



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:57 AM BST

PDB ID : 4NCO  
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122  
Authors : Julien, J.-P.; Stanfield, R.L.; Lyumkis, D.; Ward, A.B.; Wilson, I.A.  
Deposited on : 2013-10-24  
Resolution : 4.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

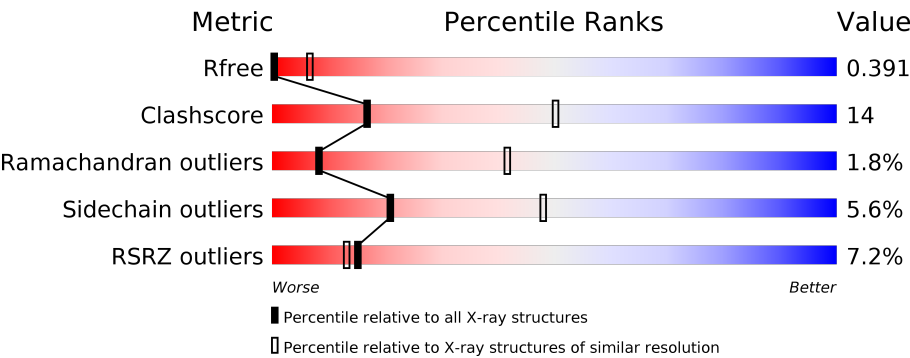
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.70 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))
$R_{free}$	130704	1085 (5.58-3.80)
Clashscore	141614	1159 (5.60-3.80)
Ramachandran outliers	138981	1094 (5.58-3.80)
Sidechain outliers	138945	1074 (5.58-3.80)
RSRZ outliers	127900	1118 (5.70-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	475	<div><div>3%</div><div><div></div><div>51%</div><div>33%</div><div>5%</div><div>12%</div></div></div>
1	E	475	<div><div>4%</div><div><div></div><div>51%</div><div>33%</div><div>5%</div><div>12%</div></div></div>
1	I	475	<div><div>3%</div><div><div></div><div>51%</div><div>33%</div><div>5%</div><div>12%</div></div></div>
2	B	78	<div><div></div><div><div></div><div>95%</div><div></div><div></div><div></div></div><div></div></div>
2	F	78	<div><div></div><div><div></div><div>95%</div><div></div><div></div><div></div></div><div></div></div>
2	J	78	<div><div></div><div><div></div><div>92%</div><div></div><div></div><div>6%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	C	211	
3	G	211	
3	K	211	
4	D	235	
4	H	235	
4	L	235	
5	M	7	
5	N	7	
5	O	7	
5	P	7	
5	S	7	
5	T	7	
5	U	7	
5	V	7	
5	Y	7	
5	Z	7	
5	a	7	
5	b	7	
6	Q	9	
6	W	9	
6	c	9	
7	R	2	
7	X	2	
7	d	2	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	M	1	-	-	-	X
5	NAG	M	2	-	-	-	X
5	BMA	M	3	-	-	-	X
5	MAN	M	4	-	-	-	X
5	MAN	M	5	-	-	-	X
5	MAN	M	6	-	-	-	X
5	MAN	M	7	-	-	-	X
5	BMA	N	3	-	-	-	X
5	MAN	N	4	-	-	-	X
5	MAN	N	5	-	-	-	X
5	MAN	N	6	-	-	-	X
5	MAN	N	7	-	-	-	X
5	NAG	O	1	-	-	-	X
5	MAN	O	4	-	-	-	X
5	MAN	O	5	-	-	-	X
5	MAN	O	6	-	-	-	X
5	BMA	P	3	-	-	-	X
5	MAN	P	4	-	-	-	X
5	MAN	P	5	-	-	-	X
5	MAN	P	6	-	-	-	X
5	MAN	P	7	-	-	-	X
5	NAG	S	1	-	-	-	X
5	NAG	S	2	-	-	-	X
5	BMA	S	3	-	-	-	X
5	MAN	S	4	-	-	-	X
5	MAN	S	5	-	-	-	X
5	MAN	S	6	-	-	-	X
5	MAN	S	7	-	-	-	X
5	MAN	T	4	-	-	-	X
5	MAN	T	5	-	-	-	X
5	MAN	T	6	-	-	-	X
5	MAN	T	7	-	-	-	X
5	NAG	U	1	-	-	-	X
5	NAG	U	2	-	-	-	X
5	MAN	U	4	-	-	-	X
5	MAN	U	5	-	-	-	X
5	MAN	U	6	-	-	-	X
5	MAN	V	4	-	-	-	X
5	MAN	V	5	-	-	-	X
5	MAN	V	6	-	-	-	X
5	NAG	Y	1	-	-	-	X
5	NAG	Y	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	Y	3	-	-	-	X
5	MAN	Y	4	-	-	-	X
5	MAN	Y	5	-	-	-	X
5	MAN	Y	6	-	-	-	X
5	MAN	Y	7	-	-	-	X
5	BMA	Z	3	-	-	-	X
5	MAN	Z	4	-	-	-	X
5	MAN	Z	5	-	-	-	X
5	MAN	Z	7	-	-	-	X
5	NAG	a	1	-	-	-	X
5	MAN	a	4	-	-	-	X
5	MAN	a	5	-	-	-	X
5	MAN	a	6	-	-	-	X
5	NAG	b	2	-	-	-	X
5	MAN	b	4	-	-	-	X
5	MAN	b	5	-	-	-	X
5	MAN	b	6	-	-	-	X
6	NAG	Q	1	-	-	-	X
6	MAN	Q	6	-	-	-	X
6	MAN	W	4	-	-	-	X
6	MAN	W	6	-	-	-	X
6	MAN	W	7	-	-	-	X
6	MAN	W	8	-	-	-	X
6	MAN	c	4	-	-	-	X
6	MAN	c	6	-	-	-	X
6	MAN	c	7	-	-	-	X
6	MAN	c	9	-	-	-	X
7	MAN	R	1	-	-	-	X
7	MAN	R	2	-	-	-	X
7	MAN	X	1	-	-	-	X
7	MAN	X	2	-	-	-	X
7	MAN	d	1	-	-	-	X
7	MAN	d	2	-	-	-	X
8	NAG	A	1088	-	-	-	X
8	NAG	A	1160	-	-	-	X
8	NAG	A	1295	-	-	-	X
8	NAG	A	1355	-	-	-	X
8	NAG	A	1386	-	-	-	X
8	NAG	A	1392	-	-	-	X
8	NAG	A	1448	-	-	-	X
8	NAG	E	1088	-	-	-	X
8	NAG	E	1160	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	E	1234	-	-	-	X
8	NAG	E	1295	-	-	-	X
8	NAG	E	1386	-	-	-	X
8	NAG	E	1392	-	-	-	X
8	NAG	E	1448	-	-	-	X
8	NAG	I	1088	-	-	-	X
8	NAG	I	1160	-	-	-	X
8	NAG	I	1234	-	-	-	X
8	NAG	I	1295	-	-	-	X
8	NAG	I	1386	-	-	-	X
8	NAG	I	1392	-	-	-	X
8	NAG	I	1448	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	E	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			
1	I	420	Total	C	N	O	S	0	0	0
			3096	1937	544	590	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	F	77	Total	C	N	O	0	0	0
			385	231	77	77			
2	J	77	Total	C	N	O	0	0	0
			385	231	77	77			

- Molecule 3 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

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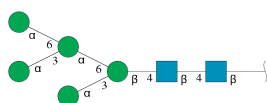
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			
3	K	202	Total	C	N	O	S	0	0	0
			1530	964	255	307	4			

- Molecule 4 is a protein called PGT122 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	H	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			
4	L	226	Total	C	N	O	S	0	0	0
			1728	1100	293	330	5			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
5	M	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	N	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	O	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	P	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	S	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	U	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	V	7	Total	C	N	O	0	0	0
			83	46	2	35			

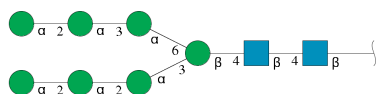
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	Z	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	a	7	Total	C	N	O	0	0	0
			83	46	2	35			
5	b	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]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
6	Q	9	Total	C	N	O	0	0	0
			105	58	2	45			
6	W	9	Total	C	N	O	0	0	0
			105	58	2	45			
6	c	9	Total	C	N	O	0	0	0
			105	58	2	45			

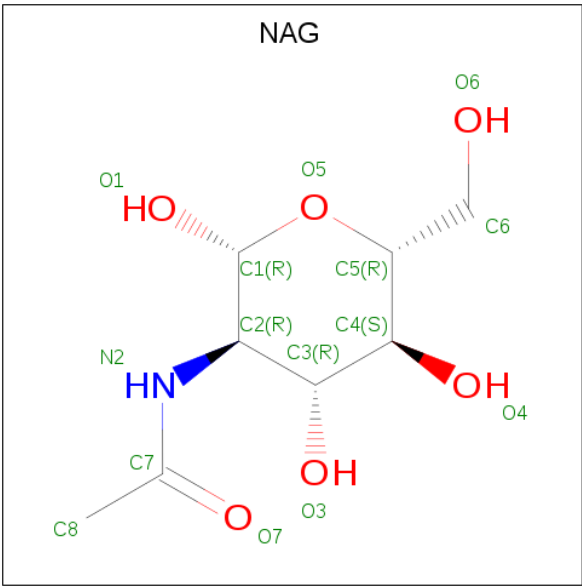
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	R	2	Total	C	O	0	0	0
			22	12	10			
7	X	2	Total	C	O	0	0	0
			22	12	10			
7	d	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



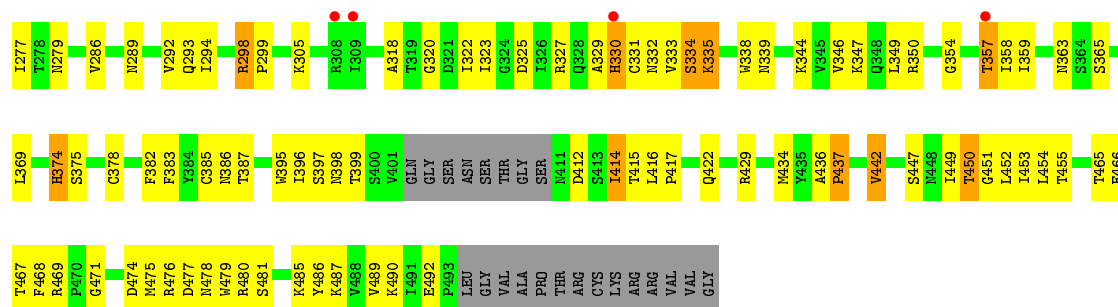
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1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

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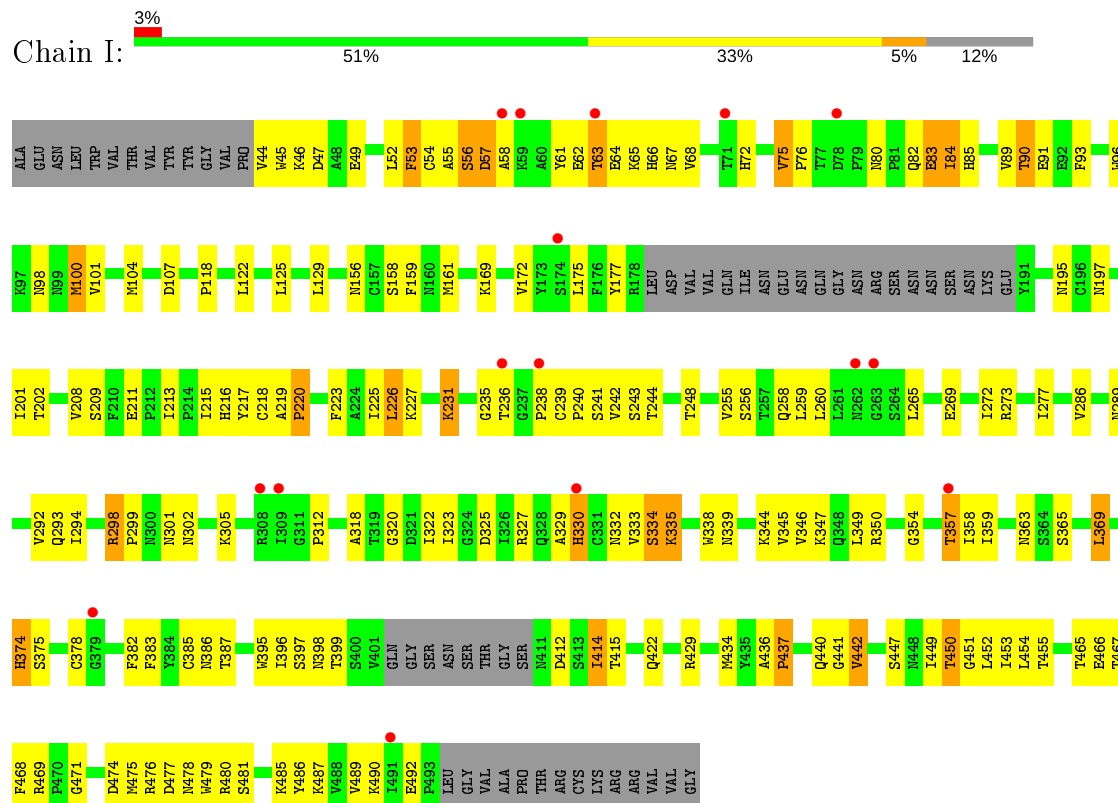
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		



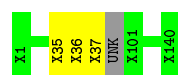


• Molecule 1: BG505 SOSIP gp120



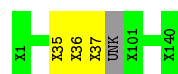
• Molecule 2: BG505 SOSIP gp41

Chain B: 95%



• Molecule 2: BG505 SOSIP gp41

Chain F: 95%




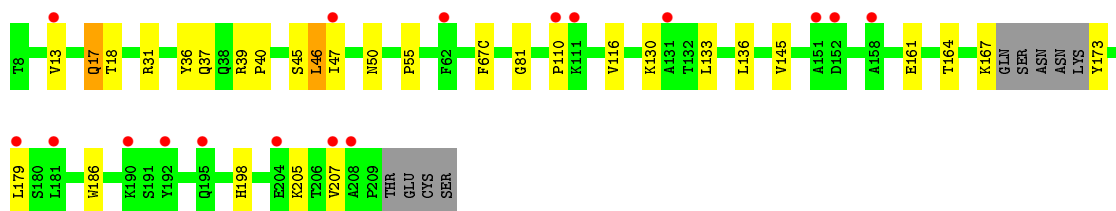
• Molecule 2: BG505 SOSIP gp41

Chain J:  92% 6%




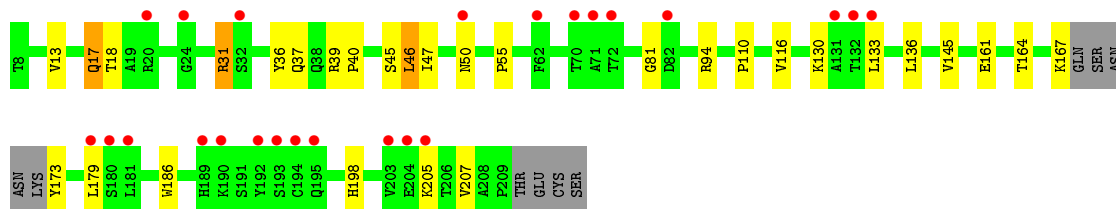
- Molecule 3: PGT122 light chain

Chain C:  8% 82% 13%




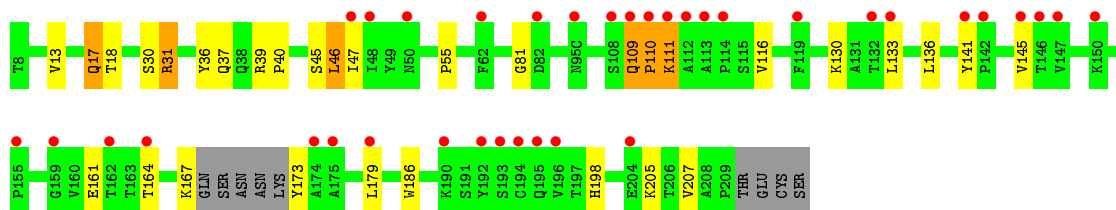
- Molecule 3: PGT122 light chain

Chain G:  11% 82% 13%




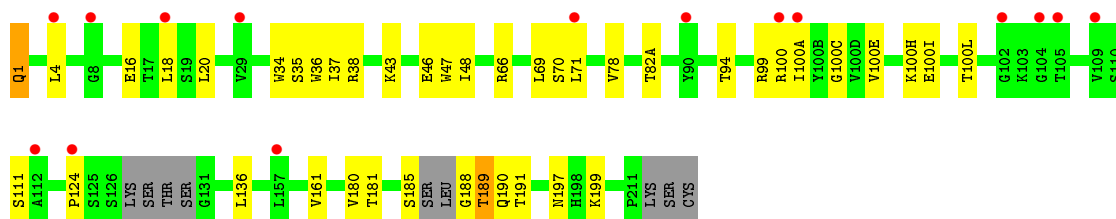
- Molecule 3: PGT122 light chain

Chain K:  17% 81% 12%

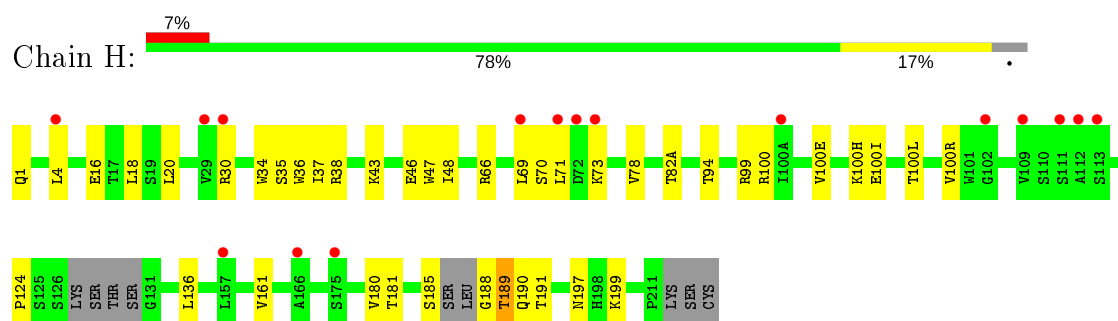


- Molecule 4: PGT122 heavy chain

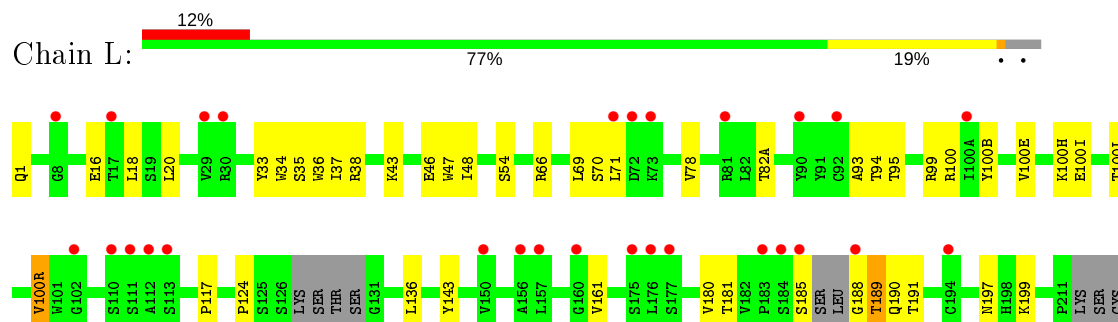
Chain D:  6% 78% 17%



- Molecule 4: PGT122 heavy chain



- Molecule 4: PGT122 heavy chain



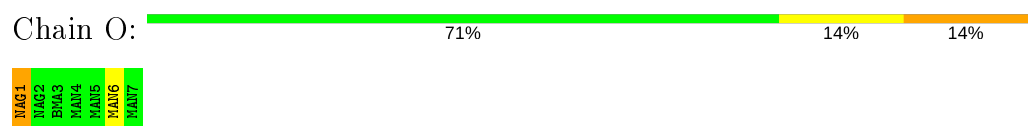
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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



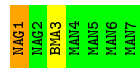
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  57% 43%



- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -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 S:  71% 14% 14%



- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -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 T:  57% 43%



- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -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 U:  71% 14% 14%



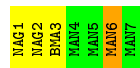
- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain V:  57% 43%



- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -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

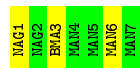
Chain Y:  43% 43% 14%





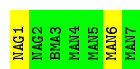
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  57% 43%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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 a:  71% 29%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[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 b:  71% 29%



