



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:35 AM UTC

PDB ID : 5EVM / pdb\_00005evm  
Title : Crystal Structure of Nipah Virus Fusion Glycoprotein in the Prefusion State  
Authors : Xu, K.; Nikolov, D.B.  
Deposited on : 2015-11-20  
Resolution : 3.37 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](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

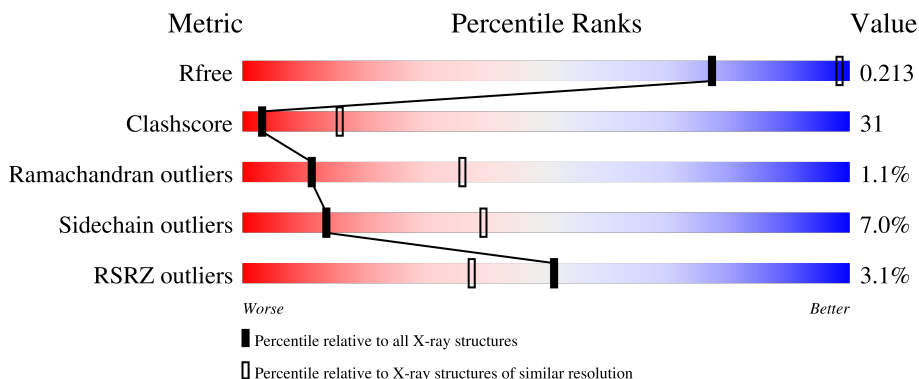
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	A	529	 2% 44% 38% 14%
1	B	529	 2% 42% 39% 5% 14%
1	C	529	 4% 39% 42% 5% 15%
1	D	529	 3% 41% 40% 5% 14%
1	E	529	 2% 41% 40% 5% 14%

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Mol	Chain	Length	Quality of chain
1	F	529	 4% 38% 42% 5% 15%
2	G	5	 40% 60%
3	H	2	 100%
3	N	2	 50% 50%
3	O	2	 50% 50%
3	U	2	 50% 50%
3	V	2	 50% 50%
4	I	3	 33% 67%
4	J	3	 67% 33%
4	K	3	 33% 67%
4	R	3	 33% 67%
4	S	3	 67% 33%
4	W	3	 67% 33%
5	L	5	 80% 20%
5	X	5	 80% 20%
6	M	5	 20% 20% 60%
7	P	4	 50% 50%
8	Q	4	 75% 25%
8	T	4	 50% 50%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21612 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3482	2204	571	687	20	0	0	0
1	B	456	3478	2202	571	685	20	0	0	0
1	C	450	3439	2178	562	679	20	0	0	0
1	D	456	3482	2204	571	687	20	0	0	0
1	E	456	3482	2204	571	687	20	0	0	0
1	F	450	3439	2178	562	679	20	0	0	0

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	engineered mutation	UNP Q9IH63
A	305	ASP	ASN	engineered mutation	UNP Q9IH63
A	532	LYS	-	expression tag	UNP Q9IH63
A	533	LEU	-	expression tag	UNP Q9IH63
A	534	MET	-	expression tag	UNP Q9IH63
A	535	LYS	-	expression tag	UNP Q9IH63
A	536	GLN	-	expression tag	UNP Q9IH63
A	537	ILE	-	expression tag	UNP Q9IH63
A	538	GLU	-	expression tag	UNP Q9IH63
A	539	ASP	-	expression tag	UNP Q9IH63
A	540	LYS	-	expression tag	UNP Q9IH63
A	541	ILE	-	expression tag	UNP Q9IH63
A	542	GLU	-	expression tag	UNP Q9IH63
A	543	GLU	-	expression tag	UNP Q9IH63
A	544	ILE	-	expression tag	UNP Q9IH63
A	545	LEU	-	expression tag	UNP Q9IH63
A	546	SER	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
A	547	LYS	-	expression tag	UNP Q9IH63
A	548	ILE	-	expression tag	UNP Q9IH63
A	549	TYR	-	expression tag	UNP Q9IH63
A	550	HIS	-	expression tag	UNP Q9IH63
A	551	ILE	-	expression tag	UNP Q9IH63
A	552	GLU	-	expression tag	UNP Q9IH63
A	553	ASN	-	expression tag	UNP Q9IH63
A	554	GLU	-	expression tag	UNP Q9IH63
A	555	ILE	-	expression tag	UNP Q9IH63
A	556	ALA	-	expression tag	UNP Q9IH63
A	557	ARG	-	expression tag	UNP Q9IH63
A	558	ILE	-	expression tag	UNP Q9IH63
A	559	LYS	-	expression tag	UNP Q9IH63
A	560	LYS	-	expression tag	UNP Q9IH63
A	561	LEU	-	expression tag	UNP Q9IH63
A	562	ILE	-	expression tag	UNP Q9IH63
A	563	GLY	-	expression tag	UNP Q9IH63
A	564	GLU	-	expression tag	UNP Q9IH63
A	565	ALA	-	expression tag	UNP Q9IH63
A	566	PRO	-	expression tag	UNP Q9IH63
A	567	GLY	-	expression tag	UNP Q9IH63
A	568	GLY	-	expression tag	UNP Q9IH63
A	569	ILE	-	expression tag	UNP Q9IH63
A	570	GLU	-	expression tag	UNP Q9IH63
A	571	GLY	-	expression tag	UNP Q9IH63
A	572	ARG	-	expression tag	UNP Q9IH63
B	67	ASP	ASN	engineered mutation	UNP Q9IH63
B	305	ASP	ASN	engineered mutation	UNP Q9IH63
B	489	LYS	-	expression tag	UNP Q9IH63
B	490	LEU	-	expression tag	UNP Q9IH63
B	491	MET	-	expression tag	UNP Q9IH63
B	492	LYS	-	expression tag	UNP Q9IH63
B	493	GLN	-	expression tag	UNP Q9IH63
B	494	ILE	-	expression tag	UNP Q9IH63
B	495	GLU	-	expression tag	UNP Q9IH63
B	496	ASP	-	expression tag	UNP Q9IH63
B	497	LYS	-	expression tag	UNP Q9IH63
B	498	ILE	-	expression tag	UNP Q9IH63
B	499	GLU	-	expression tag	UNP Q9IH63
B	500	GLU	-	expression tag	UNP Q9IH63
B	501	ILE	-	expression tag	UNP Q9IH63
B	502	LEU	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	SER	-	expression tag	UNP Q9IH63
B	504	LYS	-	expression tag	UNP Q9IH63
B	505	ILE	-	expression tag	UNP Q9IH63
B	506	TYR	-	expression tag	UNP Q9IH63
B	507	HIS	-	expression tag	UNP Q9IH63
B	508	ILE	-	expression tag	UNP Q9IH63
B	509	GLU	-	expression tag	UNP Q9IH63
B	510	ASN	-	expression tag	UNP Q9IH63
B	511	GLU	-	expression tag	UNP Q9IH63
B	512	ILE	-	expression tag	UNP Q9IH63
B	513	ALA	-	expression tag	UNP Q9IH63
B	514	ARG	-	expression tag	UNP Q9IH63
B	515	ILE	-	expression tag	UNP Q9IH63
B	516	LYS	-	expression tag	UNP Q9IH63
B	517	LYS	-	expression tag	UNP Q9IH63
B	518	LEU	-	expression tag	UNP Q9IH63
B	519	ILE	-	expression tag	UNP Q9IH63
B	520	GLY	-	expression tag	UNP Q9IH63
B	521	GLU	-	expression tag	UNP Q9IH63
B	522	ALA	-	expression tag	UNP Q9IH63
B	523	PRO	-	expression tag	UNP Q9IH63
B	524	GLY	-	expression tag	UNP Q9IH63
B	525	GLY	-	expression tag	UNP Q9IH63
B	526	ILE	-	expression tag	UNP Q9IH63
B	527	GLU	-	expression tag	UNP Q9IH63
B	528	GLY	-	expression tag	UNP Q9IH63
B	529	ARG	-	expression tag	UNP Q9IH63
C	67	ASP	ASN	engineered mutation	UNP Q9IH63
C	305	ASP	ASN	engineered mutation	UNP Q9IH63
C	489	LYS	-	expression tag	UNP Q9IH63
C	490	LEU	-	expression tag	UNP Q9IH63
C	491	MET	-	expression tag	UNP Q9IH63
C	492	LYS	-	expression tag	UNP Q9IH63
C	493	GLN	-	expression tag	UNP Q9IH63
C	494	ILE	-	expression tag	UNP Q9IH63
C	495	GLU	-	expression tag	UNP Q9IH63
C	496	ASP	-	expression tag	UNP Q9IH63
C	497	LYS	-	expression tag	UNP Q9IH63
C	498	ILE	-	expression tag	UNP Q9IH63
C	499	GLU	-	expression tag	UNP Q9IH63
C	500	GLU	-	expression tag	UNP Q9IH63
C	501	ILE	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
C	502	LEU	-	expression tag	UNP Q9IH63
C	503	SER	-	expression tag	UNP Q9IH63
C	504	LYS	-	expression tag	UNP Q9IH63
C	505	ILE	-	expression tag	UNP Q9IH63
C	506	TYR	-	expression tag	UNP Q9IH63
C	507	HIS	-	expression tag	UNP Q9IH63
C	508	ILE	-	expression tag	UNP Q9IH63
C	509	GLU	-	expression tag	UNP Q9IH63
C	510	ASN	-	expression tag	UNP Q9IH63
C	511	GLU	-	expression tag	UNP Q9IH63
C	512	ILE	-	expression tag	UNP Q9IH63
C	513	ALA	-	expression tag	UNP Q9IH63
C	514	ARG	-	expression tag	UNP Q9IH63
C	515	ILE	-	expression tag	UNP Q9IH63
C	516	LYS	-	expression tag	UNP Q9IH63
C	517	LYS	-	expression tag	UNP Q9IH63
C	518	LEU	-	expression tag	UNP Q9IH63
C	519	ILE	-	expression tag	UNP Q9IH63
C	520	GLY	-	expression tag	UNP Q9IH63
C	521	GLU	-	expression tag	UNP Q9IH63
C	522	ALA	-	expression tag	UNP Q9IH63
C	523	PRO	-	expression tag	UNP Q9IH63
C	524	GLY	-	expression tag	UNP Q9IH63
C	525	GLY	-	expression tag	UNP Q9IH63
C	526	ILE	-	expression tag	UNP Q9IH63
C	527	GLU	-	expression tag	UNP Q9IH63
C	528	GLY	-	expression tag	UNP Q9IH63
C	529	ARG	-	expression tag	UNP Q9IH63
D	67	ASP	ASN	engineered mutation	UNP Q9IH63
D	305	ASP	ASN	engineered mutation	UNP Q9IH63
D	489	LYS	-	expression tag	UNP Q9IH63
D	490	LEU	-	expression tag	UNP Q9IH63
D	491	MET	-	expression tag	UNP Q9IH63
D	492	LYS	-	expression tag	UNP Q9IH63
D	493	GLN	-	expression tag	UNP Q9IH63
D	494	ILE	-	expression tag	UNP Q9IH63
D	495	GLU	-	expression tag	UNP Q9IH63
D	496	ASP	-	expression tag	UNP Q9IH63
D	497	LYS	-	expression tag	UNP Q9IH63
D	498	ILE	-	expression tag	UNP Q9IH63
D	499	GLU	-	expression tag	UNP Q9IH63
D	500	GLU	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
D	501	ILE	-	expression tag	UNP Q9IH63
D	502	LEU	-	expression tag	UNP Q9IH63
D	503	SER	-	expression tag	UNP Q9IH63
D	504	LYS	-	expression tag	UNP Q9IH63
D	505	ILE	-	expression tag	UNP Q9IH63
D	506	TYR	-	expression tag	UNP Q9IH63
D	507	HIS	-	expression tag	UNP Q9IH63
D	508	ILE	-	expression tag	UNP Q9IH63
D	509	GLU	-	expression tag	UNP Q9IH63
D	510	ASN	-	expression tag	UNP Q9IH63
D	511	GLU	-	expression tag	UNP Q9IH63
D	512	ILE	-	expression tag	UNP Q9IH63
D	513	ALA	-	expression tag	UNP Q9IH63
D	514	ARG	-	expression tag	UNP Q9IH63
D	515	ILE	-	expression tag	UNP Q9IH63
D	516	LYS	-	expression tag	UNP Q9IH63
D	517	LYS	-	expression tag	UNP Q9IH63
D	518	LEU	-	expression tag	UNP Q9IH63
D	519	ILE	-	expression tag	UNP Q9IH63
D	520	GLY	-	expression tag	UNP Q9IH63
D	521	GLU	-	expression tag	UNP Q9IH63
D	522	ALA	-	expression tag	UNP Q9IH63
D	523	PRO	-	expression tag	UNP Q9IH63
D	524	GLY	-	expression tag	UNP Q9IH63
D	525	GLY	-	expression tag	UNP Q9IH63
D	526	ILE	-	expression tag	UNP Q9IH63
D	527	GLU	-	expression tag	UNP Q9IH63
D	528	GLY	-	expression tag	UNP Q9IH63
D	529	ARG	-	expression tag	UNP Q9IH63
E	67	ASP	ASN	engineered mutation	UNP Q9IH63
E	305	ASP	ASN	engineered mutation	UNP Q9IH63
E	489	LYS	-	expression tag	UNP Q9IH63
E	490	LEU	-	expression tag	UNP Q9IH63
E	491	MET	-	expression tag	UNP Q9IH63
E	492	LYS	-	expression tag	UNP Q9IH63
E	493	GLN	-	expression tag	UNP Q9IH63
E	494	ILE	-	expression tag	UNP Q9IH63
E	495	GLU	-	expression tag	UNP Q9IH63
E	496	ASP	-	expression tag	UNP Q9IH63
E	497	LYS	-	expression tag	UNP Q9IH63
E	498	ILE	-	expression tag	UNP Q9IH63
E	499	GLU	-	expression tag	UNP Q9IH63

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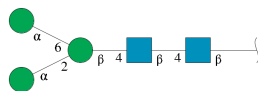
Chain	Residue	Modelled	Actual	Comment	Reference
E	500	GLU	-	expression tag	UNP Q9IH63
E	501	ILE	-	expression tag	UNP Q9IH63
E	502	LEU	-	expression tag	UNP Q9IH63
E	503	SER	-	expression tag	UNP Q9IH63
E	504	LYS	-	expression tag	UNP Q9IH63
E	505	ILE	-	expression tag	UNP Q9IH63
E	506	TYR	-	expression tag	UNP Q9IH63
E	507	HIS	-	expression tag	UNP Q9IH63
E	508	ILE	-	expression tag	UNP Q9IH63
E	509	GLU	-	expression tag	UNP Q9IH63
E	510	ASN	-	expression tag	UNP Q9IH63
E	511	GLU	-	expression tag	UNP Q9IH63
E	512	ILE	-	expression tag	UNP Q9IH63
E	513	ALA	-	expression tag	UNP Q9IH63
E	514	ARG	-	expression tag	UNP Q9IH63
E	515	ILE	-	expression tag	UNP Q9IH63
E	516	LYS	-	expression tag	UNP Q9IH63
E	517	LYS	-	expression tag	UNP Q9IH63
E	518	LEU	-	expression tag	UNP Q9IH63
E	519	ILE	-	expression tag	UNP Q9IH63
E	520	GLY	-	expression tag	UNP Q9IH63
E	521	GLU	-	expression tag	UNP Q9IH63
E	522	ALA	-	expression tag	UNP Q9IH63
E	523	PRO	-	expression tag	UNP Q9IH63
E	524	GLY	-	expression tag	UNP Q9IH63
E	525	GLY	-	expression tag	UNP Q9IH63
E	526	ILE	-	expression tag	UNP Q9IH63
E	527	GLU	-	expression tag	UNP Q9IH63
E	528	GLY	-	expression tag	UNP Q9IH63
E	529	ARG	-	expression tag	UNP Q9IH63
F	67	ASP	ASN	engineered mutation	UNP Q9IH63
F	305	ASP	ASN	engineered mutation	UNP Q9IH63
F	489	LYS	-	expression tag	UNP Q9IH63
F	490	LEU	-	expression tag	UNP Q9IH63
F	491	MET	-	expression tag	UNP Q9IH63
F	492	LYS	-	expression tag	UNP Q9IH63
F	493	GLN	-	expression tag	UNP Q9IH63
F	494	ILE	-	expression tag	UNP Q9IH63
F	495	GLU	-	expression tag	UNP Q9IH63
F	496	ASP	-	expression tag	UNP Q9IH63
F	497	LYS	-	expression tag	UNP Q9IH63
F	498	ILE	-	expression tag	UNP Q9IH63

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Chain	Residue	Modelled	Actual	Comment	Reference
F	499	GLU	-	expression tag	UNP Q9IH63
F	500	GLU	-	expression tag	UNP Q9IH63
F	501	ILE	-	expression tag	UNP Q9IH63
F	502	LEU	-	expression tag	UNP Q9IH63
F	503	SER	-	expression tag	UNP Q9IH63
F	504	LYS	-	expression tag	UNP Q9IH63
F	505	ILE	-	expression tag	UNP Q9IH63
F	506	TYR	-	expression tag	UNP Q9IH63
F	507	HIS	-	expression tag	UNP Q9IH63
F	508	ILE	-	expression tag	UNP Q9IH63
F	509	GLU	-	expression tag	UNP Q9IH63
F	510	ASN	-	expression tag	UNP Q9IH63
F	511	GLU	-	expression tag	UNP Q9IH63
F	512	ILE	-	expression tag	UNP Q9IH63
F	513	ALA	-	expression tag	UNP Q9IH63
F	514	ARG	-	expression tag	UNP Q9IH63
F	515	ILE	-	expression tag	UNP Q9IH63
F	516	LYS	-	expression tag	UNP Q9IH63
F	517	LYS	-	expression tag	UNP Q9IH63
F	518	LEU	-	expression tag	UNP Q9IH63
F	519	ILE	-	expression tag	UNP Q9IH63
F	520	GLY	-	expression tag	UNP Q9IH63
F	521	GLU	-	expression tag	UNP Q9IH63
F	522	ALA	-	expression tag	UNP Q9IH63
F	523	PRO	-	expression tag	UNP Q9IH63
F	524	GLY	-	expression tag	UNP Q9IH63
F	525	GLY	-	expression tag	UNP Q9IH63
F	526	ILE	-	expression tag	UNP Q9IH63
F	527	GLU	-	expression tag	UNP Q9IH63
F	528	GLY	-	expression tag	UNP Q9IH63
F	529	ARG	-	expression tag	UNP Q9IH63

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



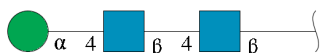
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	5	61	34	2	25	0	0	0

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



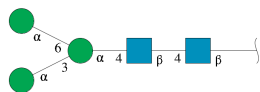
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	H	2	28	16	2	10	0	0	0
3	N	2	28	16	2	10	0	0	0
3	O	2	28	16	2	10	0	0	0
3	U	2	28	16	2	10	0	0	0
3	V	2	28	16	2	10	0	0	0

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



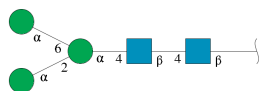
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	3	39	22	2	15	0	0	0
4	J	3	39	22	2	15	0	0	0
4	K	3	39	22	2	15	0	0	0
4	R	3	39	22	2	15	0	0	0
4	S	3	39	22	2	15	0	0	0
4	W	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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			
5	L	5	61	34	2	25	0	0	0
5	X	5	61	34	2	25	0	0	0

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



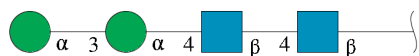
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	M	5	61	34	2	25	0	0	0

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



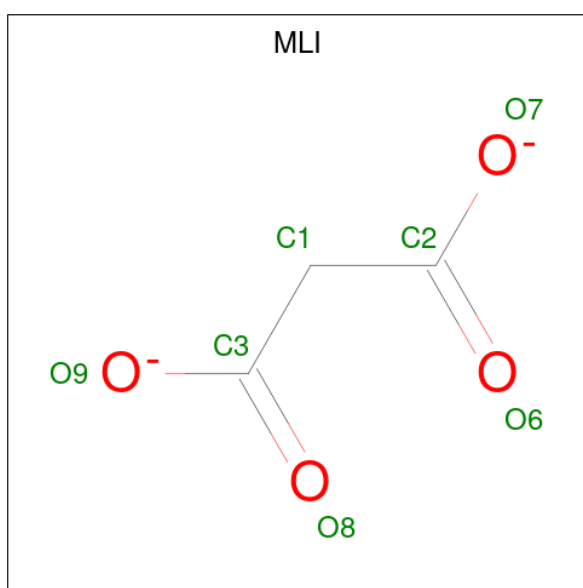
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	P	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
8	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).

