



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 5W1X / pdb_00005w1x
Title : Crystal Structure of Humanpapillomavirus18 (HPV18) Capsid L1 Pentamers
Bound to Heparin Oligosaccharides
Authors : Chen, X.S.; Dasgupta, J.
Deposited on : 2017-06-05
Resolution : 3.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

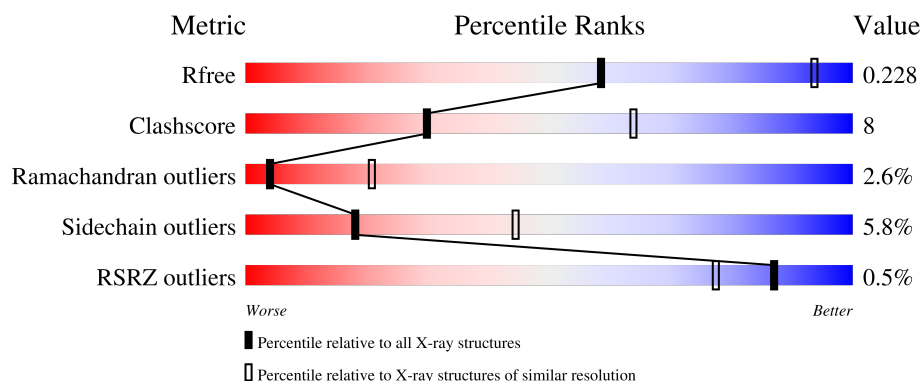
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



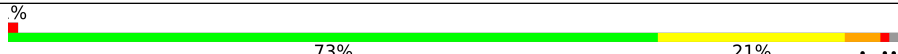
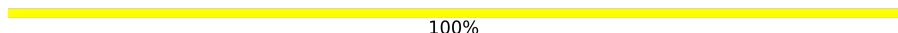
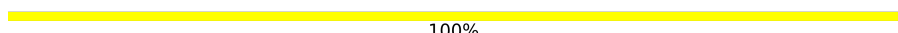
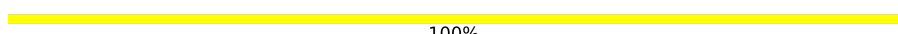
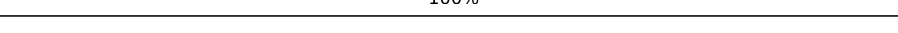
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	427	 80% 18% ..
1	B	427	 78% 19% ..
1	C	427	 77% 18% ..
1	D	427	 75% 21% ..
1	E	427	 76% 21% ..

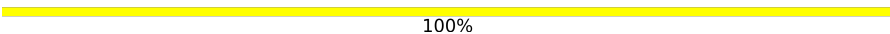
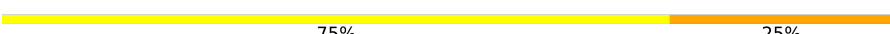
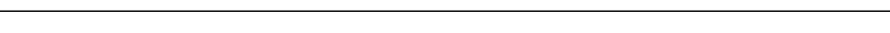
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Mol	Chain	Length	Quality of chain
1	F	427	%  76%21%..
1	G	427	%  74%21%..
1	H	427	 75%20%..
1	I	427	%  76%20%..
1	J	427	 80%17%..
1	K	427	 76%21%..
1	L	427	 72%23%..
1	M	427	%  73%21%..
1	N	427	 78%18%..
1	O	427	%  74%21%..
2	P	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 50%50%
2	W	2	 50%50%
2	Y	2	 100%
2	Z	2	 100%
2	a	2	 50%50%
2	d	2	 100%
2	i	2	 100%
2	j	2	 100%
2	k	2	 50%50%
2	l	2	 50%50%
2	m	2	 100%
2	n	2	 50%50%

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Mol	Chain	Length	Quality of chain
2	o	2	
2	q	2	
2	r	2	
2	s	2	
3	Q	4	
3	R	4	
3	V	4	
3	X	4	
3	b	4	
3	c	4	
3	g	4	
3	h	4	
3	p	4	
4	e	6	
5	f	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IDS	Y	2	-	-	X	-
2	IDS	m	2	-	-	X	-
2	JHM	n	1	-	-	X	-
2	IDS	r	2	-	-	X	-
2	JHM	s	1	-	-	X	-
3	JHM	X	1	-	-	X	-
3	IDS	h	2	-	-	X	-
4	JHM	e	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51075 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	B	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	C	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	D	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	E	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	F	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	G	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	H	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	I	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	J	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	K	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	L	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	M	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	N	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	O	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q5G244
A	47	ASP	ASN	engineered mutation	UNP Q5G244
A	175	SER	CYS	engineered mutation	UNP Q5G244
A	393	GLN	HIS	engineered mutation	UNP Q5G244
A	433	GLY	-	linker	UNP Q5G244
A	434	GLY	-	linker	UNP Q5G244
A	435	SER	-	linker	UNP Q5G244
A	436	GLY	-	linker	UNP Q5G244
A	437	GLY	-	linker	UNP Q5G244
B	20	ALA	-	expression tag	UNP Q5G244
B	47	ASP	ASN	engineered mutation	UNP Q5G244
B	175	SER	CYS	engineered mutation	UNP Q5G244
B	393	GLN	HIS	engineered mutation	UNP Q5G244
B	433	GLY	-	linker	UNP Q5G244
B	434	GLY	-	linker	UNP Q5G244
B	435	SER	-	linker	UNP Q5G244
B	436	GLY	-	linker	UNP Q5G244
B	437	GLY	-	linker	UNP Q5G244
C	20	ALA	-	expression tag	UNP Q5G244
C	47	ASP	ASN	engineered mutation	UNP Q5G244
C	175	SER	CYS	engineered mutation	UNP Q5G244
C	393	GLN	HIS	engineered mutation	UNP Q5G244
C	433	GLY	-	linker	UNP Q5G244
C	434	GLY	-	linker	UNP Q5G244
C	435	SER	-	linker	UNP Q5G244
C	436	GLY	-	linker	UNP Q5G244
C	437	GLY	-	linker	UNP Q5G244
D	20	ALA	-	expression tag	UNP Q5G244
D	47	ASP	ASN	engineered mutation	UNP Q5G244
D	175	SER	CYS	engineered mutation	UNP Q5G244
D	393	GLN	HIS	engineered mutation	UNP Q5G244
D	433	GLY	-	linker	UNP Q5G244
D	434	GLY	-	linker	UNP Q5G244
D	435	SER	-	linker	UNP Q5G244
D	436	GLY	-	linker	UNP Q5G244
D	437	GLY	-	linker	UNP Q5G244
E	20	ALA	-	expression tag	UNP Q5G244
E	47	ASP	ASN	engineered mutation	UNP Q5G244
E	175	SER	CYS	engineered mutation	UNP Q5G244
E	393	GLN	HIS	engineered mutation	UNP Q5G244
E	433	GLY	-	linker	UNP Q5G244
E	434	GLY	-	linker	UNP Q5G244
E	435	SER	-	linker	UNP Q5G244

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	linker	UNP Q5G244
E	437	GLY	-	linker	UNP Q5G244
F	20	ALA	-	expression tag	UNP Q5G244
F	47	ASP	ASN	engineered mutation	UNP Q5G244
F	175	SER	CYS	engineered mutation	UNP Q5G244
F	393	GLN	HIS	engineered mutation	UNP Q5G244
F	433	GLY	-	linker	UNP Q5G244
F	434	GLY	-	linker	UNP Q5G244
F	435	SER	-	linker	UNP Q5G244
F	436	GLY	-	linker	UNP Q5G244
F	437	GLY	-	linker	UNP Q5G244
G	20	ALA	-	expression tag	UNP Q5G244
G	47	ASP	ASN	engineered mutation	UNP Q5G244
G	175	SER	CYS	engineered mutation	UNP Q5G244
G	393	GLN	HIS	engineered mutation	UNP Q5G244
G	433	GLY	-	linker	UNP Q5G244
G	434	GLY	-	linker	UNP Q5G244
G	435	SER	-	linker	UNP Q5G244
G	436	GLY	-	linker	UNP Q5G244
G	437	GLY	-	linker	UNP Q5G244
H	20	ALA	-	expression tag	UNP Q5G244
H	47	ASP	ASN	engineered mutation	UNP Q5G244
H	175	SER	CYS	engineered mutation	UNP Q5G244
H	393	GLN	HIS	engineered mutation	UNP Q5G244
H	433	GLY	-	linker	UNP Q5G244
H	434	GLY	-	linker	UNP Q5G244
H	435	SER	-	linker	UNP Q5G244
H	436	GLY	-	linker	UNP Q5G244
H	437	GLY	-	linker	UNP Q5G244
I	20	ALA	-	expression tag	UNP Q5G244
I	47	ASP	ASN	engineered mutation	UNP Q5G244
I	175	SER	CYS	engineered mutation	UNP Q5G244
I	393	GLN	HIS	engineered mutation	UNP Q5G244
I	433	GLY	-	linker	UNP Q5G244
I	434	GLY	-	linker	UNP Q5G244
I	435	SER	-	linker	UNP Q5G244
I	436	GLY	-	linker	UNP Q5G244
I	437	GLY	-	linker	UNP Q5G244
J	20	ALA	-	expression tag	UNP Q5G244
J	47	ASP	ASN	engineered mutation	UNP Q5G244
J	175	SER	CYS	engineered mutation	UNP Q5G244
J	393	GLN	HIS	engineered mutation	UNP Q5G244

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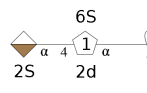
Chain	Residue	Modelled	Actual	Comment	Reference
J	433	GLY	-	linker	UNP Q5G244
J	434	GLY	-	linker	UNP Q5G244
J	435	SER	-	linker	UNP Q5G244
J	436	GLY	-	linker	UNP Q5G244
J	437	GLY	-	linker	UNP Q5G244
K	20	ALA	-	expression tag	UNP Q5G244
K	47	ASP	ASN	engineered mutation	UNP Q5G244
K	175	SER	CYS	engineered mutation	UNP Q5G244
K	393	GLN	HIS	engineered mutation	UNP Q5G244
K	433	GLY	-	linker	UNP Q5G244
K	434	GLY	-	linker	UNP Q5G244
K	435	SER	-	linker	UNP Q5G244
K	436	GLY	-	linker	UNP Q5G244
K	437	GLY	-	linker	UNP Q5G244
L	20	ALA	-	expression tag	UNP Q5G244
L	47	ASP	ASN	engineered mutation	UNP Q5G244
L	175	SER	CYS	engineered mutation	UNP Q5G244
L	393	GLN	HIS	engineered mutation	UNP Q5G244
L	433	GLY	-	linker	UNP Q5G244
L	434	GLY	-	linker	UNP Q5G244
L	435	SER	-	linker	UNP Q5G244
L	436	GLY	-	linker	UNP Q5G244
L	437	GLY	-	linker	UNP Q5G244
M	20	ALA	-	expression tag	UNP Q5G244
M	47	ASP	ASN	engineered mutation	UNP Q5G244
M	175	SER	CYS	engineered mutation	UNP Q5G244
M	393	GLN	HIS	engineered mutation	UNP Q5G244
M	433	GLY	-	linker	UNP Q5G244
M	434	GLY	-	linker	UNP Q5G244
M	435	SER	-	linker	UNP Q5G244
M	436	GLY	-	linker	UNP Q5G244
M	437	GLY	-	linker	UNP Q5G244
N	20	ALA	-	expression tag	UNP Q5G244
N	47	ASP	ASN	engineered mutation	UNP Q5G244
N	175	SER	CYS	engineered mutation	UNP Q5G244
N	393	GLN	HIS	engineered mutation	UNP Q5G244
N	433	GLY	-	linker	UNP Q5G244
N	434	GLY	-	linker	UNP Q5G244
N	435	SER	-	linker	UNP Q5G244
N	436	GLY	-	linker	UNP Q5G244
N	437	GLY	-	linker	UNP Q5G244
O	20	ALA	-	expression tag	UNP Q5G244

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Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	engineered mutation	UNP Q5G244
O	175	SER	CYS	engineered mutation	UNP Q5G244
O	393	GLN	HIS	engineered mutation	UNP Q5G244
O	433	GLY	-	linker	UNP Q5G244
O	434	GLY	-	linker	UNP Q5G244
O	435	SER	-	linker	UNP Q5G244
O	436	GLY	-	linker	UNP Q5G244
O	437	GLY	-	linker	UNP Q5G244

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



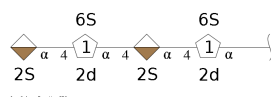
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	S	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	T	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	U	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	W	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	Y	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	Z	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	a	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	d	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	i	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	j	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	k	2	Total	C	O	S	0	0	0
			30	12	16	2			

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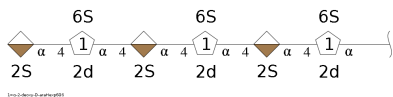
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	l	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	m	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	n	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	o	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	q	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	r	2	Total	C	O	S	0	0	0
			30	12	16	2			
2	s	2	Total	C	O	S	0	0	0
			30	12	16	2			

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



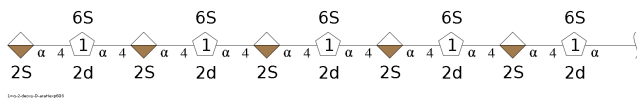
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	R	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	V	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	X	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	b	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	c	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	g	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	h	4	Total	C	O	S	0	0	0
			60	24	32	4			
3	p	4	Total	C	O	S	0	0	0
			60	24	32	4			

- Molecule 4 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	e	6	Total	C	O	S	0	0	0
			90	36	48	6			

- Molecule 5 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose.

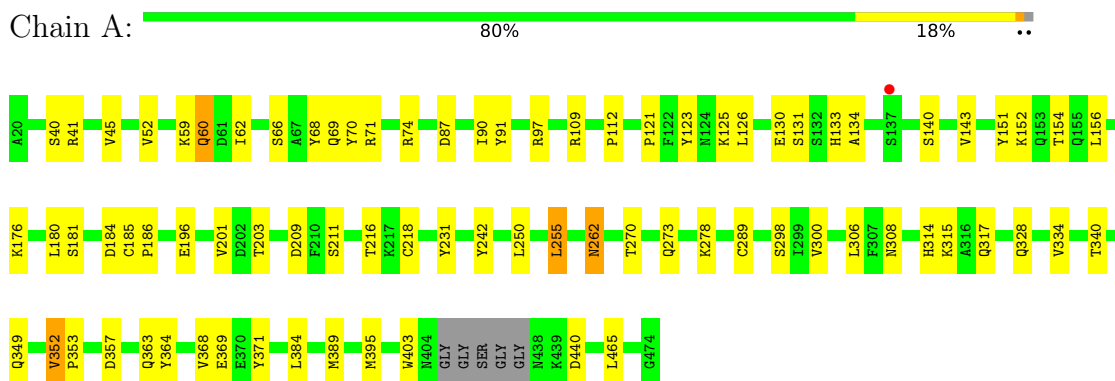


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	f	10	Total	C	O	S	0	0	0
			150	60	80	10			

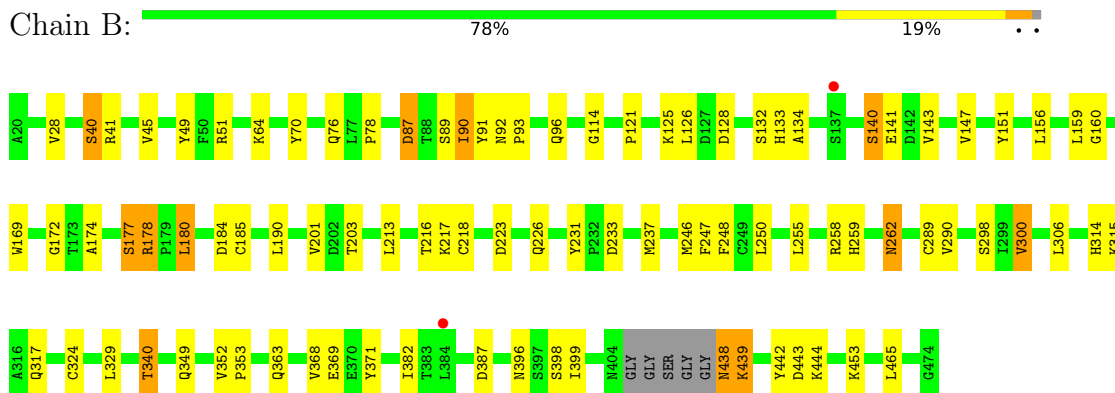
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

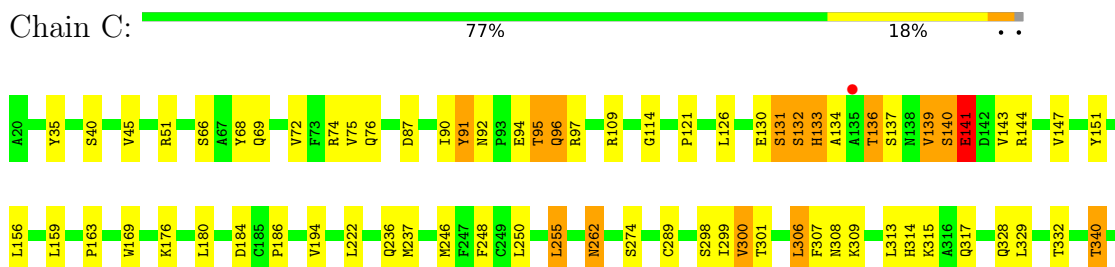
• Molecule 1: Major capsid protein L1

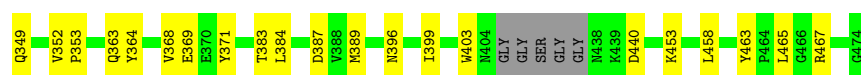


• Molecule 1: Major capsid protein L1

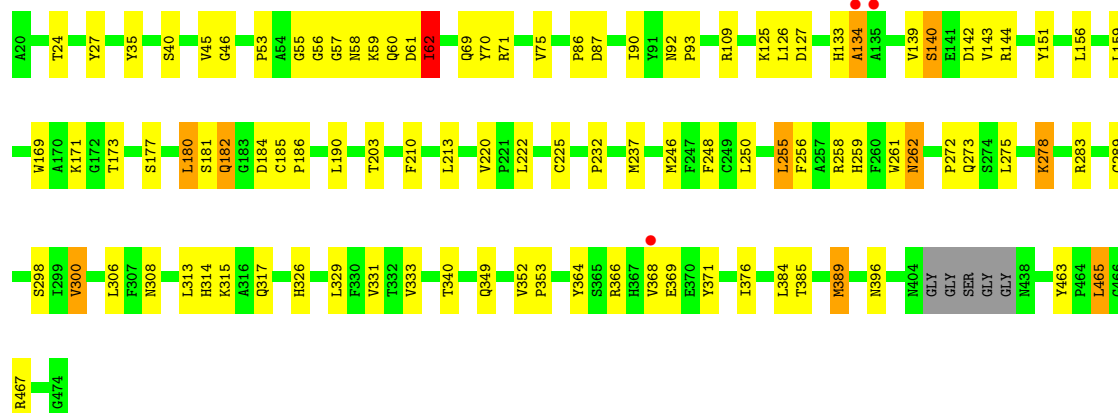
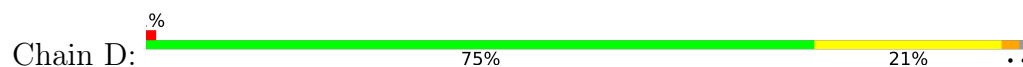


• Molecule 1: Major capsid protein L1

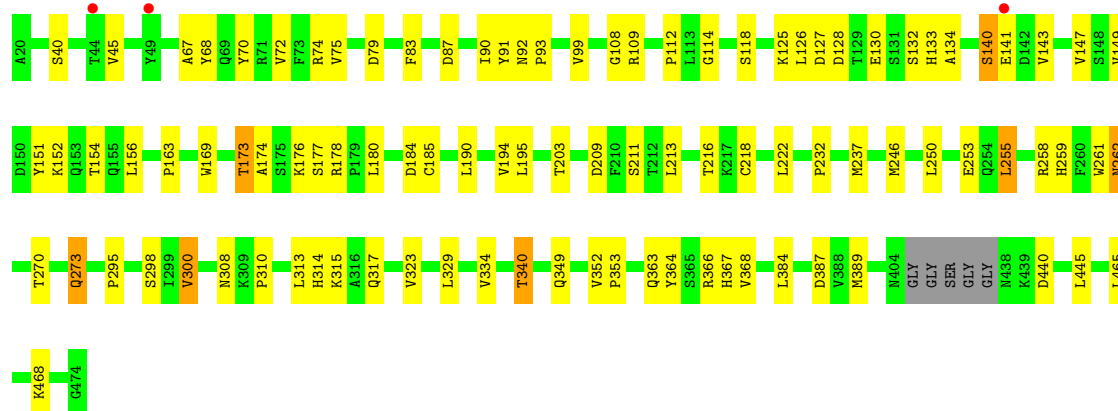
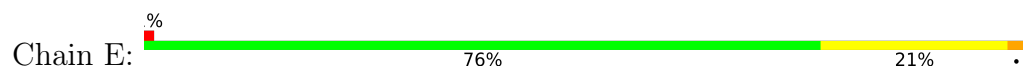




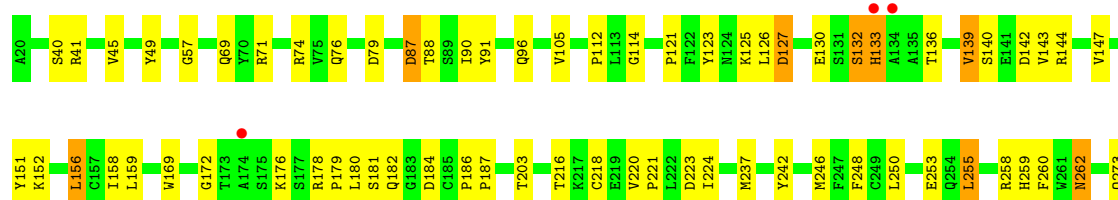
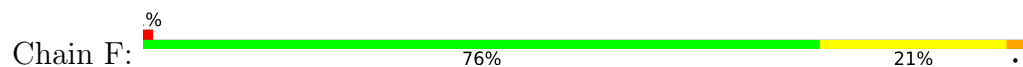
• Molecule 1: Major capsid protein L1

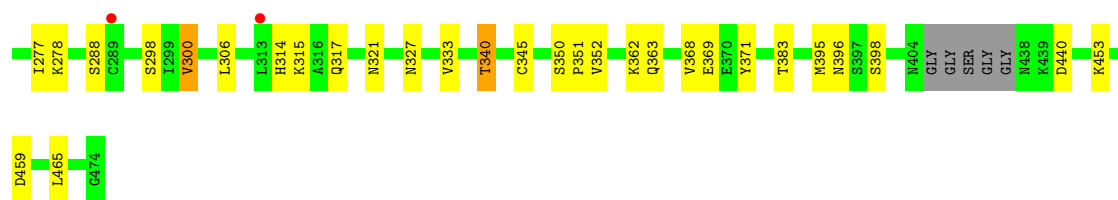


• Molecule 1: Major capsid protein L1

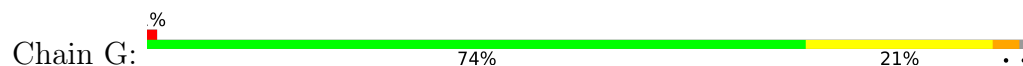


• Molecule 1: Major capsid protein L1

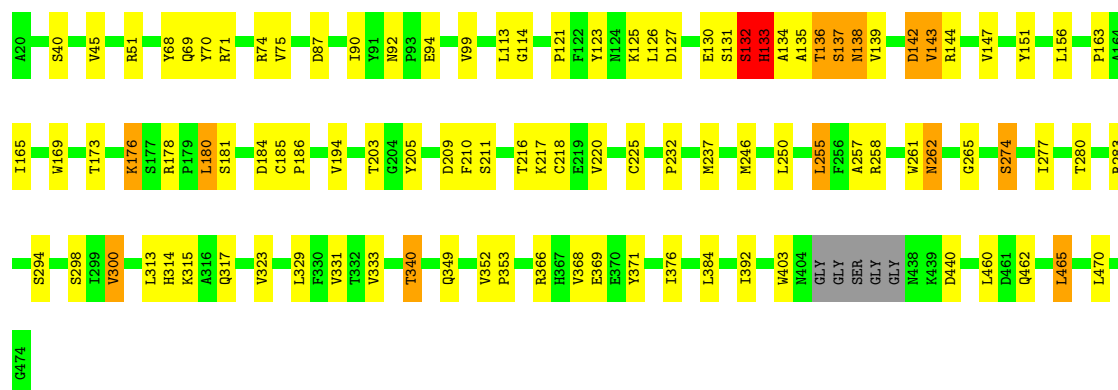
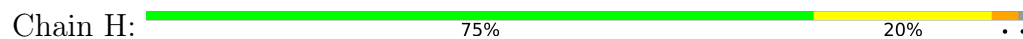




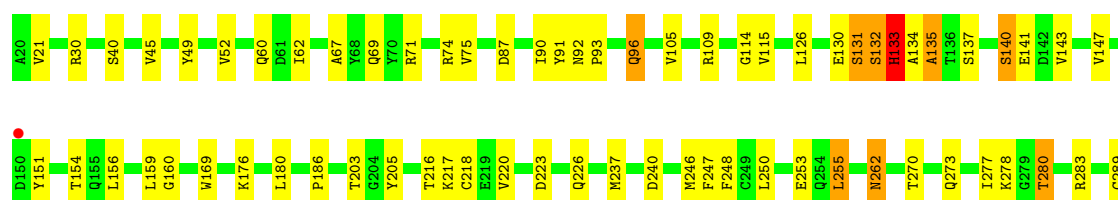
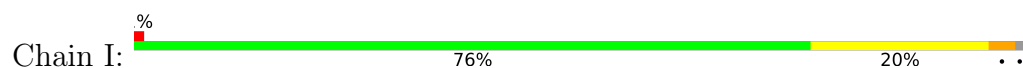
• Molecule 1: Major capsid protein L1

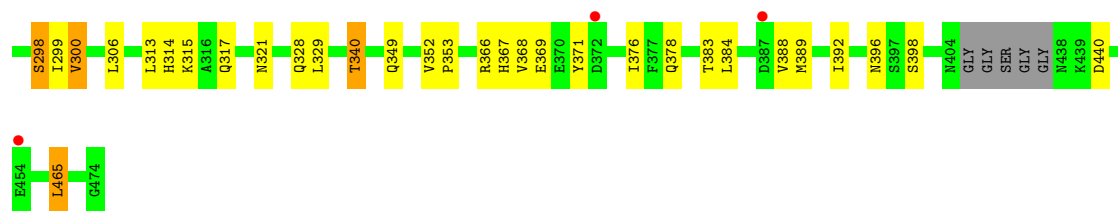


• Molecule 1: Major capsid protein L1



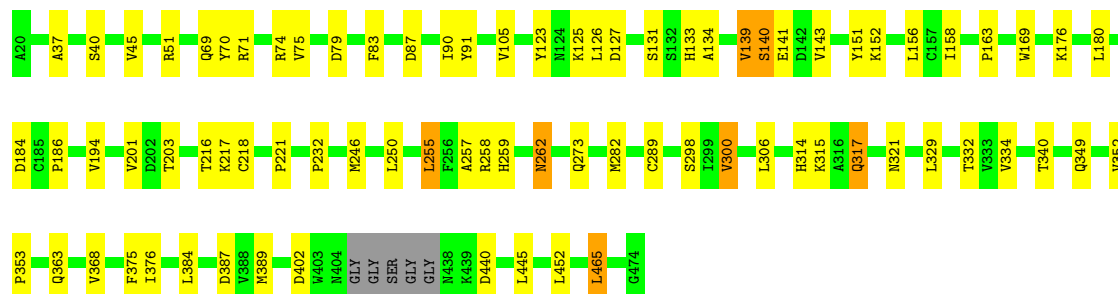
• Molecule 1: Major capsid protein L1





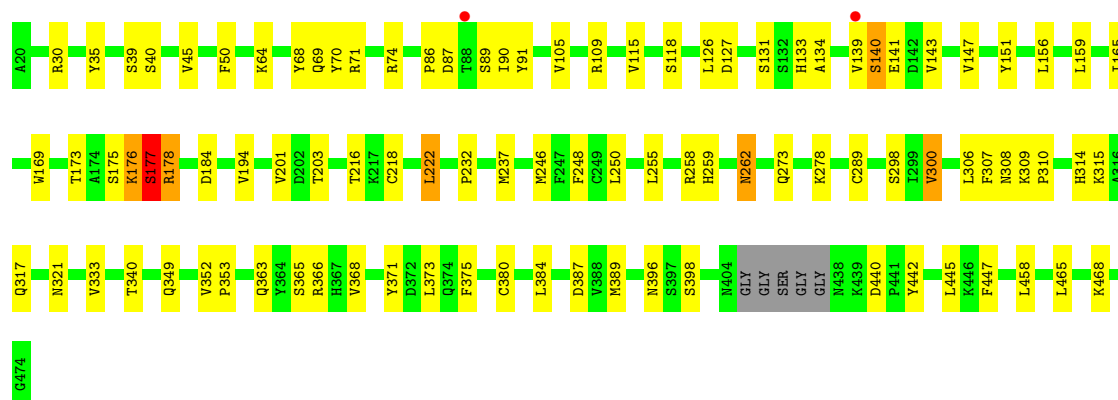
- Molecule 1: Major capsid protein L1

Chain J: 80% 17% ..



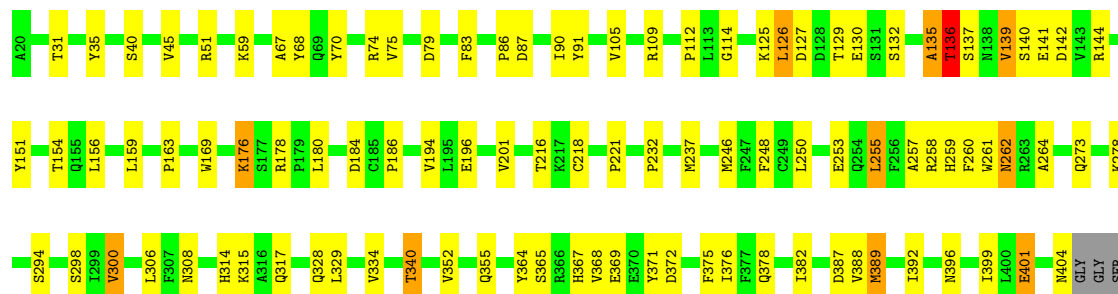
- Molecule 1: Major capsid protein L1

Chain K: 76% 21% ..



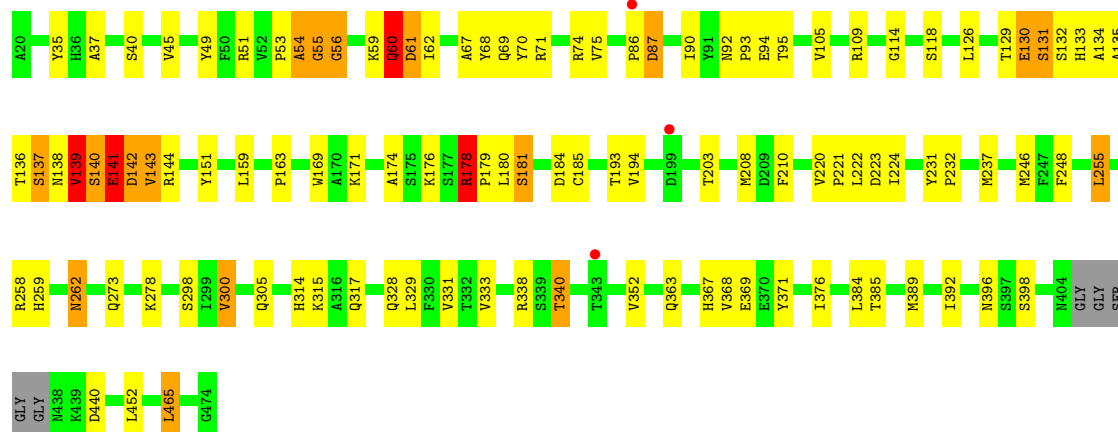
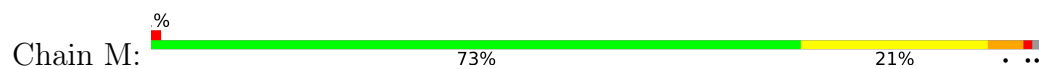
- Molecule 1: Major capsid protein L1

Chain L: 72% 23% ..

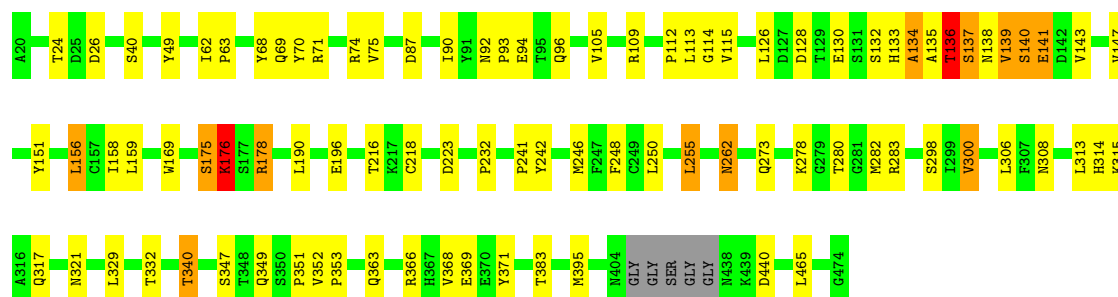
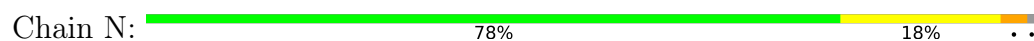




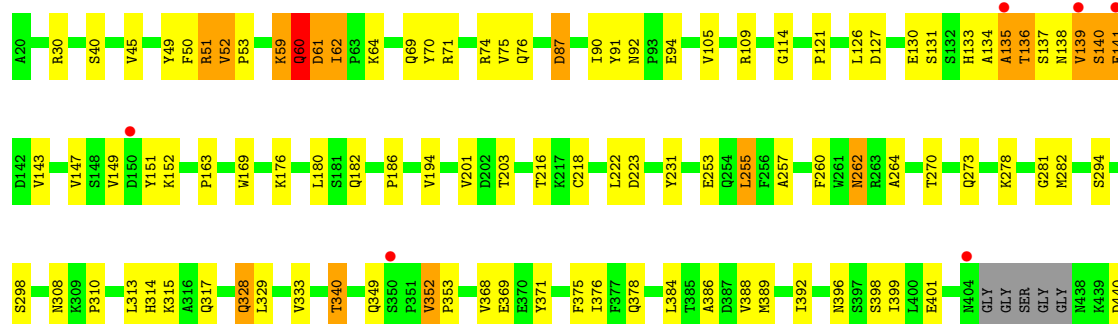
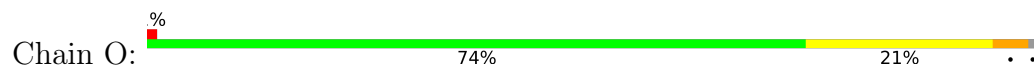
• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1

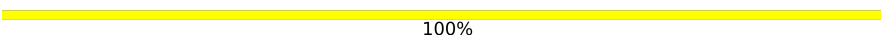


• Molecule 1: Major capsid protein L1



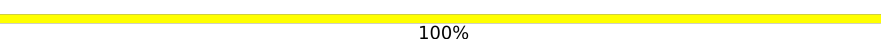


- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain P:  100%

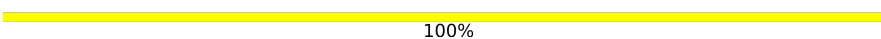


- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain S:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain T:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain U:  50% 50%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain W:  50% 50%

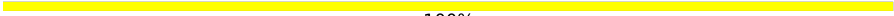


- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Y:  100%



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Z:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain a:  50% 50%

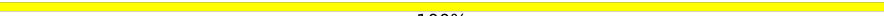
JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain d:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain i:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain j:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain k:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain l:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain m:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain n:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain o:  50% 50%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain q:  100%

JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain r:  100%

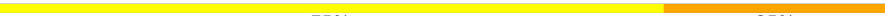
JHM1
IDS2

- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain s:  50% 50%

JHM1
IDS2

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain Q:  75% 25%



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain R:



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain V:



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain X:



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain b:

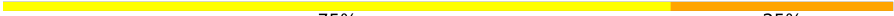


- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain c:



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain g:  75% 25%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain h:  100%

JHM1
IDS2
JHM3
IDS4

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain p:  75% 25%

JHM1
IDS2
JHM3
IDS4

- Molecule 4: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain e:  17% 83%

JHM1
IDS2
JHM3
IDS4
JHM5
IDS6

- Molecule 5: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-alpha-D-glucopyranose

Chain f:  50% 50%

JHM1
IDS2
JHM3
IDS4
JHM5
IDS6
JHM7
IDS8
JHM9
IDS10

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.99Å 106.49Å 237.66Å 88.46° 85.75° 69.02°	Depositor
Resolution (Å)	42.79 – 3.37 42.79 – 3.37	Depositor EDS
% Data completeness (in resolution range)	89.3 (42.79-3.37) 84.3 (42.79-3.37)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.171 , 0.234 0.171 , 0.228	Depositor DCC
R_{free} test set	4610 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	51075	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.29	0/3400	0.70	2/4622 (0.0%)
1	B	0.32	0/3400	0.72	1/4622 (0.0%)
1	C	0.31	0/3400	0.74	1/4622 (0.0%)
1	D	0.35	0/3400	0.74	2/4622 (0.0%)
1	E	0.30	0/3400	0.72	0/4622
1	F	0.30	0/3400	0.72	0/4622
1	G	0.30	0/3400	0.74	0/4622
1	H	0.31	0/3400	0.75	2/4622 (0.0%)
1	I	0.33	0/3400	0.74	2/4622 (0.0%)
1	J	0.30	0/3400	0.71	0/4622
1	K	0.30	0/3400	0.72	0/4622
1	L	0.32	0/3400	0.75	1/4622 (0.0%)
1	M	0.38	0/3400	0.78	3/4622 (0.1%)
1	N	0.30	0/3400	0.74	1/4622 (0.0%)
1	O	0.34	1/3400 (0.0%)	0.75	4/4622 (0.1%)
All	All	0.32	1/51000 (0.0%)	0.73	19/69330 (0.0%)

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	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	62	ILE	CA-CB	5.02	1.60	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	178	ARG	CA-C-N	-8.39	109.35	119.84
1	M	178	ARG	C-N-CA	-8.39	109.35	119.84
1	M	143	VAL	N-CA-C	-6.44	106.23	112.29
1	H	139	VAL	N-CA-C	5.77	116.51	109.30
1	C	140	SER	CB-CA-C	-5.73	108.97	115.79
1	D	62	ILE	CA-C-N	5.62	125.53	119.85
1	D	62	ILE	C-N-CA	5.62	125.53	119.85
1	A	352	VAL	CA-C-N	5.57	125.57	119.89
1	A	352	VAL	C-N-CA	5.57	125.57	119.89
1	I	240	ASP	CA-C-N	5.53	124.99	119.24
1	I	240	ASP	C-N-CA	5.53	124.99	119.24
1	H	143	VAL	N-CA-C	-5.40	106.16	111.77
1	O	352	VAL	CA-C-N	5.38	125.32	119.78
1	O	352	VAL	C-N-CA	5.38	125.32	119.78
1	O	52	VAL	CA-C-N	5.24	126.39	119.84
1	O	52	VAL	C-N-CA	5.24	126.39	119.84
1	L	137	SER	N-CA-C	5.14	116.88	109.07
1	B	90	ILE	N-CA-C	-5.10	106.95	113.22
1	N	133	HIS	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	133	HIS	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	3315	0	3181	48	0
1	B	3315	0	3181	60	0
1	C	3315	0	3180	60	0
1	D	3315	0	3181	56	0
1	E	3315	0	3181	51	0
1	F	3315	0	3181	62	0
1	G	3315	0	3181	71	0
1	H	3315	0	3181	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3315	0	3181	58	0
1	J	3315	0	3181	43	0
1	K	3315	0	3181	49	0
1	L	3315	0	3181	70	0
1	M	3315	0	3181	65	1
1	N	3315	0	3181	63	0
1	O	3315	0	3181	63	0
2	P	30	0	14	0	0
2	S	30	0	14	0	0
2	T	30	0	14	0	0
2	U	30	0	13	1	0
2	W	30	0	14	2	0
2	Y	30	0	14	10	0
2	Z	30	0	14	0	0
2	a	30	0	14	2	0
2	d	30	0	14	4	0
2	i	30	0	14	0	0
2	j	30	0	14	0	0
2	k	30	0	13	5	0
2	l	30	0	14	5	0
2	m	30	0	14	9	0
2	n	30	0	14	7	0
2	o	30	0	14	1	0
2	q	30	0	14	0	0
2	r	30	0	14	12	0
2	s	30	0	14	6	0
3	Q	60	0	26	1	0
3	R	60	0	26	2	0
3	V	60	0	26	8	0
3	X	60	0	26	11	0
3	b	60	0	26	5	0
3	c	60	0	25	6	0
3	g	60	0	26	1	0
3	h	60	0	27	12	0
3	p	60	0	26	1	0
4	e	90	0	39	14	0
5	f	150	0	62	4	1
All	All	51075	0	48313	840	1

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 8.