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

Chain Q:  44% 44% 11%



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

Chain W:  44% 56%



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

Chain c:  44% 56%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain R:  50% 50%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain X:  100%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain d:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.20Å 260.72Å 283.18Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	39.89 – 4.70 39.89 – 4.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (39.89-4.70) 89.1 (39.89-4.70)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 4.63Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.375 , 0.389 0.377 , 0.391	Depositor DCC
$R_{free}$ test set	2550 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	136.6	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 374.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	22014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	262.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.33	0/3161	0.71	4/4306 (0.1%)
1	E	0.35	0/3161	0.71	3/4306 (0.1%)
1	I	0.33	0/3161	0.71	3/4306 (0.1%)
3	C	0.27	0/1571	0.54	1/2151 (0.0%)
3	G	0.27	0/1571	0.55	1/2151 (0.0%)
3	K	0.28	0/1571	0.58	2/2151 (0.1%)
4	D	0.30	0/1774	0.57	0/2421
4	H	0.34	1/1774 (0.1%)	0.57	0/2421
4	L	0.45	1/1774 (0.1%)	0.59	1/2421 (0.0%)
All	All	0.33	2/19518 (0.0%)	0.64	15/26634 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	3
1	I	0	3
3	C	0	1
3	G	0	1
3	K	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	100(R)	VAL	C-N	13.91	1.66	1.34
4	H	100(R)	VAL	C-N	6.19	1.48	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	335	LYS	N-CA-C	6.21	127.77	111.00
1	A	335	LYS	N-CA-C	6.18	127.69	111.00
1	I	335	LYS	N-CA-C	6.10	127.48	111.00
1	I	450	THR	C-N-CA	-6.05	109.59	122.30
4	L	100(R)	VAL	O-C-N	6.04	132.37	122.70
1	E	450	THR	C-N-CA	-5.98	109.73	122.30
1	A	450	THR	C-N-CA	-5.97	109.75	122.30
1	E	334	SER	C-N-CA	5.65	135.84	121.70
3	K	111	LYS	N-CA-C	5.61	126.14	111.00
1	A	334	SER	C-N-CA	5.51	135.48	121.70
3	C	46	LEU	CA-CB-CG	5.35	127.61	115.30
3	K	46	LEU	CA-CB-CG	5.35	127.61	115.30
3	G	46	LEU	CA-CB-CG	5.35	127.60	115.30
1	I	334	SER	C-N-CA	5.32	134.99	121.70
1	A	259	LEU	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
3	C	110	PRO	Peptide
1	E	236	THR	Peptide
1	E	56	SER	Peptide
1	E	80	ASN	Peptide
3	G	110	PRO	Peptide
1	I	236	THR	Peptide
1	I	56	SER	Peptide
1	I	80	ASN	Peptide
3	K	110	PRO	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	2821	142	0
1	E	3096	0	2821	144	0
1	I	3096	0	2821	140	0
2	B	385	0	82	2	0
2	F	385	0	82	2	0
2	J	385	0	82	3	0
3	C	1530	0	1472	21	0
3	G	1530	0	1472	20	0
3	K	1530	0	1472	22	0
4	D	1728	0	1699	36	0
4	H	1728	0	1699	30	0
4	L	1728	0	1699	40	0
5	M	83	0	70	1	0
5	N	83	0	70	0	0
5	O	83	0	70	5	0
5	P	83	0	70	0	0
5	S	83	0	70	1	0
5	T	83	0	70	0	0
5	U	83	0	70	5	0
5	V	83	0	70	0	0
5	Y	83	0	70	1	0
5	Z	83	0	70	0	0
5	a	83	0	70	0	0
5	b	83	0	70	0	0
6	Q	105	0	88	2	0
6	W	105	0	88	0	0
6	c	105	0	88	0	0
7	R	22	0	19	3	0
7	X	22	0	19	1	0
7	d	22	0	19	0	0
8	A	140	0	130	3	0
8	E	140	0	130	3	0
8	I	140	0	130	2	0
All	All	22014	0	19773	580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:293:GLN:HB2	1:I:334:SER:HB3	1.33	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:GLN:HB2	1:E:334:SER:HB3	1.33	1.09
1:A:293:GLN:HB2	1:A:334:SER:HB3	1.33	1.08
1:I:91:GLU:HA	1:I:239:CYS:O	1.74	0.88
1:E:91:GLU:HA	1:E:239:CYS:O	1.74	0.86
1:A:91:GLU:HA	1:A:239:CYS:O	1.74	0.86
1:I:358:ILE:HB	1:I:465:THR:HG22	1.58	0.84
1:E:358:ILE:HB	1:E:465:THR:HG22	1.58	0.84
1:A:358:ILE:HB	1:A:465:THR:HG22	1.58	0.84
1:A:260:LEU:HB2	1:A:450:THR:O	1.78	0.83
1:I:260:LEU:HB2	1:I:450:THR:O	1.79	0.83
4:D:38:ARG:N	4:D:46:GLU:O	2.12	0.83
4:H:38:ARG:N	4:H:46:GLU:O	2.12	0.82
4:L:38:ARG:N	4:L:46:GLU:O	2.12	0.81
1:E:260:LEU:HB2	1:E:450:THR:O	1.79	0.81
4:H:38:ARG:O	4:H:46:GLU:N	2.15	0.79
4:D:38:ARG:O	4:D:46:GLU:N	2.15	0.78
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.48	0.78
1:I:269:GLU:HA	1:I:289:ASN:HD22	1.48	0.78
1:E:269:GLU:HA	1:E:289:ASN:HD22	1.48	0.77
4:L:38:ARG:O	4:L:46:GLU:N	2.15	0.76
1:E:335:LYS:HD3	1:E:414:ILE:HD11	1.67	0.76
4:D:99:ARG:HG2	4:D:100(L):THR:HG22	1.68	0.76
1:I:335:LYS:HD3	1:I:414:ILE:HD11	1.68	0.75
1:A:335:LYS:HD3	1:A:414:ILE:HD11	1.67	0.75
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.69	0.75
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.75
4:L:35:SER:HB3	4:L:47:TRP:HE1	1.51	0.74
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.69	0.74
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.69	0.74
1:E:55:ALA:HB3	1:E:216:HIS:HB2	1.68	0.74
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.68	0.74
4:L:99:ARG:HG2	4:L:100(L):THR:HG22	1.68	0.74
1:I:55:ALA:HB3	1:I:216:HIS:HB2	1.68	0.74
1:A:436:ALA:HB3	1:A:437:PRO:HD3	1.70	0.73
1:I:436:ALA:HB3	1:I:437:PRO:HD3	1.69	0.73
1:E:436:ALA:HB3	1:E:437:PRO:HD3	1.70	0.73
1:A:327:ARG:HA	4:D:100(H):LYS:HD2	1.71	0.72
1:E:327:ARG:HA	4:H:100(H):LYS:HD2	1.70	0.72
1:E:227:LYS:HE3	1:E:485:LYS:HD2	1.75	0.69
1:I:227:LYS:HE3	1:I:485:LYS:HD2	1.75	0.69
4:D:100(C):GLY:HA3	6:Q:2:NAG:H4	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HE3	1:A:485:LYS:HD2	1.75	0.69
4:L:37:ILE:HG23	4:L:47:TRP:HA	1.76	0.68
4:D:37:ILE:HG23	4:D:47:TRP:HA	1.76	0.68
4:H:38:ARG:O	4:H:46:GLU:O	2.12	0.68
1:E:294:ILE:HG23	1:E:447:SER:HB2	1.76	0.68
4:H:37:ILE:HG23	4:H:47:TRP:HA	1.76	0.67
1:A:294:ILE:HG23	1:A:447:SER:HB2	1.76	0.67
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.27	0.67
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.27	0.67
4:D:38:ARG:O	4:D:46:GLU:O	2.12	0.67
2:F:35:UNK:O	2:F:37:UNK:O	2.12	0.67
2:B:35:UNK:O	2:B:37:UNK:O	2.12	0.67
3:G:39:ARG:HG3	3:G:40:PRO:HD2	1.77	0.67
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.27	0.67
2:J:35:UNK:O	2:J:37:UNK:O	2.12	0.67
4:L:38:ARG:O	4:L:46:GLU:O	2.12	0.67
3:K:39:ARG:HG3	3:K:40:PRO:HD2	1.77	0.66
1:I:294:ILE:HG23	1:I:447:SER:HB2	1.78	0.66
3:C:39:ARG:HG3	3:C:40:PRO:HD2	1.77	0.66
1:A:350:ARG:NH2	1:A:397:SER:O	2.29	0.66
4:D:35:SER:HB3	4:D:47:TRP:HE1	1.62	0.65
1:I:350:ARG:NH2	1:I:397:SER:O	2.29	0.65
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.79	0.65
1:I:327:ARG:HA	4:L:100(H):LYS:HD2	1.78	0.65
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.79	0.65
1:E:350:ARG:NH2	1:E:397:SER:O	2.29	0.64
3:K:37:GLN:N	3:K:45:SER:O	2.31	0.64
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.63	0.64
1:A:68:VAL:O	1:A:72:HIS:ND1	2.31	0.63
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.63	0.63
1:E:330:HIS:HE1	1:E:415:THR:HG21	1.63	0.63
1:E:91:GLU:O	1:E:238:PRO:HA	1.99	0.63
1:E:68:VAL:O	1:E:72:HIS:ND1	2.31	0.63
1:I:91:GLU:O	1:I:238:PRO:HA	1.99	0.63
1:E:101:VAL:HG21	1:E:480:ARG:HG2	1.79	0.63
4:H:34:TRP:CZ3	4:H:94:THR:HG22	2.34	0.63
1:I:359:ILE:HD12	1:I:468:PHE:HE1	1.63	0.63
3:C:37:GLN:N	3:C:45:SER:O	2.31	0.62
3:G:37:GLN:N	3:G:45:SER:O	2.31	0.62
1:E:330:HIS:CG	4:H:100(E):VAL:HG23	2.34	0.62
1:A:91:GLU:O	1:A:238:PRO:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:HG3	1:A:84:ILE:H	1.65	0.62
1:I:68:VAL:O	1:I:72:HIS:ND1	2.31	0.62
1:A:363:ASN:O	1:A:469:ARG:NH1	2.33	0.62
1:I:363:ASN:O	1:I:469:ARG:NH1	2.33	0.62
1:A:100:MET:N	1:A:100:MET:SD	2.73	0.61
1:E:330:HIS:CB	4:H:100(E):VAL:HG23	2.30	0.61
1:I:100:MET:SD	1:I:100:MET:N	2.73	0.61
1:E:226:LEU:HD11	1:E:487:LYS:HB3	1.82	0.61
1:I:83:GLU:HG3	1:I:84:ILE:H	1.65	0.61
1:E:358:ILE:HG13	1:E:397:SER:H	1.66	0.61
1:A:332:ASN:HB3	8:A:1295:NAG:H82	1.82	0.61
1:E:330:HIS:CE1	1:E:415:THR:CG2	2.84	0.61
1:E:363:ASN:O	1:E:469:ARG:NH1	2.33	0.61
1:A:177:TYR:HE2	1:A:422:GLN:HE21	1.49	0.60
1:I:226:LEU:HD11	1:I:487:LYS:HB3	1.83	0.60
1:A:330:HIS:ND1	4:D:100(E):VAL:HG23	2.16	0.60
1:E:332:ASN:HB3	8:E:1295:NAG:H82	1.83	0.60
4:H:37:ILE:HG13	4:H:47:TRP:HD1	1.67	0.60
1:I:358:ILE:HG13	1:I:397:SER:H	1.66	0.60
4:L:34:TRP:CZ3	4:L:94:THR:HG22	2.37	0.60
1:E:83:GLU:HG3	1:E:84:ILE:H	1.65	0.60
1:I:177:TYR:HE2	1:I:422:GLN:HE21	1.49	0.60
1:E:226:LEU:HD11	1:E:487:LYS:HD3	1.82	0.60
3:G:37:GLN:O	3:G:45:SER:O	2.20	0.60
1:E:100:MET:SD	1:E:100:MET:N	2.73	0.59
1:I:226:LEU:HD11	1:I:487:LYS:HD3	1.82	0.59
1:A:358:ILE:HG13	1:A:397:SER:H	1.66	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HD3	1.82	0.59
1:E:52:LEU:HB3	1:E:217:TYR:HD2	1.67	0.59
1:A:226:LEU:HD11	1:A:487:LYS:HB3	1.83	0.59
1:I:52:LEU:HB3	1:I:217:TYR:HD2	1.68	0.59
3:C:37:GLN:O	3:C:45:SER:O	2.20	0.59
3:K:31:ARG:O	4:L:100:ARG:NH1	2.34	0.59
3:K:37:GLN:O	3:K:45:SER:O	2.20	0.59
4:L:54:SER:HB2	5:Y:6:MAN:O4	2.03	0.59
1:E:256:SER:HB2	1:E:374:HIS:HE1	1.68	0.59
4:L:37:ILE:HG13	4:L:47:TRP:HD1	1.66	0.59
1:E:177:TYR:HE2	1:E:422:GLN:HE21	1.49	0.59
1:I:226:LEU:CD1	1:I:487:LYS:HB3	2.33	0.59
1:I:258:GLN:O	1:I:452:LEU:HA	2.03	0.59
1:I:476:ARG:HA	1:I:479:TRP:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:ILE:HG13	4:D:47:TRP:HD1	1.67	0.58
1:E:258:GLN:O	1:E:452:LEU:HA	2.03	0.58
1:I:256:SER:HB2	1:I:374:HIS:HE1	1.68	0.58
1:E:476:ARG:HA	1:E:479:TRP:CD1	2.38	0.58
1:E:226:LEU:CD1	1:E:487:LYS:HB3	2.33	0.58
1:A:256:SER:HB2	1:A:374:HIS:HE1	1.68	0.58
4:L:33:TYR:HB2	4:L:95:THR:O	2.03	0.58
1:A:325:ASP:O	4:D:100(I):GLU:OE2	2.22	0.58
1:A:258:GLN:O	1:A:452:LEU:HA	2.03	0.58
3:K:36:TYR:HA	3:K:46:LEU:HA	1.85	0.58
4:D:4:LEU:HD11	4:D:94:THR:HG23	1.85	0.58
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.38	0.57
1:E:122:LEU:HA	1:E:201:ILE:HA	1.86	0.57
3:G:36:TYR:HA	3:G:46:LEU:HA	1.85	0.57
1:A:98:ASN:HB3	1:A:100:MET:HG2	1.87	0.57
1:I:332:ASN:HB3	8:I:1295:NAG:H82	1.85	0.57
3:C:36:TYR:HA	3:C:46:LEU:HA	1.85	0.57
1:A:122:LEU:HA	1:A:201:ILE:HA	1.86	0.57
1:A:226:LEU:CD1	1:A:487:LYS:HB3	2.33	0.57
1:A:422:GLN:O	1:A:434:MET:HA	2.05	0.57
3:C:145:VAL:HG12	3:C:198:HIS:HB2	1.86	0.57
1:I:98:ASN:HB3	1:I:100:MET:HG2	1.87	0.57
1:A:52:LEU:HB3	1:A:217:TYR:HD2	1.68	0.57
1:A:53:PHE:HB3	1:A:218:CYS:HB2	1.87	0.57
1:I:53:PHE:HB3	1:I:218:CYS:HB2	1.87	0.57
3:G:145:VAL:HG12	3:G:198:HIS:HB2	1.86	0.57
1:A:259:LEU:HB3	1:A:449:ILE:HG23	1.85	0.57
1:I:122:LEU:HA	1:I:201:ILE:HA	1.86	0.57
1:I:422:GLN:O	1:I:434:MET:HA	2.05	0.57
1:E:325:ASP:O	4:H:100(I):GLU:OE2	2.23	0.57
4:L:161:VAL:HG22	4:L:180:VAL:HG12	1.87	0.57
1:E:53:PHE:HB3	1:E:218:CYS:HB2	1.86	0.56
1:I:259:LEU:HB3	1:I:449:ILE:HG23	1.86	0.56
1:E:422:GLN:O	1:E:434:MET:HA	2.05	0.56
1:E:259:LEU:HB3	1:E:449:ILE:HG23	1.86	0.56
3:K:110:PRO:HB2	3:K:111:LYS:HB2	1.87	0.56
4:D:161:VAL:HG22	4:D:180:VAL:HG12	1.88	0.56
3:K:145:VAL:HG12	3:K:198:HIS:HB2	1.87	0.56
1:E:98:ASN:HB3	1:E:100:MET:HG2	1.86	0.56
1:E:330:HIS:HE1	1:E:415:THR:CG2	2.19	0.56
4:D:37:ILE:HG13	4:D:47:TRP:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:GLN:O	1:E:84:ILE:HG13	2.06	0.56
4:D:37:ILE:HA	4:D:47:TRP:HA	1.88	0.56
1:I:82:GLN:O	1:I:84:ILE:HG13	2.06	0.56
4:L:37:ILE:HG13	4:L:47:TRP:CD1	2.41	0.56
1:A:199:SER:HA	1:I:312:PRO:HB3	1.86	0.55
4:H:37:ILE:HA	4:H:47:TRP:HA	1.88	0.55
1:A:347:LYS:O	1:A:350:ARG:HG2	2.06	0.55
1:I:217:TYR:O	1:I:248:THR:HG23	2.07	0.55
4:H:37:ILE:HG13	4:H:47:TRP:CD1	2.41	0.55
3:C:50:ASN:OD1	4:D:100:ARG:NH2	2.36	0.55
1:I:347:LYS:O	1:I:350:ARG:HG2	2.06	0.55
1:E:217:TYR:O	1:E:248:THR:HG23	2.07	0.55
4:D:100(A):ILE:HB	7:R:1:MAN:H3	1.88	0.55
1:E:347:LYS:O	1:E:350:ARG:HG2	2.06	0.55
4:H:161:VAL:HG22	4:H:180:VAL:HG12	1.88	0.55
1:A:82:GLN:O	1:A:84:ILE:HG13	2.06	0.54
1:E:451:GLY:O	1:E:452:LEU:HD23	2.08	0.54
1:I:93:PHE:CE1	1:I:226:LEU:HD13	2.42	0.54
1:A:93:PHE:CE1	1:A:226:LEU:HD13	2.42	0.54
3:C:39:ARG:NH1	3:C:81:GLY:O	2.40	0.54
1:E:93:PHE:CE1	1:E:226:LEU:HD13	2.42	0.54
1:A:217:TYR:O	1:A:248:THR:HG23	2.07	0.54
1:A:346:VAL:HG21	1:A:395:TRP:CD1	2.43	0.54
1:E:478:ASN:O	1:E:481:SER:OG	2.20	0.54
3:K:39:ARG:NH1	3:K:81:GLY:O	2.40	0.54
1:A:396:ILE:HG22	1:A:398:ASN:H	1.73	0.54
1:E:396:ILE:HG22	1:E:398:ASN:H	1.73	0.54
4:D:34:TRP:CZ3	4:D:94:THR:HG22	2.43	0.54
1:E:344:LYS:HA	1:E:347:LYS:HE2	1.90	0.54
1:E:64:GLU:HB2	1:E:209:SER:HB3	1.90	0.54
1:I:344:LYS:HA	1:I:347:LYS:HE2	1.90	0.54
1:I:63:THR:OG1	1:I:64:GLU:N	2.40	0.54
3:G:50:ASN:ND2	7:X:2:MAN:O2	2.38	0.54
1:E:346:VAL:HG21	1:E:395:TRP:CD1	2.43	0.54
1:I:64:GLU:HB2	1:I:209:SER:HB3	1.90	0.54
1:I:82:GLN:O	1:I:84:ILE:N	2.41	0.54
4:H:4:LEU:HD11	4:H:94:THR:HG23	1.90	0.54
4:L:37:ILE:HA	4:L:47:TRP:HA	1.89	0.54
1:A:64:GLU:HB2	1:A:209:SER:HB3	1.90	0.53
1:I:451:GLY:O	1:I:452:LEU:HD23	2.07	0.53
1:A:451:GLY:O	1:A:452:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ALA:O	1:E:216:HIS:ND1	2.42	0.53
1:E:63:THR:OG1	1:E:64:GLU:N	2.40	0.53
1:A:298:ARG:HG2	1:A:383:PHE:CZ	2.43	0.53
1:A:265:LEU:HD23	1:A:450:THR:HG23	1.91	0.53
3:G:37:GLN:HB2	3:G:47:ILE:HG12	1.90	0.53
1:I:346:VAL:HG21	1:I:395:TRP:CD1	2.43	0.53
1:I:55:ALA:O	1:I:216:HIS:ND1	2.42	0.53
3:K:109:GLN:HB3	3:K:141:TYR:HE2	1.73	0.53
3:K:37:GLN:HB2	3:K:47:ILE:HG12	1.91	0.53
1:A:82:GLN:O	1:A:84:ILE:N	2.41	0.53
1:I:265:LEU:HD23	1:I:450:THR:HG23	1.90	0.53
1:A:344:LYS:HA	1:A:347:LYS:HE2	1.90	0.53
1:A:63:THR:OG1	1:A:64:GLU:N	2.40	0.53
1:E:82:GLN:O	1:E:84:ILE:N	2.41	0.53
1:I:46:LYS:HB3	1:I:490:LYS:HG3	1.90	0.53
1:A:299:PRO:HA	1:A:442:VAL:HA	1.91	0.53
1:A:378:CYS:HB2	1:A:383:PHE:CE1	2.44	0.53
3:C:37:GLN:HB2	3:C:47:ILE:HG12	1.91	0.53
1:E:46:LYS:HB3	1:E:490:LYS:HG3	1.91	0.53
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.90	0.53
4:L:35:SER:OG	4:L:95:THR:OG1	2.19	0.53
1:E:265:LEU:HD23	1:E:450:THR:HG23	1.91	0.53
4:D:100(C):GLY:CA	6:Q:2:NAG:H4	2.37	0.53
1:A:305:LYS:O	1:A:318:ALA:N	2.42	0.53
1:E:378:CYS:HB2	1:E:383:PHE:CE1	2.44	0.53
1:E:66:HIS:HB3	1:E:213:ILE:HG12	1.90	0.53
1:I:305:LYS:O	1:I:318:ALA:N	2.42	0.53
1:I:298:ARG:HG2	1:I:383:PHE:CZ	2.43	0.52
1:E:298:ARG:HG2	1:E:383:PHE:CZ	2.43	0.52
1:I:66:HIS:HB3	1:I:213:ILE:HG12	1.91	0.52
4:L:189:THR:OG1	4:L:190:GLN:N	2.42	0.52
1:E:305:LYS:O	1:E:318:ALA:N	2.42	0.52
1:I:299:PRO:HA	1:I:442:VAL:HA	1.91	0.52
3:K:133:LEU:HD12	3:K:179:LEU:HD23	1.92	0.52
1:A:55:ALA:O	1:A:216:HIS:ND1	2.42	0.52
1:E:93:PHE:HE1	1:E:226:LEU:HD13	1.75	0.52
1:I:396:ILE:HG22	1:I:398:ASN:H	1.73	0.52
1:A:93:PHE:HE1	1:A:226:LEU:HD13	1.75	0.52
3:C:133:LEU:HD12	3:C:179:LEU:HD23	1.92	0.52
4:H:189:THR:OG1	4:H:190:GLN:N	2.42	0.52
1:I:346:VAL:HA	1:I:349:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:109:GLN:HB3	3:K:141:TYR:CE2	2.45	0.52
1:I:378:CYS:HB2	1:I:383:PHE:CE1	2.44	0.52
1:I:330:HIS:ND1	4:L:100(E):VAL:HA	2.25	0.52
4:H:185:SER:O	4:H:188:GLY:N	2.44	0.51
1:E:159:PHE:HB2	1:E:172:VAL:HG23	1.93	0.51
3:G:39:ARG:NH1	3:G:81:GLY:O	2.40	0.51
1:E:299:PRO:HA	1:E:442:VAL:HA	1.91	0.51
1:E:346:VAL:HA	1:E:349:LEU:HD12	1.92	0.51
1:I:478:ASN:O	1:I:481:SER:OG	2.20	0.51
4:D:185:SER:O	4:D:188:GLY:N	2.44	0.51
4:L:185:SER:O	4:L:188:GLY:N	2.44	0.51
3:C:50:ASN:ND2	7:R:2:MAN:O2	2.38	0.51
1:E:252:LYS:HD3	5:U:1:NAG:H81	1.93	0.51
1:A:334:SER:HB2	8:A:1295:NAG:H83	1.93	0.51
1:A:346:VAL:HA	1:A:349:LEU:HD12	1.92	0.51
1:E:90:THR:HG22	1:E:91:GLU:H	1.76	0.51
1:I:64:GLU:HA	1:I:209:SER:N	2.26	0.51
1:I:90:THR:HG22	1:I:91:GLU:H	1.76	0.51
3:G:133:LEU:HD12	3:G:179:LEU:HD23	1.92	0.50
4:H:35:SER:HB3	4:H:47:TRP:HE1	1.76	0.50
1:I:248:THR:HG22	1:I:486:TYR:CE1	2.46	0.50
1:A:335:LYS:HG3	1:A:339:ASN:OD1	2.11	0.50
1:A:64:GLU:HA	1:A:209:SER:N	2.26	0.50
1:I:286:VAL:HB	1:I:452:LEU:HB2	1.94	0.50
1:I:325:ASP:O	4:L:100(I):GLU:OE2	2.29	0.50
1:I:335:LYS:HG3	1:I:339:ASN:OD1	2.12	0.50
1:A:212:PRO:HB2	5:O:1:NAG:C8	2.42	0.50
1:A:159:PHE:HB2	1:A:172:VAL:HG23	1.92	0.50
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.46	0.50
1:E:332:ASN:OD1	1:E:415:THR:HG23	2.11	0.50
1:E:64:GLU:HA	1:E:209:SER:N	2.26	0.50
1:I:159:PHE:HB2	1:I:172:VAL:HG23	1.92	0.50
1:A:252:LYS:HD3	5:O:1:NAG:H81	1.93	0.50
1:A:327:ARG:CA	4:D:100(H):LYS:HD2	2.41	0.50
4:D:189:THR:OG1	4:D:190:GLN:N	2.42	0.50
1:A:158:SER:O	1:A:159:PHE:HD1	1.94	0.49
1:A:330:HIS:CE1	4:D:100(E):VAL:HA	2.46	0.49
1:E:96:TRP:HZ2	1:E:273:ARG:HB3	1.77	0.49
1:I:93:PHE:HE1	1:I:226:LEU:HD13	1.75	0.49
1:A:226:LEU:HA	1:A:243:SER:O	2.12	0.49
1:A:90:THR:HG22	1:A:91:GLU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:LEU:HA	1:E:159:PHE:CE1	2.47	0.49
1:E:474:ASP:HB3	1:E:476:ARG:HG2	1.94	0.49
3:G:37:GLN:HB2	3:G:47:ILE:CG1	2.42	0.49
1:E:212:PRO:HB2	5:U:1:NAG:C8	2.42	0.49
1:A:96:TRP:HZ2	1:A:273:ARG:HB3	1.76	0.49
1:E:335:LYS:HG3	1:E:339:ASN:OD1	2.12	0.49
1:E:226:LEU:HA	1:E:243:SER:O	2.12	0.49
1:E:248:THR:HG22	1:E:486:TYR:CE1	2.46	0.49
1:I:96:TRP:HZ2	1:I:273:ARG:HB3	1.77	0.49
3:K:37:GLN:HB2	3:K:47:ILE:CG1	2.42	0.49
1:E:202:THR:HA	1:E:434:MET:HB2	1.95	0.49
1:I:226:LEU:HA	1:I:243:SER:O	2.12	0.49
1:A:474:ASP:HB3	1:A:476:ARG:HG2	1.94	0.49
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.94	0.49
1:E:158:SER:O	1:E:159:PHE:HD1	1.94	0.49
1:E:334:SER:HB2	8:E:1295:NAG:H83	1.94	0.48
1:I:202:THR:HA	1:I:434:MET:HB2	1.95	0.48
4:D:100(A):ILE:HB	7:R:1:MAN:C3	2.42	0.48
1:I:129:LEU:HA	1:I:159:PHE:CE1	2.48	0.48
1:I:158:SER:O	1:I:159:PHE:HD1	1.95	0.48
4:L:35:SER:CB	4:L:95:THR:OG1	2.61	0.48
1:E:129:LEU:HG	1:E:159:PHE:CZ	2.48	0.48
1:A:455:THR:HG23	1:A:471:GLY:HA3	1.95	0.48
1:A:85:HIS:CE1	1:A:241:SER:HA	2.49	0.48
1:A:46:LYS:HB3	1:A:490:LYS:HG3	1.94	0.48
1:E:129:LEU:HA	1:E:159:PHE:HE1	1.79	0.48
1:A:129:LEU:HA	1:A:159:PHE:CE1	2.47	0.48
1:A:129:LEU:HA	1:A:159:PHE:HE1	1.79	0.48
1:I:474:ASP:HB3	1:I:476:ARG:HG2	1.94	0.48
1:A:212:PRO:HB2	5:O:1:NAG:H83	1.96	0.48
1:A:478:ASN:O	1:A:481:SER:OG	2.20	0.48
3:C:37:GLN:O	3:C:45:SER:OG	2.21	0.48
3:C:37:GLN:HB2	3:C:47:ILE:CG1	2.42	0.48
3:C:36:TYR:HB3	3:C:45:SER:O	2.14	0.48
1:E:455:THR:HG23	1:E:471:GLY:HA3	1.95	0.48
1:I:85:HIS:CE1	1:I:241:SER:HA	2.49	0.48
1:I:455:THR:HG23	1:I:471:GLY:HA3	1.95	0.48
1:I:375:SER:HA	1:I:383:PHE:O	2.14	0.47
3:K:36:TYR:HB3	3:K:45:SER:O	2.14	0.47
1:A:375:SER:HA	1:A:383:PHE:O	2.14	0.47
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:365:SER:HB2	1:I:469:ARG:HD3	1.96	0.47
1:A:365:SER:HB2	1:A:469:ARG:HD3	1.96	0.47
3:G:36:TYR:HB3	3:G:45:SER:O	2.14	0.47
1:I:259:LEU:HD13	1:I:449:ILE:HD13	1.96	0.47
3:K:30:SER:HB2	4:L:100(B):TYR:OH	2.15	0.47
1:A:64:GLU:OE2	1:A:211:GLU:N	2.48	0.47
3:K:17:GLN:CD	3:K:18:THR:H	2.18	0.47
1:A:65:LYS:HG3	1:A:208:VAL:HB	1.96	0.47
1:E:85:HIS:ND1	1:E:242:VAL:O	2.36	0.47
1:E:85:HIS:CE1	1:E:241:SER:HA	2.49	0.47
1:I:55:ALA:HB3	1:I:216:HIS:CB	2.42	0.47
1:I:129:LEU:HG	1:I:159:PHE:CZ	2.49	0.47
1:I:330:HIS:CE1	1:I:415:THR:CG2	2.98	0.47
4:L:124:PRO:HG3	4:L:136:LEU:HG	1.97	0.47
1:E:212:PRO:HB2	5:U:1:NAG:H83	1.96	0.47
4:D:43:LYS:HE3	4:D:43:LYS:HB3	1.65	0.47
1:E:354:GLY:O	1:E:357:THR:OG1	2.33	0.47
1:E:365:SER:HB2	1:E:469:ARG:HD3	1.97	0.47
1:I:333:VAL:HG13	1:I:414:ILE:HD12	1.97	0.47
1:I:64:GLU:OE2	1:I:211:GLU:N	2.48	0.47
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.65	0.47
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.97	0.47
2:B:35:UNK:O	2:B:36:UNK:C	2.63	0.47
1:E:65:LYS:HG3	1:E:208:VAL:HB	1.96	0.47
1:E:64:GLU:OE2	1:E:211:GLU:N	2.48	0.47
1:E:175:LEU:HD21	1:E:320:GLY:HA3	1.97	0.47
1:E:375:SER:HA	1:E:383:PHE:O	2.15	0.47
1:A:129:LEU:HG	1:A:159:PHE:CZ	2.49	0.47
1:E:298:ARG:HB3	1:E:329:ALA:HB1	1.97	0.47
3:G:17:GLN:CD	3:G:18:THR:H	2.18	0.47
3:G:37:GLN:O	3:G:45:SER:OG	2.20	0.47
1:I:65:LYS:HG3	1:I:208:VAL:HB	1.96	0.47
1:I:332:ASN:OD1	1:I:415:THR:HG23	2.15	0.47
1:I:75:VAL:HG22	1:I:76:PRO:HD2	1.97	0.47
4:L:35:SER:HG	4:L:95:THR:CB	2.25	0.47
1:I:298:ARG:HG3	1:I:298:ARG:H	1.60	0.47
1:I:330:HIS:CE1	4:L:100(E):VAL:HA	2.50	0.47
4:L:36:TRP:HE1	4:L:78:VAL:HG12	1.80	0.47
1:A:202:THR:HA	1:A:434:MET:HB2	1.96	0.46
1:A:333:VAL:HG13	1:A:414:ILE:HD12	1.97	0.46
1:E:259:LEU:HD13	1:E:449:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:HG2	1:E:67:ASN:H	1.80	0.46
1:A:64:GLU:HG2	1:A:67:ASN:H	1.80	0.46
1:A:85:HIS:CE1	1:A:242:VAL:H	2.34	0.46
1:A:324:GLY:HA2	3:C:67(C):PHE:CZ	2.50	0.46
4:H:124:PRO:HG3	4:H:136:LEU:HG	1.98	0.46
4:H:36:TRP:HE1	4:H:78:VAL:HG12	1.80	0.46
1:E:55:ALA:HB3	1:E:216:HIS:CB	2.42	0.46
3:C:17:GLN:CD	3:C:18:THR:H	2.18	0.46
1:E:75:VAL:HG22	1:E:76:PRO:HD2	1.97	0.46
1:I:272:ILE:HG22	1:I:286:VAL:HG13	1.98	0.46
1:A:85:HIS:ND1	1:A:242:VAL:O	2.36	0.46
1:I:64:GLU:HG2	1:I:67:ASN:H	1.80	0.46
1:E:252:LYS:HD3	5:U:1:NAG:C8	2.44	0.46
1:I:175:LEU:HD21	1:I:320:GLY:HA3	1.98	0.46
1:A:252:LYS:HD3	5:O:1:NAG:C8	2.45	0.46
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.97	0.46
1:A:49:GLU:HG3	1:A:223:PHE:HE2	1.79	0.46
1:A:55:ALA:HB3	1:A:216:HIS:CB	2.42	0.46
1:I:129:LEU:HA	1:I:159:PHE:HE1	1.81	0.46
1:A:332:ASN:OD1	1:A:415:THR:HG23	2.16	0.46
1:A:96:TRP:CH2	1:A:235:GLY:HA3	2.51	0.45
4:D:36:TRP:HE1	4:D:78:VAL:HG12	1.80	0.45
2:F:35:UNK:O	2:F:36:UNK:C	2.63	0.45
1:I:330:HIS:CE1	1:I:415:THR:HG21	2.51	0.45
1:I:85:HIS:CE1	1:I:242:VAL:H	2.34	0.45
1:A:298:ARG:HB3	1:A:329:ALA:HB1	1.98	0.45
1:A:354:GLY:O	1:A:357:THR:OG1	2.34	0.45
1:A:57:ASP:OD1	1:A:58:ALA:N	2.49	0.45
4:D:47:TRP:O	4:D:48:ILE:HG13	2.16	0.45
1:E:85:HIS:CE1	1:E:242:VAL:H	2.34	0.45
1:E:298:ARG:HG2	1:E:383:PHE:HZ	1.82	0.45
3:G:31:ARG:O	4:H:100:ARG:NH1	2.45	0.45
4:H:47:TRP:O	4:H:48:ILE:HG13	2.16	0.45
1:A:175:LEU:HD21	1:A:320:GLY:HA3	1.97	0.45
1:A:272:ILE:HG22	1:A:286:VAL:HG13	1.98	0.45
1:E:223:PHE:CE2	1:E:490:LYS:HB3	2.52	0.45
1:E:49:GLU:HG3	1:E:223:PHE:HE2	1.81	0.45
1:E:96:TRP:CH2	1:E:235:GLY:HA3	2.51	0.45
1:E:57:ASP:OD1	1:E:58:ALA:N	2.48	0.45
1:A:298:ARG:HG2	1:A:383:PHE:HZ	1.82	0.45
1:I:298:ARG:HG2	1:I:383:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:35:UNK:O	2:J:36:UNK:C	2.63	0.45
1:I:49:GLU:HG3	1:I:223:PHE:HE2	1.80	0.45
1:A:65:LYS:NZ	1:A:208:VAL:HG11	2.32	0.45
4:D:124:PRO:HG3	4:D:136:LEU:HG	1.97	0.45
1:E:272:ILE:HG22	1:E:286:VAL:HG13	1.98	0.45
1:I:96:TRP:CH2	1:I:235:GLY:HA3	2.52	0.45
1:I:65:LYS:NZ	1:I:208:VAL:HG11	2.32	0.45
1:E:44:VAL:HB	1:E:492:GLU:HB2	1.99	0.45
1:A:252:LYS:HB3	5:O:1:NAG:H81	1.98	0.45
3:C:46:LEU:HD23	3:C:55:PRO:HG3	1.99	0.45
3:G:116:VAL:HG23	3:G:205:LYS:HD2	1.99	0.45
1:I:220:PRO:HG2	1:I:223:PHE:CD1	2.52	0.45
1:I:298:ARG:HB3	1:I:329:ALA:HB1	1.99	0.45
1:E:422:GLN:OE1	1:E:436:ALA:HA	2.17	0.44
4:L:66:ARG:HD2	4:L:82(A):THR:O	2.17	0.44
4:D:66:ARG:HD2	4:D:82(A):THR:O	2.17	0.44
1:I:354:GLY:O	1:I:357:THR:OG1	2.34	0.44
1:E:161:MET:HE2	1:E:172:VAL:HG11	1.99	0.44
1:E:220:PRO:HG2	1:E:223:PHE:CD1	2.52	0.44
1:E:219:ALA:HB2	1:E:225:ILE:HG13	2.00	0.44
1:E:62:GLU:O	1:E:63:THR:OG1	2.35	0.44
4:H:66:ARG:HD2	4:H:82(A):THR:O	2.17	0.44
1:I:85:HIS:ND1	1:I:242:VAL:O	2.36	0.44
4:L:47:TRP:O	4:L:48:ILE:HG13	2.16	0.44
3:K:37:GLN:O	3:K:45:SER:C	2.56	0.44
3:C:167:LYS:HE3	3:C:173:TYR:CE1	2.52	0.44
1:E:65:LYS:NZ	1:E:208:VAL:HG11	2.32	0.44
1:I:259:LEU:HA	1:I:451:GLY:O	2.18	0.44
3:K:46:LEU:HD23	3:K:55:PRO:HG3	1.99	0.44
1:I:327:ARG:CA	4:L:100(H):LYS:HD2	2.44	0.44
4:L:34:TRP:CZ3	4:L:94:THR:CG2	3.01	0.44
1:A:138:ILE:C	5:M:1:NAG:HN2	2.21	0.44
1:A:259:LEU:HA	1:A:451:GLY:O	2.18	0.44
1:A:260:LEU:HD21	1:A:481:SER:OG	2.18	0.44
1:A:369:LEU:HG	1:A:369:LEU:H	1.58	0.44
3:G:37:GLN:O	3:G:45:SER:C	2.56	0.44
1:I:260:LEU:HD21	1:I:481:SER:OG	2.17	0.44
1:I:440:GLN:HB3	1:I:441:GLY:H	1.53	0.44
1:A:219:ALA:HB2	1:A:225:ILE:HG13	2.00	0.44
3:C:37:GLN:O	3:C:45:SER:C	2.56	0.44
1:E:255:VAL:HG13	1:E:475:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:PHE:CD2	1:I:490:LYS:HB3	2.51	0.44
3:K:186:TRP:HH2	3:K:207:VAL:HG22	1.83	0.44
1:E:333:VAL:HG13	1:E:414:ILE:HD12	1.98	0.44
3:G:186:TRP:HH2	3:G:207:VAL:HG22	1.83	0.44
3:K:116:VAL:HG23	3:K:205:LYS:HD2	1.99	0.44
3:C:186:TRP:HH2	3:C:207:VAL:HG22	1.83	0.44
1:E:279:ASN:HB2	8:E:1276:NAG:O5	2.18	0.44
1:E:63:THR:O	1:E:208:VAL:HA	2.18	0.43
1:E:298:ARG:HG3	1:E:298:ARG:H	1.59	0.43
3:G:167:LYS:HE3	3:G:173:TYR:CE1	2.53	0.43
4:L:18:LEU:HD11	4:L:20:LEU:HD21	2.00	0.43
3:C:47:ILE:HD13	3:C:47:ILE:HA	1.87	0.43
1:I:369:LEU:HG	1:I:369:LEU:H	1.58	0.43
1:I:255:VAL:HG13	1:I:475:MET:SD	2.58	0.43
4:L:93:ALA:HA	4:L:100(R):VAL:O	2.18	0.43
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.58	0.43
1:I:422:GLN:OE1	1:I:436:ALA:HA	2.17	0.43
1:I:57:ASP:OD1	1:I:58:ALA:N	2.52	0.43
1:A:422:GLN:OE1	1:A:436:ALA:HA	2.17	0.43
1:E:416:LEU:HA	1:E:417:PRO:HD3	1.65	0.43
4:H:43:LYS:HE3	4:H:43:LYS:HB3	1.65	0.43
1:A:255:VAL:HG13	1:A:475:MET:SD	2.58	0.43
3:C:116:VAL:HG23	3:C:205:LYS:HD2	2.00	0.43
1:E:259:LEU:HA	1:E:451:GLY:O	2.18	0.43
1:I:219:ALA:HB2	1:I:225:ILE:HG13	2.00	0.43
4:L:38:ARG:O	4:L:46:GLU:C	2.57	0.43
1:A:330:HIS:CE1	1:A:415:THR:HG21	2.54	0.43
1:E:61:TYR:HB3	1:E:62:GLU:H	1.53	0.43
1:I:54:CYS:SG	1:I:215:ILE:HG23	2.59	0.43
3:K:167:LYS:HE3	3:K:173:TYR:CE1	2.53	0.43
1:A:63:THR:O	1:A:208:VAL:HA	2.18	0.43
1:E:129:LEU:HG	1:E:159:PHE:HZ	1.83	0.43
1:E:239:CYS:HA	1:E:240:PRO:HD3	1.46	0.43
4:D:111:SER:OG	4:D:111:SER:O	2.32	0.43
3:G:46:LEU:HD23	3:G:55:PRO:HG3	1.99	0.43
1:I:63:THR:O	1:I:208:VAL:HA	2.18	0.43
1:I:104:MET:HG3	1:I:217:TYR:OH	2.19	0.43
1:A:220:PRO:HG2	1:A:223:PHE:CD1	2.53	0.43
1:E:252:LYS:HB3	5:U:1:NAG:H81	2.01	0.43
3:K:47:ILE:HG23	3:K:47:ILE:HD12	1.80	0.43
1:E:93:PHE:HD2	1:E:239:CYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:43:LYS:HB3	4:L:43:LYS:HE3	1.65	0.43
1:A:292:VAL:HB	1:A:449:ILE:HB	2.01	0.42
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.58	0.42
1:E:260:LEU:HD21	1:E:481:SER:OG	2.18	0.42
1:I:301:ASN:O	1:I:302:ASN:ND2	2.52	0.42
4:D:38:ARG:O	4:D:46:GLU:C	2.57	0.42
1:A:298:ARG:HG3	1:A:298:ARG:H	1.58	0.42
1:A:453:ILE:O	1:A:454:LEU:HD23	2.19	0.42
1:I:335:LYS:HA	1:I:338:TRP:HB3	2.02	0.42
1:A:93:PHE:HD2	1:A:239:CYS:HB3	1.84	0.42
1:I:44:VAL:HB	1:I:492:GLU:HB2	2.00	0.42
1:A:129:LEU:HG	1:A:159:PHE:HZ	1.84	0.42
1:A:104:MET:HG3	1:A:217:TYR:OH	2.19	0.42
1:I:129:LEU:HG	1:I:159:PHE:HZ	1.85	0.42
1:I:239:CYS:HA	1:I:240:PRO:HD3	1.46	0.42
1:I:359:ILE:HD13	1:I:466:GLU:HB2	2.02	0.42
1:A:223:PHE:CE2	1:A:490:LYS:HB3	2.54	0.42
1:E:292:VAL:HB	1:E:449:ILE:HB	2.01	0.42
1:E:453:ILE:O	1:E:454:LEU:HD23	2.19	0.42
1:E:223:PHE:CD2	1:E:490:LYS:HB3	2.55	0.42
1:I:161:MET:SD	1:I:172:VAL:HG21	2.60	0.42
1:I:453:ILE:O	1:I:454:LEU:HD23	2.19	0.42
1:I:161:MET:O	1:I:169:LYS:HA	2.20	0.42
1:E:104:MET:HG3	1:E:217:TYR:OH	2.19	0.42
4:H:18:LEU:HD11	4:H:20:LEU:HD21	2.01	0.42
1:A:359:ILE:HD13	1:A:466:GLU:HB2	2.02	0.42
1:E:54:CYS:HA	1:E:216:HIS:O	2.20	0.42
1:I:45:TRP:HB3	1:I:489:VAL:HG21	2.02	0.42
1:E:138:ILE:C	5:S:1:NAG:HN2	2.23	0.42
1:A:330:HIS:CE1	1:A:415:THR:CG2	3.03	0.41
4:D:18:LEU:HD11	4:D:20:LEU:HD21	2.01	0.41
1:I:54:CYS:HA	1:I:216:HIS:O	2.20	0.41
1:E:335:LYS:O	1:E:339:ASN:N	2.48	0.41
1:E:335:LYS:HA	1:E:338:TRP:HB3	2.03	0.41
1:A:54:CYS:HA	1:A:216:HIS:O	2.20	0.41
4:D:197:ASN:OD1	4:D:199:LYS:HG3	2.21	0.41
1:E:436:ALA:CB	1:E:437:PRO:HD3	2.46	0.41
4:H:197:ASN:OD1	4:H:199:LYS:HG3	2.21	0.41
1:E:220:PRO:HB2	1:E:221:ALA:H	1.76	0.41
1:I:93:PHE:HD2	1:I:239:CYS:HB3	1.84	0.41
1:A:335:LYS:O	1:A:339:ASN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:38:ARG:HB3	4:L:48:ILE:HD11	2.03	0.41
1:A:301:ASN:O	1:A:302:ASN:ND2	2.54	0.41
1:A:385:CYS:O	1:A:387:THR:HG23	2.21	0.41
1:E:325:ASP:CB	3:G:94:ARG:HH11	2.33	0.41
1:A:231:LYS:HD3	1:A:231:LYS:H	1.85	0.41
1:A:279:ASN:HB2	8:A:1276:NAG:O5	2.21	0.41
1:A:44:VAL:HB	1:A:492:GLU:HB2	2.01	0.41
1:E:231:LYS:HD3	1:E:231:LYS:H	1.85	0.41
4:H:38:ARG:HB3	4:H:48:ILE:HD11	2.03	0.41
4:D:36:TRP:O	4:D:48:ILE:HB	2.21	0.41
1:E:359:ILE:HD13	1:E:466:GLU:HB2	2.02	0.41
4:H:46:GLU:O	4:H:47:TRP:O	2.39	0.41
4:H:36:TRP:O	4:H:48:ILE:HB	2.21	0.41
1:I:334:SER:HB2	8:I:1295:NAG:H83	2.02	0.41
1:I:335:LYS:HE2	1:I:339:ASN:ND2	2.36	0.41
1:I:385:CYS:O	1:I:387:THR:HG23	2.21	0.41
4:L:197:ASN:OD1	4:L:199:LYS:HG3	2.20	0.41
1:A:231:LYS:NZ	1:A:231:LYS:HB2	2.36	0.41
1:A:83:GLU:HA	1:A:244:THR:O	2.21	0.41
1:E:385:CYS:O	1:E:387:THR:HG23	2.21	0.41
1:I:231:LYS:H	1:I:231:LYS:HD3	1.85	0.41
1:I:231:LYS:NZ	1:I:231:LYS:HB2	2.36	0.41
1:I:62:GLU:HB3	1:I:63:THR:H	1.67	0.41
1:E:292:VAL:HG11	1:E:338:TRP:HE3	1.86	0.41
1:I:83:GLU:HA	1:I:244:THR:O	2.21	0.41
1:I:292:VAL:HB	1:I:449:ILE:HB	2.02	0.40
1:A:220:PRO:HB2	1:A:221:ALA:H	1.76	0.40
4:D:46:GLU:O	4:D:47:TRP:O	2.39	0.40
1:E:335:LYS:HE2	1:E:339:ASN:ND2	2.36	0.40
1:E:45:TRP:HB3	1:E:489:VAL:HG21	2.02	0.40
1:I:330:HIS:HB3	4:L:100(E):VAL:HG23	2.03	0.40
1:A:239:CYS:HA	1:A:240:PRO:HD3	1.46	0.40
1:E:331:CYS:SG	1:E:332:ASN:N	2.95	0.40
4:L:117:PRO:HB3	4:L:143:TYR:HB3	2.04	0.40
4:L:36:TRP:O	4:L:48:ILE:HB	2.21	0.40
4:L:35:SER:HB2	4:L:95:THR:OG1	2.21	0.40
4:H:30:ARG:HD3	4:H:73:LYS:HD3	2.04	0.40
1:I:345:VAL:O	1:I:349:LEU:HG	2.22	0.40
1:I:359:ILE:HD12	1:I:468:PHE:CE1	2.50	0.40
1:I:223:PHE:CE2	1:I:490:LYS:HB3	2.57	0.40
2:J:9:UNK:O	2:J:10:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:SD	1:A:172:VAL:HG21	2.61	0.40
1:A:335:LYS:HE2	1:A:339:ASN:ND2	2.36	0.40
1:A:335:LYS:HA	1:A:338:TRP:HB3	2.03	0.40
4:D:1:GLN:N	4:D:1:GLN:OE1	2.53	0.40
1:I:292:VAL:HG11	1:I:338:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/475 (87%)	349 (84%)	51 (12%)	14 (3%)	3	29
1	E	414/475 (87%)	348 (84%)	51 (12%)	15 (4%)	3	28
1	I	414/475 (87%)	348 (84%)	52 (13%)	14 (3%)	3	29
3	C	198/211 (94%)	191 (96%)	7 (4%)	0	100	100
3	G	198/211 (94%)	191 (96%)	7 (4%)	0	100	100
3	K	198/211 (94%)	192 (97%)	6 (3%)	0	100	100
4	D	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	29	68
4	H	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	29	68
4	L	220/235 (94%)	213 (97%)	6 (3%)	1 (0%)	29	68
All	All	2496/2763 (90%)	2258 (90%)	192 (8%)	46 (2%)	8	41

