



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 5VIY / pdb_00005viy
EMDB ID : EMD-8693
Title : BG505 SOSIP.664 in complex with broadly neutralizing antibodies BG1 and 8ANC195
Authors : Wang, H.; Bjorkman, P.J.
Deposited on : 2017-04-17
Resolution : 6.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

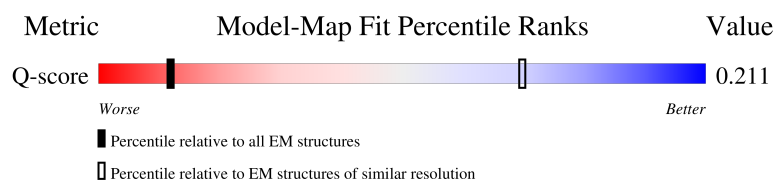
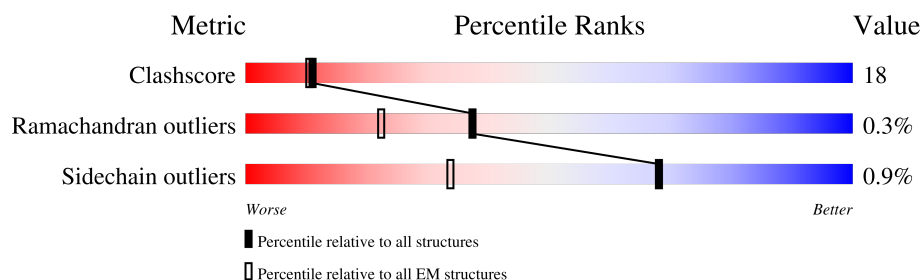
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	6% 56% 31% 13%
1	B	153	8% 56% 31% 13%
1	C	153	6% 54% 33% 13%
2	D	481	• 59% 34% • 7%

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Mol	Chain	Length	Quality of chain
2	E	481	
2	F	481	
3	G	214	
3	I	214	
4	H	233	
4	J	233	
5	K	233	
5	M	233	
5	O	233	
6	L	215	
6	N	215	
6	P	215	
7	0	5	
7	7	5	
7	Q	5	
7	R	5	
7	S	5	
7	U	5	
7	n	5	
7	v	5	
7	w	5	
8	1	2	
8	2	2	
8	3	2	
8	T	2	

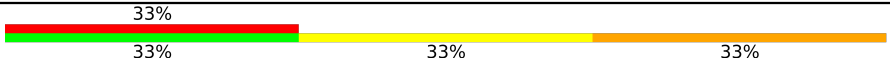
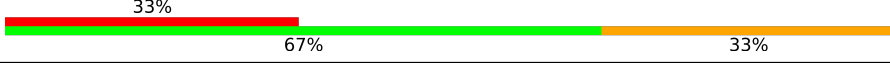
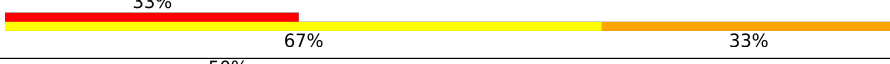
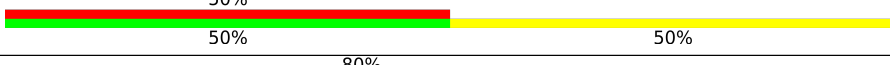
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Mol	Chain	Length	Quality of chain
8	V	2	50% 100%
8	Z	2	50% 50%
8	a	2	50% 50%
8	c	2	50% 50%
8	e	2	50% 50%
8	g	2	50% 50%
8	h	2	50% 50%
8	j	2	50% 100%
8	k	2	50% 100%
8	o	2	50% 100%
8	p	2	50% 50%
8	q	2	100%
8	u	2	50% 50%
8	x	2	50% 50%
9	W	4	25% 50% 25%
9	l	4	25% 50% 25%
9	y	4	50% 50%
10	X	7	57% 57% 29% 14%
10	m	7	43% 43% 43% 14%
10	z	7	57% 29% 71%
11	Y	4	50% 50%
11	b	4	50% 50%
12	4	3	67% 33% 67%
12	5	3	33% 33% 67%
12	6	3	33% 33% 67%

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Mol	Chain	Length	Quality of chain
12	d	3	
12	f	3	
12	i	3	
12	r	3	
13	s	2	
14	t	5	

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
7	BMA	0	3	-	-	X	-
7	BMA	n	3	-	-	X	-
7	NAG	v	1	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 32071 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1063	674	184	199	6		
1	B	133	Total	C	N	O	S	0	0
			1063	674	184	199	6		
1	C	133	Total	C	N	O	S	0	0
			1063	674	184	199	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP Q2N0S6
A	605	CYS	THR	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
C	559	PRO	ILE	conflict	UNP Q2N0S6
C	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	E	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	F	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6
D	509	ARG	GLU	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	ARG	LYS	conflict	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	GLU	conflict	UNP Q2N0S6
E	510	ARG	LYS	conflict	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	GLU	conflict	UNP Q2N0S6
F	510	ARG	LYS	conflict	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called BG1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	212	Total	C	N	O	S	0	0
			1613	1009	272	327	5		
3	I	213	Total	C	N	O	S	0	0
			1620	1014	273	328	5		

- Molecule 4 is a protein called BG1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	223	Total	C	N	O	S	0	0
			1658	1059	280	312	7		
4	J	223	Total	C	N	O	S	0	0
			1658	1059	280	312	7		

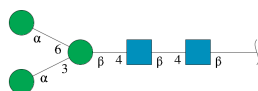
- Molecule 5 is a protein called 8ANC195 G52K5 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	227	Total	C	N	O	S	0	0
			1675	1063	282	325	5		
5	M	227	Total	C	N	O	S	0	0
			1675	1063	282	325	5		
5	O	227	Total	C	N	O	S	0	0
			1675	1063	282	325	5		

- Molecule 6 is a protein called 8ANC195 G52K5 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	214	Total	C	N	O	S	0	0
			1540	962	255	318	5		
6	N	214	Total	C	N	O	S	0	0
			1540	962	255	318	5		
6	P	214	Total	C	N	O	S	0	0
			1540	962	255	318	5		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	5	Total	C	N	O	0	0
			61	34	2	25		
7	R	5	Total	C	N	O	0	0
			61	34	2	25		
7	S	5	Total	C	N	O	0	0
			61	34	2	25		
7	U	5	Total	C	N	O	0	0
			61	34	2	25		
7	n	5	Total	C	N	O	0	0
			61	34	2	25		
7	v	5	Total	C	N	O	0	0
			61	34	2	25		
7	w	5	Total	C	N	O	0	0
			61	34	2	25		
7	0	5	Total	C	N	O	0	0
			61	34	2	25		
7	7	5	Total	C	N	O	0	0
			61	34	2	25		

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



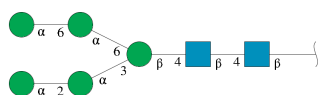
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	g	2	Total	C	N	O	0	0
			28	16	2	10		
8	h	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		
8	k	2	Total	C	N	O	0	0
			28	16	2	10		
8	o	2	Total	C	N	O	0	0
			28	16	2	10		
8	p	2	Total	C	N	O	0	0
			28	16	2	10		
8	q	2	Total	C	N	O	0	0
			28	16	2	10		
8	u	2	Total	C	N	O	0	0
			28	16	2	10		
8	x	2	Total	C	N	O	0	0
			28	16	2	10		
8	1	2	Total	C	N	O	0	0
			28	16	2	10		
8	2	2	Total	C	N	O	0	0
			28	16	2	10		
8	3	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	4	Total	C	N	O	0	0
			50	28	2	20		
9	l	4	Total	C	N	O	0	0
			50	28	2	20		
9	y	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



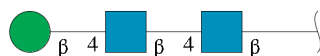
Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	7	Total	C	N	O	0	0
			83	46	2	35		
10	m	7	Total	C	N	O	0	0
			83	46	2	35		
10	z	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	4	Total	C	N	O	0	0
			50	28	2	20		
11	b	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



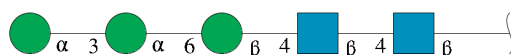
Mol	Chain	Residues	Atoms				AltConf	Trace
12	d	3	Total	C	N	O	0	0
			39	22	2	15		
12	f	3	Total	C	N	O	0	0
			39	22	2	15		
12	i	3	Total	C	N	O	0	0
			39	22	2	15		
12	r	3	Total	C	N	O	0	0
			39	22	2	15		
12	4	3	Total	C	N	O	0	0
			39	22	2	15		
12	5	3	Total	C	N	O	0	0
			39	22	2	15		
12	6	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



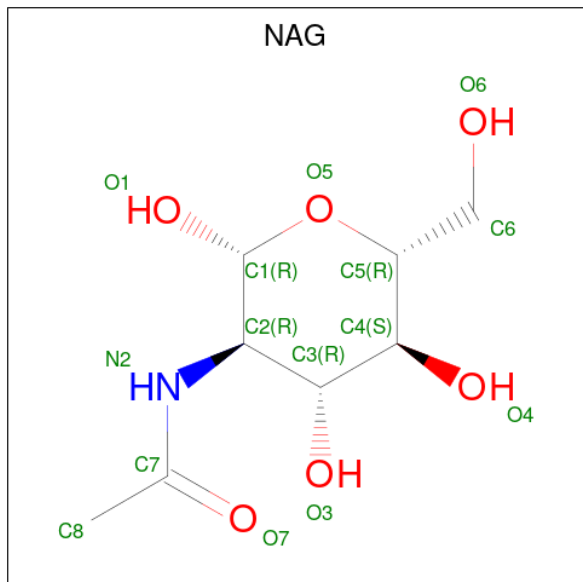
Mol	Chain	Residues	Atoms				AltConf	Trace
13	s	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	N	O	0
			14	8	1	5	
15	B	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	
15	F	1	Total	C	N	O	0
			14	8	1	5	

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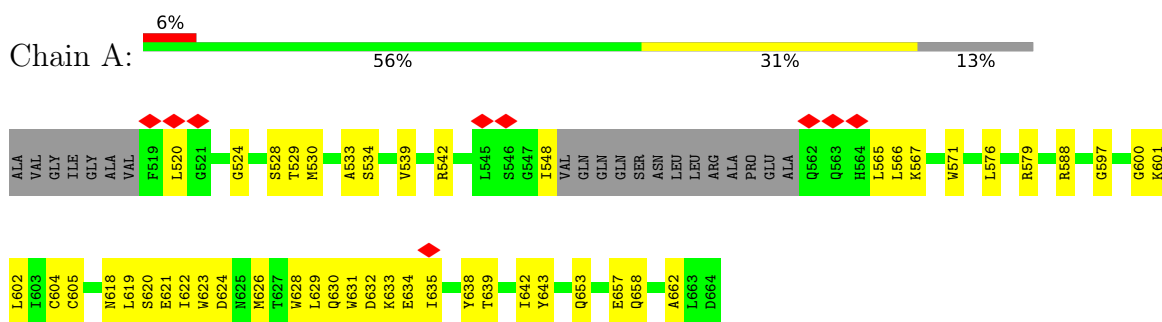
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	F	1	14	8	1	5	0

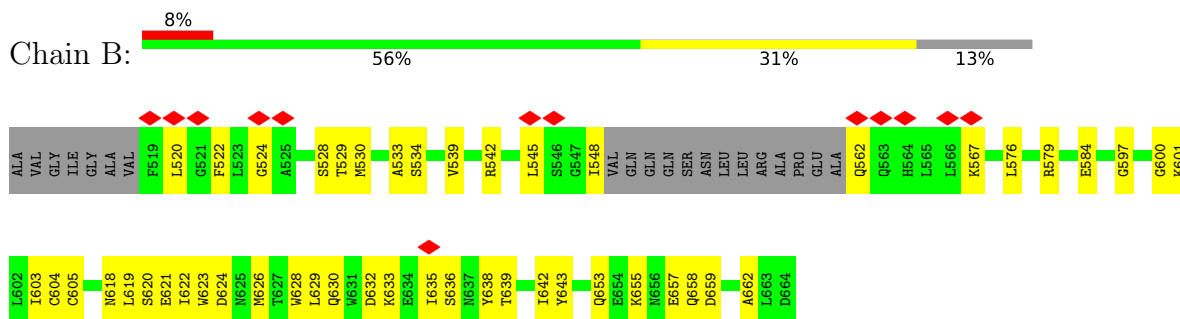
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

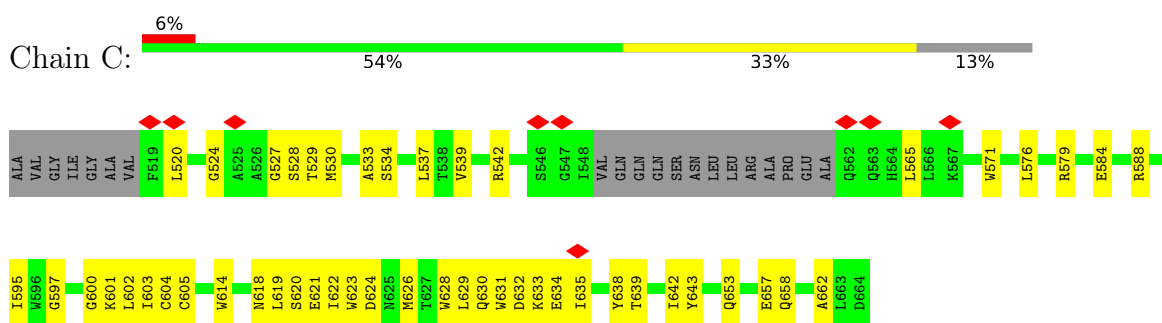
- Molecule 1: Envelope glycoprotein gp160



- Molecule 1: Envelope glycoprotein gp160

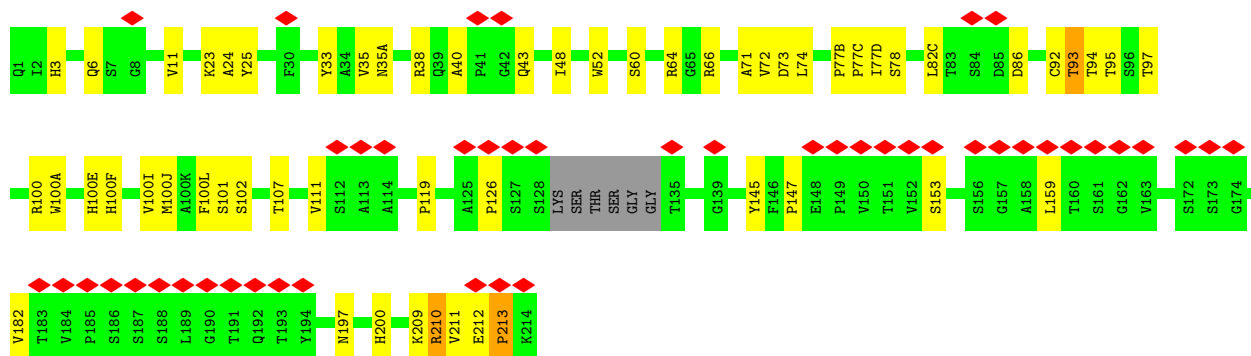


- Molecule 1: Envelope glycoprotein gp160

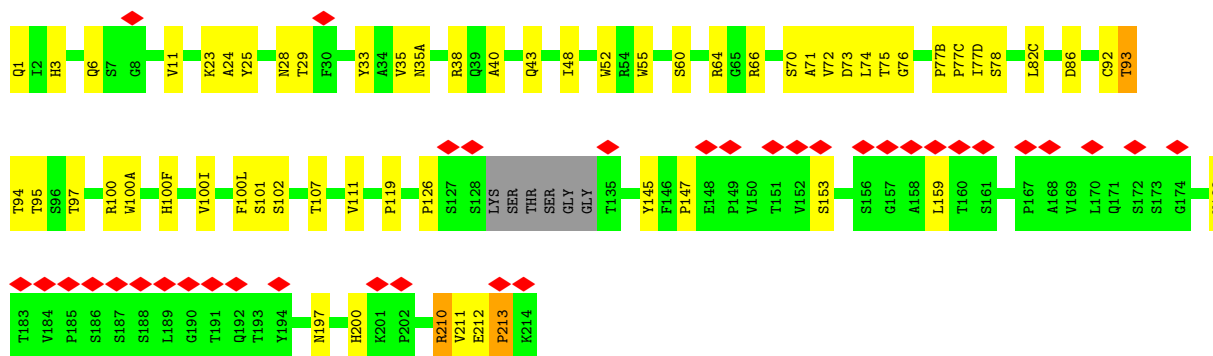


- Molecule 2: Envelope glycoprotein gp160

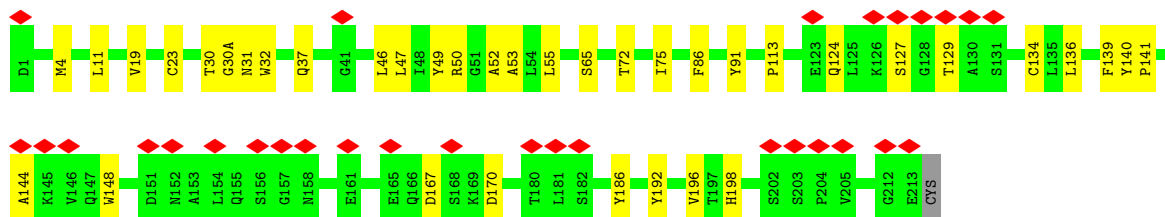
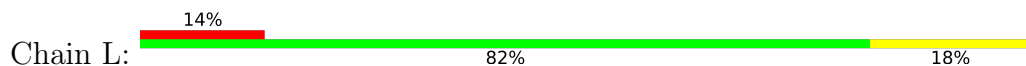




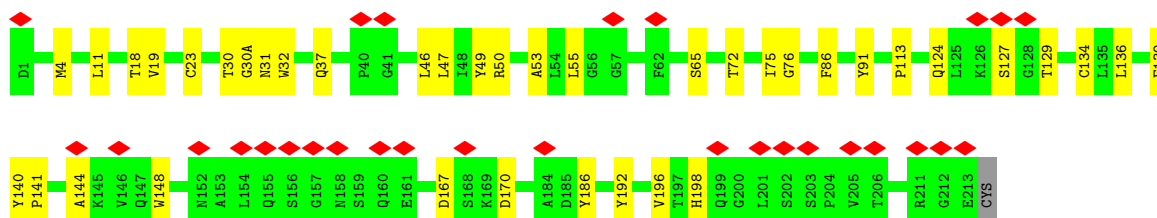
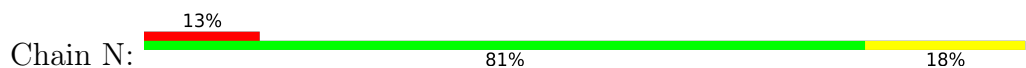
• Molecule 5: 8ANC195 G52K5 Fab heavy chain



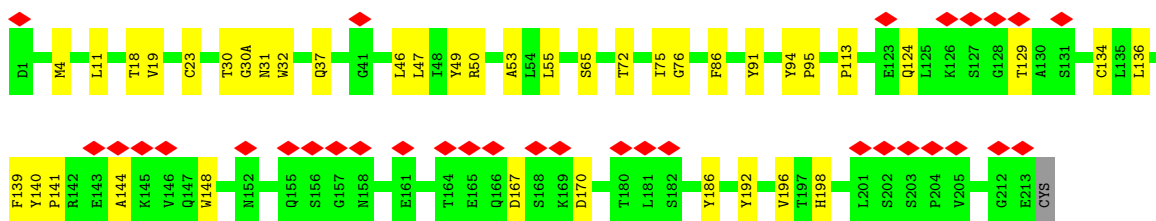
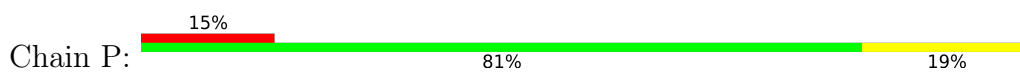
• Molecule 6: 8ANC195 G52K5 Fab light chain



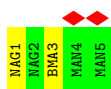
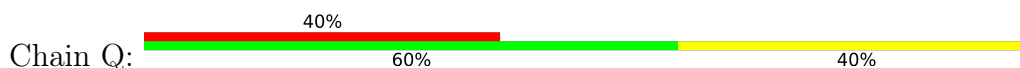
• Molecule 6: 8ANC195 G52K5 Fab light chain



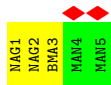
• Molecule 6: 8ANC195 G52K5 Fab light chain



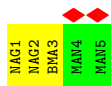
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



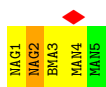
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



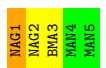
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



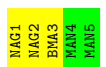
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



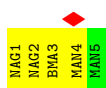
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



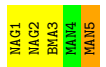
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



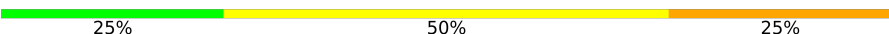
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 



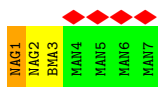
- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y: 



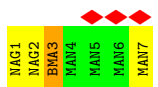
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m: 



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z: 