All (840) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:2:IDS:C4	2:s:1:JHM:H1	1.39	1.48
2:r:2:IDS:C4	2:s:1:JHM:C1	1.92	1.47
1:H:274:SER:CB	3:h:2:IDS:O6A	1.74	1.33
2:k:1:JHM:H2A	2:l:2:IDS:C6	1.61	1.29
1:H:274:SER:HB3	3:h:2:IDS:O6A	1.11	1.29
1:H:274:SER:HB3	3:h:2:IDS:C6	1.66	1.24
2:m:2:IDS:C4	2:n:1:JHM:O1	1.88	1.21
1:G:226:GLN:NE2	3:h:2:IDS:O2S	1.78	1.14
2:m:2:IDS:C4	2:n:1:JHM:C1	2.27	1.13
2:r:2:IDS:C4	2:s:1:JHM:O1	1.95	1.11
1:F:179:PRO:HB2	4:e:1:JHM:O8	1.46	1.10
3:X:1:JHM:C1	2:Y:2:IDS:C4	2.32	1.07
3:X:1:JHM:H1	2:Y:2:IDS:C4	1.85	1.07
2:a:2:IDS:O2	3:b:1:JHM:H1	1.54	1.05
1:B:217:LYS:HD3	3:V:1:JHM:O7	1.58	1.03
2:m:2:IDS:C4	2:n:1:JHM:H1	1.90	1.02
1:F:181:SER:N	4:e:1:JHM:O9	2.00	0.95
1:F:179:PRO:CB	4:e:1:JHM:O8	2.14	0.94
1:D:53:PRO:HG2	2:Y:1:JHM:O7	1.66	0.94
2:r:2:IDS:H3	2:s:1:JHM:O1	1.68	0.92
3:X:2:IDS:C6	3:X:3:JHM:C1	2.48	0.91
2:r:2:IDS:C3	2:s:1:JHM:O1	2.18	0.91
2:k:1:JHM:C2	2:l:2:IDS:C6	2.51	0.88
1:N:351:PRO:HG3	2:r:1:JHM:H4	1.57	0.87
1:N:69:GLN:HE21	1:N:71:ARG:HH12	1.24	0.86
1:G:226:GLN:O	3:h:4:IDS:O3	1.94	0.85
2:m:2:IDS:C3	2:n:1:JHM:O1	2.26	0.84
1:O:273:GLN:HB3	3:p:2:IDS:O3S	1.76	0.84
1:C:136:THR:HB	1:D:134:ALA:HB2	1.58	0.84
1:H:135:ALA:HB3	1:H:136:THR:HA	1.60	0.84
1:H:135:ALA:H	1:H:136:THR:HG22	1.42	0.82
2:m:2:IDS:H3	2:n:1:JHM:C1	2.11	0.81
1:F:178:ARG:CZ	4:e:1:JHM:H2	2.11	0.80
1:F:180:LEU:C	4:e:1:JHM:O9	2.25	0.80
2:m:2:IDS:H3	2:n:1:JHM:O5	1.81	0.80
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.64	0.79
1:H:274:SER:CA	3:h:2:IDS:O6A	2.30	0.79
1:C:139:VAL:HG22	1:C:140:SER:H	1.47	0.79
2:m:2:IDS:C3	2:n:1:JHM:C1	2.61	0.79
1:I:180:LEU:HD21	1:I:186:PRO:HA	1.66	0.78
1:B:217:LYS:CD	3:V:1:JHM:O7	2.32	0.78
1:E:174:ALA:N	3:c:3:JHM:O9	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:351:PRO:HD2	2:r:1:JHM:O9	1.85	0.76
1:B:174:ALA:HB2	1:B:180:LEU:HG	1.69	0.75
1:N:136:THR:OG1	1:N:137:SER:N	2.14	0.75
1:N:351:PRO:CG	2:r:1:JHM:H4	2.17	0.75
2:r:2:IDS:C4	2:s:1:JHM:HO1	1.96	0.75
1:F:179:PRO:CG	4:e:1:JHM:O8	2.36	0.73
1:M:139:VAL:O	1:M:141:GLU:N	2.20	0.73
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.70	0.72
1:K:258:ARG:NH1	1:L:130:GLU:OE1	2.23	0.72
2:k:1:JHM:H2A	2:l:2:IDS:C5	1.89	0.72
4:e:2:IDS:C6	4:e:3:JHM:H2A	2.18	0.72
1:I:273:GLN:HE22	1:I:278:LYS:HE2	1.53	0.72
1:L:59:LYS:HD3	1:M:178:ARG:NH1	2.04	0.72
1:D:55:GLY:O	1:D:57:GLY:N	2.23	0.72
1:J:69:GLN:HE21	1:J:71:ARG:HH12	1.37	0.71
1:O:140:SER:OG	1:O:141:GLU:N	2.20	0.71
1:N:351:PRO:HG2	2:r:1:JHM:O6	1.90	0.71
1:C:75:VAL:HB	1:C:329:LEU:HB3	1.73	0.71
1:K:273:GLN:HE22	1:K:278:LYS:HE2	1.54	0.70
1:F:179:PRO:HG2	4:e:1:JHM:O8	1.90	0.70
1:G:273:GLN:HE22	1:G:278:LYS:HE2	1.55	0.70
1:A:368:VAL:HG11	1:B:169:TRP:CZ2	2.27	0.70
2:k:1:JHM:H2A	2:l:2:IDS:O6B	1.92	0.69
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.75	0.69
1:L:178:ARG:HG2	2:m:1:JHM:O9	1.92	0.69
3:X:1:JHM:O1	2:Y:2:IDS:C4	2.41	0.69
1:L:176:LYS:HA	2:o:2:IDS:H3	1.73	0.68
1:L:125:LYS:NZ	1:M:131:SER:O	2.25	0.68
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.77	0.67
1:K:126:LEU:HB3	1:K:262:ASN:HB3	1.77	0.67
1:D:278:LYS:HE3	3:b:1:JHM:O7	1.95	0.66
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.77	0.66
1:A:180:LEU:HD21	1:A:186:PRO:HA	1.76	0.66
1:G:250:LEU:HB3	1:G:306:LEU:HD21	1.78	0.66
1:F:180:LEU:HD21	1:F:186:PRO:HA	1.78	0.66
1:L:59:LYS:HD3	1:M:178:ARG:HH11	1.58	0.66
1:D:384:LEU:HB3	1:D:389:MET:HE2	1.78	0.65
1:N:175:SER:O	1:N:176:LYS:HB3	1.94	0.65
1:A:357:ASP:HA	1:B:141:GLU:HG3	1.79	0.65
1:A:109:ARG:H	1:A:308:ASN:HD21	1.45	0.65
4:e:2:IDS:C6	4:e:3:JHM:C1	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ARG:H	1:O:308:ASN:HD21	1.42	0.65
1:G:109:ARG:H	1:G:308:ASN:HD21	1.45	0.65
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.78	0.64
1:K:384:LEU:HB3	1:K:389:MET:HE2	1.77	0.64
1:B:250:LEU:HB3	1:B:306:LEU:HD21	1.79	0.64
1:L:135:ALA:O	1:L:136:THR:OG1	2.13	0.64
1:A:273:GLN:HE22	1:A:278:LYS:HD2	1.61	0.64
2:a:2:IDS:H3	3:b:1:JHM:O5	1.89	0.64
1:L:178:ARG:CG	2:m:1:JHM:O9	2.46	0.63
3:R:2:IDS:O6B	3:R:3:JHM:O5	2.16	0.63
1:M:126:LEU:HB3	1:M:262:ASN:HB3	1.79	0.63
1:M:273:GLN:HE22	1:M:278:LYS:HE2	1.63	0.63
1:B:64:LYS:HD2	3:V:4:IDS:O2S	1.99	0.63
1:F:368:VAL:HG11	1:G:169:TRP:CZ2	2.33	0.62
1:D:142:ASP:OD2	1:D:144:ARG:NE	2.31	0.62
1:A:369:GLU:HG3	1:A:371:TYR:HE1	1.63	0.62
1:A:384:LEU:HD22	1:A:389:MET:HG3	1.81	0.62
1:B:442:TYR:O	1:B:444:LYS:N	2.32	0.62
1:F:169:TRP:CZ2	1:J:368:VAL:HG11	2.34	0.62
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.64	0.62
1:A:130:GLU:OE1	1:E:258:ARG:NH1	2.33	0.62
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.82	0.61
1:B:226:GLN:C	3:V:4:IDS:O3	2.44	0.61
1:J:384:LEU:HD22	1:J:389:MET:HG3	1.80	0.61
1:L:180:LEU:HD21	1:L:186:PRO:HA	1.82	0.61
1:B:89:SER:HB2	1:J:282:MET:HG2	1.82	0.61
1:M:114:GLY:HA3	1:M:340:THR:HG23	1.82	0.61
1:C:140:SER:OG	1:C:141:GLU:N	2.27	0.61
1:C:369:GLU:HG3	1:C:371:TYR:HE1	1.65	0.61
1:D:75:VAL:HB	1:D:329:LEU:HB3	1.83	0.61
1:N:250:LEU:HB3	1:N:306:LEU:HD21	1.82	0.60
1:G:386:ALA:HB2	1:L:355:GLN:HB2	1.83	0.60
1:M:130:GLU:O	1:M:132:SER:N	2.34	0.60
1:I:109:ARG:NH2	1:I:369:GLU:OE1	2.34	0.60
1:H:369:GLU:HG3	1:H:371:TYR:HE1	1.66	0.60
1:E:75:VAL:HB	1:E:329:LEU:HB3	1.83	0.60
1:G:142:ASP:OD2	1:G:142:ASP:N	2.34	0.60
1:I:369:GLU:HG3	1:I:371:TYR:HE1	1.66	0.60
1:M:105:VAL:HG21	1:M:159:LEU:HD11	1.82	0.60
1:O:376:ILE:HG12	1:O:465:LEU:HD13	1.84	0.59
1:E:156:LEU:HG	1:E:334:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:ASN:C	1:N:140:SER:H	2.11	0.59
1:I:133:HIS:O	1:I:135:ALA:N	2.29	0.59
1:N:175:SER:OG	1:N:178:ARG:O	2.18	0.59
1:C:274:SER:HB3	3:V:1:JHM:O3	2.01	0.59
1:G:75:VAL:HB	1:G:329:LEU:HB3	1.83	0.59
1:A:41:ARG:NH2	1:B:233:ASP:OD2	2.34	0.59
1:F:91:TYR:C	1:O:281:GLY:HA2	2.27	0.59
1:N:75:VAL:HB	1:N:329:LEU:HB3	1.85	0.59
1:L:442:TYR:C	1:L:444:LYS:H	2.11	0.59
3:h:2:IDS:O6B	3:h:3:JHM:C1	2.51	0.59
1:K:45:VAL:HG12	1:K:368:VAL:HG22	1.83	0.59
1:N:159:LEU:HB2	1:N:248:PHE:HB3	1.84	0.59
1:E:237:MET:HB3	1:E:246:MET:HG2	1.85	0.59
1:L:126:LEU:HB3	1:L:262:ASN:HB3	1.84	0.59
1:K:237:MET:HB3	1:K:246:MET:HG2	1.85	0.58
1:C:180:LEU:HD21	1:C:186:PRO:HA	1.85	0.58
1:C:369:GLU:HG3	1:C:371:TYR:CE1	2.38	0.58
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.86	0.58
1:N:140:SER:OG	1:N:141:GLU:N	2.34	0.58
1:N:368:VAL:HG11	1:O:169:TRP:CZ2	2.39	0.58
1:O:398:SER:HA	1:O:401:GLU:HB2	1.85	0.58
1:N:273:GLN:HE22	1:N:278:LYS:HE2	1.68	0.58
1:O:194:VAL:HG11	1:O:445:LEU:HD13	1.84	0.58
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.85	0.58
1:G:217:LYS:HD2	3:h:2:IDS:O1S	2.04	0.58
1:G:368:VAL:HG11	1:H:169:TRP:CZ2	2.39	0.58
1:G:178:ARG:HH12	5:f:1:JHM:H2	1.69	0.57
4:e:2:IDS:C6	4:e:3:JHM:C2	2.82	0.57
1:N:349:GLN:HB2	1:N:353:PRO:HD3	1.86	0.57
1:H:137:SER:O	1:H:138:ASN:HB2	2.03	0.57
1:G:87:ASP:O	1:G:90:ILE:HG12	2.04	0.57
1:O:75:VAL:HB	1:O:329:LEU:HB3	1.87	0.57
1:C:368:VAL:HG11	1:D:169:TRP:CZ2	2.40	0.57
1:H:45:VAL:HG12	1:H:368:VAL:HG22	1.86	0.57
1:N:105:VAL:HG21	1:N:159:LEU:HD11	1.87	0.57
1:G:273:GLN:NE2	1:G:278:LYS:HE2	2.20	0.57
1:A:369:GLU:HG3	1:A:371:TYR:CE1	2.39	0.57
1:H:142:ASP:OD2	1:H:144:ARG:NE	2.37	0.57
1:J:75:VAL:HB	1:J:329:LEU:HB3	1.87	0.57
1:L:368:VAL:HG11	1:M:169:TRP:HZ2	1.70	0.57
1:M:61:ASP:OD2	1:M:61:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ARG:NH2	4:e:1:JHM:H2	2.20	0.56
3:h:2:IDS:C6	3:h:3:JHM:C1	2.83	0.56
1:C:109:ARG:H	1:C:308:ASN:HD21	1.52	0.56
1:G:159:LEU:HB2	1:G:248:PHE:HB3	1.87	0.56
1:H:69:GLN:HE21	1:H:71:ARG:HH12	1.53	0.56
1:L:470:LEU:O	1:L:473:ALA:N	2.34	0.56
1:D:180:LEU:HD21	1:D:186:PRO:HA	1.87	0.56
1:E:45:VAL:HG12	1:E:368:VAL:HG22	1.87	0.56
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.88	0.56
1:M:369:GLU:HG3	1:M:371:TYR:HE1	1.70	0.56
1:I:314:HIS:CG	1:I:315:LYS:H	2.24	0.56
3:X:2:IDS:C6	3:X:3:JHM:H2A	2.36	0.56
1:H:176:LYS:O	1:H:176:LYS:HG3	2.06	0.56
1:K:250:LEU:HB3	1:K:306:LEU:HD21	1.87	0.55
1:B:396:ASN:ND2	1:B:398:SER:OG	2.39	0.55
1:C:274:SER:HB2	3:V:2:IDS:O5	2.06	0.55
1:O:126:LEU:HG	1:O:127:ASP:OD2	2.04	0.55
1:C:114:GLY:HA3	1:C:340:THR:HG23	1.89	0.55
1:L:368:VAL:HG11	1:M:169:TRP:CZ2	2.41	0.55
3:X:2:IDS:C6	3:X:3:JHM:C2	2.84	0.55
1:A:156:LEU:HG	1:A:334:VAL:HB	1.89	0.55
1:B:300:VAL:HG13	1:C:255:LEU:HD13	1.89	0.55
1:F:69:GLN:HE21	1:F:71:ARG:HH12	1.55	0.55
1:J:250:LEU:HB3	1:J:306:LEU:HD21	1.87	0.55
1:L:472:GLN:C	1:L:474:GLY:H	2.14	0.55
1:O:45:VAL:HG12	1:O:368:VAL:HG22	1.89	0.55
1:I:273:GLN:NE2	1:I:278:LYS:HE2	2.20	0.55
1:B:258:ARG:HG3	1:B:259:HIS:ND1	2.21	0.54
1:H:368:VAL:HG11	1:I:169:TRP:CZ2	2.41	0.54
1:A:59:LYS:HG3	1:A:60:GLN:N	2.21	0.54
1:C:250:LEU:HB3	1:C:306:LEU:HD21	1.88	0.54
1:K:349:GLN:HB2	1:K:353:PRO:HD3	1.89	0.54
1:C:87:ASP:O	1:C:90:ILE:HG12	2.07	0.54
1:D:384:LEU:HD22	1:D:389:MET:HG3	1.89	0.54
1:H:165:ILE:HD12	1:H:237:MET:HG2	1.88	0.54
1:O:369:GLU:HG3	1:O:371:TYR:HE1	1.71	0.54
1:L:45:VAL:HG12	1:L:368:VAL:HG22	1.89	0.54
5:f:2:IDS:O2	5:f:3:JHM:C1	2.56	0.54
1:C:383:THR:HG21	2:W:1:JHM:O1	2.08	0.54
1:K:396:ASN:ND2	1:K:398:SER:OG	2.41	0.54
1:F:87:ASP:O	1:F:90:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:VAL:HG11	1:H:323:VAL:HG13	1.90	0.53
1:I:140:SER:OG	1:I:141:GLU:N	2.40	0.53
4:e:4:IDS:O2S	4:e:5:JHM:O8	2.27	0.53
1:O:114:GLY:HA3	1:O:340:THR:HG23	1.89	0.53
1:F:258:ARG:NH1	1:G:130:GLU:OE1	2.40	0.53
1:H:113:LEU:HD22	1:I:253:GLU:HG3	1.89	0.53
1:O:87:ASP:O	1:O:90:ILE:HG12	2.08	0.53
1:H:180:LEU:HD21	1:H:186:PRO:HA	1.91	0.53
1:J:314:HIS:CG	1:J:315:LYS:H	2.25	0.53
1:F:250:LEU:HB3	1:F:306:LEU:HD21	1.90	0.53
1:K:35:TYR:OH	1:K:86:PRO:HD3	2.09	0.53
1:O:126:LEU:HB3	1:O:262:ASN:HB3	1.90	0.53
1:F:369:GLU:HG3	1:F:371:TYR:CE1	2.42	0.53
1:E:140:SER:OG	1:E:141:GLU:N	2.42	0.53
1:F:41:ARG:NH2	1:G:233:ASP:OD2	2.41	0.53
1:E:87:ASP:O	1:E:90:ILE:HG12	2.10	0.52
1:I:368:VAL:HG11	1:J:169:TRP:CZ2	2.44	0.52
1:N:314:HIS:CG	1:N:315:LYS:H	2.26	0.52
1:D:46:GLY:HA2	1:D:62:ILE:HG22	1.91	0.52
1:H:92:ASN:HD21	1:H:94:GLU:HB2	1.74	0.52
1:M:45:VAL:HG12	1:M:368:VAL:HG22	1.92	0.52
1:M:369:GLU:HG3	1:M:371:TYR:CE1	2.44	0.52
1:N:158:ILE:HD12	1:N:246:MET:HE2	1.92	0.52
1:I:396:ASN:ND2	1:I:398:SER:OG	2.42	0.52
1:J:180:LEU:HD21	1:J:186:PRO:HA	1.92	0.52
1:D:159:LEU:HB2	1:D:248:PHE:HB3	1.91	0.52
1:G:355:GLN:HE22	1:I:280:THR:HG23	1.74	0.52
1:B:442:TYR:C	1:B:444:LYS:H	2.18	0.52
1:D:87:ASP:O	1:D:90:ILE:HG12	2.09	0.52
1:H:369:GLU:HG3	1:H:371:TYR:CE1	2.45	0.52
1:I:69:GLN:HE21	1:I:71:ARG:HH12	1.58	0.52
1:E:99:VAL:HG11	1:E:323:VAL:HG13	1.92	0.52
1:F:258:ARG:HG3	1:F:259:HIS:ND1	2.25	0.52
1:M:132:SER:O	1:M:132:SER:OG	2.25	0.51
1:O:180:LEU:HD21	1:O:186:PRO:HA	1.93	0.51
3:c:1:JHM:O5	2:d:2:IDS:O6B	2.27	0.51
1:D:53:PRO:CG	2:Y:1:JHM:O7	2.50	0.51
1:D:272:PRO:HD2	1:D:275:LEU:HD12	1.92	0.51
1:H:151:TYR:CD2	1:H:203:THR:HB	2.45	0.51
1:F:273:GLN:HE22	1:F:278:LYS:HE2	1.76	0.51
3:c:1:JHM:O5	2:d:2:IDS:C6	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:VAL:HG11	1:G:445:LEU:HD13	1.92	0.51
1:J:105:VAL:HG22	1:J:375:PHE:HD2	1.75	0.51
1:L:139:VAL:O	1:L:141:GLU:N	2.36	0.51
1:A:87:ASP:O	1:A:90:ILE:HG12	2.10	0.51
1:H:132:SER:O	1:H:134:ALA:N	2.40	0.51
1:H:135:ALA:N	1:H:136:THR:HG22	2.19	0.51
1:F:96:GLN:HB3	1:F:383:THR:HA	1.91	0.51
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.92	0.51
1:N:92:ASN:HD21	1:N:94:GLU:HB2	1.75	0.51
1:I:216:THR:HG22	1:I:218:CYS:HB2	1.92	0.51
1:A:52:VAL:HB	1:A:62:ILE:HB	1.93	0.51
1:B:368:VAL:HG11	1:C:169:TRP:CZ2	2.46	0.51
1:N:273:GLN:NE2	1:N:278:LYS:HE2	2.26	0.51
1:D:250:LEU:HB3	1:D:306:LEU:HD21	1.92	0.50
1:G:158:ILE:HB	1:G:332:THR:HB	1.93	0.50
1:A:368:VAL:HG11	1:B:169:TRP:HZ2	1.73	0.50
1:A:384:LEU:HB3	1:A:389:MET:HE2	1.92	0.50
1:I:159:LEU:HB2	1:I:248:PHE:HB3	1.93	0.50
1:I:369:GLU:HG3	1:I:371:TYR:CE1	2.44	0.50
1:M:368:VAL:HG11	1:N:169:TRP:CZ2	2.46	0.50
1:N:126:LEU:HB3	1:N:262:ASN:HB3	1.93	0.50
1:B:49:TYR:HA	1:B:223:ASP:HB3	1.93	0.50
1:H:274:SER:OG	3:h:2:IDS:O6A	2.27	0.50
4:e:2:IDS:O6B	4:e:3:JHM:H2A	2.12	0.50
1:O:50:PHE:HD1	1:O:51:ARG:O	1.95	0.50
1:D:368:VAL:HG11	1:E:169:TRP:CZ2	2.46	0.50
1:E:151:TYR:CG	1:E:203:THR:HB	2.47	0.50
1:A:349:GLN:HB2	1:A:353:PRO:HD3	1.93	0.50
1:H:261:TRP:CZ3	1:H:294:SER:HB3	2.47	0.50
1:L:470:LEU:O	1:L:472:GLN:N	2.44	0.50
1:M:141:GLU:O	1:M:143:VAL:HG23	2.12	0.50
1:N:87:ASP:O	1:N:90:ILE:HG12	2.12	0.50
1:B:226:GLN:O	3:V:4:IDS:O3	2.29	0.50
1:E:310:PRO:HG3	1:E:468:LYS:HD3	1.93	0.50
1:F:169:TRP:HZ2	1:J:368:VAL:HG11	1.75	0.50
1:I:298:SER:OG	1:I:299:ILE:N	2.44	0.50
1:L:87:ASP:O	1:L:90:ILE:HG12	2.12	0.50
1:N:158:ILE:HB	1:N:332:THR:HB	1.93	0.50
1:O:74:ARG:NH2	1:O:328:GLN:OE1	2.40	0.50
1:C:72:VAL:HG22	1:C:332:THR:HG23	1.93	0.49
1:D:180:LEU:C	1:D:182:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:LYS:NZ	3:c:4:IDS:O6B	2.45	0.49
1:E:209:ASP:OD2	1:E:211:SER:OG	2.29	0.49
1:G:387:ASP:HB3	1:N:280:THR:HG22	1.92	0.49
1:I:74:ARG:HH22	1:I:440:ASP:CG	2.20	0.49
1:L:194:VAL:HG11	1:L:445:LEU:HD13	1.94	0.49
3:X:1:JHM:O5	2:Y:2:IDS:H3	2.12	0.49
1:L:105:VAL:HG22	1:L:375:PHE:HD2	1.77	0.49
1:B:159:LEU:HB2	1:B:248:PHE:HB3	1.93	0.49
1:L:109:ARG:H	1:L:308:ASN:HD21	1.59	0.49
1:A:121:PRO:HG3	1:B:289:CYS:SG	2.53	0.49
1:F:273:GLN:NE2	1:F:278:LYS:HE2	2.28	0.49
1:L:258:ARG:HG3	1:L:259:HIS:ND1	2.28	0.49
1:L:442:TYR:O	1:L:444:LYS:N	2.43	0.49
1:G:156:LEU:HA	1:G:250:LEU:O	2.12	0.49
1:K:70:TYR:OH	1:K:232:PRO:HD3	2.12	0.49
1:M:69:GLN:HE21	1:M:71:ARG:HH12	1.59	0.49
1:M:273:GLN:NE2	1:M:278:LYS:HE2	2.26	0.49
1:O:163:PRO:HB2	1:O:194:VAL:HG13	1.95	0.49
1:J:163:PRO:HB2	1:J:194:VAL:HG13	1.94	0.49
1:K:194:VAL:HG11	1:K:445:LEU:HD13	1.95	0.49
1:G:109:ARG:H	1:G:308:ASN:ND2	2.10	0.49
1:L:130:GLU:HB2	1:L:260:PHE:HB2	1.95	0.49
1:D:45:VAL:HG12	1:D:368:VAL:HG22	1.94	0.49
1:E:349:GLN:HB2	1:E:353:PRO:HD3	1.94	0.49
1:G:173:THR:OG1	1:G:174:ALA:N	2.46	0.49
1:H:135:ALA:CB	1:H:136:THR:HA	2.37	0.49
1:J:140:SER:OG	1:J:141:GLU:N	2.46	0.49
1:M:151:TYR:CD2	1:M:203:THR:HB	2.47	0.49
1:N:369:GLU:HG3	1:N:371:TYR:CE1	2.48	0.49
1:O:105:VAL:HG22	1:O:375:PHE:HD2	1.77	0.49
1:O:138:ASN:O	1:O:140:SER:N	2.45	0.49
1:I:376:ILE:HG12	1:I:465:LEU:HD13	1.95	0.49
1:F:152:LYS:HE3	1:F:253:GLU:HB2	1.95	0.48
1:F:396:ASN:ND2	1:F:398:SER:OG	2.46	0.48
1:G:181:SER:OG	1:G:184:ASP:OD2	2.27	0.48
1:H:121:PRO:HG3	1:I:289:CYS:SG	2.53	0.48
1:J:349:GLN:HB2	1:J:353:PRO:HD3	1.94	0.48
1:N:368:VAL:HG11	1:O:169:TRP:HZ2	1.77	0.48
1:C:97:ARG:HE	1:C:403:TRP:HB3	1.78	0.48
1:C:97:ARG:HG3	1:C:403:TRP:CD2	2.48	0.48
1:C:121:PRO:HG3	1:D:289:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:MET:HE3	1:G:246:MET:HE3	1.95	0.48
1:C:139:VAL:HG22	1:C:140:SER:N	2.24	0.48
1:F:182:GLN:O	4:e:3:JHM:O8	2.31	0.48
1:F:237:MET:HB3	1:F:246:MET:HG2	1.95	0.48
1:H:132:SER:C	1:H:134:ALA:N	2.72	0.48
1:N:156:LEU:HA	1:N:250:LEU:O	2.13	0.48
1:O:396:ASN:HB3	1:O:399:ILE:HG13	1.95	0.48
1:E:216:THR:HG22	1:E:218:CYS:HB2	1.94	0.48
1:G:134:ALA:HB3	1:H:133:HIS:CE1	2.49	0.48
1:I:151:TYR:CD2	1:I:203:THR:HB	2.48	0.48
1:K:87:ASP:O	1:K:90:ILE:HG12	2.13	0.48
1:K:87:ASP:OD2	1:K:89:SER:OG	2.29	0.48
1:A:123:TYR:HD2	1:A:125:LYS:HB2	1.78	0.48
1:B:349:GLN:HB2	1:B:353:PRO:HD3	1.94	0.48
1:F:216:THR:HG22	1:F:218:CYS:HB2	1.94	0.48
1:H:300:VAL:HG13	1:I:255:LEU:HD13	1.95	0.48
2:k:1:JHM:H1	2:l:2:IDS:O2	2.12	0.48
1:C:131:SER:O	1:C:133:HIS:N	2.46	0.48
1:F:351:PRO:HD2	3:g:3:JHM:O7	2.14	0.48
1:K:105:VAL:HG22	1:K:375:PHE:HD2	1.78	0.48
1:L:261:TRP:CZ3	1:L:294:SER:HB3	2.49	0.48
1:N:315:LYS:HA	1:N:321:ASN:HD21	1.79	0.48
1:O:134:ALA:O	1:O:136:THR:N	2.46	0.48
1:G:333:VAL:HG11	1:G:371:TYR:HE2	1.78	0.48
1:N:216:THR:HG22	1:N:218:CYS:HB2	1.95	0.48
1:L:105:VAL:HG22	1:L:375:PHE:CD2	2.49	0.48
1:L:273:GLN:HE22	1:L:278:LYS:HE2	1.78	0.48
1:A:152:LYS:HB2	1:A:255:LEU:HB3	1.96	0.48
1:O:349:GLN:HB2	1:O:353:PRO:HD3	1.96	0.48
1:A:262:ASN:HD22	1:A:262:ASN:HA	1.51	0.47
1:C:74:ARG:HH22	1:C:440:ASP:CG	2.21	0.47
1:C:136:THR:OG1	1:C:137:SER:N	2.44	0.47
1:F:126:LEU:HG	1:F:127:ASP:OD2	2.15	0.47
1:F:350:SER:HB3	1:F:351:PRO:HD3	1.96	0.47
1:G:35:TYR:OH	1:G:86:PRO:HD3	2.14	0.47
1:M:92:ASN:ND2	1:M:95:THR:OG1	2.47	0.47
1:C:349:GLN:HB2	1:C:353:PRO:HD3	1.96	0.47
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.14	0.47
1:G:37:ALA:HB1	1:G:452:LEU:HD13	1.96	0.47
1:K:368:VAL:HG11	1:L:169:TRP:CZ2	2.50	0.47
1:L:369:GLU:HG3	1:L:371:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:237:MET:HB3	1:M:246:MET:HG2	1.95	0.47
3:c:1:JHM:H6A	2:d:2:IDS:O6A	2.15	0.47
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.97	0.47
1:A:181:SER:OG	1:A:184:ASP:OD1	2.31	0.47
1:E:163:PRO:HB2	1:E:194:VAL:HG13	1.96	0.47
1:M:300:VAL:HG13	1:N:255:LEU:HD13	1.97	0.47
1:O:369:GLU:HG3	1:O:371:TYR:CE1	2.50	0.47
1:A:68:TYR:CE2	1:A:151:TYR:HB2	2.50	0.47
1:B:180:LEU:H	1:B:180:LEU:HD12	1.80	0.47
1:D:314:HIS:CG	1:D:315:LYS:H	2.32	0.47
1:J:376:ILE:HG12	1:J:465:LEU:HD13	1.97	0.47
1:E:109:ARG:H	1:E:308:ASN:HD21	1.62	0.47
1:H:87:ASP:O	1:H:90:ILE:HG12	2.14	0.47
1:H:368:VAL:HG11	1:I:169:TRP:HZ2	1.79	0.47
1:I:67:ALA:HB2	1:I:367:HIS:CE1	2.50	0.47
1:J:79:ASP:O	1:J:83:PHE:HB2	2.14	0.47
1:K:262:ASN:HD22	1:K:262:ASN:HA	1.54	0.47
1:L:389:MET:HB2	1:L:389:MET:HE3	1.58	0.47
1:M:138:ASN:OD1	1:M:138:ASN:C	2.58	0.47
1:O:69:GLN:HE21	1:O:71:ARG:HH12	1.62	0.47
1:O:333:VAL:HG11	1:O:371:TYR:HE2	1.79	0.47
1:E:384:LEU:HB3	1:E:389:MET:HE2	1.96	0.47
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.97	0.47
1:I:237:MET:HB3	1:I:246:MET:HG2	1.97	0.47
1:I:384:LEU:HD22	1:I:389:MET:HG3	1.96	0.47
1:J:151:TYR:CD2	1:J:203:THR:HB	2.49	0.47
1:B:439:LYS:HA	1:B:439:LYS:HD3	1.58	0.47
1:O:105:VAL:HG22	1:O:375:PHE:CD2	2.50	0.47
1:O:126:LEU:HD13	1:O:264:ALA:HB2	1.97	0.47
3:V:2:IDS:C6	3:V:3:JHM:O5	2.63	0.47
1:B:87:ASP:O	1:B:90:ILE:HG12	2.15	0.47
1:L:159:LEU:HB2	1:L:248:PHE:HB3	1.97	0.47
1:N:169:TRP:CE2	1:N:190:LEU:HD13	2.49	0.47
1:O:92:ASN:ND2	1:O:94:GLU:HB2	2.30	0.47
1:B:237:MET:HB3	1:B:246:MET:HG2	1.96	0.46
1:D:151:TYR:CD2	1:D:203:THR:HB	2.49	0.46
1:F:221:PRO:HD2	1:F:224:ILE:HD11	1.97	0.46
1:I:315:LYS:HA	1:I:321:ASN:HD21	1.79	0.46
1:K:333:VAL:HG11	1:K:371:TYR:HE2	1.80	0.46
1:M:258:ARG:HG3	1:M:259:HIS:ND1	2.30	0.46
1:A:74:ARG:NH2	1:A:328:GLN:OE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA3	1:B:340:THR:HG23	1.97	0.46
1:B:396:ASN:HB3	1:B:399:ILE:HG13	1.97	0.46
1:E:156:LEU:HA	1:E:250:LEU:O	2.15	0.46
1:G:114:GLY:HA3	1:G:340:THR:HG23	1.97	0.46
1:G:314:HIS:CG	1:G:315:LYS:H	2.33	0.46
1:G:358:ALA:O	1:H:265:GLY:HA2	2.15	0.46
1:M:396:ASN:ND2	1:M:398:SER:OG	2.49	0.46
1:K:69:GLN:HE21	1:K:71:ARG:HH12	1.63	0.46
1:K:300:VAL:HG13	1:L:255:LEU:HD13	1.97	0.46
1:A:97:ARG:HG3	1:A:403:TRP:CE3	2.51	0.46
1:I:87:ASP:O	1:I:90:ILE:HG12	2.16	0.46
1:M:87:ASP:O	1:M:90:ILE:HG12	2.14	0.46
1:B:177:SER:OG	1:B:178:ARG:N	2.49	0.46
1:F:121:PRO:HG3	1:G:289:CYS:SG	2.56	0.46
1:J:258:ARG:HG3	1:J:259:HIS:ND1	2.30	0.46
1:K:140:SER:OG	1:K:141:GLU:N	2.48	0.46
1:N:105:VAL:HG21	1:N:159:LEU:CD1	2.44	0.46
1:H:258:ARG:NH1	1:I:130:GLU:OE1	2.49	0.46
1:B:76:GLN:HG3	1:B:453:LYS:HE3	1.97	0.46
1:D:273:GLN:HE22	1:D:278:LYS:HE3	1.81	0.46
1:F:151:TYR:CG	1:F:203:THR:HB	2.51	0.46
1:I:45:VAL:HG12	1:I:368:VAL:HG22	1.96	0.46
1:L:388:VAL:O	1:L:392:ILE:HG13	2.16	0.46
1:M:305:GLN:OE1	1:M:338:ARG:NH1	2.45	0.46
1:L:75:VAL:HB	1:L:329:LEU:HB3	1.97	0.46
1:L:126:LEU:HD13	1:L:264:ALA:HB2	1.98	0.46
1:M:210:PHE:CE2	1:M:220:VAL:HG11	2.51	0.46
1:N:74:ARG:HH22	1:N:440:ASP:CG	2.24	0.46
1:D:237:MET:HB3	1:D:246:MET:HG2	1.98	0.46
1:G:452:LEU:HA	1:G:455:LYS:HG3	1.97	0.46
1:J:87:ASP:O	1:J:90:ILE:HG12	2.16	0.46
1:K:74:ARG:HH22	1:K:440:ASP:CG	2.23	0.46
1:L:364:TYR:CD2	1:M:185:CYS:HB2	2.50	0.46
1:O:152:LYS:HE3	1:O:253:GLU:HB2	1.98	0.46
1:O:384:LEU:HD22	1:O:389:MET:HG3	1.96	0.46
1:A:151:TYR:CD2	1:A:203:THR:HB	2.51	0.46
1:B:125:LYS:NZ	1:C:132:SER:HB3	2.30	0.46
1:C:262:ASN:HD22	1:C:262:ASN:HA	1.50	0.46
1:D:180:LEU:O	1:D:182:GLN:N	2.48	0.46
1:D:326:HIS:HE1	1:D:396:ASN:OD1	1.99	0.46
1:F:315:LYS:HA	1:F:321:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:TYR:CD2	1:G:203:THR:HB	2.51	0.46
1:H:70:TYR:OH	1:H:232:PRO:HD3	2.16	0.46
1:O:92:ASN:HD21	1:O:94:GLU:HB2	1.81	0.46
1:A:255:LEU:HD13	1:E:300:VAL:HG13	1.98	0.45
1:G:30:ARG:NH2	1:G:321:ASN:O	2.48	0.45
1:K:39:SER:HG	1:K:373:LEU:H	1.64	0.45
1:K:442:TYR:HB3	1:K:447:PHE:HE1	1.81	0.45
1:B:258:ARG:NH1	1:C:130:GLU:OE1	2.49	0.45
1:C:307:PHE:C	1:C:309:LYS:H	2.25	0.45
1:G:76:GLN:HG3	1:G:453:LYS:HE3	1.99	0.45
1:O:151:TYR:CD2	1:O:203:THR:HB	2.52	0.45
1:B:217:LYS:HG2	1:B:226:GLN:OE1	2.17	0.45
1:F:123:TYR:HD2	1:F:125:LYS:HB2	1.82	0.45
1:G:369:GLU:HG3	1:G:371:TYR:CE1	2.51	0.45
1:M:75:VAL:HB	1:M:329:LEU:HB3	1.99	0.45
1:O:76:GLN:HG3	1:O:453:LYS:HE3	1.98	0.45
1:O:216:THR:HG22	1:O:218:CYS:HB2	1.98	0.45
1:A:45:VAL:HG12	1:A:368:VAL:HG22	1.97	0.45
1:D:109:ARG:H	1:D:308:ASN:HD21	1.63	0.45
1:G:258:ARG:HG3	1:G:259:HIS:ND1	2.32	0.45
1:G:261:TRP:CZ3	1:G:294:SER:HB3	2.52	0.45
1:K:273:GLN:NE2	1:K:278:LYS:HE2	2.27	0.45
1:L:300:VAL:HG13	1:M:255:LEU:HD13	1.98	0.45
1:N:96:GLN:HB3	1:N:383:THR:HA	1.98	0.45
1:O:127:ASP:CG	1:O:136:THR:HG21	2.40	0.45
1:E:68:TYR:CE2	1:E:151:TYR:HB2	2.51	0.45
1:I:105:VAL:HG21	1:I:159:LEU:HD11	1.98	0.45
1:I:133:HIS:ND1	1:I:133:HIS:N	2.64	0.45
1:I:300:VAL:HG13	1:J:255:LEU:HD13	1.97	0.45
1:M:384:LEU:HD22	1:M:389:MET:HG3	1.98	0.45
1:B:28:VAL:HG22	1:B:382:ILE:HD11	1.99	0.45
1:D:262:ASN:HD22	1:D:262:ASN:HA	1.58	0.45
1:H:237:MET:HB3	1:H:246:MET:HG2	1.99	0.45
1:O:273:GLN:HE22	1:O:278:LYS:HE2	1.82	0.45
1:B:368:VAL:HG11	1:C:169:TRP:HZ2	1.82	0.45
1:B:369:GLU:HG3	1:B:371:TYR:HE1	1.81	0.45
1:D:300:VAL:HG13	1:E:255:LEU:HD13	1.98	0.45
1:E:445:LEU:HD21	2:d:1:JHM:H2A	1.99	0.45
1:G:369:GLU:HG3	1:G:371:TYR:HE1	1.82	0.45
1:I:52:VAL:HB	1:I:62:ILE:HB	1.99	0.45
1:M:67:ALA:HB2	1:M:367:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:HB2	1:B:96:GLN:HG3	1.98	0.45
1:I:349:GLN:HB2	1:I:353:PRO:HD3	1.98	0.45
3:X:1:JHM:C1	2:Y:2:IDS:C3	2.92	0.45
1:A:250:LEU:HB3	1:A:306:LEU:HD21	1.99	0.45
1:E:92:ASN:HA	1:E:93:PRO:HD2	1.86	0.45
1:H:366:ARG:HA	1:H:366:ARG:HD3	1.87	0.45
1:J:70:TYR:OH	1:J:232:PRO:HD3	2.16	0.45
1:F:114:GLY:HA3	1:F:340:THR:HG23	1.99	0.44
1:J:262:ASN:HD22	1:J:262:ASN:HA	1.58	0.44
1:K:151:TYR:CD2	1:K:203:THR:HB	2.52	0.44
1:M:144:ARG:O	1:N:283:ARG:HD3	2.17	0.44
1:A:112:PRO:HB3	1:B:231:TYR:CE1	2.52	0.44
1:A:231:TYR:CE1	1:E:112:PRO:HB3	2.53	0.44
1:F:49:TYR:HA	1:F:223:ASP:HB3	2.00	0.44
1:G:172:GLY:O	1:G:174:ALA:N	2.51	0.44
1:L:142:ASP:OD2	1:L:144:ARG:HG3	2.17	0.44
1:M:258:ARG:NH1	1:N:130:GLU:OE1	2.50	0.44
1:N:49:TYR:HA	1:N:223:ASP:HB3	1.99	0.44
1:F:45:VAL:HG12	1:F:368:VAL:HG22	1.97	0.44
1:G:366:ARG:HA	1:G:366:ARG:HD3	1.82	0.44
1:K:30:ARG:HD3	1:K:380:CYS:SG	2.57	0.44
1:K:368:VAL:HG11	1:L:169:TRP:HZ2	1.82	0.44
1:D:258:ARG:HG3	1:D:259:HIS:ND1	2.32	0.44
1:E:114:GLY:HA3	1:E:340:THR:HG23	1.99	0.44
1:B:140:SER:OG	1:B:141:GLU:N	2.49	0.44
1:C:76:GLN:HG3	1:C:453:LYS:HE3	2.00	0.44
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.98	0.44
1:F:76:GLN:HG3	1:F:453:LYS:HE3	1.98	0.44
1:F:127:ASP:OD2	1:F:136:THR:HB	2.17	0.44
1:H:384:LEU:HD21	1:H:403:TRP:HZ3	1.82	0.44
1:I:159:LEU:O	1:I:246:MET:HA	2.18	0.44
1:J:105:VAL:HG22	1:J:375:PHE:CD2	2.53	0.44
1:L:216:THR:HG22	1:L:218:CYS:HB2	1.99	0.44
1:L:237:MET:HB3	1:L:246:MET:HG2	1.99	0.44
1:M:105:VAL:HG21	1:M:159:LEU:CD1	2.47	0.44
1:O:384:LEU:HB3	1:O:389:MET:HE2	1.98	0.44
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.52	0.44
1:A:349:GLN:NE2	3:Q:3:JHM:H6	2.33	0.44
1:C:95:THR:HG21	2:W:1:JHM:H6A	1.99	0.44
1:D:220:VAL:HG23	1:D:225:CYS:HA	1.98	0.44
1:I:75:VAL:HB	1:I:329:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:GLY:HA3	1:I:340:THR:HG23	2.00	0.44
1:K:115:VAL:HG21	1:L:257:ALA:HB2	2.00	0.44
1:O:30:ARG:NH1	1:O:378:GLN:OE1	2.42	0.44
1:A:278:LYS:HD3	2:U:2:IDS:O3S	2.17	0.44
1:G:176:LYS:HA	1:G:176:LYS:HD3	1.90	0.44
1:J:70:TYR:CE1	1:J:201:VAL:HG12	2.53	0.44
1:L:401:GLU:O	1:L:404:ASN:N	2.32	0.44
1:H:460:LEU:HD12	1:H:470:LEU:HD21	1.99	0.44
1:E:74:ARG:HH22	1:E:440:ASP:CG	2.25	0.44
1:E:173:THR:HA	3:c:3:JHM:O8	2.18	0.44
1:F:105:VAL:HG21	1:F:159:LEU:HD11	1.99	0.44
1:F:314:HIS:CG	1:F:315:LYS:H	2.36	0.44
1:J:156:LEU:HG	1:J:334:VAL:HB	2.00	0.44
1:L:439:LYS:HD2	1:L:439:LYS:O	2.18	0.44
1:M:70:TYR:OH	1:M:232:PRO:HD3	2.17	0.44
1:B:169:TRP:CZ2	1:B:190:LEU:HD13	2.53	0.43
1:C:237:MET:HB3	1:C:246:MET:HG2	1.99	0.43
1:D:24:THR:HA	1:D:27:TYR:CE2	2.52	0.43
1:O:70:TYR:CZ	1:O:201:VAL:HG12	2.53	0.43
3:R:2:IDS:O6B	3:R:3:JHM:C1	2.65	0.43
1:M:35:TYR:OH	1:M:86:PRO:HD3	2.18	0.43
1:M:159:LEU:O	1:M:246:MET:HA	2.18	0.43
1:N:242:TYR:CZ	1:N:395:MET:HA	2.53	0.43
1:C:384:LEU:HB3	1:C:389:MET:HE2	2.01	0.43
1:D:366:ARG:HA	1:D:366:ARG:HD3	1.78	0.43
1:G:300:VAL:HG13	1:H:255:LEU:HD13	1.98	0.43
1:H:217:LYS:HD3	1:I:277:ILE:HD11	1.99	0.43
1:I:109:ARG:HA	1:I:109:ARG:HD2	1.89	0.43
1:K:237:MET:HE3	1:K:246:MET:HE3	2.00	0.43
1:N:128:ASP:O	1:N:132:SER:HB3	2.18	0.43
1:D:92:ASN:HA	1:D:93:PRO:HD2	1.80	0.43
1:K:315:LYS:HA	1:K:321:ASN:HD21	1.83	0.43
1:O:149:VAL:HG21	1:O:294:SER:HB2	1.99	0.43
3:X:1:JHM:O1	2:Y:2:IDS:C3	2.66	0.43
1:A:209:ASP:OD2	1:A:211:SER:OG	2.29	0.43
1:B:70:TYR:CE1	1:B:201:VAL:HG12	2.53	0.43
1:C:109:ARG:H	1:C:308:ASN:ND2	2.16	0.43
1:E:314:HIS:CG	1:E:315:LYS:H	2.36	0.43
1:G:242:TYR:CZ	1:G:395:MET:HA	2.53	0.43
1:H:131:SER:O	1:H:132:SER:C	2.61	0.43
1:I:366:ARG:HA	1:I:366:ARG:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:310:PRO:HG3	1:K:468:LYS:HD3	2.01	0.43
1:L:35:TYR:OH	1:L:86:PRO:HD3	2.18	0.43
1:M:37:ALA:HB1	1:M:452:LEU:HD13	2.00	0.43
1:B:128:ASP:O	1:B:132:SER:HB3	2.19	0.43
1:F:333:VAL:HG11	1:F:371:TYR:HE2	1.83	0.43
1:I:96:GLN:HB3	1:I:383:THR:HA	2.01	0.43
1:F:172:GLY:HA3	1:F:187:PRO:HG2	2.00	0.43
1:H:68:TYR:CE2	1:H:151:TYR:HB2	2.54	0.43
1:N:300:VAL:HG13	1:O:255:LEU:HD13	2.01	0.43
1:N:347:SER:O	1:O:182:GLN:NE2	2.52	0.43
1:O:396:ASN:ND2	1:O:398:SER:OG	2.52	0.43
3:X:1:JHM:O5	2:Y:2:IDS:C4	2.67	0.43
1:A:70:TYR:CE1	1:A:201:VAL:HG12	2.53	0.43
1:B:442:TYR:C	1:B:444:LYS:N	2.77	0.43
1:C:66:SER:H	1:C:69:GLN:NE2	2.15	0.43
1:E:273:GLN:HE21	1:E:273:GLN:HB3	1.53	0.43
1:G:74:ARG:HH22	1:G:440:ASP:CG	2.26	0.43
1:H:384:LEU:HD21	1:H:403:TRP:CZ3	2.54	0.43
1:M:314:HIS:CG	1:M:315:LYS:H	2.37	0.43
1:B:92:ASN:HA	1:B:93:PRO:HD2	1.87	0.43
1:C:368:VAL:HG11	1:D:169:TRP:HZ2	1.81	0.43
1:H:216:THR:HG22	1:H:218:CYS:HB2	1.99	0.43
1:L:376:ILE:HG12	1:L:465:LEU:HD13	2.01	0.43
1:L:440:ASP:C	1:L:442:TYR:H	2.27	0.43
1:M:54:ALA:HB2	1:M:61:ASP:OD1	2.19	0.43
1:M:92:ASN:C	1:M:94:GLU:H	2.27	0.43
1:N:175:SER:OG	1:N:176:LYS:N	2.50	0.43
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.53	0.43
1:B:438:ASN:OD1	1:B:438:ASN:N	2.51	0.43
1:G:96:GLN:HB3	1:G:383:THR:HA	2.01	0.43
1:L:74:ARG:NH2	1:L:328:GLN:OE1	2.49	0.43
1:N:68:TYR:CE2	1:N:151:TYR:HB2	2.53	0.43
1:O:388:VAL:O	1:O:392:ILE:HG13	2.18	0.43
1:C:92:ASN:HD21	1:C:94:GLU:HB2	1.84	0.42
1:D:369:GLU:HG3	1:D:371:TYR:CE1	2.54	0.42
1:F:156:LEU:HA	1:F:250:LEU:O	2.19	0.42
1:G:368:VAL:HG11	1:H:169:TRP:HZ2	1.81	0.42
1:J:37:ALA:HB1	1:J:452:LEU:HD13	2.00	0.42
1:J:317:GLN:HE21	1:J:317:GLN:HB2	1.66	0.42
1:K:86:PRO:HB3	1:K:458:LEU:HD11	2.00	0.42
1:K:366:ARG:HA	1:K:366:ARG:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:438:ASN:HB2	1:L:439:LYS:H	1.53	0.42
1:O:74:ARG:HH22	1:O:440:ASP:CG	2.27	0.42
1:H:462:GLN:HE22	1:I:21:VAL:HB	1.84	0.42
1:I:250:LEU:HB3	1:I:306:LEU:HD21	2.01	0.42
1:L:114:GLY:HA3	1:L:340:THR:HG23	2.01	0.42
1:L:440:ASP:HB3	1:L:443:ASP:OD1	2.18	0.42
1:M:208:MET:HE2	1:M:210:PHE:CD2	2.55	0.42
1:B:444:LYS:HE2	1:B:444:LYS:HA	2.01	0.42
1:C:97:ARG:HG3	1:C:403:TRP:CE3	2.54	0.42
1:C:131:SER:O	1:C:132:SER:C	2.62	0.42
1:C:300:VAL:HG13	1:D:255:LEU:HD13	2.00	0.42
1:D:70:TYR:OH	1:D:232:PRO:HD3	2.19	0.42
1:D:376:ILE:HG12	1:D:465:LEU:HD13	2.00	0.42
1:E:366:ARG:HA	1:E:366:ARG:HD3	1.86	0.42
1:F:130:GLU:HB2	1:F:260:PHE:HB2	2.01	0.42
1:G:70:TYR:CE1	1:G:201:VAL:HG12	2.54	0.42
1:G:142:ASP:HB2	1:H:283:ARG:HD2	2.01	0.42
1:L:67:ALA:HB2	1:L:367:HIS:CE1	2.55	0.42
1:L:79:ASP:O	1:L:83:PHE:HB2	2.19	0.42
1:O:92:ASN:C	1:O:94:GLU:H	2.26	0.42
5:f:4:IDS:C6	5:f:5:JHM:C1	2.97	0.42
1:E:67:ALA:HB2	1:E:367:HIS:CE1	2.55	0.42
1:H:125:LYS:HD2	1:H:261:TRP:NE1	2.35	0.42
1:I:49:TYR:HA	1:I:223:ASP:HB3	2.02	0.42
1:K:289:CYS:SG	1:O:121:PRO:HG3	2.60	0.42
1:L:369:GLU:HG3	1:L:371:TYR:HE1	1.85	0.42
1:N:113:LEU:HD22	1:O:253:GLU:HG3	2.02	0.42
1:C:237:MET:HE3	1:C:246:MET:HE3	2.02	0.42
1:C:314:HIS:O	1:C:315:LYS:HG3	2.20	0.42
1:G:317:GLN:HE21	1:G:317:GLN:HB2	1.65	0.42
1:G:364:TYR:CD2	1:H:185:CYS:HB2	2.54	0.42
1:I:115:VAL:HG21	1:J:257:ALA:HB2	2.00	0.42
1:M:109:ARG:HA	1:M:109:ARG:HD2	1.89	0.42
1:F:74:ARG:HH22	1:F:440:ASP:CG	2.26	0.42
1:F:79:ASP:HA	1:F:327:ASN:ND2	2.35	0.42
1:F:300:VAL:HG13	1:G:255:LEU:HD13	2.02	0.42
1:G:109:ARG:HA	1:G:109:ARG:HD2	1.90	0.42
1:H:114:GLY:HA3	1:H:340:THR:HG23	2.02	0.42
1:I:388:VAL:O	1:I:392:ILE:HG12	2.20	0.42
1:J:314:HIS:CG	1:J:315:LYS:N	2.87	0.42
1:K:105:VAL:HG22	1:K:375:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:LEU:HB2	1:K:248:PHE:HB3	2.00	0.42
1:L:151:TYR:OH	1:L:221:PRO:HB2	2.20	0.42
1:M:60:GLN:HE21	1:M:60:GLN:HB2	1.66	0.42
1:M:138:ASN:OD1	1:M:140:SER:N	2.42	0.42
1:N:314:HIS:CG	1:N:315:LYS:N	2.88	0.42
1:B:160:GLY:HA2	1:B:247:PHE:CE2	2.54	0.42
1:D:278:LYS:HB2	3:b:1:JHM:O7	2.20	0.42
1:H:209:ASP:OD2	1:H:211:SER:OG	2.37	0.42
1:I:384:LEU:HB3	1:I:389:MET:HE2	2.01	0.42
1:J:158:ILE:HB	1:J:332:THR:HB	2.01	0.42
1:C:35:TYR:CE2	1:C:458:LEU:HG	2.55	0.42
1:C:133:HIS:HB3	1:C:134:ALA:H	1.53	0.42
1:G:178:ARG:NH1	5:f:1:JHM:H2	2.34	0.42
1:J:194:VAL:HG11	1:J:445:LEU:HD13	2.02	0.42
1:L:70:TYR:CE1	1:L:201:VAL:HG12	2.55	0.42
1:L:163:PRO:HB2	1:L:194:VAL:HG13	2.01	0.42
1:M:74:ARG:HH22	1:M:440:ASP:CG	2.27	0.42
1:O:60:GLN:HB3	1:O:61:ASP:H	1.74	0.42
1:B:78:PRO:HD3	1:B:453:LYS:HA	2.02	0.42
1:D:210:PHE:CE2	1:D:220:VAL:HG11	2.55	0.42
1:F:255:LEU:HD13	1:J:300:VAL:HG13	2.02	0.42
1:F:277:ILE:HD11	1:J:217:LYS:HD3	2.02	0.42
1:J:402:ASP:OD2	1:J:402:ASP:N	2.53	0.42
1:N:134:ALA:O	1:N:136:THR:N	2.52	0.42
1:D:125:LYS:HG3	1:D:261:TRP:CG	2.54	0.42
1:F:262:ASN:HD22	1:F:262:ASN:HA	1.55	0.42
1:F:345:CYS:HA	1:F:362:LYS:O	2.19	0.42
1:F:459:ASP:OD2	1:F:459:ASP:N	2.53	0.42
1:H:74:ARG:HH22	1:H:440:ASP:CG	2.28	0.42
1:H:210:PHE:CE2	1:H:220:VAL:HG11	2.54	0.42
1:H:376:ILE:HG12	1:H:465:LEU:HD13	2.01	0.42
1:I:30:ARG:HB3	1:I:378:GLN:NE2	2.35	0.42
1:K:109:ARG:H	1:K:308:ASN:HD21	1.68	0.42
1:K:222:LEU:HD12	1:K:222:LEU:HA	1.89	0.42
1:L:112:PRO:HB3	1:M:231:TYR:CD1	2.55	0.42
1:M:141:GLU:HB2	1:M:142:ASP:H	1.61	0.42
1:N:369:GLU:HG3	1:N:371:TYR:HE1	1.84	0.42
1:A:66:SER:H	1:A:69:GLN:NE2	2.18	0.41
1:B:40:SER:OG	1:B:41:ARG:N	2.53	0.41
1:G:172:GLY:O	1:G:173:THR:C	2.63	0.41
1:L:31:THR:O	1:L:378:GLN:NE2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:PRO:HB2	1:M:194:VAL:HG13	2.02	0.41
1:N:114:GLY:HA3	1:N:340:THR:HG23	2.02	0.41
1:C:74:ARG:NH2	1:C:328:GLN:OE1	2.48	0.41
1:C:163:PRO:HB2	1:C:194:VAL:HG13	2.01	0.41
1:D:463:TYR:O	1:D:467:ARG:HG3	2.20	0.41
1:E:79:ASP:O	1:E:83:PHE:HB2	2.20	0.41
1:G:133:HIS:CD2	1:G:133:HIS:N	2.88	0.41
1:G:151:TYR:CG	1:G:203:THR:HB	2.55	0.41
1:M:68:TYR:CE2	1:M:151:TYR:HB2	2.55	0.41
1:M:141:GLU:O	1:M:143:VAL:N	2.52	0.41
1:N:262:ASN:HD22	1:N:262:ASN:HA	1.58	0.41
1:N:351:PRO:HG3	2:r:2:IDS:C1	2.50	0.41
1:N:351:PRO:HG2	2:r:1:JHM:H4	1.99	0.41
1:A:363:GLN:HB3	1:B:290:VAL:HG21	2.01	0.41
1:A:364:TYR:CD2	1:B:185:CYS:HB2	2.55	0.41
1:C:159:LEU:HB2	1:C:248:PHE:HB3	2.01	0.41
1:E:149:VAL:HG21	1:E:295:PRO:HD2	2.02	0.41
1:F:242:TYR:CZ	1:F:395:MET:HA	2.55	0.41
1:G:70:TYR:OH	1:G:232:PRO:HD3	2.20	0.41
1:H:123:TYR:HD2	1:H:125:LYS:HB2	1.85	0.41
1:H:349:GLN:HB2	1:H:353:PRO:HD3	2.02	0.41
1:K:216:THR:HG22	1:K:218:CYS:HB2	2.01	0.41
1:O:310:PRO:HG3	1:O:468:LYS:HD3	2.02	0.41
1:C:68:TYR:CE2	1:C:151:TYR:HB2	2.55	0.41
1:C:109:ARG:NH2	1:C:369:GLU:OE1	2.53	0.41
1:D:364:TYR:CD2	1:E:185:CYS:HB2	2.55	0.41
1:H:75:VAL:HB	1:H:329:LEU:HB3	2.01	0.41
1:H:144:ARG:O	1:I:283:ARG:HD3	2.21	0.41
1:J:216:THR:HG22	1:J:218:CYS:HB2	2.01	0.41
1:K:165:ILE:HD12	1:K:237:MET:HG2	2.02	0.41
1:L:396:ASN:HB3	1:L:399:ILE:HG13	2.03	0.41
1:D:331:VAL:HG12	1:D:333:VAL:HG23	2.03	0.41
1:E:72:VAL:HG21	1:E:195:LEU:O	2.20	0.41
1:E:389:MET:HE3	1:E:389:MET:HB2	1.81	0.41
1:G:120:HIS:HA	1:G:121:PRO:HD3	1.90	0.41
1:J:315:LYS:HA	1:J:321:ASN:HD21	1.85	0.41
1:K:50:PHE:HA	1:K:64:LYS:HD2	2.03	0.41
1:M:221:PRO:HD2	1:M:224:ILE:HD11	2.02	0.41
1:N:92:ASN:ND2	1:N:94:GLU:HB2	2.36	0.41
1:O:262:ASN:HD22	1:O:262:ASN:HA	1.60	0.41
1:B:151:TYR:CD2	1:B:203:THR:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LYS:CE	3:b:1:JHM:O7	2.67	0.41
1:E:128:ASP:O	1:E:132:SER:HB3	2.21	0.41
1:E:262:ASN:HD22	1:E:262:ASN:HA	1.52	0.41
1:J:74:ARG:HH22	1:J:440:ASP:CG	2.29	0.41
1:K:177:SER:HB2	1:K:178:ARG:H	1.63	0.41
1:L:70:TYR:OH	1:L:232:PRO:HD3	2.20	0.41
1:N:24:THR:C	1:N:26:ASP:H	2.28	0.41
1:N:112:PRO:HB3	1:O:231:TYR:CD1	2.56	0.41
1:N:282:MET:HE3	1:N:282:MET:HB2	1.78	0.41
1:E:258:ARG:HG3	1:E:259:HIS:ND1	2.36	0.41
1:H:314:HIS:CG	1:H:315:LYS:H	2.38	0.41
1:K:258:ARG:HG3	1:K:259:HIS:ND1	2.35	0.41
1:M:49:TYR:HA	1:M:223:ASP:HB3	2.03	0.41
1:M:151:TYR:CG	1:M:203:THR:HB	2.56	0.41
1:D:169:TRP:CE2	1:D:190:LEU:HD13	2.56	0.41
1:G:262:ASN:HD22	1:G:262:ASN:HA	1.54	0.41
1:H:163:PRO:HB2	1:H:194:VAL:HG13	2.03	0.41
1:H:331:VAL:HG12	1:H:333:VAL:HG23	2.02	0.41
1:J:123:TYR:HD2	1:J:125:LYS:HB2	1.86	0.41
1:K:68:TYR:CE2	1:K:151:TYR:HB2	2.55	0.41
1:L:314:HIS:CG	1:L:315:LYS:H	2.38	0.41
1:M:55:GLY:O	1:M:56:GLY:C	2.64	0.41
1:N:92:ASN:C	1:N:94:GLU:H	2.29	0.41
1:B:216:THR:HG22	1:B:218:CYS:HB2	2.02	0.41
1:C:463:TYR:O	1:C:467:ARG:HG3	2.21	0.41
1:E:125:LYS:HD2	1:E:261:TRP:NE1	2.35	0.41
1:G:333:VAL:HG11	1:G:371:TYR:CE2	2.55	0.41
1:H:205:TYR:CD2	1:H:220:VAL:HG12	2.55	0.41
1:H:237:MET:HE3	1:H:246:MET:HE3	2.03	0.41
1:I:74:ARG:NE	1:I:328:GLN:OE1	2.49	0.41
1:J:246:MET:O	1:J:246:MET:HG3	2.21	0.41
1:K:169:TRP:HZ2	1:O:368:VAL:HG11	1.85	0.41
1:K:314:HIS:CG	1:K:315:LYS:H	2.39	0.41
1:L:68:TYR:CE2	1:L:151:TYR:HB2	2.56	0.41
1:M:331:VAL:HG12	1:M:333:VAL:HG23	2.02	0.41
1:M:376:ILE:HG12	1:M:465:LEU:HD13	2.02	0.41
1:O:180:LEU:HD12	1:O:180:LEU:HA	1.94	0.41
1:A:69:GLN:HE21	1:A:71:ARG:HH12	1.68	0.41
1:A:216:THR:HG22	1:A:218:CYS:HB2	2.01	0.41
1:A:314:HIS:CG	1:A:315:LYS:H	2.39	0.41
1:C:364:TYR:CG	1:D:185:CYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:HA	1:D:180:LEU:HD12	1.74	0.41
1:F:112:PRO:HB3	1:G:231:TYR:CD1	2.56	0.41
1:F:262:ASN:OD1	1:F:288:SER:HB3	2.20	0.41
1:G:216:THR:HG22	1:G:218:CYS:HB2	2.02	0.41
1:I:160:GLY:HA2	1:I:247:PHE:CE2	2.56	0.41
1:M:159:LEU:HB2	1:M:248:PHE:HB3	2.03	0.41
1:O:130:GLU:HB2	1:O:260:PHE:HB2	2.03	0.41
1:O:151:TYR:CG	1:O:203:THR:HB	2.56	0.41
1:O:314:HIS:CG	1:O:315:LYS:H	2.39	0.41
1:A:74:ARG:HH22	1:A:440:ASP:CG	2.29	0.40
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.91	0.40
1:C:396:ASN:HB3	1:C:399:ILE:HG13	2.03	0.40
1:G:226:GLN:C	3:h:4:IDS:O3	2.63	0.40
1:H:277:ILE:CD1	3:h:1:JHM:O7	2.69	0.40
1:I:92:ASN:HA	1:I:93:PRO:HD2	1.85	0.40
1:J:45:VAL:HG12	1:J:368:VAL:HG13	2.02	0.40
1:M:54:ALA:HB2	1:M:61:ASP:CG	2.45	0.40
1:M:74:ARG:NH2	1:M:328:GLN:OE1	2.48	0.40
3:X:1:JHM:O1	2:Y:2:IDS:O3	2.28	0.40
1:B:324:CYS:SG	1:B:329:LEU:HD13	2.61	0.40
1:E:169:TRP:CE2	1:E:190:LEU:HD13	2.55	0.40
1:F:142:ASP:OD2	1:F:144:ARG:NE	2.53	0.40
1:G:349:GLN:HB2	1:G:353:PRO:HD3	2.03	0.40
1:H:220:VAL:HG23	1:H:225:CYS:HA	2.02	0.40
1:I:205:TYR:CD2	1:I:220:VAL:HG12	2.56	0.40
1:J:151:TYR:OH	1:J:221:PRO:HB2	2.21	0.40
1:K:70:TYR:CE1	1:K:201:VAL:HG12	2.56	0.40
1:L:154:THR:HG23	1:L:253:GLU:HB3	2.03	0.40
1:N:115:VAL:HG21	1:O:257:ALA:HB2	2.02	0.40
1:O:49:TYR:HA	1:O:223:ASP:HB3	2.03	0.40
1:A:242:TYR:CZ	1:A:395:MET:HA	2.56	0.40
1:B:237:MET:HE3	1:B:246:MET:HE3	2.03	0.40
1:C:144:ARG:O	1:D:283:ARG:HD3	2.21	0.40
1:D:259:HIS:HE1	1:E:130:GLU:OE1	2.03	0.40
1:E:152:LYS:HE3	1:E:253:GLU:HB2	2.03	0.40
1:L:156:LEU:HA	1:L:250:LEU:O	2.21	0.40
1:N:62:ILE:HA	1:N:63:PRO:HD3	1.94	0.40
1:N:109:ARG:H	1:N:308:ASN:HD21	1.68	0.40
1:B:121:PRO:HG3	1:C:289:CYS:SG	2.60	0.40
1:D:69:GLN:HE21	1:D:71:ARG:HH12	1.68	0.40
1:E:108:GLY:HA2	1:E:308:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ARG:H	1:E:308:ASN:ND2	2.19	0.40
1:G:115:VAL:HG21	1:H:257:ALA:HB2	2.03	0.40
1:I:131:SER:OG	1:I:132:SER:N	2.53	0.40
1:L:125:LYS:HD2	1:L:261:TRP:NE1	2.36	0.40
1:N:70:TYR:OH	1:N:232:PRO:HD3	2.21	0.40
1:N:366:ARG:HA	1:N:366:ARG:HD3	1.88	0.40
1:O:135:ALA:HB1	1:O:282:MET:SD	2.61	0.40
1:A:185:CYS:HB2	1:E:364:TYR:CG	2.56	0.40
1:B:314:HIS:CG	1:B:315:LYS:H	2.39	0.40
1:C:91:TYR:HB2	1:C:96:GLN:HG3	2.03	0.40
1:C:299:ILE:HA	1:D:256:PHE:HB3	2.04	0.40
1:D:35:TYR:OH	1:D:86:PRO:HD3	2.22	0.40
1:D:349:GLN:HB2	1:D:353:PRO:HD3	2.02	0.40
1:F:159:LEU:HB2	1:F:248:PHE:HB3	2.03	0.40
1:I:217:LYS:HE3	1:I:226:GLN:NE2	2.36	0.40
1:K:307:PHE:C	1:K:309:LYS:H	2.29	0.40
1:L:156:LEU:HG	1:L:334:VAL:HB	2.03	0.40
1:L:469:PHE:O	1:L:469:PHE:CG	2.73	0.40
1:M:137:SER:C	1:M:139:VAL:H	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:53:PRO:CB	5:f:3:JHM:O8[1_655]	1.92	0.28

