



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:17 AM UTC

PDB ID : 7BJ4 / pdb_00007bj4
Title : Inulosucrase from Halalkalicoccus jeotgali bound to kestose
Authors : Ghauri, K.; Pijning, T.; Munawar, N.; Ali, H.; Ghauri, M.A.; Anwar, M.A.; Wallis, R.
Deposited on : 2021-01-14
Resolution : 2.72 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

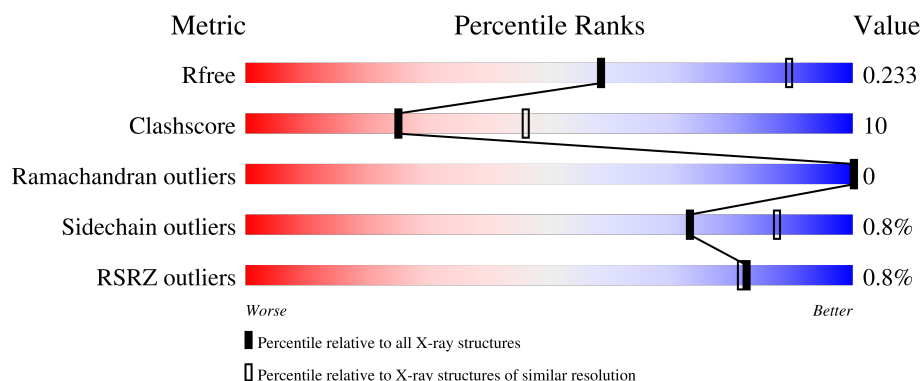
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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.



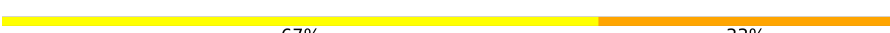
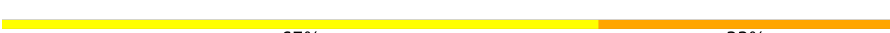
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	428	 85% 9% 5%
1	B	428	 79% 15% 5%
1	C	428	 84% 11% 5%
1	D	428	 82% 13% 5%
1	E	428	 84% 11% 5%

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Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	
2	K	3	
2	L	3	
2	M	3	
2	N	3	
2	O	3	
2	P	3	
2	Q	3	
2	R	3	
2	T	3	
2	U	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	M	3	-	-	X	-
2	GLC	Q	1	-	-	X	-
2	FRU	Q	3	-	-	X	-
2	FRU	T	3	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32221 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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	B	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	C	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	D	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	E	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	F	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	G	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	H	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	I	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	J	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	3	Total	C	O	0	0	0
			34	18	16			
2	L	3	Total	C	O	0	0	0
			34	18	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	3	Total 34	C 18	O 16	0	0	0
2	N	3	Total 34	C 18	O 16	0	0	0
2	O	3	Total 34	C 18	O 16	0	0	0
2	P	3	Total 34	C 18	O 16	0	0	0
2	Q	3	Total 34	C 18	O 16	0	0	0
2	R	3	Total 34	C 18	O 16	0	0	0
2	T	3	Total 34	C 18	O 16	0	0	0
2	U	3	Total 34	C 18	O 16	0	0	0

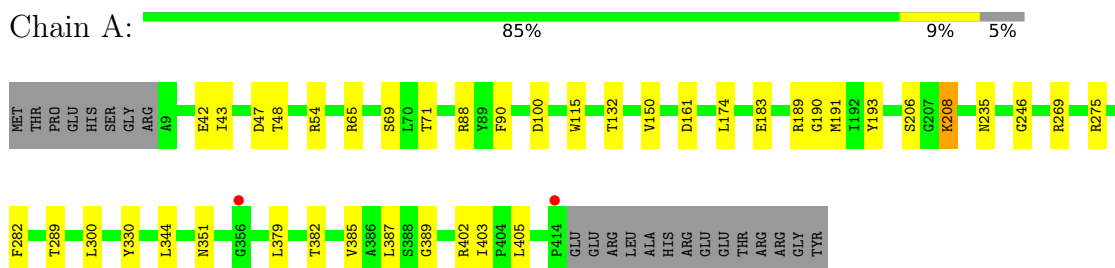
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	9	Total 9	O 9	0	0
3	C	5	Total 5	O 5	0	0
3	D	8	Total 8	O 8	0	0
3	E	10	Total 10	O 10	0	0
3	F	8	Total 8	O 8	0	0
3	G	9	Total 9	O 9	0	0
3	H	10	Total 10	O 10	0	0
3	I	10	Total 10	O 10	0	0
3	J	10	Total 10	O 10	0	0

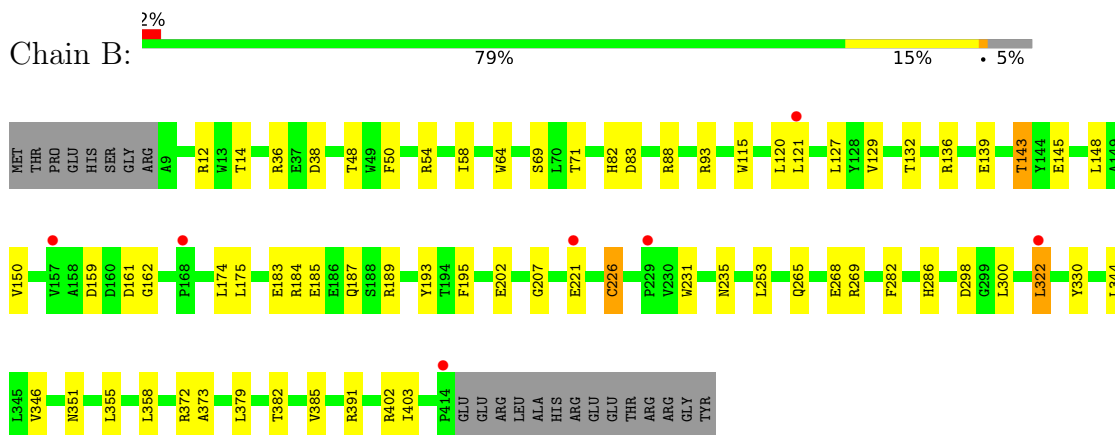
3 Residue-property plots [i](#)

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.

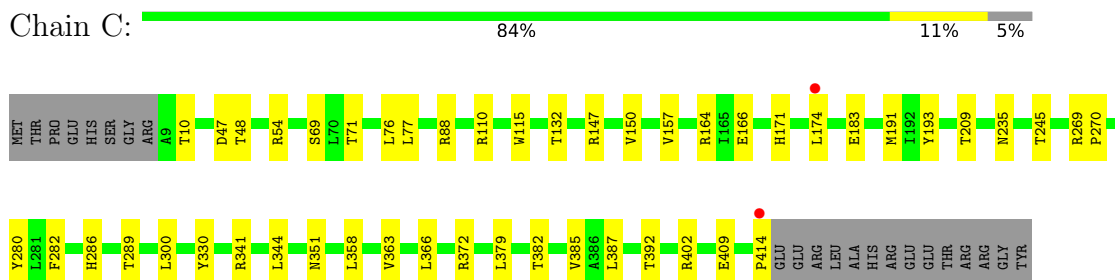
• Molecule 1: Levansucrase



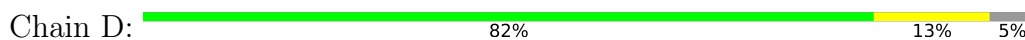
• Molecule 1: Levansucrase

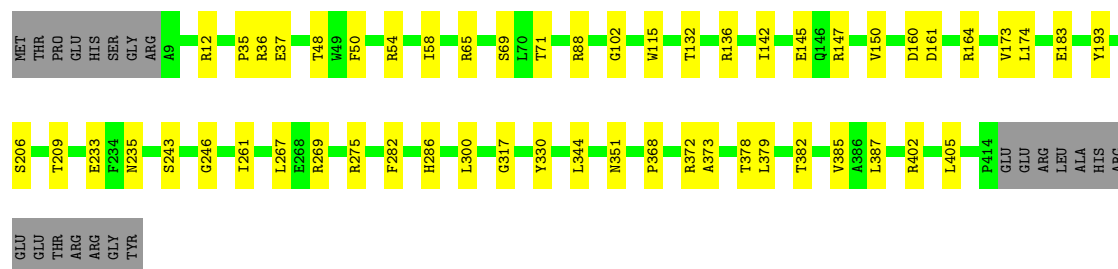


• Molecule 1: Levansucrase



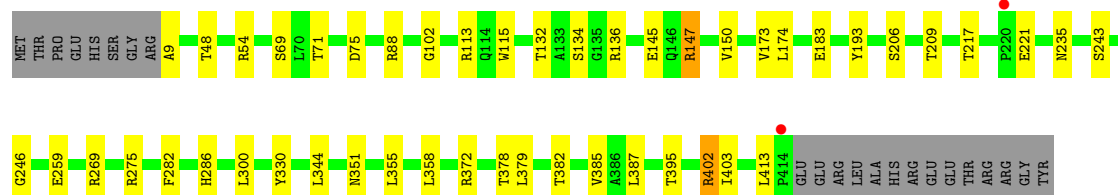
• Molecule 1: Levansucrase





• Molecule 1: Levansucrase

Chain E: 84% 11% 5%



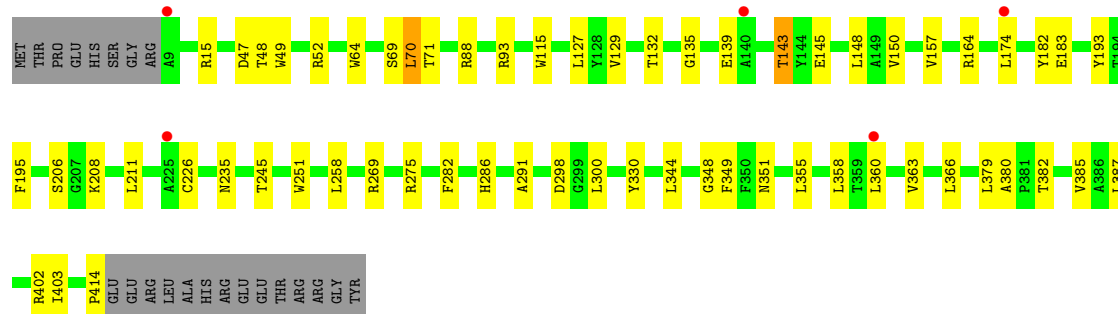
• Molecule 1: Levansucrase

Chain F: 82% 13% 5%



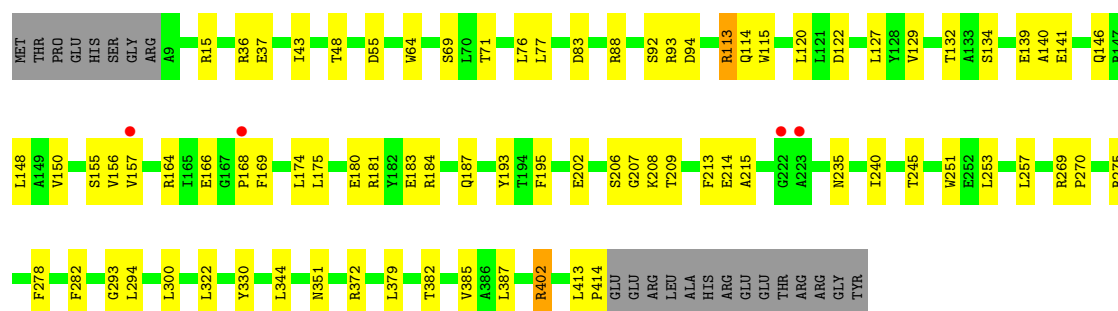
• Molecule 1: Levansucrase

Chain G: 81% 14% 5%

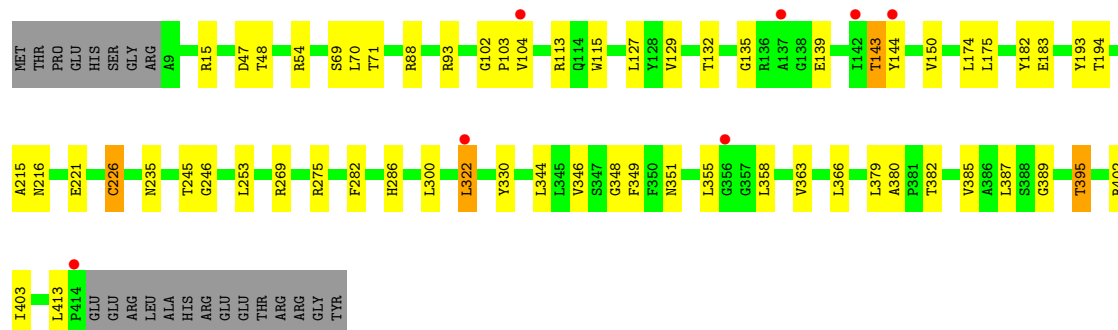
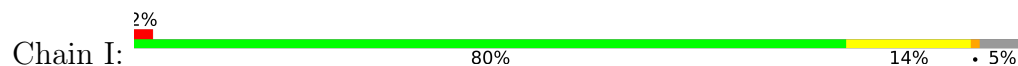


