	U	2	MAN	C1-O5-C5	3.88	117.45	112.19
9	A	5	MAN	C1-O5-C5	3.85	117.41	112.19
11	I	5	MAN	C1-O5-C5	3.50	116.94	112.19
9	A	3	BMA	O3-C3-C2	3.36	116.43	109.99
9	A	4	MAN	C1-O5-C5	3.11	116.41	112.19
8	T	4	MAN	C1-O5-C5	2.95	116.18	112.19
10	S	1	NAG	C3-C4-C5	2.85	115.33	110.24
11	I	4	MAN	C1-O5-C5	2.81	116.00	112.19
9	A	4	MAN	O3-C3-C2	2.78	115.32	109.99
12	J	3	BMA	C1-C2-C3	-2.71	106.34	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	2	NAG	O4-C4-C3	2.62	116.41	110.35
7	U	1	MAN	C1-C2-C3	2.55	112.80	109.67
10	S	1	NAG	O4-C4-C5	-2.40	103.35	109.30
13	M	4	MAN	C1-O5-C5	2.33	115.35	112.19
8	T	6	MAN	C1-O5-C5	2.33	115.35	112.19
9	A	5	MAN	O2-C2-C3	-2.33	105.47	110.14
9	A	4	MAN	O3-C3-C4	2.28	115.62	110.35
7	U	1	MAN	C1-O5-C5	2.28	115.28	112.19
8	T	4	MAN	O2-C2-C3	-2.28	105.57	110.14
13	M	4	MAN	O2-C2-C3	-2.28	105.58	110.14
8	T	6	MAN	O2-C2-C3	-2.26	105.60	110.14
11	I	4	MAN	O2-C2-C3	-2.25	105.64	110.14
11	I	5	MAN	O2-C2-C3	-2.24	105.66	110.14
8	T	5	MAN	O2-C2-C3	-2.23	105.66	110.14
7	U	1	MAN	O5-C1-C2	2.21	114.19	110.77
9	A	6	MAN	O2-C2-C3	-2.17	105.79	110.14
12	J	4	MAN	O2-C2-C3	-2.15	105.82	110.14
9	A	7	MAN	C1-O5-C5	2.12	115.07	112.19
12	J	4	MAN	C1-C2-C3	2.11	112.26	109.67
12	J	3	BMA	O3-C3-C2	2.08	113.97	109.99
9	A	3	BMA	C1-C2-C3	-2.07	107.12	109.67
7	U	3	MAN	O2-C2-C3	-2.05	106.03	110.14
13	M	3	BMA	C1-O5-C5	2.05	114.96	112.19
8	T	3	BMA	C1-O5-C5	2.02	114.92	112.19
9	A	7	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Q	1	NAG	O5-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
10	C	2	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
9	A	3	BMA	O5-C5-C6-O6
10	F	2	NAG	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
13	M	3	BMA	O5-C5-C6-O6
10	Q	1	NAG	C4-C5-C6-O6
9	A	3	BMA	C4-C5-C6-O6
10	P	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	I	3	BMA	O5-C5-C6-O6
10	F	1	NAG	O5-C5-C6-O6
10	C	2	NAG	C4-C5-C6-O6
10	F	2	NAG	C4-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
13	M	3	BMA	C4-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
11	I	3	BMA	C4-C5-C6-O6
10	C	2	NAG	C8-C7-N2-C2
10	C	2	NAG	O7-C7-N2-C2
10	N	1	NAG	C8-C7-N2-C2
10	N	1	NAG	O7-C7-N2-C2
10	P	1	NAG	C8-C7-N2-C2
10	P	1	NAG	O7-C7-N2-C2
10	Q	1	NAG	C8-C7-N2-C2
10	Q	1	NAG	O7-C7-N2-C2
12	J	1	NAG	C8-C7-N2-C2
12	J	1	NAG	O7-C7-N2-C2
13	M	1	NAG	C8-C7-N2-C2
13	M	1	NAG	O7-C7-N2-C2
10	F	1	NAG	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
9	A	2	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
9	A	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
9	A	5	MAN	O5-C5-C6-O6
8	T	5	MAN	O5-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
11	I	4	MAN	O5-C5-C6-O6
12	J	2	NAG	C4-C5-C6-O6
11	I	5	MAN	O5-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
12	J	3	BMA	O5-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
9	A	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	M	2	NAG	O5-C5-C6-O6
8	T	4	MAN	C4-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
11	I	1	NAG	O5-C5-C6-O6
8	T	2	NAG	C3-C2-N2-C7
10	F	2	NAG	C3-C2-N2-C7
10	R	1	NAG	C3-C2-N2-C7
8	T	4	MAN	O5-C5-C6-O6
9	A	1	NAG	C4-C5-C6-O6
9	A	1	NAG	O5-C5-C6-O6
7	U	2	MAN	C4-C5-C6-O6

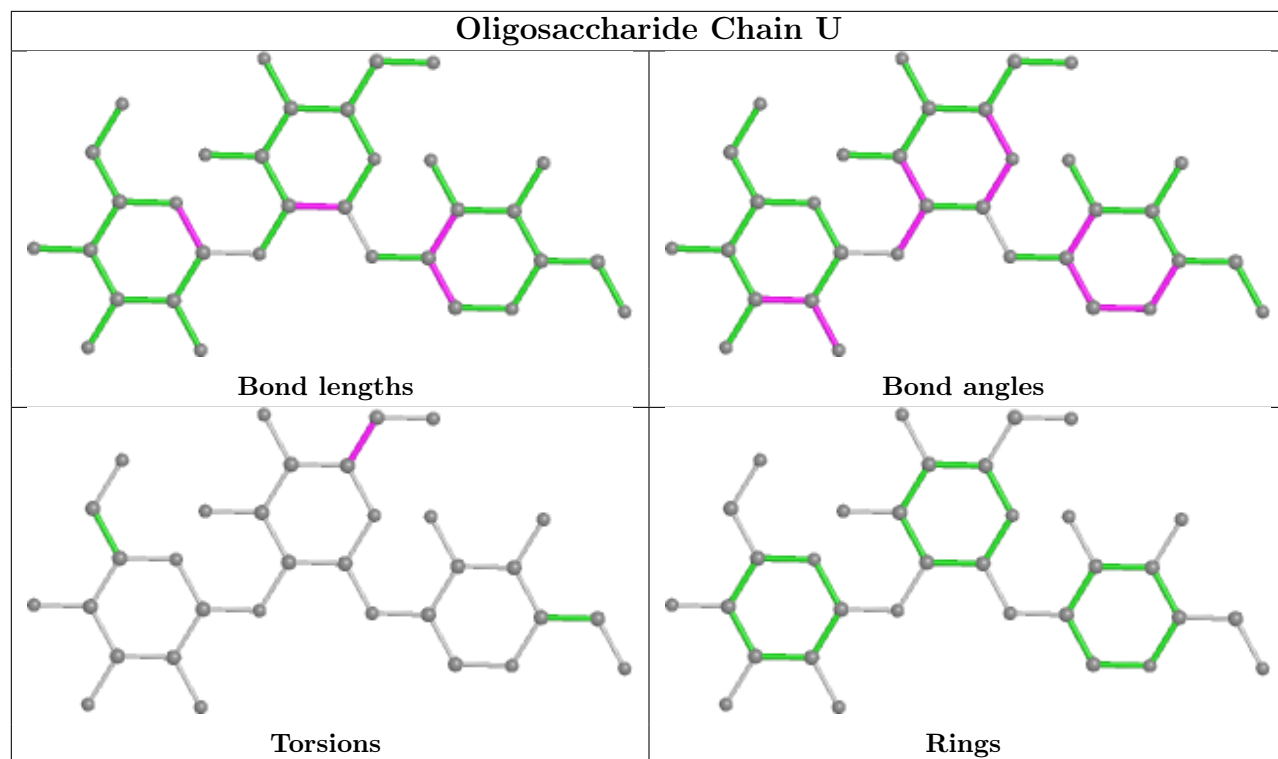
All (3) ring outliers are listed below:

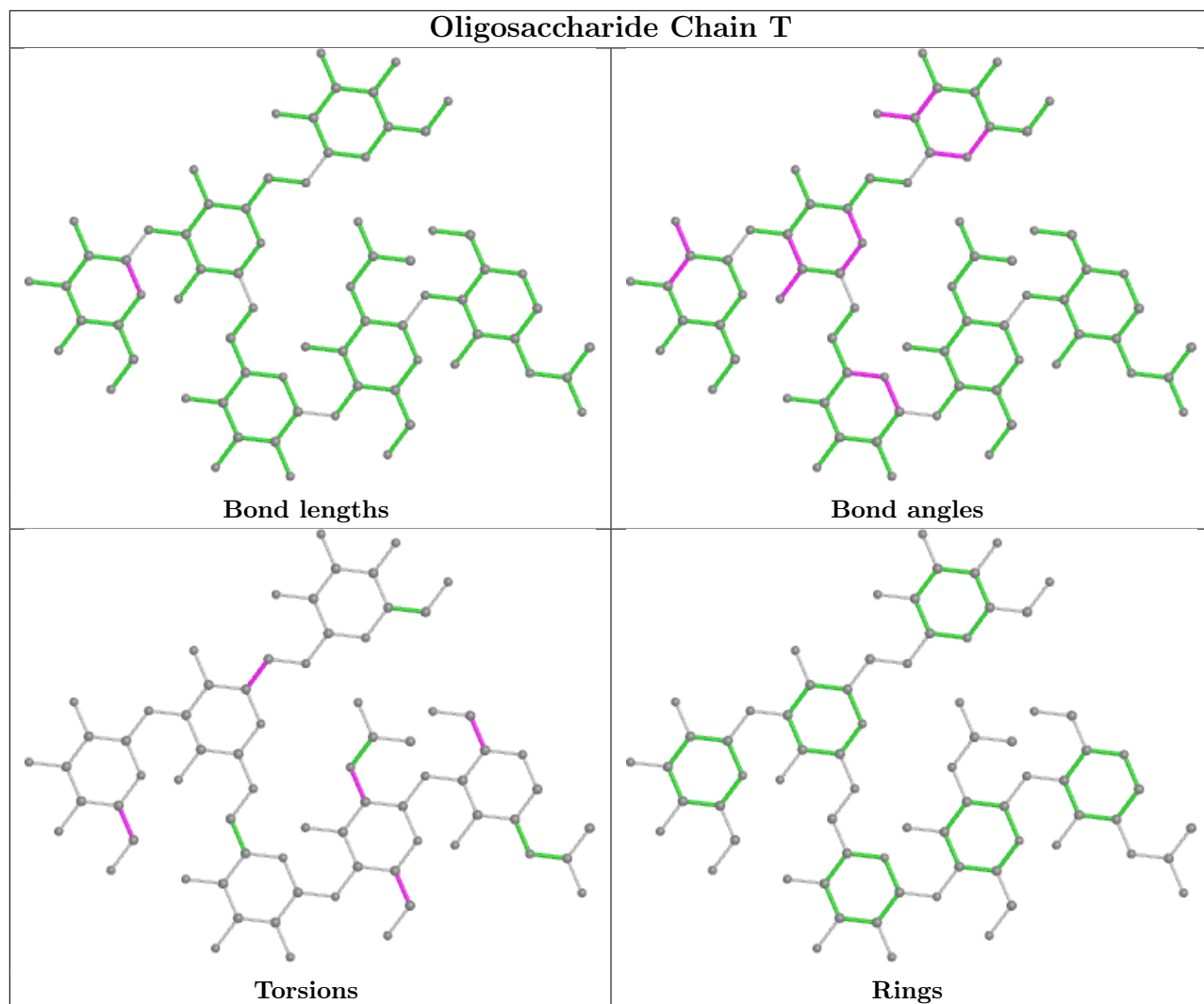
Mol	Chain	Res	Type	Atoms
9	A	7	MAN	C1-C2-C3-C4-C5-O5
9	A	5	MAN	C1-C2-C3-C4-C5-O5
11	I	5	MAN	C1-C2-C3-C4-C5-O5