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	418/427 (98%)	383 (92%)	28 (7%)	7 (2%)	7 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	418/427 (98%)	380 (91%)	30 (7%)	8 (2%)	6	25
1	C	418/427 (98%)	379 (91%)	31 (7%)	8 (2%)	6	25
1	D	418/427 (98%)	376 (90%)	32 (8%)	10 (2%)	4	22
1	E	418/427 (98%)	382 (91%)	31 (7%)	5 (1%)	10	34
1	F	418/427 (98%)	382 (91%)	28 (7%)	8 (2%)	6	25
1	G	418/427 (98%)	372 (89%)	30 (7%)	16 (4%)	2	15
1	H	418/427 (98%)	371 (89%)	37 (9%)	10 (2%)	4	22
1	I	418/427 (98%)	378 (90%)	29 (7%)	11 (3%)	4	21
1	J	418/427 (98%)	383 (92%)	28 (7%)	7 (2%)	7	27
1	K	418/427 (98%)	382 (91%)	28 (7%)	8 (2%)	6	25
1	L	418/427 (98%)	372 (89%)	31 (7%)	15 (4%)	2	16
1	M	418/427 (98%)	374 (90%)	23 (6%)	21 (5%)	1	10
1	N	418/427 (98%)	377 (90%)	27 (6%)	14 (3%)	3	17
1	O	418/427 (98%)	372 (89%)	34 (8%)	12 (3%)	3	18
All	All	6270/6405 (98%)	5663 (90%)	447 (7%)	160 (3%)	4	21

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	SER
1	B	177	SER
1	C	132	SER
1	C	133	HIS
1	C	139	VAL
1	C	298	SER
1	D	56	GLY
1	D	60	GLN
1	D	177	SER
1	F	40	SER
1	G	40	SER
1	G	131	SER
1	G	142	ASP
1	G	173	THR
1	G	298	SER
1	H	40	SER
1	H	138	ASN
1	I	40	SER

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Mol	Chain	Res	Type
1	I	132	SER
1	I	133	HIS
1	I	134	ALA
1	I	137	SER
1	J	40	SER
1	K	40	SER
1	K	176	LYS
1	L	40	SER
1	L	135	ALA
1	L	139	VAL
1	L	140	SER
1	L	471	VAL
1	M	40	SER
1	M	55	GLY
1	M	131	SER
1	M	136	THR
1	M	140	SER
1	M	142	ASP
1	N	40	SER
1	N	135	ALA
1	N	136	THR
1	N	137	SER
1	N	176	LYS
1	O	40	SER
1	O	137	SER
1	O	139	VAL
1	A	40	SER
1	A	298	SER
1	B	172	GLY
1	B	298	SER
1	B	443	ASP
1	C	40	SER
1	C	131	SER
1	D	40	SER
1	D	181	SER
1	D	298	SER
1	E	40	SER
1	E	134	ALA
1	F	133	HIS
1	F	298	SER
1	G	135	ALA
1	G	141	GLU

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Mol	Chain	Res	Type
1	G	172	GLY
1	G	181	SER
1	G	182	GLN
1	H	132	SER
1	H	133	HIS
1	H	137	SER
1	H	173	THR
1	I	131	SER
1	I	135	ALA
1	I	298	SER
1	J	134	ALA
1	J	140	SER
1	K	177	SER
1	K	298	SER
1	L	126	LEU
1	L	136	THR
1	L	298	SER
1	L	470	LEU
1	L	473	ALA
1	M	54	ALA
1	M	56	GLY
1	M	134	ALA
1	M	137	SER
1	M	139	VAL
1	N	134	ALA
1	N	141	GLU
1	N	298	SER
1	O	135	ALA
1	O	298	SER
1	A	134	ALA
1	B	134	ALA
1	B	140	SER
1	D	140	SER
1	D	182	GLN
1	E	140	SER
1	E	298	SER
1	F	132	SER
1	F	140	SER
1	G	132	SER
1	I	140	SER
1	J	131	SER
1	J	298	SER

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Mol	Chain	Res	Type
1	K	131	SER
1	K	140	SER
1	L	132	SER
1	L	443	ASP
1	M	130	GLU
1	M	179	PRO
1	M	298	SER
1	N	139	VAL
1	N	140	SER
1	N	175	SER
1	O	60	GLN
1	O	131	SER
1	O	141	GLU
1	A	140	SER
1	C	141	GLU
1	G	175	SER
1	H	142	ASP
1	H	298	SER
1	K	134	ALA
1	L	401	GLU
1	M	60	GLN
1	M	141	GLU
1	M	181	SER
1	O	53	PRO
1	O	59	LYS
1	A	131	SER
1	B	352	VAL
1	D	134	ALA
1	E	352	VAL
1	G	174	ALA
1	H	130	GLU
1	I	60	GLN
1	M	135	ALA
1	M	174	ALA
1	N	352	VAL
1	O	386	ALA
1	A	60	GLN
1	A	352	VAL
1	C	352	VAL
1	G	60	GLN
1	G	352	VAL
1	H	352	VAL

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Mol	Chain	Res	Type
1	J	352	VAL
1	L	352	VAL
1	M	352	VAL
1	D	352	VAL
1	F	352	VAL
1	J	139	VAL
1	M	93	PRO
1	N	93	PRO
1	I	352	VAL
1	K	352	VAL
1	F	139	VAL
1	L	441	PRO
1	N	241	PRO
1	F	57	GLY
1	G	57	GLY
1	O	352	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/370 (100%)	355 (96%)	14 (4%)	29	54
1	B	369/370 (100%)	349 (95%)	20 (5%)	20	47
1	C	369/370 (100%)	345 (94%)	24 (6%)	15	42
1	D	369/370 (100%)	343 (93%)	26 (7%)	14	39
1	E	369/370 (100%)	344 (93%)	25 (7%)	14	40
1	F	369/370 (100%)	349 (95%)	20 (5%)	20	47
1	G	369/370 (100%)	351 (95%)	18 (5%)	22	49
1	H	369/370 (100%)	346 (94%)	23 (6%)	16	43
1	I	369/370 (100%)	352 (95%)	17 (5%)	24	50
1	J	369/370 (100%)	350 (95%)	19 (5%)	21	48
1	K	369/370 (100%)	345 (94%)	24 (6%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	369/370 (100%)	345 (94%)	24 (6%)	15	42
1	M	369/370 (100%)	341 (92%)	28 (8%)	12	38
1	N	369/370 (100%)	353 (96%)	16 (4%)	26	51
1	O	369/370 (100%)	344 (93%)	25 (7%)	14	40
All	All	5535/5550 (100%)	5212 (94%)	323 (6%)	18	44

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
1	A	133	HIS
1	A	143	VAL
1	A	154	THR
1	A	176	LYS
1	A	196	GLU
1	A	255	LEU
1	A	262	ASN
1	A	270	THR
1	A	289	CYS
1	A	300	VAL
1	A	317	GLN
1	A	340	THR
1	A	465	LEU
1	B	51	ARG
1	B	87	ASP
1	B	133	HIS
1	B	143	VAL
1	B	147	VAL
1	B	156	LEU
1	B	178	ARG
1	B	180	LEU
1	B	184	ASP
1	B	213	LEU
1	B	255	LEU
1	B	262	ASN
1	B	300	VAL
1	B	317	GLN
1	B	340	THR
1	B	363	GLN
1	B	387	ASP
1	B	438	ASN

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Mol	Chain	Res	Type
1	B	439	LYS
1	B	465	LEU
1	C	51	ARG
1	C	91	TYR
1	C	95	THR
1	C	96	GLN
1	C	136	THR
1	C	141	GLU
1	C	143	VAL
1	C	147	VAL
1	C	156	LEU
1	C	176	LYS
1	C	184	ASP
1	C	222	LEU
1	C	236	GLN
1	C	255	LEU
1	C	262	ASN
1	C	300	VAL
1	C	301	THR
1	C	306	LEU
1	C	313	LEU
1	C	317	GLN
1	C	340	THR
1	C	363	GLN
1	C	387	ASP
1	C	465	LEU
1	D	58	ASN
1	D	59	LYS
1	D	61	ASP
1	D	62	ILE
1	D	127	ASP
1	D	133	HIS
1	D	139	VAL
1	D	140	SER
1	D	143	VAL
1	D	156	LEU
1	D	171	LYS
1	D	173	THR
1	D	180	LEU
1	D	184	ASP
1	D	213	LEU
1	D	222	LEU

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Mol	Chain	Res	Type
1	D	255	LEU
1	D	262	ASN
1	D	278	LYS
1	D	300	VAL
1	D	313	LEU
1	D	317	GLN
1	D	340	THR
1	D	385	THR
1	D	389	MET
1	D	465	LEU
1	E	91	TYR
1	E	118	SER
1	E	127	ASP
1	E	133	HIS
1	E	143	VAL
1	E	147	VAL
1	E	154	THR
1	E	173	THR
1	E	177	SER
1	E	178	ARG
1	E	180	LEU
1	E	184	ASP
1	E	213	LEU
1	E	222	LEU
1	E	255	LEU
1	E	262	ASN
1	E	270	THR
1	E	273	GLN
1	E	300	VAL
1	E	313	LEU
1	E	317	GLN
1	E	340	THR
1	E	363	GLN
1	E	387	ASP
1	E	465	LEU
1	F	87	ASP
1	F	88	THR
1	F	127	ASP
1	F	132	SER
1	F	133	HIS
1	F	139	VAL
1	F	143	VAL

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Mol	Chain	Res	Type
1	F	147	VAL
1	F	156	LEU
1	F	158	ILE
1	F	176	LYS
1	F	184	ASP
1	F	220	VAL
1	F	255	LEU
1	F	262	ASN
1	F	300	VAL
1	F	317	GLN
1	F	340	THR
1	F	363	GLN
1	F	465	LEU
1	G	91	TYR
1	G	132	SER
1	G	133	HIS
1	G	136	THR
1	G	139	VAL
1	G	142	ASP
1	G	143	VAL
1	G	156	LEU
1	G	175	SER
1	G	180	LEU
1	G	181	SER
1	G	222	LEU
1	G	255	LEU
1	G	262	ASN
1	G	300	VAL
1	G	317	GLN
1	G	340	THR
1	G	465	LEU
1	H	51	ARG
1	H	127	ASP
1	H	132	SER
1	H	136	THR
1	H	143	VAL
1	H	147	VAL
1	H	156	LEU
1	H	176	LYS
1	H	178	ARG
1	H	180	LEU
1	H	181	SER

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Mol	Chain	Res	Type
1	H	184	ASP
1	H	250	LEU
1	H	255	LEU
1	H	262	ASN
1	H	274	SER
1	H	280	THR
1	H	300	VAL
1	H	313	LEU
1	H	317	GLN
1	H	340	THR
1	H	392	ILE
1	H	465	LEU
1	I	91	TYR
1	I	96	GLN
1	I	133	HIS
1	I	143	VAL
1	I	147	VAL
1	I	154	THR
1	I	156	LEU
1	I	176	LYS
1	I	255	LEU
1	I	262	ASN
1	I	270	THR
1	I	280	THR
1	I	300	VAL
1	I	313	LEU
1	I	317	GLN
1	I	340	THR
1	I	465	LEU
1	J	51	ARG
1	J	91	TYR
1	J	127	ASP
1	J	133	HIS
1	J	139	VAL
1	J	143	VAL
1	J	152	LYS
1	J	176	LYS
1	J	184	ASP
1	J	255	LEU
1	J	262	ASN
1	J	273	GLN
1	J	289	CYS

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Mol	Chain	Res	Type
1	J	300	VAL
1	J	317	GLN
1	J	340	THR
1	J	363	GLN
1	J	387	ASP
1	J	465	LEU
1	K	91	TYR
1	K	118	SER
1	K	127	ASP
1	K	133	HIS
1	K	139	VAL
1	K	143	VAL
1	K	147	VAL
1	K	156	LEU
1	K	173	THR
1	K	175	SER
1	K	176	LYS
1	K	177	SER
1	K	178	ARG
1	K	184	ASP
1	K	222	LEU
1	K	255	LEU
1	K	262	ASN
1	K	300	VAL
1	K	317	GLN
1	K	340	THR
1	K	363	GLN
1	K	365	SER
1	K	387	ASP
1	K	465	LEU
1	L	51	ARG
1	L	91	TYR
1	L	127	ASP
1	L	129	THR
1	L	136	THR
1	L	176	LYS
1	L	184	ASP
1	L	196	GLU
1	L	255	LEU
1	L	262	ASN
1	L	300	VAL
1	L	306	LEU

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Mol	Chain	Res	Type
1	L	317	GLN
1	L	340	THR
1	L	365	SER
1	L	372	ASP
1	L	382	ILE
1	L	387	ASP
1	L	389	MET
1	L	438	ASN
1	L	439	LYS
1	L	444	LYS
1	L	465	LEU
1	L	472	GLN
1	M	51	ARG
1	M	59	LYS
1	M	60	GLN
1	M	61	ASP
1	M	62	ILE
1	M	87	ASP
1	M	118	SER
1	M	129	THR
1	M	133	HIS
1	M	139	VAL
1	M	141	GLU
1	M	171	LYS
1	M	176	LYS
1	M	178	ARG
1	M	180	LEU
1	M	181	SER
1	M	184	ASP
1	M	193	THR
1	M	222	LEU
1	M	255	LEU
1	M	262	ASN
1	M	300	VAL
1	M	317	GLN
1	M	340	THR
1	M	363	GLN
1	M	385	THR
1	M	392	ILE
1	M	465	LEU
1	N	136	THR
1	N	139	VAL

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Mol	Chain	Res	Type
1	N	143	VAL
1	N	147	VAL
1	N	156	LEU
1	N	176	LYS
1	N	178	ARG
1	N	196	GLU
1	N	255	LEU
1	N	262	ASN
1	N	300	VAL
1	N	313	LEU
1	N	317	GLN
1	N	340	THR
1	N	363	GLN
1	N	465	LEU
1	O	51	ARG
1	O	52	VAL
1	O	59	LYS
1	O	60	GLN
1	O	61	ASP
1	O	62	ILE
1	O	64	LYS
1	O	87	ASP
1	O	91	TYR
1	O	133	HIS
1	O	136	THR
1	O	139	VAL
1	O	140	SER
1	O	143	VAL
1	O	147	VAL
1	O	176	LYS
1	O	222	LEU
1	O	255	LEU
1	O	262	ASN
1	O	270	THR
1	O	313	LEU
1	O	317	GLN
1	O	328	GLN
1	O	340	THR
1	O	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	69	GLN
1	A	153	GLN
1	A	182	GLN
1	A	262	ASN
1	A	273	GLN
1	A	308	ASN
1	A	317	GLN
1	A	319	HIS
1	A	326	HIS
1	A	327	ASN
1	A	341	ASN
1	A	349	GLN
1	A	367	HIS
1	A	396	ASN
1	B	69	GLN
1	B	92	ASN
1	B	153	GLN
1	B	262	ASN
1	B	308	ASN
1	B	317	GLN
1	B	326	HIS
1	B	327	ASN
1	B	367	HIS
1	B	396	ASN
1	C	69	GLN
1	C	76	GLN
1	C	92	ASN
1	C	182	GLN
1	C	226	GLN
1	C	262	ASN
1	C	273	GLN
1	C	308	ASN
1	C	317	GLN
1	C	326	HIS
1	C	327	ASN
1	C	367	HIS
1	C	396	ASN
1	C	462	GLN
1	D	58	ASN
1	D	69	GLN
1	D	138	ASN
1	D	262	ASN

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Mol	Chain	Res	Type
1	D	273	GLN
1	D	308	ASN
1	D	317	GLN
1	D	326	HIS
1	D	341	ASN
1	D	367	HIS
1	D	396	ASN
1	E	36	HIS
1	E	69	GLN
1	E	92	ASN
1	E	153	GLN
1	E	182	GLN
1	E	262	ASN
1	E	308	ASN
1	E	317	GLN
1	E	319	HIS
1	E	326	HIS
1	E	327	ASN
1	E	367	HIS
1	E	396	ASN
1	E	449	ASN
1	E	462	GLN
1	F	69	GLN
1	F	92	ASN
1	F	153	GLN
1	F	155	GLN
1	F	182	GLN
1	F	254	GLN
1	F	262	ASN
1	F	273	GLN
1	F	308	ASN
1	F	317	GLN
1	F	321	ASN
1	F	326	HIS
1	F	327	ASN
1	F	367	HIS
1	F	396	ASN
1	F	462	GLN
1	G	69	GLN
1	G	92	ASN
1	G	133	HIS
1	G	153	GLN

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Mol	Chain	Res	Type
1	G	262	ASN
1	G	273	GLN
1	G	308	ASN
1	G	317	GLN
1	G	326	HIS
1	G	327	ASN
1	G	341	ASN
1	G	367	HIS
1	G	396	ASN
1	G	462	GLN
1	H	69	GLN
1	H	92	ASN
1	H	133	HIS
1	H	153	GLN
1	H	182	GLN
1	H	262	ASN
1	H	273	GLN
1	H	308	ASN
1	H	317	GLN
1	H	319	HIS
1	H	326	HIS
1	H	327	ASN
1	H	367	HIS
1	H	396	ASN
1	H	462	GLN
1	I	69	GLN
1	I	92	ASN
1	I	153	GLN
1	I	182	GLN
1	I	226	GLN
1	I	262	ASN
1	I	273	GLN
1	I	308	ASN
1	I	317	GLN
1	I	319	HIS
1	I	321	ASN
1	I	327	ASN
1	I	341	ASN
1	I	367	HIS
1	I	396	ASN
1	I	462	GLN
1	J	69	GLN

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Mol	Chain	Res	Type
1	J	92	ASN
1	J	153	GLN
1	J	182	GLN
1	J	254	GLN
1	J	262	ASN
1	J	308	ASN
1	J	317	GLN
1	J	319	HIS
1	J	321	ASN
1	J	326	HIS
1	J	327	ASN
1	J	341	ASN
1	J	349	GLN
1	J	367	HIS
1	J	396	ASN
1	J	462	GLN
1	K	69	GLN
1	K	92	ASN
1	K	153	GLN
1	K	182	GLN
1	K	254	GLN
1	K	262	ASN
1	K	308	ASN
1	K	317	GLN
1	K	321	ASN
1	K	326	HIS
1	K	327	ASN
1	K	349	GLN
1	K	367	HIS
1	K	396	ASN
1	L	69	GLN
1	L	92	ASN
1	L	153	GLN
1	L	182	GLN
1	L	254	GLN
1	L	262	ASN
1	L	273	GLN
1	L	308	ASN
1	L	317	GLN
1	L	319	HIS
1	L	321	ASN
1	L	326	HIS

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Mol	Chain	Res	Type
1	L	327	ASN
1	L	341	ASN
1	L	349	GLN
1	L	367	HIS
1	L	396	ASN
1	L	438	ASN
1	M	60	GLN
1	M	69	GLN
1	M	76	GLN
1	M	92	ASN
1	M	182	GLN
1	M	226	GLN
1	M	273	GLN
1	M	308	ASN
1	M	317	GLN
1	M	321	ASN
1	M	326	HIS
1	M	327	ASN
1	M	341	ASN
1	M	367	HIS
1	M	396	ASN
1	N	69	GLN
1	N	76	GLN
1	N	92	ASN
1	N	153	GLN
1	N	182	GLN
1	N	192	ASN
1	N	262	ASN
1	N	273	GLN
1	N	308	ASN
1	N	317	GLN
1	N	319	HIS
1	N	321	ASN
1	N	326	HIS
1	N	327	ASN
1	N	341	ASN
1	N	367	HIS
1	N	378	GLN
1	N	396	ASN
1	N	462	GLN
1	O	23	ASN
1	O	69	GLN

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Mol	Chain	Res	Type
1	O	92	ASN
1	O	138	ASN
1	O	153	GLN
1	O	182	GLN
1	O	259	HIS
1	O	262	ASN
1	O	273	GLN
1	O	308	ASN
1	O	317	GLN
1	O	319	HIS
1	O	321	ASN
1	O	327	ASN
1	O	367	HIS
1	O	396	ASN
1	O	462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

