



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 5UTF / pdb\_00005utf  
Title : Crystal Structure of a Stabilized DS-SOSIP.6mut BG505 gp140 HIV-1 Env Trimer, Containing Mutations I201C-P433C (DS), L154M, Y177W, N300M, N302M, T320L, I420M in Complex with Human Antibodies PGT122 and 35O22 at 4.3 Å  
Authors : Pancera, M.; Chuang, G.-Y.; Xu, K.; Kwong, P.D.  
Deposited on : 2017-02-14  
Resolution : 3.50 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](mailto: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>.

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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

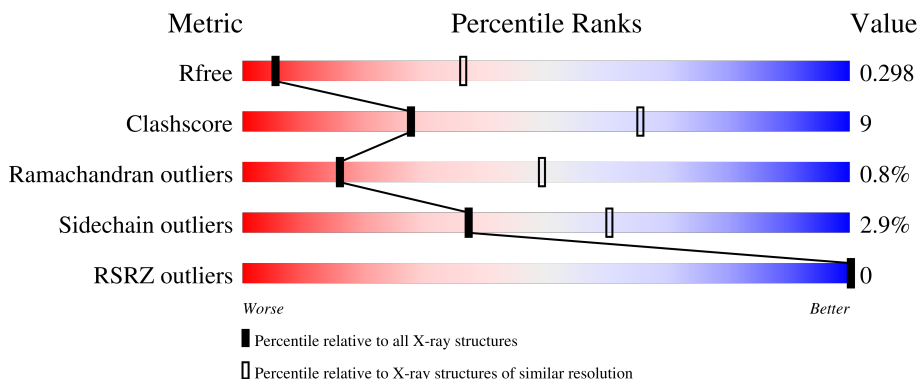
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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  $\geq 3$ , 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	481	
2	B	153	
3	L	213	
4	H	235	

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Mol	Chain	Length	Quality of chain
5	D	243	 80% 19%
6	E	216	 77% 21%
7	A	10	 10% 40% 50%
8	C	3	 67% 33%
9	F	2	 100%
9	J	2	 100%
9	K	2	 100%
9	M	2	 50% 50%
9	N	2	 50% 50%
9	P	2	 50% 50%
9	Q	2	 100%
9	R	2	 100%
9	S	2	 100%
10	I	6	 33% 67%
11	O	5	 60% 40%
12	T	10	 10% 70% 20%

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 11964 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	439	3464	2179	609	642	34	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	154	MET	LEU	engineered mutation	UNP Q2N0S6
G	177	TRP	TYR	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	300	MET	ASN	engineered mutation	UNP Q2N0S6
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	420	MET	ILE	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	engineered mutation	UNP Q2N0S6
G	510	ARG	LYS	engineered mutation	UNP Q2N0S6
G	512	ARG	ALA	engineered mutation	UNP Q2N0S6
G	513	ARG	VAL	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	123	980	620	169	185	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	208	1577	990	265	318	4	0	0	0

- Molecule 4 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	228	1742	1109	295	333	5	0	0	0

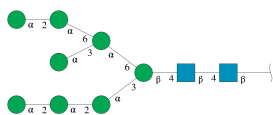
- Molecule 5 is a protein called 35022 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	242	1832	1165	306	353	8	0	0	0

- Molecule 6 is a protein called 35022 Light Chain.

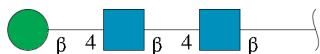
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	213	1615	1012	267	328	8	0	0	0

- Molecule 7 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-(1-6)-[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			
7	A	10	116	64	2	50	0	0	0

- Molecule 8 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.



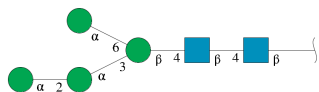
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	3	39	22	2	15	0	0	0

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



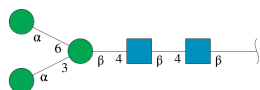
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	2	28	16	2	10	0	0	0
9	J	2	28	16	2	10	0	0	0
9	K	2	28	16	2	10	0	0	0
9	M	2	28	16	2	10	0	0	0
9	N	2	28	16	2	10	0	0	0
9	P	2	28	16	2	10	0	0	0
9	Q	2	28	16	2	10	0	0	0
9	R	2	28	16	2	10	0	0	0
9	S	2	28	16	2	10	0	0	0

- 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.



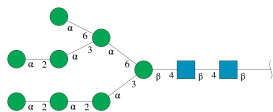
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	6	72	40	2	30	0	0	0

- 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	O	5	61	34	2	25	0	0	0

- 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
			Total	C	N	O			
12	T	10	116	64	2	50	0	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

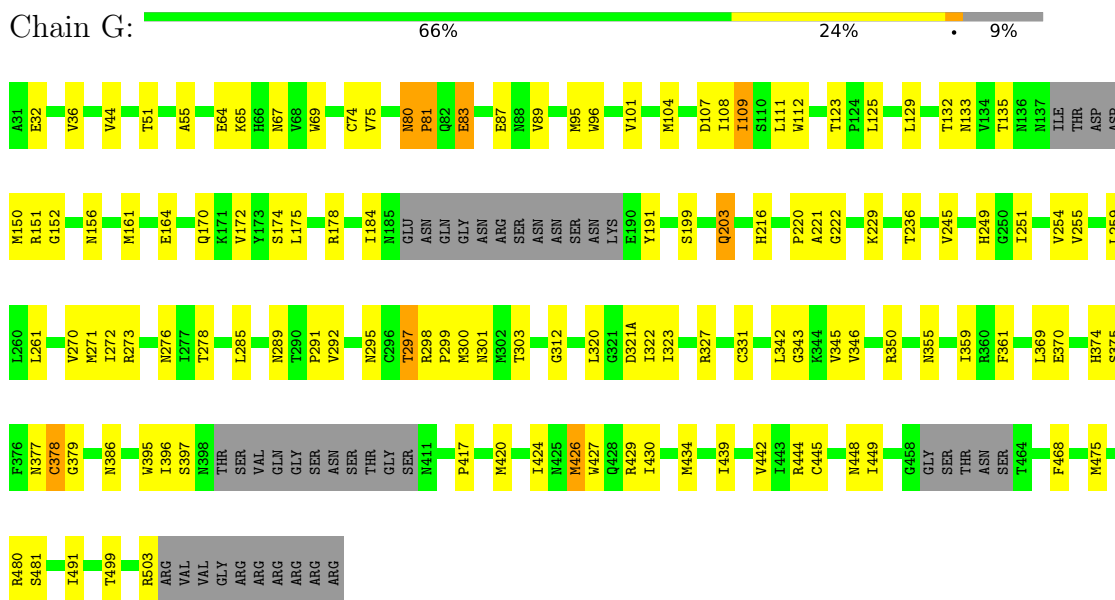


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	G	1	Total 14	8	1	5	0	0
13	B	1	Total 14	8	1	5	0	0
13	B	1	Total 14	8	1	5	0	0
13	B	1	Total 14	8	1	5	0	0

### 3 Residue-property plots

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

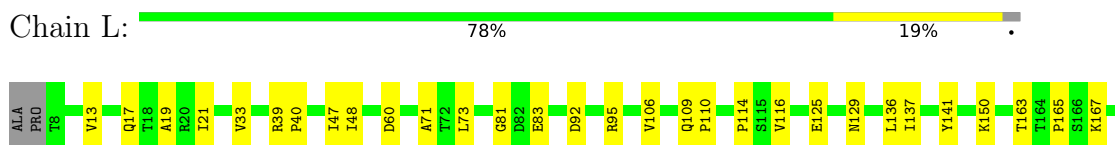
- Molecule 1: Envelope glycoprotein gp120



- Molecule 2: Envelope glycoprotein gp41



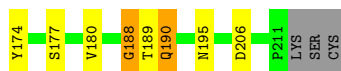
- Molecule 3: PGT122 Light chain





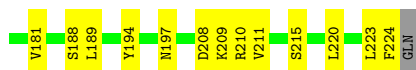
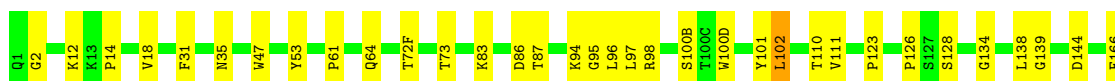
- Molecule 4: PGT122 Heavy chain

Chain H: 81% 14%



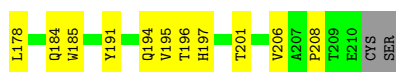
- Molecule 5: 35022 Heavy chain

Chain D: 80% 19%



- Molecule 6: 35022 Light Chain

Chain E: 77% 21%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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: 10% 40% 50%



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

Chain C: 67% 33%

MAG1  
MAG2  
BMA3

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

Chain F:  100%


MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain M:  50% 50%

MAG1  
MAG2

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

Chain N:  50% 50%

MAG1  
MAG2

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

Chain P:  50% 50%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  100%

MAG1  
MAG2

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

Chain S:  100%

MAG1  
MAG2

- 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 I:  33% 67%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- 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 O:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- 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 T:  10% 70% 20%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.38Å 128.38Å 313.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.98 – 3.50 38.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	50.8 (38.98-3.50) 50.9 (38.98-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.215 , 0.299 0.219 , 0.298	Depositor DCC
$R_{free}$ test set	951 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.7	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 23.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.156 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	G	0.18	0/3537	0.40	0/4796
2	B	0.17	0/998	0.41	0/1353
3	L	0.18	0/1619	0.36	0/2217
4	H	0.13	0/1789	0.34	0/2443
5	D	0.15	0/1880	0.33	0/2560
6	E	0.14	0/1659	0.33	0/2269
All	All	0.16	0/11482	0.36	0/15638

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	3464	0	3394	79	0
2	B	980	0	955	27	0
3	L	1577	0	1518	26	0
4	H	1742	0	1716	29	0
5	D	1832	0	1806	32	0
6	E	1615	0	1542	33	0
7	A	116	0	97	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	39	0	34	0	0
9	F	28	0	25	1	0
9	J	28	0	25	0	0
9	K	28	0	25	1	0
9	M	28	0	25	1	0
9	N	28	0	25	2	0
9	P	28	0	25	1	0
9	Q	28	0	25	0	0
9	R	28	0	25	0	0
9	S	28	0	25	0	0
10	I	72	0	61	2	0
11	O	61	0	52	0	0
12	T	116	0	97	2	0
13	B	42	0	39	3	0
13	G	56	0	52	2	0
All	All	11964	0	11588	211	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 9.

