



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:52 AM UTC

PDB ID : 8IKW / pdb_00008ikw
Title : A complex structure of PGIP-PG
Authors : Xiao, Y.; Chai, J.
Deposited on : 2023-03-01
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

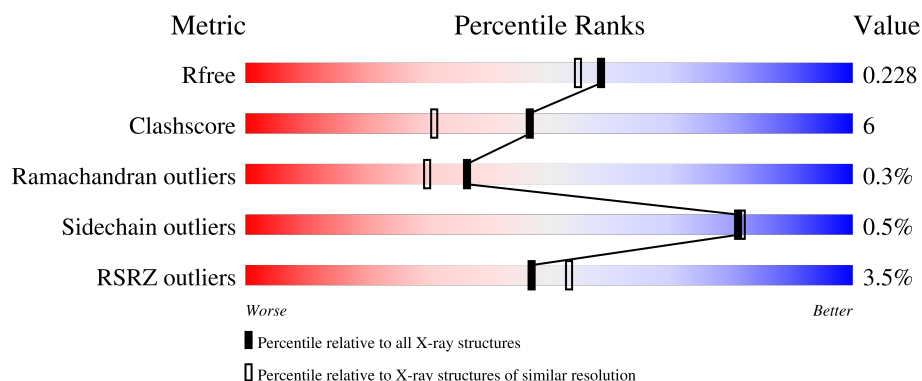
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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.



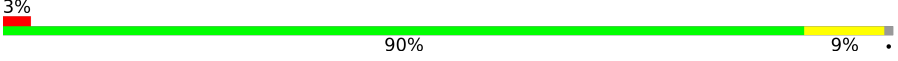
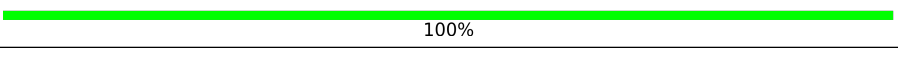
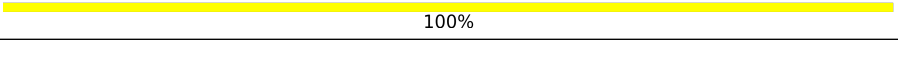
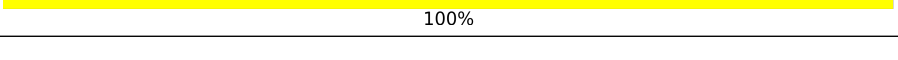
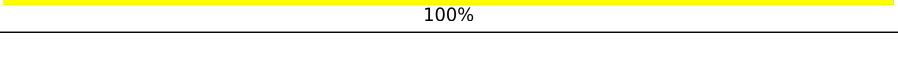
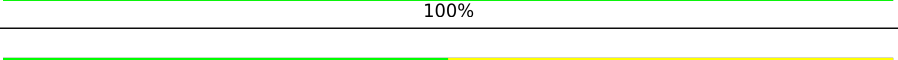
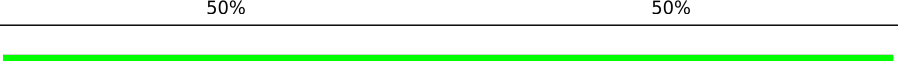
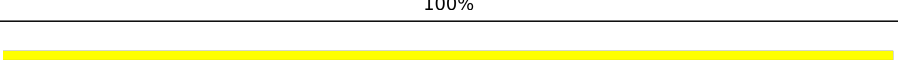
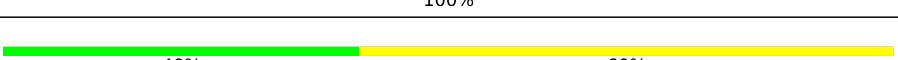
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	 3% 89% 11%
1	C	313	 3% 91% 9%
1	E	313	 4% 88% 12%
1	G	313	 4% 86% 14%
2	B	349	 2% 87% 12% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	349	
2	F	349	
2	H	349	
3	I	3	
4	J	4	
5	K	2	
5	L	2	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	S	2	
5	T	2	
6	Q	3	
7	R	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22453 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 Polygalacturonase inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	C	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	E	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			
1	G	313	Total	C	N	O	S	0	0	0
			2392	1524	405	453	10			

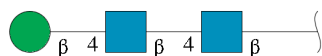
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ASP	ASN	engineered mutation	UNP P58822
C	274	ASP	ASN	engineered mutation	UNP P58822
E	274	ASP	ASN	engineered mutation	UNP P58822
G	274	ASP	ASN	engineered mutation	UNP P58822

- Molecule 2 is a protein called Endo-polygalacturonase.

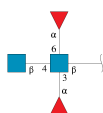
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	D	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	F	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			
2	H	346	Total	C	N	O	S	0	0	0
			2520	1543	436	530	11			

- Molecule 3 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
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			48	28	2	18			

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



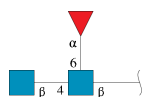
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

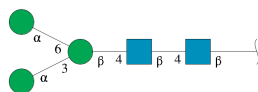
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Q	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	298	Total	O	0	0
			298	298		
8	B	338	Total	O	0	0
			338	338		
8	C	298	Total	O	0	0
			298	298		
8	E	305	Total	O	0	0
			305	305		
8	G	285	Total	O	0	0
			285	285		
8	D	278	Total	O	0	0
			278	278		

Continued on next page...

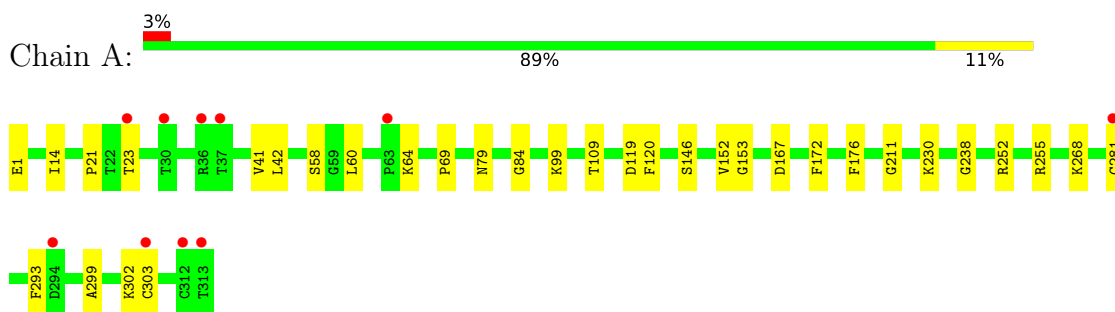
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	321	Total 321	O 321	0	0
8	H	272	Total 272	O 272	0	0

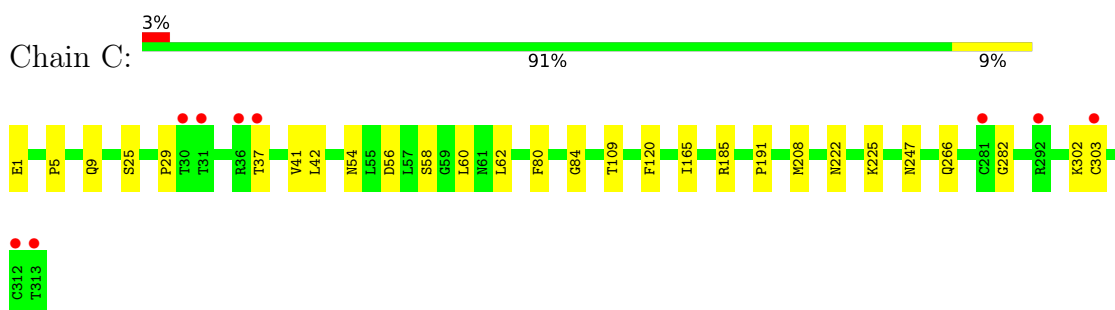
3 Residue-property plots [i](#)

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.

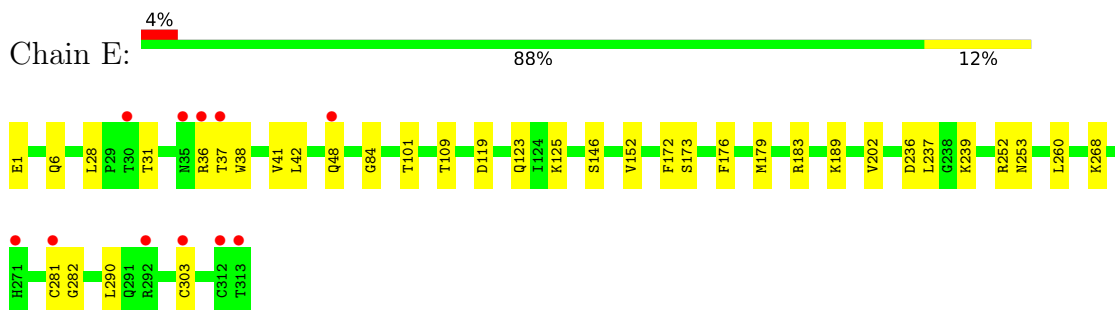
- Molecule 1: Polygalacturonase inhibitor 2



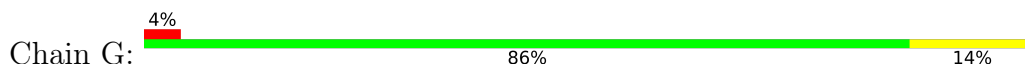
- Molecule 1: Polygalacturonase inhibitor 2

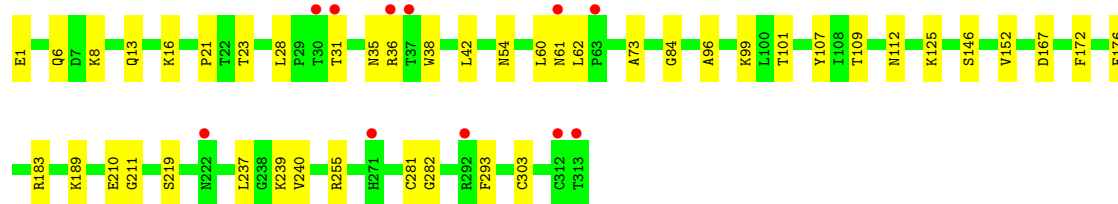


- Molecule 1: Polygalacturonase inhibitor 2

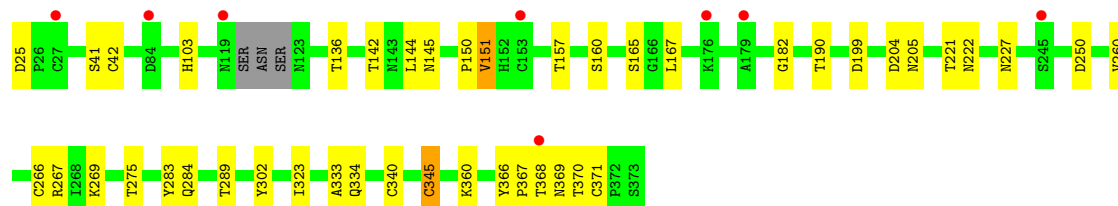
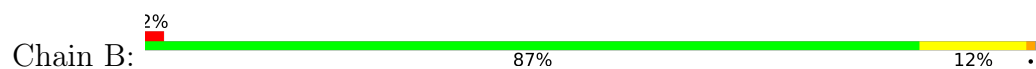


- Molecule 1: Polygalacturonase inhibitor 2

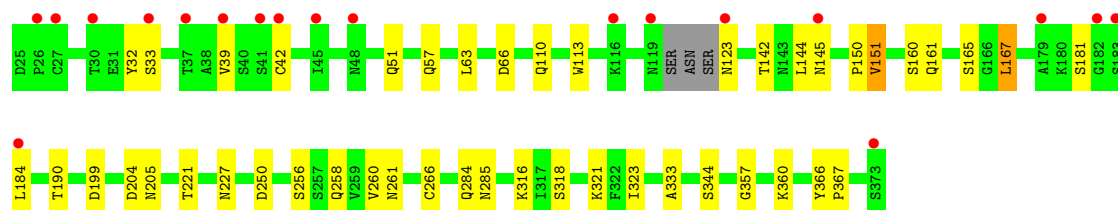
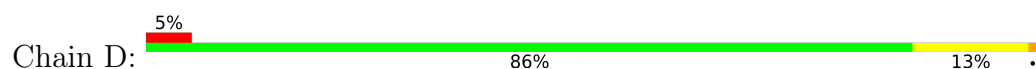