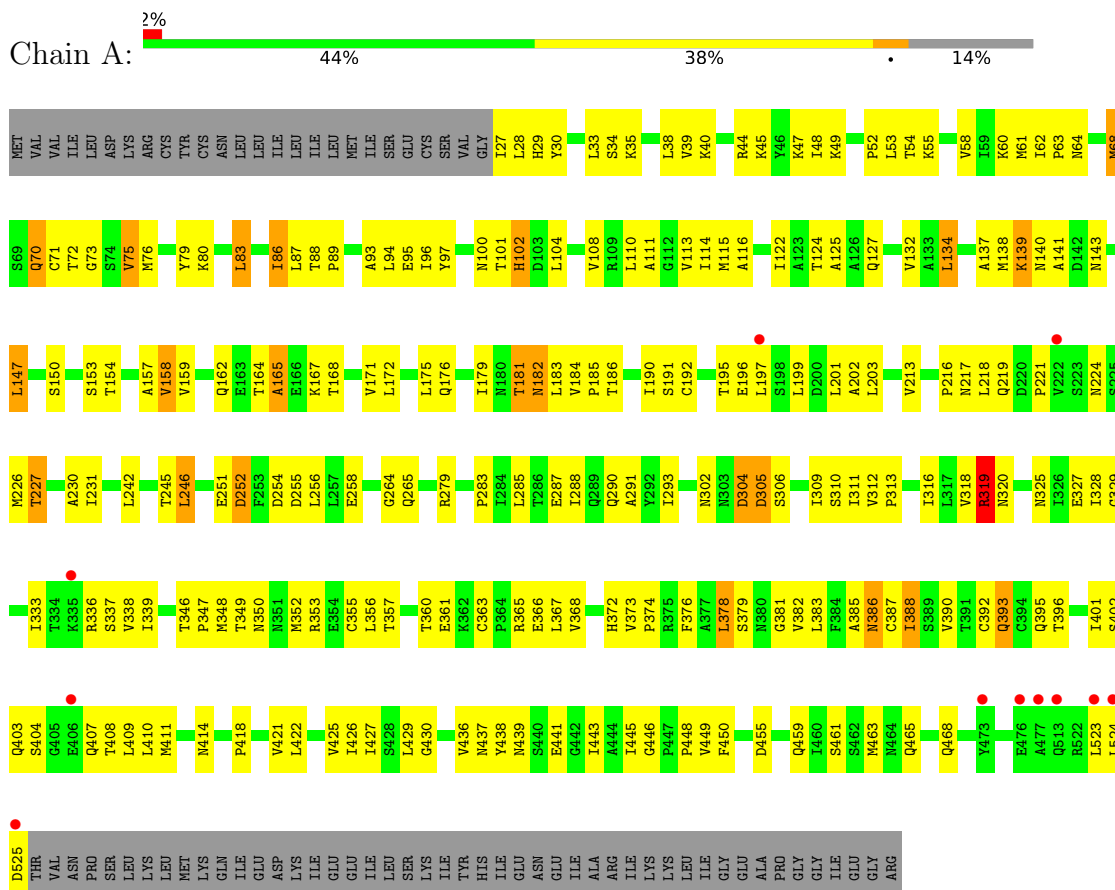


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	3	4		
9	B	1	Total	C	O	0	0
			7	3	4		
9	C	1	Total	C	O	0	0
			7	3	4		
9	D	1	Total	C	O	0	0
			7	3	4		
9	E	1	Total	C	O	0	0
			7	3	4		
9	F	1	Total	C	O	0	0
			7	3	4		

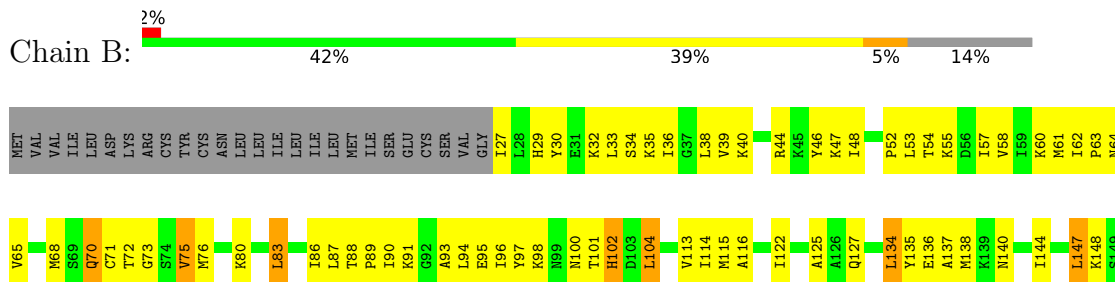
### 3 Residue-property plots

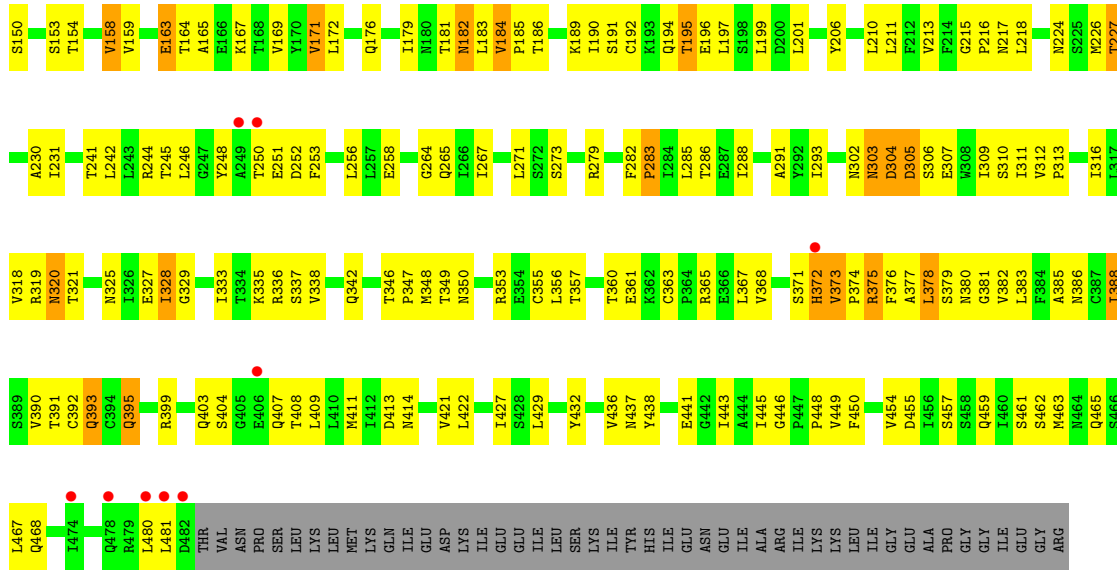
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fusion glycoprotein F0

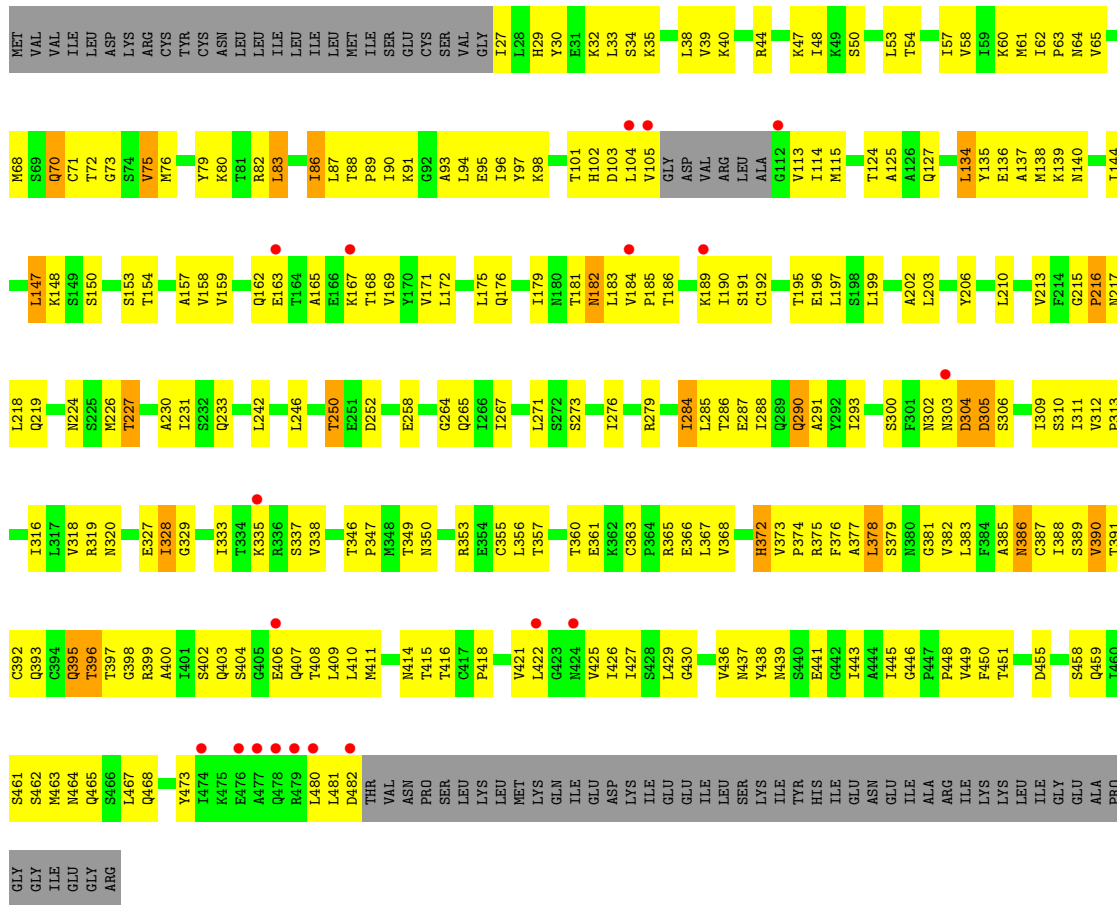


- Molecule 1: Fusion glycoprotein F0

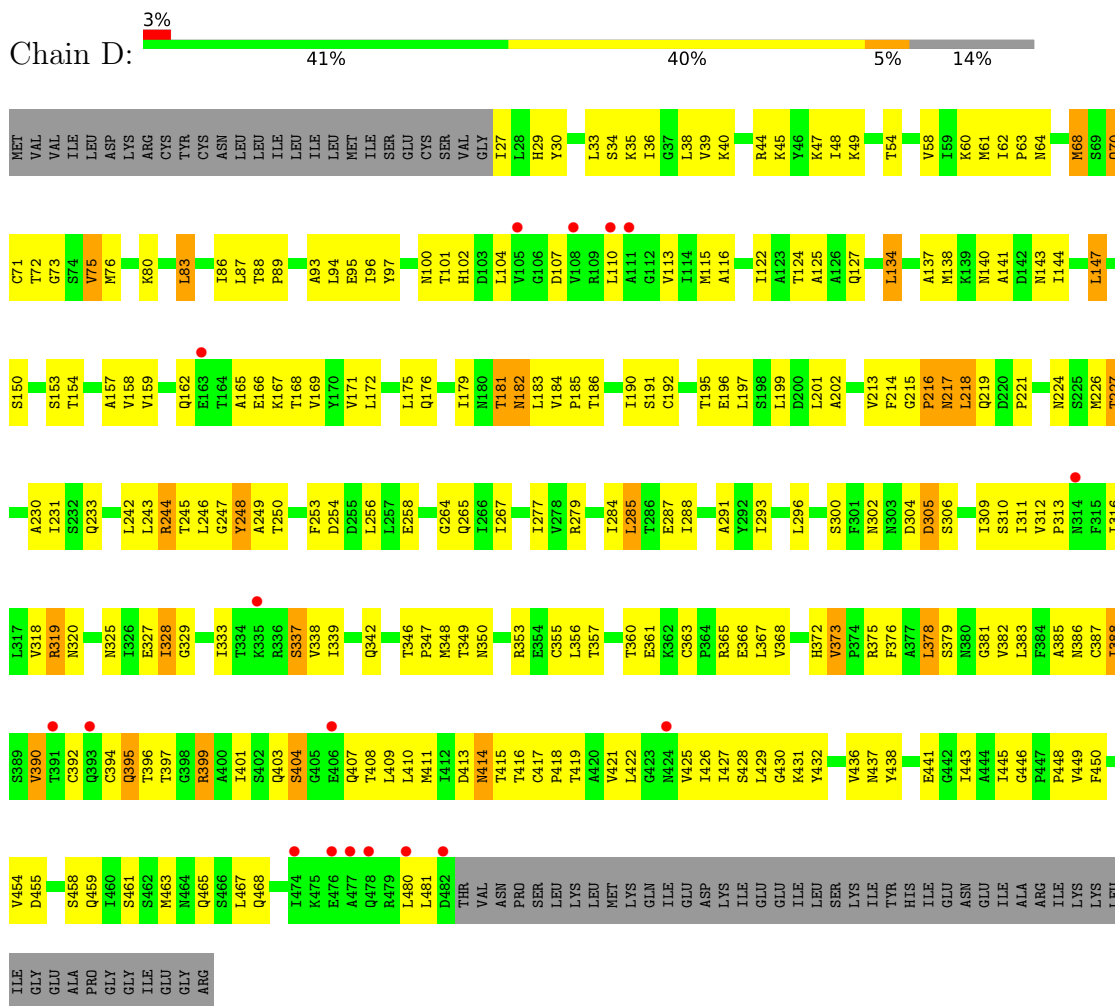




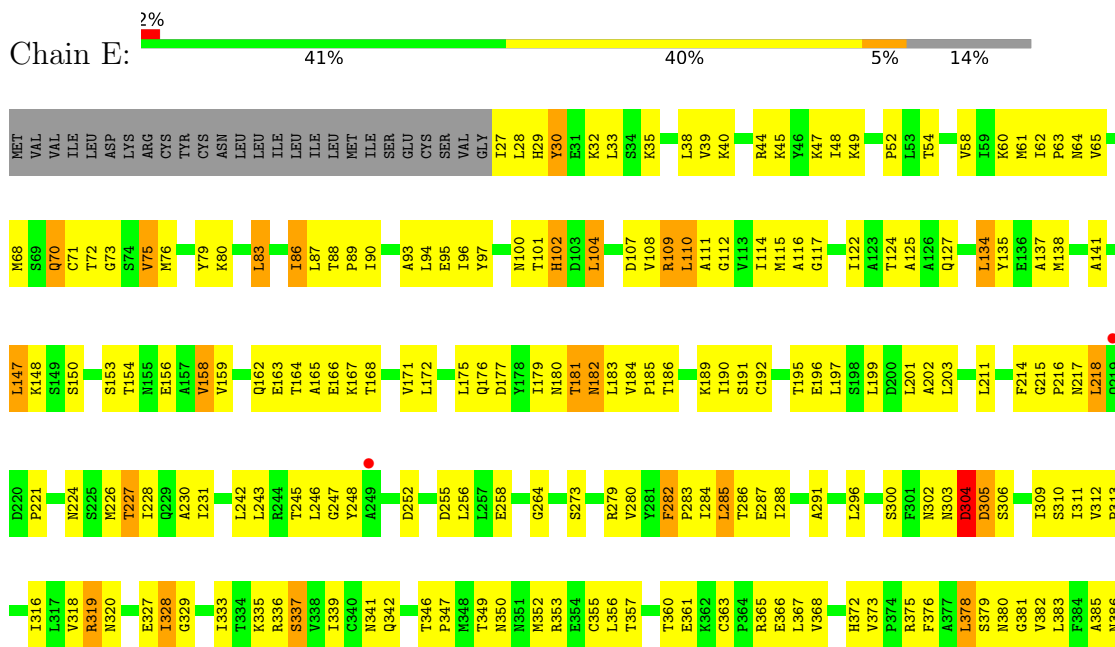
• Molecule 1: Fusion glycoprotein F0




• Molecule 1: Fusion glycoprotein F0



● Molecule 1: Fusion glycoprotein F0





Chain H:  100%


MAG1  
MAG2

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

Chain N:  50% 50%

MAG1  
MAG2

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

Chain O:  50% 50%

MAG1  
MAG2

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

Chain U:  50% 50%


MAG1  
MAG2

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

Chain V:  50% 50%

MAG1  
MAG2

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

Chain I:  33% 67%

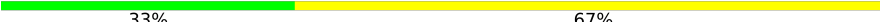
MAG1  
MAG2  
MAN3

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

Chain J:  67% 33%

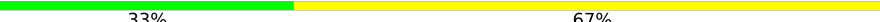
MAG1  
MAG2  
MAN3

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

Chain K:  33% 67%



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

Chain R:  33% 67%



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

Chain S:  67% 33%

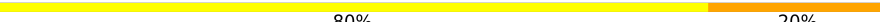


- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  67% 33%




- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  80% 20%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  80% 20%



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

nose

Chain M:  20% 20% 60%


MAG1  
MAG2  
MAN3  
MAN4  
MAN5

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

Chain P:  50% 50%


MAG1  
MAG2  
MAN3  
MAN4

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

Chain Q:  75% 25%

MAG1  
MAG2  
MAN3  
MAN4

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

Chain T:  50% 50%

MAG1  
MAG2  
MAN3  
MAN4

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	355.75Å 355.75Å 168.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.16 – 3.37 43.16 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.16-3.37) 99.3 (43.16-3.37)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.213 , 0.220 (Not available) , 0.213	Depositor DCC
$R_{free}$ test set	5593 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.8	Xtrriage
Anisotropy	0.678	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 96.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: NAG, MAN, BMA, MLI

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	0.58	0/3531	1.08	22/4800 (0.5%)
1	B	0.59	1/3527 (0.0%)	1.08	24/4795 (0.5%)
1	C	0.59	0/3487	1.05	18/4739 (0.4%)
1	D	0.58	0/3531	1.05	19/4800 (0.4%)
1	E	0.58	0/3531	1.09	29/4800 (0.6%)
1	F	0.57	0/3487	1.15	31/4739 (0.7%)
All	All	0.58	1/21094 (0.0%)	1.08	143/28673 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	VAL	CA-CB	5.07	1.57	1.54

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	ASN	N-CA-C	12.17	128.85	113.88
1	F	394	CYS	N-CA-CB	-12.09	90.43	110.37
1	E	182	ASN	N-CA-C	11.62	128.18	113.88
1	F	375	ARG	NE-CZ-NH2	11.46	129.51	119.20
1	F	182	ASN	N-CA-CB	-11.30	95.56	110.59

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	3482	0	3510	216	0
1	B	3478	0	3506	236	0
1	C	3439	0	3463	255	0
1	D	3482	0	3510	248	0
1	E	3482	0	3510	234	0
1	F	3439	0	3464	257	0
2	G	61	0	52	4	0
3	H	28	0	25	0	0
3	N	28	0	25	3	0
3	O	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
4	I	39	0	34	1	0
4	J	39	0	34	1	0
4	K	39	0	34	0	0
4	R	39	0	34	0	0
4	S	39	0	34	2	0
4	W	39	0	34	2	0
5	L	61	0	52	6	0
5	X	61	0	52	2	0
6	M	61	0	52	2	0
7	P	50	0	43	4	0
8	Q	50	0	43	2	0
8	T	50	0	43	8	0
9	A	7	0	2	0	0
9	B	7	0	2	0	0
9	C	7	0	2	0	0
9	D	7	0	2	0	0
9	E	7	0	2	1	0
9	F	7	0	2	0	0
All	All	21612	0	21641	1336	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 31.