All (211) 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:163:THR:HG22	4:H:167:VAL:HB	1.58	0.84
4:H:100(D):VAL:HA	12:T:2:NAG:H2	1.59	0.82
1:G:350:ARG:NH2	1:G:396:ILE:O	2.13	0.81
13:B:702:NAG:H83	6:E:54:ARG:HH21	1.52	0.73
2:B:536:THR:O	2:B:540:GLN:NE2	2.23	0.72
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.73	0.71
1:G:291:PRO:HG3	9:N:1:NAG:H61	1.73	0.70
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.75	0.67
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.58	0.67
3:L:137:ILE:HB	3:L:175:ALA:HB3	1.78	0.66
6:E:37:GLN:HB2	6:E:47:ILE:HD11	1.77	0.65
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.77	0.65
3:L:39:ARG:NH1	3:L:81:GLY:O	2.30	0.65
1:G:298:ARG:NH2	1:G:439:ILE:O	2.30	0.65
3:L:116:VAL:HG12	3:L:137:ILE:HG23	1.80	0.64
1:G:175:LEU:HB3	1:G:320:LEU:HB2	1.80	0.63
5:D:12:LYS:HG3	5:D:18:VAL:HB	1.80	0.63
5:D:72(F):THR:HG1	5:D:73:THR:HG1	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:VAL:HG13	2:B:542:ARG:HH22	1.63	0.63
3:L:170:ASN:HB3	3:L:172:LYS:H	1.63	0.63
4:H:11:LEU:HB2	4:H:145:PRO:HG3	1.83	0.61
5:D:72(F):THR:OG1	5:D:73:THR:OG1	2.20	0.59
2:B:625:ASN:HB2	5:D:97:LEU:HD22	1.84	0.59
4:H:100(D):VAL:O	4:H:100(F):ALA:N	2.34	0.58
1:G:426:MET:HB3	1:G:427:TRP:CE3	2.39	0.58
7:A:2:NAG:H3	7:A:2:NAG:H83	1.86	0.58
1:G:109:ILE:HG12	1:G:430:ILE:HG21	1.85	0.58
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.86	0.58
13:G:622:NAG:H3	13:G:622:NAG:H83	1.86	0.57
5:D:35:ASN:HD21	5:D:100(D):TRP:HE3	1.50	0.57
1:G:292:VAL:HB	1:G:449:ILE:HB	1.86	0.57
1:G:261:LEU:HD11	1:G:374:HIS:CE1	2.39	0.56
9:P:2:NAG:H3	9:P:2:NAG:H83	1.87	0.56
3:L:13:VAL:HG21	3:L:19:ALA:HA	1.88	0.56
1:G:261:LEU:HD11	1:G:374:HIS:HE1	1.71	0.55
6:E:165:SER:O	6:E:173:ALA:N	2.37	0.55
1:G:379:GLY:N	10:I:2:NAG:O6	2.39	0.55
4:H:188:GLY:HA3	4:H:190:GLN:N	2.21	0.55
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.89	0.55
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.89	0.54
1:G:83:GLU:HG2	1:G:245:VAL:HG22	1.90	0.54
1:G:297:THR:HG23	1:G:444:ARG:HG3	1.88	0.54
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.90	0.54
2:B:598:CYS:O	2:B:600:GLY:N	2.40	0.54
1:G:132:THR:HA	13:G:633:NAG:H82	1.89	0.54
1:G:108:ILE:HD13	1:G:111:LEU:HD12	1.90	0.54
1:G:503:ARG:HD2	2:B:605:CYS:O	2.07	0.54
5:D:100(B):SER:HG	6:E:91:TYR:HH	1.56	0.54
6:E:93:HIS:NE2	7:A:6:MAN:H5	2.23	0.54
6:E:145:THR:OG1	6:E:196:THR:HB	2.08	0.54
4:H:20:LEU:HB2	4:H:80:LEU:HB3	1.89	0.53
1:G:503:ARG:NH1	2:B:597:GLY:HA3	2.23	0.53
4:H:99:ARG:HD3	4:H:100(J):TRP:CZ3	2.43	0.53
1:G:270:VAL:HG12	1:G:289:ASN:H	1.74	0.53
4:H:21:THR:HG23	4:H:77:LEU:HD13	1.90	0.53
3:L:92:ASP:HB3	3:L:95:ARG:HB2	1.90	0.53
1:G:396:ILE:HG22	1:G:397:SER:H	1.73	0.53
4:H:157:LEU:HD21	4:H:180:VAL:HG11	1.90	0.53
6:E:127:ALA:N	6:E:128:ASN:HA	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:22:CYS:HB3	4:H:78:VAL:HB	1.91	0.52
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.91	0.52
1:G:96:TRP:HH2	1:G:285:LEU:HG	1.74	0.52
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.90	0.52
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.92	0.52
2:B:634:GLU:HA	13:B:703:NAG:H82	1.91	0.51
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.91	0.51
13:B:702:NAG:H62	6:E:53:GLU:HG2	1.93	0.51
6:E:54:ARG:HD2	6:E:58:ILE:HG22	1.93	0.51
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.92	0.51
1:G:272:ILE:HD11	1:G:345:VAL:HG13	1.92	0.51
4:H:31:ASP:N	4:H:31:ASP:OD1	2.43	0.51
5:D:2:GLY:H	5:D:102:LEU:HD11	1.76	0.51
5:D:96:LEU:HD13	5:D:101:TYR:HB2	1.94	0.50
1:G:152:GLY:C	1:G:178:ARG:HH21	2.19	0.50
1:G:295:ASN:O	1:G:331:CYS:HA	2.11	0.50
1:G:222:GLY:HA3	2:B:585:ARG:HD3	1.94	0.50
6:E:144:VAL:HG12	6:E:197:HIS:HB2	1.92	0.50
4:H:161:VAL:HG22	4:H:180:VAL:HG22	1.93	0.49
6:E:185:TRP:CZ3	6:E:208:PRO:HG3	2.47	0.49
3:L:125:GLU:OE1	4:H:141:LYS:NZ	2.45	0.49
1:G:448:ASN:HD22	9:N:1:NAG:H83	1.76	0.49
5:D:134:GLY:HA2	5:D:223:LEU:HD13	1.94	0.49
2:B:529:THR:O	2:B:533:ALA:N	2.40	0.49
1:G:174:SER:OG	1:G:175:LEU:N	2.46	0.48
6:E:46:LEU:HG	6:E:55:ALA:HB2	1.96	0.48
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.95	0.48
1:G:350:ARG:HD3	1:G:355:ASN:O	2.14	0.47
6:E:93:HIS:CG	7:A:4:MAN:H2	2.49	0.47
6:E:27(C):CYS:HA	6:E:28:CYS:HA	1.65	0.47
1:G:95:MET:SD	1:G:273:ARG:HD3	2.53	0.47
3:L:167:LYS:HB3	3:L:173:TYR:CZ	2.49	0.47
2:B:618:ASN:OD1	2:B:619:LEU:N	2.44	0.47
4:H:106:SER:HB3	4:H:147:PRO:HD3	1.96	0.47
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.96	0.47
4:H:6:GLU:N	4:H:6:GLU:OE1	2.47	0.47
5:D:31:PHE:HA	7:A:1:NAG:O6	2.15	0.46
5:D:47:TRP:CZ3	6:E:95(A):GLY:HA3	2.50	0.46
1:G:51:THR:HB	2:B:578:ALA:HB2	1.97	0.46
1:G:424:ILE:HD11	1:G:434:MET:HE2	1.97	0.46
4:H:100(D):VAL:HG21	4:H:100(G):PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:THR:HG22	2:B:626:MET:H	1.79	0.46
6:E:132:LEU:HD12	6:E:178:LEU:HD23	1.96	0.46
3:L:129:ASN:HA	3:L:183:PRO:HG2	1.98	0.46
1:G:420:MET:HE3	1:G:420:MET:HB2	1.83	0.46
6:E:27(B):VAL:O	6:E:90:SER:OG	2.19	0.46
6:E:165:SER:N	6:E:173:ALA:O	2.33	0.46
1:G:361:PHE:HE2	1:G:395:TRP:CD1	2.33	0.46
1:G:271:MET:HG2	1:G:273:ARG:CZ	2.46	0.45
1:G:427:TRP:CD1	1:G:475:MET:HG3	2.51	0.45
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.45	0.45
5:D:138:LEU:HD13	5:D:211:VAL:HG11	1.97	0.45
1:G:164:GLU:HG3	1:G:312:GLY:HA3	1.99	0.45
1:G:270:VAL:HG12	1:G:289:ASN:N	2.31	0.45
1:G:303:THR:OG1	1:G:321(A):ASP:O	2.27	0.45
5:D:61:PRO:HA	5:D:64:GLN:HB2	1.97	0.45
5:D:194:TYR:O	5:D:210:ARG:HD2	2.16	0.45
1:G:255:VAL:HG21	1:G:426:MET:HE1	1.97	0.45
3:L:167:LYS:HB3	3:L:173:TYR:CE2	2.52	0.45
1:G:74:CYS:SG	1:G:75:VAL:N	2.90	0.45
9:F:1:NAG:H62	9:F:2:NAG:C7	2.47	0.45
1:G:377:ASN:OD1	1:G:378:CYS:N	2.50	0.45
3:L:60:ASP:OD1	3:L:60:ASP:N	2.50	0.45
3:L:165:PRO:HA	3:L:174:ALA:O	2.17	0.45
6:E:196:THR:HA	6:E:201:THR:HA	1.98	0.45
1:G:300:MET:HE2	1:G:322:ILE:HG21	2.00	0.44
1:G:161:MET:HB3	1:G:170:GLN:HB3	2.00	0.44
4:H:195:ASN:ND2	4:H:206:ASP:OD1	2.48	0.44
5:D:14:PRO:HG3	5:D:111:VAL:HG12	2.00	0.44
4:H:157:LEU:O	4:H:161:VAL:HG21	2.18	0.44
2:B:642:ILE:O	2:B:646:LEU:HD12	2.18	0.44
5:D:100(B):SER:OG	6:E:91:TYR:OH	2.28	0.44
5:D:139:GLY:HA3	5:D:181:VAL:HA	1.98	0.44
5:D:188:SER:HG	5:D:194:TYR:HH	1.58	0.44
6:E:117:LEU:HD23	6:E:206:VAL:HG13	1.99	0.44
1:G:370:GLU:H	1:G:370:GLU:CD	2.25	0.44
1:G:132:THR:OG1	1:G:133:ASN:N	2.51	0.44
2:B:570:VAL:HG12	2:B:571:TRP:H	1.83	0.44
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.53	0.44
7:A:3:BMA:H61	7:A:7:MAN:H2	1.42	0.44
1:G:343:GLY:HA2	1:G:346:VAL:HG12	1.99	0.43
6:E:83:GLU:O	6:E:166:LYS:NZ	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:148:TRP:CD1	6:E:159:VAL:HG13	2.53	0.43
1:G:156:ASN:HA	1:G:175:LEU:HD12	2.00	0.43
1:G:299:PRO:HA	1:G:442:VAL:HG22	2.00	0.43
1:G:491:ILE:O	2:B:585:ARG:NH2	2.43	0.43
3:L:109:GLN:HG3	3:L:141:TYR:CZ	2.52	0.43
1:G:80:ASN:O	1:G:81:PRO:C	2.62	0.43
1:G:426:MET:HE3	1:G:427:TRP:CH2	2.53	0.43
1:G:259:LEU:HD12	1:G:374:HIS:CD2	2.54	0.43
4:H:18:LEU:HB3	4:H:82:LEU:HB3	2.00	0.43
4:H:188:GLY:HA3	4:H:190:GLN:H	1.83	0.43
1:G:276:ASN:OD1	1:G:278:THR:OG1	2.35	0.43
1:G:87:GLU:C	1:G:89:VAL:H	2.26	0.43
5:D:100(D):TRP:CZ2	6:E:91:TYR:HB2	2.54	0.43
6:E:27:ASN:HA	6:E:27(C):CYS:O	2.19	0.43
1:G:44:VAL:HA	2:B:629:LEU:HD23	2.00	0.42
1:G:359:ILE:HD12	1:G:468:PHE:HE2	1.84	0.42
1:G:203:GLN:HE21	1:G:203:GLN:HB3	1.59	0.42
3:L:174:ALA:HB1	4:H:164:PHE:CD2	2.54	0.42
12:T:8:MAN:H2	12:T:9:MAN:H2	1.71	0.42
2:B:529:THR:HG23	5:D:98:ARG:HD2	2.00	0.42
6:E:167:GLN:OE1	6:E:173:ALA:HB2	2.19	0.42
3:L:114:PRO:HG2	3:L:203:VAL:HG21	2.02	0.42
4:H:6:GLU:OE2	4:H:92:CYS:N	2.51	0.42
5:D:94:LYS:HD3	5:D:102:LEU:HB2	2.02	0.42
9:K:1:NAG:H61	9:K:2:NAG:N2	2.35	0.42
1:G:107:ASP:O	1:G:111:LEU:HG	2.20	0.42
5:D:87:THR:HG23	5:D:110:THR:HA	2.02	0.42
5:D:220:LEU:HD12	5:D:223:LEU:HD12	2.02	0.42
1:G:221:ALA:HB1	2:B:544:LEU:O	2.20	0.42
1:G:327:ARG:HG2	4:H:100(I):GLU:CD	2.44	0.42
3:L:95:ARG:HD3	3:L:95:ARG:HA	1.77	0.42
6:E:146:VAL:HG22	6:E:195:VAL:HG22	2.01	0.42
1:G:503:ARG:HH12	2:B:597:GLY:HA3	1.84	0.41
4:H:188:GLY:HA3	4:H:189:THR:C	2.44	0.41
3:L:208:ALA:HA	3:L:209:PRO:HD3	1.94	0.41
6:E:146:VAL:HA	6:E:194:GLN:O	2.20	0.41
6:E:184:GLN:O	6:E:191:TYR:OH	2.37	0.41
1:G:301:ASN:HB3	1:G:323:ILE:O	2.19	0.41
4:H:144:PHE:HA	4:H:145:PRO:HA	1.86	0.41
3:L:83:GLU:HB2	3:L:106:VAL:HG23	2.01	0.41
5:D:166:PHE:CZ	6:E:135:LEU:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:197:ASN:ND2	5:D:208:ASP:OD1	2.50	0.41
6:E:161:THR:HG23	6:E:176:SER:HB2	2.01	0.41
1:G:109:ILE:HG23	1:G:430:ILE:HG12	2.03	0.41
1:G:261:LEU:HA	1:G:448:ASN:O	2.20	0.41
9:M:1:NAG:H4	9:M:2:NAG:N2	2.35	0.41
1:G:64:GLU:HG3	1:G:65:LYS:H	1.86	0.41
2:B:535:MET:H	2:B:535:MET:HG2	1.65	0.41
2:B:592:LEU:HD22	2:B:596:TRP:CZ2	2.55	0.41
1:G:108:ILE:HG22	1:G:427:TRP:CZ2	2.55	0.41
1:G:112:TRP:CG	1:G:427:TRP:HZ3	2.38	0.41
1:G:150:MET:HE3	1:G:151:ARG:H	1.85	0.41
5:D:83:LYS:N	5:D:86:ASP:OD2	2.52	0.41
1:G:104:MET:O	1:G:108:ILE:HG12	2.21	0.41
1:G:129:LEU:O	1:G:191:TYR:N	2.51	0.41
1:G:170:GLN:HG2	1:G:172:VAL:HG13	2.03	0.41
1:G:249:HIS:O	1:G:251:ILE:HG13	2.21	0.41
4:H:100(D):VAL:HG22	4:H:100(I):GLU:OE1	2.20	0.41
4:H:167:VAL:O	4:H:174:TYR:HA	2.21	0.41
5:D:189:LEU:HD21	5:D:224:PHE:HE1	1.86	0.41
6:E:28:CYS:HB3	6:E:66:LYS:HD2	2.03	0.41
1:G:83:GLU:OE1	1:G:229:LYS:HD3	2.20	0.41
1:G:101:VAL:HG21	1:G:480:ARG:HG2	2.03	0.41
5:D:53:TYR:CD2	7:A:1:NAG:H5	2.56	0.41
2:B:661:LEU:HA	2:B:661:LEU:HD13	1.82	0.40
3:L:13:VAL:HG13	3:L:17:GLN:HB2	2.03	0.40
5:D:94:LYS:HG2	5:D:95:GLY:O	2.21	0.40
6:E:161:THR:HA	6:E:176:SER:HA	2.03	0.40
1:G:445:CYS:HB3	10:I:2:NAG:H61	2.03	0.40
3:L:136:LEU:HD11	4:H:177:SER:HB2	2.02	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	429/481 (89%)	371 (86%)	52 (12%)	6 (1%)	9	38
2	B	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	7	35
3	L	206/213 (97%)	187 (91%)	18 (9%)	1 (0%)	24	57
4	H	224/235 (95%)	207 (92%)	15 (7%)	2 (1%)	14	47
5	D	240/243 (99%)	223 (93%)	16 (7%)	1 (0%)	30	62
6	E	211/216 (98%)	191 (90%)	20 (10%)	0	100	100
All	All	1429/1541 (93%)	1284 (90%)	133 (9%)	12 (1%)	16	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	81	PRO
2	B	599	SER
3	L	110	PRO
4	H	190	GLN
1	G	67	ASN
1	G	69	TRP
2	B	615	SER
1	G	80	ASN
1	G	135	THR
4	H	188	GLY
5	D	144	ASP
1	G	220	PRO

### 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	392/429 (91%)	374 (95%)	18 (5%)	24	50
2	B	106/129 (82%)	92 (87%)	14 (13%)	4	20
3	L	177/181 (98%)	176 (99%)	1 (1%)	78	79
4	H	198/205 (97%)	197 (100%)	1 (0%)	81	80
5	D	205/206 (100%)	204 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	E	186/189 (98%)	184 (99%)	2 (1%)	65 74
All	All	1264/1339 (94%)	1227 (97%)	37 (3%)	37 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	32	GLU
1	G	83	GLU
1	G	109	ILE
1	G	123	THR
1	G	125	LEU
1	G	184	ILE
1	G	199	SER
1	G	203	GLN
1	G	236	THR
1	G	297	THR
1	G	342	LEU
1	G	369	LEU
1	G	375	SER
1	G	378	CYS
1	G	426	MET
1	G	429	ARG
1	G	481	SER
1	G	499	THR
2	B	529	THR
2	B	535	MET
2	B	570	VAL
2	B	573	ILE
2	B	576	LEU
2	B	581	LEU
2	B	604	CYS
2	B	619	LEU
2	B	626	MET
2	B	635	ILE
2	B	639	THR
2	B	645	LEU
2	B	658	GLN
2	B	661	LEU
3	L	180	SER
4	H	31	ASP
5	D	102	LEU
6	E	89	CYS

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Mol	Chain	Res	Type
6	E	96	CYS

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

Mol	Chain	Res	Type
1	G	80	ASN
1	G	85	HIS
1	G	94	ASN
1	G	99	ASN
1	G	105	HIS
1	G	195	ASN
1	G	203	GLN
2	B	658	GLN
3	L	198	HIS
4	H	97	HIS
4	H	197	ASN
5	D	35	ASN
6	E	197	HIS

### 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](#)

52 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	1	7,1	14,14,15	0.17	0	17,19,21	0.75	1 (5%)
7	MAN	A	10	7	11,11,12	0.73	0	15,15,17	1.28	2 (13%)
7	NAG	A	2	7	14,14,15	0.48	0	17,19,21	1.44	3 (17%)
7	BMA	A	3	7	11,11,12	0.79	0	15,15,17	0.90	0
7	MAN	A	4	7	11,11,12	0.72	0	15,15,17	1.11	2 (13%)
7	MAN	A	5	7	11,11,12	0.71	0	15,15,17	0.85	0
7	MAN	A	6	7	11,11,12	0.73	0	15,15,17	1.37	2 (13%)
7	MAN	A	7	7	11,11,12	1.31	1 (9%)	15,15,17	1.68	4 (26%)
7	MAN	A	8	7	11,11,12	0.87	0	15,15,17	1.24	1 (6%)
7	MAN	A	9	7	11,11,12	1.01	0	15,15,17	1.19	2 (13%)
8	NAG	C	1	8,1	14,14,15	0.46	0	17,19,21	0.46	0
8	NAG	C	2	8	14,14,15	0.39	0	17,19,21	0.41	0
8	BMA	C	3	8	11,11,12	0.51	0	15,15,17	0.89	1 (6%)
9	NAG	F	1	9,1	14,14,15	0.29	0	17,19,21	0.46	0
9	NAG	F	2	9	14,14,15	0.36	0	17,19,21	0.56	0
10	NAG	I	1	10,1	14,14,15	0.30	0	17,19,21	0.54	0
10	NAG	I	2	10	14,14,15	0.41	0	17,19,21	0.45	0
10	BMA	I	3	10	11,11,12	0.95	0	15,15,17	0.84	0
10	MAN	I	4	10	11,11,12	0.95	0	15,15,17	0.92	1 (6%)
10	MAN	I	5	10	11,11,12	0.93	1 (9%)	15,15,17	1.21	2 (13%)
10	MAN	I	6	10	11,11,12	0.77	0	15,15,17	0.99	2 (13%)
9	NAG	J	1	9,1	14,14,15	0.38	0	17,19,21	0.52	0
9	NAG	J	2	9	14,14,15	0.17	0	17,19,21	0.58	0
9	NAG	K	1	9,1	14,14,15	0.35	0	17,19,21	0.58	0
9	NAG	K	2	9	14,14,15	0.44	0	17,19,21	0.60	0
9	NAG	M	1	9,1	14,14,15	0.25	0	17,19,21	0.57	0
9	NAG	M	2	9	14,14,15	0.74	1 (7%)	17,19,21	0.71	1 (5%)
9	NAG	N	1	9,1	14,14,15	0.19	0	17,19,21	0.57	0
9	NAG	N	2	9	14,14,15	0.22	0	17,19,21	0.46	0
11	NAG	O	1	11,1	14,14,15	0.24	0	17,19,21	0.55	0
11	NAG	O	2	11	14,14,15	0.25	0	17,19,21	0.48	0
11	BMA	O	3	11	11,11,12	0.73	0	15,15,17	0.69	0
11	MAN	O	4	11	11,11,12	0.79	0	15,15,17	1.16	1 (6%)
11	MAN	O	5	11	11,11,12	0.65	0	15,15,17	1.42	2 (13%)
9	NAG	P	1	9,1	14,14,15	0.27	0	17,19,21	0.53	0
9	NAG	P	2	9	14,14,15	0.62	0	17,19,21	1.41	2 (11%)
9	NAG	Q	1	9,1	14,14,15	0.18	0	17,19,21	0.43	0
9	NAG	Q	2	9	14,14,15	0.34	0	17,19,21	0.49	0
9	NAG	R	1	9,1	14,14,15	0.32	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	R	2	9	14,14,15	0.22	0	17,19,21	0.43	0
9	NAG	S	1	9,1	14,14,15	0.38	0	17,19,21	0.33	0
9	NAG	S	2	9	14,14,15	0.16	0	17,19,21	0.53	0
12	NAG	T	1	12,1	14,14,15	0.38	0	17,19,21	0.42	0
12	MAN	T	10	12	11,11,12	0.76	0	15,15,17	0.93	2 (13%)
12	NAG	T	2	12	14,14,15	0.30	0	17,19,21	0.76	0
12	BMA	T	3	12	11,11,12	1.01	0	15,15,17	1.20	1 (6%)
12	MAN	T	4	12	11,11,12	0.85	0	15,15,17	1.05	1 (6%)
12	MAN	T	5	12	11,11,12	0.79	0	15,15,17	1.19	2 (13%)
12	MAN	T	6	12	11,11,12	0.59	0	15,15,17	1.26	1 (6%)
12	MAN	T	7	12	11,11,12	1.06	1 (9%)	15,15,17	0.77	1 (6%)
12	MAN	T	8	12	11,11,12	0.74	0	15,15,17	0.98	1 (6%)
12	MAN	T	9	12	11,11,12	0.92	0	15,15,17	1.12	2 (13%)