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	83	GLU
1	A	323	ILE

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Mol	Chain	Res	Type
1	A	429	ARG
1	E	57	ASP
1	E	83	GLU
1	E	323	ILE
1	E	429	ARG
1	I	57	ASP
1	I	83	GLU
1	I	323	ILE
1	I	429	ARG
1	A	195	ASN
1	A	322	ILE
4	D	189	THR
1	E	195	ASN
1	E	322	ILE
4	H	189	THR
1	I	195	ASN
1	I	322	ILE
4	L	189	THR
1	A	56	SER
1	E	56	SER
1	I	56	SER
1	A	63	THR
1	A	220	PRO
1	E	63	THR
1	E	220	PRO
1	I	63	THR
1	I	220	PRO
1	A	84	ILE
1	A	118	PRO
1	E	84	ILE
1	E	118	PRO
1	I	84	ILE
1	I	89	VAL
1	I	118	PRO
1	A	89	VAL
1	A	437	PRO
1	E	89	VAL
1	E	437	PRO
1	I	437	PRO
1	A	442	VAL
1	E	442	VAL
1	I	442	VAL

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Mol	Chain	Res	Type
1	E	194	ILE

### 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	317/422 (75%)	293 (92%)	24 (8%)	13	39
1	E	317/422 (75%)	293 (92%)	24 (8%)	13	39
1	I	317/422 (75%)	293 (92%)	24 (8%)	13	39
3	C	171/180 (95%)	164 (96%)	7 (4%)	30	56
3	G	171/180 (95%)	164 (96%)	7 (4%)	30	56
3	K	171/180 (95%)	163 (95%)	8 (5%)	26	52
4	D	196/205 (96%)	189 (96%)	7 (4%)	35	59
4	H	196/205 (96%)	189 (96%)	7 (4%)	35	59
4	L	196/205 (96%)	189 (96%)	7 (4%)	35	59
All	All	2052/2421 (85%)	1937 (94%)	115 (6%)	21	48

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	53	PHE
1	A	61	TYR
1	A	75	VAL
1	A	90	THR
1	A	100	MET
1	A	107	ASP
1	A	125	LEU
1	A	156	ASN
1	A	197	ASN
1	A	226	LEU
1	A	231	LYS
1	A	277	ILE

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Mol	Chain	Res	Type
1	A	298	ARG
1	A	330	HIS
1	A	357	THR
1	A	369	LEU
1	A	374	HIS
1	A	382	PHE
1	A	386	ASN
1	A	399	THR
1	A	412	ASP
1	A	414	ILE
1	A	467	THR
3	C	13	VAL
3	C	17	GLN
3	C	31	ARG
3	C	130	LYS
3	C	136	LEU
3	C	161	GLU
3	C	164	THR
4	D	1	GLN
4	D	16	GLU
4	D	69	LEU
4	D	70	SER
4	D	71	LEU
4	D	181	THR
4	D	191	THR
1	E	47	ASP
1	E	53	PHE
1	E	61	TYR
1	E	75	VAL
1	E	90	THR
1	E	100	MET
1	E	107	ASP
1	E	125	LEU
1	E	156	ASN
1	E	197	ASN
1	E	226	LEU
1	E	231	LYS
1	E	277	ILE
1	E	298	ARG
1	E	330	HIS
1	E	357	THR
1	E	369	LEU

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Mol	Chain	Res	Type
1	E	374	HIS
1	E	382	PHE
1	E	386	ASN
1	E	399	THR
1	E	412	ASP
1	E	414	ILE
1	E	467	THR
3	G	13	VAL
3	G	17	GLN
3	G	31	ARG
3	G	130	LYS
3	G	136	LEU
3	G	161	GLU
3	G	164	THR
4	H	1	GLN
4	H	16	GLU
4	H	69	LEU
4	H	70	SER
4	H	71	LEU
4	H	181	THR
4	H	191	THR
1	I	47	ASP
1	I	53	PHE
1	I	61	TYR
1	I	75	VAL
1	I	90	THR
1	I	100	MET
1	I	107	ASP
1	I	125	LEU
1	I	156	ASN
1	I	197	ASN
1	I	226	LEU
1	I	231	LYS
1	I	277	ILE
1	I	298	ARG
1	I	330	HIS
1	I	357	THR
1	I	369	LEU
1	I	374	HIS
1	I	382	PHE
1	I	386	ASN
1	I	399	THR

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Mol	Chain	Res	Type
1	I	412	ASP
1	I	414	ILE
1	I	467	THR
3	K	13	VAL
3	K	17	GLN
3	K	31	ARG
3	K	109	GLN
3	K	130	LYS
3	K	136	LEU
3	K	161	GLU
3	K	164	THR
4	L	1	GLN
4	L	16	GLU
4	L	69	LEU
4	L	70	SER
4	L	71	LEU
4	L	181	THR
4	L	191	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	374	HIS
1	E	289	ASN
1	E	330	HIS
1	E	374	HIS
1	I	289	ASN
1	I	374	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

