



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:17 PM EDT

PDB ID : 6OM1 / pdb_00006om1
Title : Crystal structure of an atypical integrin
Authors : Wang, J.C.; Springer, T.A.
Deposited on : 2019-04-17
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

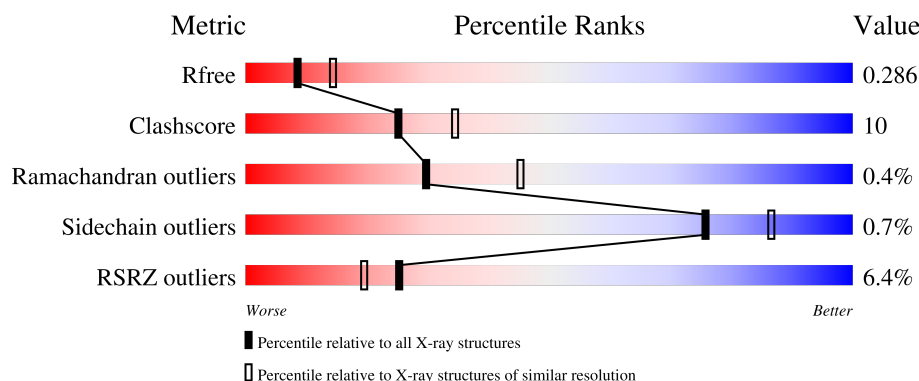
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	599	4% 85% 13% ..
1	C	599	4% 84% 15% .
1	E	599	7% 80% 18% .
1	G	599	5% 84% 15% ..
2	B	456	6% 53% 20% 27% .

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Mol	Chain	Length	Quality of chain
2	D	456	
2	F	456	
2	H	456	
3	I	4	
3	K	4	
3	O	4	
3	Q	4	
3	S	4	
3	a	4	
3	d	4	
4	J	5	
4	U	5	
4	X	5	
5	L	6	
6	M	2	
6	N	2	
6	T	2	
6	V	2	
6	Y	2	
6	Z	2	
6	e	2	
6	f	2	
6	g	2	
7	P	6	
7	R	6	

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Mol	Chain	Length	Quality of chain
7	W	6	 50% 50%
8	b	6	 33% 67%
9	c	4	 50% 50%

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
3	NAG	I	2	-	-	X	-
3	BMA	I	3	-	-	X	-
3	BMA	Q	3	-	-	X	-
6	NAG	e	2	-	-	X	-
7	BMA	R	3	-	-	X	-
7	BMA	W	3	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 57933 atoms, of which 27345 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	592	Total	C	H	N	O	S	0	0	0
			8954	2905	4374	776	878	21			
1	C	595	Total	C	H	N	O	S	0	0	0
			9011	2918	4409	780	883	21			
1	E	593	Total	C	H	N	O	S	0	0	0
			8984	2905	4399	778	881	21			
1	G	596	Total	C	H	N	O	S	0	0	0
			9006	2922	4395	783	885	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	engineered mutation	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
A	599	LEU	-	expression tag	UNP P06756
C	400	GLY	-	insertion	UNP P06756
C	401	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756
C	599	LEU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	engineered mutation	UNP P06756
E	596	THR	-	expression tag	UNP P06756
E	597	GLY	-	expression tag	UNP P06756
E	598	GLY	-	expression tag	UNP P06756
E	599	LEU	-	expression tag	UNP P06756
G	400	GLY	-	insertion	UNP P06756
G	401	CYS	MET	engineered mutation	UNP P06756
G	596	THR	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
G	597	GLY	-	expression tag	UNP P06756
G	598	GLY	-	expression tag	UNP P06756
G	599	LEU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	333	Total	C	H	N	O	S	0	0	0
			5068	1658	2455	447	491	17			
2	D	312	Total	C	H	N	O	S	0	0	0
			4742	1559	2291	416	462	14			
2	F	332	Total	C	H	N	O	S	0	0	0
			5069	1648	2470	448	488	15			
2	H	336	Total	C	H	N	O	S	0	0	0
			5181	1667	2552	453	491	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	CYS	VAL	engineered mutation	UNP P26012
D	259	CYS	VAL	engineered mutation	UNP P26012
F	259	CYS	VAL	engineered mutation	UNP P26012
H	259	CYS	VAL	engineered mutation	UNP P26012

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



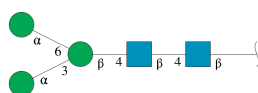
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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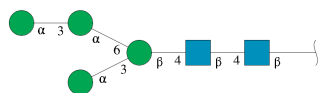
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	a	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



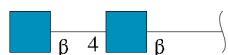
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



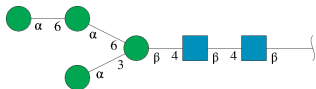
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



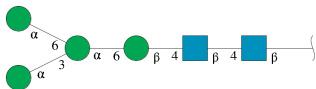
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	P	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	R	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



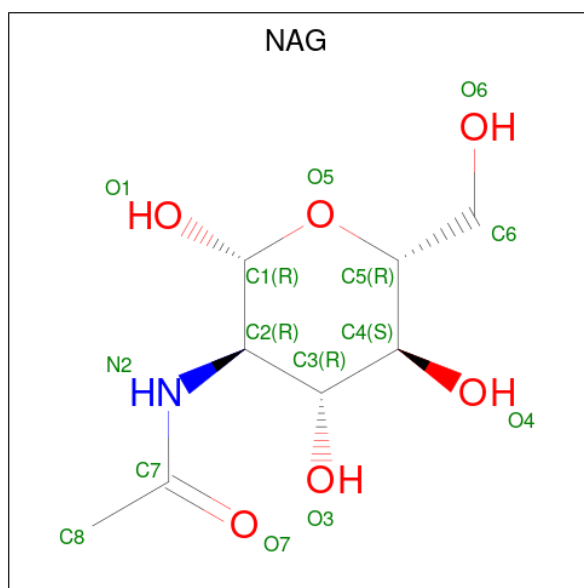
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	b	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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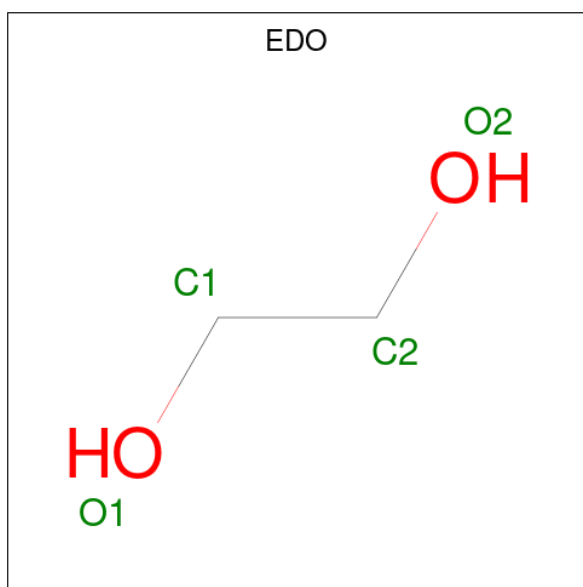
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	Ca	0	0
			4	4		
11	B	1	Total	Ca	0	0
			1	1		
11	C	4	Total	Ca	0	0
			4	4		
11	D	1	Total	Ca	0	0
			1	1		
11	E	4	Total	Ca	0	0
			4	4		
11	F	1	Total	Ca	0	0
			1	1		
11	G	4	Total	Ca	0	0
			4	4		
11	H	1	Total	Ca	0	0
			1	1		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

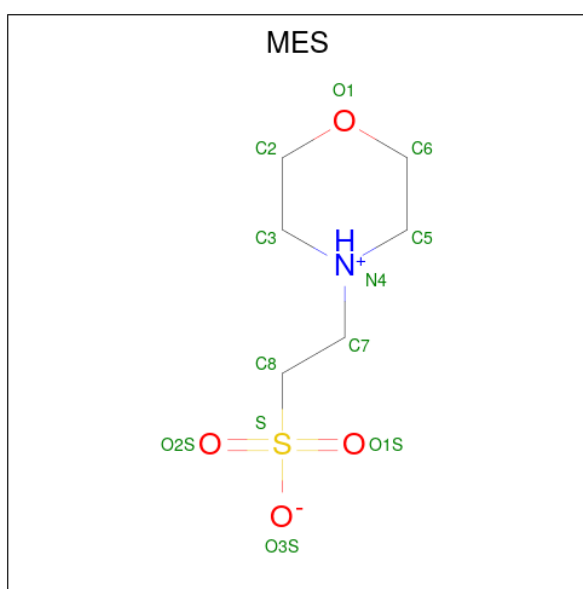


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	F	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Mg	0	0
			1	1		
13	D	1	Total	Mg	0	0
			1	1		
13	F	1	Total	Mg	0	0
			1	1		
13	H	1	Total	Mg	0	0
			1	1		

- Molecule 14 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
14	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
14	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
14	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	137	Total	O	0	0
			137	137		

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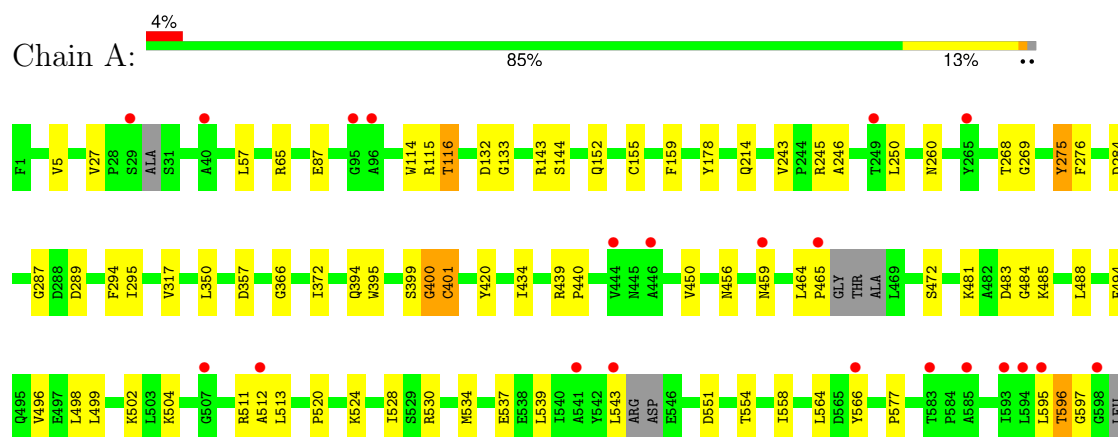
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	25	Total 25	O 25	0	0
15	C	108	Total 108	O 108	0	0
15	D	14	Total 14	O 14	0	0
15	E	47	Total 47	O 47	0	0
15	F	23	Total 23	O 23	0	0
15	G	62	Total 62	O 62	0	0
15	H	15	Total 15	O 15	0	0

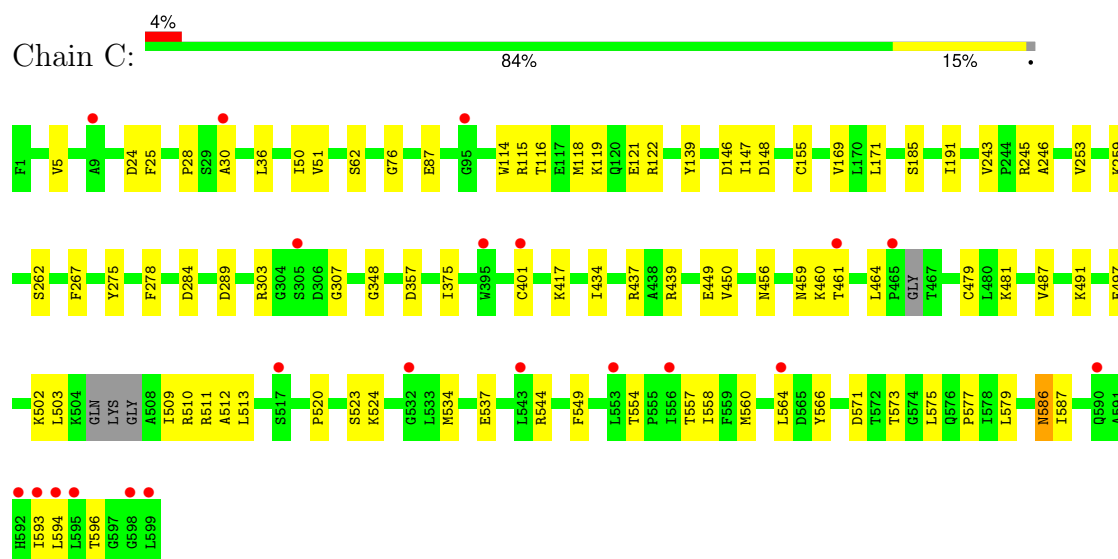
3 Residue-property plots [i](#)

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.

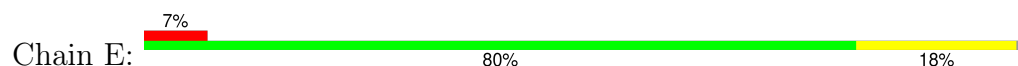
• Molecule 1: Integrin alpha-V

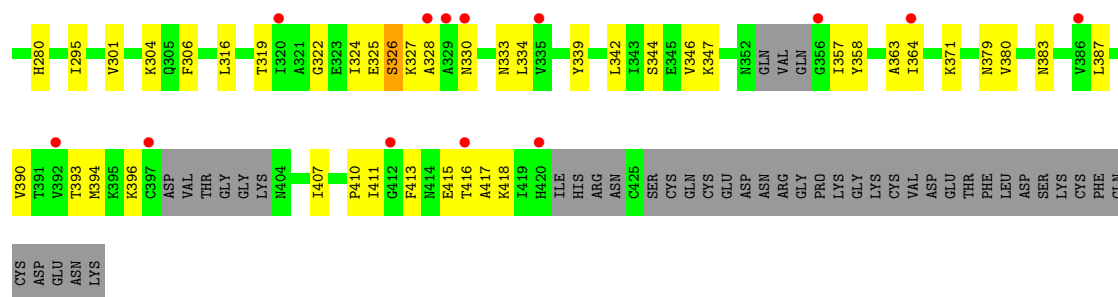


• Molecule 1: Integrin alpha-V

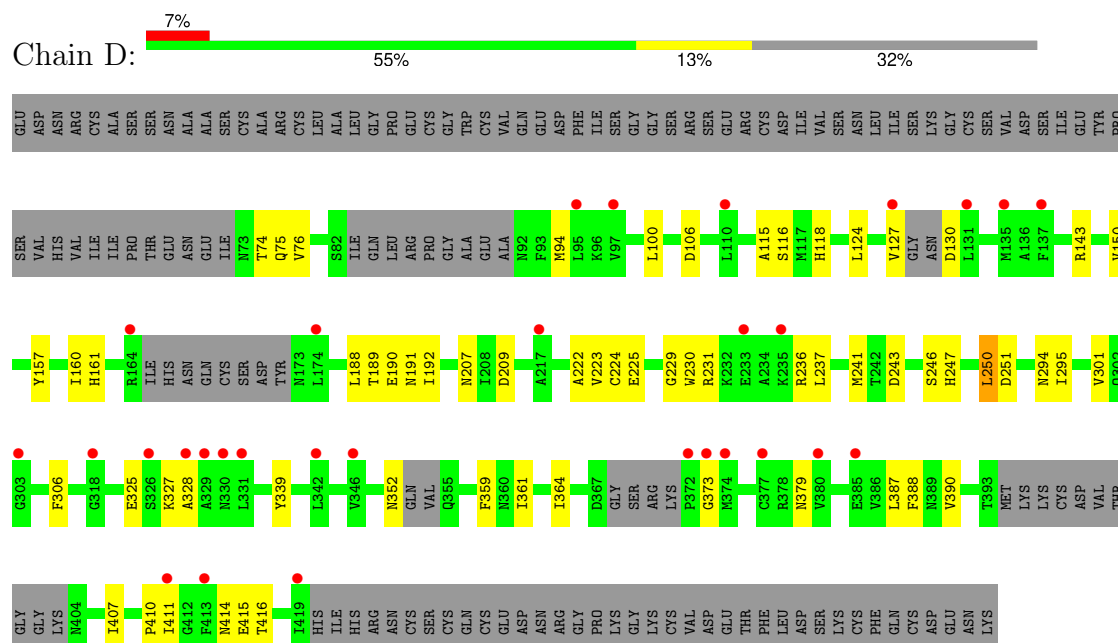


• Molecule 1: Integrin alpha-V

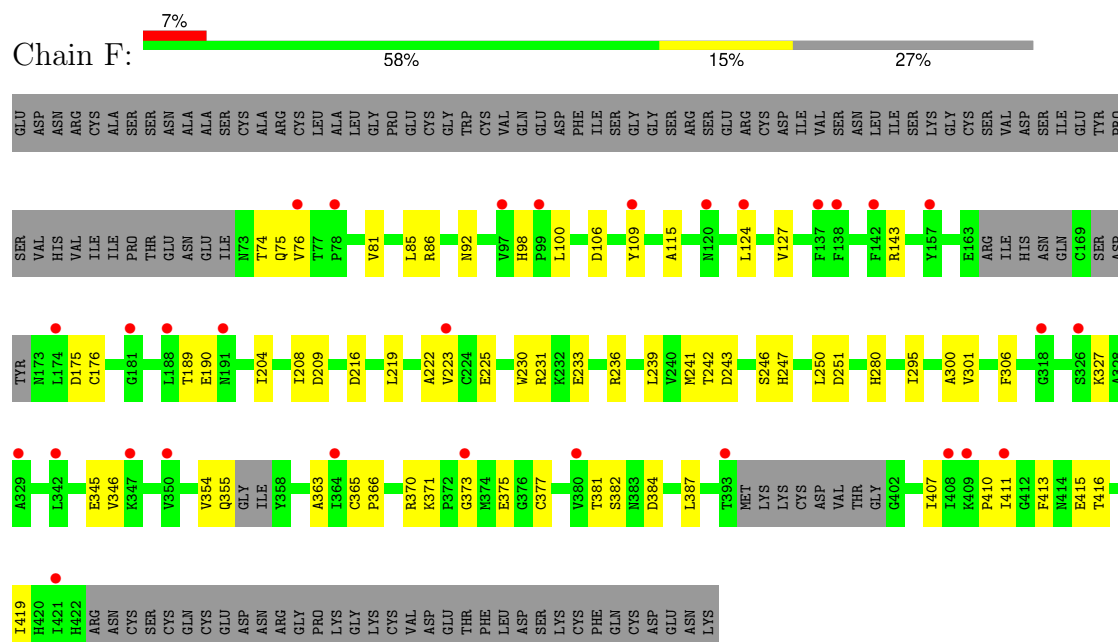




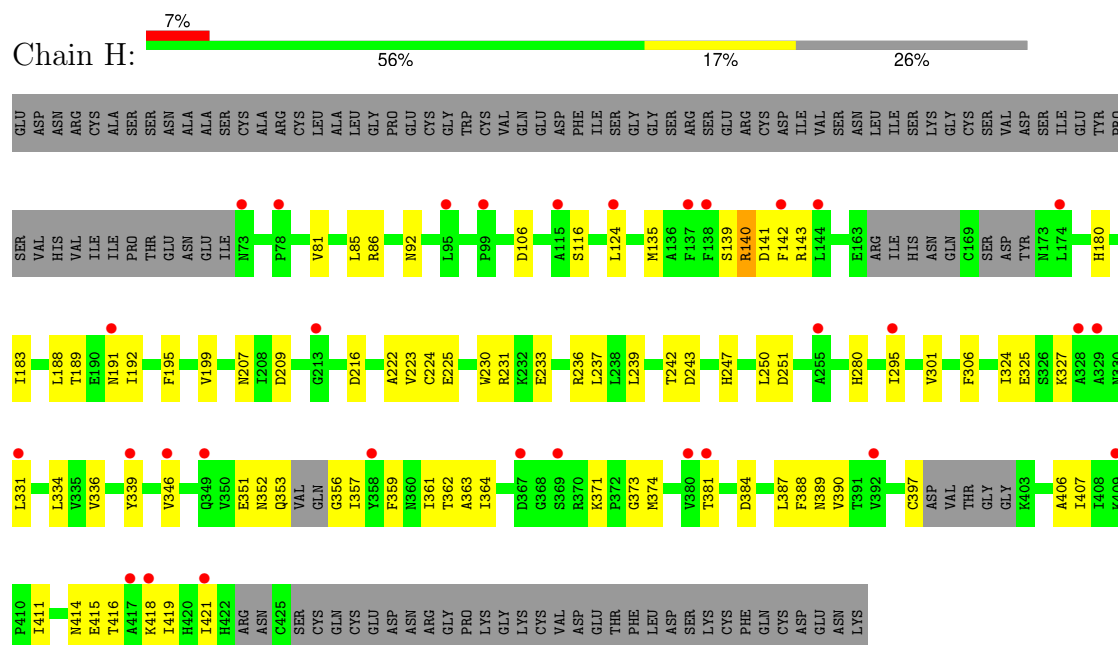
• Molecule 2: Integrin beta-8



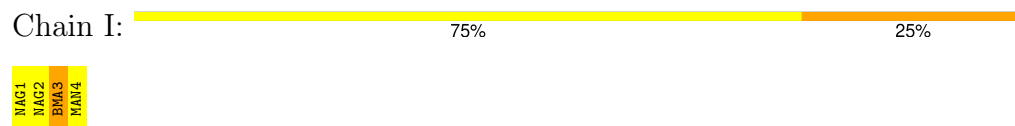
• Molecule 2: Integrin beta-8



- Molecule 2: Integrin beta-8



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



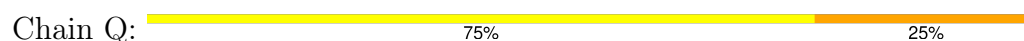
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





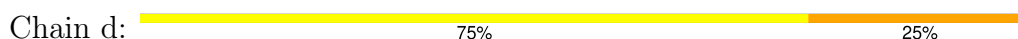
- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



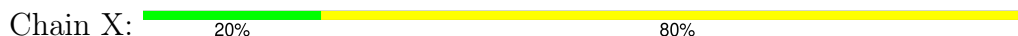
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



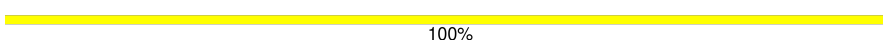


- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 



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

Chain M: 

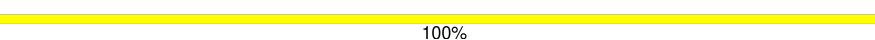


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

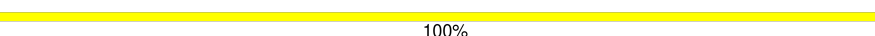


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

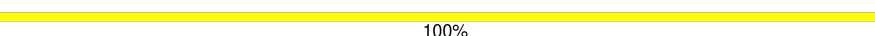


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain Y: 

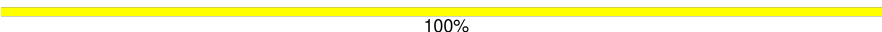


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 



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

Chain e: 



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

Chain f: 



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

Chain g: 



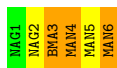
- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 



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

Chain R: 



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

ido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%



• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 67%



• Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	144.24Å 55.07Å 175.07Å 90.37° 107.00° 90.01°	Depositor
Resolution (Å)	48.07 – 2.66 48.07 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.07-2.66) 95.6 (48.07-2.66)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.248 , 0.280 0.256 , 0.286	Depositor DCC
R_{free} test set	2001 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57933	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/4681	0.29	0/6332
1	C	0.12	0/4704	0.30	0/6367
1	E	0.12	0/4687	0.29	0/6343
1	G	0.12	0/4713	0.30	0/6377
2	B	0.12	0/2662	0.30	0/3600
2	D	0.13	0/2497	0.30	0/3378
2	F	0.12	0/2650	0.29	0/3587
2	H	0.13	0/2679	0.30	0/3621
All	All	0.12	0/29273	0.30	0/39605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4580	4374	4429	65	1
1	C	4602	4409	4450	67	2
1	E	4585	4399	4427	82	0
1	G	4611	4395	4458	71	0
2	B	2613	2455	2600	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2451	2291	2431	53	0
2	F	2599	2470	2580	52	0
2	H	2629	2552	2615	62	0
3	I	50	0	43	11	1
3	K	50	0	43	2	0
3	O	50	0	43	2	0
3	Q	50	0	43	10	0
3	S	50	0	43	2	0
3	a	50	0	43	2	0
3	d	50	0	43	9	0
4	J	61	0	52	0	0
4	U	61	0	52	1	0
4	X	61	0	52	1	0
5	L	72	0	61	8	0
6	M	28	0	25	1	0
6	N	28	0	25	0	0
6	T	28	0	25	2	0
6	V	28	0	25	1	0
6	Y	28	0	25	5	0
6	Z	28	0	25	1	0
6	e	28	0	25	8	0
6	f	28	0	25	6	0
6	g	28	0	25	4	0
7	P	72	0	61	1	0
7	R	72	0	61	7	0
7	W	72	0	61	7	0
8	b	72	0	61	6	0
9	c	50	0	43	1	0
10	A	14	0	13	0	0
10	B	14	0	13	0	0
10	C	28	0	26	1	0
10	D	28	0	26	3	0
10	E	28	0	26	1	0
10	F	28	0	26	1	0
10	G	28	0	26	3	0
11	A	4	0	0	0	0
11	B	1	0	0	0	0
11	C	4	0	0	0	0
11	D	1	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
11	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1	0	0	0	0
12	A	4	0	6	0	0
12	B	8	0	12	0	0
12	C	12	0	18	0	0
12	E	4	0	6	0	0
12	F	4	0	6	0	0
12	G	16	0	24	2	0
12	H	4	0	6	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	H	1	0	0	0	0
14	B	12	0	13	3	0
14	D	12	0	13	3	0
14	F	12	0	13	4	0
14	H	12	0	13	2	0
15	A	137	0	0	3	1
15	B	25	0	0	5	0
15	C	108	0	0	4	1
15	D	14	0	0	1	0
15	E	47	0	0	3	0
15	F	23	0	0	1	0
15	G	62	0	0	4	1
15	H	15	0	0	2	1
All	All	30588	27345	29306	575	4

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.