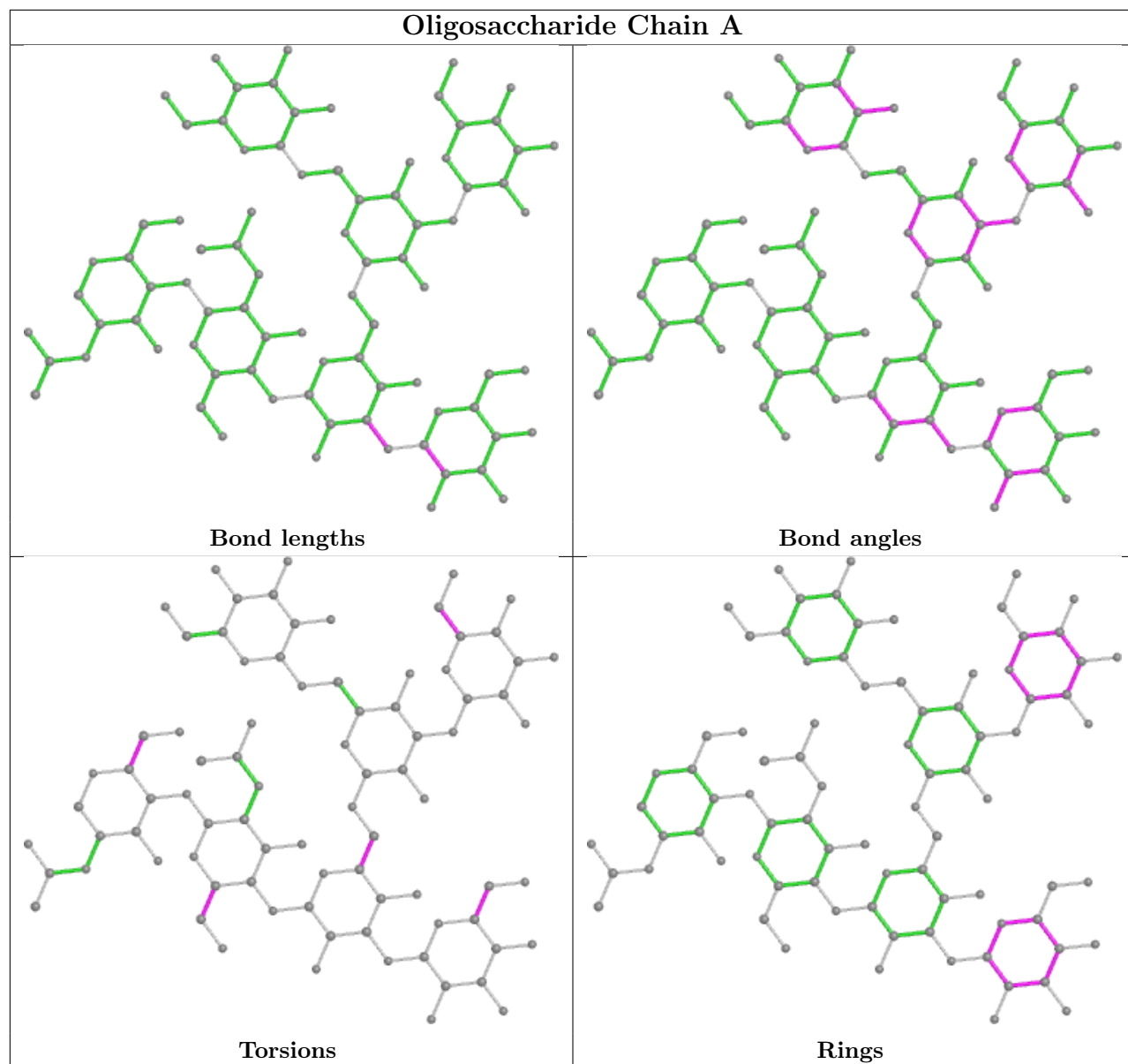
5 monomers are involved in 4 short contacts:

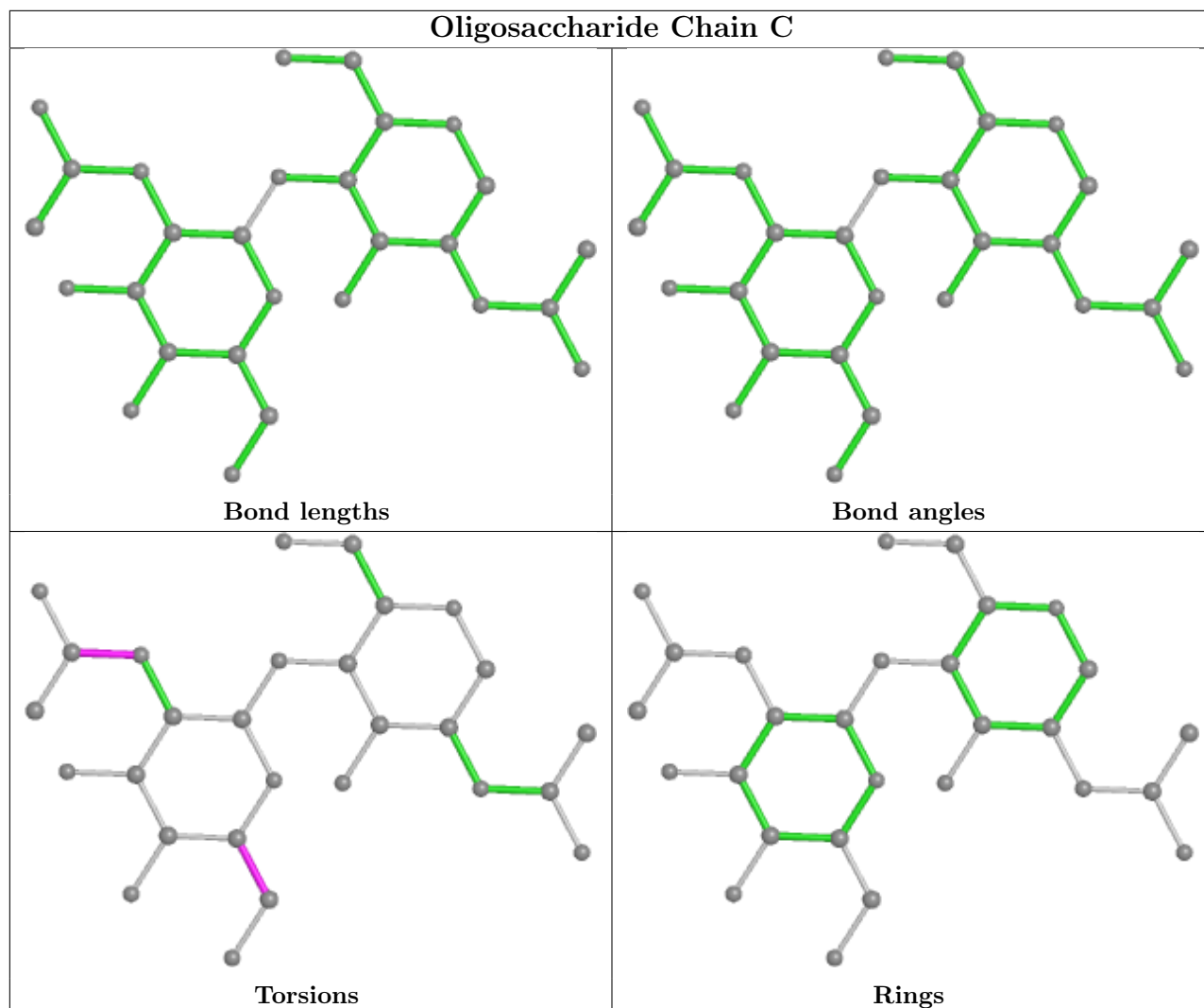
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	1	NAG	1	0
9	A	6	MAN	1	0
10	P	1	NAG	1	0
9	A	4	MAN	2	0
11	I	2	NAG	1	0

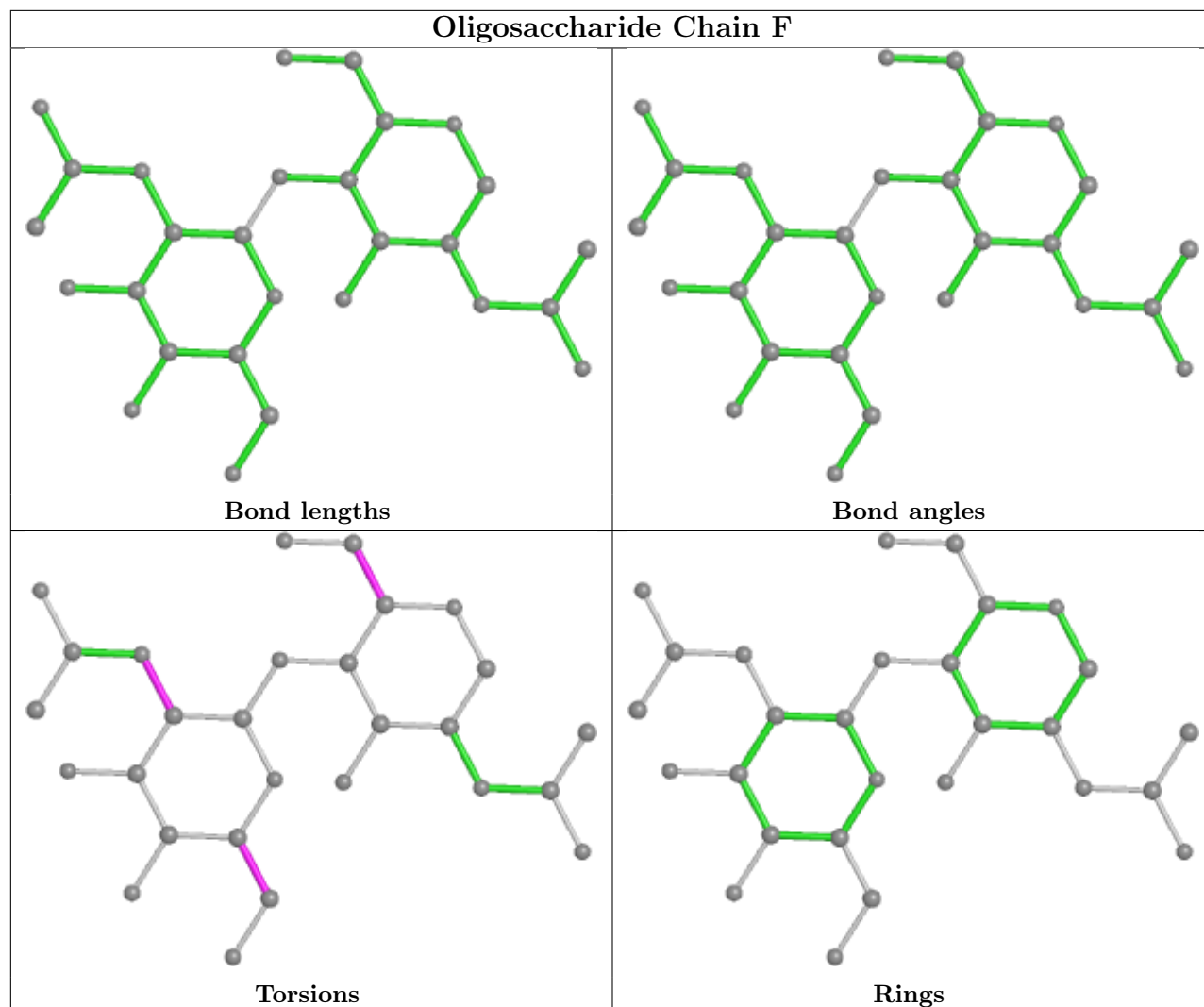
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