The worst 5 of 1336 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:258:GLU:HG3	1:C:216:PRO:HD2	1.28	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:THR:HG21	1:A:443:ILE:HD11	1.29	1.09
1:B:468:GLN:HE21	5:L:1:NAG:H62	1.13	1.08
1:C:360:THR:HG21	1:C:443:ILE:HD11	1.35	1.08
1:A:437:ASN:O	1:A:441:GLU:HG2	1.53	1.07

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	454/529 (86%)	398 (88%)	52 (12%)	4 (1%)	14	41
1	B	454/529 (86%)	396 (87%)	53 (12%)	5 (1%)	11	36
1	C	446/529 (84%)	384 (86%)	57 (13%)	5 (1%)	11	36
1	D	454/529 (86%)	390 (86%)	60 (13%)	4 (1%)	14	41
1	E	454/529 (86%)	392 (86%)	58 (13%)	4 (1%)	14	41
1	F	446/529 (84%)	379 (85%)	59 (13%)	8 (2%)	6	26
All	All	2708/3174 (85%)	2339 (86%)	339 (12%)	30 (1%)	11	36

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	166	GLU
1	F	398	GLY
1	A	381	GLY
1	B	320	ASN
1	C	320	ASN

### 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	397/471 (84%)	368 (93%)	29 (7%)	13	39
1	B	396/471 (84%)	370 (93%)	26 (7%)	15	42
1	C	393/471 (83%)	367 (93%)	26 (7%)	15	42
1	D	397/471 (84%)	367 (92%)	30 (8%)	12	38
1	E	397/471 (84%)	365 (92%)	32 (8%)	11	36
1	F	393/471 (83%)	371 (94%)	22 (6%)	19	46
All	All	2373/2826 (84%)	2208 (93%)	165 (7%)	14	40

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	104	LEU
1	F	70	GLN
1	E	147	LEU
1	E	304	ASP
1	F	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	217	ASN
1	E	70	GLN
1	F	459	GLN
1	D	224	ASN
1	D	395	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

60 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	NAG	G	1	2,1	14,14,15	0.71	0	17,19,21	0.79	1 (5%)
2	NAG	G	2	2	14,14,15	0.51	0	17,19,21	0.66	0
2	BMA	G	3	2	11,11,12	1.33	2 (18%)	15,15,17	1.30	2 (13%)
2	MAN	G	4	2	11,11,12	0.88	0	15,15,17	0.92	2 (13%)
2	MAN	G	5	2	11,11,12	0.91	0	15,15,17	0.89	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.90	0	17,19,21	1.07	2 (11%)
3	NAG	H	2	3	14,14,15	1.13	1 (7%)	17,19,21	0.77	0
4	NAG	I	1	4,1	14,14,15	0.73	0	17,19,21	0.78	0
4	NAG	I	2	4	14,14,15	0.76	0	17,19,21	0.89	0
4	MAN	I	3	4	11,11,12	0.89	0	15,15,17	1.19	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.70	0	17,19,21	0.81	0
4	NAG	J	2	4	14,14,15	0.99	0	17,19,21	1.00	1 (5%)
4	MAN	J	3	4	11,11,12	1.01	0	15,15,17	1.21	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.77	0	17,19,21	0.86	1 (5%)
4	NAG	K	2	4	14,14,15	0.88	0	17,19,21	0.86	0
4	MAN	K	3	4	11,11,12	0.91	0	15,15,17	0.73	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.62	0	17,19,21	0.89	0
5	NAG	L	2	5	14,14,15	0.74	0	17,19,21	0.79	0
5	MAN	L	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.63	3 (20%)
5	MAN	L	4	5	11,11,12	0.72	0	15,15,17	0.78	1 (6%)
5	MAN	L	5	5	11,11,12	0.69	0	15,15,17	0.81	1 (6%)
6	NAG	M	1	1,6	14,14,15	0.70	0	17,19,21	1.61	3 (17%)
6	NAG	M	2	6	14,14,15	0.78	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	M	3	6	11,11,12	1.05	0	15,15,17	0.56	0
6	MAN	M	4	6	11,11,12	0.75	0	15,15,17	0.80	1 (6%)
6	MAN	M	5	6	11,11,12	0.63	0	15,15,17	0.65	1 (6%)
3	NAG	N	1	1,3	14,14,15	0.68	0	17,19,21	0.81	0
3	NAG	N	2	3	14,14,15	0.91	0	17,19,21	0.80	0
3	NAG	O	1	1,3	14,14,15	0.79	0	17,19,21	1.27	2 (11%)
3	NAG	O	2	3	14,14,15	0.93	1 (7%)	17,19,21	0.60	0
7	NAG	P	1	7,1	14,14,15	0.76	1 (7%)	17,19,21	0.86	1 (5%)
7	NAG	P	2	7	14,14,15	0.78	0	17,19,21	0.93	1 (5%)
7	MAN	P	3	7	11,11,12	0.82	0	15,15,17	0.72	1 (6%)
7	MAN	P	4	7	11,11,12	0.76	0	15,15,17	0.85	1 (6%)
8	NAG	Q	1	1,8	14,14,15	0.60	0	17,19,21	0.74	0
8	NAG	Q	2	8	14,14,15	0.86	0	17,19,21	1.03	2 (11%)
8	MAN	Q	3	8	11,11,12	0.89	0	15,15,17	0.93	1 (6%)
8	MAN	Q	4	8	11,11,12	0.84	0	15,15,17	0.67	0
4	NAG	R	1	4,1	14,14,15	0.68	0	17,19,21	0.86	1 (5%)
4	NAG	R	2	4	14,14,15	0.74	0	17,19,21	0.79	0
4	MAN	R	3	4	11,11,12	1.11	1 (9%)	15,15,17	0.94	1 (6%)
4	NAG	S	1	4,1	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
4	NAG	S	2	4	14,14,15	0.75	0	17,19,21	0.97	1 (5%)
4	MAN	S	3	4	11,11,12	0.92	0	15,15,17	0.81	1 (6%)
8	NAG	T	1	1,8	14,14,15	0.57	0	17,19,21	0.60	0
8	NAG	T	2	8	14,14,15	0.60	0	17,19,21	0.89	0
8	MAN	T	3	8	11,11,12	1.14	1 (9%)	15,15,17	0.86	1 (6%)
8	MAN	T	4	8	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
3	NAG	U	1	1,3	14,14,15	0.81	0	17,19,21	0.69	0
3	NAG	U	2	3	14,14,15	0.97	1 (7%)	17,19,21	0.61	0
3	NAG	V	1	1,3	14,14,15	0.86	0	17,19,21	0.93	1 (5%)
3	NAG	V	2	3	14,14,15	0.76	0	17,19,21	0.73	0
4	NAG	W	1	4,1	14,14,15	0.53	0	17,19,21	0.73	0
4	NAG	W	2	4	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
4	MAN	W	3	4	11,11,12	0.87	0	15,15,17	0.86	1 (6%)
5	NAG	X	1	1,5	14,14,15	0.62	0	17,19,21	0.89	1 (5%)
5	NAG	X	2	5	14,14,15	0.71	0	17,19,21	0.74	1 (5%)
5	MAN	X	3	5	11,11,12	1.17	1 (9%)	15,15,17	0.55	0
5	MAN	X	4	5	11,11,12	0.85	0	15,15,17	0.84	1 (6%)
5	MAN	X	5	5	11,11,12	0.90	0	15,15,17	0.69	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	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	1/2/19/22	0/1/1/1
2	MAN	G	5	2	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	3/6/23/26	0/1/1/1
4	MAN	I	3	4	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	3	4	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	MAN	K	3	4	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	MAN	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	2/2/19/22	0/1/1/1
5	MAN	L	5	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	0/1/1/1
6	MAN	M	3	6	-	2/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	1/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
7	NAG	P	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	MAN	P	3	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	P	4	7	-	2/2/19/22	0/1/1/1
8	NAG	Q	1	1,8	-	5/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	MAN	Q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	2/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	MAN	R	3	4	-	2/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	4/6/23/26	0/1/1/1
4	MAN	S	3	4	-	1/2/19/22	1/1/1/1
8	NAG	T	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	MAN	T	3	8	-	2/2/19/22	0/1/1/1
8	MAN	T	4	8	-	2/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	MAN	W	3	4	-	2/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	4/6/23/26	0/1/1/1
5	MAN	X	3	5	-	0/2/19/22	0/1/1/1
5	MAN	X	4	5	-	2/2/19/22	0/1/1/1
5	MAN	X	5	5	-	2/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C1-C2	3.33	1.56	1.52
2	G	3	BMA	C2-C3	2.81	1.56	1.52
4	R	3	MAN	C2-C3	2.60	1.56	1.52
3	O	2	NAG	C1-C2	2.50	1.55	1.52
7	P	1	NAG	C1-C2	2.46	1.55	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	3	MAN	C3-C4-C5	4.70	118.76	110.23
6	M	2	NAG	C4-C3-C2	-3.97	105.20	111.02
6	M	1	NAG	C4-C3-C2	3.93	116.78	111.02
3	O	1	NAG	C4-C3-C2	3.73	116.49	111.02
6	M	1	NAG	C3-C4-C5	3.56	116.69	110.23

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	4	MAN	C1-C2-C3-C4-C5-O5
4	S	3	MAN	C1-C2-C3-C4-C5-O5

28 monomers are involved in 38 short contacts:

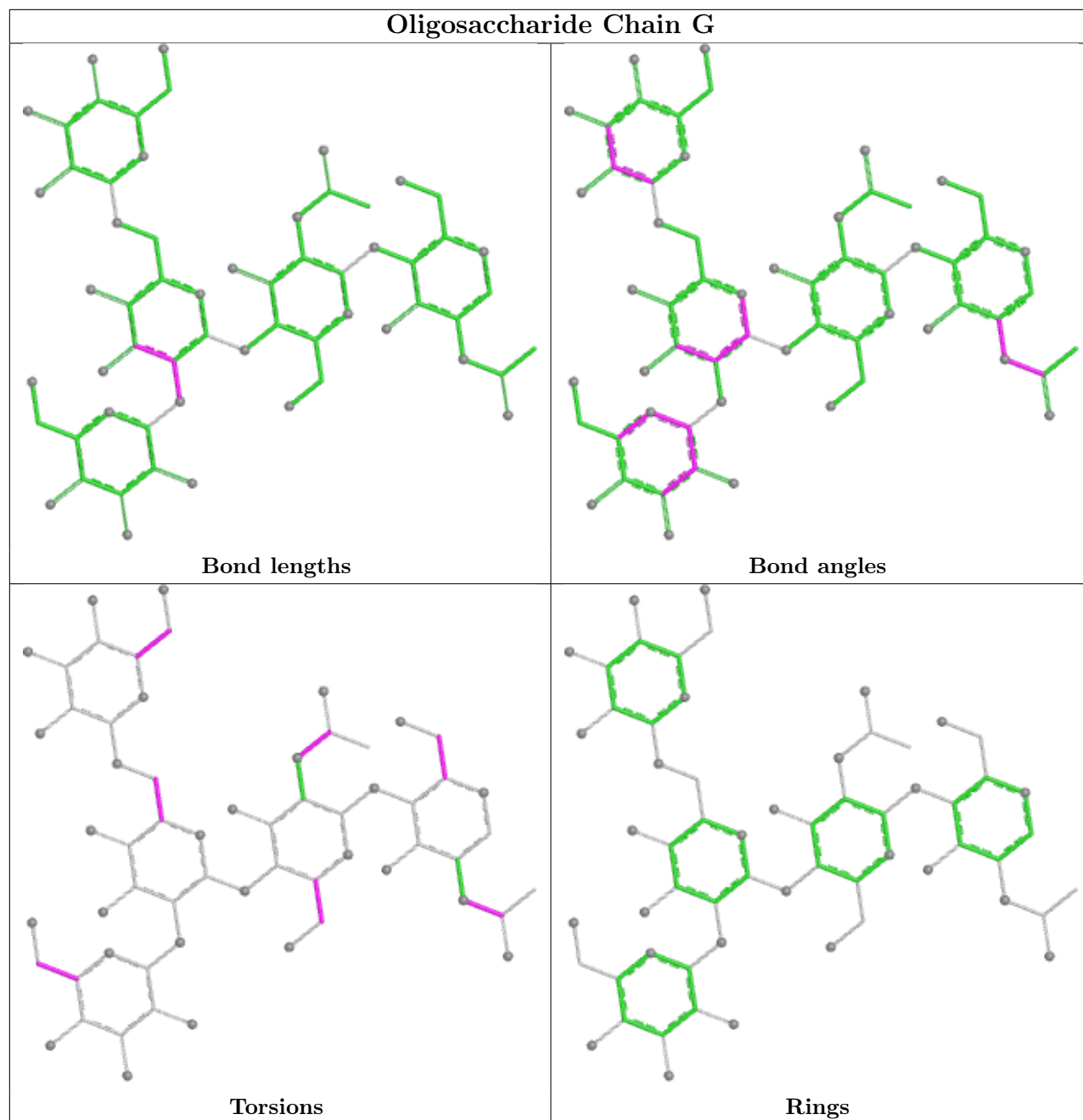
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Q	3	MAN	1	0
6	M	4	MAN	1	0
4	S	1	NAG	2	0
2	G	3	BMA	2	0
8	Q	1	NAG	1	0
4	W	1	NAG	2	0
8	T	1	NAG	2	0
7	P	2	NAG	4	0
3	O	1	NAG	1	0
8	T	2	NAG	5	0
4	W	2	NAG	2	0
5	L	3	MAN	2	0
6	M	2	NAG	1	0
4	J	2	NAG	1	0
7	P	1	NAG	4	0
4	I	1	NAG	1	0

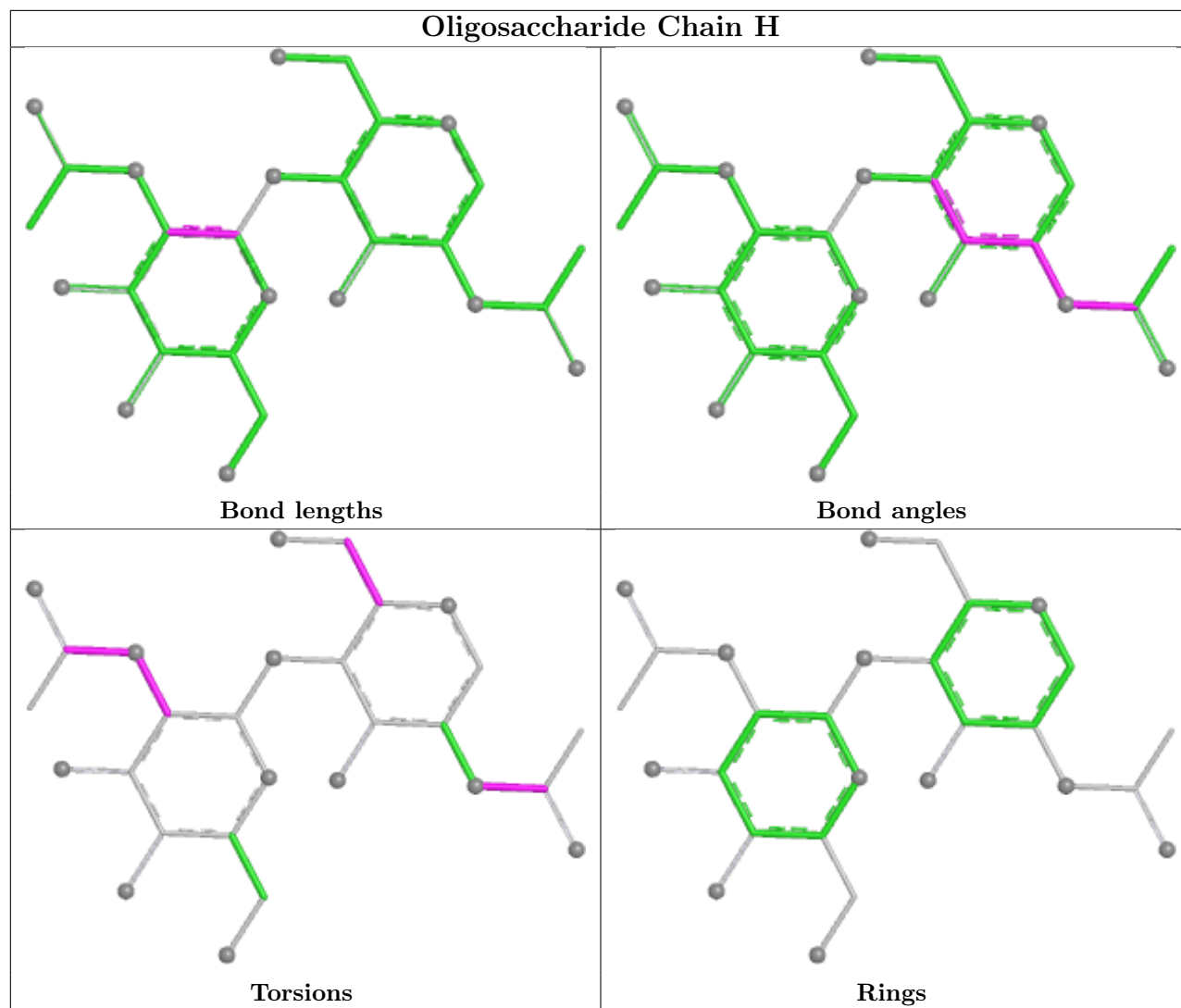
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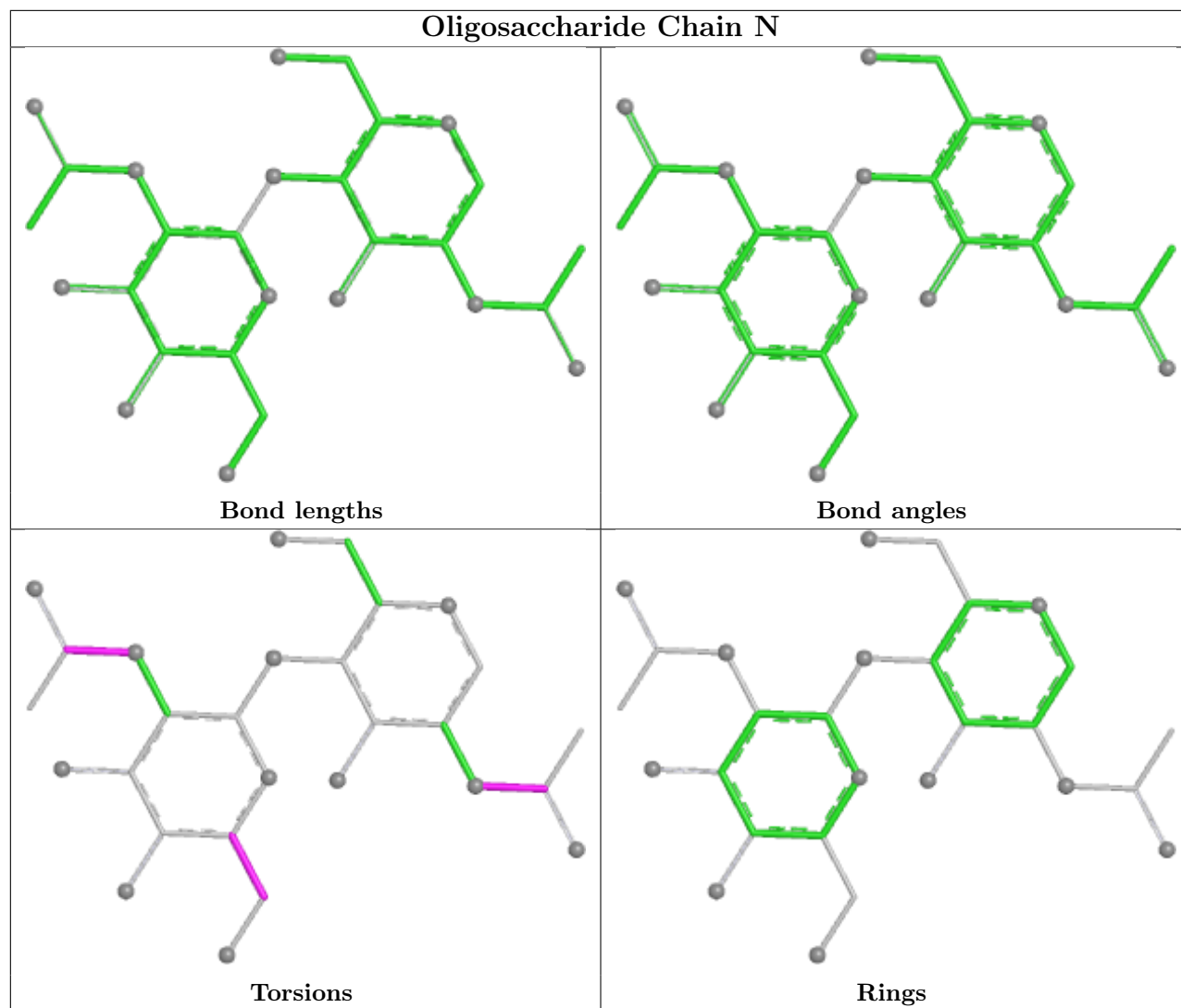
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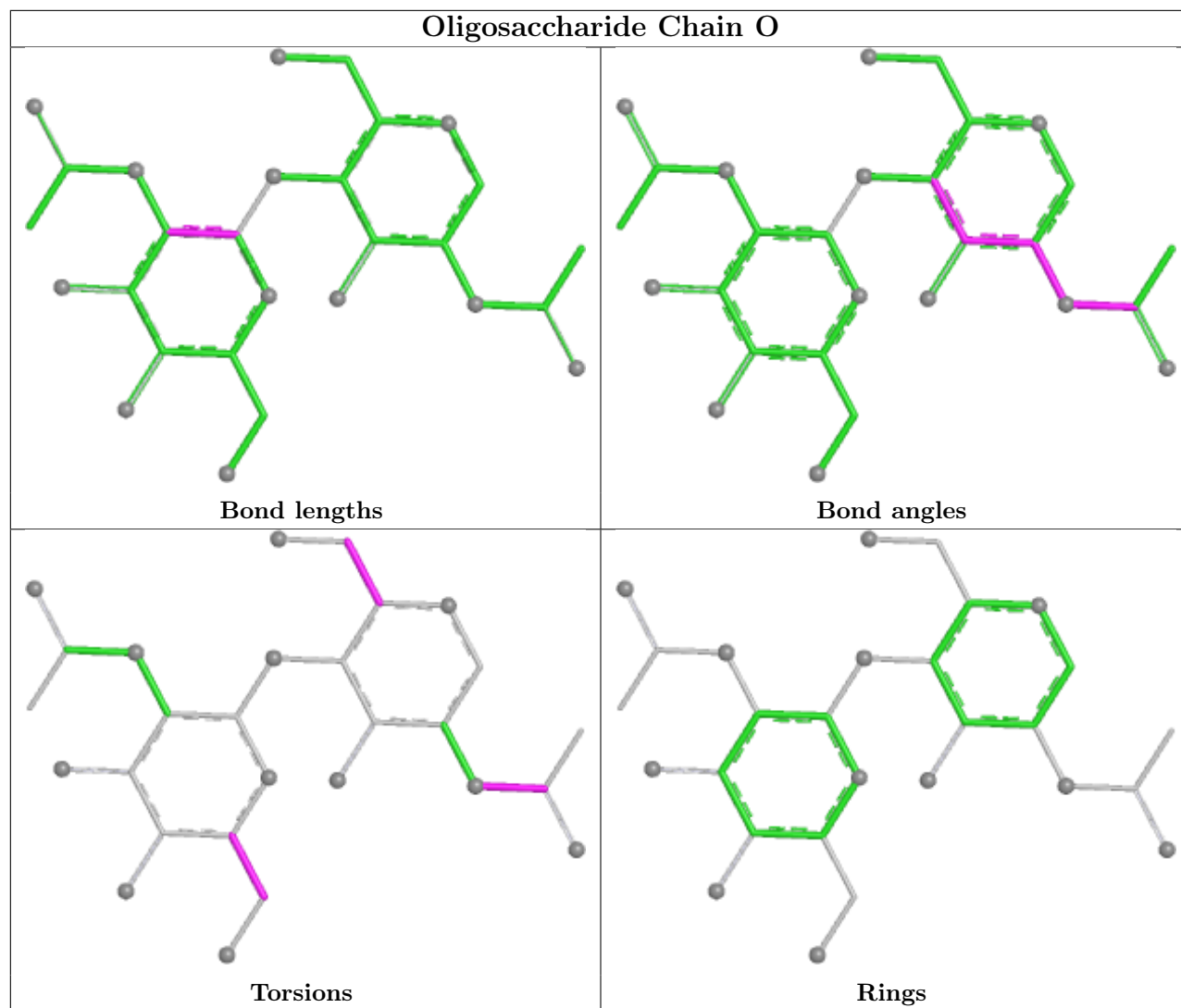
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	NAG	3	0
8	T	4	MAN	1	0
8	Q	4	MAN	1	0
4	J	1	NAG	1	0
2	G	5	MAN	1	0
3	N	1	NAG	3	0
5	L	1	NAG	4	0
6	M	1	NAG	1	0
2	G	1	NAG	2	0
8	T	3	MAN	1	0
5	X	1	NAG	2	0
2	G	2	NAG	2	0