All (575) 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)
2:D:325:GLU:HG2	2:D:327:LYS:HE2	1.26	1.12
3:I:2:NAG:O3	3:I:3:BMA:O5	1.78	1.02
2:B:66:ILE:HB	2:B:67:PRO:HD3	1.44	0.98
2:H:352:ASN:HB3	2:H:406:ALA:HB1	1.44	0.97
6:g:2:NAG:H83	6:g:2:NAG:H3	1.52	0.91
7:R:2:NAG:H61	7:R:3:BMA:H2	1.56	0.87
1:A:287:GLY:O	1:C:259:LYS:NZ	2.08	0.86
6:e:2:NAG:H83	6:e:2:NAG:H3	1.55	0.86
1:E:416:ASP:OD2	15:E:702:HOH:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:O	1:A:116:THR:OG1	1.97	0.83
2:B:66:ILE:HB	2:B:67:PRO:CD	2.10	0.82
2:H:243:ASP:OD1	15:H:601:HOH:O	1.97	0.82
2:B:70:ASN:ND2	15:B:2101:HOH:O	2.10	0.81
1:G:115:ARG:O	1:G:116:THR:OG1	1.97	0.81
2:D:325:GLU:HG3	2:D:327:LYS:HG2	1.61	0.81
15:C:701:HOH:O	3:Q:2:NAG:O7	1.99	0.81
1:C:115:ARG:O	1:C:116:THR:OG1	1.99	0.80
7:W:2:NAG:H61	7:W:3:BMA:O2	1.82	0.79
5:L:2:NAG:H61	5:L:3:BMA:H2	1.64	0.77
1:C:449:GLU:OE1	3:S:4:MAN:O4	2.01	0.77
2:F:208:ILE:O	14:F:510:MES:H31	1.83	0.77
3:I:1:NAG:H61	3:I:2:NAG:HN2	1.52	0.75
2:B:394:MET:HE2	2:B:396:LYS:O	1.86	0.74
1:C:502:LYS:O	15:C:702:HOH:O	2.04	0.74
2:D:325:GLU:HG2	2:D:327:LYS:CE	2.11	0.74
2:D:325:GLU:CG	2:D:327:LYS:HG2	2.17	0.74
3:Q:2:NAG:H62	3:Q:3:BMA:H2	1.69	0.74
1:G:126:GLY:O	15:G:2101:HOH:O	2.06	0.73
1:C:459:ASN:OD1	1:C:461:THR:OG1	2.07	0.73
2:F:243:ASP:OD1	15:F:601:HOH:O	2.05	0.73
2:H:140:ARG:HH21	6:f:2:NAG:H83	1.53	0.73
2:H:301:VAL:HG21	2:H:306:PHE:HA	1.70	0.73
1:E:495:GLN:OE1	10:E:624:NAG:O6	2.07	0.73
2:B:98:HIS:NE2	2:B:383:ASN:O	2.22	0.73
1:C:115:ARG:NH2	1:E:118:MET:O	2.23	0.72
1:E:456:ASN:HB3	1:E:459:ASN:HB2	1.70	0.72
3:Q:3:BMA:O2	3:Q:4:MAN:O5	2.07	0.71
1:E:444:VAL:N	15:E:703:HOH:O	2.19	0.71
2:B:208:ILE:O	14:B:2014:MES:H31	1.90	0.71
1:G:564:LEU:HD22	1:G:579:LEU:HD11	1.71	0.71
1:G:84:ASP:OD1	15:G:2102:HOH:O	2.09	0.71
1:E:275:TYR:OH	2:F:251:ASP:OD1	2.06	0.71
2:H:352:ASN:HB3	2:H:406:ALA:CB	2.18	0.70
1:G:31:SER:OG	15:G:2103:HOH:O	2.10	0.70
2:B:301:VAL:HG21	2:B:306:PHE:HA	1.73	0.70
1:G:511:ARG:NH2	1:G:554:THR:O	2.25	0.70
1:C:439:ARG:NH1	1:C:577:PRO:O	2.24	0.70
2:H:233:GLU:HG2	6:f:1:NAG:H2	1.74	0.70
1:G:439:ARG:NH1	1:G:577:PRO:O	2.24	0.69
1:A:524:LYS:NZ	1:A:537:GLU:OE1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LYS:NZ	1:C:537:GLU:OE1	2.24	0.69
2:B:163:GLU:O	15:B:2102:HOH:O	2.11	0.69
2:D:209:ASP:OD2	2:D:247:HIS:NE2	2.26	0.68
1:E:465:PRO:O	1:E:518:ARG:NH1	2.27	0.68
2:F:100:LEU:HD22	6:Y:2:NAG:H81	1.74	0.68
1:G:450:VAL:HG21	1:G:558:ILE:HD12	1.76	0.68
2:H:362:THR:OG1	2:H:389:ASN:HB3	1.93	0.68
5:L:4:MAN:H2	5:L:5:MAN:H2	1.74	0.68
1:A:597:GLY:O	15:A:701:HOH:O	2.11	0.67
1:C:456:ASN:HB3	1:C:459:ASN:HB2	1.77	0.67
1:G:524:LYS:NZ	1:G:537:GLU:OE1	2.22	0.66
1:A:260:ASN:HD22	3:K:1:NAG:H83	1.59	0.66
2:D:94:MET:HE1	10:D:502:NAG:O3	1.95	0.66
2:B:74:THR:OG1	15:B:2103:HOH:O	2.14	0.66
6:e:1:NAG:H62	6:e:2:NAG:H82	1.77	0.65
2:F:363:ALA:HB2	2:F:373:GLY:HA2	1.78	0.65
3:d:1:NAG:H62	3:d:2:NAG:C7	2.27	0.65
1:C:284:ASP:OD2	1:C:289:ASP:N	2.30	0.65
2:B:106:ASP:OD1	2:B:143:ARG:NH1	2.30	0.64
1:C:586:ASN:OD1	10:C:601:NAG:N2	2.30	0.64
1:G:145:GLN:OE1	1:G:145:GLN:N	2.30	0.64
1:E:439:ARG:NH1	1:E:577:PRO:O	2.30	0.64
1:G:243:VAL:CG1	1:G:246:ALA:HB2	2.28	0.64
7:R:2:NAG:H61	7:R:3:BMA:C2	2.28	0.64
2:B:69:GLU:HG2	2:B:80:GLU:HB2	1.79	0.64
8:b:1:NAG:H62	8:b:2:NAG:H82	1.80	0.64
3:I:2:NAG:HO3	3:I:3:BMA:C1	2.06	0.64
1:E:178:TYR:CE1	14:F:510:MES:H22	2.33	0.63
1:A:394:GLN:N	1:A:394:GLN:OE1	2.31	0.63
2:H:361:ILE:HD12	2:H:390:VAL:HG22	1.79	0.63
1:E:61:TRP:O	1:E:62:SER:OG	2.13	0.62
2:B:72:ILE:HG13	2:B:73:ASN:H	1.63	0.62
6:e:1:NAG:H62	6:e:2:NAG:C8	2.30	0.62
1:E:450:VAL:HG21	1:E:558:ILE:HD12	1.82	0.62
2:F:365:CYS:HB3	2:F:366:PRO:HD2	1.82	0.62
2:H:374:MET:SD	2:H:374:MET:N	2.73	0.62
1:E:24:ASP:OD1	1:E:25:PHE:N	2.30	0.62
1:G:178:TYR:OH	14:H:510:MES:H22	2.00	0.62
1:C:560:MET:CE	1:C:587:ILE:HD11	2.31	0.61
2:D:124:LEU:HD12	2:D:241:MET:HE1	1.82	0.61
2:F:233:GLU:HB2	6:Y:1:NAG:H4	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ALA:C	2:B:364:ILE:HD12	2.26	0.61
1:A:512:ALA:O	1:A:513:LEU:HD23	1.99	0.60
2:B:243:ASP:OD1	15:B:2105:HOH:O	2.15	0.60
1:G:308:LYS:NZ	2:H:351:GLU:OE1	2.34	0.60
14:D:507:MES:H22	15:D:609:HOH:O	2.00	0.60
2:F:233:GLU:OE2	2:F:233:GLU:N	2.33	0.60
7:W:3:BMA:O4	7:W:6:MAN:H3	2.00	0.60
1:G:144:SER:OG	1:G:152:GLN:OE1	2.19	0.60
6:Y:1:NAG:O3	6:Y:2:NAG:O5	2.17	0.60
2:B:180:HIS:CD2	2:B:183:ILE:HD12	2.37	0.60
1:G:24:ASP:OD1	1:G:25:PHE:N	2.33	0.60
6:g:2:NAG:H3	6:g:2:NAG:C8	2.28	0.60
2:B:237:LEU:HD11	2:B:339:TYR:CD1	2.37	0.59
1:E:440:PRO:HB2	1:E:488:LEU:HD21	1.84	0.59
2:B:275:SER:OG	15:B:2104:HOH:O	2.15	0.59
2:B:363:ALA:HB3	2:B:371:LYS:H	1.67	0.59
2:D:106:ASP:HB3	2:D:188:LEU:HD13	1.83	0.59
1:G:24:ASP:OD2	1:G:99:ARG:NH1	2.35	0.59
1:G:449:GLU:OE2	3:d:4:MAN:H62	2.03	0.59
2:D:115:ALA:O	2:D:118:HIS:ND1	2.31	0.59
2:H:301:VAL:O	2:H:324:ILE:N	2.35	0.59
1:A:357:ASP:O	15:A:702:HOH:O	2.17	0.59
1:A:485:LYS:HE2	3:Q:3:BMA:H61	1.84	0.59
1:E:214:GLN:HE21	7:W:3:BMA:H61	1.68	0.59
1:A:395:TRP:CZ3	1:A:434:ILE:HD11	2.37	0.58
2:F:371:LYS:HD2	2:F:375:GLU:CB	2.33	0.58
1:A:596:THR:OG1	1:A:597:GLY:N	2.33	0.58
1:C:456:ASN:HA	1:C:594:LEU:HD23	1.85	0.58
2:F:301:VAL:HG21	2:F:306:PHE:HA	1.85	0.58
3:Q:3:BMA:H4	3:Q:4:MAN:H3	1.84	0.58
1:C:481:LYS:HB2	1:C:534:MET:HG2	1.86	0.58
1:C:564:LEU:HD21	1:C:566:TYR:CE1	2.38	0.58
2:D:301:VAL:HG21	2:D:306:PHE:HA	1.85	0.58
2:D:74:THR:HG23	2:D:415:GLU:HB3	1.86	0.58
6:g:1:NAG:O3	6:g:2:NAG:O5	2.18	0.57
1:E:524:LYS:NZ	1:E:537:GLU:OE1	2.31	0.57
2:H:81:VAL:HB	2:H:419:ILE:HG22	1.86	0.57
6:V:1:NAG:H62	6:V:2:NAG:C7	2.35	0.57
2:D:237:LEU:HD11	2:D:339:TYR:HD2	1.69	0.57
2:B:107:LEU:HD12	2:B:237:LEU:HB2	1.88	0.56
2:D:94:MET:HE3	10:D:502:NAG:O5	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:TYR:CG	2:B:250:LEU:HD12	2.40	0.56
3:I:2:NAG:C3	3:I:3:BMA:O5	2.53	0.56
3:d:1:NAG:O4	3:d:2:NAG:O7	2.23	0.56
1:A:512:ALA:C	1:A:513:LEU:HD23	2.30	0.56
2:D:116:SER:OG	2:D:243:ASP:OD2	2.12	0.56
1:E:545:ASP:OD1	1:E:546:GLU:N	2.39	0.56
6:e:1:NAG:H62	6:e:2:NAG:C7	2.36	0.56
2:D:294:ASN:ND2	2:D:414:ASN:HA	2.20	0.56
2:B:222:ALA:HA	2:B:295:ILE:CD1	2.36	0.56
2:H:233:GLU:HA	2:H:414:ASN:HD22	1.70	0.56
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.36	0.56
3:I:1:NAG:O7	3:I:1:NAG:O3	2.18	0.56
1:G:505:GLN:HA	1:G:510:ARG:HE	1.70	0.55
2:H:116:SER:OG	2:H:243:ASP:OD2	2.18	0.55
3:I:2:NAG:HO3	3:I:3:BMA:C5	2.08	0.55
2:D:157:TYR:OH	2:D:251:ASP:O	2.24	0.55
1:E:2:ASN:O	1:E:439:ARG:N	2.36	0.55
1:E:504:LYS:O	1:E:510:ARG:NE	2.39	0.55
6:e:2:NAG:H3	6:e:2:NAG:C8	2.31	0.55
1:C:24:ASP:OD1	1:C:25:PHE:N	2.38	0.55
7:R:2:NAG:H61	7:R:3:BMA:C1	2.36	0.55
1:G:42:LYS:O	3:a:1:NAG:H82	2.07	0.55
1:C:564:LEU:HD23	1:C:564:LEU:H	1.72	0.55
1:G:243:VAL:HG12	1:G:246:ALA:HB2	1.87	0.55
2:B:330:ASN:OD1	2:B:333:ASN:HB2	2.07	0.55
1:E:494:PHE:CE1	1:E:528:ILE:HD11	2.41	0.55
1:A:214:GLN:NE2	5:L:3:BMA:O5	2.38	0.54
5:L:4:MAN:H2	5:L:5:MAN:C2	2.37	0.54
1:A:456:ASN:HB3	1:A:459:ASN:HB2	1.89	0.54
1:E:214:GLN:NE2	7:W:3:BMA:H61	2.22	0.54
1:A:144:SER:OG	1:A:152:GLN:OE1	2.23	0.54
2:B:325:GLU:O	2:B:328:ALA:N	2.36	0.54
2:B:357:ILE:HD12	2:B:358:TYR:H	1.72	0.54
1:A:260:ASN:ND2	3:K:1:NAG:H83	2.22	0.54
1:E:24:ASP:OD2	1:E:99:ARG:NH1	2.38	0.54
1:E:464:LEU:HD12	1:E:465:PRO:HD2	1.88	0.54
2:F:74:THR:HB	2:F:415:GLU:HB3	1.88	0.54
3:Q:2:NAG:H62	3:Q:3:BMA:C2	2.36	0.54
1:C:245:ARG:NH2	2:D:246:SER:O	2.41	0.54
2:B:66:ILE:CB	2:B:67:PRO:HD3	2.27	0.54
2:H:230:TRP:HB3	2:H:236:ARG:NE	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:370:ARG:O	2:F:371:LYS:HB2	2.06	0.54
2:H:92:ASN:HD22	6:e:1:NAG:H5	1.72	0.53
3:I:1:NAG:C6	3:I:2:NAG:HN2	2.20	0.53
2:B:75:GLN:N	2:B:415:GLU:OE1	2.39	0.53
2:D:387:LEU:C	2:D:387:LEU:HD12	2.34	0.53
1:E:63:SER:O	1:E:64:THR:OG1	2.23	0.53
2:H:363:ALA:C	2:H:364:ILE:HD12	2.33	0.53
1:G:138:GLU:OE2	1:G:143:ARG:NH2	2.39	0.53
2:F:371:LYS:HD2	2:F:375:GLU:HB3	1.90	0.53
1:E:115:ARG:HG3	1:E:116:THR:O	2.08	0.53
1:G:586:ASN:OD1	10:G:2024:NAG:N2	2.41	0.53
1:E:127:THR:HG22	1:E:128:CYS:N	2.24	0.53
7:R:2:NAG:C6	7:R:3:BMA:H2	2.35	0.53
1:E:501:ASP:OD2	1:E:511:ARG:NH1	2.42	0.53
2:F:216:ASP:OD1	2:F:280:HIS:ND1	2.40	0.53
8:b:4:MAN:H2	8:b:5:MAN:C5	2.39	0.53
2:H:106:ASP:OD2	2:H:143:ARG:NH2	2.41	0.52
1:A:513:LEU:HD22	1:A:520:PRO:HG3	1.90	0.52
2:H:223:VAL:O	2:H:225:GLU:N	2.42	0.52
2:B:69:GLU:HG3	2:B:80:GLU:O	2.09	0.52
2:F:76:VAL:HG11	2:F:410:PRO:HG2	1.92	0.52
3:Q:3:BMA:HO2	3:Q:4:MAN:C1	2.21	0.52
1:A:420:TYR:OH	1:A:485:LYS:O	2.14	0.52
1:C:510:ARG:O	1:C:544:ARG:NH1	2.43	0.52
2:H:209:ASP:OD2	2:H:247:HIS:NE2	2.39	0.52
2:D:94:MET:SD	2:D:94:MET:N	2.82	0.52
1:A:250:LEU:HD21	1:A:269:GLY:O	2.10	0.52
6:e:2:NAG:H82	6:e:2:NAG:C1	2.40	0.52
1:C:115:ARG:HA	1:C:121:GLU:O	2.09	0.52
2:D:76:VAL:HG23	2:D:76:VAL:O	2.09	0.52
2:B:216:ASP:OD1	2:B:280:HIS:ND1	2.41	0.52
2:D:76:VAL:HG11	2:D:410:PRO:HG2	1.90	0.52
6:Y:1:NAG:O4	6:Y:2:NAG:O7	2.28	0.52
2:D:222:ALA:HA	2:D:295:ILE:CD1	2.40	0.51
4:X:2:NAG:H62	4:X:3:BMA:C1	2.40	0.51
1:A:65:ARG:NH2	15:A:709:HOH:O	2.42	0.51
1:A:132:ASP:OD1	1:A:133:GLY:N	2.43	0.51
1:A:399:SER:O	1:A:401:CYS:N	2.43	0.51
1:C:511:ARG:NH2	1:C:554:THR:O	2.43	0.51
2:D:223:VAL:O	2:D:225:GLU:N	2.41	0.51
1:G:338:ALA:HB1	1:G:362:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:363:ALA:HB2	2:H:388:PHE:CE2	2.45	0.51
1:A:395:TRP:CH2	1:A:434:ILE:HD11	2.45	0.51
1:C:118:MET:HE2	1:C:119:LYS:CG	2.41	0.51
1:C:560:MET:HE2	1:C:587:ILE:HD11	1.93	0.51
2:F:124:LEU:HG	2:F:127:VAL:HG22	1.91	0.51
1:A:250:LEU:CD2	1:A:268:THR:HG22	2.40	0.51
1:E:250:LEU:CD2	1:E:268:THR:HG22	2.41	0.51
3:d:2:NAG:H62	3:d:3:BMA:C1	2.40	0.51
2:F:85:LEU:HD23	2:F:86:ARG:O	2.10	0.51
5:L:4:MAN:C2	5:L:5:MAN:H2	2.38	0.51
1:E:250:LEU:HD21	1:E:269:GLY:O	2.11	0.51
2:F:407:ILE:HD11	2:F:416:THR:CG2	2.40	0.51
2:H:85:LEU:HD23	2:H:86:ARG:O	2.11	0.51
1:A:440:PRO:HB2	1:A:488:LEU:HD21	1.93	0.50
1:C:303:ARG:NE	1:C:307:GLY:O	2.41	0.50
1:G:464:LEU:HD23	1:G:465:PRO:HD2	1.93	0.50
2:B:66:ILE:CB	2:B:67:PRO:CD	2.85	0.50
1:C:147:ILE:HD12	1:C:148:ASP:HB2	1.92	0.50
2:B:209:ASP:OD2	2:B:247:HIS:NE2	2.39	0.50
1:E:564:LEU:HD23	1:E:564:LEU:H	1.75	0.50
1:A:564:LEU:HD23	1:A:564:LEU:H	1.75	0.50
2:F:124:LEU:HG	2:F:127:VAL:CG2	2.41	0.50
2:F:92:ASN:OD1	10:F:502:NAG:H2	2.12	0.50
1:G:5:VAL:HG12	1:G:5:VAL:O	2.12	0.50
1:G:314:GLN:NE2	1:G:332:ASN:OD1	2.39	0.50
2:H:207:ASN:O	14:H:510:MES:H72	2.11	0.50
2:B:364:ILE:HD13	2:B:387:LEU:HD12	1.94	0.50
2:F:242:THR:O	2:F:301:VAL:HA	2.12	0.50
1:G:564:LEU:HD23	1:G:564:LEU:H	1.76	0.50
1:A:539:LEU:N	1:A:539:LEU:HD23	2.27	0.49
2:H:141:ASP:OD1	2:H:142:PHE:N	2.44	0.49
2:B:76:VAL:HG11	2:B:410:PRO:HG2	1.95	0.49
2:D:189:THR:HG22	2:D:190:GLU:N	2.27	0.49
1:E:78:ARG:HD3	1:E:87:GLU:OE1	2.12	0.49
1:E:199:VAL:O	1:E:202:ILE:HD11	2.12	0.49
2:F:124:LEU:HD13	2:F:241:MET:HE1	1.94	0.49
1:G:525:ASN:CB	10:G:2023:NAG:O5	2.59	0.49
2:H:222:ALA:HA	2:H:295:ILE:CD1	2.43	0.49
1:A:564:LEU:HD21	1:A:566:TYR:CE1	2.47	0.49
2:B:357:ILE:HD11	2:B:393:THR:H	1.76	0.49
1:C:303:ARG:NH2	1:C:307:GLY:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:LEU:HD11	2:D:339:TYR:CD2	2.47	0.49
1:E:415:ILE:HG21	1:E:435:LEU:HD21	1.94	0.49
2:H:421:ILE:N	2:H:421:ILE:HD12	2.28	0.49
2:D:361:ILE:CD1	2:D:390:VAL:HG23	2.41	0.49
1:E:275:TYR:CG	2:F:250:LEU:HD12	2.48	0.49
6:g:2:NAG:C1	6:g:2:NAG:H82	2.42	0.49
2:H:363:ALA:N	2:H:371:LYS:O	2.39	0.49
1:A:115:ARG:O	1:A:116:THR:CB	2.61	0.49
1:A:243:VAL:HG12	1:A:246:ALA:HB2	1.95	0.49
2:D:94:MET:CG	2:D:387:LEU:HD13	2.42	0.49
2:B:92:ASN:HA	2:B:390:VAL:O	2.13	0.49
1:C:512:ALA:O	1:C:513:LEU:HD23	2.13	0.49
1:G:178:TYR:HB2	12:G:2025:EDO:H21	1.94	0.49
2:H:364:ILE:HD12	2:H:364:ILE:N	2.27	0.49
6:T:2:NAG:O7	6:T:2:NAG:O3	2.28	0.49
1:E:42:LYS:O	4:U:1:NAG:H82	2.11	0.49
1:A:178:TYR:HE2	14:B:2014:MES:H22	1.77	0.48
1:E:476:VAL:HG22	1:E:558:ILE:HD13	1.95	0.48
1:G:334:PHE:O	12:G:2026:EDO:H11	2.13	0.48
1:E:571:ASP:OD1	1:E:575:LEU:N	2.45	0.48
2:D:361:ILE:O	2:D:373:GLY:HA3	2.13	0.48
1:E:115:ARG:O	1:E:116:THR:HB	2.13	0.48
2:F:106:ASP:OD1	2:F:143:ARG:NH1	2.47	0.48
1:G:564:LEU:HD21	1:G:566:TYR:CE1	2.48	0.48
1:A:450:VAL:HG21	1:A:558:ILE:HD12	1.95	0.48
2:H:415:GLU:HG2	6:f:1:NAG:H82	1.94	0.48
3:d:1:NAG:H62	3:d:2:NAG:N2	2.28	0.48
1:C:87:GLU:HA	1:C:114:TRP:HA	1.96	0.48
1:E:335:GLU:OE1	1:E:366:GLY:N	2.45	0.48
2:F:143:ARG:NH2	2:F:231:ARG:HG2	2.28	0.48
1:G:449:GLU:CD	3:d:4:MAN:H62	2.39	0.48
1:E:178:TYR:HE1	14:F:510:MES:H22	1.78	0.48
1:G:243:VAL:HG11	1:G:246:ALA:HB2	1.95	0.48
1:E:583:THR:HG21	15:E:703:HOH:O	2.13	0.48
2:H:192:ILE:O	2:H:195:PHE:N	2.44	0.48
1:A:496:VAL:HG12	1:A:498:LEU:CD1	2.44	0.47
2:B:71:GLU:O	2:B:72:ILE:C	2.57	0.47
1:E:284:ASP:OD2	1:E:289:ASP:N	2.43	0.47
6:Z:1:NAG:O7	6:Z:1:NAG:O3	2.24	0.47
1:A:543:LEU:N	1:A:543:LEU:HD12	2.28	0.47
1:C:513:LEU:HD22	1:C:520:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ASN:ND2	14:D:507:MES:O1S	2.47	0.47
2:F:381:THR:OG1	2:F:384:ASP:OD2	2.32	0.47
3:O:1:NAG:H62	3:O:2:NAG:C1	2.43	0.47
1:C:564:LEU:HD22	1:C:579:LEU:HD11	1.96	0.47
1:E:1:PHE:HA	1:E:389:GLN:HB2	1.96	0.47
1:E:202:ILE:HD12	1:E:202:ILE:H	1.79	0.47
1:G:481:LYS:HB3	1:G:534:MET:HA	1.95	0.47
2:F:76:VAL:O	2:F:76:VAL:HG23	2.14	0.47
2:H:189:THR:HG22	2:H:191:ASN:H	1.79	0.47
5:L:3:BMA:H61	5:L:4:MAN:H2	1.56	0.47
2:B:239:LEU:C	2:B:239:LEU:HD23	2.39	0.47
1:C:262:SER:HB2	3:Q:1:NAG:HN2	1.79	0.47
2:D:94:MET:HG3	2:D:387:LEU:HD13	1.95	0.47
2:H:247:HIS:O	15:H:602:HOH:O	2.20	0.47
2:B:233:GLU:HG2	3:O:2:NAG:H61	1.96	0.47
2:B:237:LEU:HD11	2:B:339:TYR:HD1	1.79	0.47
1:C:51:VAL:HG13	7:P:1:NAG:H5	1.95	0.47
1:G:559:PHE:CE2	1:G:586:ASN:HB2	2.50	0.47
2:H:231:ARG:C	2:H:236:ARG:HH11	2.23	0.47
1:A:294:PHE:CE2	1:A:317:VAL:HG13	2.50	0.47
1:E:116:THR:HG22	1:E:117:GLU:N	2.29	0.47
2:H:124:LEU:HD12	2:H:331:LEU:HD12	1.96	0.47
1:A:595:LEU:O	1:A:597:GLY:N	2.47	0.47
1:E:348:GLY:O	1:E:357:ASP:N	2.41	0.47
1:E:580:ASN:HB3	1:E:583:THR:HG23	1.97	0.47
2:F:346:VAL:O	2:F:346:VAL:HG23	2.14	0.47
2:B:223:VAL:O	2:B:225:GLU:N	2.47	0.46
2:B:327:LYS:O	2:B:328:ALA:HB3	2.15	0.46
2:B:134:LYS:NZ	2:B:333:ASN:OD1	2.47	0.46
1:G:494:PHE:CE1	1:G:528:ILE:HD11	2.50	0.46
2:D:190:GLU:O	2:D:192:ILE:N	2.49	0.46
2:F:354:VAL:O	2:F:355:GLN:C	2.58	0.46
2:H:239:LEU:HD23	2:H:239:LEU:C	2.40	0.46
2:D:75:GLN:HG3	2:D:100:LEU:HD11	1.98	0.46
2:D:352:ASN:HB3	2:D:359:PHE:CE1	2.51	0.46
2:B:357:ILE:HD12	2:B:358:TYR:N	2.31	0.46
1:E:234:ASP:OD1	1:E:235:GLY:N	2.49	0.46
2:F:223:VAL:O	2:F:225:GLU:N	2.49	0.46
2:H:414:ASN:ND2	6:f:1:NAG:O7	2.48	0.46
2:D:74:THR:HG22	2:D:76:VAL:HG22	1.98	0.46
2:D:387:LEU:HD12	2:D:388:PHE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:THR:HG21	1:E:147:ILE:HD13	1.98	0.46
6:T:1:NAG:H4	6:T:2:NAG:H2	1.83	0.46
1:C:118:MET:HA	1:E:118:MET:HA	1.96	0.46
1:E:27:VAL:O	1:E:27:VAL:HG13	2.15	0.46
2:H:124:LEU:HD23	2:H:199:VAL:HG11	1.98	0.46
2:D:222:ALA:HA	2:D:295:ILE:HD13	1.98	0.46
2:F:363:ALA:HB3	2:F:370:ARG:O	2.16	0.46
1:G:118:MET:HE2	1:G:119:LYS:HB2	1.98	0.46
1:A:245:ARG:NH2	2:B:246:SER:O	2.48	0.45
2:D:230:TRP:HB3	2:D:236:ARG:NE	2.31	0.45
2:D:364:ILE:HD12	2:D:387:LEU:HD11	1.98	0.45
1:E:564:LEU:HD22	1:E:579:LEU:HD11	1.98	0.45
2:F:75:GLN:HG3	2:F:100:LEU:HD11	1.98	0.45
1:C:479:CYS:CB	1:C:534:MET:HE2	2.47	0.45
2:D:188:LEU:HD12	2:D:229:GLY:O	2.16	0.45
2:D:411:ILE:HD12	2:D:411:ILE:O	2.17	0.45
2:H:327:LYS:HD2	2:H:327:LYS:HA	1.75	0.45
3:I:2:NAG:O3	3:I:2:NAG:O7	2.33	0.45
1:A:178:TYR:CE2	14:B:2014:MES:H22	2.51	0.45
1:C:594:LEU:N	1:C:594:LEU:HD22	2.31	0.45
1:E:437:ARG:NH2	1:E:573:THR:OG1	2.44	0.45
15:G:2104:HOH:O	9:c:1:NAG:O4	2.21	0.45
2:H:140:ARG:NH2	6:f:2:NAG:H83	2.26	0.45
2:B:325:GLU:O	2:B:326:SER:C	2.60	0.45
2:F:231:ARG:C	2:F:236:ARG:HH11	2.24	0.45
1:G:437:ARG:NH2	1:G:573:THR:OG1	2.43	0.45
2:H:216:ASP:OD1	2:H:280:HIS:ND1	2.44	0.45
6:M:1:NAG:H61	6:M:2:NAG:H82	1.98	0.45
3:a:2:NAG:O3	3:a:3:BMA:O5	2.28	0.45
1:A:5:VAL:O	1:A:5:VAL:HG12	2.17	0.45
1:G:275:TYR:OH	2:H:251:ASP:OD1	2.20	0.45
1:A:350:LEU:N	1:A:357:ASP:OD2	2.50	0.45
1:E:60:ASP:OD1	1:E:61:TRP:N	2.48	0.45
1:E:243:VAL:CG1	1:E:246:ALA:HB2	2.47	0.45
1:A:464:LEU:C	1:A:464:LEU:HD23	2.42	0.45
1:C:118:MET:HE2	1:C:119:LYS:HG2	1.99	0.45
1:G:418:ASN:ND2	1:G:438:ALA:O	2.50	0.45
2:B:174:LEU:O	2:B:175:ASP:C	2.59	0.45
1:E:410:LYS:O	1:E:423:LEU:HD12	2.17	0.45
7:W:3:BMA:O4	7:W:6:MAN:H5	2.16	0.45
2:B:74:THR:HG22	2:B:76:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LEU:HD23	2:B:334:LEU:C	2.42	0.45
1:E:347:LEU:HD11	1:E:359:ALA:HB2	1.98	0.45
2:H:407:ILE:HD11	2:H:416:THR:CG2	2.47	0.45
1:A:483:ASP:OD1	1:A:484:GLY:N	2.45	0.44
2:D:75:GLN:N	2:D:415:GLU:OE1	2.31	0.44
2:F:109:TYR:CE2	2:F:124:LEU:HD11	2.53	0.44
1:G:275:TYR:CG	2:H:250:LEU:HD12	2.52	0.44
2:F:222:ALA:HA	2:F:295:ILE:CD1	2.46	0.44
2:F:346:VAL:HG12	2:F:413:PHE:CE1	2.51	0.44
2:B:357:ILE:HD11	2:B:393:THR:N	2.32	0.44
1:C:122:ARG:CD	2:D:160:ILE:HG13	2.47	0.44
2:D:327:LYS:O	2:D:328:ALA:HB3	2.17	0.44
2:F:81:VAL:HB	2:F:419:ILE:HG22	1.98	0.44
1:G:473:CYS:O	3:d:1:NAG:O6	2.34	0.44
1:A:439:ARG:NH1	1:A:577:PRO:O	2.51	0.44
1:A:511:ARG:NH2	1:A:554:THR:O	2.50	0.44
1:C:481:LYS:CB	1:C:534:MET:HG2	2.47	0.44
1:G:543:LEU:CD2	1:G:593:ILE:HD11	2.47	0.44
7:R:4:MAN:H61	7:R:5:MAN:H2	1.40	0.44
1:A:494:PHE:CE1	1:A:528:ILE:HD11	2.53	0.44
1:G:115:ARG:HA	1:G:121:GLU:O	2.18	0.44
1:A:27:VAL:HG13	1:A:27:VAL:O	2.18	0.44
1:A:276:PHE:CZ	1:A:295:ILE:HG21	2.52	0.44
2:B:231:ARG:C	2:B:236:ARG:HH11	2.25	0.44
2:F:124:LEU:CD1	2:F:241:MET:HE1	2.48	0.44
2:F:209:ASP:OD2	2:F:247:HIS:NE2	2.50	0.44
2:F:98:HIS:NE2	2:F:382:SER:O	2.50	0.44
1:G:464:LEU:HB3	1:G:465:PRO:HD2	2.00	0.44
2:H:415:GLU:CG	6:f:1:NAG:H82	2.48	0.44
5:L:2:NAG:H61	5:L:3:BMA:C2	2.42	0.44
3:S:2:NAG:O3	3:S:3:BMA:O5	2.30	0.44
2:B:346:VAL:HG23	2:B:346:VAL:O	2.17	0.44
2:B:316:LEU:O	2:B:319:THR:OG1	2.32	0.44
1:C:171:LEU:C	1:C:171:LEU:HD23	2.42	0.44
1:E:115:ARG:O	1:E:116:THR:CB	2.66	0.44
2:F:115:ALA:N	14:F:510:MES:O2S	2.40	0.44
2:D:143:ARG:HB3	2:D:188:LEU:HB3	1.98	0.43
1:E:190:GLU:OE1	1:E:205:ASN:N	2.51	0.43
2:F:230:TRP:HB3	2:F:236:ARG:NE	2.34	0.43
2:H:346:VAL:HG23	2:H:346:VAL:O	2.18	0.43
2:F:189:THR:HG22	2:F:190:GLU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:242:THR:O	2:H:301:VAL:HA	2.18	0.43
1:A:488:LEU:HB2	1:A:530:ARG:NH1	2.33	0.43
2:B:230:TRP:HB3	2:B:236:ARG:NE	2.32	0.43
2:B:380:VAL:O	2:B:380:VAL:HG13	2.17	0.43
2:D:231:ARG:C	2:D:236:ARG:HH11	2.26	0.43
1:E:593:ILE:HG22	1:E:594:LEU:H	1.83	0.43
2:F:411:ILE:O	2:F:411:ILE:HD12	2.19	0.43
1:G:372:ILE:HG22	1:G:373:VAL:N	2.34	0.43
7:R:3:BMA:O4	7:R:6:MAN:H2	2.19	0.43
1:C:487:VAL:O	1:C:487:VAL:HG13	2.17	0.43
1:G:115:ARG:C	1:G:116:THR:HG1	2.09	0.43
1:G:539:LEU:N	1:G:539:LEU:HD23	2.34	0.43
8:b:4:MAN:H2	8:b:5:MAN:H61	2.00	0.43
1:E:116:THR:HG23	1:E:147:ILE:HG21	2.00	0.43
1:G:411:GLY:O	1:G:412:ALA:HB3	2.18	0.43
1:G:471:VAL:HG21	1:G:542:TYR:CG	2.54	0.43
5:L:4:MAN:C2	5:L:5:MAN:C2	2.96	0.43
2:B:344:SER:O	2:B:379:ASN:N	2.52	0.43
1:C:571:ASP:OD1	1:C:575:LEU:N	2.48	0.43
1:G:60:ASP:OD1	1:G:61:TRP:N	2.51	0.43
1:G:234:ASP:HB3	8:b:2:NAG:C8	2.49	0.43
6:Y:1:NAG:HO3	6:Y:2:NAG:C1	2.30	0.43
1:A:87:GLU:HA	1:A:114:TRP:HA	2.00	0.43
2:B:72:ILE:HG13	2:B:73:ASN:N	2.31	0.43
2:B:411:ILE:HD12	2:B:411:ILE:C	2.43	0.43
2:B:416:THR:HG22	2:B:417:ALA:N	2.34	0.43
1:C:278:PHE:CD1	2:D:250:LEU:CD1	3.02	0.43
2:D:127:VAL:O	2:D:130:ASP:N	2.52	0.43
2:H:237:LEU:HD11	2:H:339:TYR:CD1	2.54	0.43
1:C:28:PRO:HB2	1:C:30:ALA:O	2.19	0.43
1:E:243:VAL:HG12	1:E:246:ALA:HB2	2.01	0.43
2:H:387:LEU:HD12	2:H:387:LEU:C	2.44	0.43
1:A:481:LYS:HB3	1:A:534:MET:HA	2.00	0.43
1:C:593:ILE:HG22	1:C:594:LEU:N	2.34	0.43
2:H:356:GLY:O	2:H:357:ILE:HG23	2.19	0.43
1:A:464:LEU:HG	1:A:465:PRO:HD2	2.00	0.42
1:C:278:PHE:CD1	2:D:250:LEU:HD12	2.54	0.42
1:C:459:ASN:HB3	15:C:705:HOH:O	2.18	0.42
1:E:503:LEU:HD21	1:E:557:THR:HG23	2.00	0.42
1:C:243:VAL:CG1	1:C:246:ALA:HB2	2.49	0.42
1:G:27:VAL:HG13	1:G:27:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:GLU:O	2:D:328:ALA:N	2.48	0.42
1:E:118:MET:HE2	1:E:119:LYS:HG3	2.00	0.42
1:G:375:ILE:HD12	1:G:375:ILE:N	2.35	0.42
1:C:139:TYR:CD1	1:C:191:ILE:HG12	2.54	0.42
1:C:450:VAL:HG21	1:C:558:ILE:HD12	2.01	0.42
1:G:143:ARG:NE	1:G:200:TYR:O	2.51	0.42
1:G:449:GLU:OE2	3:d:4:MAN:H4	2.20	0.42
2:B:322:GLY:C	2:B:334:LEU:HD11	2.43	0.42
1:C:434:ILE:N	1:C:434:ILE:HD12	2.34	0.42
1:G:278:PHE:CD1	2:H:250:LEU:HD13	2.54	0.42
1:G:571:ASP:OD1	1:G:575:LEU:N	2.52	0.42
2:H:334:LEU:C	2:H:334:LEU:HD23	2.44	0.42
3:I:1:NAG:C6	3:I:2:NAG:N2	2.83	0.42
1:C:459:ASN:O	1:C:460:LYS:C	2.62	0.42
1:E:450:VAL:CG2	1:E:558:ILE:HD12	2.49	0.42
1:G:553:LEU:N	1:G:553:LEU:HD22	2.35	0.42
2:B:407:ILE:HD13	2:B:418:LYS:HG2	2.00	0.42
1:E:481:LYS:HB2	1:E:534:MET:CB	2.50	0.42
7:R:3:BMA:H62	7:R:4:MAN:H2	1.82	0.42
7:W:3:BMA:H3	7:W:6:MAN:H2	1.30	0.42
1:A:132:ASP:OD1	1:A:132:ASP:C	2.62	0.42
1:C:5:VAL:HG12	1:C:5:VAL:O	2.19	0.42
1:E:375:ILE:HD12	1:E:375:ILE:N	2.35	0.42
1:G:494:PHE:HE1	1:G:528:ILE:HD11	1.84	0.42
3:Q:3:BMA:H4	3:Q:4:MAN:H5	2.02	0.42
1:A:284:ASP:OD2	1:A:289:ASP:N	2.49	0.42
1:A:472:SER:HB3	1:A:543:LEU:HD13	2.02	0.42
2:B:249:ALA:HA	2:B:280:HIS:HB2	2.02	0.42
2:H:135:MET:O	2:H:139:SER:N	2.52	0.42
1:E:303:ARG:NH1	1:E:307:GLY:O	2.52	0.41
2:B:191:ASN:OD1	2:B:193:THR:HG22	2.20	0.41
2:B:347:LYS:O	2:B:410:PRO:HA	2.20	0.41
1:C:497:GLU:OE2	1:C:523:SER:OG	2.32	0.41
1:G:525:ASN:HD21	10:G:2023:NAG:C7	2.33	0.41
6:e:2:NAG:C8	6:e:2:NAG:C1	2.98	0.41
1:A:57:LEU:N	1:A:57:LEU:HD12	2.36	0.41
1:A:275:TYR:OH	2:B:251:ASP:OD1	2.29	0.41
1:C:594:LEU:O	1:C:596:THR:N	2.49	0.41
1:E:539:LEU:HD23	1:E:539:LEU:N	2.36	0.41
2:F:76:VAL:HG11	2:F:410:PRO:CG	2.49	0.41
2:F:387:LEU:HD12	2:F:387:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:HIS:ND1	2:H:183:ILE:HD12	2.35	0.41
2:H:411:ILE:O	2:H:411:ILE:HD12	2.20	0.41
1:C:169:VAL:O	1:C:185:SER:HA	2.20	0.41
1:E:411:GLY:O	1:E:412:ALA:HB3	2.20	0.41
2:F:239:LEU:HD11	2:F:300:ALA:HB2	2.02	0.41
1:C:36:LEU:HD12	1:C:36:LEU:N	2.36	0.41
1:C:503:LEU:HD21	1:C:557:THR:HG23	2.02	0.41
1:E:28:PRO:HB2	1:E:31:SER:HB3	2.02	0.41
1:E:248:ARG:O	1:E:249:THR:OG1	2.36	0.41
1:E:439:ARG:NH2	1:E:578:ILE:HD13	2.35	0.41
1:E:564:LEU:HD22	1:E:579:LEU:CD1	2.51	0.41
1:G:85:PRO:O	1:G:115:ARG:HD2	2.21	0.41
1:G:496:VAL:HG12	1:G:524:LYS:O	2.21	0.41
2:B:145:GLY:N	2:B:188:LEU:HD23	2.35	0.41
1:C:121:GLU:OE2	2:D:161:HIS:HB2	2.20	0.41
1:E:87:GLU:HA	1:E:114:TRP:HA	2.02	0.41
1:G:284:ASP:OD2	1:G:289:ASP:N	2.50	0.41
3:Q:3:BMA:C4	3:Q:4:MAN:H3	2.51	0.41
1:A:275:TYR:CB	2:B:250:LEU:HD12	2.50	0.41
2:D:411:ILE:HD12	2:D:411:ILE:C	2.46	0.41
1:E:254:TYR:OH	7:W:1:NAG:H62	2.21	0.41
2:F:345:GLU:HA	2:F:377:CYS:O	2.20	0.41
1:G:1:PHE:HA	1:G:389:GLN:HB2	2.02	0.41
2:H:407:ILE:HD13	2:H:418:LYS:HD2	2.02	0.41
1:A:504:LYS:NZ	1:A:551:ASP:OD2	2.52	0.41
2:B:74:THR:CG2	2:B:76:VAL:HG22	2.51	0.41
2:B:219:LEU:C	2:B:219:LEU:HD23	2.45	0.41
1:C:146:ASP:OD1	15:C:703:HOH:O	2.21	0.41
1:G:505:GLN:O	1:G:506:LYS:C	2.63	0.41
1:G:564:LEU:HD21	1:G:566:TYR:HE1	1.85	0.41
2:H:361:ILE:O	2:H:373:GLY:N	2.45	0.41
1:A:143:ARG:O	1:A:143:ARG:CG	2.69	0.41
1:A:159:PHE:CE1	2:B:254:LEU:HD23	2.55	0.41
1:A:499:LEU:CD1	1:A:502:LYS:HB2	2.51	0.41
1:C:464:LEU:HD23	1:C:464:LEU:C	2.46	0.41
1:C:503:LEU:HD22	1:C:557:THR:OG1	2.20	0.41
2:H:106:ASP:HB3	2:H:188:LEU:HD13	2.03	0.41
2:H:135:MET:SD	2:H:336:VAL:HG12	2.61	0.41
2:H:351:GLU:HB3	2:H:407:ILE:HG23	2.03	0.41
2:H:381:THR:OG1	2:H:384:ASP:OD2	2.39	0.41
2:B:102:LYS:HB2	2:B:140:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:VAL:HG12	2:B:413:PHE:CE1	2.56	0.41
1:C:253:VAL:HB	1:C:267:PHE:HB2	2.03	0.41
1:E:496:VAL:HG12	1:E:524:LYS:O	2.21	0.41
2:F:115:ALA:HA	2:F:204:ILE:HG21	2.03	0.41
1:G:594:LEU:C	1:G:594:LEU:HD12	2.45	0.41
2:H:357:ILE:HB	2:H:359:PHE:CE1	2.56	0.41
8:b:4:MAN:C2	8:b:5:MAN:C5	2.98	0.41
1:E:58:LYS:HB2	1:E:70:ILE:HD11	2.02	0.40
1:A:366:GLY:CA	1:A:372:ILE:HD11	2.52	0.40
1:A:399:SER:O	1:A:400:GLY:C	2.65	0.40
1:C:50:ILE:HD11	1:C:76:GLY:HA2	2.03	0.40
1:C:348:GLY:O	1:C:357:ASP:N	2.42	0.40
1:C:375:ILE:HD12	1:C:375:ILE:N	2.37	0.40
2:D:379:ASN:OD1	10:D:501:NAG:H2	2.20	0.40
2:D:407:ILE:HD11	2:D:416:THR:CG2	2.51	0.40
1:E:116:THR:HG21	1:E:147:ILE:CD1	2.52	0.40
3:I:2:NAG:O3	3:I:3:BMA:H61	2.20	0.40
2:B:301:VAL:O	2:B:324:ILE:N	2.32	0.40
1:C:509:ILE:HD11	1:C:549:PHE:CB	2.51	0.40
1:E:19:PHE:CZ	1:E:38:VAL:HG11	2.57	0.40
2:F:175:ASP:OD1	2:F:176:CYS:N	2.55	0.40
2:F:219:LEU:C	2:F:219:LEU:HD23	2.46	0.40
8:b:4:MAN:H2	8:b:5:MAN:C6	2.51	0.40
3:d:1:NAG:H5	3:d:2:NAG:O7	2.22	0.40
1:E:5:VAL:O	1:E:5:VAL:HG12	2.20	0.40
1:G:57:LEU:HD12	1:G:57:LEU:N	2.37	0.40
1:G:234:ASP:OD1	1:G:235:GLY:N	2.54	0.40
1:C:437:ARG:NH2	1:C:573:THR:OG1	2.48	0.40
14:D:507:MES:H82	14:D:507:MES:H51	1.75	0.40
1:E:169:VAL:O	1:E:185:SER:HA	2.22	0.40
1:E:245:ARG:NH2	2:F:246:SER:O	2.54	0.40
1:G:224:TYR:OH	2:H:250:LEU:O	2.39	0.40
3:I:1:NAG:HO3	3:I:1:NAG:C7	2.25	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:809:HOH:O	15:C:731:HOH:O[1_545]	2.01	0.19
15:G:2123:HOH:O	15:H:603:HOH:O[1_565]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ARG:O	1:C:417:LYS:NZ[1_545]	2.08	0.12
1:C:491:LYS:NZ	3:I:3:BMA:O6[1_565]	2.19	0.01