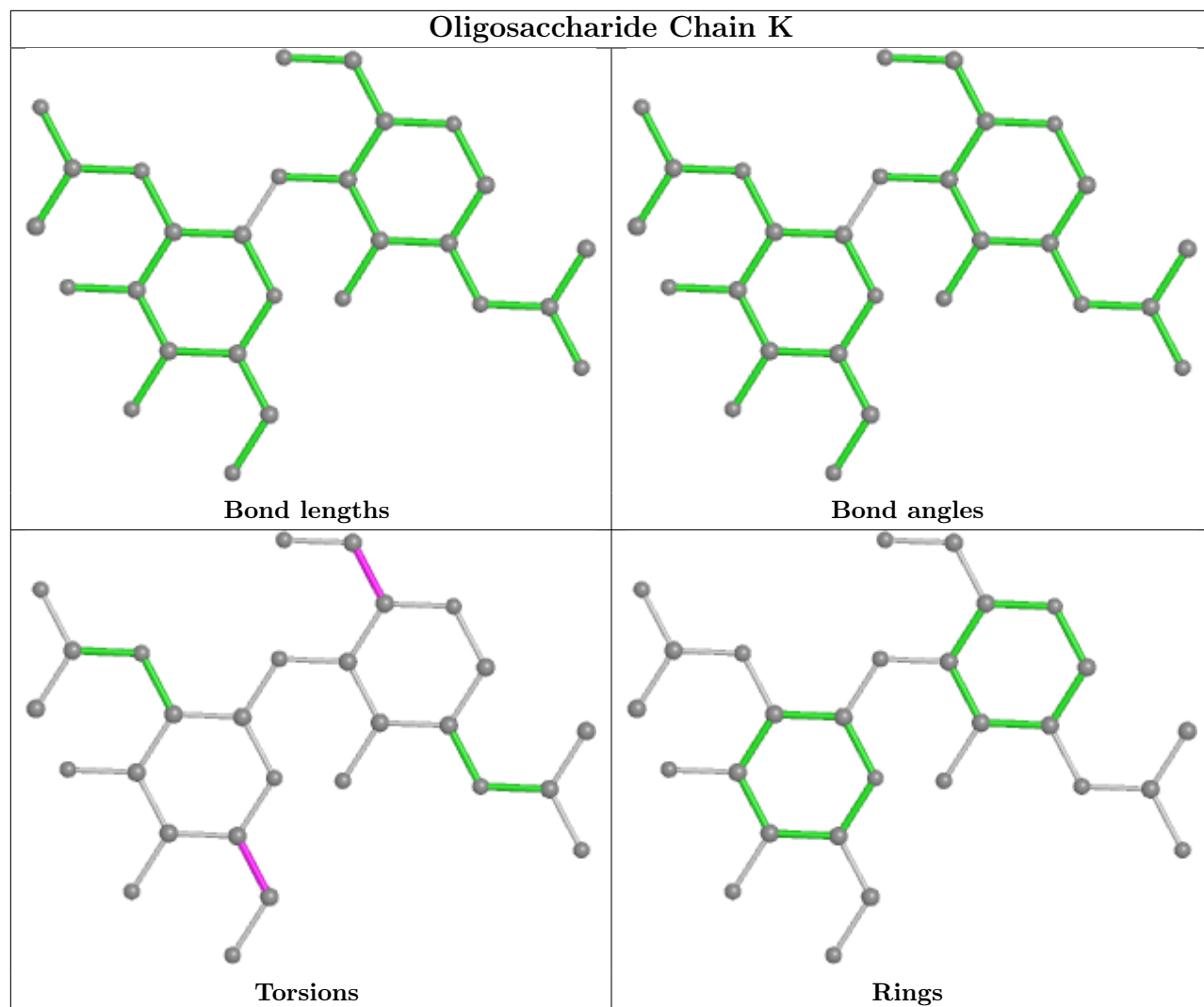


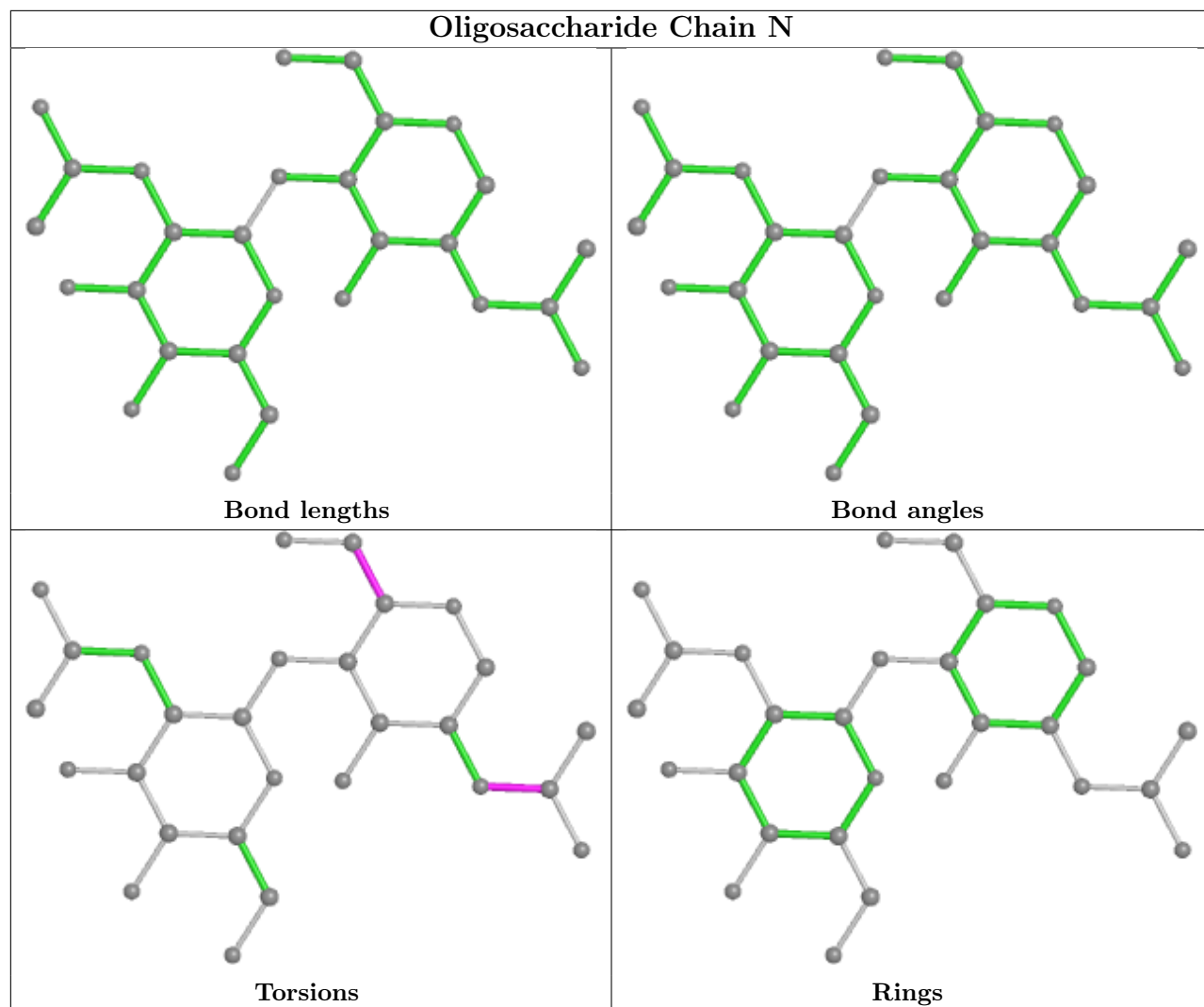


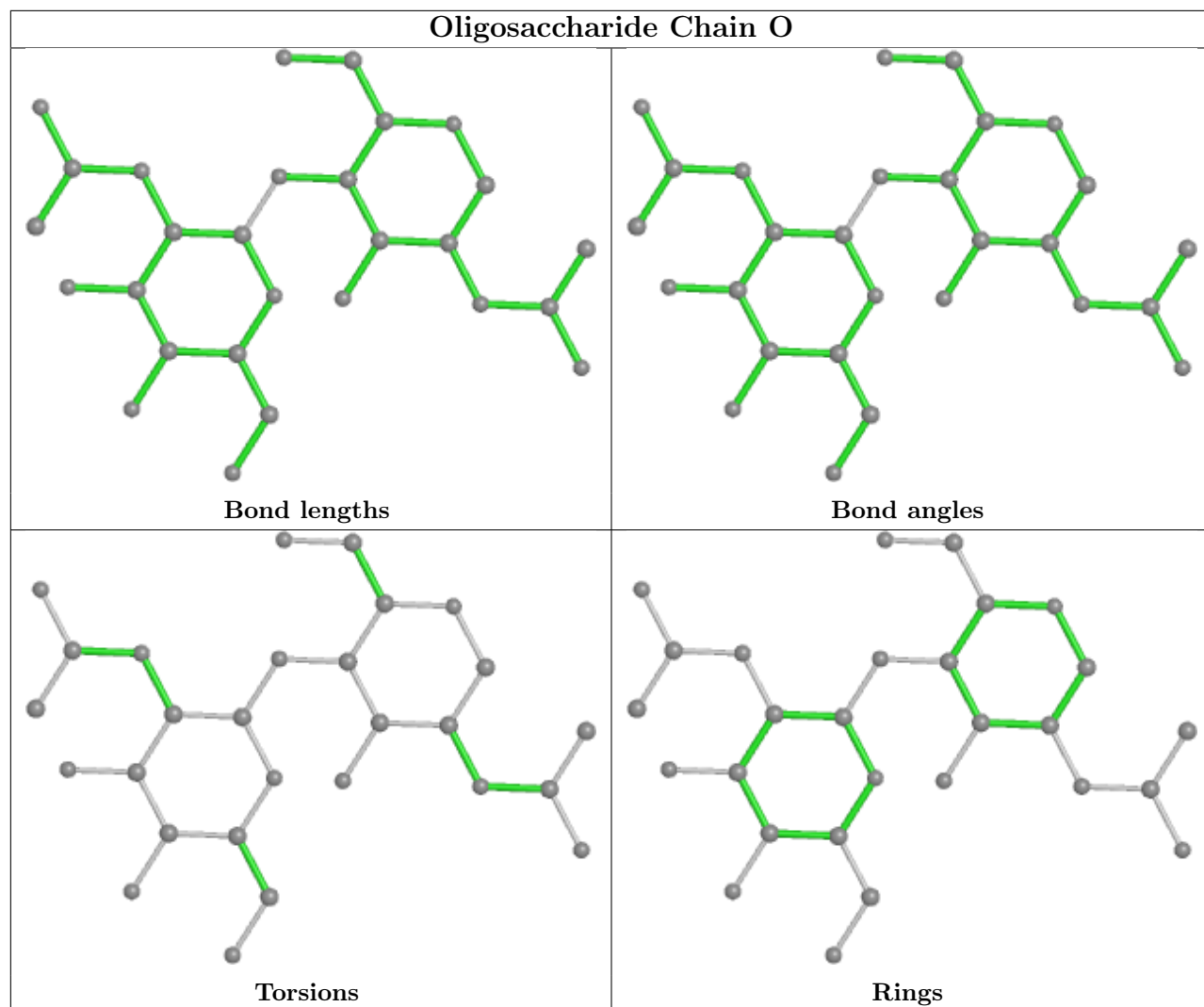


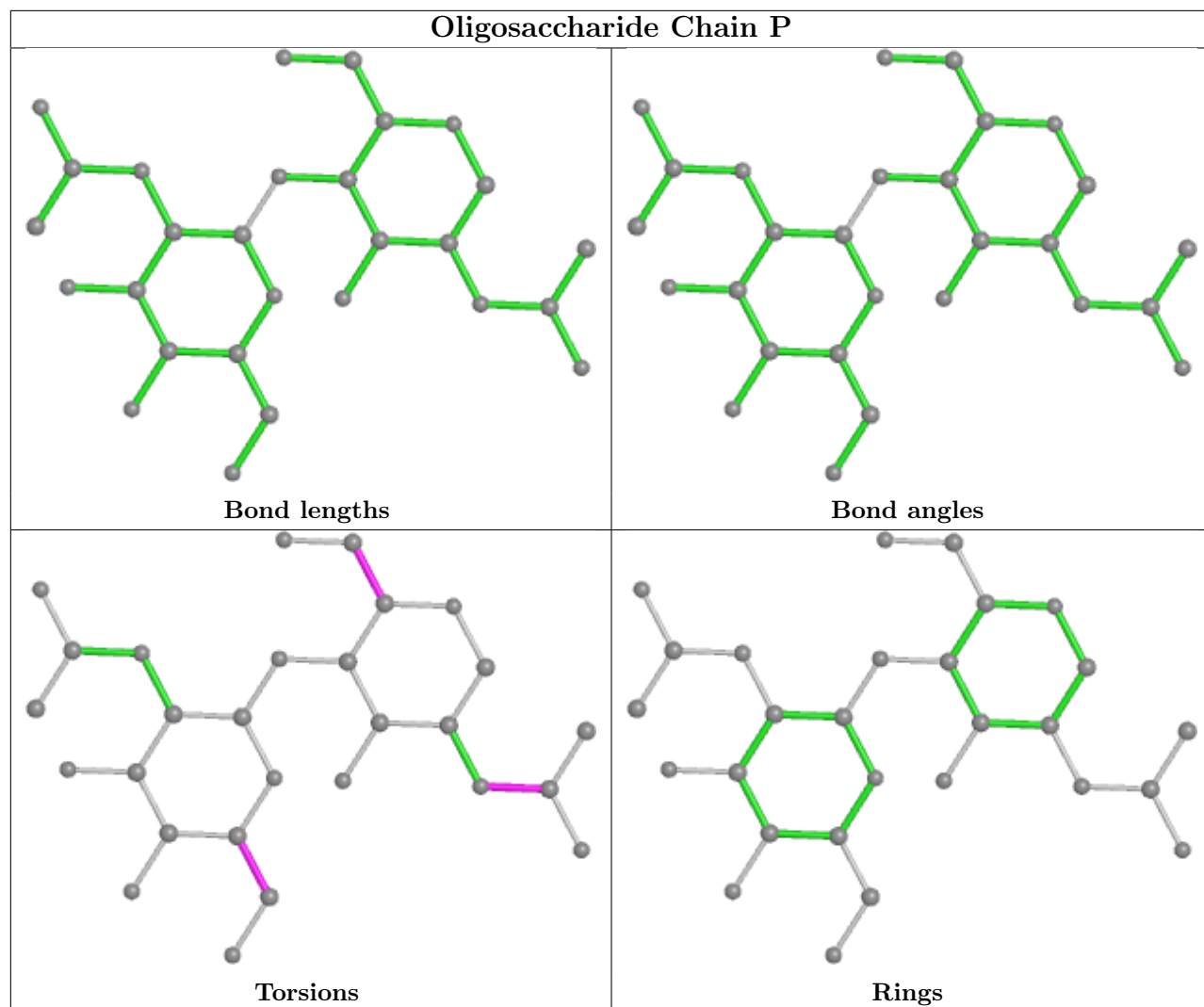


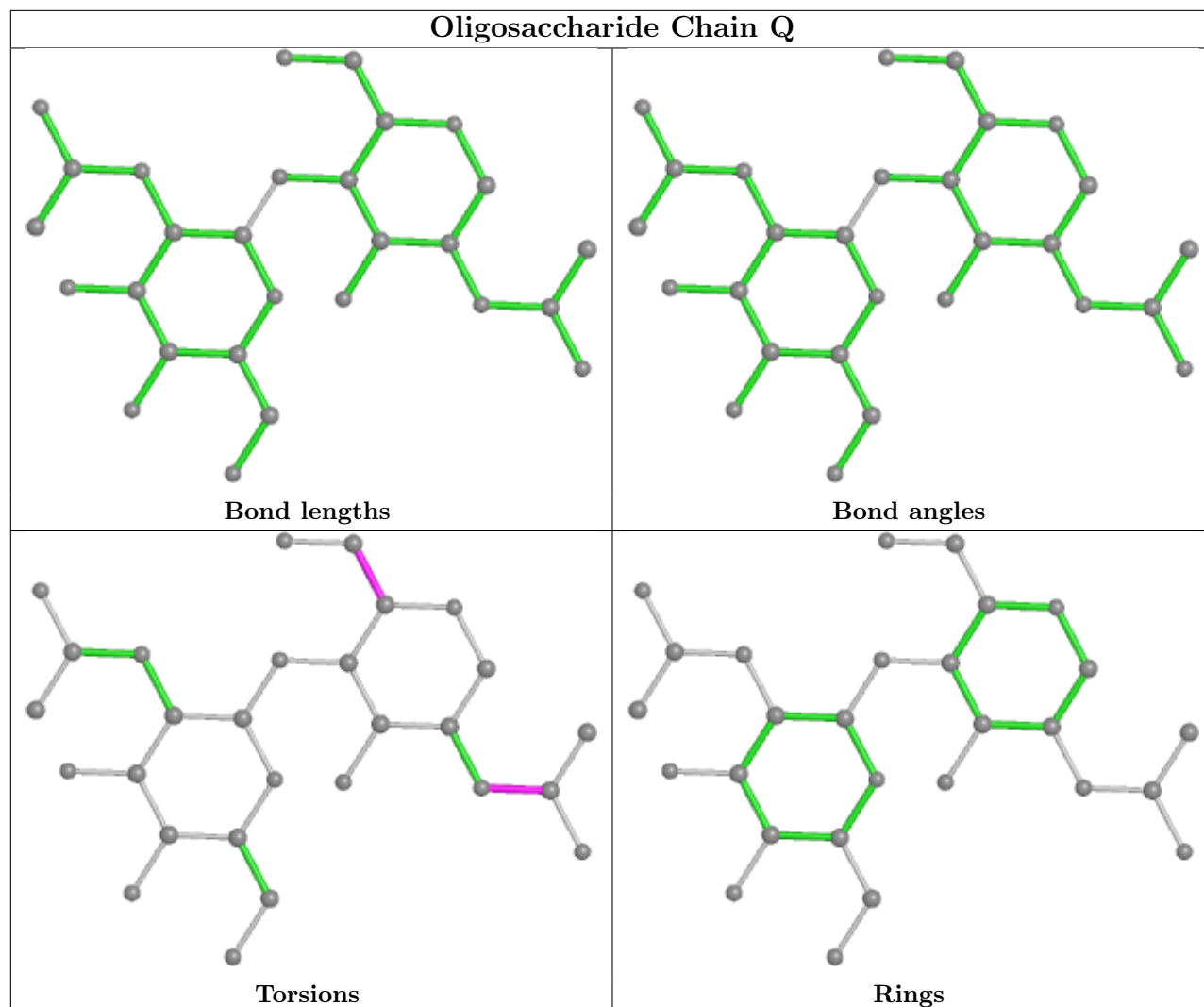


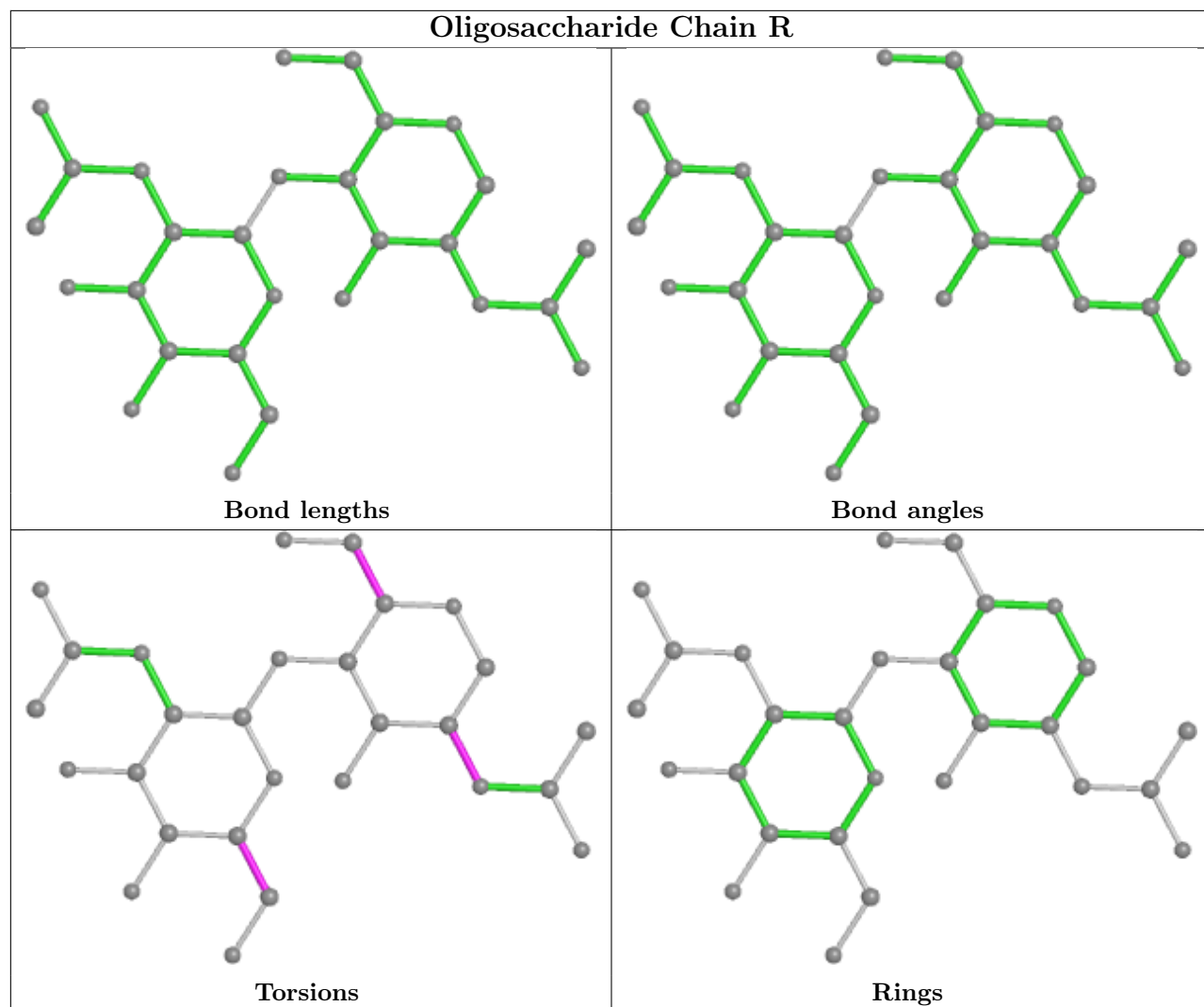


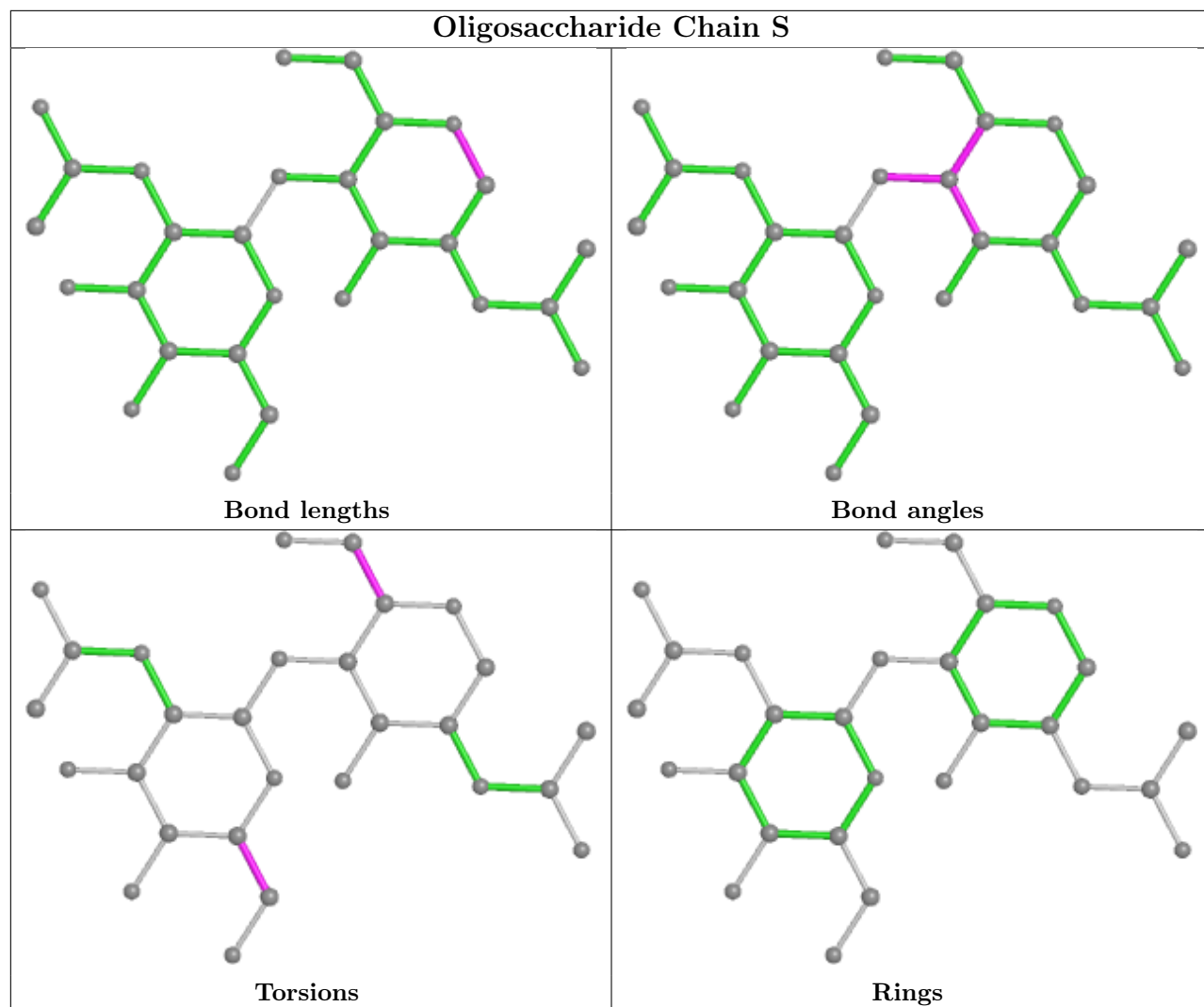


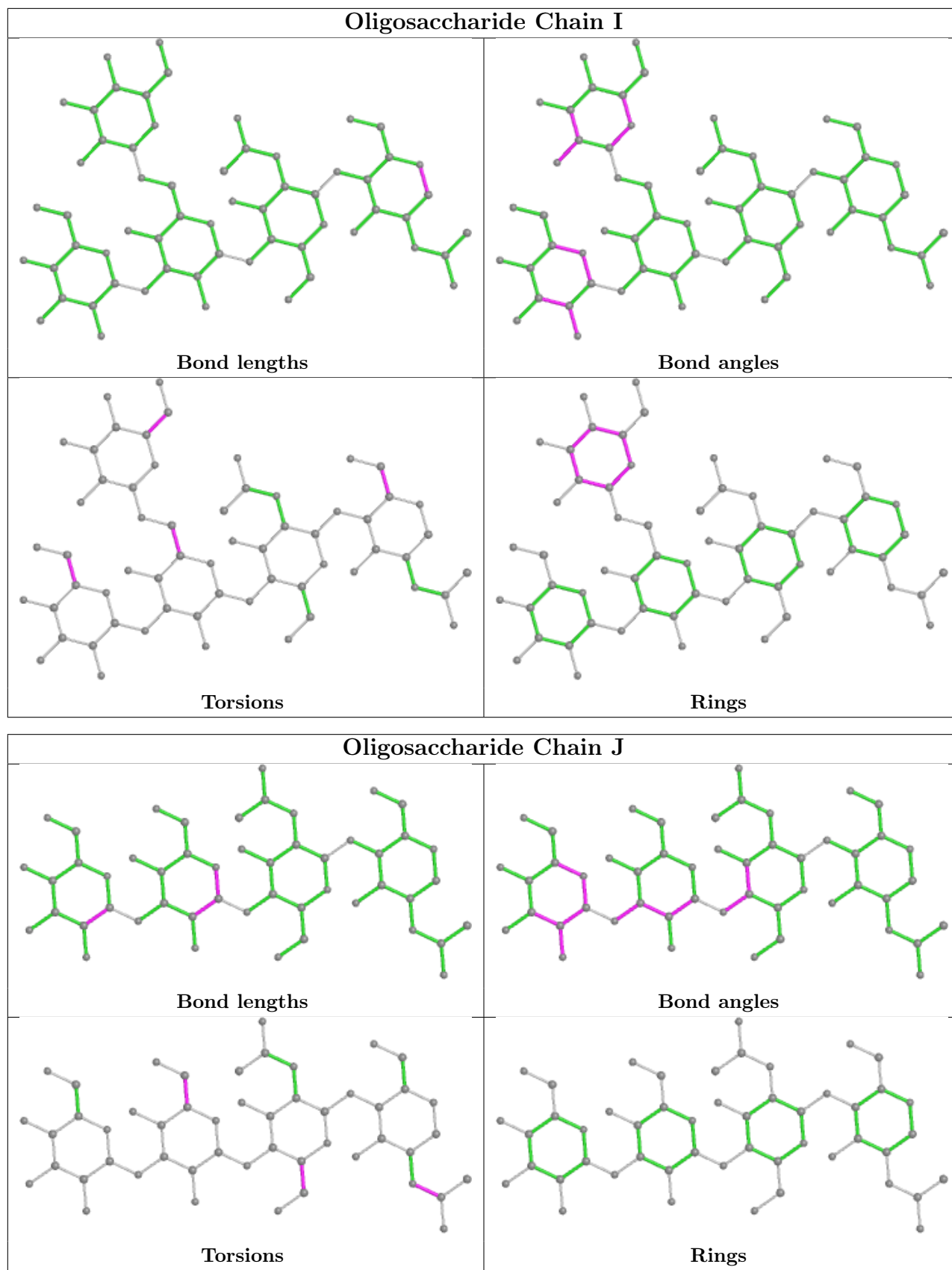


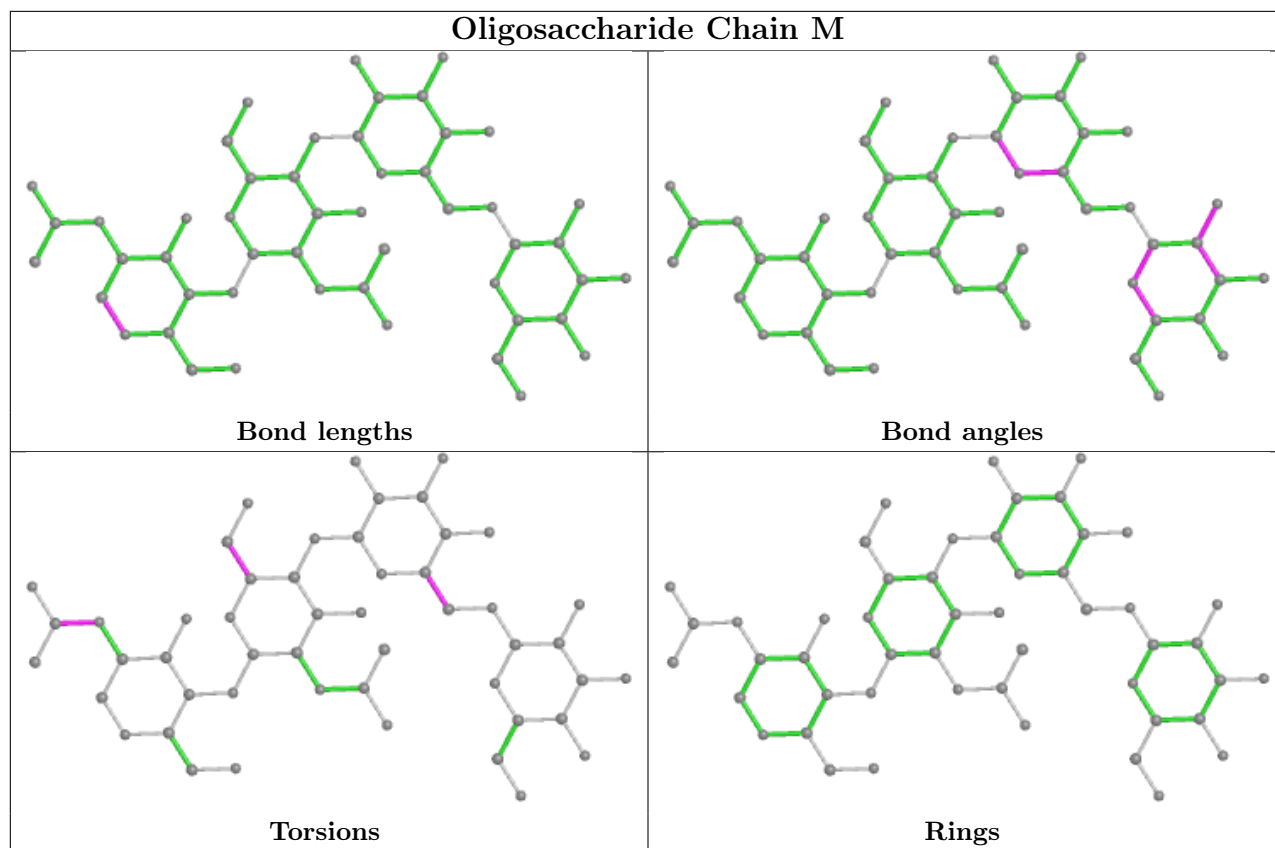












5.6 Ligand geometry [i](#)

6 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	G	601	1	14,14,15	0.18	0	17,19,21	0.53	0
14	NAG	G	605	1	14,14,15	0.35	0	17,19,21	0.61	0
14	NAG	B	701	2	14,14,15	0.20	0	17,19,21	0.40	0