- Molecule 11: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 



- Molecule 11: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



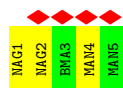
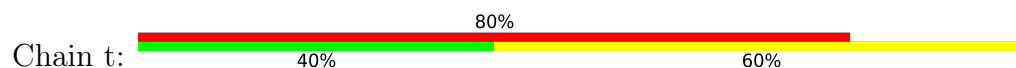
- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0342	Depositor
Map size (Å)	321.30002, 321.30002, 321.30002	wwPDB
Map dimensions	238, 238, 238	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/1082	0.70	2/1466 (0.1%)
1	B	0.29	0/1082	0.70	2/1466 (0.1%)
1	C	0.29	0/1082	0.70	2/1466 (0.1%)
2	D	0.23	0/3605	0.53	0/4895
2	E	0.23	0/3605	0.54	0/4895
2	F	0.23	0/3605	0.54	0/4895
3	G	0.21	0/1650	0.50	0/2249
3	I	0.22	0/1658	0.50	0/2262
4	H	0.21	0/1705	0.51	0/2329
4	J	0.22	0/1705	0.51	0/2329
5	K	0.28	2/1720 (0.1%)	0.47	2/2359 (0.1%)
5	M	0.28	2/1720 (0.1%)	0.46	2/2359 (0.1%)
5	O	0.28	2/1720 (0.1%)	0.46	2/2359 (0.1%)
6	L	0.15	0/1574	0.35	0/2159
6	N	0.15	0/1574	0.35	0/2159
6	P	0.15	0/1574	0.35	0/2159
All	All	0.23	6/30661 (0.0%)	0.51	12/41806 (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
2	D	0	1
2	E	0	1
2	F	0	1
3	G	0	1
3	I	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	212	GLU	C-N	5.92	1.40	1.33
5	K	212	GLU	C-N	5.90	1.40	1.33
5	O	212	GLU	C-N	5.86	1.40	1.33
5	O	213	PRO	N-CD	5.35	1.55	1.47
5	M	213	PRO	N-CD	5.29	1.55	1.47
5	K	213	PRO	N-CD	5.25	1.55	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	212	GLU	CA-C-N	-6.74	113.36	120.03
5	K	212	GLU	C-N-CA	-6.74	113.36	120.03
5	M	212	GLU	CA-C-N	-6.71	113.39	120.03
5	M	212	GLU	C-N-CA	-6.71	113.39	120.03
5	O	212	GLU	CA-C-N	-6.67	113.43	120.03
5	O	212	GLU	C-N-CA	-6.67	113.43	120.03
1	B	600	GLY	CA-C-N	5.68	131.93	121.70
1	B	600	GLY	C-N-CA	5.68	131.93	121.70
1	C	600	GLY	CA-C-N	5.68	131.92	121.70
1	C	600	GLY	C-N-CA	5.68	131.92	121.70
1	A	600	GLY	CA-C-N	5.67	131.91	121.70
1	A	600	GLY	C-N-CA	5.67	131.91	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	68	VAL	Peptide
2	E	68	VAL	Peptide
2	F	68	VAL	Peptide
3	G	29	ILE	Peptide
3	I	29	ILE	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	1063	0	1048	54	0
1	B	1063	0	1048	44	0
1	C	1063	0	1048	64	0
2	D	3532	0	3462	169	0
2	E	3532	0	3460	199	0
2	F	3532	0	3460	173	0
3	G	1613	0	1524	54	0
3	I	1620	0	1534	57	0
4	H	1658	0	1550	53	0
4	J	1658	0	1550	60	0
5	K	1675	0	1601	91	0
5	M	1675	0	1601	77	0
5	O	1675	0	1601	105	0
6	L	1540	0	1382	26	0
6	N	1540	0	1382	23	0
6	P	1540	0	1382	32	0
7	0	61	0	52	11	0
7	7	61	0	51	2	0
7	Q	61	0	52	0	0
7	R	61	0	52	5	0
7	S	61	0	52	0	0
7	U	61	0	52	3	0
7	n	61	0	52	22	0
7	v	61	0	52	8	0
7	w	61	0	52	0	0
8	1	28	0	25	0	0
8	2	28	0	25	0	0
8	3	28	0	25	0	0
8	T	28	0	25	1	0
8	V	28	0	25	0	0
8	Z	28	0	25	0	0
8	a	28	0	25	0	0
8	c	28	0	25	1	0
8	e	28	0	25	0	0
8	g	28	0	25	1	0
8	h	28	0	25	0	0
8	j	28	0	25	0	0
8	k	28	0	25	0	0
8	o	28	0	25	0	0
8	p	28	0	25	0	0
8	q	28	0	25	0	0
8	u	28	0	25	0	0
8	x	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	50	0	43	7	0
9	l	50	0	43	5	0
9	y	50	0	43	2	0
10	X	83	0	70	1	0
10	m	83	0	70	2	0
10	z	83	0	70	0	0
11	Y	50	0	43	1	0
11	b	50	0	43	0	0
12	4	39	0	34	0	0
12	5	39	0	34	0	0
12	6	39	0	34	1	0
12	d	39	0	34	1	0
12	f	39	0	34	1	0
12	i	39	0	34	3	0
12	r	39	0	34	4	0
13	s	24	0	22	0	0
14	t	61	0	52	0	0
15	A	14	0	13	0	0
15	B	14	0	13	0	0
15	C	14	0	13	2	0
15	D	42	0	39	0	0
15	E	42	0	39	2	0
15	F	56	0	52	0	0
All	All	32071	0	30456	1140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1140) 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)
5:O:3:HIS:CE1	7:n:3:BMA:H3	1.09	1.58
2:F:304:ARG:NH2	2:F:318:TYR:CD1	1.74	1.52
1:A:629:LEU:HD21	5:M:100:ARG:CD	1.35	1.52
1:A:629:LEU:CD2	5:M:100:ARG:CD	1.89	1.49
2:E:183:GLN:CA	2:E:191:TYR:HB3	1.41	1.49
5:O:3:HIS:CE1	7:n:3:BMA:C3	1.94	1.45
2:E:183:GLN:HA	2:E:191:TYR:CB	1.46	1.44
5:O:3:HIS:CE1	7:n:4:MAN:C1	1.98	1.43
2:D:46:LYS:NZ	5:K:100(A):TRP:CE2	1.85	1.42
1:C:630:GLN:NE2	5:O:100(F):HIS:ND1	1.71	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3:HIS:ND1	7:n:3:BMA:H3	1.37	1.34
5:O:3:HIS:NE2	7:n:4:MAN:C1	1.87	1.34
5:K:3:HIS:O	5:K:4:LEU:CG	1.77	1.31
2:E:46:LYS:NZ	5:O:100(A):TRP:CE2	1.99	1.27
2:D:278:THR:HG21	5:K:74:LEU:CD1	1.65	1.26
2:D:188:ASN:OD1	4:J:57:GLY:O	1.54	1.25
1:A:629:LEU:CD2	5:M:100:ARG:HD2	1.56	1.24
2:D:278:THR:HG22	5:K:75:THR:O	1.31	1.24
1:A:629:LEU:CD2	5:M:100:ARG:HD3	1.55	1.24
2:E:278:THR:HG22	5:O:75:THR:O	1.31	1.23
1:C:629:LEU:HD21	5:O:100:ARG:CD	1.68	1.22
2:D:159:PHE:CZ	2:D:172:VAL:HG23	1.73	1.22
1:B:629:LEU:CD2	5:K:100:ARG:HD3	1.71	1.21
2:F:160:ASN:HA	2:F:171:LYS:HB2	1.26	1.18
2:D:278:THR:CG2	5:K:74:LEU:HD11	1.74	1.17
2:D:159:PHE:CZ	2:D:172:VAL:CG2	2.29	1.14
2:D:46:LYS:NZ	5:K:100(A):TRP:NE1	1.95	1.13
1:C:629:LEU:HD21	5:O:100:ARG:HD3	1.31	1.12
2:E:160:ASN:HA	2:E:171:LYS:HB2	1.27	1.11
2:D:129:LEU:HD12	2:D:191:TYR:O	1.48	1.11
5:M:3:HIS:CE1	7:O:3:BMA:H3	1.85	1.10
1:A:629:LEU:HD22	5:M:100:ARG:CD	1.82	1.09
1:B:629:LEU:HD21	5:K:100:ARG:HD3	1.32	1.09
1:C:630:GLN:OE1	5:O:100(F):HIS:CE1	2.04	1.08
5:K:3:HIS:O	5:K:4:LEU:HG	0.91	1.08
1:B:629:LEU:CD2	5:K:100:ARG:CD	2.30	1.08
2:F:183:GLN:CA	2:F:191:TYR:HB3	1.84	1.07
2:F:192:ARG:HD2	2:F:193:LEU:H	1.16	1.06
2:F:165:LEU:HD12	2:F:168:LYS:HG3	1.37	1.06
1:A:630:GLN:OE1	5:M:100(F):HIS:CE1	2.08	1.06
2:D:317:PHE:CE2	2:D:319:ALA:HB2	1.90	1.06
2:E:317:PHE:CE2	2:E:319:ALA:HB2	1.90	1.06
2:E:46:LYS:NZ	5:O:100(A):TRP:NE1	2.03	1.05
2:E:278:THR:HG21	5:O:74:LEU:HD11	1.07	1.03
2:F:183:GLN:HA	2:F:191:TYR:CB	1.89	1.02
5:K:72:VAL:HG22	9:W:4:MAN:H62	1.42	1.01
2:E:278:THR:HG21	5:O:74:LEU:CD1	1.90	1.00
2:F:304:ARG:NH2	2:F:318:TYR:CG	2.26	1.00
2:D:46:LYS:NZ	5:K:100(A):TRP:CZ2	2.29	1.00
2:F:173:TYR:CZ	7:v:1:NAG:H3	1.96	0.99
2:D:159:PHE:CE1	2:D:172:VAL:HG23	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HD22	5:K:100:ARG:CD	1.96	0.96
2:F:173:TYR:OH	7:v:1:NAG:H3	1.66	0.95
1:B:629:LEU:HD22	5:K:100:ARG:HD3	1.48	0.94
2:D:46:LYS:HZ3	5:K:100(A):TRP:NE1	1.59	0.94
2:E:278:THR:CG2	5:O:74:LEU:HD11	1.97	0.94
2:D:170:GLN:HE22	2:D:307:ILE:HG23	1.32	0.93
2:F:304:ARG:NH2	2:F:318:TYR:HD1	1.47	0.93
2:E:278:THR:CG2	5:O:75:THR:O	2.16	0.92
5:K:70:SER:HB2	9:W:4:MAN:O2	1.70	0.92
5:M:3:HIS:HE1	7:O:3:BMA:H3	1.31	0.92
2:E:165:LEU:HD12	2:E:168:LYS:HG3	1.52	0.91
2:E:183:GLN:HB3	2:E:191:TYR:HD2	1.33	0.91
2:E:197:ASN:HA	2:F:164:GLU:OE2	1.71	0.91
5:O:3:HIS:HE1	7:n:4:MAN:C1	1.82	0.90
5:K:3:HIS:C	5:K:4:LEU:HG	1.95	0.90
2:D:183:GLN:HB3	2:D:191:TYR:CE2	2.07	0.90
1:C:629:LEU:HD21	5:O:100:ARG:HD2	1.54	0.90
2:D:183:GLN:HB3	2:D:191:TYR:CD2	2.07	0.90
2:F:46:LYS:NZ	5:M:100(A):TRP:CE2	2.39	0.90
2:F:183:GLN:HA	2:F:191:TYR:HB3	0.94	0.90
1:B:630:GLN:OE1	5:K:100(F):HIS:CE1	2.25	0.89
1:C:629:LEU:CD2	5:O:100:ARG:CD	2.50	0.89
2:D:159:PHE:CE2	2:D:172:VAL:CG2	2.55	0.89
5:K:55:TRP:CD1	9:W:2:NAG:O7	2.26	0.89
2:F:131:CYS:SG	2:F:191:TYR:HE1	1.95	0.88
5:O:55:TRP:CD1	9:l:2:NAG:O7	2.26	0.88
1:C:630:GLN:CD	6:P:32:TRP:CZ2	2.51	0.88
5:M:3:HIS:CE1	7:O:3:BMA:C3	2.57	0.87
2:D:46:LYS:HZ1	5:K:100(A):TRP:NE1	1.72	0.87
1:C:630:GLN:CD	5:O:100(F):HIS:ND1	2.32	0.87
2:F:160:ASN:CA	2:F:171:LYS:HB2	2.04	0.86
2:E:474:ASP:OD1	2:E:476:ARG:NH1	2.08	0.86
2:E:46:LYS:HZ1	5:O:100(A):TRP:NE1	1.70	0.85
2:E:160:ASN:CA	2:E:171:LYS:HB2	2.05	0.85
2:F:474:ASP:OD1	2:F:476:ARG:NH1	2.08	0.85
2:D:129:LEU:CD1	2:D:191:TYR:O	2.24	0.85
2:D:474:ASP:OD1	2:D:476:ARG:NH1	2.08	0.85
5:O:3:HIS:NE2	7:n:4:MAN:C2	2.39	0.85
1:A:638:TYR:O	1:A:642:ILE:HB	1.78	0.84
1:C:638:TYR:O	1:C:642:ILE:HB	1.78	0.84
2:F:160:ASN:HA	2:F:171:LYS:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:ASN:OD1	2:E:173:TYR:HD1	1.60	0.84
1:A:633:LYS:NZ	5:M:100(A):TRP:HA	1.92	0.84
1:A:629:LEU:HD23	5:M:100:ARG:HD2	1.60	0.84
2:D:156:ASN:OD1	2:D:173:TYR:HD1	1.60	0.84
2:D:278:THR:CG2	5:K:74:LEU:CD1	2.43	0.84
5:M:3:HIS:CE1	7:O:4:MAN:C1	2.60	0.84
2:D:192:ARG:HD2	2:D:193:LEU:H	1.41	0.84
2:E:101:VAL:O	2:E:105:HIS:HB2	1.78	0.84
2:F:101:VAL:O	2:F:105:HIS:HB2	1.78	0.84
1:A:629:LEU:HD21	5:M:100:ARG:HD3	0.85	0.84
2:F:156:ASN:OD1	2:F:173:TYR:HD1	1.60	0.84
2:F:165:LEU:HB2	2:F:168:LYS:HG2	1.60	0.84
2:D:278:THR:CG2	5:K:75:THR:O	2.23	0.83
2:D:101:VAL:O	2:D:105:HIS:HB2	1.77	0.83
2:F:170:GLN:HE22	2:F:307:ILE:HG23	1.42	0.83
2:E:46:LYS:HZ3	5:O:100(A):TRP:NE1	1.71	0.83
2:E:170:GLN:HE22	2:E:307:ILE:HG23	1.41	0.83
1:A:629:LEU:HD22	5:M:100:ARG:CG	2.09	0.83
1:B:629:LEU:HD21	5:K:100:ARG:CD	2.03	0.83
5:M:3:HIS:HE1	7:O:4:MAN:C1	1.92	0.83
1:B:638:TYR:O	1:B:642:ILE:HB	1.78	0.82
2:D:421:LYS:NZ	2:D:423:ILE:O	2.13	0.82
5:O:3:HIS:CD2	7:n:3:BMA:O4	2.33	0.82
1:B:630:GLN:OE1	5:K:100(F):HIS:HE1	1.60	0.82
2:E:156:ASN:OD1	2:E:173:TYR:CD1	2.33	0.82
5:K:210:ARG:HH11	5:K:210:ARG:HG2	1.45	0.82
5:M:210:ARG:HH11	5:M:210:ARG:HG2	1.45	0.82
1:C:630:GLN:HE22	5:O:100(F):HIS:CG	1.98	0.81
2:D:156:ASN:OD1	2:D:173:TYR:CD1	2.33	0.81
2:E:421:LYS:NZ	2:E:423:ILE:O	2.13	0.81
2:F:421:LYS:NZ	2:F:423:ILE:O	2.13	0.81
1:A:620:SER:O	1:A:624:ASP:HB2	1.81	0.81
5:O:210:ARG:HG2	5:O:210:ARG:HH11	1.45	0.81
1:C:630:GLN:OE1	5:O:100(F):HIS:HE1	1.60	0.81
2:F:156:ASN:OD1	2:F:173:TYR:CD1	2.33	0.81
1:B:620:SER:O	1:B:624:ASP:HB2	1.81	0.81
1:B:629:LEU:CD2	5:K:100:ARG:HD2	2.09	0.81
2:F:131:CYS:SG	2:F:191:TYR:CE1	2.74	0.80
2:E:165:LEU:HB2	2:E:168:LYS:HG2	1.62	0.80
2:E:46:LYS:HZ1	5:O:100(A):TRP:CD1	1.99	0.80
2:F:192:ARG:HD2	2:F:193:LEU:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:ASN:HA	2:E:171:LYS:CB	2.08	0.80
5:O:72:VAL:HG22	9:I:4:MAN:H62	1.64	0.80
1:C:620:SER:O	1:C:624:ASP:HB2	1.81	0.80
5:O:3:HIS:ND1	7:n:3:BMA:C3	2.24	0.79
2:D:159:PHE:CZ	2:D:172:VAL:HG21	2.16	0.79
5:O:3:HIS:HE1	7:n:3:BMA:H3	1.35	0.79
5:M:11:VAL:HG21	5:M:147:PRO:HG3	1.64	0.79
2:D:192:ARG:HD2	2:D:193:LEU:N	1.98	0.78
1:A:630:GLN:OE1	5:M:100(F):HIS:ND1	2.14	0.78
2:D:165:LEU:HB2	2:D:168:LYS:HG2	1.66	0.78
2:F:304:ARG:HH21	2:F:318:TYR:HB3	1.48	0.78
5:M:38:ARG:HB3	5:M:48:ILE:HD11	1.66	0.78
5:O:11:VAL:HG21	5:O:147:PRO:HG3	1.64	0.78
1:C:630:GLN:CD	5:O:100(F):HIS:CE1	2.61	0.77
5:K:11:VAL:HG21	5:K:147:PRO:HG3	1.64	0.77
5:K:38:ARG:HB3	5:K:48:ILE:HD11	1.66	0.77
5:O:1:GLN:O	7:n:2:NAG:O6	2.02	0.77
2:D:278:THR:HG23	5:K:74:LEU:HG	1.65	0.77
2:F:131:CYS:HB2	2:F:191:TYR:OH	1.84	0.77
5:M:3:HIS:CE1	7:O:3:BMA:O4	2.38	0.77
2:D:317:PHE:HE2	2:D:319:ALA:HB2	1.48	0.77
5:K:3:HIS:O	5:K:4:LEU:CB	2.34	0.76
1:C:605:CYS:HG	2:E:501:CYS:HG	1.33	0.76
5:O:38:ARG:HB3	5:O:48:ILE:HD11	1.66	0.76
3:I:108:ARG:NH1	3:I:109:THR:O	2.18	0.76
2:E:317:PHE:HE2	2:E:319:ALA:HB2	1.47	0.75
1:A:630:GLN:OE1	5:M:100(F):HIS:HE1	1.66	0.75
2:D:91:GLU:OE1	5:K:100:ARG:NH2	2.20	0.75
3:G:108:ARG:NH1	3:G:109:THR:O	2.18	0.75
2:D:278:THR:HG21	5:K:74:LEU:HD11	0.81	0.75
5:K:6:GLN:HE21	5:K:107:THR:HG23	1.52	0.75
2:E:182:VAL:O	2:E:191:TYR:HB2	1.87	0.75
2:F:159:PHE:CZ	2:F:172:VAL:HG23	2.21	0.74
1:C:629:LEU:CD2	5:O:100:ARG:HD2	2.14	0.74
2:E:159:PHE:CZ	2:E:172:VAL:HG23	2.23	0.74
2:E:181:VAL:HG12	2:E:193:LEU:CD2	2.18	0.74
2:D:188:ASN:CG	4:J:57:GLY:O	2.30	0.74
2:D:181:VAL:HG12	2:D:193:LEU:CD2	2.17	0.74
2:D:365:SER:OG	2:D:469:ARG:NH1	2.20	0.74
2:E:129:LEU:HD12	2:E:191:TYR:O	1.88	0.74
5:M:6:GLN:HE21	5:M:107:THR:HG23	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:VAL:HG12	2:F:193:LEU:CD2	2.18	0.74
5:O:70:SER:HB2	9:I:4:MAN:O2	1.85	0.74
2:F:365:SER:OG	2:F:469:ARG:NH1	2.20	0.74
5:O:6:GLN:HE21	5:O:107:THR:HG23	1.52	0.74
2:D:304:ARG:HD3	2:D:318:TYR:CD1	2.23	0.74
5:K:72:VAL:CG2	9:W:4:MAN:H62	2.17	0.74
2:E:46:LYS:NZ	5:O:100(A):TRP:CD2	2.56	0.73
2:F:129:LEU:HD12	2:F:191:TYR:O	1.87	0.73
1:B:619:LEU:O	1:B:623:TRP:HB2	1.89	0.72
2:E:197:ASN:CA	2:F:164:GLU:OE2	2.36	0.72
1:A:629:LEU:HD22	5:M:100:ARG:HG2	1.70	0.72
5:O:55:TRP:NE1	9:I:2:NAG:O7	2.23	0.72
1:A:619:LEU:O	1:A:623:TRP:HB2	1.89	0.72
3:I:55:GLN:HE22	4:J:102:GLN:HE22	1.35	0.72
3:I:14:SER:N	3:I:17:ASP:OD2	2.21	0.72
1:C:619:LEU:O	1:C:623:TRP:HB2	1.89	0.71
5:O:3:HIS:CE1	7:n:3:BMA:O3	2.42	0.71
2:D:165:LEU:HB2	2:D:168:LYS:CG	2.20	0.71
2:D:278:THR:CG2	5:K:74:LEU:CG	2.68	0.71
2:E:192:ARG:HD2	2:E:193:LEU:H	1.54	0.71
1:A:630:GLN:NE2	5:M:100(F):HIS:ND1	2.38	0.71
5:O:3:HIS:CG	7:n:3:BMA:O4	2.44	0.71
5:K:2:ILE:HG23	5:K:25:TYR:O	1.91	0.71
2:E:180:ASP:O	2:E:423:ILE:HD12	1.91	0.71
2:D:180:ASP:O	2:D:423:ILE:HD12	1.91	0.70
2:F:303:THR:HB	2:F:321:GLY:HA3	1.74	0.70
2:F:180:ASP:O	2:F:423:ILE:HD12	1.91	0.70
3:G:14:SER:N	3:G:17:ASP:OD2	2.21	0.70
2:D:278:THR:HG23	5:K:74:LEU:CG	2.20	0.70
2:F:165:LEU:HB2	2:F:168:LYS:CG	2.21	0.70
2:E:365:SER:OG	2:E:469:ARG:NH1	2.25	0.70
2:F:165:LEU:O	2:F:167:ASP:N	2.25	0.70
5:M:66:ARG:NH1	5:M:86:ASP:OD2	2.25	0.69
2:D:165:LEU:HD12	2:D:168:LYS:HG3	1.75	0.69
2:E:165:LEU:HB2	2:E:168:LYS:CG	2.21	0.69
5:O:66:ARG:NH1	5:O:86:ASP:OD2	2.25	0.69
5:O:3:HIS:HB2	7:n:3:BMA:H5	1.72	0.69
2:F:163:THR:HG22	2:F:170:GLN:OE1	1.93	0.69
6:N:30(A):GLY:O	6:N:50:ARG:NH1	2.26	0.69
5:K:66:ARG:NH1	5:K:86:ASP:OD2	2.25	0.68
3:G:136:LEU:HB2	3:G:175:LEU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LYS:HG2	5:K:100(A):TRP:CH2	2.28	0.68
2:E:184:ILE:HG22	2:E:190:GLU:O	1.93	0.68
6:L:30(A):GLY:O	6:L:50:ARG:NH1	2.26	0.68
1:A:605:CYS:HG	2:F:501:CYS:HG	0.70	0.68
6:P:30(A):GLY:O	6:P:50:ARG:NH1	2.26	0.68
2:D:165:LEU:O	2:D:167:ASP:N	2.28	0.67
3:I:136:LEU:HB2	3:I:175:LEU:HB3	1.76	0.67
5:M:119:PRO:HB3	5:M:145:TYR:HB3	1.77	0.67
2:D:190:GLU:C	2:D:191:TYR:CD1	2.73	0.67
2:E:36:VAL:HA	2:E:498:PRO:HA	1.77	0.67
2:E:192:ARG:HD2	2:E:193:LEU:N	2.09	0.67
2:F:172:VAL:HG21	2:F:307:ILE:HD13	1.77	0.67
2:D:129:LEU:HB2	2:D:191:TYR:O	1.95	0.67
2:E:172:VAL:HG21	2:E:307:ILE:HD13	1.77	0.67
2:E:303:THR:HB	2:E:321:GLY:HA3	1.75	0.67
5:K:119:PRO:HB3	5:K:145:TYR:HB3	1.76	0.67
2:F:165:LEU:O	2:F:168:LYS:N	2.26	0.67
2:F:173:TYR:CE2	7:v:1:NAG:H5	2.30	0.67
5:O:3:HIS:CG	7:n:3:BMA:H5	2.29	0.67
2:D:36:VAL:HA	2:D:498:PRO:HA	1.77	0.67
2:F:36:VAL:HA	2:F:498:PRO:HA	1.77	0.67
1:C:630:GLN:CD	6:P:32:TRP:HZ2	2.01	0.67
5:K:55:TRP:NE1	9:W:2:NAG:O7	2.27	0.67
3:G:132:VAL:HB	3:G:179:LEU:HB3	1.77	0.66
1:B:530:MET:O	1:B:534:SER:HB3	1.95	0.66
1:C:530:MET:O	1:C:534:SER:HB3	1.95	0.66
1:A:633:LYS:HZ1	5:M:100(A):TRP:HA	1.56	0.66
2:E:165:LEU:O	2:E:167:ASP:N	2.29	0.66
2:F:159:PHE:O	2:F:171:LYS:CA	2.43	0.66
5:O:73:ASP:OD1	5:O:74:LEU:N	2.26	0.66
5:K:73:ASP:OD1	5:K:74:LEU:N	2.26	0.66
2:E:159:PHE:O	2:E:171:LYS:CA	2.44	0.66
5:M:74:LEU:HD13	5:M:77(C):PRO:HD3	1.78	0.66
5:K:52:TRP:NE1	5:K:97:THR:HG21	2.11	0.66
2:E:165:LEU:O	2:E:168:LYS:N	2.27	0.66
5:O:52:TRP:NE1	5:O:97:THR:HG21	2.11	0.65
1:A:530:MET:O	1:A:534:SER:HB3	1.95	0.65
3:I:132:VAL:HB	3:I:179:LEU:HB3	1.77	0.65
5:O:94:THR:HB	5:O:102:SER:HB2	1.78	0.65
1:A:630:GLN:CD	5:M:100(F):HIS:ND1	2.54	0.65
2:D:173:TYR:CE2	7:U:1:NAG:H5	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:119:PRO:HB3	5:O:145:TYR:HB3	1.76	0.65
5:K:94:THR:HB	5:K:102:SER:HB2	1.78	0.65
2:D:183:GLN:CB	2:D:191:TYR:CD2	2.79	0.65
5:O:74:LEU:HD13	5:O:77(C):PRO:HD3	1.78	0.65
2:D:131:CYS:HB3	2:D:155:LYS:HB3	1.79	0.65
2:E:183:GLN:CB	2:E:191:TYR:HD2	2.08	0.65
5:M:52:TRP:NE1	5:M:97:THR:HG21	2.11	0.65
2:F:159:PHE:O	2:F:171:LYS:HA	1.98	0.64
2:E:46:LYS:NZ	5:O:100(A):TRP:CD1	2.60	0.64
2:E:362:ALA:HB3	2:E:467:THR:CG2	2.27	0.64
6:P:136:LEU:HD21	6:P:196:VAL:HG21	1.79	0.64
2:E:131:CYS:HB3	2:E:155:LYS:HB3	1.79	0.64
2:F:131:CYS:HB3	2:F:155:LYS:HB3	1.79	0.64
5:K:74:LEU:HD13	5:K:77(C):PRO:HD3	1.78	0.64
5:M:94:THR:HB	5:M:102:SER:HB2	1.78	0.64
6:N:136:LEU:HD21	6:N:196:VAL:HG21	1.79	0.64
4:J:162:VAL:HB	4:J:198:LEU:HB3	1.80	0.64
5:M:73:ASP:OD1	5:M:74:LEU:N	2.26	0.64
5:K:2:ILE:HG12	5:K:26:GLY:C	2.22	0.64
2:E:179:LEU:O	2:E:421:LYS:HE2	1.98	0.63
6:L:136:LEU:HD21	6:L:196:VAL:HG21	1.79	0.63
2:D:165:LEU:O	2:D:168:LYS:N	2.27	0.63
1:C:639:THR:O	1:C:643:TYR:HB2	1.98	0.63
5:O:72:VAL:CG2	9:l:4:MAN:H62	2.27	0.63
1:C:630:GLN:NE2	6:P:32:TRP:CZ2	2.66	0.63
2:E:159:PHE:O	2:E:171:LYS:HA	1.97	0.63
3:I:30:ALA:HA	3:I:68:GLY:HA2	1.80	0.63
1:B:639:THR:O	1:B:643:TYR:HB2	1.99	0.63
2:F:179:LEU:O	2:F:421:LYS:HE2	1.99	0.63
4:H:71:ALA:HB3	4:H:84:ASP:HB2	1.81	0.63
2:D:46:LYS:HZ1	5:K:100(A):TRP:CD1	2.16	0.63
1:A:576:LEU:HD23	1:A:579:ARG:HD3	1.81	0.63
1:C:576:LEU:HD23	1:C:579:ARG:HD3	1.81	0.63
2:E:173:TYR:CE2	12:i:1:NAG:H5	2.33	0.63
2:F:171:LYS:O	2:F:171:LYS:HG2	1.99	0.63
3:I:147:GLN:HB3	3:I:195:GLU:HB3	1.81	0.63
2:E:170:GLN:NE2	2:E:307:ILE:HG23	2.13	0.62
3:G:30:ALA:HA	3:G:68:GLY:HA2	1.80	0.62
1:B:576:LEU:HD23	1:B:579:ARG:HD3	1.81	0.62
2:E:181:VAL:HG12	2:E:193:LEU:HD23	1.81	0.62
4:H:18:LEU:HB3	4:H:85:VAL:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:162:VAL:HB	4:H:198:LEU:HB3	1.80	0.62
2:E:163:THR:HG22	2:E:170:GLN:OE1	2.00	0.62
2:F:170:GLN:NE2	2:F:307:ILE:HG23	2.12	0.62
3:G:147:GLN:HB3	3:G:195:GLU:HB3	1.80	0.62
1:C:565:LEU:HD22	2:E:66:HIS:HA	1.81	0.62
1:C:629:LEU:HD22	5:O:100:ARG:HG2	1.80	0.62
2:D:179:LEU:O	2:D:421:LYS:HE2	1.98	0.62
2:F:192:ARG:NH2	2:F:193:LEU:O	2.32	0.62
5:O:23:LYS:HA	5:O:77(D):ILE:HG12	1.80	0.62
1:A:639:THR:O	1:A:643:TYR:HB2	1.99	0.62
2:D:181:VAL:HG12	2:D:193:LEU:HD23	1.81	0.62
2:F:304:ARG:NH2	2:F:318:TYR:HB3	2.15	0.62
5:O:3:HIS:ND1	7:n:3:BMA:H5	2.15	0.62
2:D:129:LEU:CG	2:D:191:TYR:O	2.47	0.62
2:F:175:LEU:HD21	7:v:1:NAG:H82	1.81	0.62
3:I:145:LYS:HB3	3:I:197:THR:HB	1.82	0.62
5:M:23:LYS:HA	5:M:77(D):ILE:HG12	1.81	0.62
2:E:196:CYS:O	2:F:164:GLU:HB3	2.00	0.62
2:E:317:PHE:CE2	2:E:319:ALA:CB	2.76	0.62
4:H:5:VAL:HB	4:H:23:SER:HB2	1.81	0.62
5:K:23:LYS:HA	5:K:77(D):ILE:HG12	1.81	0.62
4:H:52:ARG:HH11	4:H:59:SER:HB3	1.64	0.62
4:J:71:ALA:HB3	4:J:84:ASP:HB2	1.81	0.62
2:E:91:GLU:OE1	5:O:100:ARG:NH2	2.33	0.62
2:E:171:LYS:O	2:E:171:LYS:HG2	2.00	0.62
2:F:304:ARG:NH2	2:F:318:TYR:CB	2.63	0.61
1:C:527:GLY:HA3	2:E:88:ASN:HB2	1.82	0.61
3:G:59:PRO:HG2	3:G:61:ARG:HH12	1.65	0.61
2:E:184:ILE:CG2	2:E:190:GLU:O	2.49	0.61
1:A:634:GLU:OE2	6:N:30(A):GLY:HA2	1.99	0.61
2:F:479:TRP:O	2:F:483:LEU:HB2	2.01	0.61
4:J:5:VAL:HB	4:J:23:SER:HB2	1.81	0.61
2:E:183:GLN:HB3	2:E:191:TYR:CD2	2.25	0.61
2:F:292:VAL:HB	2:F:449:ILE:HB	1.83	0.61
4:J:52:ARG:HH11	4:J:59:SER:HB3	1.64	0.61
2:E:479:TRP:O	2:E:483:LEU:HB2	2.01	0.61