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	584/599 (98%)	550 (94%)	31 (5%)	3 (0%)	24	39
1	C	589/599 (98%)	556 (94%)	32 (5%)	1 (0%)	43	60
1	E	587/599 (98%)	538 (92%)	48 (8%)	1 (0%)	43	60
1	G	590/599 (98%)	546 (92%)	43 (7%)	1 (0%)	43	60
2	B	322/456 (71%)	290 (90%)	28 (9%)	4 (1%)	10	17
2	D	298/456 (65%)	266 (89%)	29 (10%)	3 (1%)	12	20
2	F	323/456 (71%)	288 (89%)	35 (11%)	0	100	100
2	H	326/456 (72%)	293 (90%)	31 (10%)	2 (1%)	21	34
All	All	3619/4220 (86%)	3327 (92%)	277 (8%)	15 (0%)	30	45

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	GLY
2	B	326	SER
1	A	596	THR
2	B	72	ILE
2	B	175	ASP
2	D	191	ASN
1	C	62	SER
2	D	150	VAL
2	D	224	CYS
1	G	465	PRO

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Mol	Chain	Res	Type
2	H	140	ARG
2	H	224	CYS
1	A	116	THR
1	E	276	PHE
2	B	150	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/489 (99%)	482 (99%)	3 (1%)	78	88
1	C	487/489 (100%)	483 (99%)	4 (1%)	73	85
1	E	485/489 (99%)	482 (99%)	3 (1%)	78	88
1	G	488/489 (100%)	482 (99%)	6 (1%)	63	79
2	B	296/402 (74%)	294 (99%)	2 (1%)	76	86
2	D	277/402 (69%)	276 (100%)	1 (0%)	84	93
2	F	292/402 (73%)	291 (100%)	1 (0%)	86	94
2	H	296/402 (74%)	293 (99%)	3 (1%)	68	81
All	All	3106/3564 (87%)	3083 (99%)	23 (1%)	76	86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	CYS
1	A	275	TYR
1	A	401	CYS
2	B	304	LYS
2	B	342	LEU
1	C	155	CYS
1	C	275	TYR
1	C	401	CYS
1	C	586	ASN
2	D	250	LEU

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Mol	Chain	Res	Type
1	E	155	CYS
1	E	190	GLU
1	E	275	TYR
2	F	327	LYS
1	G	155	CYS
1	G	275	TYR
1	G	401	CYS
1	G	463	SER
1	G	464	LEU
1	G	538	GLU
2	H	325	GLU
2	H	353	GLN
2	H	397	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	356	ASN
2	B	92	ASN
2	B	180	HIS
2	B	200	HIS
1	C	92	GLN
1	C	198	ASN
1	C	457	GLN
2	D	92	ASN
2	D	120	ASN
1	E	68	GLN
1	E	131	GLN
1	E	475	ASN
2	F	180	HIS
1	G	113	HIS
1	G	206	ASN
1	G	310	GLN
1	G	445	ASN
2	H	75	GLN
2	H	120	ASN
2	H	352	ASN
2	H	360	ASN

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 ⓘ

95 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	I	1	1,3	14,14,15	0.35	0	17,19,21	0.41	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	BMA	I	3	3	11,11,12	0.49	0	15,15,17	1.33	1 (6%)
3	MAN	I	4	3	11,11,12	0.82	1 (9%)	15,15,17	0.83	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	J	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	BMA	J	3	4	11,11,12	0.54	0	15,15,17	0.80	0
4	MAN	J	4	4	11,11,12	0.68	0	15,15,17	0.95	2 (13%)
4	MAN	J	5	4	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.30	0	17,19,21	0.38	0
3	NAG	K	2	3	14,14,15	0.29	0	17,19,21	0.40	0
3	BMA	K	3	3	11,11,12	0.67	0	15,15,17	0.96	0
3	MAN	K	4	3	11,11,12	0.74	0	15,15,17	1.27	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	L	2	5	14,14,15	0.24	0	17,19,21	0.49	0
5	BMA	L	3	5	11,11,12	0.70	0	15,15,17	1.04	1 (6%)
5	MAN	L	4	5	11,11,12	1.12	1 (9%)	15,15,17	1.53	4 (26%)
5	MAN	L	5	5	11,11,12	0.77	1 (9%)	15,15,17	1.05	2 (13%)
5	MAN	L	6	5	11,11,12	1.27	1 (9%)	15,15,17	0.84	1 (6%)
6	NAG	M	1	6,2	14,14,15	0.20	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	N	1	6,2	14,14,15	0.18	0	17,19,21	0.41	0
6	NAG	N	2	6	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	O	1	3,2	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.43	0
3	BMA	O	3	3	11,11,12	0.48	0	15,15,17	0.84	0
3	MAN	O	4	3	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
7	NAG	P	1	7,1	14,14,15	0.44	0	17,19,21	0.45	0
7	NAG	P	2	7	14,14,15	0.33	0	17,19,21	0.41	0
7	BMA	P	3	7	11,11,12	0.91	1 (9%)	15,15,17	0.89	0
7	MAN	P	4	7	11,11,12	0.63	0	15,15,17	1.29	2 (13%)
7	MAN	P	5	7	11,11,12	0.76	0	15,15,17	0.80	1 (6%)
7	MAN	P	6	7	11,11,12	0.72	0	15,15,17	1.02	2 (13%)
3	NAG	Q	1	1,3	14,14,15	0.41	0	17,19,21	0.43	0
3	NAG	Q	2	3	14,14,15	0.25	0	17,19,21	0.41	0
3	BMA	Q	3	3	11,11,12	0.67	0	15,15,17	0.87	0
3	MAN	Q	4	3	11,11,12	1.15	1 (9%)	15,15,17	2.09	4 (26%)
7	NAG	R	1	7,1	14,14,15	0.42	0	17,19,21	0.52	0
7	NAG	R	2	7	14,14,15	0.28	0	17,19,21	0.45	0
7	BMA	R	3	7	11,11,12	0.75	0	15,15,17	1.10	1 (6%)
7	MAN	R	4	7	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
7	MAN	R	5	7	11,11,12	0.73	0	15,15,17	0.93	0
7	MAN	R	6	7	11,11,12	1.10	1 (9%)	15,15,17	1.07	2 (13%)
3	NAG	S	1	1,3	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	S	2	3	14,14,15	0.22	0	17,19,21	0.47	0
3	BMA	S	3	3	11,11,12	0.90	1 (9%)	15,15,17	1.11	1 (6%)
3	MAN	S	4	3	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
6	NAG	T	1	6,2	14,14,15	0.28	0	17,19,21	0.53	0
6	NAG	T	2	6	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	U	1	4,1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	U	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	BMA	U	3	4	11,11,12	0.51	0	15,15,17	0.84	0
4	MAN	U	4	4	11,11,12	0.62	0	15,15,17	1.07	2 (13%)
4	MAN	U	5	4	11,11,12	0.79	1 (9%)	15,15,17	1.27	2 (13%)
6	NAG	V	1	6,1	14,14,15	0.33	0	17,19,21	0.46	0
6	NAG	V	2	6	14,14,15	0.21	0	17,19,21	0.45	0
7	NAG	W	1	7,1	14,14,15	0.56	1 (7%)	17,19,21	0.50	0
7	NAG	W	2	7	14,14,15	0.53	0	17,19,21	0.52	0
7	BMA	W	3	7	11,11,12	1.17	1 (9%)	15,15,17	1.72	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	W	4	7	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
7	MAN	W	5	7	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
7	MAN	W	6	7	11,11,12	1.47	2 (18%)	15,15,17	1.54	3 (20%)
4	NAG	X	1	4,1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	X	2	4	14,14,15	0.27	0	17,19,21	0.49	0
4	BMA	X	3	4	11,11,12	0.78	0	15,15,17	0.82	0
4	MAN	X	4	4	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
4	MAN	X	5	4	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
6	NAG	Y	1	6,2	14,14,15	0.27	0	17,19,21	0.47	0
6	NAG	Y	2	6	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	Z	1	6,2	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
6	NAG	Z	2	6	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	a	1	1,3	14,14,15	0.50	0	17,19,21	0.48	0
3	NAG	a	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	BMA	a	3	3	11,11,12	0.50	0	15,15,17	0.97	0
3	MAN	a	4	3	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
8	NAG	b	1	8,1	14,14,15	0.83	2 (14%)	17,19,21	0.64	1 (5%)
8	NAG	b	2	8	14,14,15	0.76	1 (7%)	17,19,21	1.59	3 (17%)
8	BMA	b	3	8	11,11,12	0.68	0	15,15,17	0.87	1 (6%)
8	MAN	b	4	8	11,11,12	1.30	2 (18%)	15,15,17	1.17	2 (13%)
8	MAN	b	5	8	11,11,12	0.88	1 (9%)	15,15,17	1.01	2 (13%)
8	MAN	b	6	8	11,11,12	1.50	3 (27%)	15,15,17	1.75	4 (26%)
9	NAG	c	1	1,9	14,14,15	0.37	0	17,19,21	0.46	0
9	NAG	c	2	9	14,14,15	0.24	0	17,19,21	0.45	0
9	BMA	c	3	9	11,11,12	0.58	0	15,15,17	0.68	0
9	MAN	c	4	9	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
3	NAG	d	1	1,3	14,14,15	0.52	0	17,19,21	0.52	0
3	NAG	d	2	3	14,14,15	0.42	0	17,19,21	0.44	0
3	BMA	d	3	3	11,11,12	0.73	0	15,15,17	0.66	0
3	MAN	d	4	3	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
6	NAG	e	1	6,2	14,14,15	0.52	0	17,19,21	0.48	0
6	NAG	e	2	6	14,14,15	0.25	0	17,19,21	0.58	0
6	NAG	f	1	6,2	14,14,15	0.38	0	17,19,21	0.56	0
6	NAG	f	2	6	14,14,15	0.18	0	17,19,21	0.76	1 (5%)
6	NAG	g	1	6,2	14,14,15	0.56	1 (7%)	17,19,21	0.53	0
6	NAG	g	2	6	14,14,15	0.31	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	1/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	MAN	L	5	5	-	0/2/19/22	0/1/1/1
5	MAN	L	6	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	2/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
7	MAN	P	5	7	-	0/2/19/22	0/1/1/1
7	MAN	P	6	7	-	1/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	a	3	3	-	2/2/19/22	0/1/1/1
3	MAN	a	4	3	-	0/2/19/22	1/1/1/1
8	NAG	b	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	2/2/19/22	0/1/1/1
8	MAN	b	4	8	-	2/2/19/22	0/1/1/1
8	MAN	b	5	8	-	2/2/19/22	0/1/1/1
8	MAN	b	6	8	-	0/2/19/22	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	BMA	d	3	3	-	0/2/19/22	0/1/1/1
3	MAN	d	4	3	-	1/2/19/22	0/1/1/1
6	NAG	e	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	4/6/23/26	0/1/1/1
6	NAG	f	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	5/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	6	MAN	O5-C1	-3.71	1.37	1.43
7	W	6	MAN	C2-C3	3.46	1.57	1.52
8	b	6	MAN	C4-C5	2.74	1.58	1.53
7	R	6	MAN	O5-C1	-2.74	1.39	1.43
8	b	6	MAN	O5-C5	2.68	1.48	1.43
7	W	6	MAN	C1-C2	2.53	1.58	1.52
3	Q	4	MAN	C1-C2	2.51	1.58	1.52
8	b	2	NAG	O5-C1	-2.49	1.39	1.43
5	L	4	MAN	O5-C1	-2.45	1.39	1.43
8	b	4	MAN	O5-C1	-2.44	1.39	1.43
3	I	4	MAN	O5-C1	-2.39	1.39	1.43
8	b	6	MAN	C2-C3	-2.34	1.48	1.52
5	L	5	MAN	C1-C2	2.27	1.57	1.52
7	P	3	BMA	O5-C1	-2.25	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	1	NAG	O5-C1	2.23	1.47	1.43
8	b	4	MAN	C2-C3	2.15	1.55	1.52
8	b	5	MAN	C1-C2	2.12	1.57	1.52
7	W	3	BMA	C1-C2	2.11	1.57	1.52
8	b	1	NAG	C1-C2	2.08	1.55	1.52
4	U	5	MAN	C1-C2	2.06	1.57	1.52
7	W	1	NAG	O5-C1	-2.05	1.40	1.43
6	g	1	NAG	O5-C1	-2.01	1.40	1.43
3	S	3	BMA	O5-C1	-2.00	1.40	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	4	MAN	C1-O5-C5	6.13	120.40	112.19
8	b	6	MAN	C1-O5-C5	4.58	118.32	112.19
3	I	3	BMA	C1-O5-C5	4.43	118.12	112.19
7	W	3	BMA	C1-C2-C3	4.41	116.07	109.64
8	b	2	NAG	O4-C4-C5	-3.98	99.52	109.32
8	b	2	NAG	C3-C4-C5	3.64	116.83	110.23
7	W	6	MAN	C1-C2-C3	3.55	114.81	109.64
7	P	4	MAN	C1-O5-C5	3.53	116.92	112.19
5	L	4	MAN	C1-O5-C5	3.47	116.83	112.19
7	R	4	MAN	C1-O5-C5	3.36	116.68	112.19
3	Q	4	MAN	O5-C1-C2	3.20	118.41	110.79
8	b	6	MAN	C1-C2-C3	-3.06	105.19	109.64
3	K	4	MAN	C1-O5-C5	2.97	116.16	112.19
4	U	4	MAN	C1-O5-C5	2.96	116.15	112.19
3	S	4	MAN	C1-O5-C5	2.88	116.05	112.19
7	R	6	MAN	C1-C2-C3	-2.85	105.49	109.64
4	U	5	MAN	C1-O5-C5	2.76	115.89	112.19
3	a	4	MAN	C1-O5-C5	2.63	115.71	112.19
4	J	5	MAN	C1-O5-C5	2.58	115.64	112.19
7	W	5	MAN	C1-O5-C5	2.56	115.61	112.19
5	L	4	MAN	O6-C6-C5	-2.55	102.64	111.33
8	b	4	MAN	C1-O5-C5	2.54	115.58	112.19
7	P	6	MAN	C1-O5-C5	2.46	115.49	112.19
4	X	4	MAN	C1-O5-C5	2.46	115.48	112.19
7	W	3	BMA	O5-C1-C2	2.44	116.62	110.79
7	W	3	BMA	O2-C2-C3	-2.44	105.10	110.15
6	f	2	NAG	C1-O5-C5	2.43	115.45	112.19
4	X	5	MAN	C1-O5-C5	2.42	115.43	112.19
8	b	2	NAG	O4-C4-C3	-2.41	104.70	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	5	MAN	O5-C1-C2	2.41	116.53	110.79
7	R	3	BMA	C1-O5-C5	2.41	115.41	112.19
5	L	5	MAN	C1-O5-C5	2.40	115.41	112.19
7	W	3	BMA	O5-C5-C4	-2.37	105.06	110.83
7	P	4	MAN	O2-C2-C3	-2.31	105.38	110.15
3	Q	4	MAN	C3-C4-C5	-2.30	106.06	110.23
3	O	4	MAN	C1-O5-C5	2.28	115.25	112.19
7	R	4	MAN	O2-C2-C3	-2.26	105.46	110.15
8	b	1	NAG	C1-O5-C5	2.26	115.22	112.19
9	c	4	MAN	C1-O5-C5	2.24	115.19	112.19
5	L	5	MAN	O2-C2-C3	-2.24	105.51	110.15
7	W	6	MAN	O5-C5-C4	-2.24	105.39	110.83
4	X	5	MAN	O2-C2-C3	-2.23	105.52	110.15
3	O	4	MAN	O2-C2-C3	-2.23	105.53	110.15
3	d	4	MAN	O2-C2-C3	-2.22	105.55	110.15
3	Q	4	MAN	O2-C2-C3	-2.22	105.56	110.15
8	b	6	MAN	C3-C4-C5	2.22	114.25	110.23
5	L	4	MAN	O3-C3-C2	2.21	114.57	110.05
4	J	4	MAN	C1-O5-C5	2.21	115.15	112.19
7	W	4	MAN	C1-O5-C5	2.18	115.11	112.19
4	X	4	MAN	O2-C2-C3	-2.16	105.67	110.15
7	P	6	MAN	O2-C2-C3	-2.16	105.68	110.15
8	b	6	MAN	O2-C2-C3	-2.16	105.68	110.15
7	W	6	MAN	O5-C1-C2	2.15	115.92	110.79
7	W	5	MAN	O2-C2-C3	-2.14	105.72	110.15
3	S	3	BMA	C1-C2-C3	2.13	112.75	109.64
7	R	6	MAN	O2-C2-C3	-2.12	105.75	110.15
3	a	4	MAN	O2-C2-C3	-2.12	105.76	110.15
7	P	5	MAN	O2-C2-C3	-2.12	105.76	110.15
3	S	4	MAN	O2-C2-C3	-2.11	105.77	110.15
4	J	5	MAN	O2-C2-C3	-2.11	105.79	110.15
5	L	3	BMA	C1-O5-C5	2.08	114.98	112.19
3	I	4	MAN	O2-C2-C3	-2.08	105.84	110.15
4	J	4	MAN	O2-C2-C3	-2.07	105.86	110.15
5	L	4	MAN	O2-C2-C3	-2.05	105.90	110.15
8	b	4	MAN	O2-C2-C3	-2.05	105.90	110.15
7	W	4	MAN	O2-C2-C3	-2.04	105.92	110.15
8	b	3	BMA	C1-O5-C5	2.03	114.91	112.19
6	Z	1	NAG	C1-O5-C5	2.02	114.90	112.19
4	U	5	MAN	O2-C2-C3	-2.02	105.97	110.15
5	L	6	MAN	O2-C2-C3	-2.02	105.97	110.15
8	b	5	MAN	O2-C2-C3	-2.01	106.00	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	4	MAN	O2-C2-C3	-2.01	106.00	110.15

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	2	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
4	X	4	MAN	C4-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	3	BMA	O5-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
3	O	4	MAN	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
8	b	4	MAN	O5-C5-C6-O6
8	b	5	MAN	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
7	R	6	MAN	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
6	e	2	NAG	C8-C7-N2-C2
6	e	2	NAG	O7-C7-N2-C2
6	g	2	NAG	C8-C7-N2-C2
6	g	2	NAG	O7-C7-N2-C2
3	S	4	MAN	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
4	X	5	MAN	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
8	b	3	BMA	C4-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	a	3	BMA	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	R	3	BMA	C4-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
3	a	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
7	W	3	BMA	C4-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
7	R	6	MAN	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
4	U	5	MAN	C4-C5-C6-O6
8	b	2	NAG	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
4	U	5	MAN	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
3	d	4	MAN	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
7	R	4	MAN	O5-C5-C6-O6
4	X	5	MAN	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
8	b	4	MAN	C4-C5-C6-O6
3	S	4	MAN	C4-C5-C6-O6
4	U	3	BMA	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	d	2	NAG	C1-C2-N2-C7
8	b	5	MAN	C4-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	d	2	NAG	C3-C2-N2-C7
6	Z	1	NAG	C3-C2-N2-C7
6	e	2	NAG	C3-C2-N2-C7
6	g	2	NAG	C3-C2-N2-C7
4	J	4	MAN	O5-C5-C6-O6
7	P	6	MAN	C4-C5-C6-O6
7	W	5	MAN	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
6	Y	2	NAG	C1-C2-N2-C7
6	e	2	NAG	C1-C2-N2-C7
6	g	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
9	c	4	MAN	C4-C5-C6-O6
4	U	4	MAN	C4-C5-C6-O6
3	Q	4	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	4	MAN	C1-C2-C3-C4-C5-O5
3	a	4	MAN	C1-C2-C3-C4-C5-O5

57 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	3	BMA	4	0
6	Y	1	NAG	4	0
3	S	3	BMA	1	0
3	a	1	NAG	1	0
6	f	1	NAG	4	0
6	M	2	NAG	1	0
4	X	3	BMA	1	0
6	Z	1	NAG	1	0
8	b	4	MAN	4	0
7	R	3	BMA	6	0
5	L	4	MAN	5	0
3	Q	1	NAG	1	0
7	P	1	NAG	1	0
6	M	1	NAG	1	0