• Molecule 1: Levansucrase

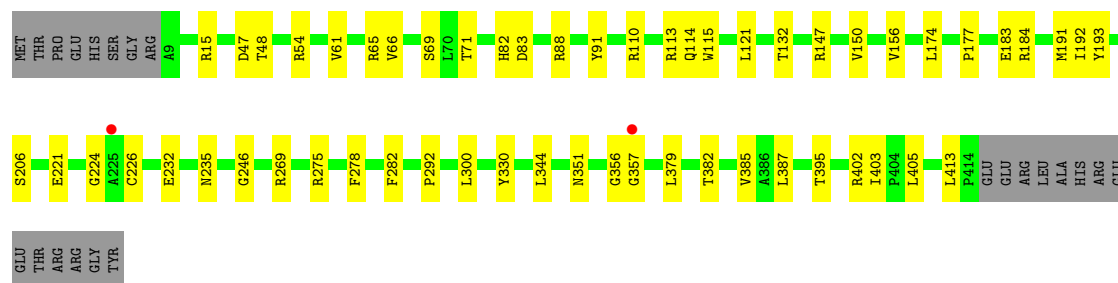
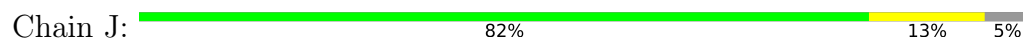
Chain H: 76% 18% 5%



• Molecule 1: Levansucrase



• Molecule 1: Levansucrase



• Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose





- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P: 67% 33%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain R: 100%



- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  67% 33%

GLC1
FRU2
FRU3

- Molecule 2: beta-D-fructofuranose-(2-1)-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:  67% 33%

GLC3
FRU2
FRU3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.30Å 142.97Å 172.87Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	106.54 – 2.72 106.54 – 2.72	Depositor EDS
% Data completeness (in resolution range)	59.0 (106.54-2.72) 59.2 (106.54-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.197 , 0.225 0.209 , 0.233	Depositor DCC
R_{free} test set	4758 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32221	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 35.34 % 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 5.9255e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, FRU

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	0.97	0/3274	1.25	1/4466 (0.0%)
1	B	0.98	0/3274	1.28	3/4466 (0.1%)
1	C	0.97	0/3274	1.26	3/4466 (0.1%)
1	D	0.98	0/3274	1.26	2/4466 (0.0%)
1	E	0.96	0/3274	1.26	2/4466 (0.0%)
1	F	0.97	0/3274	1.24	1/4466 (0.0%)
1	G	0.98	0/3274	1.27	3/4466 (0.1%)
1	H	0.99	0/3274	1.28	2/4466 (0.0%)
1	I	0.97	0/3274	1.28	5/4466 (0.1%)
1	J	0.98	0/3274	1.25	0/4466
All	All	0.98	0/32740	1.26	22/44660 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	245	THR	CA-C-O	-7.43	113.04	121.81
1	H	245	THR	CA-C-O	-7.42	113.05	121.81
1	C	245	THR	CA-C-O	-7.33	113.16	121.81
1	G	245	THR	CA-C-O	-7.29	113.21	121.81
1	I	221	GLU	CA-C-O	-6.44	114.06	120.82

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	A	3180	0	2977	31	0
1	B	3180	0	2977	69	0
1	C	3180	0	2977	41	0
1	D	3180	0	2977	40	0
1	E	3180	0	2977	42	0
1	F	3180	0	2977	75	0
1	G	3180	0	2977	66	0
1	H	3180	0	2977	91	0
1	I	3180	0	2977	72	0
1	J	3180	0	2977	56	0
2	K	34	0	31	4	0
2	L	34	0	31	5	0
2	M	34	0	31	10	0
2	N	34	0	31	4	0
2	O	34	0	31	6	0
2	P	34	0	31	5	0
2	Q	34	0	31	14	0
2	R	34	0	31	4	0
2	T	34	0	31	9	0
2	U	34	0	31	3	0
3	A	2	0	0	4	0
3	B	9	0	0	20	0
3	C	5	0	0	7	0
3	D	8	0	0	9	0
3	E	10	0	0	10	0
3	F	8	0	0	39	0
3	G	9	0	0	21	0
3	H	10	0	0	27	0
3	I	10	0	0	24	0
3	J	10	0	0	25	0
All	All	32221	0	30080	601	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 10.

The worst 5 of 601 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:B:14:THR:HG23	3:B:503:HOH:O	1.17	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:PHE:HA	3:I:501:HOH:O	1.31	1.26
1:J:91:TYR:HA	3:J:501:HOH:O	1.35	1.26
1:F:170:ALA:HB3	3:F:506:HOH:O	1.35	1.24
1:H:155:SER:HA	3:H:503:HOH:O	1.27	1.24

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/428 (94%)	383 (95%)	21 (5%)	0	100	100
1	B	404/428 (94%)	385 (95%)	19 (5%)	0	100	100
1	C	404/428 (94%)	384 (95%)	20 (5%)	0	100	100
1	D	404/428 (94%)	384 (95%)	20 (5%)	0	100	100
1	E	404/428 (94%)	383 (95%)	21 (5%)	0	100	100
1	F	404/428 (94%)	383 (95%)	21 (5%)	0	100	100
1	G	404/428 (94%)	385 (95%)	19 (5%)	0	100	100
1	H	404/428 (94%)	383 (95%)	21 (5%)	0	100	100
1	I	404/428 (94%)	384 (95%)	20 (5%)	0	100	100
1	J	404/428 (94%)	380 (94%)	24 (6%)	0	100	100
All	All	4040/4280 (94%)	3834 (95%)	206 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/348 (94%)	328 (100%)	1 (0%)	86	93
1	B	329/348 (94%)	327 (99%)	2 (1%)	78	90
1	C	329/348 (94%)	327 (99%)	2 (1%)	78	90
1	D	329/348 (94%)	326 (99%)	3 (1%)	70	86
1	E	329/348 (94%)	325 (99%)	4 (1%)	63	82
1	F	329/348 (94%)	327 (99%)	2 (1%)	78	90
1	G	329/348 (94%)	325 (99%)	4 (1%)	63	82
1	H	329/348 (94%)	326 (99%)	3 (1%)	70	86
1	I	329/348 (94%)	325 (99%)	4 (1%)	63	82
1	J	329/348 (94%)	327 (99%)	2 (1%)	78	90
All	All	3290/3480 (94%)	3263 (99%)	27 (1%)	73	87

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	70	LEU
1	G	258	LEU
1	I	395	THR
1	G	226	CYS
1	H	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	351	ASN
1	J	82	HIS
1	E	242	HIS
1	E	114	GLN
1	J	242	HIS

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 ⓘ

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	K	1	2	11,11,12	0.26	0	15,15,17	0.53	0
2	FRU	K	2	2	11,12,12	0.54	0	10,18,18	0.92	0
2	FRU	K	3	2	11,11,12	0.39	0	15,15,18	1.17	1 (6%)
2	GLC	L	1	2	11,11,12	0.26	0	15,15,17	0.53	0
2	FRU	L	2	2	11,12,12	0.54	0	10,18,18	0.87	0
2	FRU	L	3	2	11,11,12	0.40	0	15,15,18	1.16	1 (6%)
2	GLC	M	1	2	11,11,12	0.25	0	15,15,17	0.50	0
2	FRU	M	2	2	11,12,12	0.57	0	10,18,18	0.87	0
2	FRU	M	3	2	11,11,12	0.39	0	15,15,18	1.18	1 (6%)
2	GLC	N	1	2	11,11,12	0.26	0	15,15,17	0.56	0
2	FRU	N	2	2	11,12,12	0.54	0	10,18,18	0.90	0
2	FRU	N	3	2	11,11,12	0.40	0	15,15,18	1.17	1 (6%)
2	GLC	O	1	2	11,11,12	0.25	0	15,15,17	0.51	0
2	FRU	O	2	2	11,12,12	0.58	0	10,18,18	0.88	0
2	FRU	O	3	2	11,11,12	0.39	0	15,15,18	1.17	1 (6%)
2	GLC	P	1	2	11,11,12	0.25	0	15,15,17	0.52	0
2	FRU	P	2	2	11,12,12	0.53	0	10,18,18	0.91	0
2	FRU	P	3	2	11,11,12	0.40	0	15,15,18	1.17	1 (6%)
2	GLC	Q	1	2	11,11,12	0.26	0	15,15,17	0.53	0
2	FRU	Q	2	2	11,12,12	0.58	0	10,18,18	0.87	0
2	FRU	Q	3	2	11,11,12	0.40	0	15,15,18	1.15	0
2	GLC	R	1	2	11,11,12	0.26	0	15,15,17	0.55	0
2	FRU	R	2	2	11,12,12	0.57	0	10,18,18	0.91	0
2	FRU	R	3	2	11,11,12	0.40	0	15,15,18	1.13	0
2	GLC	T	1	2	11,11,12	0.26	0	15,15,17	0.53	0
2	FRU	T	2	2	11,12,12	0.54	0	10,18,18	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FRU	T	3	2	11,11,12	0.39	0	15,15,18	1.14	1 (6%)
2	GLC	U	1	2	11,11,12	0.26	0	15,15,17	0.55	0
2	FRU	U	2	2	11,12,12	0.57	0	10,18,18	0.92	0
2	FRU	U	3	2	11,11,12	0.40	0	15,15,18	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	FRU	K	2	2	-	3/5/24/24	0/1/1/1
2	FRU	K	3	2	-	3/4/20/24	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	5/5/24/24	0/1/1/1
2	FRU	L	3	2	-	3/4/20/24	0/1/1/1
2	GLC	M	1	2	-	1/2/19/22	0/1/1/1
2	FRU	M	2	2	-	4/5/24/24	0/1/1/1
2	FRU	M	3	2	-	0/4/20/24	0/1/1/1
2	GLC	N	1	2	-	2/2/19/22	0/1/1/1
2	FRU	N	2	2	-	5/5/24/24	0/1/1/1
2	FRU	N	3	2	-	4/4/20/24	0/1/1/1
2	GLC	O	1	2	-	2/2/19/22	0/1/1/1
2	FRU	O	2	2	-	3/5/24/24	0/1/1/1
2	FRU	O	3	2	-	0/4/20/24	0/1/1/1
2	GLC	P	1	2	-	2/2/19/22	0/1/1/1
2	FRU	P	2	2	-	3/5/24/24	0/1/1/1
2	FRU	P	3	2	-	2/4/20/24	0/1/1/1
2	GLC	Q	1	2	-	2/2/19/22	0/1/1/1
2	FRU	Q	2	2	-	3/5/24/24	0/1/1/1
2	FRU	Q	3	2	-	3/4/20/24	0/1/1/1
2	GLC	R	1	2	-	2/2/19/22	0/1/1/1
2	FRU	R	2	2	-	3/5/24/24	0/1/1/1
2	FRU	R	3	2	-	2/4/20/24	0/1/1/1
2	GLC	T	1	2	-	0/2/19/22	0/1/1/1
2	FRU	T	2	2	-	5/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	T	3	2	-	3/4/20/24	0/1/1/1
2	GLC	U	1	2	-	2/2/19/22	0/1/1/1
2	FRU	U	2	2	-	4/5/24/24	0/1/1/1
2	FRU	U	3	2	-	2/4/20/24	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	FRU	C1-C2-C3	-2.08	110.18	115.10
2	K	3	FRU	C1-C2-C3	-2.06	110.22	115.10
2	O	3	FRU	C1-C2-C3	-2.05	110.27	115.10
2	N	3	FRU	C1-C2-C3	-2.04	110.27	115.10
2	P	3	FRU	C1-C2-C3	-2.04	110.27	115.10