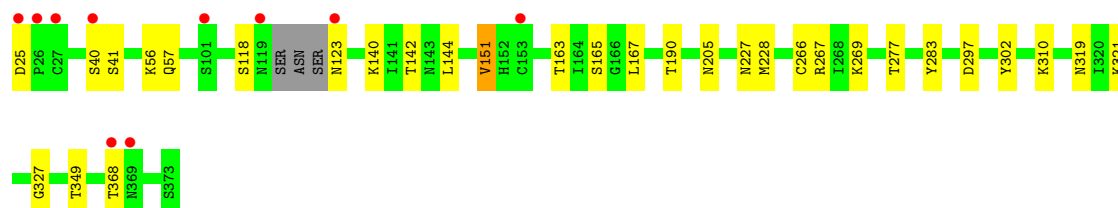
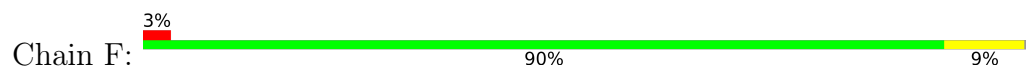
• Molecule 2: Endo-polygalacturonase



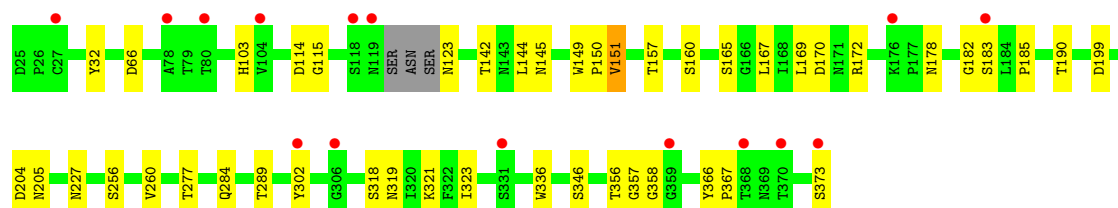
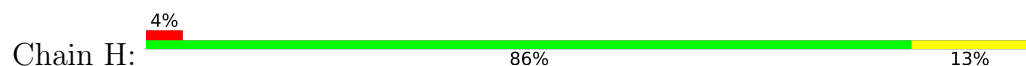
• Molecule 2: Endo-polygalacturonase



• Molecule 2: Endo-polygalacturonase



• Molecule 2: Endo-polygalacturonase



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

Chain I:  67% 33%

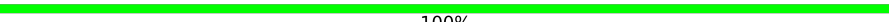
NAG1
NAG2
BMA3

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

Chain J:  75% 25%

NAG1
FUC2
NAG3
FUC4

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

Chain K:  100%

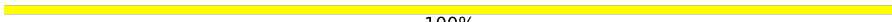
NAG1
NAG2

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

Chain L:  50% 50%

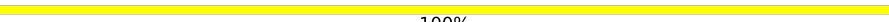
NAG1
NAG2

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

Chain M:  100%

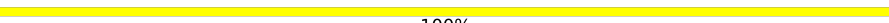
NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2
FUC3

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

Chain R:  40% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.73Å 105.22Å 113.82Å 63.93° 89.12° 86.27°	Depositor
Resolution (Å)	34.29 – 1.94 34.29 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.4 (34.29-1.94) 95.3 (34.29-1.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.94Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.192 , 0.233 0.192 , 0.228	Depositor DCC
R_{free} test set	10111 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22453	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8638e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	A	0.70	0/2444	0.73	4/3333 (0.1%)
1	C	0.58	0/2444	0.72	4/3333 (0.1%)
1	E	0.57	0/2444	0.73	3/3333 (0.1%)
1	G	0.67	0/2444	0.73	3/3333 (0.1%)
2	B	0.65	1/2562 (0.0%)	0.73	2/3487 (0.1%)
2	D	0.68	2/2562 (0.1%)	0.76	7/3487 (0.2%)
2	F	0.52	1/2562 (0.0%)	0.67	1/3487 (0.0%)
2	H	0.52	0/2562	0.68	3/3487 (0.1%)
All	All	0.61	4/20024 (0.0%)	0.72	27/27280 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	33	SER	C-O	-5.33	1.17	1.24
2	F	40	SER	C-O	-5.26	1.17	1.24
2	D	32	TYR	C-O	-5.20	1.17	1.24
2	B	345	CYS	C-O	-5.20	1.17	1.24

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	333	ALA	N-CA-C	8.27	122.58	110.59
2	D	333	ALA	N-CA-C	8.23	121.15	110.53
1	A	211	GLY	N-CA-C	8.08	126.27	112.22
2	D	184	LEU	N-CA-C	7.53	120.47	110.08
2	H	358	GLY	N-CA-C	7.35	121.33	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2412	23	0
1	C	2392	0	2412	18	0
1	E	2392	0	2410	37	0
1	G	2392	0	2412	40	0
2	B	2520	0	2400	29	0
2	D	2520	0	2398	27	0
2	F	2520	0	2398	20	0
2	H	2520	0	2398	33	0
3	I	39	0	34	0	0
4	J	48	0	43	1	0
5	K	28	0	25	0	0
5	L	28	0	25	2	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	S	28	0	25	1	0
5	T	28	0	25	0	0
6	Q	38	0	34	1	0
7	R	61	0	52	0	0
8	A	298	0	0	9	0
8	B	338	0	0	7	0
8	C	298	0	0	11	2
8	D	278	0	0	9	1
8	E	305	0	0	19	1
8	F	321	0	0	6	0
8	G	285	0	0	21	1
8	H	272	0	0	13	1
All	All	22453	0	19603	225	3

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.

The worst 5 of 225 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:THR:HG23	1:E:38:TRP:HE1	1.06	1.18
1:A:281:CYS:SG	8:A:666:HOH:O	2.14	1.04
1:E:36:ARG:NH1	8:E:401:HOH:O	1.93	1.02
2:B:371:CYS:SG	8:B:568:HOH:O	2.20	0.98
1:G:61:ASN:O	8:G:401:HOH:O	1.84	0.95

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:673:HOH:O	8:G:649:HOH:O[1_645]	1.97	0.23
8:D:525:HOH:O	8:H:452:HOH:O[1_655]	2.08	0.12
8:C:656:HOH:O	8:E:693:HOH:O[1_554]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
1	C	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
1	E	311/313 (99%)	294 (94%)	17 (6%)	0	100	100
1	G	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
2	B	342/349 (98%)	328 (96%)	12 (4%)	2 (1%)	21	11
2	D	342/349 (98%)	328 (96%)	12 (4%)	2 (1%)	21	11
2	F	342/349 (98%)	329 (96%)	12 (4%)	1 (0%)	36	30
2	H	342/349 (98%)	329 (96%)	11 (3%)	2 (1%)	21	11
All	All	2612/2648 (99%)	2487 (95%)	118 (4%)	7 (0%)	36	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	151	VAL
2	D	151	VAL
2	F	151	VAL
2	H	151	VAL
2	H	150	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	273 (100%)	1 (0%)	84	84
1	C	274/274 (100%)	271 (99%)	3 (1%)	65	60
1	E	274/274 (100%)	272 (99%)	2 (1%)	76	74
1	G	274/274 (100%)	274 (100%)	0	100	100
2	B	289/292 (99%)	289 (100%)	0	100	100
2	D	289/292 (99%)	286 (99%)	3 (1%)	68	64
2	F	289/292 (99%)	287 (99%)	2 (1%)	76	74
2	H	289/292 (99%)	288 (100%)	1 (0%)	86	86
All	All	2252/2264 (100%)	2240 (100%)	12 (0%)	81	82

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	258	GLN
2	D	260	VAL
2	H	356	THR
2	F	41	SER
1	C	303	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	51	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	279	ASN
2	F	128	HIS
2	H	86	ASN
1	C	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

31 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	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.63	0	17,19,21	0.81	0
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	0.77	0
3	BMA	I	3	3	11,11,12	0.86	0	15,15,17	1.09	1 (6%)
4	NAG	J	1	2,4	14,14,15	1.77	1 (7%)	17,19,21	1.53	4 (23%)
4	FUC	J	2	4	10,10,11	1.11	1 (10%)	14,14,16	1.02	0
4	NAG	J	3	4	14,14,15	0.44	0	17,19,21	0.42	0
4	FUC	J	4	4	10,10,11	1.65	1 (10%)	14,14,16	1.14	2 (14%)
5	NAG	K	1	2,5	14,14,15	0.58	0	17,19,21	0.73	0
5	NAG	K	2	5	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	L	1	1,5	14,14,15	0.39	0	17,19,21	0.73	0
5	NAG	L	2	5	14,14,15	0.60	0	17,19,21	0.62	0
5	NAG	M	1	1,5	14,14,15	0.48	0	17,19,21	0.90	2 (11%)
5	NAG	M	2	5	14,14,15	0.29	0	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	N	1	1,5	14,14,15	0.53	0	17,19,21	0.91	2 (11%)
5	NAG	N	2	5	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
5	NAG	O	1	2,5	14,14,15	0.56	0	17,19,21	0.79	1 (5%)
5	NAG	O	2	5	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
5	NAG	P	1	2,5	14,14,15	0.62	0	17,19,21	0.79	0
5	NAG	P	2	5	14,14,15	0.40	0	17,19,21	0.58	0
6	NAG	Q	1	2,6	14,14,15	0.63	1 (7%)	17,19,21	1.20	2 (11%)
6	NAG	Q	2	6	14,14,15	0.55	0	17,19,21	0.56	0
6	FUC	Q	3	6	10,10,11	0.98	1 (10%)	14,14,16	0.62	0
7	NAG	R	1	2,7	14,14,15	0.47	0	17,19,21	0.61	0
7	NAG	R	2	7	14,14,15	0.33	0	17,19,21	0.60	0
7	BMA	R	3	7	11,11,12	0.86	0	15,15,17	1.11	2 (13%)
7	MAN	R	4	7	11,11,12	1.01	1 (9%)	15,15,17	1.05	1 (6%)
7	MAN	R	5	7	11,11,12	1.17	1 (9%)	15,15,17	1.37	2 (13%)
5	NAG	S	1	2,5	14,14,15	0.49	0	17,19,21	0.61	0
5	NAG	S	2	5	14,14,15	0.40	0	17,19,21	0.48	0
5	NAG	T	1	2,5	14,14,15	0.28	0	17,19,21	0.82	0
5	NAG	T	2	5	14,14,15	0.40	0	17,19,21	0.39	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
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
4	NAG	J	3	4	-	1/6/23/26	0/1/1/1
4	FUC	J	4	4	-	-	0/1/1/1
5	NAG	K	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	-6.40	1.32	1.43
4	J	4	FUC	C1-C2	3.90	1.61	1.52
4	J	2	FUC	C2-C3	2.82	1.56	1.52
7	R	5	MAN	C1-C2	2.19	1.57	1.52
6	Q	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	5	MAN	C1-O5-C5	4.12	117.71	112.19
4	J	1	NAG	C1-O5-C5	3.57	116.96	112.19
7	R	3	BMA	C1-O5-C5	3.29	116.60	112.19
3	I	3	BMA	C1-O5-C5	3.24	116.53	112.19
4	J	1	NAG	O5-C5-C6	-3.23	101.39	107.66