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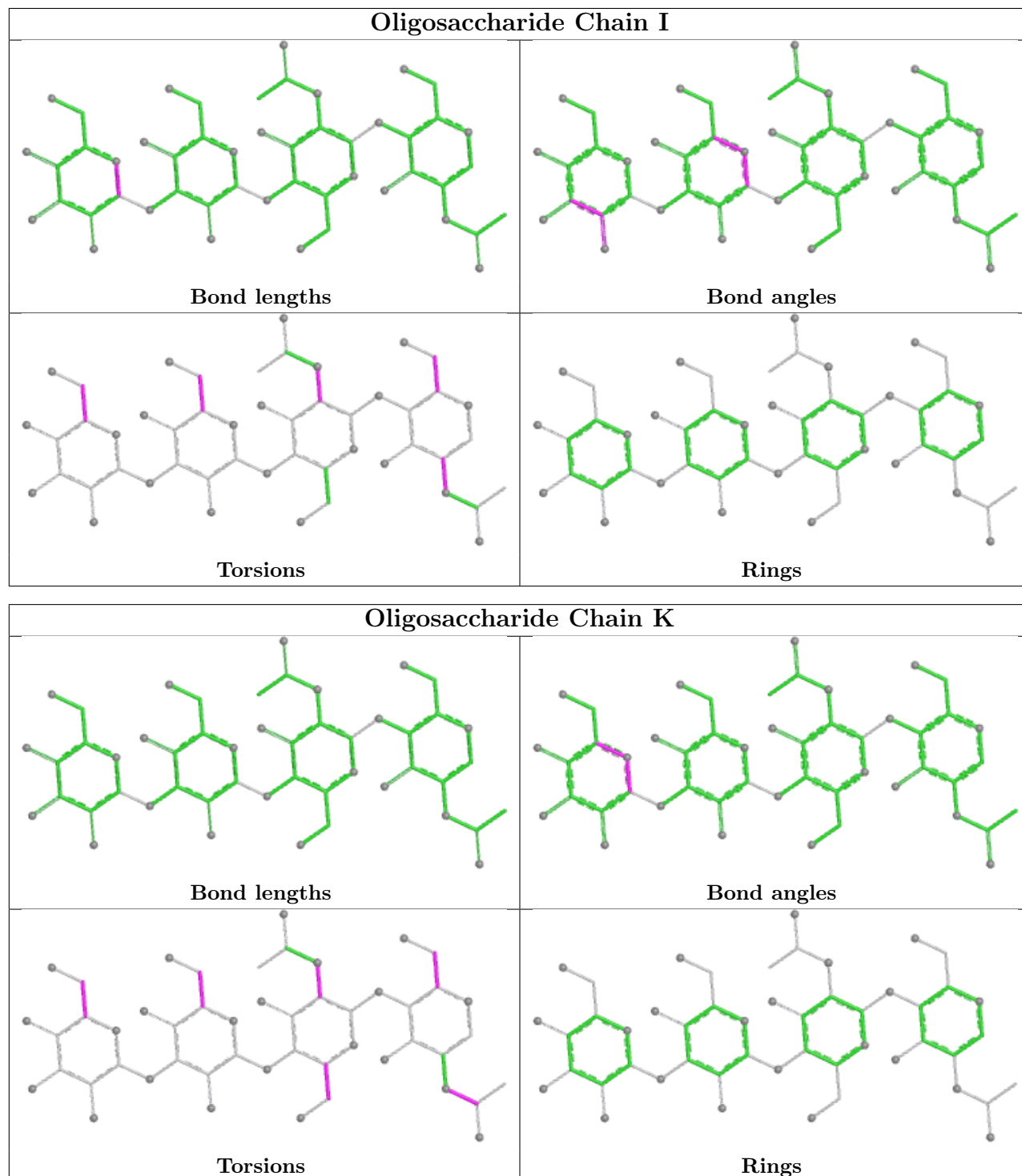
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	e	2	NAG	7	0
6	e	1	NAG	4	0
3	a	2	NAG	1	0
8	b	2	NAG	2	0
7	W	3	BMA	6	0
3	d	3	BMA	1	0
7	R	5	MAN	1	0
3	K	1	NAG	2	0
4	X	2	NAG	1	0
3	d	1	NAG	5	0
6	g	2	NAG	4	0
5	L	2	NAG	2	0
6	Y	2	NAG	4	0
3	d	2	NAG	5	0
3	Q	3	BMA	8	0
3	I	3	BMA	5	1
3	S	2	NAG	1	0
7	R	2	NAG	4	0
6	V	1	NAG	1	0
8	b	1	NAG	1	0
3	Q	4	MAN	5	0
6	V	2	NAG	1	0
3	O	2	NAG	2	0
6	g	1	NAG	1	0
3	I	1	NAG	5	0
6	T	2	NAG	2	0
3	S	4	MAN	1	0
3	I	2	NAG	9	0
7	R	4	MAN	2	0
7	W	2	NAG	1	0
7	W	1	NAG	1	0
3	a	3	BMA	1	0
9	c	1	NAG	1	0
7	W	6	MAN	3	0
6	T	1	NAG	1	0
3	d	4	MAN	3	0
8	b	5	MAN	4	0
5	L	5	MAN	4	0
3	Q	2	NAG	3	0
3	O	1	NAG	1	0
6	f	2	NAG	2	0
4	U	1	NAG	1	0

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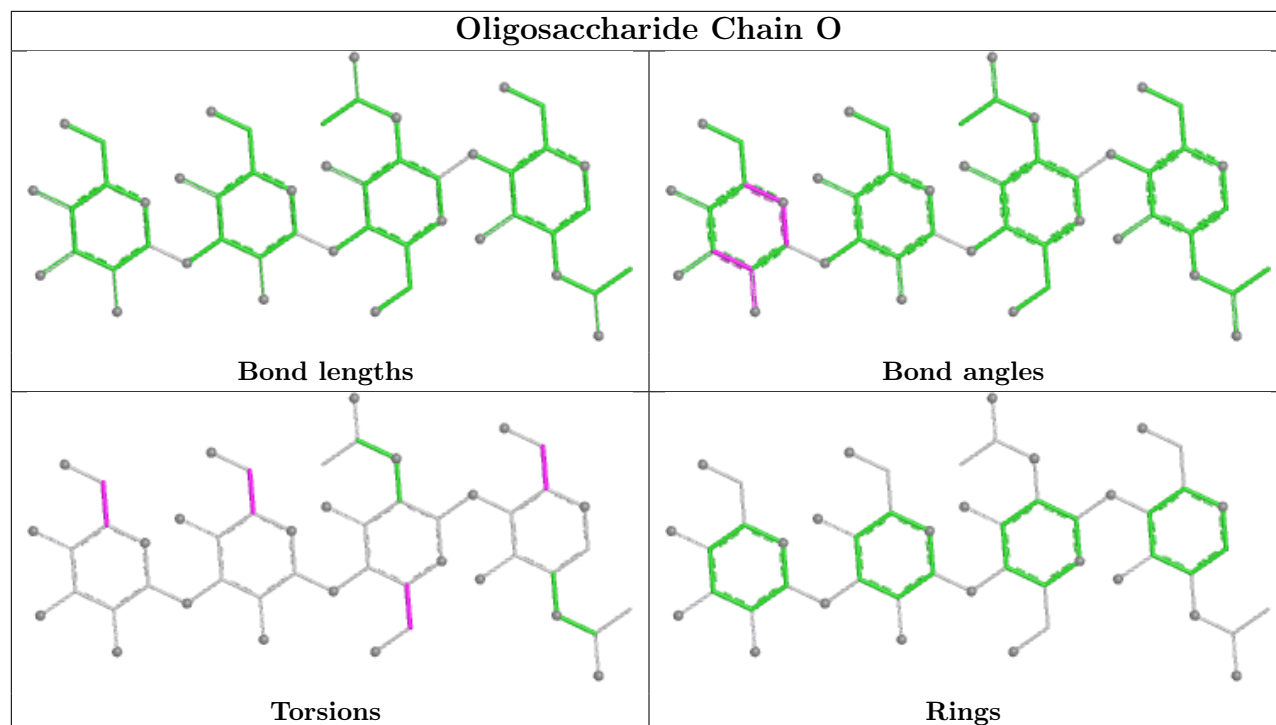
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	6	MAN	1	0

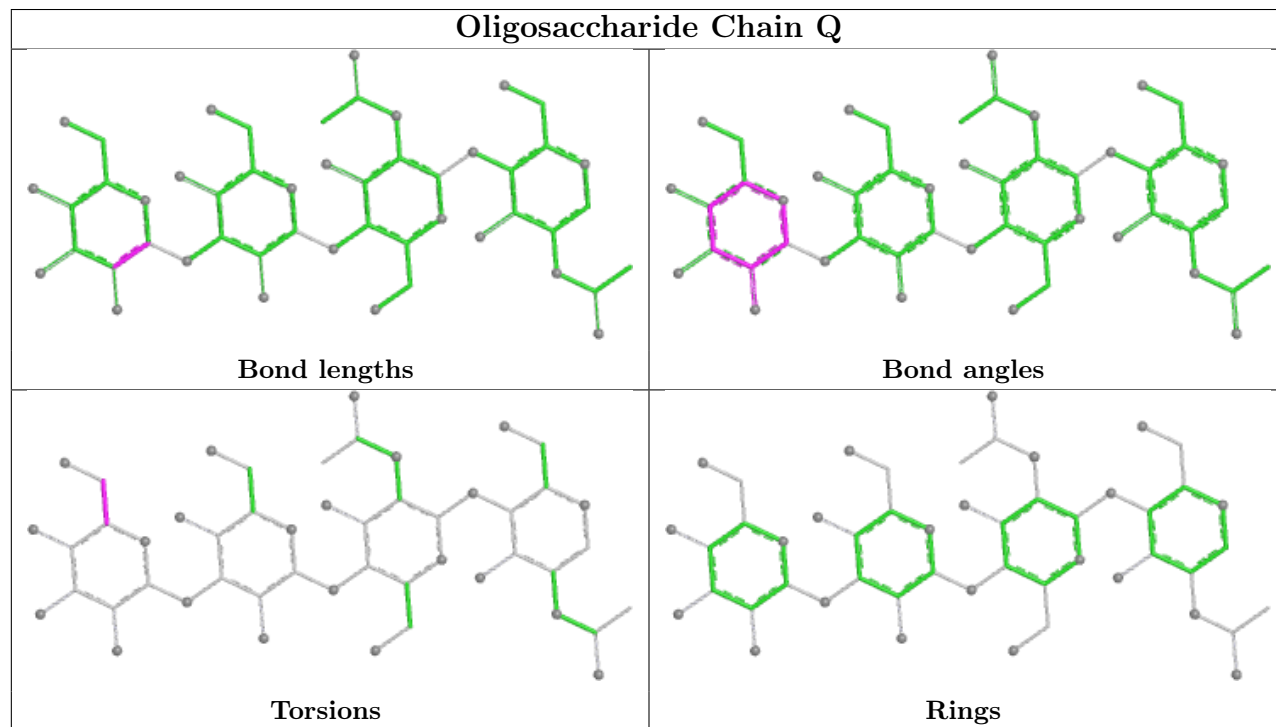
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

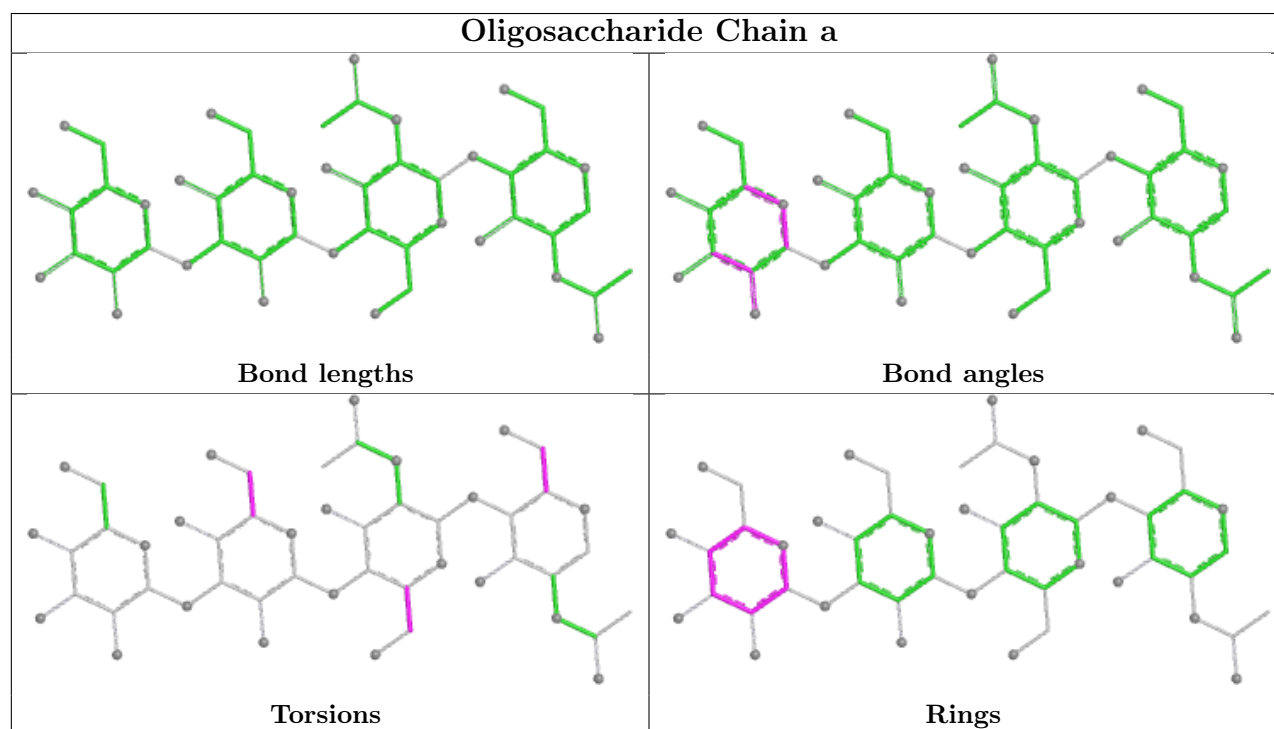
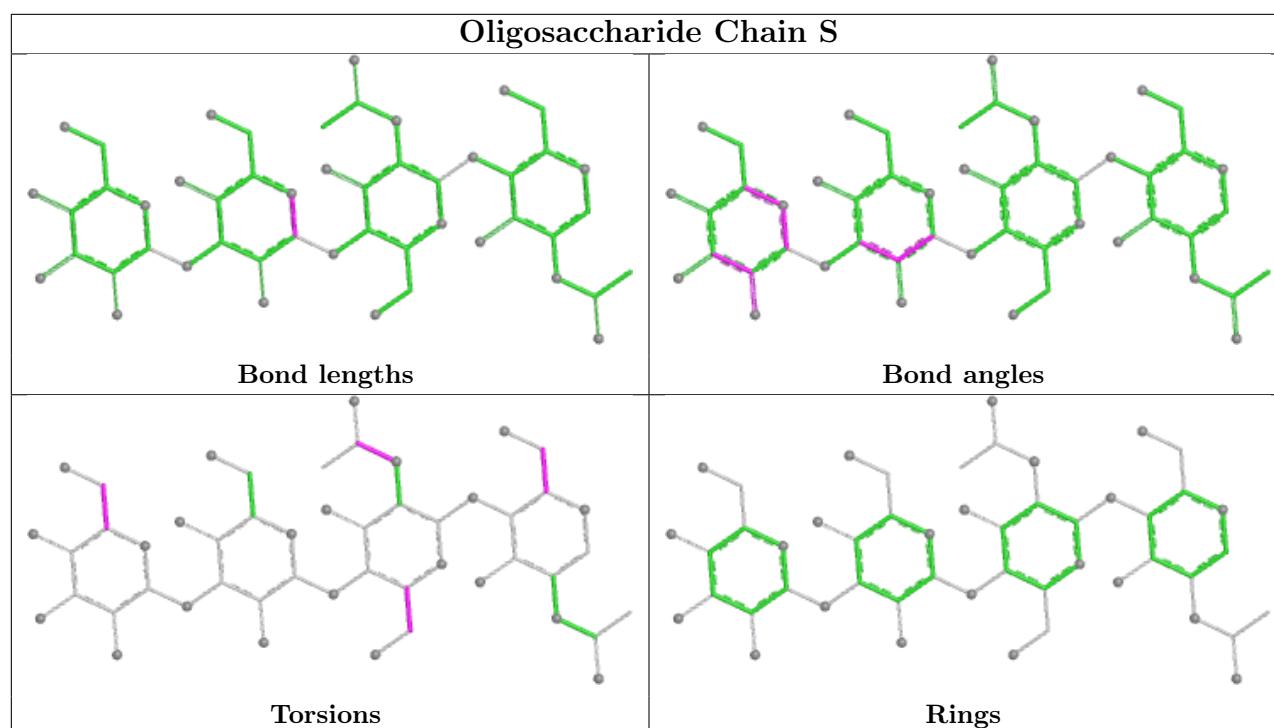


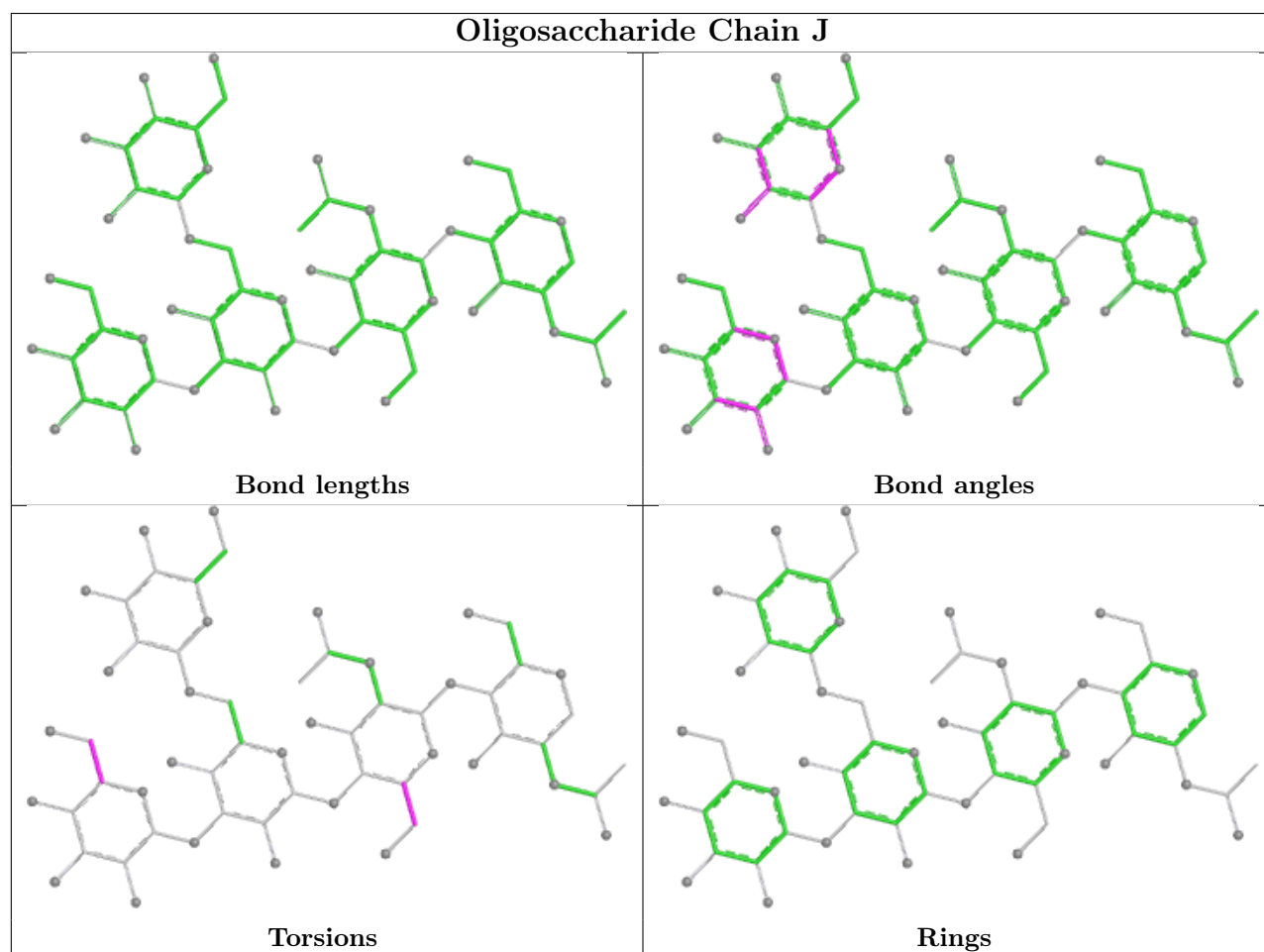
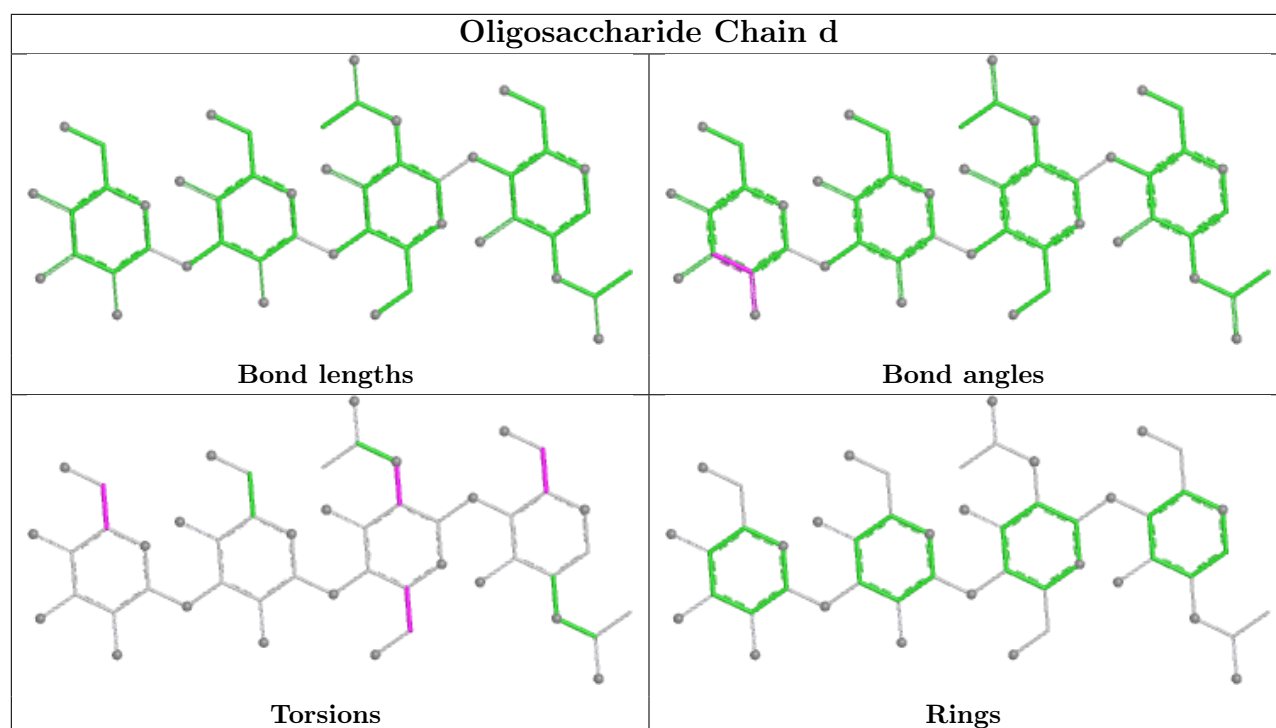
Oligosaccharide Chain O