90 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	JHM	P	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.20	2 (10%)
2	IDS	P	2	2	15,15,17	2.00	1 (6%)	14,22,26	1.50	3 (21%)
3	JHM	Q	1	3	15,15,15	1.05	1 (6%)	19,22,22	1.22	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IDS	Q	2	3	16,16,17	2.18	3 (18%)	16,24,26	4.93	4 (25%)
3	JHM	Q	3	3	14,14,15	0.95	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	Q	4	3	15,15,17	2.03	2 (13%)	14,22,26	1.56	3 (21%)
3	JHM	R	1	3	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
3	IDS	R	2	3	16,16,17	2.13	3 (18%)	16,24,26	3.68	3 (18%)
3	JHM	R	3	3	14,14,15	0.96	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	R	4	3	15,15,17	2.02	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	S	1	2	15,15,15	1.06	1 (6%)	19,22,22	1.20	2 (10%)
2	IDS	S	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.53	3 (21%)
2	JHM	T	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	T	2	2	15,15,17	2.01	2 (13%)	14,22,26	1.56	3 (21%)
2	JHM	U	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.22	2 (10%)
2	IDS	U	2	2	15,15,17	2.01	2 (13%)	14,22,26	1.54	3 (21%)
3	JHM	V	1	3	15,15,15	1.03	1 (6%)	19,22,22	1.20	2 (10%)
3	IDS	V	2	3	16,16,17	2.07	2 (12%)	16,24,26	2.78	3 (18%)
3	JHM	V	3	3	14,14,15	0.94	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	V	4	3	15,15,17	2.02	2 (13%)	14,22,26	1.53	3 (21%)
2	JHM	W	1	2	15,15,15	1.02	0	19,22,22	1.21	2 (10%)
2	IDS	W	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.55	3 (21%)
3	JHM	X	1	3	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
3	IDS	X	2	3	16,16,17	1.96	2 (12%)	16,24,26	3.48	3 (18%)
3	JHM	X	3	3	14,14,15	0.95	1 (7%)	19,20,22	1.38	3 (15%)
3	IDS	X	4	3	15,15,17	2.01	2 (13%)	14,22,26	1.56	3 (21%)
2	JHM	Y	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.20	2 (10%)
2	IDS	Y	2	2	15,15,17	1.99	1 (6%)	14,22,26	1.50	3 (21%)
2	JHM	Z	1	2	15,15,15	1.06	1 (6%)	19,22,22	1.22	2 (10%)
2	IDS	Z	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.55	3 (21%)
2	JHM	a	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	a	2	2	15,15,17	2.01	2 (13%)	14,22,26	1.51	3 (21%)
3	JHM	b	1	3	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)
3	IDS	b	2	3	16,16,17	1.94	1 (6%)	16,24,26	2.49	2 (12%)
3	JHM	b	3	3	14,14,15	0.98	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	b	4	3	15,15,17	2.02	2 (13%)	14,22,26	1.51	3 (21%)
3	JHM	c	1	3	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)
3	IDS	c	2	3	16,16,17	2.27	3 (18%)	16,24,26	5.37	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	JHM	c	3	3	14,14,15	0.95	0	19,20,22	1.40	3 (15%)
3	IDS	c	4	3	15,15,17	2.01	2 (13%)	14,22,26	1.53	3 (21%)
2	JHM	d	1	2	15,15,15	1.02	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	d	2	2	15,15,17	1.99	2 (13%)	14,22,26	1.51	3 (21%)
4	JHM	e	1	4	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)
4	IDS	e	2	4	16,16,17	2.29	3 (18%)	16,24,26	2.69	4 (25%)
4	JHM	e	3	4	14,14,15	0.95	1 (7%)	19,20,22	1.38	3 (15%)
4	IDS	e	4	4	16,16,17	1.98	2 (12%)	16,24,26	2.53	4 (25%)
4	JHM	e	5	4	14,14,15	0.95	1 (7%)	19,20,22	1.39	3 (15%)
4	IDS	e	6	4	15,15,17	2.03	2 (13%)	14,22,26	1.54	3 (21%)
5	JHM	f	1	5	15,15,15	1.04	1 (6%)	19,22,22	1.20	2 (10%)
5	IDS	f	10	5	15,15,17	1.99	1 (6%)	14,22,26	1.52	3 (21%)
5	IDS	f	2	5	16,16,17	2.27	2 (12%)	16,24,26	3.12	2 (12%)
5	JHM	f	3	5	14,14,15	0.97	1 (7%)	19,20,22	1.38	3 (15%)
5	IDS	f	4	5	16,16,17	2.22	2 (12%)	16,24,26	2.77	2 (12%)
5	JHM	f	5	5	14,14,15	0.95	1 (7%)	19,20,22	1.40	3 (15%)
5	IDS	f	6	5	16,16,17	1.93	2 (12%)	16,24,26	3.20	2 (12%)
5	JHM	f	7	5	14,14,15	0.96	1 (7%)	19,20,22	1.38	3 (15%)
5	IDS	f	8	5	16,16,17	2.07	2 (12%)	16,24,26	3.17	2 (12%)
5	JHM	f	9	5	14,14,15	0.95	1 (7%)	19,20,22	1.39	3 (15%)
3	JHM	g	1	3	15,15,15	1.02	1 (6%)	19,22,22	1.20	2 (10%)
3	IDS	g	2	3	16,16,17	1.94	1 (6%)	16,24,26	3.75	3 (18%)
3	JHM	g	3	3	14,14,15	0.96	1 (7%)	19,20,22	1.39	3 (15%)
3	IDS	g	4	3	15,15,17	1.99	1 (6%)	14,22,26	1.50	3 (21%)
3	JHM	h	1	3	15,15,15	1.04	1 (6%)	19,22,22	1.19	2 (10%)
3	IDS	h	2	3	16,16,17	1.92	2 (12%)	16,24,26	2.22	3 (18%)
3	JHM	h	3	3	14,14,15	0.96	1 (7%)	19,20,22	1.40	3 (15%)
3	IDS	h	4	3	15,15,17	1.99	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	i	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	i	2	2	15,15,17	2.04	2 (13%)	14,22,26	1.55	3 (21%)
2	JHM	j	1	2	15,15,15	1.02	1 (6%)	19,22,22	1.20	2 (10%)
2	IDS	j	2	2	15,15,17	2.00	2 (13%)	14,22,26	1.52	3 (21%)
2	JHM	k	1	2	15,15,15	1.03	0	19,22,22	1.21	2 (10%)
2	IDS	k	2	2	15,15,17	1.98	2 (13%)	14,22,26	1.50	3 (21%)
2	JHM	l	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IDS	l	2	2	15,15,17	1.99	2 (13%)	14,22,26	1.48	3 (21%)
2	JHM	m	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	m	2	2	15,15,17	2.01	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	n	1	2	15,15,15	1.04	0	19,22,22	1.21	2 (10%)
2	IDS	n	2	2	15,15,17	1.98	1 (6%)	14,22,26	1.51	3 (21%)
2	JHM	o	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.20	2 (10%)
2	IDS	o	2	2	15,15,17	1.99	1 (6%)	14,22,26	1.52	3 (21%)
3	JHM	p	1	3	15,15,15	1.03	1 (6%)	19,22,22	1.21	2 (10%)
3	IDS	p	2	3	16,16,17	2.00	2 (12%)	16,24,26	2.45	3 (18%)
3	JHM	p	3	3	14,14,15	0.94	0	19,20,22	1.39	3 (15%)
3	IDS	p	4	3	15,15,17	2.01	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	q	1	2	15,15,15	1.03	1 (6%)	19,22,22	1.22	2 (10%)
2	IDS	q	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	r	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	r	2	2	15,15,17	2.02	2 (13%)	14,22,26	1.54	3 (21%)
2	JHM	s	1	2	15,15,15	1.04	1 (6%)	19,22,22	1.21	2 (10%)
2	IDS	s	2	2	15,15,17	2.03	2 (13%)	14,22,26	1.54	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JHM	P	1	2	-	1/6/22/22	0/1/1/1
2	IDS	P	2	2	-	0/9/22/29	0/1/1/1
3	JHM	Q	1	3	-	0/6/22/22	0/1/1/1
3	IDS	Q	2	3	-	0/9/26/29	0/1/1/1
3	JHM	Q	3	3	-	0/6/20/22	0/1/1/1
3	IDS	Q	4	3	-	0/9/22/29	0/1/1/1
3	JHM	R	1	3	-	1/6/22/22	0/1/1/1
3	IDS	R	2	3	-	0/9/26/29	0/1/1/1
3	JHM	R	3	3	-	0/6/20/22	0/1/1/1
3	IDS	R	4	3	-	0/9/22/29	0/1/1/1
2	JHM	S	1	2	-	0/6/22/22	0/1/1/1
2	IDS	S	2	2	-	0/9/22/29	0/1/1/1
2	JHM	T	1	2	-	0/6/22/22	0/1/1/1
2	IDS	T	2	2	-	0/9/22/29	0/1/1/1
2	JHM	U	1	2	-	0/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDS	U	2	2	-	0/9/22/29	0/1/1/1
3	JHM	V	1	3	-	1/6/22/22	0/1/1/1
3	IDS	V	2	3	-	0/9/26/29	0/1/1/1
3	JHM	V	3	3	-	0/6/20/22	0/1/1/1
3	IDS	V	4	3	-	0/9/22/29	0/1/1/1
2	JHM	W	1	2	-	0/6/22/22	0/1/1/1
2	IDS	W	2	2	-	0/9/22/29	0/1/1/1
3	JHM	X	1	3	-	0/6/22/22	0/1/1/1
3	IDS	X	2	3	-	0/9/26/29	0/1/1/1
3	JHM	X	3	3	-	1/6/20/22	0/1/1/1
3	IDS	X	4	3	-	0/9/22/29	0/1/1/1
2	JHM	Y	1	2	-	1/6/22/22	0/1/1/1
2	IDS	Y	2	2	-	0/9/22/29	0/1/1/1
2	JHM	Z	1	2	-	0/6/22/22	0/1/1/1
2	IDS	Z	2	2	-	0/9/22/29	0/1/1/1
2	JHM	a	1	2	-	1/6/22/22	0/1/1/1
2	IDS	a	2	2	-	0/9/22/29	0/1/1/1
3	JHM	b	1	3	-	1/6/22/22	0/1/1/1
3	IDS	b	2	3	-	0/9/26/29	0/1/1/1
3	JHM	b	3	3	-	1/6/20/22	0/1/1/1
3	IDS	b	4	3	-	0/9/22/29	0/1/1/1
3	JHM	c	1	3	-	0/6/22/22	0/1/1/1
3	IDS	c	2	3	-	0/9/26/29	0/1/1/1
3	JHM	c	3	3	-	0/6/20/22	0/1/1/1
3	IDS	c	4	3	-	0/9/22/29	0/1/1/1
2	JHM	d	1	2	-	1/6/22/22	0/1/1/1
2	IDS	d	2	2	-	0/9/22/29	0/1/1/1
4	JHM	e	1	4	-	0/6/22/22	0/1/1/1
4	IDS	e	2	4	-	0/9/26/29	0/1/1/1
4	JHM	e	3	4	-	0/6/20/22	0/1/1/1
4	IDS	e	4	4	-	0/9/26/29	0/1/1/1
4	JHM	e	5	4	-	0/6/20/22	0/1/1/1
4	IDS	e	6	4	-	0/9/22/29	0/1/1/1
5	JHM	f	1	5	-	1/6/22/22	0/1/1/1
5	IDS	f	10	5	-	0/9/22/29	0/1/1/1
5	IDS	f	2	5	-	0/9/26/29	0/1/1/1
5	JHM	f	3	5	-	1/6/20/22	0/1/1/1
5	IDS	f	4	5	-	0/9/26/29	0/1/1/1
5	JHM	f	5	5	-	0/6/20/22	0/1/1/1
5	IDS	f	6	5	-	0/9/26/29	0/1/1/1
5	JHM	f	7	5	-	1/6/20/22	0/1/1/1
5	IDS	f	8	5	-	0/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JHM	f	9	5	-	1/6/20/22	0/1/1/1
3	JHM	g	1	3	-	1/6/22/22	0/1/1/1
3	IDS	g	2	3	-	0/9/26/29	0/1/1/1
3	JHM	g	3	3	-	0/6/20/22	0/1/1/1
3	IDS	g	4	3	-	0/9/22/29	0/1/1/1
3	JHM	h	1	3	-	1/6/22/22	0/1/1/1
3	IDS	h	2	3	-	0/9/26/29	0/1/1/1
3	JHM	h	3	3	-	0/6/20/22	0/1/1/1
3	IDS	h	4	3	-	0/9/22/29	0/1/1/1
2	JHM	i	1	2	-	0/6/22/22	0/1/1/1
2	IDS	i	2	2	-	0/9/22/29	0/1/1/1
2	JHM	j	1	2	-	0/6/22/22	0/1/1/1
2	IDS	j	2	2	-	0/9/22/29	0/1/1/1
2	JHM	k	1	2	-	0/6/22/22	0/1/1/1
2	IDS	k	2	2	-	0/9/22/29	0/1/1/1
2	JHM	l	1	2	-	0/6/22/22	0/1/1/1
2	IDS	l	2	2	-	0/9/22/29	0/1/1/1
2	JHM	m	1	2	-	0/6/22/22	0/1/1/1
2	IDS	m	2	2	-	0/9/22/29	0/1/1/1
2	JHM	n	1	2	-	0/6/22/22	0/1/1/1
2	IDS	n	2	2	-	0/9/22/29	0/1/1/1
2	JHM	o	1	2	-	1/6/22/22	0/1/1/1
2	IDS	o	2	2	-	0/9/22/29	0/1/1/1
3	JHM	p	1	3	-	0/6/22/22	0/1/1/1
3	IDS	p	2	3	-	0/9/26/29	0/1/1/1
3	JHM	p	3	3	-	0/6/20/22	0/1/1/1
3	IDS	p	4	3	-	0/9/22/29	0/1/1/1
2	JHM	q	1	2	-	0/6/22/22	0/1/1/1
2	IDS	q	2	2	-	0/9/22/29	0/1/1/1
2	JHM	r	1	2	-	0/6/22/22	0/1/1/1
2	IDS	r	2	2	-	0/9/22/29	0/1/1/1
2	JHM	s	1	2	-	0/6/22/22	0/1/1/1
2	IDS	s	2	2	-	0/9/22/29	0/1/1/1

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	IDS	O2-C2	-6.80	1.37	1.47
2	i	2	IDS	O2-C2	-6.80	1.37	1.47
3	Q	4	IDS	O2-C2	-6.78	1.37	1.47
2	m	2	IDS	O2-C2	-6.77	1.37	1.47
3	b	4	IDS	O2-C2	-6.76	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	IDS	O2-C2	-6.76	1.37	1.47
4	e	2	IDS	O2-C2	-6.76	1.37	1.47
2	a	2	IDS	O2-C2	-6.75	1.37	1.47
3	b	2	IDS	O2-C2	-6.75	1.37	1.47
4	e	4	IDS	O2-C2	-6.74	1.37	1.47
3	R	2	IDS	O2-C2	-6.73	1.37	1.47
5	f	2	IDS	O2-C2	-6.73	1.37	1.47
2	s	2	IDS	O2-C2	-6.73	1.37	1.47
3	p	2	IDS	O2-C2	-6.73	1.37	1.47
5	f	6	IDS	O2-C2	-6.73	1.37	1.47
2	W	2	IDS	O2-C2	-6.72	1.37	1.47
2	j	2	IDS	O2-C2	-6.72	1.37	1.47
2	Z	2	IDS	O2-C2	-6.72	1.37	1.47
4	e	6	IDS	O2-C2	-6.72	1.37	1.47
2	o	2	IDS	O2-C2	-6.72	1.37	1.47
2	r	2	IDS	O2-C2	-6.71	1.37	1.47
5	f	4	IDS	O2-C2	-6.71	1.37	1.47
3	V	4	IDS	O2-C2	-6.71	1.37	1.47
3	h	4	IDS	O2-C2	-6.71	1.37	1.47
3	h	2	IDS	O2-C2	-6.70	1.37	1.47
2	l	2	IDS	O2-C2	-6.69	1.37	1.47
3	g	4	IDS	O2-C2	-6.69	1.37	1.47
2	n	2	IDS	O2-C2	-6.68	1.37	1.47
3	R	4	IDS	O2-C2	-6.68	1.37	1.47
5	f	10	IDS	O2-C2	-6.68	1.37	1.47
3	X	4	IDS	O2-C2	-6.67	1.37	1.47
3	X	2	IDS	O2-C2	-6.67	1.37	1.47
3	c	2	IDS	O2-C2	-6.67	1.37	1.47
3	c	4	IDS	O2-C2	-6.66	1.37	1.47
2	Y	2	IDS	O2-C2	-6.66	1.37	1.47
2	k	2	IDS	O2-C2	-6.66	1.37	1.47
3	Q	2	IDS	O2-C2	-6.66	1.37	1.47
2	U	2	IDS	O2-C2	-6.65	1.37	1.47
5	f	8	IDS	O2-C2	-6.65	1.37	1.47
3	p	4	IDS	O2-C2	-6.65	1.37	1.47
3	V	2	IDS	O2-C2	-6.64	1.37	1.47
2	d	2	IDS	O2-C2	-6.64	1.37	1.47
2	q	2	IDS	O2-C2	-6.64	1.37	1.47
2	S	2	IDS	O2-C2	-6.63	1.37	1.47
2	T	2	IDS	O2-C2	-6.63	1.37	1.47
5	f	2	IDS	O4-C4	4.81	1.54	1.43
4	e	2	IDS	O4-C4	4.71	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	2	IDS	O4-C4	4.70	1.54	1.43
5	f	4	IDS	O4-C4	4.43	1.53	1.43
3	Q	2	IDS	O4-C4	4.02	1.52	1.43
3	R	2	IDS	O4-C4	3.62	1.51	1.43
3	V	2	IDS	O4-C4	3.18	1.50	1.43
5	f	8	IDS	O4-C4	3.15	1.50	1.43
4	e	4	IDS	O6B-C6	-2.30	1.23	1.30
3	X	2	IDS	O6B-C6	-2.28	1.23	1.30
2	W	2	IDS	O6B-C6	-2.28	1.23	1.30
4	e	6	IDS	O6B-C6	-2.28	1.23	1.30
3	c	2	IDS	O6B-C6	-2.27	1.23	1.30
3	p	4	IDS	O6B-C6	-2.27	1.23	1.30
2	Z	2	IDS	O6B-C6	-2.27	1.23	1.30
3	V	4	IDS	O6B-C6	-2.27	1.23	1.30
2	s	2	IDS	O6B-C6	-2.26	1.23	1.30
2	q	2	IDS	O6B-C6	-2.26	1.23	1.30
4	e	2	IDS	O6B-C6	-2.26	1.23	1.30
2	S	2	IDS	O6B-C6	-2.26	1.23	1.30
3	R	4	IDS	O6B-C6	-2.25	1.23	1.30
2	r	2	IDS	O6B-C6	-2.25	1.23	1.30
3	X	4	IDS	O6B-C6	-2.25	1.23	1.30
2	i	2	IDS	O6B-C6	-2.24	1.23	1.30
2	T	2	IDS	O6B-C6	-2.24	1.23	1.30
3	Q	4	IDS	O6B-C6	-2.24	1.23	1.30
3	Q	2	IDS	O6B-C6	-2.24	1.23	1.30
3	c	4	IDS	O6B-C6	-2.23	1.23	1.30
2	U	2	IDS	O6B-C6	-2.23	1.23	1.30
3	b	3	JHM	C3-C4	2.17	1.55	1.52
3	Q	1	JHM	C3-C4	2.14	1.55	1.52
2	Z	1	JHM	C3-C4	2.11	1.55	1.52
3	R	3	JHM	C3-C4	2.10	1.55	1.52
5	f	1	JHM	C3-C4	2.10	1.55	1.52
4	e	5	JHM	C3-C4	2.08	1.55	1.52
3	h	3	JHM	C3-C4	2.07	1.55	1.52
2	Y	1	JHM	C3-C4	2.07	1.55	1.52
2	U	1	JHM	C3-C4	2.07	1.55	1.52
3	X	1	JHM	C3-C4	2.07	1.55	1.52
5	f	7	JHM	C3-C4	2.07	1.55	1.52
3	c	1	JHM	C3-C4	2.07	1.55	1.52
3	p	2	IDS	O4-C4	2.07	1.48	1.43
5	f	3	JHM	C3-C4	2.06	1.55	1.52
2	a	1	JHM	C3-C4	2.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	1	JHM	C3-C4	2.05	1.55	1.52
2	T	1	JHM	C3-C4	2.05	1.55	1.52
2	P	1	JHM	C3-C4	2.05	1.55	1.52
3	V	1	JHM	C3-C4	2.05	1.55	1.52
4	e	3	JHM	C3-C4	2.04	1.55	1.52
5	f	5	JHM	C3-C4	2.04	1.55	1.52
2	S	1	JHM	C3-C4	2.04	1.55	1.52
3	X	3	JHM	C3-C4	2.04	1.55	1.52
3	g	3	JHM	C3-C4	2.04	1.55	1.52
2	d	1	JHM	C3-C4	2.03	1.55	1.52
2	l	1	JHM	C3-C4	2.03	1.55	1.52
2	s	1	JHM	C3-C4	2.03	1.55	1.52
3	R	1	JHM	C3-C4	2.03	1.55	1.52
3	V	3	JHM	C3-C4	2.02	1.55	1.52
2	d	2	IDS	O6B-C6	-2.02	1.24	1.30
3	b	4	IDS	O6B-C6	-2.02	1.24	1.30
3	Q	3	JHM	C3-C4	2.02	1.55	1.52
2	i	1	JHM	C3-C4	2.02	1.55	1.52
4	e	1	JHM	C3-C4	2.02	1.55	1.52
3	g	1	JHM	C3-C4	2.02	1.55	1.52
2	a	2	IDS	O6B-C6	-2.02	1.24	1.30
2	q	1	JHM	C3-C4	2.02	1.55	1.52
2	r	1	JHM	C3-C4	2.01	1.55	1.52
3	R	2	IDS	O6B-C6	-2.01	1.24	1.30
5	f	6	IDS	O6B-C6	-2.01	1.24	1.30
2	o	1	JHM	C3-C4	2.01	1.55	1.52
3	p	1	JHM	C3-C4	2.01	1.55	1.52
2	m	1	JHM	C3-C4	2.01	1.55	1.52
2	k	2	IDS	O6B-C6	-2.00	1.24	1.30
3	h	2	IDS	O6B-C6	-2.00	1.24	1.30
2	l	2	IDS	O6B-C6	-2.00	1.24	1.30
2	j	2	IDS	O6B-C6	-2.00	1.24	1.30
2	j	1	JHM	C3-C4	2.00	1.55	1.52
3	h	1	JHM	C3-C4	2.00	1.55	1.52
5	f	9	JHM	C3-C4	2.00	1.55	1.52

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	2	IDS	O4-C4-C5	19.82	155.01	109.76
3	Q	2	IDS	O4-C4-C5	17.78	150.35	109.76
3	R	2	IDS	O4-C4-C3	13.84	143.00	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	2	IDS	O4-C4-C5	13.27	140.07	109.76
3	X	2	IDS	O4-C4-C3	13.09	141.24	110.38
5	f	6	IDS	O4-C4-C5	12.01	137.18	109.76
5	f	8	IDS	O4-C4-C5	11.72	136.52	109.76
5	f	2	IDS	O4-C4-C5	11.61	136.26	109.76
5	f	4	IDS	O4-C4-C5	10.08	132.78	109.76
4	e	2	IDS	O4-C4-C3	9.34	132.40	110.38
3	V	2	IDS	O4-C4-C5	8.88	130.04	109.76
3	b	2	IDS	O4-C4-C5	8.86	130.00	109.76
3	p	2	IDS	O4-C4-C5	8.41	128.97	109.76
4	e	4	IDS	O4-C4-C5	7.66	127.24	109.76
3	Q	2	IDS	O4-C4-C3	-7.21	93.39	110.38
3	c	2	IDS	O4-C4-C3	-7.07	93.71	110.38
3	h	2	IDS	O4-C4-C3	6.63	126.00	110.38
3	g	2	IDS	O4-C4-C3	-5.41	97.63	110.38
3	V	2	IDS	O4-C4-C3	-4.90	98.82	110.38
4	e	4	IDS	O4-C4-C3	4.87	121.86	110.38
3	h	2	IDS	O4-C4-C5	3.87	118.59	109.76
5	f	5	JHM	C2-C3-C4	-3.52	107.13	111.16
3	p	3	JHM	C2-C3-C4	-3.51	107.14	111.16
5	f	9	JHM	C2-C3-C4	-3.51	107.15	111.16
5	f	3	JHM	C2-C3-C4	-3.51	107.15	111.16
3	h	3	JHM	C2-C3-C4	-3.50	107.16	111.16
3	g	3	JHM	C2-C3-C4	-3.50	107.16	111.16
5	f	7	JHM	C2-C3-C4	-3.49	107.17	111.16
3	Q	3	JHM	C2-C3-C4	-3.48	107.17	111.16
3	b	3	JHM	C2-C3-C4	-3.48	107.18	111.16
4	e	5	JHM	C2-C3-C4	-3.47	107.19	111.16
3	R	3	JHM	C2-C3-C4	-3.47	107.20	111.16
3	c	3	JHM	C2-C3-C4	-3.46	107.20	111.16
3	V	3	JHM	C2-C3-C4	-3.46	107.21	111.16
3	X	3	JHM	C2-C3-C4	-3.45	107.21	111.16
4	e	3	JHM	C2-C3-C4	-3.43	107.23	111.16
3	R	1	JHM	C3-C4-C5	-3.34	106.64	109.99
3	Q	1	JHM	C3-C4-C5	-3.33	106.65	109.99
3	b	1	JHM	C3-C4-C5	-3.33	106.65	109.99
3	b	3	JHM	C3-C4-C5	-3.32	106.66	109.99
2	d	1	JHM	C3-C4-C5	-3.31	106.67	109.99
2	a	1	JHM	C3-C4-C5	-3.30	106.68	109.99
2	Z	1	JHM	C3-C4-C5	-3.30	106.69	109.99
2	o	1	JHM	C3-C4-C5	-3.28	106.70	109.99
2	U	1	JHM	C3-C4-C5	-3.28	106.70	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	1	JHM	C3-C4-C5	-3.28	106.70	109.99
3	R	3	JHM	C3-C4-C5	-3.27	106.71	109.99
2	P	1	JHM	C3-C4-C5	-3.27	106.71	109.99
2	W	1	JHM	C3-C4-C5	-3.26	106.72	109.99
3	h	3	JHM	C3-C4-C5	-3.26	106.72	109.99
2	q	1	JHM	C3-C4-C5	-3.26	106.72	109.99
2	m	1	JHM	C3-C4-C5	-3.25	106.73	109.99
2	Y	1	JHM	C3-C4-C5	-3.25	106.73	109.99
3	c	3	JHM	C3-C4-C5	-3.24	106.74	109.99
2	i	1	JHM	C3-C4-C5	-3.24	106.74	109.99
5	f	9	JHM	C3-C4-C5	-3.24	106.74	109.99
3	p	3	JHM	C3-C4-C5	-3.24	106.74	109.99
5	f	5	JHM	C3-C4-C5	-3.23	106.75	109.99
2	r	1	JHM	C3-C4-C5	-3.23	106.75	109.99
3	V	1	JHM	C3-C4-C5	-3.23	106.75	109.99
3	X	1	JHM	C3-C4-C5	-3.23	106.75	109.99
3	g	1	JHM	C3-C4-C5	-3.23	106.75	109.99
4	e	3	JHM	C3-C4-C5	-3.23	106.75	109.99
4	e	5	JHM	C3-C4-C5	-3.22	106.76	109.99
2	s	1	JHM	C3-C4-C5	-3.22	106.76	109.99
2	n	1	JHM	C3-C4-C5	-3.22	106.76	109.99
3	X	3	JHM	C3-C4-C5	-3.22	106.76	109.99
2	T	1	JHM	C3-C4-C5	-3.22	106.76	109.99
3	Q	3	JHM	C3-C4-C5	-3.22	106.76	109.99
2	W	2	IDS	O6B-C6-C5	3.22	121.07	112.71
2	S	1	JHM	C3-C4-C5	-3.21	106.77	109.99
3	c	1	JHM	C3-C4-C5	-3.21	106.77	109.99
4	e	1	JHM	C3-C4-C5	-3.21	106.77	109.99
2	q	2	IDS	O6B-C6-C5	3.20	121.04	112.71
2	k	1	JHM	C3-C4-C5	-3.20	106.78	109.99
2	Z	2	IDS	O6B-C6-C5	3.20	121.03	112.71
5	f	7	JHM	C3-C4-C5	-3.20	106.78	109.99
3	V	3	JHM	C3-C4-C5	-3.20	106.78	109.99
3	p	1	JHM	C3-C4-C5	-3.19	106.79	109.99
3	p	4	IDS	O6B-C6-C5	3.19	121.02	112.71
4	e	6	IDS	O6B-C6-C5	3.19	121.01	112.71
3	h	1	JHM	C3-C4-C5	-3.19	106.79	109.99
3	g	3	JHM	C3-C4-C5	-3.19	106.80	109.99
2	s	2	IDS	O6B-C6-C5	3.18	120.99	112.71
3	Q	4	IDS	O6B-C6-C5	3.18	120.99	112.71
2	r	2	IDS	O6B-C6-C5	3.18	120.99	112.71
5	f	3	JHM	C3-C4-C5	-3.18	106.80	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	2	IDS	O6B-C6-C5	3.18	120.98	112.71
2	l	1	JHM	C3-C4-C5	-3.18	106.80	109.99
3	X	4	IDS	O6B-C6-C5	3.17	120.97	112.71
3	R	4	IDS	O6B-C6-C5	3.17	120.96	112.71
3	V	4	IDS	O6B-C6-C5	3.17	120.96	112.71
3	c	4	IDS	O6B-C6-C5	3.17	120.95	112.71
2	U	2	IDS	O6B-C6-C5	3.17	120.95	112.71
2	T	2	IDS	O6B-C6-C5	3.16	120.94	112.71
2	S	2	IDS	O6B-C6-C5	3.16	120.92	112.71
2	j	1	JHM	C3-C4-C5	-3.13	106.85	109.99
2	o	2	IDS	O6B-C6-C5	2.95	120.38	112.71
2	j	2	IDS	O6B-C6-C5	2.94	120.35	112.71
2	n	2	IDS	O6B-C6-C5	2.93	120.34	112.71
3	h	4	IDS	O6B-C6-C5	2.93	120.32	112.71
5	f	10	IDS	O6B-C6-C5	2.92	120.31	112.71
2	k	2	IDS	O6B-C6-C5	2.92	120.31	112.71
3	b	4	IDS	O6B-C6-C5	2.91	120.28	112.71
2	a	2	IDS	O6B-C6-C5	2.91	120.28	112.71
2	m	2	IDS	O6B-C6-C5	2.91	120.28	112.71
3	g	4	IDS	O6B-C6-C5	2.90	120.26	112.71
2	d	2	IDS	O6B-C6-C5	2.90	120.26	112.71
2	P	2	IDS	O6B-C6-C5	2.90	120.25	112.71
2	l	2	IDS	O6B-C6-C5	2.90	120.25	112.71
2	Y	2	IDS	O6B-C6-C5	2.89	120.23	112.71
4	e	2	IDS	O4-C4-C5	2.88	116.34	109.76
2	k	2	IDS	C1-C2-C3	2.80	113.78	109.84
2	Z	2	IDS	C1-C2-C3	2.78	113.76	109.84
3	X	4	IDS	C1-C2-C3	2.77	113.75	109.84
2	Y	2	IDS	C1-C2-C3	2.77	113.74	109.84
2	U	2	IDS	C1-C2-C3	2.76	113.73	109.84
2	W	2	IDS	C1-C2-C3	2.76	113.73	109.84
3	p	4	IDS	C1-C2-C3	2.76	113.73	109.84
2	a	2	IDS	C1-C2-C3	2.75	113.71	109.84
2	T	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	o	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	r	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	j	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	m	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	S	2	IDS	C1-C2-C3	2.74	113.70	109.84
2	n	2	IDS	C1-C2-C3	2.74	113.70	109.84
3	R	4	IDS	C1-C2-C3	2.74	113.70	109.84
4	e	6	IDS	C1-C2-C3	2.74	113.70	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	4	IDS	C1-C2-C3	2.74	113.70	109.84
5	f	10	IDS	C1-C2-C3	2.74	113.70	109.84
2	l	2	IDS	C1-C2-C3	2.74	113.69	109.84
2	d	2	IDS	C1-C2-C3	2.73	113.69	109.84
3	h	4	IDS	C1-C2-C3	2.73	113.69	109.84
3	c	4	IDS	C1-C2-C3	2.73	113.69	109.84
2	P	2	IDS	C1-C2-C3	2.73	113.68	109.84
3	g	4	IDS	C1-C2-C3	2.73	113.68	109.84
3	V	4	IDS	C1-C2-C3	2.71	113.66	109.84
3	Q	4	IDS	C1-C2-C3	2.71	113.65	109.84
2	s	2	IDS	C1-C2-C3	2.70	113.64	109.84
2	i	2	IDS	C1-C2-C3	2.69	113.63	109.84
2	q	2	IDS	C1-C2-C3	2.68	113.62	109.84
4	e	1	JHM	C2-C3-C4	-2.45	107.14	110.67
2	j	1	JHM	C2-C3-C4	-2.44	107.15	110.67
2	Z	1	JHM	C2-C3-C4	-2.44	107.15	110.67
3	p	1	JHM	C2-C3-C4	-2.44	107.15	110.67
3	X	1	JHM	C2-C3-C4	-2.43	107.16	110.67
3	V	1	JHM	C2-C3-C4	-2.43	107.16	110.67
2	l	1	JHM	C2-C3-C4	-2.43	107.16	110.67
2	d	1	JHM	C2-C3-C4	-2.43	107.16	110.67
2	T	1	JHM	C2-C3-C4	-2.43	107.17	110.67
3	g	1	JHM	C2-C3-C4	-2.43	107.17	110.67
3	h	1	JHM	C2-C3-C4	-2.42	107.18	110.67
3	Q	1	JHM	C2-C3-C4	-2.41	107.19	110.67
3	c	1	JHM	C2-C3-C4	-2.41	107.19	110.67
3	b	1	JHM	C2-C3-C4	-2.41	107.19	110.67
2	P	1	JHM	C2-C3-C4	-2.41	107.20	110.67
2	n	2	IDS	O6B-C6-O6A	-2.40	118.63	124.08
2	m	2	IDS	O6B-C6-O6A	-2.40	118.63	124.08
2	k	1	JHM	C2-C3-C4	-2.40	107.20	110.67
2	s	1	JHM	C2-C3-C4	-2.40	107.20	110.67
2	U	1	JHM	C2-C3-C4	-2.40	107.20	110.67
2	q	1	JHM	C2-C3-C4	-2.40	107.21	110.67
2	q	2	IDS	O6B-C6-O6A	-2.40	118.64	124.08
5	f	1	JHM	C2-C3-C4	-2.40	107.21	110.67
2	r	1	JHM	C2-C3-C4	-2.40	107.21	110.67
2	r	2	IDS	O6B-C6-O6A	-2.40	118.64	124.08
4	e	2	IDS	O6B-C6-O6A	-2.39	118.65	124.08
2	Y	1	JHM	C2-C3-C4	-2.39	107.21	110.67
2	a	1	JHM	C2-C3-C4	-2.39	107.22	110.67
2	i	2	IDS	O6B-C6-O6A	-2.38	118.67	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	1	JHM	C2-C3-C4	-2.38	107.23	110.67
2	m	1	JHM	C2-C3-C4	-2.38	107.23	110.67
3	p	2	IDS	O6B-C6-O6A	-2.38	118.67	124.08
2	o	2	IDS	O6B-C6-O6A	-2.38	118.67	124.08
2	s	2	IDS	O6B-C6-O6A	-2.38	118.67	124.08
2	n	1	JHM	C2-C3-C4	-2.38	107.23	110.67
2	W	2	IDS	O6B-C6-O6A	-2.38	118.68	124.08
2	j	2	IDS	O6B-C6-O6A	-2.38	118.68	124.08
2	S	1	JHM	C2-C3-C4	-2.38	107.24	110.67
2	W	1	JHM	C2-C3-C4	-2.38	107.24	110.67
3	R	2	IDS	O6B-C6-O6A	-2.38	118.69	124.08
3	R	1	JHM	C2-C3-C4	-2.38	107.24	110.67
3	R	4	IDS	O6B-C6-O6A	-2.38	118.69	124.08
3	V	2	IDS	O6B-C6-O6A	-2.37	118.69	124.08
2	k	2	IDS	O6B-C6-O6A	-2.37	118.69	124.08
3	h	4	IDS	O6B-C6-O6A	-2.37	118.69	124.08
2	o	1	JHM	C2-C3-C4	-2.37	107.24	110.67
3	p	4	IDS	O6B-C6-O6A	-2.37	118.70	124.08
5	f	2	IDS	O6B-C6-O6A	-2.37	118.70	124.08
3	V	4	IDS	O6B-C6-O6A	-2.37	118.71	124.08
3	X	2	IDS	O6B-C6-O6A	-2.37	118.71	124.08
4	e	4	IDS	O6B-C6-O6A	-2.37	118.71	124.08
4	e	6	IDS	O6B-C6-O6A	-2.37	118.71	124.08
3	Q	4	IDS	O6B-C6-O6A	-2.37	118.71	124.08
5	f	4	IDS	O6B-C6-O6A	-2.37	118.71	124.08
5	f	10	IDS	O6B-C6-O6A	-2.36	118.72	124.08
2	Z	2	IDS	O6B-C6-O6A	-2.36	118.72	124.08
2	T	2	IDS	O6B-C6-O6A	-2.36	118.74	124.08
3	b	2	IDS	O6B-C6-O6A	-2.35	118.74	124.08
3	g	2	IDS	O6B-C6-O6A	-2.35	118.74	124.08
2	U	2	IDS	O6B-C6-O6A	-2.35	118.74	124.08
5	f	6	IDS	O6B-C6-O6A	-2.35	118.75	124.08
3	h	2	IDS	O6B-C6-O6A	-2.35	118.75	124.08
2	Y	2	IDS	O6B-C6-O6A	-2.35	118.76	124.08
3	c	4	IDS	O6B-C6-O6A	-2.35	118.76	124.08
3	g	4	IDS	O6B-C6-O6A	-2.35	118.76	124.08
3	b	4	IDS	O6B-C6-O6A	-2.34	118.76	124.08
3	X	4	IDS	O6B-C6-O6A	-2.34	118.77	124.08
2	l	2	IDS	O6B-C6-O6A	-2.34	118.78	124.08
3	Q	2	IDS	O6B-C6-O6A	-2.34	118.78	124.08
2	S	2	IDS	O6B-C6-O6A	-2.34	118.78	124.08
2	P	2	IDS	O6B-C6-O6A	-2.33	118.79	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	2	IDS	O6B-C6-O6A	-2.33	118.80	124.08
2	d	2	IDS	O6B-C6-O6A	-2.32	118.81	124.08
5	f	8	IDS	O6B-C6-O6A	-2.32	118.81	124.08
3	c	2	IDS	O6B-C6-O6A	-2.31	118.83	124.08
3	c	3	JHM	C1-C2-C3	-2.25	106.95	110.61
5	f	3	JHM	C1-C2-C3	-2.23	106.99	110.61
3	g	3	JHM	C1-C2-C3	-2.21	107.02	110.61
3	b	3	JHM	C1-C2-C3	-2.21	107.02	110.61
4	e	5	JHM	C1-C2-C3	-2.21	107.02	110.61
3	R	3	JHM	C1-C2-C3	-2.21	107.02	110.61
3	X	3	JHM	C1-C2-C3	-2.21	107.02	110.61
5	f	7	JHM	C1-C2-C3	-2.20	107.03	110.61
5	f	9	JHM	C1-C2-C3	-2.19	107.05	110.61
3	Q	3	JHM	C1-C2-C3	-2.19	107.06	110.61
5	f	5	JHM	C1-C2-C3	-2.19	107.06	110.61
3	V	3	JHM	C1-C2-C3	-2.19	107.06	110.61
4	e	3	JHM	C1-C2-C3	-2.19	107.06	110.61
3	h	3	JHM	C1-C2-C3	-2.17	107.08	110.61
3	p	2	IDS	O4-C4-C3	2.16	115.46	110.38
3	R	2	IDS	O4-C4-C5	-2.15	104.85	109.76
3	p	3	JHM	C1-C2-C3	-2.13	107.15	110.61
4	e	2	IDS	O6B-C6-C5	2.06	121.09	113.64
4	e	4	IDS	O6B-C6-C5	2.06	121.09	113.64
3	X	2	IDS	O6B-C6-C5	2.06	121.06	113.64
3	Q	2	IDS	O6B-C6-C5	2.02	120.94	113.64
3	c	2	IDS	O6B-C6-C5	2.02	120.93	113.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1	JHM	C6-O6-S-O8
2	Y	1	JHM	C6-O6-S-O8
2	a	1	JHM	C6-O6-S-O8
2	d	1	JHM	C6-O6-S-O8
2	o	1	JHM	C6-O6-S-O8
3	R	1	JHM	C6-O6-S-O8
3	V	1	JHM	C6-O6-S-O8
3	X	3	JHM	C6-O6-S-O8
3	b	1	JHM	C6-O6-S-O8
3	b	3	JHM	C6-O6-S-O8
3	g	1	JHM	C6-O6-S-O8

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Mol	Chain	Res	Type	Atoms
3	h	1	JHM	C6-O6-S-O8
5	f	1	JHM	C6-O6-S-O8
5	f	3	JHM	C6-O6-S-O8
5	f	7	JHM	C6-O6-S-O8
5	f	9	JHM	C6-O6-S-O8

There are no ring outliers.