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

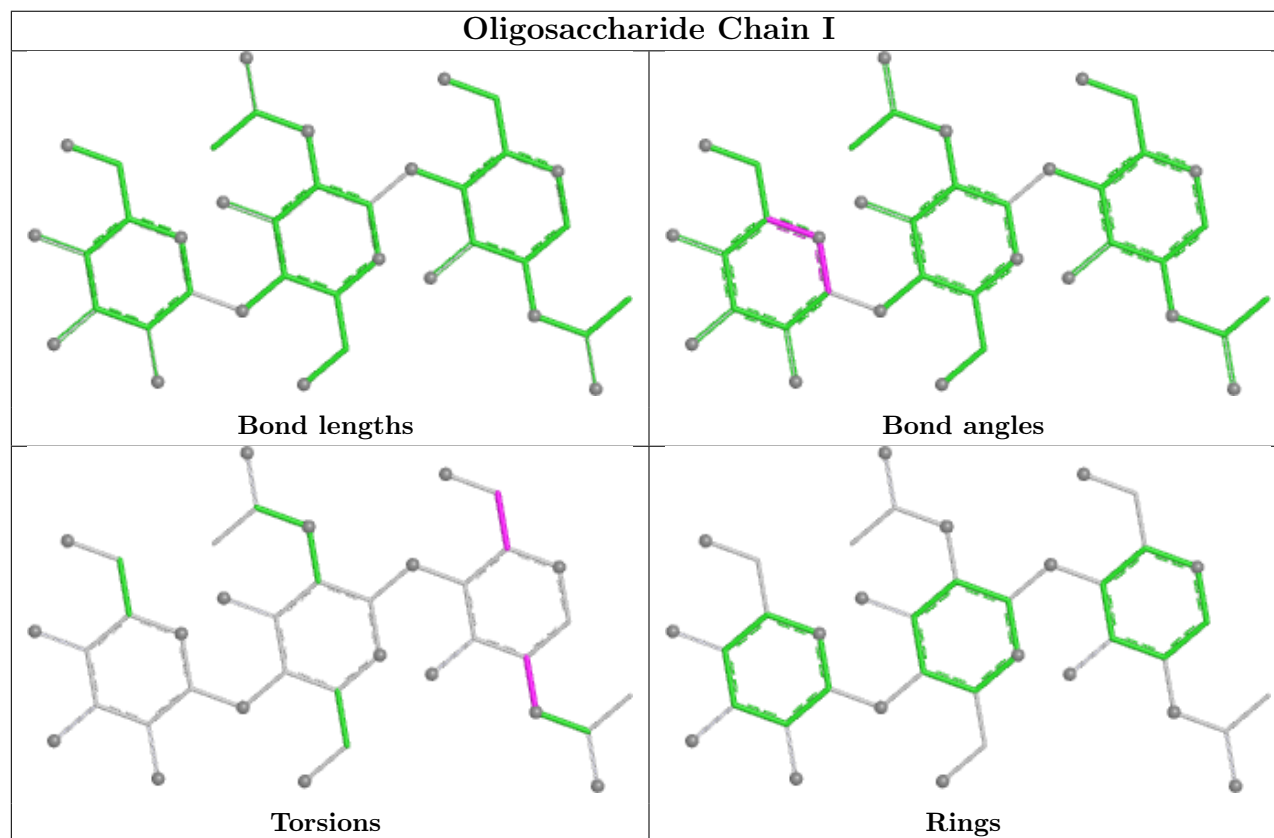
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	3	NAG	O5-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6

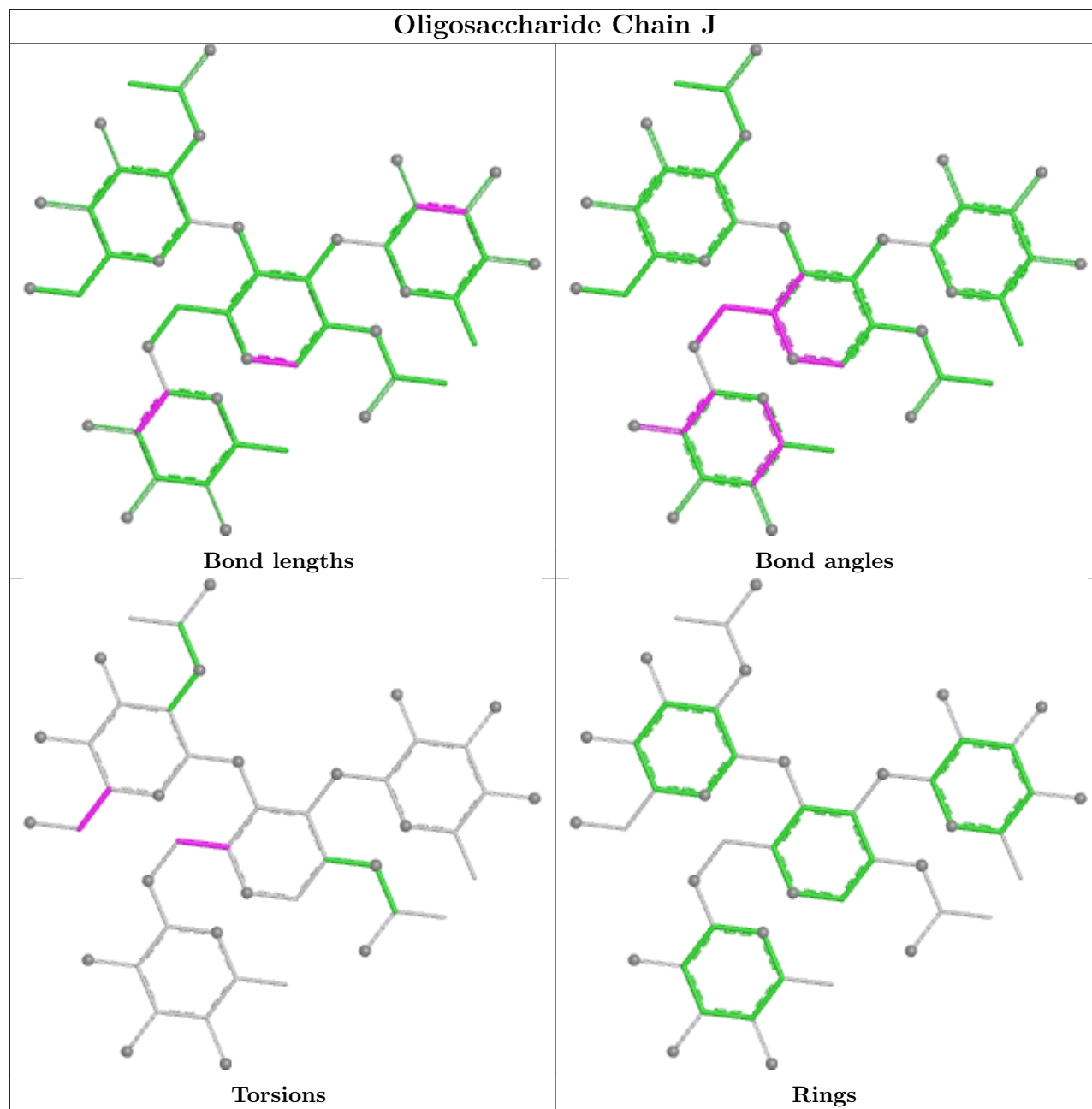
There are no ring outliers.

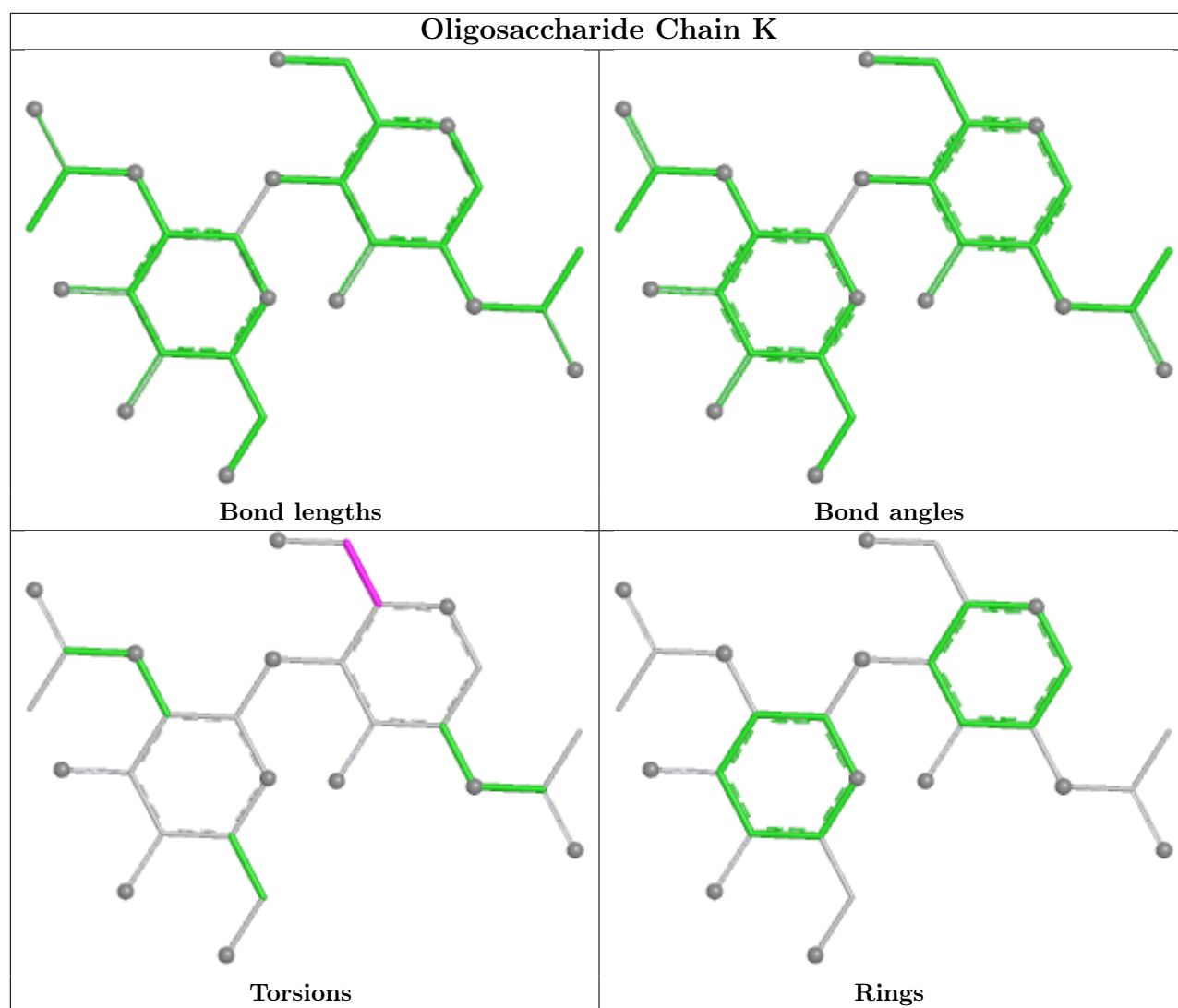
5 monomers are involved in 5 short contacts:

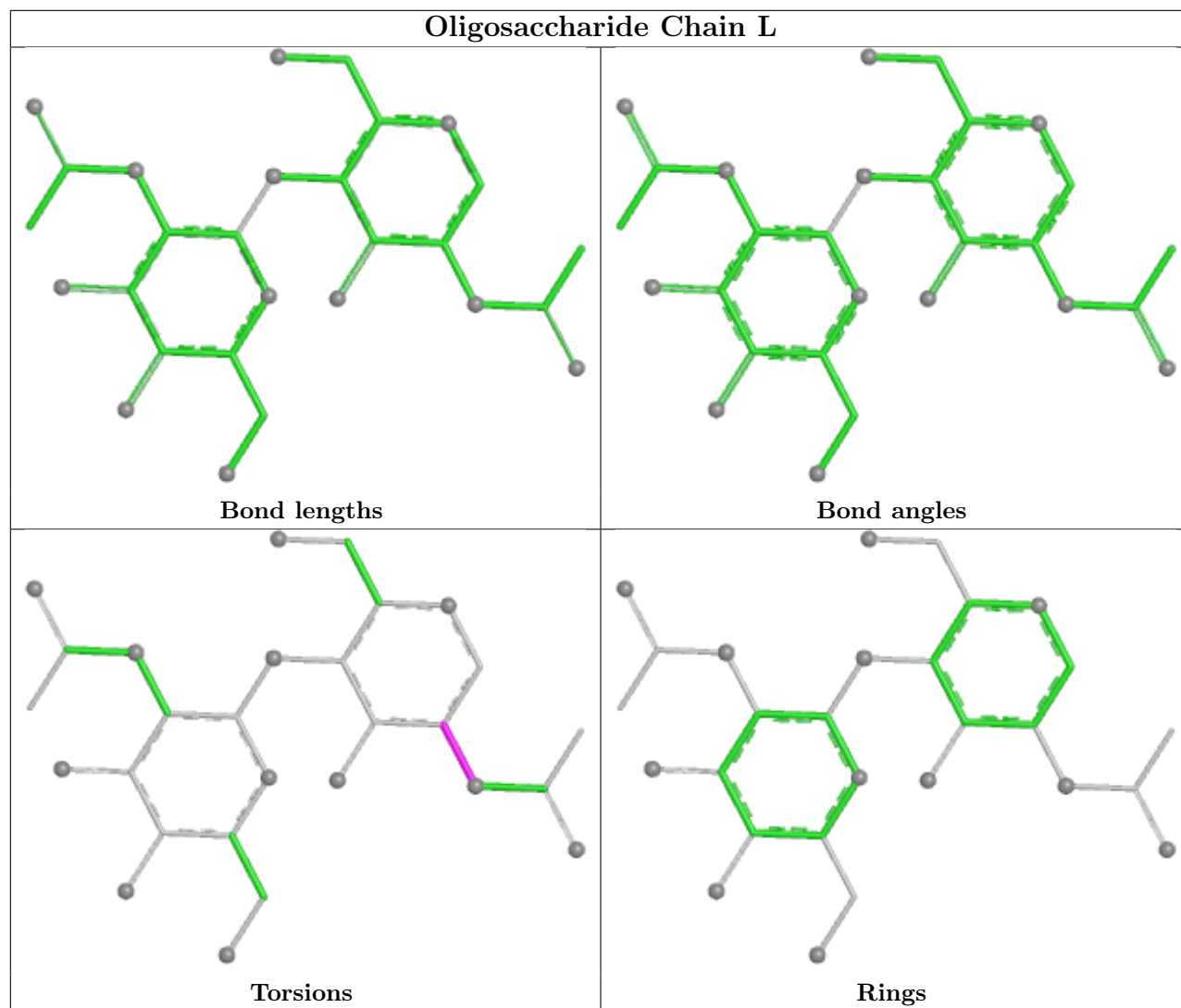
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	NAG	2	0
4	J	4	FUC	1	0
4	J	3	NAG	1	0
5	S	1	NAG	1	0
6	Q	2	NAG	1	0