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	FRU	O1-C1-C2-C3
2	K	2	FRU	O1-C1-C2-O2
2	L	2	FRU	O1-C1-C2-C3
2	L	2	FRU	O1-C1-C2-O2
2	M	2	FRU	O1-C1-C2-C3

There are no ring outliers.

28 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	GLC	1	0
2	Q	2	FRU	5	0
2	L	1	GLC	2	0
2	N	1	GLC	1	0
2	P	3	FRU	4	0
2	P	2	FRU	1	0
2	O	2	FRU	2	0
2	R	1	GLC	1	0
2	M	3	FRU	6	0
2	R	3	FRU	3	0
2	M	2	FRU	3	0

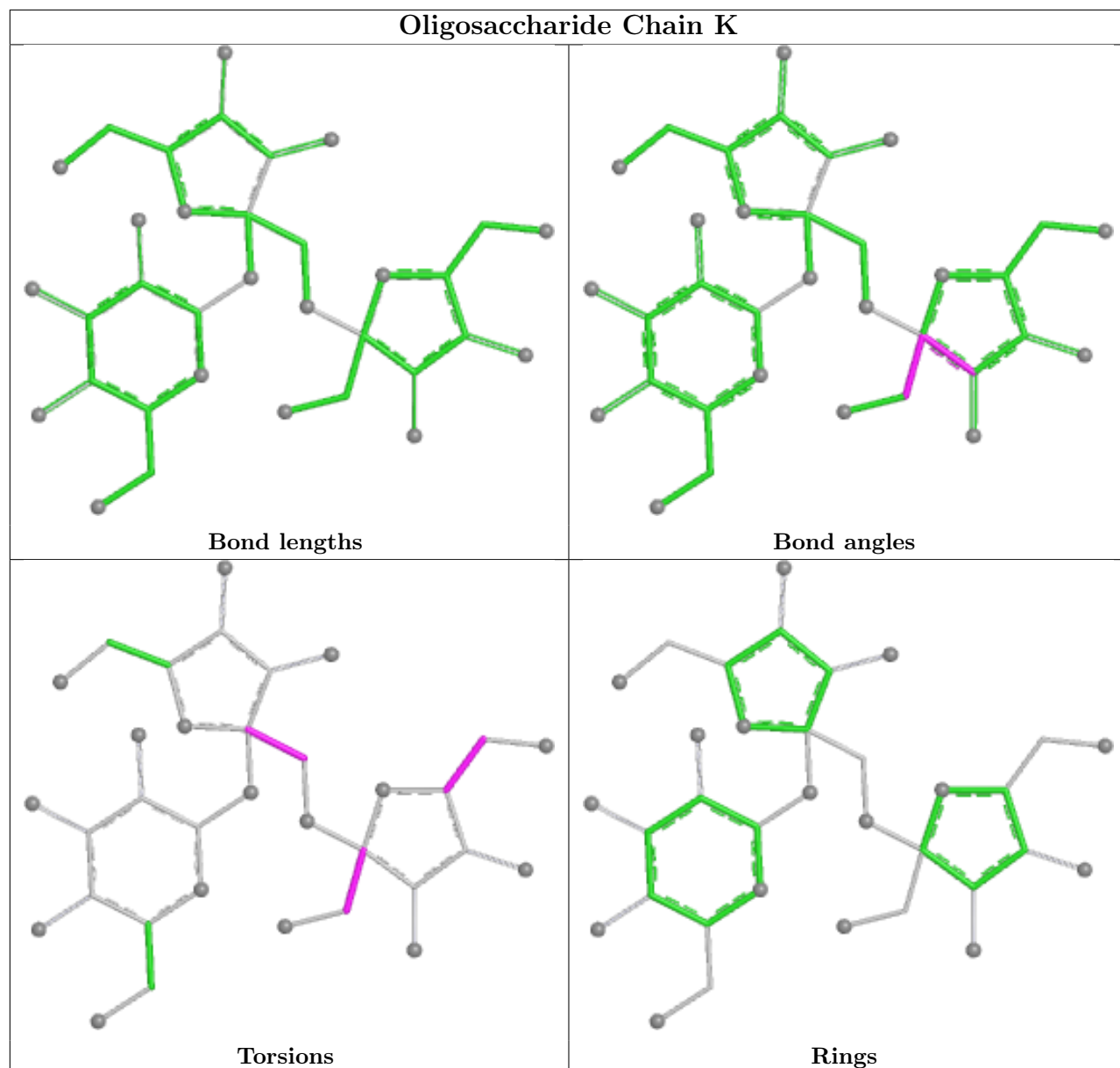
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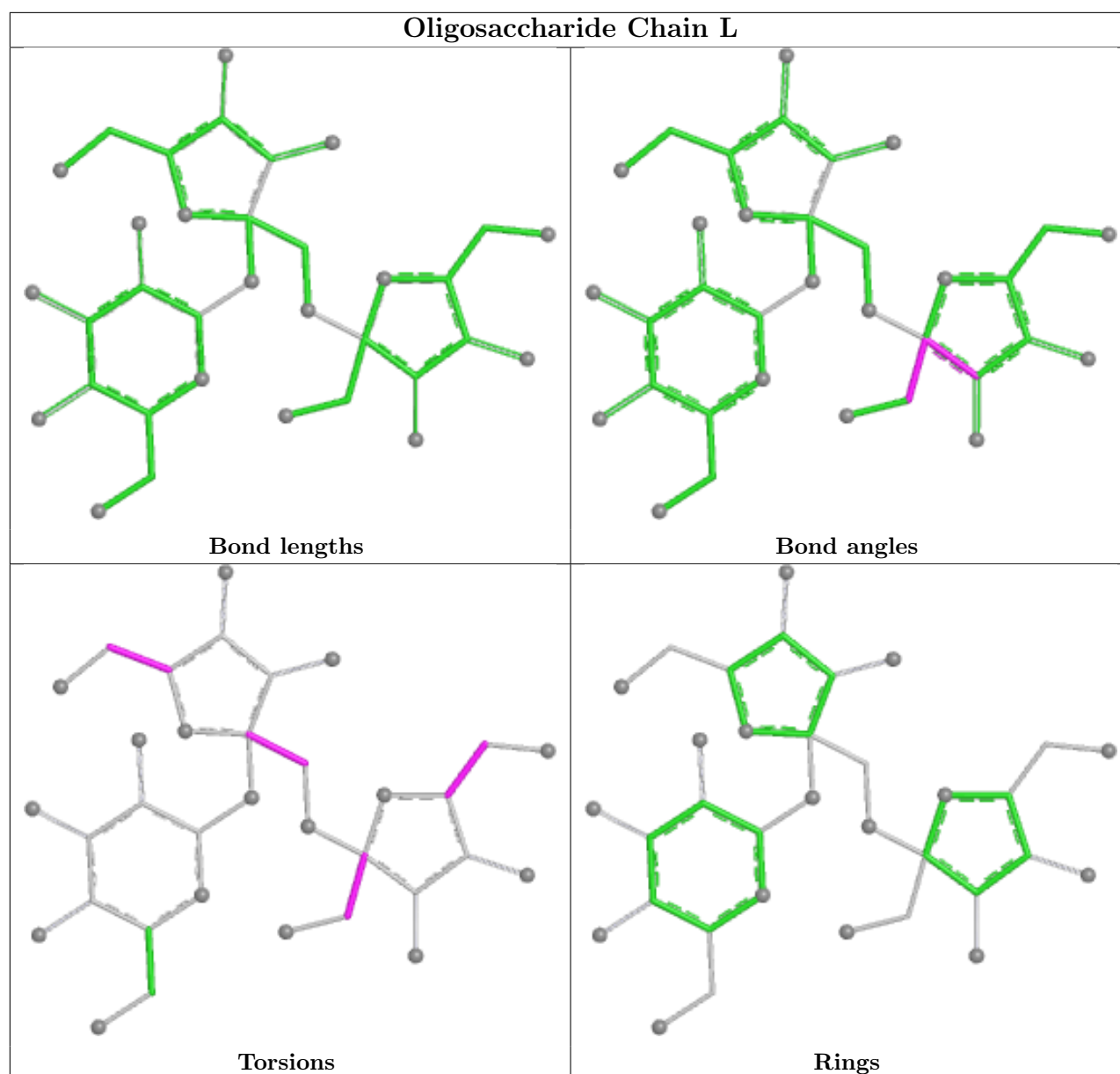
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	GLC	1	0
2	L	2	FRU	3	0
2	N	2	FRU	1	0
2	O	1	GLC	3	0
2	R	2	FRU	2	0
2	Q	3	FRU	7	0
2	O	3	FRU	3	0
2	U	3	FRU	3	0
2	T	1	GLC	1	0
2	T	3	FRU	6	0
2	T	2	FRU	4	0
2	K	2	FRU	1	0
2	K	3	FRU	3	0
2	L	3	FRU	2	0
2	N	3	FRU	3	0
2	M	1	GLC	4	0
2	Q	1	GLC	7	0