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. <sup>2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,1	-	3/6/23/26	0/1/1/1
7	MAN	A	10	7	-	0/2/19/22	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	1/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	1/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
7	MAN	A	8	7	-	1/2/19/22	0/1/1/1
7	MAN	A	9	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
10	NAG	I	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	2/2/19/22	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	7	MAN	C1-C2	3.75	1.61	1.52
12	T	7	MAN	O5-C1	-2.89	1.38	1.43
10	I	5	MAN	O5-C5	2.19	1.47	1.43
9	M	2	NAG	C1-C2	2.04	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	2	NAG	C2-N2-C7	4.70	129.20	122.90
7	A	2	NAG	C2-N2-C7	4.66	129.15	122.90
7	A	6	MAN	C1-O5-C5	4.36	118.03	112.19
11	O	5	MAN	C1-O5-C5	4.01	117.56	112.19
12	T	6	MAN	C1-O5-C5	3.91	117.43	112.19
7	A	10	MAN	C1-O5-C5	3.91	117.43	112.19
7	A	7	MAN	C1-O5-C5	3.63	117.05	112.19
7	A	8	MAN	C1-O5-C5	3.53	116.91	112.19
10	I	5	MAN	C1-O5-C5	3.45	116.81	112.19
7	A	9	MAN	C1-O5-C5	3.27	116.57	112.19
12	T	9	MAN	C1-O5-C5	3.14	116.40	112.19
7	A	7	MAN	C1-C2-C3	3.00	114.02	109.64
12	T	5	MAN	C1-O5-C5	2.99	116.19	112.19
11	O	4	MAN	C1-O5-C5	2.90	116.08	112.19
7	A	4	MAN	C1-O5-C5	2.88	116.05	112.19
12	T	4	MAN	C1-O5-C5	2.72	115.84	112.19
12	T	8	MAN	C1-O5-C5	2.68	115.78	112.19
7	A	4	MAN	O2-C2-C3	-2.51	104.94	110.15
9	M	2	NAG	C1-O5-C5	2.50	115.54	112.19
7	A	7	MAN	O2-C2-C3	-2.46	105.06	110.15
7	A	1	NAG	C1-O5-C5	2.42	115.42	112.19
10	I	5	MAN	O2-C2-C3	-2.39	105.20	110.15
8	C	3	BMA	C1-O5-C5	2.39	115.39	112.19
10	I	6	MAN	C1-O5-C5	2.35	115.33	112.19
9	P	2	NAG	C1-C2-N2	2.33	114.10	110.43
7	A	2	NAG	C1-C2-N2	2.27	114.02	110.43
12	T	10	MAN	C1-O5-C5	2.26	115.21	112.19
7	A	10	MAN	O2-C2-C3	-2.23	105.53	110.15
7	A	7	MAN	O5-C1-C2	2.22	116.07	110.79
12	T	10	MAN	O2-C2-C3	-2.21	105.57	110.15
12	T	9	MAN	O2-C2-C3	-2.16	105.67	110.15
10	I	4	MAN	C1-O5-C5	2.15	115.07	112.19
7	A	6	MAN	O2-C2-C3	-2.15	105.70	110.15
12	T	3	BMA	C1-O5-C5	2.12	115.03	112.19
12	T	7	MAN	O2-C2-C3	-2.09	105.82	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	NAG	C1-O5-C5	2.07	114.96	112.19
11	O	5	MAN	O2-C2-C3	-2.06	105.88	110.15
7	A	9	MAN	O2-C2-C3	-2.04	105.93	110.15
10	I	6	MAN	O2-C2-C3	-2.02	105.96	110.15
12	T	5	MAN	O3-C3-C2	2.01	114.16	110.05

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	2	NAG	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
10	I	6	MAN	O5-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
10	I	4	MAN	O5-C5-C6-O6
12	T	2	NAG	O5-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
9	S	2	NAG	O5-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6
12	T	4	MAN	O5-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
10	I	6	MAN	C4-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6
11	O	2	NAG	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
9	S	2	NAG	C4-C5-C6-O6
12	T	4	MAN	C4-C5-C6-O6
12	T	6	MAN	O5-C5-C6-O6
12	T	7	MAN	O5-C5-C6-O6
11	O	1	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
9	K	1	NAG	C4-C5-C6-O6
12	T	2	NAG	C4-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
10	I	4	MAN	C4-C5-C6-O6
11	O	5	MAN	C4-C5-C6-O6
12	T	7	MAN	C4-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	N	1	NAG	C4-C5-C6-O6
11	O	2	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
9	N	1	NAG	C8-C7-N2-C2
9	N	1	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	P	2	NAG	C8-C7-N2-C2
9	P	2	NAG	O7-C7-N2-C2
9	Q	1	NAG	C8-C7-N2-C2
9	Q	1	NAG	O7-C7-N2-C2
7	A	3	BMA	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
11	O	5	MAN	O5-C5-C6-O6
11	O	3	BMA	C4-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
11	O	3	BMA	O5-C5-C6-O6
7	A	9	MAN	C4-C5-C6-O6
10	I	5	MAN	C4-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
7	A	6	MAN	O5-C5-C6-O6
9	Q	2	NAG	C4-C5-C6-O6
9	P	2	NAG	C4-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
9	M	1	NAG	C4-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
7	A	8	MAN	C4-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
7	A	9	MAN	O5-C5-C6-O6
12	T	6	MAN	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
9	K	1	NAG	C3-C2-N2-C7
12	T	2	NAG	C3-C2-N2-C7
10	I	5	MAN	O5-C5-C6-O6
9	P	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C1-C2-N2-C7
7	A	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C1-C2-N2-C7
9	K	1	NAG	C1-C2-N2-C7
9	P	2	NAG	C1-C2-N2-C7
12	T	2	NAG	C1-C2-N2-C7
8	C	3	BMA	O5-C5-C6-O6
9	P	2	NAG	C3-C2-N2-C7
9	Q	1	NAG	C4-C5-C6-O6
9	S	1	NAG	C4-C5-C6-O6

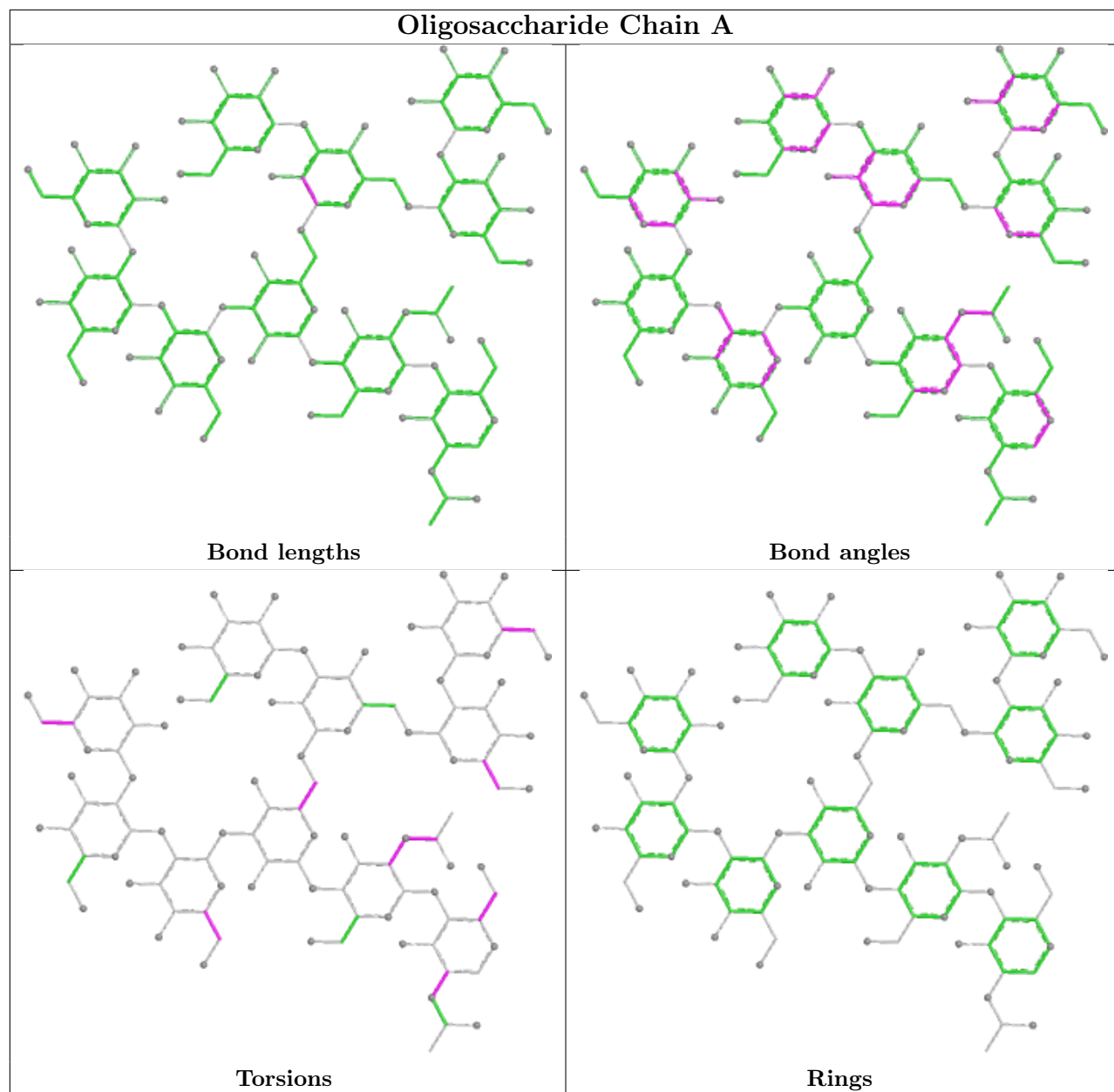
All (2) ring outliers are listed below:

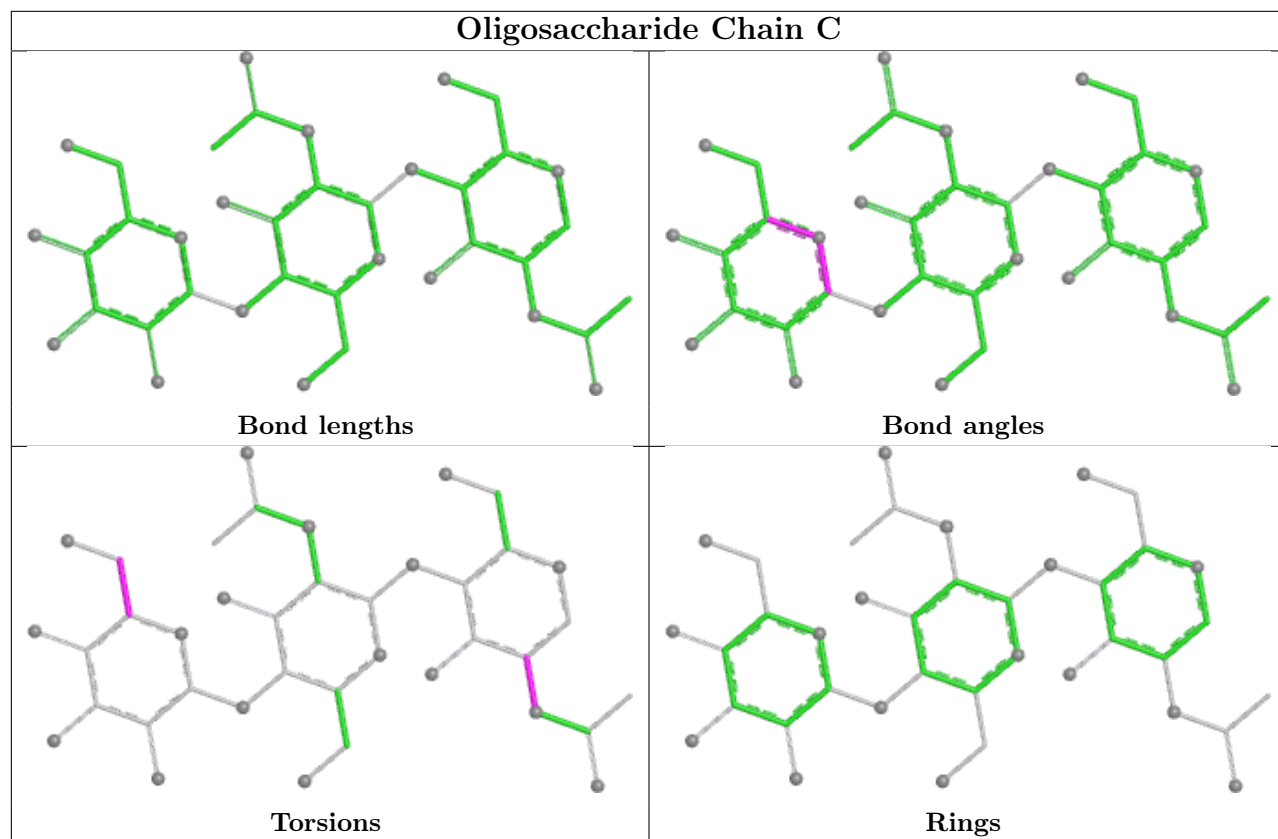
Mol	Chain	Res	Type	Atoms
12	T	9	MAN	C1-C2-C3-C4-C5-O5
10	I	5	MAN	C1-C2-C3-C4-C5-O5