117 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
5	NAG	M	1	1,5	14,14,15	0.57	0	17,19,21	1.37	1 (5%)
5	NAG	M	2	5	14,14,15	0.55	0	17,19,21	0.83	0
5	BMA	M	3	5	11,11,12	0.69	0	15,15,17	0.87	1 (6%)
5	MAN	M	4	5	11,11,12	0.71	0	15,15,17	0.87	0
5	MAN	M	5	5	11,11,12	0.64	0	15,15,17	0.66	0
5	MAN	M	6	5	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
5	MAN	M	7	5	11,11,12	0.60	0	15,15,17	0.68	0
5	NAG	N	1	1,5	14,14,15	0.61	0	17,19,21	1.43	3 (17%)
5	NAG	N	2	5	14,14,15	0.57	0	17,19,21	0.88	0
5	BMA	N	3	5	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
5	MAN	N	4	5	11,11,12	0.73	0	15,15,17	1.09	0
5	MAN	N	5	5	11,11,12	0.64	0	15,15,17	0.68	0
5	MAN	N	6	5	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
5	MAN	N	7	5	11,11,12	0.59	0	15,15,17	0.71	0
5	NAG	O	1	1,5	14,14,15	0.76	1 (7%)	17,19,21	1.45	3 (17%)
5	NAG	O	2	5	14,14,15	0.56	0	17,19,21	0.78	0
5	BMA	O	3	5	11,11,12	0.75	0	15,15,17	0.73	0
5	MAN	O	4	5	11,11,12	0.70	0	15,15,17	0.92	0
5	MAN	O	5	5	11,11,12	0.64	0	15,15,17	0.65	0
5	MAN	O	6	5	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	MAN	O	7	5	11,11,12	0.59	0	15,15,17	0.69	0
5	NAG	P	1	1,5	14,14,15	0.61	0	17,19,21	1.20	1 (5%)
5	NAG	P	2	5	14,14,15	0.59	0	17,19,21	0.79	0
5	BMA	P	3	5	11,11,12	0.73	0	15,15,17	0.79	1 (6%)
5	MAN	P	4	5	11,11,12	0.71	0	15,15,17	0.92	0
5	MAN	P	5	5	11,11,12	0.63	0	15,15,17	0.65	0
5	MAN	P	6	5	11,11,12	0.70	0	15,15,17	0.90	1 (6%)
5	MAN	P	7	5	11,11,12	0.59	0	15,15,17	0.68	0
6	NAG	Q	1	1,6	14,14,15	0.62	0	17,19,21	1.51	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	Q	2	6	14,14,15	0.53	0	17,19,21	1.16	2 (11%)
6	BMA	Q	3	6	11,11,12	0.71	0	15,15,17	1.37	1 (6%)
6	MAN	Q	4	6	11,11,12	0.53	0	15,15,17	0.83	0
6	MAN	Q	5	6	11,11,12	0.61	0	15,15,17	0.81	0
6	MAN	Q	6	6	11,11,12	0.66	0	15,15,17	0.74	1 (6%)
6	MAN	Q	7	6	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
6	MAN	Q	8	6	11,11,12	0.62	0	15,15,17	0.66	0
6	MAN	Q	9	6	11,11,12	0.63	0	15,15,17	0.62	0
7	MAN	R	1	7	11,11,12	0.72	0	15,15,17	1.35	2 (13%)
7	MAN	R	2	7	11,11,12	0.70	0	15,15,17	0.71	0
5	NAG	S	1	1,5	14,14,15	0.58	0	17,19,21	1.38	1 (5%)
5	NAG	S	2	5	14,14,15	0.54	0	17,19,21	0.84	0
5	BMA	S	3	5	11,11,12	0.70	0	15,15,17	0.87	1 (6%)
5	MAN	S	4	5	11,11,12	0.71	0	15,15,17	0.88	0
5	MAN	S	5	5	11,11,12	0.62	0	15,15,17	0.66	0
5	MAN	S	6	5	11,11,12	0.70	0	15,15,17	0.87	0
5	MAN	S	7	5	11,11,12	0.61	0	15,15,17	0.67	0
5	NAG	T	1	1,5	14,14,15	0.61	0	17,19,21	1.41	3 (17%)
5	NAG	T	2	5	14,14,15	0.56	0	17,19,21	0.89	0
5	BMA	T	3	5	11,11,12	0.78	0	15,15,17	0.84	1 (6%)
5	MAN	T	4	5	11,11,12	0.75	0	15,15,17	1.09	0
5	MAN	T	5	5	11,11,12	0.63	0	15,15,17	0.68	0
5	MAN	T	6	5	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	MAN	T	7	5	11,11,12	0.59	0	15,15,17	0.71	0
5	NAG	U	1	1,5	14,14,15	0.75	1 (7%)	17,19,21	1.44	3 (17%)
5	NAG	U	2	5	14,14,15	0.55	0	17,19,21	0.76	0
5	BMA	U	3	5	11,11,12	0.75	0	15,15,17	0.73	0
5	MAN	U	4	5	11,11,12	0.71	0	15,15,17	0.91	0
5	MAN	U	5	5	11,11,12	0.64	0	15,15,17	0.65	0
5	MAN	U	6	5	11,11,12	0.70	0	15,15,17	0.90	1 (6%)
5	MAN	U	7	5	11,11,12	0.60	0	15,15,17	0.69	0
5	NAG	V	1	1,5	14,14,15	0.62	0	17,19,21	1.13	1 (5%)
5	NAG	V	2	5	14,14,15	0.57	0	17,19,21	0.78	0
5	BMA	V	3	5	11,11,12	0.72	0	15,15,17	0.81	1 (6%)
5	MAN	V	4	5	11,11,12	0.71	0	15,15,17	0.92	0
5	MAN	V	5	5	11,11,12	0.65	0	15,15,17	0.66	0
5	MAN	V	6	5	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	MAN	V	7	5	11,11,12	0.61	0	15,15,17	0.68	0
6	NAG	W	1	1,6	14,14,15	0.64	0	17,19,21	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	W	2	6	14,14,15	0.58	0	17,19,21	0.84	1 (5%)
6	BMA	W	3	6	11,11,12	0.76	0	15,15,17	0.97	1 (6%)
6	MAN	W	4	6	11,11,12	0.53	0	15,15,17	0.80	0
6	MAN	W	5	6	11,11,12	0.60	0	15,15,17	0.82	0
6	MAN	W	6	6	11,11,12	0.67	0	15,15,17	0.74	1 (6%)
6	MAN	W	7	6	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
6	MAN	W	8	6	11,11,12	0.63	0	15,15,17	0.65	0
6	MAN	W	9	6	11,11,12	0.64	0	15,15,17	0.63	0
7	MAN	X	1	7	11,11,12	0.66	0	15,15,17	1.25	2 (13%)
7	MAN	X	2	7	11,11,12	0.66	0	15,15,17	0.87	0
5	NAG	Y	1	1,5	14,14,15	0.56	0	17,19,21	1.44	1 (5%)
5	NAG	Y	2	5	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	BMA	Y	3	5	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
5	MAN	Y	4	5	11,11,12	0.70	0	15,15,17	0.86	0
5	MAN	Y	5	5	11,11,12	0.64	0	15,15,17	0.65	0
5	MAN	Y	6	5	11,11,12	0.69	0	15,15,17	1.18	2 (13%)
5	MAN	Y	7	5	11,11,12	0.60	0	15,15,17	0.67	0
5	NAG	Z	1	1,5	14,14,15	0.63	0	17,19,21	1.47	2 (11%)
5	NAG	Z	2	5	14,14,15	0.59	0	17,19,21	0.88	0
5	BMA	Z	3	5	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
5	MAN	Z	4	5	11,11,12	0.75	0	15,15,17	1.10	0
5	MAN	Z	5	5	11,11,12	0.64	0	15,15,17	0.68	0
5	MAN	Z	6	5	11,11,12	0.70	0	15,15,17	0.90	1 (6%)
5	MAN	Z	7	5	11,11,12	0.57	0	15,15,17	0.71	0
5	NAG	a	1	1,5	14,14,15	0.72	0	17,19,21	1.48	3 (17%)
5	NAG	a	2	5	14,14,15	0.57	0	17,19,21	0.78	0
5	BMA	a	3	5	11,11,12	0.75	0	15,15,17	0.73	0
5	MAN	a	4	5	11,11,12	0.70	0	15,15,17	0.92	0
5	MAN	a	5	5	11,11,12	0.64	0	15,15,17	0.65	0
5	MAN	a	6	5	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	MAN	a	7	5	11,11,12	0.59	0	15,15,17	0.69	0
5	NAG	b	1	1,5	14,14,15	0.68	0	17,19,21	1.19	1 (5%)
5	NAG	b	2	5	14,14,15	0.59	0	17,19,21	0.81	0
5	BMA	b	3	5	11,11,12	0.74	0	15,15,17	0.79	0
5	MAN	b	4	5	11,11,12	0.71	0	15,15,17	0.92	0
5	MAN	b	5	5	11,11,12	0.64	0	15,15,17	0.66	0
5	MAN	b	6	5	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
5	MAN	b	7	5	11,11,12	0.60	0	15,15,17	0.68	0
6	NAG	c	1	1,6	14,14,15	0.57	0	17,19,21	1.57	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	c	2	6	14,14,15	0.58	0	17,19,21	1.19	1 (5%)
6	BMA	c	3	6	11,11,12	0.71	0	15,15,17	1.44	1 (6%)
6	MAN	c	4	6	11,11,12	0.52	0	15,15,17	0.83	0
6	MAN	c	5	6	11,11,12	0.60	0	15,15,17	0.82	0
6	MAN	c	6	6	11,11,12	0.67	0	15,15,17	0.75	1 (6%)
6	MAN	c	7	6	11,11,12	0.67	0	15,15,17	1.19	1 (6%)
6	MAN	c	8	6	11,11,12	0.62	0	15,15,17	0.65	0
6	MAN	c	9	6	11,11,12	0.64	0	15,15,17	0.62	0
7	MAN	d	1	7	11,11,12	0.73	0	15,15,17	1.34	2 (13%)
7	MAN	d	2	7	11,11,12	0.75	0	15,15,17	0.84	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
5	NAG	M	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	MAN	N	4	5	-	1/2/19/22	0/1/1/1
5	MAN	N	5	5	-	0/2/19/22	0/1/1/1
5	MAN	N	6	5	-	0/2/19/22	0/1/1/1
5	MAN	N	7	5	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	2/2/19/22	0/1/1/1
5	MAN	O	5	5	-	0/2/19/22	0/1/1/1
5	MAN	O	6	5	-	0/2/19/22	0/1/1/1
5	MAN	O	7	5	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	P	4	5	-	2/2/19/22	0/1/1/1
5	MAN	P	5	5	-	0/2/19/22	0/1/1/1
5	MAN	P	6	5	-	0/2/19/22	0/1/1/1
5	MAN	P	7	5	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	6	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	7	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	8	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	9	6	-	0/2/19/22	0/1/1/1
7	MAN	R	1	7	-	2/2/19/22	0/1/1/1
7	MAN	R	2	7	-	0/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	MAN	S	4	5	-	0/2/19/22	0/1/1/1
5	MAN	S	5	5	-	0/2/19/22	0/1/1/1
5	MAN	S	6	5	-	0/2/19/22	0/1/1/1
5	MAN	S	7	5	-	0/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	MAN	T	4	5	-	1/2/19/22	0/1/1/1
5	MAN	T	5	5	-	0/2/19/22	0/1/1/1
5	MAN	T	6	5	-	0/2/19/22	0/1/1/1
5	MAN	T	7	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
5	MAN	U	4	5	-	2/2/19/22	0/1/1/1
5	MAN	U	5	5	-	0/2/19/22	0/1/1/1
5	MAN	U	6	5	-	0/2/19/22	0/1/1/1
5	MAN	U	7	5	-	0/2/19/22	0/1/1/1
5	NAG	V	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	BMA	V	3	5	-	0/2/19/22	0/1/1/1
5	MAN	V	4	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	V	5	5	-	0/2/19/22	0/1/1/1
5	MAN	V	6	5	-	0/2/19/22	0/1/1/1
5	MAN	V	7	5	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	2/2/19/22	0/1/1/1
6	MAN	W	6	6	-	0/2/19/22	0/1/1/1
6	MAN	W	7	6	-	2/2/19/22	0/1/1/1
6	MAN	W	8	6	-	0/2/19/22	0/1/1/1
6	MAN	W	9	6	-	0/2/19/22	0/1/1/1
7	MAN	X	1	7	-	2/2/19/22	1/1/1/1
7	MAN	X	2	7	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	5	5	-	0/2/19/22	0/1/1/1
5	MAN	Y	6	5	-	2/2/19/22	0/1/1/1
5	MAN	Y	7	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	1/2/19/22	0/1/1/1
5	MAN	Z	5	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	6	5	-	0/2/19/22	0/1/1/1
5	MAN	Z	7	5	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	MAN	a	4	5	-	2/2/19/22	0/1/1/1
5	MAN	a	5	5	-	0/2/19/22	0/1/1/1
5	MAN	a	6	5	-	0/2/19/22	0/1/1/1
5	MAN	a	7	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	b	6	5	-	0/2/19/22	0/1/1/1
5	MAN	b	7	5	-	0/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	0/2/19/22	0/1/1/1
6	MAN	c	5	6	-	2/2/19/22	0/1/1/1
6	MAN	c	6	6	-	0/2/19/22	0/1/1/1
6	MAN	c	7	6	-	2/2/19/22	0/1/1/1
6	MAN	c	8	6	-	0/2/19/22	0/1/1/1
6	MAN	c	9	6	-	0/2/19/22	0/1/1/1
7	MAN	d	1	7	-	2/2/19/22	0/1/1/1
7	MAN	d	2	7	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	1	NAG	O5-C1	-2.02	1.40	1.43
5	O	1	NAG	O5-C1	-2.01	1.40	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	c	3	BMA	C1-C2-C3	4.35	115.01	109.67
6	Q	3	BMA	C1-C2-C3	4.13	114.75	109.67
5	Y	1	NAG	C4-C3-C2	4.11	117.05	111.02
5	S	1	NAG	C4-C3-C2	3.87	116.69	111.02
5	M	1	NAG	C4-C3-C2	3.84	116.65	111.02
7	d	1	MAN	O5-C1-C2	3.65	116.40	110.77
7	X	1	MAN	O5-C1-C2	3.63	116.37	110.77
6	W	1	NAG	C3-C4-C5	3.53	116.53	110.24
6	c	1	NAG	C3-C4-C5	3.52	116.52	110.24
5	O	1	NAG	C3-C4-C5	3.50	116.47	110.24
5	a	1	NAG	C3-C4-C5	3.49	116.47	110.24
6	c	1	NAG	O5-C1-C2	-3.45	105.83	111.29
7	R	1	MAN	O5-C1-C2	3.45	116.10	110.77
6	Q	1	NAG	C3-C4-C5	3.43	116.36	110.24
5	U	1	NAG	C3-C4-C5	3.39	116.28	110.24
5	Z	1	NAG	C3-C4-C5	3.38	116.27	110.24
6	W	1	NAG	O5-C1-C2	-3.30	106.08	111.29
5	T	1	NAG	O5-C1-C2	-3.21	106.22	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	1	NAG	O5-C1-C2	-3.21	106.23	111.29
5	Z	1	NAG	O5-C1-C2	-3.16	106.29	111.29
5	N	1	NAG	O5-C1-C2	-3.15	106.31	111.29
6	c	7	MAN	O5-C5-C6	2.97	111.87	107.20
5	N	1	NAG	C3-C4-C5	2.96	115.53	110.24
5	U	1	NAG	C4-C3-C2	2.89	115.26	111.02
5	O	1	NAG	C4-C3-C2	2.84	115.18	111.02
5	T	1	NAG	C3-C4-C5	2.81	115.26	110.24
5	a	1	NAG	C4-C3-C2	2.81	115.14	111.02
6	W	3	BMA	C1-C2-C3	2.77	113.08	109.67
5	Y	3	BMA	C1-C2-C3	2.75	113.05	109.67
6	W	7	MAN	O5-C5-C6	2.70	111.43	107.20
6	Q	7	MAN	O5-C5-C6	2.67	111.38	107.20
5	b	1	NAG	C4-C3-C2	2.60	114.83	111.02
5	V	1	NAG	C4-C3-C2	2.59	114.81	111.02
5	Y	6	MAN	O5-C5-C6	2.54	111.19	107.20
5	P	1	NAG	C4-C3-C2	2.50	114.68	111.02
5	T	6	MAN	O5-C1-C2	-2.47	106.96	110.77
5	Z	6	MAN	O5-C1-C2	-2.46	106.97	110.77
5	N	6	MAN	O5-C1-C2	-2.46	106.97	110.77
5	O	6	MAN	O5-C1-C2	-2.46	106.97	110.77
6	c	2	NAG	C3-C4-C5	2.45	114.61	110.24
5	a	6	MAN	O5-C1-C2	-2.45	106.99	110.77
7	d	1	MAN	O5-C5-C6	2.45	111.04	107.20
5	V	6	MAN	O5-C1-C2	-2.44	107.01	110.77
5	Y	6	MAN	C2-C3-C4	-2.43	106.69	110.89
5	P	6	MAN	O5-C1-C2	-2.42	107.03	110.77
5	U	6	MAN	O5-C1-C2	-2.41	107.04	110.77
5	S	3	BMA	C1-C2-C3	2.41	112.63	109.67
6	Q	1	NAG	C4-C3-C2	2.41	114.55	111.02
5	b	6	MAN	O5-C1-C2	-2.41	107.06	110.77
6	c	1	NAG	C4-C3-C2	2.39	114.52	111.02
5	M	3	BMA	C1-C2-C3	2.37	112.58	109.67
7	R	1	MAN	O5-C5-C6	2.31	110.83	107.20
5	a	1	NAG	O5-C1-C2	-2.31	107.64	111.29
6	W	1	NAG	C4-C3-C2	2.29	114.38	111.02
6	Q	2	NAG	C3-C4-C5	2.27	114.29	110.24
5	U	1	NAG	O5-C1-C2	-2.25	107.73	111.29
5	T	3	BMA	C1-C2-C3	2.22	112.39	109.67
5	O	1	NAG	O5-C1-C2	-2.18	107.85	111.29
5	M	6	MAN	C2-C3-C4	-2.15	107.17	110.89
5	V	3	BMA	C1-C2-C3	2.13	112.28	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	2	NAG	O5-C5-C6	2.13	110.54	107.20
5	N	3	BMA	C1-C2-C3	2.13	112.28	109.67
5	M	6	MAN	O5-C5-C6	2.12	110.53	107.20
5	T	1	NAG	C4-C3-C2	2.10	114.10	111.02
6	Q	2	NAG	O5-C5-C6	2.10	110.50	107.20
5	Z	3	BMA	C1-C2-C3	2.05	112.19	109.67
6	c	6	MAN	O5-C1-C2	-2.05	107.61	110.77
7	X	1	MAN	O5-C5-C6	2.05	110.42	107.20
6	W	6	MAN	O5-C1-C2	-2.04	107.62	110.77
5	Y	2	NAG	O5-C1-C2	-2.03	108.08	111.29
6	Q	6	MAN	O5-C1-C2	-2.03	107.64	110.77
5	N	1	NAG	C4-C3-C2	2.03	113.99	111.02
5	P	3	BMA	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
7	X	1	MAN	O5-C5-C6-O6
7	R	1	MAN	O5-C5-C6-O6
7	d	1	MAN	O5-C5-C6-O6
6	W	7	MAN	C4-C5-C6-O6
6	Q	7	MAN	C4-C5-C6-O6
6	c	7	MAN	C4-C5-C6-O6
6	W	5	MAN	O5-C5-C6-O6
6	Q	5	MAN	O5-C5-C6-O6
5	Y	1	NAG	C8-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
6	c	5	MAN	O5-C5-C6-O6
7	X	1	MAN	C4-C5-C6-O6
7	R	1	MAN	C4-C5-C6-O6
5	M	1	NAG	O7-C7-N2-C2
7	d	1	MAN	C4-C5-C6-O6
6	W	7	MAN	O5-C5-C6-O6
6	Q	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	c	7	MAN	O5-C5-C6-O6
5	Y	1	NAG	O7-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
6	Q	5	MAN	C4-C5-C6-O6
5	U	4	MAN	O5-C5-C6-O6
5	O	4	MAN	O5-C5-C6-O6
5	a	4	MAN	O5-C5-C6-O6
6	W	5	MAN	C4-C5-C6-O6
6	c	5	MAN	C4-C5-C6-O6
5	V	4	MAN	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
5	Y	6	MAN	C4-C5-C6-O6
5	Y	6	MAN	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
5	T	4	MAN	O5-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	S	1	NAG	C1-C2-N2-C7
5	Y	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C4-C5-C6-O6
5	U	4	MAN	C4-C5-C6-O6
5	O	4	MAN	C4-C5-C6-O6
5	a	4	MAN	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
5	V	4	MAN	C4-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6
5	P	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	1	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 19 short contacts:

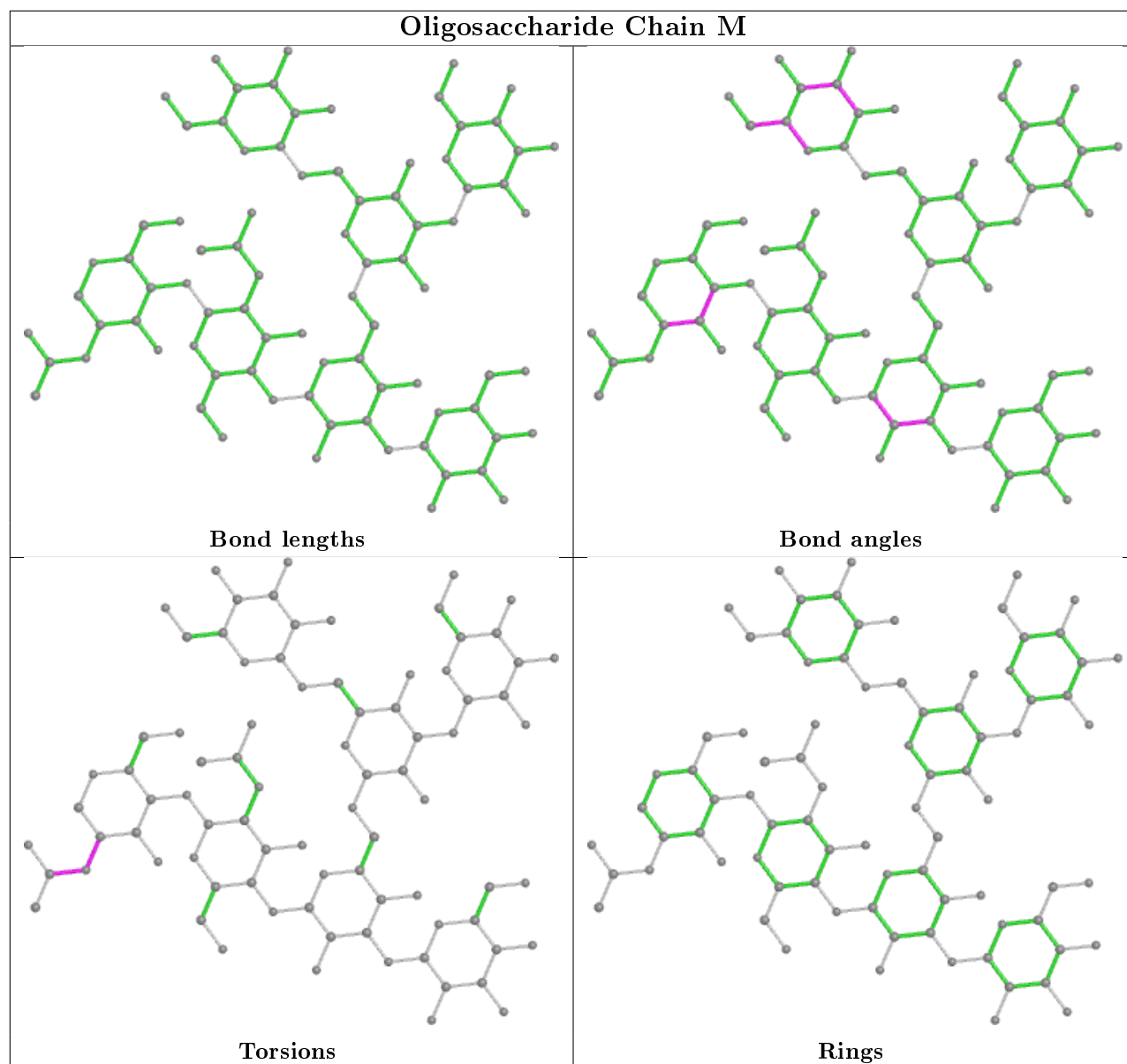
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	2	NAG	2	0
5	Y	6	MAN	1	0
5	U	1	NAG	5	0