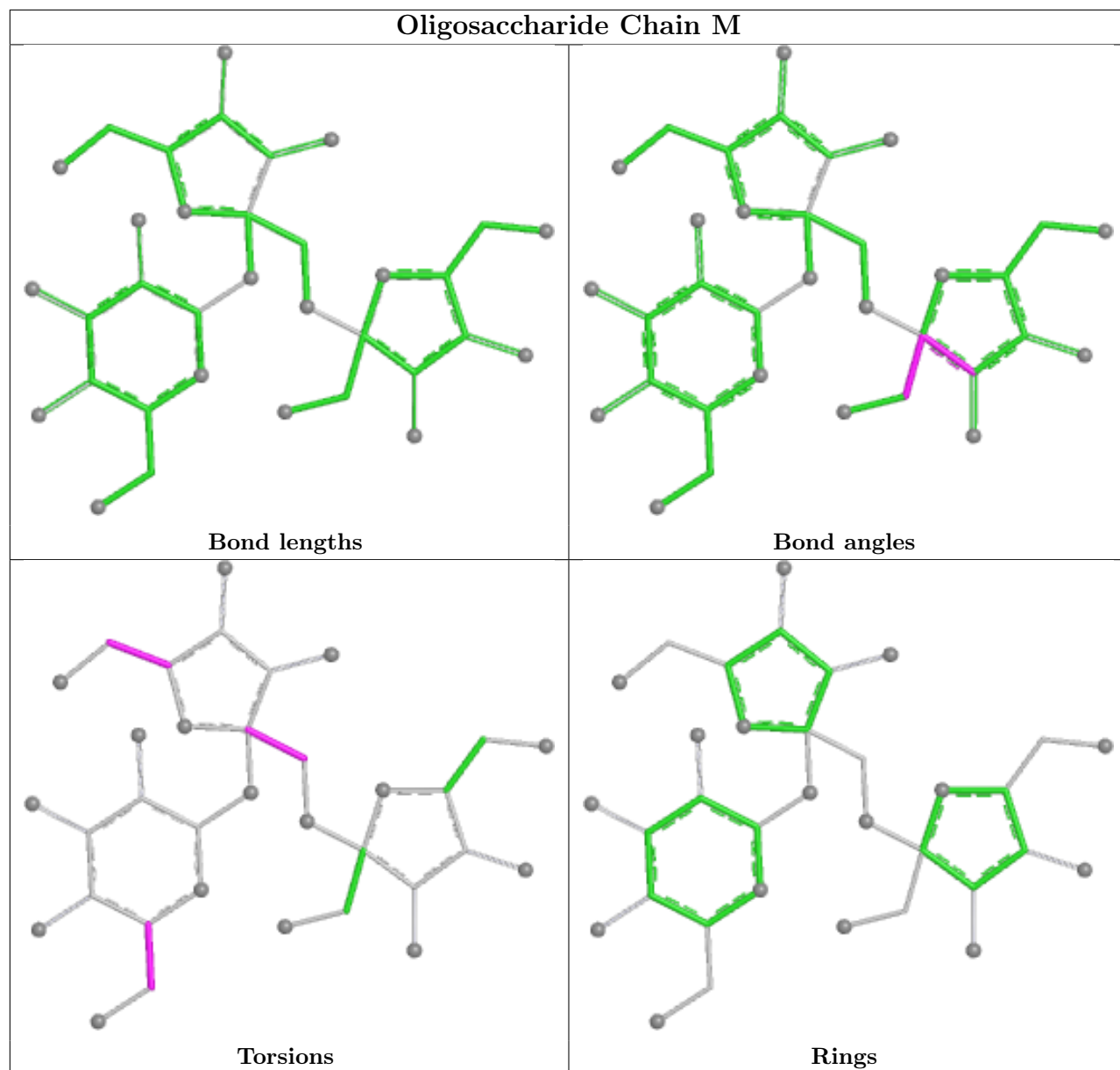
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