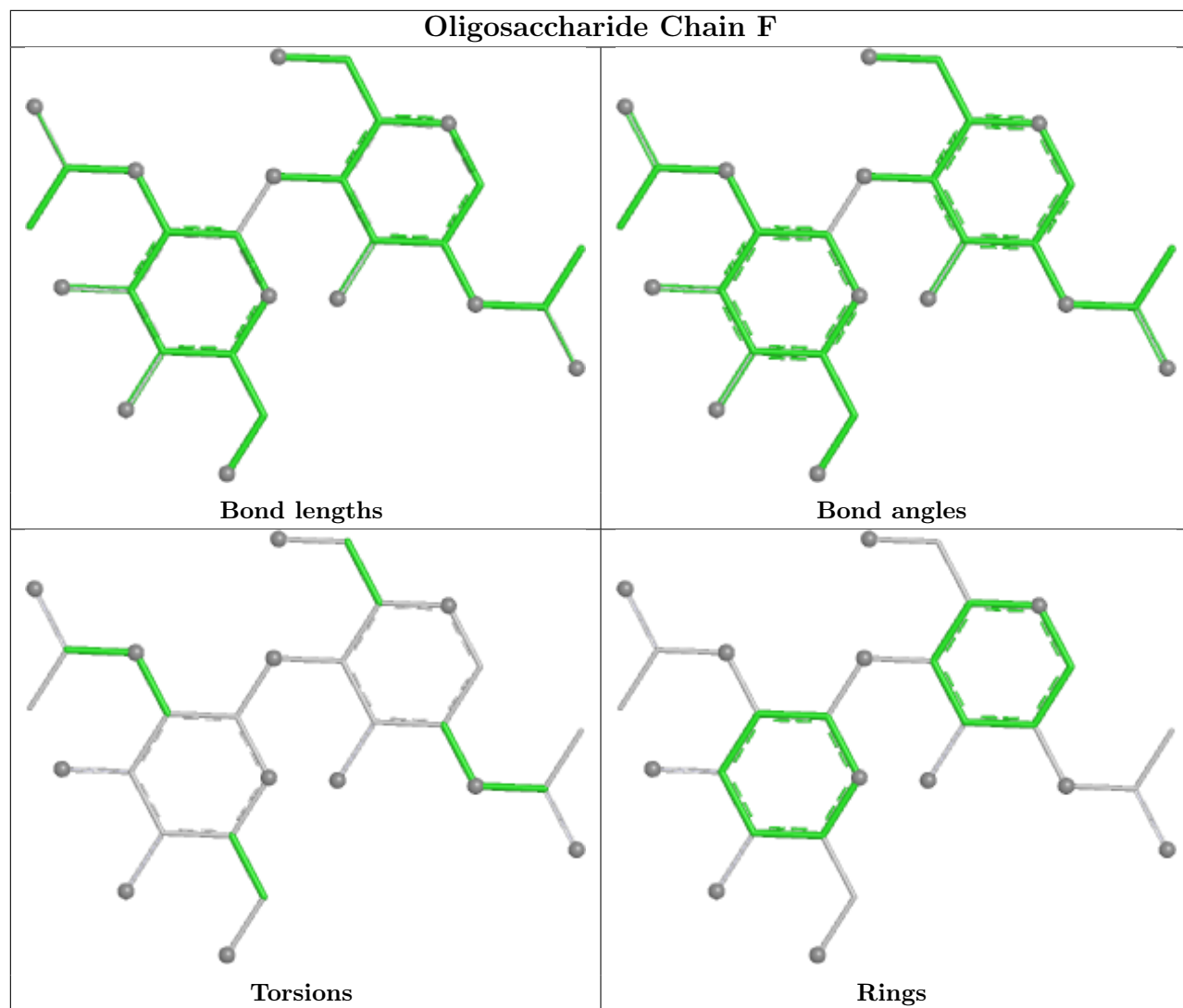
18 monomers are involved in 16 short contacts:

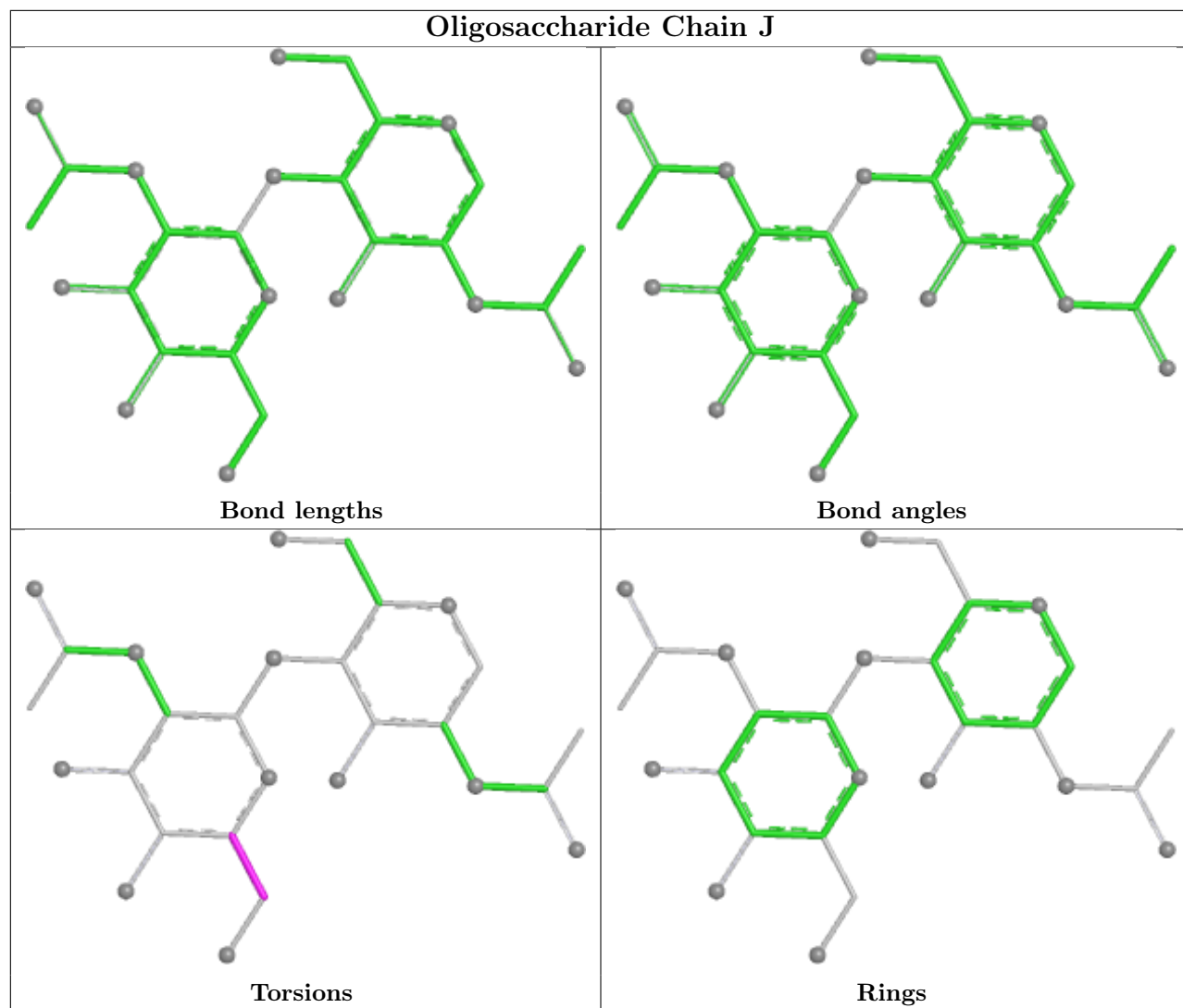
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	9	MAN	1	0
7	A	7	MAN	1	0
9	P	2	NAG	1	0
9	F	1	NAG	1	0
9	K	2	NAG	1	0
7	A	1	NAG	2	0
9	N	1	NAG	2	0
9	M	2	NAG	1	0
9	F	2	NAG	1	0
9	M	1	NAG	1	0
7	A	3	BMA	1	0
10	I	2	NAG	2	0
7	A	4	MAN	1	0
7	A	2	NAG	1	0
7	A	6	MAN	1	0
12	T	2	NAG	1	0
9	K	1	NAG	1	0
12	T	8	MAN	1	0

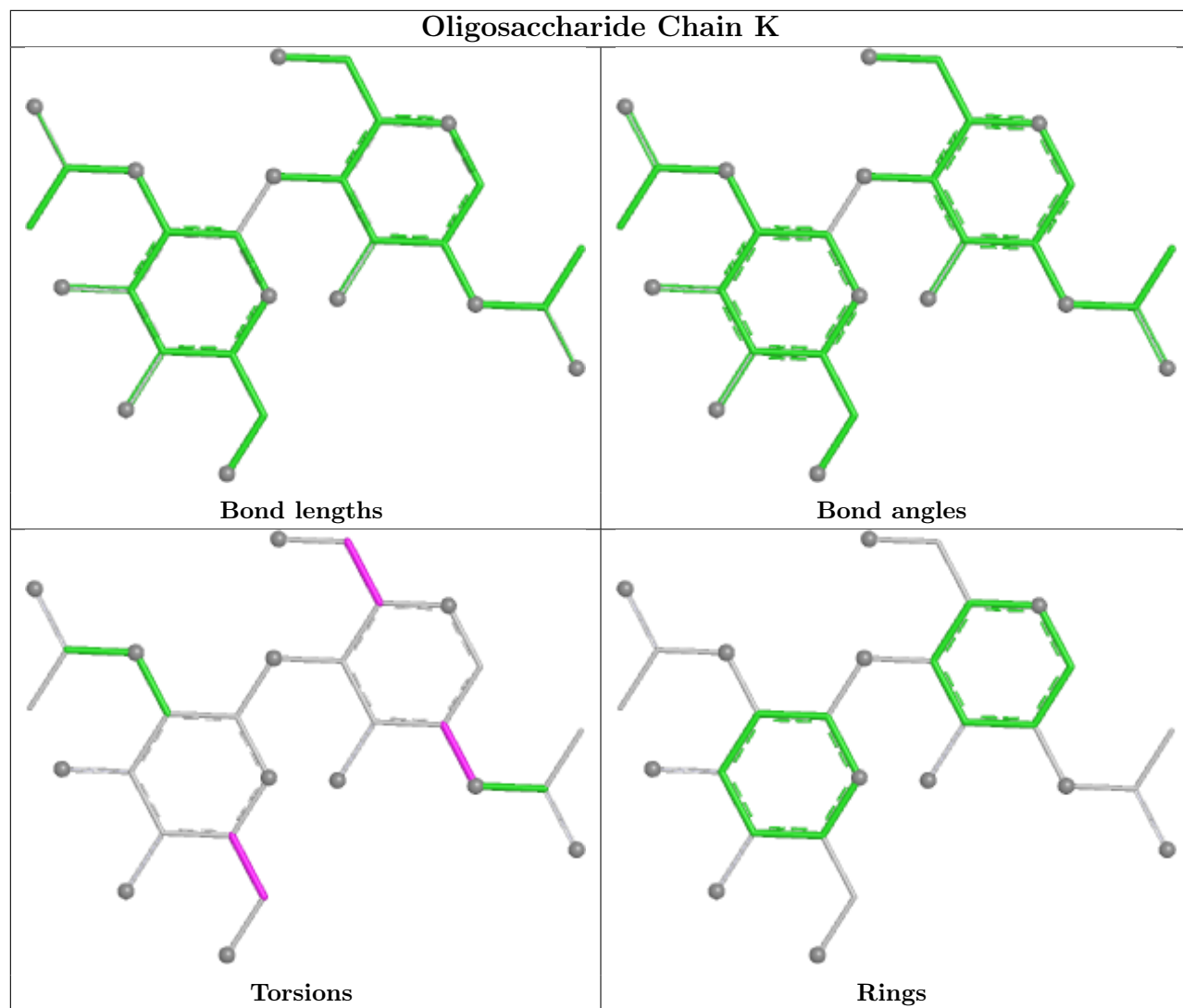
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