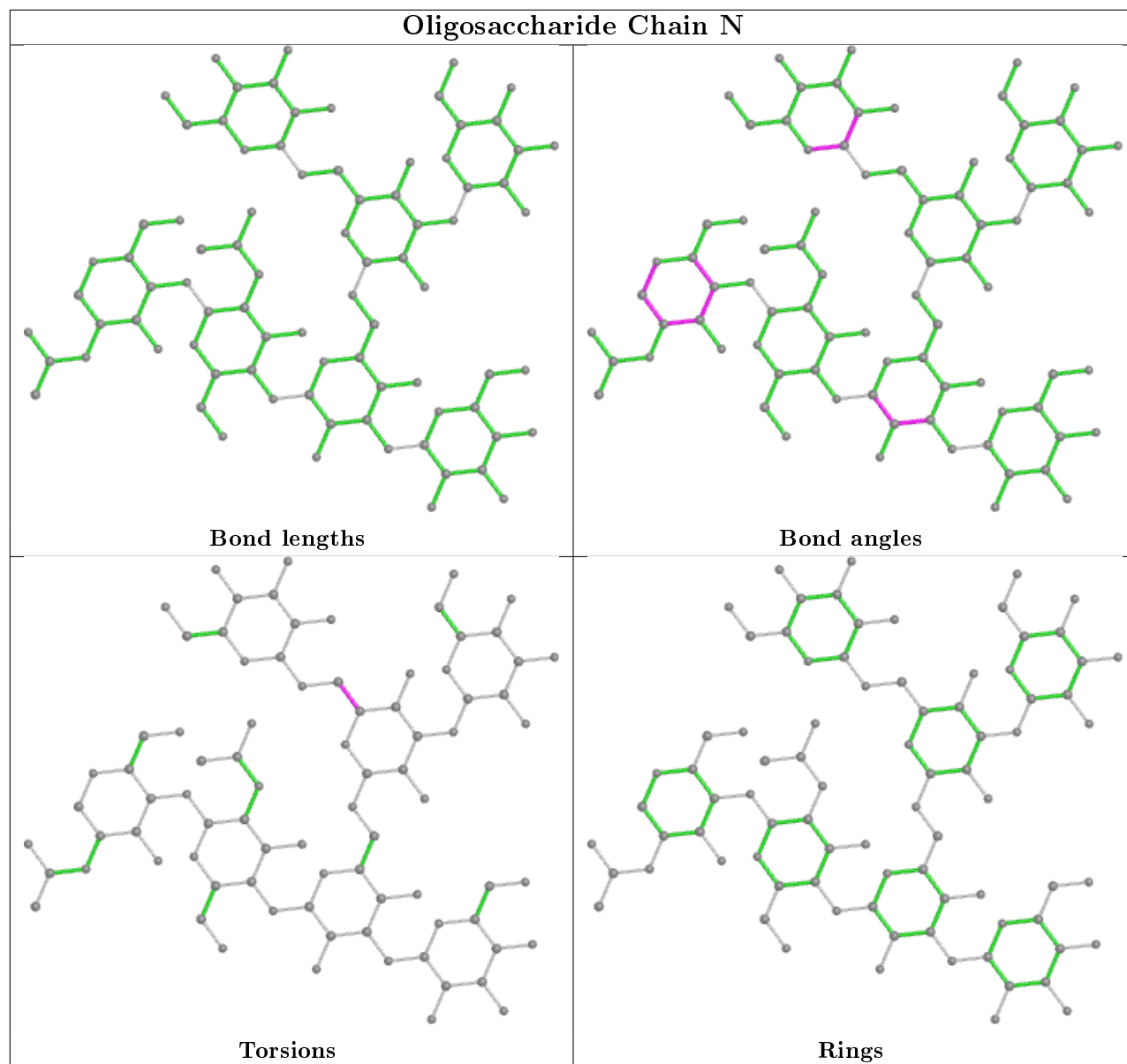
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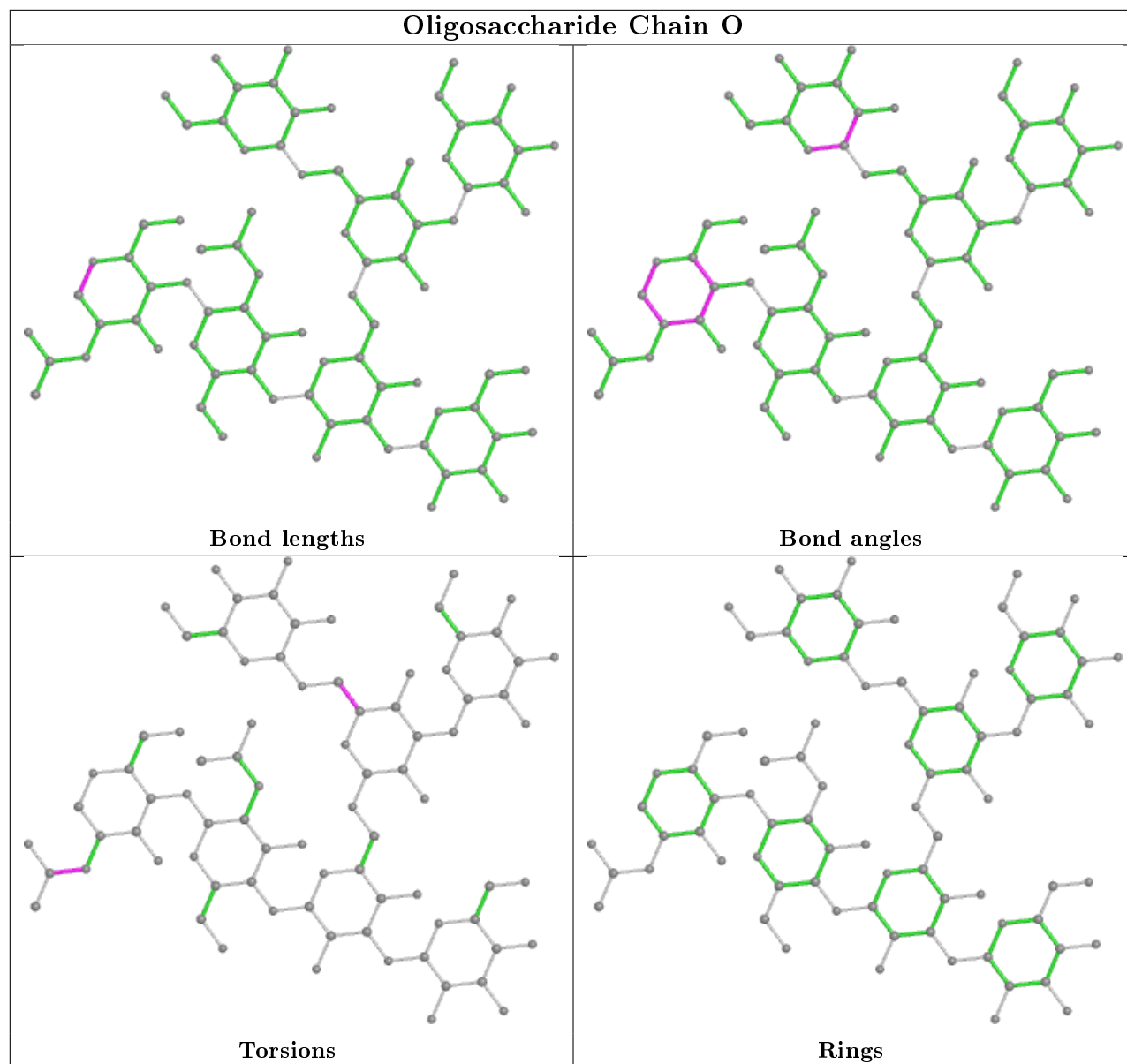
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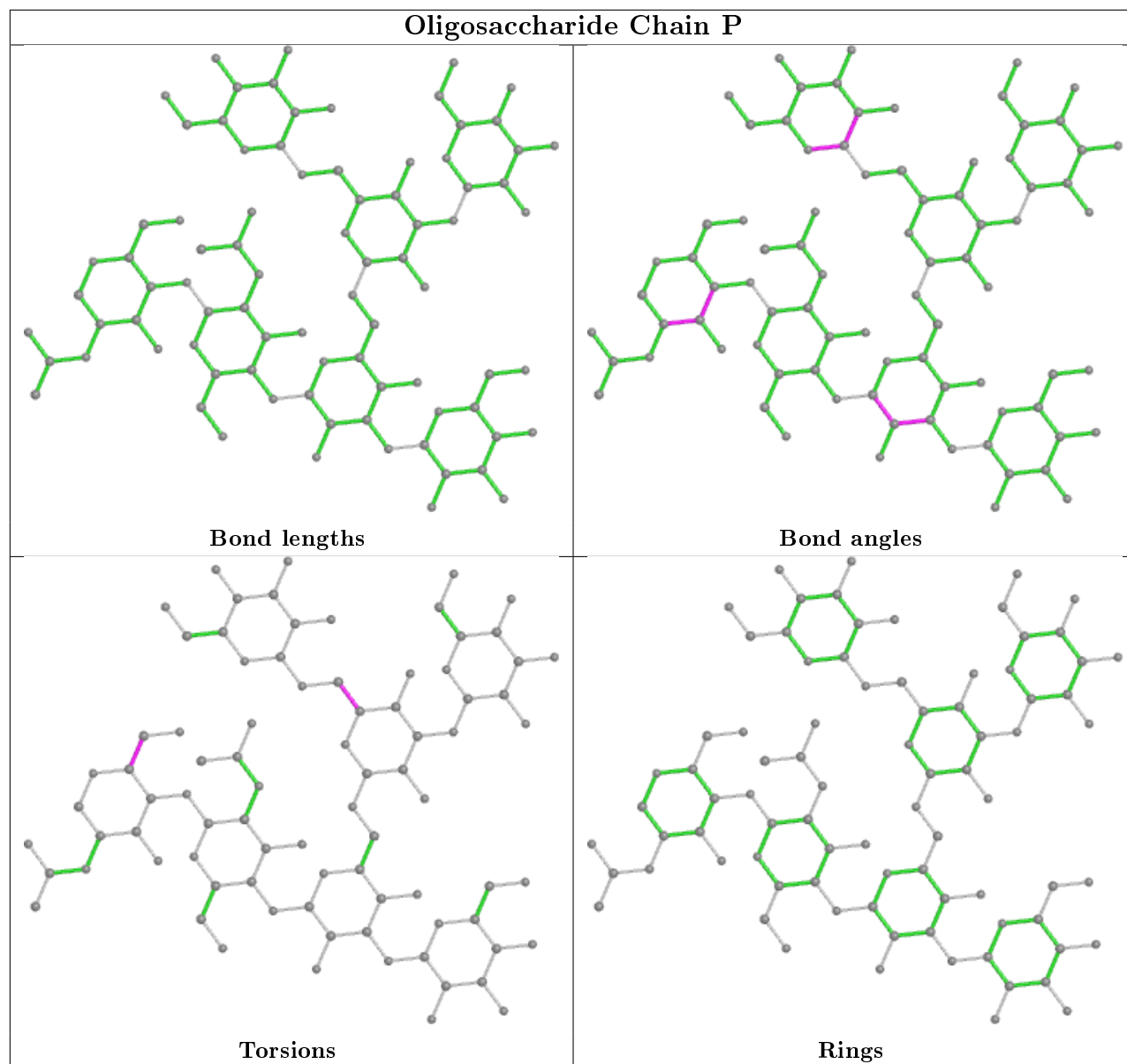
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	1	NAG	1	0
7	X	2	MAN	1	0
7	R	1	MAN	2	0
7	R	2	MAN	1	0
5	O	1	NAG	5	0
5	M	1	NAG	1	0