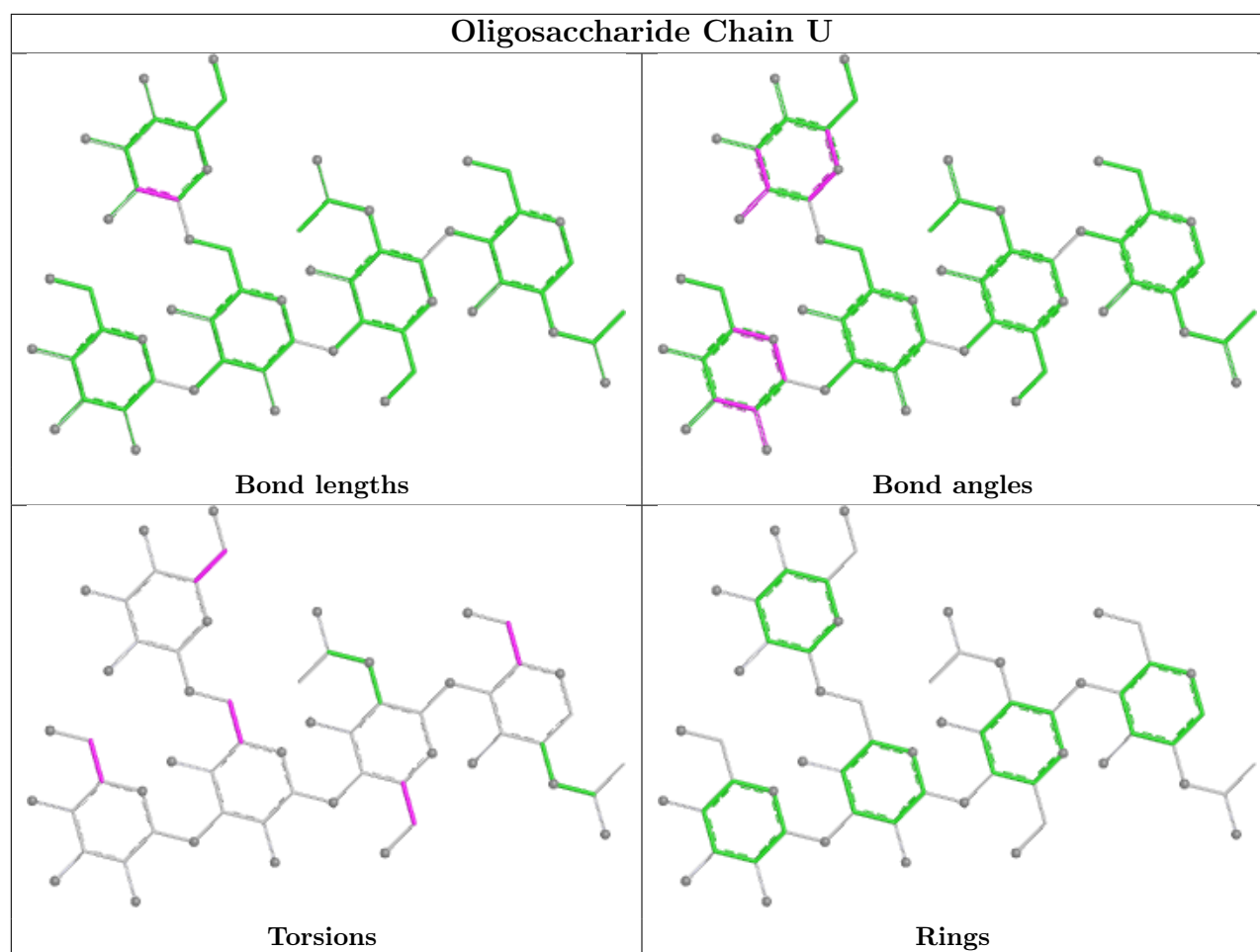


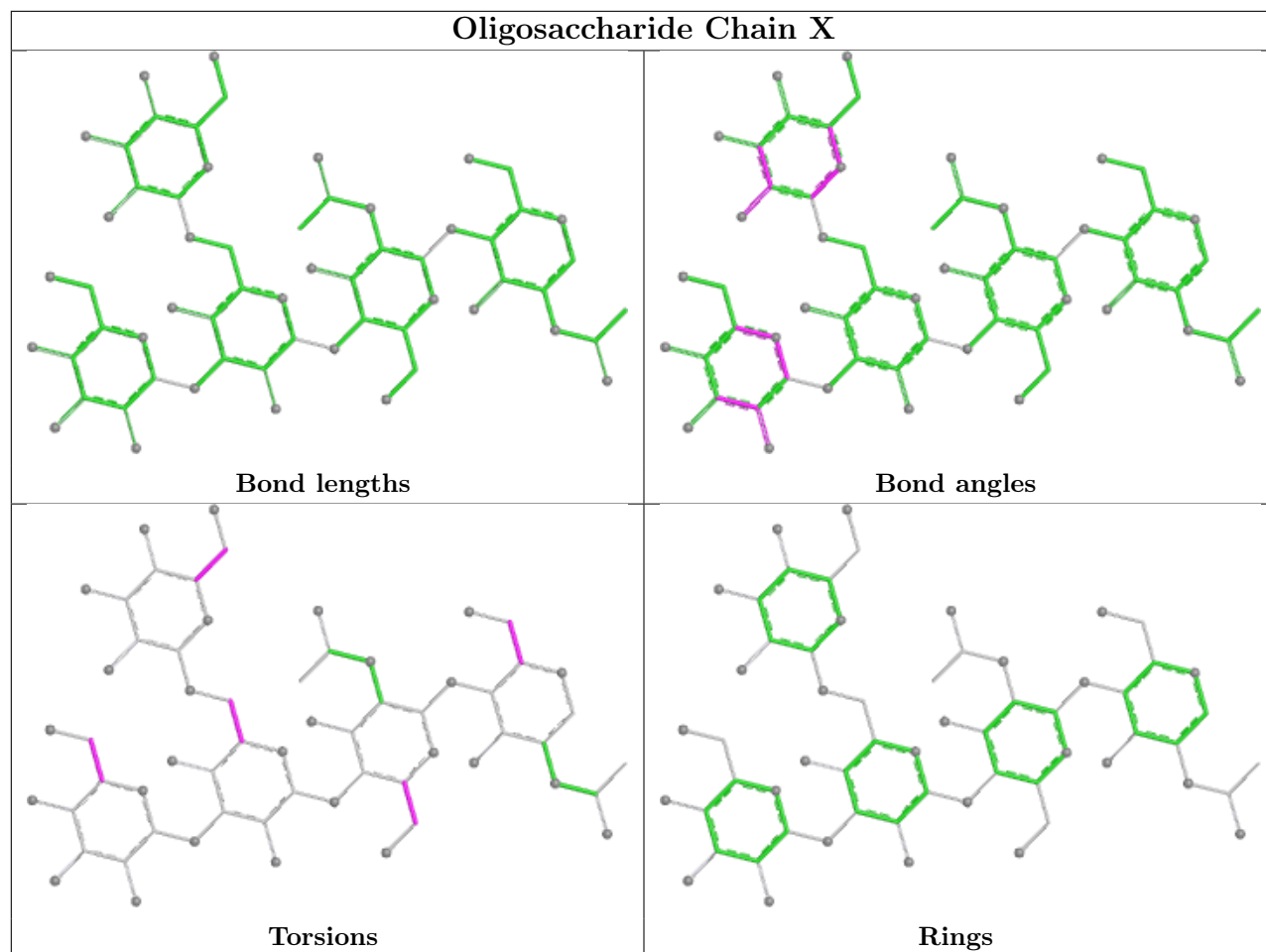
Oligosaccharide Chain Q

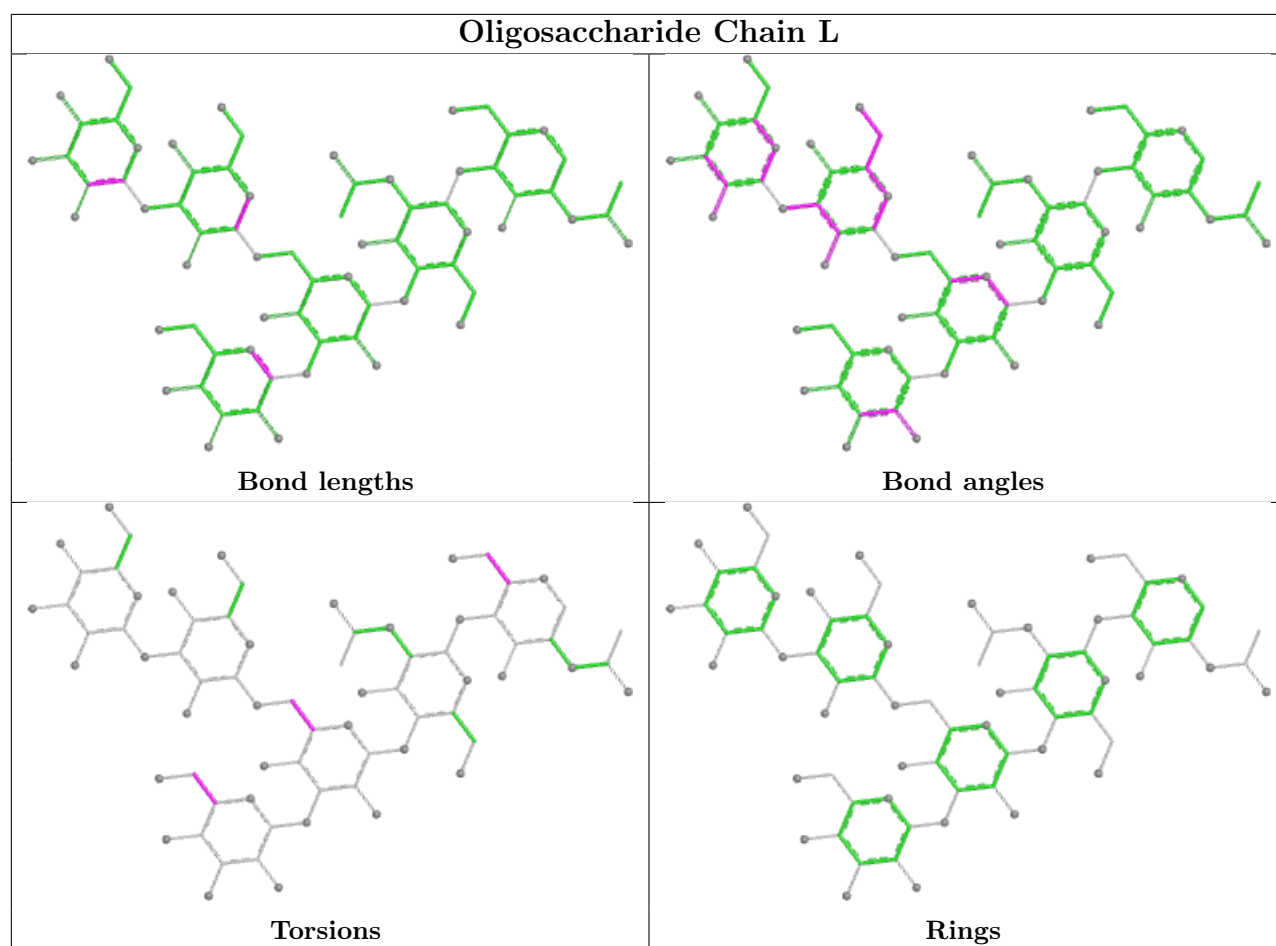


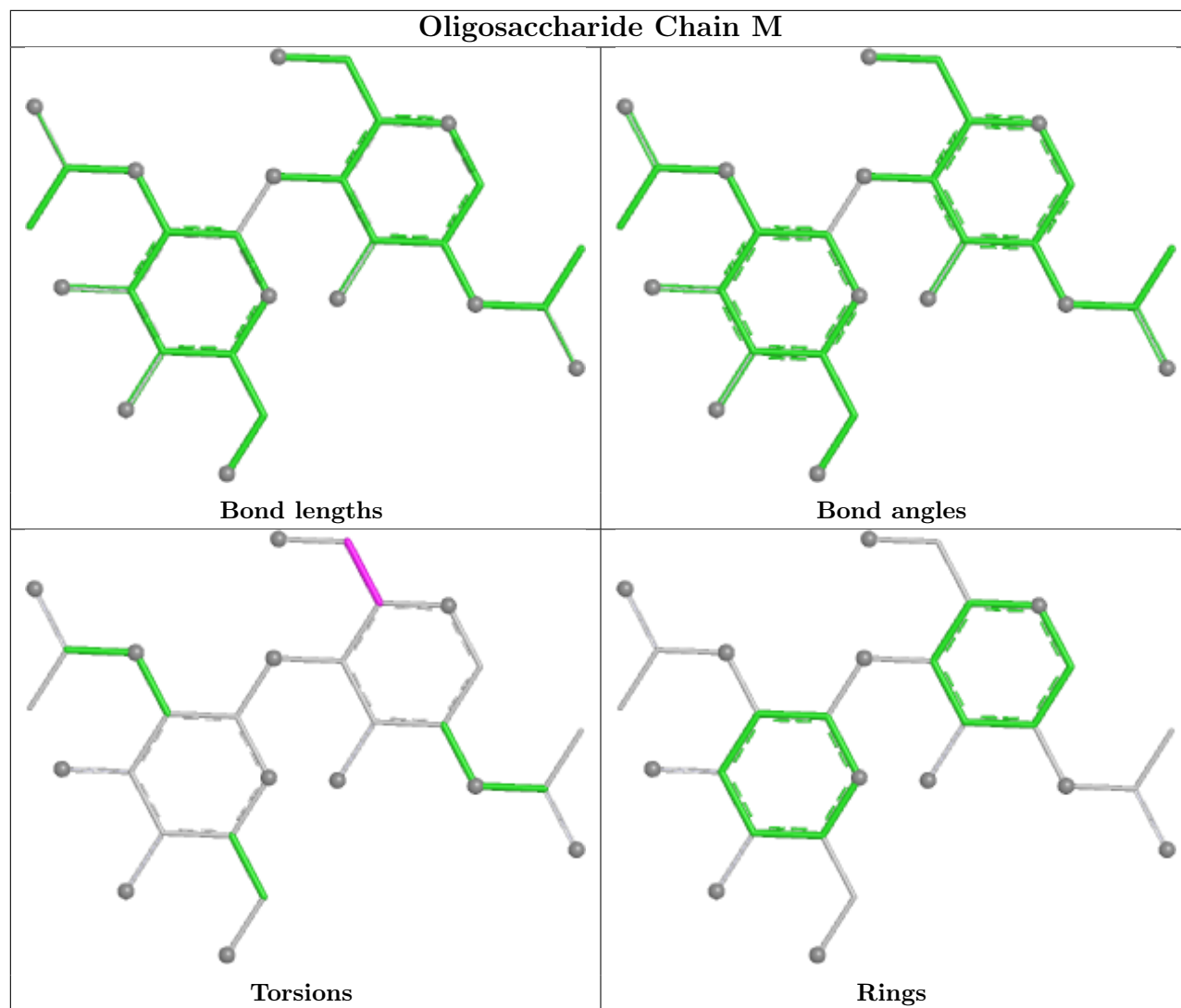


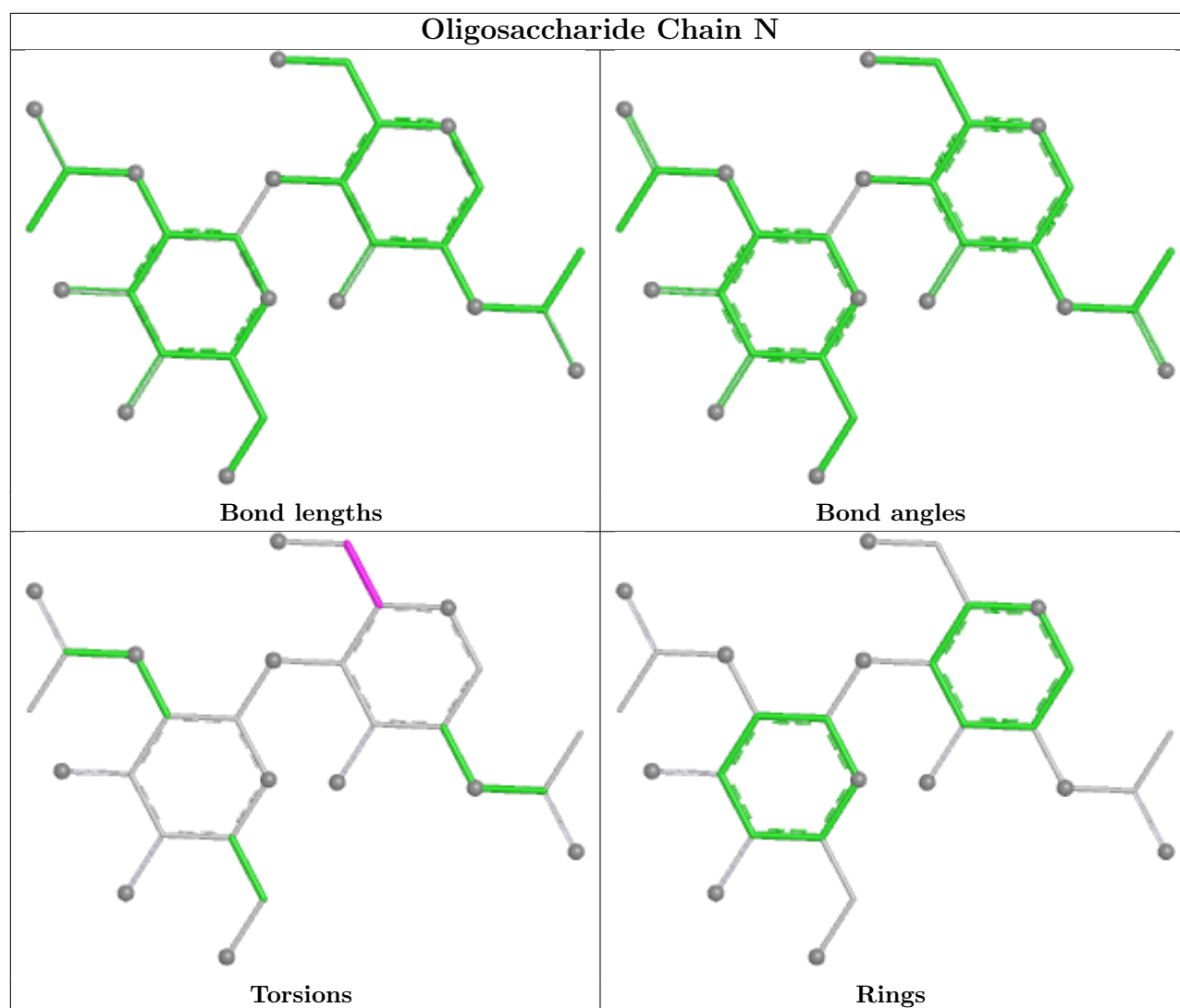


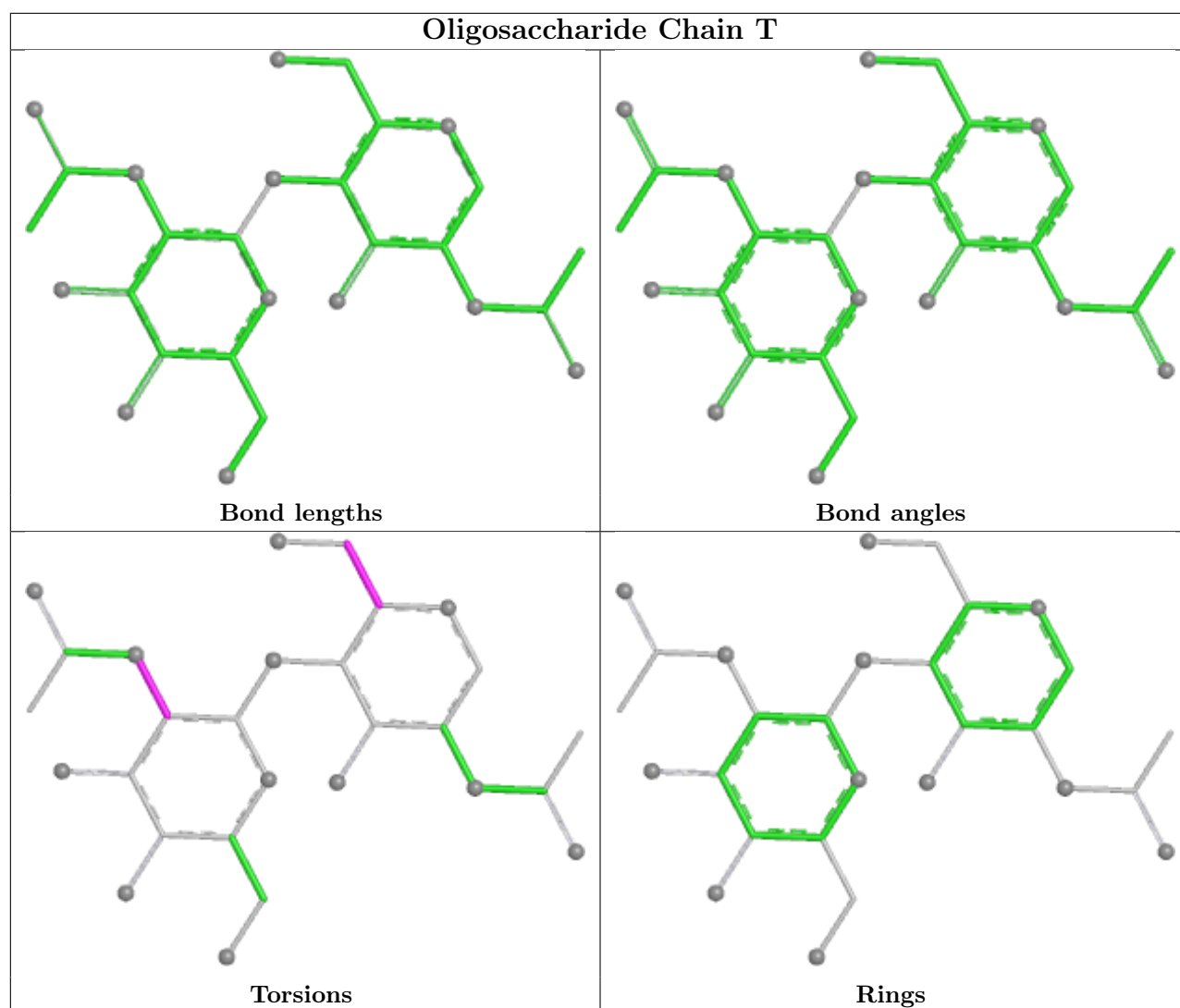


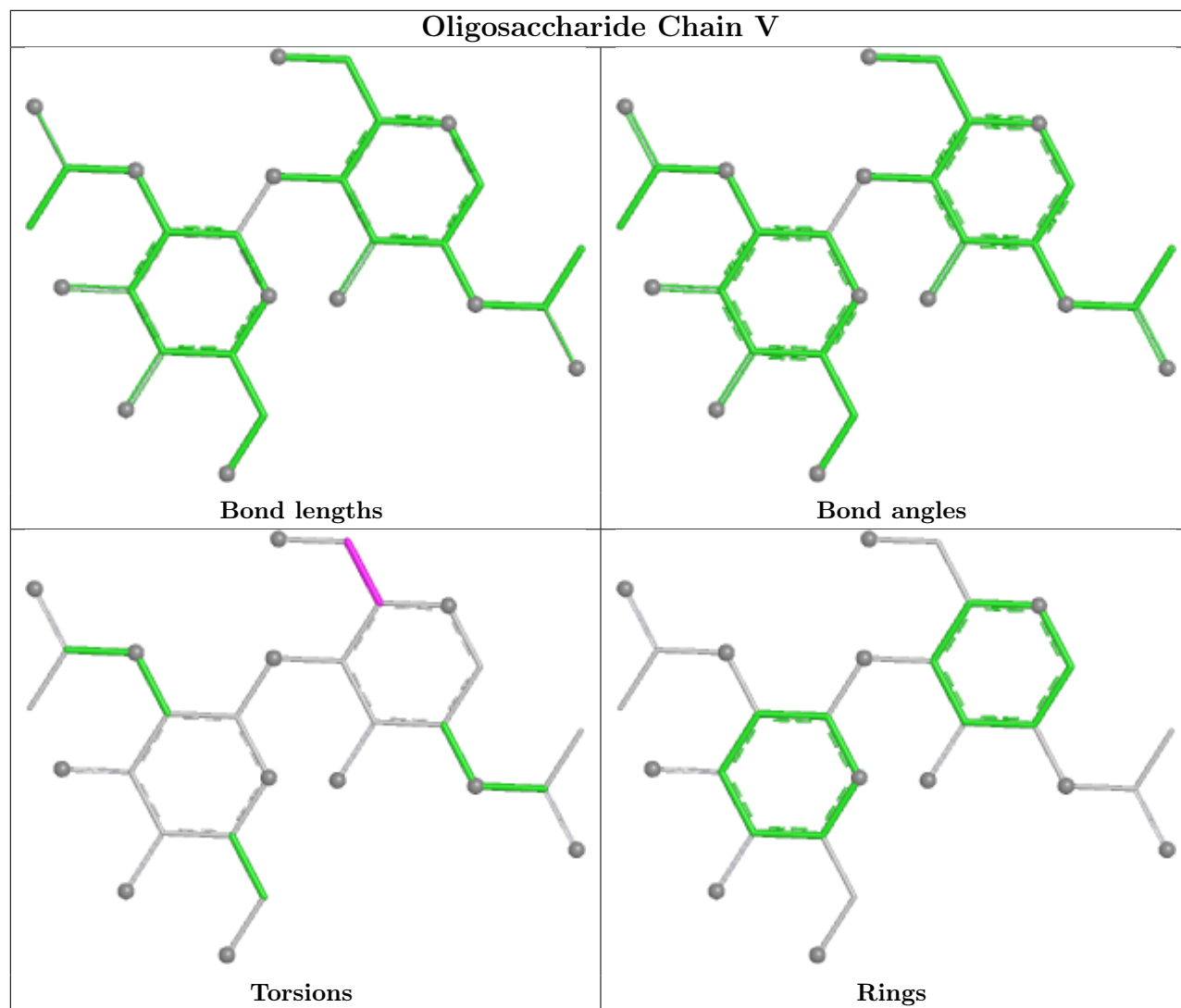


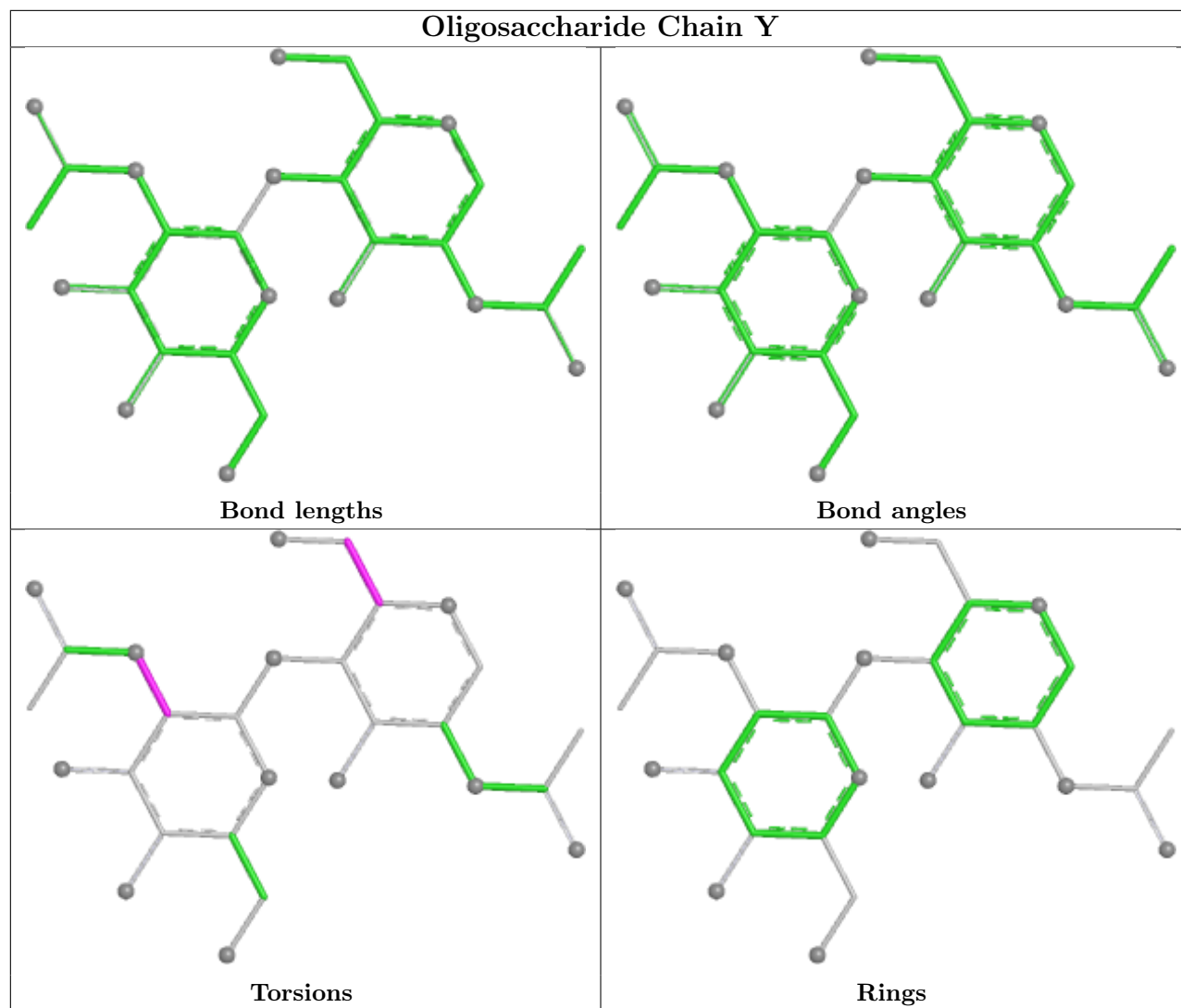


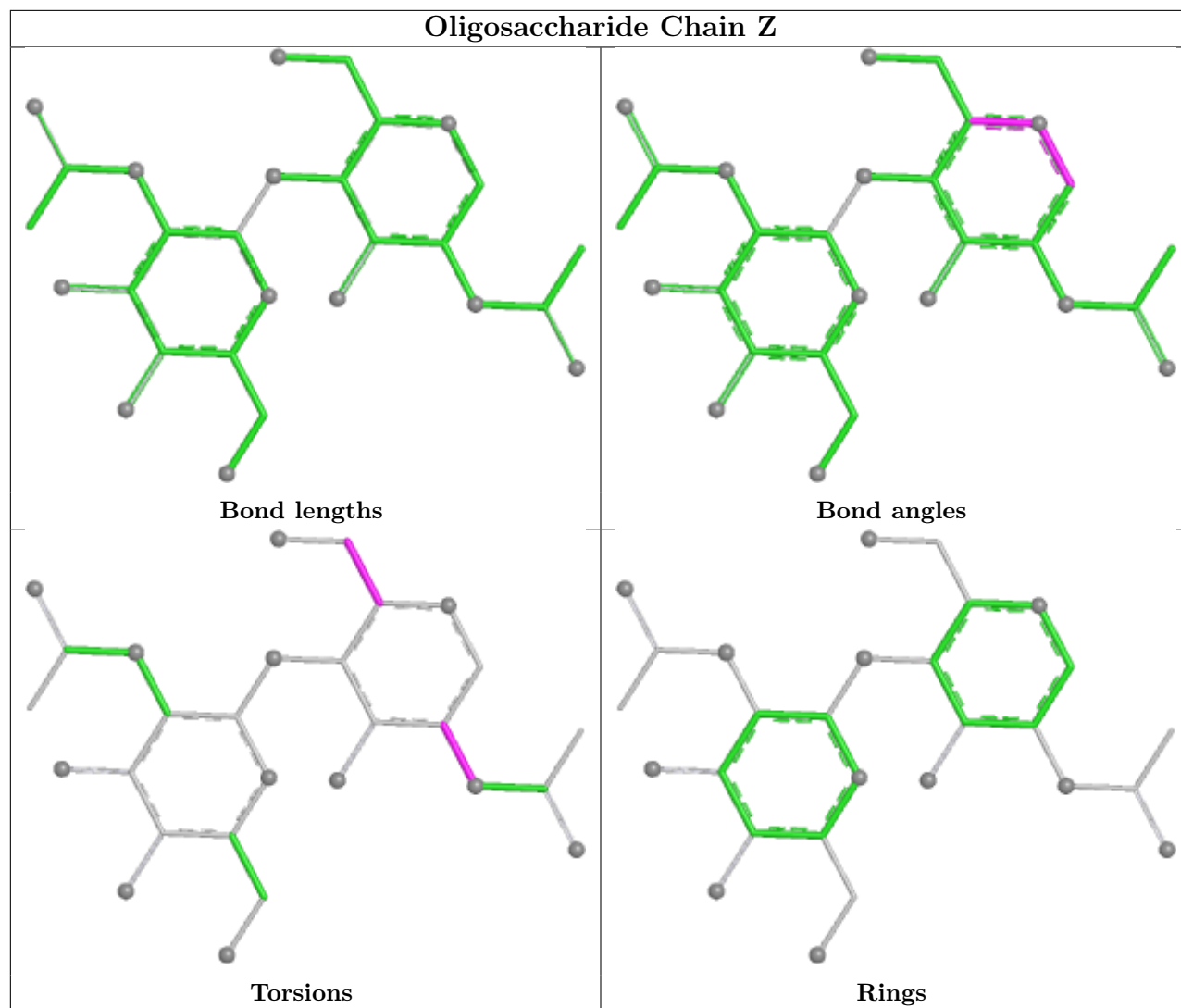


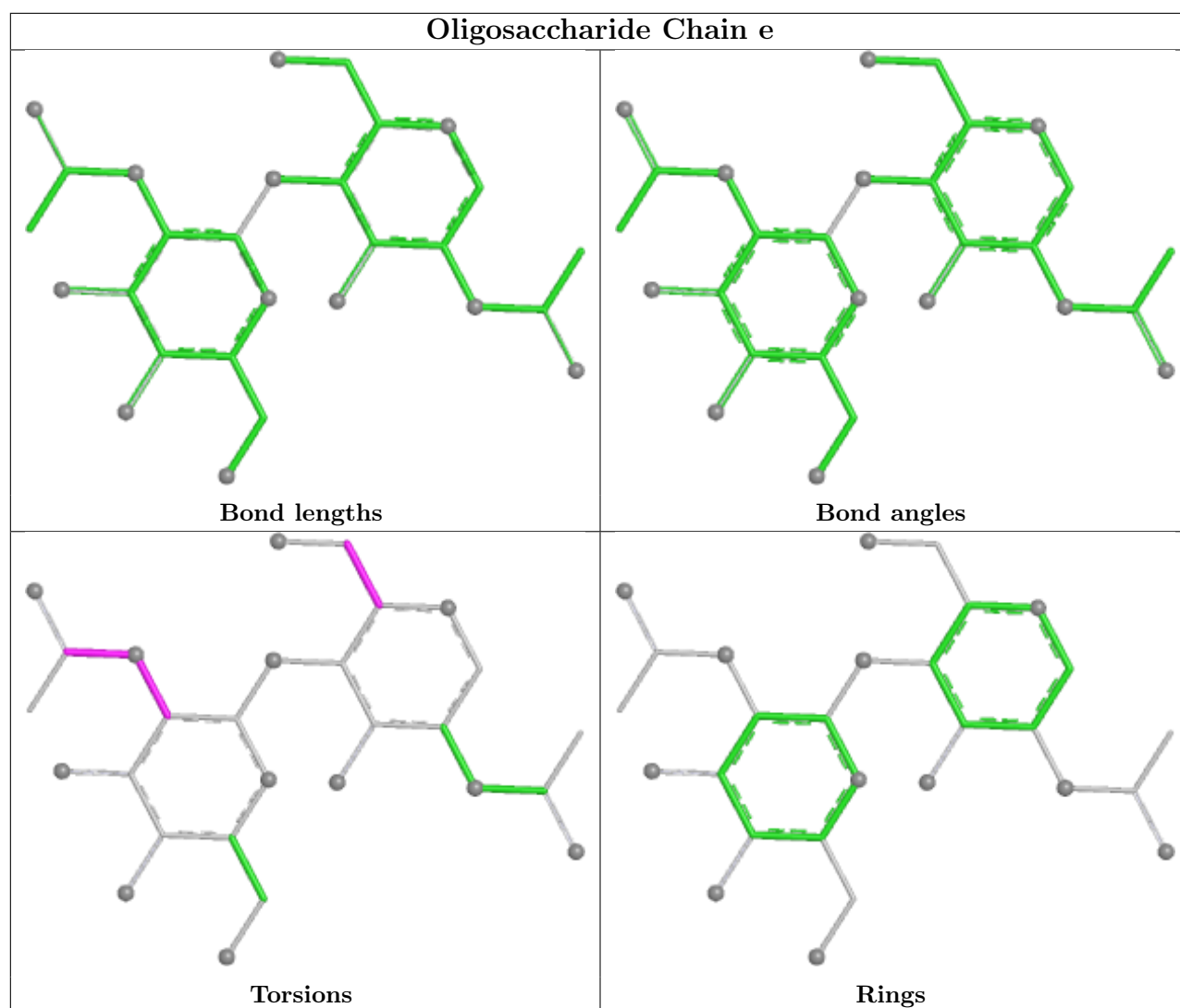


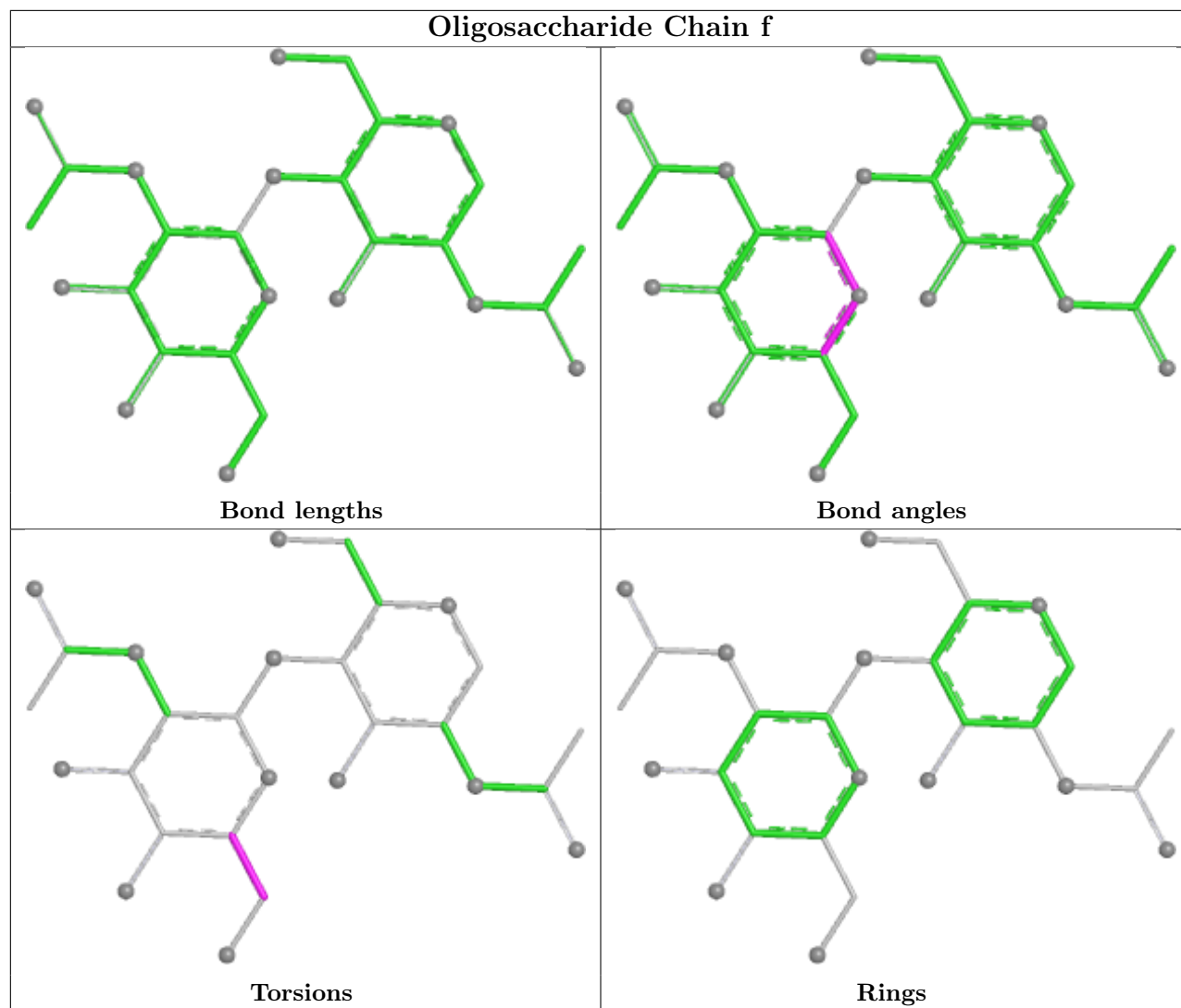


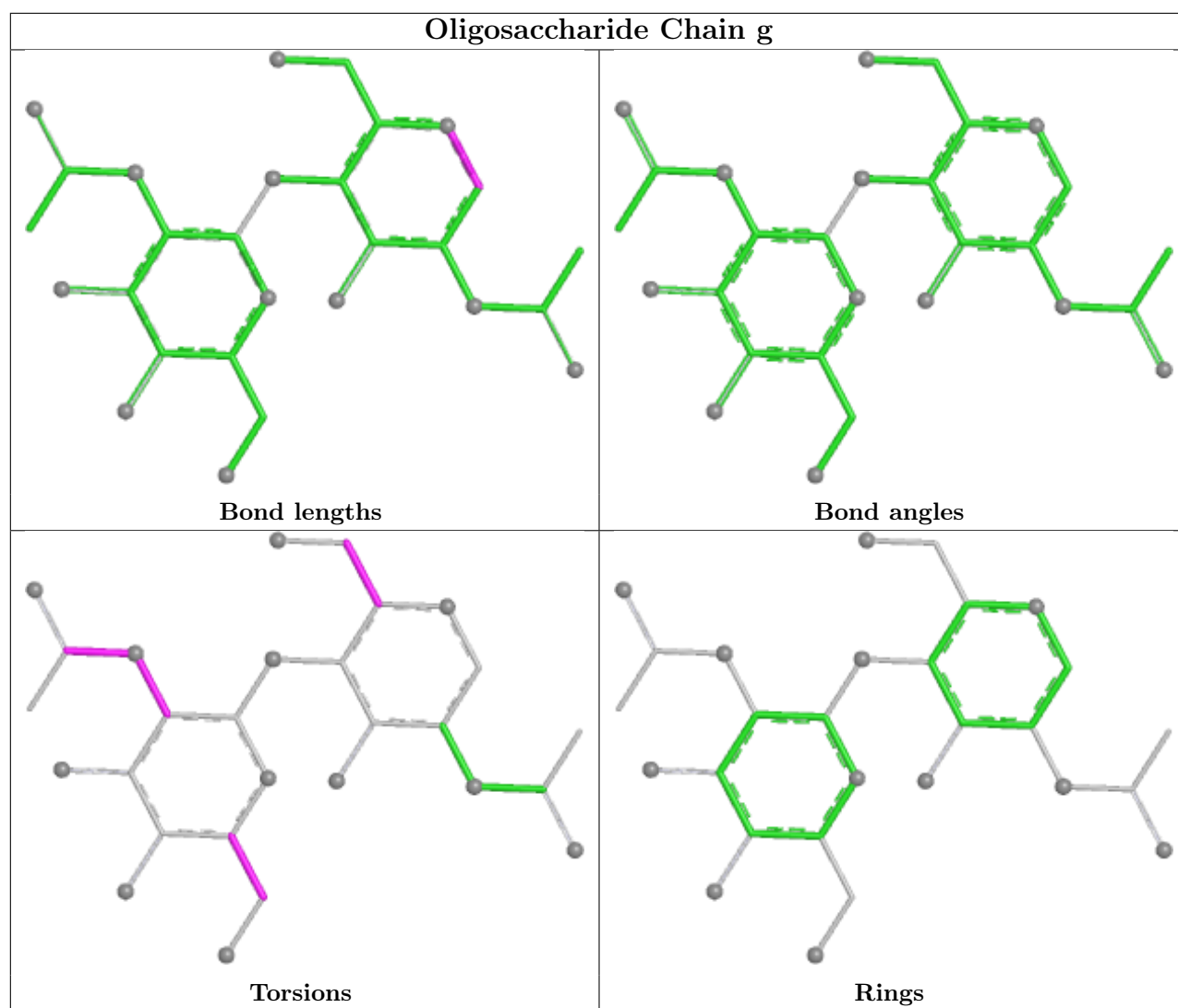


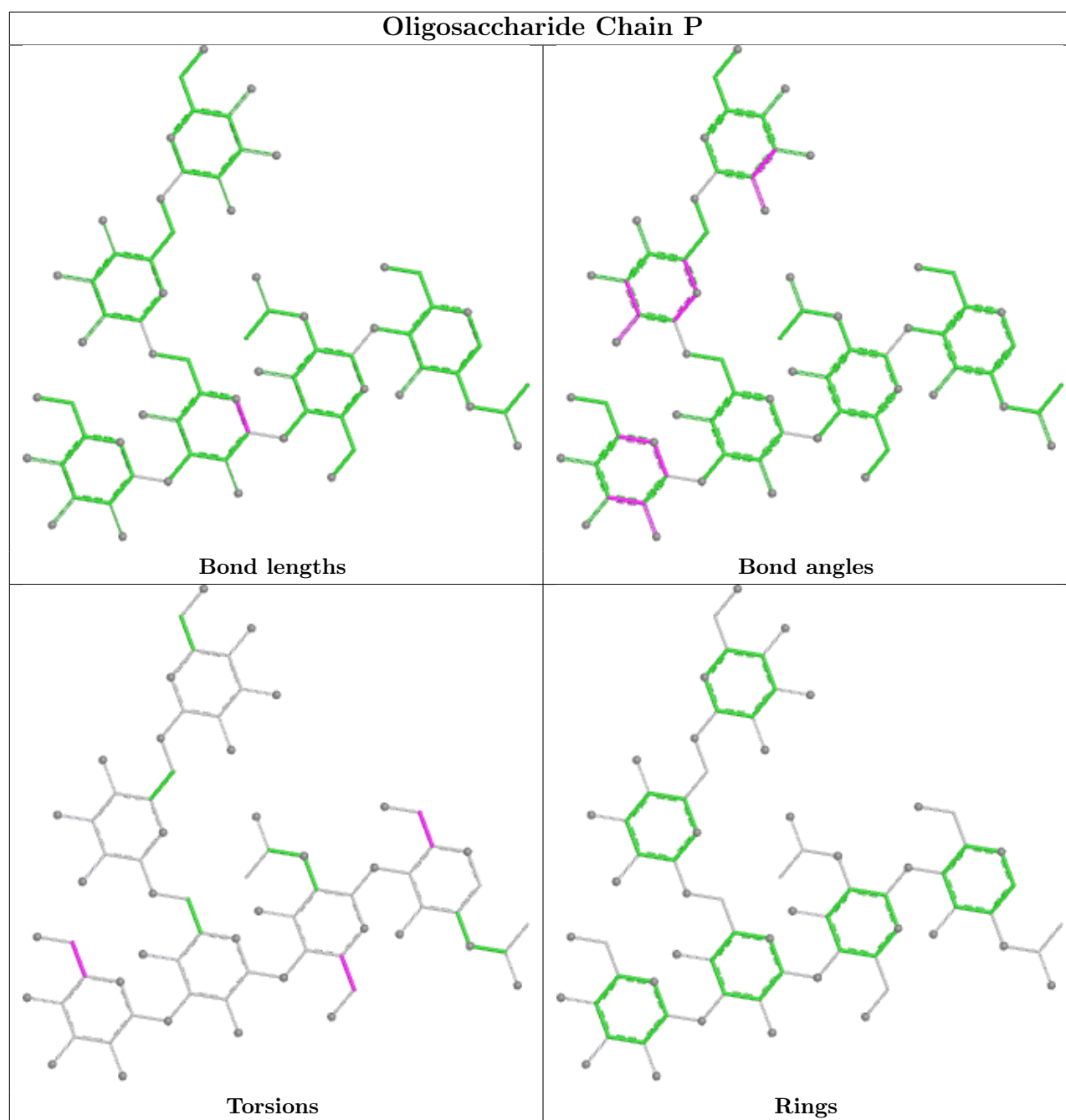


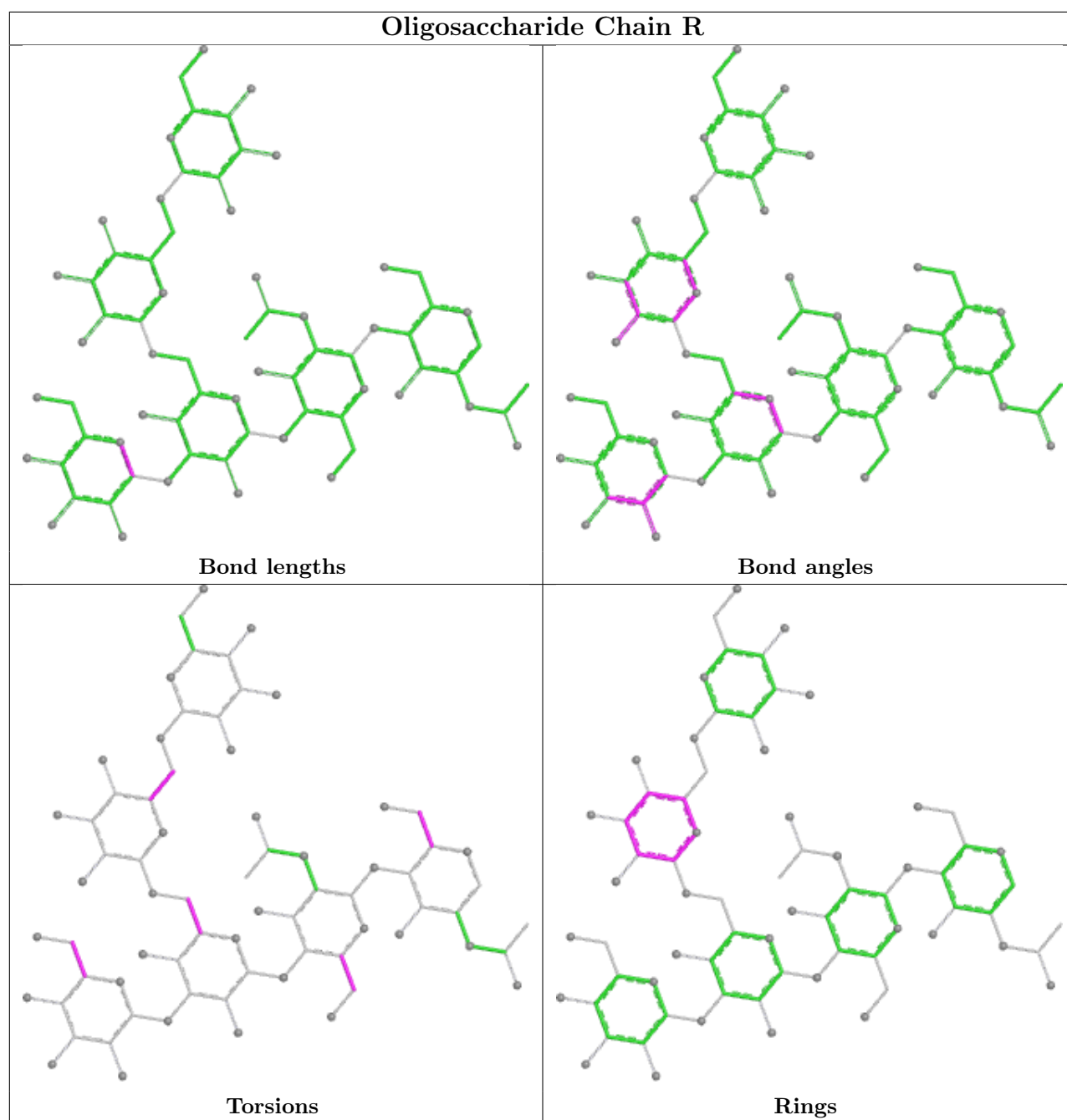


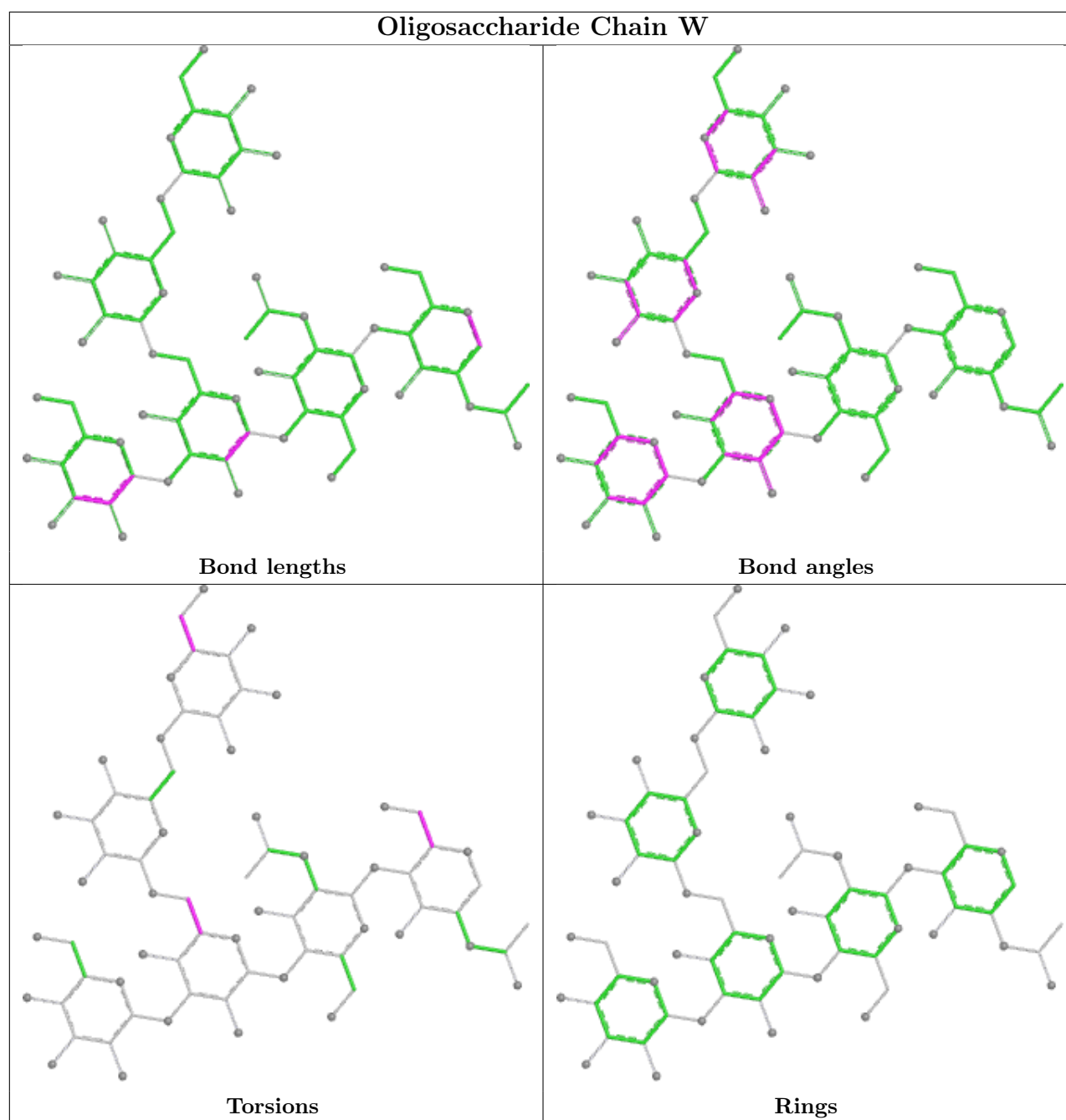


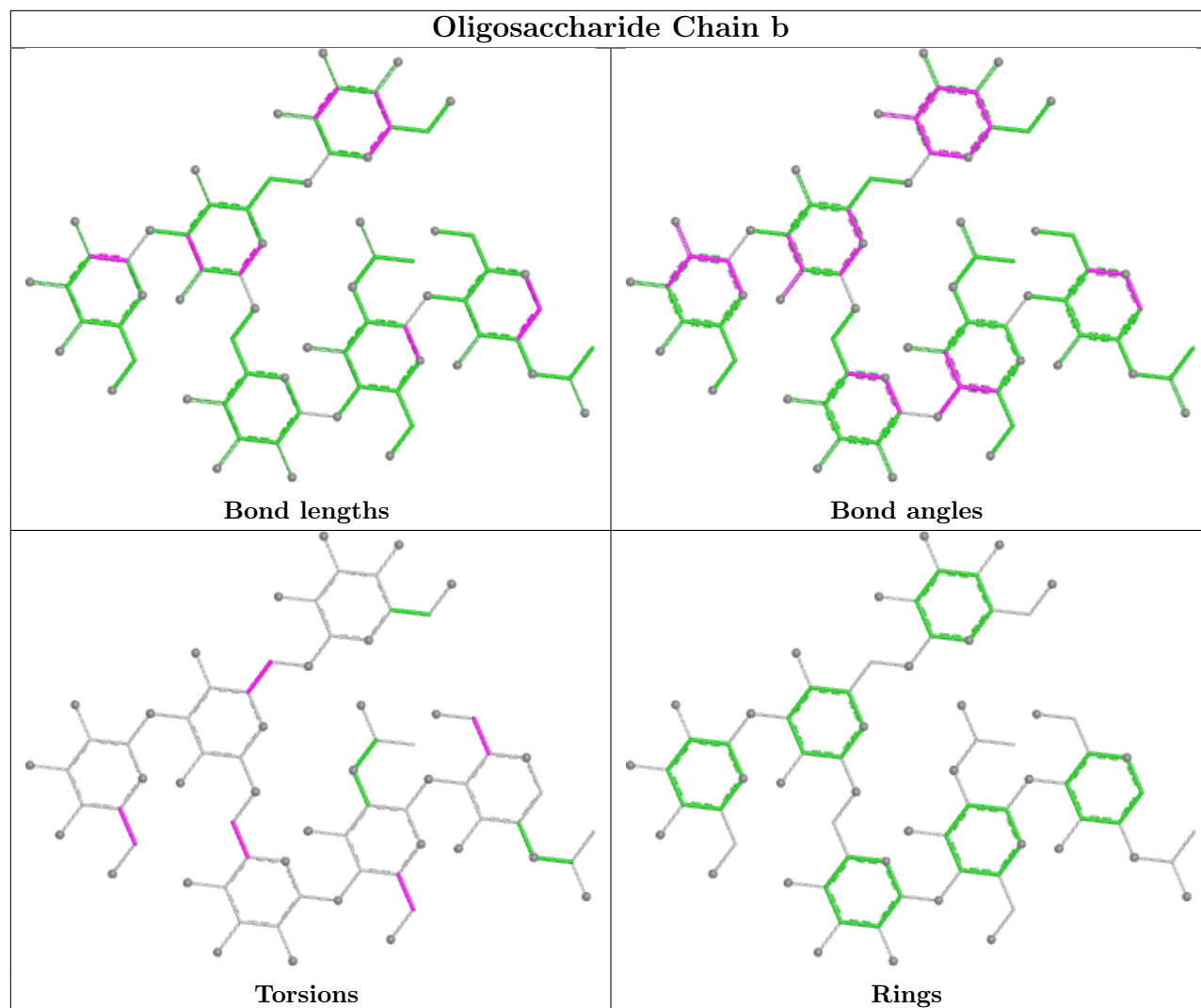


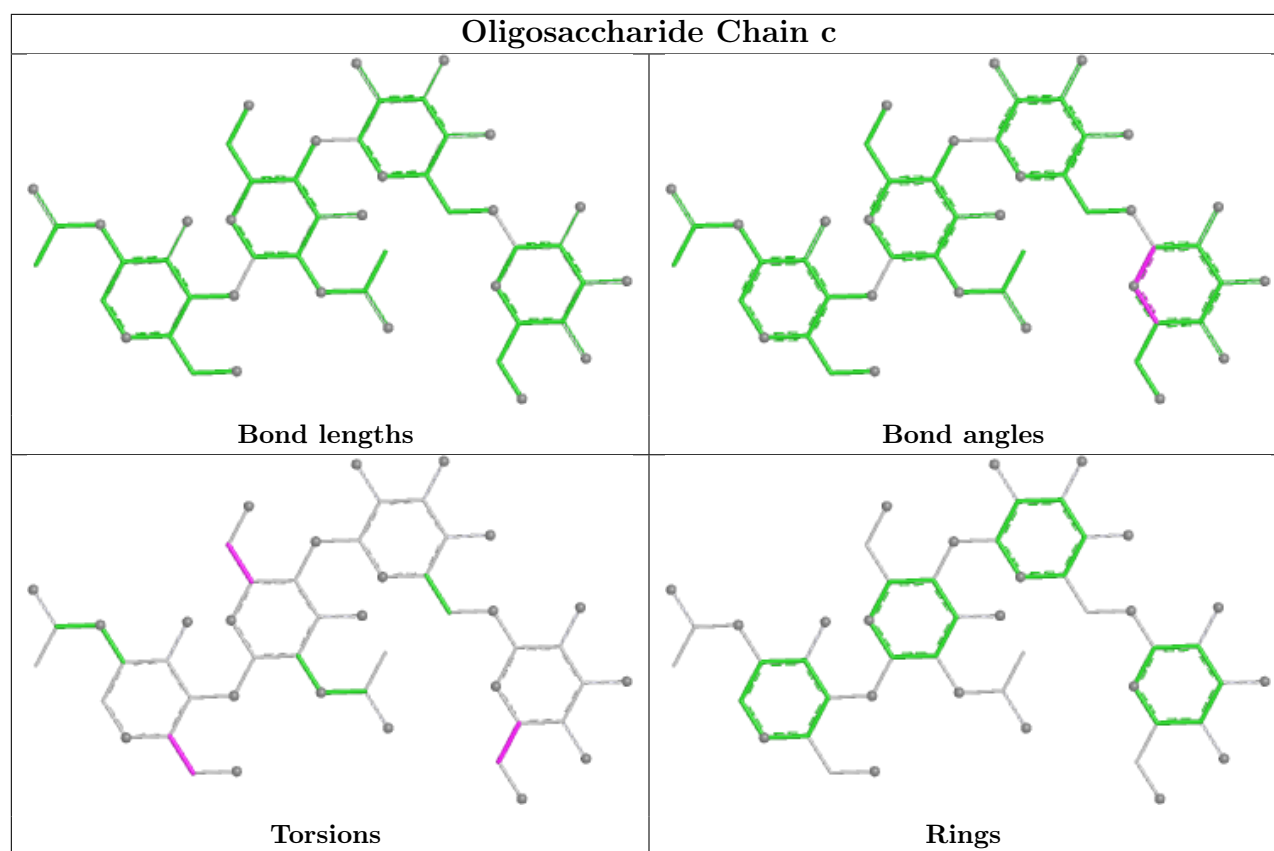












5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 24 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	MES	H	510	13	12,12,12	1.71	3 (25%)	15,16,16	1.73	4 (26%)
10	NAG	A	601	1	14,14,15	0.22	0	17,19,21	0.43	0
12	EDO	A	625	-	3,3,3	0.44	0	2,2,2	0.34	0
10	NAG	D	501	2	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
10	NAG	C	626	1	14,14,15	0.39	0	17,19,21	0.52	0
10	NAG	B	2005	2	14,14,15	0.24	0	17,19,21	0.40	0
10	NAG	E	601	-	14,14,15	0.95	1 (7%)	17,19,21	1.51	2 (11%)
12	EDO	E	625	-	3,3,3	0.42	0	2,2,2	0.40	0
12	EDO	G	2027	-	3,3,3	0.42	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EDO	H	509	-	3,3,3	0.43	0	2,2,2	0.35	0
14	MES	B	2014	13	12,12,12	1.70	2 (16%)	15,16,16	1.71	3 (20%)
10	NAG	F	501	2	14,14,15	0.18	0	17,19,21	0.39	0
10	NAG	C	601	1	14,14,15	0.29	0	17,19,21	0.48	0
10	NAG	E	624	1	14,14,15	0.30	0	17,19,21	0.50	0
12	EDO	C	628	-	3,3,3	0.42	0	2,2,2	0.40	0
14	MES	D	507	13	12,12,12	1.65	3 (25%)	15,16,16	1.76	4 (26%)
12	EDO	C	627	-	3,3,3	0.42	0	2,2,2	0.38	0
12	EDO	G	2026	-	3,3,3	0.43	0	2,2,2	0.33	0
10	NAG	G	2023	1	14,14,15	0.26	0	17,19,21	0.43	0
10	NAG	F	502	2	14,14,15	0.30	0	17,19,21	0.36	0
12	EDO	B	2013	-	3,3,3	0.44	0	2,2,2	0.39	0
12	EDO	F	509	-	3,3,3	0.44	0	2,2,2	0.34	0
10	NAG	G	2024	1	14,14,15	0.32	0	17,19,21	0.35	0
14	MES	F	510	13	12,12,12	1.63	3 (25%)	15,16,16	1.71	4 (26%)
12	EDO	C	629	-	3,3,3	0.41	0	2,2,2	0.40	0
12	EDO	G	2028	-	3,3,3	0.43	0	2,2,2	0.39	0
12	EDO	G	2025	-	3,3,3	0.43	0	2,2,2	0.35	0
10	NAG	D	502	2	14,14,15	0.78	1 (7%)	17,19,21	0.71	0
12	EDO	B	2012	-	3,3,3	0.43	0	2,2,2	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MES	H	510	13	-	3/6/14/14	0/1/1/1
10	NAG	A	601	1	-	0/6/23/26	0/1/1/1
12	EDO	A	625	-	-	0/1/1/1	-
10	NAG	D	501	2	-	3/6/23/26	0/1/1/1
10	NAG	C	626	1	-	2/6/23/26	0/1/1/1
10	NAG	B	2005	2	-	0/6/23/26	0/1/1/1
10	NAG	E	601	-	-	4/6/23/26	0/1/1/1
12	EDO	E	625	-	-	0/1/1/1	-
12	EDO	G	2027	-	-	0/1/1/1	-
12	EDO	H	509	-	-	0/1/1/1	-
14	MES	B	2014	13	-	4/6/14/14	0/1/1/1
10	NAG	F	501	2	-	0/6/23/26	0/1/1/1
10	NAG	C	601	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	E	624	1	-	2/6/23/26	0/1/1/1
12	EDO	C	628	-	-	0/1/1/1	-