3:G:89:GLN:NE2	3:G:90:GLN:O	2.34	0.61
3:I:89:GLN:NE2	3:I:90:GLN:O	2.34	0.61
4:J:18:LEU:HB3	4:J:85:VAL:HB	1.81	0.61
3:I:59:PRO:HG2	3:I:61:ARG:HH12	1.65	0.61
2:D:173:TYR:CZ	7:U:1:NAG:H5	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:149:LYS:HB2	3:I:193:ALA:HB3	1.83	0.60
2:D:479:TRP:O	2:D:483:LEU:HB2	2.00	0.60
2:F:173:TYR:CZ	7:v:1:NAG:H5	2.36	0.60
3:G:149:LYS:HB2	3:G:193:ALA:HB3	1.83	0.60
3:I:46:LEU:HD21	3:I:49:PHE:HB3	1.83	0.60
2:F:425:ASN:HD21	2:F:430:ILE:HA	1.66	0.60
2:E:173:TYR:CZ	12:i:1:NAG:H5	2.36	0.60
2:F:181:VAL:HG12	2:F:193:LEU:HD23	1.81	0.60
2:D:170:GLN:NE2	2:D:307:ILE:HG23	2.09	0.60
2:D:292:VAL:HB	2:D:449:ILE:HB	1.83	0.60
3:G:145:LYS:HB3	3:G:197:THR:HB	1.82	0.60
2:E:304:ARG:NH2	2:E:318:TYR:CG	2.69	0.60
2:E:278:THR:HA	5:O:76:GLY:HA2	1.84	0.60
2:E:292:VAL:HB	2:E:449:ILE:HB	1.83	0.60
15:E:639:NAG:O4	12:r:1:NAG:O4	2.19	0.60
2:F:257:THR:O	2:F:374:HIS:ND1	2.28	0.60
3:G:46:LEU:HD21	3:G:49:PHE:HB3	1.83	0.60
4:J:13:PRO:HD2	4:J:16:ARG:HE	1.67	0.60
2:E:183:GLN:HA	2:E:191:TYR:CA	2.29	0.60
4:J:38:ARG:NH1	4:J:92:ASP:OD1	2.34	0.60
1:A:633:LYS:CE	5:M:100(A):TRP:HA	2.32	0.59
2:D:304:ARG:HD3	2:D:318:TYR:HB3	1.84	0.59
2:E:278:THR:CG2	5:O:74:LEU:CD1	2.68	0.59
2:D:159:PHE:CE2	2:D:172:VAL:HG23	2.29	0.59
3:I:24:ARG:HA	3:I:70:GLU:HA	1.85	0.59
5:O:3:HIS:CB	7:n:3:BMA:H5	2.31	0.59
1:C:630:GLN:NE2	5:O:100(F):HIS:CE1	2.61	0.59
2:E:257:THR:O	2:E:374:HIS:ND1	2.29	0.59
2:E:475:MET:SD	2:E:478:ASN:ND2	2.76	0.59
2:E:285:LEU:HD21	2:E:477:ASP:HB3	1.85	0.59
3:I:114:SER:HB2	3:I:137:ASN:HB3	1.85	0.59
3:G:24:ARG:HA	3:G:70:GLU:HA	1.84	0.59
2:F:173:TYR:CE1	7:v:1:NAG:H3	2.37	0.59
2:D:257:THR:O	2:D:374:HIS:ND1	2.29	0.59
2:D:475:MET:SD	2:D:478:ASN:ND2	2.76	0.59
4:H:13:PRO:HD2	4:H:16:ARG:HE	1.67	0.59
2:D:130:GLN:OE1	2:D:188:ASN:ND2	2.35	0.58
2:D:317:PHE:CE2	2:D:319:ALA:CB	2.76	0.58
2:D:425:ASN:HD21	2:D:430:ILE:HA	1.66	0.58
2:F:285:LEU:HD21	2:F:477:ASP:HB3	1.85	0.58
2:E:342:LEU:HD22	2:E:361:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:425:ASN:HD21	2:E:430:ILE:HA	1.66	0.58
2:D:278:THR:HA	5:K:76:GLY:HA2	1.85	0.58
3:G:114:SER:HB2	3:G:137:ASN:HB3	1.85	0.58
5:O:93:THR:HG21	5:O:100(L):PHE:CD1	2.39	0.58
2:F:475:MET:SD	2:F:478:ASN:ND2	2.76	0.58
3:I:116:PHE:HB2	3:I:135:LEU:HB3	1.84	0.58
5:K:93:THR:HG21	5:K:100(L):PHE:CD1	2.39	0.58
2:D:258:GLN:NE2	2:D:371:VAL:O	2.37	0.58
3:G:116:PHE:HB2	3:G:135:LEU:HB3	1.84	0.58
3:I:48:ILE:HG21	3:I:64:ALA:HB3	1.84	0.58
2:F:161:MET:HB3	2:F:170:GLN:O	2.04	0.58
5:M:3:HIS:CE1	7:O:3:BMA:HO4	2.22	0.58
5:O:126:PRO:HG2	5:O:213:PRO:HB3	1.86	0.58
2:D:285:LEU:HD21	2:D:477:ASP:HB3	1.85	0.58
2:E:130:GLN:OE1	2:E:188:ASN:ND2	2.35	0.57
2:F:130:GLN:OE1	2:F:188:ASN:ND2	2.35	0.57
2:F:304:ARG:HH21	2:F:318:TYR:CB	2.16	0.57
2:E:258:GLN:NE2	2:E:371:VAL:O	2.37	0.57
5:O:6:GLN:OE1	5:O:92:CYS:N	2.37	0.57
2:D:181:VAL:HG12	2:D:193:LEU:HD21	1.86	0.57
5:K:6:GLN:OE1	5:K:92:CYS:N	2.37	0.57
2:F:192:ARG:CD	2:F:193:LEU:H	2.04	0.57
2:F:258:GLN:NE2	2:F:371:VAL:O	2.37	0.57
5:K:126:PRO:HG2	5:K:213:PRO:HB3	1.86	0.57
5:M:93:THR:HG21	5:M:100(L):PHE:CD1	2.39	0.57
2:F:159:PHE:O	2:F:171:LYS:CB	2.52	0.57
5:M:6:GLN:OE1	5:M:92:CYS:N	2.37	0.57
5:M:52:TRP:HE1	5:M:97:THR:HG21	1.69	0.57
3:G:48:ILE:HG21	3:G:64:ALA:HB3	1.84	0.57
4:H:92:ASP:O	4:H:96:TYR:OH	2.23	0.57
2:E:364:SER:O	12:r:1:NAG:H82	2.05	0.57
5:K:52:TRP:HE1	5:K:97:THR:HG21	1.69	0.57
5:O:52:TRP:HE1	5:O:97:THR:HG21	1.69	0.57
1:A:567:LYS:NZ	2:E:106:THR:HB	2.19	0.57
2:F:129:LEU:HB2	2:F:191:TYR:O	2.04	0.57
5:M:3:HIS:ND1	7:O:3:BMA:H5	2.19	0.57
5:M:25:TYR:CE1	5:M:77(B):PRO:HG3	2.39	0.57
3:G:68:GLY:H	3:G:71:PHE:HE1	1.52	0.57
2:F:299:PRO:HA	2:F:442:VAL:HG13	1.87	0.57
10:m:3:BMA:H61	10:m:7:MAN:H2	1.87	0.57
2:D:268:GLU:O	2:D:289:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:GLU:O	2:E:289:ASN:ND2	2.38	0.56
2:F:268:GLU:O	2:F:289:ASN:ND2	2.38	0.56
5:K:25:TYR:CE1	5:K:77(B):PRO:HG3	2.39	0.56
5:M:126:PRO:HG2	5:M:213:PRO:HB3	1.86	0.56
2:D:299:PRO:HA	2:D:442:VAL:HG13	1.87	0.56
2:E:182:VAL:O	2:E:191:TYR:CB	2.52	0.56
2:E:197:ASN:CB	2:F:164:GLU:OE2	2.53	0.56
2:E:299:PRO:HA	2:E:442:VAL:HG13	1.87	0.56
2:E:361:PHE:HB2	2:E:393:SER:H	1.69	0.56
4:H:38:ARG:NH1	4:H:92:ASP:OD1	2.33	0.56
4:H:93:THR:HG23	4:H:130:VAL:HA	1.87	0.56
6:N:31:ASN:O	6:N:50:ARG:HA	2.05	0.56
2:F:131:CYS:HB2	2:F:191:TYR:CZ	2.41	0.56
5:O:25:TYR:CE1	5:O:77(B):PRO:HG3	2.39	0.56
6:P:31:ASN:O	6:P:50:ARG:HA	2.06	0.56
3:I:39:LYS:NZ	3:I:81:GLU:O	2.39	0.56
4:J:92:ASP:O	4:J:96:TYR:OH	2.23	0.56
2:E:161:MET:HB3	2:E:170:GLN:O	2.05	0.56
1:B:630:GLN:NE2	5:K:100(F):HIS:ND1	2.54	0.56
5:K:2:ILE:CG2	5:K:27:VAL:HG23	2.36	0.56
6:P:49:TYR:O	6:P:53:ALA:HB3	2.06	0.56
2:F:80:ASN:HB3	2:F:82:GLN:HE21	1.71	0.56
2:E:181:VAL:HG12	2:E:193:LEU:HD21	1.86	0.56
2:E:159:PHE:O	2:E:171:LYS:CB	2.54	0.56
2:E:245:VAL:HG12	2:E:247:CYS:H	1.71	0.56
2:F:165:LEU:HD12	2:F:168:LYS:CG	2.24	0.56
6:L:49:TYR:O	6:L:53:ALA:HB3	2.06	0.56
2:F:181:VAL:HG12	2:F:193:LEU:HD21	1.86	0.55
1:C:633:LYS:HD3	6:P:50:ARG:NH2	2.21	0.55
2:D:133:ASN:OD1	2:D:155:LYS:NZ	2.29	0.55
3:G:39:LYS:NZ	3:G:81:GLU:O	2.39	0.55
5:O:3:HIS:HE1	7:n:3:BMA:C3	2.00	0.55
2:F:286:VAL:HB	2:F:452:LEU:HB2	1.88	0.55
2:D:80:ASN:HB3	2:D:82:GLN:HE21	1.71	0.55
2:F:173:TYR:CE1	7:v:1:NAG:C1	2.89	0.55
2:F:245:VAL:HG12	2:F:247:CYS:H	1.71	0.55
2:F:297:THR:HG22	2:F:444:ARG:HG2	1.89	0.55
4:J:93:THR:HG23	4:J:130:VAL:HA	1.87	0.55
2:D:165:LEU:O	2:D:166:ARG:C	2.50	0.55
2:E:362:ALA:O	2:E:363:ASN:O	2.25	0.55
6:L:31:ASN:O	6:L:50:ARG:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3:HIS:ND1	7:n:3:BMA:C4	2.69	0.55
2:E:286:VAL:HB	2:E:452:LEU:HB2	1.88	0.55
2:E:131:CYS:SG	2:E:191:TYR:HE1	2.29	0.55
2:D:297:THR:HG22	2:D:444:ARG:HG2	1.89	0.55
2:E:278:THR:HG23	5:O:74:LEU:HG	1.88	0.55
2:E:362:ALA:HB3	2:E:467:THR:HG23	1.88	0.55
2:E:362:ALA:O	2:E:469:ARG:HG2	2.07	0.55
5:M:159:LEU:HD21	5:M:182:VAL:HG11	1.89	0.55
5:O:159:LEU:HD21	5:O:182:VAL:HG11	1.89	0.55
2:E:80:ASN:HB3	2:E:82:GLN:HE21	1.71	0.54
2:F:165:LEU:O	2:F:166:ARG:C	2.49	0.54
6:L:52:ALA:HB3	7:R:2:NAG:C6	2.37	0.54
1:A:548:ILE:C	1:C:588:ARG:HH12	2.14	0.54
3:I:68:GLY:H	3:I:71:PHE:HE1	1.52	0.54
6:N:49:TYR:O	6:N:53:ALA:HB3	2.06	0.54
1:B:530:MET:O	1:B:534:SER:CB	2.55	0.54
2:E:297:THR:HG22	2:E:444:ARG:HG2	1.89	0.54
2:D:286:VAL:HB	2:D:452:LEU:HB2	1.88	0.54
2:E:74:CYS:SG	2:E:75:VAL:N	2.80	0.54
2:E:165:LEU:O	2:E:166:ARG:C	2.50	0.54
2:E:182:VAL:C	2:E:191:TYR:HB2	2.33	0.54
2:F:270:VAL:HG23	2:F:348:GLN:HG3	1.90	0.54
1:C:537:LEU:HD13	2:E:42:VAL:HA	1.90	0.54
2:D:298:ARG:NH2	2:D:441:GLY:O	2.35	0.54
2:E:362:ALA:CB	2:E:467:THR:HG23	2.37	0.54
3:G:19:VAL:HB	3:G:75:ILE:HB	1.90	0.54
5:K:210:ARG:HH11	5:K:210:ARG:CG	2.16	0.54
2:D:245:VAL:HG12	2:D:247:CYS:H	1.71	0.54
2:E:385:CYS:HA	2:E:418:CYS:HA	1.90	0.54
1:A:530:MET:O	1:A:534:SER:CB	2.55	0.54
1:A:653:GLN:HA	1:A:657:GLU:H	1.72	0.54
2:F:318:TYR:O	2:F:438:PRO:HD2	2.08	0.54
4:H:167:PRO:O	4:H:220:HIS:NE2	2.40	0.54
5:M:3:HIS:CE1	7:O:3:BMA:C4	2.90	0.54
1:C:530:MET:O	1:C:534:SER:CB	2.56	0.53
2:F:74:CYS:SG	2:F:75:VAL:N	2.81	0.53
2:F:133:ASN:OD1	2:F:155:LYS:NZ	2.29	0.53
3:I:92:HIS:O	7:7:5:MAN:O3	2.22	0.53
6:N:37:GLN:HB2	6:N:47:LEU:HD11	1.90	0.53
2:E:270:VAL:HG23	2:E:348:GLN:HG3	1.90	0.53
1:B:653:GLN:HA	1:B:657:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:ASN:OD1	2:D:278:THR:OG1	2.26	0.53
4:H:35:ALA:HA	4:H:50:PHE:HA	1.90	0.53
5:K:159:LEU:HD21	5:K:182:VAL:HG11	1.89	0.53
6:P:37:GLN:HB2	6:P:47:LEU:HD11	1.90	0.53
2:D:74:CYS:SG	2:D:75:VAL:N	2.81	0.53
2:D:191:TYR:CD1	2:D:191:TYR:N	2.76	0.53
1:B:520:LEU:HB3	1:B:524:GLY:HA3	1.90	0.53
2:D:100:MET:O	2:D:104:MET:HB2	2.09	0.53
2:D:170:GLN:HE22	2:D:307:ILE:CG2	2.13	0.53
2:E:170:GLN:HE22	2:E:307:ILE:CG2	2.19	0.53
2:E:361:PHE:CD2	2:E:393:SER:HB2	2.44	0.53
3:I:39:LYS:HB2	3:I:42:LYS:HD2	1.91	0.53
4:J:167:PRO:O	4:J:220:HIS:NE2	2.40	0.53
2:F:41:GLY:N	2:F:493:PRO:O	2.42	0.53
2:F:179:LEU:HD12	2:F:420:ILE:O	2.09	0.53
5:K:211:VAL:HG12	5:K:211:VAL:O	2.08	0.53
5:O:3:HIS:CG	7:n:3:BMA:C4	2.92	0.53
2:D:41:GLY:N	2:D:493:PRO:O	2.42	0.53
2:D:158:SER:HA	2:D:172:VAL:O	2.09	0.53
2:F:159:PHE:O	2:F:171:LYS:HG3	2.08	0.53
4:J:35:ALA:HA	4:J:50:PHE:HA	1.90	0.53
1:C:520:LEU:HB3	1:C:524:GLY:HA3	1.90	0.53
1:C:653:GLN:HA	1:C:657:GLU:H	1.73	0.53
2:E:41:GLY:N	2:E:493:PRO:O	2.42	0.53
5:M:211:VAL:HG12	5:M:211:VAL:O	2.08	0.53
1:B:628:TRP:O	1:B:632:ASP:N	2.41	0.53
2:D:101:VAL:O	2:D:105:HIS:CB	2.54	0.53
2:D:179:LEU:HD12	2:D:420:ILE:O	2.09	0.53
2:F:100:MET:O	2:F:104:MET:HB2	2.09	0.53
2:F:385:CYS:HA	2:F:418:CYS:HA	1.90	0.53
2:D:192:ARG:CD	2:D:193:LEU:H	2.16	0.52
2:D:385:CYS:HA	2:D:418:CYS:HA	1.90	0.52
3:I:19:VAL:HB	3:I:75:ILE:HB	1.90	0.52
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.90	0.52
5:O:211:VAL:HG12	5:O:211:VAL:O	2.08	0.52
6:P:186:TYR:HA	6:P:192:TYR:OH	2.10	0.52
1:C:630:GLN:CG	6:P:32:TRP:HZ2	2.23	0.52
2:F:293:GLN:HE22	2:F:446:VAL:HG13	1.74	0.52
5:K:1:GLN:O	11:Y:2:NAG:H61	2.09	0.52
2:E:100:MET:O	2:E:104:MET:HB2	2.09	0.52
3:G:39:LYS:HB2	3:G:42:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:155:GLN:OE1	3:I:158:ASN:ND2	2.42	0.52
2:D:270:VAL:HG23	2:D:348:GLN:HG3	1.90	0.52
2:E:180:ASP:OD2	2:E:422:GLN:HB2	2.10	0.52
4:J:74:ARG:HA	4:J:81:VAL:HA	1.91	0.52
6:N:186:TYR:HA	6:N:192:TYR:OH	2.09	0.52
2:E:101:VAL:O	2:E:105:HIS:CB	2.54	0.52
2:E:293:GLN:HE22	2:E:446:VAL:HG13	1.74	0.52
6:P:19:VAL:HG12	6:P:75:ILE:HB	1.92	0.52
2:D:180:ASP:OD2	2:D:422:GLN:HB2	2.10	0.52
2:E:46:LYS:HG2	5:O:100(A):TRP:CH2	2.45	0.52
2:F:298:ARG:NH2	2:F:441:GLY:O	2.35	0.52
1:A:520:LEU:HB3	1:A:524:GLY:HA3	1.90	0.52
1:B:562:GLN:HG3	2:D:61:TYR:CZ	2.45	0.52
2:E:298:ARG:NH2	2:E:441:GLY:O	2.35	0.52
2:F:101:VAL:O	2:F:105:HIS:CB	2.54	0.52
4:J:41:PRO:HD3	4:J:94:GLY:HA2	1.92	0.52
3:G:136:LEU:HD13	3:G:175:LEU:HD22	1.92	0.52
3:G:155:GLN:OE1	3:G:158:ASN:ND2	2.42	0.52
4:H:41:PRO:HD3	4:H:94:GLY:HA2	1.92	0.52
4:H:162:VAL:HG11	4:H:170:VAL:HG21	1.91	0.52
3:I:6:GLN:NE2	3:I:86:TYR:O	2.43	0.52
6:L:186:TYR:HA	6:L:192:TYR:OH	2.09	0.52
4:J:162:VAL:HG11	4:J:170:VAL:HG21	1.91	0.52
6:L:19:VAL:HG12	6:L:75:ILE:HB	1.92	0.52
1:A:628:TRP:O	1:A:632:ASP:N	2.41	0.51
2:F:192:ARG:O	2:F:193:LEU:HD23	2.09	0.51
1:A:635:ILE:O	1:A:639:THR:OG1	2.21	0.51
2:D:293:GLN:HE22	2:D:446:VAL:HG13	1.74	0.51
3:G:67:ASP:OD1	3:G:70:GLU:N	2.44	0.51
4:J:12:VAL:HG11	4:J:18:LEU:HD13	1.92	0.51
8:c:2:NAG:H62	12:d:2:NAG:H5	1.91	0.51
2:E:179:LEU:HD12	2:E:420:ILE:O	2.09	0.51
2:F:122:LEU:HD11	2:F:203:GLN:HB3	1.93	0.51
4:H:12:VAL:HG11	4:H:18:LEU:HD13	1.92	0.51
4:H:74:ARG:HA	4:H:81:VAL:HA	1.91	0.51
4:H:185:THR:HA	4:H:200:SER:HA	1.93	0.51
2:D:501:CYS:SG	2:D:502:LYS:N	2.84	0.51
2:E:501:CYS:SG	2:E:502:LYS:N	2.84	0.51
6:N:19:VAL:HG12	6:N:75:ILE:HB	1.92	0.51
2:D:278:THR:CG2	5:K:74:LEU:HG	2.33	0.51
2:F:165:LEU:C	2:F:167:ASP:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:185:THR:HA	4:J:200:SER:HA	1.93	0.51
1:A:622:ILE:HA	1:A:626:MET:HB3	1.93	0.51
2:D:260:LEU:HD12	2:D:451:GLY:HA3	1.93	0.51
2:E:122:LEU:HD11	2:E:203:GLN:HB3	1.93	0.51
1:B:635:ILE:O	1:B:639:THR:OG1	2.21	0.51
1:C:629:LEU:CD2	5:O:100:ARG:HG2	2.41	0.51
2:E:362:ALA:CB	2:E:467:THR:CG2	2.89	0.51
2:F:180:ASP:OD2	2:F:422:GLN:HB2	2.10	0.51
2:F:260:LEU:HD12	2:F:451:GLY:HA3	1.93	0.51
1:B:633:LYS:NZ	5:K:100:ARG:O	2.42	0.51
2:D:99:ASN:HD21	2:D:483:LEU:HB3	1.76	0.51
3:G:6:GLN:NE2	3:G:86:TYR:O	2.43	0.51
3:I:67:ASP:OD1	3:I:70:GLU:N	2.44	0.51
4:J:22:CYS:HB3	4:J:81:VAL:HB	1.93	0.51
5:K:100(I):VAL:HG12	6:L:91:TYR:HB2	1.93	0.51
2:E:175:LEU:O	2:E:320:THR:OG1	2.27	0.51
1:C:635:ILE:O	1:C:639:THR:OG1	2.21	0.50
2:E:133:ASN:OD1	2:E:155:LYS:NZ	2.29	0.50
6:L:65:SER:OG	6:L:72:THR:OG1	2.29	0.50
2:E:183:GLN:N	2:E:191:TYR:HB3	2.15	0.50
1:B:567:LYS:NZ	2:F:106:THR:HB	2.26	0.50
2:D:87:GLU:HG2	8:T:1:NAG:HN2	1.75	0.50
2:E:159:PHE:O	2:E:171:LYS:HG3	2.11	0.50
2:F:99:ASN:HD21	2:F:483:LEU:HB3	1.76	0.50
4:H:22:CYS:HB3	4:H:81:VAL:HB	1.93	0.50
5:O:74:LEU:CD1	5:O:77(B):PRO:HA	2.42	0.50
2:E:289:ASN:HB3	2:E:344:LYS:NZ	2.27	0.50
4:J:141:VAL:HG21	4:J:218:VAL:HG21	1.94	0.50
2:D:165:LEU:C	2:D:167:ASP:N	2.70	0.50
2:D:289:ASN:HB3	2:D:344:LYS:NZ	2.26	0.50
2:F:289:ASN:HB3	2:F:344:LYS:NZ	2.26	0.50
4:H:141:VAL:HG21	4:H:218:VAL:HG21	1.94	0.50
4:H:155:THR:HA	4:H:206:SER:H	1.76	0.50
3:I:161:GLU:HA	3:I:177:SER:HA	1.93	0.50
5:O:100(I):VAL:HG12	6:P:91:TYR:HB2	1.94	0.50
5:O:210:ARG:HG2	5:O:210:ARG:NH1	2.20	0.50
6:P:65:SER:OG	6:P:72:THR:OG1	2.29	0.50
1:C:622:ILE:HA	1:C:626:MET:HB3	1.93	0.50
1:C:628:TRP:O	1:C:632:ASP:N	2.41	0.50
1:C:629:LEU:CD2	5:O:100:ARG:CG	2.89	0.50
2:D:170:GLN:HG2	2:D:172:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:136:LEU:HD13	3:I:175:LEU:HD22	1.93	0.50
5:M:74:LEU:CD1	5:M:77(B):PRO:HA	2.42	0.50
1:B:622:ILE:HA	1:B:626:MET:HB3	1.93	0.50
2:D:192:ARG:O	2:D:193:LEU:HD23	2.12	0.50
2:E:99:ASN:HD21	2:E:483:LEU:HB3	1.76	0.50
2:F:55:ALA:HB3	2:F:216:HIS:HB2	1.94	0.50
2:F:64:GLU:O	2:F:68:VAL:N	2.41	0.50
2:F:501:CYS:SG	2:F:502:LYS:N	2.84	0.50
2:D:122:LEU:HD11	2:D:203:GLN:HB3	1.93	0.50
2:D:129:LEU:CB	2:D:191:TYR:O	2.59	0.50
2:E:55:ALA:HB3	2:E:216:HIS:HB2	1.94	0.50
4:J:155:THR:HA	4:J:206:SER:H	1.76	0.50
5:M:210:ARG:HH11	5:M:210:ARG:CG	2.16	0.50
6:N:65:SER:OG	6:N:72:THR:OG1	2.29	0.50
2:F:161:MET:O	2:F:170:GLN:N	2.45	0.49
1:A:530:MET:HA	1:A:533:ALA:HB3	1.94	0.49
1:C:530:MET:HA	1:C:533:ALA:HB3	1.94	0.49
2:D:175:LEU:O	2:D:320:THR:OG1	2.27	0.49
2:F:184:ILE:HG22	2:F:190:GLU:O	2.13	0.49
3:G:161:GLU:HA	3:G:177:SER:HA	1.93	0.49
1:B:658:GLN:O	1:B:662:ALA:HB2	2.12	0.49
2:D:46:LYS:HG2	5:K:100(A):TRP:CZ2	2.47	0.49
4:H:186:PHE:HB2	4:H:199:SER:HB2	1.94	0.49
3:I:186:TYR:O	3:I:192:TYR:OH	2.29	0.49
4:J:143:PRO:HA	4:J:160:CYS:HA	1.94	0.49
1:B:530:MET:HA	1:B:533:ALA:HB3	1.94	0.49
1:C:571:TRP:HZ2	2:E:111:LEU:HD12	1.78	0.49
4:J:164:ASP:HA	4:J:195:LEU:HB3	1.94	0.49
5:K:74:LEU:HB2	5:K:77(C):PRO:HG3	1.95	0.49
2:D:55:ALA:HB3	2:D:216:HIS:HB2	1.94	0.49
2:D:384:TYR:N	2:D:419:ARG:O	2.42	0.49
2:E:161:MET:O	2:E:170:GLN:N	2.45	0.49
4:J:176:SER:N	4:J:217:ASN:OD1	2.46	0.49
4:J:186:PHE:HB2	4:J:199:SER:HB2	1.94	0.49
1:A:658:GLN:O	1:A:662:ALA:HB2	2.12	0.49
4:H:30:PRO:HB2	4:H:54:TRP:HE1	1.78	0.49
4:J:7:SER:OG	4:J:21:SER:OG	2.29	0.49
5:K:210:ARG:HG2	5:K:210:ARG:NH1	2.20	0.49
5:M:3:HIS:HE1	7:O:3:BMA:C3	2.10	0.49
5:O:210:ARG:HH11	5:O:210:ARG:CG	2.16	0.49
1:B:601:LYS:HB3	1:B:604:CYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:126:PRO:HD2	5:O:213:PRO:HA	1.95	0.49
2:E:165:LEU:C	2:E:167:ASP:N	2.70	0.49
2:E:260:LEU:HD12	2:E:451:GLY:HA3	1.93	0.49
4:H:7:SER:OG	4:H:21:SER:OG	2.29	0.49
5:K:74:LEU:CD1	5:K:77(B):PRO:HA	2.42	0.49
5:M:74:LEU:HB2	5:M:77(C):PRO:HG3	1.95	0.49
1:A:601:LYS:HB3	1:A:604:CYS:HB3	1.94	0.49
5:O:74:LEU:HB2	5:O:77(C):PRO:HG3	1.94	0.49
6:L:52:ALA:HB3	7:R:2:NAG:H62	1.94	0.49
1:C:633:LYS:HB3	6:P:50:ARG:HH21	1.77	0.48
4:H:143:PRO:HA	4:H:160:CYS:HA	1.95	0.48
5:O:147:PRO:O	5:O:200:HIS:NE2	2.38	0.48
3:G:144:ALA:HB2	3:G:198:HIS:HD2	1.79	0.48
5:K:6:GLN:NE2	5:K:107:THR:HG23	2.26	0.48
5:K:126:PRO:HD2	5:K:213:PRO:HA	1.95	0.48
5:M:126:PRO:HD2	5:M:213:PRO:HA	1.95	0.48
1:C:658:GLN:O	1:C:662:ALA:HB2	2.12	0.48
2:E:342:LEU:HD22	2:E:361:PHE:HE2	1.76	0.48
4:H:164:ASP:HA	4:H:195:LEU:HB3	1.94	0.48
3:I:118:PHE:HZ	4:J:157:ALA:HB3	1.77	0.48
5:M:100(I):VAL:HG12	6:N:91:TYR:HB2	1.93	0.48
2:E:214:PRO:HG3	2:E:252:LYS:HD2	1.95	0.48
2:E:304:ARG:NH1	2:E:318:TYR:CD1	2.82	0.48
3:G:163:VAL:HG22	3:G:175:LEU:HG	1.96	0.48
4:J:30:PRO:HB2	4:J:54:TRP:HE1	1.78	0.48
5:K:70:SER:HB2	9:W:4:MAN:HO2	1.72	0.48
1:C:601:LYS:HB3	1:C:604:CYS:HB3	1.95	0.48
2:F:138:ILE:HA	2:F:141:ASP:HB3	1.96	0.48
4:H:176:SER:N	4:H:217:ASN:OD1	2.46	0.48
3:I:13:ALA:O	3:I:107:LYS:N	2.43	0.48
5:K:33:TYR:CD2	5:K:94:THR:HG22	2.49	0.48
1:A:631:TRP:HZ2	2:F:497:ALA:HA	1.79	0.48
1:A:633:LYS:HE2	5:M:100(A):TRP:HA	1.94	0.48
2:D:138:ILE:HA	2:D:141:ASP:HB3	1.96	0.48
2:D:173:TYR:CE1	7:U:1:NAG:C1	2.97	0.48
5:M:35(A):ASN:O	5:M:93:THR:HB	2.14	0.48
1:B:597:GLY:O	1:B:601:LYS:NZ	2.40	0.48
2:D:64:GLU:O	2:D:68:VAL:N	2.41	0.48
2:E:294:ILE:HD12	2:E:449:ILE:HD11	1.96	0.48
2:F:294:ILE:HD12	2:F:449:ILE:HD11	1.96	0.48
5:M:33:TYR:CD2	5:M:94:THR:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:3:HIS:ND1	7:n:3:BMA:C5	2.76	0.48
2:D:318:TYR:O	2:D:438:PRO:HD2	2.13	0.48
4:H:20:LEU:HB2	4:H:83:LEU:HB3	1.96	0.48
3:I:37:GLN:HB2	3:I:47:LEU:HD11	1.96	0.48
5:K:35(A):ASN:O	5:K:93:THR:HB	2.14	0.48
5:M:60:SER:O	5:M:64:ARG:N	2.47	0.48
1:A:579:ARG:NH2	1:C:584:GLU:OE1	2.47	0.47
2:E:138:ILE:HA	2:E:141:ASP:HB3	1.96	0.47
2:F:214:PRO:HG3	2:F:252:LYS:HD2	1.95	0.47
2:F:384:TYR:N	2:F:419:ARG:O	2.43	0.47
5:O:60:SER:O	5:O:64:ARG:N	2.47	0.47
2:F:163:THR:CG2	2:F:170:GLN:HB3	2.44	0.47
3:I:163:VAL:HG22	3:I:175:LEU:HG	1.96	0.47
2:D:302:ASN:H	2:D:441:GLY:H	1.63	0.47
2:E:197:ASN:CB	2:F:164:GLU:CD	2.87	0.47
2:E:276:ASN:OD1	2:E:278:THR:OG1	2.26	0.47
2:E:304:ARG:NH2	2:E:318:TYR:CD2	2.82	0.47
3:I:144:ALA:HB2	3:I:198:HIS:HD2	1.78	0.47
4:J:20:LEU:HB2	4:J:83:LEU:HB3	1.97	0.47
1:A:597:GLY:O	1:A:601:LYS:NZ	2.40	0.47
2:D:214:PRO:HG3	2:D:252:LYS:HD2	1.95	0.47
2:E:318:TYR:O	2:E:438:PRO:HD2	2.13	0.47
2:E:334:SER:HA	2:E:413:SER:HA	1.96	0.47
4:H:158:LEU:HB2	4:H:231:VAL:HG11	1.96	0.47
3:I:61:ARG:NH2	3:I:82:ASP:OD1	2.45	0.47
5:O:33:TYR:CD2	5:O:94:THR:HG22	2.49	0.47
5:O:35(A):ASN:O	5:O:93:THR:HB	2.14	0.47
2:E:289:ASN:HB3	2:E:344:LYS:HZ2	1.80	0.47
3:G:37:GLN:N	3:G:45:THR:O	2.47	0.47
3:I:151:ASP:HA	3:I:191:VAL:HB	1.97	0.47
2:D:159:PHE:CE2	2:D:172:VAL:HG22	2.49	0.47
2:D:298:ARG:N	2:D:443:ILE:O	2.42	0.47
3:G:61:ARG:NH2	3:G:82:ASP:OD1	2.45	0.47
5:K:210:ARG:CG	5:K:210:ARG:NH1	2.75	0.47
5:O:3:HIS:CG	7:n:3:BMA:C5	2.97	0.47
1:B:659:ASP:OD2	1:C:603:ILE:HD11	2.15	0.47
2:D:161:MET:O	2:D:170:GLN:N	2.47	0.47
2:D:192:ARG:NH2	2:D:193:LEU:O	2.46	0.47
2:D:358:ILE:HG12	2:D:396:ILE:HG12	1.97	0.47
2:E:358:ILE:HG12	2:E:396:ILE:HG12	1.97	0.47
2:E:384:TYR:N	2:E:419:ARG:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:276:ASN:OD1	2:F:278:THR:OG1	2.26	0.47