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

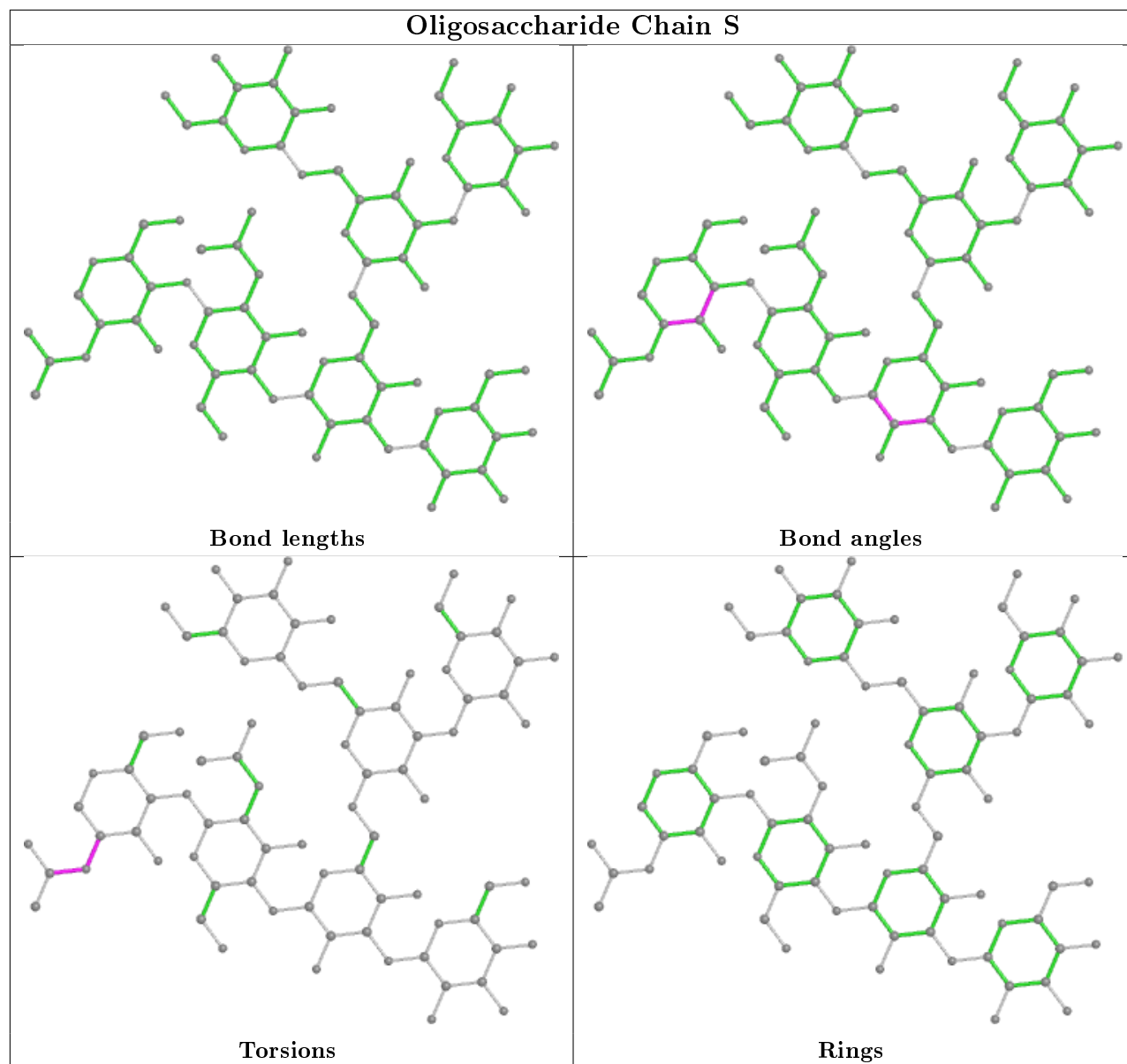


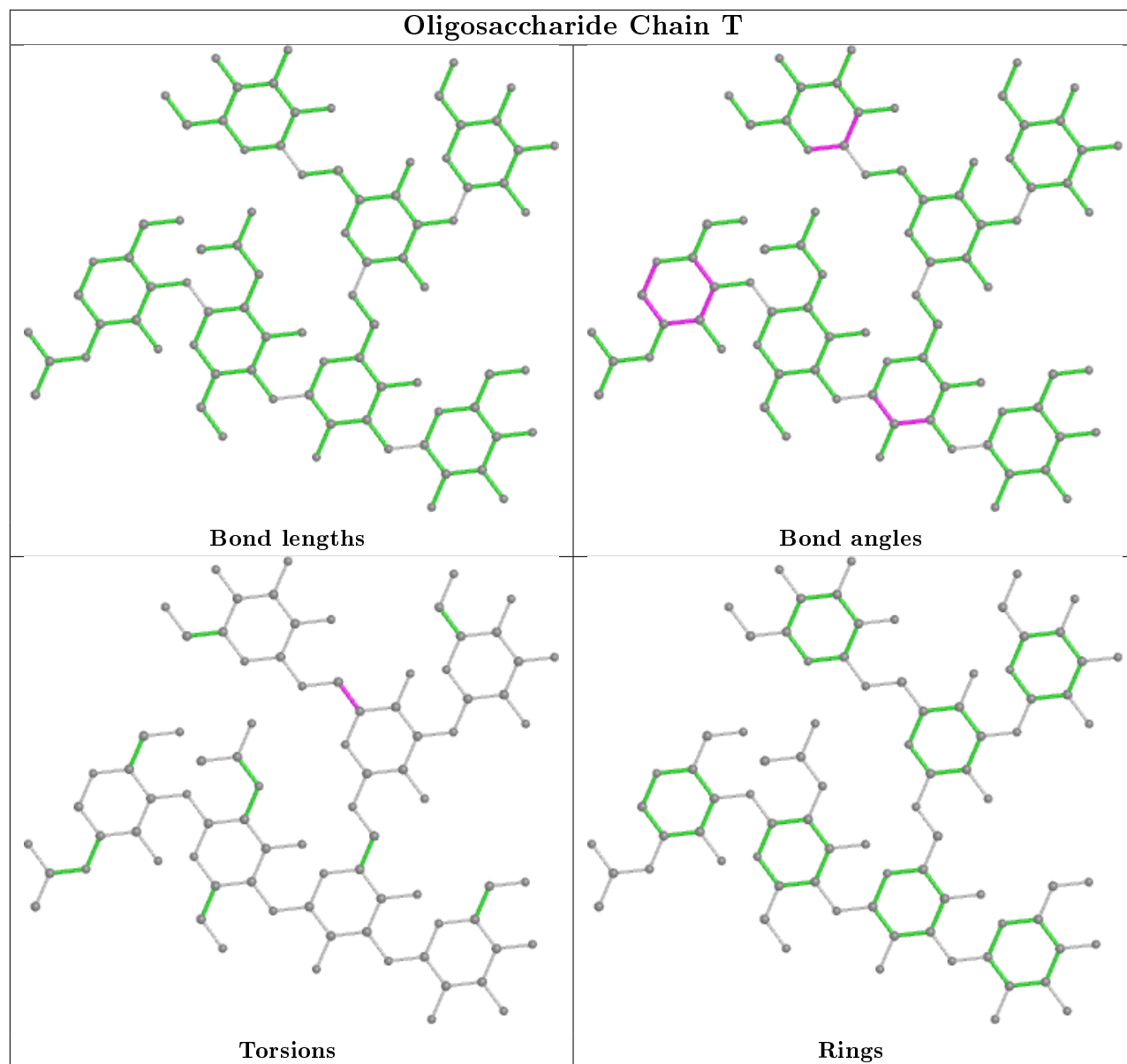


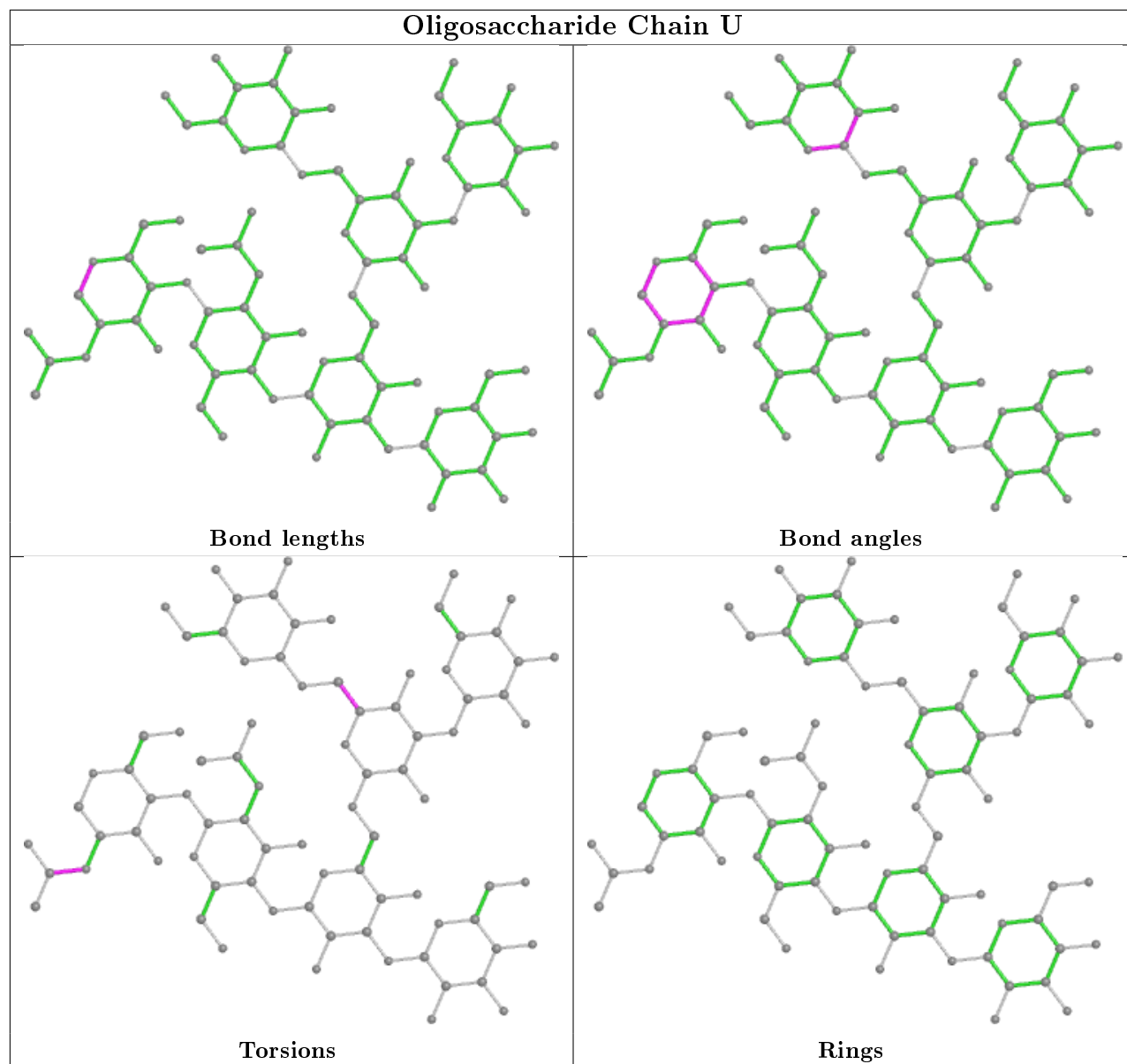


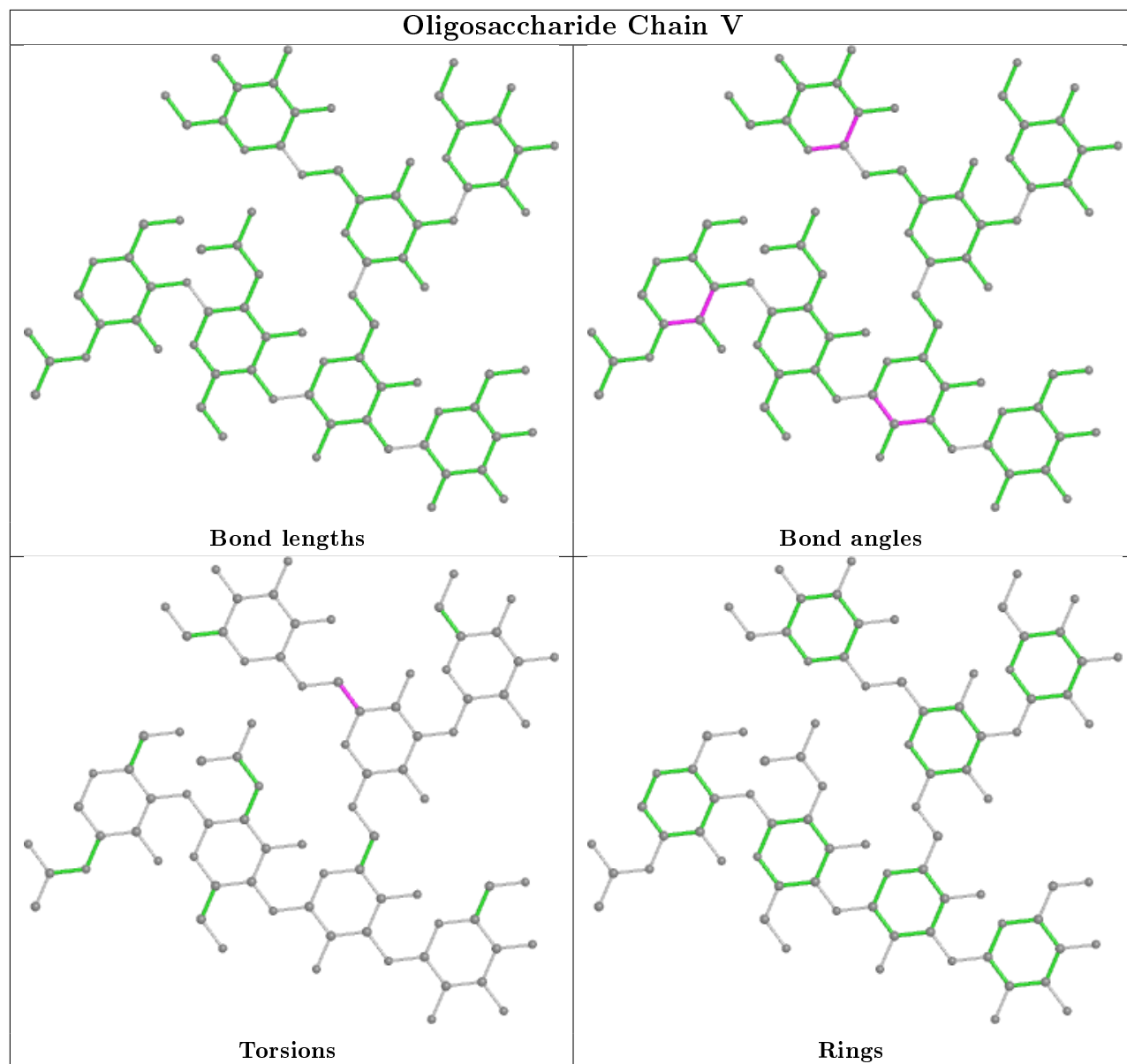


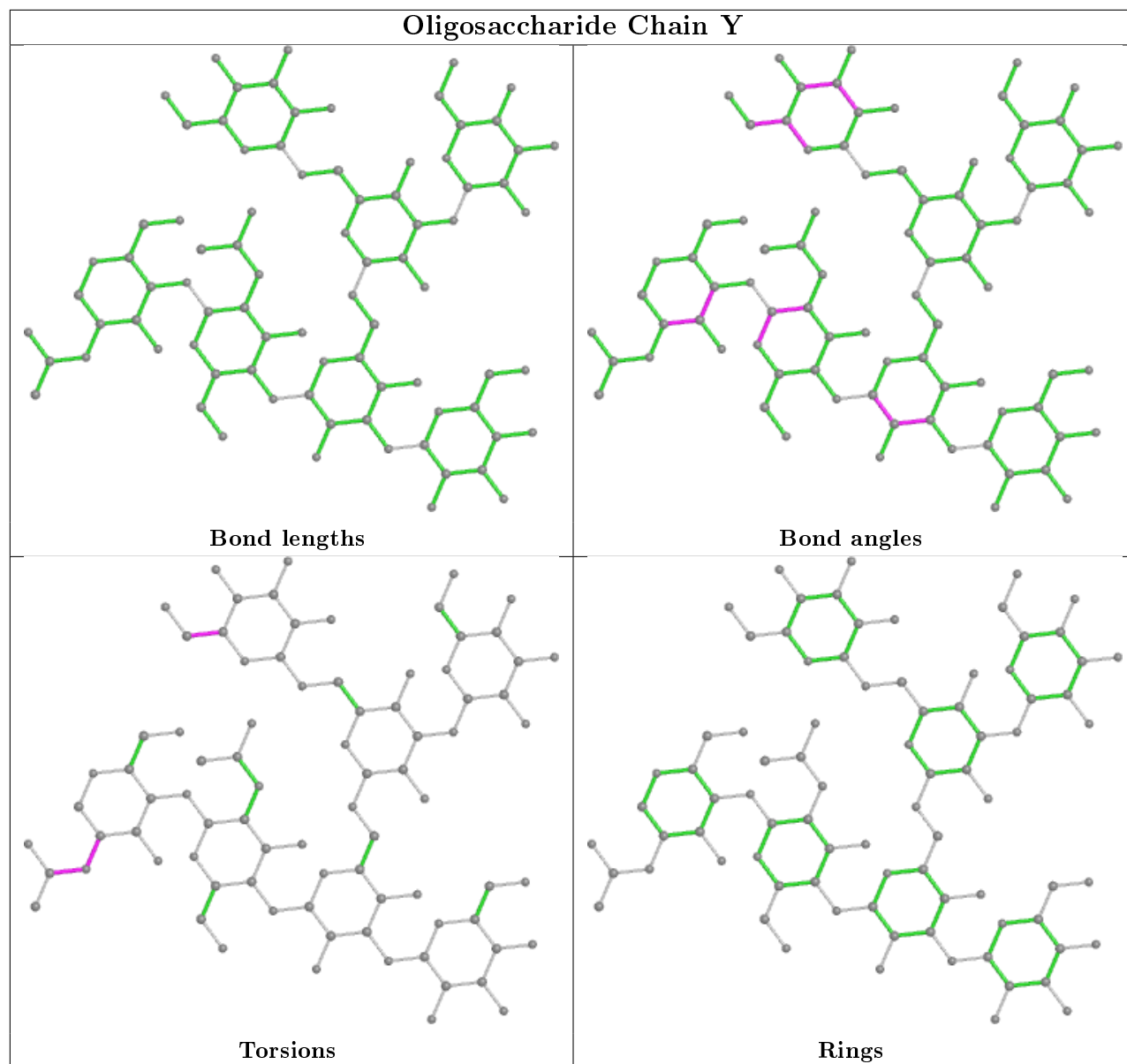


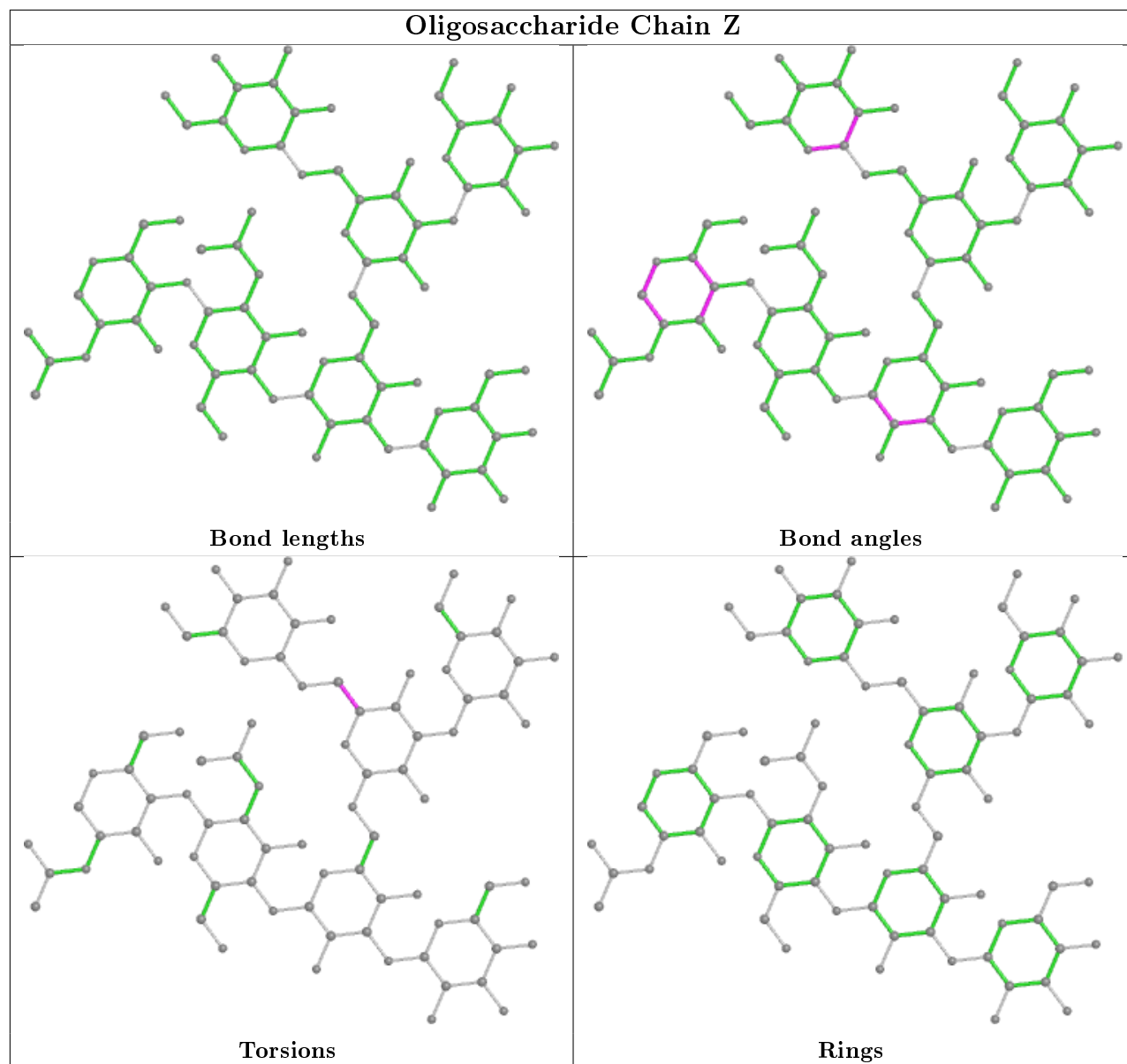


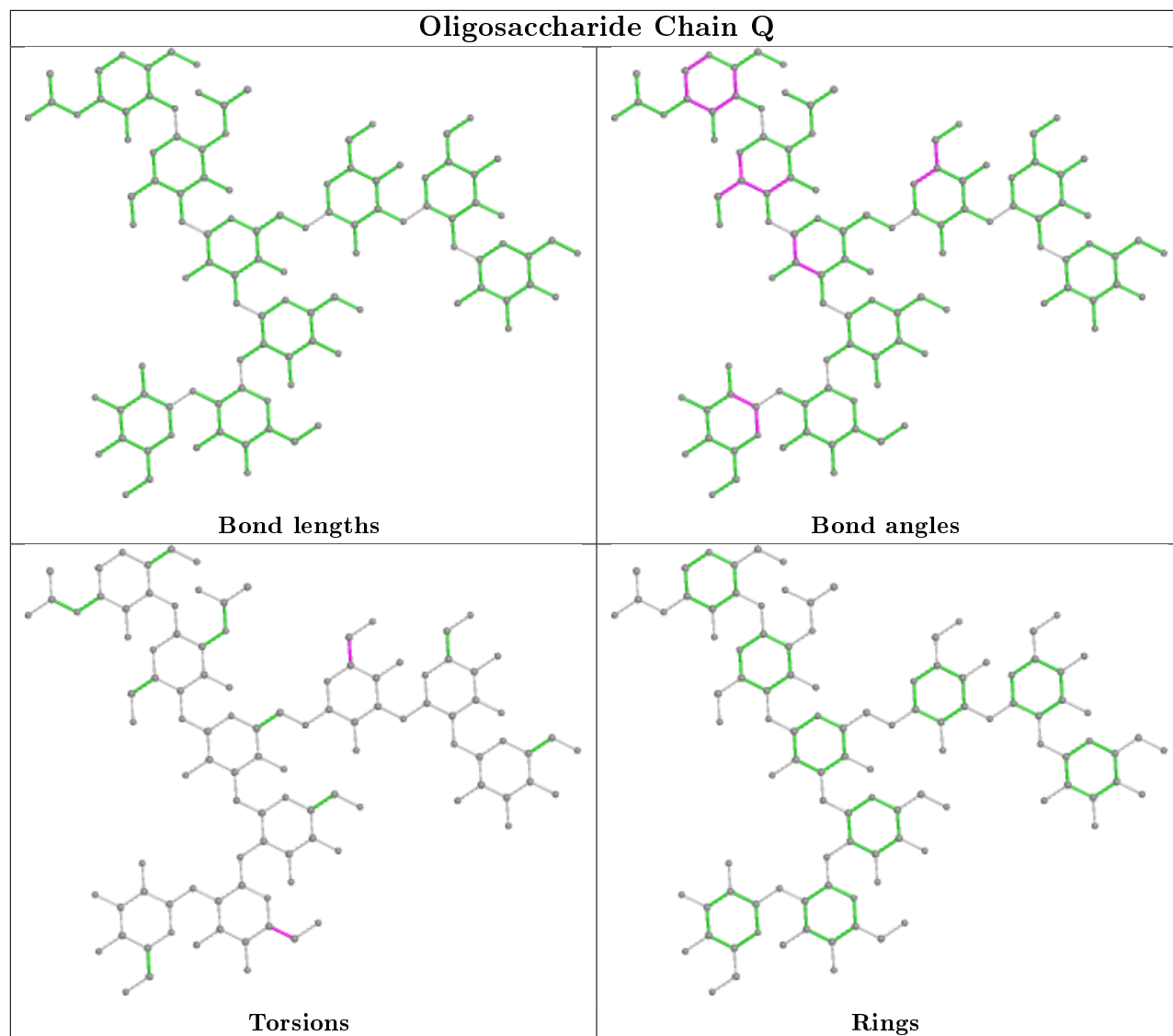


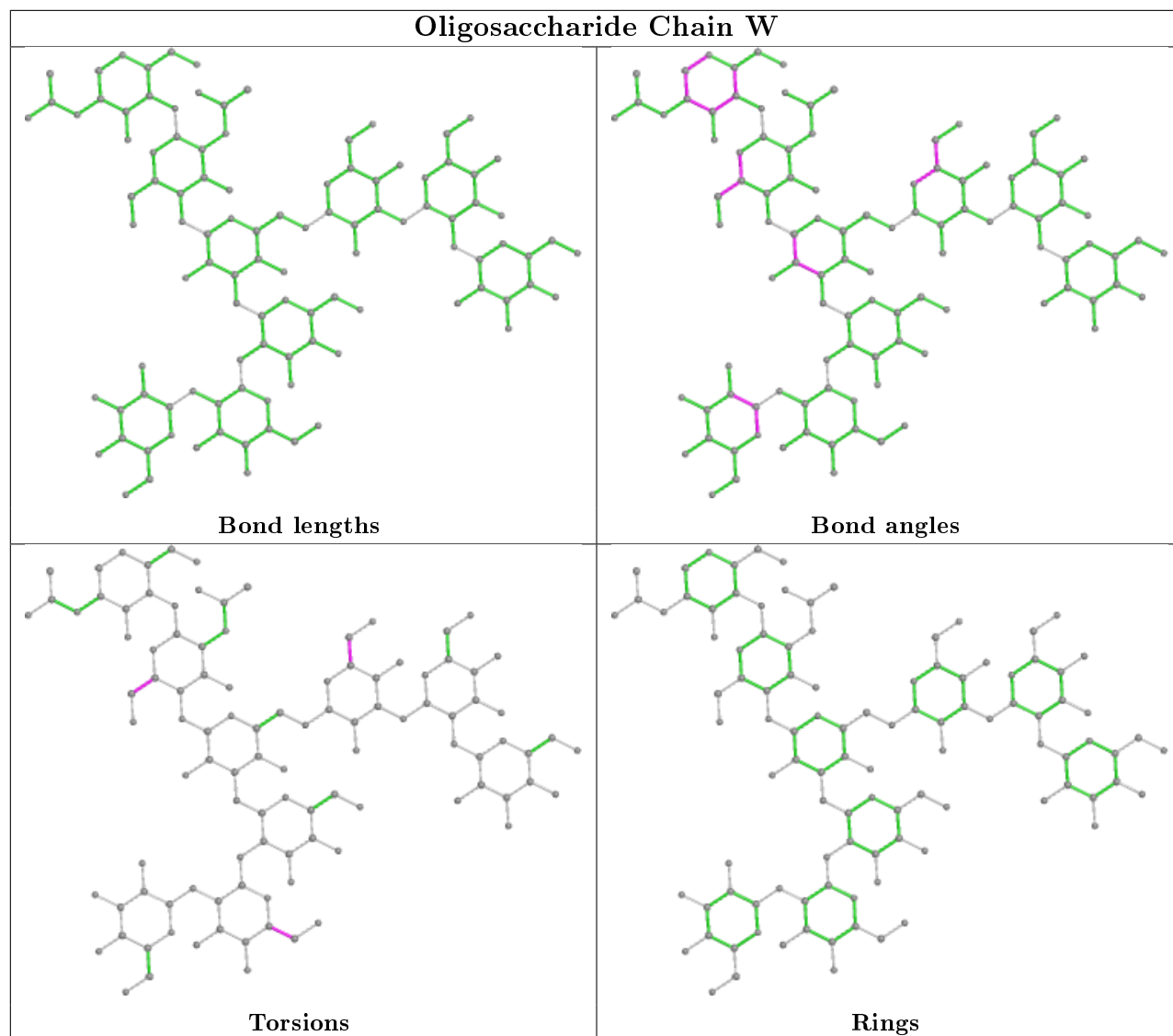




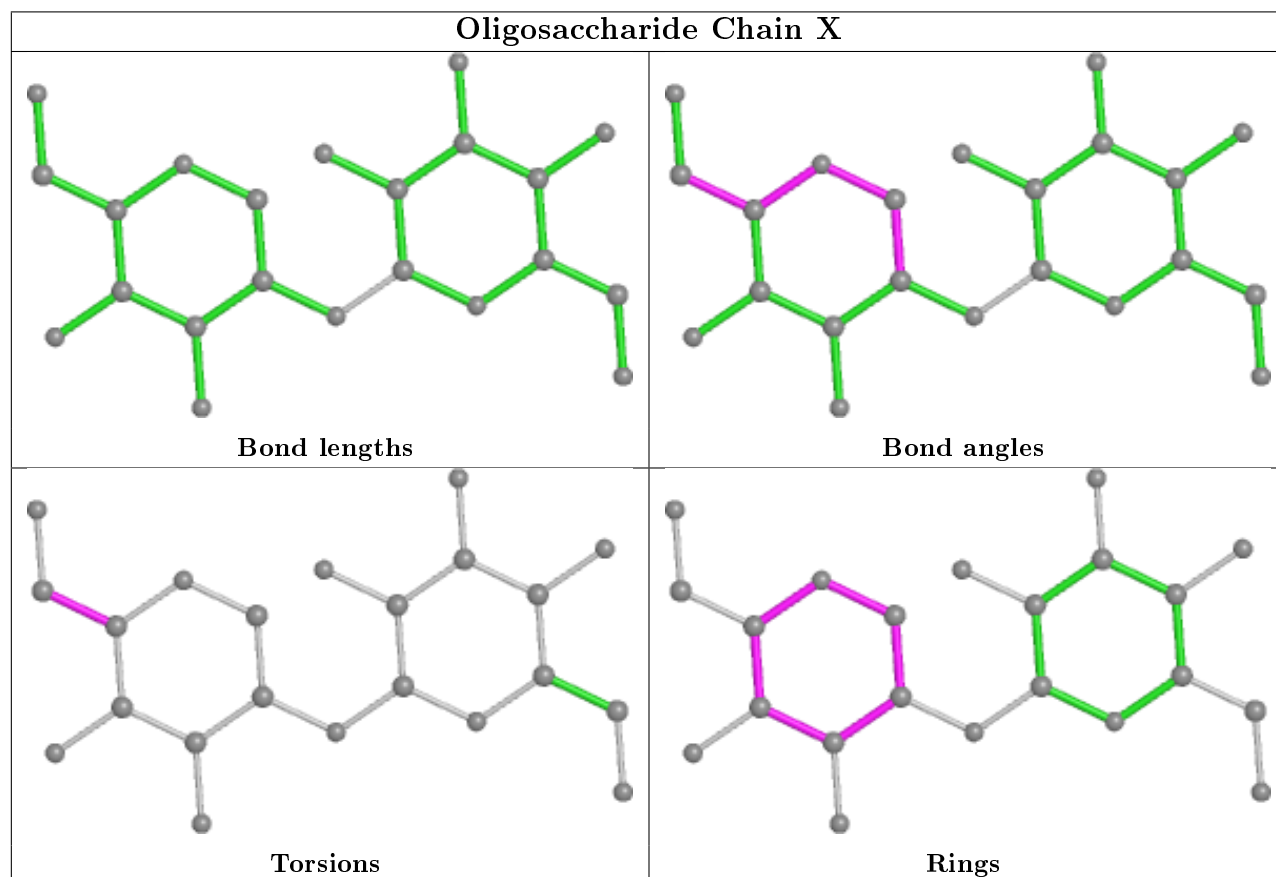
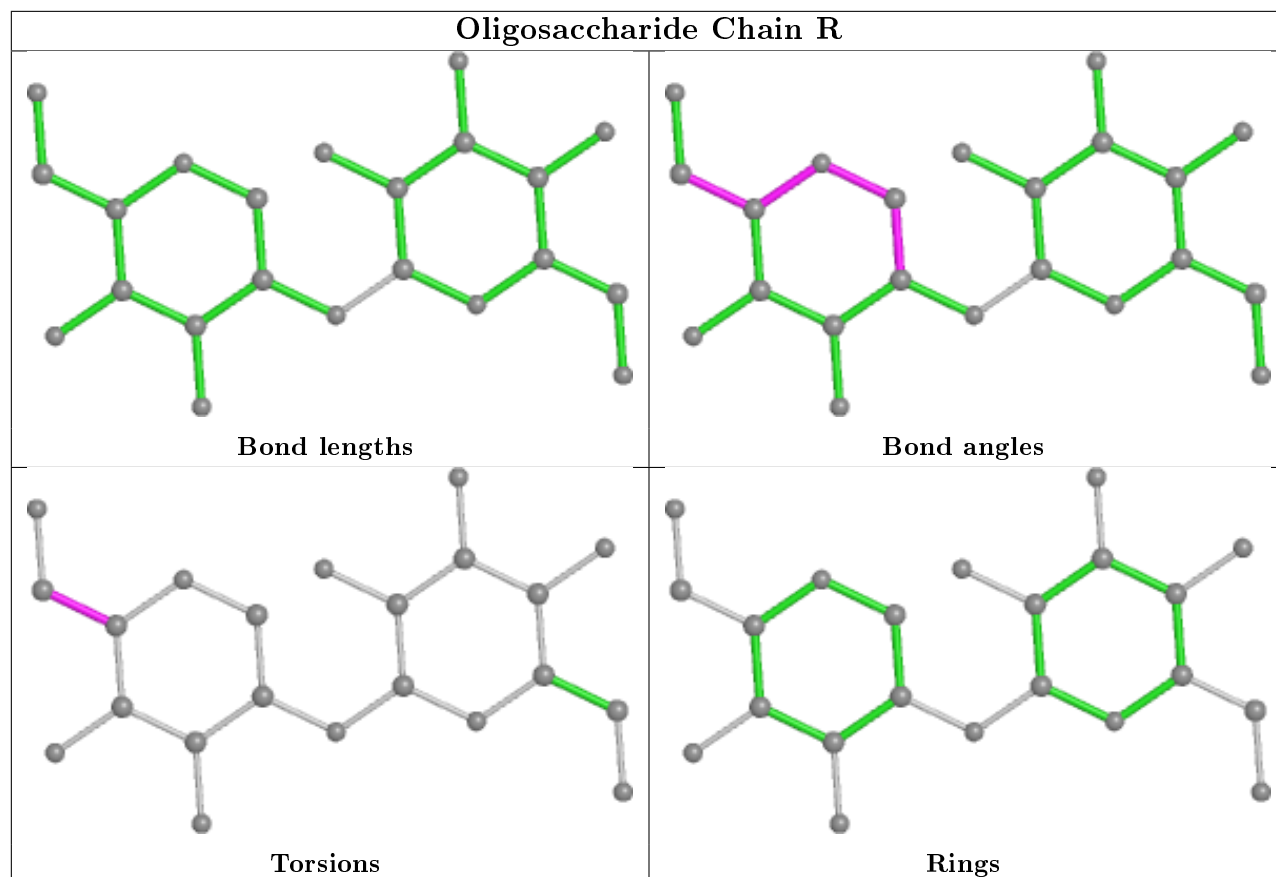












## 5.6 Ligand geometry

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	I	1386	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
8	NAG	I	1088	1	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
8	NAG	E	1355	1	14,14,15	0.51	0	17,19,21	0.75	0
8	NAG	E	1386	1	14,14,15	0.58	0	17,19,21	0.76	0
8	NAG	A	1088	1	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
8	NAG	A	1160	1	14,14,15	0.50	0	17,19,21	0.78	0
8	NAG	I	1448	1	14,14,15	0.46	0	17,19,21	1.56	3 (17%)
8	NAG	I	1197	1	14,14,15	0.50	0	17,19,21	0.83	0
8	NAG	E	1276	1	14,14,15	0.45	0	17,19,21	1.25	2 (11%)
8	NAG	A	1295	1	14,14,15	0.54	0	17,19,21	0.74	0
8	NAG	I	1234	1	14,14,15	0.47	0	17,19,21	1.18	2 (11%)
8	NAG	E	1392	1	14,14,15	0.49	0	17,19,21	0.71	0
8	NAG	E	1088	1	14,14,15	0.56	0	17,19,21	0.75	0
8	NAG	A	1234	1	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
8	NAG	A	1392	1	14,14,15	0.46	0	17,19,21	0.75	0
8	NAG	E	1234	1	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
8	NAG	A	1197	1	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
8	NAG	I	1392	1	14,14,15	0.43	0	17,19,21	0.80	0
8	NAG	I	1276	1	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
8	NAG	E	1448	1	14,14,15	0.50	0	17,19,21	1.53	3 (17%)
8	NAG	E	1197	1	14,14,15	0.47	0	17,19,21	0.82	0
8	NAG	I	1355	1	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
8	NAG	I	1295	1	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
8	NAG	E	1160	1	14,14,15	0.50	0	17,19,21	0.73	0
8	NAG	E	1295	1	14,14,15	0.51	0	17,19,21	0.77	0
8	NAG	A	1386	1	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
8	NAG	A	1276	1	14,14,15	0.41	0	17,19,21	1.19	1 (5%)
8	NAG	A	1355	1	14,14,15	0.50	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	A	1448	1	14,14,15	0.51	0	17,19,21	1.47	3 (17%)
8	NAG	I	1160	1	14,14,15	0.42	0	17,19,21	0.91	1 (5%)

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
8	NAG	I	1386	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1386	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1160	1	-	2/6/23/26	0/1/1/1
8	NAG	I	1448	1	-	4/6/23/26	0/1/1/1
8	NAG	I	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1088	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1234	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1392	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1448	1	-	4/6/23/26	0/1/1/1
8	NAG	E	1197	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	I	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	E	1160	1	-	2/6/23/26	0/1/1/1
8	NAG	E	1295	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1386	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1276	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1448	1	-	4/6/23/26	0/1/1/1
8	NAG	I	1160	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1448	NAG	C1-O5-C5	3.33	116.71	112.19
8	E	1448	NAG	C1-O5-C5	3.31	116.68	112.19
8	A	1448	NAG	C1-O5-C5	3.09	116.38	112.19
8	A	1276	NAG	C1-O5-C5	2.99	116.25	112.19
8	E	1276	NAG	C1-O5-C5	2.97	116.21	112.19
8	I	1448	NAG	O5-C1-C2	-2.81	106.86	111.29
8	E	1448	NAG	O5-C1-C2	-2.80	106.87	111.29
8	A	1448	NAG	O5-C1-C2	-2.69	107.04	111.29
8	A	1234	NAG	C1-O5-C5	2.61	115.73	112.19
8	I	1276	NAG	C1-O5-C5	2.53	115.62	112.19
8	A	1088	NAG	C1-O5-C5	2.42	115.47	112.19
8	I	1088	NAG	C1-O5-C5	2.41	115.46	112.19
8	I	1448	NAG	C2-N2-C7	-2.39	119.50	122.90
8	E	1448	NAG	C2-N2-C7	-2.30	119.64	122.90
8	I	1234	NAG	O5-C1-C2	-2.28	107.68	111.29
8	A	1197	NAG	C1-O5-C5	2.25	115.25	112.19
8	E	1234	NAG	O5-C1-C2	-2.24	107.74	111.29
8	A	1448	NAG	C2-N2-C7	-2.24	119.71	122.90
8	I	1160	NAG	C1-O5-C5	2.23	115.21	112.19
8	E	1276	NAG	O5-C1-C2	-2.16	107.88	111.29
8	I	1234	NAG	C1-O5-C5	2.12	115.06	112.19
8	A	1234	NAG	O5-C1-C2	-2.09	107.99	111.29
8	E	1234	NAG	C1-O5-C5	2.08	115.00	112.19
8	A	1386	NAG	C1-O5-C5	2.07	114.99	112.19
8	I	1355	NAG	C1-O5-C5	2.04	114.95	112.19
8	I	1386	NAG	C1-O5-C5	2.04	114.95	112.19
8	I	1295	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	1160	NAG	C8-C7-N2-C2
8	A	1160	NAG	C8-C7-N2-C2
8	E	1160	NAG	O7-C7-N2-C2
8	I	1160	NAG	C8-C7-N2-C2
8	I	1160	NAG	O7-C7-N2-C2
8	A	1448	NAG	O5-C5-C6-O6
8	E	1448	NAG	O5-C5-C6-O6
8	I	1448	NAG	O5-C5-C6-O6
8	I	1448	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	A	1160	NAG	O7-C7-N2-C2
8	A	1448	NAG	C8-C7-N2-C2
8	I	1448	NAG	O7-C7-N2-C2
8	E	1448	NAG	C8-C7-N2-C2
8	A	1448	NAG	O7-C7-N2-C2
8	E	1448	NAG	O7-C7-N2-C2
8	A	1448	NAG	C4-C5-C6-O6
8	E	1448	NAG	C4-C5-C6-O6
8	I	1448	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1276	NAG	1	0
8	A	1295	NAG	2	0
8	I	1295	NAG	2	0
8	E	1295	NAG	2	0
8	A	1276	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	100(R):VAL	C	101:TRP	N	1.66