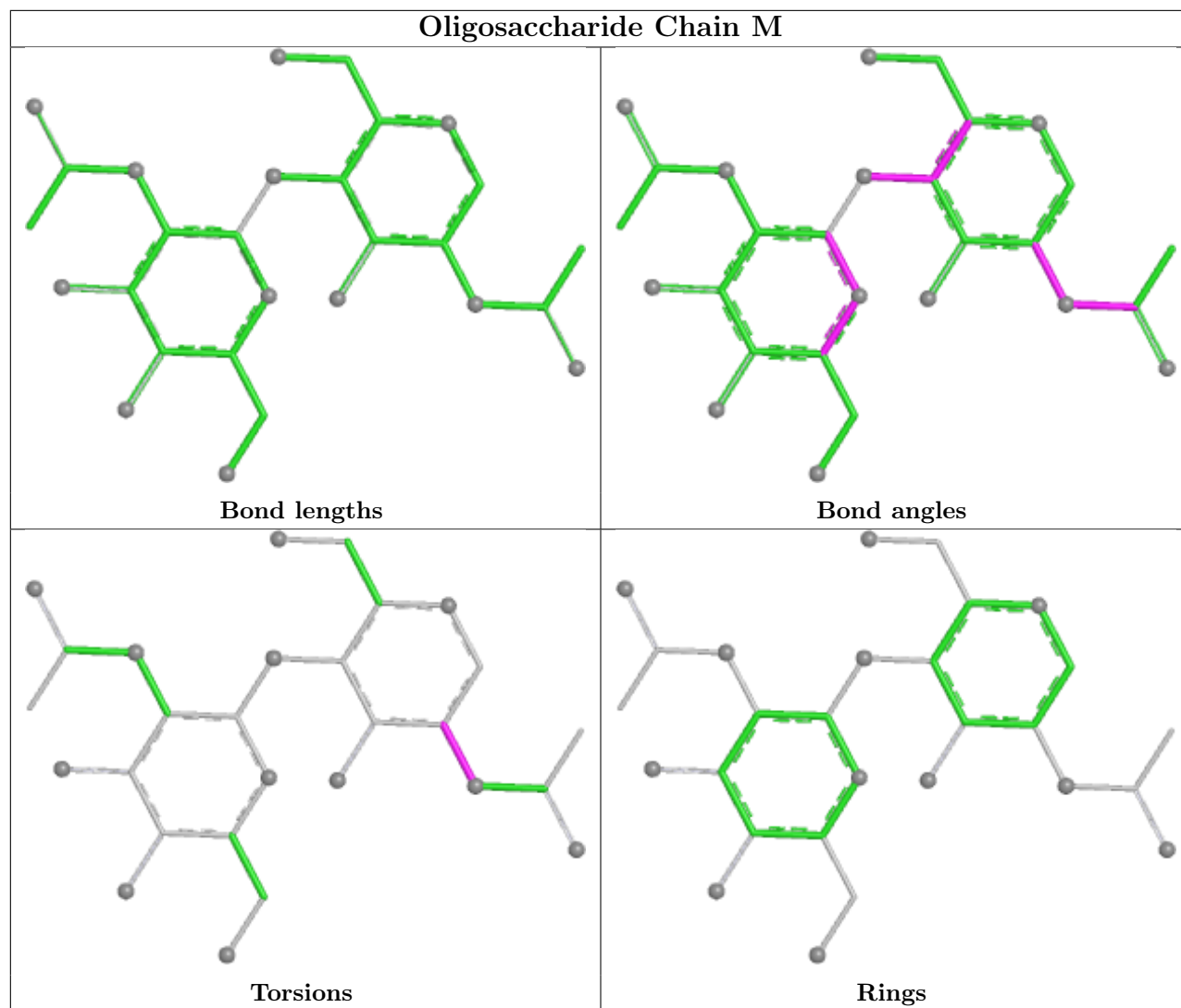
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