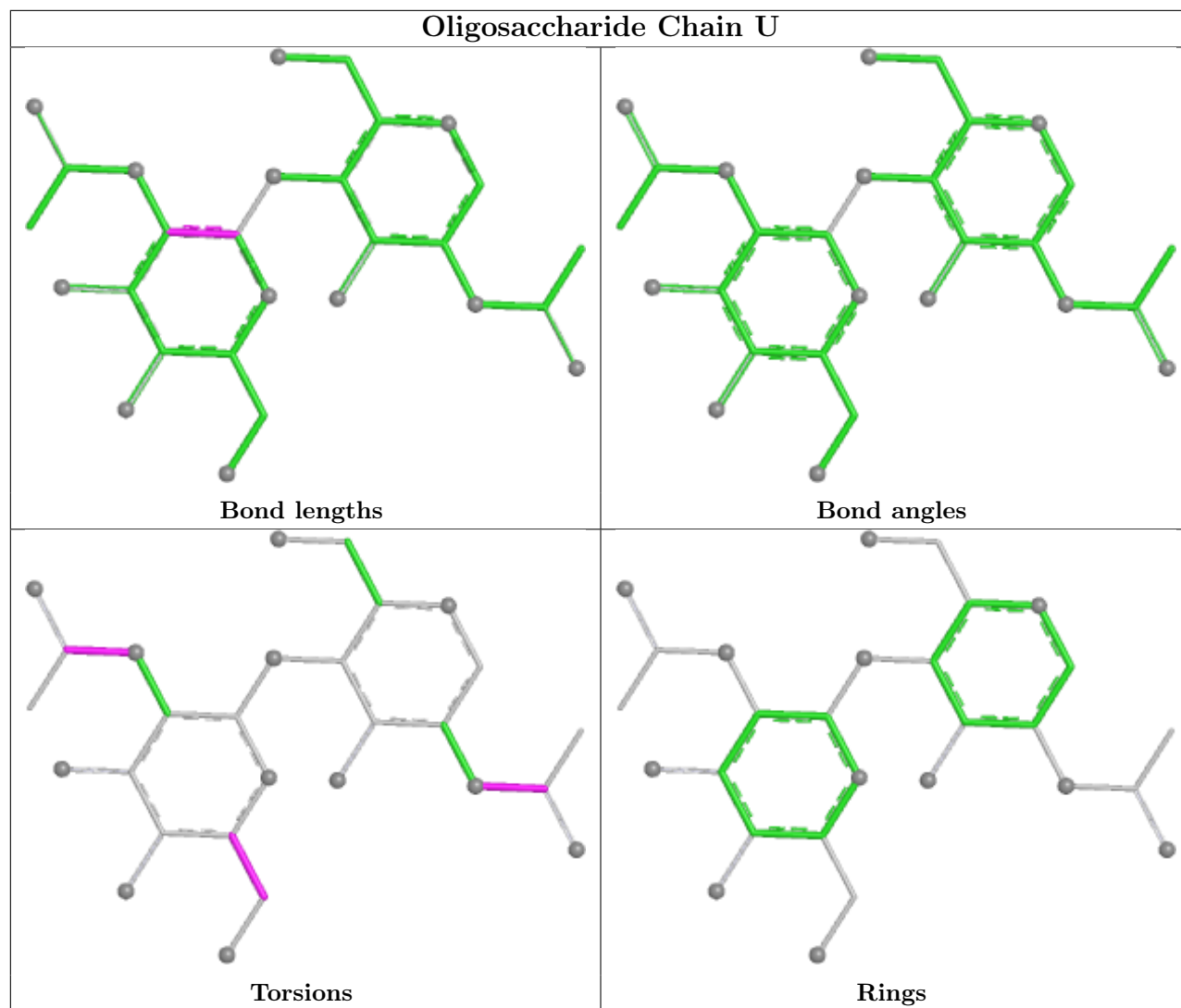
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

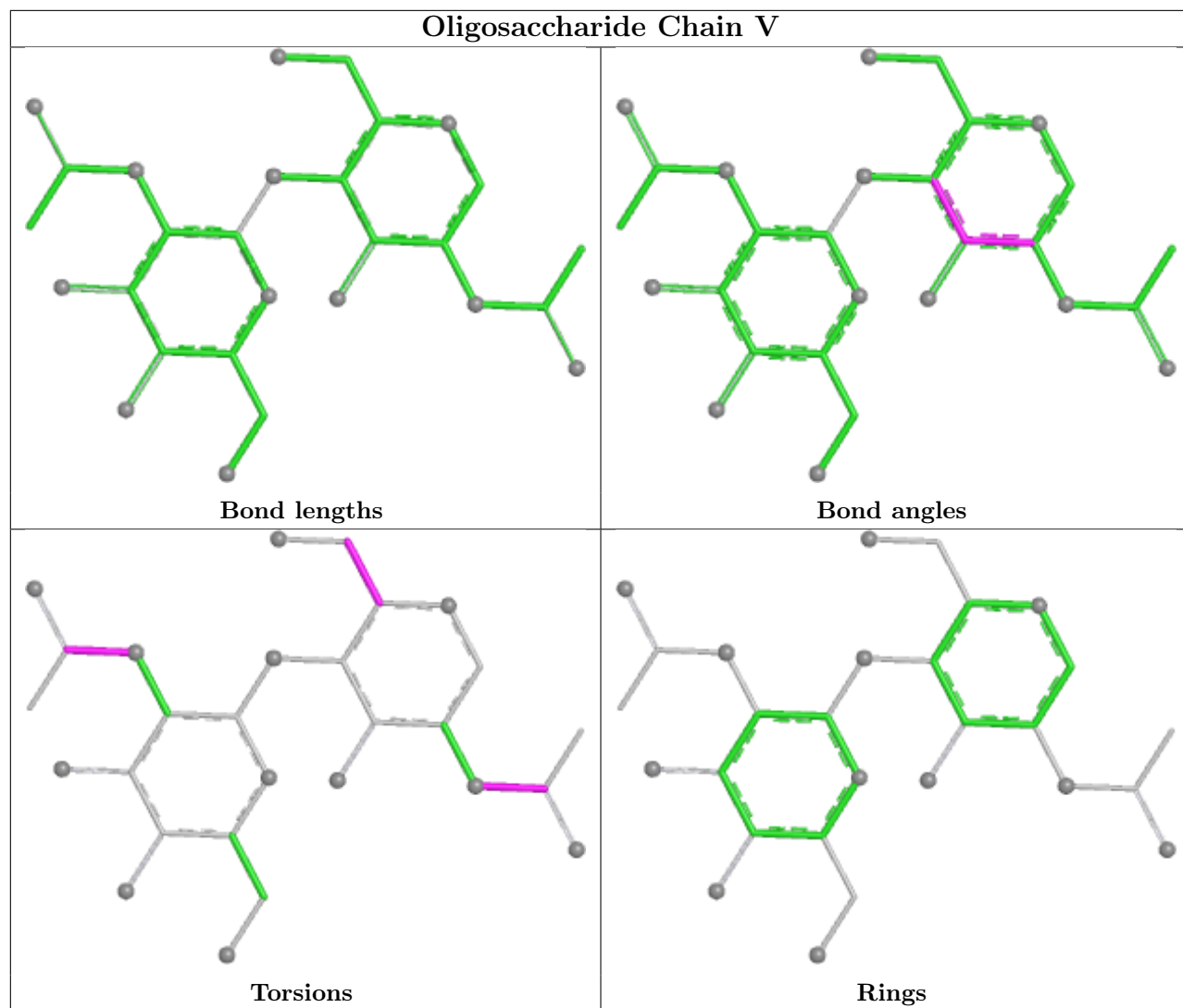


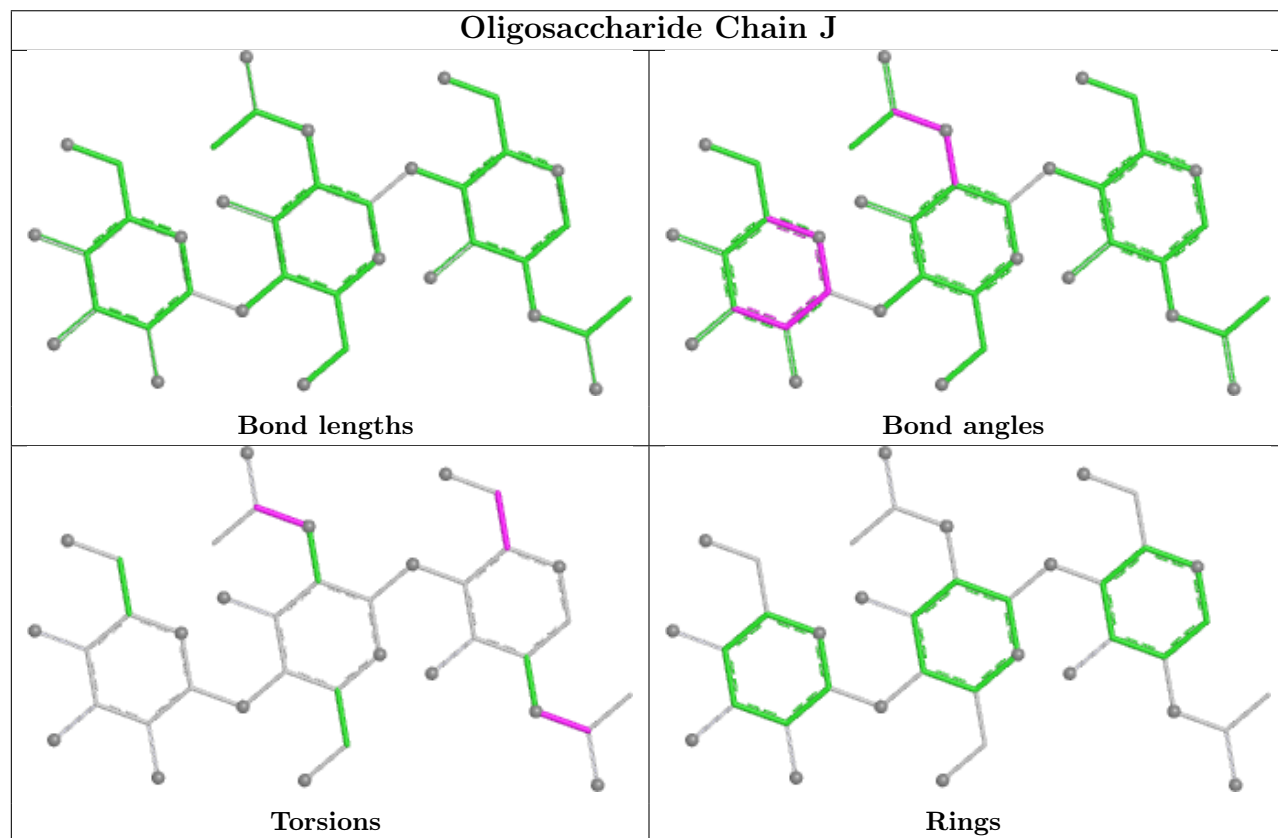
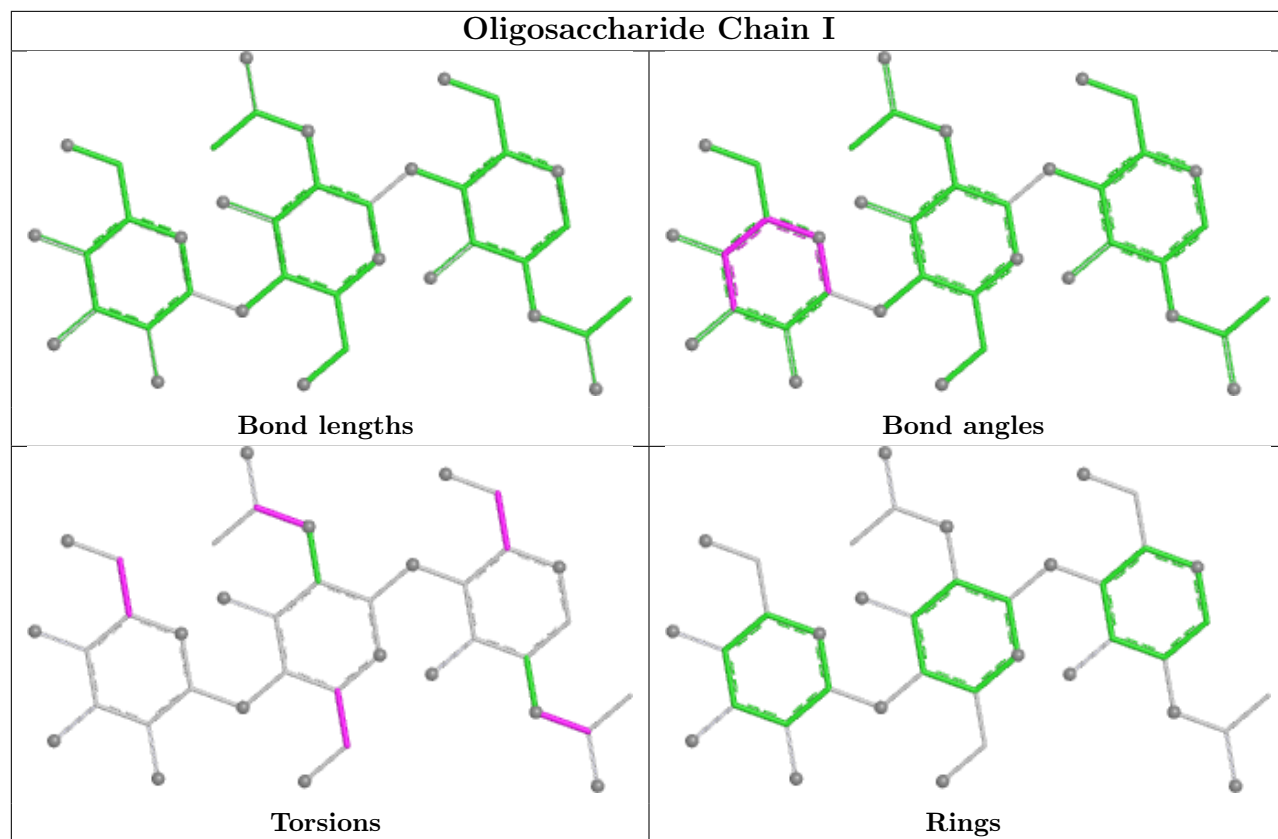