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	420/475 (88%)	0.03	13 (3%)	49	39	7, 227, 434, 596	0
1	E	420/475 (88%)	0.06	18 (4%)	35	30	16, 221, 423, 559	0
1	I	420/475 (88%)	0.08	16 (3%)	40	33	25, 216, 434, 550	0
2	B	0/78	-	-	-	-	-	-
2	F	0/78	-	-	-	-	-	-
2	J	0/78	-	-	-	-	-	-
3	C	202/211 (95%)	0.41	17 (8%)	11	10	74, 234, 422, 563	0
3	G	202/211 (95%)	0.46	24 (11%)	4	5	43, 229, 392, 572	0
3	K	202/211 (95%)	0.77	36 (17%)	1	2	47, 291, 454, 533	0
4	D	226/235 (96%)	0.42	15 (6%)	18	15	67, 232, 488, 582	0
4	H	226/235 (96%)	0.30	16 (7%)	16	13	56, 232, 421, 563	0
4	L	226/235 (96%)	0.65	28 (12%)	4	5	71, 287, 466, 582	0
All	All	2544/2997 (84%)	0.28	183 (7%)	15	13	7, 236, 440, 596	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	100(A)	ILE	6.9
3	K	204	GLU	6.5
4	L	111	SER	6.2
4	D	29	VAL	6.1
3	K	147	VAL	5.6
3	G	204	GLU	5.6
4	L	112	ALA	5.6
4	L	188	GLY	5.2
4	H	112	ALA	5.0
4	D	112	ALA	5.0
3	C	111	LYS	5.0
3	K	193	SER	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	L	177	SER	5.0
3	K	179	LEU	4.8
4	L	184	SER	4.7
3	K	145	VAL	4.7
3	G	133	LEU	4.7
3	K	108	SER	4.7
3	K	175	ALA	4.6
3	K	159	GLY	4.6
4	H	100(A)	ILE	4.4
3	K	133	LEU	4.4
4	L	185	SER	4.2
4	H	71	LEU	4.2
3	G	190	LYS	4.2
4	D	102	GLY	4.1
4	L	102	GLY	4.1
3	K	192	TYR	4.0
4	L	100(A)	ILE	3.9
4	L	71	LEU	3.9
4	D	109	VAL	3.9
4	L	29	VAL	3.7
4	L	92	CYS	3.7
3	G	71	ALA	3.7
3	K	47	ILE	3.7
1	A	59	LYS	3.6
3	K	174	ALA	3.6
1	I	309	ILE	3.6
4	L	176	LEU	3.6
4	D	71	LEU	3.5
3	G	203	VAL	3.5
3	K	50	ASN	3.5
3	G	192	TYR	3.4
3	C	207	VAL	3.4
4	H	175	SER	3.4
3	K	132	THR	3.4
4	D	105	THR	3.4
1	I	262	ASN	3.4
1	E	262	ASN	3.4
3	G	132	THR	3.3
3	G	189	HIS	3.3
4	H	102	GLY	3.3
4	L	183	PRO	3.3
1	E	309	ILE	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	L	73	LYS	3.3
1	E	357	THR	3.2
4	D	104	GLY	3.2
3	G	70	THR	3.2
3	C	181	LEU	3.2
3	K	190	LYS	3.2
3	C	13	VAL	3.2
3	C	151	ALA	3.2
4	L	160	GLY	3.2
4	H	73	LYS	3.2
1	E	237	GLY	3.2
1	I	357	THR	3.1
4	D	100	ARG	3.1
3	K	162	THR	3.1
1	E	59	LYS	3.1
4	H	111	SER	3.1
3	K	82	ASP	3.1
1	I	59	LYS	3.0
3	C	47	ILE	3.0
3	K	113	ALA	3.0
3	C	204	GLU	3.0
3	C	158	ALA	2.9
1	E	238	PRO	2.9
3	C	110	PRO	2.9
3	K	111	LYS	2.9
3	K	164	THR	2.9
3	K	146	THR	2.9
4	L	156	ALA	2.8
4	H	30	ARG	2.8
4	L	72	ASP	2.8
3	K	141	TYR	2.8
4	L	150	VAL	2.8
3	C	190	LYS	2.8
4	D	90	TYR	2.8
1	E	137	ASN	2.8
1	E	236	THR	2.7
4	L	175	SER	2.7
3	G	180	SER	2.7
1	E	78	ASP	2.7
4	H	72	ASP	2.7
3	C	62	PHE	2.7
1	A	137	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	157	LEU	2.7
1	E	94	ASN	2.7
3	G	179	LEU	2.7
4	D	8	GLY	2.7
1	I	238	PRO	2.7
1	A	256	SER	2.7
3	G	50	ASN	2.6
3	G	131	ALA	2.6
4	L	110	SER	2.6
4	H	113	SER	2.6
3	C	152	ASP	2.6
3	C	179	LEU	2.6
3	C	192	TYR	2.6
1	I	263	GLY	2.6
3	C	131	ALA	2.5
3	K	114	PRO	2.5
3	C	208	ALA	2.5
4	H	109	VAL	2.5
3	G	32	SER	2.5
3	G	193	SER	2.5
3	G	205	LYS	2.5
3	K	194	CYS	2.4
3	K	150	LYS	2.4
1	I	78	ASP	2.4
3	G	62	PHE	2.4
3	K	155	PRO	2.4
3	G	72	THR	2.4
1	A	392	ASN	2.4
3	K	195	GLN	2.4
1	A	263	GLY	2.4
1	I	63	THR	2.4
4	D	157	LEU	2.4
3	K	110	PRO	2.4
4	L	30	ARG	2.4
3	G	195	GLN	2.3
4	L	8	GLY	2.3
4	D	18	LEU	2.3
1	I	308	ARG	2.3
3	K	109	GLN	2.3
1	A	262	ASN	2.3
4	D	124	PRO	2.3
1	E	330	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	PRO	2.3
1	E	70	ALA	2.3
3	G	82	ASP	2.3
4	H	166	ALA	2.3
1	I	491	ILE	2.3
4	L	194	CYS	2.3
1	E	308	ARG	2.3
1	I	174	SER	2.3
4	L	113	SER	2.3
4	H	69	LEU	2.3
4	H	157	LEU	2.2
3	K	196	VAL	2.2
4	H	4	LEU	2.2
3	K	142	PRO	2.2
4	L	17	THR	2.2
3	K	62	PHE	2.2
4	D	4	LEU	2.2
1	A	63	THR	2.2
1	A	357	THR	2.2
3	G	20	ARG	2.2
1	I	71	THR	2.2
3	G	181	LEU	2.2
1	I	236	THR	2.2
3	C	195	GLN	2.2
4	H	29	VAL	2.2
3	K	119	PHE	2.2
1	E	45	TRP	2.1
1	E	85	HIS	2.1
1	I	330	HIS	2.1
3	K	95(C)	ASN	2.1
1	A	70	ALA	2.1
1	E	171	LYS	2.1
3	G	24	GLY	2.1
4	L	90	TYR	2.1
1	E	191	TYR	2.1
1	A	462	ASN	2.1
1	I	379	GLY	2.1
4	L	81	ARG	2.0
1	E	219	ALA	2.0
3	K	112	ALA	2.0
1	A	57	ASP	2.0
1	A	149	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	K	48	ILE	2.0
3	G	194	CYS	2.0
1	I	58	ALA	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	a	6	11/12	-0.36	1.46	532,532,532,532	0
5	MAN	Z	7	11/12	-0.35	2.15	550,550,550,550	0
5	MAN	Y	4	11/12	-0.27	0.99	550,550,550,550	0
7	MAN	R	2	11/12	-0.25	2.17	489,489,489,489	0
5	MAN	S	5	11/12	-0.16	1.74	550,550,550,550	0
5	NAG	S	1	14/15	-0.13	1.36	550,550,550,550	0
5	MAN	S	4	11/12	-0.09	1.23	550,550,550,550	0
7	MAN	X	2	11/12	-0.07	1.31	545,545,545,545	0
7	MAN	X	1	11/12	-0.07	1.12	427,427,427,427	0
7	MAN	R	1	11/12	-0.06	1.94	550,550,550,550	0
5	MAN	S	6	11/12	-0.05	1.53	497,497,497,497	0
5	MAN	U	5	11/12	-0.05	1.40	550,550,550,550	0
5	MAN	O	6	11/12	-0.03	0.70	455,455,455,455	0
7	MAN	d	2	11/12	-0.01	1.83	550,550,550,550	0
5	MAN	Y	5	11/12	0.03	1.50	477,477,477,477	0
5	MAN	b	4	11/12	0.06	0.40	467,467,467,467	0
5	MAN	U	6	11/12	0.07	0.82	515,515,515,515	0
5	MAN	U	4	11/12	0.09	0.72	550,550,550,550	0
5	MAN	S	7	11/12	0.09	1.10	518,518,518,518	0
5	MAN	M	5	11/12	0.10	1.53	481,481,481,481	0
5	MAN	V	6	11/12	0.12	0.97	454,454,454,454	0
5	MAN	P	6	11/12	0.15	0.78	470,470,470,470	0
5	MAN	P	7	11/12	0.17	1.17	447,447,447,447	0
5	MAN	N	6	11/12	0.18	0.72	464,464,464,464	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MAN	d	1	11/12	0.27	1.13	408,408,408,408	0
5	MAN	a	5	11/12	0.28	1.14	507,507,507,507	0
5	NAG	Y	1	14/15	0.29	0.77	530,530,530,530	0
5	BMA	V	3	11/12	0.31	0.27	492,492,492,492	0
5	MAN	O	5	11/12	0.32	1.00	468,468,468,468	0
5	MAN	V	5	11/12	0.33	1.21	495,495,495,495	0
5	MAN	Y	6	11/12	0.34	1.48	494,494,494,494	0
6	MAN	W	6	11/12	0.35	0.63	452,452,452,452	0
5	MAN	P	5	11/12	0.35	0.96	418,418,418,418	0
5	BMA	S	3	11/12	0.36	1.00	500,500,500,500	0
5	NAG	U	1	14/15	0.39	0.67	408,408,408,408	0
5	BMA	Y	3	11/12	0.39	0.41	402,402,402,402	0
5	MAN	V	4	11/12	0.39	0.61	471,471,471,471	0
5	MAN	M	4	11/12	0.40	0.82	517,517,517,517	0
5	NAG	M	1	14/15	0.40	0.58	439,439,439,439	0
5	MAN	a	4	11/12	0.40	0.72	545,545,545,545	0
5	BMA	N	3	11/12	0.41	0.47	483,483,483,483	0
5	MAN	Y	7	11/12	0.42	0.74	520,520,520,520	0
6	MAN	Q	5	11/12	0.44	0.35	302,302,302,302	0
5	MAN	Z	6	11/12	0.45	0.32	428,428,428,428	0
5	BMA	Z	3	11/12	0.45	0.56	491,491,491,491	0
5	MAN	M	7	11/12	0.46	0.49	451,451,451,451	0
5	MAN	N	7	11/12	0.46	1.55	498,498,498,498	0
5	MAN	T	6	11/12	0.46	0.52	446,446,446,446	0
5	MAN	O	4	11/12	0.48	0.60	550,550,550,550	0
5	MAN	Z	4	11/12	0.50	0.57	550,550,550,550	0
5	MAN	N	4	11/12	0.51	0.83	550,550,550,550	0
5	NAG	O	1	14/15	0.52	0.65	423,423,423,423	0
6	BMA	W	3	11/12	0.53	0.35	400,400,400,400	0
6	MAN	W	5	11/12	0.53	0.37	330,330,330,330	0
5	MAN	b	6	11/12	0.54	0.89	474,474,474,474	0
6	MAN	W	7	11/12	0.54	0.63	418,418,418,418	0
6	MAN	Q	6	11/12	0.54	0.49	422,422,422,422	0
5	NAG	a	1	14/15	0.54	0.70	437,437,437,437	0
6	MAN	Q	9	11/12	0.55	0.38	303,303,303,303	0
5	MAN	T	7	11/12	0.56	1.41	542,542,542,542	0
5	MAN	N	5	11/12	0.56	0.45	329,329,329,329	0
5	MAN	T	4	11/12	0.57	0.54	550,550,550,550	0
5	NAG	Y	2	14/15	0.57	0.55	460,460,460,460	0
6	MAN	c	6	11/12	0.58	0.51	436,436,436,436	0
5	BMA	U	3	11/12	0.58	0.27	340,340,340,340	0

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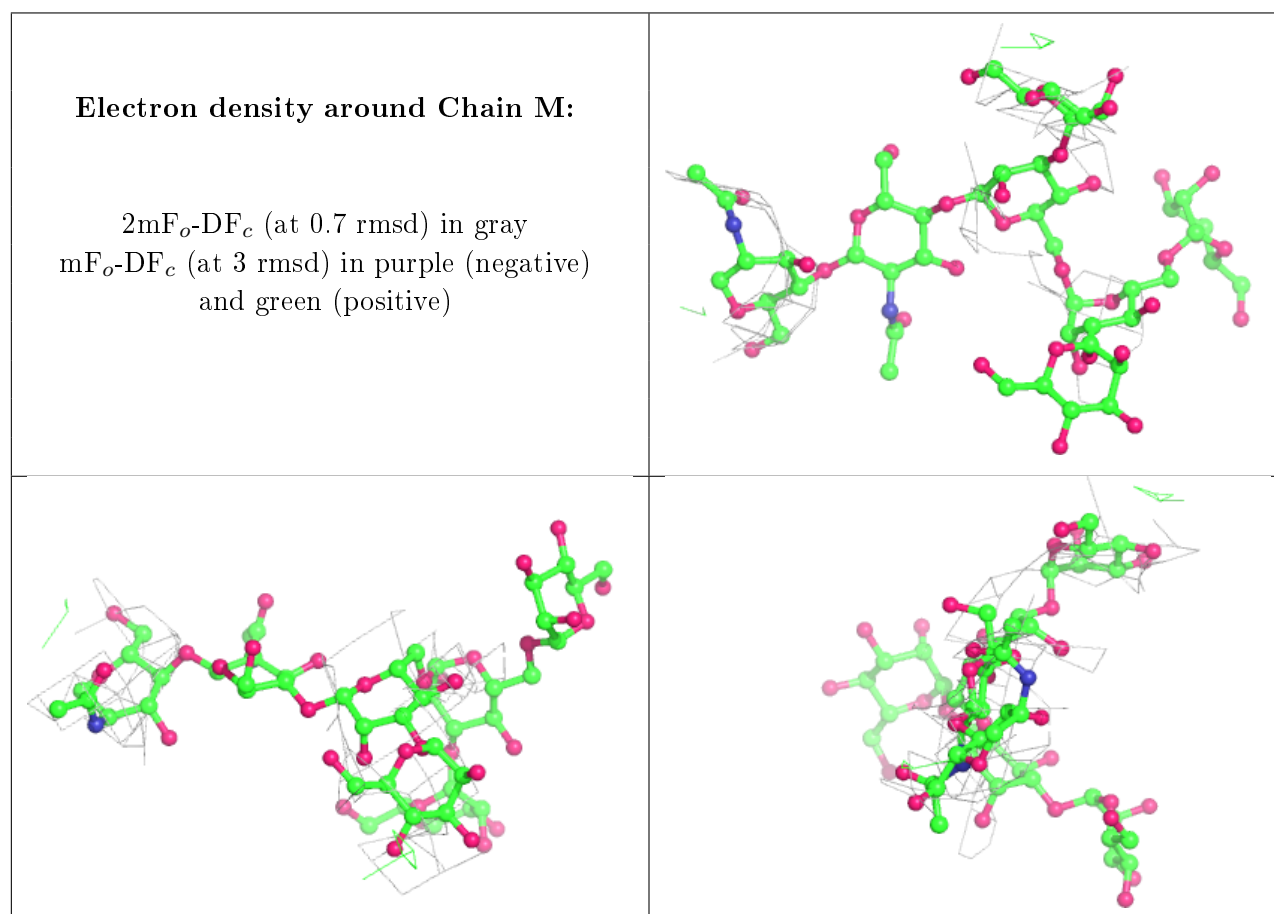
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	O	3	11/12	0.59	0.22	506,506,506,506	0
6	MAN	W	4	11/12	0.59	0.62	550,550,550,550	0
5	BMA	T	3	11/12	0.59	0.31	466,466,466,466	0
5	BMA	b	3	11/12	0.60	0.34	474,474,474,474	0
5	MAN	M	6	11/12	0.60	1.15	434,434,434,434	0
5	BMA	P	3	11/12	0.60	0.54	455,455,455,455	0
5	MAN	b	5	11/12	0.61	1.07	482,482,482,482	0
5	MAN	T	5	11/12	0.62	0.60	422,422,422,422	0
5	BMA	M	3	11/12	0.62	0.44	356,356,356,356	0
5	MAN	P	4	11/12	0.62	0.66	483,483,483,483	0
5	NAG	M	2	14/15	0.64	0.97	519,519,519,519	0
6	MAN	Q	7	11/12	0.66	0.34	309,309,309,309	0
5	NAG	b	2	14/15	0.66	0.47	382,382,382,382	0
6	NAG	Q	1	14/15	0.68	0.54	366,366,366,366	0
5	NAG	S	2	14/15	0.69	1.08	488,488,488,488	0
5	MAN	b	7	11/12	0.69	0.36	330,330,330,330	0
5	MAN	Z	5	11/12	0.70	0.47	410,410,410,410	0
6	MAN	c	5	11/12	0.70	0.29	277,277,277,277	0
6	MAN	c	9	11/12	0.71	0.52	362,362,362,362	0
6	MAN	c	7	11/12	0.71	0.47	382,382,382,382	0
5	NAG	U	2	14/15	0.72	0.42	310,310,310,310	0
6	NAG	c	1	14/15	0.75	0.37	292,292,292,292	0
6	MAN	c	4	11/12	0.75	0.68	550,550,550,550	0
5	NAG	V	2	14/15	0.77	0.31	335,335,335,335	0
6	NAG	W	1	14/15	0.77	0.35	302,302,302,302	0
5	NAG	P	2	14/15	0.77	0.26	307,307,307,307	0
6	NAG	W	2	14/15	0.78	0.39	388,388,388,388	0
5	NAG	Z	1	14/15	0.78	0.36	337,337,337,337	0
5	MAN	V	7	11/12	0.78	0.38	377,377,377,377	0
6	MAN	W	8	11/12	0.78	0.81	491,491,491,491	0
5	NAG	b	1	14/15	0.78	0.36	276,276,276,276	0
5	MAN	O	7	11/12	0.80	0.20	229,229,229,229	0
5	NAG	Z	2	14/15	0.81	0.38	375,375,375,375	0
6	BMA	Q	3	11/12	0.82	0.36	292,292,292,292	0
5	MAN	U	7	11/12	0.82	0.30	195,195,195,195	0
5	NAG	P	1	14/15	0.82	0.29	202,202,202,202	0
5	MAN	a	7	11/12	0.83	0.26	197,197,197,197	0
6	NAG	Q	2	14/15	0.84	0.35	258,258,258,258	0
6	MAN	Q	4	11/12	0.84	0.35	550,550,550,550	0
6	MAN	W	9	11/12	0.84	0.55	335,335,335,335	0
5	NAG	V	1	14/15	0.84	0.30	242,242,242,242	0
5	NAG	a	2	14/15	0.84	0.29	231,231,231,231	0

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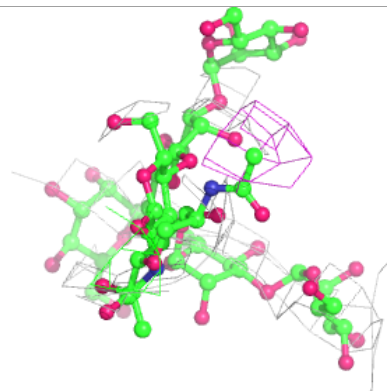
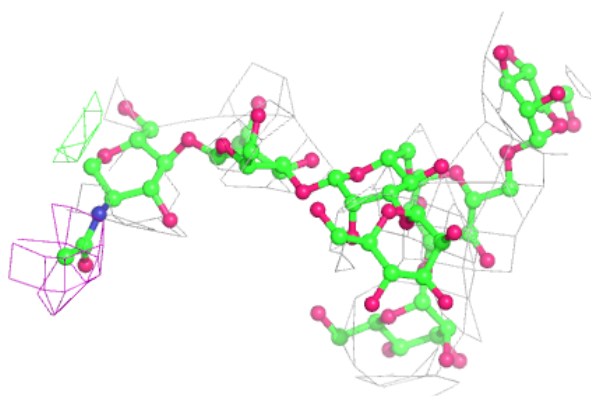
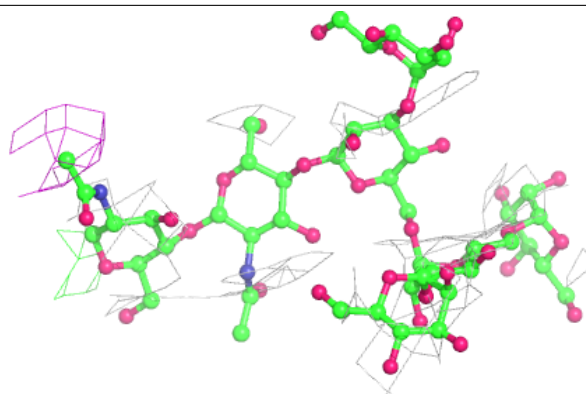
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	a	3	11/12	0.85	0.15	297,297,297,297	0
5	NAG	T	1	14/15	0.85	0.31	186,186,186,186	0
6	MAN	c	8	11/12	0.85	0.83	507,507,507,507	0
5	NAG	N	1	14/15	0.87	0.34	356,356,356,356	0
5	NAG	O	2	14/15	0.88	0.31	410,410,410,410	0
5	NAG	N	2	14/15	0.89	0.28	310,310,310,310	0
6	MAN	Q	8	11/12	0.91	0.82	500,500,500,500	0
6	BMA	c	3	11/12	0.91	0.25	345,345,345,345	0
5	NAG	T	2	14/15	0.92	0.28	301,301,301,301	0
6	NAG	c	2	14/15	0.96	0.22	213,213,213,213	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.