14	NAG	G	602	1	14,14,15	0.21	0	17,19,21	0.43	0
14	NAG	G	603	1	14,14,15	0.36	0	17,19,21	0.56	0
14	NAG	G	604	1	14,14,15	0.23	0	17,19,21	0.44	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	G	601	1	-	1/6/23/26	0/1/1/1
14	NAG	G	605	1	-	3/6/23/26	0/1/1/1
14	NAG	B	701	2	-	2/6/23/26	0/1/1/1
14	NAG	G	602	1	-	0/6/23/26	0/1/1/1
14	NAG	G	603	1	-	0/6/23/26	0/1/1/1
14	NAG	G	604	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	605	NAG	C4-C5-C6-O6
14	G	605	NAG	O5-C5-C6-O6
14	G	604	NAG	C8-C7-N2-C2
14	G	604	NAG	O7-C7-N2-C2
14	B	701	NAG	O5-C5-C6-O6
14	B	701	NAG	C4-C5-C6-O6
14	G	605	NAG	C3-C2-N2-C7
14	G	601	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	601	NAG	1	0
14	B	701	NAG	1	0
14	G	603	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	6
3	D	3
4	E	2
2	B	1
6	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	550:GLN	C	566:LEU	N	23.34
1	D	151:THR	C	163:VAL	N	13.94
1	G	58:ALA	C	68:VAL	N	13.00
1	E	149:THR	C	164:GLU	N	11.15
1	G	398:THR	C	408:THR	N	11.07
1	G	458:GLY	C	465:LYS	N	10.27
1	D	180:SER	C	196:CYS	N	9.69
1	H	126:PRO	C	132:SER	N	8.90
1	D	123:PRO	C	138:LEU	N	8.72
1	G	206:PRO	C	210:PHE	N	8.42
1	G	185:GLY	C	188:SER	N	7.86
1	G	134:VAL	C	151:GLN	N	7.43
1	E	200:THR	C	204:SER	N	6.03