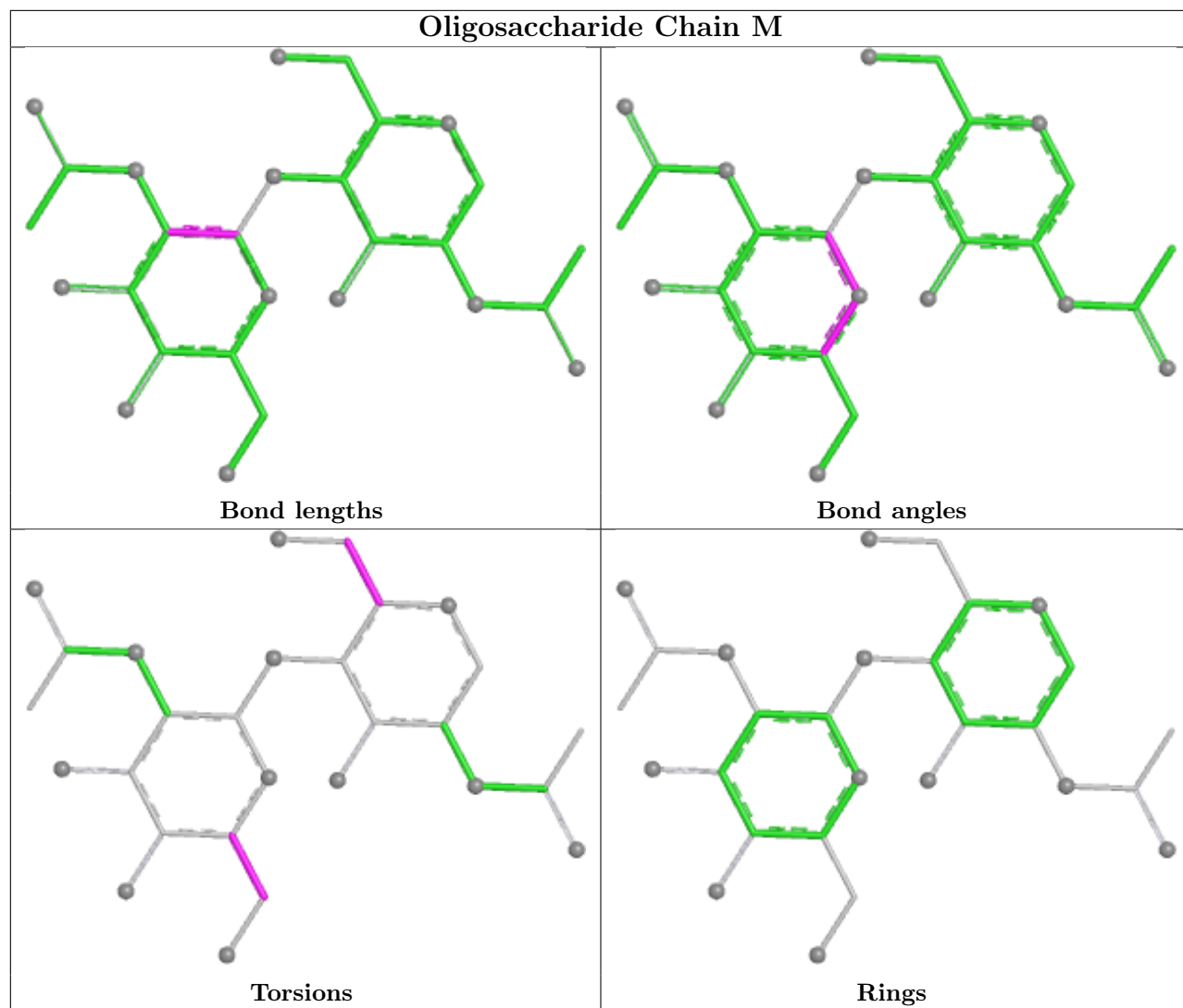




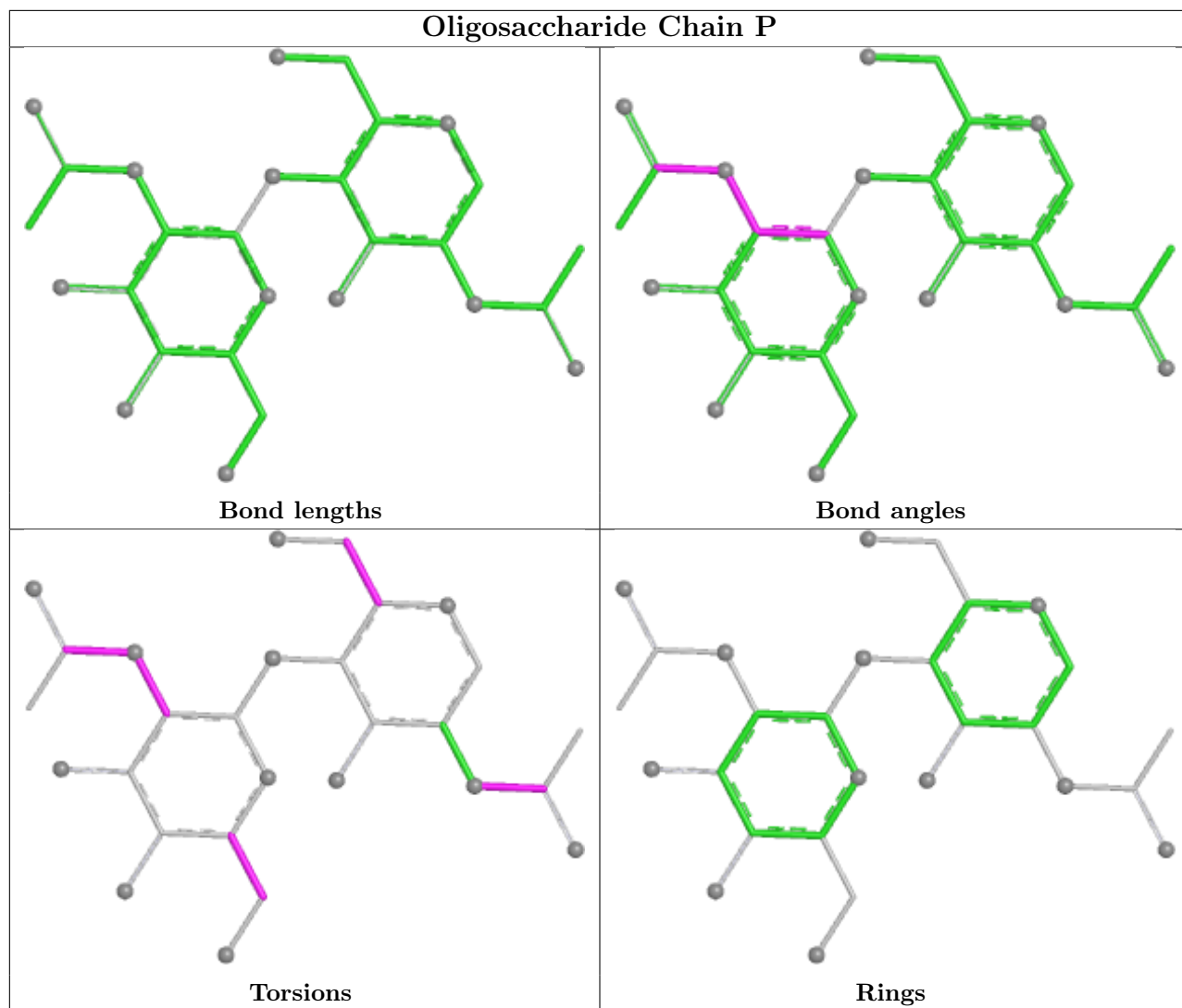


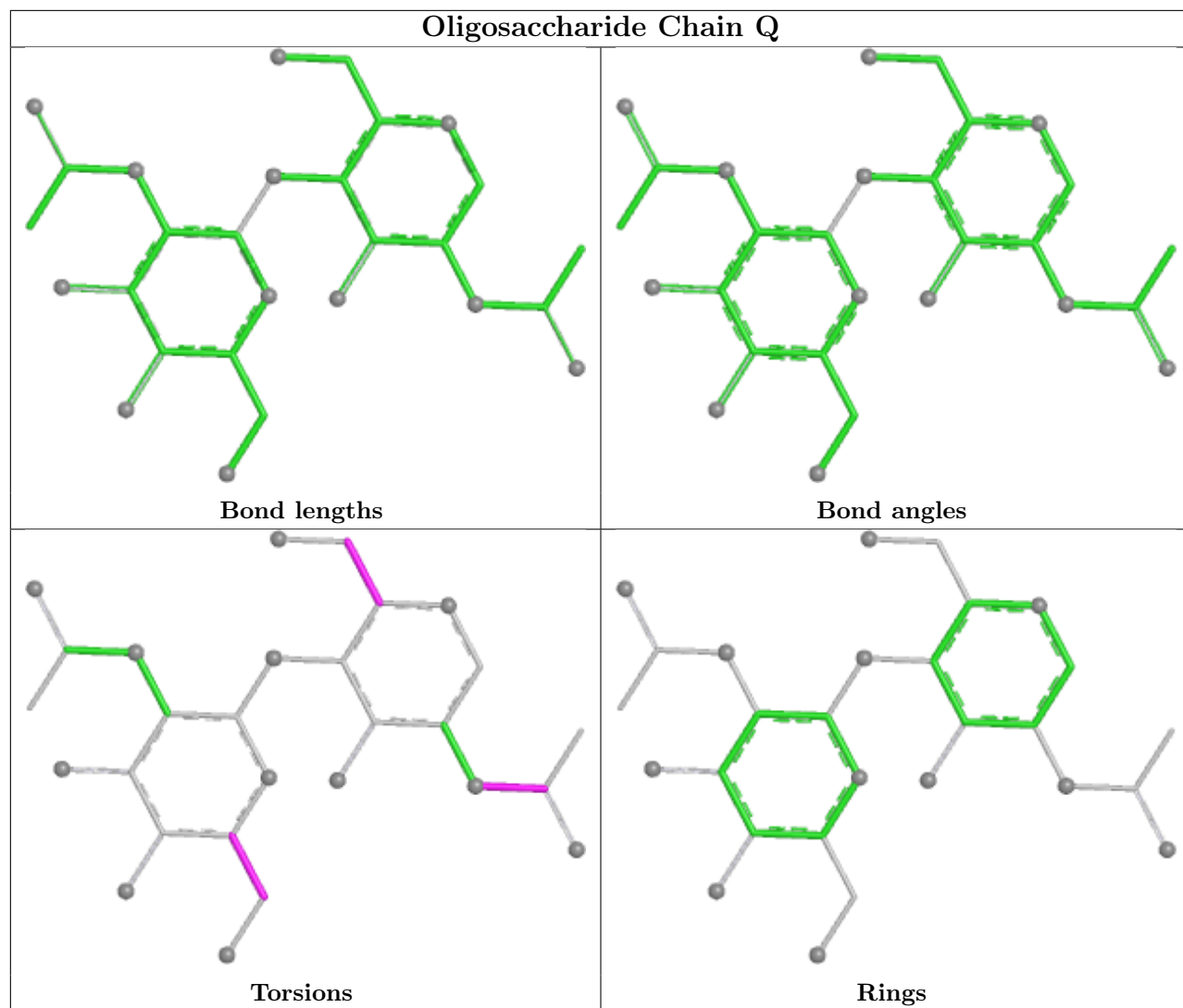


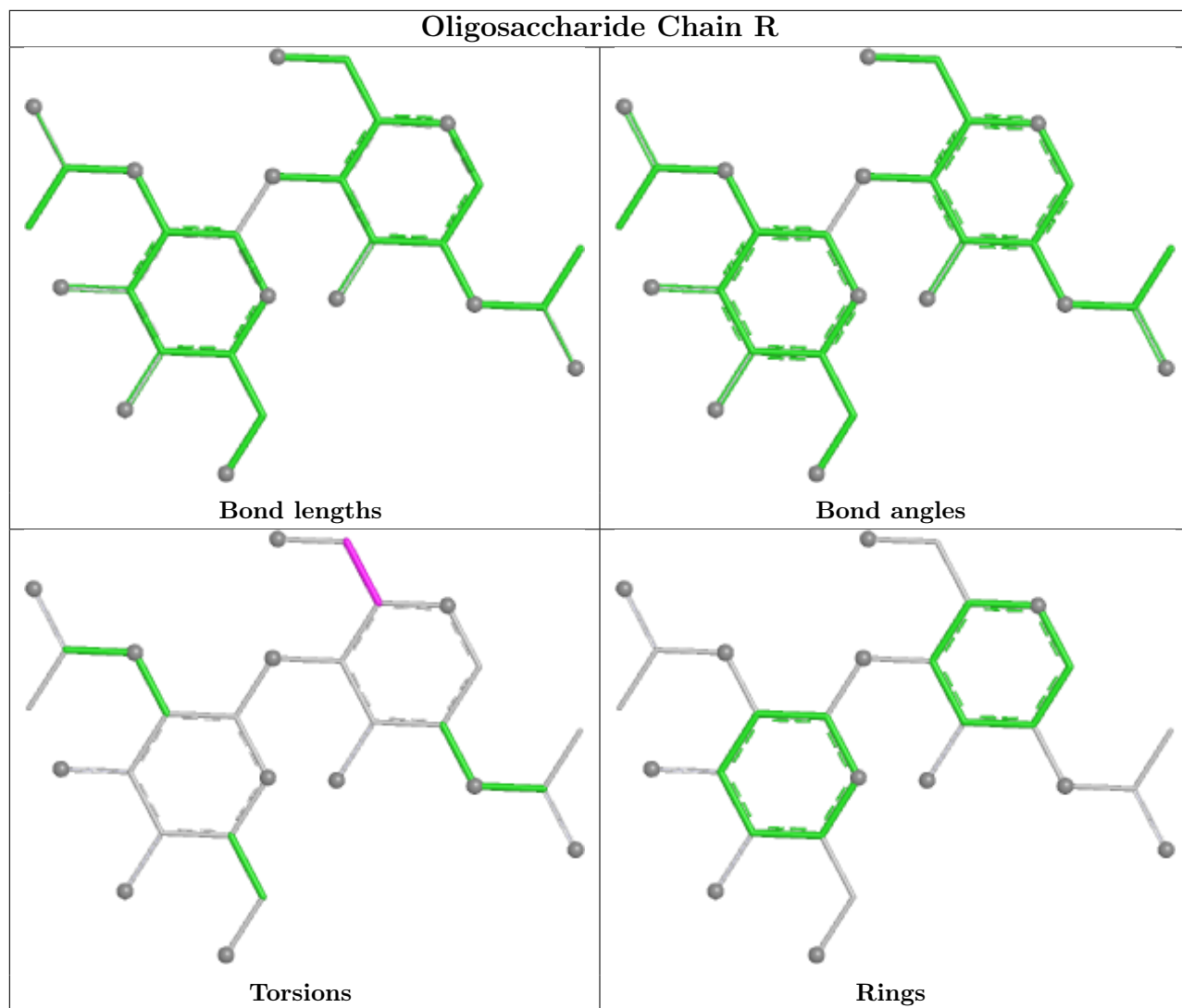


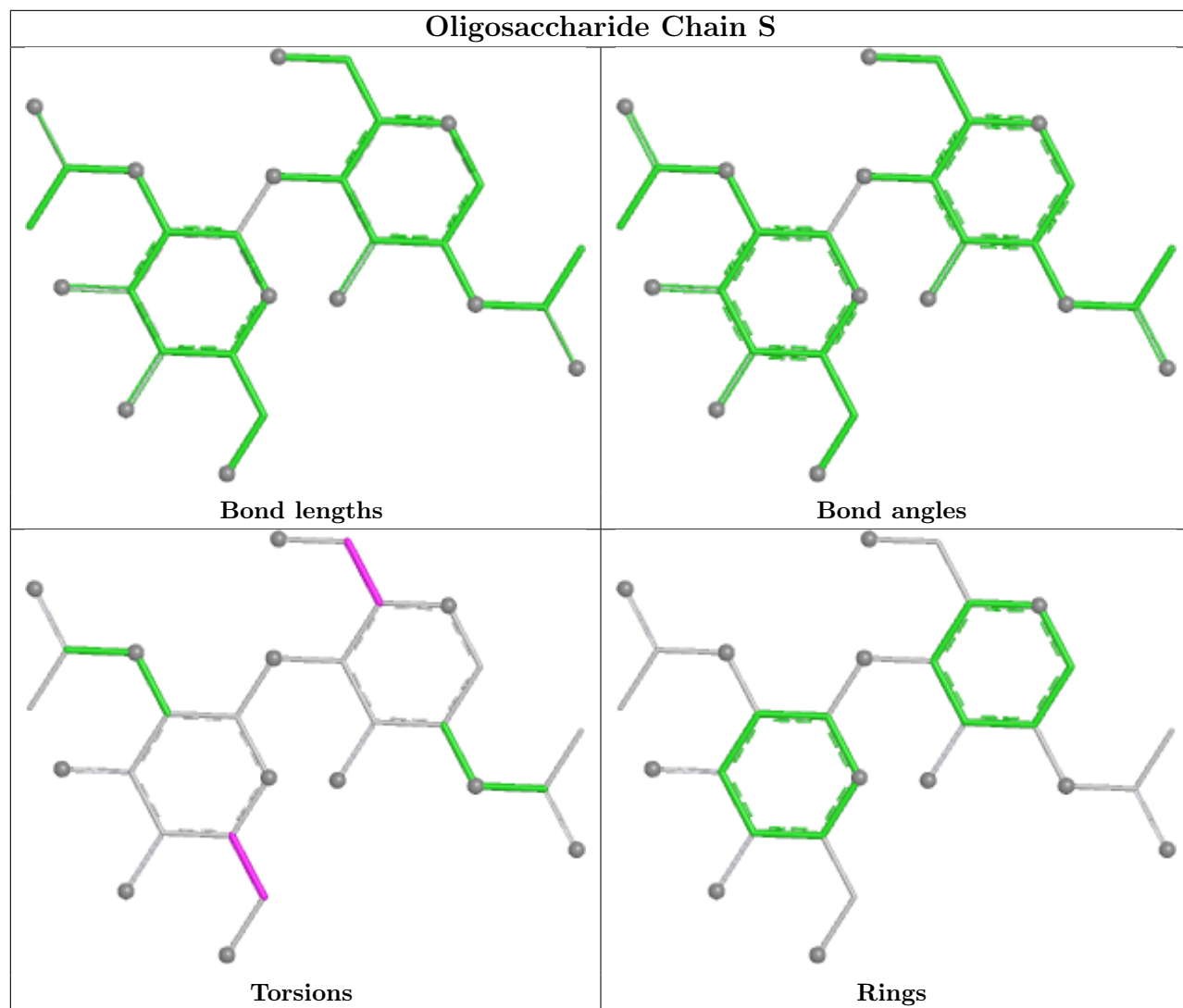


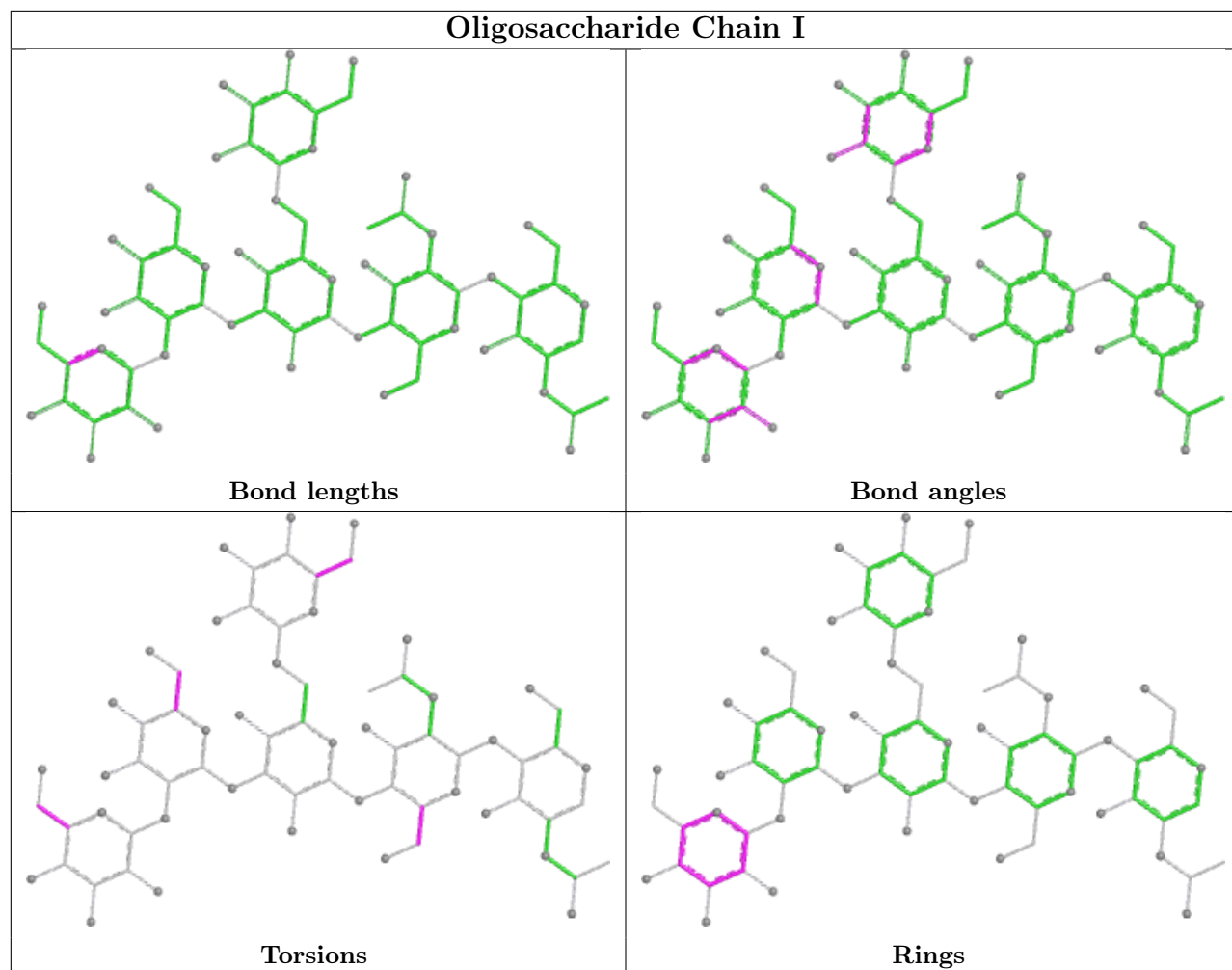


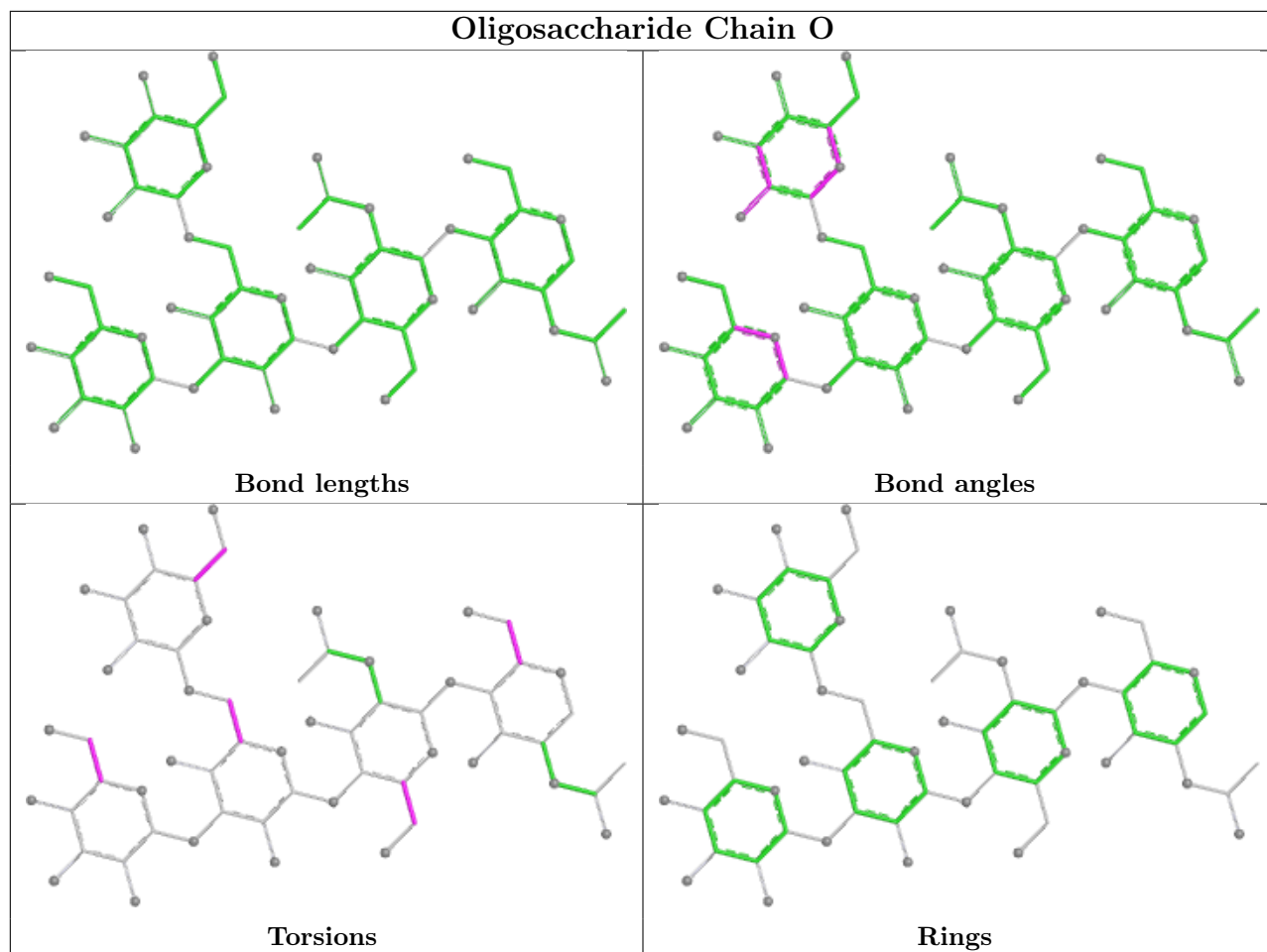


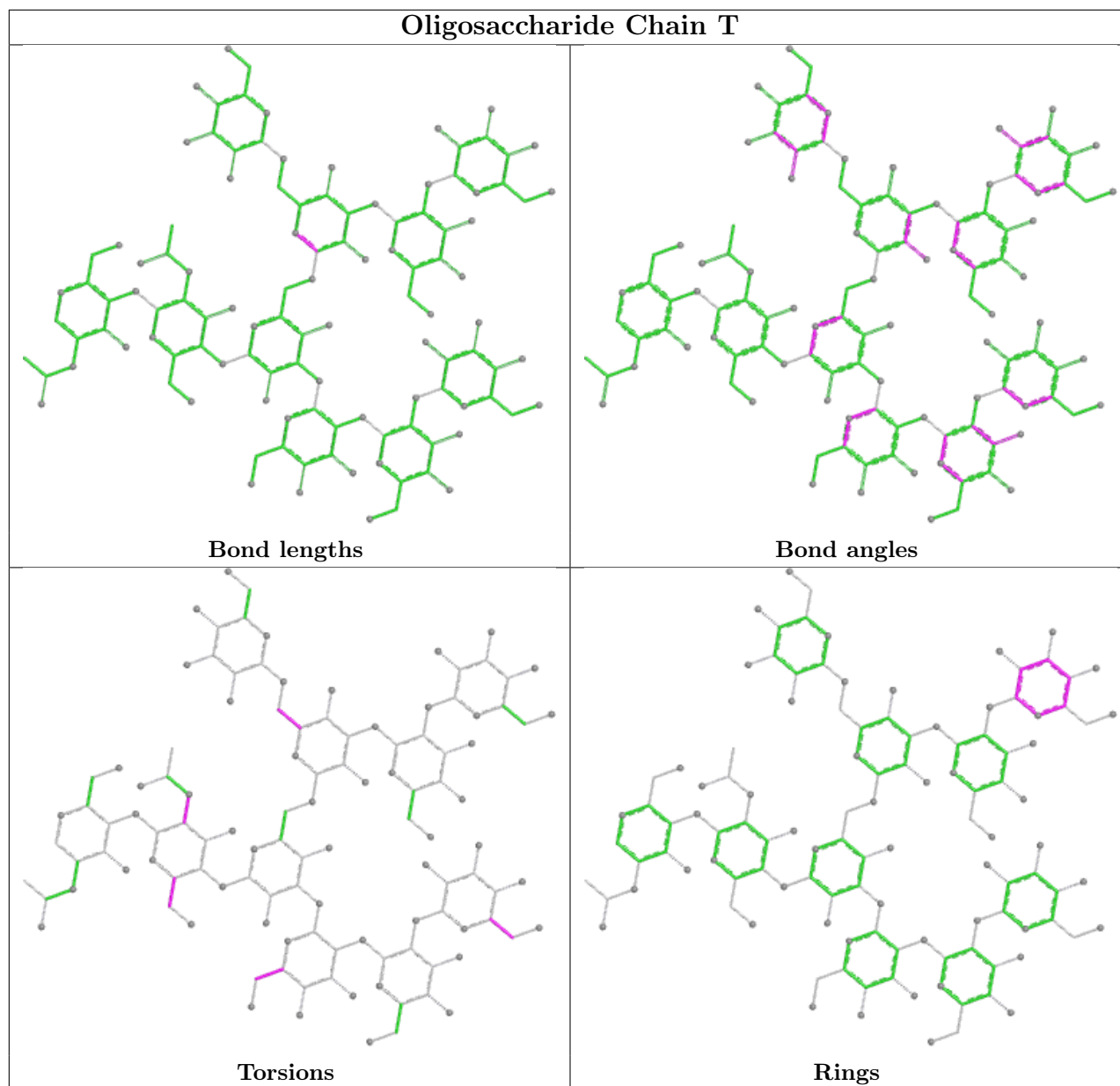












## 5.6 Ligand geometry [i](#)

7 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
13	NAG	B	703	2	14,14,15	0.45	0	17,19,21	0.42	0
13	NAG	G	624	1	14,14,15	0.21	0	17,19,21	0.53	0
13	NAG	B	701	2	14,14,15	0.33	0	17,19,21	0.60	0
13	NAG	B	702	2	14,14,15	0.34	0	17,19,21	0.38	0
13	NAG	G	622	1	14,14,15	0.62	1 (7%)	17,19,21	1.31	1 (5%)
13	NAG	G	633	1	14,14,15	0.46	0	17,19,21	0.66	1 (5%)
13	NAG	G	623	1	14,14,15	0.44	0	17,19,21	0.41	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
13	NAG	B	703	2	-	1/6/23/26	0/1/1/1
13	NAG	G	624	1	-	4/6/23/26	0/1/1/1
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
13	NAG	B	702	2	-	1/6/23/26	0/1/1/1
13	NAG	G	622	1	-	6/6/23/26	0/1/1/1
13	NAG	G	633	1	-	1/6/23/26	0/1/1/1
13	NAG	G	623	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	622	NAG	C1-C2	2.02	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	622	NAG	C2-N2-C7	4.54	128.98	122.90
13	G	633	NAG	C1-O5-C5	2.33	115.31	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	624	NAG	O5-C5-C6-O6
13	G	622	NAG	O5-C5-C6-O6
13	G	622	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	G	624	NAG	C4-C5-C6-O6
13	G	622	NAG	C8-C7-N2-C2
13	G	622	NAG	O7-C7-N2-C2
13	G	624	NAG	C8-C7-N2-C2
13	G	624	NAG	O7-C7-N2-C2
13	G	633	NAG	O5-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	G	622	NAG	C1-C2-N2-C7
13	B	703	NAG	O5-C5-C6-O6
13	G	622	NAG	C3-C2-N2-C7
13	G	623	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	703	NAG	1	0
13	B	702	NAG	2	0
13	G	622	NAG	1	0
13	G	633	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	439/481 (91%)	-1.18	0 100 100	23, 80, 145, 229	0
2	B	123/153 (80%)	-1.26	0 100 100	32, 69, 128, 181	0
3	L	208/213 (97%)	-1.02	0 100 100	52, 105, 158, 211	0
4	H	228/235 (97%)	-0.98	0 100 100	52, 124, 172, 217	0
5	D	242/243 (99%)	-1.00	0 100 100	64, 135, 240, 310	0
6	E	213/216 (98%)	-0.79	0 100 100	73, 152, 227, 271	0