4:J:140:SER:N	4:J:163:LYS:O	2.45	0.47
4:J:158:LEU:HB2	4:J:231:VAL:HG11	1.97	0.47
4:J:206:SER:HA	4:J:209:LEU:HG	1.97	0.47
5:O:210:ARG:NH1	5:O:210:ARG:CG	2.75	0.47
2:D:183:GLN:CB	2:D:191:TYR:CE2	2.90	0.47
2:D:303:THR:O	2:D:321:GLY:N	2.39	0.47
2:F:182:VAL:O	2:F:191:TYR:HB2	2.14	0.47
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.96	0.47
3:G:151:ASP:HA	3:G:191:VAL:HB	1.97	0.47
3:I:37:GLN:O	3:I:45:THR:N	2.48	0.47
5:K:60:SER:O	5:K:64:ARG:N	2.47	0.47
5:M:100(F):HIS:HB2	6:N:32:TRP:CE3	2.50	0.47
5:O:100(F):HIS:HB2	6:P:32:TRP:CE3	2.50	0.47
1:B:633:LYS:O	1:B:636:SER:OG	2.26	0.47
2:D:230:ASP:OD2	2:D:233:PHE:HB2	2.15	0.47
2:D:334:SER:HA	2:D:413:SER:HA	1.97	0.47
2:E:230:ASP:OD2	2:E:233:PHE:HB2	2.15	0.47
4:H:104:ASN:OD1	4:H:108:ARG:N	2.48	0.47
3:I:47:LEU:HA	3:I:58:VAL:HG21	1.96	0.47
4:J:52:ARG:HD3	4:J:56:TYR:HB3	1.97	0.47
5:M:210:ARG:HG2	5:M:210:ARG:NH1	2.20	0.47
1:A:588:ARG:HH12	1:B:548:ILE:C	2.23	0.47
1:B:603:ILE:HG22	2:D:40:TYR:H	1.80	0.47
1:C:614:TRP:NE1	15:C:701:NAG:HN2	2.13	0.47
2:D:294:ILE:HD12	2:D:449:ILE:HD11	1.96	0.47
2:E:160:ASN:OD1	2:E:171:LYS:CB	2.63	0.47
2:E:302:ASN:H	2:E:441:GLY:H	1.63	0.47
2:E:390:LEU:HG	2:E:416:LEU:HD11	1.97	0.47
2:F:298:ARG:N	2:F:443:ILE:O	2.42	0.47
3:G:37:GLN:O	3:G:45:THR:N	2.48	0.47
6:L:11:LEU:HD13	6:L:19:VAL:HG21	1.97	0.47
2:D:304:ARG:CD	2:D:318:TYR:HB3	2.45	0.46
2:E:278:THR:CG2	5:O:74:LEU:CG	2.93	0.46
2:F:170:GLN:HE22	2:F:307:ILE:CG2	2.20	0.46
6:N:11:LEU:HD13	6:N:19:VAL:HG21	1.97	0.46
2:F:276:ASN:HB3	2:F:282:LYS:HG3	1.97	0.46
2:F:358:ILE:HG12	2:F:396:ILE:HG12	1.96	0.46
3:G:47:LEU:HA	3:G:58:VAL:HG21	1.97	0.46
5:M:93:THR:HA	5:M:102:SER:O	2.15	0.46
5:O:82(C):LEU:HB3	5:O:111:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:GLU:OE2	2:D:229:LYS:HD3	2.16	0.46
2:D:231:LYS:HA	2:D:267:GLU:HG3	1.97	0.46
4:H:206:SER:HA	4:H:209:LEU:HG	1.97	0.46
4:J:104:ASN:OD1	4:J:108:ARG:N	2.48	0.46
5:K:93:THR:HA	5:K:102:SER:O	2.15	0.46
2:E:91:GLU:HG2	2:E:487:LYS:NZ	2.31	0.46
2:E:270:VAL:HG12	2:E:288:PHE:HA	1.98	0.46
2:F:231:LYS:HA	2:F:267:GLU:HG3	1.97	0.46
2:F:334:SER:HA	2:F:413:SER:HA	1.96	0.46
4:H:163:LYS:HA	4:H:197:SER:HA	1.98	0.46
2:E:231:LYS:HA	2:E:267:GLU:HG3	1.97	0.46
5:K:100(F):HIS:HB2	6:L:32:TRP:CE3	2.50	0.46
2:E:182:VAL:C	2:E:191:TYR:CB	2.88	0.46
2:E:266:ALA:N	2:E:288:PHE:O	2.42	0.46
2:F:342:LEU:HD22	2:F:361:PHE:HE2	1.80	0.46
4:J:20:LEU:HD12	4:J:83:LEU:HD23	1.98	0.46
5:M:82(C):LEU:HB3	5:M:111:VAL:HG21	1.97	0.46
5:M:40:ALA:HB3	5:M:43:GLN:HB2	1.98	0.46
2:F:230:ASP:OD2	2:F:233:PHE:HB2	2.15	0.46
2:F:302:ASN:H	2:F:441:GLY:H	1.63	0.46
4:J:78:ARG:NH1	4:J:82:TYR:OH	2.49	0.46
1:C:614:TRP:HE1	15:C:701:NAG:HN2	1.64	0.46
2:D:342:LEU:HD22	2:D:361:PHE:HE2	1.80	0.46
2:E:276:ASN:HB3	2:E:282:LYS:HG3	1.97	0.46
2:F:160:ASN:OD1	2:F:171:LYS:CB	2.64	0.46
2:F:180:ASP:OD1	2:F:423:ILE:N	2.34	0.46
2:F:182:VAL:O	2:F:191:TYR:CB	2.63	0.46
6:L:144:ALA:HB2	6:L:198:HIS:HD2	1.81	0.46
5:M:6:GLN:NE2	5:M:107:THR:HG23	2.26	0.46
6:P:11:LEU:HD13	6:P:19:VAL:HG21	1.97	0.46
1:A:565:LEU:HD11	2:F:61:TYR:HE1	1.81	0.46
2:E:64:GLU:O	2:E:68:VAL:N	2.41	0.46
2:E:160:ASN:OD1	2:E:171:LYS:HB2	2.15	0.46
2:E:197:ASN:HB2	2:F:164:GLU:OE2	2.15	0.46
2:F:160:ASN:OD1	2:F:171:LYS:HB2	2.15	0.46
2:F:270:VAL:HG12	2:F:288:PHE:HA	1.98	0.46
4:H:78:ARG:NH1	4:H:82:TYR:OH	2.49	0.46
5:K:2:ILE:HG21	5:K:27:VAL:HG23	1.98	0.46
5:K:82(C):LEU:HB3	5:K:111:VAL:HG21	1.97	0.46
6:L:124:GLN:O	6:L:127:SER:OG	2.31	0.46
5:O:93:THR:HA	5:O:102:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:GLY:HA2	2:D:315:GLN:HB2	1.98	0.45
2:E:163:THR:CG2	2:E:170:GLN:HB3	2.46	0.45
2:F:390:LEU:HG	2:F:416:LEU:HD11	1.97	0.45
4:H:52:ARG:HD3	4:H:56:TYR:HB3	1.97	0.45
5:K:24:ALA:O	5:K:77(B):PRO:HB2	2.16	0.45
6:L:52:ALA:CB	7:R:2:NAG:C6	2.93	0.45
5:M:3:HIS:ND1	7:O:3:BMA:O4	2.49	0.45
6:N:124:GLN:O	6:N:127:SER:OG	2.31	0.45
6:N:134:CYS:HB2	6:N:148:TRP:CH2	2.51	0.45
1:C:632:ASP:HA	1:C:635:ILE:HG12	1.99	0.45
2:D:304:ARG:HD3	2:D:318:TYR:CG	2.51	0.45
2:E:312:GLY:HA2	2:E:315:GLN:HB2	1.98	0.45
3:G:59:PRO:HG2	3:G:61:ARG:NH1	2.31	0.45
3:I:37:GLN:N	3:I:45:THR:O	2.47	0.45
6:L:52:ALA:HB3	7:R:2:NAG:H61	1.97	0.45
6:L:124:GLN:HG2	6:L:129:THR:O	2.17	0.45
2:D:259:LEU:HB2	2:D:374:HIS:CE1	2.52	0.45
2:D:270:VAL:HG12	2:D:288:PHE:HA	1.98	0.45
2:F:36:VAL:HG12	2:F:498:PRO:HB3	1.98	0.45
2:F:83:GLU:OE2	2:F:229:LYS:HD3	2.16	0.45
3:G:19:VAL:O	3:G:75:ILE:N	2.41	0.45
4:H:140:SER:N	4:H:163:LYS:O	2.45	0.45
4:J:163:LYS:HA	4:J:197:SER:HA	1.98	0.45
2:D:390:LEU:HG	2:D:416:LEU:HD11	1.97	0.45
2:F:175:LEU:O	2:F:320:THR:OG1	2.27	0.45
1:B:655:LYS:NZ	1:C:601:LYS:HA	2.32	0.45
2:D:91:GLU:HG2	2:D:487:LYS:NZ	2.31	0.45
2:F:91:GLU:HG2	2:F:487:LYS:NZ	2.31	0.45
2:F:259:LEU:HB2	2:F:374:HIS:CE1	2.52	0.45
3:G:129:THR:HG21	4:H:163:LYS:HE2	1.98	0.45
3:G:147:GLN:O	3:G:195:GLU:N	2.47	0.45
4:H:20:LEU:HD12	4:H:83:LEU:HD23	1.98	0.45
6:N:144:ALA:HB2	6:N:198:HIS:HD2	1.81	0.45
6:P:144:ALA:HB2	6:P:198:HIS:HD2	1.81	0.45
2:D:93:PHE:HE2	2:D:228:CYS:HB2	1.82	0.45
4:H:50:PHE:HE2	4:H:52:ARG:HG3	1.82	0.45
3:I:89:GLN:HE21	3:I:96:VAL:HG13	1.82	0.45
2:D:276:ASN:HB3	2:D:282:LYS:HG3	1.97	0.45
2:E:36:VAL:HG12	2:E:498:PRO:HB3	1.98	0.45
2:E:83:GLU:OE2	2:E:229:LYS:HD3	2.16	0.45
4:H:8:GLY:HA3	4:H:20:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:19:VAL:O	3:I:75:ILE:N	2.41	0.45
5:O:24:ALA:O	5:O:77(B):PRO:HB2	2.16	0.45
5:O:40:ALA:HB3	5:O:43:GLN:HB2	1.98	0.45
6:P:167:ASP:HB3	6:P:170:ASP:OD1	2.17	0.45
1:B:584:GLU:OE1	1:C:579:ARG:NH2	2.50	0.45
2:D:305:LYS:O	2:D:319:ALA:N	2.43	0.45
2:E:278:THR:HG23	5:O:74:LEU:CG	2.45	0.45
3:I:59:PRO:HG2	3:I:61:ARG:NH1	2.31	0.45
5:M:210:ARG:CG	5:M:210:ARG:NH1	2.75	0.45
1:C:630:GLN:CG	6:P:32:TRP:CZ2	2.99	0.45
2:E:106:THR:O	2:E:110:SER:HB3	2.17	0.45
2:E:183:GLN:CB	2:E:191:TYR:HB3	2.32	0.45
2:E:259:LEU:HB2	2:E:374:HIS:CE1	2.52	0.45
2:F:131:CYS:HB2	2:F:191:TYR:CE1	2.51	0.45
3:G:76:ASN:HA	3:G:77:THR:HA	1.64	0.45
5:K:71:ALA:HA	5:K:78:SER:HA	1.98	0.45
5:M:35:VAL:HA	5:M:93:THR:O	2.17	0.45
5:M:71:ALA:HA	5:M:78:SER:HA	1.98	0.45
5:O:6:GLN:NE2	5:O:107:THR:HG23	2.26	0.45
6:P:37:GLN:HB2	6:P:86:PHE:CE1	2.52	0.45
1:A:632:ASP:HA	1:A:635:ILE:HG12	1.99	0.45
2:D:106:THR:O	2:D:110:SER:HB3	2.17	0.45
2:F:106:THR:O	2:F:110:SER:HB3	2.17	0.45
4:H:6:GLU:OE2	4:H:124:GLY:HA3	2.18	0.45
5:M:24:ALA:O	5:M:77(B):PRO:HB2	2.16	0.45
6:N:167:ASP:HB3	6:N:170:ASP:OD1	2.17	0.45
6:P:134:CYS:HB2	6:P:148:TRP:CH2	2.51	0.45
1:B:605:CYS:SG	2:D:501:CYS:SG	3.12	0.44
2:F:93:PHE:HE2	2:F:228:CYS:HB2	1.82	0.44
3:I:147:GLN:O	3:I:195:GLU:N	2.47	0.44
5:K:40:ALA:HB3	5:K:43:GLN:HB2	1.98	0.44
5:K:147:PRO:O	5:K:200:HIS:NE2	2.38	0.44
6:L:37:GLN:HB2	6:L:86:PHE:CE1	2.52	0.44
6:N:124:GLN:HG2	6:N:129:THR:O	2.17	0.44
1:B:632:ASP:HA	1:B:635:ILE:HG12	1.99	0.44
2:F:312:GLY:HA2	2:F:315:GLN:HB2	1.98	0.44
3:G:160:GLN:HE22	4:H:191:GLN:HG2	1.82	0.44
4:H:146:PRO:HG3	4:H:158:LEU:HB3	1.99	0.44
3:I:76:ASN:HA	3:I:77:THR:HA	1.64	0.44
6:P:124:GLN:HG2	6:P:129:THR:O	2.17	0.44
1:B:528:SER:OG	1:B:529:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:120:VAL:HG11	2:E:203:GLN:HE21	1.83	0.44
2:F:131:CYS:CB	2:F:191:TYR:CE1	3.00	0.44
4:J:6:GLU:OE2	4:J:124:GLY:HA3	2.17	0.44
4:J:146:PRO:HG3	4:J:158:LEU:HB3	1.99	0.44
6:L:134:CYS:HB2	6:L:148:TRP:CH2	2.52	0.44
1:C:528:SER:OG	1:C:529:THR:N	2.51	0.44
2:F:359:ILE:O	2:F:395:TRP:N	2.47	0.44
4:H:19:ARG:NE	4:H:84:ASP:OD1	2.51	0.44
4:H:172:VAL:HA	4:H:218:VAL:HA	2.00	0.44
2:D:447:SER:OG	10:X:1:NAG:N2	2.50	0.44
2:F:120:VAL:HG11	2:F:203:GLN:HE21	1.83	0.44
2:F:192:ARG:O	2:F:193:LEU:HG	2.18	0.44
3:I:21:ILE:O	3:I:73:LEU:N	2.48	0.44
6:N:37:GLN:HB2	6:N:86:PHE:CE1	2.52	0.44
2:E:93:PHE:HE2	2:E:228:CYS:HB2	1.82	0.44
2:F:159:PHE:O	2:F:171:LYS:CG	2.66	0.44
3:G:13:ALA:O	3:G:107:LYS:N	2.43	0.44
4:H:161:LEU:HG	4:H:163:LYS:HB2	2.00	0.44
2:D:153:GLU:OE2	2:D:177:TYR:HB3	2.18	0.44
2:D:163:THR:CG2	2:D:170:GLN:HB2	2.48	0.44
2:E:173:TYR:CE1	12:i:1:NAG:C1	3.00	0.44
2:E:184:ILE:HG22	2:E:191:TYR:HA	1.99	0.44
2:E:298:ARG:N	2:E:443:ILE:O	2.42	0.44
2:F:266:ALA:N	2:F:288:PHE:O	2.42	0.44
4:J:8:GLY:HA3	4:J:20:LEU:HD23	1.98	0.44
4:J:19:ARG:NE	4:J:84:ASP:OD1	2.51	0.44
4:J:161:LEU:HG	4:J:163:LYS:HB2	2.00	0.44
6:L:52:ALA:CB	7:R:2:NAG:H62	2.48	0.44
6:L:167:ASP:HB3	6:L:170:ASP:OD1	2.17	0.44
12:f:1:NAG:H4	12:f:2:NAG:H2	1.83	0.44
2:D:226:LEU:HD12	2:D:487:LYS:HD3	1.99	0.44
2:E:183:GLN:CB	2:E:191:TYR:CD2	2.94	0.44
3:G:89:GLN:HE21	3:G:96:VAL:HG13	1.82	0.44
2:D:36:VAL:HG12	2:D:498:PRO:HB3	1.98	0.43
2:E:137:ASN:HB2	2:E:326:ILE:HB	2.00	0.43
2:F:153:GLU:OE2	2:F:177:TYR:HB3	2.18	0.43
2:F:226:LEU:HD12	2:F:487:LYS:HD3	2.00	0.43
5:O:35:VAL:HA	5:O:93:THR:O	2.17	0.43
1:B:658:GLN:O	1:B:662:ALA:CB	2.66	0.43
2:D:137:ASN:HB2	2:D:326:ILE:HB	2.00	0.43
2:D:192:ARG:H	2:D:192:ARG:HG3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:ASN:HD22	2:E:326:ILE:H	1.66	0.43
2:E:160:ASN:HA	2:E:171:LYS:CA	2.48	0.43
2:F:137:ASN:HD22	2:F:326:ILE:H	1.67	0.43
2:F:289:ASN:HB3	2:F:344:LYS:HZ1	1.82	0.43
3:I:46:LEU:HD22	4:J:119:GLY:HA3	1.99	0.43
1:A:528:SER:OG	1:A:529:THR:N	2.51	0.43
1:C:603:ILE:HG22	2:E:40:TYR:H	1.84	0.43
4:J:220:HIS:O	4:J:224:ASN:N	2.51	0.43
5:K:35:VAL:HA	5:K:93:THR:O	2.17	0.43
5:O:71:ALA:HA	5:O:78:SER:HA	1.98	0.43
1:A:658:GLN:O	1:A:662:ALA:CB	2.66	0.43
1:C:633:LYS:CD	6:P:50:ARG:NH2	2.81	0.43
1:C:658:GLN:O	1:C:662:ALA:CB	2.66	0.43
2:D:137:ASN:HD22	2:D:326:ILE:H	1.67	0.43
2:E:192:ARG:H	2:E:192:ARG:HG3	1.64	0.43
3:G:150:VAL:HG13	3:G:192:TYR:HE1	1.84	0.43
5:O:25:TYR:CD1	5:O:77(B):PRO:HG3	2.54	0.43
1:C:631:TRP:CH2	2:E:498:PRO:HD2	2.53	0.43
4:H:220:HIS:O	4:H:224:ASN:N	2.51	0.43
5:K:2:ILE:HG21	5:K:27:VAL:CG2	2.49	0.43
2:D:46:LYS:NZ	5:K:100(A):TRP:CD2	2.68	0.43
2:D:359:ILE:O	2:D:395:TRP:N	2.47	0.43
2:E:153:GLU:OE2	2:E:177:TYR:HB3	2.18	0.43
4:H:219:ASN:HA	4:H:226:LYS:HA	2.01	0.43
5:M:25:TYR:CD1	5:M:77(B):PRO:HG3	2.54	0.43
5:M:72:VAL:HG22	9:y:4:MAN:H62	2.00	0.43
5:M:147:PRO:O	5:M:200:HIS:NE2	2.38	0.43
2:F:137:ASN:HB2	2:F:326:ILE:HB	2.00	0.43
2:F:192:ARG:O	2:F:193:LEU:CD2	2.67	0.43
4:J:50:PHE:HE2	4:J:52:ARG:HG3	1.82	0.43
4:J:172:VAL:HA	4:J:218:VAL:HA	2.00	0.43
5:M:33:TYR:HD2	5:M:94:THR:HG22	1.84	0.43
1:B:618:ASN:HB2	1:B:621:GLU:HG3	2.00	0.43
2:E:373:THR:OG1	2:E:375:SER:OG	2.36	0.43
15:E:639:NAG:HO4	12:r:1:NAG:C4	2.31	0.43
2:F:160:ASN:HA	2:F:171:LYS:CA	2.48	0.43
3:G:20:THR:HA	3:G:74:SER:HA	2.01	0.43
4:H:188:ALA:HA	4:H:198:LEU:HA	2.01	0.43
5:K:3:HIS:C	5:K:4:LEU:CG	2.63	0.43
2:F:159:PHE:C	2:F:171:LYS:HG3	2.44	0.43
3:G:137:ASN:OD1	3:G:174:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:20:THR:HA	3:I:74:SER:HA	2.01	0.43
1:C:618:ASN:HB2	1:C:621:GLU:HG3	2.00	0.42
2:D:55:ALA:N	2:D:216:HIS:O	2.52	0.42
2:D:120:VAL:HG11	2:D:203:GLN:HE21	1.83	0.42
5:K:25:TYR:CD1	5:K:77(B):PRO:HG3	2.54	0.42
4:H:188:ALA:HB2	4:H:198:LEU:HD12	2.01	0.42
3:I:150:VAL:HG13	3:I:192:TYR:HE1	1.84	0.42
1:A:539:VAL:HG22	1:A:542:ARG:NH1	2.34	0.42
1:C:539:VAL:HG22	1:C:542:ARG:NH1	2.34	0.42
2:E:55:ALA:N	2:E:216:HIS:O	2.52	0.42
2:E:362:ALA:C	2:E:363:ASN:O	2.61	0.42
2:E:447:SER:OG	10:m:1:NAG:N2	2.52	0.42
2:F:91:GLU:HG2	2:F:487:LYS:HZ2	1.85	0.42
3:G:108:ARG:NE	3:G:170:ASP:O	2.53	0.42
2:D:266:ALA:N	2:D:288:PHE:O	2.43	0.42
2:E:180:ASP:OD1	2:E:423:ILE:N	2.34	0.42
2:E:226:LEU:HD12	2:E:487:LYS:HD3	2.00	0.42
2:F:55:ALA:N	2:F:216:HIS:O	2.52	0.42
2:F:129:LEU:CD1	2:F:191:TYR:O	2.62	0.42
2:F:261:LEU:HD23	2:F:449:ILE:HA	2.02	0.42
6:P:140:TYR:CD1	6:P:141:PRO:HA	2.55	0.42
3:G:17:ASP:H	3:G:78:LEU:HB3	1.84	0.42
4:H:73:SER:O	4:H:82:TYR:N	2.45	0.42
2:D:261:LEU:HD23	2:D:449:ILE:HA	2.02	0.42
1:B:539:VAL:HG22	1:B:542:ARG:NH1	2.34	0.42
1:C:597:GLY:O	1:C:601:LYS:NZ	2.40	0.42
2:D:163:THR:HG22	2:D:170:GLN:OE1	2.18	0.42
2:D:189:LYS:HB2	2:D:191:TYR:OH	2.19	0.42
2:F:46:LYS:NZ	5:M:100(A):TRP:NE1	2.66	0.42
3:G:187:GLU:HA	3:G:211:ARG:HG3	2.01	0.42
6:P:94:TYR:HA	6:P:95:PRO:HA	1.91	0.42
1:A:618:ASN:HB2	1:A:621:GLU:HG3	2.00	0.42
1:A:631:TRP:CH2	2:F:498:PRO:HD2	2.55	0.42
1:B:655:LYS:HE2	1:C:602:LEU:HB2	2.00	0.42
2:D:96:TRP:CE2	2:D:275:GLU:HB2	2.55	0.42
3:I:17:ASP:H	3:I:78:LEU:HB3	1.84	0.42
3:I:17:ASP:O	3:I:77:THR:OG1	2.36	0.42
6:L:46:LEU:HD23	6:L:55:LEU:HD22	2.02	0.42
2:D:305:LYS:HG3	2:D:321:GLY:HA2	2.01	0.42
2:E:261:LEU:HD23	2:E:449:ILE:HA	2.02	0.42
3:I:11:LEU:HB3	3:I:104:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:219:ASN:HA	4:J:226:LYS:HA	2.01	0.42
5:M:72:VAL:HG13	9:y:4:MAN:H62	2.02	0.42
6:P:4:MET:HE3	6:P:23:CYS:SG	2.60	0.42
1:C:634:GLU:OE2	6:P:30(A):GLY:HA2	2.20	0.42
3:I:187:GLU:HA	3:I:211:ARG:HG3	2.01	0.42
6:L:140:TYR:CD1	6:L:141:PRO:HA	2.55	0.42
1:C:633:LYS:HB3	6:P:50:ARG:NH2	2.35	0.41
6:L:4:MET:HE3	6:L:23:CYS:SG	2.60	0.41
1:C:631:TRP:HZ2	2:E:497:ALA:HA	1.85	0.41
2:D:180:ASP:OD1	2:D:423:ILE:N	2.34	0.41
2:F:373:THR:OG1	2:F:375:SER:OG	2.36	0.41
5:M:209:LYS:HD2	5:M:209:LYS:HA	1.91	0.41
1:B:522:PHE:HB3	2:D:84:ILE:HD13	2.02	0.41
2:F:192:ARG:NH1	8:x:1:NAG:O7	2.52	0.41
4:J:114:PHE:HB2	7:7:5:MAN:O3	2.21	0.41
5:K:33:TYR:HD2	5:K:94:THR:HG22	1.84	0.41
6:N:140:TYR:CD1	6:N:141:PRO:HA	2.55	0.41
1:A:571:TRP:HZ3	2:F:74:CYS:HB2	1.85	0.41
2:E:388:SER:HB3	12:r:1:NAG:O7	2.19	0.41
3:G:64:ALA:HA	3:G:73:LEU:HA	2.02	0.41
4:H:121:ASP:OD1	4:H:121:ASP:N	2.53	0.41
3:I:108:ARG:NE	3:I:170:ASP:O	2.53	0.41
4:J:188:ALA:HA	4:J:198:LEU:HA	2.01	0.41
6:P:46:LEU:HD23	6:P:55:LEU:HD22	2.02	0.41
3:G:11:LEU:HB3	3:G:104:VAL:HG22	2.02	0.41
4:J:121:ASP:OD1	4:J:121:ASP:N	2.53	0.41
6:N:4:MET:HE3	6:N:23:CYS:SG	2.60	0.41
2:D:159:PHE:CE2	2:D:172:VAL:HG21	2.46	0.41
2:F:96:TRP:CE2	2:F:275:GLU:HB2	2.55	0.41
2:F:257:THR:OG1	2:F:375:SER:N	2.48	0.41
12:6:1:NAG:H4	12:6:2:NAG:H2	1.88	0.41
1:A:602:LEU:HD21	1:C:595:ILE:HA	2.02	0.41
2:D:104:MET:HA	2:D:107:ASP:HB2	2.02	0.41
2:E:96:TRP:CE2	2:E:275:GLU:HB2	2.55	0.41
4:H:37:VAL:HG22	4:H:47:TRP:HD1	1.86	0.41
4:J:188:ALA:HB2	4:J:198:LEU:HD12	2.01	0.41
5:K:100(E):HIS:HA	5:K:100(J):MET:HB3	2.03	0.41
6:N:46:LEU:HD23	6:N:55:LEU:HD22	2.02	0.41
1:A:567:LYS:HZ2	2:E:106:THR:HB	1.84	0.41
4:H:62:PHE:HB3	4:H:66:ALA:HB3	2.03	0.41
3:I:195:GLU:HA	3:I:206:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:13:PRO:HD2	4:J:16:ARG:HH21	1.86	0.41
4:J:37:VAL:HA	4:J:47:TRP:HA	2.02	0.41
5:M:100(E):HIS:HA	5:M:100(J):MET:HB3	2.03	0.41
1:A:539:VAL:HG22	1:A:542:ARG:HH12	1.86	0.41
1:C:539:VAL:HG22	1:C:542:ARG:HH12	1.86	0.41
2:D:122:LEU:HB2	2:D:201:ILE:HG23	2.03	0.41
2:D:373:THR:OG1	2:D:375:SER:OG	2.36	0.41
2:E:362:ALA:O	2:E:363:ASN:C	2.64	0.41
2:F:165:LEU:CD1	2:F:168:LYS:HG3	2.27	0.41
3:G:195:GLU:HA	3:G:206:THR:HA	2.02	0.41
3:I:130:ALA:HB3	3:I:181:LEU:HB2	2.03	0.41
4:J:62:PHE:HB3	4:J:66:ALA:HB3	2.02	0.41
6:L:113:PRO:HB3	6:L:139:PHE:HB3	2.02	0.41
6:N:113:PRO:HB3	6:N:139:PHE:HB3	2.02	0.41
5:O:28:ASN:OD1	5:O:29:THR:N	2.54	0.41
2:E:55:ALA:HB1	2:E:77:THR:HA	2.03	0.41
2:E:164:GLU:HA	2:E:312:GLY:O	2.21	0.41
2:F:173:TYR:CD2	7:v:1:NAG:H5	2.56	0.41
2:F:309:ILE:HD11	2:F:317:PHE:HB2	2.03	0.41
5:K:95:THR:HA	5:K:101:SER:OG	2.21	0.41
5:M:153:SER:O	5:M:197:ASN:N	2.42	0.41
1:A:588:ARG:HE	1:B:545:LEU:HD13	1.86	0.40
2:D:164:GLU:HA	2:D:312:GLY:O	2.20	0.40
2:E:46:LYS:NZ	5:O:100(A):TRP:CG	2.89	0.40
2:E:165:LEU:HD12	2:E:168:LYS:CG	2.37	0.40
2:E:359:ILE:O	2:E:395:TRP:N	2.47	0.40
2:F:192:ARG:C	2:F:193:LEU:HG	2.45	0.40
4:J:168:GLU:HA	4:J:169:PRO:HA	1.92	0.40
5:O:95:THR:HA	5:O:101:SER:OG	2.21	0.40
6:P:18:THR:HA	6:P:76:GLY:HA2	2.03	0.40
2:D:189:LYS:CB	2:D:191:TYR:OH	2.69	0.40
2:E:91:GLU:HG2	2:E:487:LYS:HZ2	1.86	0.40
2:E:104:MET:HA	2:E:107:ASP:HB2	2.02	0.40
2:F:55:ALA:HB1	2:F:77:THR:HA	2.03	0.40
3:I:64:ALA:HA	3:I:73:LEU:HA	2.02	0.40
3:I:137:ASN:OD1	3:I:174:SER:OG	2.29	0.40
5:K:70:SER:HB2	9:W:4:MAN:C2	2.51	0.40
6:P:113:PRO:HB3	6:P:139:PHE:HB3	2.02	0.40
2:E:304:ARG:CZ	2:E:318:TYR:CG	3.03	0.40
3:G:24:ARG:HB3	3:G:70:GLU:HG3	2.03	0.40
3:G:130:ALA:HB3	3:G:181:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:179:LEU:HD22	4:J:214:TYR:CD1	2.57	0.40
5:O:153:SER:O	5:O:197:ASN:N	2.42	0.40
1:A:566:LEU:HG	2:F:72:HIS:CE1	2.56	0.40
2:D:234:ASN:HA	2:D:273:ARG:HG2	2.02	0.40
2:E:122:LEU:HB2	2:E:201:ILE:HG23	2.03	0.40
2:F:234:ASN:HA	2:F:273:ARG:HG2	2.02	0.40
3:G:161:GLU:OE2	3:G:175:LEU:HD11	2.22	0.40
3:G:186:TYR:O	3:G:192:TYR:OH	2.29	0.40
4:H:37:VAL:HA	4:H:47:TRP:HA	2.03	0.40
3:I:158:ASN:O	3:I:180:THR:N	2.54	0.40
3:I:161:GLU:OE2	3:I:175:LEU:HD11	2.22	0.40
4:J:37:VAL:HG22	4:J:47:TRP:HD1	1.86	0.40
4:J:73:SER:O	4:J:82:TYR:N	2.45	0.40
2:E:87:GLU:HB3	8:g:1:NAG:H82	2.02	0.40
2:E:101:VAL:HG22	2:E:479:TRP:HB3	2.04	0.40
3:G:21:ILE:O	3:G:73:LEU:N	2.48	0.40
4:H:30:PRO:HB3	4:H:76:ASP:OD2	2.21	0.40
4:J:13:PRO:HA	4:J:14:PRO:HD3	1.97	0.40
5:M:95:THR:HA	5:M:101:SER:OG	2.21	0.40
5:M:97:THR:HG22	5:M:97:THR:O	2.22	0.40
6:N:18:THR:HA	6:N:76:GLY:HA2	2.03	0.40
5:O:33:TYR:HD2	5:O:94:THR:HG22	1.84	0.40
5:O:97:THR:HG22	5:O:97:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	129/153 (84%)	108 (84%)	21 (16%)	0	100	100
1	B	129/153 (84%)	108 (84%)	21 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	129/153 (84%)	108 (84%)	21 (16%)	0	100	100
2	D	441/481 (92%)	397 (90%)	42 (10%)	2 (0%)	24	63
2	E	441/481 (92%)	395 (90%)	42 (10%)	4 (1%)	14	50
2	F	441/481 (92%)	393 (89%)	45 (10%)	3 (1%)	18	56
3	G	208/214 (97%)	193 (93%)	14 (7%)	1 (0%)	24	63
3	I	211/214 (99%)	195 (92%)	15 (7%)	1 (0%)	24	63
4	H	217/233 (93%)	202 (93%)	15 (7%)	0	100	100
4	J	217/233 (93%)	202 (93%)	15 (7%)	0	100	100
5	K	223/233 (96%)	212 (95%)	10 (4%)	1 (0%)	30	67
5	M	223/233 (96%)	214 (96%)	9 (4%)	0	100	100
5	O	223/233 (96%)	214 (96%)	9 (4%)	0	100	100
6	L	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	N	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
6	P	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
All	All	3868/4140 (93%)	3565 (92%)	291 (8%)	12 (0%)	37	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	166	ARG
2	E	166	ARG
2	E	170	GLN
2	E	363	ASN
2	F	166	ARG
2	F	170	GLN
5	K	4	LEU
2	D	165	LEU
2	E	165	LEU
2	F	165	LEU
3	G	30	ALA
3	I	30	ALA