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	427/427 (100%)	0.20	8 (1%) 66 59	97, 168, 236, 298	0
2	B	131/131 (100%)	0.05	2 (1%) 73 66	100, 132, 199, 227	0
3	D	187/187 (100%)	-0.03	2 (1%) 80 74	109, 157, 201, 214	0
4	E	192/192 (100%)	0.15	11 (5%) 23 19	109, 163, 229, 244	0
5	L	210/210 (100%)	0.02	5 (2%) 59 50	122, 166, 186, 196	0
6	H	226/226 (100%)	0.07	2 (0%) 84 78	108, 167, 215, 238	0
All	All	1373/1373 (100%)	0.10	30 (2%) 62 53	97, 164, 222, 298	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	290	GLU	3.5
5	L	141	PRO	3.2
3	D	179	SER	3.2
4	E	123	PRO	3.0
4	E	184	LEU	2.9
1	G	360	LYS	2.9
4	E	136	LEU	2.9
5	L	143	ALA	2.9
4	E	137	VAL	2.8
1	G	396	ASN	2.8
1	G	344	ARG	2.8
4	E	138	CYS	2.8
1	G	269	ASP	2.7
4	E	207	GLU	2.6
5	L	14	ALA	2.5
2	B	567	GLN	2.5
4	E	179	SER	2.5
1	G	347	GLU	2.4
4	E	114	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
5	L	30	SER	2.4
4	E	210	VAL	2.4
4	E	121	LEU	2.4
3	D	10	GLU	2.4
5	L	18	THR	2.3
2	B	571	TRP	2.2
6	H	184	VAL	2.2
1	G	321(A)	GLU	2.1
1	G	287	HIS	2.1
6	H	121	VAL	2.1
4	E	198	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	C	2	14/15	0.57	0.58	222,222,222,222	0
9	MAN	A	5	11/12	0.58	0.55	218,218,218,218	0
11	MAN	I	4	11/12	0.59	0.46	239,239,239,239	0
9	MAN	A	4	11/12	0.61	0.33	201,201,201,201	0
11	BMA	I	3	11/12	0.63	0.28	235,235,235,235	0
10	NAG	S	2	14/15	0.64	0.58	237,237,237,237	0
11	MAN	I	5	11/12	0.64	0.23	261,261,261,261	0
13	NAG	M	2	14/15	0.70	0.31	251,251,251,251	0
11	NAG	I	2	14/15	0.71	0.25	197,197,197,197	0
13	BMA	M	3	11/12	0.72	0.53	273,273,273,273	0
10	NAG	C	1	14/15	0.73	0.32	208,208,208,208	0
10	NAG	Q	2	14/15	0.74	0.28	215,215,215,215	0
8	MAN	T	5	11/12	0.74	0.45	192,194,200,200	11
10	NAG	P	2	14/15	0.75	0.27	199,199,199,199	0
8	MAN	T	6	11/12	0.75	0.46	206,210,213,215	0
9	MAN	A	6	11/12	0.75	0.33	197,197,197,197	0
7	MAN	U	1	11/12	0.76	0.34	174,177,178,179	0

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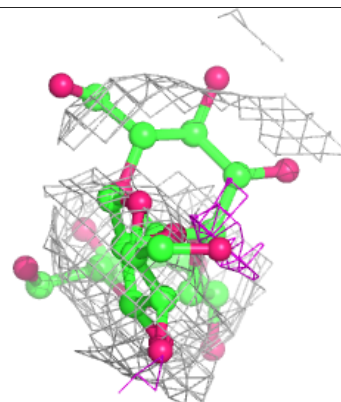
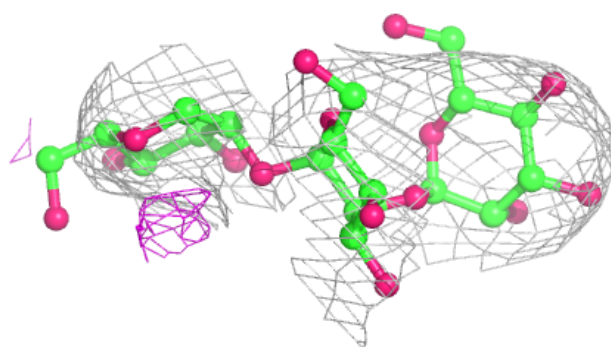
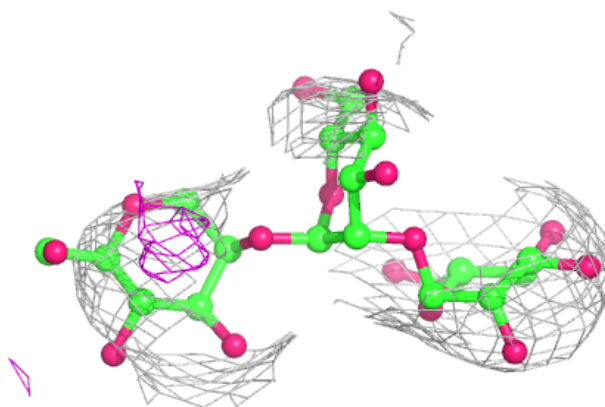
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NAG	K	2	14/15	0.77	0.36	203,203,203,203	0
8	MAN	T	4	11/12	0.77	0.31	192,194,197,199	0
10	NAG	S	1	14/15	0.79	0.43	212,212,212,212	0
10	NAG	F	2	14/15	0.80	0.16	224,224,224,224	0
10	NAG	N	1	14/15	0.82	0.19	193,193,193,193	0
12	NAG	J	2	14/15	0.83	0.31	190,190,190,190	0
9	BMA	A	3	11/12	0.83	0.23	168,168,168,168	0
10	NAG	R	2	14/15	0.83	0.37	211,211,211,211	0
12	BMA	J	3	11/12	0.84	0.17	183,183,183,183	0
10	NAG	K	1	14/15	0.84	0.19	197,197,197,197	0
10	NAG	N	2	14/15	0.84	0.42	234,234,234,234	0
12	MAN	J	4	11/12	0.85	0.19	169,169,169,169	0
13	MAN	M	4	11/12	0.85	0.30	273,273,273,273	0
10	NAG	Q	1	14/15	0.86	0.22	201,201,201,201	0
8	NAG	T	1	14/15	0.87	0.35	145,163,168,178	0
10	NAG	R	1	14/15	0.87	0.32	172,172,172,172	0
8	BMA	T	3	11/12	0.87	0.15	150,168,182,194	0
9	NAG	A	2	14/15	0.88	0.26	133,133,133,133	0
10	NAG	F	1	14/15	0.88	0.20	206,206,206,206	0
10	NAG	O	2	14/15	0.89	0.30	217,217,217,217	0
9	MAN	A	7	11/12	0.89	0.22	154,154,154,154	0
7	MAN	U	3	11/12	0.90	0.28	193,195,198,201	0
11	NAG	I	1	14/15	0.90	0.21	165,165,165,165	0
12	NAG	J	1	14/15	0.90	0.29	158,158,158,158	0
8	NAG	T	2	14/15	0.91	0.22	132,160,180,188	0
10	NAG	P	1	14/15	0.91	0.29	172,172,172,172	0
10	NAG	O	1	14/15	0.91	0.19	182,182,182,182	0
13	NAG	M	1	14/15	0.92	0.18	207,207,207,207	0
7	MAN	U	2	11/12	0.92	0.15	174,176,179,181	0
9	NAG	A	1	14/15	0.94	0.22	124,124,124,124	0

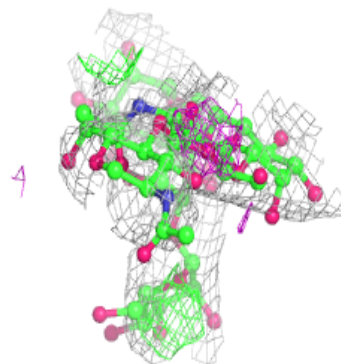
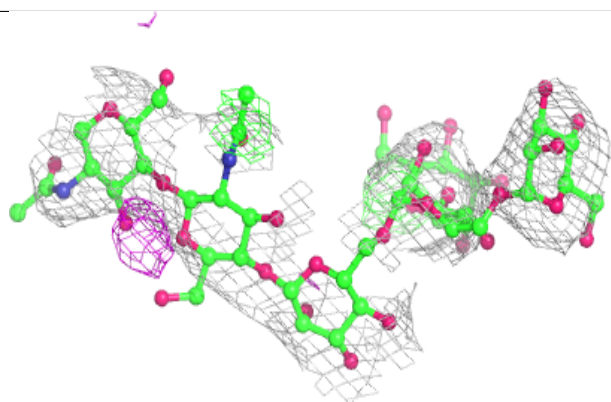
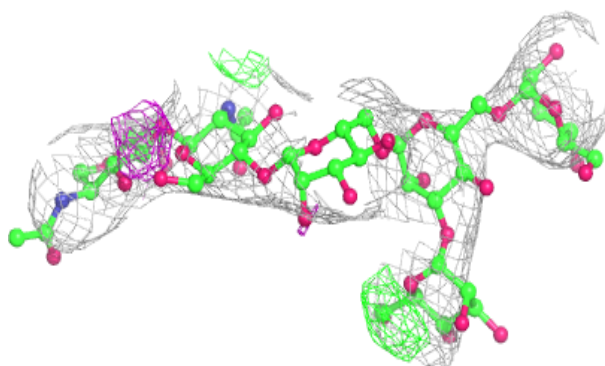
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

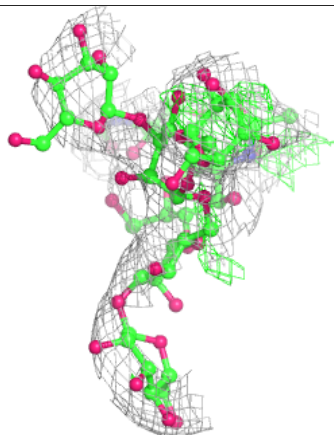
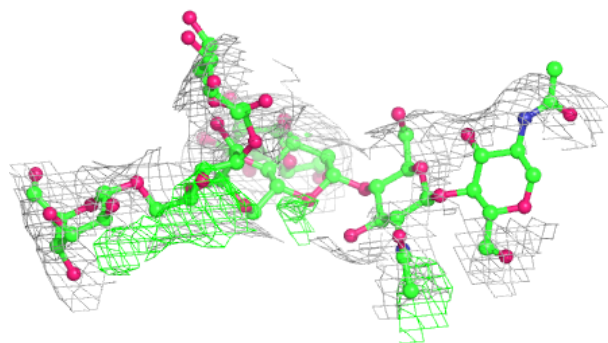
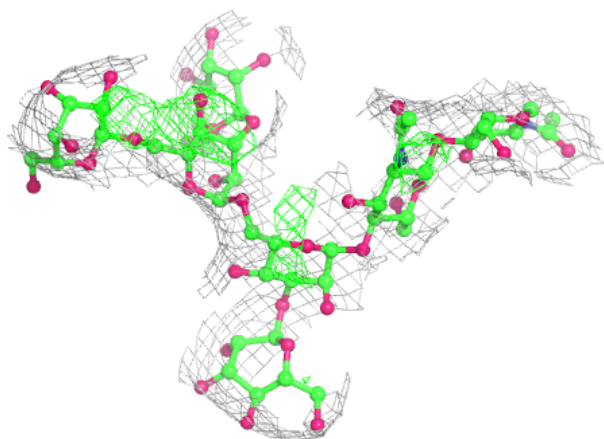
**Electron density around Chain T:**