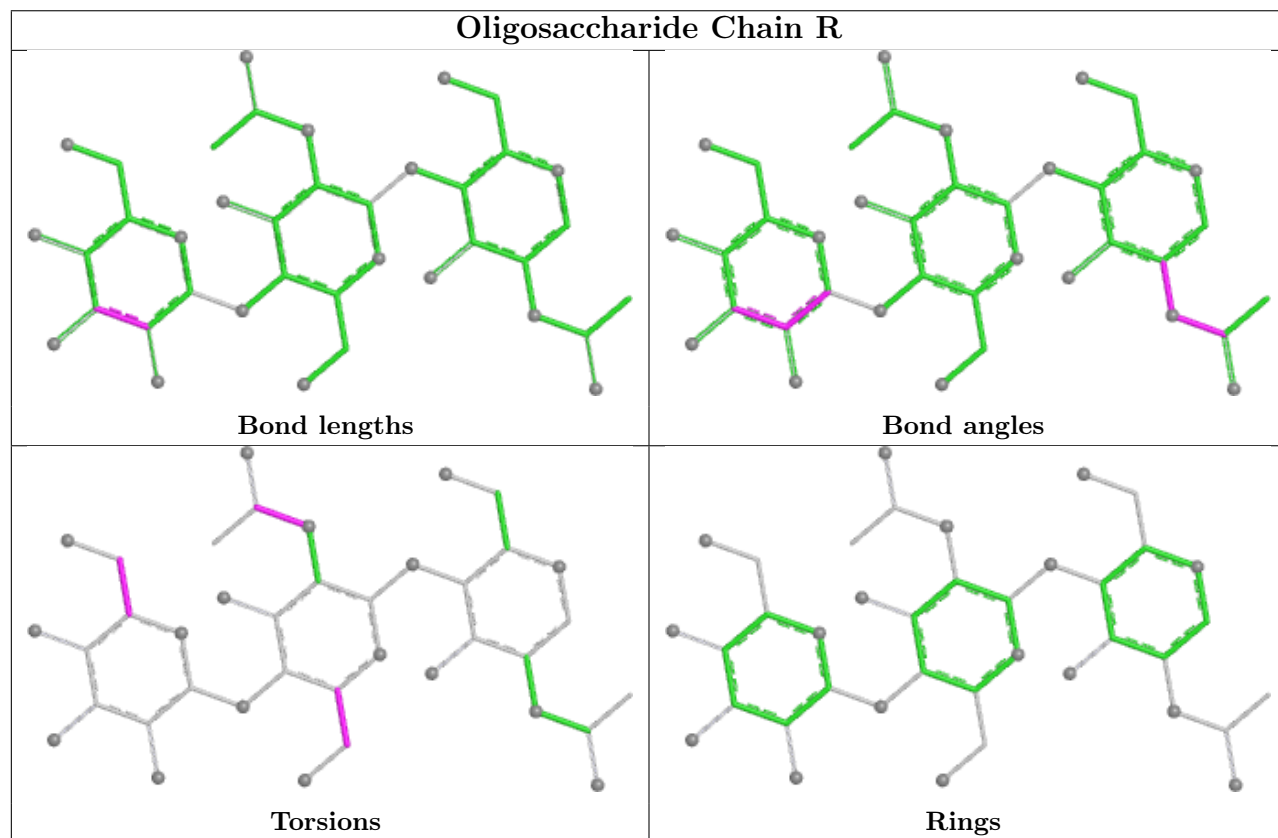
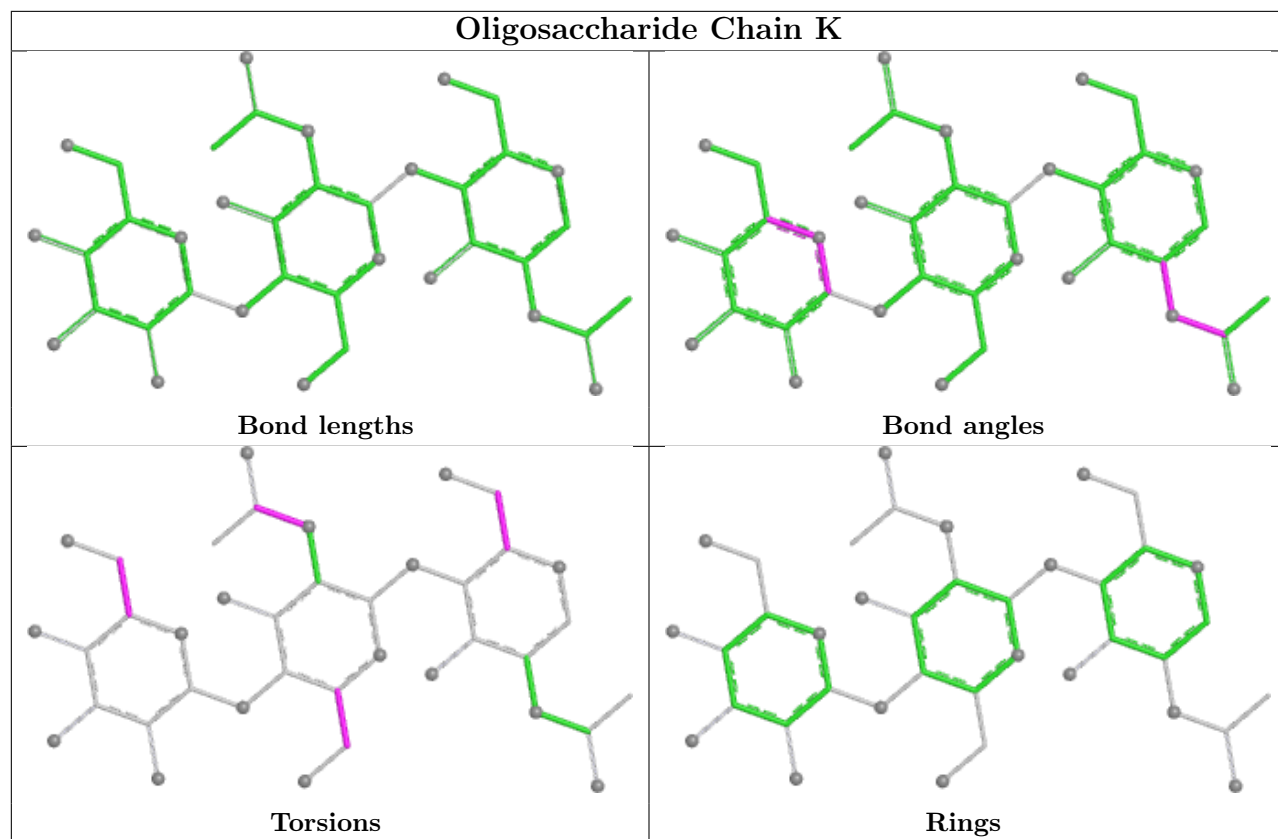


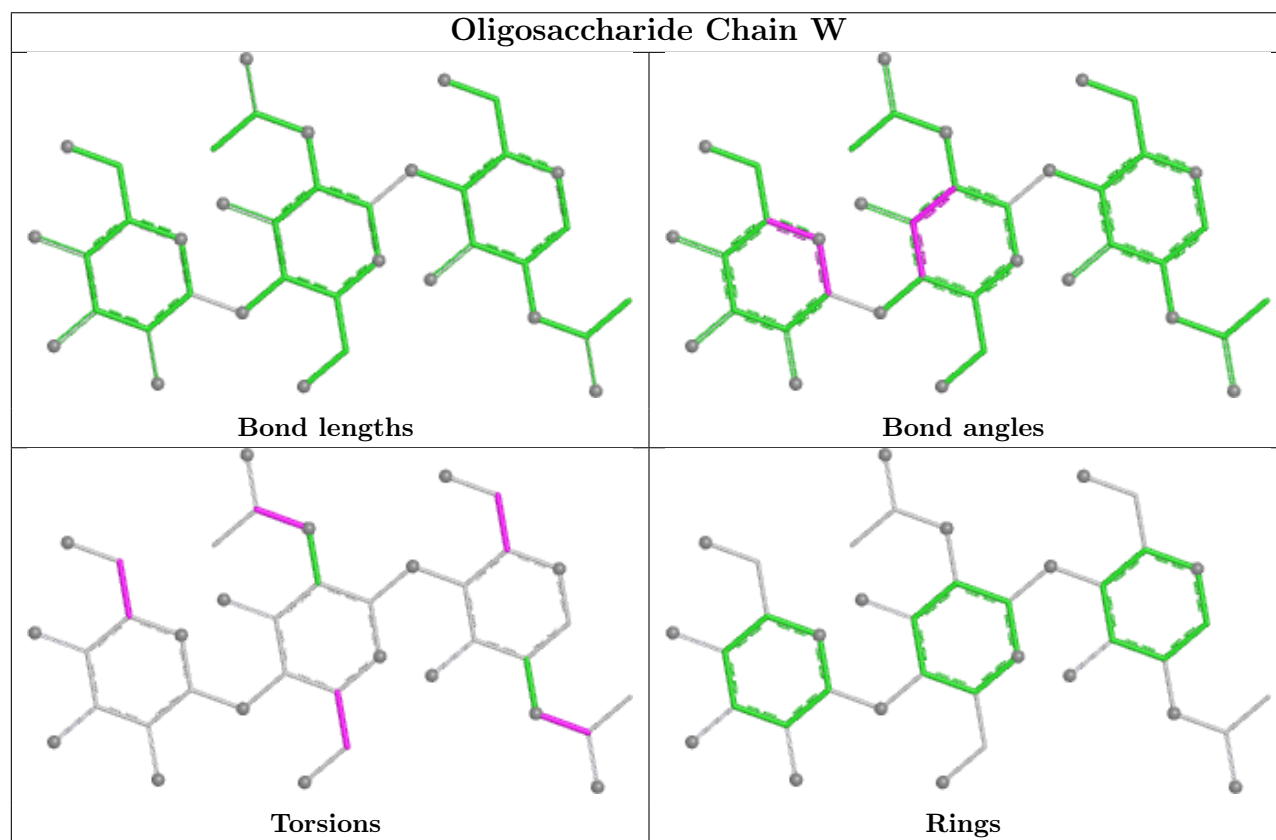
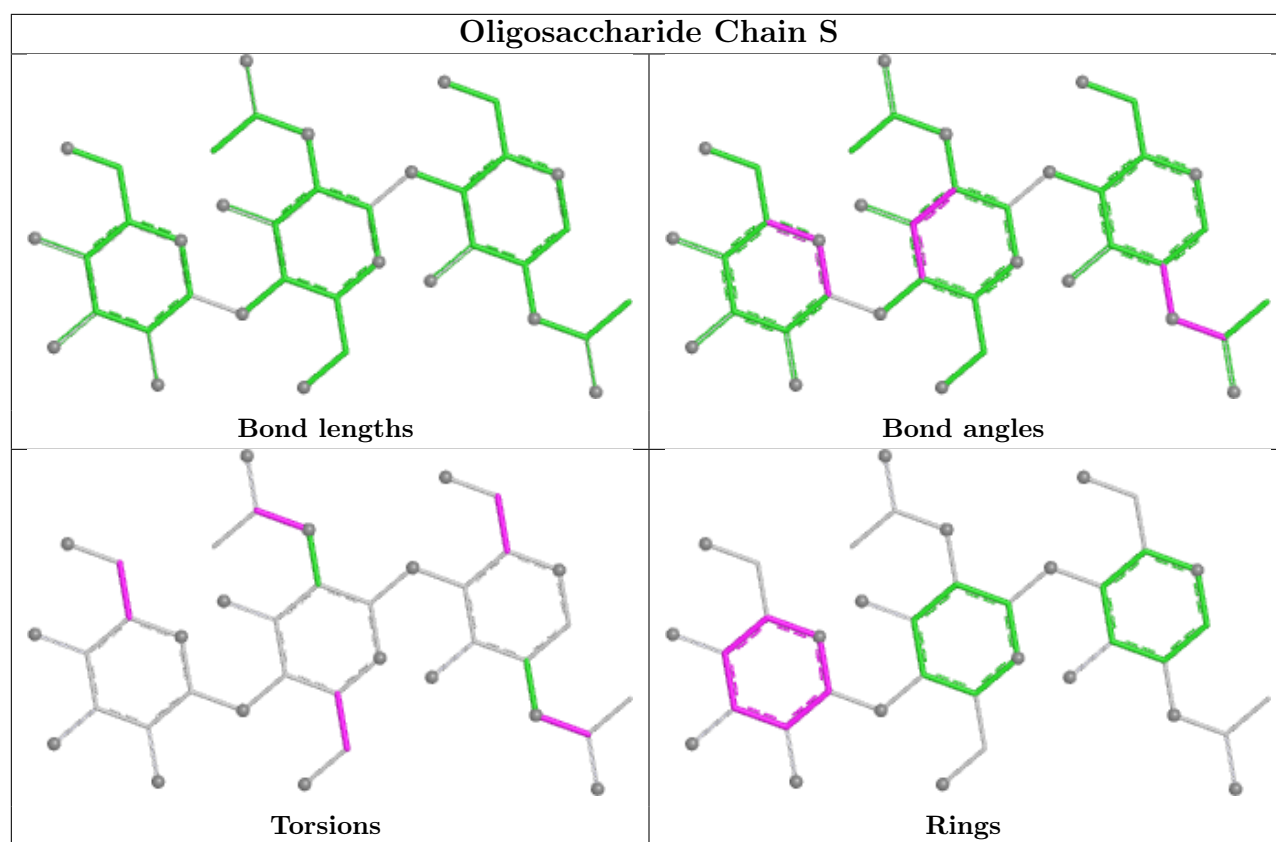