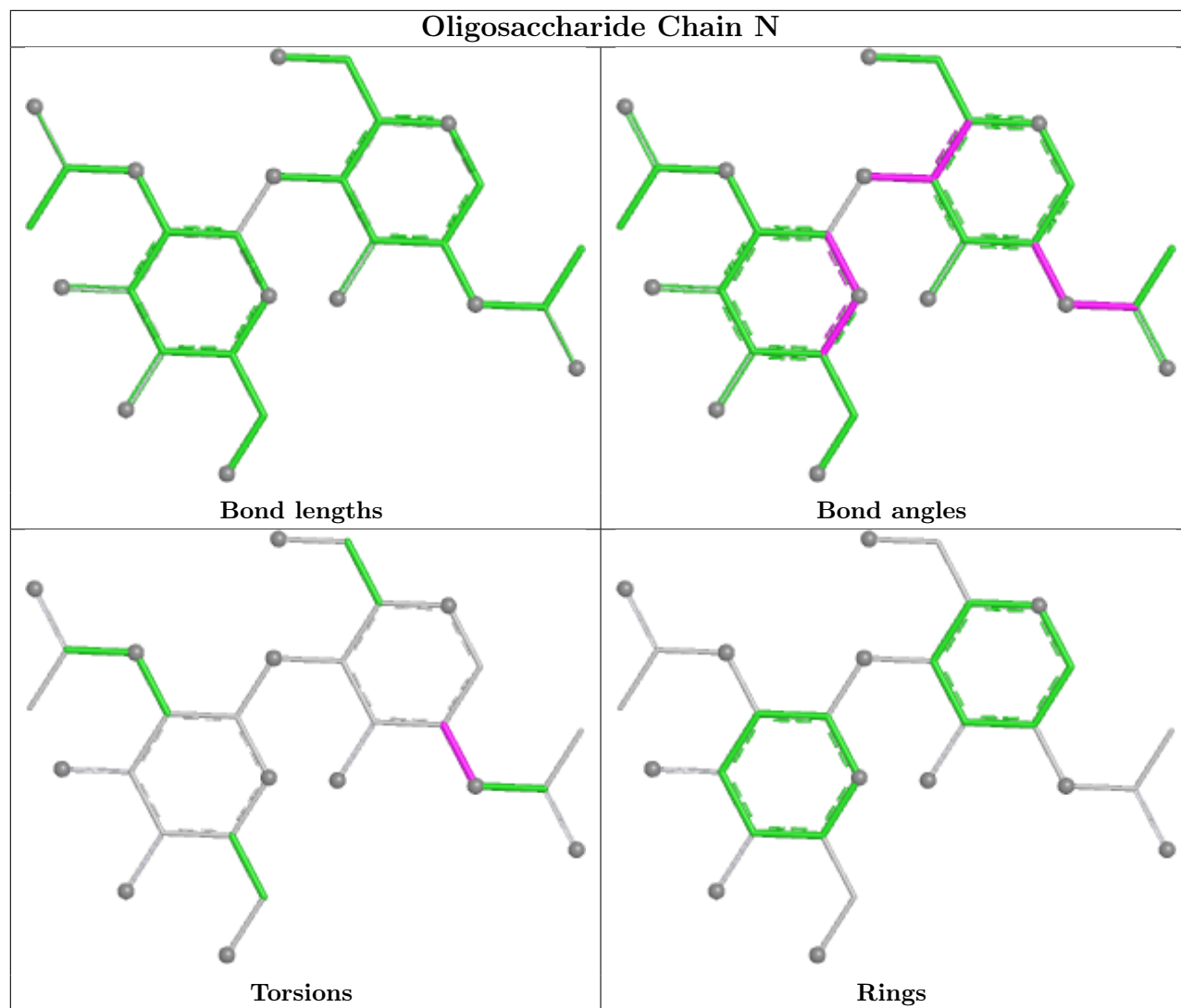


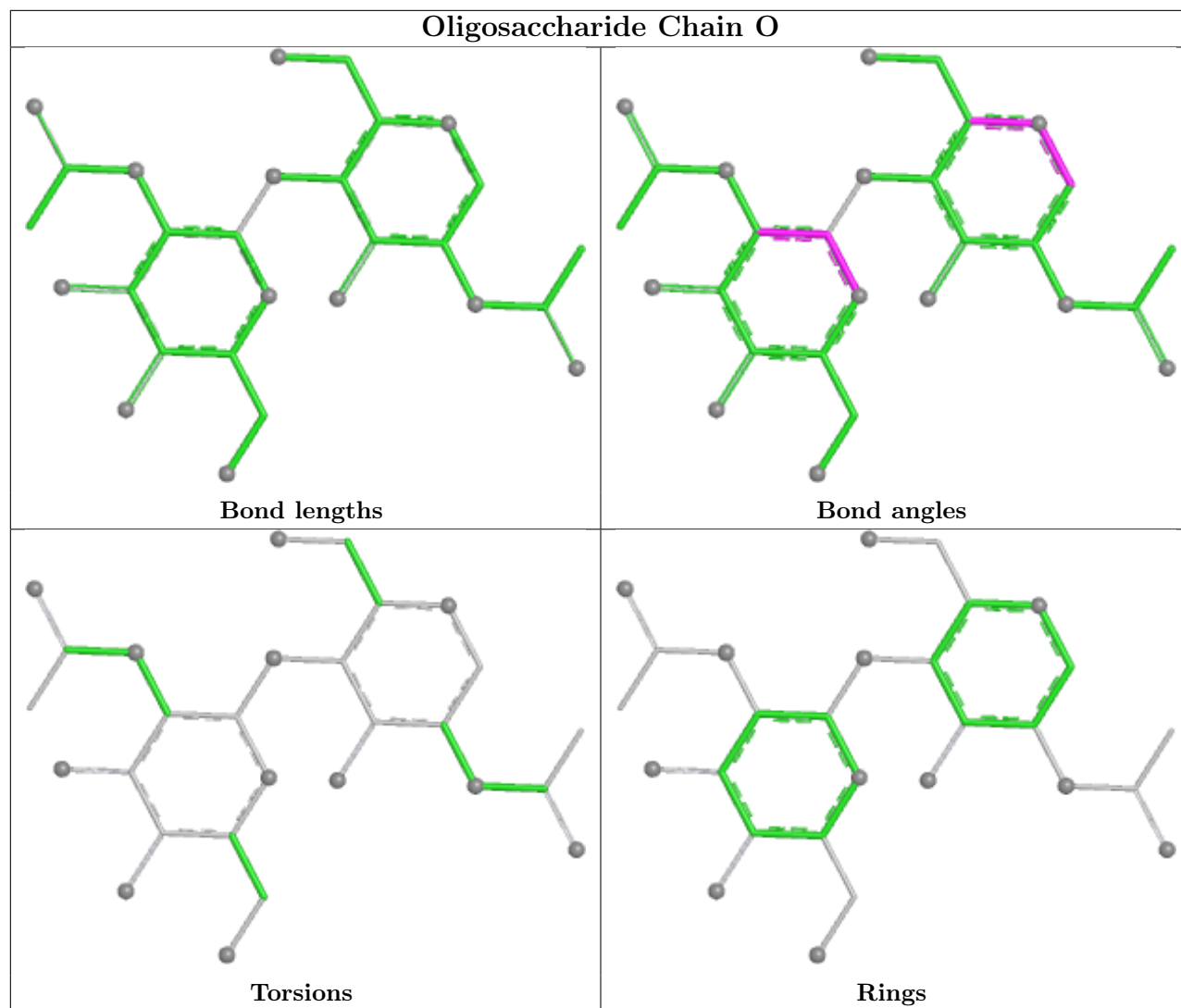


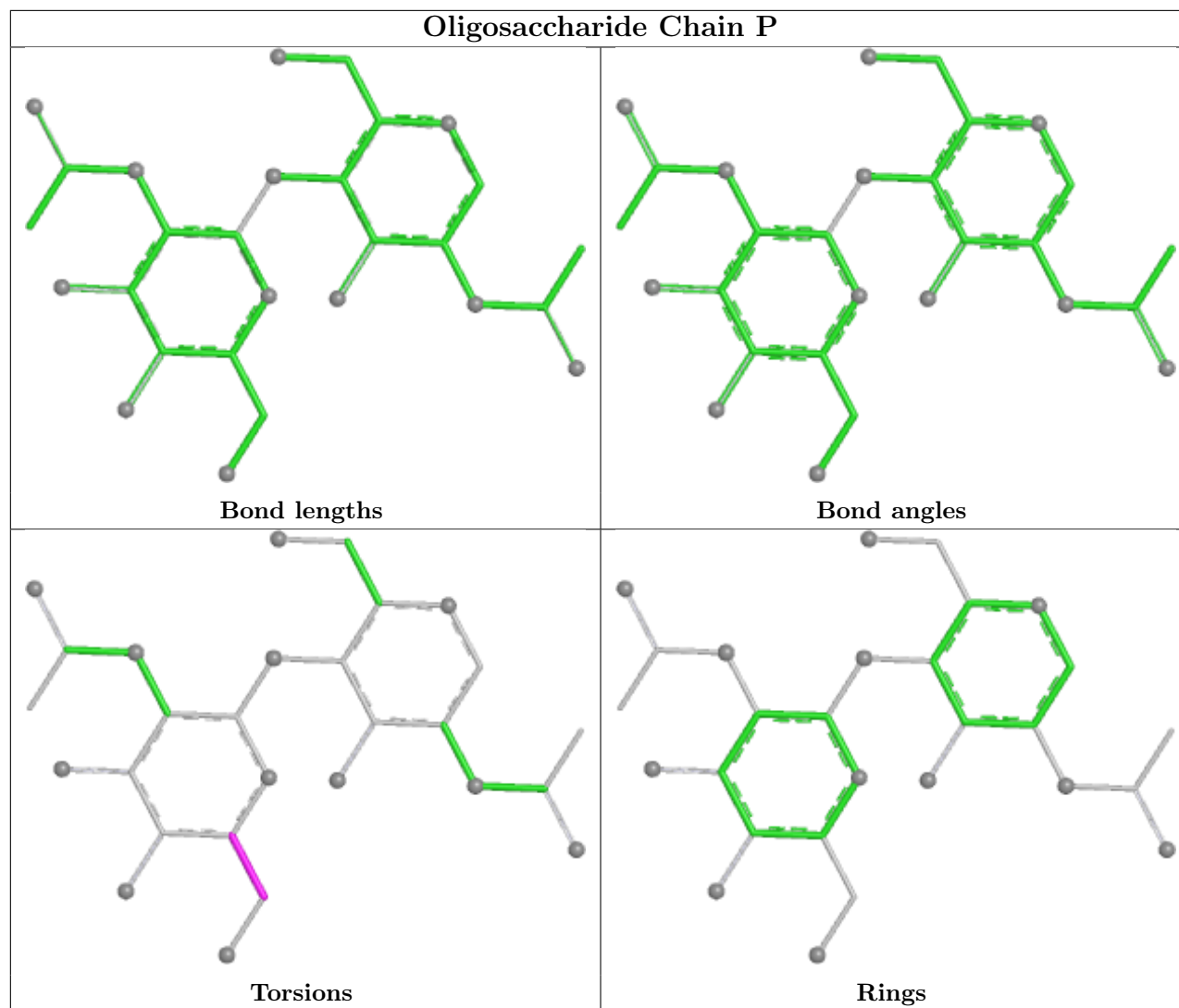


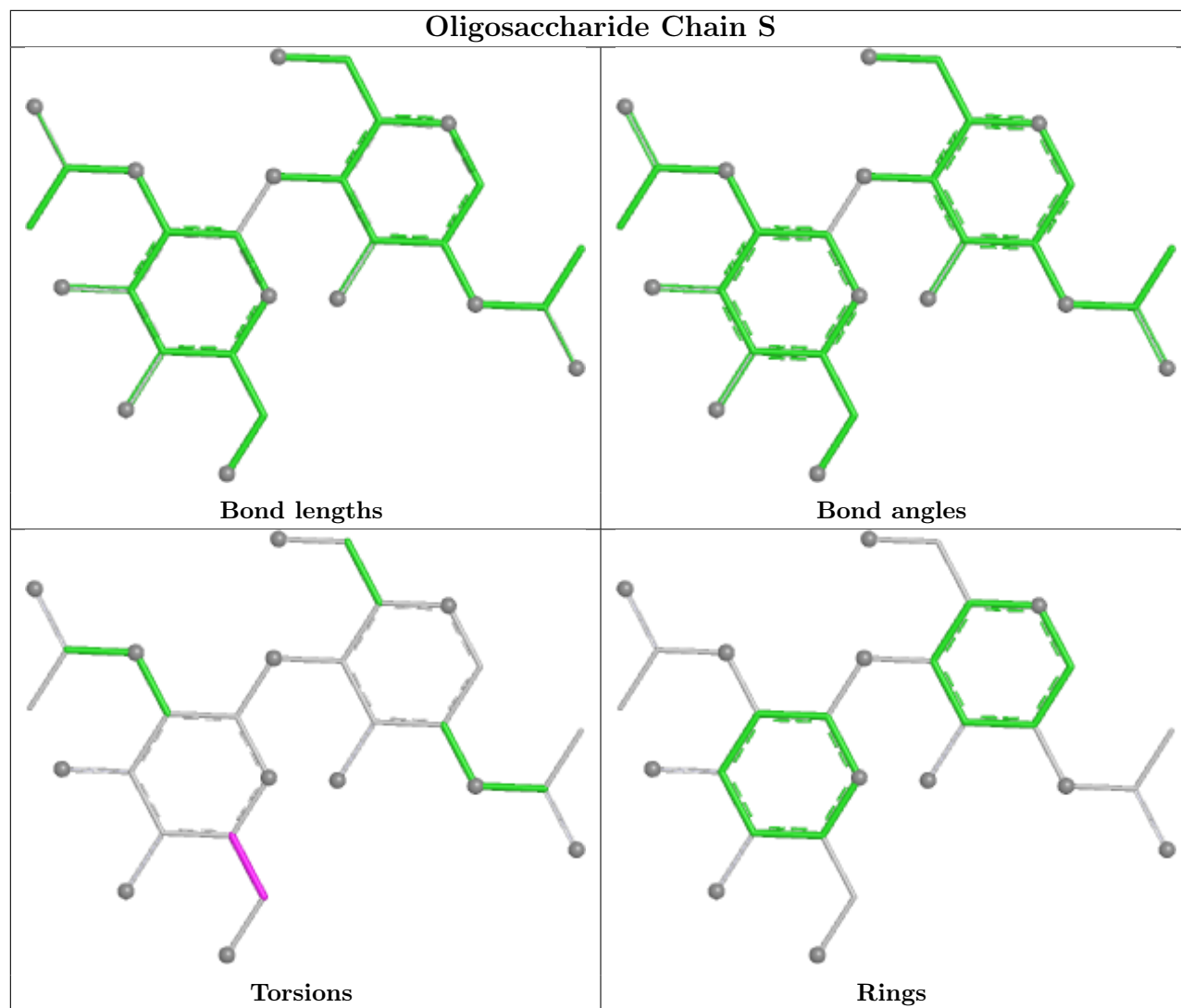


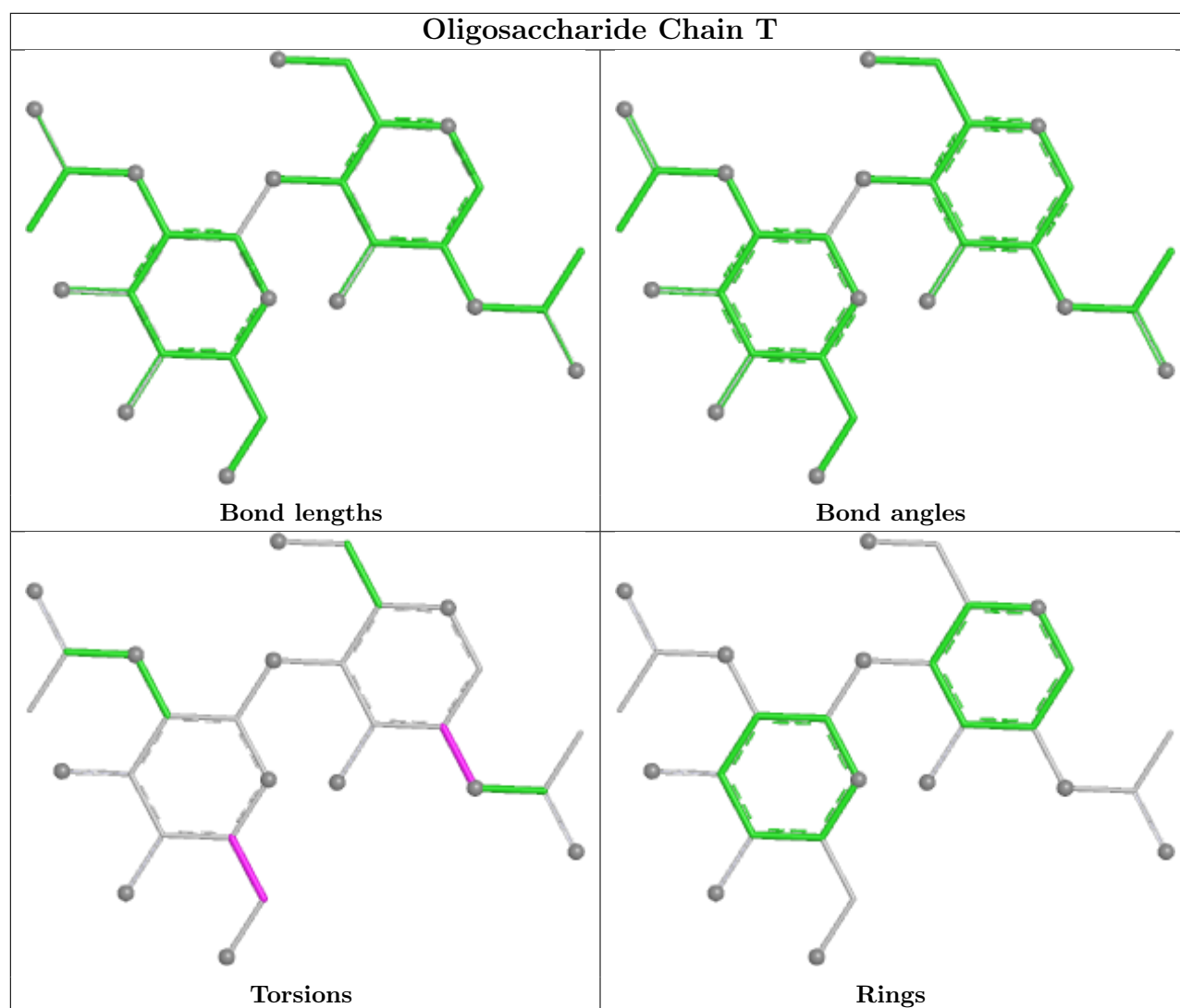


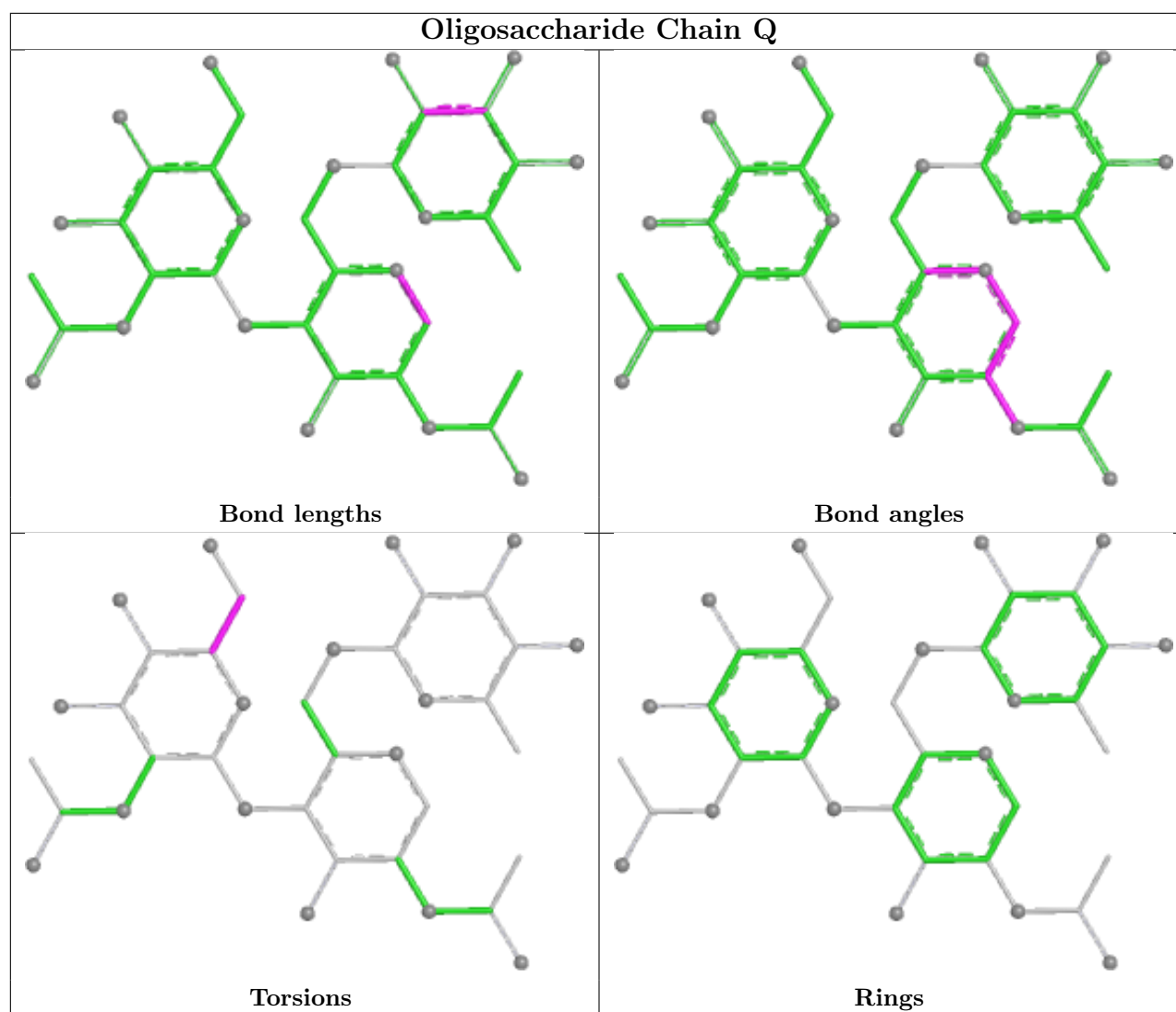


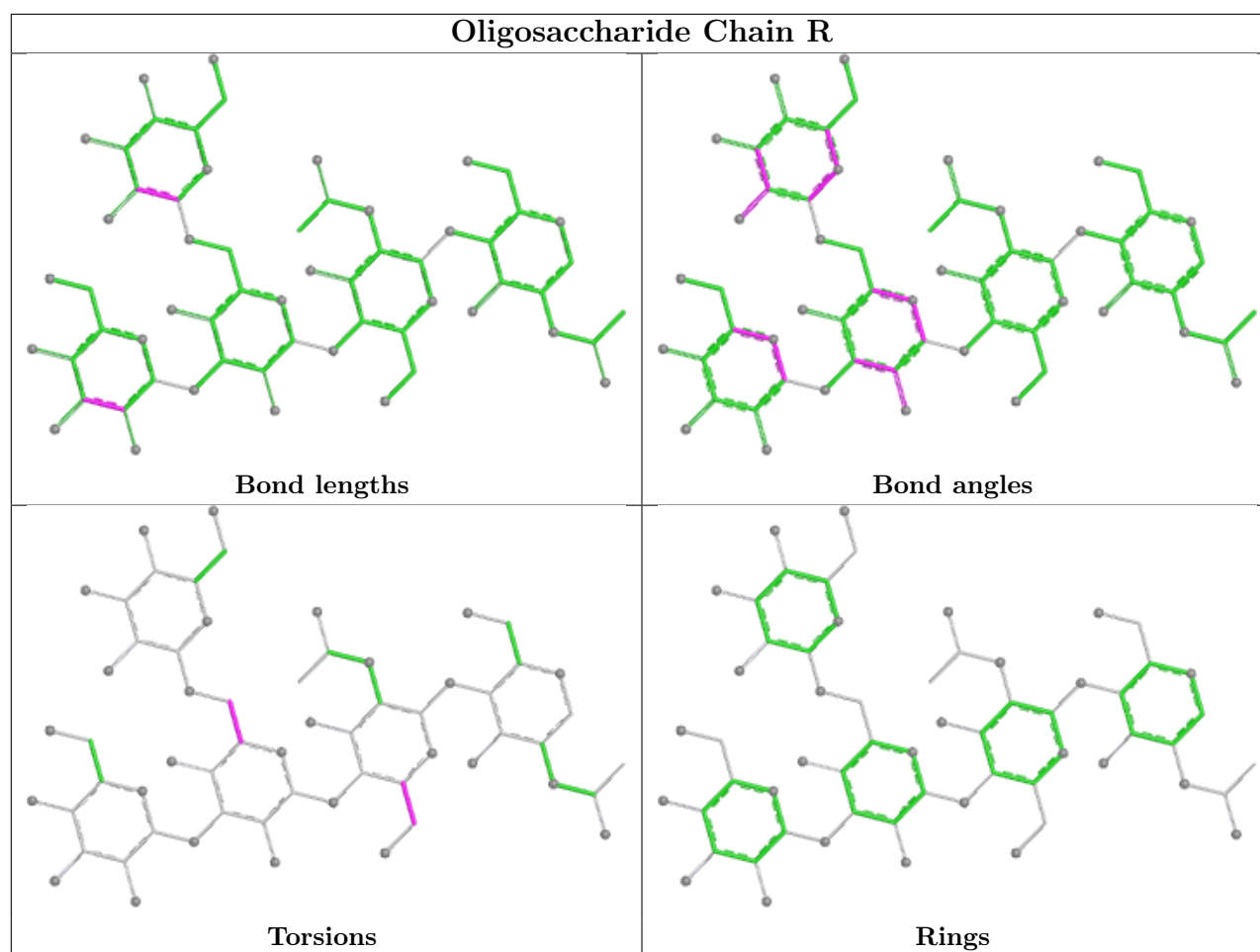












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	313/313 (100%)	0.20	10 (3%) 50 56	9, 20, 35, 50	0
1	C	313/313 (100%)	0.24	9 (2%) 53 60	11, 21, 35, 53	0
1	E	313/313 (100%)	0.20	11 (3%) 47 53	11, 20, 35, 56	0
1	G	313/313 (100%)	0.28	11 (3%) 47 53	10, 21, 36, 54	0
2	B	346/349 (99%)	0.22	8 (2%) 61 68	12, 22, 33, 51	0
2	D	346/349 (99%)	0.57	19 (5%) 30 34	12, 26, 42, 57	0
2	F	346/349 (99%)	0.30	10 (2%) 53 60	13, 22, 35, 60	0
2	H	346/349 (99%)	0.60	15 (4%) 40 44	13, 26, 39, 63	0
All	All	2636/2648 (99%)	0.33	93 (3%) 47 53	9, 22, 37, 63	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	302	TYR	5.7
1	E	292	ARG	5.2
1	A	36	ARG	4.5
2	F	119	ASN	4.3
2	H	119	ASN	4.2

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,

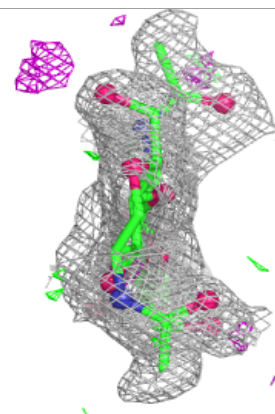
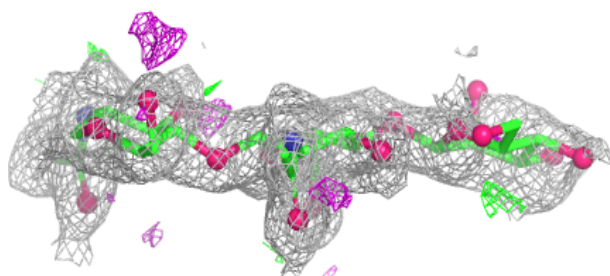
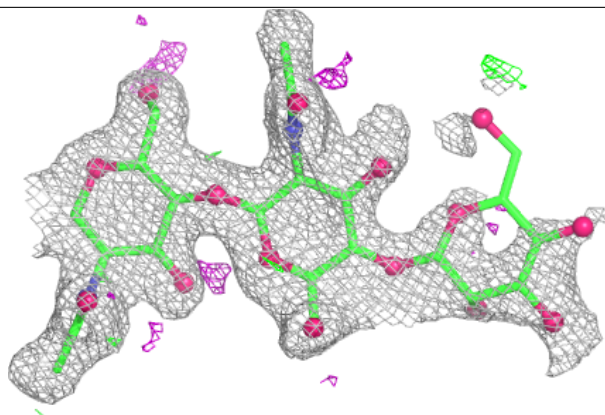
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	I	3	11/12	0.68	0.18	49,57,63,66	0