All	All	1453/1541 (94%)	-1.05	0 100 100	23, 106, 210, 310	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	A	1	14/15	-	-	40,52,82,84	0
7	NAG	A	2	14/15	-	-	51,87,102,114	0
7	BMA	A	3	11/12	-	-	88,98,104,109	0
7	MAN	A	4	11/12	-	-	57,63,83,99	0
7	MAN	A	5	11/12	-	-	112,121,130,131	0
7	MAN	A	6	11/12	-	-	131,141,151,153	0

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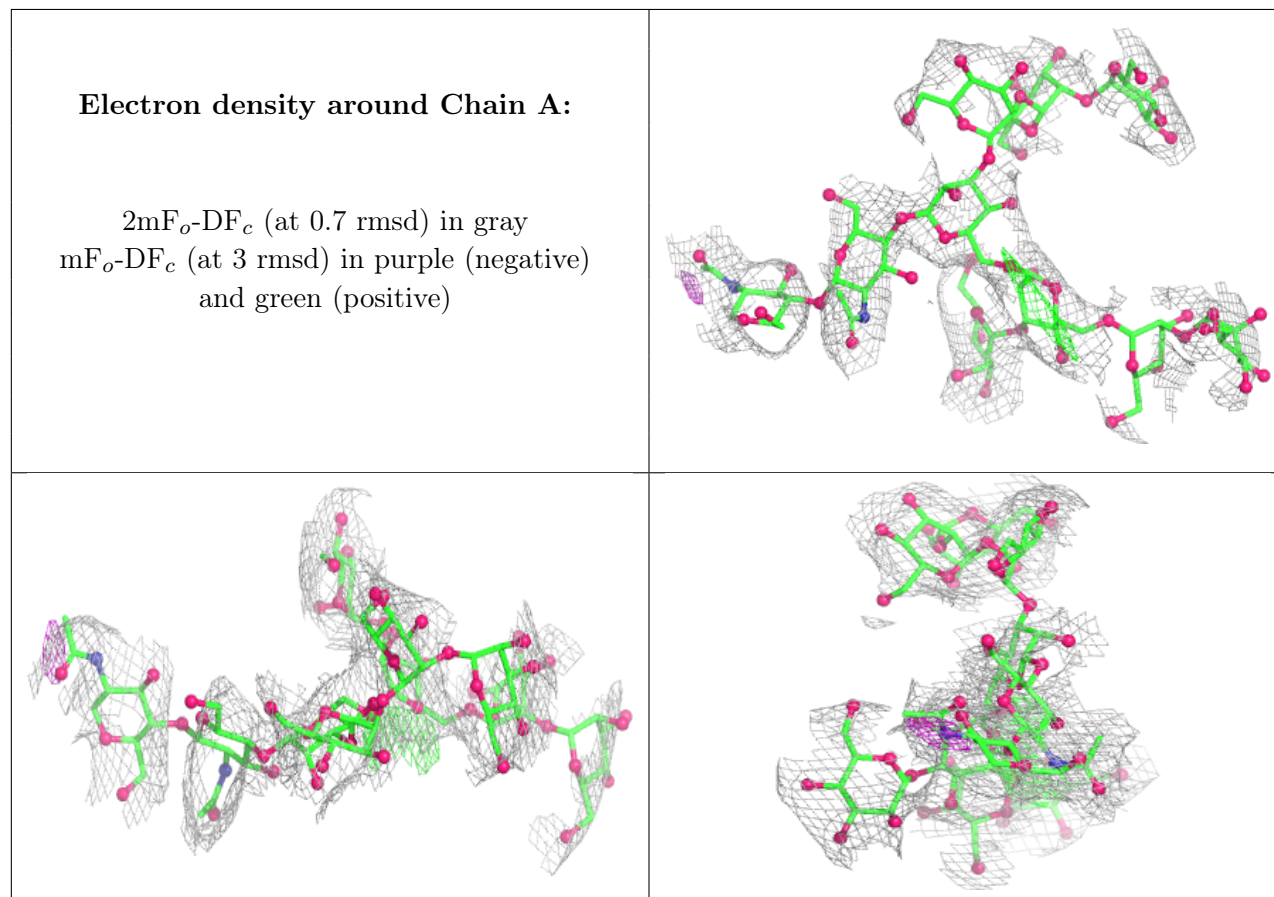
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MAN	A	7	11/12	-	-	87,94,101,101	0
7	MAN	A	8	11/12	-	-	64,87,104,106	0
7	MAN	A	9	11/12	-	-	114,128,136,141	0
7	MAN	A	10	11/12	-	-	78,96,105,105	0
8	NAG	C	1	14/15	-	-	77,115,139,154	0
8	NAG	C	2	14/15	-	-	134,150,157,160	0
8	BMA	C	3	11/12	-	-	134,145,159,163	0
9	NAG	F	1	14/15	-	-	78,91,119,126	0
9	NAG	F	2	14/15	-	-	133,141,148,148	0
9	NAG	P	2	14/15	0.96	0.04	131,143,147,149	0
11	MAN	O	4	11/12	0.96	0.04	129,134,138,139	0
9	NAG	K	2	14/15	0.97	0.04	73,86,91,91	0
9	NAG	S	2	14/15	0.97	0.04	102,127,140,147	0
9	NAG	M	2	14/15	0.97	0.05	182,188,193,194	0
12	MAN	T	7	11/12	0.97	0.06	109,119,130,135	0
12	MAN	T	8	11/12	0.97	0.05	136,148,156,159	0
12	MAN	T	9	11/12	0.97	0.05	149,160,162,163	0
9	NAG	N	1	14/15	0.98	0.04	95,113,133,145	0
10	NAG	I	1	14/15	0.98	0.07	35,46,74,81	0
10	NAG	I	2	14/15	0.98	0.06	64,81,99,108	0
9	NAG	N	2	14/15	0.98	0.05	141,151,158,159	0
11	MAN	O	5	11/12	0.98	0.03	119,125,131,137	0
12	MAN	T	6	11/12	0.98	0.04	71,84,97,106	0
9	NAG	P	1	14/15	0.98	0.05	77,94,120,139	0
9	NAG	M	1	14/15	0.98	0.06	135,151,173,185	0
9	NAG	R	2	14/15	0.98	0.03	111,132,138,138	0
11	NAG	O	2	14/15	0.99	0.03	100,112,116,116	0
10	BMA	I	3	11/12	-	-	85,101,124,129	0
10	MAN	I	4	11/12	-	-	137,146,157,161	0
10	MAN	I	5	11/12	-	-	120,129,138,142	0
10	MAN	I	6	11/12	-	-	127,133,142,147	0
11	BMA	O	3	11/12	0.99	0.02	112,115,119,124	0
9	NAG	K	1	14/15	0.99	0.03	54,82,104,107	0
9	NAG	S	1	14/15	0.99	0.04	69,90,104,106	0
12	NAG	T	1	14/15	0.99	0.03	51,64,85,88	0
12	NAG	T	2	14/15	0.99	0.03	63,81,85,87	0
12	BMA	T	3	11/12	0.99	0.03	72,82,94,100	0
12	MAN	T	5	11/12	0.99	0.04	52,70,81,84	0
9	NAG	Q	1	14/15	0.99	0.06	130,153,164,168	0
9	NAG	Q	2	14/15	0.99	0.04	164,173,193,196	0
9	NAG	R	1	14/15	0.99	0.03	66,84,105,119	0
11	NAG	O	1	14/15	0.99	0.05	47,65,79,90	0