46 monomers are involved in 99 short contacts:

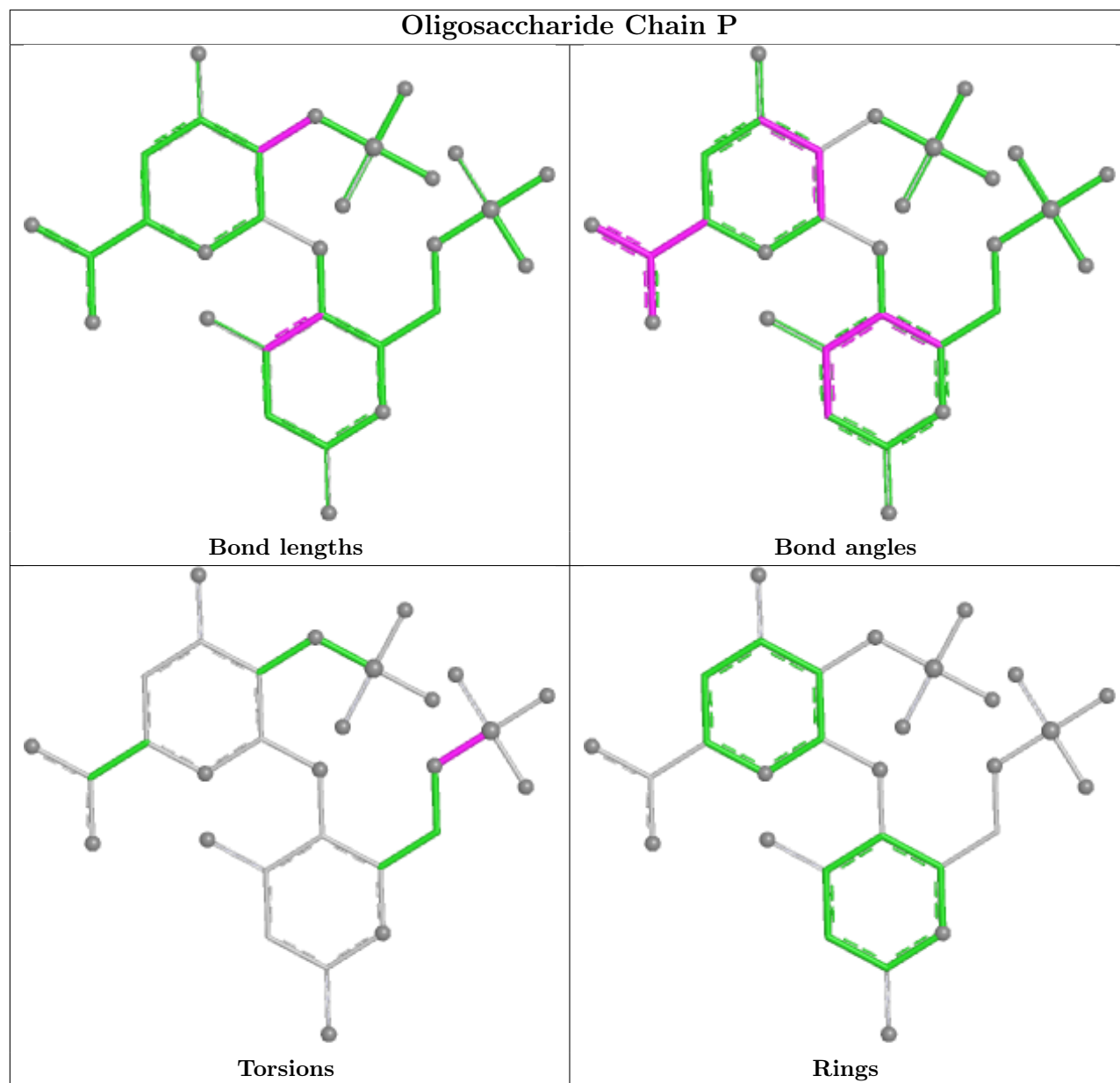
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	h	1	JHM	1	0
3	V	1	JHM	3	0
5	f	2	IDS	1	0
5	f	5	JHM	1	0
3	V	2	IDS	2	0
3	Q	3	JHM	1	0
4	e	4	IDS	1	0
5	f	4	IDS	1	0
3	b	1	JHM	5	0
2	l	2	IDS	5	0
3	V	4	IDS	3	0
2	n	1	JHM	7	0
2	m	1	JHM	2	0
2	r	1	JHM	5	0
3	X	1	JHM	8	0
3	c	4	IDS	1	0
4	e	5	JHM	1	0
3	g	3	JHM	1	0
2	d	2	IDS	3	0
2	o	2	IDS	1	0
3	c	3	JHM	2	0
2	r	2	IDS	7	0
3	R	2	IDS	2	0
4	e	3	JHM	5	0
3	V	3	JHM	1	0
3	c	1	JHM	3	0
2	s	1	JHM	6	0
3	h	3	JHM	2	0
2	Y	2	IDS	8	0
3	h	2	IDS	9	0
3	X	3	JHM	3	0
4	e	1	JHM	8	0

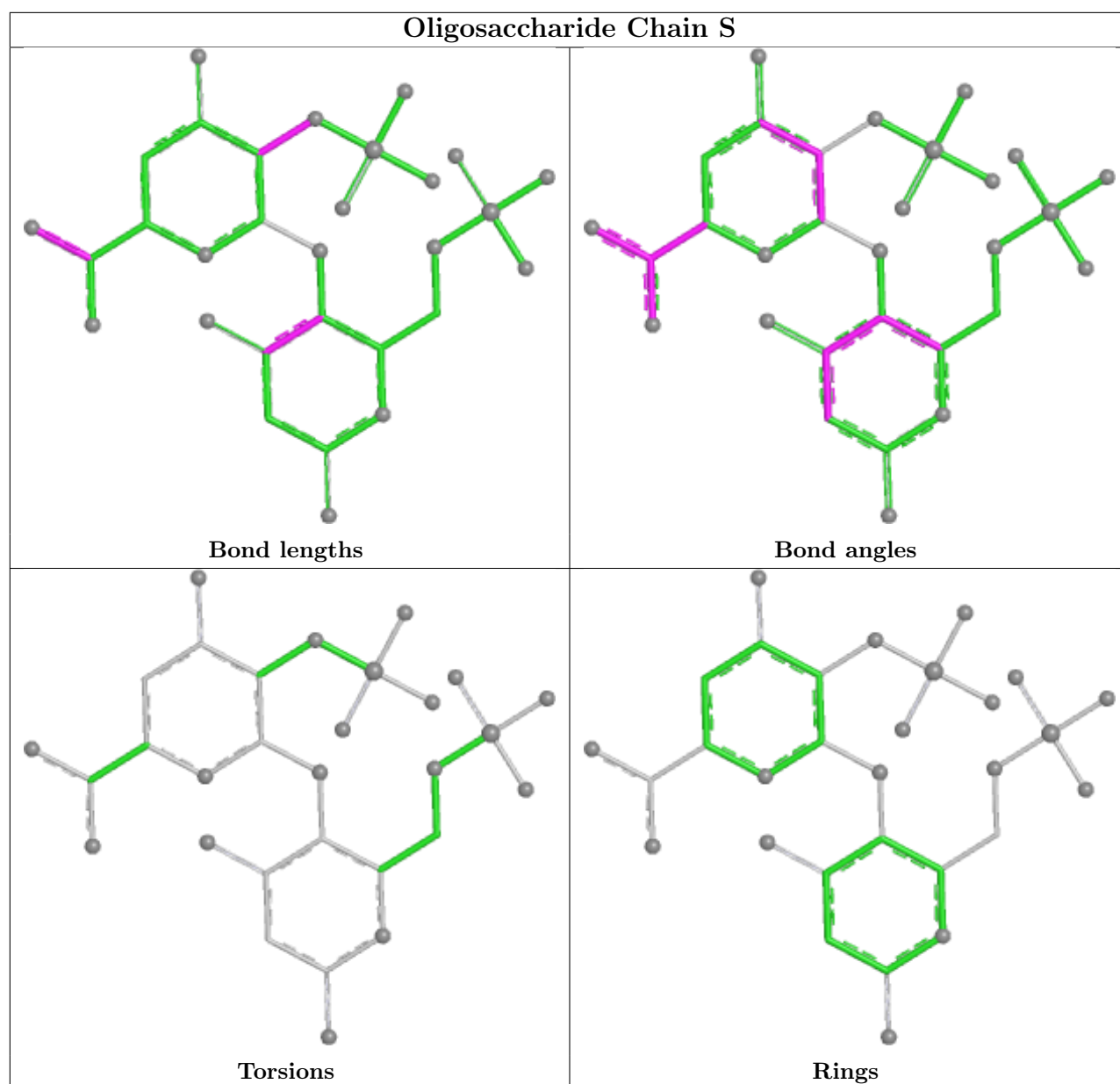
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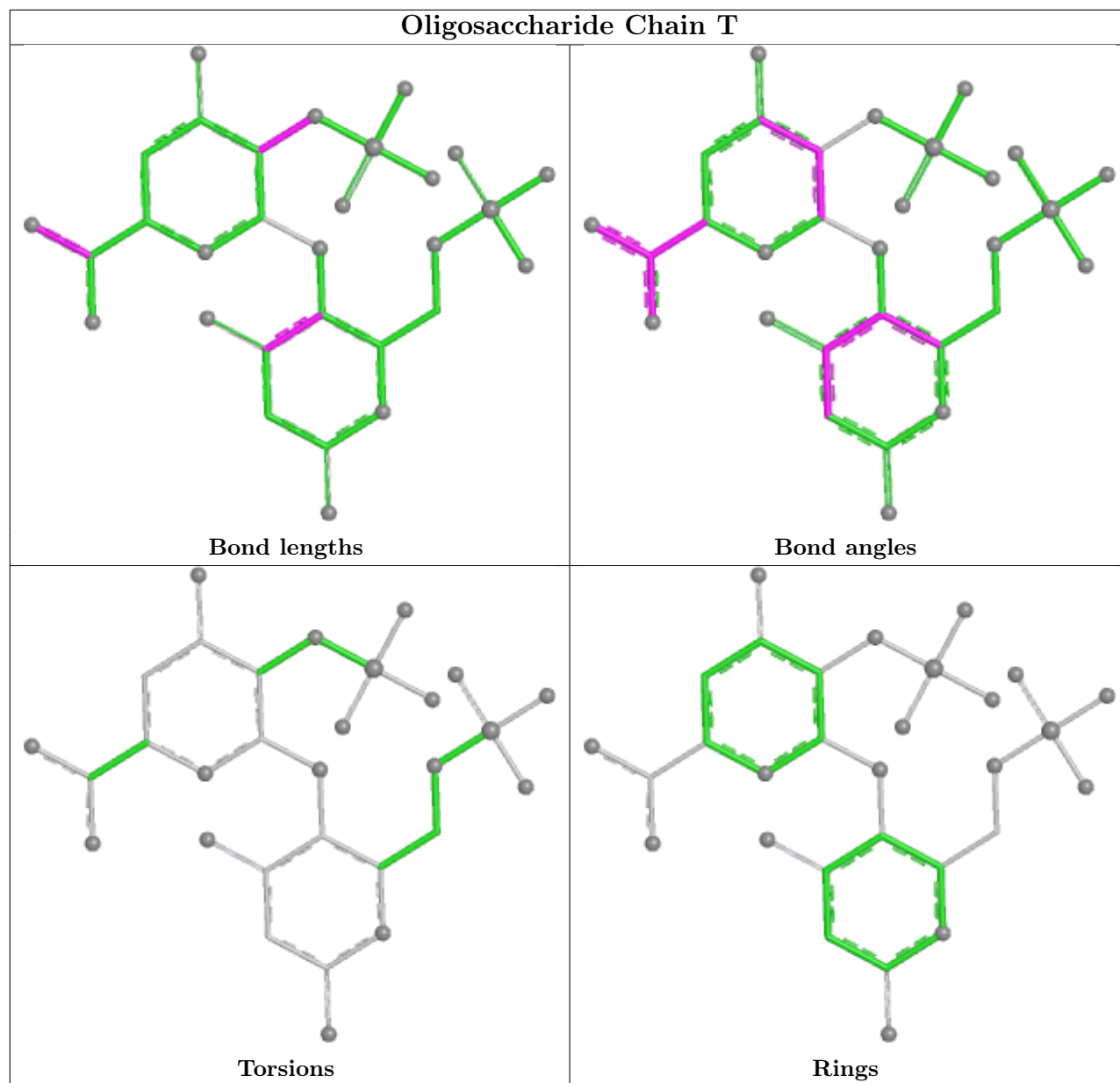
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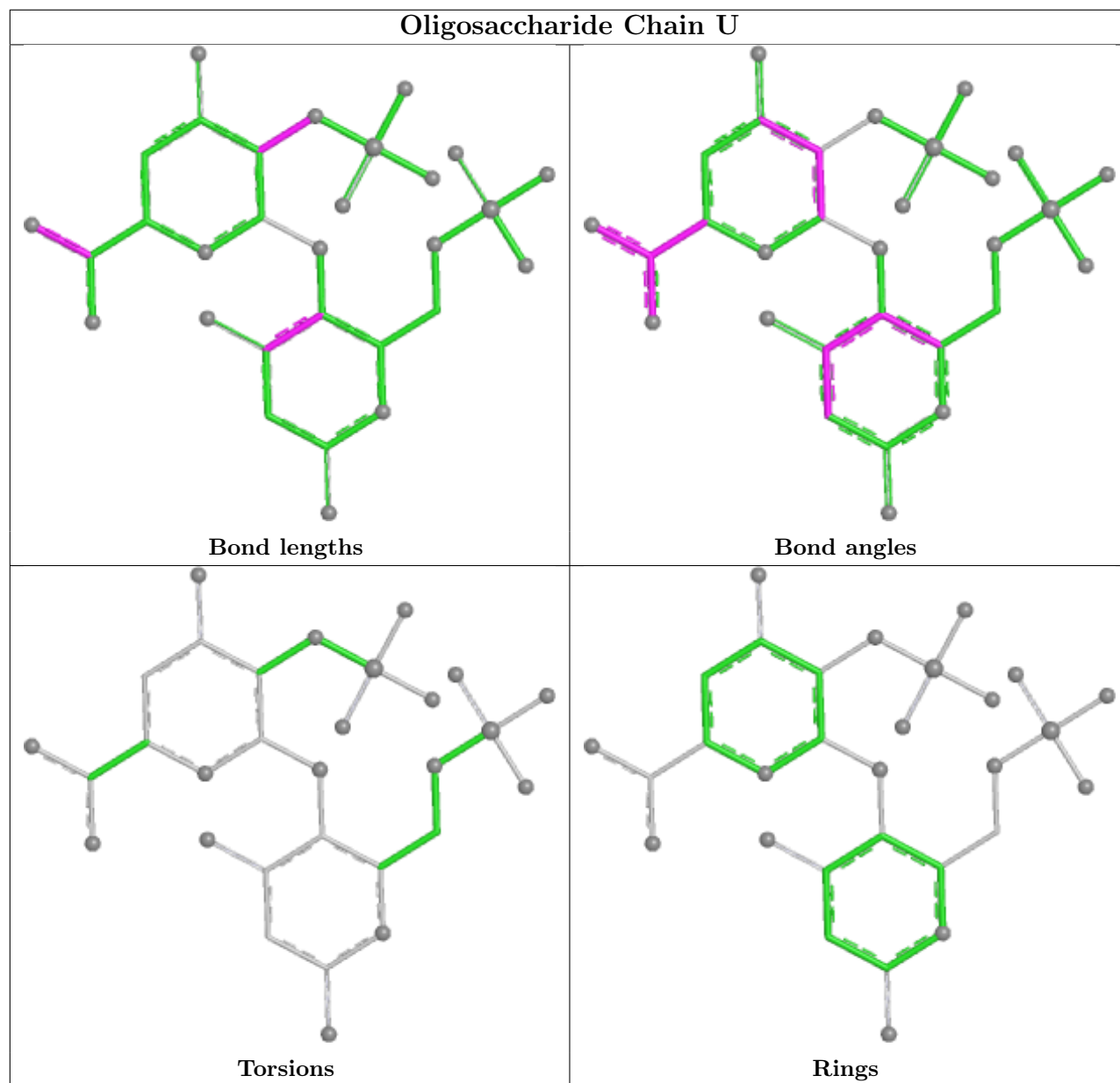
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	k	1	JHM	5	0
2	m	2	IDS	7	0
2	d	1	JHM	1	0
2	W	1	JHM	2	0
4	e	2	IDS	4	0
3	R	3	JHM	2	0
2	U	2	IDS	1	0
5	f	1	JHM	2	0
5	f	3	JHM	1	1
2	a	2	IDS	2	0
3	h	4	IDS	2	0
2	Y	1	JHM	2	0
3	X	2	IDS	3	0
3	p	2	IDS	1	0