4	FUC	J	2	10/11	0.69	0.19	53,55,58,60	0
4	FUC	J	4	10/11	0.69	0.22	48,56,64,65	0
5	NAG	M	2	14/15	0.73	0.17	32,46,54,56	0
5	NAG	O	1	14/15	0.73	0.17	40,47,57,58	0
6	FUC	Q	3	10/11	0.73	0.15	48,52,58,60	0
6	NAG	Q	1	14/15	0.74	0.13	47,51,55,58	0
6	NAG	Q	2	14/15	0.74	0.18	47,55,61,68	0
5	NAG	P	2	14/15	0.74	0.14	46,50,54,55	0
5	NAG	K	2	14/15	0.76	0.14	43,49,57,66	0
5	NAG	O	2	14/15	0.76	0.15	45,55,61,63	0
5	NAG	S	2	14/15	0.77	0.14	45,50,55,56	0
5	NAG	T	2	14/15	0.78	0.17	42,48,57,64	0
5	NAG	L	2	14/15	0.78	0.14	31,42,52,53	0
4	NAG	J	1	14/15	0.79	0.15	35,42,51,56	0
5	NAG	T	1	14/15	0.79	0.16	31,38,48,58	0
7	MAN	R	4	11/12	0.79	0.13	38,44,51,57	0
5	NAG	S	1	14/15	0.80	0.13	34,42,47,47	0
4	NAG	J	3	14/15	0.80	0.15	46,52,56,61	0
3	NAG	I	2	14/15	0.83	0.13	24,35,43,47	0
7	MAN	R	5	11/12	0.83	0.14	38,43,50,51	0
5	NAG	P	1	14/15	0.84	0.12	39,43,48,53	0
7	BMA	R	3	11/12	0.84	0.12	38,43,49,50	0
7	NAG	R	1	14/15	0.86	0.12	31,34,40,41	0
5	NAG	K	1	14/15	0.87	0.10	28,35,41,42	0
5	NAG	N	2	14/15	0.87	0.10	27,35,43,48	0
7	NAG	R	2	14/15	0.87	0.12	33,40,46,55	0
5	NAG	L	1	14/15	0.90	0.10	20,23,30,30	0
3	NAG	I	1	14/15	0.90	0.10	17,22,28,29	0
5	NAG	M	1	14/15	0.90	0.10	17,23,33,34	0
5	NAG	N	1	14/15	0.91	0.10	19,25,27,32	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.