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 PDB entries followed by that with respect to all EM entries.

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	115/129 (89%)	115 (100%)	0	100	100
1	B	115/129 (89%)	115 (100%)	0	100	100
1	C	115/129 (89%)	115 (100%)	0	100	100
2	D	401/428 (94%)	397 (99%)	4 (1%)	68	78
2	E	401/428 (94%)	395 (98%)	6 (2%)	57	72
2	F	401/428 (94%)	392 (98%)	9 (2%)	45	64
3	G	181/189 (96%)	181 (100%)	0	100	100
3	I	182/189 (96%)	182 (100%)	0	100	100
4	H	170/187 (91%)	170 (100%)	0	100	100
4	J	170/187 (91%)	170 (100%)	0	100	100
5	K	185/199 (93%)	183 (99%)	2 (1%)	65	76
5	M	185/199 (93%)	183 (99%)	2 (1%)	65	76
5	O	185/199 (93%)	183 (99%)	2 (1%)	65	76
6	L	157/182 (86%)	156 (99%)	1 (1%)	78	83
6	N	157/182 (86%)	156 (99%)	1 (1%)	78	83
6	P	157/182 (86%)	156 (99%)	1 (1%)	78	83
All	All	3277/3566 (92%)	3249 (99%)	28 (1%)	68	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	171	LYS
2	D	182	VAL
2	D	191	TYR
2	D	309	ILE
2	E	171	LYS
2	E	182	VAL
2	E	191	TYR
2	E	192	ARG
2	E	304	ARG
2	E	309	ILE
2	F	164	GLU
2	F	171	LYS
2	F	182	VAL
2	F	190	GLU

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Mol	Chain	Res	Type
2	F	191	TYR
2	F	192	ARG
2	F	304	ARG
2	F	305	LYS
2	F	309	ILE
5	K	93	THR
5	K	210	ARG
6	L	30	THR
5	M	93	THR
5	M	210	ARG
6	N	30	THR
5	O	93	THR
5	O	210	ARG
6	P	30	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	GLN
1	A	650	GLN
1	A	651	ASN
1	B	575	GLN
1	B	630	GLN
1	C	575	GLN
2	D	67	ASN
2	D	82	GLN
2	D	137	ASN
2	D	170	GLN
2	D	203	GLN
2	D	289	ASN
2	D	293	GLN
2	D	425	ASN
2	E	67	ASN
2	E	82	GLN
2	E	137	ASN
2	E	170	GLN
2	E	203	GLN
2	E	289	ASN
2	E	293	GLN
2	E	425	ASN
2	F	67	ASN
2	F	82	GLN

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Mol	Chain	Res	Type
2	F	137	ASN
2	F	170	GLN
2	F	203	GLN
2	F	289	ASN
2	F	293	GLN
2	F	425	ASN
3	G	55	GLN
3	G	89	GLN
3	G	160	GLN
4	H	191	GLN
3	I	3	HIS
3	I	55	GLN
3	I	89	GLN
3	I	92	HIS
4	J	191	GLN
5	K	100(F)	HIS
5	M	3	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

150 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	$\# Z > 2$
7	NAG	0	1	7,2	14,14,15	0.33	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	0	2	7	14,14,15	0.35	0	17,19,21	1.10	1 (5%)
7	BMA	0	3	7	11,11,12	0.23	0	15,15,17	0.91	0
7	MAN	0	4	7	11,11,12	0.29	0	15,15,17	0.61	0
7	MAN	0	5	7	11,11,12	0.29	0	15,15,17	0.72	0
8	NAG	1	1	8,2	14,14,15	0.31	0	17,19,21	0.83	0
8	NAG	1	2	8	14,14,15	0.29	0	17,19,21	0.53	0
8	NAG	2	1	8,2	14,14,15	0.31	0	17,19,21	1.90	2 (11%)
8	NAG	2	2	8	14,14,15	0.28	0	17,19,21	0.64	0
8	NAG	3	1	8,2	14,14,15	0.35	0	17,19,21	1.12	2 (11%)
8	NAG	3	2	8	14,14,15	0.30	0	17,19,21	1.53	2 (11%)
12	NAG	4	1	2,12	14,14,15	0.46	0	17,19,21	2.58	6 (35%)
12	NAG	4	2	12	14,14,15	0.36	0	17,19,21	1.65	4 (23%)
12	BMA	4	3	12	11,11,12	0.28	0	15,15,17	0.56	0
12	NAG	5	1	2,12	14,14,15	0.35	0	17,19,21	1.12	1 (5%)
12	NAG	5	2	12	14,14,15	0.56	0	17,19,21	2.23	6 (35%)
12	BMA	5	3	12	11,11,12	0.29	0	15,15,17	0.65	0
12	NAG	6	1	2,12	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
12	NAG	6	2	12	14,14,15	0.59	0	17,19,21	2.94	7 (41%)
12	BMA	6	3	12	11,11,12	0.35	0	15,15,17	0.79	0
7	NAG	7	1	7,2	14,14,15	0.46	0	17,19,21	1.85	4 (23%)
7	NAG	7	2	7	14,14,15	0.67	0	17,19,21	3.25	6 (35%)
7	BMA	7	3	7	11,11,12	0.49	0	15,15,17	1.44	4 (26%)
7	MAN	7	4	7	11,11,12	0.30	0	15,15,17	0.62	0
7	MAN	7	5	7	11,11,12	0.84	1 (9%)	15,15,17	2.12	6 (40%)
7	NAG	Q	1	1,7	14,14,15	0.34	0	17,19,21	1.14	1 (5%)
7	NAG	Q	2	7	14,14,15	0.38	0	17,19,21	0.88	0
7	BMA	Q	3	7	11,11,12	0.35	0	15,15,17	1.15	1 (6%)
7	MAN	Q	4	7	11,11,12	0.35	0	15,15,17	0.65	0
7	MAN	Q	5	7	11,11,12	0.33	0	15,15,17	0.69	0
7	NAG	R	1	1,7	14,14,15	0.46	0	17,19,21	1.57	3 (17%)
7	NAG	R	2	7	14,14,15	0.34	0	17,19,21	0.84	0
7	BMA	R	3	7	11,11,12	0.33	0	15,15,17	1.06	1 (6%)
7	MAN	R	4	7	11,11,12	0.35	0	15,15,17	0.60	0
7	MAN	R	5	7	11,11,12	0.31	0	15,15,17	0.65	0
7	NAG	S	1	1,7	14,14,15	0.34	0	17,19,21	1.15	1 (5%)
7	NAG	S	2	7	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
7	BMA	S	3	7	11,11,12	0.43	0	15,15,17	0.99	1 (6%)
7	MAN	S	4	7	11,11,12	0.37	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	S	5	7	11,11,12	0.31	0	15,15,17	0.68	0
8	NAG	T	1	8,2	14,14,15	0.39	0	17,19,21	1.05	2 (11%)
8	NAG	T	2	8	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
7	NAG	U	1	7,2	14,14,15	0.32	0	17,19,21	1.12	2 (11%)
7	NAG	U	2	7	14,14,15	0.31	0	17,19,21	0.83	1 (5%)
7	BMA	U	3	7	11,11,12	0.24	0	15,15,17	0.93	1 (6%)
7	MAN	U	4	7	11,11,12	0.29	0	15,15,17	0.79	0
7	MAN	U	5	7	11,11,12	0.30	0	15,15,17	0.66	0
8	NAG	V	1	8,2	14,14,15	0.38	0	17,19,21	1.74	4 (23%)
8	NAG	V	2	8	14,14,15	0.53	0	17,19,21	0.95	1 (5%)
9	NAG	W	1	2,9	14,14,15	0.30	0	17,19,21	1.50	3 (17%)
9	NAG	W	2	9	14,14,15	0.38	0	17,19,21	1.25	2 (11%)
9	BMA	W	3	9	11,11,12	0.27	0	15,15,17	0.79	0
9	MAN	W	4	9	11,11,12	0.31	0	15,15,17	0.94	0
10	NAG	X	1	2,10	14,14,15	0.36	0	17,19,21	1.08	3 (17%)
10	NAG	X	2	10	14,14,15	0.29	0	17,19,21	1.88	5 (29%)
10	BMA	X	3	10	11,11,12	0.42	0	15,15,17	1.36	1 (6%)
10	MAN	X	4	10	11,11,12	0.29	0	15,15,17	0.72	0
10	MAN	X	5	10	11,11,12	0.30	0	15,15,17	0.68	0
10	MAN	X	6	10	11,11,12	0.34	0	15,15,17	0.78	0
10	MAN	X	7	10	11,11,12	0.35	0	15,15,17	0.68	0
11	NAG	Y	1	11,2	14,14,15	0.33	0	17,19,21	1.38	2 (11%)
11	NAG	Y	2	11	14,14,15	0.32	0	17,19,21	0.93	0
11	BMA	Y	3	11	11,11,12	0.18	0	15,15,17	0.89	0
11	MAN	Y	4	11	11,11,12	0.28	0	15,15,17	0.65	0
8	NAG	Z	1	8,2	14,14,15	0.31	0	17,19,21	0.93	2 (11%)
8	NAG	Z	2	8	14,14,15	0.32	0	17,19,21	0.65	0
8	NAG	a	1	8,2	14,14,15	0.35	0	17,19,21	1.88	2 (11%)
8	NAG	a	2	8	14,14,15	0.25	0	17,19,21	0.52	0
11	NAG	b	1	11,2	14,14,15	0.33	0	17,19,21	1.05	1 (5%)
11	NAG	b	2	11	14,14,15	0.31	0	17,19,21	1.67	4 (23%)
11	BMA	b	3	11	11,11,12	0.29	0	15,15,17	0.96	0
11	MAN	b	4	11	11,11,12	0.31	0	15,15,17	0.73	0
8	NAG	c	1	8,2	14,14,15	0.40	0	17,19,21	2.57	6 (35%)
8	NAG	c	2	8	14,14,15	0.34	0	17,19,21	1.15	2 (11%)
12	NAG	d	1	2,12	14,14,15	0.33	0	17,19,21	1.07	2 (11%)
12	NAG	d	2	12	14,14,15	0.53	0	17,19,21	2.07	7 (41%)
12	BMA	d	3	12	11,11,12	0.30	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	e	1	8,2	14,14,15	0.36	0	17,19,21	1.21	2 (11%)
8	NAG	e	2	8	14,14,15	0.32	0	17,19,21	0.68	0
12	NAG	f	1	2,12	14,14,15	0.41	0	17,19,21	1.42	3 (17%)
12	NAG	f	2	12	14,14,15	0.64	1 (7%)	17,19,21	1.99	6 (35%)
12	BMA	f	3	12	11,11,12	0.35	0	15,15,17	0.72	0
8	NAG	g	1	8,2	14,14,15	0.39	0	17,19,21	1.22	2 (11%)
8	NAG	g	2	8	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
8	NAG	h	1	8,2	14,14,15	0.45	0	17,19,21	2.24	6 (35%)
8	NAG	h	2	8	14,14,15	0.37	0	17,19,21	0.82	0
12	NAG	i	1	2,12	14,14,15	0.35	0	17,19,21	1.18	1 (5%)
12	NAG	i	2	12	14,14,15	0.38	0	17,19,21	0.90	0
12	BMA	i	3	12	11,11,12	0.30	0	15,15,17	0.71	0
8	NAG	j	1	8,2	14,14,15	0.29	0	17,19,21	1.29	1 (5%)
8	NAG	j	2	8	14,14,15	0.49	0	17,19,21	2.97	5 (29%)
8	NAG	k	1	8,2	14,14,15	0.39	0	17,19,21	1.81	4 (23%)
8	NAG	k	2	8	14,14,15	0.58	0	17,19,21	1.01	1 (5%)
9	NAG	l	1	2,9	14,14,15	0.36	0	17,19,21	1.38	3 (17%)
9	NAG	l	2	9	14,14,15	0.38	0	17,19,21	1.19	2 (11%)
9	BMA	l	3	9	11,11,12	0.24	0	15,15,17	0.75	0
9	MAN	l	4	9	11,11,12	0.35	0	15,15,17	0.79	0
10	NAG	m	1	2,10	14,14,15	0.36	0	17,19,21	0.84	0
10	NAG	m	2	10	14,14,15	0.29	0	17,19,21	1.85	5 (29%)
10	BMA	m	3	10	11,11,12	0.49	0	15,15,17	1.76	2 (13%)
10	MAN	m	4	10	11,11,12	0.28	0	15,15,17	0.95	0
10	MAN	m	5	10	11,11,12	0.34	0	15,15,17	0.71	0
10	MAN	m	6	10	11,11,12	0.35	0	15,15,17	0.88	0
10	MAN	m	7	10	11,11,12	0.37	0	15,15,17	0.74	0
7	NAG	n	1	7,2	14,14,15	0.30	0	17,19,21	1.22	2 (11%)
7	NAG	n	2	7	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
7	BMA	n	3	7	11,11,12	0.23	0	15,15,17	0.86	0
7	MAN	n	4	7	11,11,12	0.33	0	15,15,17	0.77	0
7	MAN	n	5	7	11,11,12	0.30	0	15,15,17	0.55	0
8	NAG	o	1	8,2	14,14,15	0.34	0	17,19,21	0.95	1 (5%)
8	NAG	o	2	8	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
8	NAG	p	1	8,2	14,14,15	0.40	0	17,19,21	2.10	6 (35%)
8	NAG	p	2	8	14,14,15	0.32	0	17,19,21	0.67	0
8	NAG	q	1	8	14,14,15	0.40	0	17,19,21	1.24	1 (5%)
8	NAG	q	2	8	14,14,15	0.36	0	17,19,21	1.64	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	r	1	2,12	14,14,15	0.54	0	17,19,21	2.18	4 (23%)
12	NAG	r	2	12	14,14,15	0.46	0	17,19,21	1.83	3 (17%)
12	BMA	r	3	12	11,11,12	0.40	0	15,15,17	1.04	1 (6%)
13	NAG	s	1	13,2	14,14,15	0.35	0	17,19,21	0.87	0
13	FUC	s	2	13	10,10,11	0.73	0	14,14,16	0.85	1 (7%)
14	NAG	t	1	14,2	14,14,15	0.36	0	17,19,21	1.39	2 (11%)
14	NAG	t	2	14	14,14,15	0.63	1 (7%)	17,19,21	2.84	8 (47%)
14	BMA	t	3	14	11,11,12	0.37	0	15,15,17	1.00	0
14	MAN	t	4	14	11,11,12	0.35	0	15,15,17	0.97	1 (6%)
14	MAN	t	5	14	11,11,12	0.34	0	15,15,17	0.70	0
8	NAG	u	1	8,2	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
8	NAG	u	2	8	14,14,15	0.29	0	17,19,21	0.77	0
7	NAG	v	1	7,2	14,14,15	0.39	0	17,19,21	1.61	4 (23%)
7	NAG	v	2	7	14,14,15	0.40	0	17,19,21	1.01	2 (11%)
7	BMA	v	3	7	11,11,12	0.26	0	15,15,17	1.22	2 (13%)
7	MAN	v	4	7	11,11,12	0.29	0	15,15,17	0.67	0
7	MAN	v	5	7	11,11,12	0.37	0	15,15,17	0.71	0
7	NAG	w	1	7,2	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
7	NAG	w	2	7	14,14,15	0.64	0	17,19,21	3.22	6 (35%)
7	BMA	w	3	7	11,11,12	0.40	0	15,15,17	1.06	1 (6%)
7	MAN	w	4	7	11,11,12	0.32	0	15,15,17	0.79	0
7	MAN	w	5	7	11,11,12	0.26	0	15,15,17	0.88	0
8	NAG	x	1	8,2	14,14,15	0.43	0	17,19,21	1.54	3 (17%)
8	NAG	x	2	8	14,14,15	0.43	0	17,19,21	0.89	2 (11%)
9	NAG	y	1	2,9	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
9	NAG	y	2	9	14,14,15	0.33	0	17,19,21	0.87	0
9	BMA	y	3	9	11,11,12	0.28	0	15,15,17	0.72	0
9	MAN	y	4	9	11,11,12	0.33	0	15,15,17	0.66	0
10	NAG	z	1	2,10	14,14,15	0.38	0	17,19,21	1.26	3 (17%)
10	NAG	z	2	10	14,14,15	0.30	0	17,19,21	1.81	5 (29%)
10	BMA	z	3	10	11,11,12	0.45	0	15,15,17	2.02	5 (33%)
10	MAN	z	4	10	11,11,12	0.29	0	15,15,17	1.03	1 (6%)
10	MAN	z	5	10	11,11,12	0.33	0	15,15,17	0.72	0
10	MAN	z	6	10	11,11,12	0.34	0	15,15,17	1.06	2 (13%)
10	MAN	z	7	10	11,11,12	0.36	0	15,15,17	0.74	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	0	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	BMA	0	3	7	-	0/2/19/22	0/1/1/1
7	MAN	0	4	7	-	1/2/19/22	0/1/1/1
7	MAN	0	5	7	-	0/2/19/22	0/1/1/1
8	NAG	1	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	NAG	2	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	2	2	8	-	1/6/23/26	0/1/1/1
8	NAG	3	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	3	2	8	-	2/6/23/26	0/1/1/1
12	NAG	4	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	4	2	12	-	2/6/23/26	0/1/1/1
12	BMA	4	3	12	-	0/2/19/22	0/1/1/1
12	NAG	5	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	5	2	12	-	3/6/23/26	0/1/1/1
12	BMA	5	3	12	-	0/2/19/22	0/1/1/1
12	NAG	6	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	6	2	12	-	2/6/23/26	0/1/1/1
12	BMA	6	3	12	-	0/2/19/22	0/1/1/1
7	NAG	7	1	7,2	-	3/6/23/26	0/1/1/1
7	NAG	7	2	7	-	5/6/23/26	0/1/1/1
7	BMA	7	3	7	-	2/2/19/22	0/1/1/1
7	MAN	7	4	7	-	0/2/19/22	0/1/1/1
7	MAN	7	5	7	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
7	NAG	R	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
7	MAN	R	4	7	-	1/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	1/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	S	5	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
7	NAG	U	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	1/6/23/26	0/1/1/1
7	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	2/2/19/22	0/1/1/1
7	MAN	U	5	7	-	0/2/19/22	0/1/1/1
8	NAG	V	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	V	2	8	-	0/6/23/26	0/1/1/1
9	NAG	W	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
9	BMA	W	3	9	-	1/2/19/22	0/1/1/1
9	MAN	W	4	9	-	1/2/19/22	0/1/1/1
10	NAG	X	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
10	BMA	X	3	10	-	1/2/19/22	0/1/1/1
10	MAN	X	4	10	-	0/2/19/22	0/1/1/1
10	MAN	X	5	10	-	1/2/19/22	0/1/1/1
10	MAN	X	6	10	-	2/2/19/22	0/1/1/1
10	MAN	X	7	10	-	0/2/19/22	0/1/1/1
11	NAG	Y	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	0/2/19/22	0/1/1/1
11	MAN	Y	4	11	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	NAG	a	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
11	NAG	b	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	b	2	11	-	2/6/23/26	0/1/1/1
11	BMA	b	3	11	-	0/2/19/22	0/1/1/1
11	MAN	b	4	11	-	0/2/19/22	0/1/1/1
8	NAG	c	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	1/6/23/26	0/1/1/1
12	NAG	d	1	2,12	-	1/6/23/26	0/1/1/1
12	NAG	d	2	12	-	2/6/23/26	0/1/1/1
12	BMA	d	3	12	-	0/2/19/22	0/1/1/1
8	NAG	e	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	f	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	2/6/23/26	0/1/1/1
12	BMA	f	3	12	-	2/2/19/22	0/1/1/1
8	NAG	g	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	NAG	h	1	8,2	-	1/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
12	NAG	i	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	1/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
8	NAG	j	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	5/6/23/26	0/1/1/1
8	NAG	k	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
9	NAG	l	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1
9	BMA	l	3	9	-	1/2/19/22	0/1/1/1
9	MAN	l	4	9	-	1/2/19/22	0/1/1/1
10	NAG	m	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	m	2	10	-	2/6/23/26	0/1/1/1
10	BMA	m	3	10	-	0/2/19/22	0/1/1/1
10	MAN	m	4	10	-	0/2/19/22	0/1/1/1
10	MAN	m	5	10	-	1/2/19/22	0/1/1/1
10	MAN	m	6	10	-	2/2/19/22	0/1/1/1
10	MAN	m	7	10	-	2/2/19/22	0/1/1/1
7	NAG	n	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
7	BMA	n	3	7	-	0/2/19/22	0/1/1/1
7	MAN	n	4	7	-	1/2/19/22	0/1/1/1
7	MAN	n	5	7	-	0/2/19/22	0/1/1/1
8	NAG	o	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	o	2	8	-	1/6/23/26	0/1/1/1
8	NAG	p	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	p	2	8	-	0/6/23/26	0/1/1/1
8	NAG	q	1	8	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
12	NAG	r	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	r	2	12	-	2/6/23/26	0/1/1/1
12	BMA	r	3	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	s	1	13,2	-	0/6/23/26	0/1/1/1
13	FUC	s	2	13	-	-	0/1/1/1
14	NAG	t	1	14,2	-	0/6/23/26	0/1/1/1
14	NAG	t	2	14	-	2/6/23/26	0/1/1/1
14	BMA	t	3	14	-	2/2/19/22	0/1/1/1
14	MAN	t	4	14	-	0/2/19/22	0/1/1/1
14	MAN	t	5	14	-	0/2/19/22	0/1/1/1
8	NAG	u	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	u	2	8	-	0/6/23/26	0/1/1/1
7	NAG	v	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	1/6/23/26	0/1/1/1
7	BMA	v	3	7	-	2/2/19/22	0/1/1/1
7	MAN	v	4	7	-	0/2/19/22	0/1/1/1
7	MAN	v	5	7	-	0/2/19/22	0/1/1/1
7	NAG	w	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	5/6/23/26	0/1/1/1
7	BMA	w	3	7	-	0/2/19/22	0/1/1/1
7	MAN	w	4	7	-	2/2/19/22	0/1/1/1
7	MAN	w	5	7	-	0/2/19/22	0/1/1/1
8	NAG	x	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	x	2	8	-	0/6/23/26	0/1/1/1
9	NAG	y	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	y	3	9	-	2/2/19/22	0/1/1/1
9	MAN	y	4	9	-	1/2/19/22	0/1/1/1
10	NAG	z	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	z	5	10	-	1/2/19/22	0/1/1/1
10	MAN	z	6	10	-	2/2/19/22	0/1/1/1
10	MAN	z	7	10	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	5	MAN	O4-C4	2.45	1.49	1.43
12	f	2	NAG	C1-C2	2.18	1.55	1.52
14	t	2	NAG	C1-C2	2.10	1.55	1.52