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

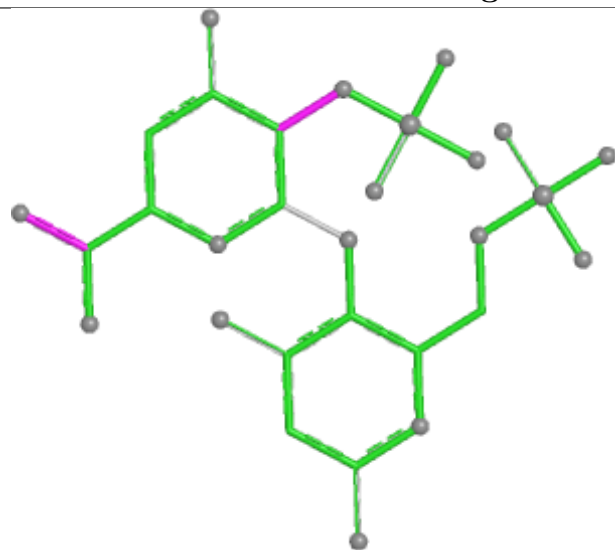




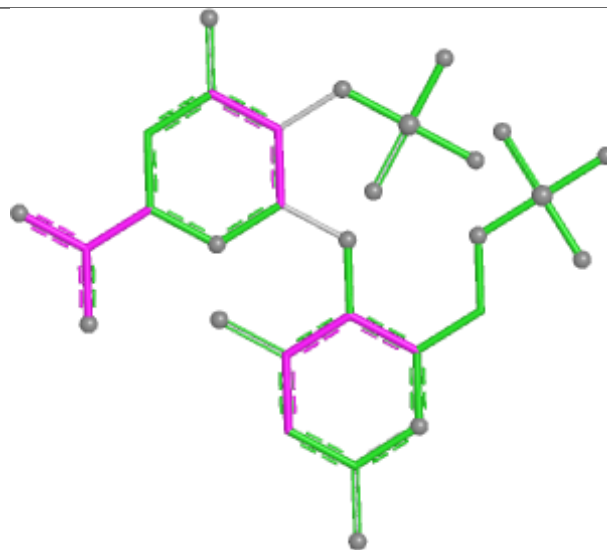




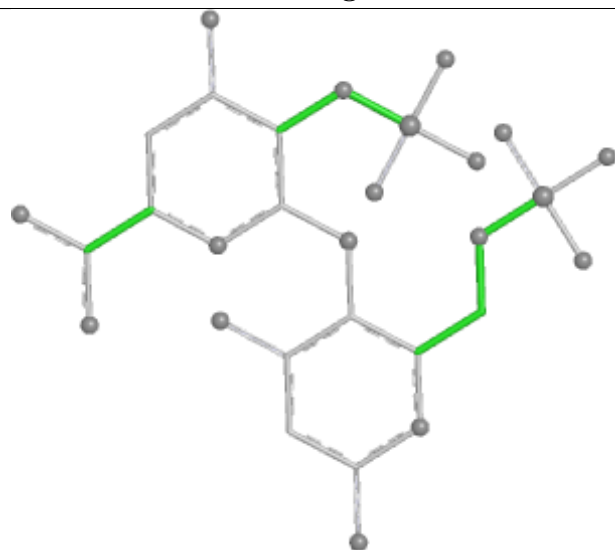
Oligosaccharide Chain W



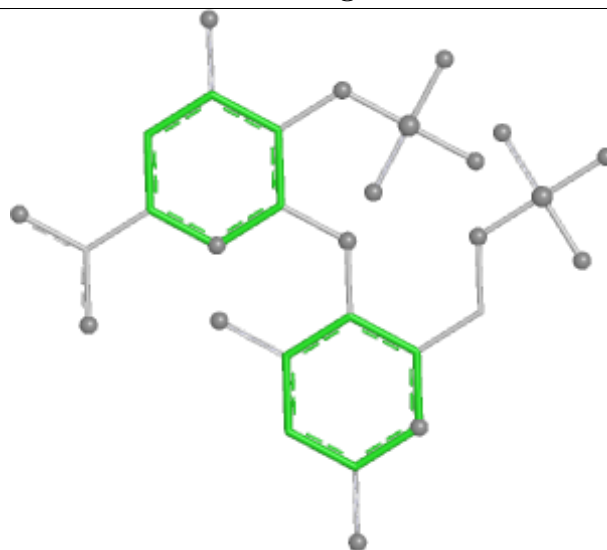
Bond lengths



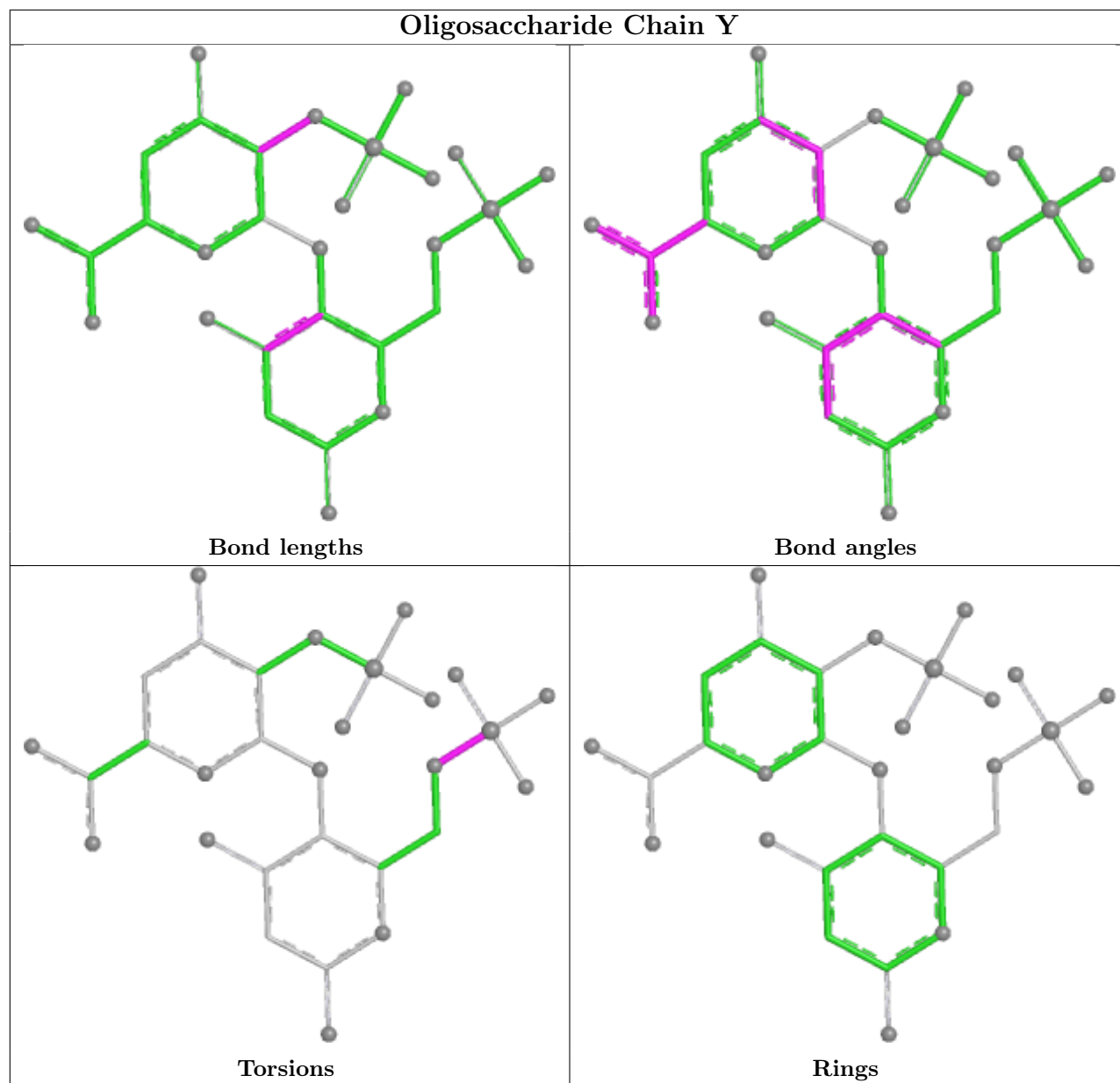
Bond angles

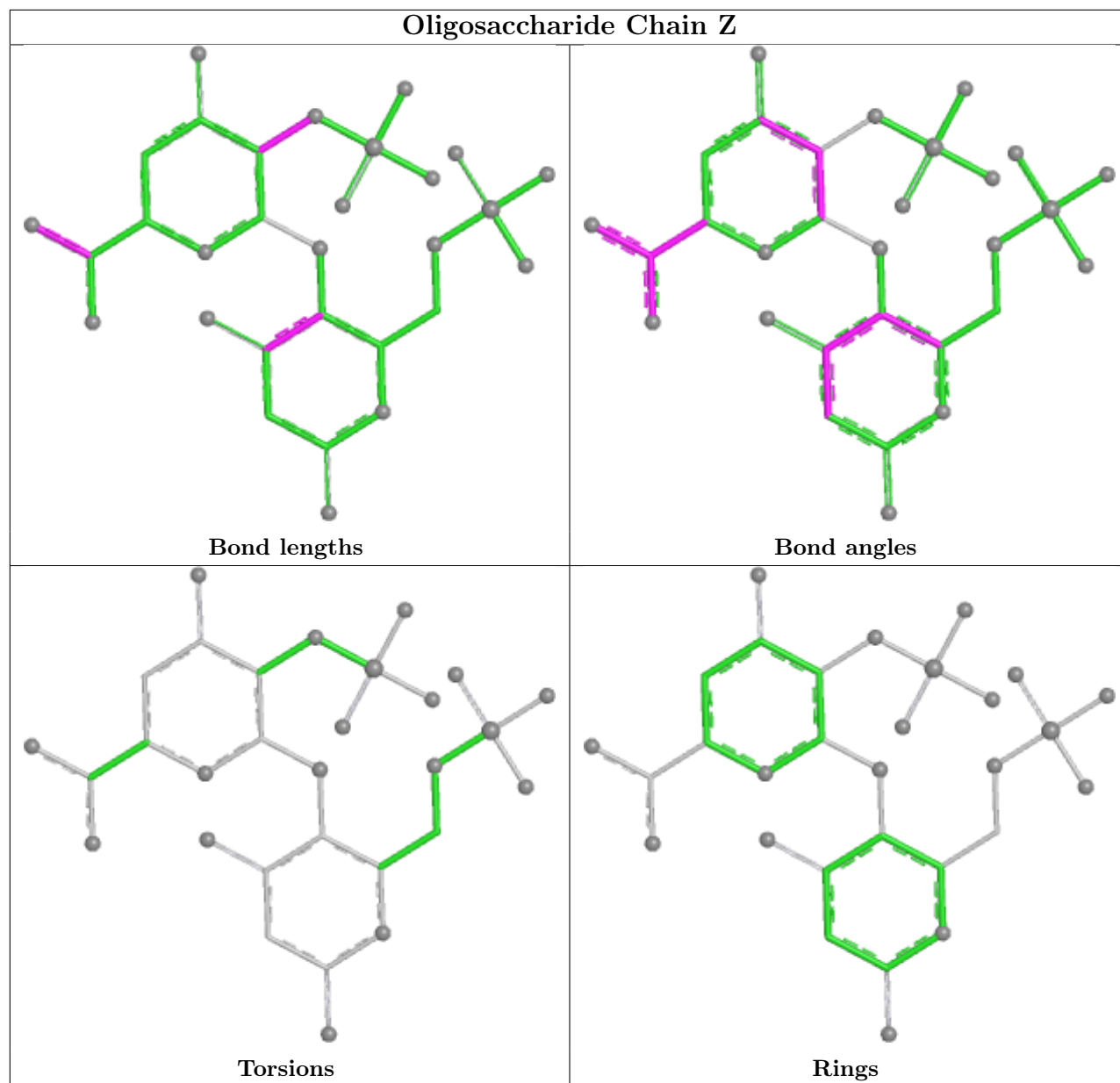


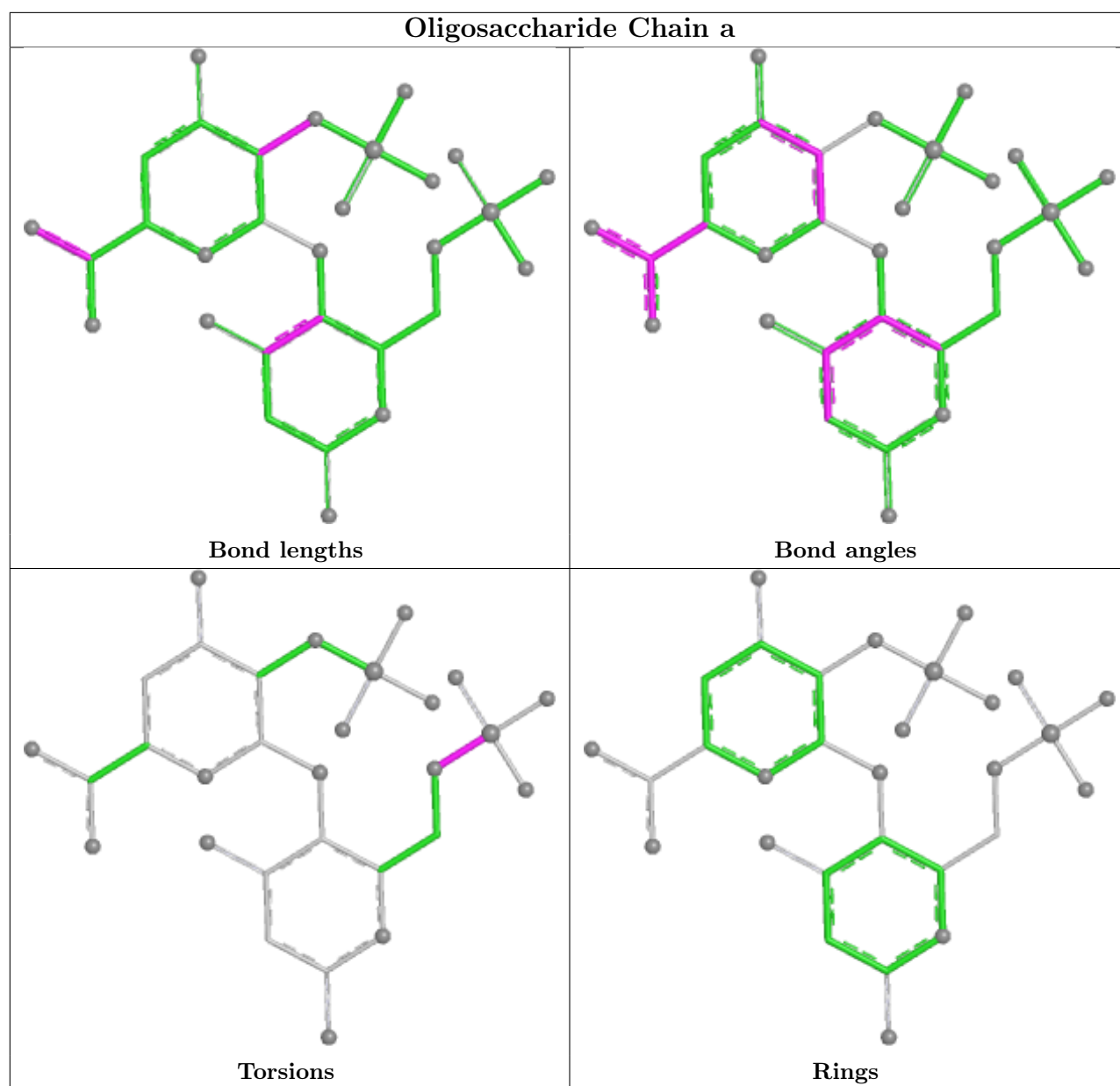
Torsions

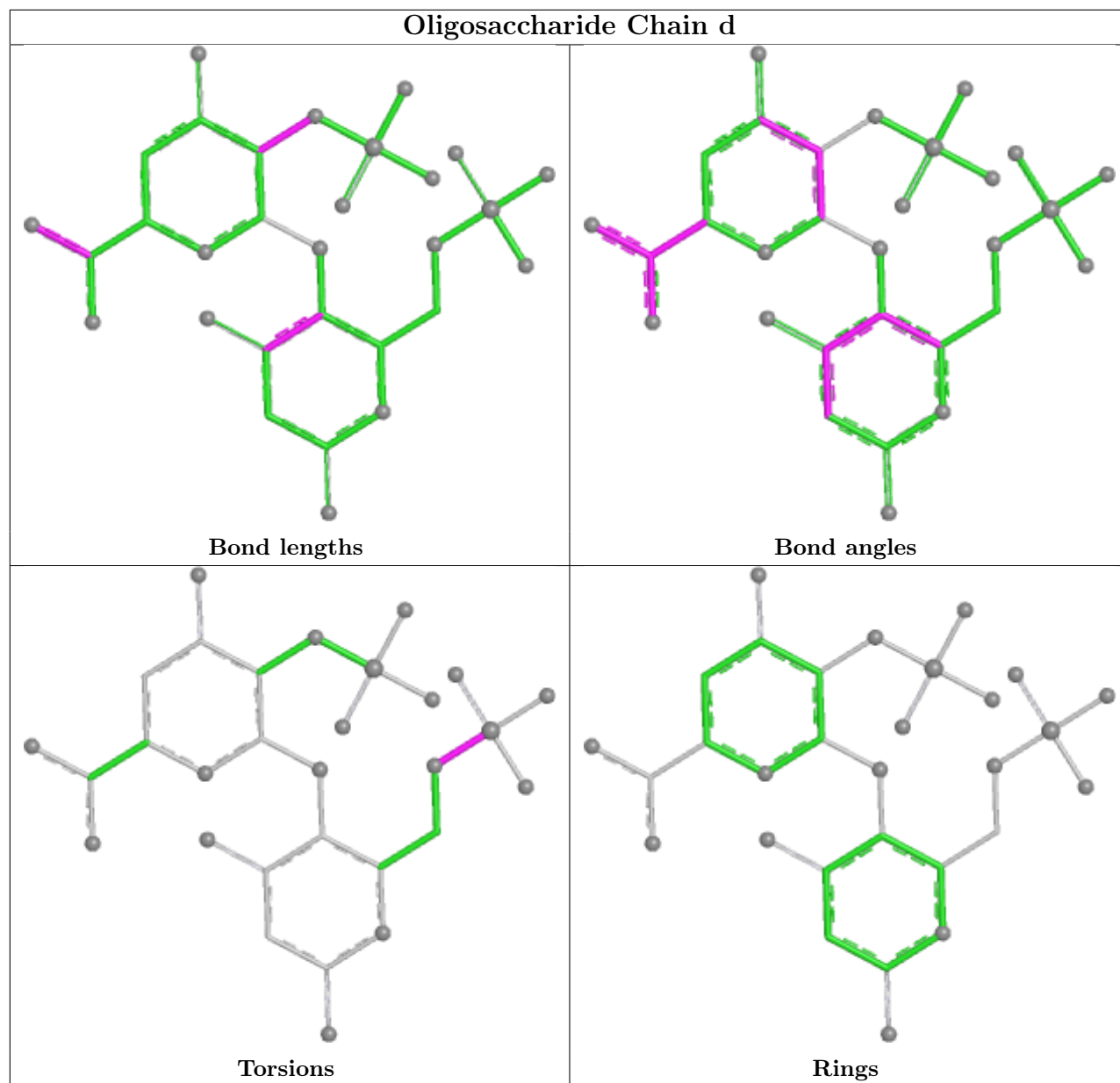


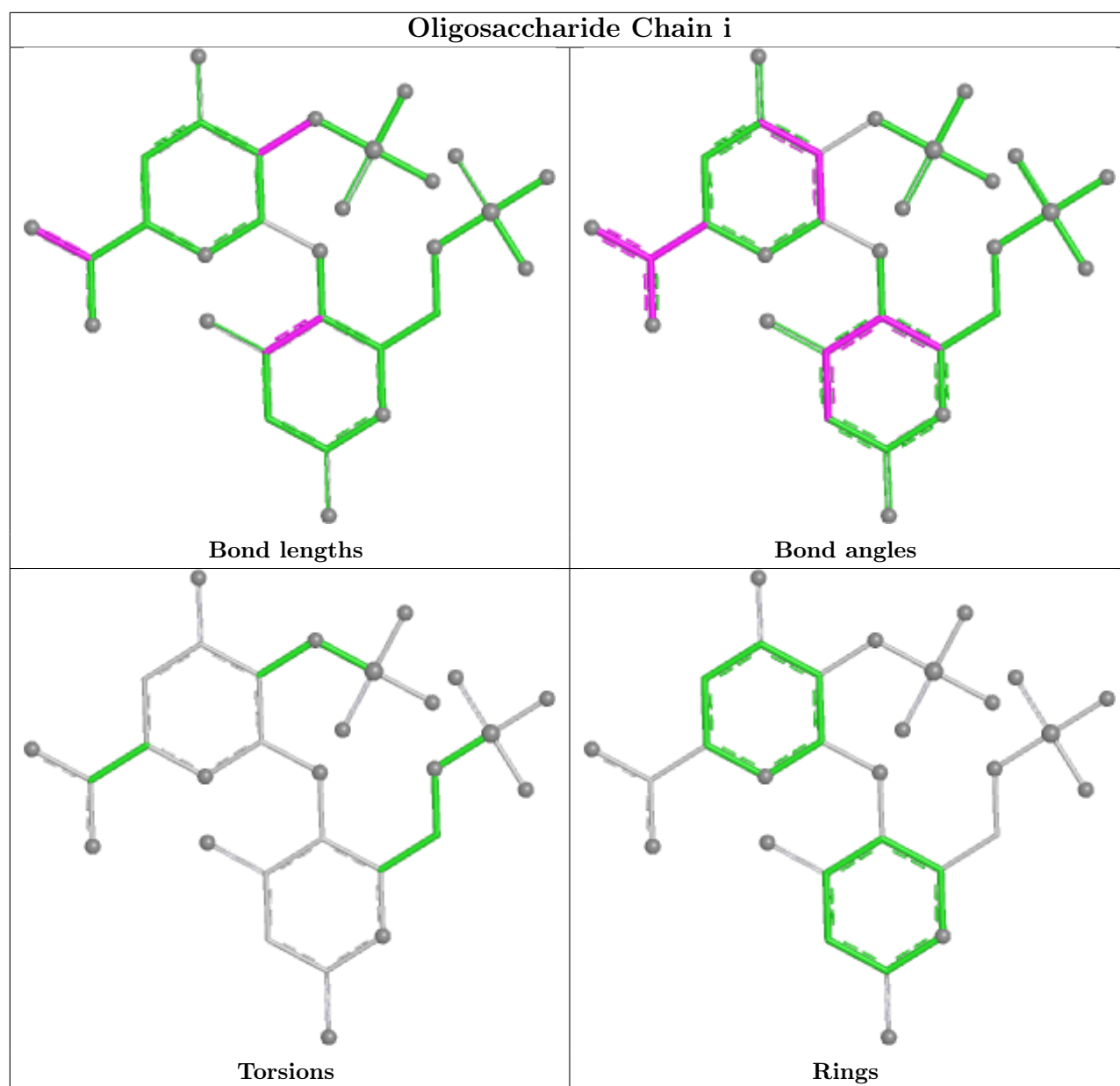
Rings

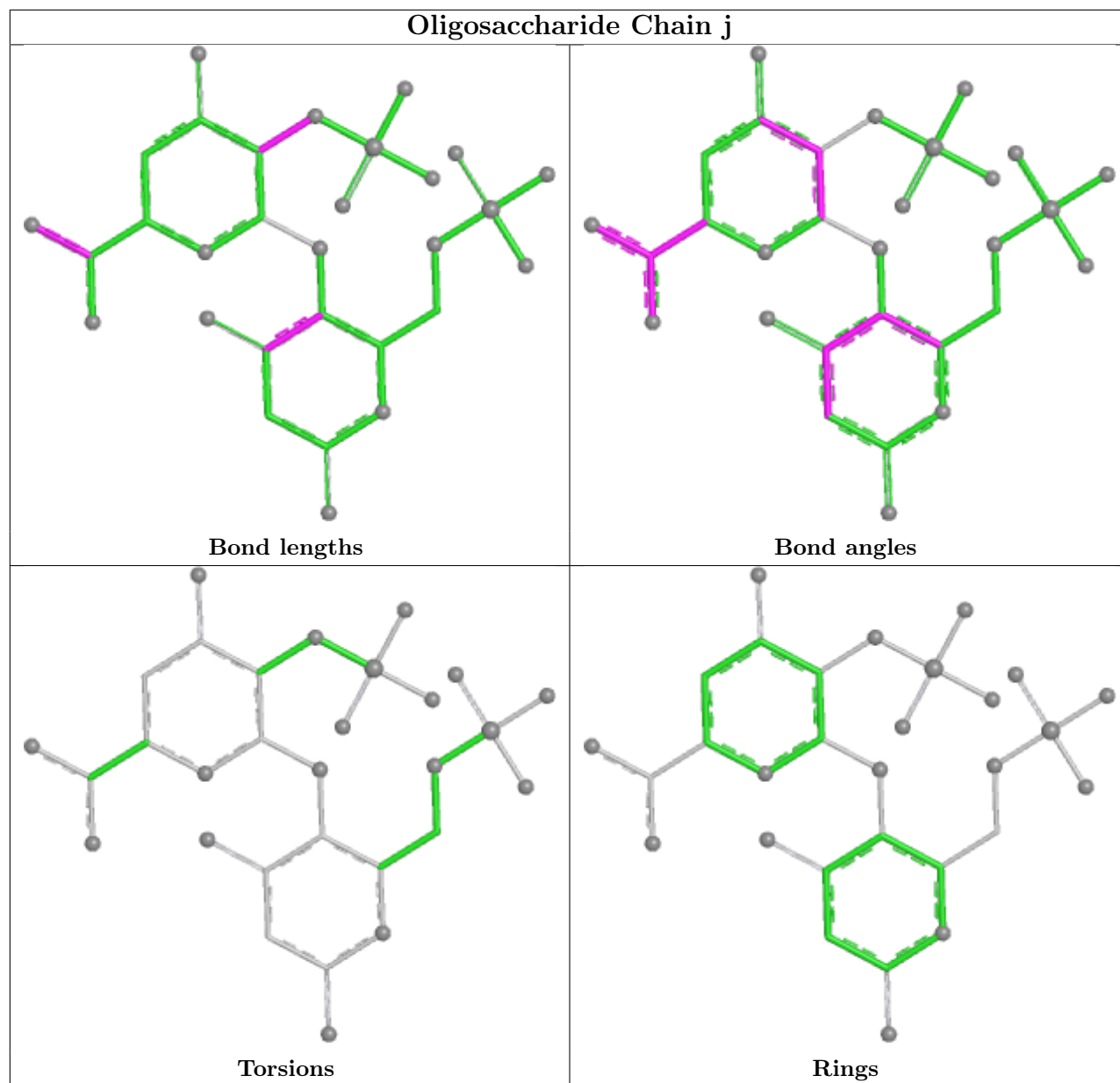


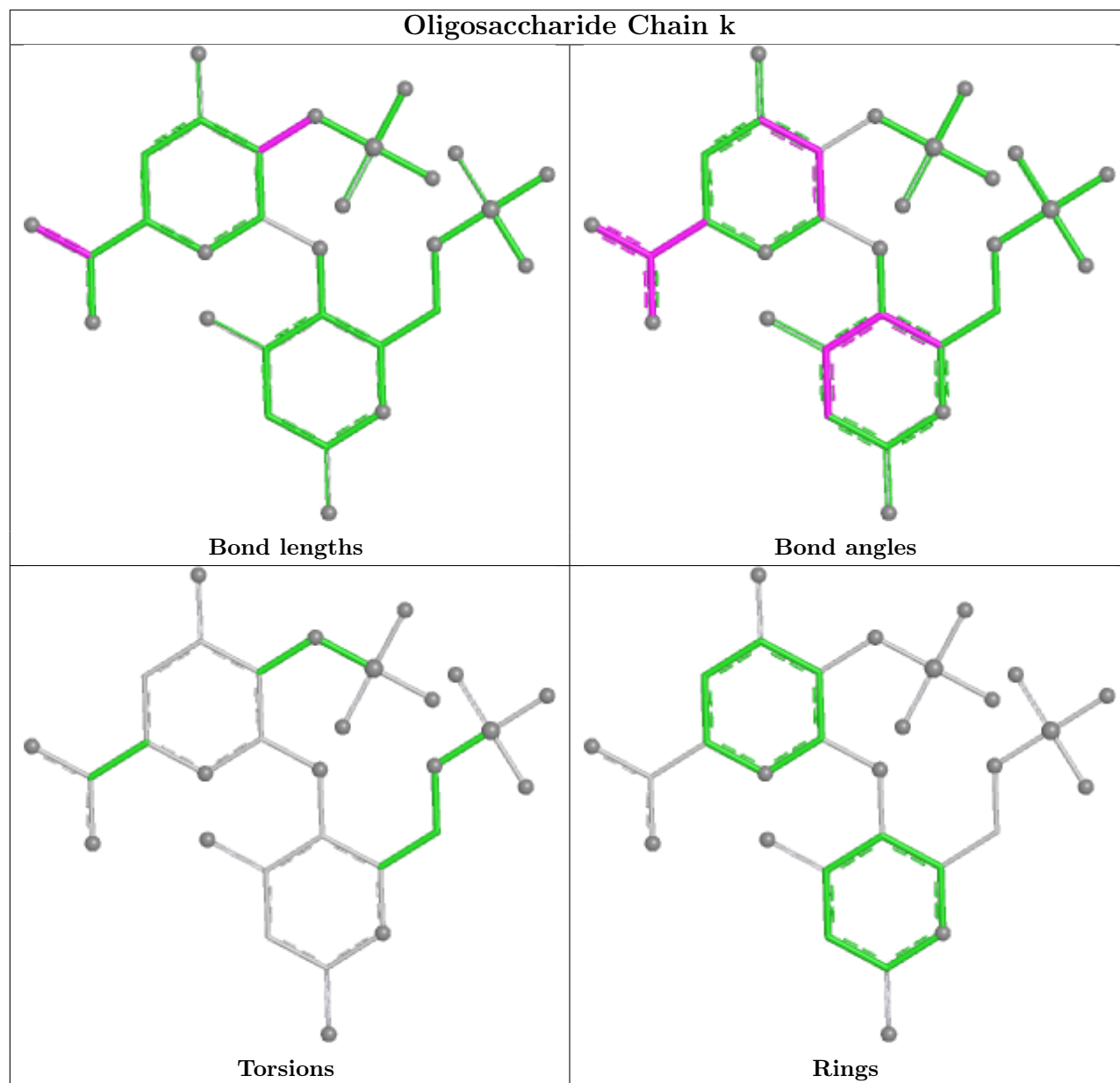


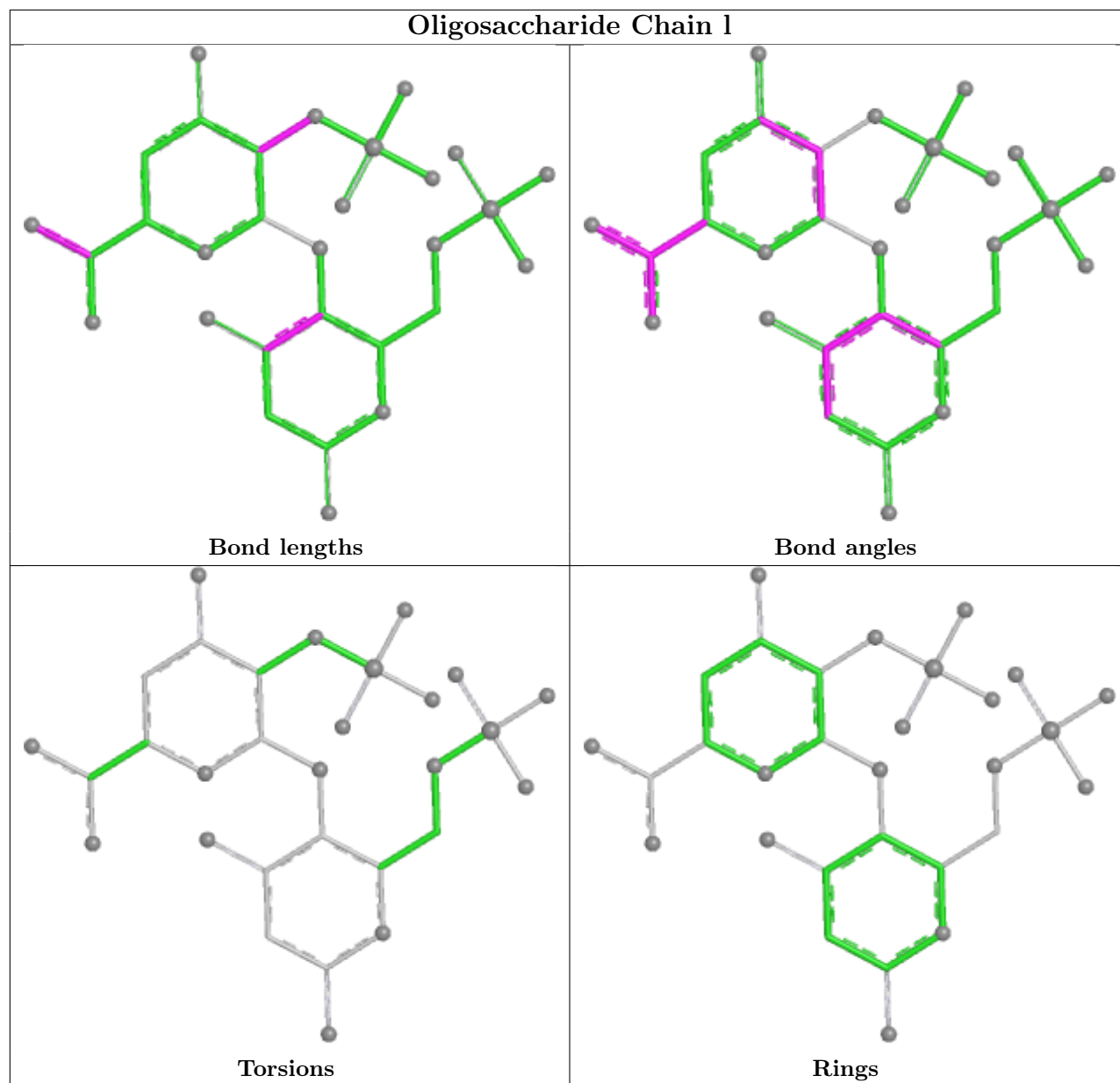


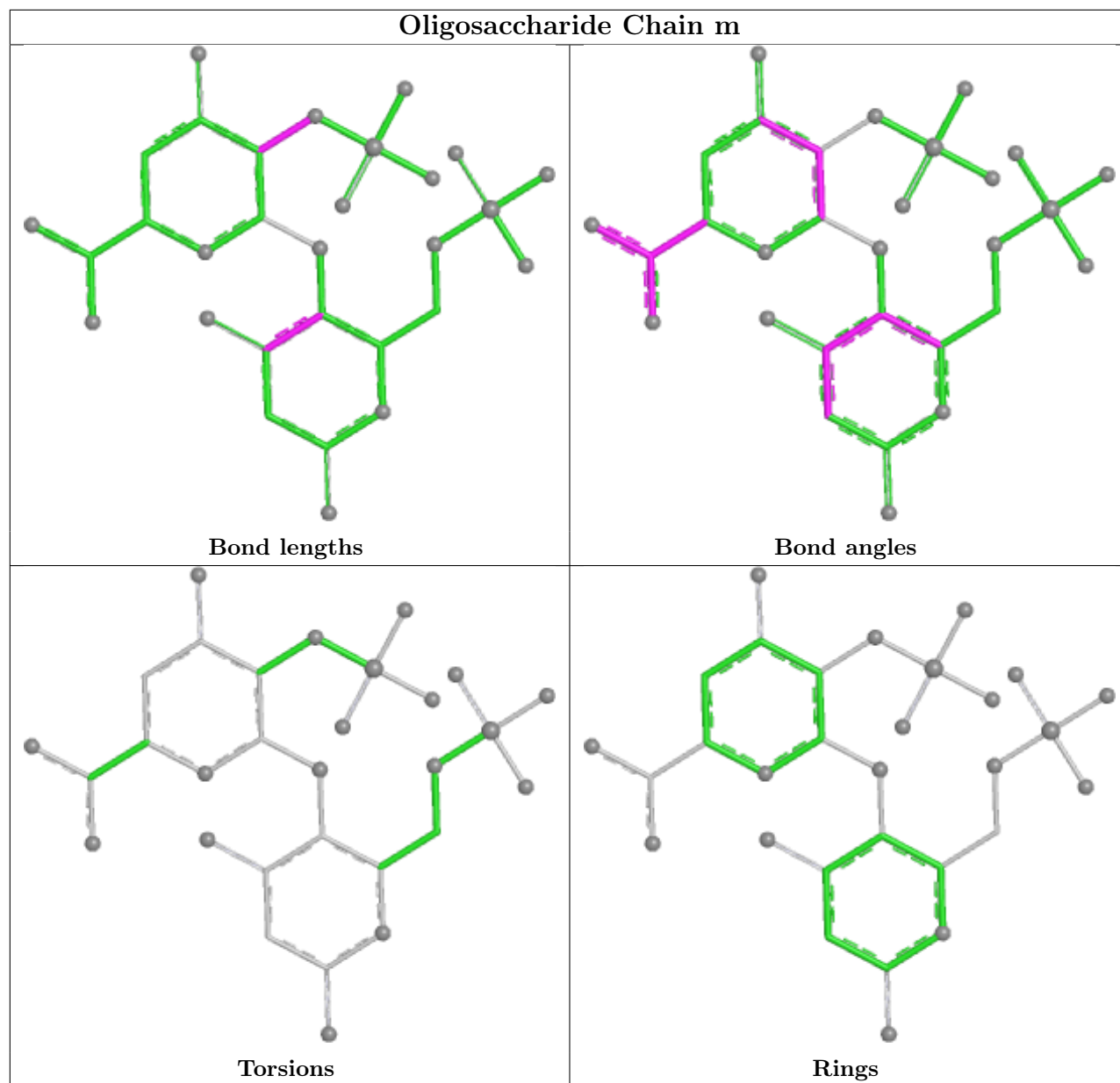


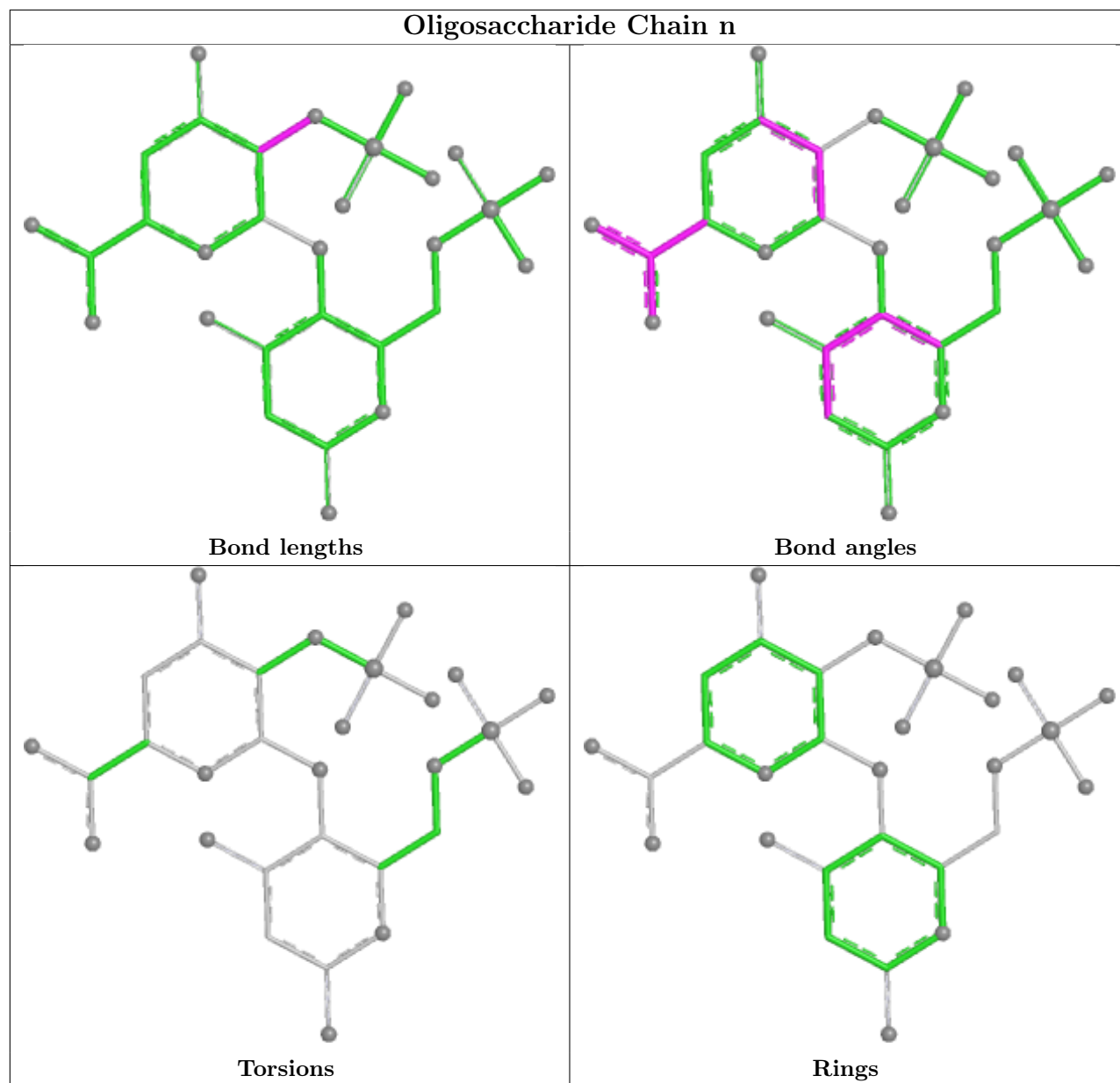


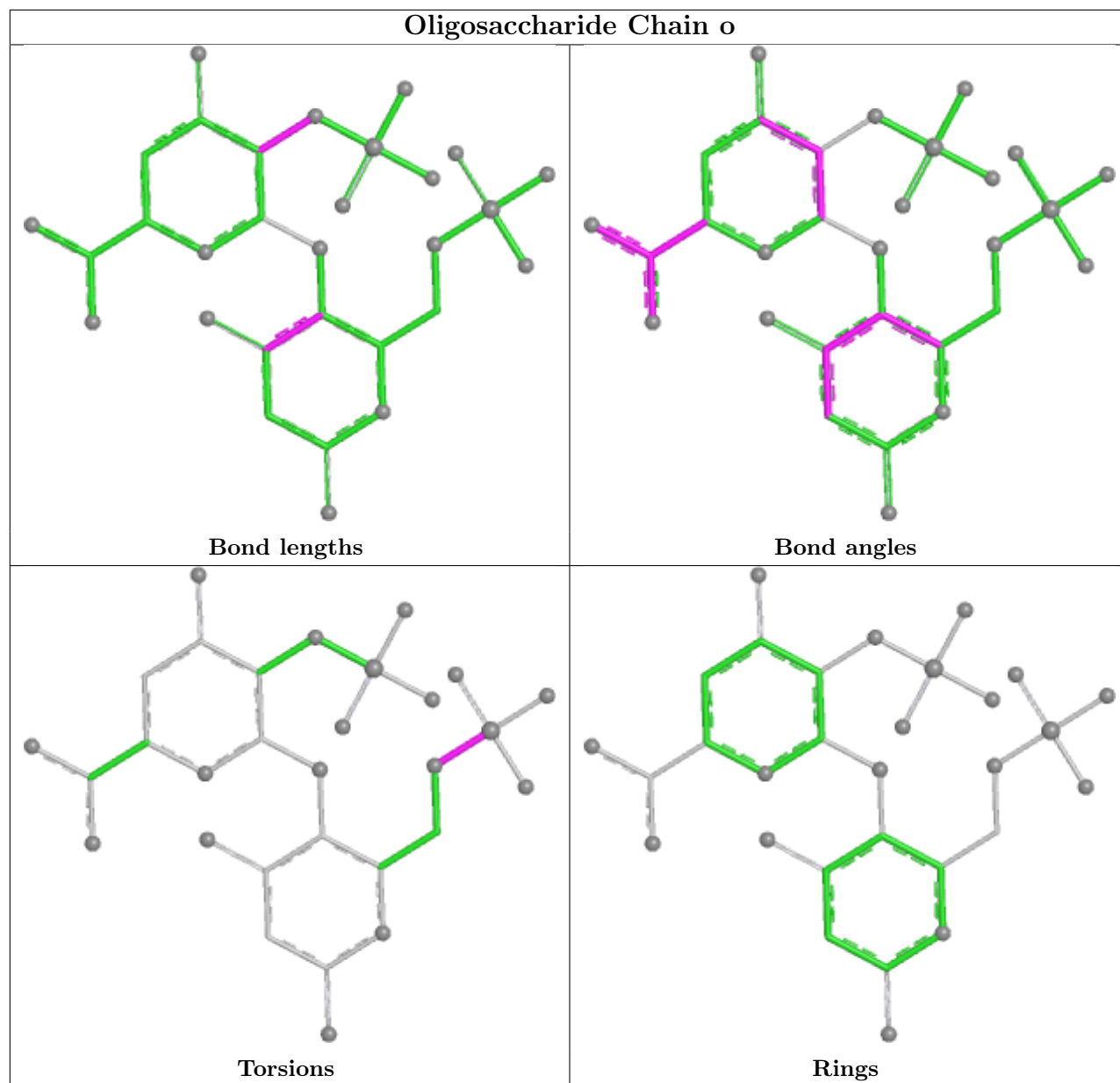


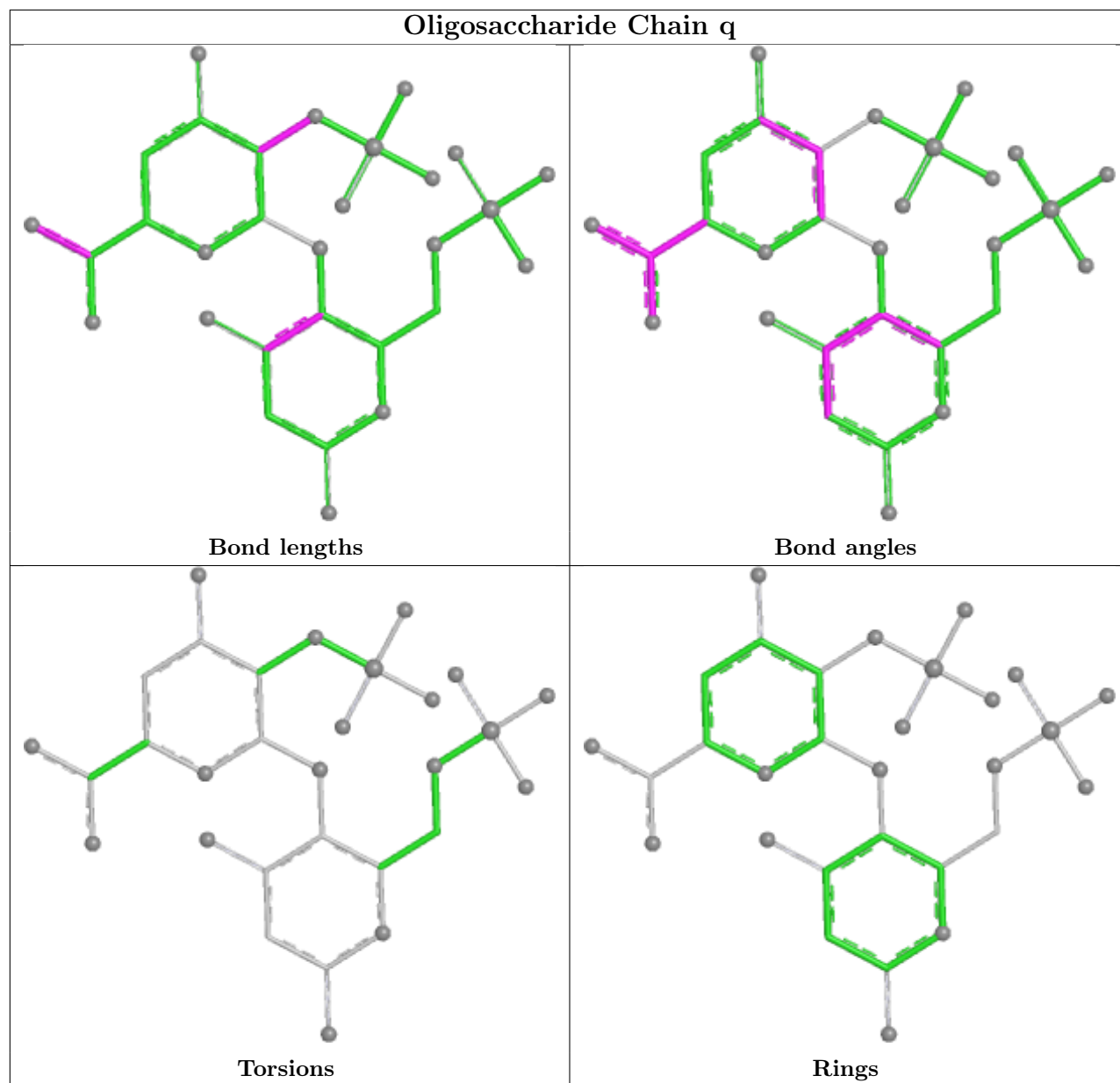


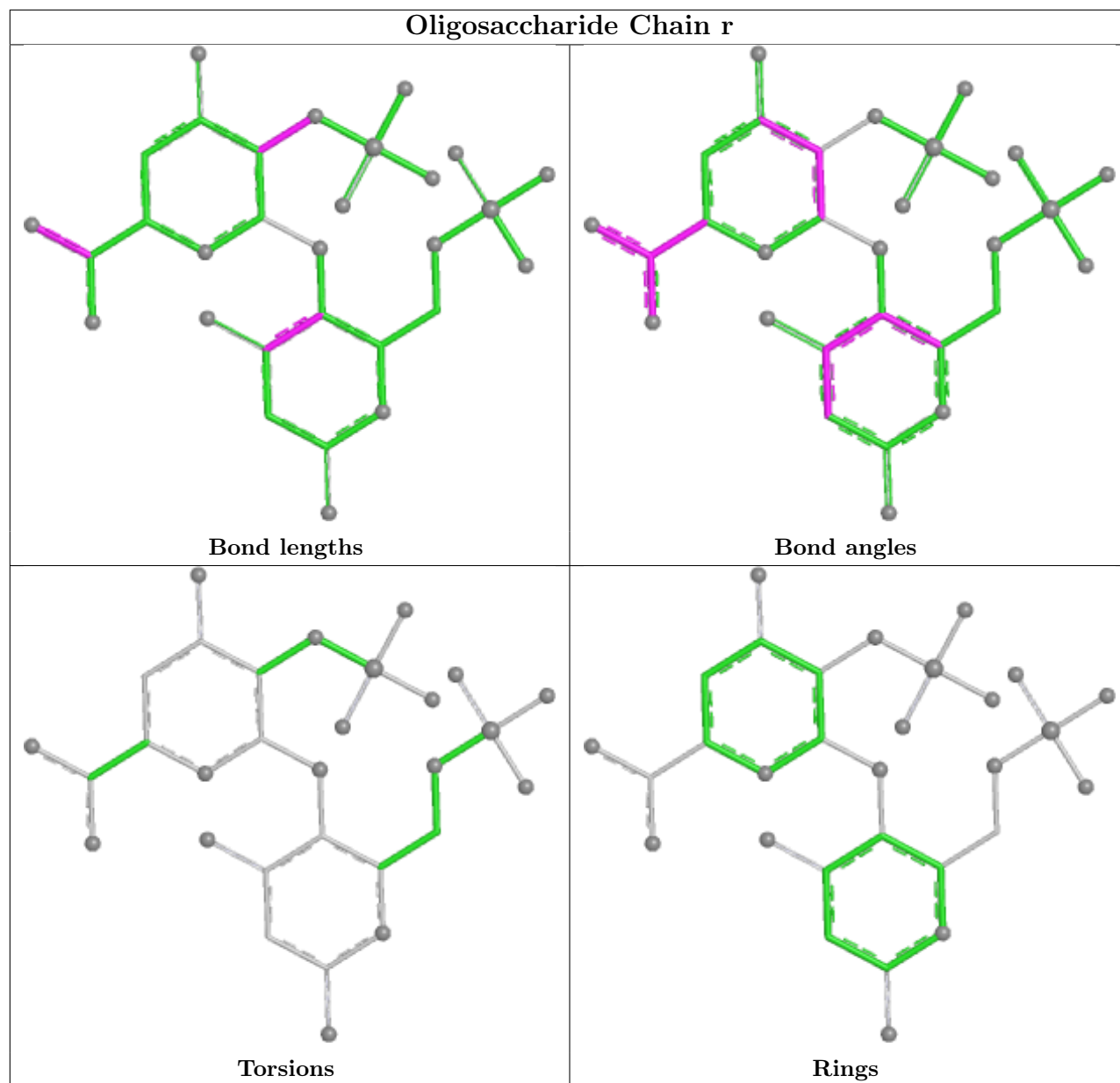


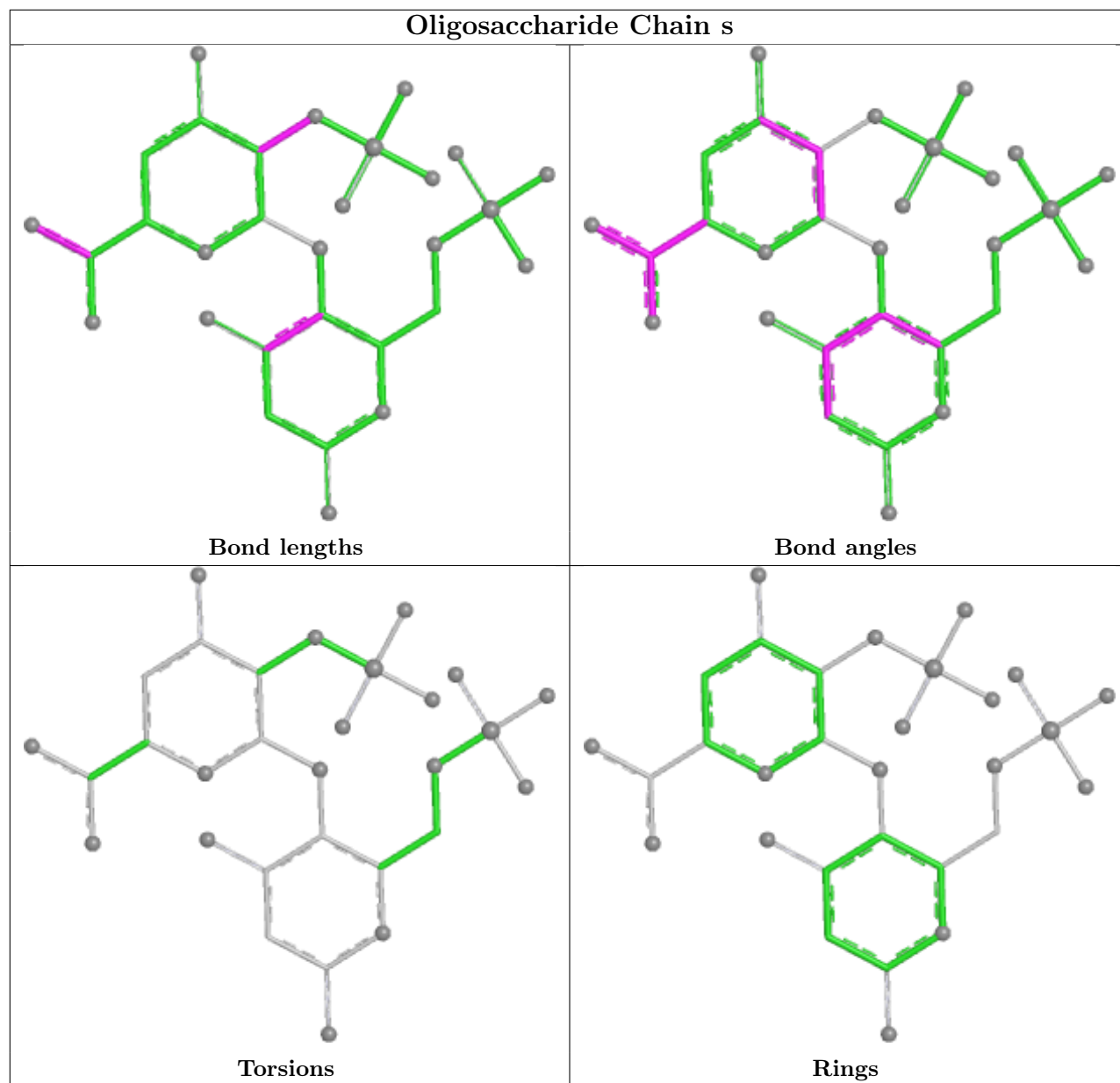




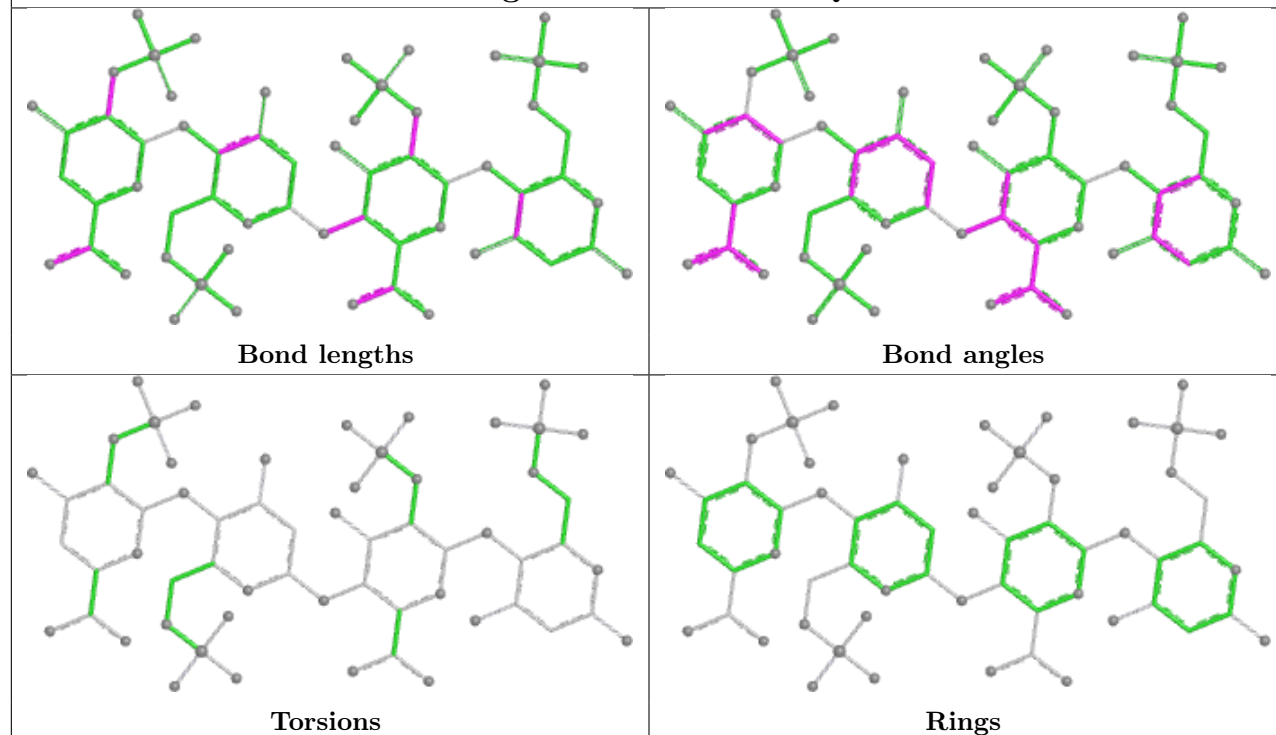




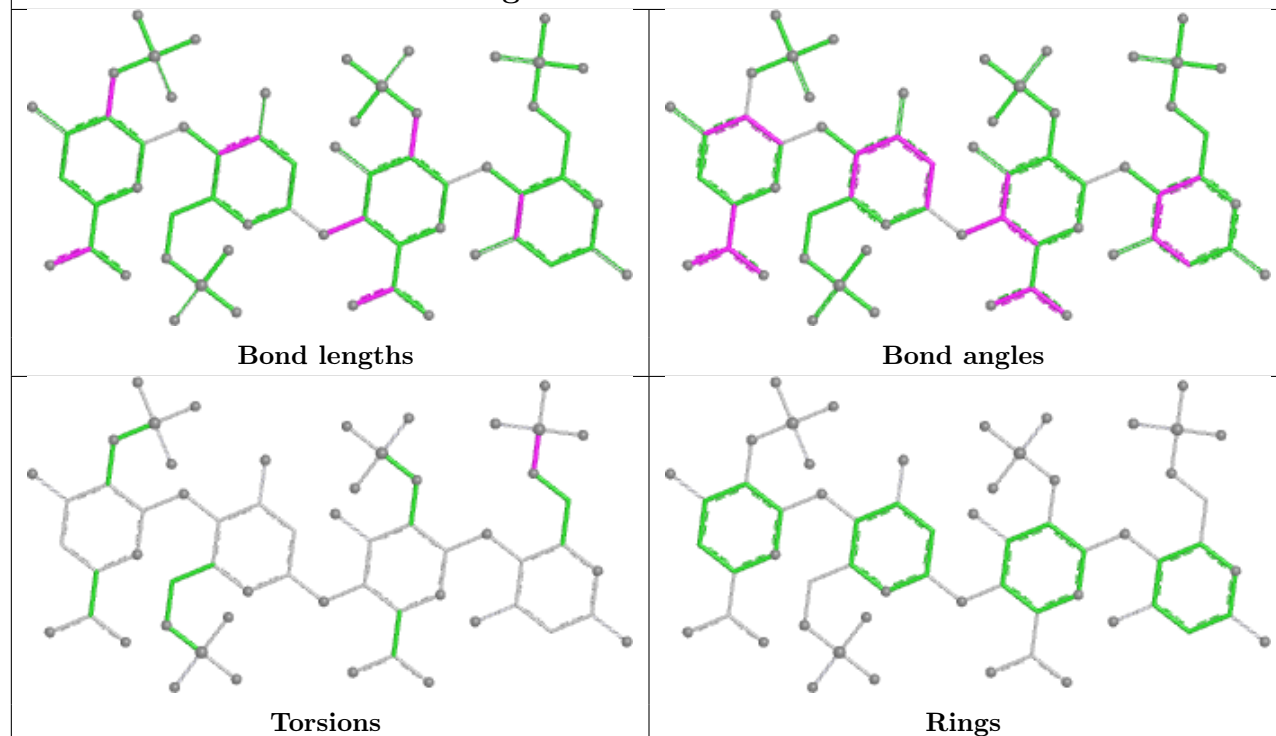


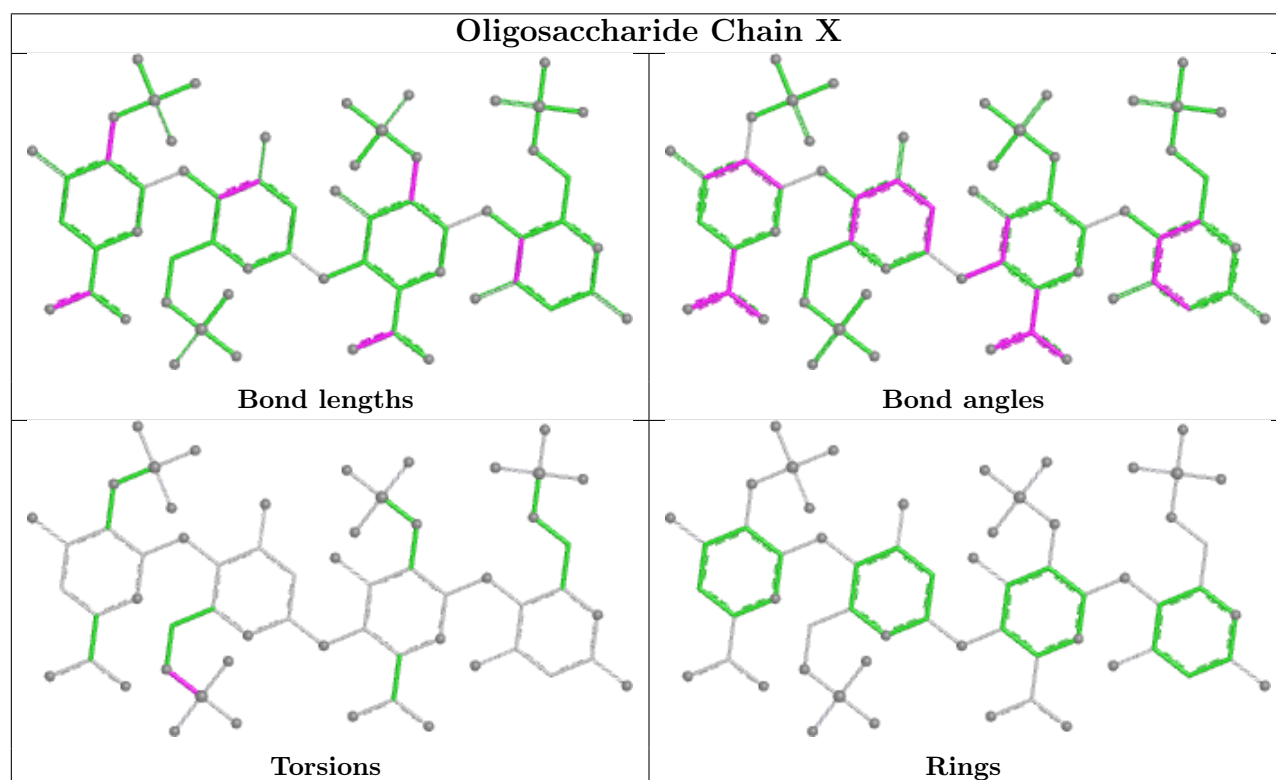
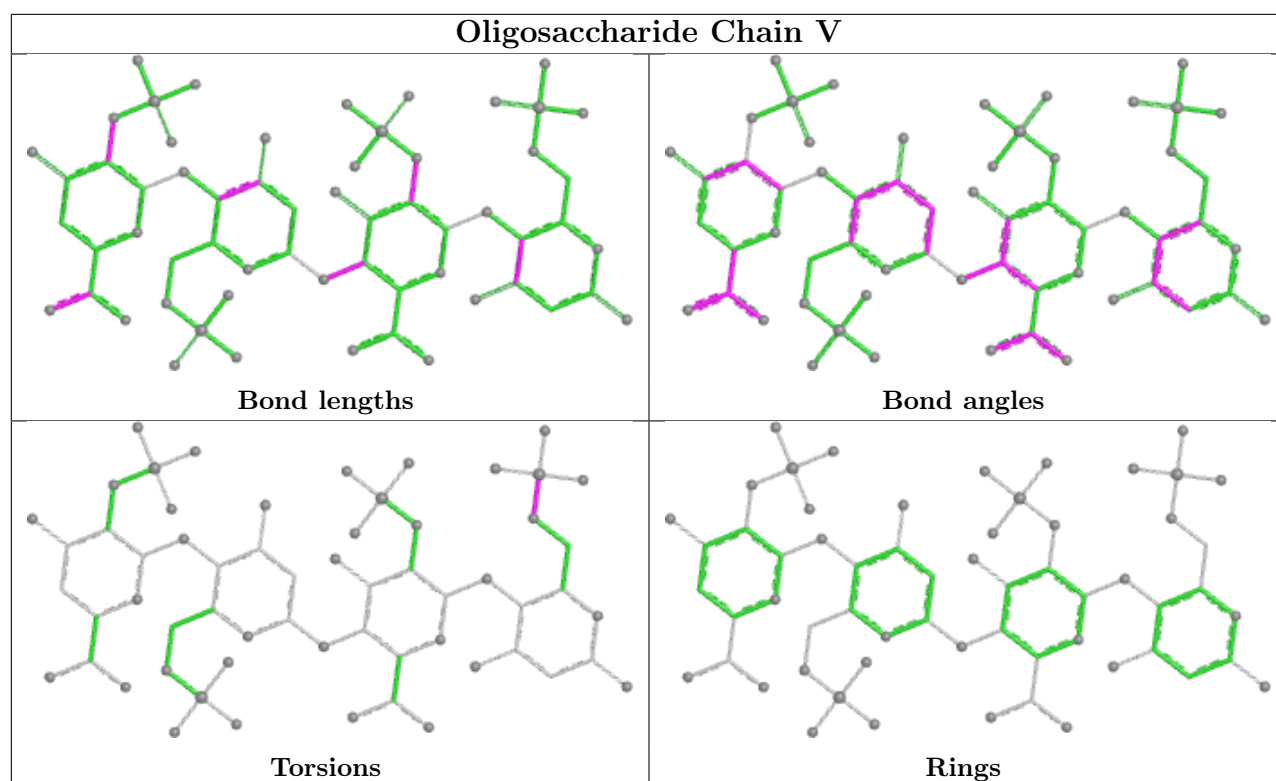


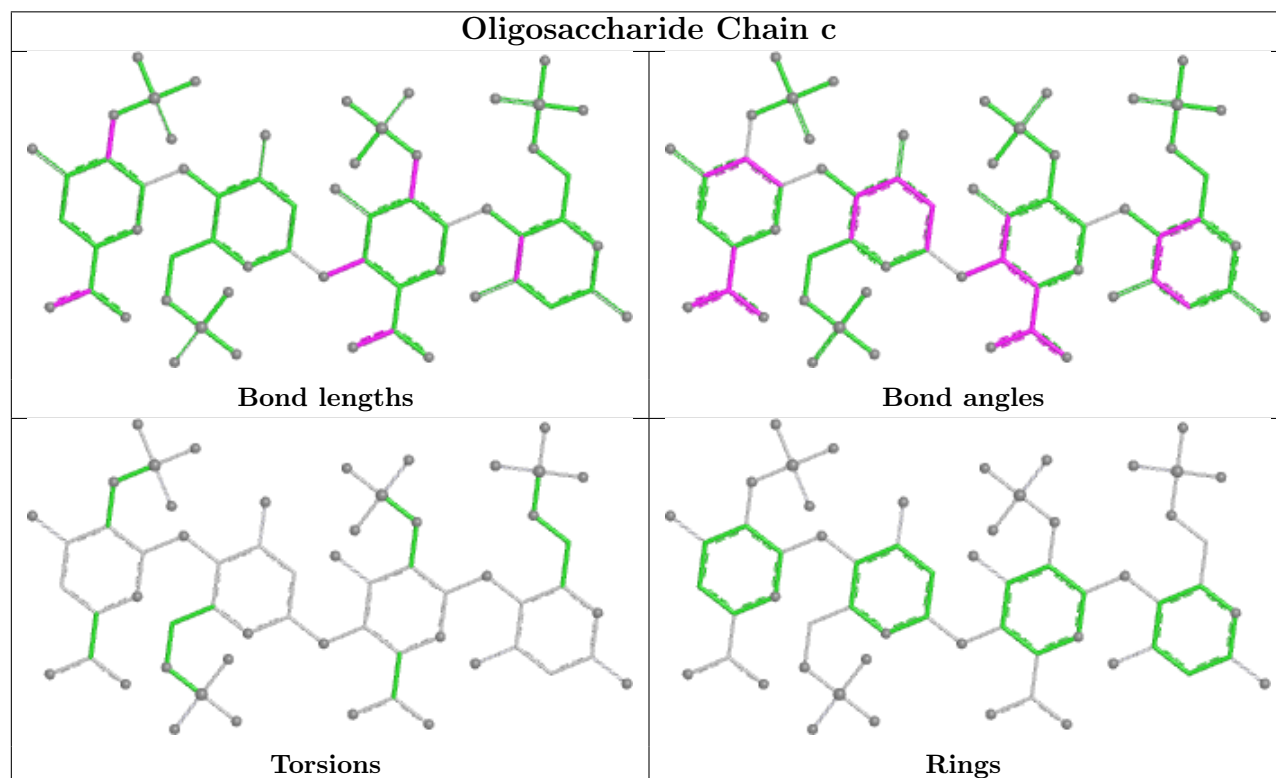
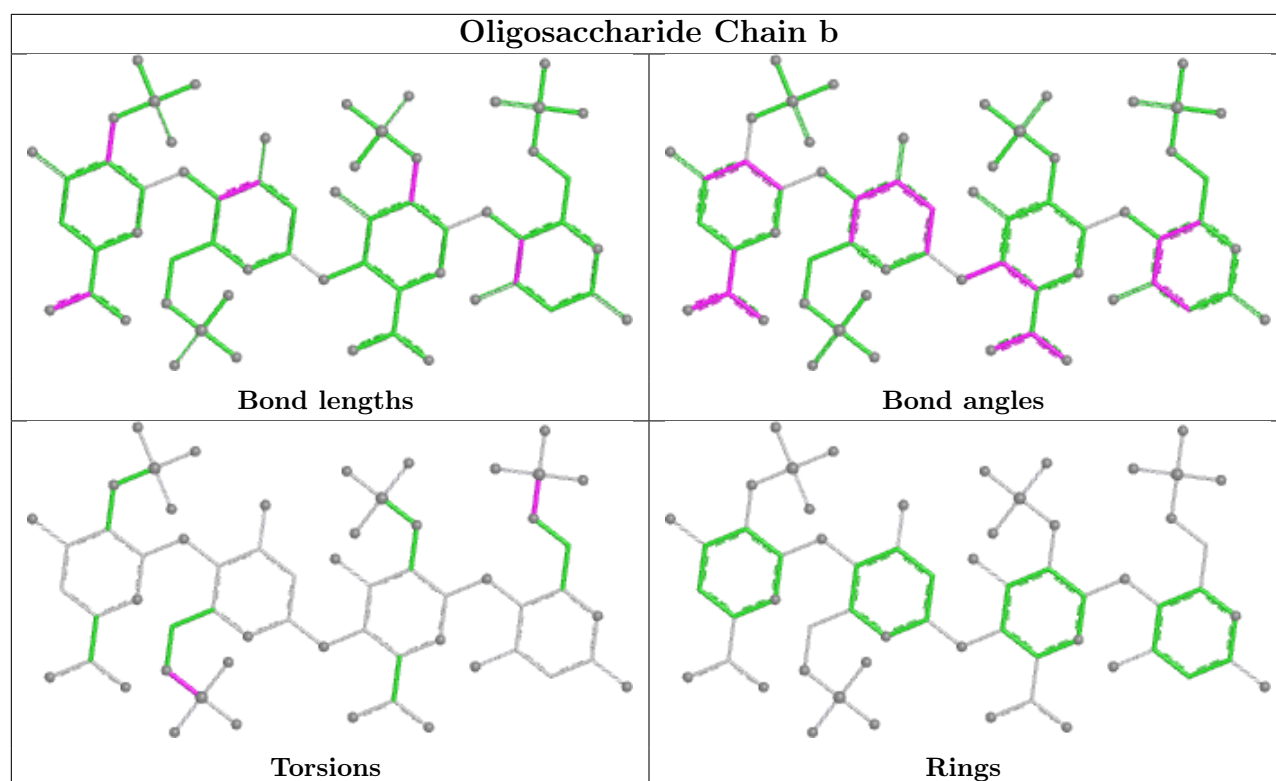
Oligosaccharide Chain Q