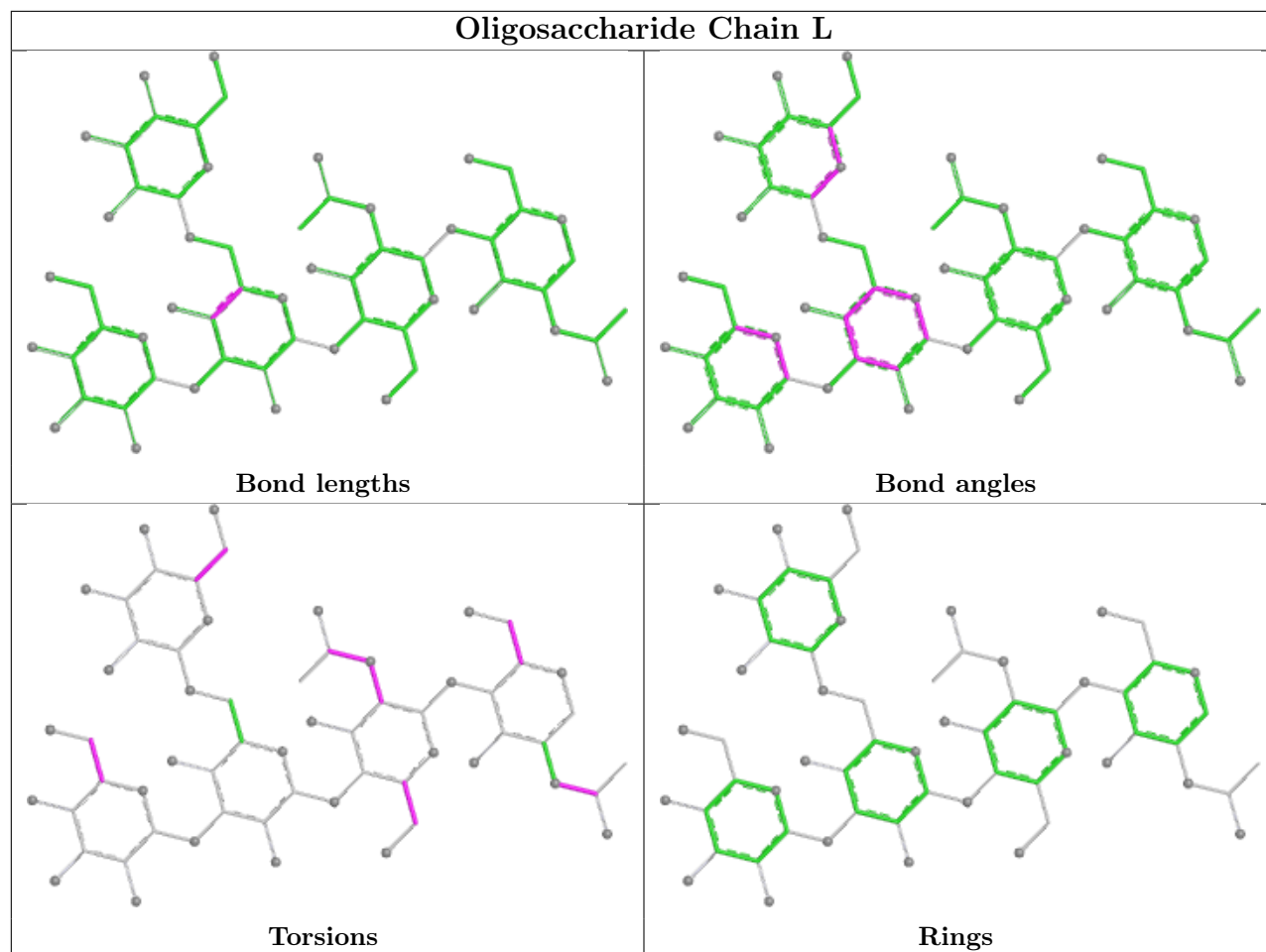


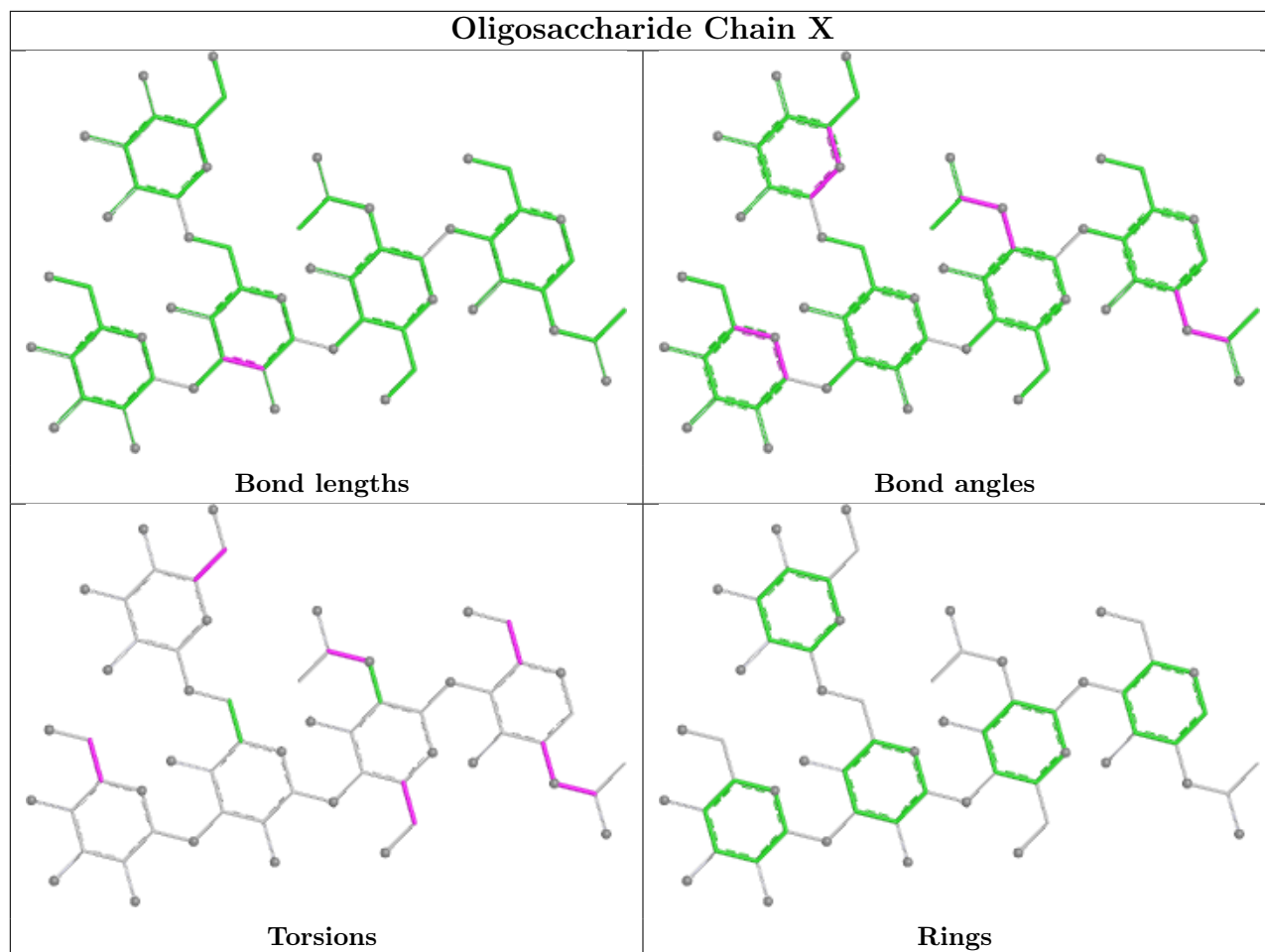


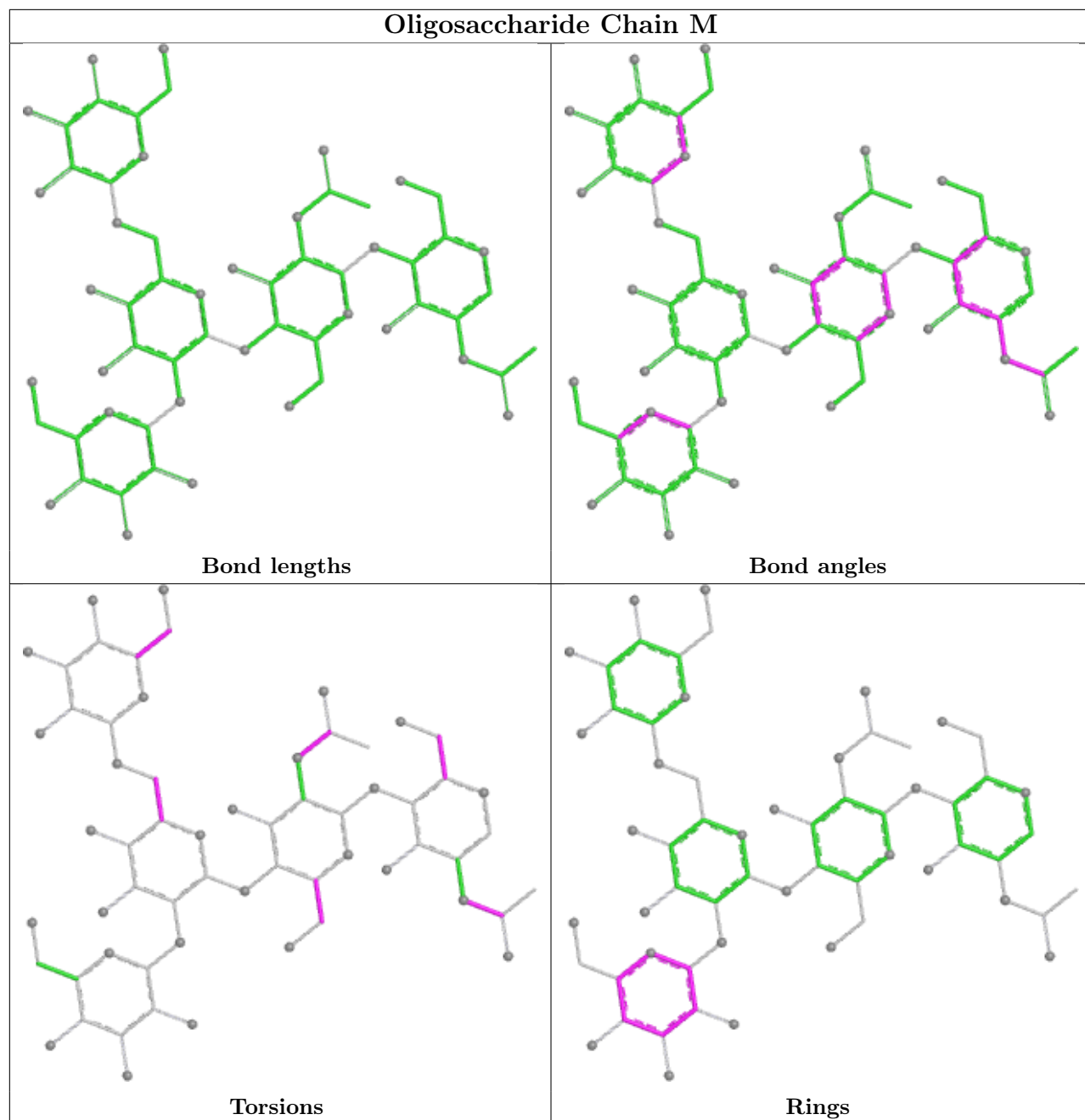


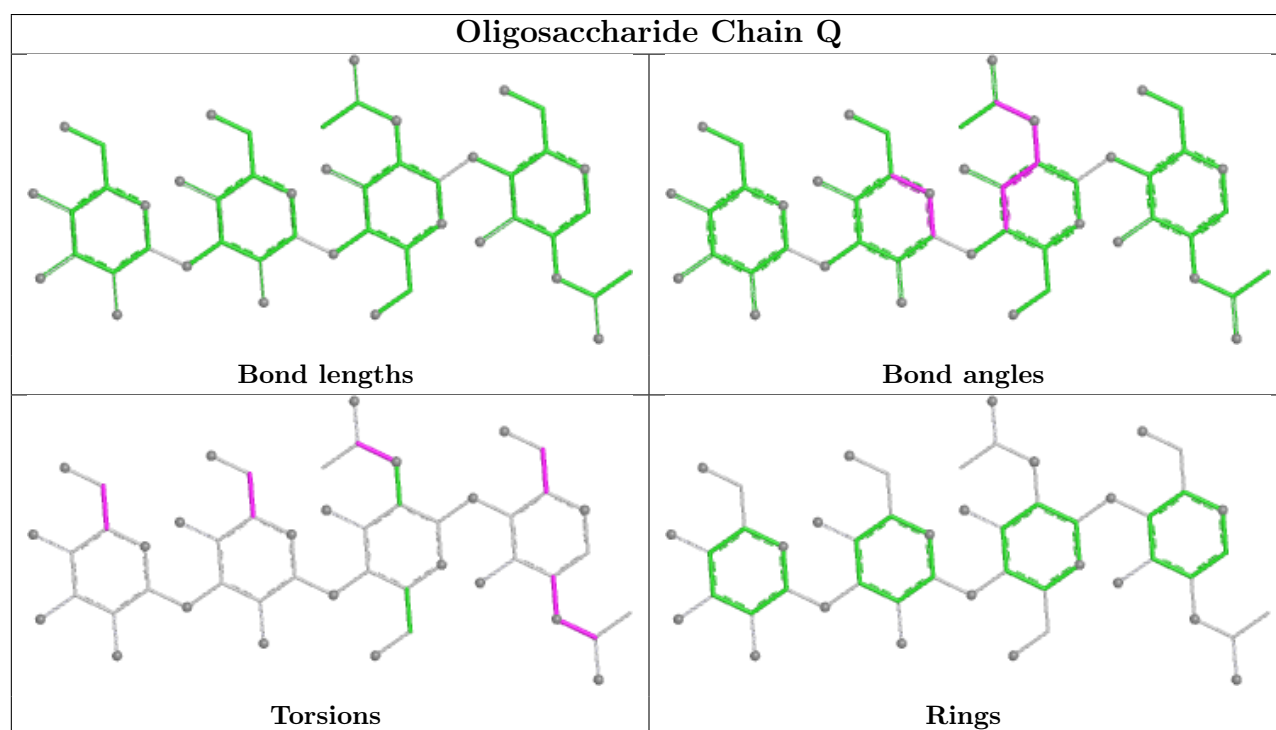
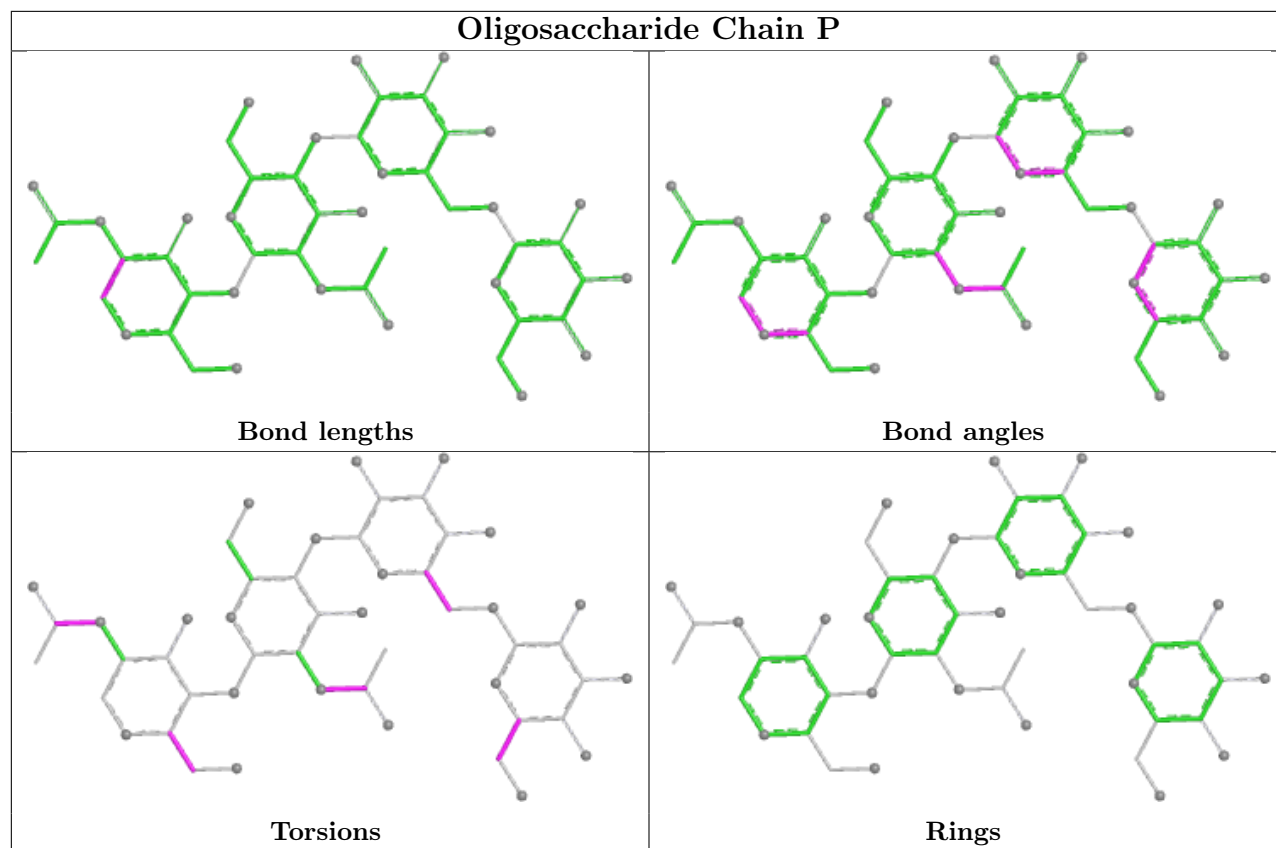


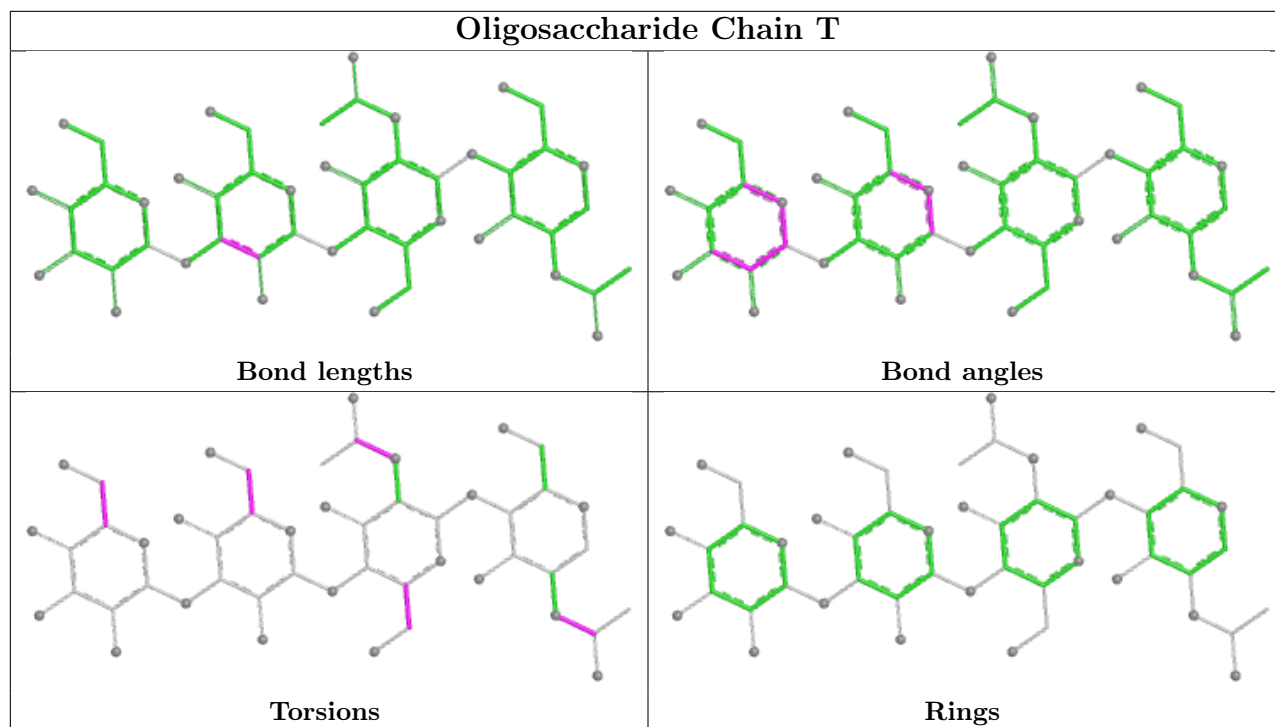












## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	MLI	D	612	-	6,6,6	1.53	2 (33%)	7,7,7	1.70	2 (28%)
9	MLI	E	610	-	6,6,6	1.47	2 (33%)	7,7,7	1.44	1 (14%)
9	MLI	A	611	-	6,6,6	1.56	2 (33%)	7,7,7	1.67	2 (28%)
9	MLI	B	612	-	6,6,6	1.45	2 (33%)	7,7,7	1.58	2 (28%)
9	MLI	F	611	-	6,6,6	1.61	2 (33%)	7,7,7	1.47	1 (14%)
9	MLI	C	610	-	6,6,6	1.70	2 (33%)	7,7,7	1.41	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MLI	D	612	-	-	0/4/4/4	-
9	MLI	E	610	-	-	0/4/4/4	-
9	MLI	A	611	-	-	0/4/4/4	-
9	MLI	B	612	-	-	0/4/4/4	-
9	MLI	F	611	-	-	0/4/4/4	-
9	MLI	C	610	-	-	0/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	610	MLI	O9-C3	-2.74	1.21	1.30
9	E	610	MLI	O7-C2	-2.62	1.22	1.30
9	F	611	MLI	O7-C2	-2.55	1.22	1.30
9	B	612	MLI	O7-C2	-2.50	1.22	1.30
9	C	610	MLI	O7-C2	-2.44	1.22	1.30

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	612	MLI	O7-C2-C1	2.50	122.27	114.51
9	E	610	MLI	O9-C3-C1	2.48	122.19	114.51
9	F	611	MLI	O9-C3-C1	2.45	122.12	114.51
9	A	611	MLI	O9-C3-C1	2.44	122.08	114.51
9	D	612	MLI	O9-C3-C1	2.38	121.88	114.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	610	MLI	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	A	456/529 (86%)	0.24	11 (2%) 59 44	63, 116, 150, 186	0
1	B	456/529 (86%)	0.22	9 (1%) 65 48	61, 116, 150, 186	0
1	C	450/529 (85%)	0.29	19 (4%) 40 28	52, 116, 152, 186	1 (0%)
1	D	456/529 (86%)	0.33	17 (3%) 45 32	65, 117, 152, 185	0
1	E	456/529 (86%)	0.24	9 (1%) 65 48	62, 116, 150, 186	0
1	F	450/529 (85%)	0.34	20 (4%) 39 28	70, 117, 155, 185	0
All	All	2724/3174 (85%)	0.28	85 (3%) 51 38	52, 116, 151, 186	1 (0%)

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	105	VAL	6.0
1	D	406	GLU	5.9
1	A	406	GLU	5.5
1	E	406	GLU	5.4
1	B	406	GLU	5.4

### 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( $\text{\AA}^2$ )	Q<0.9
4	MAN	W	3	11/12	0.03	0.19	183,183,183,183	0
3	NAG	V	2	14/15	0.07	0.18	173,173,173,173	0
5	MAN	L	4	11/12	0.12	0.15	190,190,190,190	0
8	MAN	Q	3	11/12	0.15	0.17	178,178,178,178	0
3	NAG	U	2	14/15	0.16	0.17	164,164,164,164	0
2	MAN	G	5	11/12	0.22	0.13	182,182,182,182	0
5	MAN	L	5	11/12	0.23	0.17	189,189,189,189	0
3	NAG	O	2	14/15	0.28	0.16	171,171,171,171	0
4	MAN	J	3	11/12	0.29	0.14	171,171,171,171	0
5	MAN	X	3	11/12	0.30	0.13	183,183,183,183	0
8	MAN	T	4	11/12	0.30	0.13	180,180,180,180	0
2	NAG	G	2	14/15	0.33	0.16	171,171,171,171	0
5	MAN	L	3	11/12	0.37	0.13	187,187,187,187	0
2	MAN	G	4	11/12	0.37	0.14	177,177,177,177	0
4	NAG	I	2	14/15	0.37	0.19	173,173,173,173	0
4	MAN	K	3	11/12	0.38	0.14	176,176,176,176	0
4	MAN	S	3	11/12	0.39	0.15	179,179,179,179	0
4	MAN	I	3	11/12	0.39	0.16	179,179,179,179	0
4	NAG	R	2	14/15	0.41	0.15	163,163,163,163	0
5	MAN	X	4	11/12	0.41	0.13	187,187,187,187	0
4	MAN	R	3	11/12	0.45	0.13	169,169,169,169	0
4	NAG	J	2	14/15	0.45	0.17	166,166,166,166	0
3	NAG	N	2	14/15	0.46	0.21	157,157,157,157	0
8	MAN	Q	4	11/12	0.47	0.12	181,181,181,181	0
6	MAN	M	4	11/12	0.47	0.13	188,188,188,188	0
4	NAG	S	2	14/15	0.49	0.17	172,172,172,172	0
3	NAG	H	2	14/15	0.51	0.13	162,162,162,162	0
8	MAN	T	3	11/12	0.52	0.14	178,178,178,178	0
5	MAN	X	5	11/12	0.53	0.12	186,186,186,186	0
5	NAG	L	2	14/15	0.55	0.16	177,177,177,177	0
4	NAG	W	2	14/15	0.56	0.15	176,176,176,176	0
7	MAN	P	3	11/12	0.57	0.10	180,180,180,180	0
8	NAG	Q	2	14/15	0.57	0.16	171,171,171,171	0
6	NAG	M	2	14/15	0.57	0.14	173,173,173,173	0
6	MAN	M	3	11/12	0.59	0.11	185,185,185,185	0
4	NAG	J	1	14/15	0.59	0.17	154,154,154,154	0
7	MAN	P	4	11/12	0.61	0.12	184,184,184,184	0
3	NAG	U	1	14/15	0.62	0.15	159,159,159,159	0
2	BMA	G	3	11/12	0.62	0.12	177,177,177,177	0
4	NAG	K	2	14/15	0.62	0.12	172,172,172,172	0
3	NAG	V	1	14/15	0.64	0.15	166,166,166,166	0
5	NAG	X	2	14/15	0.65	0.14	170,170,170,170	0
8	NAG	T	2	14/15	0.65	0.16	170,170,170,170	0

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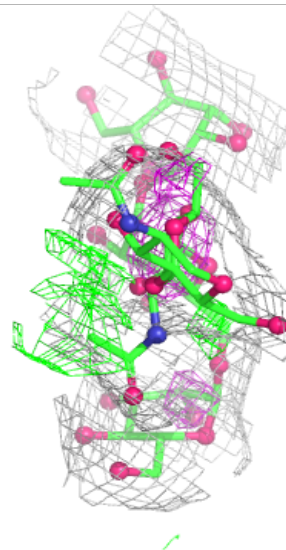
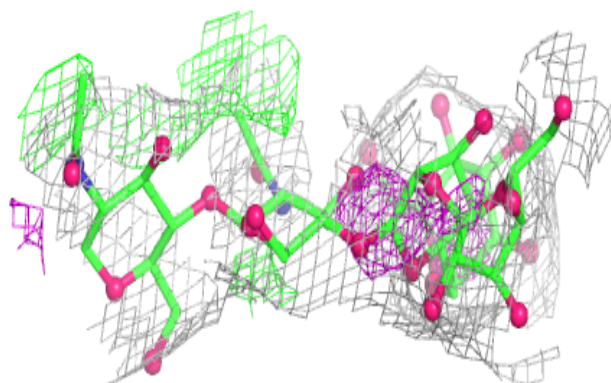
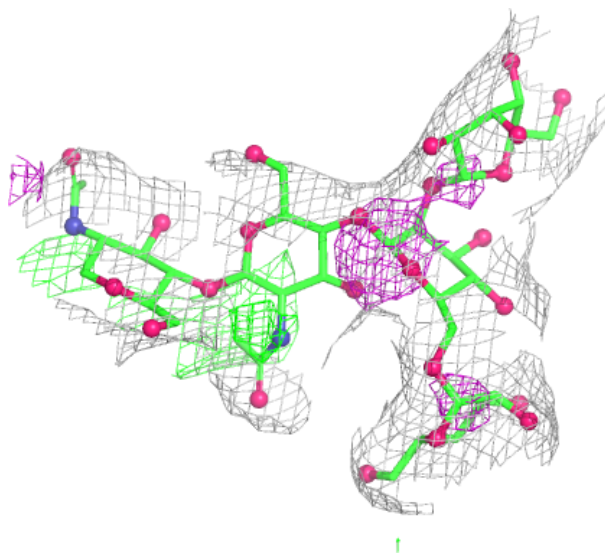
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	M	5	11/12	0.66	0.10	188,188,188,188	0
6	NAG	M	1	14/15	0.69	0.16	160,160,160,160	0
5	NAG	X	1	14/15	0.72	0.15	162,162,162,162	0
3	NAG	H	1	14/15	0.74	0.15	158,158,158,158	0
7	NAG	P	2	14/15	0.74	0.12	170,170,170,170	0
4	NAG	K	1	14/15	0.75	0.16	163,163,163,163	0
3	NAG	O	1	14/15	0.75	0.14	164,164,164,164	0
7	NAG	P	1	14/15	0.76	0.17	160,160,160,160	0
4	NAG	S	1	14/15	0.78	0.16	159,159,159,159	0
2	NAG	G	1	14/15	0.81	0.14	157,157,157,157	0
4	NAG	R	1	14/15	0.83	0.13	155,155,155,155	0
8	NAG	T	1	14/15	0.87	0.12	157,157,157,157	0
4	NAG	W	1	14/15	0.87	0.14	162,162,162,162	0
8	NAG	Q	1	14/15	0.88	0.12	160,160,160,160	0
3	NAG	N	1	14/15	0.88	0.12	152,152,152,152	0
4	NAG	I	1	14/15	0.90	0.10	160,160,160,160	0
5	NAG	L	1	14/15	0.91	0.15	163,163,163,163	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.