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	2	NAG	C2-N2-C7	10.24	136.62	122.90
8	j	2	NAG	C2-N2-C7	10.23	136.61	122.90
7	w	2	NAG	C2-N2-C7	9.98	136.27	122.90
12	6	2	NAG	O4-C4-C3	-7.06	93.73	110.38
12	4	1	NAG	O4-C4-C5	6.55	125.46	109.32
14	t	2	NAG	O4-C4-C3	-6.35	95.40	110.38
12	r	1	NAG	O4-C4-C5	6.23	124.68	109.32
8	c	1	NAG	O4-C4-C5	6.20	124.60	109.32
7	7	2	NAG	C8-C7-N2	6.00	126.07	116.12
7	w	2	NAG	C8-C7-N2	5.85	125.83	116.12
8	a	1	NAG	O4-C4-C3	-5.41	97.62	110.38
8	2	1	NAG	O4-C4-C3	-5.30	97.88	110.38
14	t	2	NAG	C2-N2-C7	5.26	129.95	122.90
12	5	2	NAG	C2-N2-C7	5.11	129.74	122.90
12	6	2	NAG	C2-N2-C7	5.03	129.64	122.90
12	f	2	NAG	C2-N2-C7	4.93	129.51	122.90
8	j	2	NAG	C8-C7-N2	4.88	124.21	116.12
8	h	1	NAG	C1-O5-C5	4.88	118.72	112.19
7	7	1	NAG	C1-O5-C5	4.78	118.59	112.19
8	k	1	NAG	O4-C4-C3	-4.77	99.12	110.38
12	d	2	NAG	C2-N2-C7	4.71	129.21	122.90
8	c	1	NAG	C1-O5-C5	4.65	118.42	112.19
10	m	2	NAG	C2-N2-C7	4.57	129.03	122.90
8	p	1	NAG	O5-C1-C2	-4.57	104.22	111.29
11	b	2	NAG	C2-N2-C7	4.50	128.94	122.90
12	4	1	NAG	C1-O5-C5	4.49	118.21	112.19
10	z	2	NAG	C2-N2-C7	4.49	128.91	122.90
10	X	2	NAG	C2-N2-C7	4.48	128.91	122.90
8	3	2	NAG	C2-N2-C7	4.47	128.89	122.90
14	t	2	NAG	C4-C3-C2	4.46	117.55	111.02
12	6	2	NAG	C4-C3-C2	4.36	117.41	111.02
8	q	2	NAG	C2-N2-C7	4.35	128.73	122.90
8	h	1	NAG	C2-N2-C7	-4.34	117.09	122.90
12	r	2	NAG	O4-C4-C5	4.24	119.77	109.32
8	V	1	NAG	O4-C4-C3	-4.21	100.45	110.38
8	p	1	NAG	O4-C4-C3	-4.10	100.72	110.38
12	4	2	NAG	C1-O5-C5	4.07	117.64	112.19
8	2	1	NAG	C4-C3-C2	4.06	116.96	111.02
10	z	3	BMA	O5-C5-C6	-4.04	99.80	107.66
9	W	1	NAG	C1-O5-C5	4.03	117.59	112.19
7	R	1	NAG	C1-O5-C5	4.00	117.55	112.19
8	a	1	NAG	C4-C3-C2	4.00	116.88	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	x	1	NAG	O4-C4-C3	-3.99	100.96	110.38
8	h	1	NAG	C4-C3-C2	-3.99	105.18	111.02
12	5	2	NAG	O4-C4-C5	-3.96	99.57	109.32
10	z	3	BMA	O3-C3-C2	-3.89	102.12	110.05
14	t	2	NAG	C1-C2-N2	3.84	116.48	110.43
10	m	3	BMA	O3-C3-C2	-3.81	102.28	110.05
7	S	1	NAG	C1-O5-C5	3.79	117.26	112.19
12	r	1	NAG	C1-O5-C5	3.76	117.23	112.19
12	6	2	NAG	C1-C2-N2	3.76	116.36	110.43
8	c	1	NAG	C2-N2-C7	-3.76	117.86	122.90
8	c	1	NAG	O5-C5-C6	-3.75	100.36	107.66
12	6	2	NAG	O5-C1-C2	-3.73	105.52	111.29
12	r	2	NAG	C1-O5-C5	3.73	117.18	112.19
8	V	1	NAG	C4-C3-C2	3.68	116.41	111.02
7	Q	1	NAG	C1-O5-C5	3.68	117.11	112.19
11	Y	1	NAG	C2-N2-C7	-3.65	118.01	122.90
12	r	2	NAG	O4-C4-C3	3.59	118.83	110.38
9	l	1	NAG	C1-O5-C5	3.54	116.93	112.19
12	4	1	NAG	C2-N2-C7	-3.52	118.18	122.90
7	R	1	NAG	O5-C5-C6	-3.52	100.81	107.66
7	v	1	NAG	C2-N2-C7	-3.51	118.20	122.90
7	n	1	NAG	C2-N2-C7	-3.49	118.23	122.90
8	q	1	NAG	O5-C1-C2	-3.47	105.92	111.29
9	W	2	NAG	C2-N2-C7	-3.47	118.25	122.90
7	7	1	NAG	O5-C5-C6	-3.45	100.94	107.66
12	d	2	NAG	O4-C4-C5	-3.42	100.91	109.32
7	7	5	MAN	C3-C4-C5	-3.40	104.06	110.23
14	t	1	NAG	O4-C4-C3	-3.37	102.43	110.38
12	5	2	NAG	O5-C1-C2	-3.34	106.13	111.29
12	4	1	NAG	O5-C5-C6	-3.26	101.32	107.66
7	7	2	NAG	O7-C7-C8	-3.23	116.30	122.05
14	t	2	NAG	O5-C1-C2	-3.22	106.31	111.29
7	w	2	NAG	O4-C4-C5	-3.21	101.42	109.32
10	X	3	BMA	O3-C3-C2	-3.20	103.52	110.05
7	v	3	BMA	O3-C3-C2	-3.20	103.52	110.05
8	c	2	NAG	C1-O5-C5	3.20	116.47	112.19
8	p	1	NAG	O5-C5-C6	-3.17	101.49	107.66
10	m	3	BMA	O5-C5-C6	-3.17	101.50	107.66
7	7	5	MAN	O4-C4-C5	3.17	117.12	109.32
9	l	2	NAG	C2-N2-C7	-3.16	118.67	122.90
7	7	5	MAN	C1-C2-C3	-3.15	105.06	109.64
8	j	1	NAG	C2-N2-C7	3.13	127.10	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	1	NAG	O5-C1-C2	-3.12	106.47	111.29
12	5	2	NAG	C1-C2-N2	3.12	115.34	110.43
9	y	1	NAG	O5-C1-C2	-3.08	106.52	111.29
12	4	2	NAG	O4-C4-C3	3.06	117.59	110.38
12	d	2	NAG	C1-C2-N2	3.01	115.17	110.43
10	m	2	NAG	O4-C4-C5	-3.00	101.94	109.32
10	z	2	NAG	C1-C2-N2	3.00	115.16	110.43
7	w	2	NAG	O7-C7-C8	-3.00	116.72	122.05
8	c	1	NAG	C4-C3-C2	-2.99	106.63	111.02
7	v	1	NAG	O5-C5-C6	2.97	113.45	107.66
12	4	2	NAG	O4-C4-C5	2.96	116.61	109.32
8	V	1	NAG	O4-C4-C5	-2.91	102.16	109.32
8	k	2	NAG	O5-C1-C2	-2.91	106.79	111.29
12	4	1	NAG	O5-C1-C2	-2.88	106.84	111.29
12	6	2	NAG	O5-C5-C6	-2.85	102.12	107.66
10	X	2	NAG	C1-C2-N2	2.85	114.92	110.43
12	d	2	NAG	O5-C1-C2	-2.83	106.91	111.29
14	t	2	NAG	O7-C7-N2	2.83	126.97	121.98
7	7	5	MAN	C1-O5-C5	2.82	115.97	112.19
8	p	1	NAG	C1-O5-C5	2.82	115.97	112.19
12	5	1	NAG	O4-C4-C3	-2.82	103.73	110.38
7	0	2	NAG	C2-N2-C7	-2.82	119.12	122.90
7	7	5	MAN	O5-C5-C6	-2.80	102.21	107.66
8	k	1	NAG	C4-C3-C2	2.79	115.11	111.02
7	v	1	NAG	O5-C1-C2	-2.79	106.98	111.29
12	f	2	NAG	O4-C4-C3	-2.78	103.81	110.38
12	f	1	NAG	O5-C1-C2	-2.78	106.99	111.29
9	W	1	NAG	O5-C1-C2	-2.77	107.00	111.29
12	f	2	NAG	O7-C7-N2	2.76	126.86	121.98
12	r	1	NAG	C4-C3-C2	-2.75	106.98	111.02
8	c	2	NAG	C2-N2-C7	-2.73	119.24	122.90
7	7	3	BMA	C6-C5-C4	-2.73	106.32	113.02
12	f	2	NAG	C1-C2-N2	2.72	114.72	110.43
12	i	1	NAG	O5-C1-C2	-2.71	107.09	111.29
12	6	2	NAG	O7-C7-N2	2.70	126.76	121.98
8	p	1	NAG	C2-N2-C7	-2.70	119.28	122.90
7	U	1	NAG	C2-N2-C7	-2.70	119.28	122.90
10	X	2	NAG	O4-C4-C5	-2.69	102.71	109.32
8	q	2	NAG	C1-C2-N2	2.69	114.67	110.43
12	r	1	NAG	O5-C1-C2	-2.68	107.15	111.29
8	k	1	NAG	O5-C1-C2	-2.67	107.16	111.29
7	w	3	BMA	C6-C5-C4	-2.67	106.46	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	z	1	NAG	C1-O5-C5	2.66	115.75	112.19
8	h	1	NAG	O5-C1-C2	-2.66	107.18	111.29
7	7	5	MAN	O4-C4-C3	2.65	116.63	110.38
12	4	1	NAG	C4-C3-C2	-2.63	107.16	111.02
8	V	2	NAG	O5-C1-C2	-2.63	107.23	111.29
8	e	1	NAG	O5-C1-C2	-2.61	107.25	111.29
10	X	2	NAG	O7-C7-N2	2.61	126.60	121.98
8	h	1	NAG	O4-C4-C5	2.61	115.76	109.32
9	y	1	NAG	C1-O5-C5	2.60	115.68	112.19
9	l	1	NAG	O5-C5-C6	-2.60	102.61	107.66
10	m	2	NAG	O7-C7-N2	2.58	126.55	121.98
8	g	1	NAG	O5-C1-C2	-2.58	107.30	111.29
7	w	2	NAG	O7-C7-N2	-2.56	117.45	121.98
12	6	1	NAG	O4-C4-C3	-2.55	104.36	110.38
12	f	1	NAG	C1-O5-C5	2.55	115.61	112.19
7	U	3	BMA	O3-C3-C2	-2.55	104.85	110.05
8	q	2	NAG	C1-O5-C5	2.54	115.60	112.19
8	3	2	NAG	O7-C7-N2	2.52	126.44	121.98
10	z	6	MAN	C1-O5-C5	2.52	115.56	112.19
7	n	2	NAG	C1-O5-C5	2.52	115.56	112.19
8	k	1	NAG	O4-C4-C5	-2.50	103.17	109.32
7	Q	3	BMA	C6-C5-C4	-2.47	106.97	113.02
7	7	2	NAG	O7-C7-N2	-2.46	117.63	121.98
14	t	4	MAN	C1-C2-C3	-2.44	106.09	109.64
7	v	1	NAG	C1-C2-N2	2.44	114.28	110.43
10	z	3	BMA	O6-C6-C5	-2.42	103.09	111.33
12	r	3	BMA	C1-C2-C3	2.42	113.16	109.64
11	b	2	NAG	C1-C2-N2	2.41	114.23	110.43
8	T	1	NAG	O5-C1-C2	-2.41	107.56	111.29
11	b	2	NAG	O7-C7-N2	2.41	126.24	121.98
8	x	1	NAG	C4-C3-C2	2.40	114.54	111.02
12	f	2	NAG	C4-C3-C2	2.40	114.53	111.02
8	j	2	NAG	O7-C7-N2	-2.39	117.77	121.98
10	z	2	NAG	O7-C7-N2	2.36	126.16	121.98
8	o	1	NAG	C1-O5-C5	2.36	115.35	112.19
7	S	2	NAG	O5-C1-C2	-2.36	107.64	111.29
10	z	2	NAG	O5-C1-C2	-2.35	107.65	111.29
11	b	1	NAG	O5-C1-C2	-2.34	107.68	111.29
14	t	1	NAG	O5-C1-C2	-2.33	107.68	111.29
12	5	2	NAG	O7-C7-N2	2.33	126.10	121.98
10	z	1	NAG	O5-C1-C2	-2.33	107.68	111.29
12	5	2	NAG	C4-C3-C2	2.33	114.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	2	NAG	C1-O5-C5	2.33	115.31	112.19
8	x	1	NAG	O4-C4-C5	-2.32	103.60	109.32
7	7	3	BMA	O6-C6-C5	-2.32	103.42	111.33
7	w	2	NAG	O5-C1-C2	-2.32	107.70	111.29
8	c	1	NAG	O5-C1-C2	-2.32	107.71	111.29
10	X	1	NAG	C1-O5-C5	2.31	115.28	112.19
7	0	1	NAG	C2-N2-C7	-2.31	119.81	122.90
10	z	3	BMA	C1-O5-C5	2.31	115.28	112.19
10	X	2	NAG	O5-C1-C2	-2.30	107.72	111.29
12	f	2	NAG	O5-C1-C2	-2.30	107.73	111.29
10	z	3	BMA	C6-C5-C4	-2.30	107.38	113.02
7	7	1	NAG	C3-C4-C5	-2.29	106.07	110.23
10	m	2	NAG	C1-C2-N2	2.29	114.04	110.43
8	3	1	NAG	O5-C1-C2	-2.29	107.75	111.29
12	d	2	NAG	O7-C7-N2	2.29	126.02	121.98
9	W	2	NAG	C1-O5-C5	2.28	115.25	112.19
10	z	4	MAN	O2-C2-C3	-2.28	105.42	110.15
10	z	1	NAG	C2-N2-C7	-2.28	119.84	122.90
13	s	2	FUC	C1-O5-C5	2.28	118.34	112.97
8	q	2	NAG	O7-C7-N2	2.28	126.01	121.98
8	j	2	NAG	O7-C7-C8	-2.27	118.02	122.05
12	d	2	NAG	O4-C4-C3	-2.26	105.06	110.38
8	T	2	NAG	C1-O5-C5	2.25	115.20	112.19
7	7	2	NAG	C4-C3-C2	2.24	114.30	111.02
7	7	2	NAG	O4-C4-C5	-2.24	103.82	109.32
7	R	3	BMA	C6-C5-C4	-2.23	107.54	113.02
12	f	1	NAG	O4-C4-C3	-2.23	105.12	110.38
10	z	2	NAG	O4-C4-C5	-2.23	103.84	109.32
7	v	2	NAG	O5-C1-C2	-2.22	107.85	111.29
8	x	2	NAG	O5-C1-C2	-2.22	107.86	111.29
10	X	1	NAG	C2-N2-C7	-2.22	119.92	122.90
12	d	1	NAG	O4-C4-C3	-2.21	105.17	110.38
8	g	1	NAG	C1-O5-C5	2.21	115.15	112.19
8	V	1	NAG	O5-C1-C2	-2.20	107.89	111.29
7	U	1	NAG	O5-C1-C2	-2.19	107.90	111.29
8	e	1	NAG	O4-C4-C3	-2.18	105.23	110.38
8	p	1	NAG	O4-C4-C5	-2.15	104.02	109.32
12	4	2	NAG	C2-N2-C7	-2.15	120.01	122.90
9	W	1	NAG	C2-N2-C7	-2.15	120.03	122.90
8	j	2	NAG	C1-C2-N2	2.14	113.81	110.43
14	t	2	NAG	O4-C4-C5	-2.14	104.06	109.32
8	Z	1	NAG	O5-C1-C2	-2.13	108.00	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	1	NAG	C1-C2-N2	2.13	113.79	110.43
10	z	6	MAN	O5-C1-C2	-2.13	105.72	110.79
12	d	2	NAG	C4-C3-C2	2.12	114.13	111.02
7	w	1	NAG	C2-N2-C7	2.11	125.73	122.90
7	n	1	NAG	C1-C2-N2	2.11	113.76	110.43
7	7	3	BMA	O5-C5-C6	2.11	111.77	107.66
7	S	3	BMA	C6-C5-C4	-2.11	107.84	113.02
8	T	1	NAG	C1-O5-C5	2.11	115.01	112.19
9	l	2	NAG	O5-C1-C2	-2.10	108.04	111.29
8	x	2	NAG	C2-N2-C7	-2.10	120.09	122.90
9	l	1	NAG	O5-C1-C2	-2.09	108.05	111.29
11	b	2	NAG	O4-C4-C5	-2.09	104.18	109.32
10	X	1	NAG	O5-C1-C2	-2.09	108.06	111.29
7	v	2	NAG	C2-N2-C7	-2.09	120.10	122.90
7	7	3	BMA	C1-C2-C3	2.08	112.68	109.64
7	n	2	NAG	C2-N2-C7	-2.08	120.11	122.90
8	3	1	NAG	C1-O5-C5	2.08	114.97	112.19
10	m	2	NAG	O5-C1-C2	-2.08	108.07	111.29
14	t	2	NAG	O5-C5-C6	-2.06	103.65	107.66
7	v	3	BMA	O3-C3-C4	-2.06	105.52	110.38
8	u	1	NAG	C1-O5-C5	2.06	114.94	112.19
12	d	1	NAG	C1-O5-C5	2.05	114.93	112.19
11	Y	1	NAG	O3-C3-C2	-2.04	105.17	109.40
7	U	2	NAG	C1-O5-C5	2.02	114.90	112.19
8	Z	1	NAG	C1-O5-C5	2.02	114.89	112.19
8	o	2	NAG	C1-O5-C5	2.02	114.89	112.19
8	h	1	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	6	2	NAG	C1-C2-N2-C7
14	t	2	NAG	C1-C2-N2-C7
9	W	2	NAG	O5-C5-C6-O6
10	X	6	MAN	O5-C5-C6-O6
10	m	6	MAN	O5-C5-C6-O6
10	z	6	MAN	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
10	m	6	MAN	C4-C5-C6-O6
7	v	3	BMA	C4-C5-C6-O6
10	X	6	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	S	1	NAG	O5-C5-C6-O6
7	v	1	NAG	O5-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6
7	7	3	BMA	C4-C5-C6-O6
10	z	6	MAN	C4-C5-C6-O6
7	v	1	NAG	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
7	7	3	BMA	O5-C5-C6-O6
7	w	1	NAG	C8-C7-N2-C2
7	w	1	NAG	O7-C7-N2-C2
7	w	2	NAG	C8-C7-N2-C2
7	w	2	NAG	O7-C7-N2-C2
7	7	1	NAG	C8-C7-N2-C2
7	7	1	NAG	O7-C7-N2-C2
7	7	2	NAG	C8-C7-N2-C2
7	7	2	NAG	O7-C7-N2-C2
8	j	1	NAG	C8-C7-N2-C2
8	j	1	NAG	O7-C7-N2-C2
8	j	2	NAG	C8-C7-N2-C2
8	j	2	NAG	O7-C7-N2-C2
7	7	2	NAG	O5-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6
7	U	4	MAN	C4-C5-C6-O6
12	4	2	NAG	O5-C5-C6-O6
9	l	4	MAN	O5-C5-C6-O6
7	v	3	BMA	O5-C5-C6-O6
12	r	2	NAG	O5-C5-C6-O6
12	f	3	BMA	O5-C5-C6-O6
9	y	1	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
7	U	3	BMA	C4-C5-C6-O6
9	y	4	MAN	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
14	t	3	BMA	C4-C5-C6-O6
12	f	3	BMA	C4-C5-C6-O6
7	Q	4	MAN	O5-C5-C6-O6
7	w	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	m	7	MAN	O5-C5-C6-O6
7	0	4	MAN	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
8	j	2	NAG	O5-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
7	v	2	NAG	O5-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
10	m	7	MAN	C4-C5-C6-O6
7	n	4	MAN	O5-C5-C6-O6
10	z	5	MAN	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	S	4	MAN	O5-C5-C6-O6
10	X	5	MAN	O5-C5-C6-O6
12	i	2	NAG	O5-C5-C6-O6
9	y	1	NAG	C4-C5-C6-O6
7	R	4	MAN	O5-C5-C6-O6
10	m	5	MAN	O5-C5-C6-O6
12	4	2	NAG	C4-C5-C6-O6
12	r	2	NAG	C4-C5-C6-O6
9	y	3	BMA	C4-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
8	3	2	NAG	C1-C2-N2-C7
10	X	2	NAG	C1-C2-N2-C7
10	m	2	NAG	C1-C2-N2-C7
10	z	2	NAG	C1-C2-N2-C7
11	b	2	NAG	C1-C2-N2-C7
12	d	2	NAG	C1-C2-N2-C7
12	f	2	NAG	C1-C2-N2-C7
8	e	1	NAG	O5-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
7	w	4	MAN	O5-C5-C6-O6
7	w	2	NAG	C3-C2-N2-C7
7	7	2	NAG	C3-C2-N2-C7
10	X	2	NAG	C3-C2-N2-C7
10	m	2	NAG	C3-C2-N2-C7
10	z	2	NAG	C3-C2-N2-C7
12	d	2	NAG	C3-C2-N2-C7

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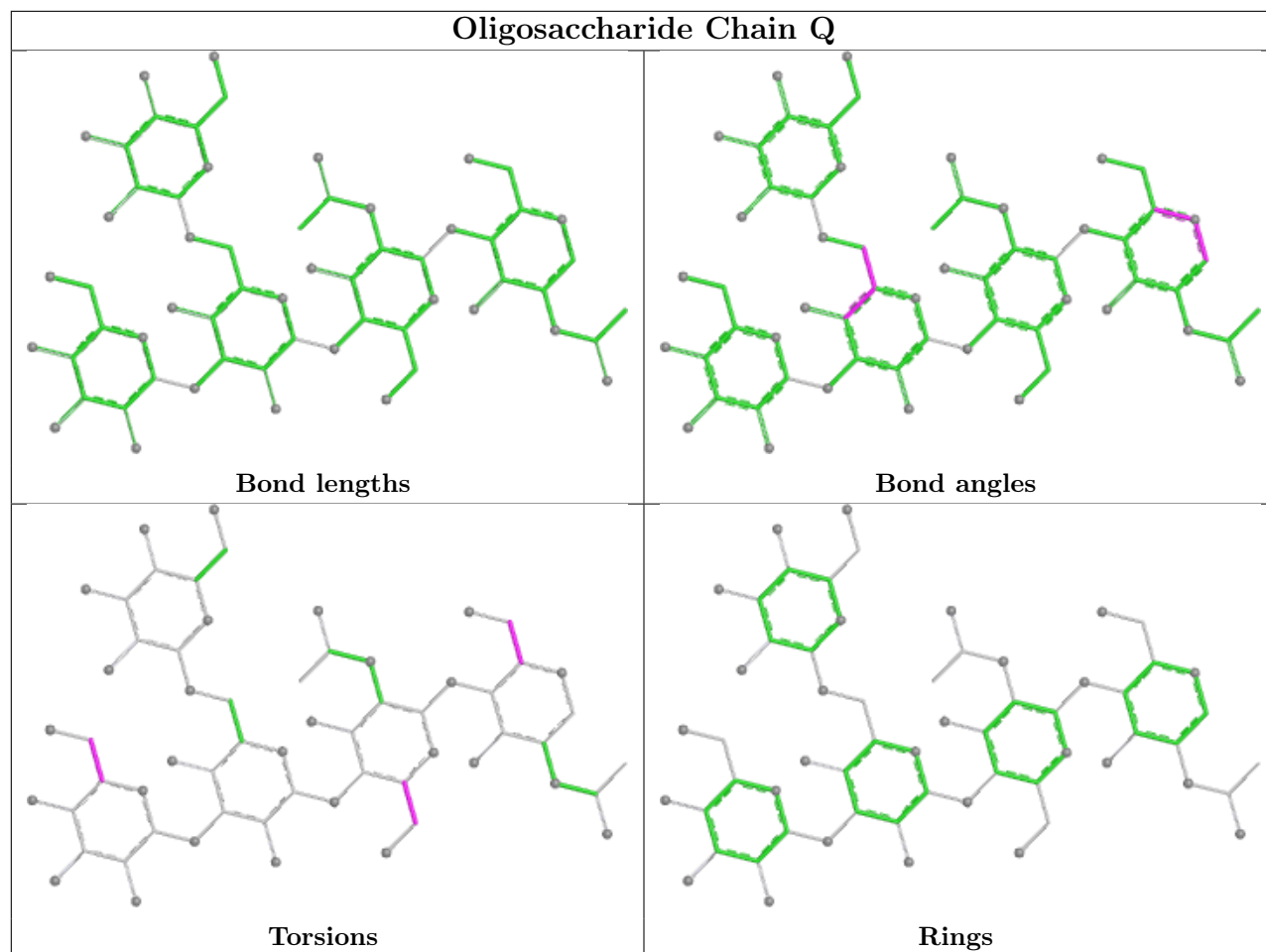
Mol	Chain	Res	Type	Atoms
12	5	2	NAG	C3-C2-N2-C7
12	6	2	NAG	C3-C2-N2-C7
7	Q	1	NAG	C4-C5-C6-O6
10	X	3	BMA	C4-C5-C6-O6
14	t	3	BMA	O5-C5-C6-O6
8	2	2	NAG	O5-C5-C6-O6
7	7	2	NAG	C4-C5-C6-O6
12	5	2	NAG	O5-C5-C6-O6
7	7	1	NAG	O5-C5-C6-O6
7	w	2	NAG	C1-C2-N2-C7
8	V	1	NAG	C1-C2-N2-C7
8	e	2	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
8	o	1	NAG	C1-C2-N2-C7
8	o	2	NAG	C1-C2-N2-C7
8	q	2	NAG	C1-C2-N2-C7
9	W	1	NAG	C1-C2-N2-C7
9	l	1	NAG	C1-C2-N2-C7
11	b	1	NAG	C1-C2-N2-C7
12	5	2	NAG	C1-C2-N2-C7
8	g	1	NAG	O5-C5-C6-O6
9	y	3	BMA	O5-C5-C6-O6
12	d	1	NAG	C4-C5-C6-O6
8	j	2	NAG	C3-C2-N2-C7
8	q	2	NAG	C3-C2-N2-C7
8	3	2	NAG	C3-C2-N2-C7
11	b	2	NAG	C3-C2-N2-C7
12	f	2	NAG	C3-C2-N2-C7
14	t	2	NAG	C3-C2-N2-C7
9	W	3	BMA	C4-C5-C6-O6
8	e	1	NAG	C4-C5-C6-O6
8	2	1	NAG	O5-C5-C6-O6
9	l	3	BMA	C4-C5-C6-O6
7	w	4	MAN	C4-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6
8	o	1	NAG	O5-C5-C6-O6

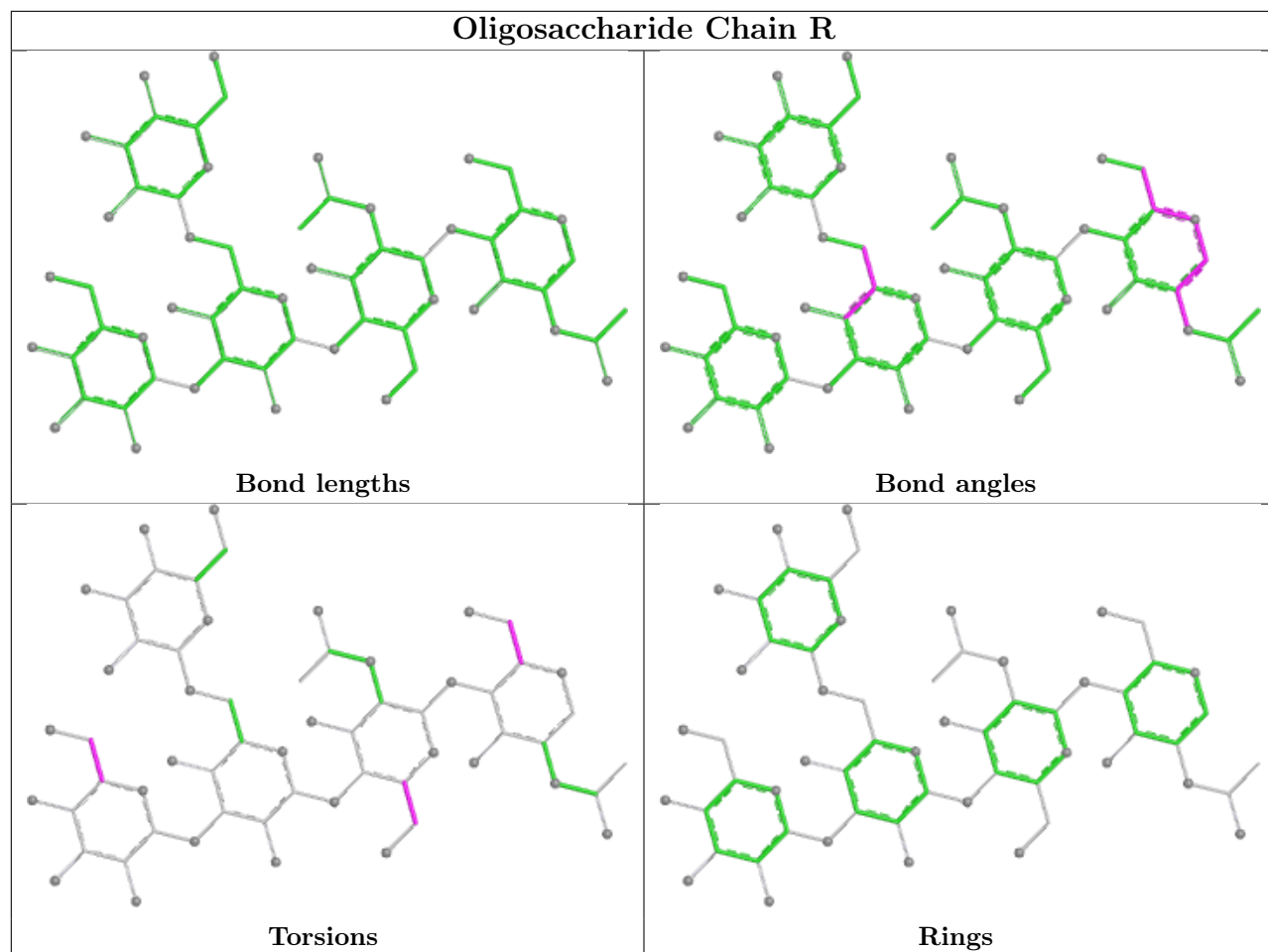
There are no ring outliers.