14	MES	D	507	13	-	2/6/14/14	0/1/1/1
12	EDO	C	627	-	-	0/1/1/1	-
12	EDO	G	2026	-	-	0/1/1/1	-
10	NAG	G	2023	1	-	1/6/23/26	0/1/1/1
10	NAG	F	502	2	-	1/6/23/26	0/1/1/1
12	EDO	B	2013	-	-	0/1/1/1	-
12	EDO	F	509	-	-	0/1/1/1	-
10	NAG	G	2024	1	-	2/6/23/26	0/1/1/1
14	MES	F	510	13	-	0/6/14/14	0/1/1/1
12	EDO	C	629	-	-	0/1/1/1	-
12	EDO	G	2028	-	-	0/1/1/1	-
12	EDO	G	2025	-	-	0/1/1/1	-
10	NAG	D	502	2	-	3/6/23/26	0/1/1/1
12	EDO	B	2012	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2014	MES	C8-S	3.64	1.82	1.77
14	D	507	MES	C8-S	3.49	1.82	1.77
14	H	510	MES	C8-S	3.43	1.82	1.77
14	F	510	MES	C8-S	3.06	1.81	1.77
14	H	510	MES	O2S-S	2.97	1.53	1.45
14	B	2014	MES	O1S-S	2.94	1.53	1.45
14	F	510	MES	O2S-S	2.89	1.53	1.45
14	H	510	MES	O1S-S	2.70	1.52	1.45
14	D	507	MES	O1S-S	2.69	1.52	1.45
14	F	510	MES	O1S-S	2.66	1.52	1.45
10	E	601	NAG	C2-N2	-2.13	1.42	1.46
10	D	502	NAG	C1-C2	2.13	1.55	1.52
14	D	507	MES	O2S-S	2.02	1.50	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	601	NAG	C2-N2-C7	-4.00	117.53	122.90
14	F	510	MES	O3S-S-O1S	-4.00	101.39	111.40
14	B	2014	MES	O3S-S-O2S	-3.97	101.46	111.40
14	D	507	MES	O2S-S-O1S	-3.97	100.91	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	510	MES	O3S-S-O1S	-3.74	102.04	111.40
14	B	2014	MES	O2S-S-C8	3.05	111.34	106.73
14	D	507	MES	O2S-S-C8	2.95	111.19	106.73
14	H	510	MES	O1S-S-C8	2.91	111.13	106.73
14	B	2014	MES	O3S-S-C8	2.90	111.69	106.00
14	D	507	MES	O1S-S-C8	2.86	111.05	106.73
14	F	510	MES	O1S-S-C8	2.65	110.74	106.73
10	E	601	NAG	C4-C3-C2	2.64	114.89	111.02
14	H	510	MES	O3S-S-C8	2.64	111.17	106.00
14	F	510	MES	O2S-S-C8	2.46	110.44	106.73
14	F	510	MES	O3S-S-C8	2.43	110.76	106.00
14	D	507	MES	O3S-S-C8	2.31	110.53	106.00
10	D	501	NAG	C1-O5-C5	2.30	115.27	112.19
14	H	510	MES	O2S-S-C8	2.08	109.87	106.73

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	502	NAG	C1-C2-N2-C7
14	B	2014	MES	N4-C7-C8-S
14	D	507	MES	C8-C7-N4-C5
14	H	510	MES	C8-C7-N4-C5
14	H	510	MES	N4-C7-C8-S
10	E	601	NAG	C8-C7-N2-C2
10	E	601	NAG	O7-C7-N2-C2
10	C	626	NAG	O5-C5-C6-O6
10	D	501	NAG	O5-C5-C6-O6
10	C	626	NAG	C4-C5-C6-O6
10	D	502	NAG	O5-C5-C6-O6
10	D	501	NAG	C4-C5-C6-O6
10	C	601	NAG	O5-C5-C6-O6
10	E	601	NAG	O5-C5-C6-O6
14	B	2014	MES	C7-C8-S-O3S
10	E	624	NAG	O5-C5-C6-O6
10	G	2024	NAG	C4-C5-C6-O6
10	C	601	NAG	C4-C5-C6-O6
10	G	2024	NAG	O5-C5-C6-O6
10	E	601	NAG	C4-C5-C6-O6
10	D	502	NAG	C4-C5-C6-O6
10	E	624	NAG	C4-C5-C6-O6
14	B	2014	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
14	B	2014	MES	C7-C8-S-O2S
10	D	501	NAG	C3-C2-N2-C7
14	D	507	MES	C8-C7-N4-C3
10	F	502	NAG	C3-C2-N2-C7
14	H	510	MES	C8-C7-N4-C3
10	G	2023	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	510	MES	2	0
10	D	501	NAG	1	0
14	B	2014	MES	3	0
10	C	601	NAG	1	0
10	E	624	NAG	1	0
14	D	507	MES	3	0
12	G	2026	EDO	1	0
10	G	2023	NAG	2	0
10	F	502	NAG	1	0
10	G	2024	NAG	1	0
14	F	510	MES	4	0
12	G	2025	EDO	1	0
10	D	502	NAG	2	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