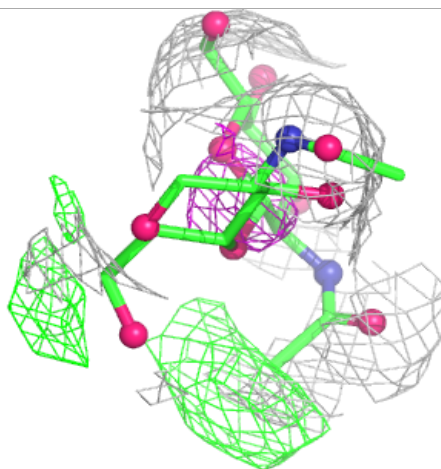
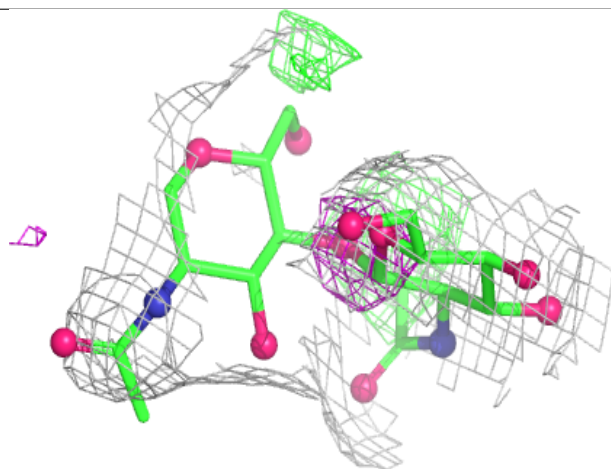
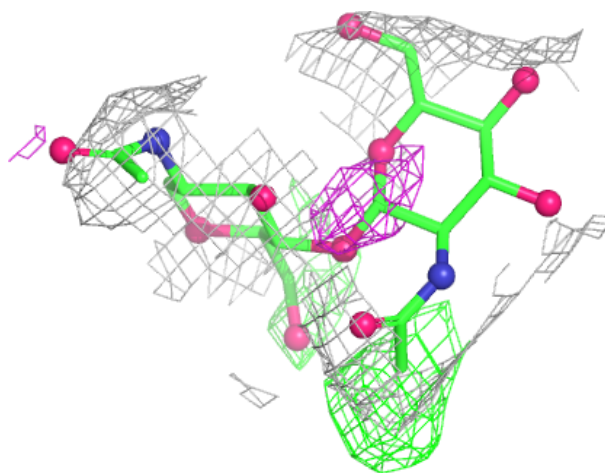
**Electron density around Chain G:**

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



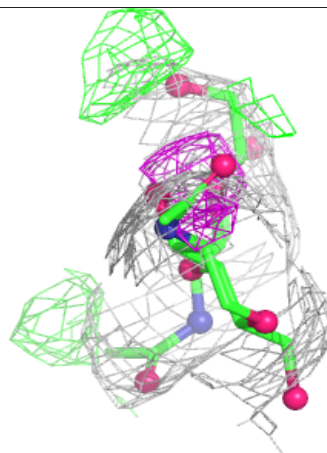
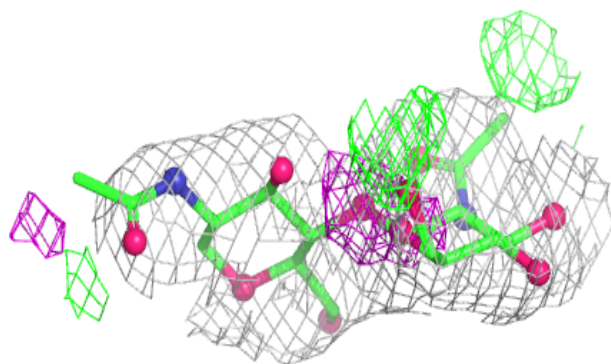
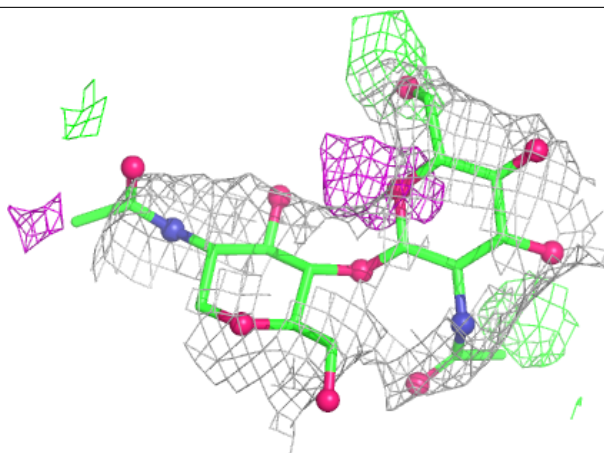
**Electron density around Chain H:**

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



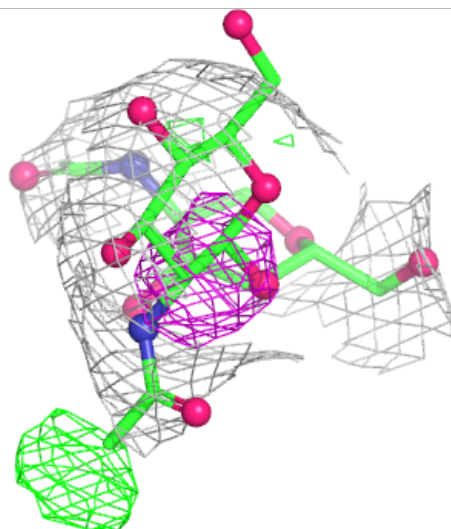
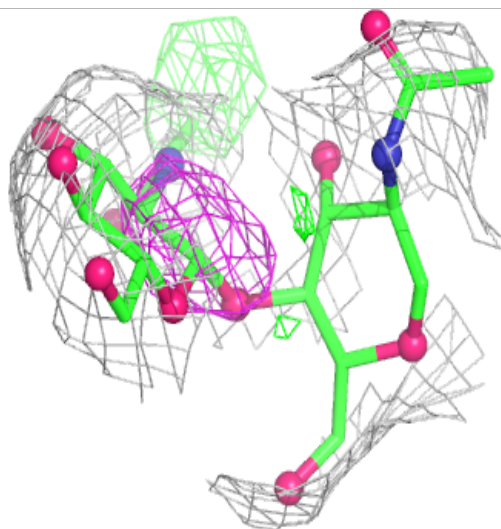
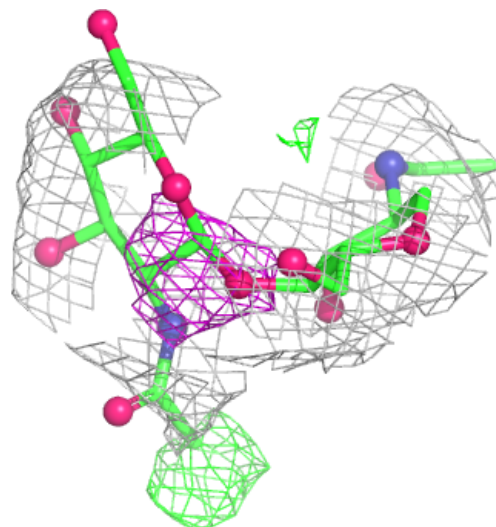
**Electron density around Chain N:**

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



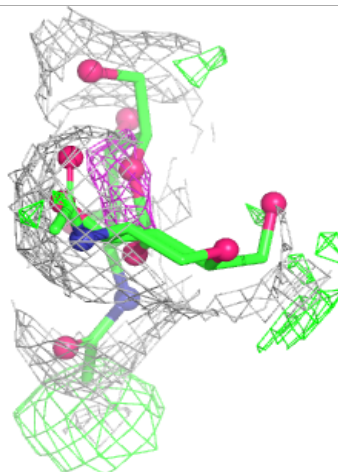
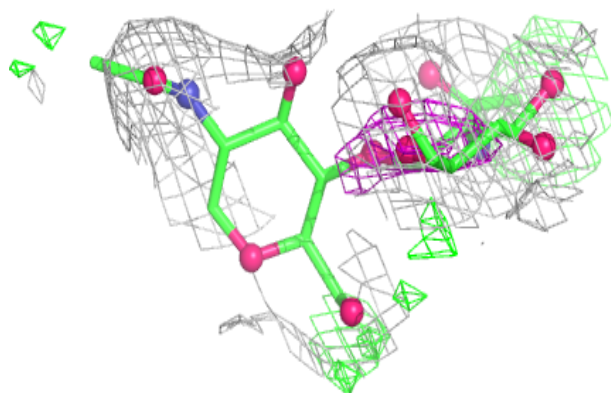
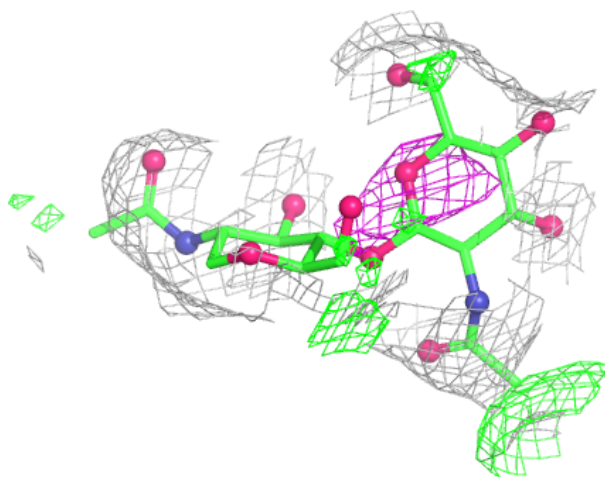
**Electron density around Chain O:**

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



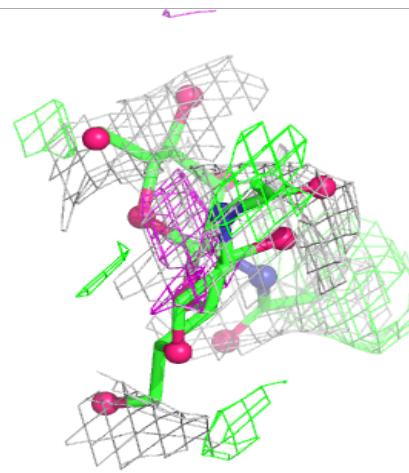
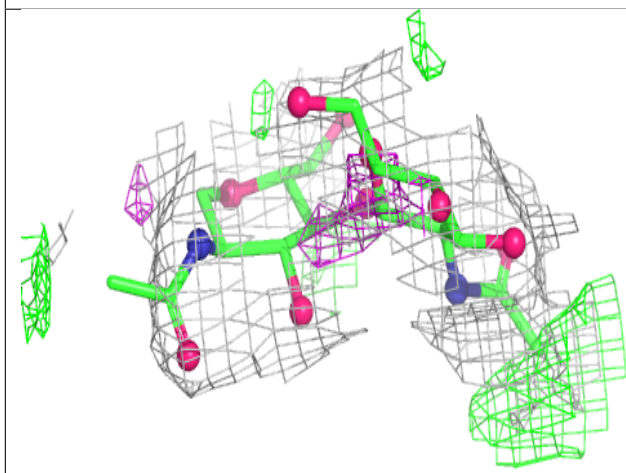
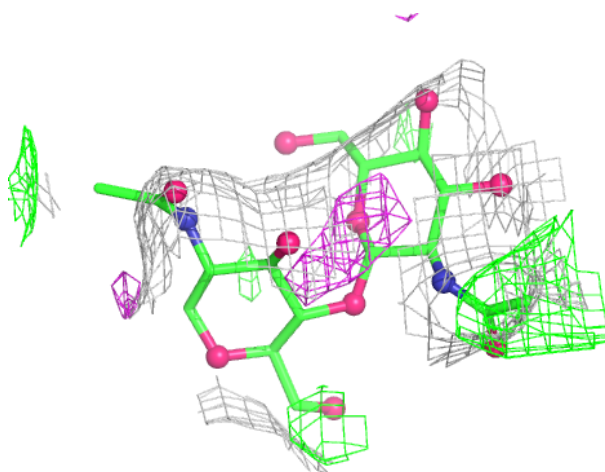
**Electron density around Chain U:**

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



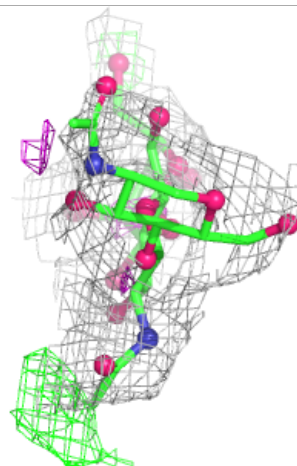
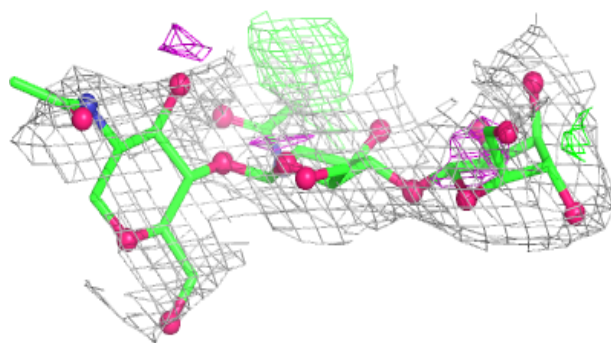
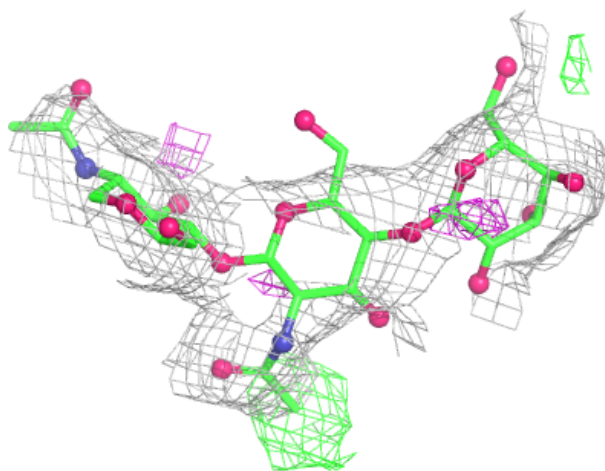
**Electron density around Chain V:**

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



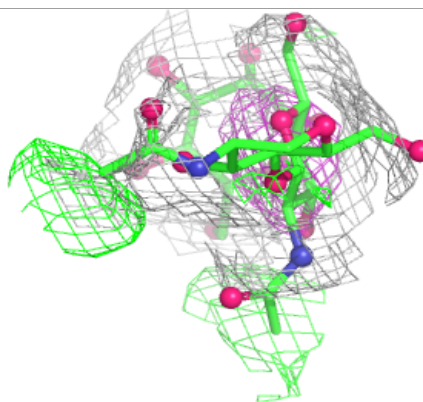
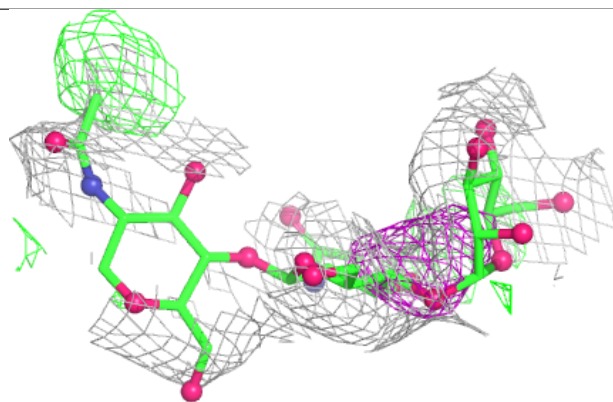
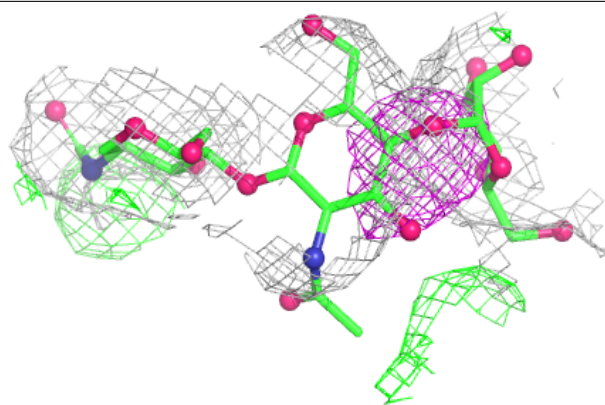
**Electron density around Chain I:**

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

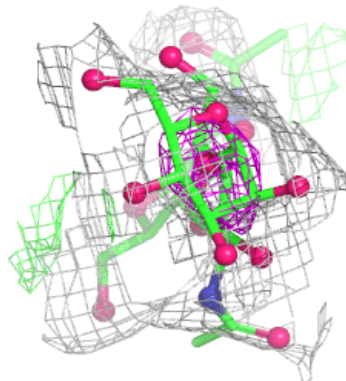
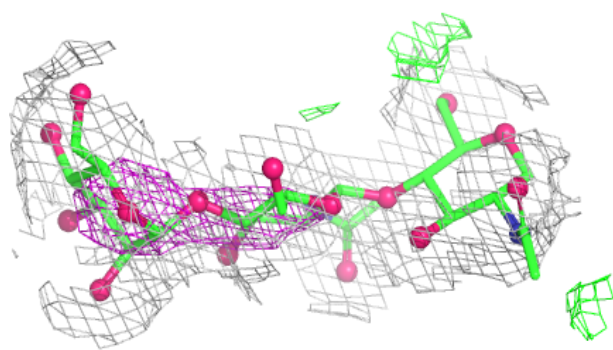
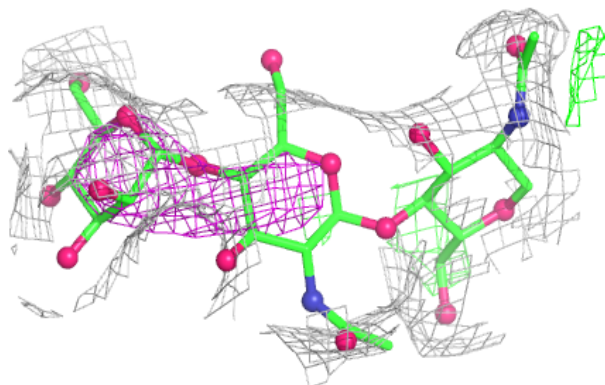