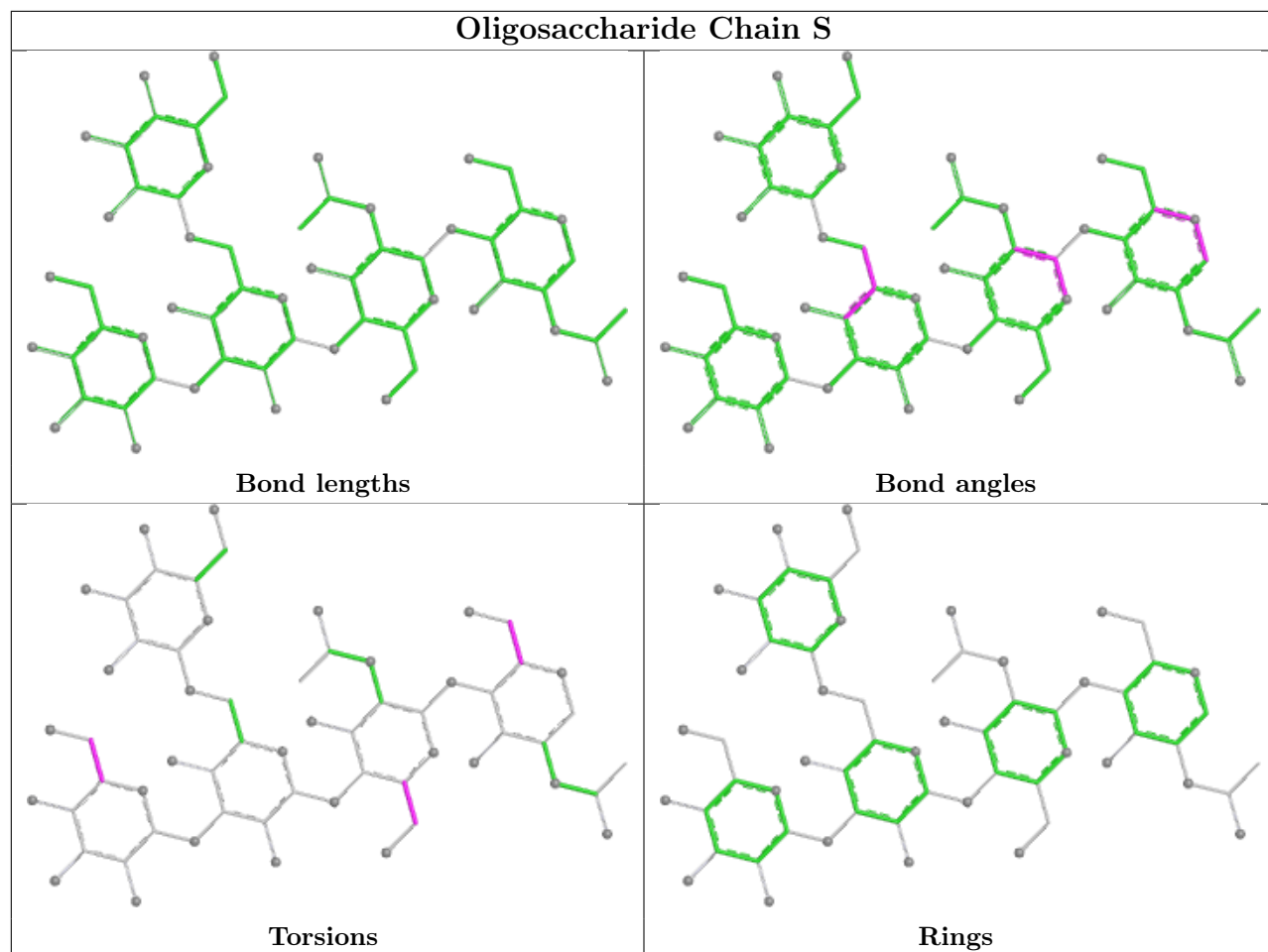
30 monomers are involved in 82 short contacts:

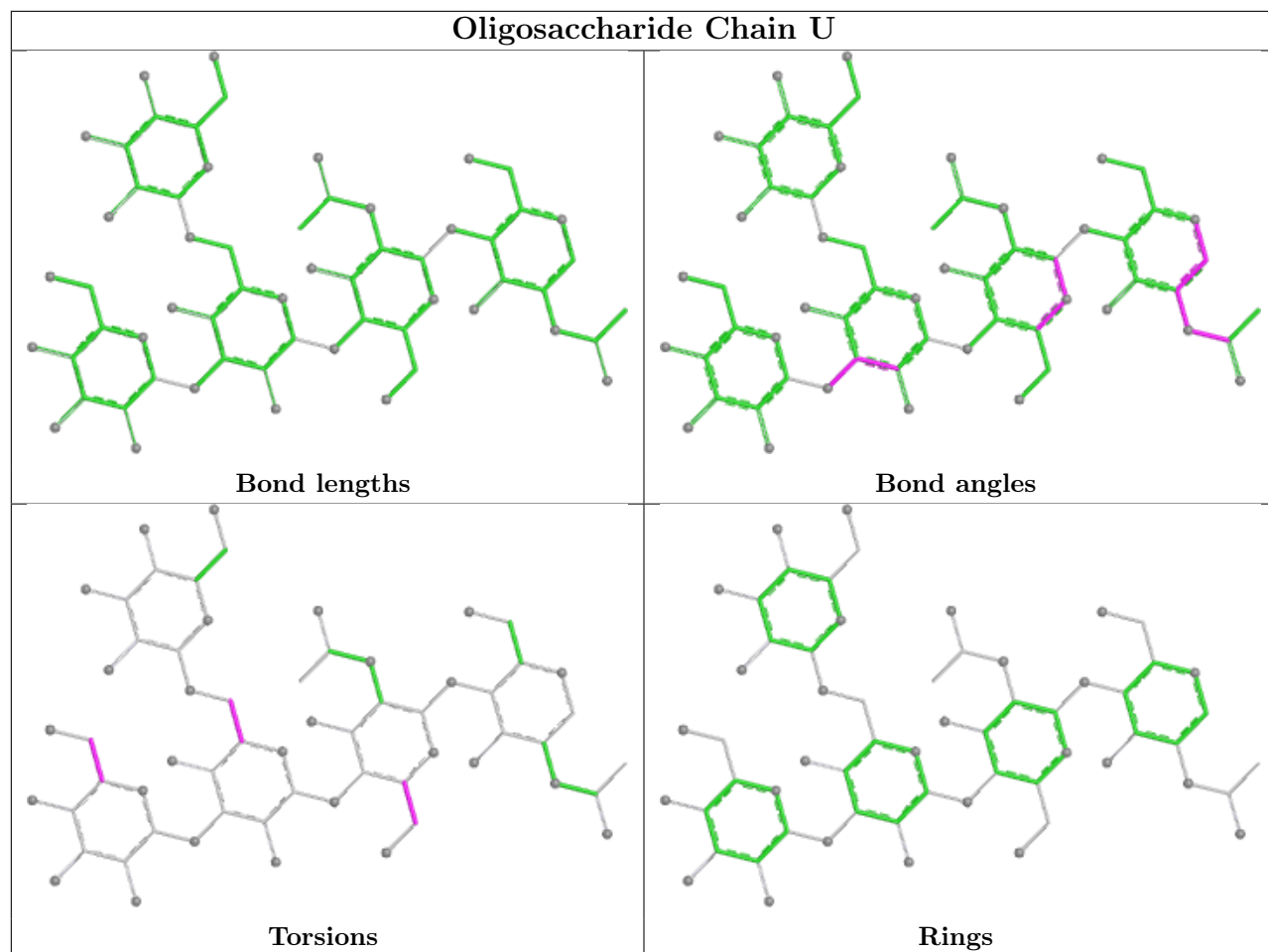
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	2	NAG	5	0
10	m	3	BMA	1	0
10	m	7	MAN	1	0
12	r	1	NAG	4	0
8	g	1	NAG	1	0
12	6	1	NAG	1	0
8	x	1	NAG	1	0
7	0	4	MAN	2	0
7	7	5	MAN	2	0
10	X	1	NAG	1	0
9	l	4	MAN	3	0
7	n	3	BMA	17	0
9	y	4	MAN	2	0
7	n	4	MAN	4	0
12	d	2	NAG	1	0
12	i	1	NAG	3	0
7	n	2	NAG	1	0
7	0	3	BMA	9	0
9	W	2	NAG	2	0
12	f	2	NAG	1	0
11	Y	2	NAG	1	0
9	l	2	NAG	2	0
12	f	1	NAG	1	0
8	T	1	NAG	1	0
12	6	2	NAG	1	0
9	W	4	MAN	5	0
10	m	1	NAG	1	0
8	c	2	NAG	1	0
7	U	1	NAG	3	0
7	v	1	NAG	8	0

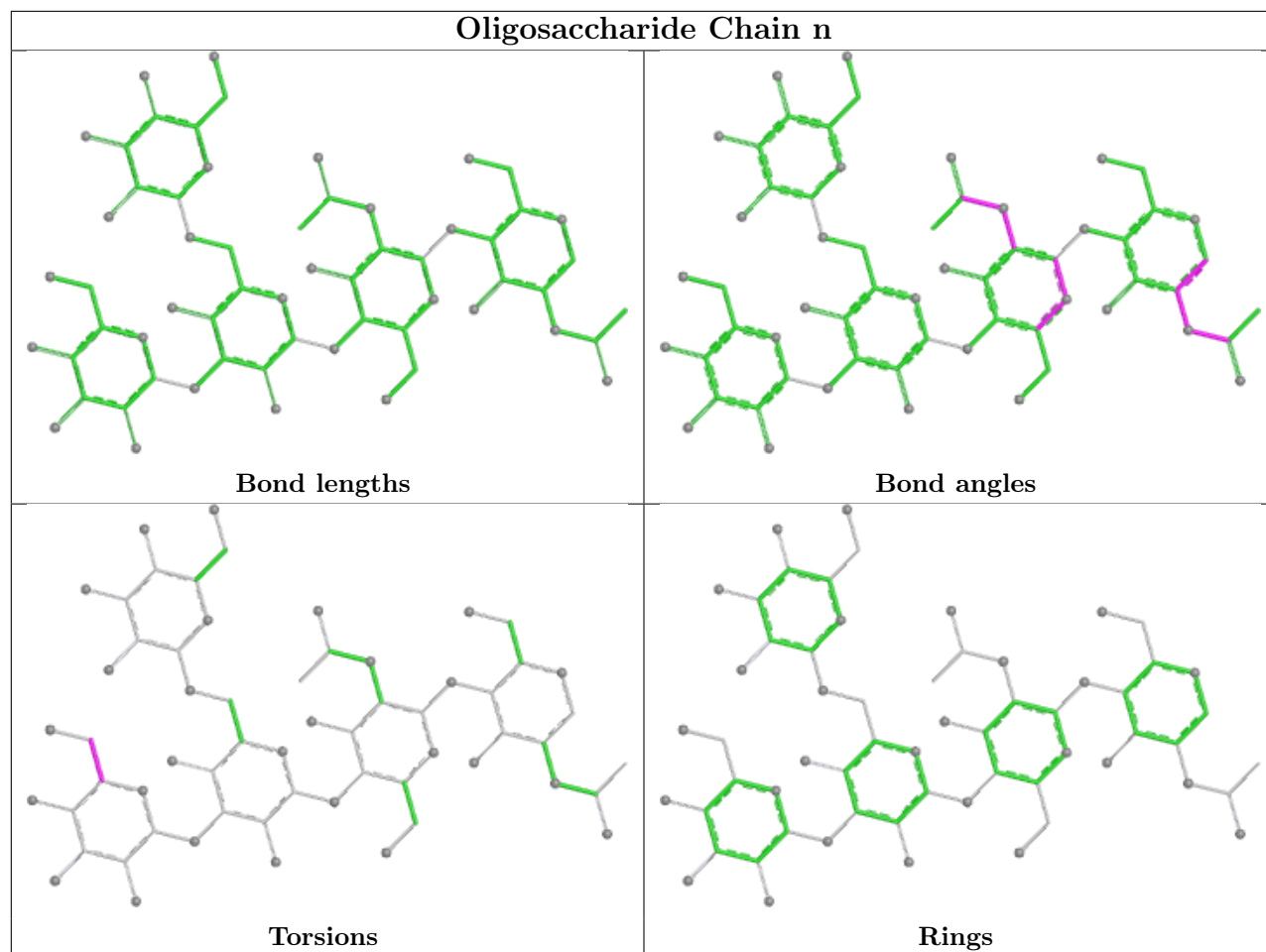
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