6.1 Protein, DNA and RNA chains

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	592/599 (98%)	0.42	21 (3%)	47	38	53, 84, 148, 191	0
1	C	595/599 (99%)	0.42	21 (3%)	47	38	55, 86, 163, 219	0
1	E	593/599 (98%)	0.63	42 (7%)	22	16	67, 109, 174, 226	0
1	G	596/599 (99%)	0.75	32 (5%)	31	25	78, 113, 166, 215	0
2	B	333/456 (73%)	0.77	29 (8%)	16	12	67, 132, 177, 244	0
2	D	312/456 (68%)	0.82	30 (9%)	13	11	66, 146, 196, 237	0
2	F	332/456 (72%)	0.92	30 (9%)	15	12	72, 139, 193, 211	0
2	H	336/456 (73%)	0.90	31 (9%)	14	11	80, 149, 199, 270	0
All	All	3689/4220 (87%)	0.66	236 (6%)	25	19	53, 111, 180, 270	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PRO	5.3
1	G	594	LEU	4.8
2	B	364	ILE	4.6
1	A	593	ILE	4.4
2	B	66	ILE	4.1
1	G	107	ALA	4.1
1	G	598	GLY	4.0
2	D	95	LEU	3.9
1	C	599	LEU	3.8
1	C	553	LEU	3.8
1	G	552	LYS	3.7
1	E	588	SER	3.6
2	H	418	LYS	3.6
1	G	593	ILE	3.6
2	D	97	VAL	3.5
2	B	72	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	328	ALA	3.5
1	A	595	LEU	3.5
1	E	487	VAL	3.5
2	F	138	PHE	3.4
1	G	562	TYR	3.3
2	H	392	VAL	3.3
1	A	594	LEU	3.2
2	H	95	LEU	3.2
1	E	512	ALA	3.2
2	D	164	ARG	3.2
2	H	174	LEU	3.2
1	G	465	PRO	3.2
1	E	543	LEU	3.2
2	B	95	LEU	3.2
2	H	331	LEU	3.2
2	B	397	CYS	3.2
1	G	512	ALA	3.2
1	E	593	ILE	3.2
1	A	566	TYR	3.2
1	C	595	LEU	3.1
1	G	553	LEU	3.0
1	C	95	GLY	3.0
1	E	587	ILE	3.0
1	E	482	ALA	3.0
1	G	446	ALA	3.0
2	F	97	VAL	3.0
1	E	464	LEU	3.0
2	F	347	LYS	3.0
2	F	174	LEU	2.9
2	D	127	VAL	2.9
1	C	594	LEU	2.9
1	E	594	LEU	2.9
2	H	115	ALA	2.9
1	C	465	PRO	2.8
1	E	61	TRP	2.8
1	E	523	SER	2.8
2	H	213	GLY	2.8
1	E	444	VAL	2.8
2	H	142	PHE	2.8
1	G	584	PRO	2.8
1	C	543	LEU	2.8
1	G	264	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	549	PHE	2.8
1	A	446	ALA	2.8
2	B	328	ALA	2.8
2	H	144	LEU	2.7
1	E	532	GLY	2.7
1	G	249	THR	2.7
2	H	358	TYR	2.7
2	D	411	ILE	2.7
2	F	318	GLY	2.7
1	A	444	VAL	2.7
1	G	468	ALA	2.7
2	D	380	VAL	2.7
2	H	137	PHE	2.7
1	G	554	THR	2.7
2	H	99	PRO	2.7
1	C	598	GLY	2.7
2	F	373	GLY	2.7
1	E	502	LYS	2.7
1	C	401	CYS	2.6
1	E	462	CYS	2.6
1	E	304	GLY	2.6
1	A	95	GLY	2.6
1	C	532	GLY	2.6
2	B	330	ASN	2.6
1	G	41	PRO	2.6
1	E	264	LEU	2.6
2	F	109	TYR	2.6
2	F	409	LYS	2.6
1	G	95	GLY	2.6
2	B	356	GLY	2.6
1	A	40	ALA	2.6
1	A	96	ALA	2.6
2	H	138	PHE	2.6
1	A	249	THR	2.6
1	C	564	LEU	2.6
1	E	542	TYR	2.6
2	H	339	TYR	2.6
2	D	372	PRO	2.6
2	F	380	VAL	2.6
2	H	329	ALA	2.6
1	C	395	TRP	2.5
1	C	556	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	543	LEU	2.5
2	D	329	ALA	2.5
2	F	137	PHE	2.5
1	C	461	THR	2.5
2	H	367	ASP	2.5
1	A	265	TYR	2.5
2	D	374	MET	2.5
2	H	349	GLN	2.5
1	G	467	THR	2.4
1	E	66	ARG	2.4
1	A	543	LEU	2.4
1	A	29	SER	2.4
2	D	318	GLY	2.4
2	D	373	GLY	2.4
2	B	97	VAL	2.4
2	D	174	LEU	2.4
2	F	76	VAL	2.4
1	C	30	ALA	2.4
1	G	105	ILE	2.4
2	B	124	LEU	2.4
2	F	411	ILE	2.4
2	F	421	ILE	2.4
2	H	381	THR	2.4
2	D	330	ASN	2.4
1	A	585	ALA	2.4
2	D	217	ALA	2.4
1	A	459	ASN	2.4
2	H	73	ASN	2.4
1	A	507	GLY	2.4
1	G	466	GLY	2.4
2	H	328	ALA	2.4
1	E	221	TYR	2.3
1	E	533	LEU	2.3
2	B	83	ILE	2.3
1	E	443	THR	2.3
1	C	517	SER	2.3
2	D	377	CYS	2.3
1	E	486	GLY	2.3
2	B	412	GLY	2.3
1	G	579	LEU	2.3
1	G	585	ALA	2.3
2	B	329	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	44	ASN	2.3
1	E	529	SER	2.3
1	E	584	PRO	2.3
1	A	598	GLY	2.3
2	H	346	VAL	2.3
2	D	137	PHE	2.3
2	F	408	ILE	2.3
1	C	592	HIS	2.3
2	F	157	TYR	2.3
2	F	99	PRO	2.3
2	H	78	PRO	2.3
2	B	85	LEU	2.3
1	G	396	ALA	2.3
2	B	320	ILE	2.3
2	D	385	GLU	2.3
1	G	44	ASN	2.3
1	E	325	ASP	2.3
1	E	553	LEU	2.3
2	H	124	LEU	2.3
1	A	541	ALA	2.2
1	C	593	ILE	2.2
2	F	181	GLY	2.2
1	E	27	VAL	2.2
1	G	130	LEU	2.2
2	B	267	LEU	2.2
1	E	585	ALA	2.2
1	A	583	THR	2.2
1	E	562	TYR	2.2
2	F	191	ASN	2.2
2	D	331	LEU	2.2
2	D	342	LEU	2.2
2	B	335	VAL	2.2
2	H	409	LYS	2.2
1	C	9	ALA	2.2
1	E	258	GLY	2.2
2	F	342	LEU	2.2
1	G	578	ILE	2.2
2	F	364	ILE	2.2
1	A	512	ALA	2.2
1	E	573	THR	2.2
2	B	416	THR	2.2
2	B	70	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	235	LYS	2.2
2	F	188	LEU	2.2
2	B	386	VAL	2.2
2	D	346	VAL	2.2
2	F	350	VAL	2.2
2	H	380	VAL	2.2
1	E	582	PHE	2.2
2	B	115	ALA	2.1
2	H	417	ALA	2.1
2	F	393	THR	2.1
2	F	78	PRO	2.1
2	F	120	ASN	2.1
1	G	533	LEU	2.1
2	D	303	GLY	2.1
1	C	305	SER	2.1
2	D	326	SER	2.1
2	F	223	VAL	2.1
2	D	413	PHE	2.1
1	E	589	ARG	2.1
1	E	554	THR	2.1
2	B	68	THR	2.1
2	H	191	ASN	2.1
1	E	566	TYR	2.1
2	B	420	HIS	2.1
2	H	421	ILE	2.1
1	C	590	GLN	2.1
2	D	135	MET	2.1
2	D	131	LEU	2.1
2	B	264	ASN	2.1
1	E	556	ILE	2.1
2	B	392	VAL	2.1
2	H	295	ILE	2.1
2	B	137	PHE	2.1
2	F	326	SER	2.1
2	B	164	ARG	2.1
1	E	564	LEU	2.1
1	G	564	LEU	2.1
2	D	110	LEU	2.1
1	E	525	ASN	2.1
1	E	364	TYR	2.1
2	D	419	ILE	2.1
2	B	82	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	221	ALA	2.0
2	F	329	ALA	2.0
1	E	509	ILE	2.0
2	D	233	GLU	2.0
2	F	142	PHE	2.0
1	G	506	LYS	2.0
1	G	508	ALA	2.0
2	H	255	ALA	2.0
2	H	369	SER	2.0
2	F	124	LEU	2.0

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	O	3	11/12	0.23	0.14	143,144,150,150	0
7	MAN	P	4	11/12	0.40	0.14	133,136,141,141	0
6	NAG	M	1	14/15	0.44	0.14	115,130,138,144	0
7	BMA	W	3	11/12	0.44	0.14	110,118,123,126	0
3	MAN	I	4	11/12	0.46	0.16	187,189,190,191	0
4	MAN	U	5	11/12	0.47	0.20	140,143,149,151	0
3	BMA	I	3	11/12	0.48	0.17	142,178,189,201	0
7	MAN	W	5	11/12	0.49	0.15	92,109,119,121	0
5	MAN	L	4	11/12	0.53	0.18	123,128,133,135	0
3	MAN	O	4	11/12	0.55	0.12	148,149,151,152	0
6	NAG	N	1	14/15	0.55	0.15	127,151,154,156	0
6	NAG	N	2	14/15	0.55	0.12	154,157,161,164	0
7	MAN	W	4	11/12	0.57	0.15	116,120,127,129	0
4	MAN	U	4	11/12	0.58	0.13	136,144,147,149	0
6	NAG	Z	2	14/15	0.58	0.11	143,150,154,157	0
6	NAG	T	2	14/15	0.59	0.12	175,180,185,186	0
3	NAG	I	2	14/15	0.59	0.17	169,174,179,181	0
5	BMA	L	3	11/12	0.60	0.14	104,108,115,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	K	3	11/12	0.60	0.12	115,122,125,126	0
5	MAN	L	5	11/12	0.60	0.16	124,131,133,134	0
3	NAG	a	1	14/15	-	-	62,81,89,90	0
3	NAG	a	2	14/15	-	-	89,99,106,115	0
3	BMA	a	3	11/12	-	-	126,133,138,142	0
3	MAN	a	4	11/12	-	-	149,157,160,165	0
3	NAG	d	1	14/15	-	-	97,120,127,128	0
3	NAG	d	2	14/15	-	-	136,141,150,150	0
3	BMA	d	3	11/12	-	-	120,127,133,135	0
3	MAN	d	4	11/12	-	-	124,127,130,130	0
4	BMA	J	3	11/12	0.60	0.12	119,125,127,128	0
7	MAN	P	6	11/12	0.61	0.11	128,130,134,136	0
4	MAN	X	5	11/12	0.61	0.14	130,134,141,142	0
7	MAN	R	5	11/12	0.62	0.16	130,131,134,135	0
7	MAN	P	5	11/12	0.62	0.16	133,135,139,142	0
7	BMA	P	3	11/12	0.62	0.13	106,117,127,130	0
7	MAN	R	4	11/12	0.62	0.17	111,113,124,128	0
6	NAG	M	2	14/15	0.64	0.12	153,159,169,172	0
3	BMA	Q	3	11/12	0.64	0.17	136,142,143,143	0
6	NAG	V	2	14/15	0.65	0.14	114,121,128,130	0
7	MAN	W	6	11/12	0.65	0.11	113,118,122,126	0
4	MAN	J	4	11/12	0.67	0.11	131,137,142,142	0
3	NAG	S	2	14/15	0.67	0.15	116,119,124,130	0
3	NAG	K	2	14/15	0.67	0.17	116,122,125,131	0
3	BMA	S	3	11/12	0.68	0.13	108,111,118,121	0
6	NAG	Y	2	14/15	0.69	0.13	135,140,144,148	0
3	MAN	S	4	11/12	0.69	0.12	78,96,105,106	0
5	MAN	L	6	11/12	0.69	0.14	101,106,114,116	0
4	MAN	X	4	11/12	0.71	0.14	108,111,114,116	0
3	NAG	O	2	14/15	0.71	0.13	130,134,142,148	0
3	NAG	K	1	14/15	0.72	0.13	82,94,109,110	0
7	MAN	R	6	11/12	0.72	0.13	114,117,125,127	0
3	MAN	Q	4	11/12	0.72	0.16	142,144,145,147	0
6	NAG	V	1	14/15	0.73	0.12	93,106,119,120	0
3	NAG	Q	2	14/15	0.74	0.17	110,118,130,138	0
6	NAG	T	1	14/15	0.74	0.12	146,163,166,171	0
3	NAG	S	1	14/15	0.74	0.16	94,108,115,116	0
6	NAG	Z	1	14/15	0.74	0.12	124,136,138,139	0
7	BMA	R	3	11/12	0.76	0.12	98,103,109,111	0
4	BMA	U	3	11/12	0.76	0.14	113,124,133,137	0
4	NAG	X	1	14/15	0.78	0.16	87,106,114,114	0
4	MAN	J	5	11/12	0.78	0.10	111,114,116,118	0

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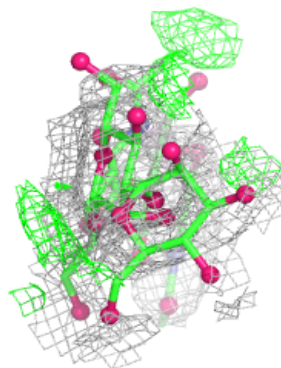
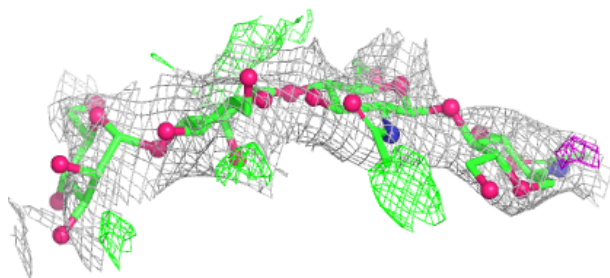
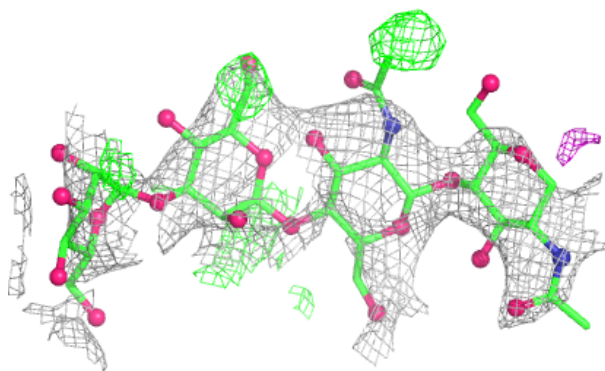
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	K	4	11/12	0.79	0.10	75,91,104,105	0
6	NAG	e	1	14/15	-	-	128,147,150,156	0
6	NAG	e	2	14/15	-	-	157,165,176,176	0
6	NAG	f	1	14/15	-	-	143,159,177,178	0
6	NAG	f	2	14/15	-	-	165,166,177,178	0
6	NAG	g	1	14/15	-	-	126,146,152,161	0
6	NAG	g	2	14/15	-	-	161,168,174,175	0
4	BMA	X	3	11/12	0.80	0.13	106,117,121,125	0
4	NAG	J	2	14/15	0.80	0.14	99,105,115,120	0
3	NAG	O	1	14/15	0.83	0.16	102,124,127,132	0
3	NAG	Q	1	14/15	0.84	0.12	65,79,89,105	0
7	NAG	R	2	14/15	0.84	0.14	63,76,83,90	0
4	NAG	X	2	14/15	0.85	0.13	117,120,122,124	0
7	NAG	W	1	14/15	0.85	0.12	62,77,80,86	0
7	NAG	P	2	14/15	0.86	0.10	87,93,97,101	0
5	NAG	L	2	14/15	0.86	0.14	80,84,88,96	0
3	NAG	I	1	14/15	0.86	0.16	122,139,150,159	0
7	NAG	W	2	14/15	0.87	0.10	70,84,91,100	0
4	NAG	U	2	14/15	0.88	0.13	81,86,96,102	0
7	NAG	P	1	14/15	0.88	0.13	55,75,81,82	0
4	NAG	U	1	14/15	0.89	0.16	53,69,82,82	0
6	NAG	Y	1	14/15	0.89	0.13	106,129,133,138	0
7	NAG	R	1	14/15	0.91	0.10	46,58,68,71	0
4	NAG	J	1	14/15	0.91	0.13	52,70,78,84	0
5	NAG	L	1	14/15	0.95	0.09	51,60,67,76	0
8	NAG	b	1	14/15	-	-	87,107,115,129	0
8	NAG	b	2	14/15	-	-	141,145,153,156	0
8	BMA	b	3	11/12	-	-	144,148,156,159	0
8	MAN	b	4	11/12	-	-	157,161,164,165	0
8	MAN	b	5	11/12	-	-	156,159,161,163	0
8	MAN	b	6	11/12	-	-	155,160,164,164	0
9	NAG	c	1	14/15	-	-	56,67,71,75	0
9	NAG	c	2	14/15	-	-	58,74,83,91	0
9	BMA	c	3	11/12	-	-	94,100,106,110	0
9	MAN	c	4	11/12	-	-	109,113,116,117	0

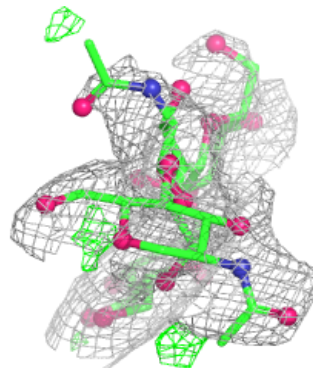
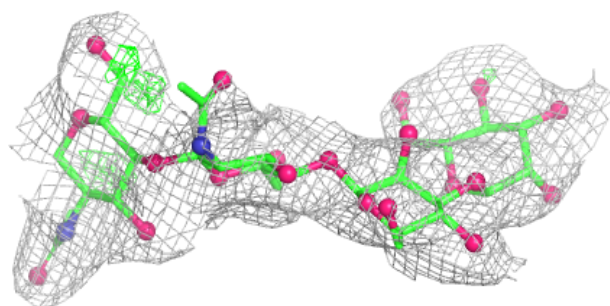
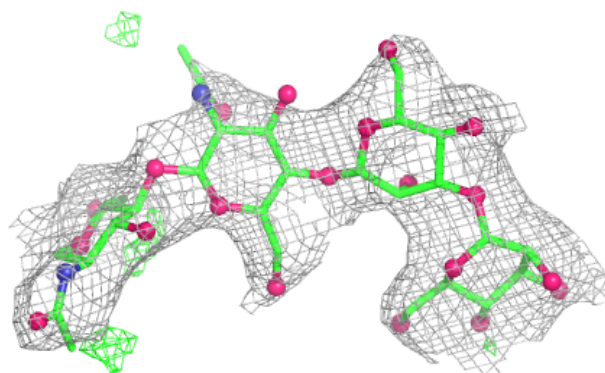
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

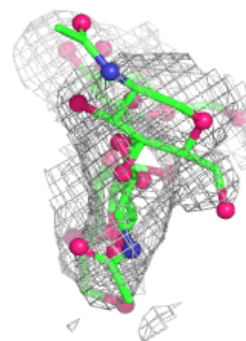
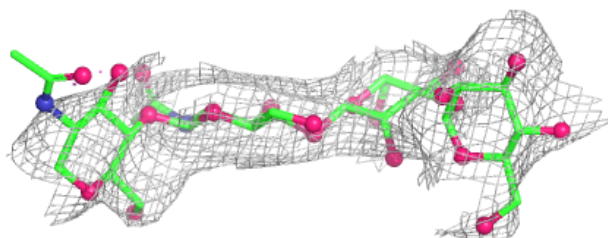
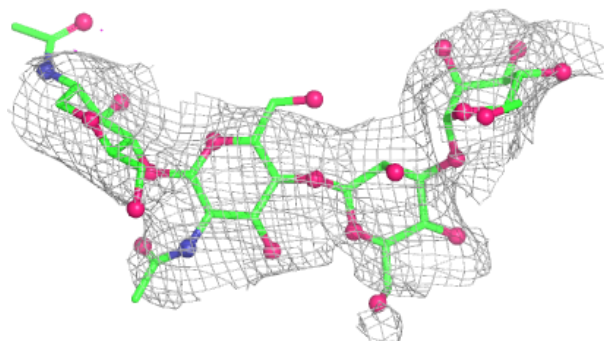
**Electron density around Chain K:**

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

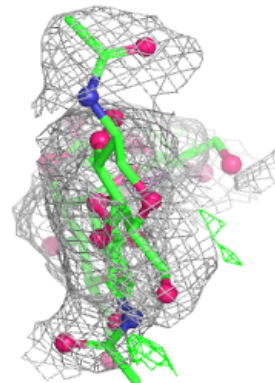
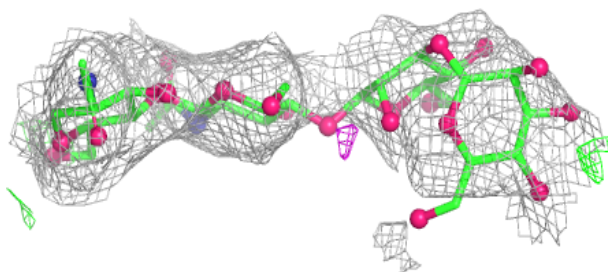
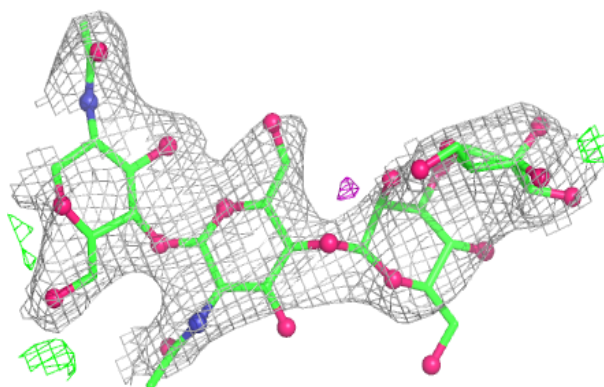


Electron density around Chain O:

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

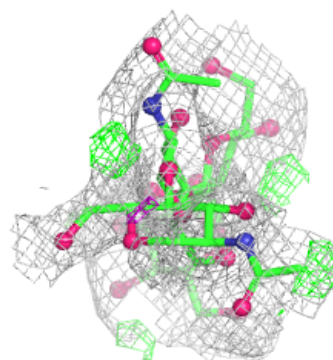
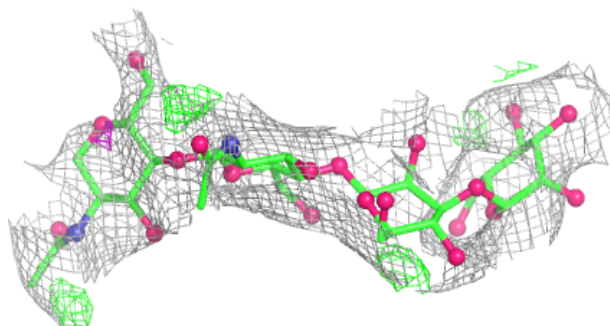
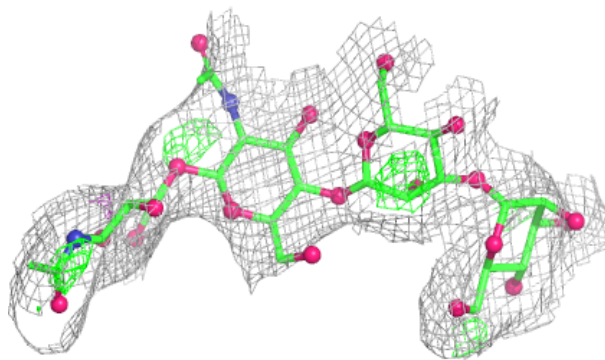
**Electron density around Chain Q:**

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

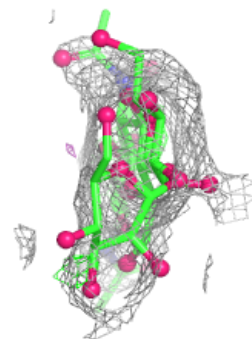
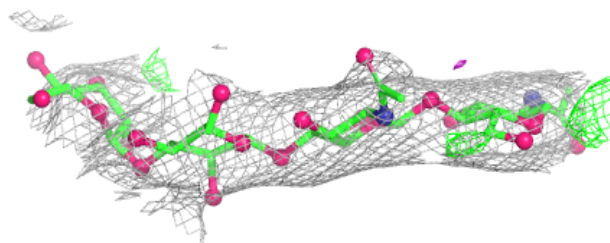
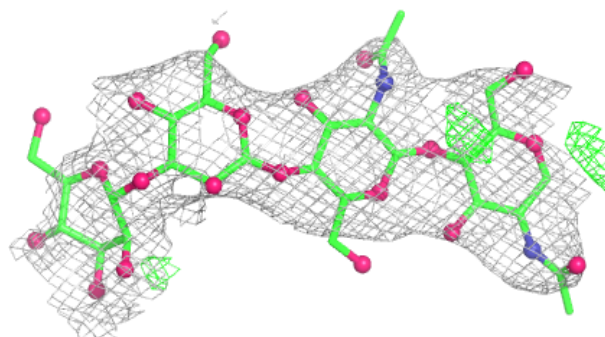


Electron density around Chain S:

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

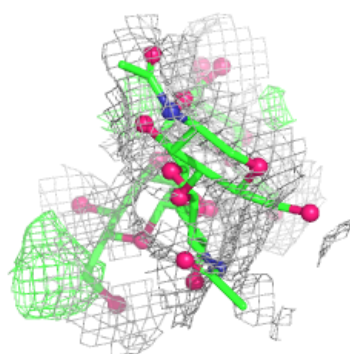
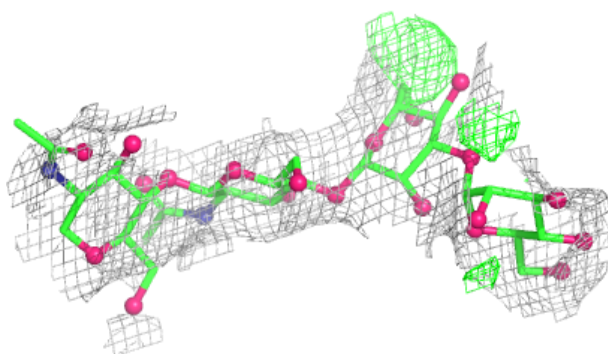
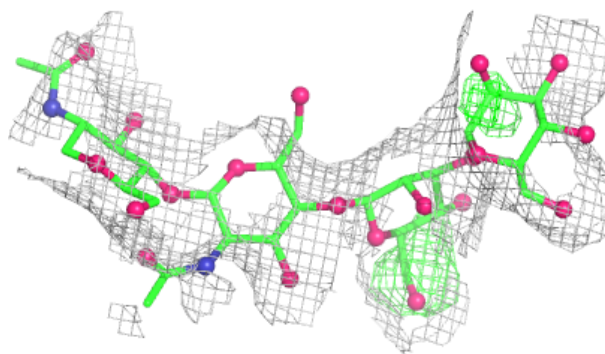
**Electron density around Chain a:**

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

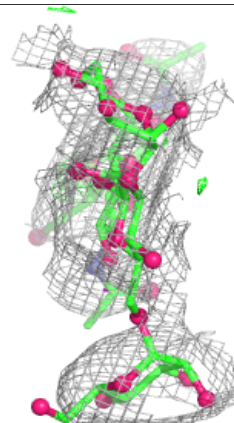
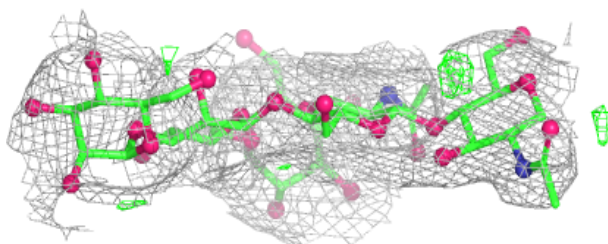
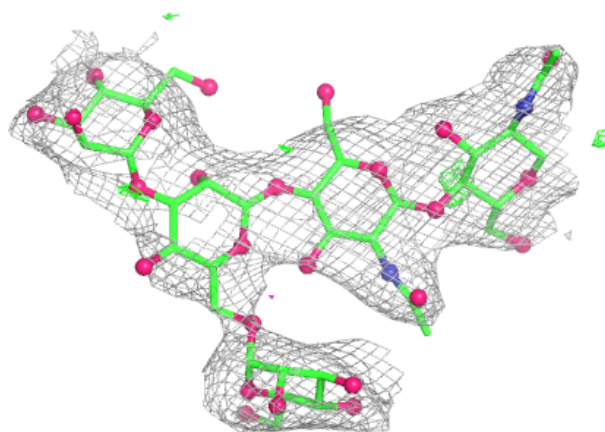


Electron density around Chain d:

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

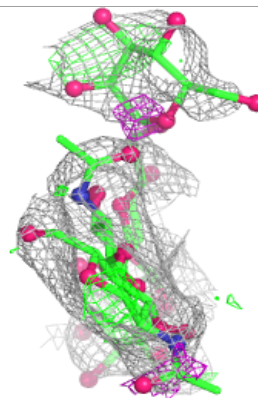
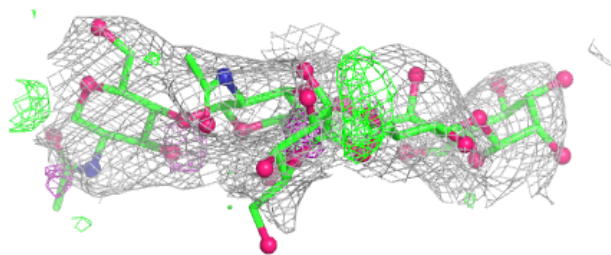
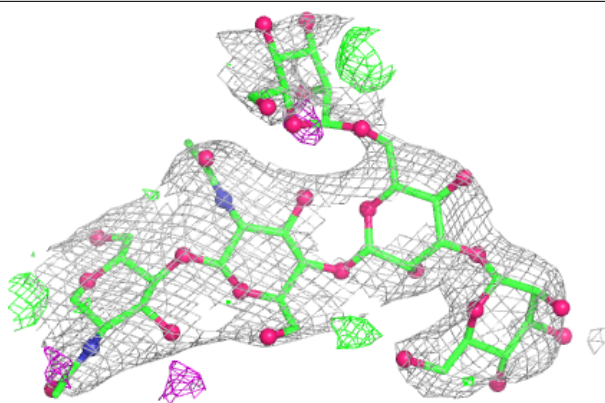
**Electron density around Chain J:**

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



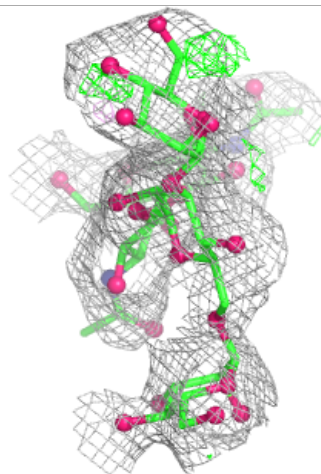
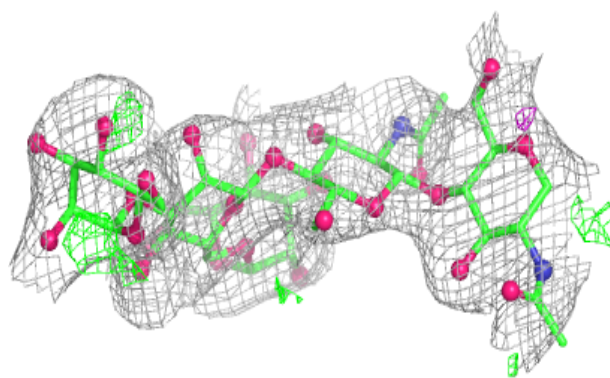
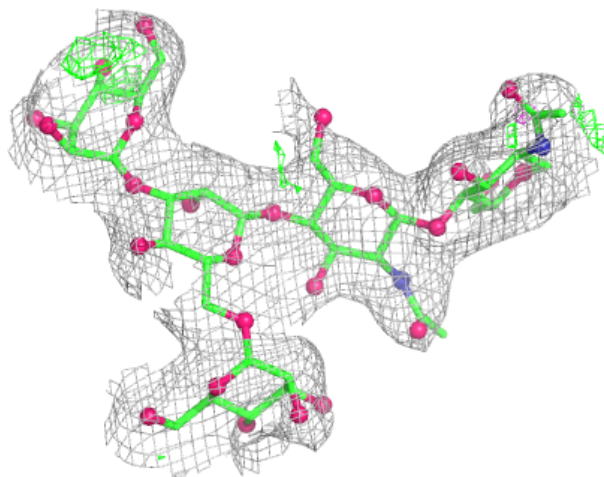
Electron density around Chain U:

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



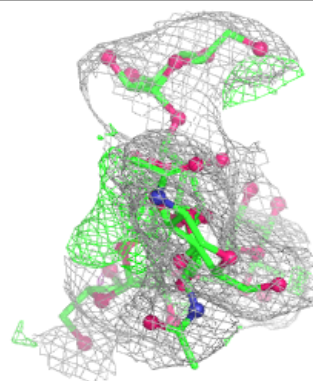
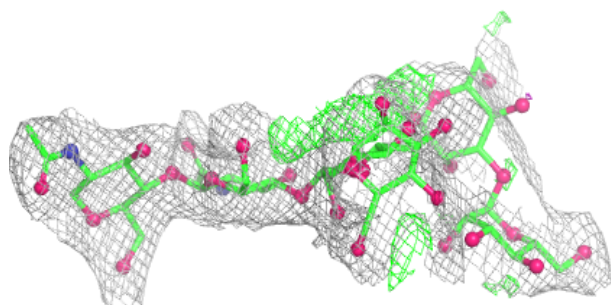
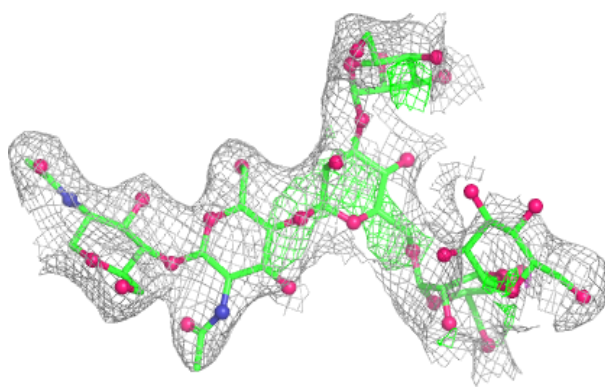
Electron density around Chain X:

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

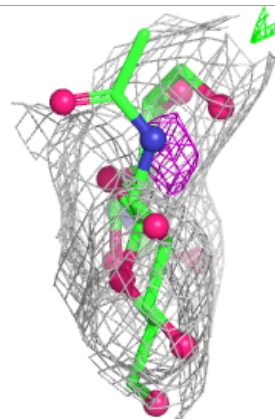
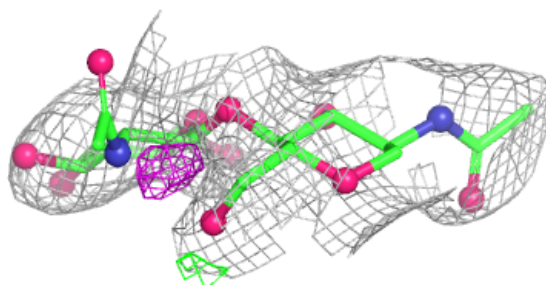
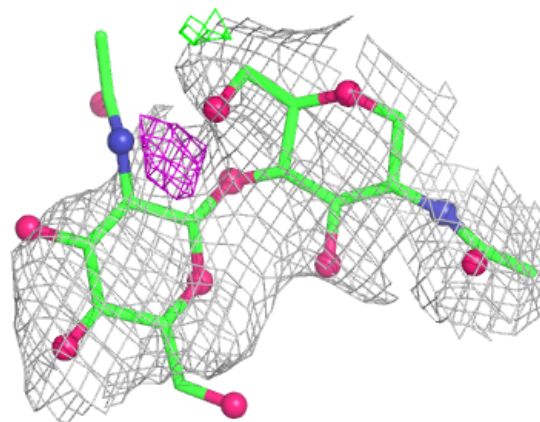


Electron density around Chain L:

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

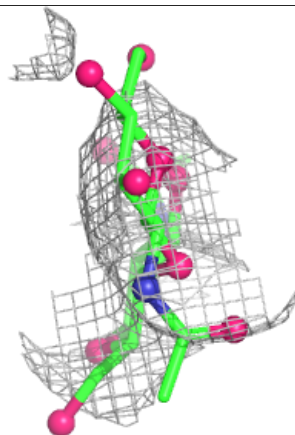
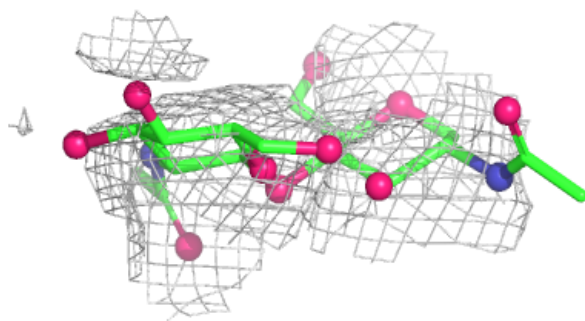
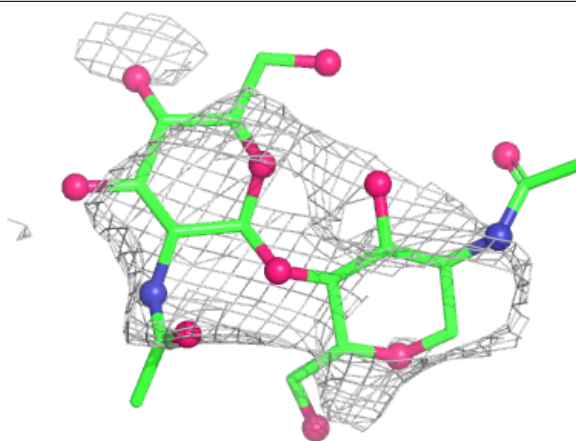
**Electron density around Chain M:**

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



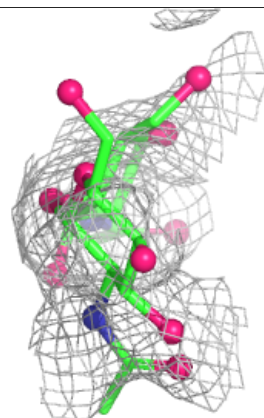
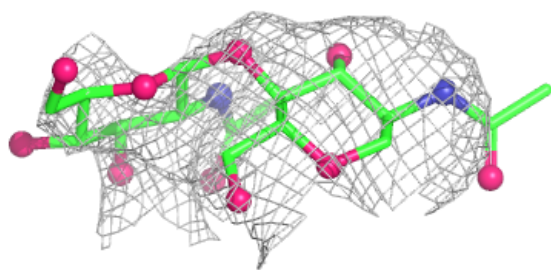
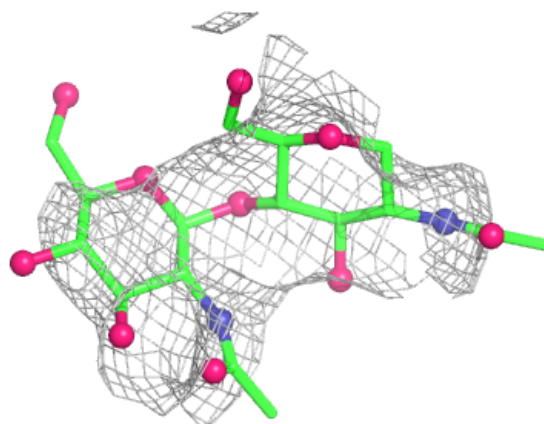
Electron density around Chain N:

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

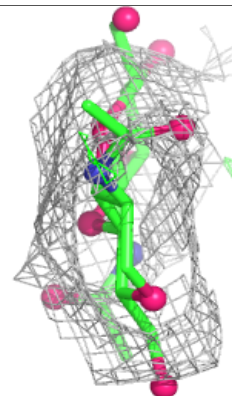
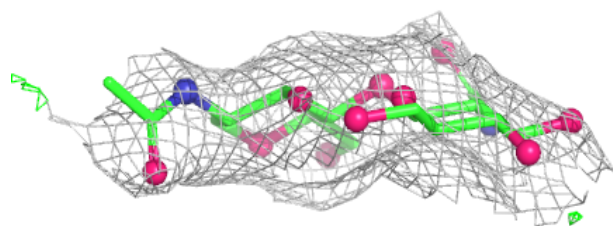
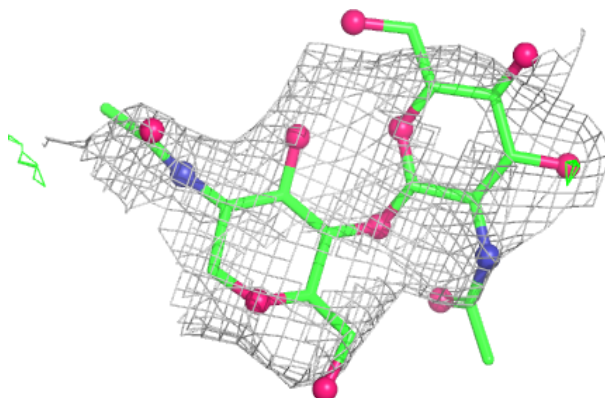


Electron density around Chain T:

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

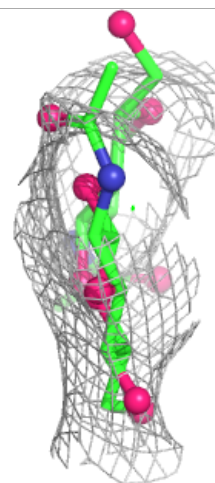
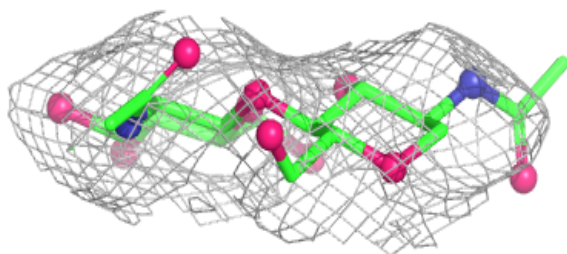
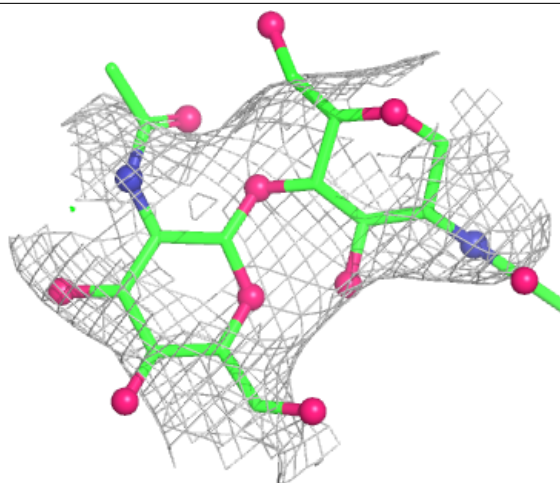
**Electron density around Chain V:**

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



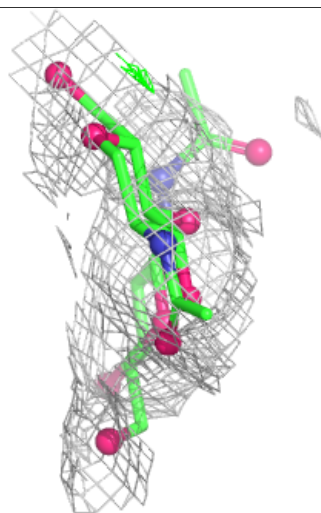
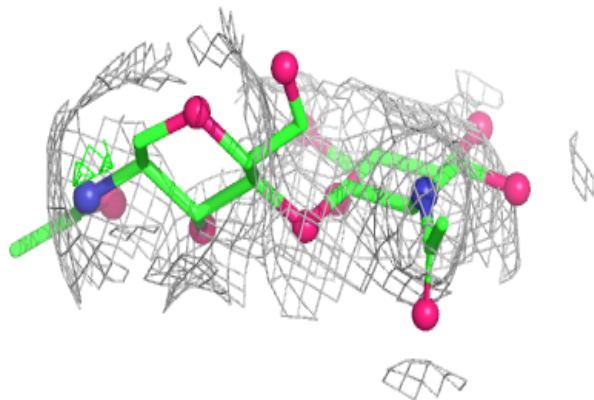
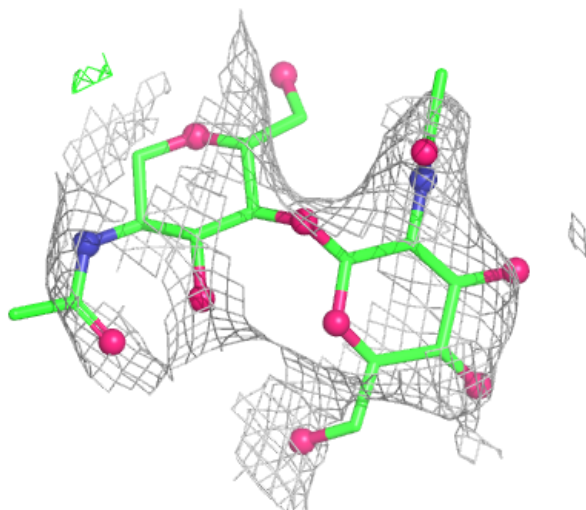
Electron density around Chain Y:

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



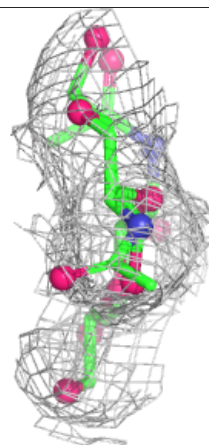
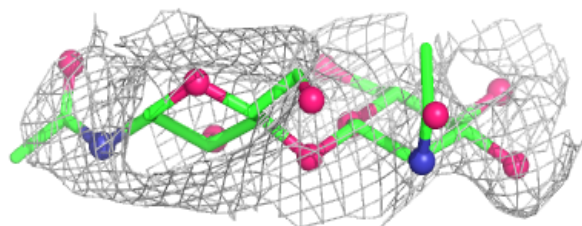
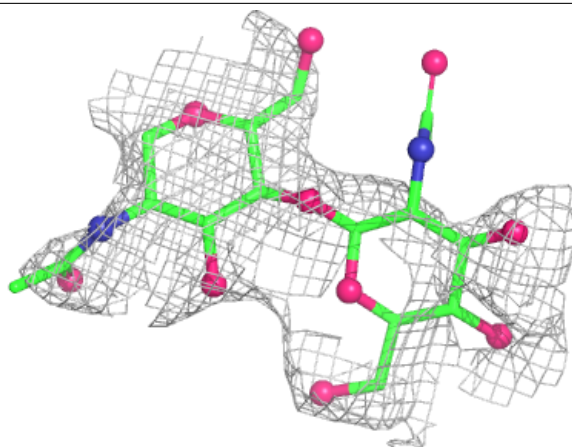
Electron density around Chain Z:

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



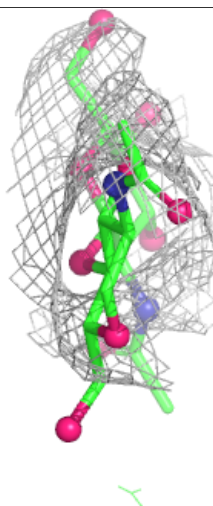
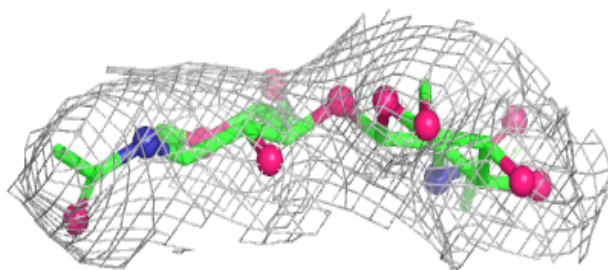
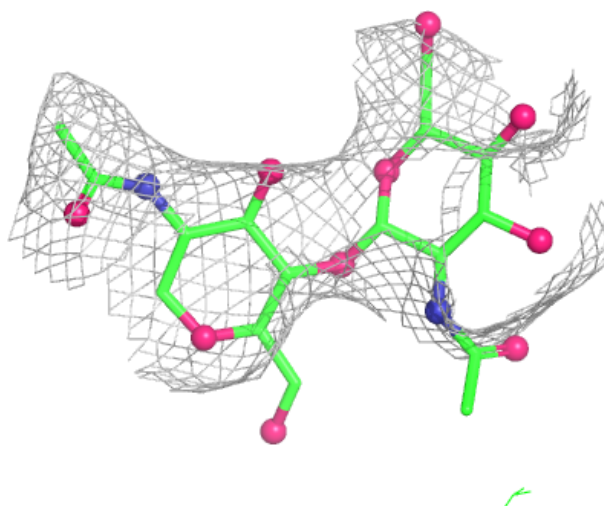
Electron density around Chain e:

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



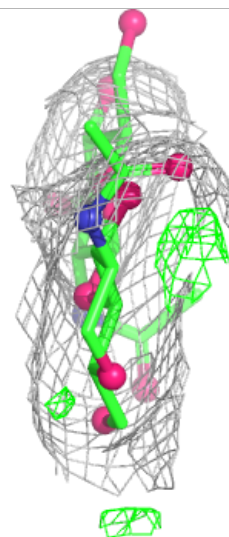
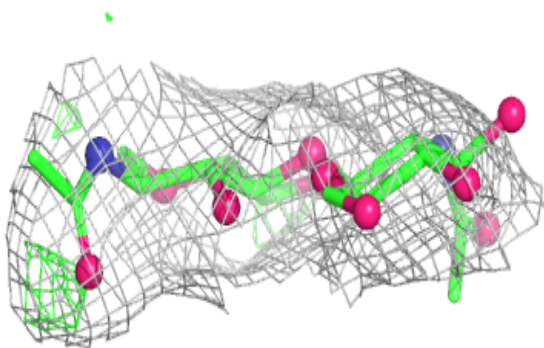
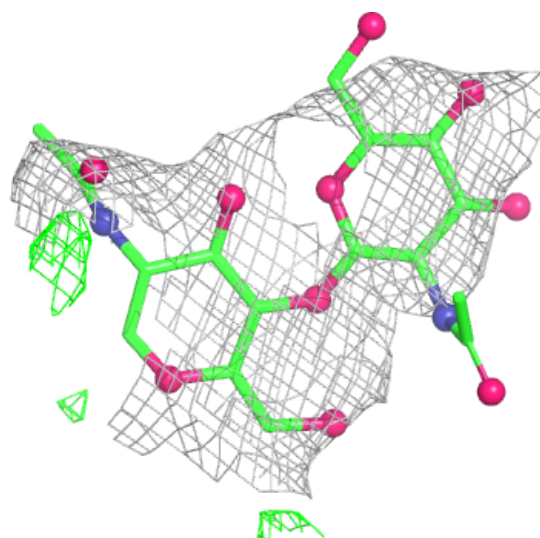
Electron density around Chain f:

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



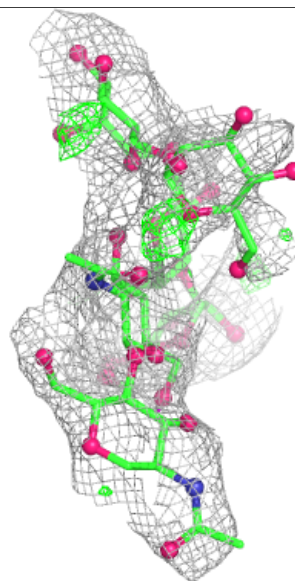
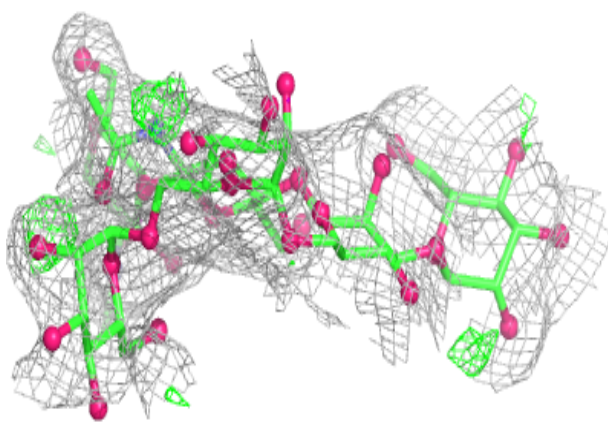
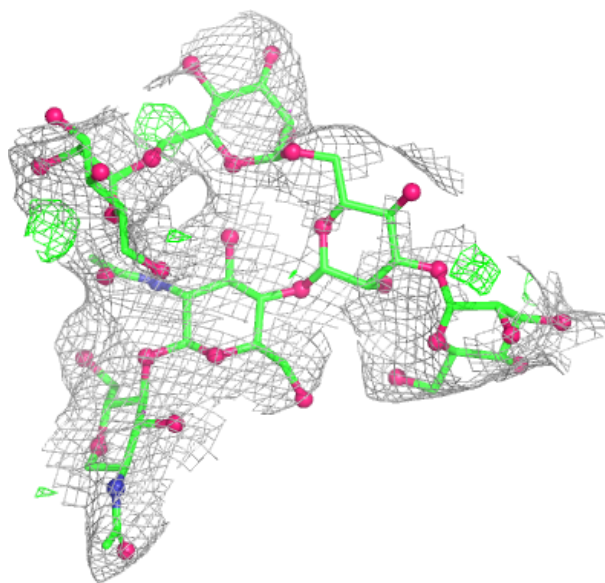
Electron density around Chain g:

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



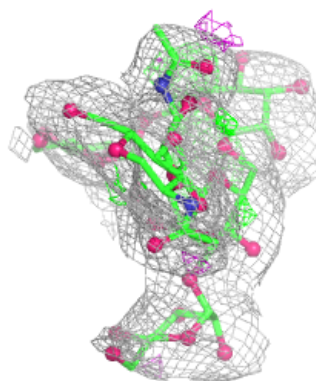
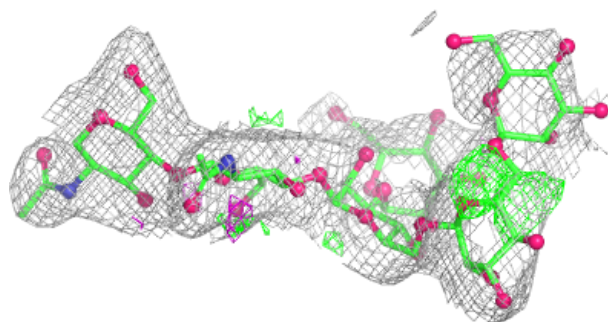
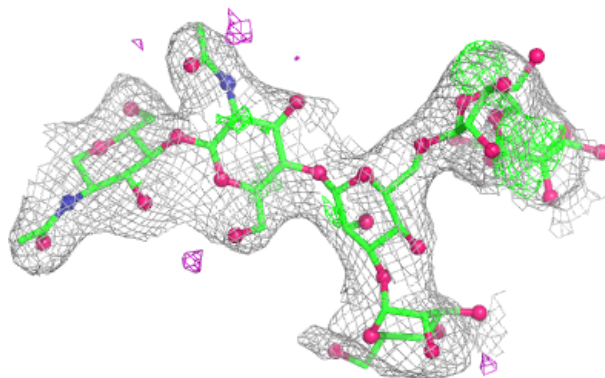
Electron density around Chain P:

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

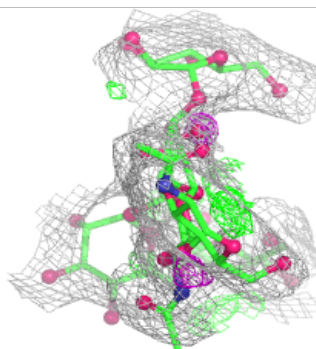
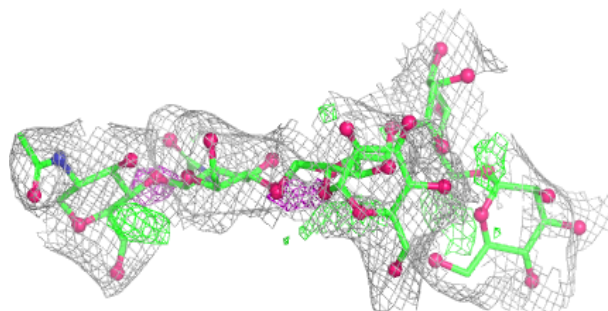
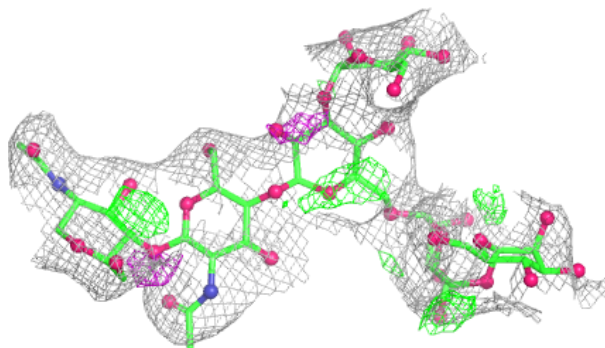


Electron density around Chain R:

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

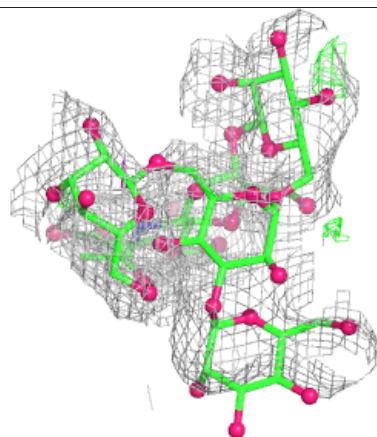
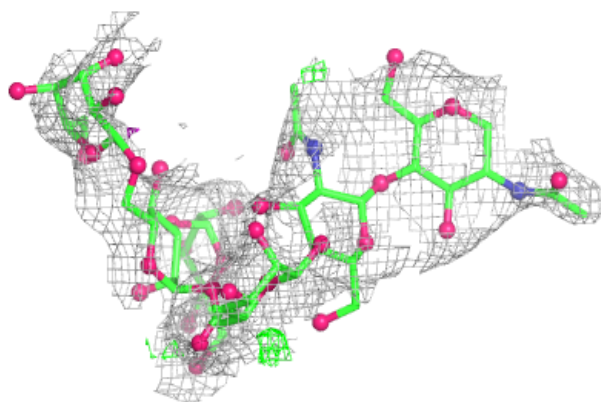
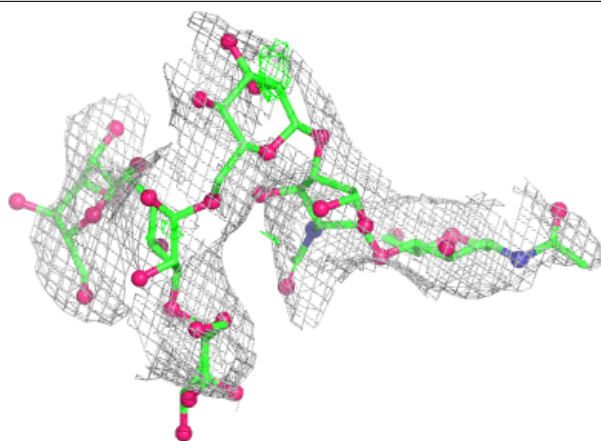
**Electron density around Chain W:**

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

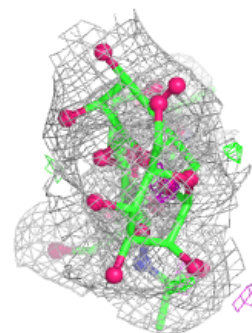
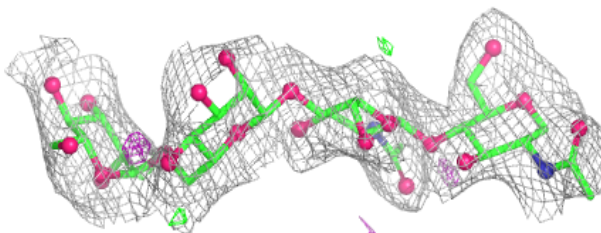
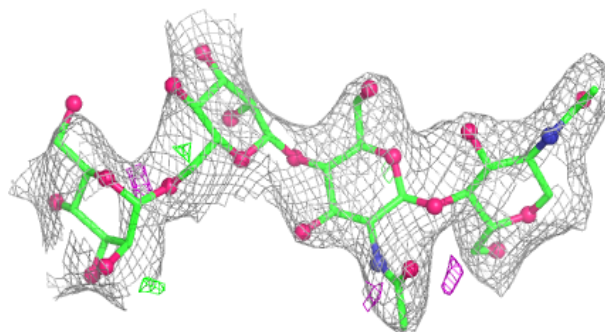


Electron density around Chain b:

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

**Electron density around Chain c:**

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	G	2023	14/15	0.04	0.20	125,140,148,155	0
12	EDO	B	2012	4/4	0.42	0.17	82,83,84,85	0
10	NAG	C	601	14/15	0.44	0.14	111,129,131,131	0
10	NAG	E	624	14/15	0.49	0.16	111,128,144,145	0
10	NAG	G	2024	14/15	0.50	0.17	140,153,166,169	0
10	NAG	F	501	14/15	0.52	0.18	125,142,159,163	0
10	NAG	D	501	14/15	0.54	0.15	134,158,162,162	0
10	NAG	D	502	14/15	0.55	0.11	118,133,138,141	0
12	EDO	F	509	4/4	0.56	0.18	95,97,98,99	0
10	NAG	A	601	14/15	0.57	0.14	95,105,115,118	0
12	EDO	C	627	4/4	0.60	0.15	89,90,90,92	0
10	NAG	C	626	14/15	0.63	0.15	113,129,138,138	0
12	EDO	G	2028	4/4	0.67	0.18	85,88,89,90	0
10	NAG	B	2005	14/15	0.68	0.09	103,123,133,135	0
12	EDO	G	2027	4/4	0.68	0.13	84,86,89,91	0
12	EDO	C	628	4/4	0.68	0.19	86,88,93,97	0
12	EDO	H	509	4/4	0.72	0.11	95,98,102,105	0
12	EDO	A	625	4/4	0.73	0.15	80,82,82,83	0
10	NAG	F	502	14/15	0.77	0.11	118,136,146,146	0
12	EDO	G	2026	4/4	0.78	0.13	88,89,92,94	0
14	MES	D	507	12/12	0.83	0.15	82,91,100,100	0
12	EDO	C	629	4/4	0.87	0.15	85,85,85,86	0
10	NAG	E	601	14/15	0.89	0.28	20,20,20,20	0
14	MES	F	510	12/12	0.89	0.14	89,99,109,111	0
14	MES	B	2014	12/12	0.90	0.13	73,103,110,111	0
12	EDO	E	625	4/4	0.91	0.10	58,59,63,67	0
13	MG	F	505	1/1	0.92	0.08	82,82,82,82	0
12	EDO	G	2025	4/4	0.92	0.11	78,80,80,80	0
14	MES	H	510	12/12	0.92	0.10	75,89,91,91	0
12	EDO	B	2013	4/4	0.95	0.14	62,65,66,68	0
13	MG	D	503	1/1	0.96	0.06	66,66,66,66	0
11	CA	D	504	1/1	0.96	0.07	60,60,60,60	0
11	CA	E	603	1/1	0.96	0.05	84,84,84,84	0
11	CA	E	604	1/1	0.96	0.07	98,98,98,98	0
11	CA	B	2002	1/1	0.96	0.05	77,77,77,77	0
13	MG	B	2001	1/1	0.96	0.05	57,57,57,57	0
11	CA	G	2001	1/1	0.97	0.06	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CA	G	2002	1/1	0.97	0.05	61,61,61,61	0
11	CA	E	605	1/1	0.97	0.05	102,102,102,102	0
13	MG	H	505	1/1	0.97	0.05	60,60,60,60	0
11	CA	A	609	1/1	0.98	0.04	55,55,55,55	0
11	CA	F	506	1/1	0.98	0.08	53,53,53,53	0
11	CA	A	607	1/1	0.98	0.05	54,54,54,54	0
11	CA	C	604	1/1	0.98	0.04	69,69,69,69	0
11	CA	G	2003	1/1	0.98	0.05	63,63,63,63	0
11	CA	G	2004	1/1	0.98	0.04	83,83,83,83	0
11	CA	H	506	1/1	0.98	0.05	68,68,68,68	0
11	CA	C	602	1/1	0.99	0.02	62,62,62,62	0
11	CA	C	603	1/1	0.99	0.04	56,56,56,56	0
11	CA	A	606	1/1	0.99	0.05	61,61,61,61	0
11	CA	C	605	1/1	0.99	0.05	58,58,58,58	0
11	CA	A	608	1/1	0.99	0.02	44,44,44,44	0
11	CA	E	602	1/1	0.99	0.03	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.