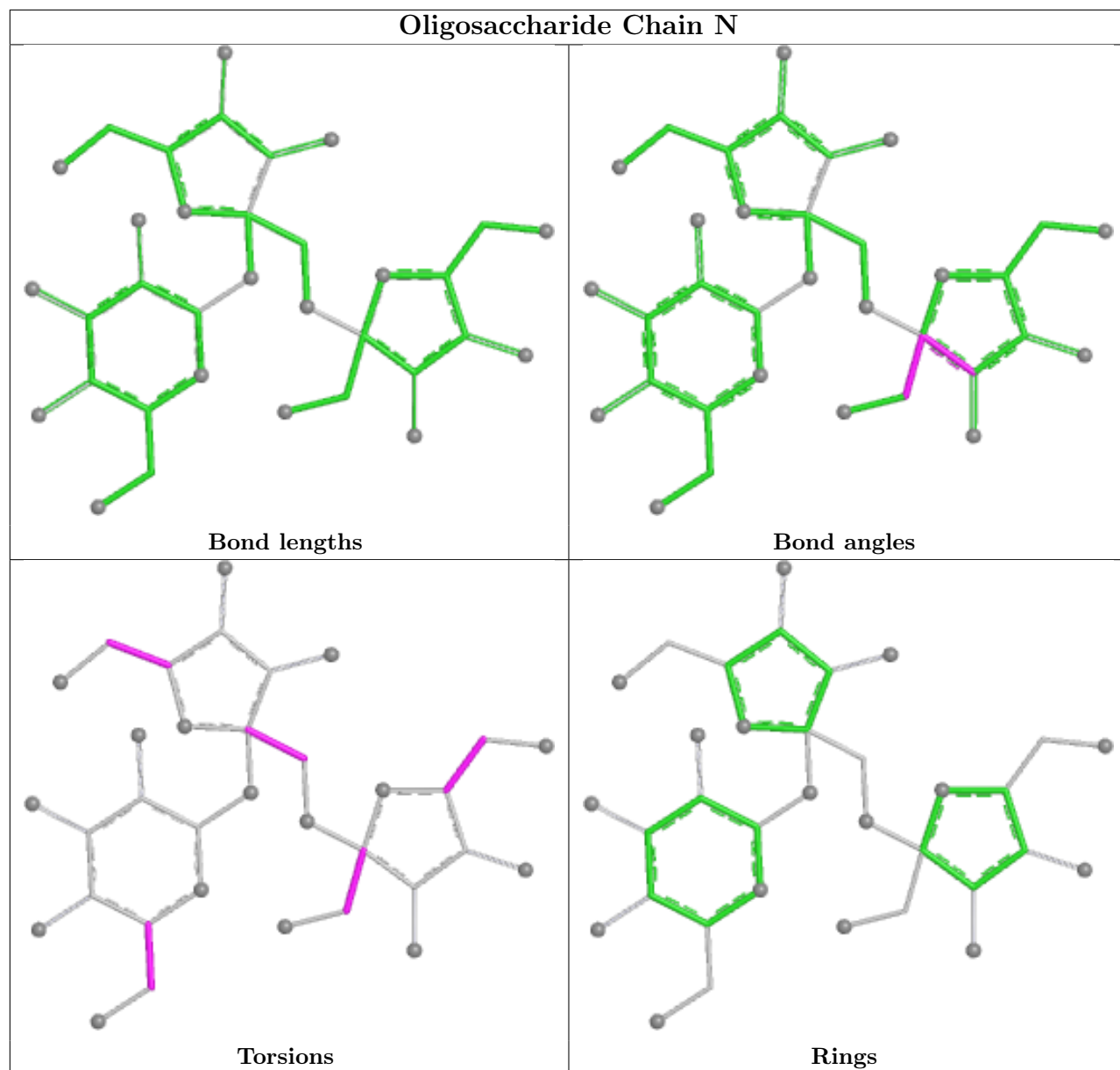
Oligosaccharide Chain K

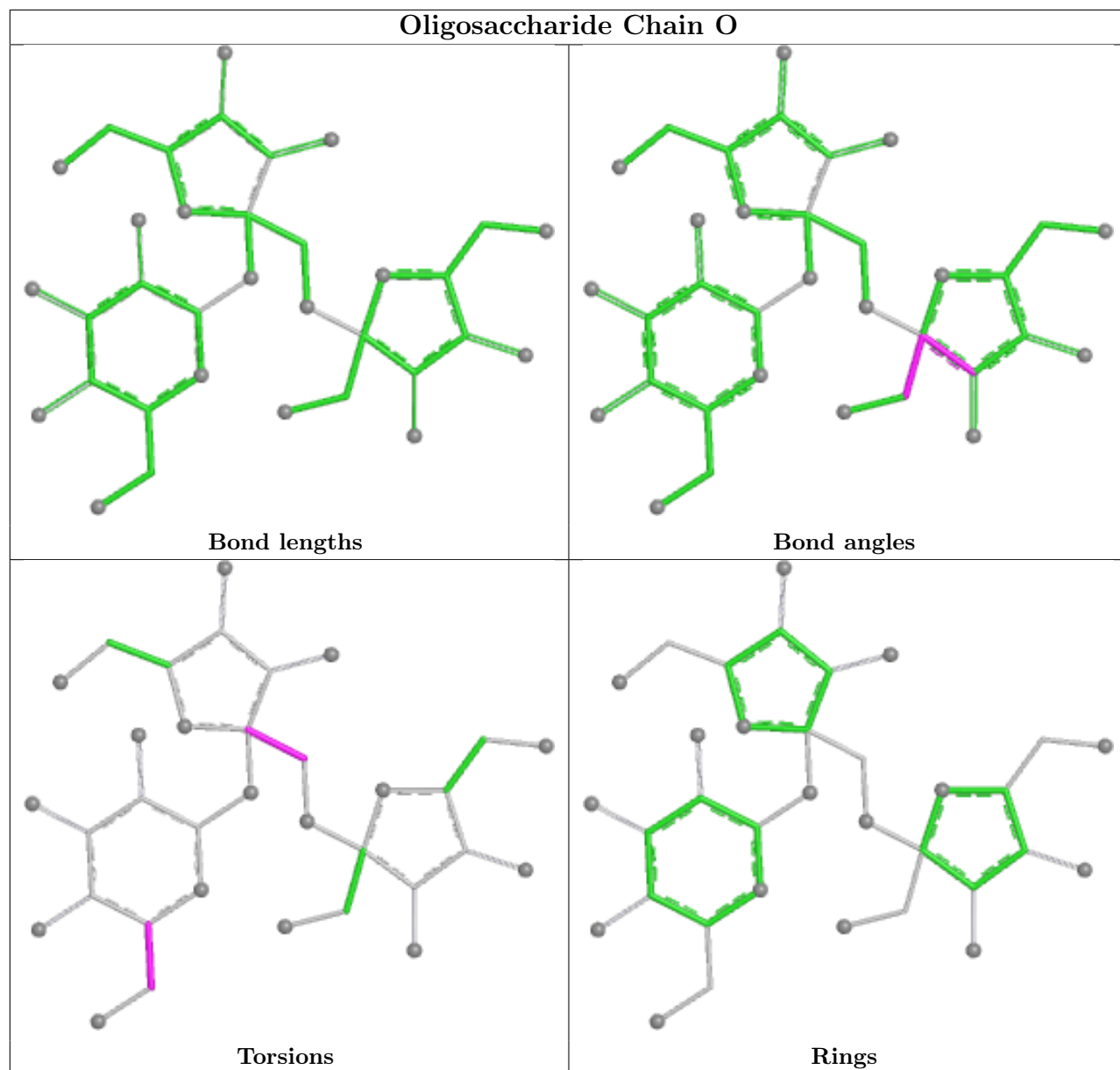


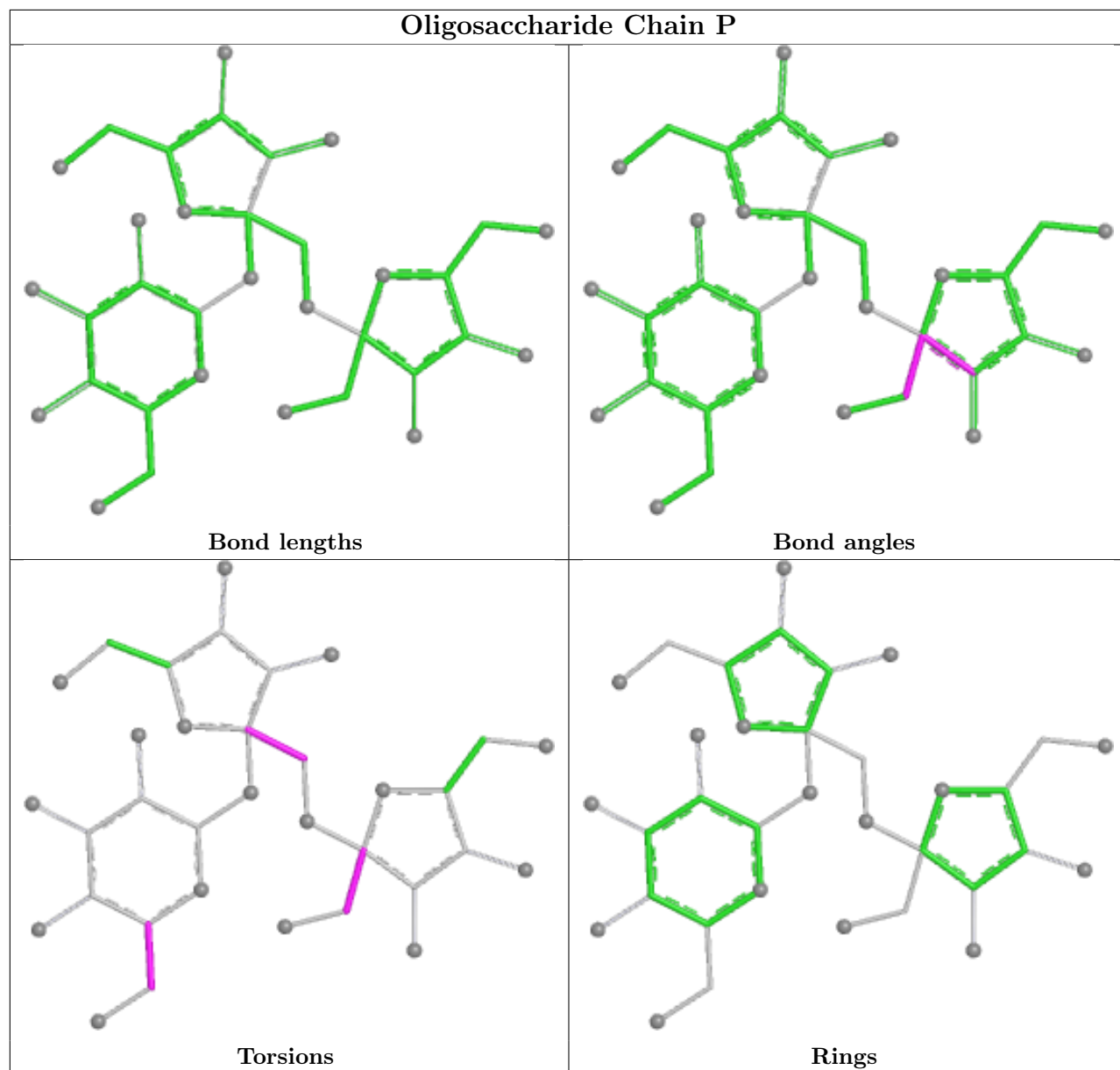


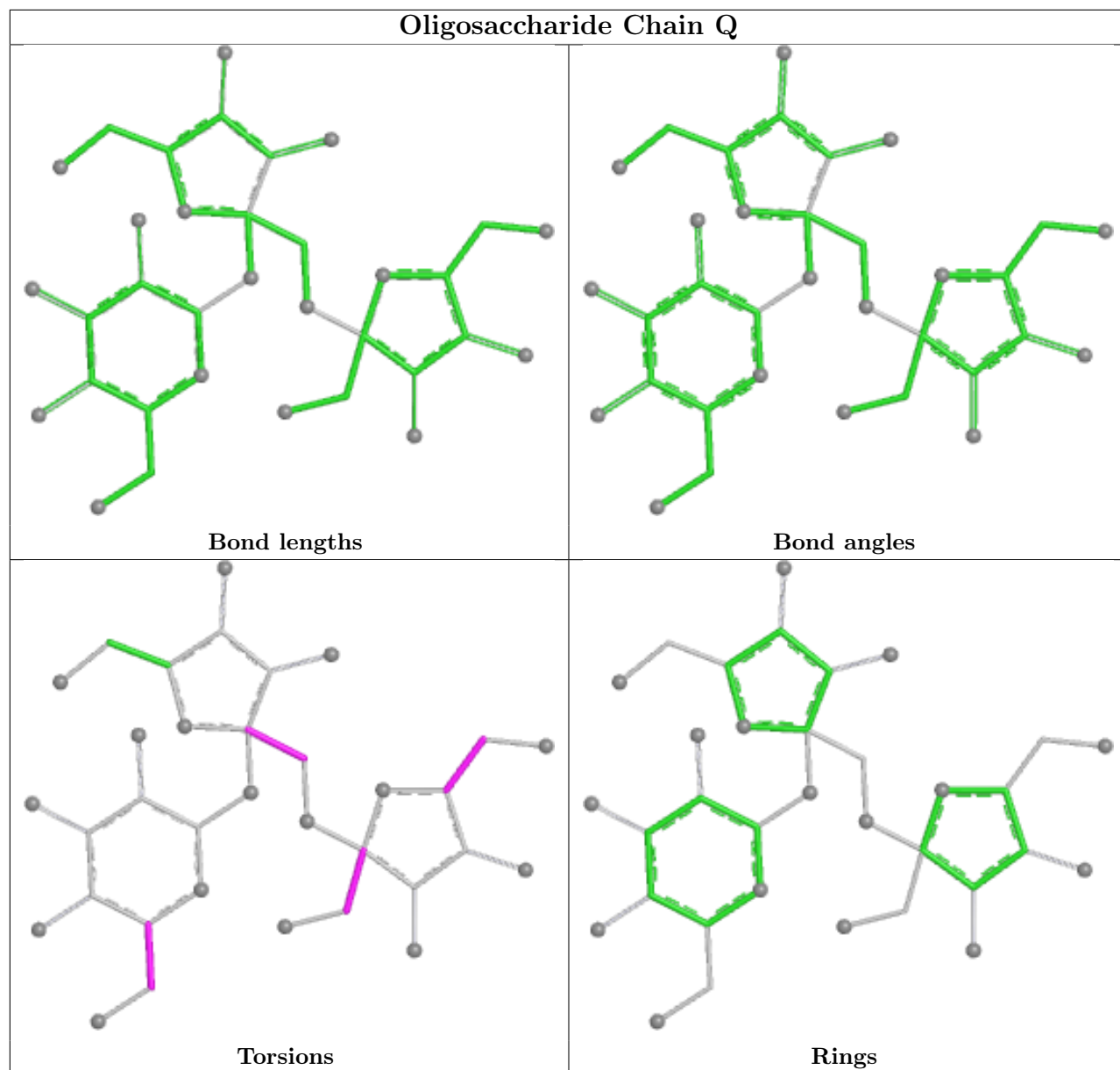
Oligosaccharide Chain M

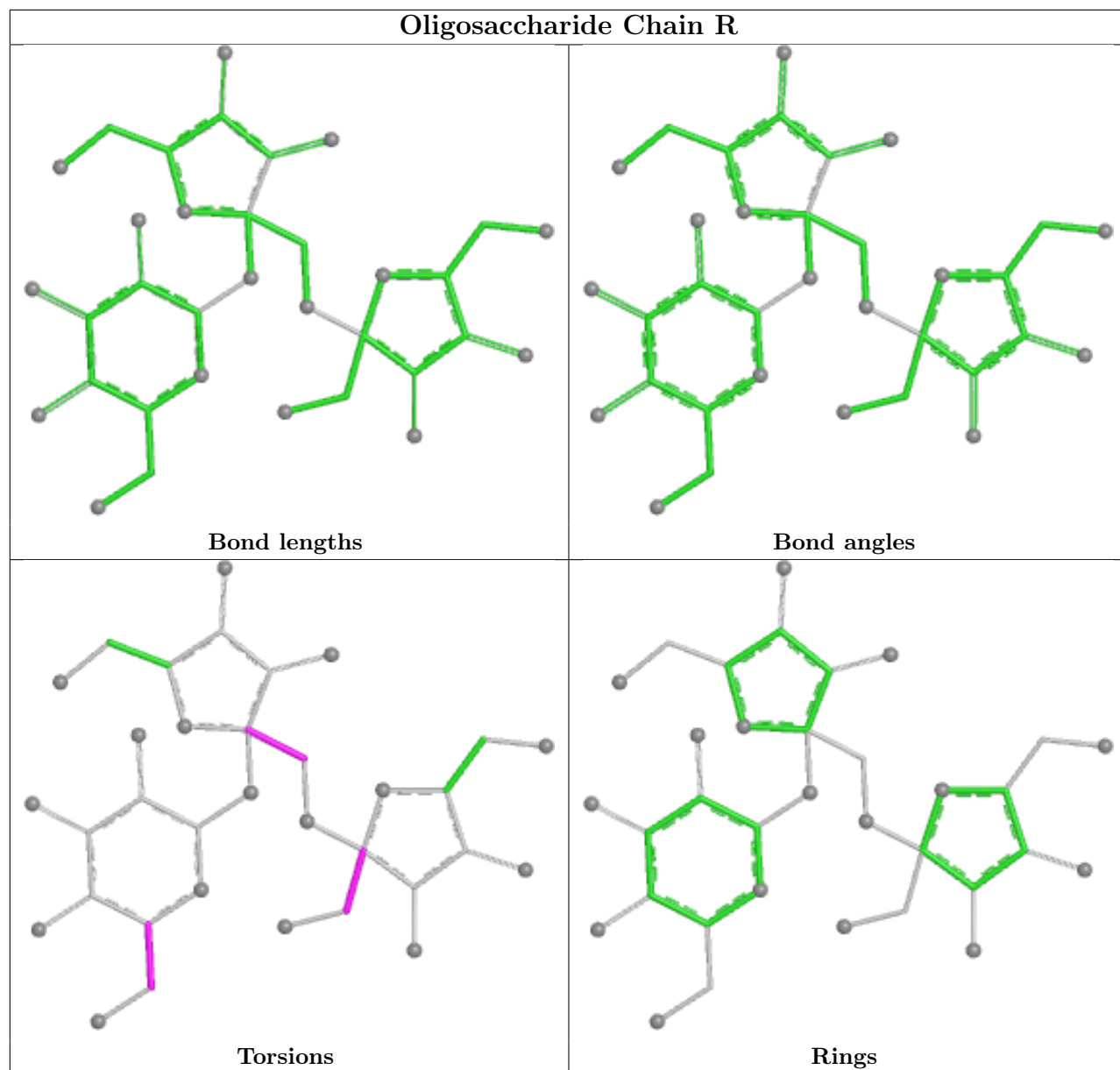


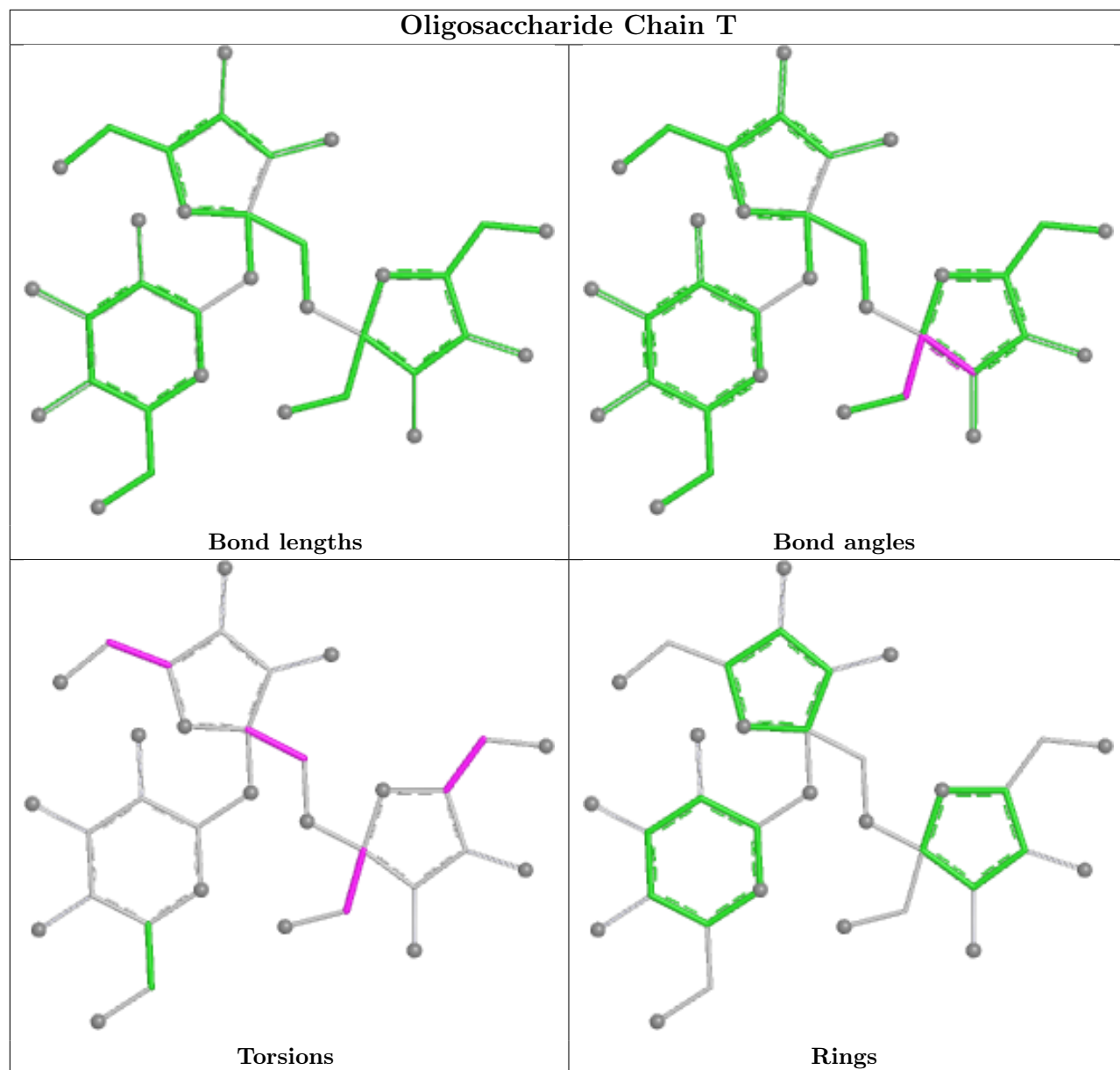


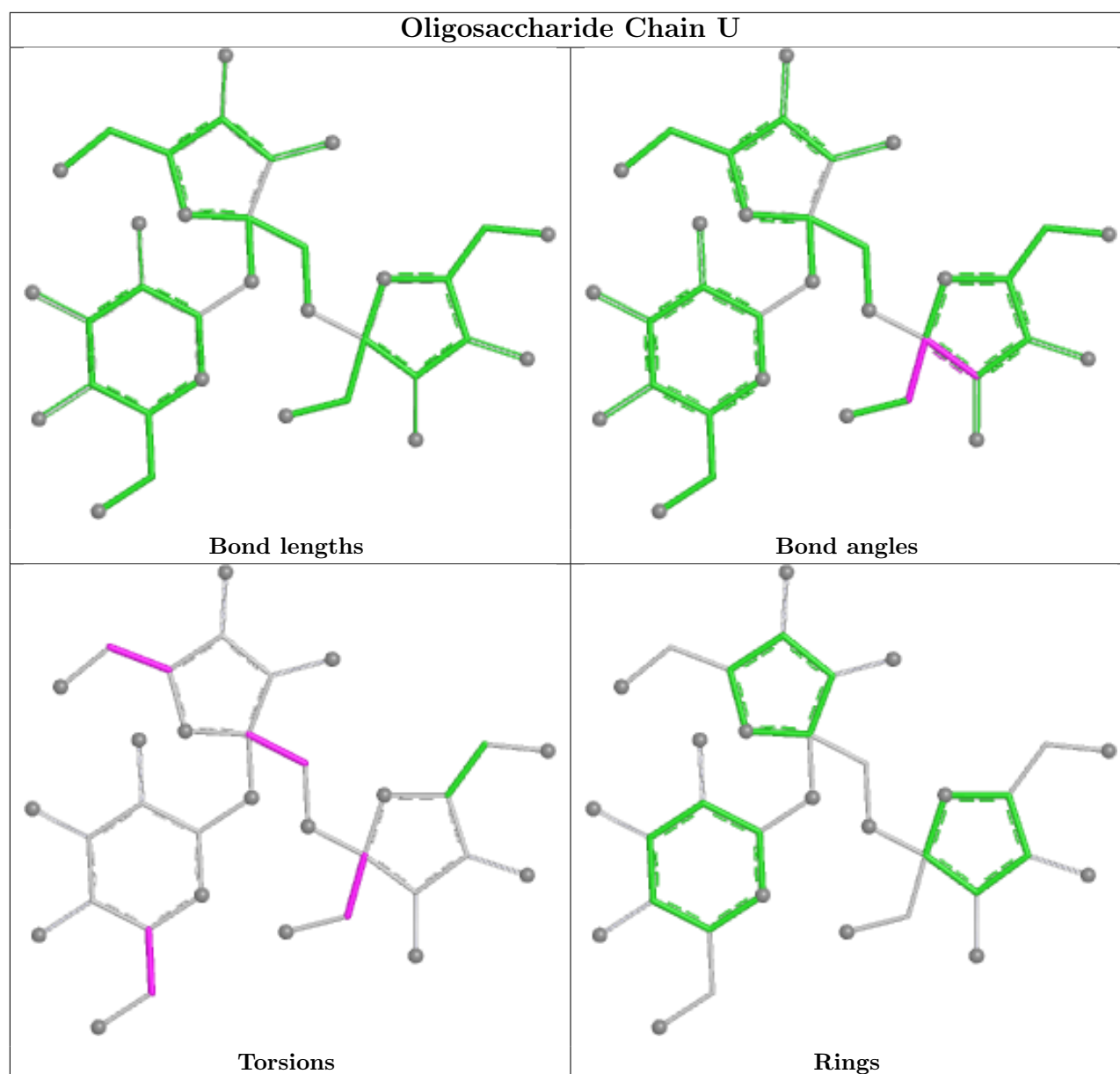












5.6 Ligand geometry [i](#)

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	406/428 (94%)	-0.34	2 (0%) 87 86	34, 51, 77, 94	0
1	B	406/428 (94%)	0.14	7 (1%) 69 66	43, 77, 118, 135	0
1	C	406/428 (94%)	-0.31	2 (0%) 87 86	37, 56, 81, 93	0
1	D	406/428 (94%)	-0.41	0 100 100	28, 47, 70, 89	0
1	E	406/428 (94%)	-0.35	2 (0%) 87 86	28, 50, 81, 104	0
1	F	406/428 (94%)	-0.23	2 (0%) 87 86	37, 57, 83, 106	0
1	G	406/428 (94%)	-0.00	5 (1%) 76 75	43, 73, 109, 128	0
1	H	406/428 (94%)	0.04	4 (0%) 79 78	37, 72, 113, 136	0
1	I	406/428 (94%)	0.02	7 (1%) 69 66	44, 72, 103, 121	0
1	J	406/428 (94%)	-0.24	2 (0%) 87 86	37, 54, 77, 94	0
All	All	4060/4280 (94%)	-0.17	33 (0%) 82 81	28, 58, 102, 136	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	PRO	4.1
1	A	414	PRO	3.7
1	C	414	PRO	3.1
1	G	360	LEU	3.1
1	B	168	PRO	3.0

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

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

6.3 Carbohydrates ⓘ

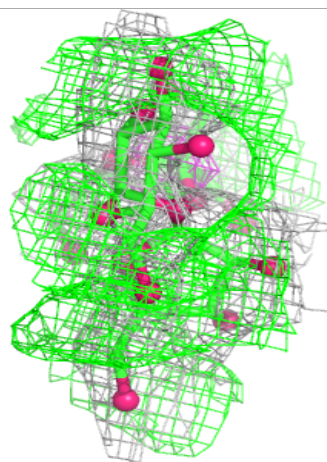
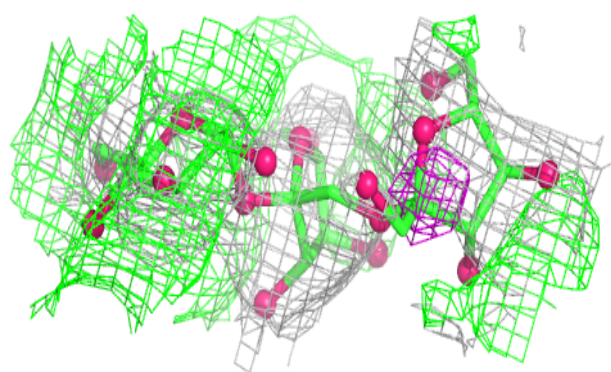