**Electron density around Chain J:**

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

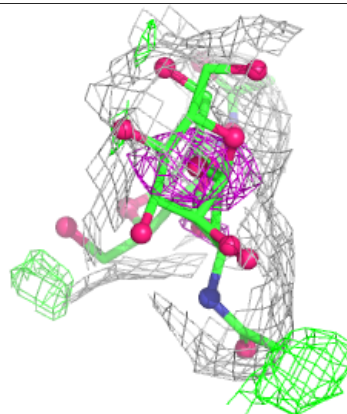
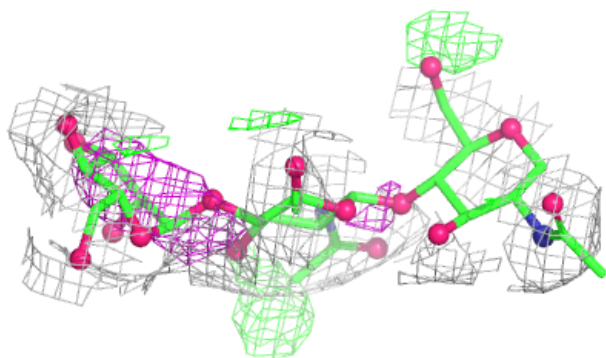
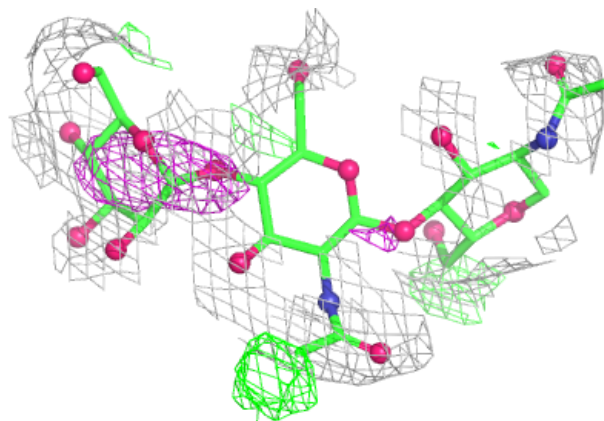
**Electron density around Chain K:**

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

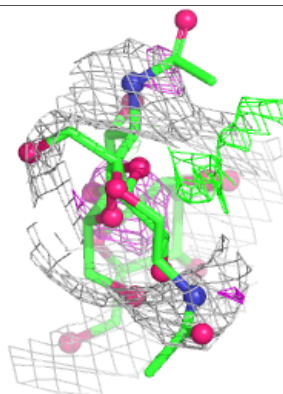
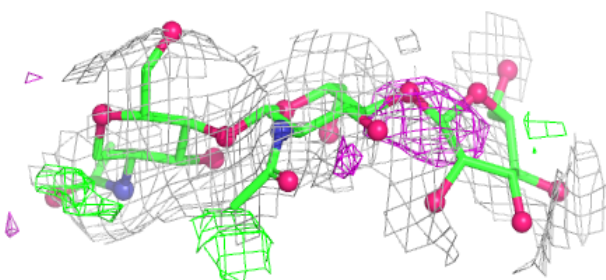
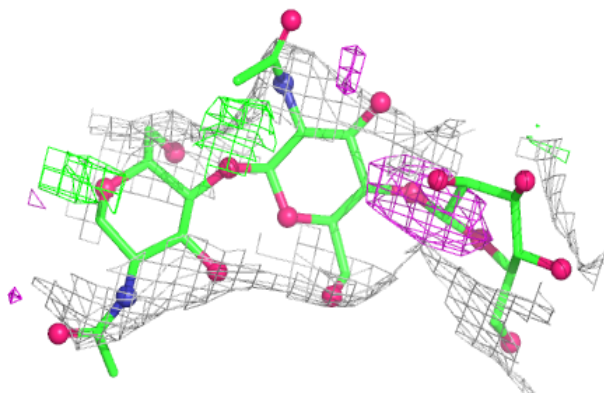


**Electron density around Chain R:**

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

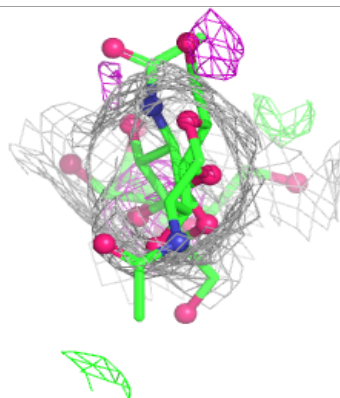
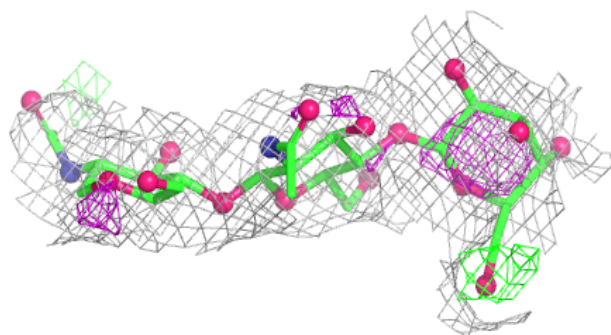
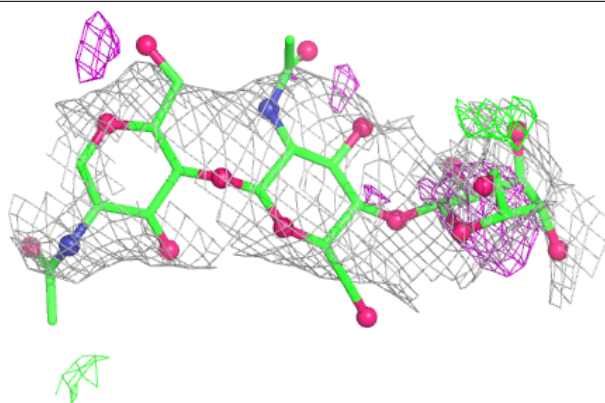
**Electron density around Chain S:**

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



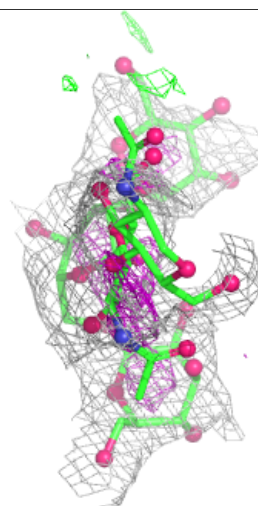
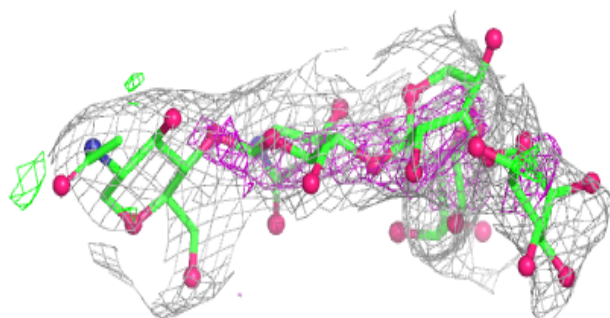
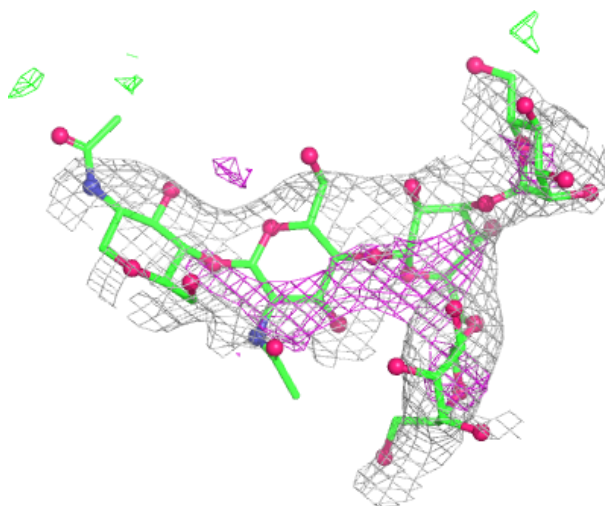
**Electron density around Chain W:**

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



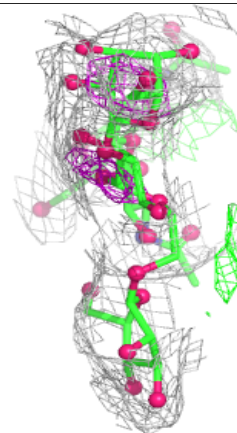
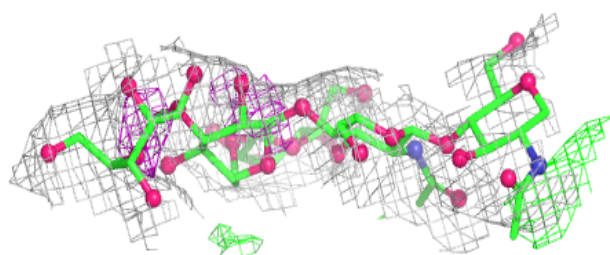
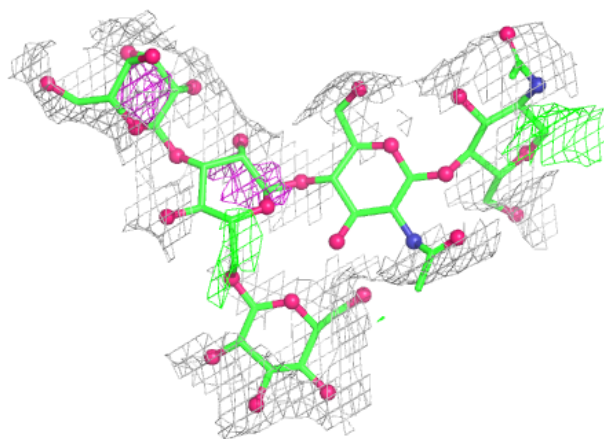
**Electron density around Chain L:**

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



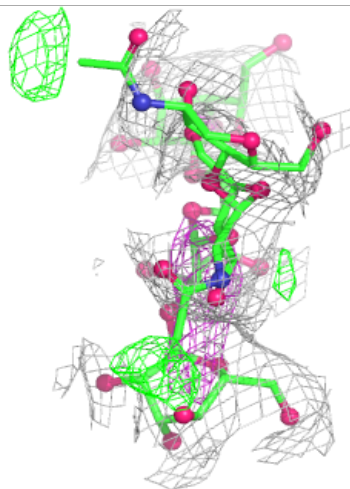
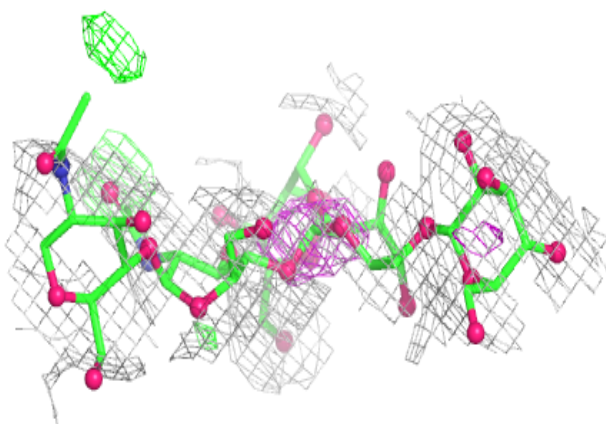
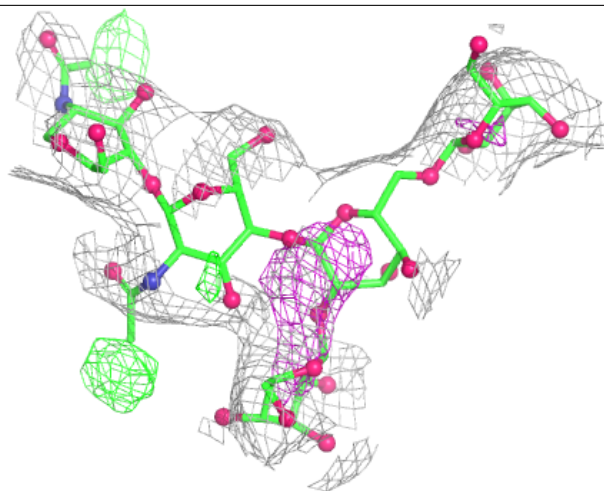
**Electron density around Chain X:**

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



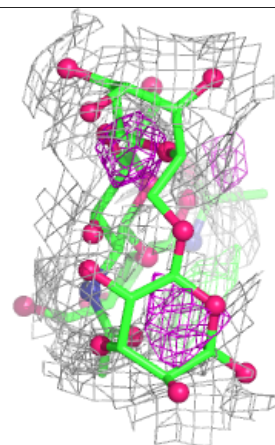
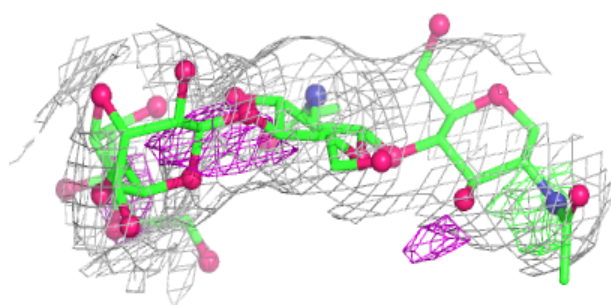
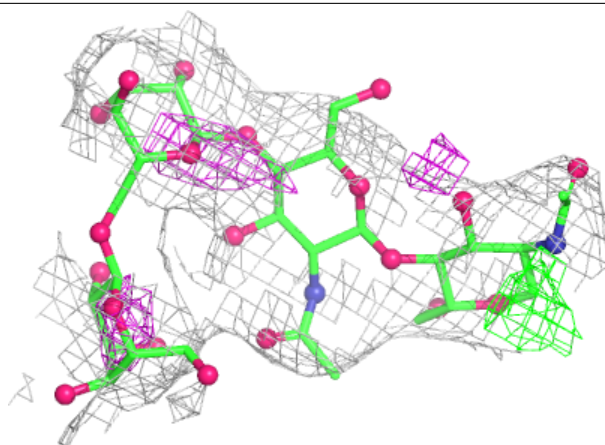
**Electron density around Chain M:**

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

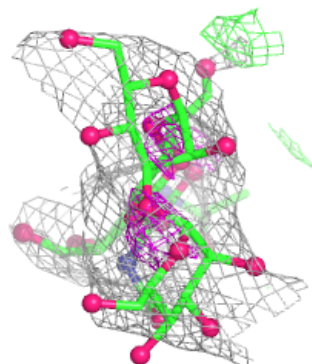
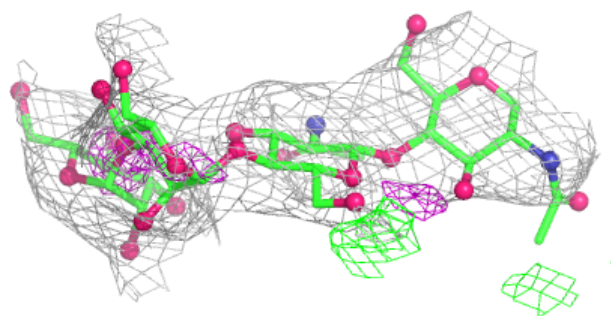
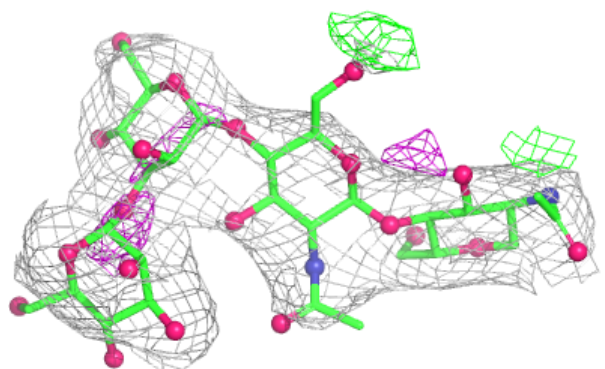


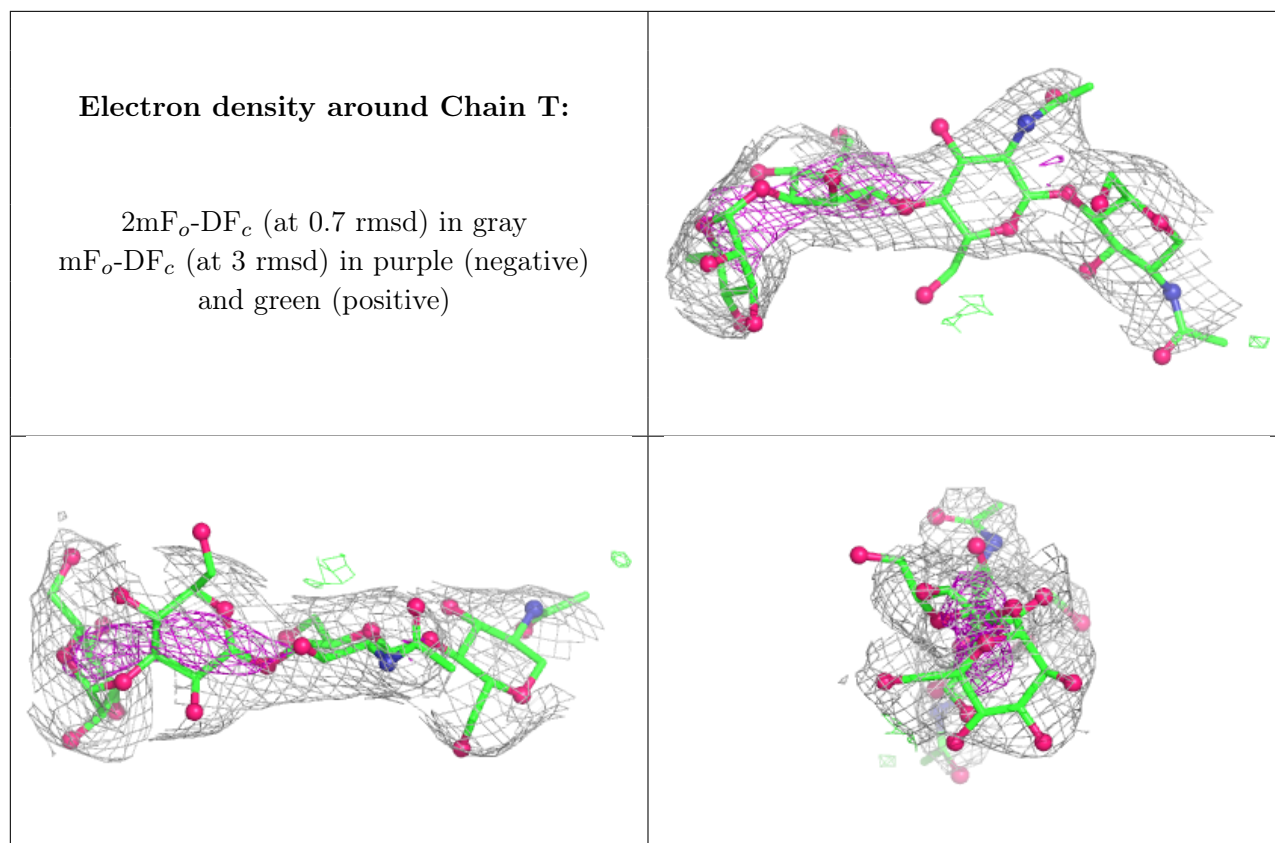
**Electron density around Chain P:**

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

**Electron density around Chain Q:**

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





## 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
9	MLI	F	611	7/7	0.84	0.23	133,134,134,135	0
9	MLI	B	612	7/7	0.88	0.20	143,144,144,144	0
9	MLI	C	610	7/7	0.89	0.21	140,141,142,143	0
9	MLI	E	610	7/7	0.91	0.16	142,142,142,143	0
9	MLI	D	612	7/7	0.92	0.18	134,134,136,136	0
9	MLI	A	611	7/7	0.95	0.15	135,136,136,137	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.