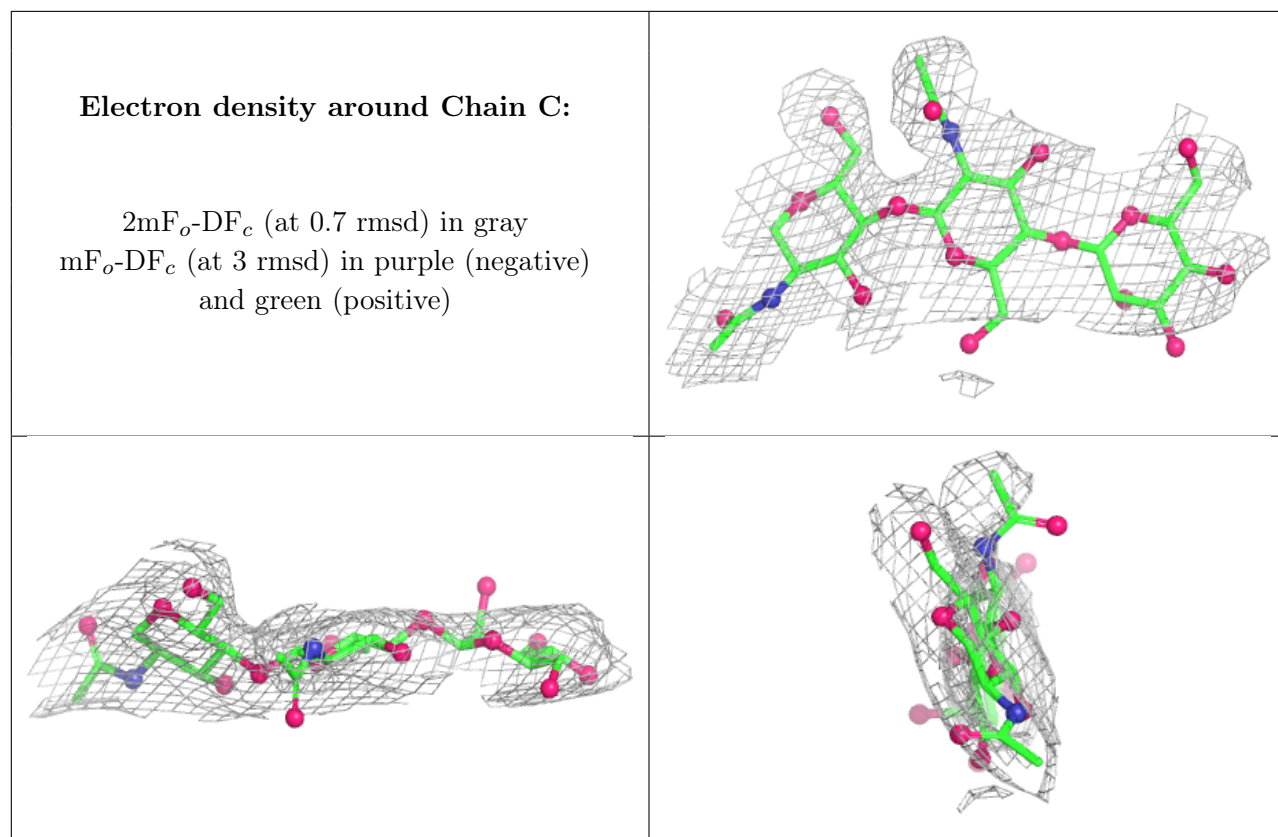
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	MAN	T	10	11/12	0.99	0.06	97,118,129,131	0
9	NAG	J	1	14/15	1.00	0.03	66,87,98,105	0
9	NAG	J	2	14/15	1.00	0.04	79,104,121,125	0
12	MAN	T	4	11/12	1.00	0.04	58,74,87,89	0

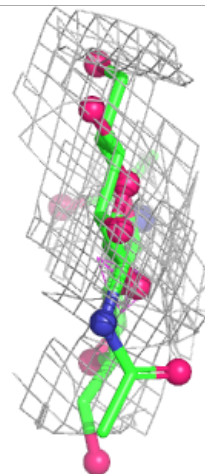
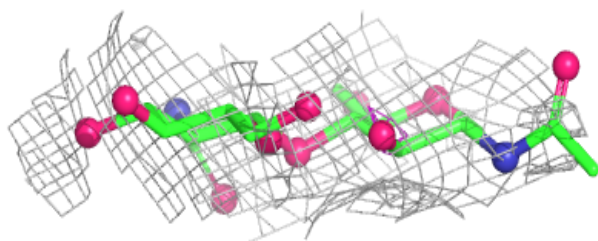
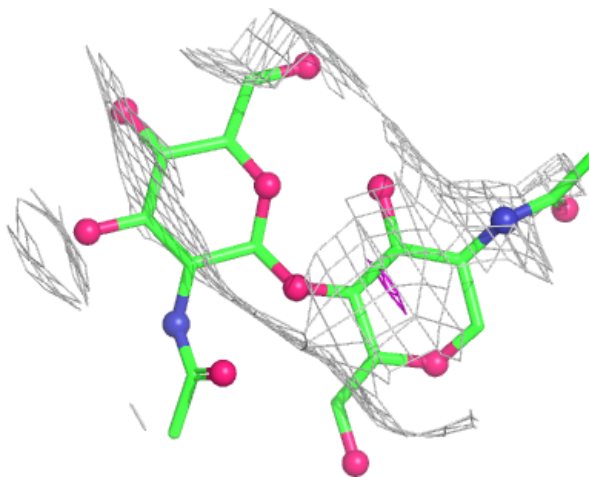
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





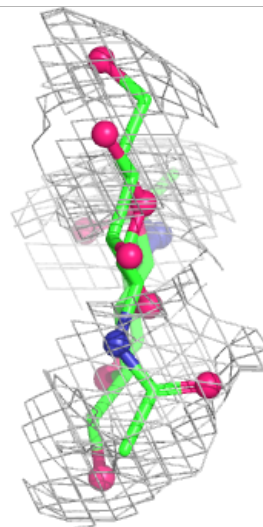
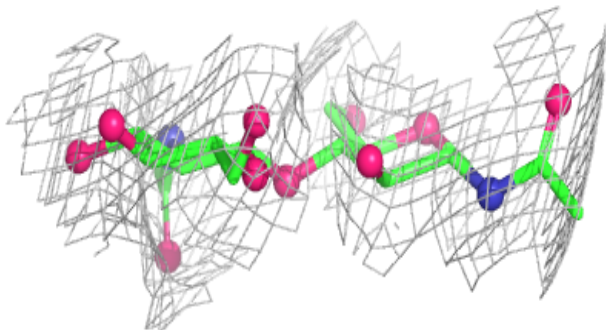
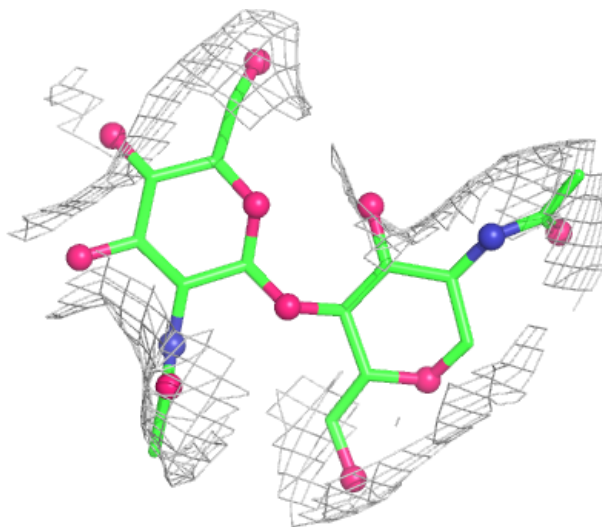
**Electron density around Chain F:**

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



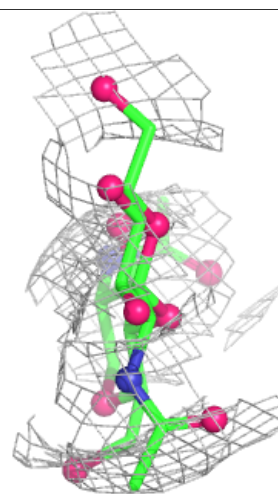
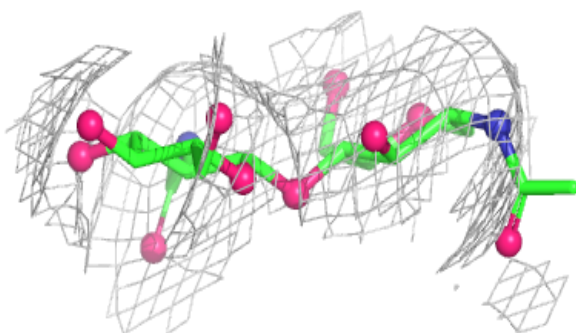
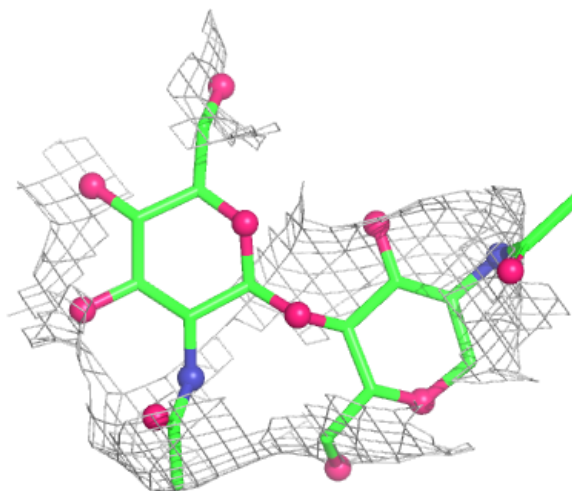
**Electron density around Chain J:**

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and green (positive)



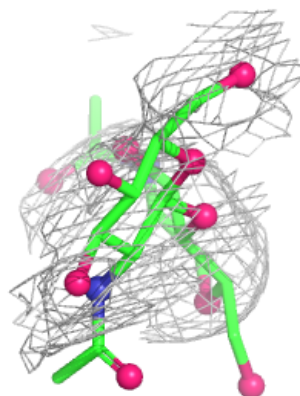
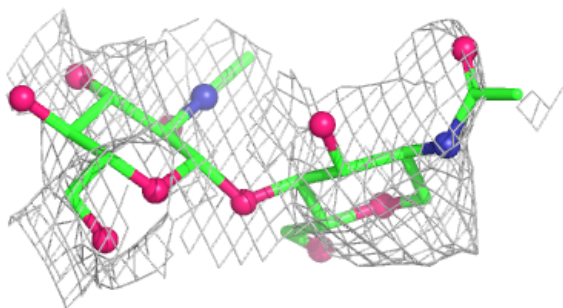
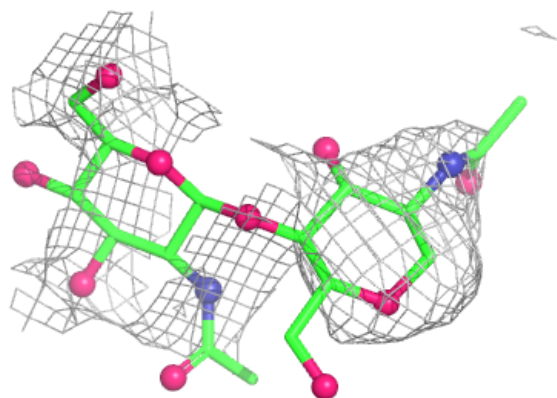
**Electron density around Chain K:**

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and green (positive)

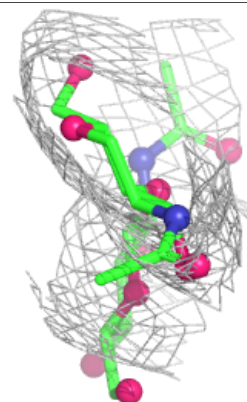
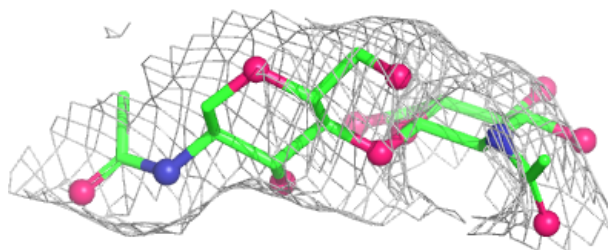
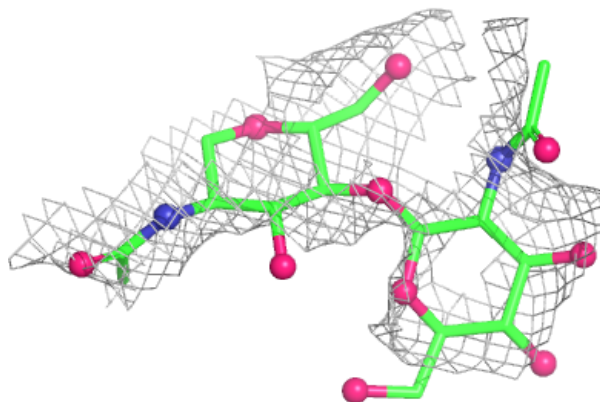


**Electron density around Chain M:**

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and green (positive)