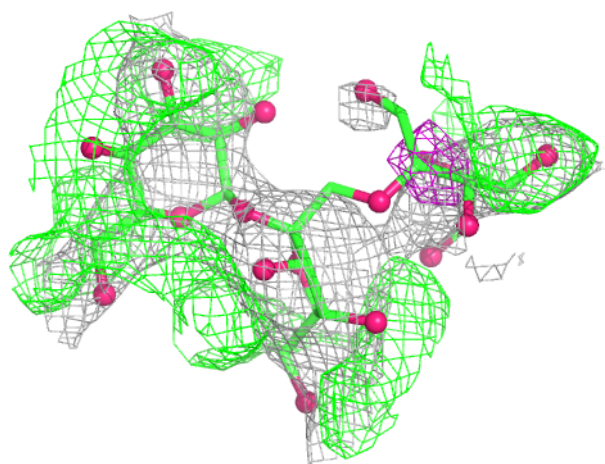
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	R	2	12/12	0.59	0.23	45,49,62,63	12
2	GLC	N	1	11/12	0.60	0.31	45,58,75,83	11
2	GLC	T	1	11/12	0.60	0.29	45,49,63,70	11
2	GLC	M	1	11/12	0.61	0.27	45,53,63,69	11
2	GLC	O	1	11/12	0.63	0.33	45,45,66,70	11
2	GLC	P	1	11/12	0.63	0.29	45,51,63,73	11
2	FRU	O	2	12/12	0.65	0.22	45,54,66,70	12
2	GLC	R	1	11/12	0.65	0.26	45,45,56,61	11
2	GLC	K	1	11/12	0.68	0.28	45,46,65,78	11
2	FRU	K	2	12/12	0.68	0.18	45,50,63,64	12
2	FRU	L	2	12/12	0.70	0.17	45,56,62,65	12
2	FRU	T	2	12/12	0.70	0.20	45,53,62,66	12
2	GLC	L	1	11/12	0.73	0.24	45,47,62,63	11
2	GLC	Q	1	11/12	0.73	0.27	45,52,65,66	11
2	FRU	N	2	12/12	0.75	0.18	45,47,57,61	12
2	FRU	M	3	11/12	0.76	0.25	45,47,57,58	11
2	FRU	Q	3	11/12	0.76	0.30	45,54,69,72	11
2	FRU	Q	2	12/12	0.77	0.23	47,57,67,70	12
2	FRU	K	3	11/12	0.78	0.23	45,48,62,64	11
2	FRU	M	2	12/12	0.82	0.15	45,50,60,61	12
2	FRU	T	3	11/12	0.82	0.24	45,49,58,60	11
2	FRU	R	3	11/12	0.85	0.19	45,49,54,55	11
2	FRU	P	2	12/12	0.85	0.18	45,54,60,64	12
2	FRU	P	3	11/12	0.86	0.21	45,50,63,73	11
2	FRU	O	3	11/12	0.86	0.23	45,45,60,63	11
2	FRU	N	3	11/12	0.88	0.19	45,45,52,54	11
2	FRU	L	3	11/12	0.88	0.23	45,54,70,75	11
2	GLC	U	1	11/12	-	-	45,46,66,68	11
2	FRU	U	2	12/12	-	-	45,54,58,60	12
2	FRU	U	3	11/12	-	-	45,51,57,60	11

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.