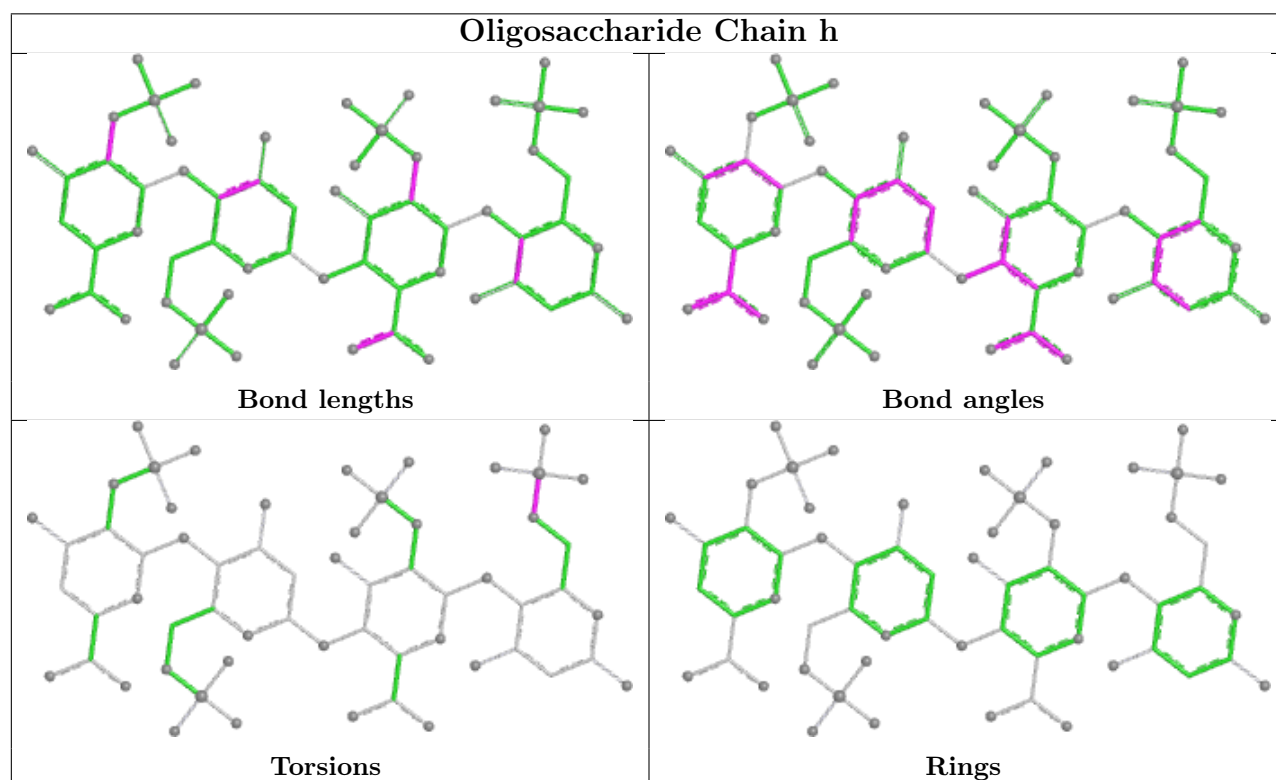
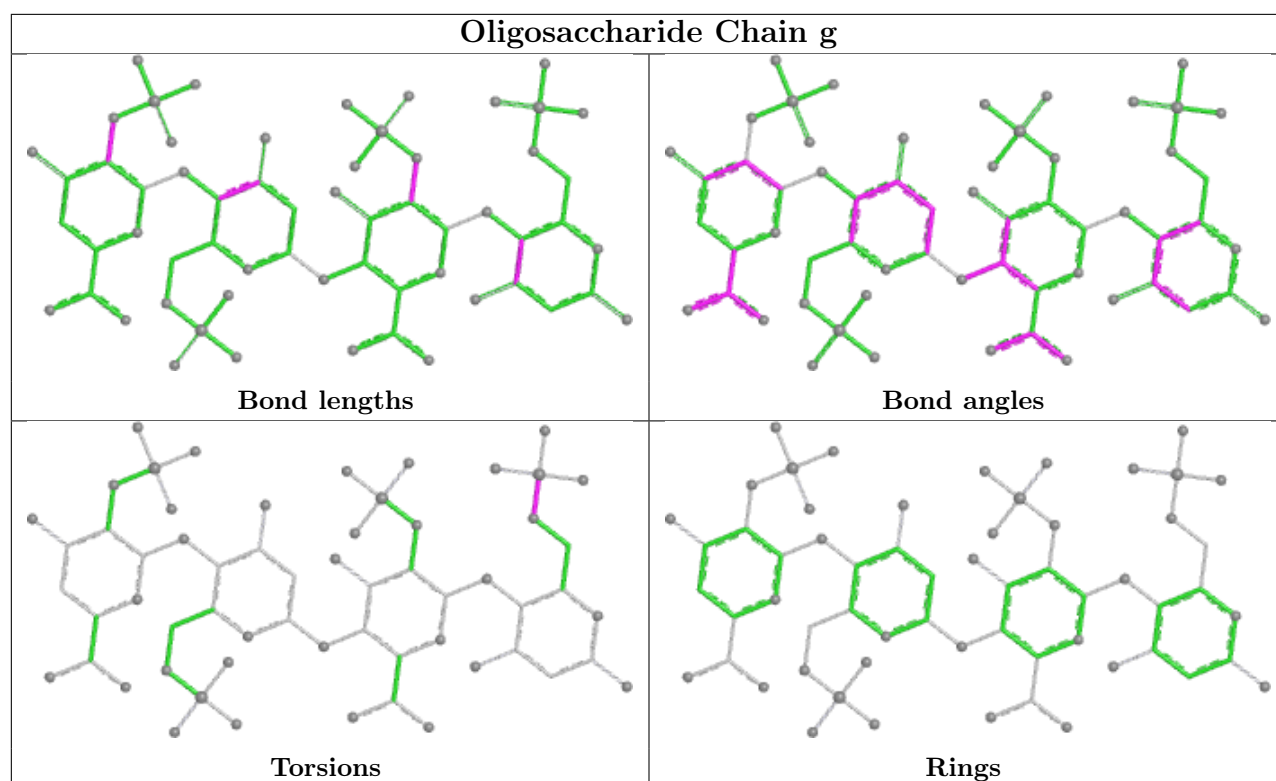


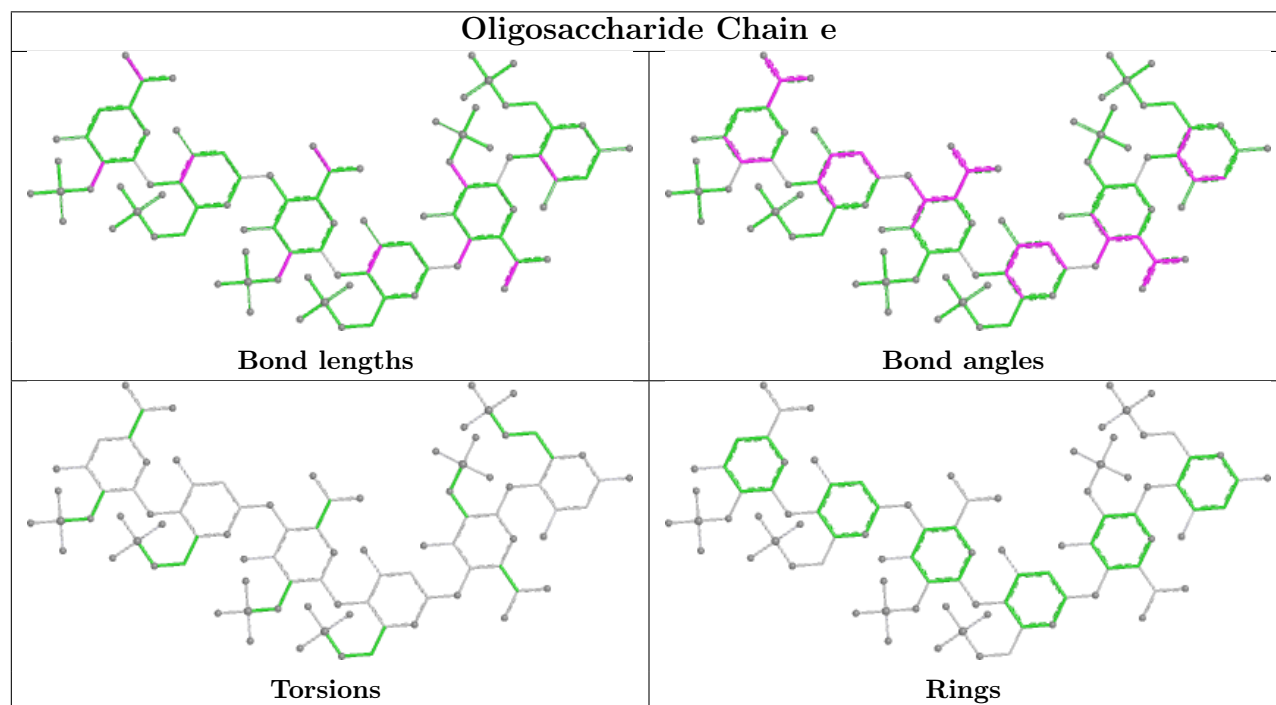
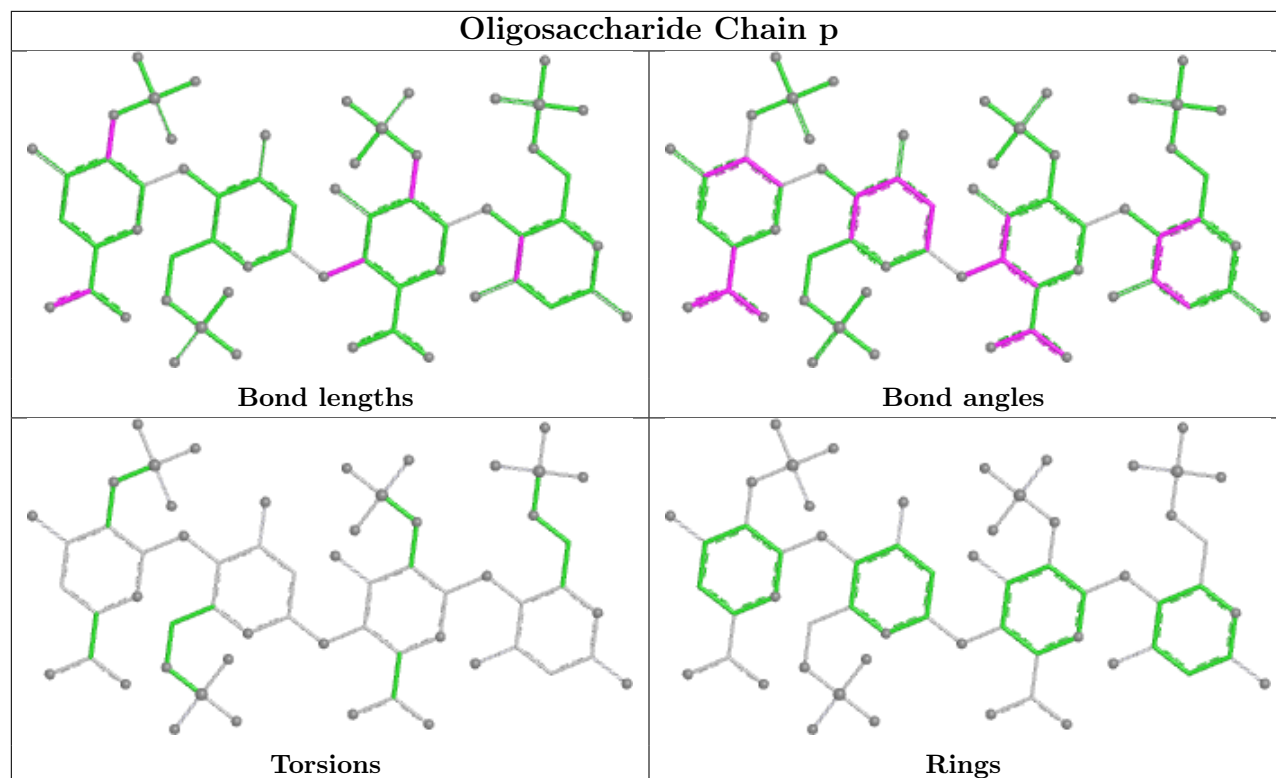
Oligosaccharide Chain R

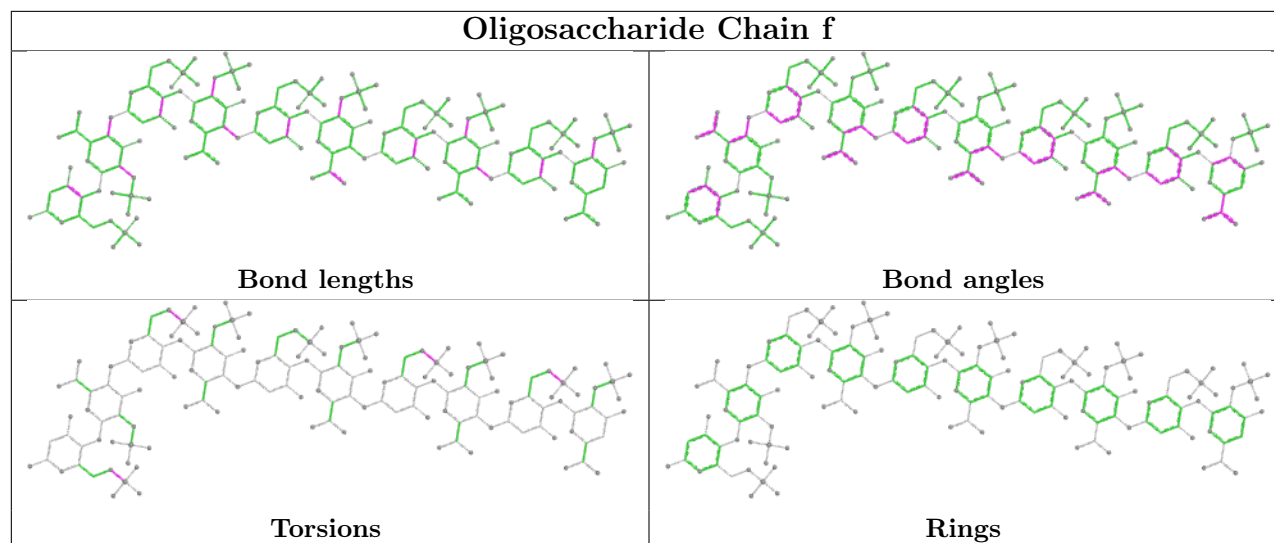












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/427 (98%)	-0.22	1 (0%) 91 87	37, 75, 133, 159	0
1	B	422/427 (98%)	-0.21	2 (0%) 87 77	34, 72, 130, 174	0
1	C	422/427 (98%)	-0.24	1 (0%) 91 87	26, 63, 122, 162	0
1	D	422/427 (98%)	-0.28	3 (0%) 84 72	30, 64, 129, 174	0
1	E	422/427 (98%)	-0.23	3 (0%) 84 72	30, 66, 125, 160	0
1	F	422/427 (98%)	-0.19	5 (1%) 76 62	34, 75, 131, 166	0
1	G	422/427 (98%)	-0.17	4 (0%) 81 68	36, 77, 134, 203	0
1	H	422/427 (98%)	-0.25	0 100 100	31, 64, 118, 150	0
1	I	422/427 (98%)	-0.23	4 (0%) 81 68	30, 64, 122, 143	0
1	J	422/427 (98%)	-0.21	0 100 100	33, 70, 137, 164	0
1	K	422/427 (98%)	-0.22	2 (0%) 87 77	38, 74, 129, 168	0
1	L	422/427 (98%)	-0.24	0 100 100	43, 72, 128, 157	0
1	M	422/427 (98%)	-0.20	3 (0%) 84 72	44, 76, 128, 147	0
1	N	422/427 (98%)	-0.16	0 100 100	43, 79, 128, 151	0
1	O	422/427 (98%)	-0.12	6 (1%) 73 59	40, 77, 136, 169	0
All	All	6330/6405 (98%)	-0.21	34 (0%) 87 77	26, 71, 129, 203	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	141	GLU	4.4
1	B	384	LEU	3.6
1	O	404	ASN	3.6
1	G	145	ASP	3.3
1	K	88	THR	3.2
1	D	135	ALA	3.2
1	I	387	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	134	ALA	3.0
1	O	350	SER	2.9
1	I	454	GLU	2.9
1	E	141	GLU	2.8
1	I	372	ASP	2.8
1	B	137	SER	2.7
1	D	368	VAL	2.7
1	F	133	HIS	2.7
1	M	199	ASP	2.6
1	O	135	ALA	2.6
1	M	86	PRO	2.6
1	E	44	THR	2.6
1	O	150	ASP	2.6
1	G	384	LEU	2.5
1	M	343	THR	2.5
1	F	289	CYS	2.5
1	O	139	VAL	2.4
1	G	382	ILE	2.3
1	C	135	ALA	2.2
1	K	139	VAL	2.2
1	F	134	ALA	2.2
1	F	174	ALA	2.2
1	A	137	SER	2.2
1	F	313	LEU	2.1
1	G	138	ASN	2.0
1	E	49	TYR	2.0
1	I	150	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JHM	X	1	15/15	0.10	0.12	206,226,248,249	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JHM	R	3	14/15	0.16	0.12	232,253,274,274	0
3	JHM	Q	1	15/15	0.26	0.12	194,215,236,236	0
3	IDS	R	4	15/17	0.28	0.13	238,240,249,252	0
3	IDS	X	4	15/17	0.28	0.13	230,232,239,243	0
2	JHM	W	1	15/15	0.29	0.14	223,243,265,266	0
2	JHM	T	1	15/15	0.29	0.14	203,225,247,247	0
2	JHM	Y	1	15/15	0.34	0.13	235,255,276,277	0
2	IDS	Y	2	15/17	0.39	0.11	226,227,235,239	0
3	JHM	R	1	15/15	0.44	0.12	224,245,267,269	0
3	IDS	V	2	16/17	0.44	0.12	234,267,274,278	0
2	JHM	S	1	15/15	0.45	0.10	258,278,299,300	0
3	JHM	X	3	14/15	0.48	0.10	200,219,242,243	0
3	IDS	R	2	16/17	0.49	0.10	255,258,263,267	0
2	JHM	a	1	15/15	-	-	193,214,235,235	0
2	IDS	a	2	15/17	-	-	211,213,221,225	0
2	JHM	d	1	15/15	-	-	201,221,243,244	0
2	IDS	d	2	15/17	-	-	223,225,232,236	0
2	JHM	i	1	15/15	-	-	228,247,270,272	0
2	IDS	i	2	15/17	-	-	261,264,269,273	0
2	JHM	j	1	15/15	-	-	212,232,254,254	0
2	IDS	j	2	15/17	-	-	247,248,256,260	0
2	JHM	k	1	15/15	-	-	218,238,261,261	0
2	IDS	k	2	15/17	-	-	226,227,235,239	0
2	JHM	l	1	15/15	-	-	224,244,266,266	0
2	IDS	l	2	15/17	-	-	260,261,269,274	0
2	JHM	m	1	15/15	-	-	207,227,248,249	0
2	IDS	m	2	15/17	-	-	249,251,259,263	0
2	JHM	n	1	15/15	-	-	185,205,226,227	0
2	IDS	n	2	15/17	-	-	245,247,254,258	0
2	JHM	o	1	15/15	-	-	220,240,261,262	0
2	IDS	o	2	15/17	-	-	214,215,224,228	0
2	JHM	q	1	15/15	-	-	235,255,277,278	0
2	IDS	q	2	15/17	-	-	261,263,271,275	0
2	JHM	r	1	15/15	-	-	198,219,240,240	0
2	IDS	r	2	15/17	-	-	270,272,280,283	0
2	JHM	s	1	15/15	-	-	210,231,252,253	0
2	IDS	s	2	15/17	-	-	227,229,237,241	0
3	JHM	V	1	15/15	0.51	0.14	233,254,275,276	0
2	IDS	U	2	15/17	0.52	0.12	260,261,269,273	0
2	IDS	T	2	15/17	0.52	0.12	255,256,264,268	0
3	IDS	Q	2	16/17	0.57	0.10	219,222,234,236	0
2	IDS	W	2	15/17	0.57	0.10	219,221,228,231	0

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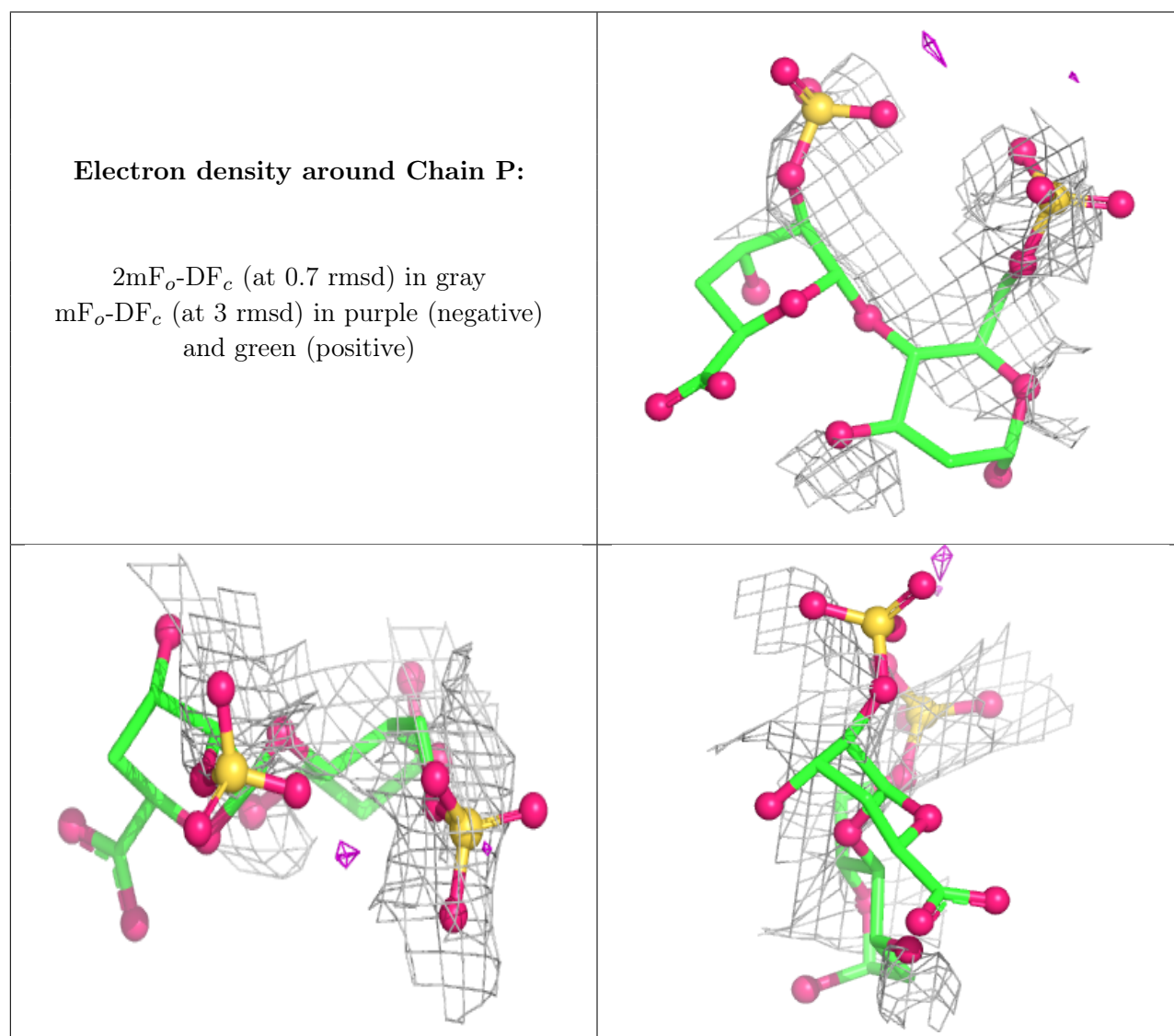
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JHM	Q	3	14/15	0.60	0.09	213,233,255,255	0
3	IDS	X	2	16/17	0.61	0.09	222,227,235,239	0
2	JHM	Z	1	15/15	0.63	0.11	206,227,248,249	0
2	IDS	S	2	15/17	0.63	0.09	281,283,290,294	0
2	JHM	U	1	15/15	0.64	0.11	235,256,278,278	0
2	IDS	Z	2	15/17	0.65	0.10	252,254,262,266	0
3	JHM	V	3	14/15	0.67	0.13	210,231,253,254	0
3	IDS	Q	4	15/17	0.71	0.08	264,265,274,278	0
2	JHM	P	1	15/15	0.76	0.13	192,212,234,235	0
3	IDS	V	4	15/17	0.76	0.17	273,275,282,286	0
2	IDS	P	2	15/17	0.79	0.12	267,270,276,279	0
3	JHM	b	1	15/15	-	-	254,274,294,296	0
3	IDS	b	2	16/17	-	-	241,271,279,282	0
3	JHM	b	3	14/15	-	-	217,237,258,259	0
3	IDS	b	4	15/17	-	-	235,237,245,248	0
3	JHM	c	1	15/15	-	-	204,224,246,247	0
3	IDS	c	2	16/17	-	-	221,223,233,237	0
3	JHM	c	3	14/15	-	-	214,234,257,257	0
3	IDS	c	4	15/17	-	-	231,233,240,244	0
3	JHM	g	1	15/15	-	-	217,238,258,259	0
3	IDS	g	2	16/17	-	-	251,264,272,276	0
3	JHM	g	3	14/15	-	-	228,248,270,270	0
3	IDS	g	4	15/17	-	-	238,240,248,252	0
3	JHM	h	1	15/15	-	-	245,266,287,288	0
3	IDS	h	2	16/17	-	-	293,295,301,305	0
3	JHM	h	3	14/15	-	-	271,292,314,314	0
3	IDS	h	4	15/17	-	-	261,263,270,274	0
3	JHM	p	1	15/15	-	-	222,243,265,265	0
3	IDS	p	2	16/17	-	-	227,266,274,278	0
3	JHM	p	3	14/15	-	-	204,224,246,246	0
3	IDS	p	4	15/17	-	-	221,222,230,234	0
4	JHM	e	1	15/15	-	-	264,284,305,307	0
4	IDS	e	2	16/17	-	-	251,281,287,291	0
4	JHM	e	3	14/15	-	-	227,248,268,270	0
4	IDS	e	4	16/17	-	-	249,286,292,296	0
4	JHM	e	5	14/15	-	-	226,246,268,269	0
4	IDS	e	6	15/17	-	-	239,241,247,251	0
5	JHM	f	1	15/15	-	-	234,255,276,277	0
5	IDS	f	2	16/17	-	-	248,255,262,265	0
5	JHM	f	3	14/15	-	-	225,245,267,268	0
5	IDS	f	4	16/17	-	-	238,318,323,327	0
5	JHM	f	5	14/15	-	-	214,234,255,256	0

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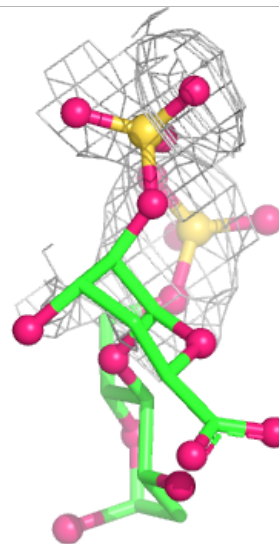
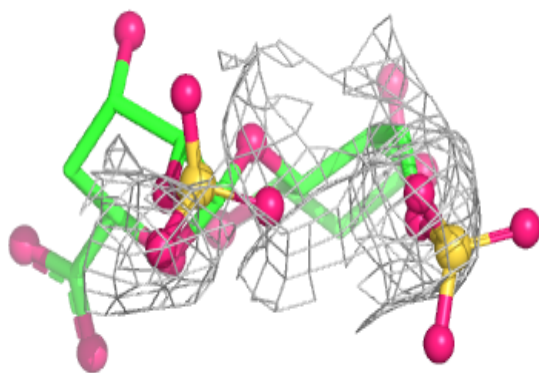
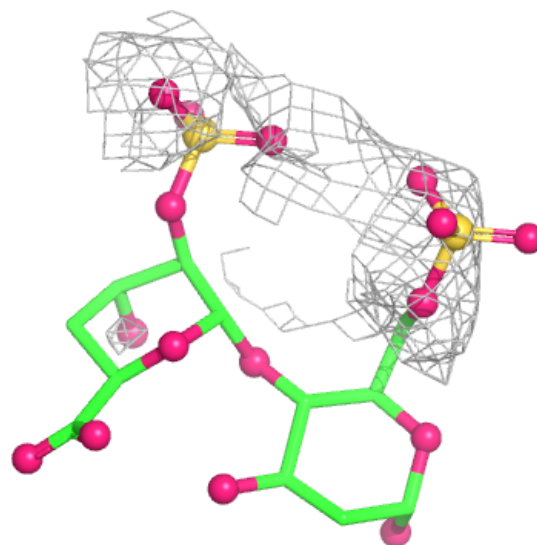
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IDS	f	6	16/17	-	-	209,212,222,240	0
5	JHM	f	7	14/15	-	-	216,237,260,261	0
5	IDS	f	8	16/17	-	-	186,189,199,262	0
5	JHM	f	9	14/15	-	-	238,259,280,282	0
5	IDS	f	10	15/17	-	-	227,229,236,239	0

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.



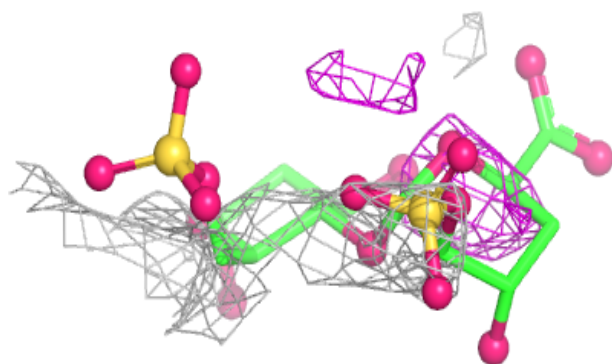
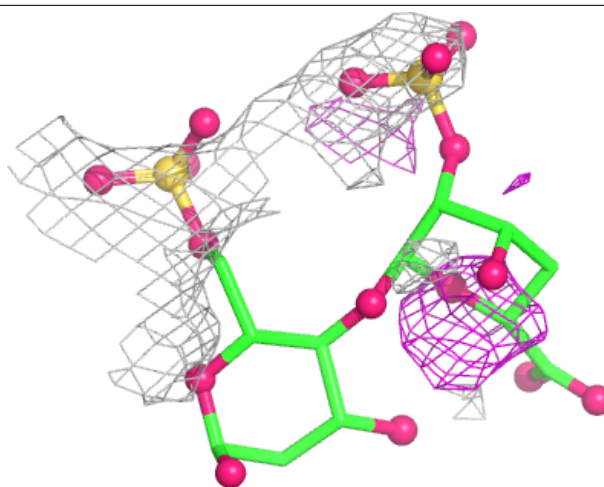
Electron density around Chain S:

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



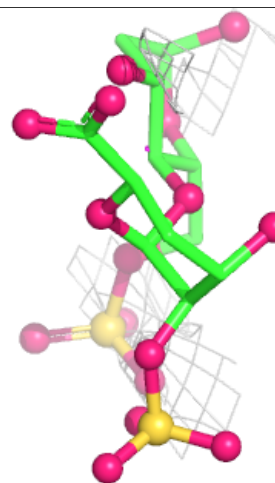
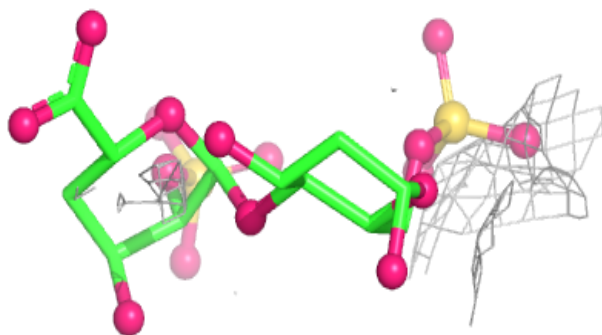
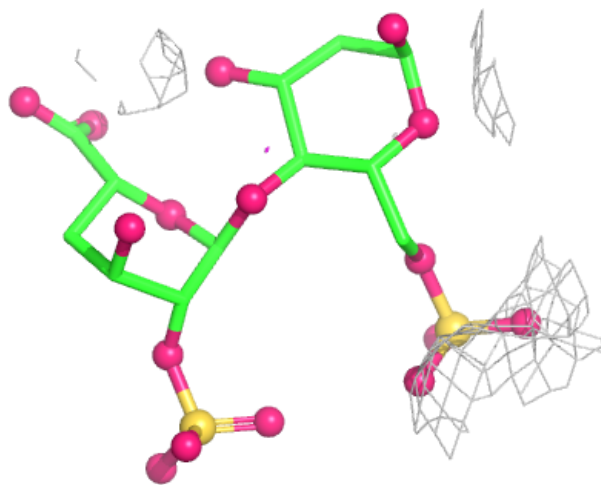
Electron density around Chain T:

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



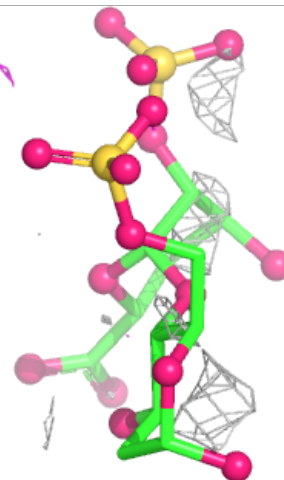
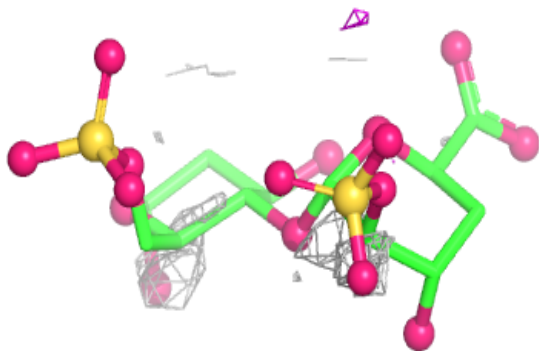
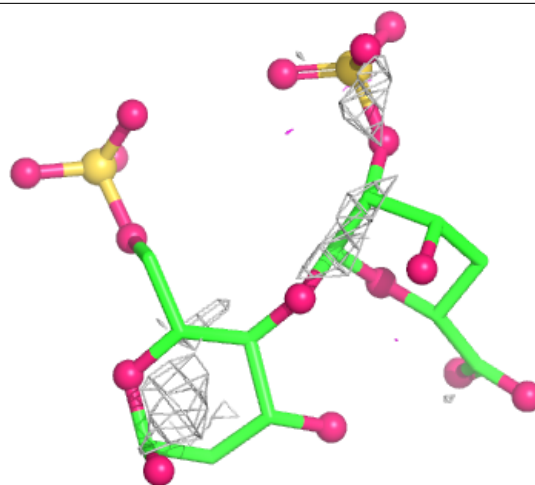
Electron density around Chain U:

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



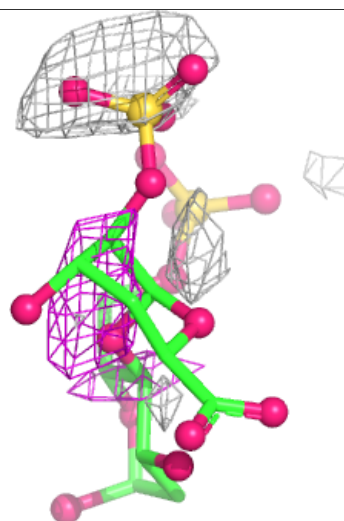
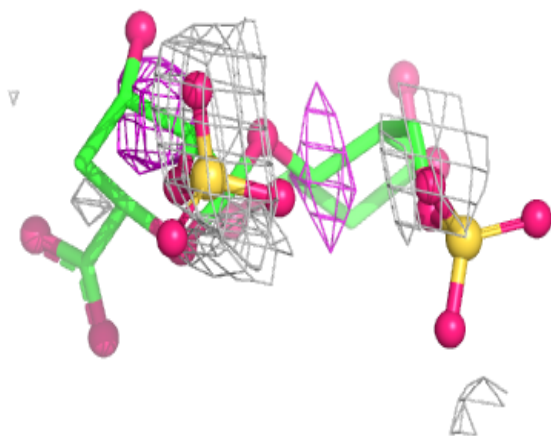
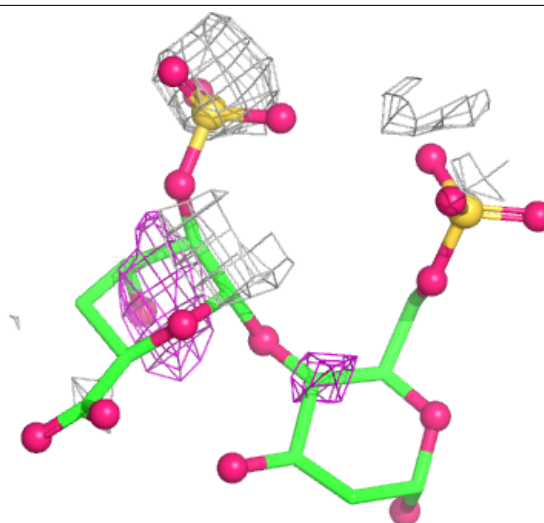
Electron density around Chain W:

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



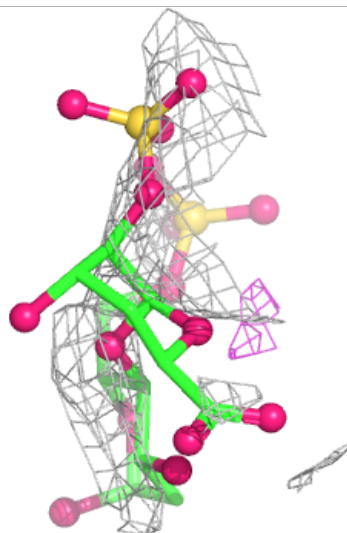
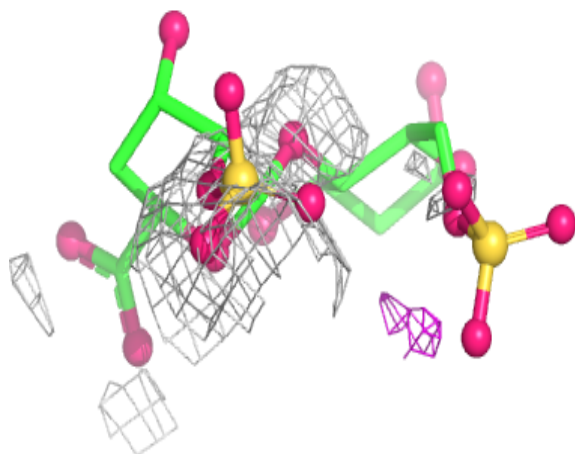
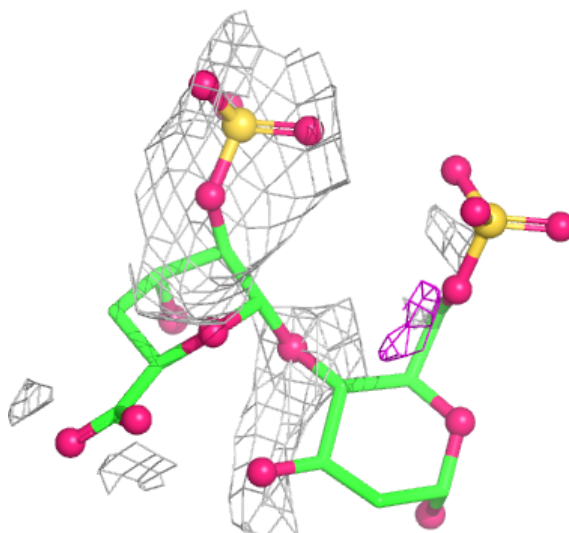
Electron density around Chain Y:

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



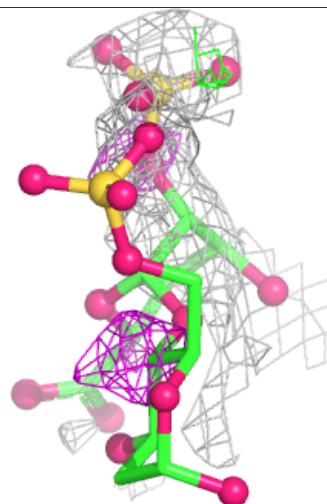
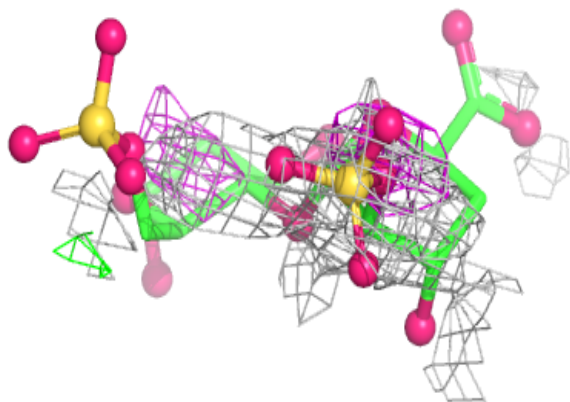
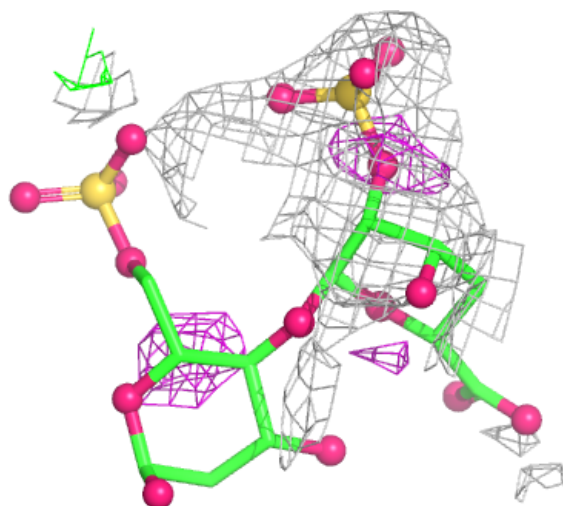
Electron density around Chain Z:

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



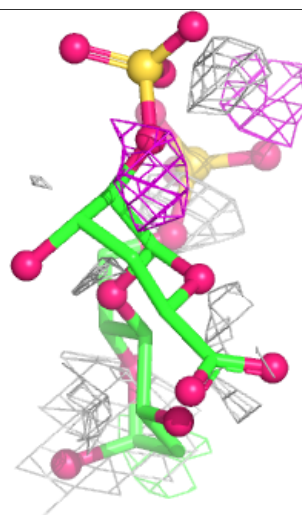
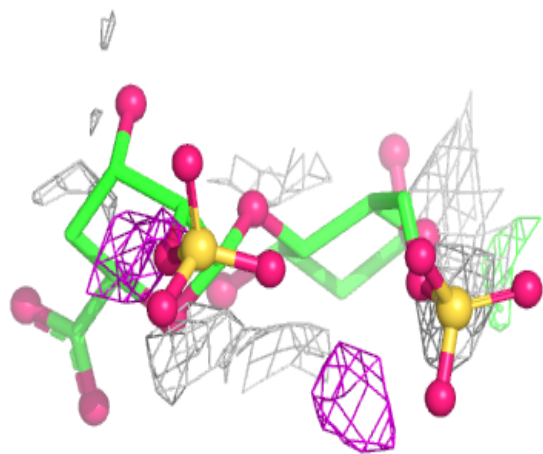
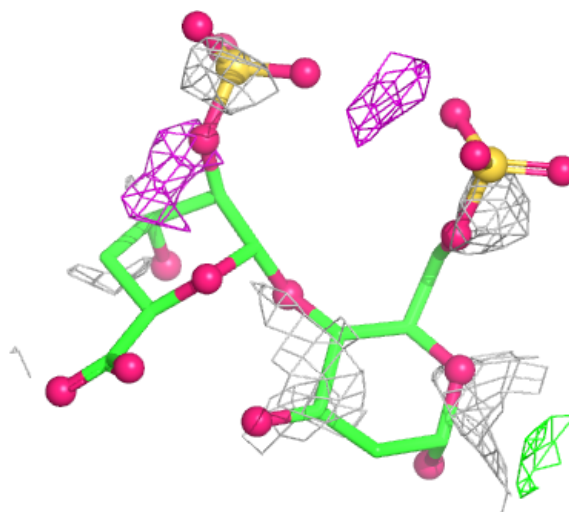
Electron density around Chain a:

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



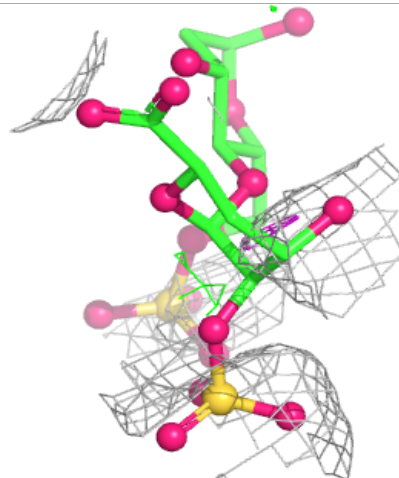
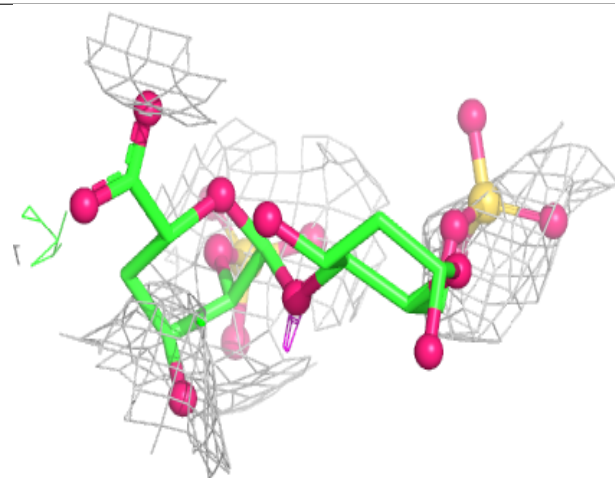
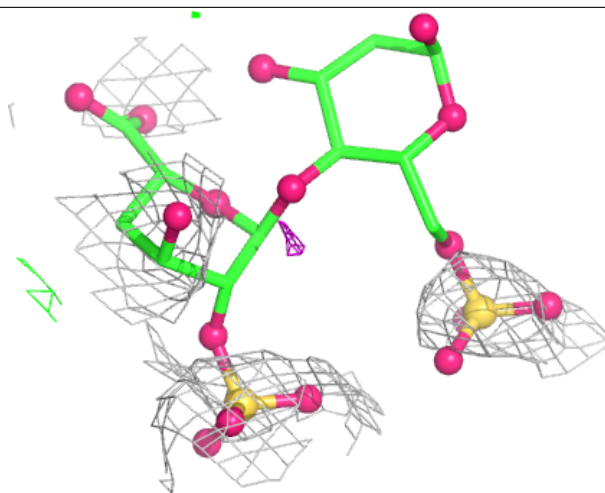
Electron density around Chain d:

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



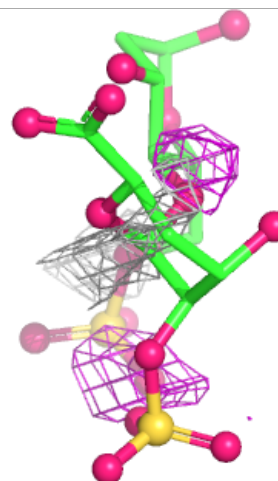
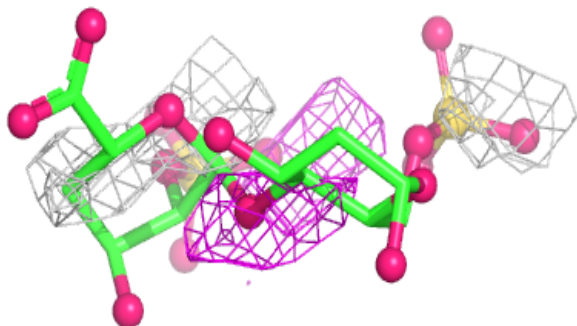
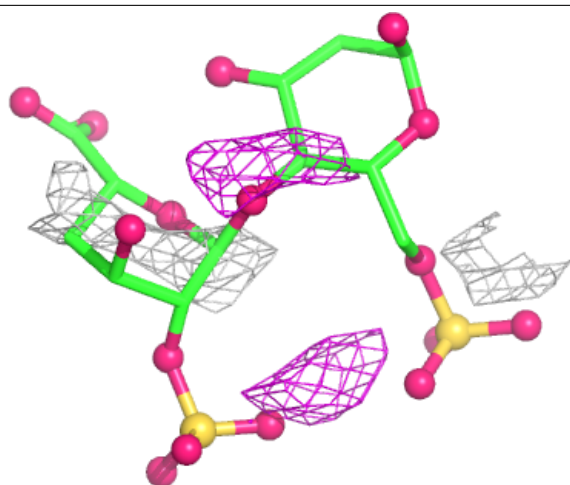
Electron density around Chain i:

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



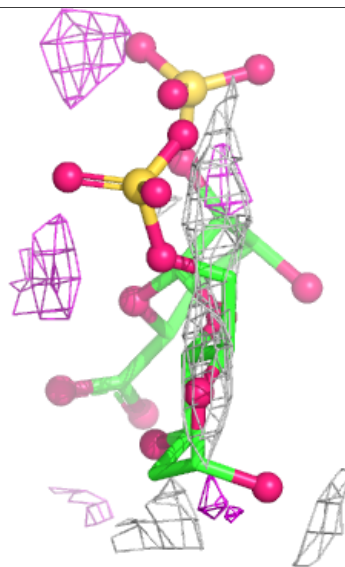
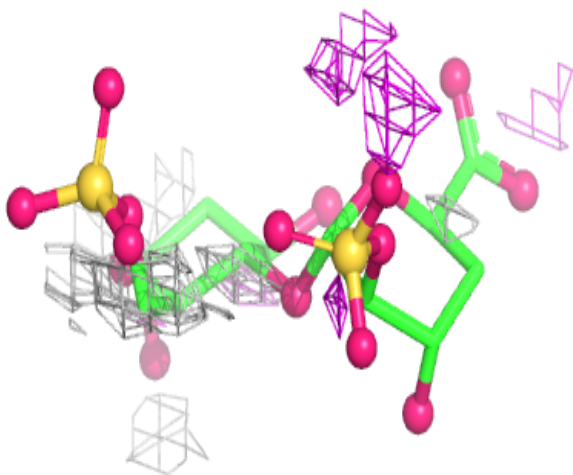
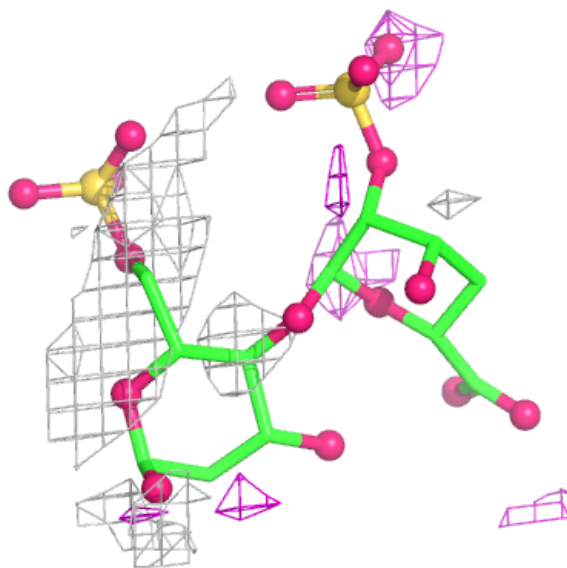
Electron density around Chain j:

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



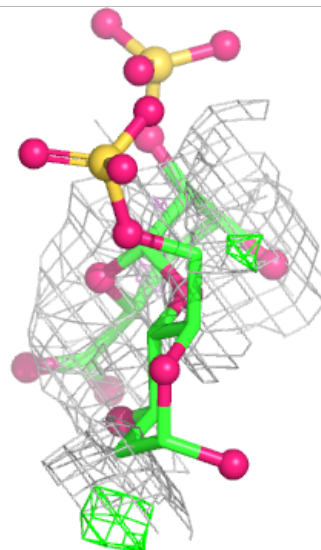
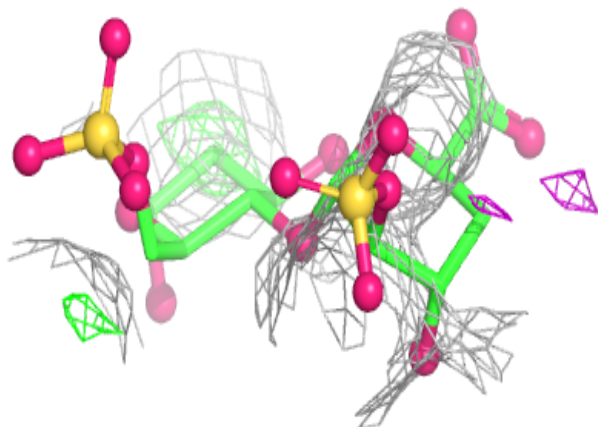
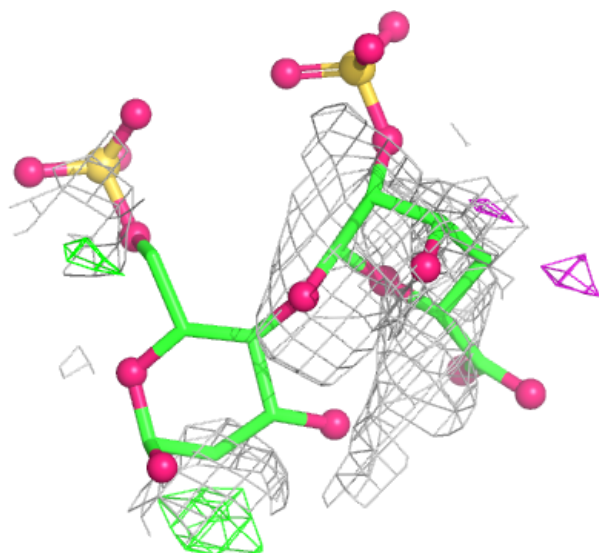
Electron density around Chain k:

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



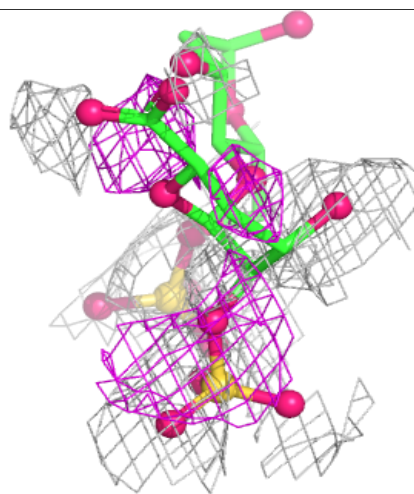
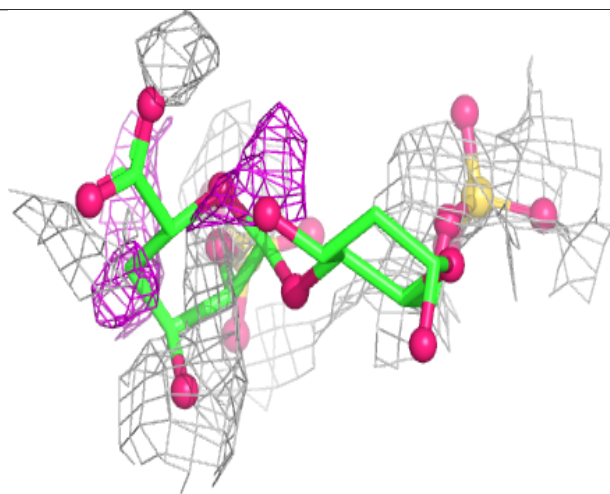
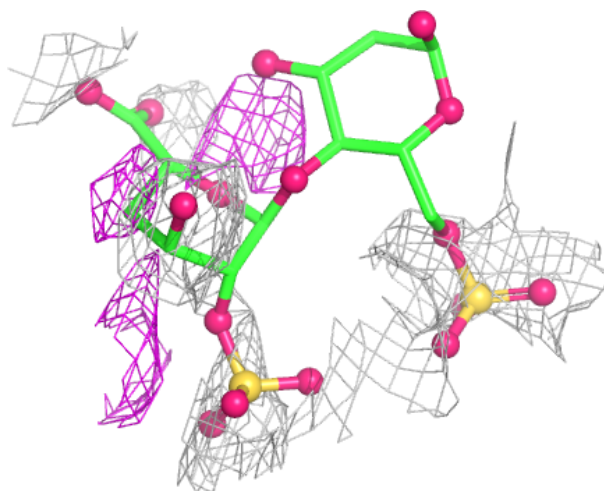
Electron density around Chain 1:

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



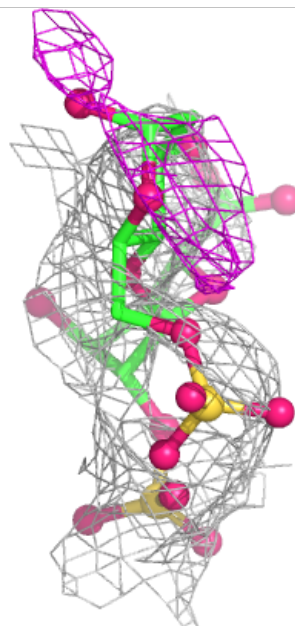
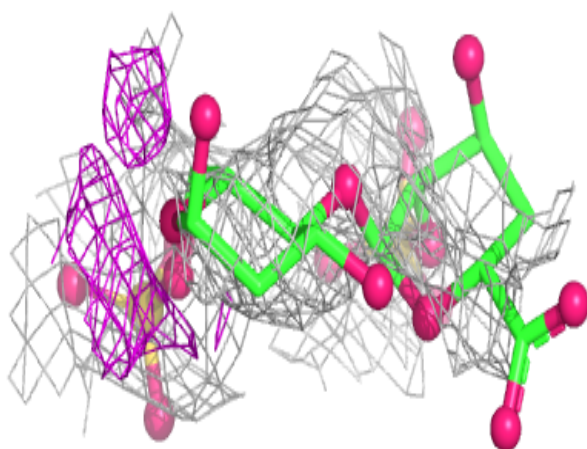
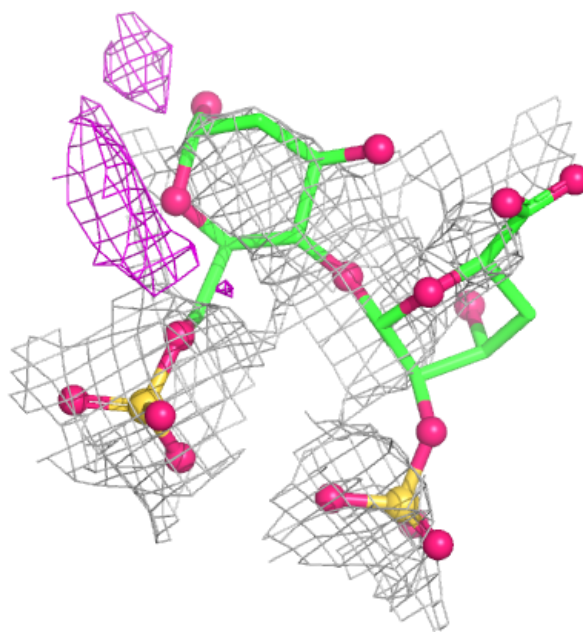
Electron density around Chain m:

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



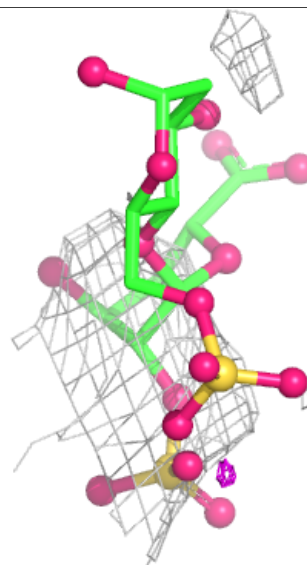
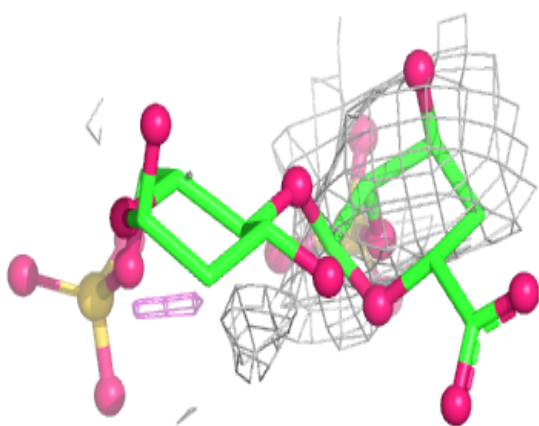
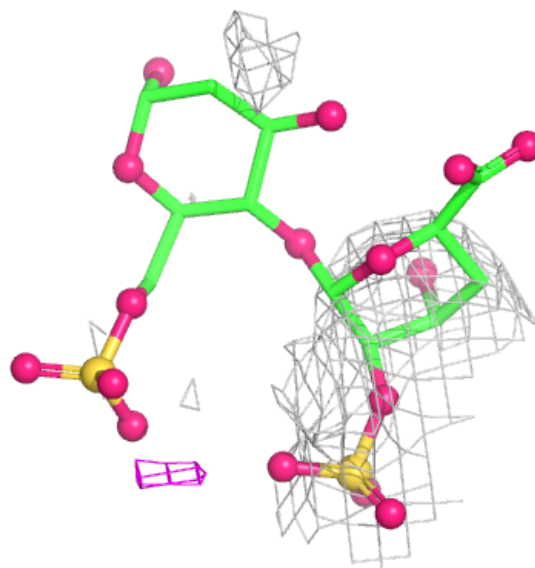
Electron density around Chain n:

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



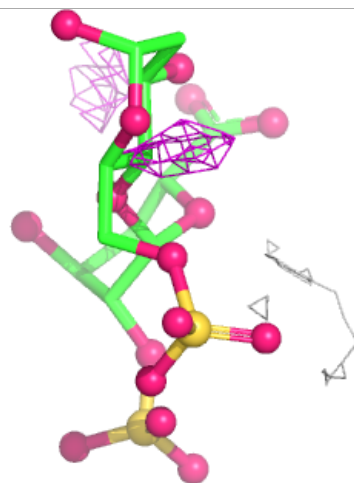
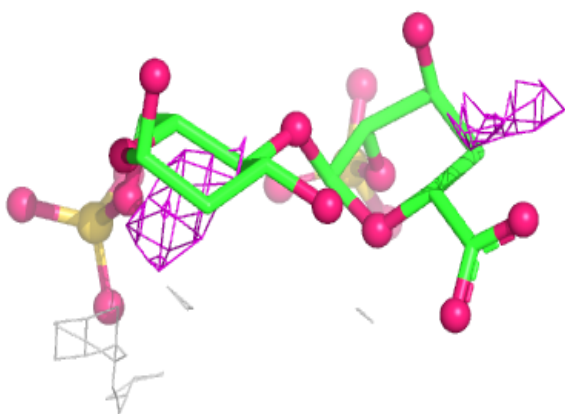
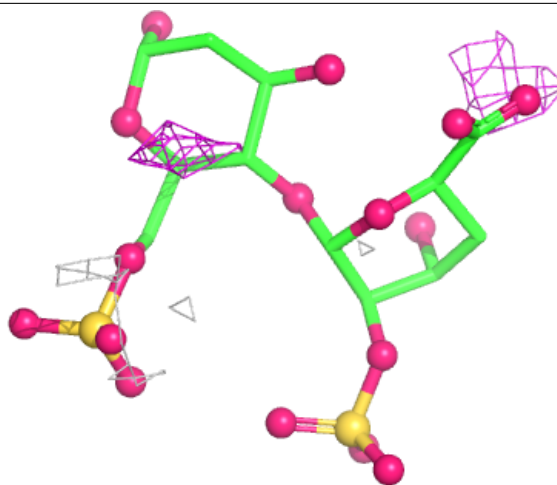
Electron density around Chain o:

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



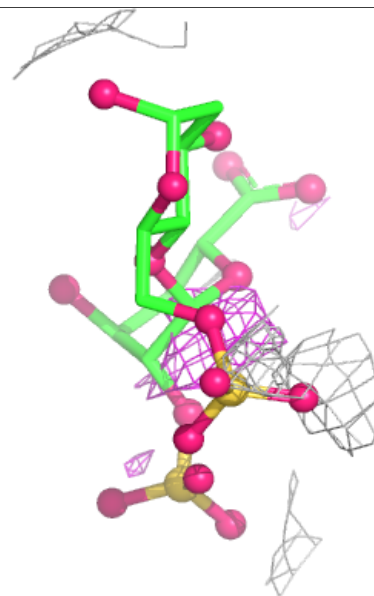
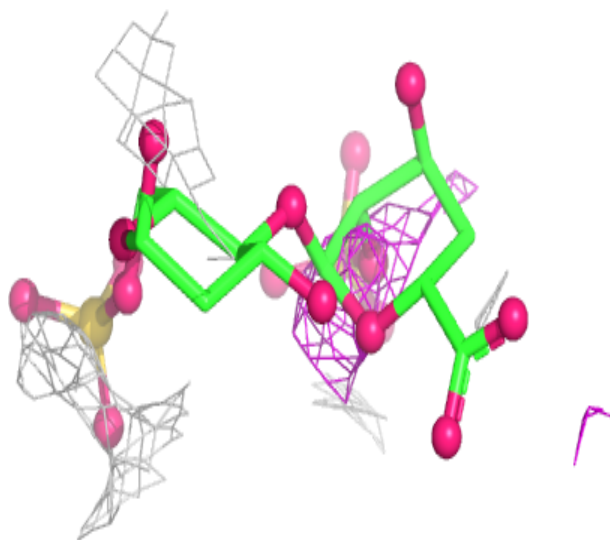
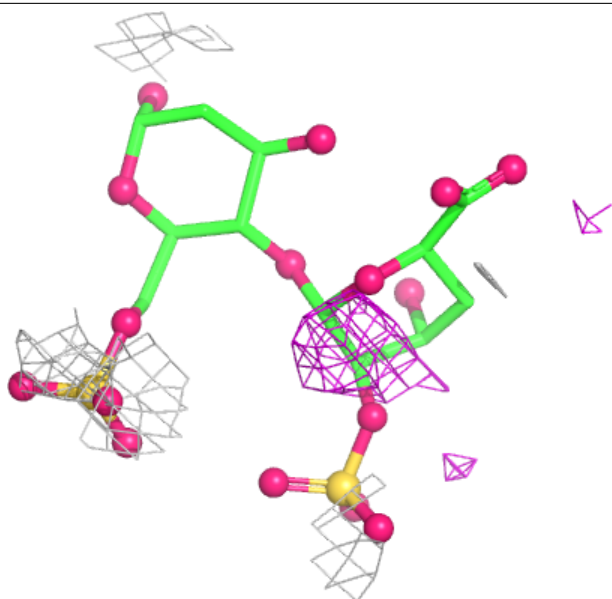
Electron density around Chain q:

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



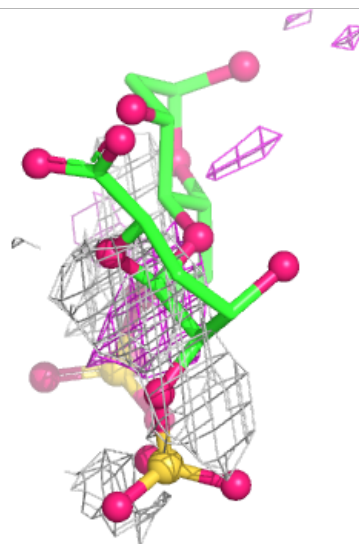
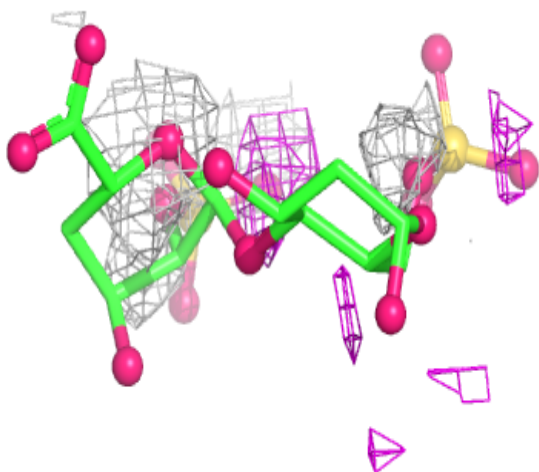
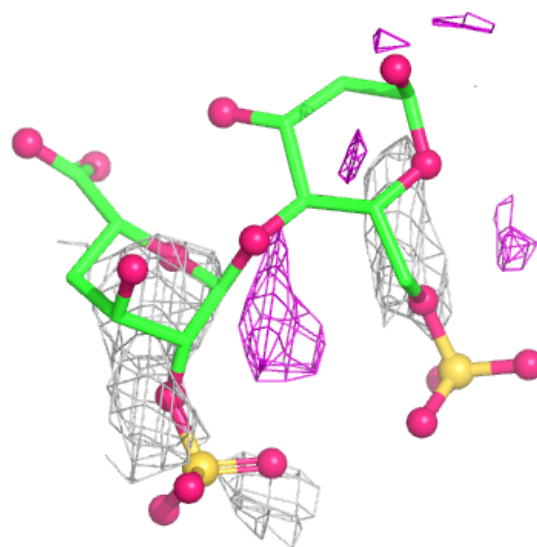
Electron density around Chain r:

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



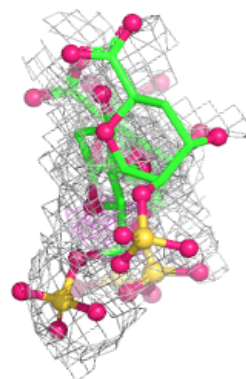
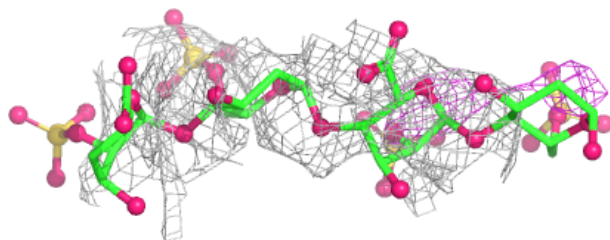
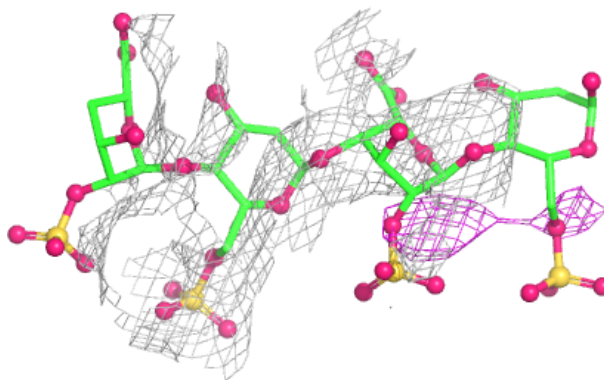
Electron density around Chain s:

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

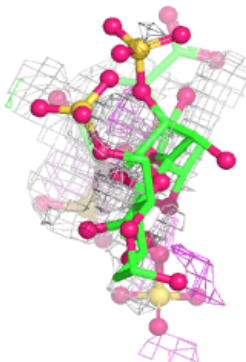
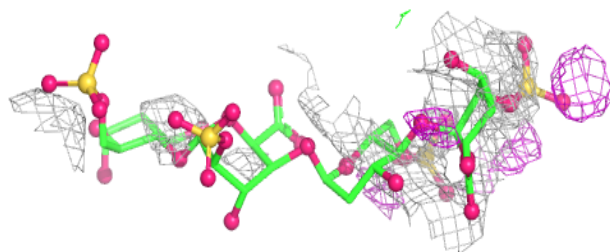
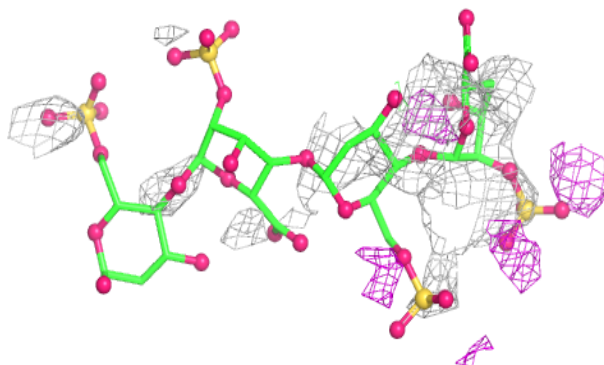


Electron density around Chain Q:

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

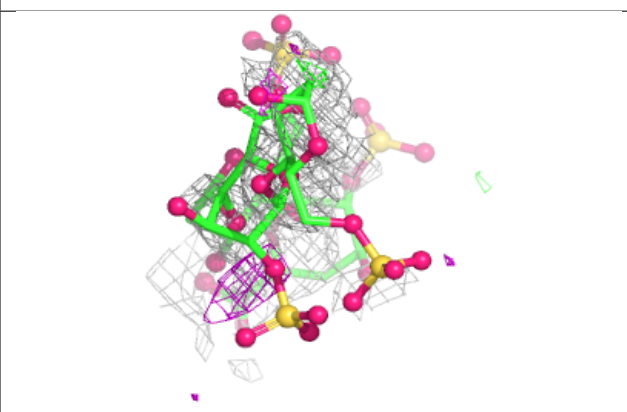
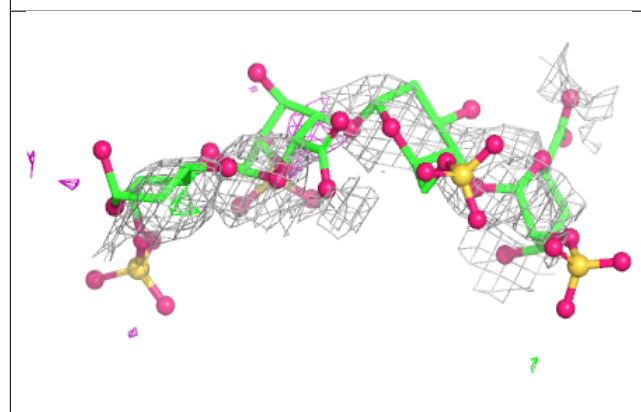
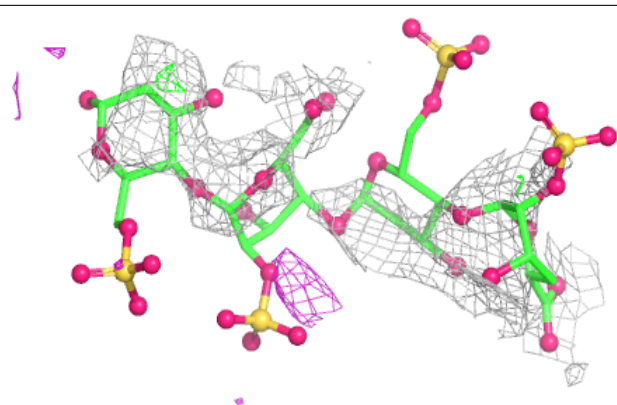
**Electron density around Chain R:**

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

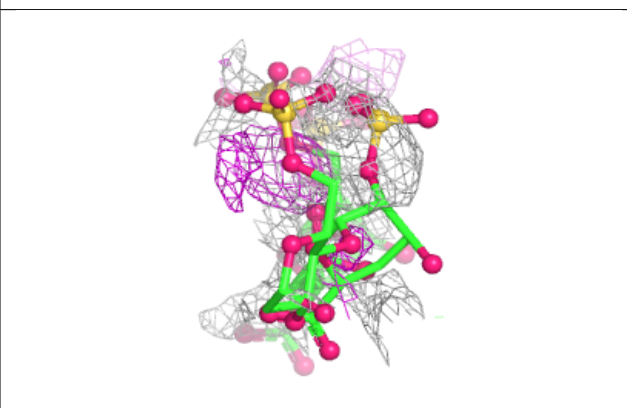
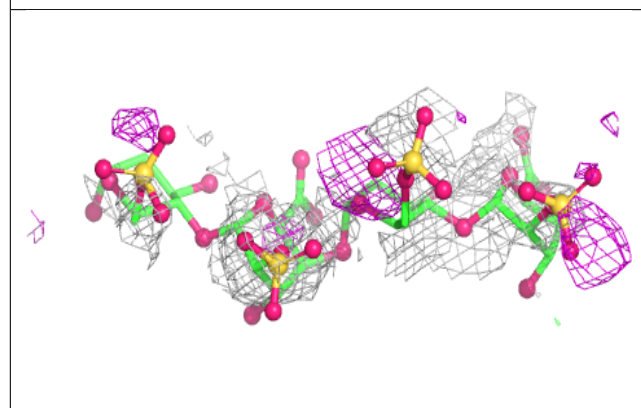
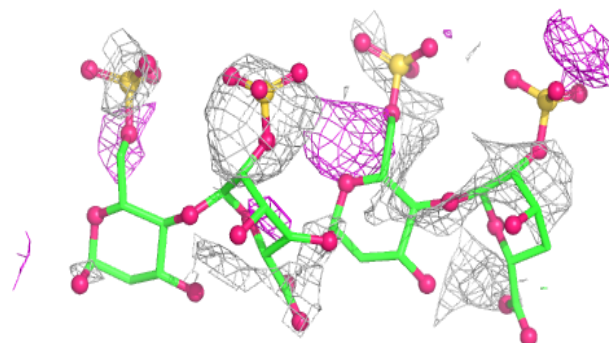


Electron density around Chain V:

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

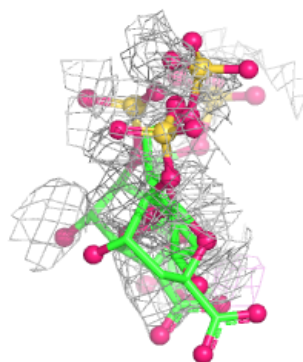
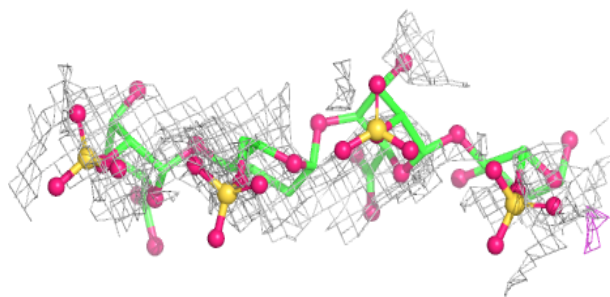
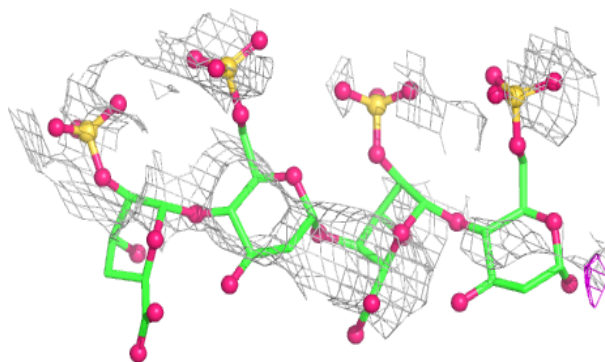
**Electron density around Chain X:**

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

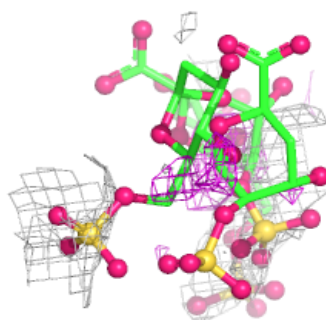
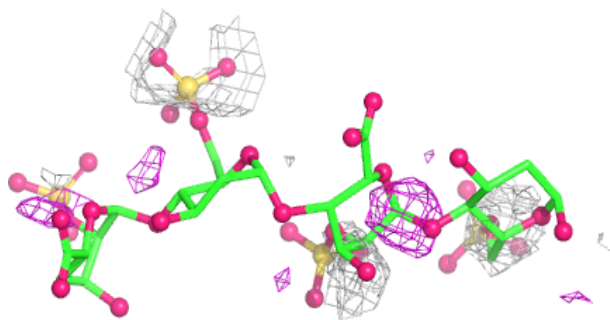
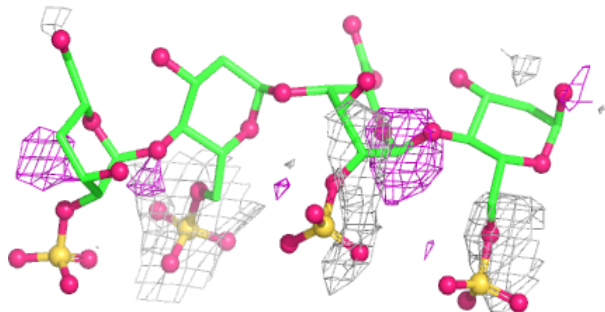


Electron density around Chain b:

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

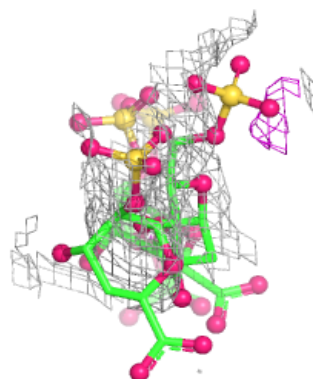
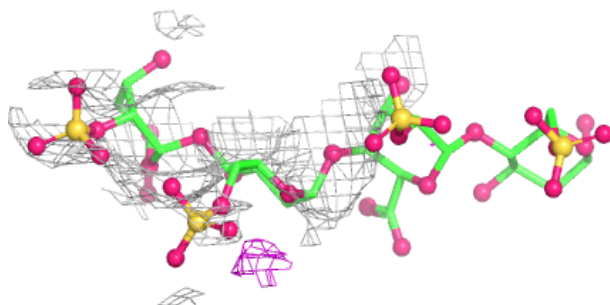
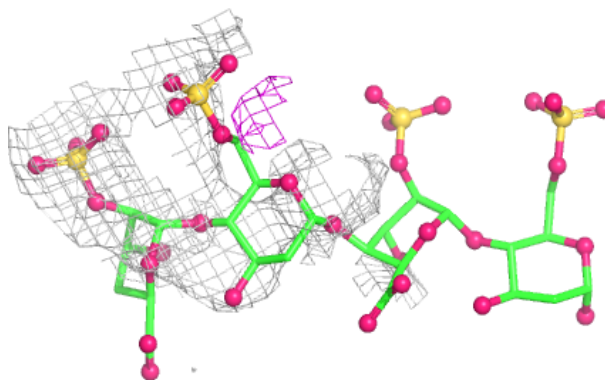
**Electron density around Chain c:**

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

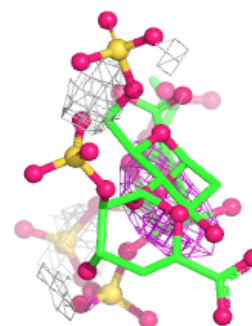
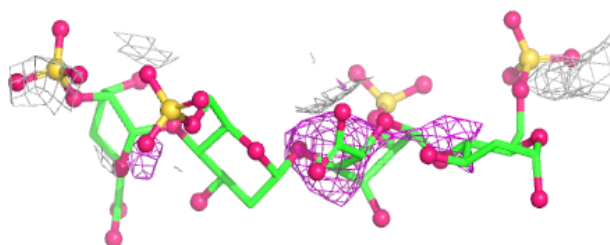
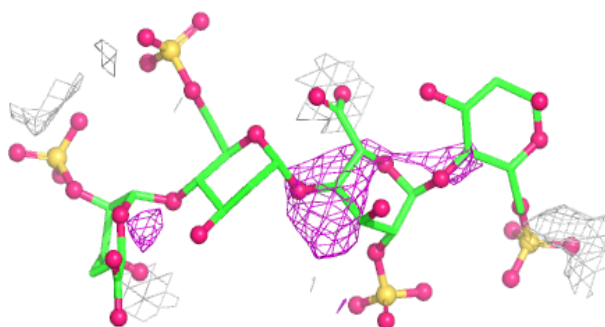


Electron density around Chain g:

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

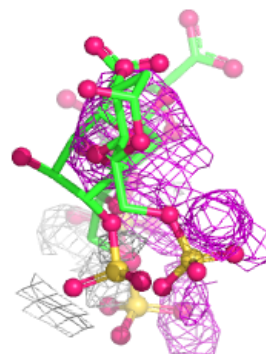
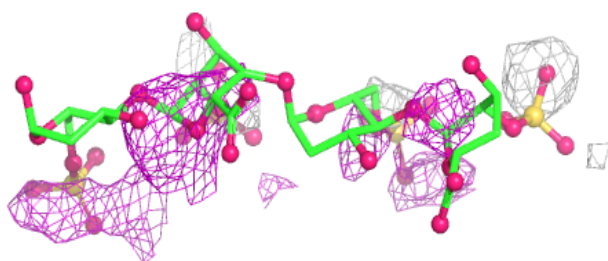
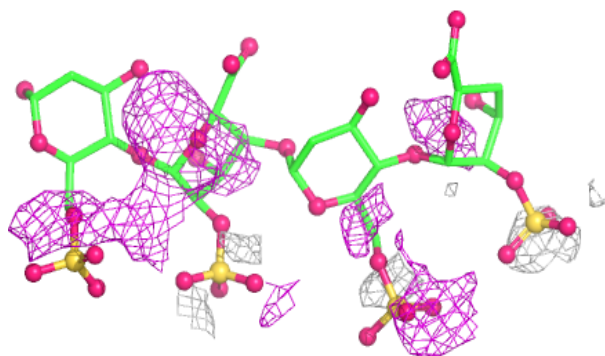
**Electron density around Chain h:**

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

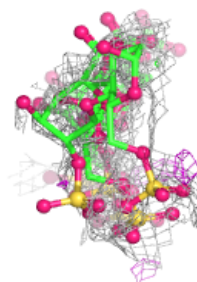
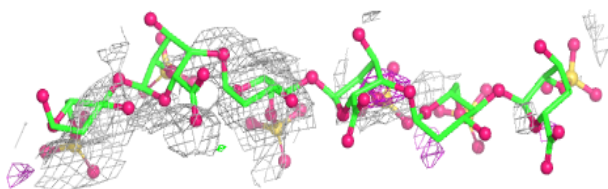
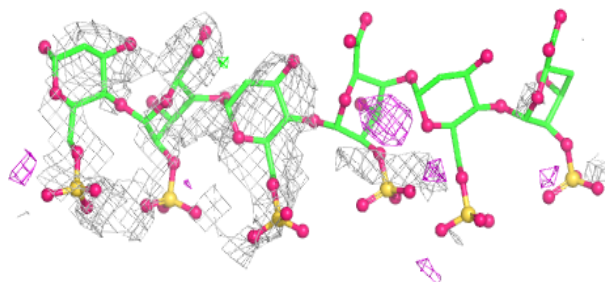


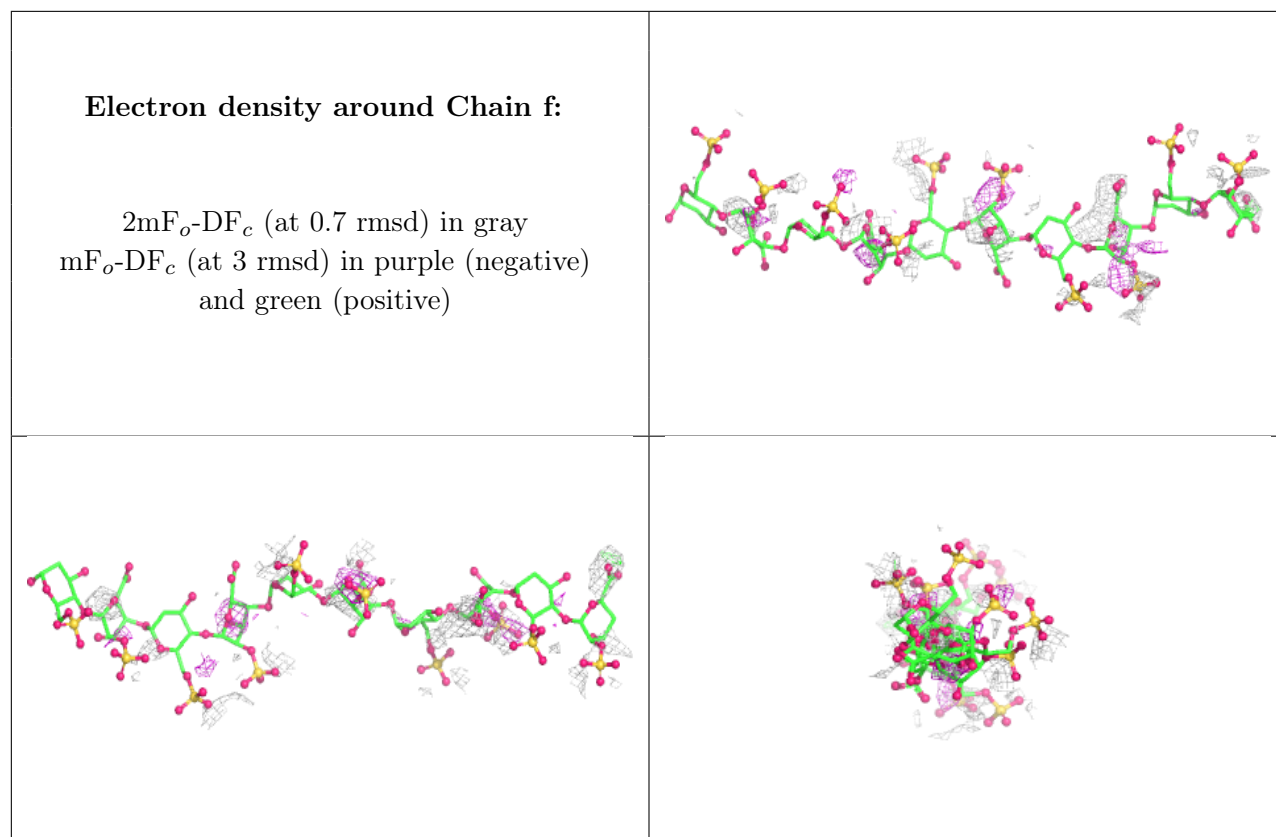
Electron density around Chain p:

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

**Electron density around Chain e:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.