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



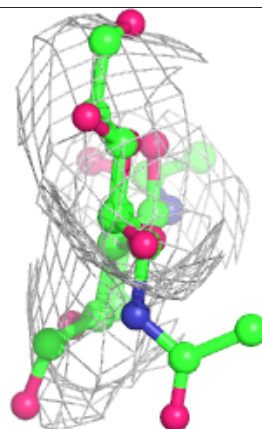
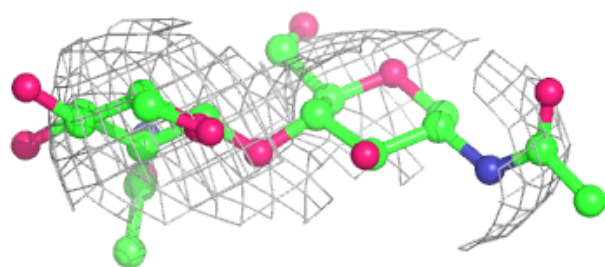
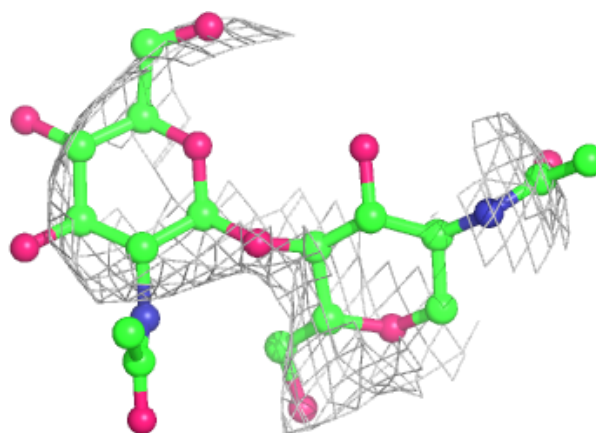
Electron density around Chain A:

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

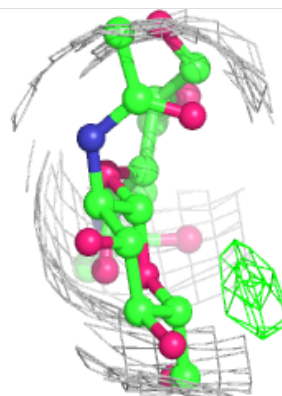
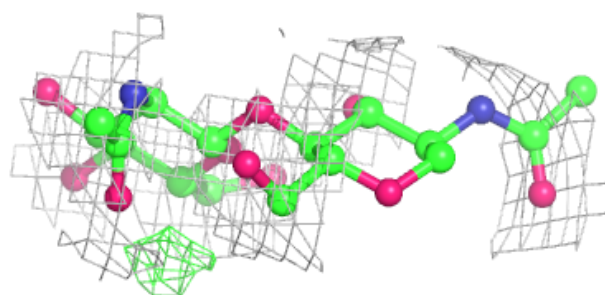
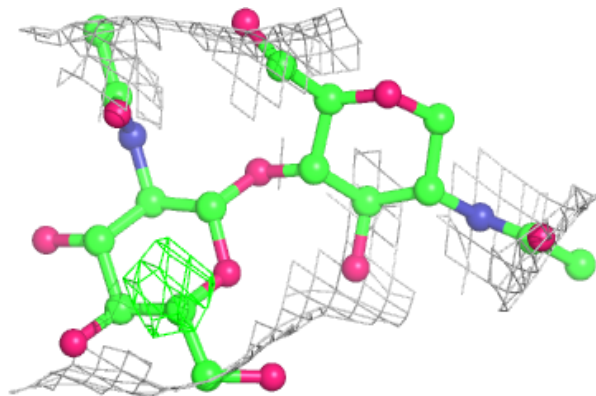


Electron density around Chain C:

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

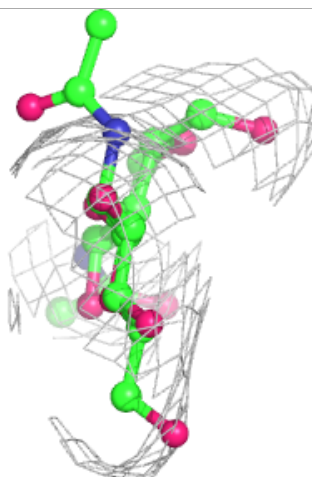
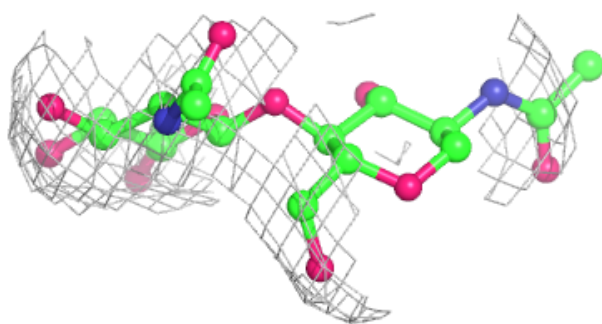
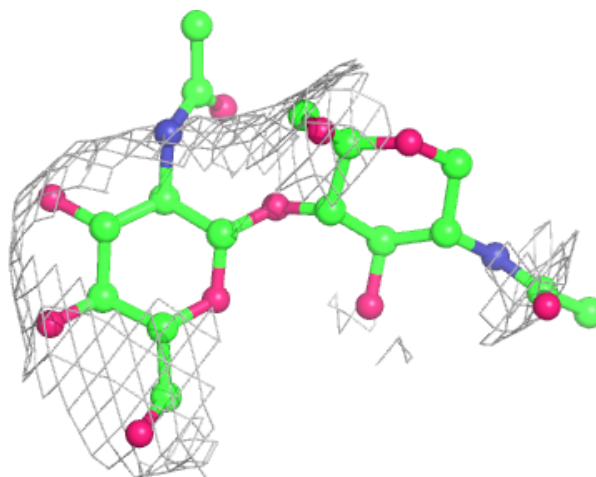
**Electron density around Chain F:**

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



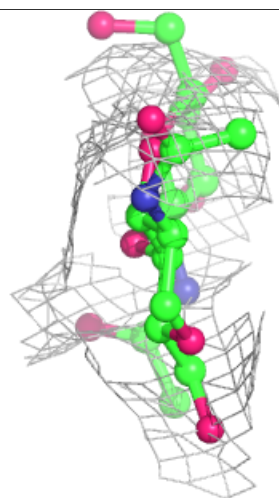
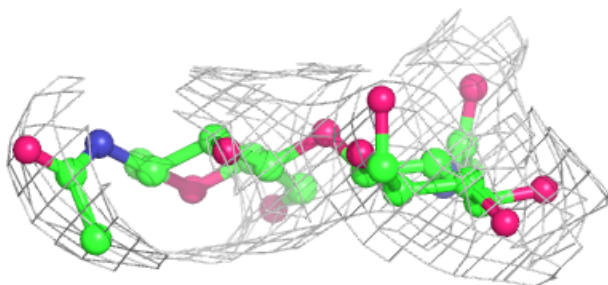
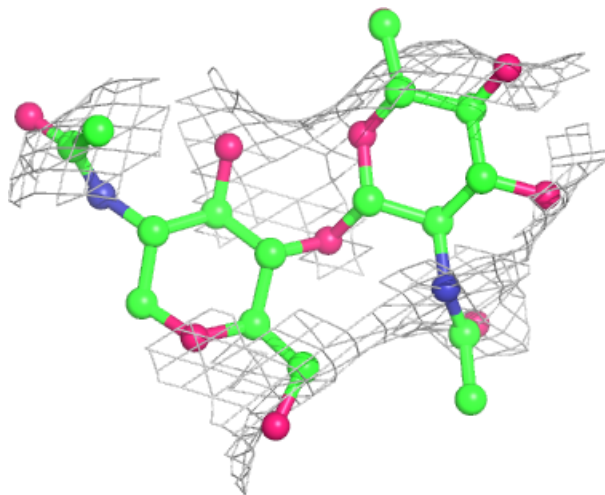
Electron density around Chain K:

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



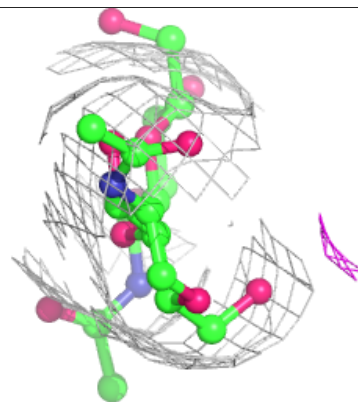
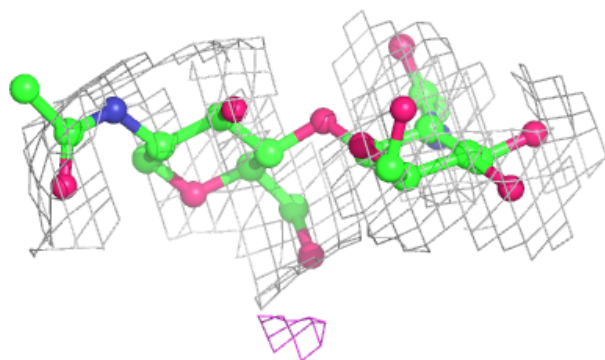
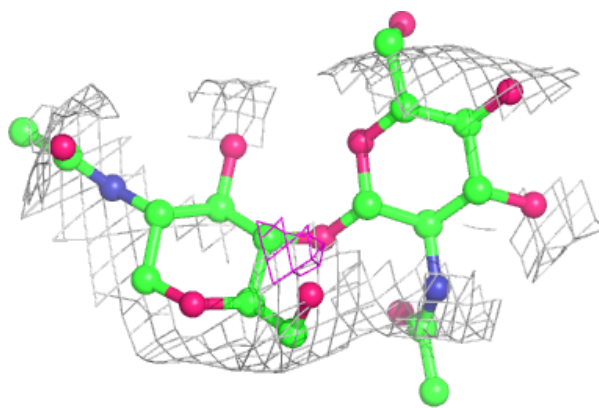
Electron density around Chain N:

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



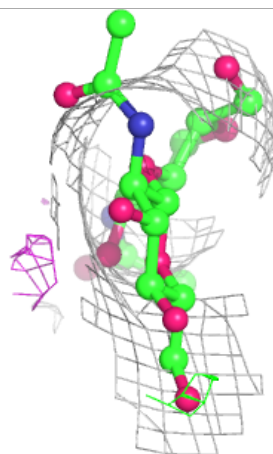
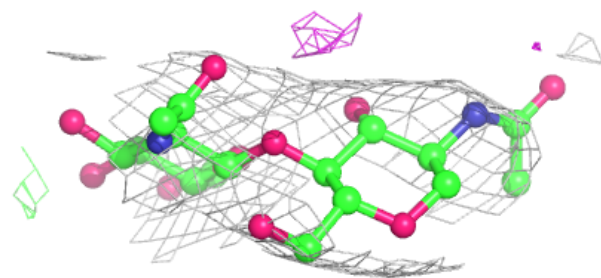
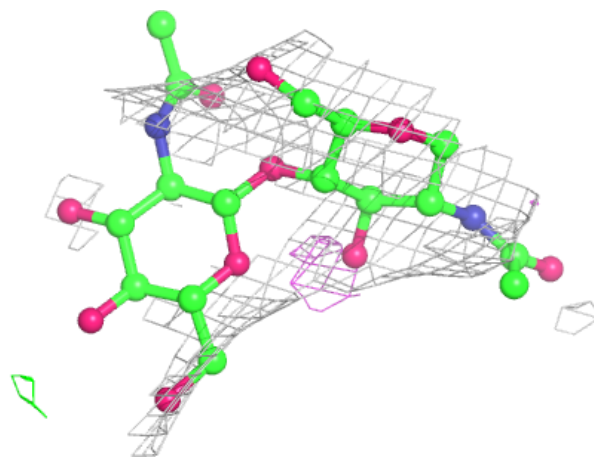
Electron density around Chain O:

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



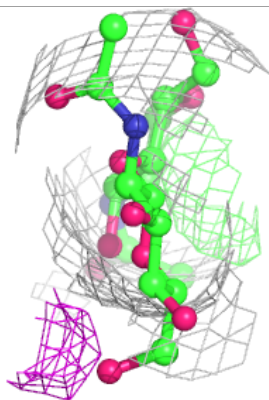
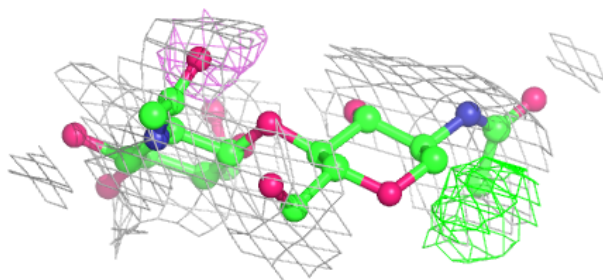
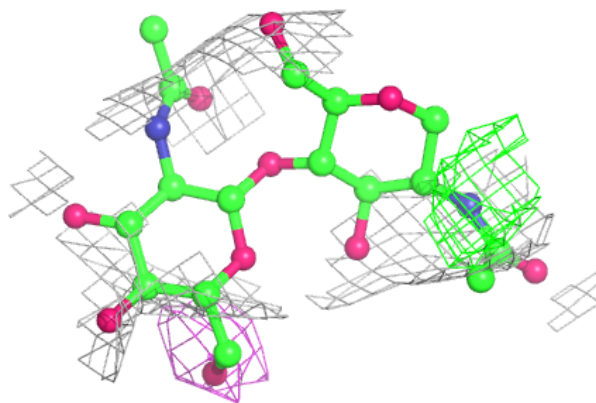
Electron density around Chain P:

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

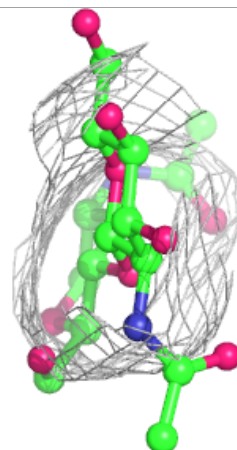
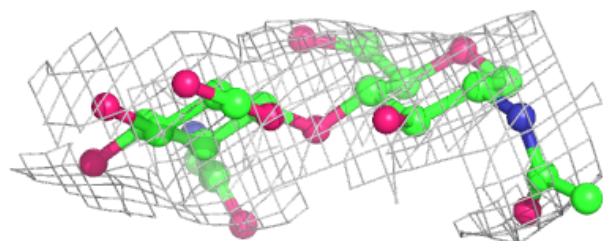
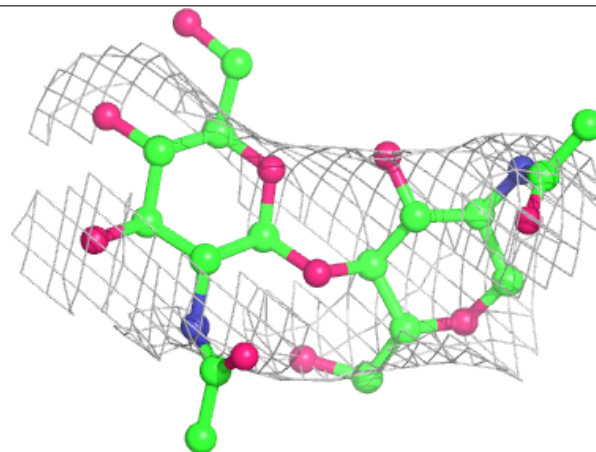


Electron density around Chain Q:

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

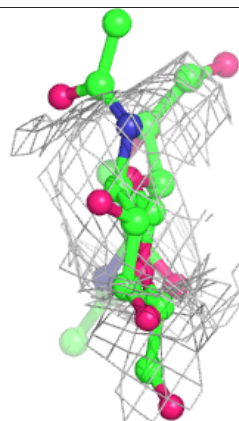
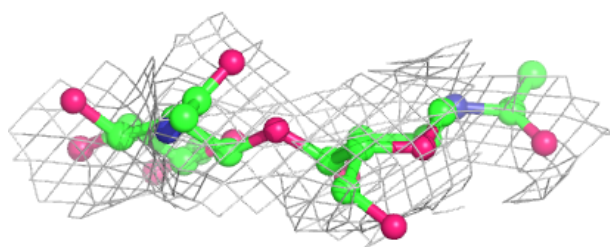
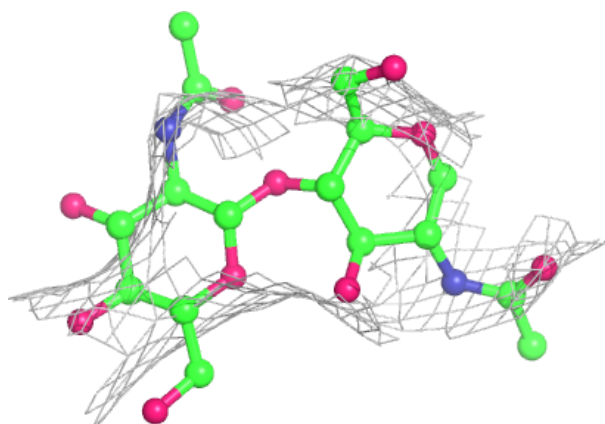
**Electron density around Chain R:**

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



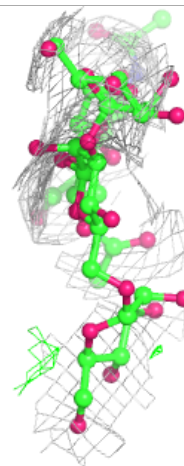
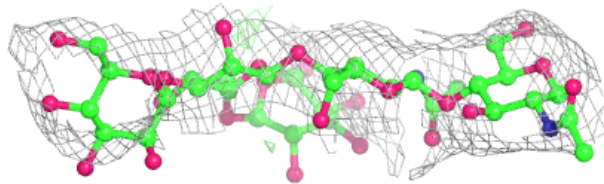
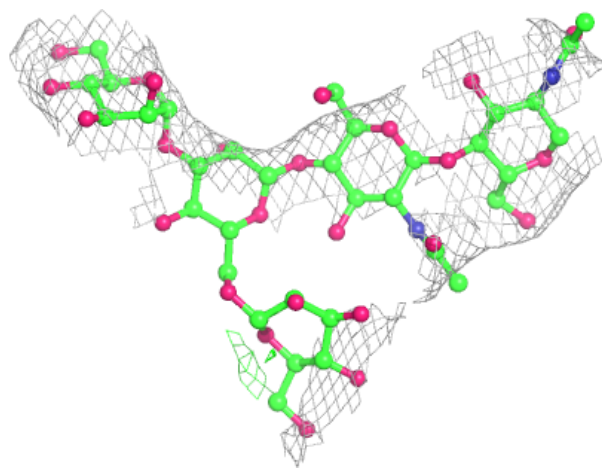
Electron density around Chain S:

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



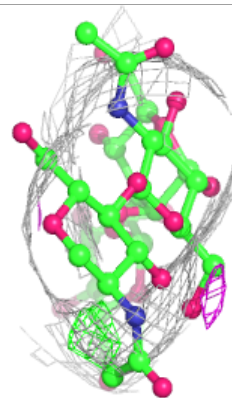
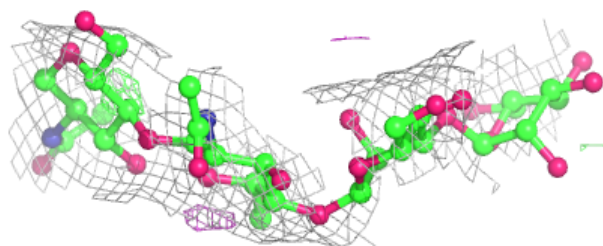
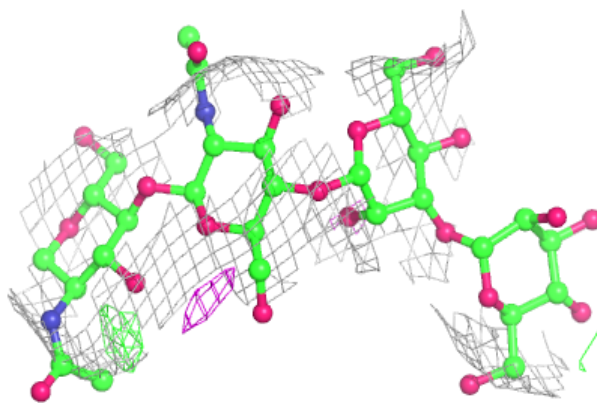
Electron density around Chain I:

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

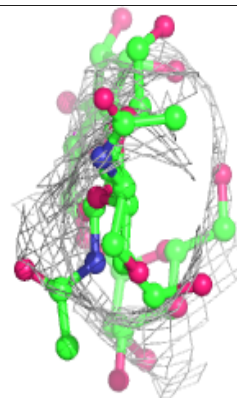
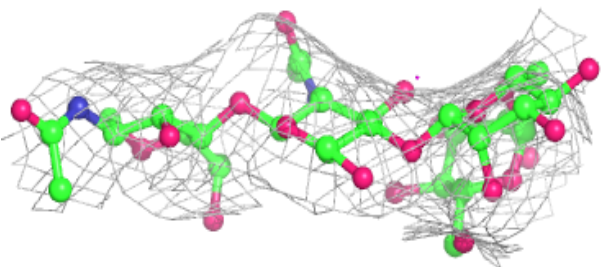
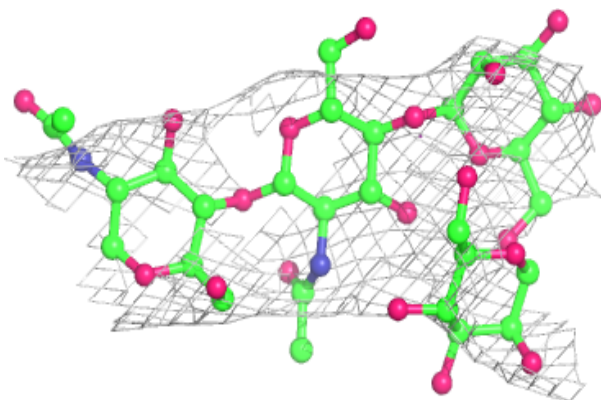


Electron density around Chain J:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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	G	605	14/15	0.69	0.25	196,196,196,196	0
14	NAG	G	603	14/15	0.72	0.32	205,205,205,205	0
14	NAG	G	601	14/15	0.76	0.30	209,209,209,209	0
14	NAG	G	604	14/15	0.80	0.45	194,194,194,194	0
14	NAG	G	602	14/15	0.85	0.24	142,142,142,142	0
14	NAG	B	701	14/15	0.92	0.27	199,199,199,199	0

6.5 Other polymers [i](#)

There are no such residues in this entry.