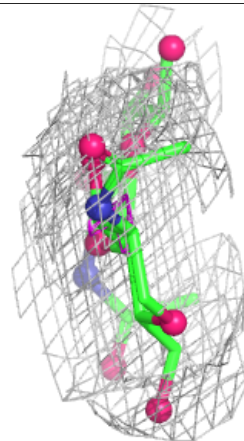
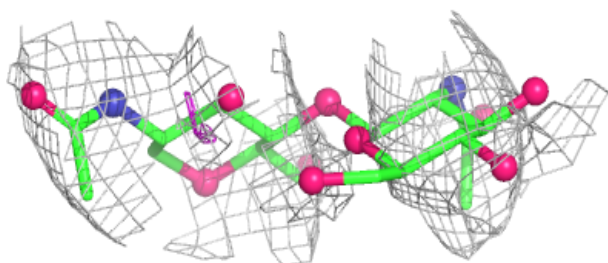
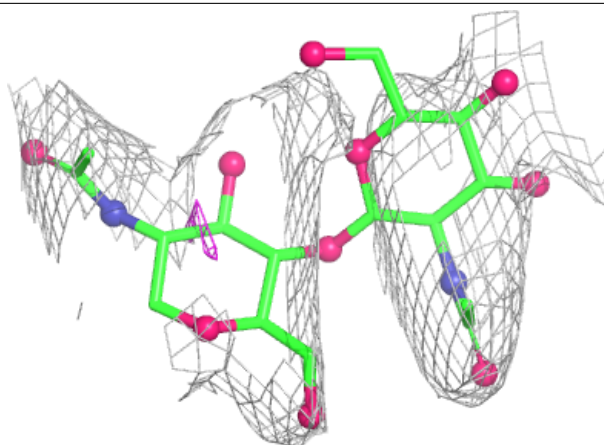
**Electron density around Chain N:**

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and green (positive)



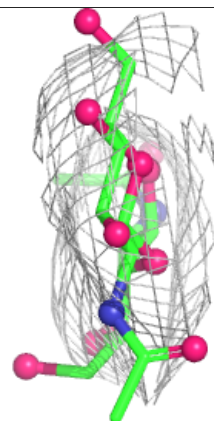
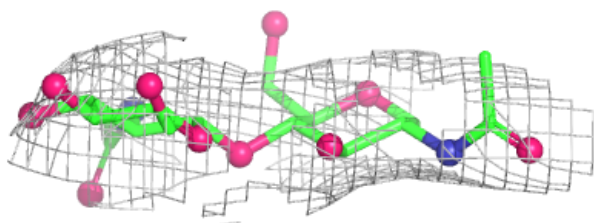
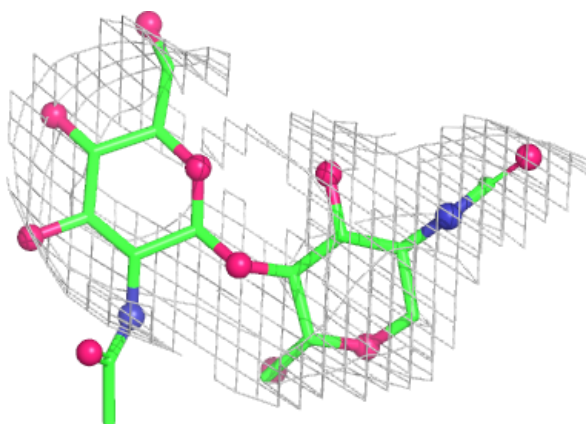
**Electron density around Chain P:**

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and green (positive)

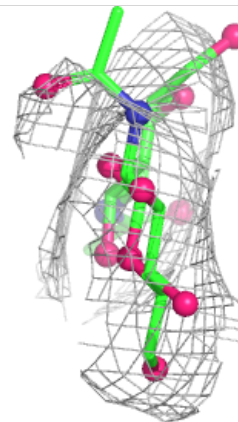
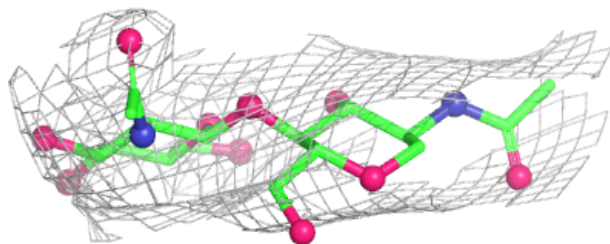
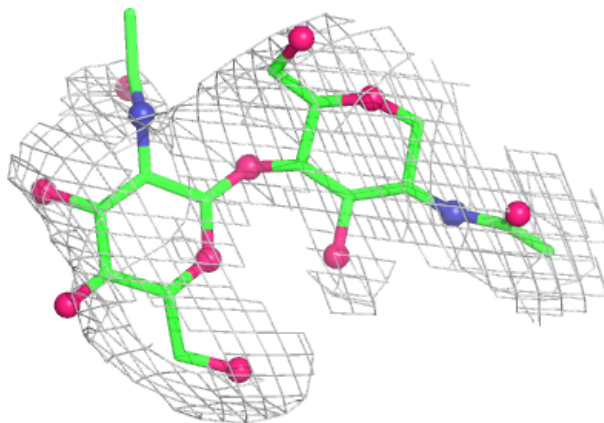


**Electron density around Chain Q:**

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

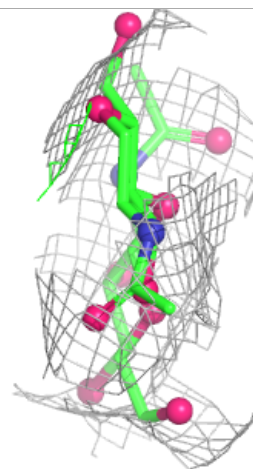
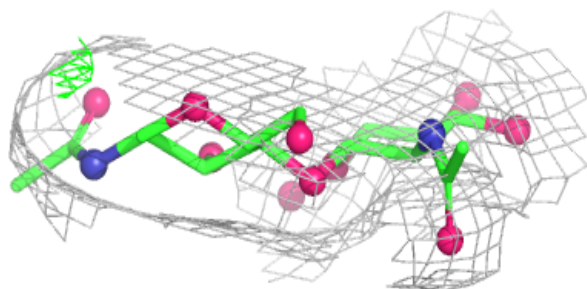
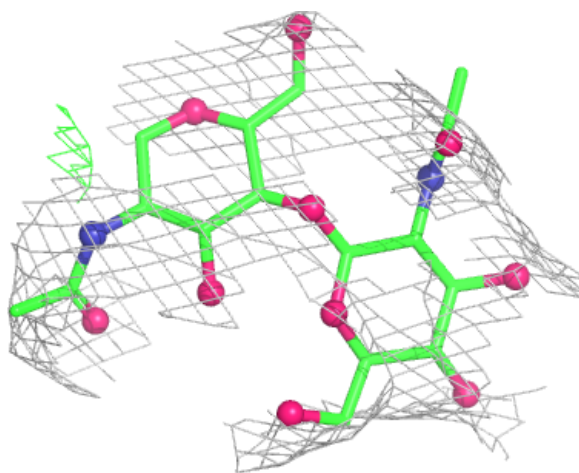
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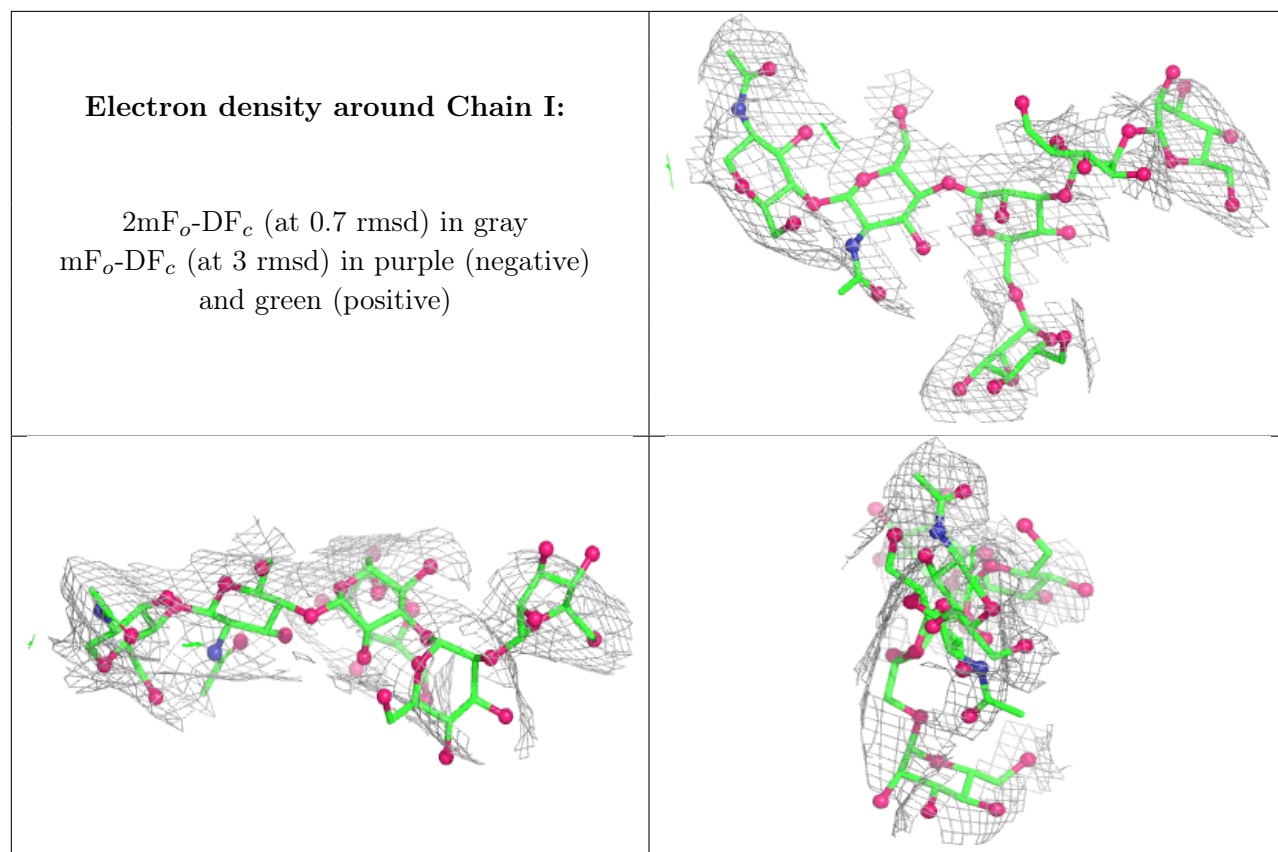
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and green (positive)



**Electron density around Chain S:**

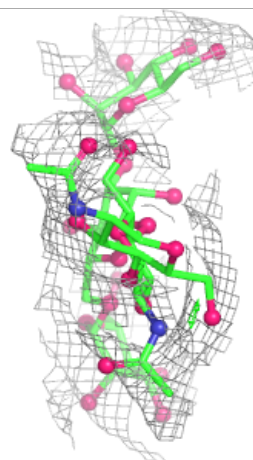
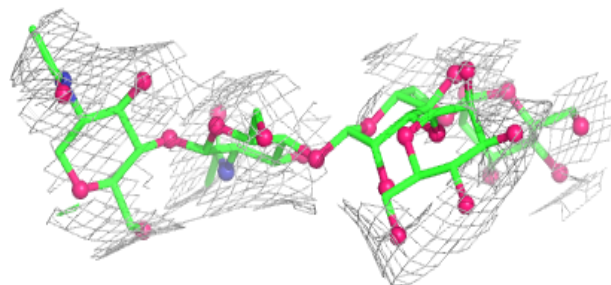
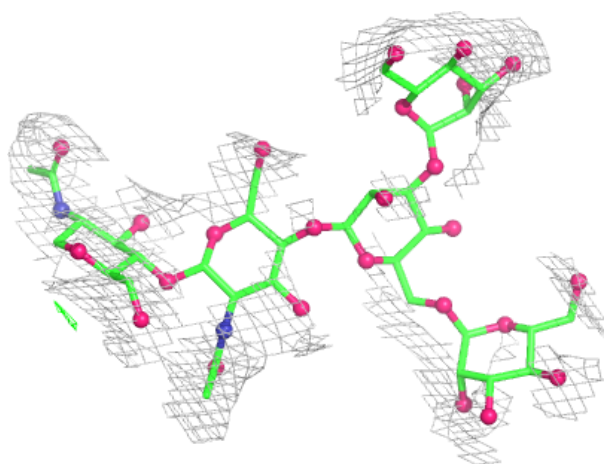
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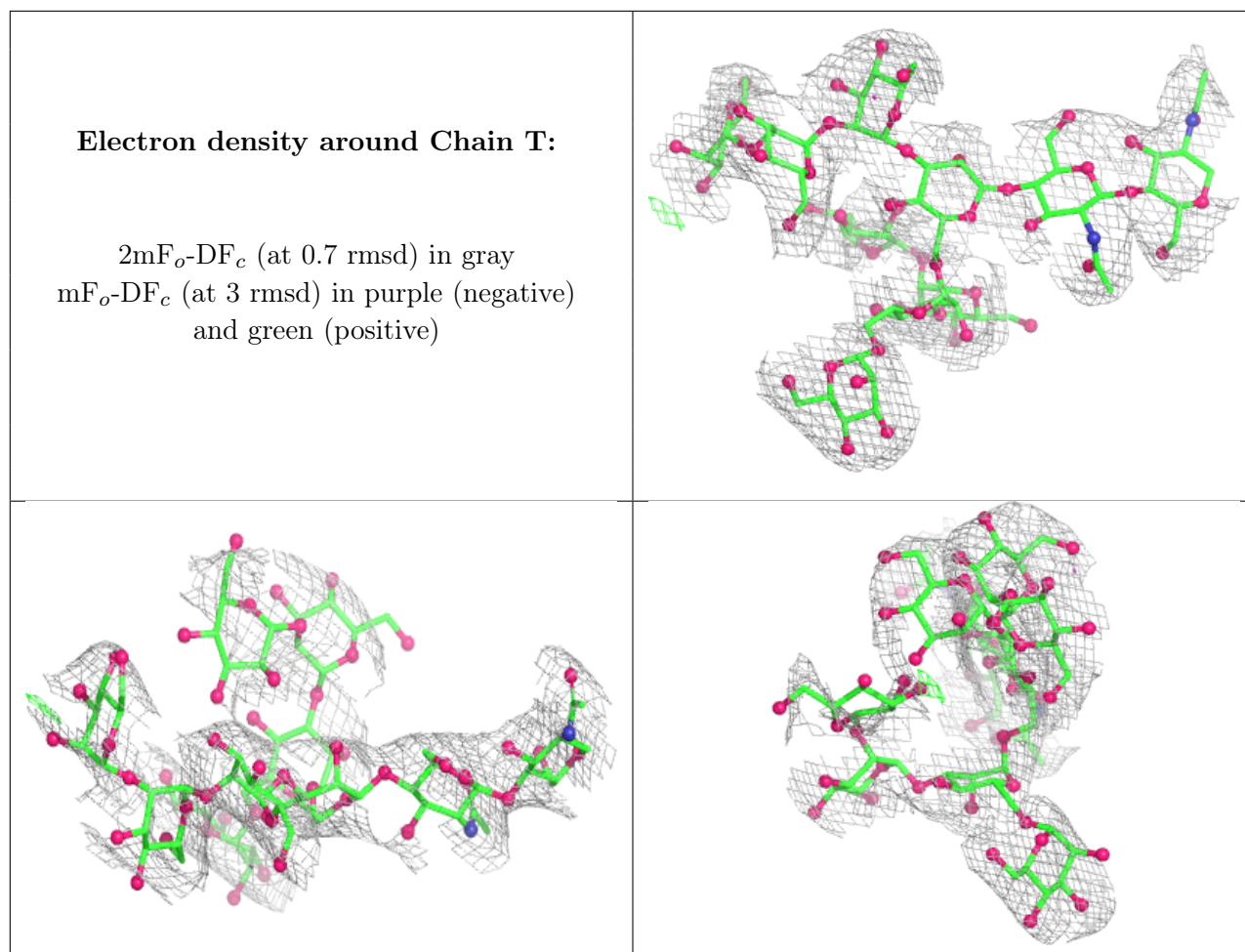




**Electron density around Chain O:**

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





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
13	NAG	G	622	14/15	0.96	0.05	94,99,101,102	0
13	NAG	G	633	14/15	0.96	0.07	120,140,153,155	0
13	NAG	B	702	14/15	0.96	0.07	120,125,132,132	0
13	NAG	G	623	14/15	0.97	0.05	79,108,130,137	0
13	NAG	G	624	14/15	0.97	0.05	147,163,168,171	0
13	NAG	B	701	14/15	0.98	0.06	127,140,159,161	0
13	NAG	B	703	14/15	0.98	0.04	94,102,111,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.