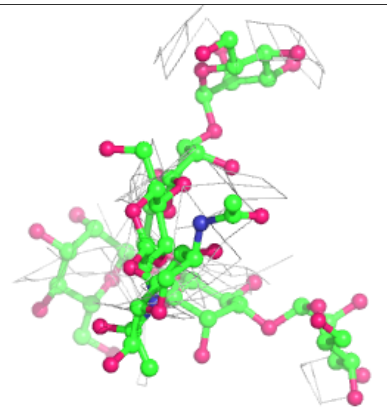
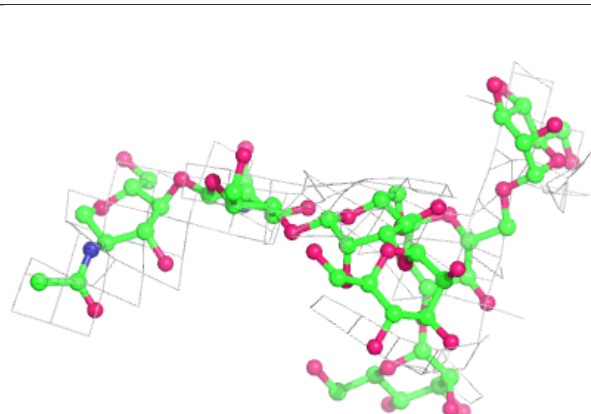
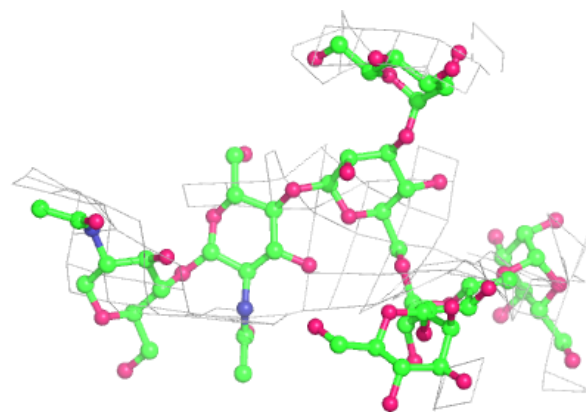


**Electron density around Chain N:**

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

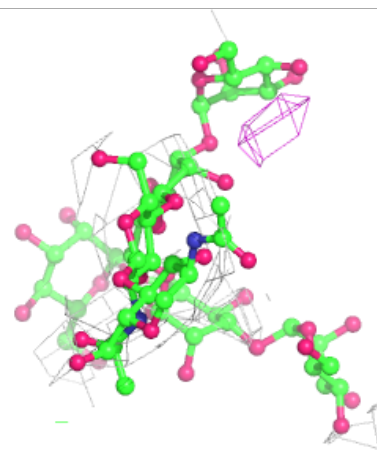
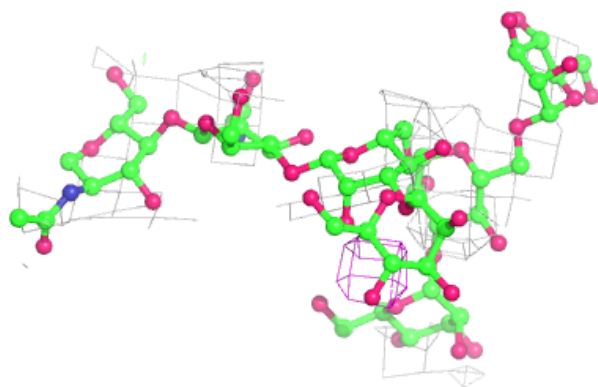
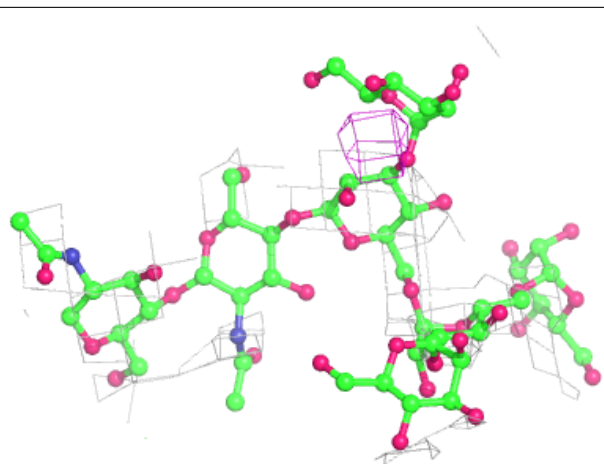
**Electron density around Chain O:**

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



**Electron density around Chain P:**

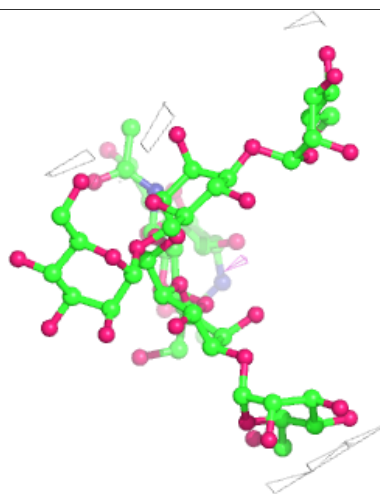
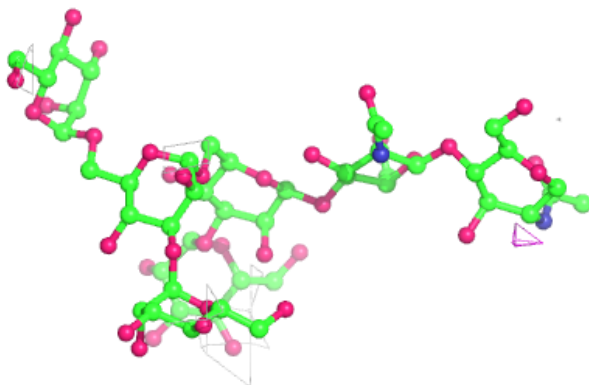
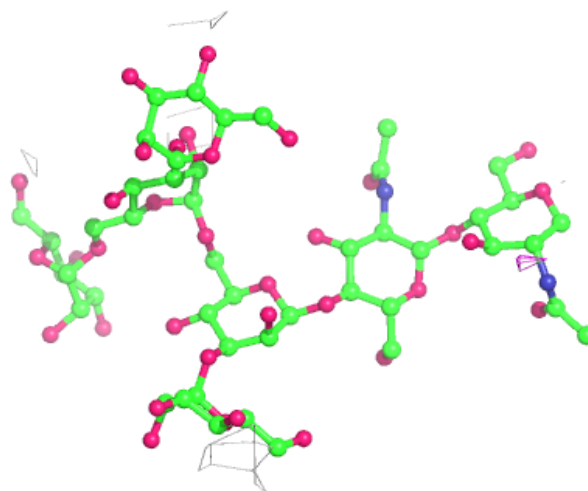
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





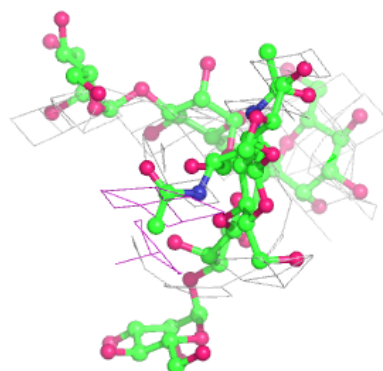
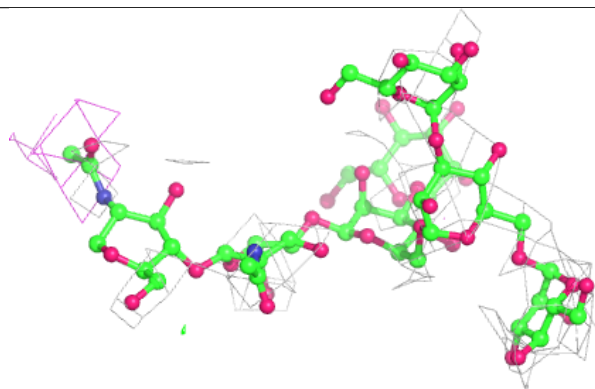
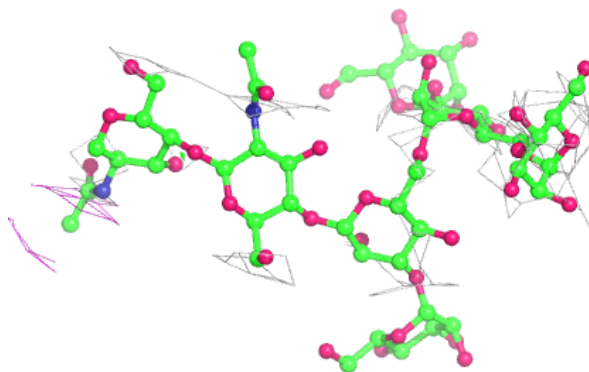
**Electron density around Chain S:**

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



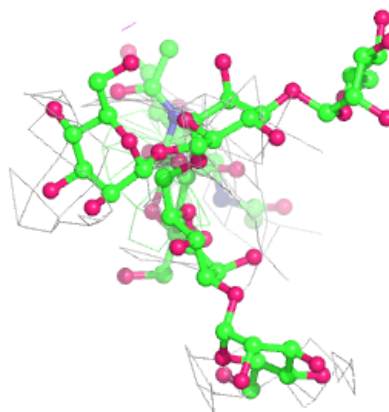
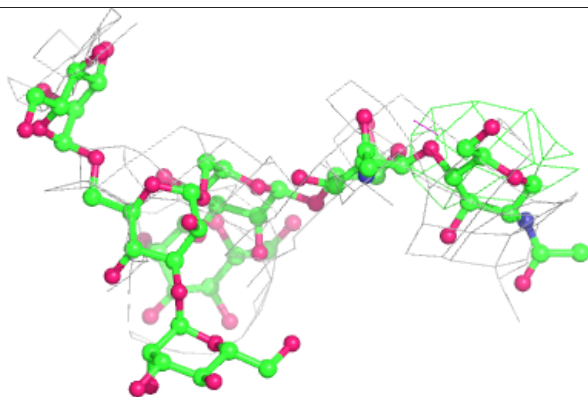
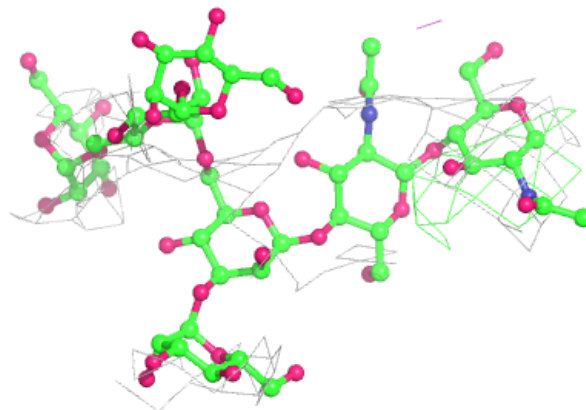
**Electron density around Chain T:**

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



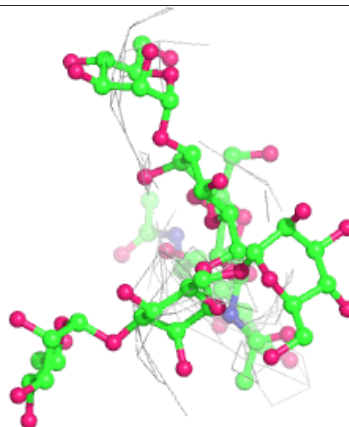
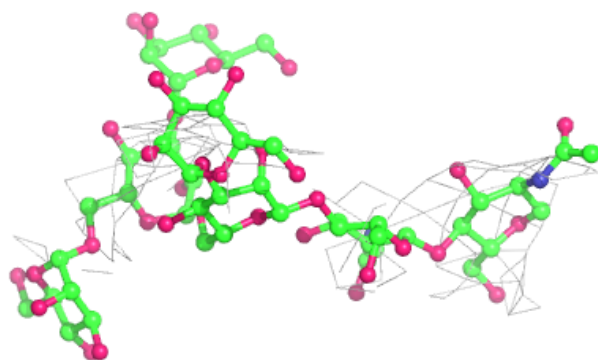
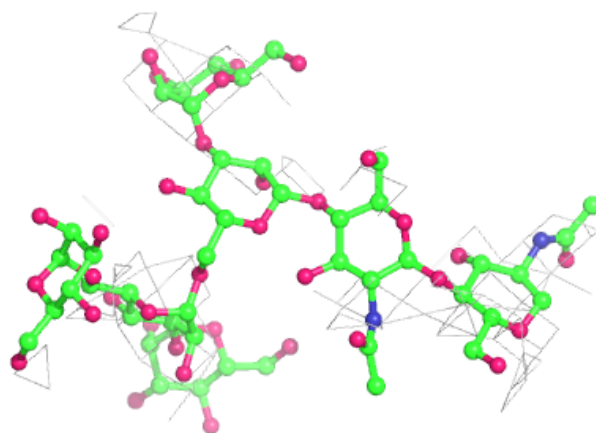
**Electron density around Chain U:**

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



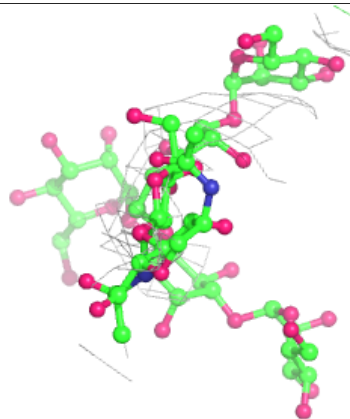
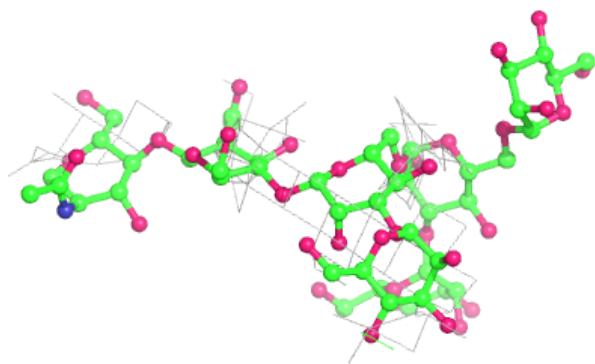
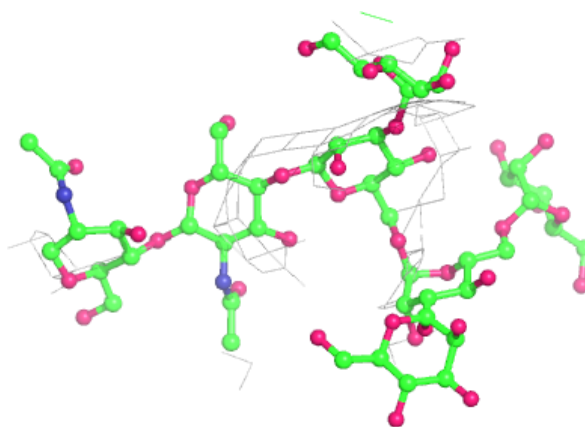
**Electron density around Chain V:**

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



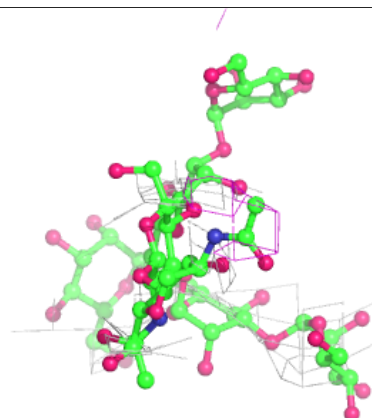
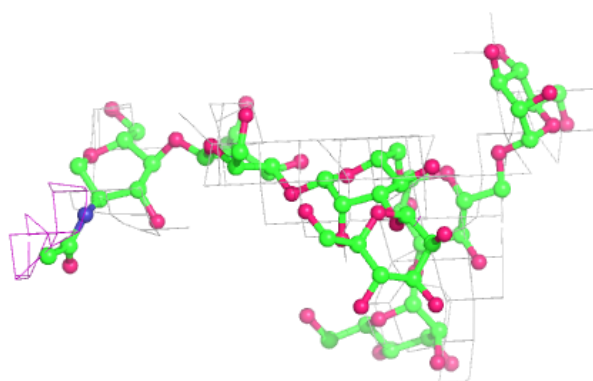
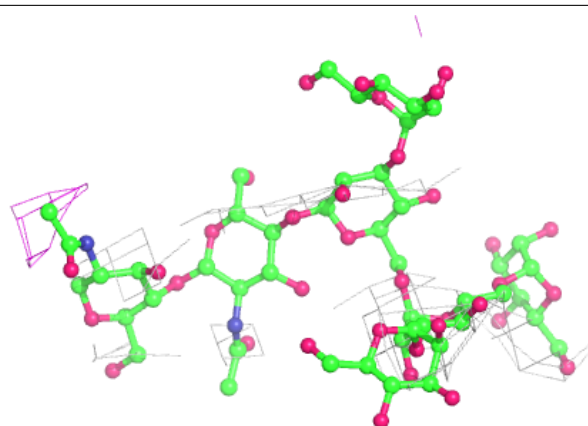
**Electron density around Chain Y:**

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

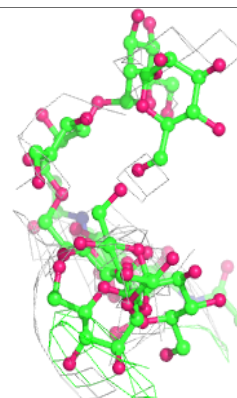
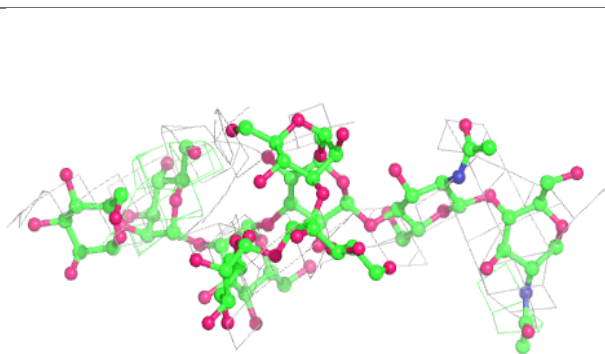
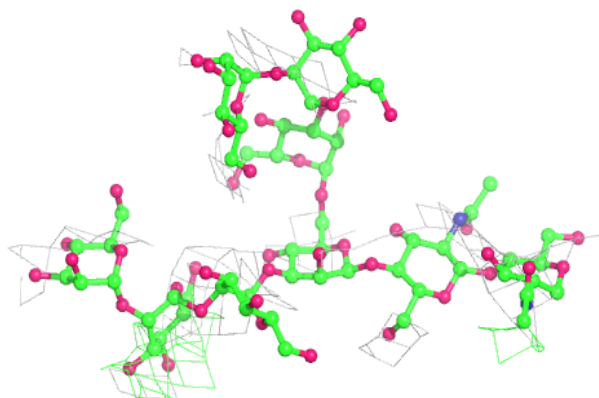


**Electron density around Chain Z:**

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

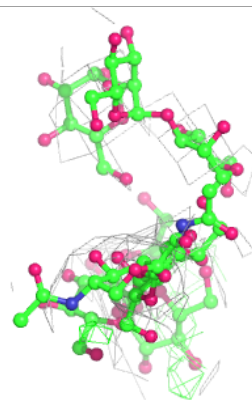
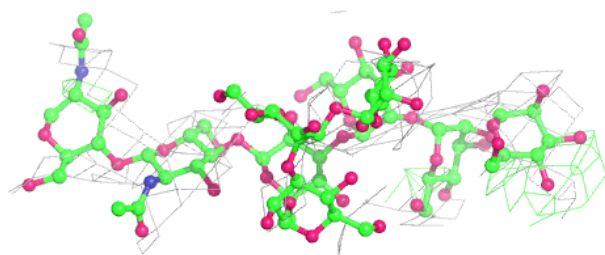
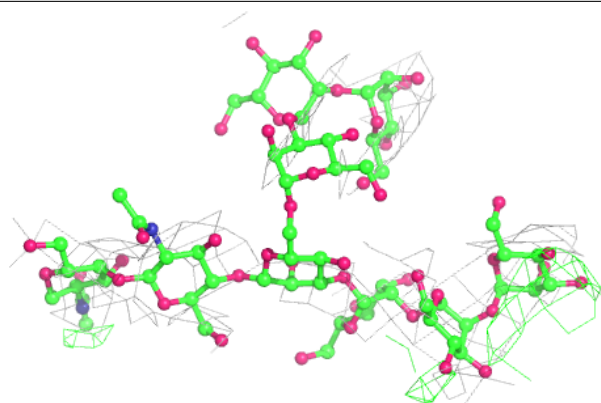
**Electron density around Chain Q:**

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



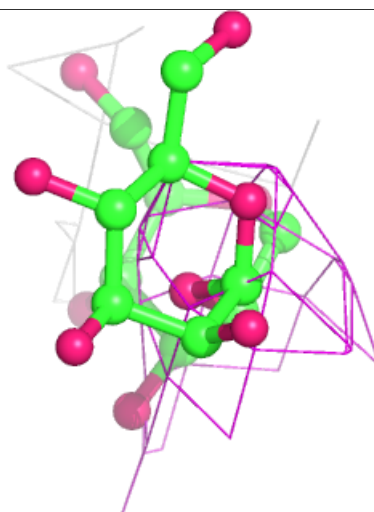
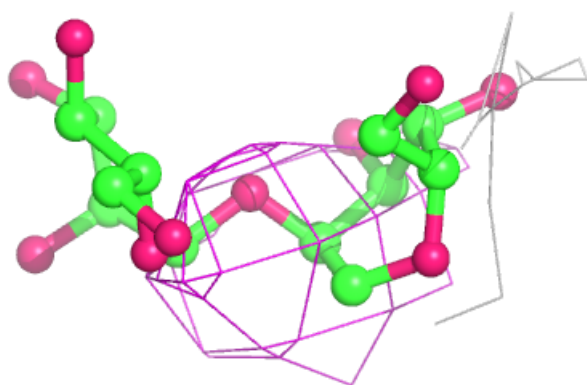
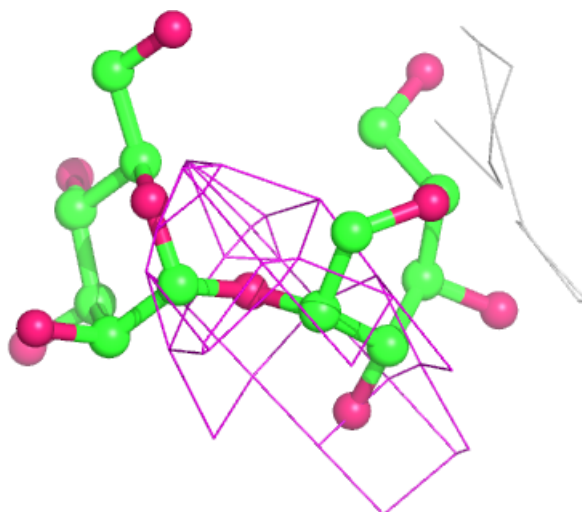
**Electron density around Chain W:**

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

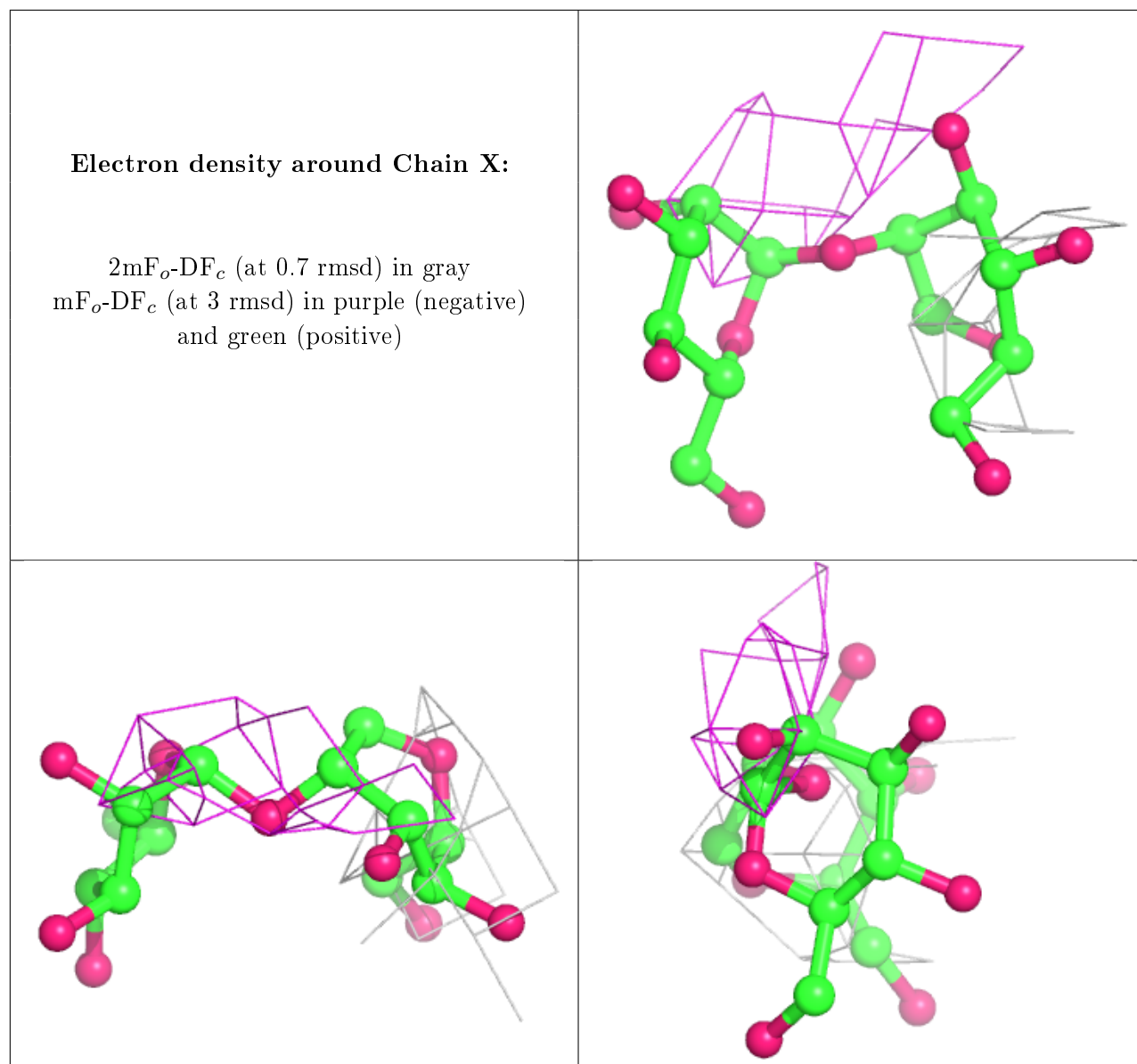


**Electron density around Chain R:**

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







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	A	1392	14/15	0.17	0.93	386,386,386,386	0
8	NAG	E	1295	14/15	0.25	0.70	356,356,356,356	0
8	NAG	I	1160	14/15	0.26	1.07	362,362,362,362	0
8	NAG	A	1088	14/15	0.38	0.69	474,474,474,474	0
8	NAG	E	1392	14/15	0.39	0.78	305,305,305,305	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	I	1088	14/15	0.40	0.75	503,503,503,503	0
8	NAG	A	1295	14/15	0.40	0.61	330,330,330,330	0
8	NAG	I	1392	14/15	0.44	0.68	345,345,345,345	0
8	NAG	E	1160	14/15	0.49	0.69	245,245,245,245	0
8	NAG	A	1448	14/15	0.54	0.61	279,279,279,279	0
8	NAG	E	1448	14/15	0.56	0.54	361,361,361,361	0
8	NAG	I	1295	14/15	0.58	0.44	323,323,323,323	0
8	NAG	I	1355	14/15	0.59	0.35	266,266,266,266	0
8	NAG	E	1088	14/15	0.61	0.64	486,486,486,486	0
8	NAG	I	1448	14/15	0.63	0.49	287,287,287,287	0
8	NAG	I	1234	14/15	0.65	0.46	345,345,345,345	0
8	NAG	E	1386	14/15	0.67	0.67	427,427,427,427	0
8	NAG	A	1386	14/15	0.69	0.58	356,356,356,356	0
8	NAG	E	1234	14/15	0.71	0.49	405,405,405,405	0
8	NAG	A	1160	14/15	0.71	0.56	267,267,267,267	0
8	NAG	E	1355	14/15	0.73	0.34	411,411,411,411	0
8	NAG	I	1386	14/15	0.73	0.50	331,331,331,331	0
8	NAG	A	1355	14/15	0.76	0.40	238,238,238,238	0
8	NAG	E	1276	14/15	0.80	0.43	313,313,313,313	0
8	NAG	I	1197	14/15	0.83	0.23	304,304,304,304	0
8	NAG	E	1197	14/15	0.84	0.33	288,288,288,288	0
8	NAG	A	1197	14/15	0.85	0.27	302,302,302,302	0
8	NAG	A	1234	14/15	0.88	0.28	431,431,431,431	0
8	NAG	A	1276	14/15	0.90	0.30	288,288,288,288	0
8	NAG	I	1276	14/15	0.91	0.37	281,281,281,281	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.