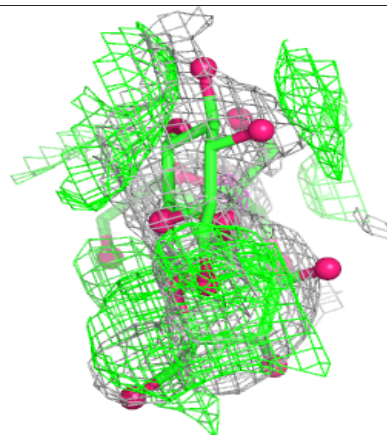
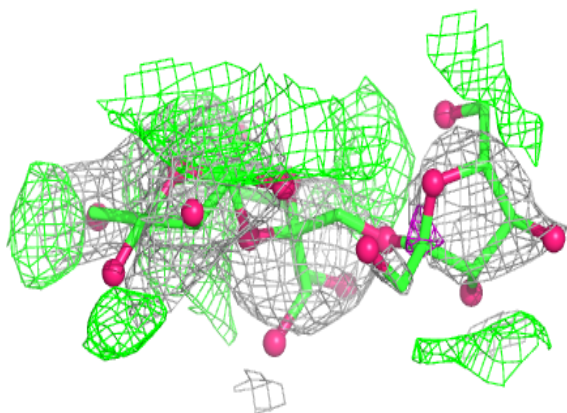
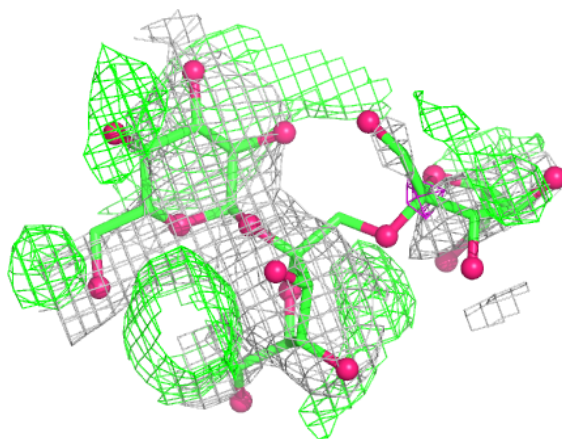
Electron density around Chain K:

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



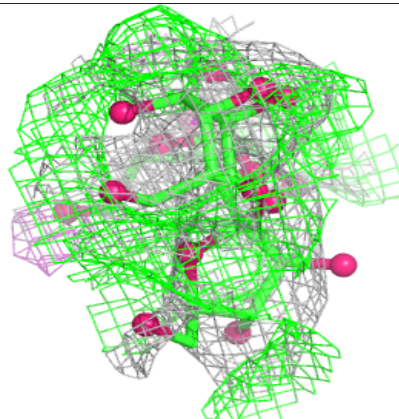
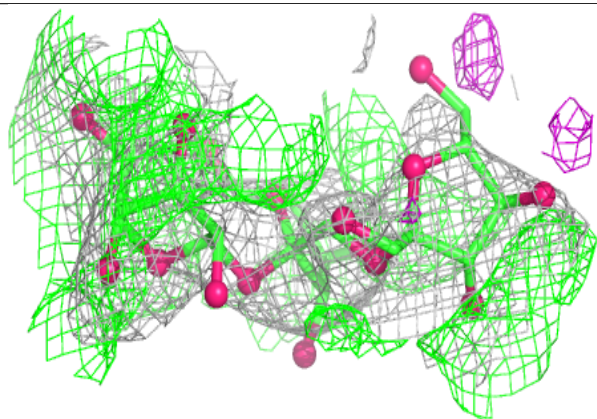
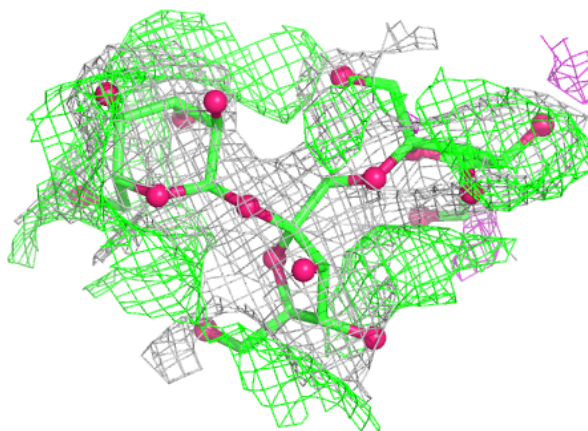
Electron density around Chain L:

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and green (positive)



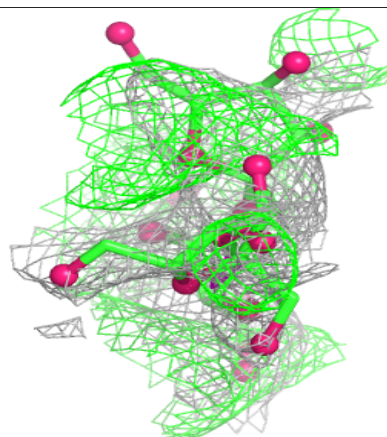
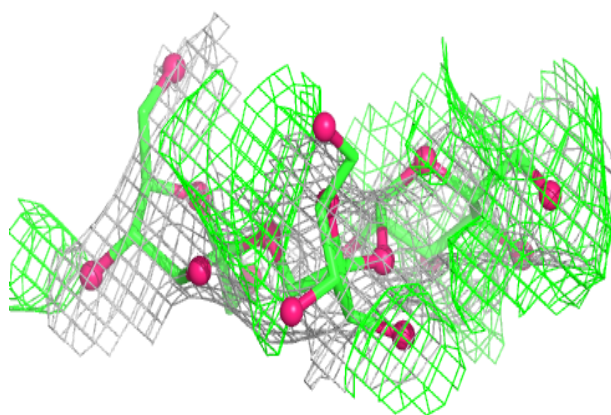
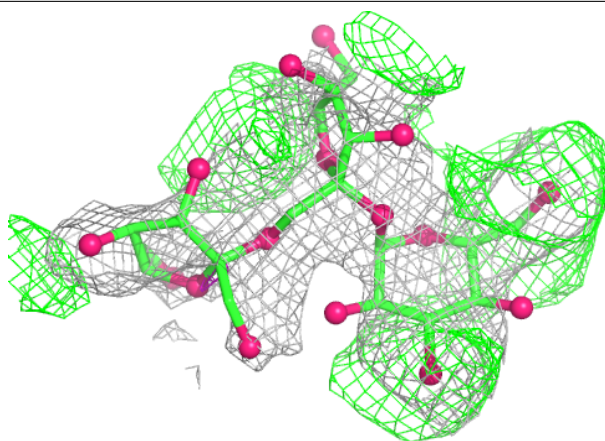
Electron density around Chain M:

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



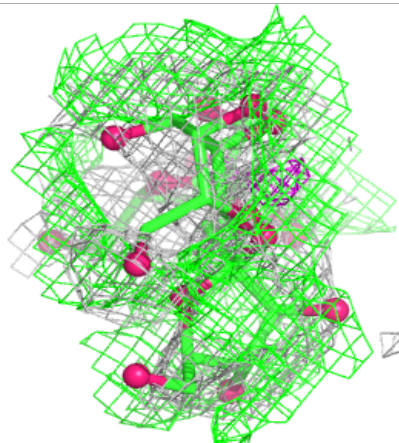
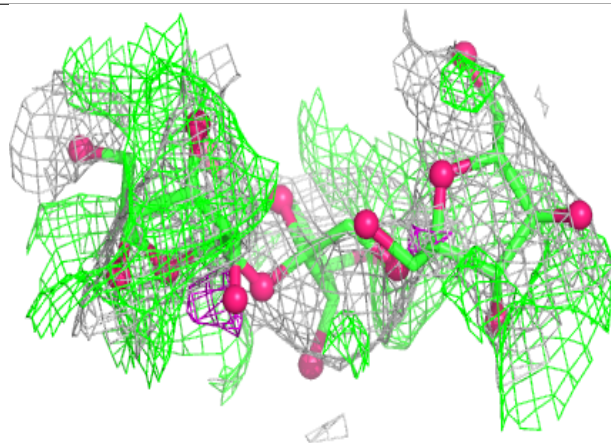
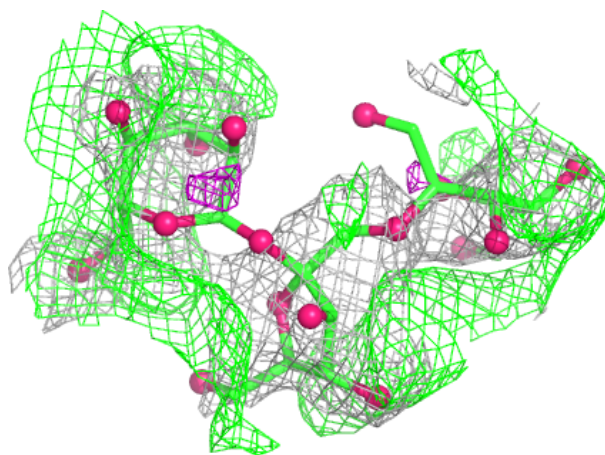
Electron density around Chain N:

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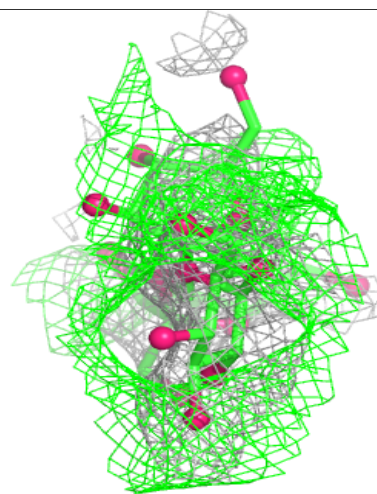
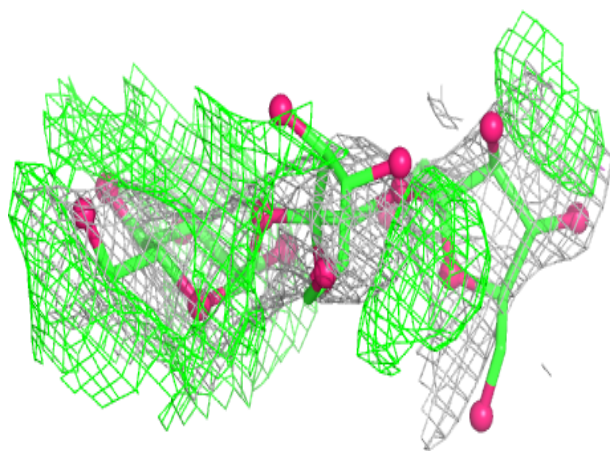
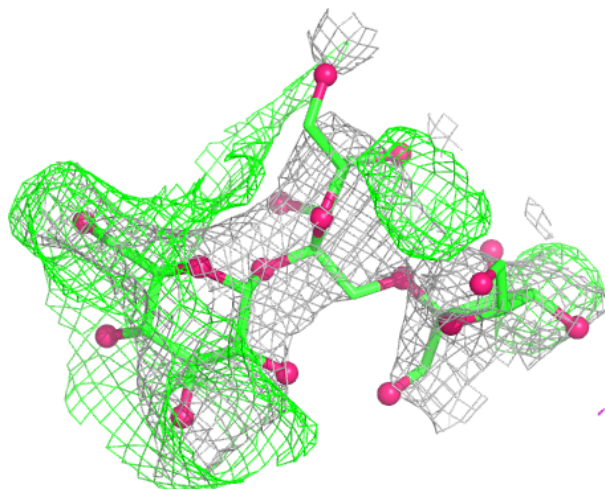
Electron density around Chain O:

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



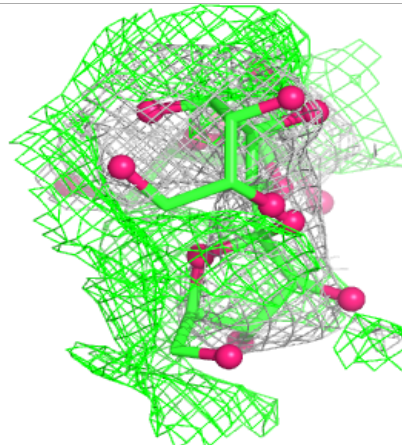
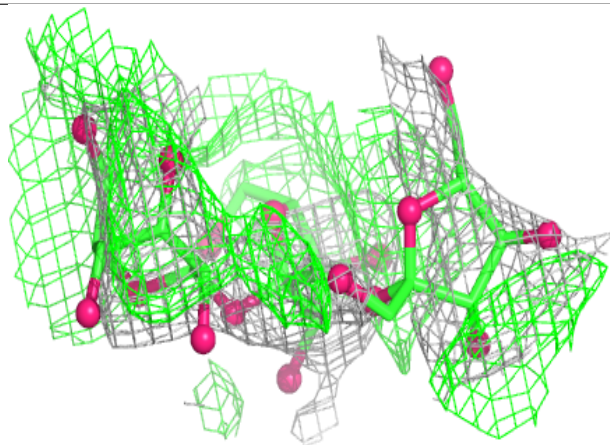
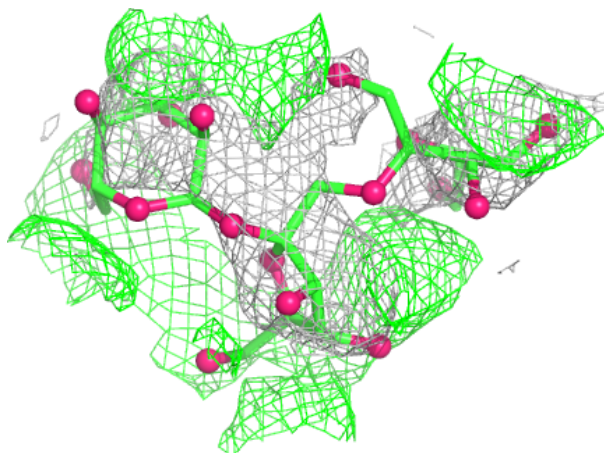
Electron density around Chain P:

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and green (positive)



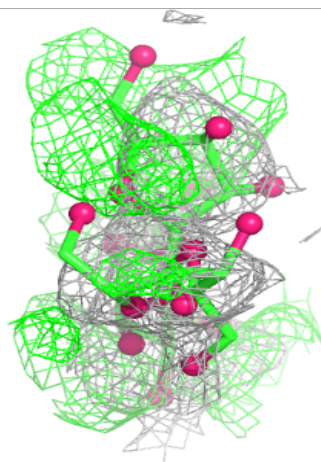
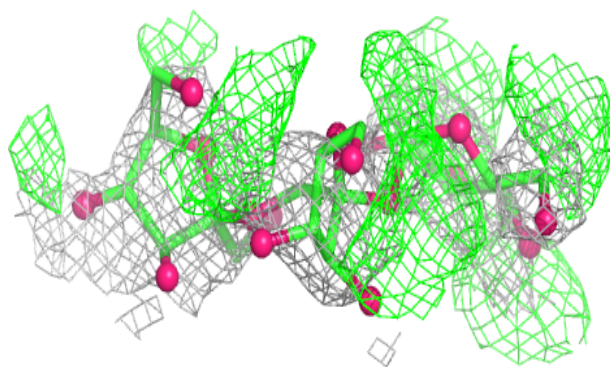
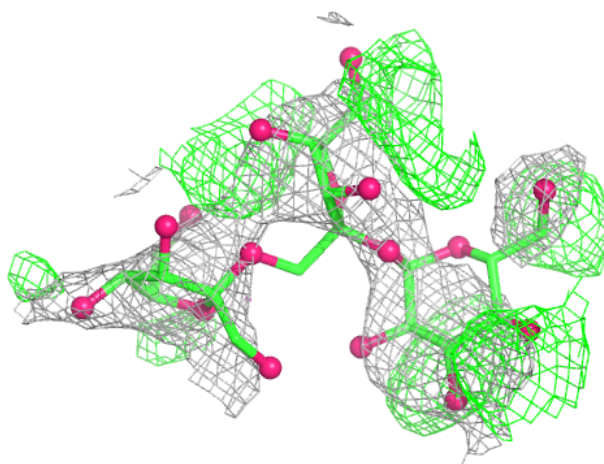
Electron density around Chain Q:

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and green (positive)



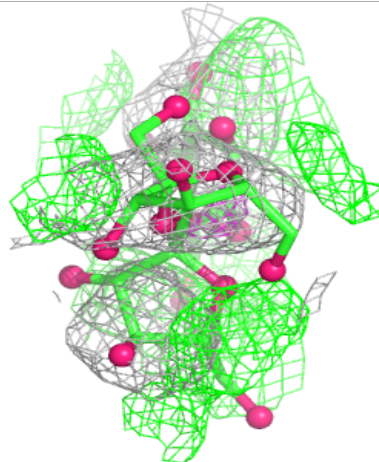
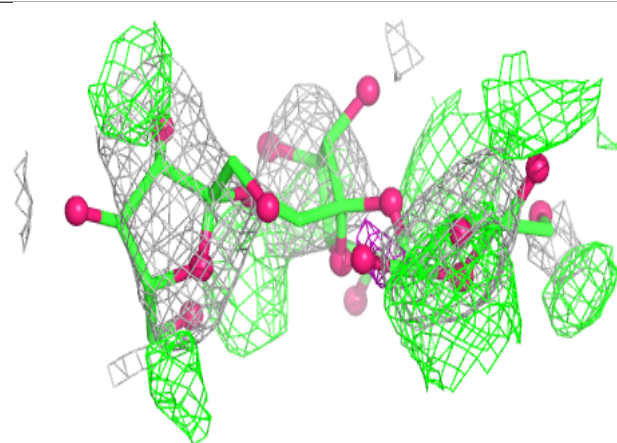
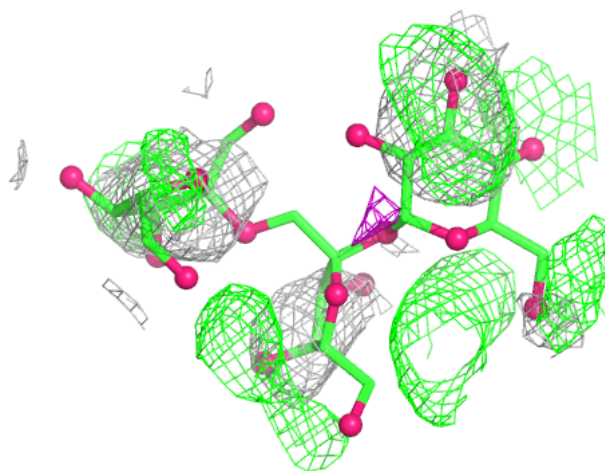
Electron density around Chain R:

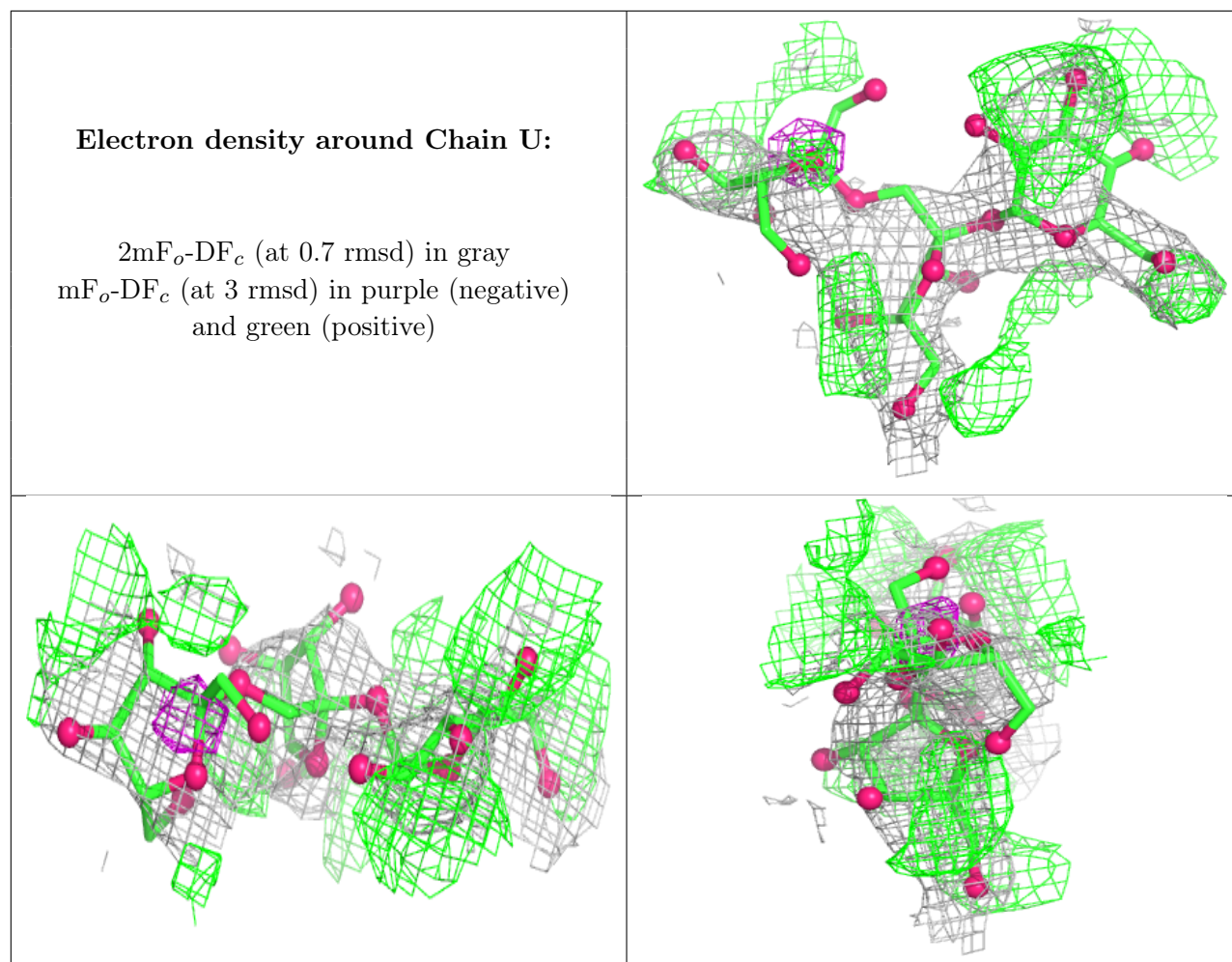
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.