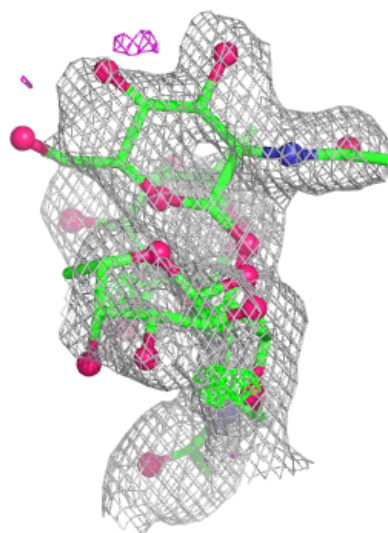
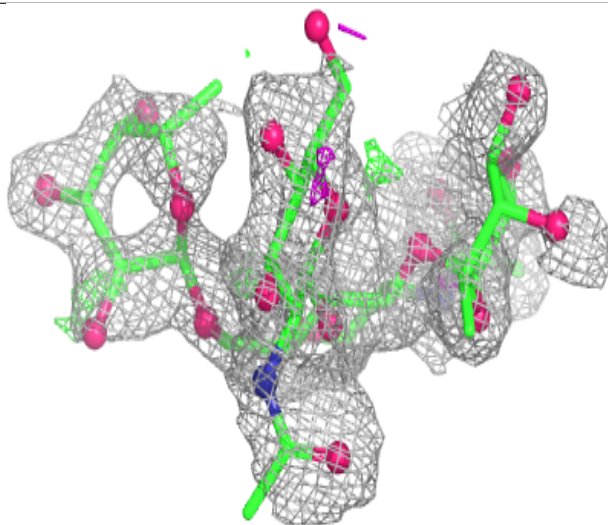
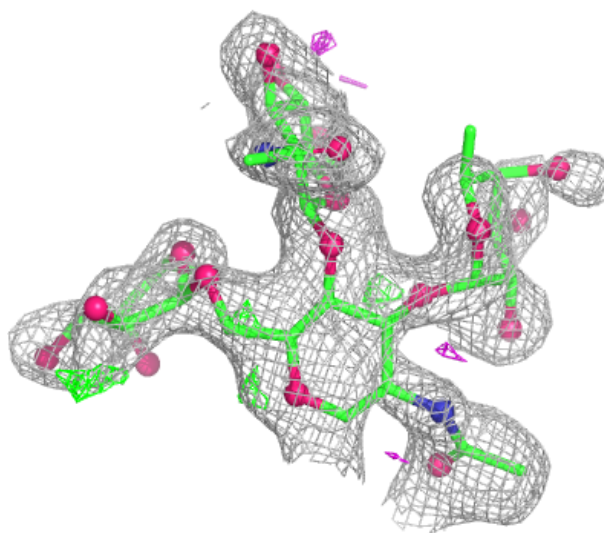
Electron density around Chain I:

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



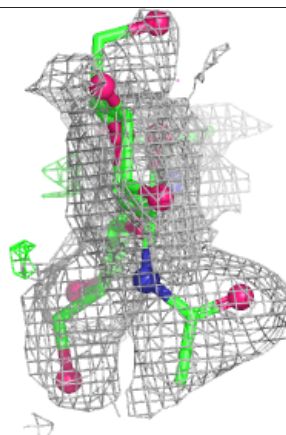
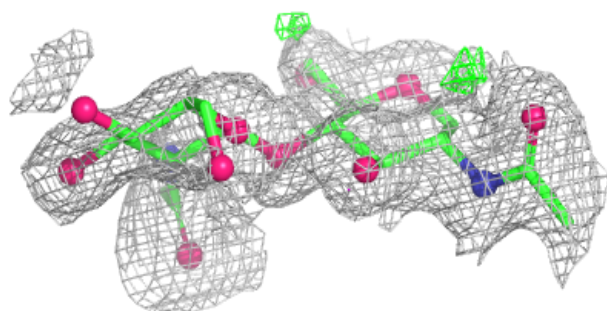
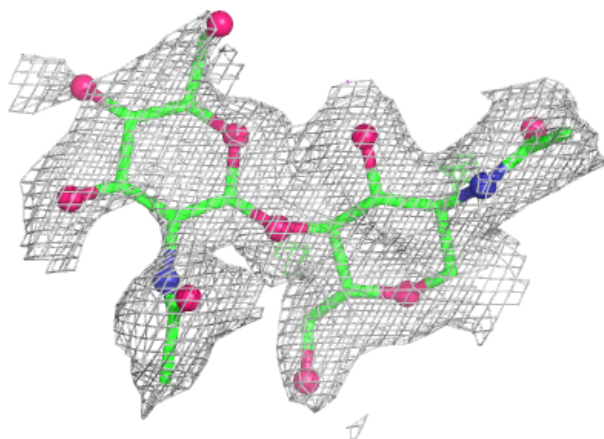
Electron density around Chain J:

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



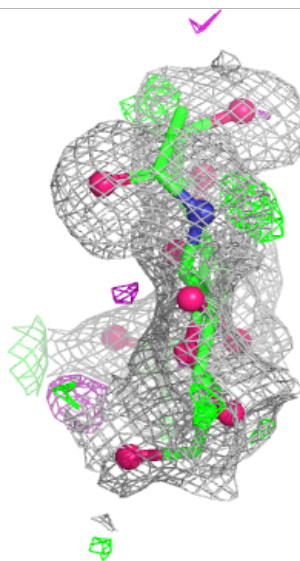
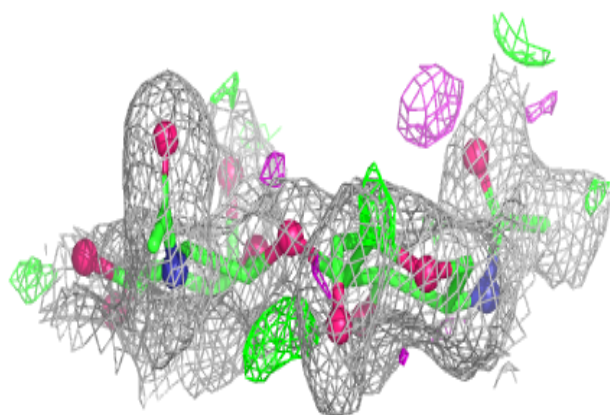
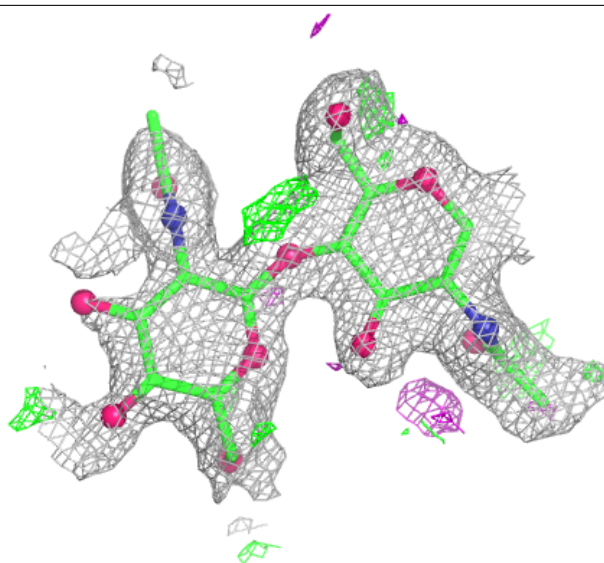
Electron density around Chain K:

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



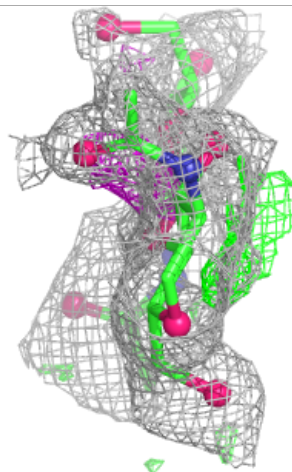
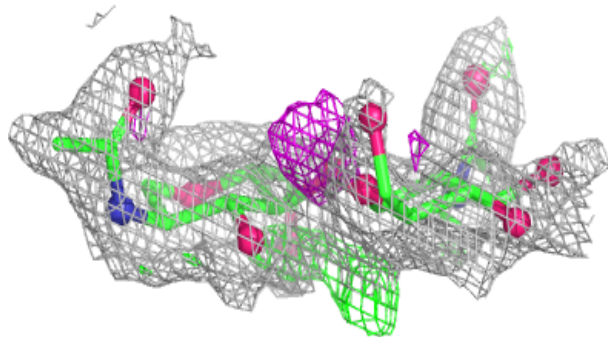
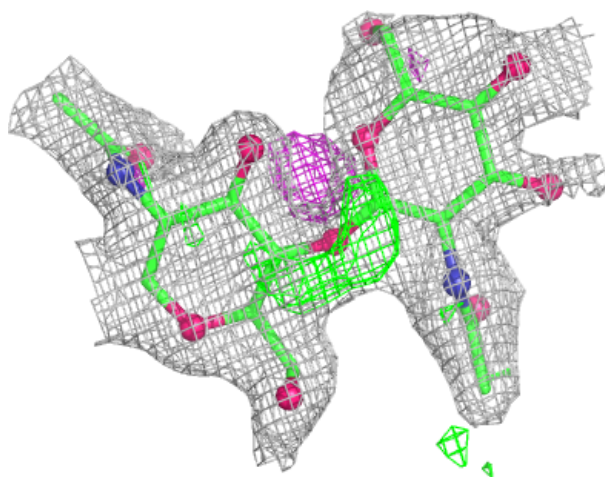
Electron density around Chain L:

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



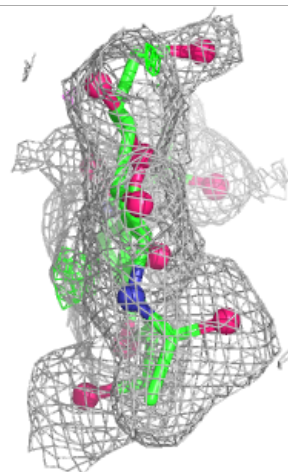
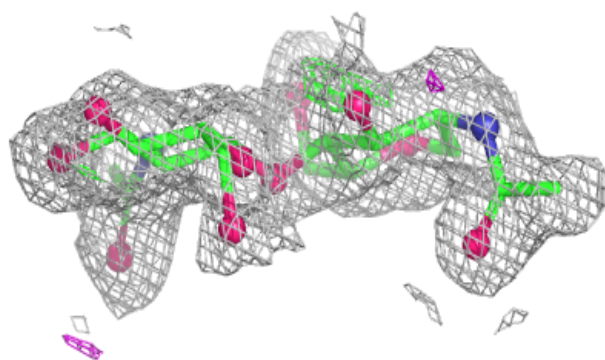
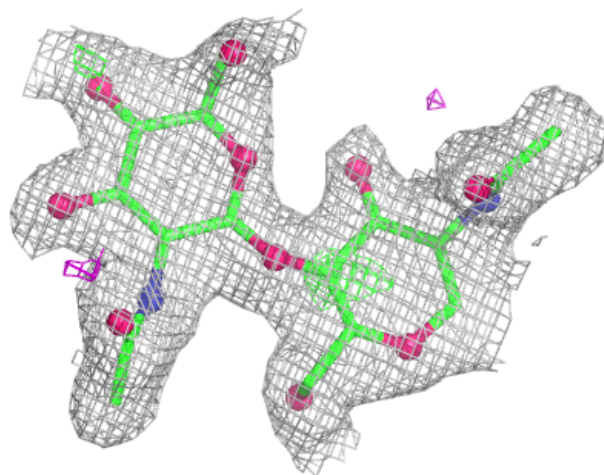
Electron density around Chain M:

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



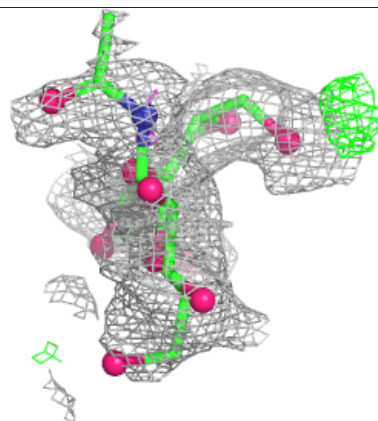
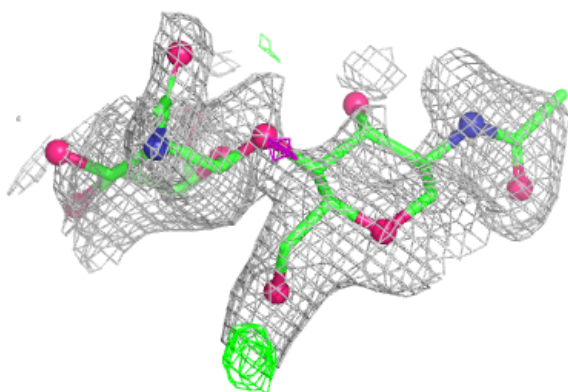
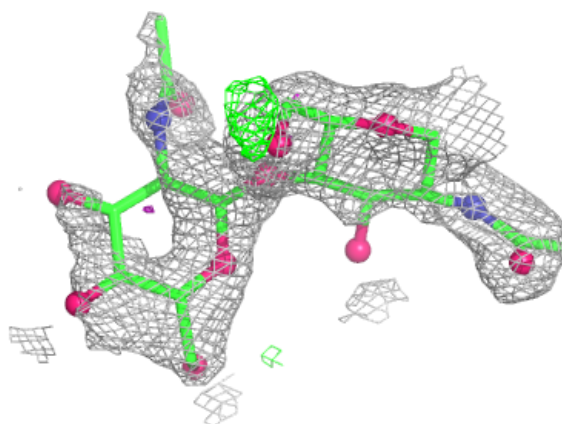
Electron density around Chain N:

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



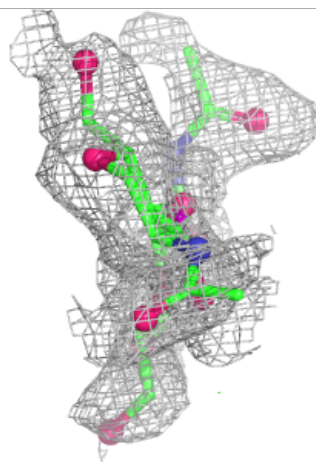
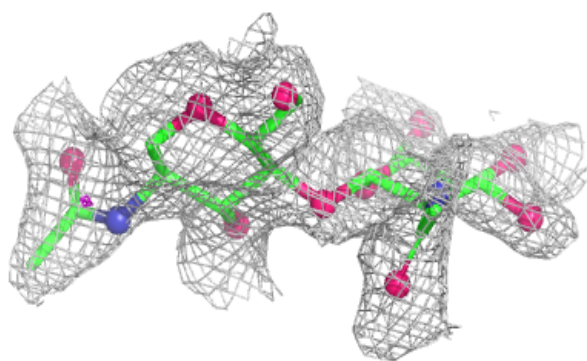
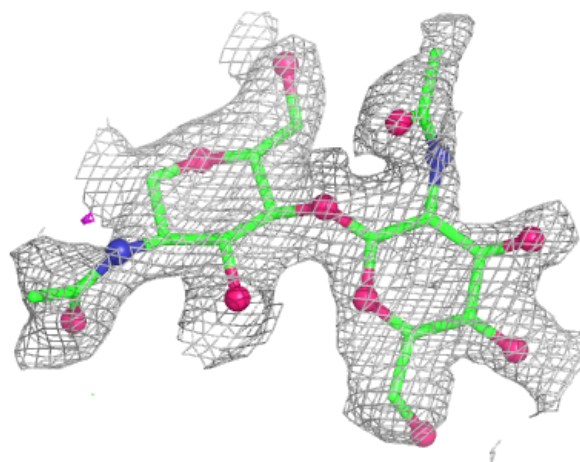
Electron density around Chain O:

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



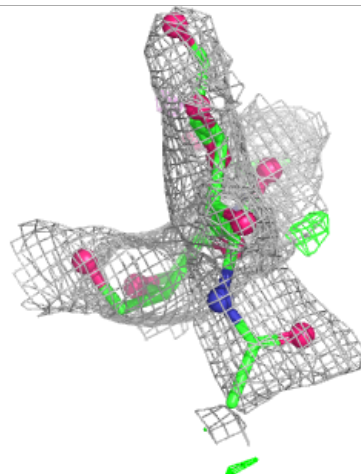
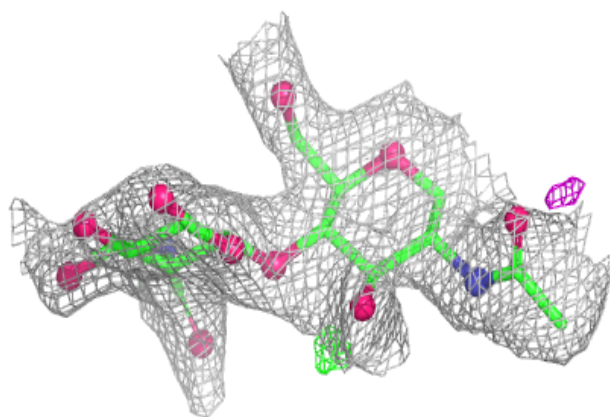
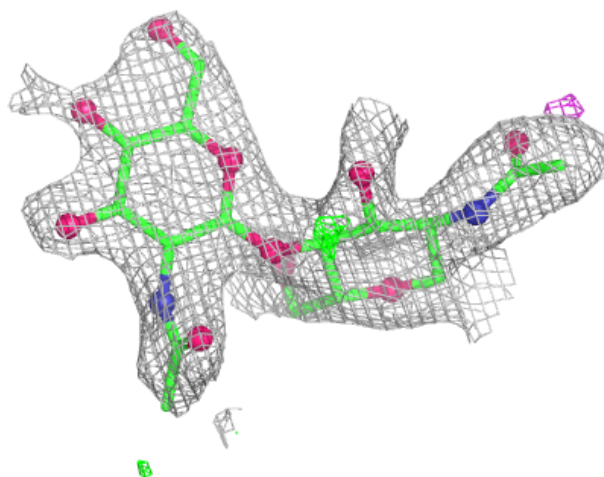
Electron density around Chain P:

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



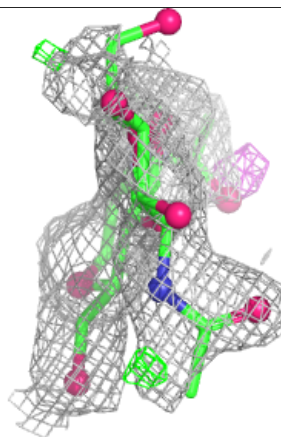
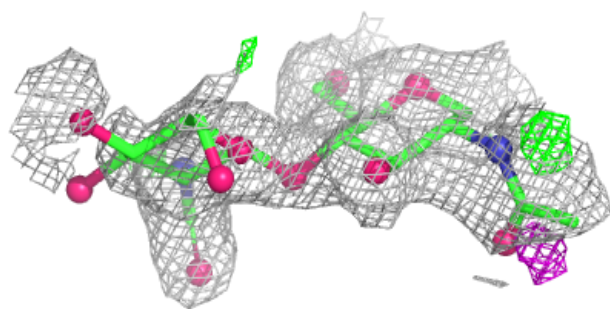
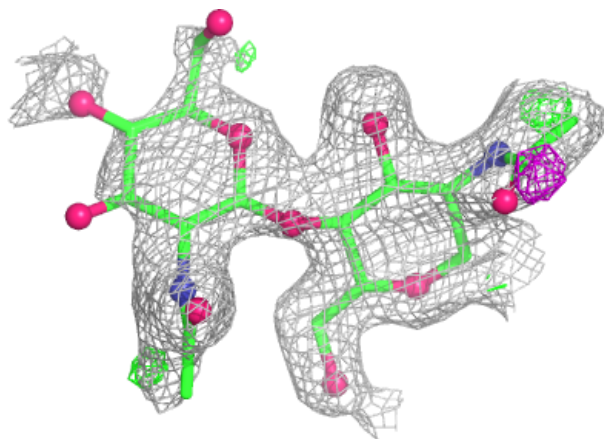
Electron density around Chain S:

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



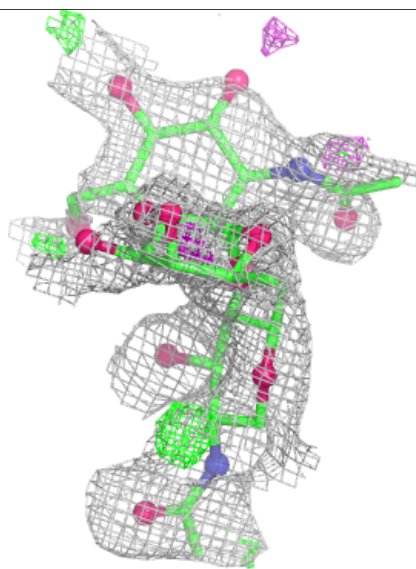
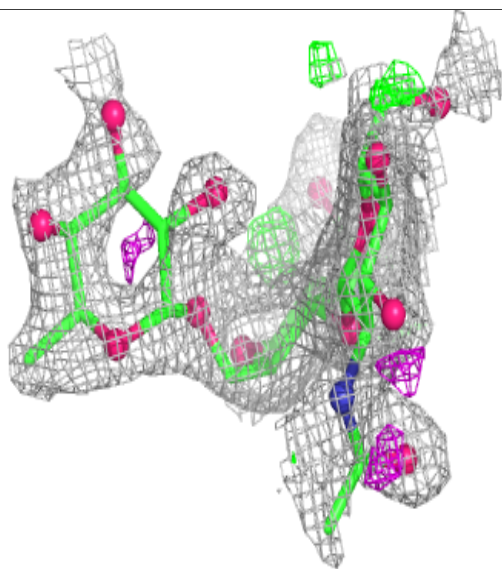
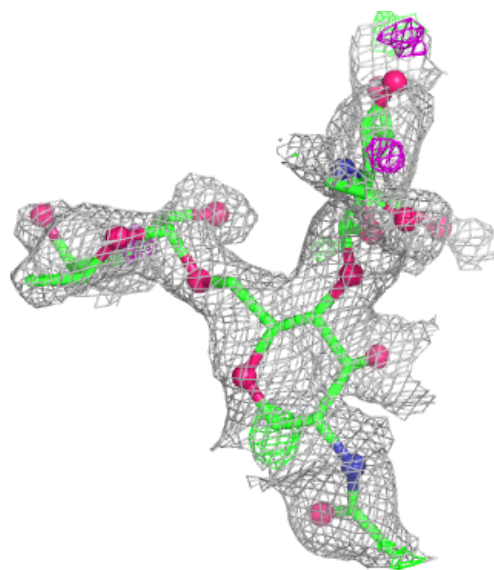
Electron density around Chain T:

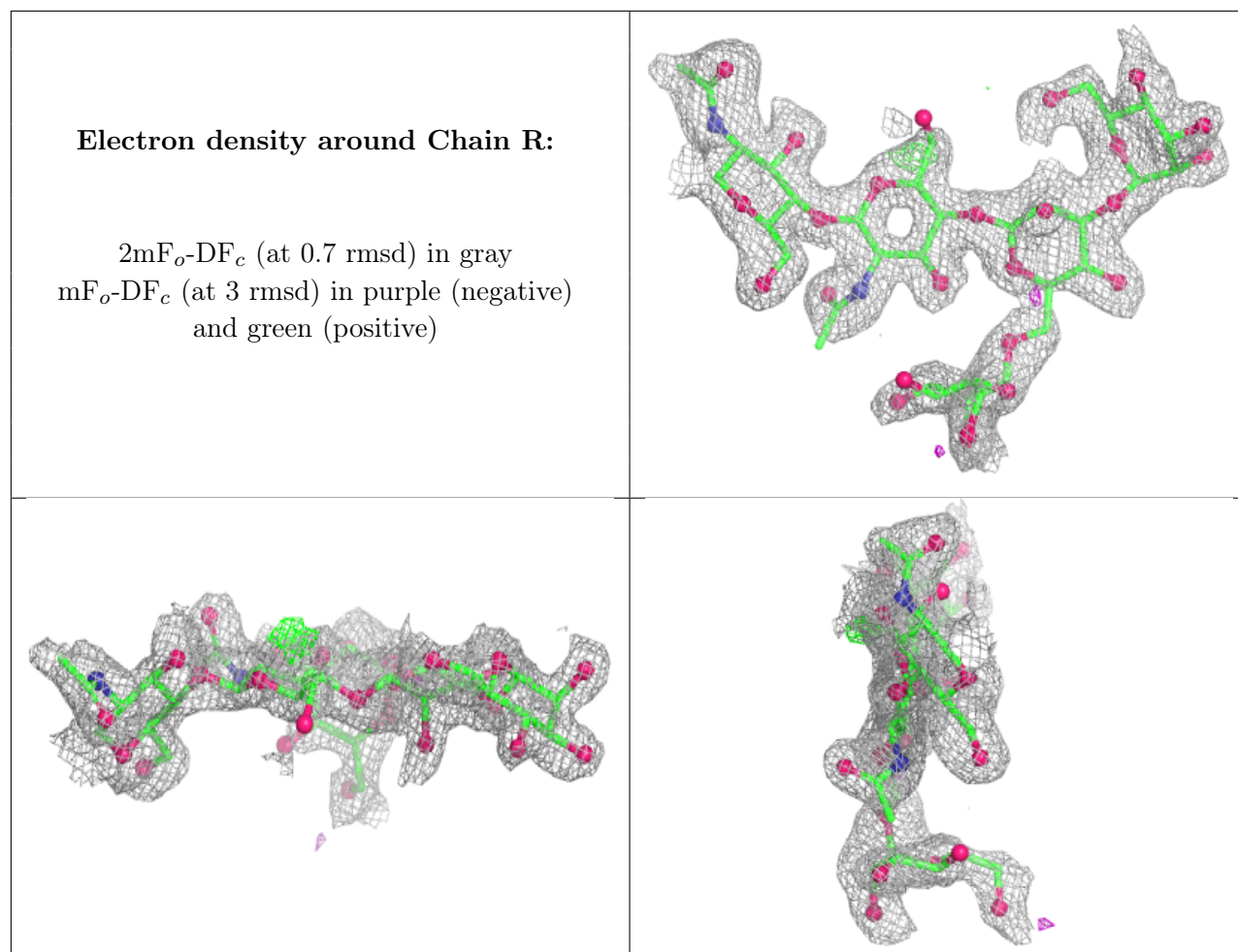
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.