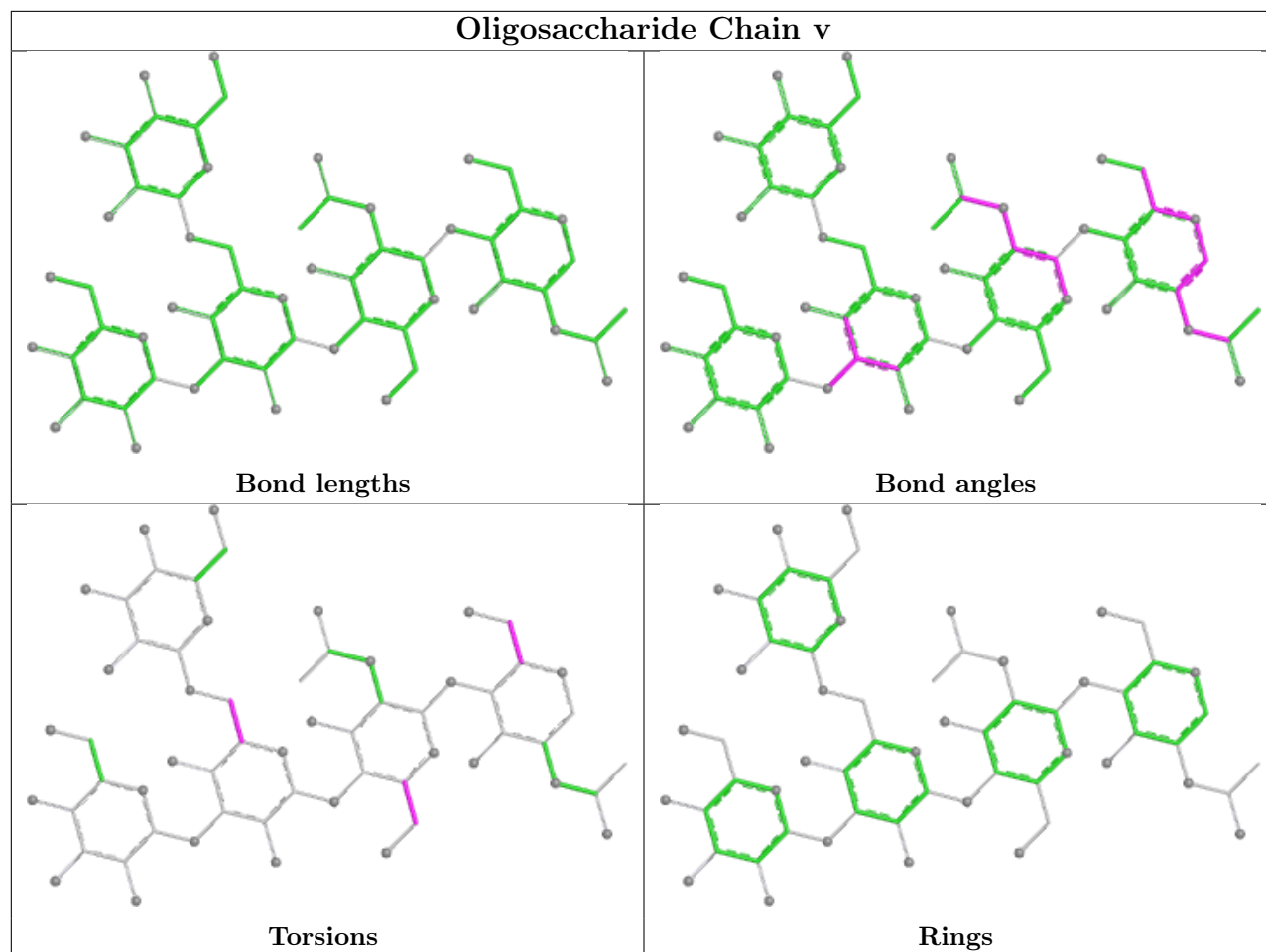


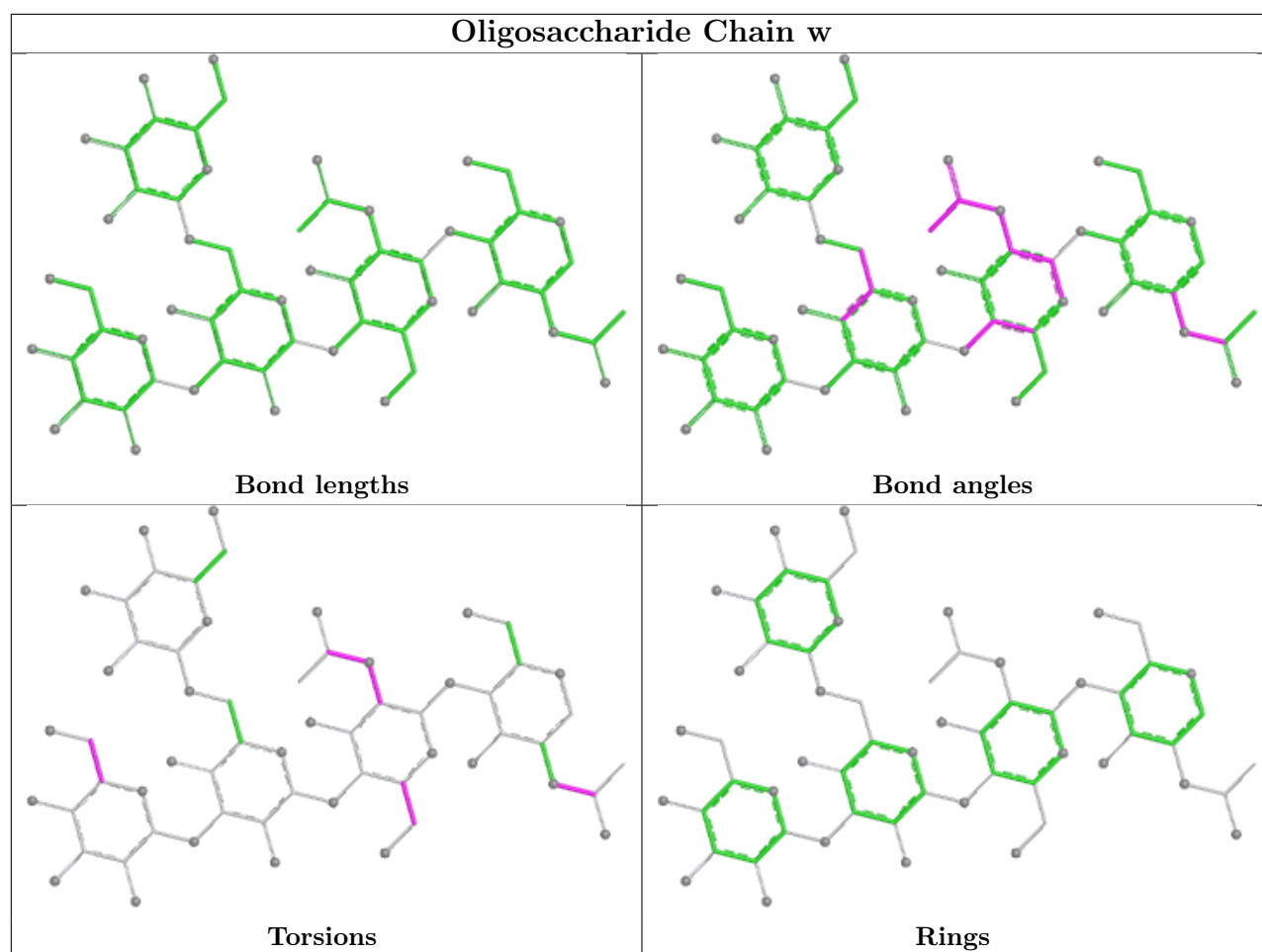


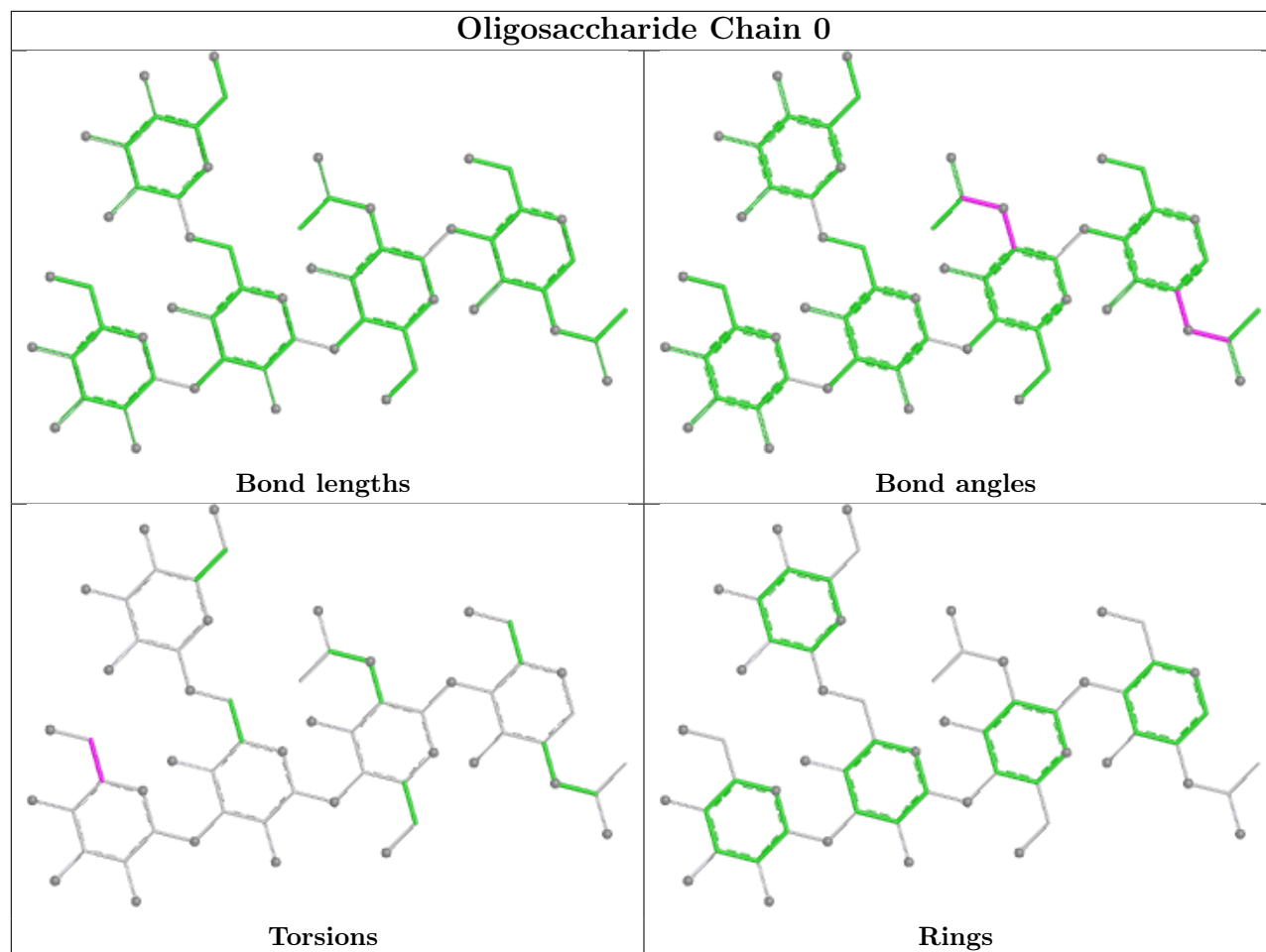


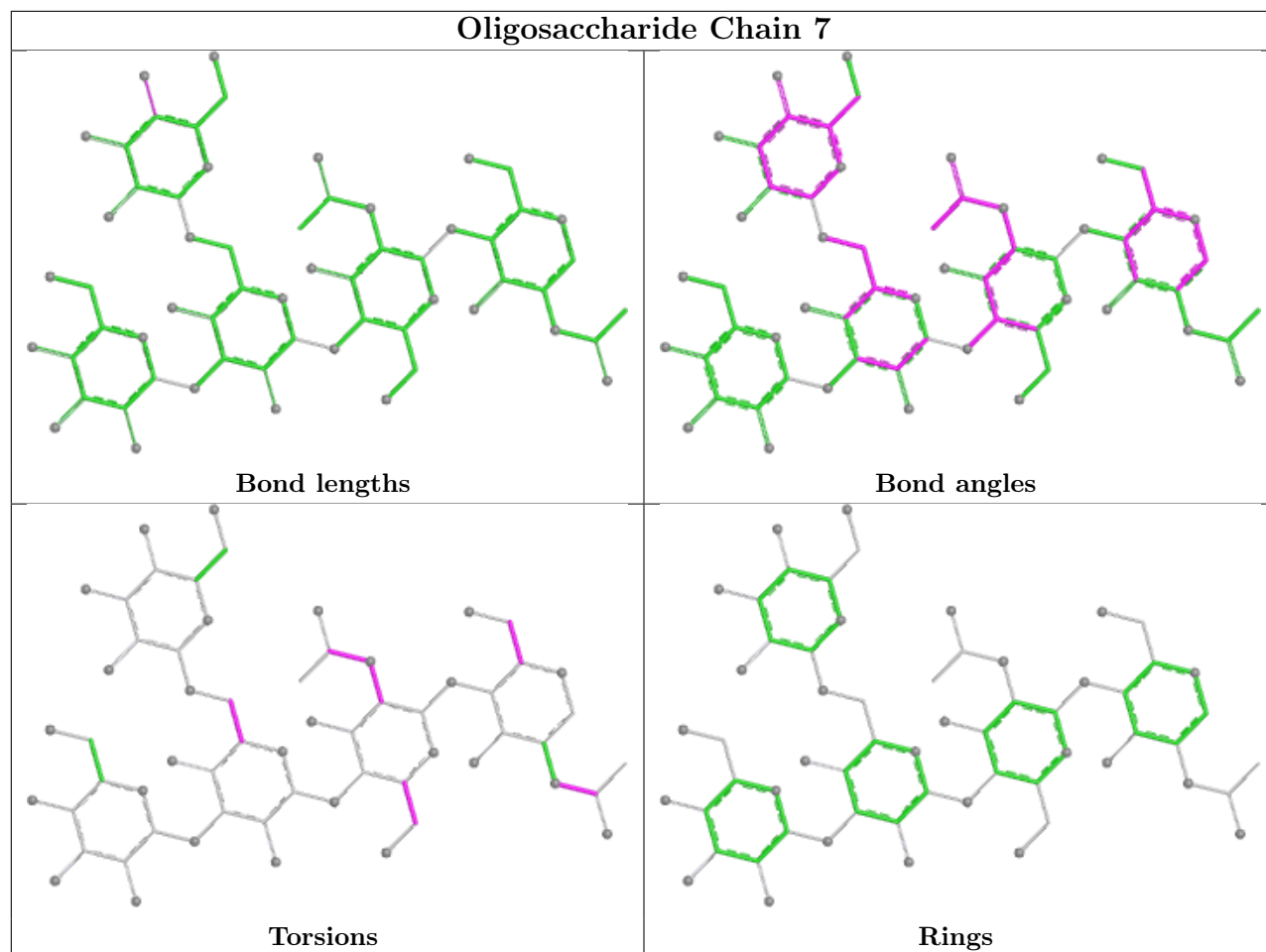


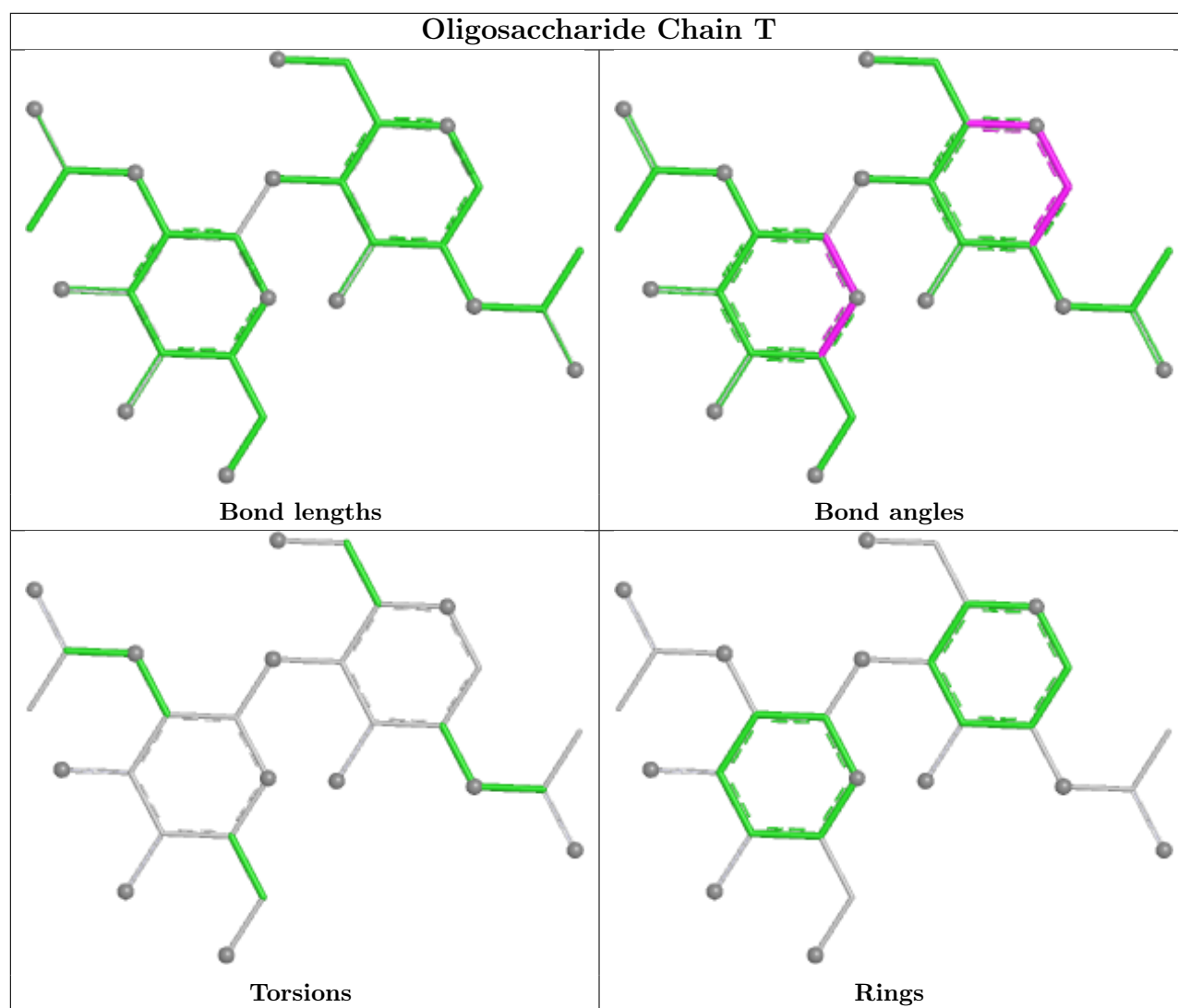


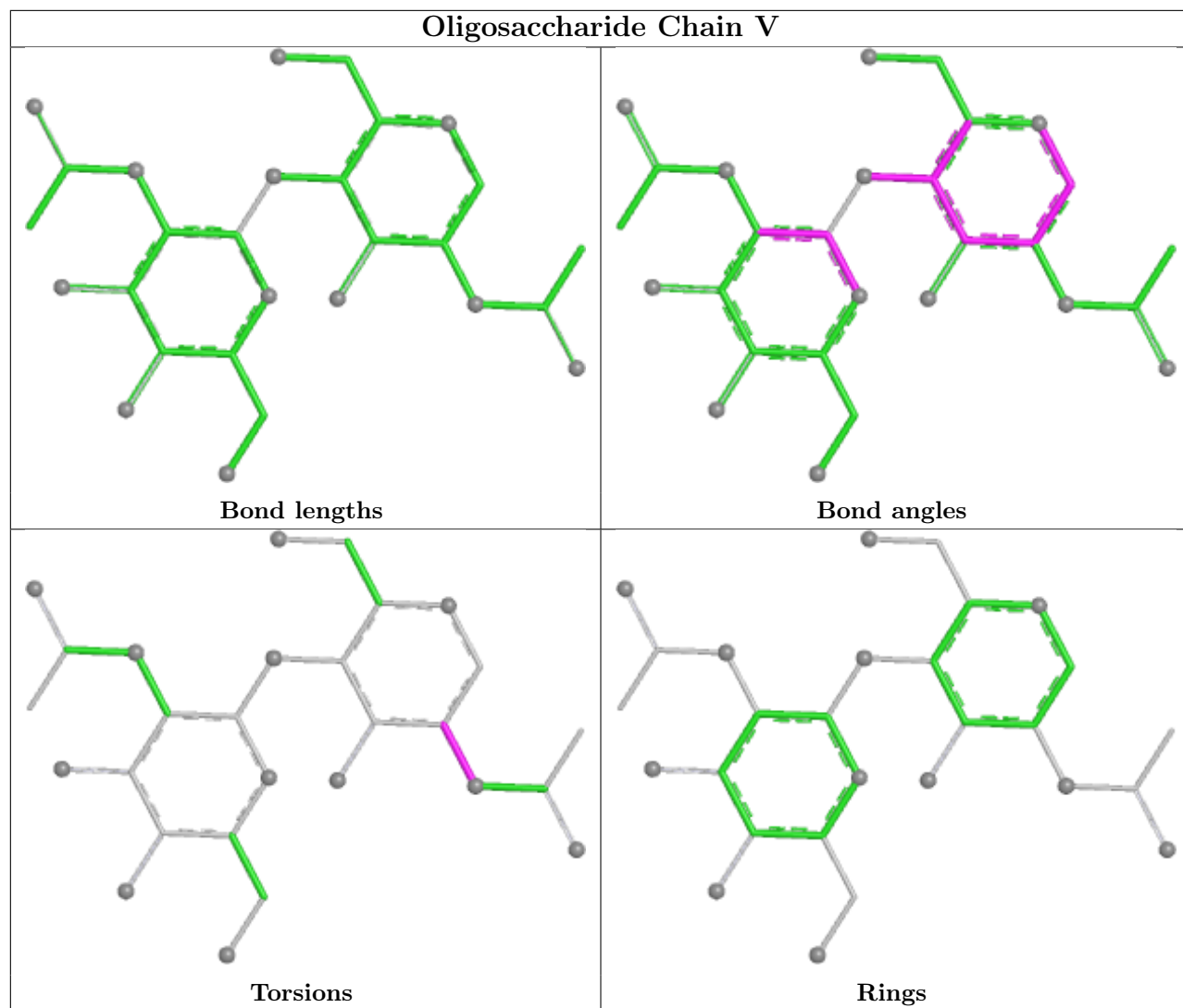


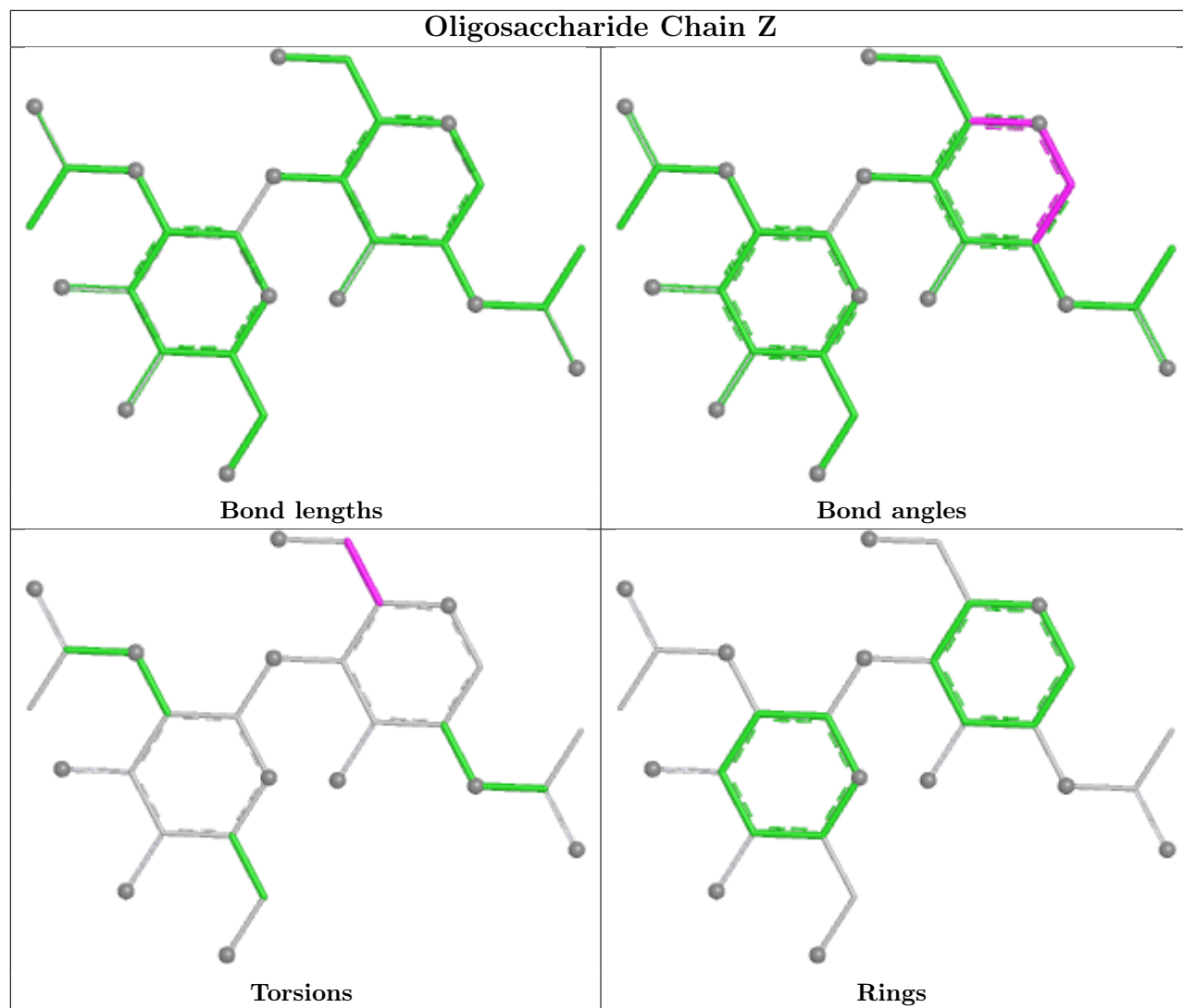


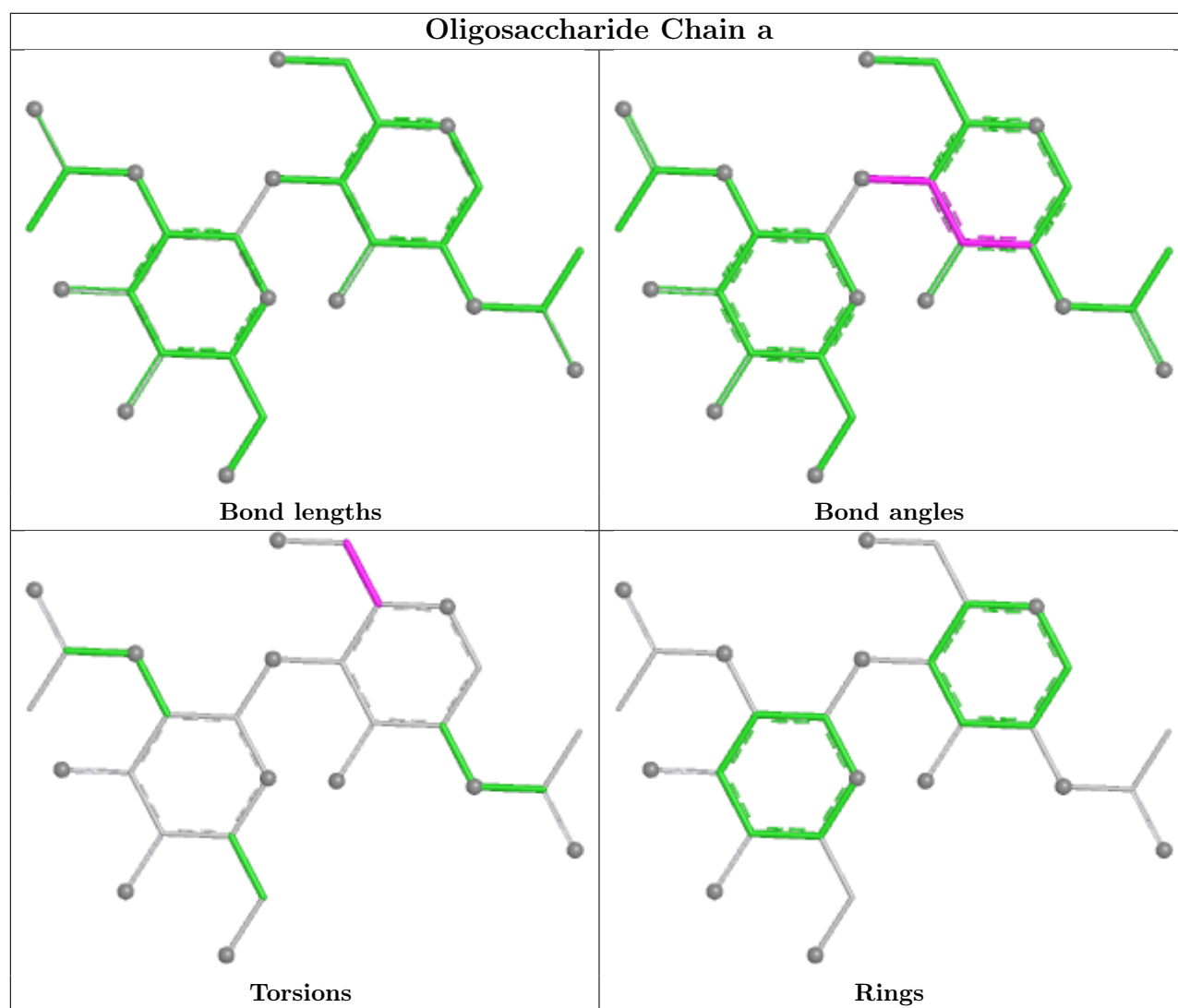


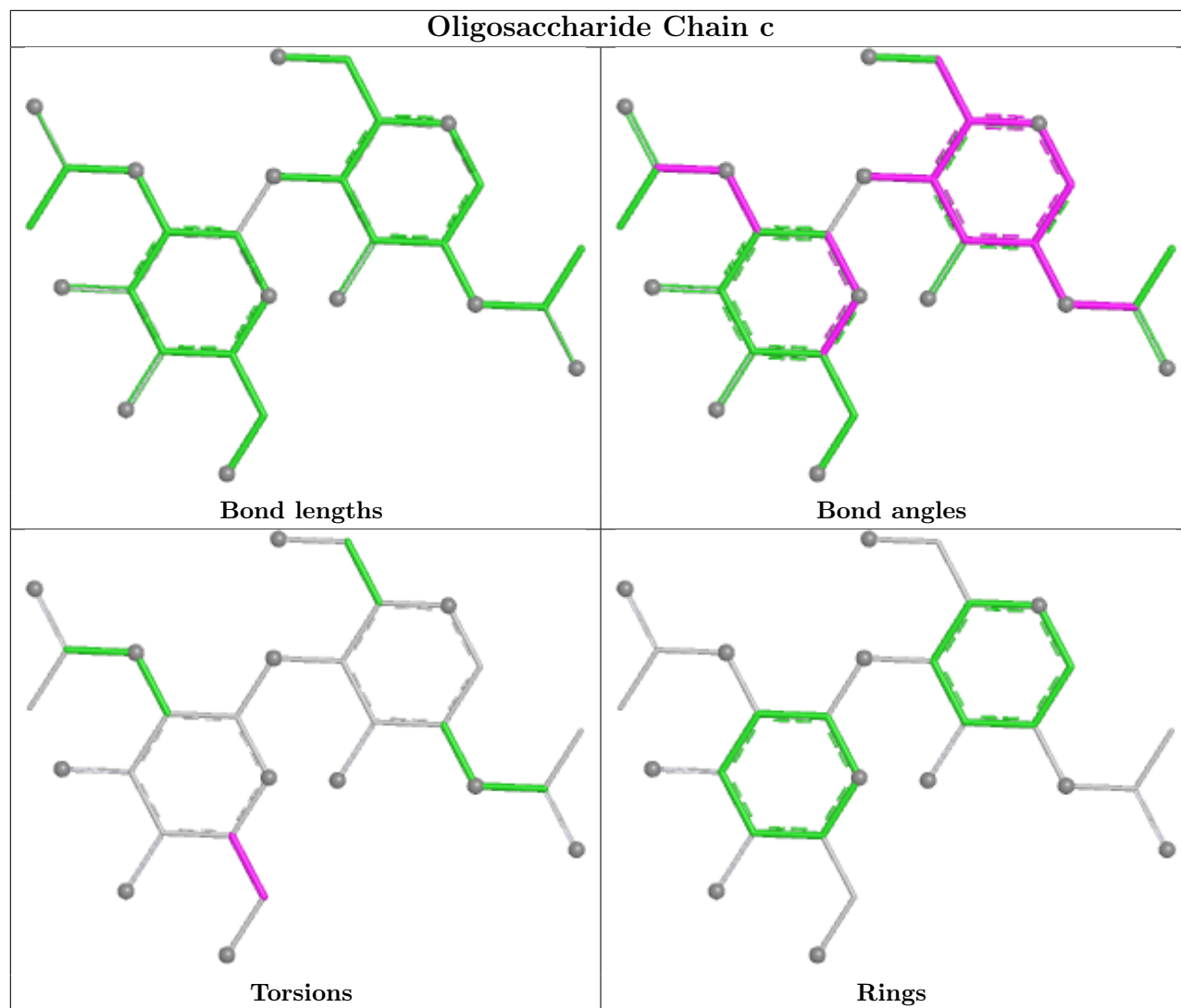


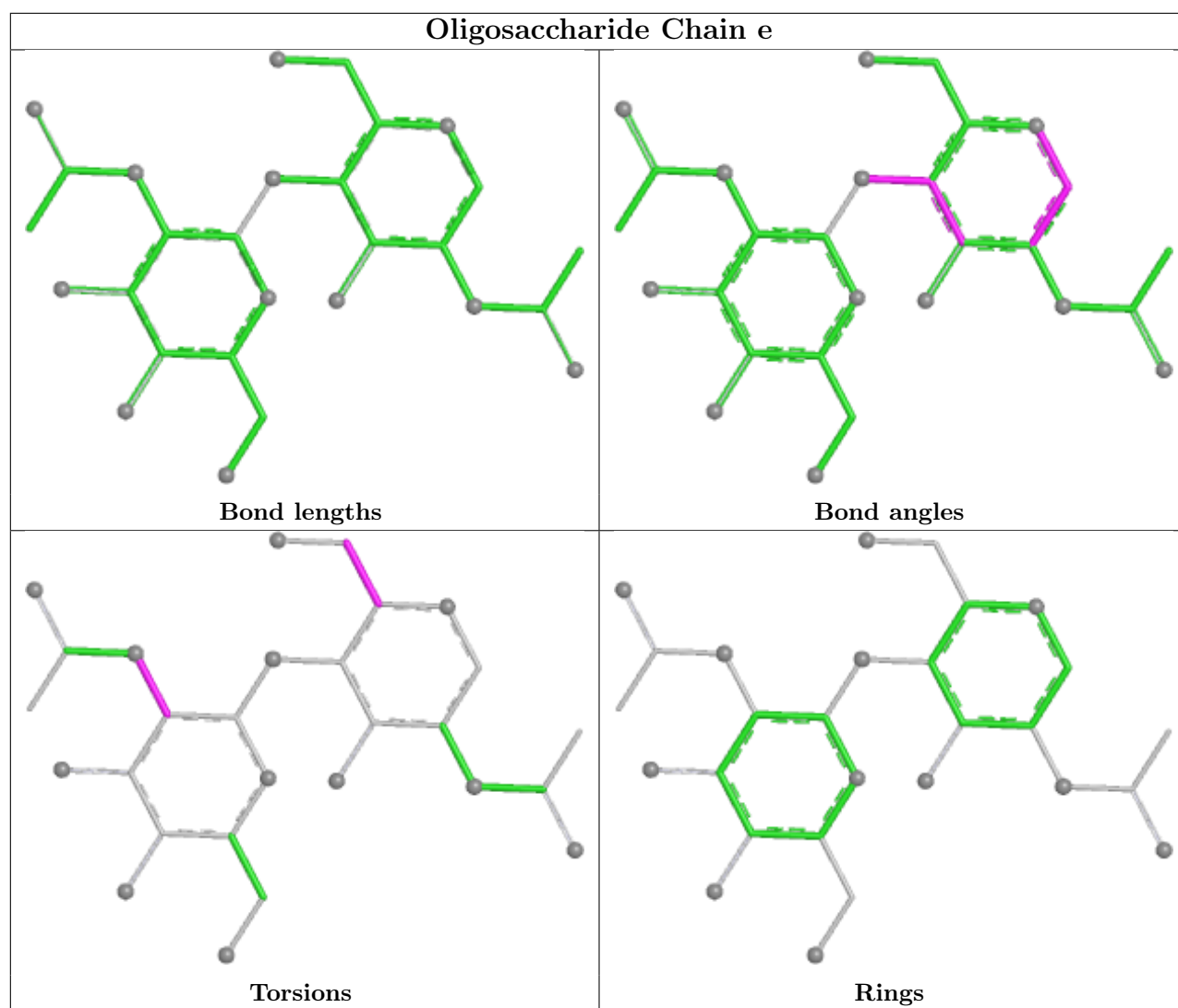


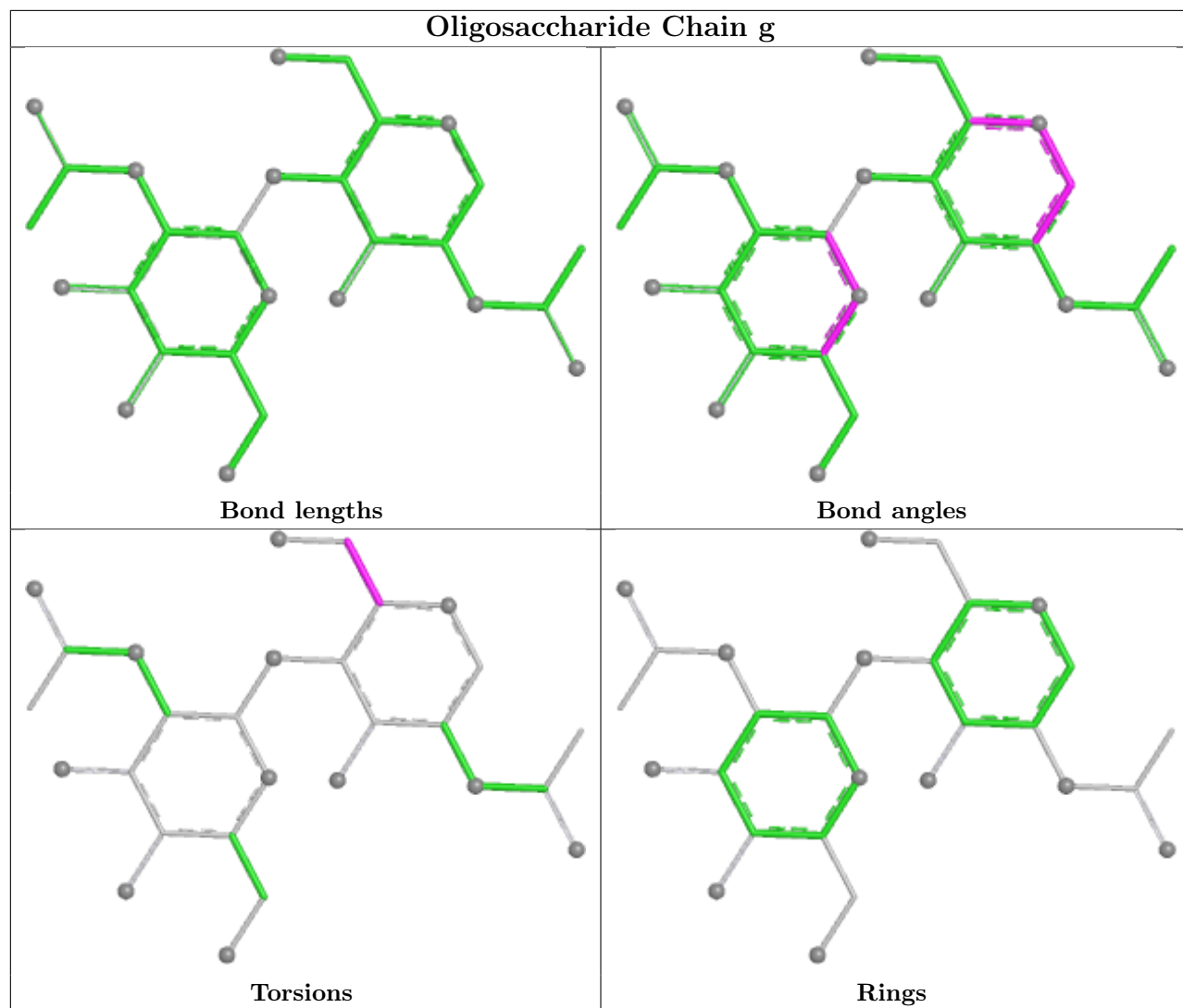


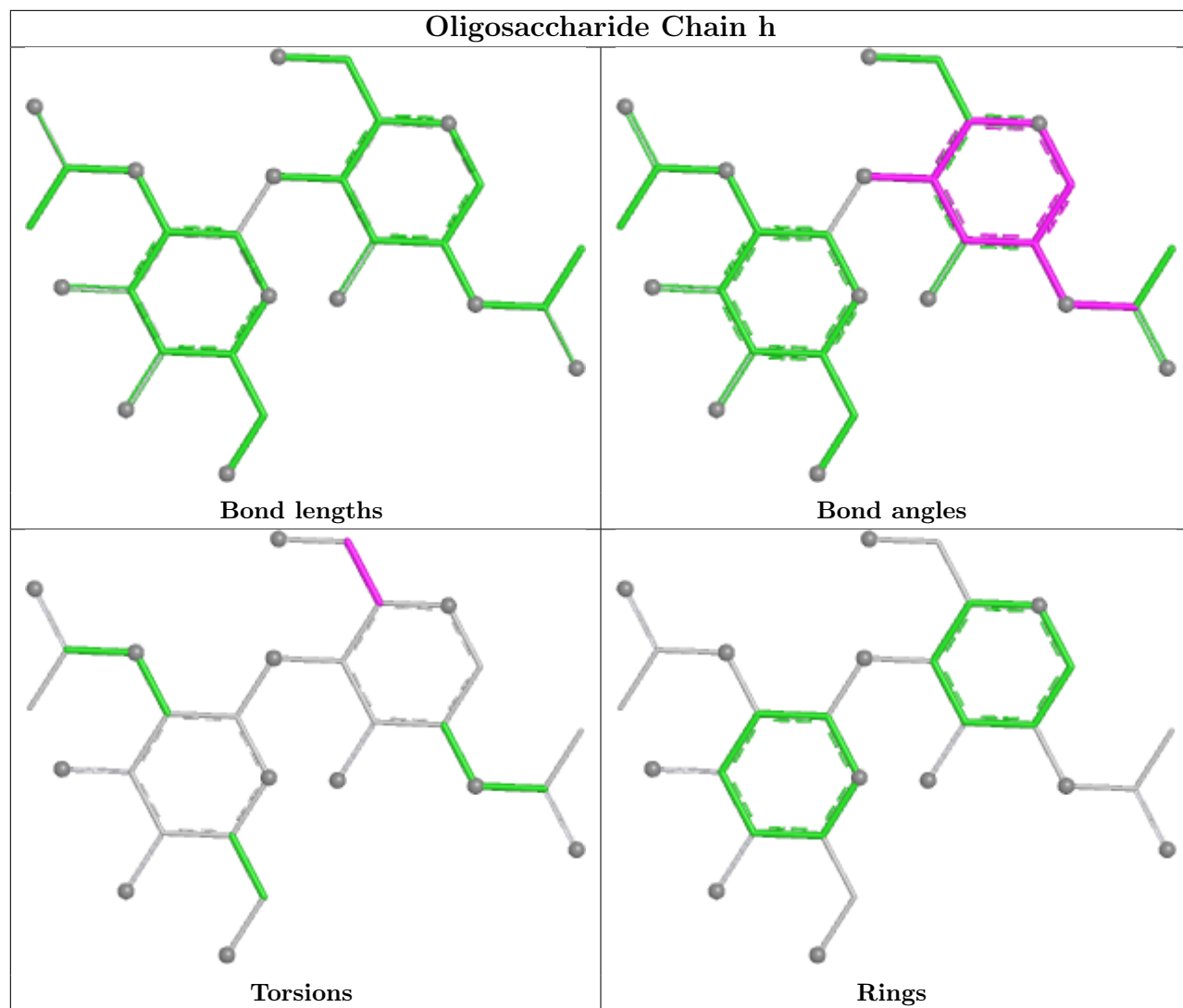


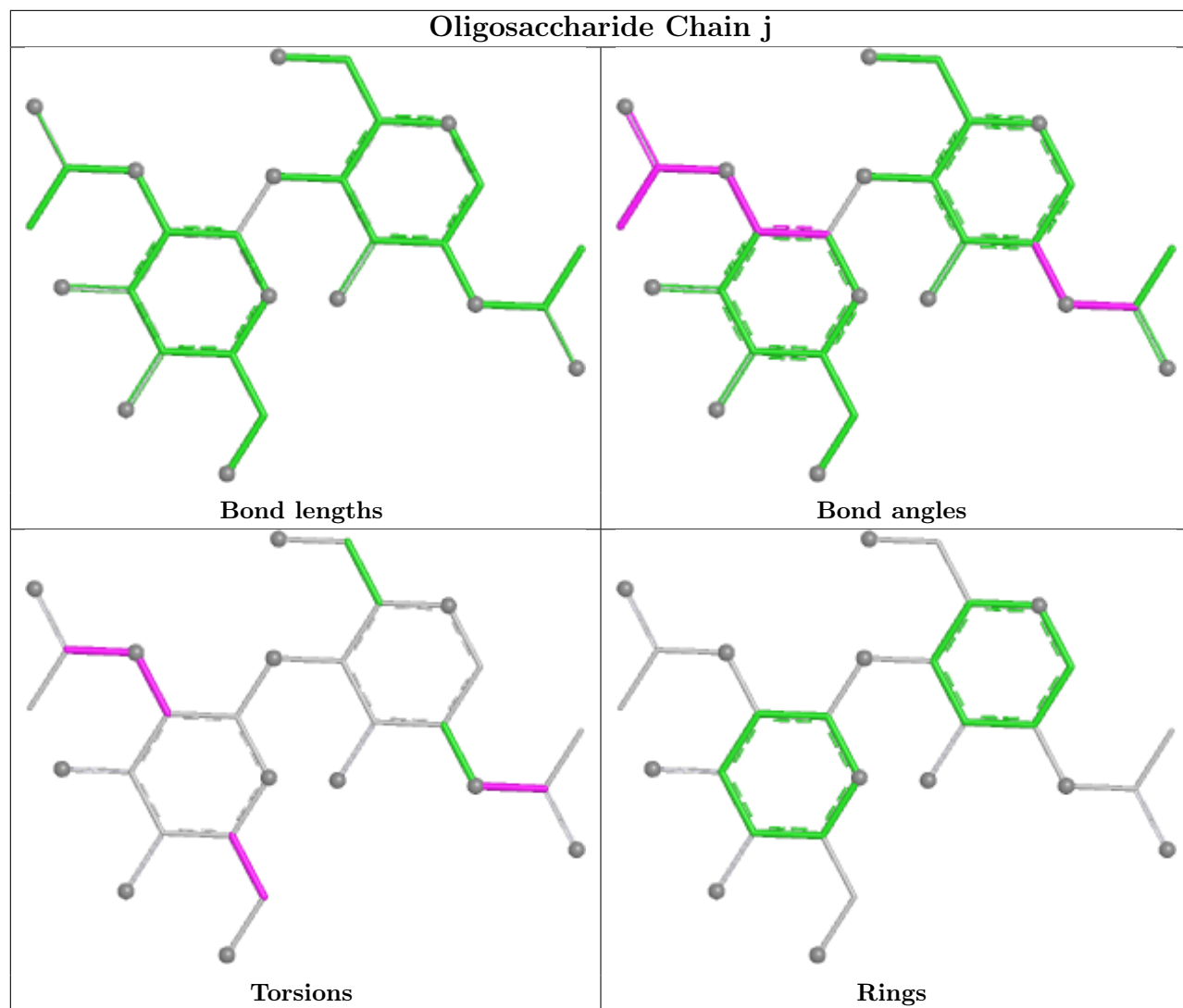


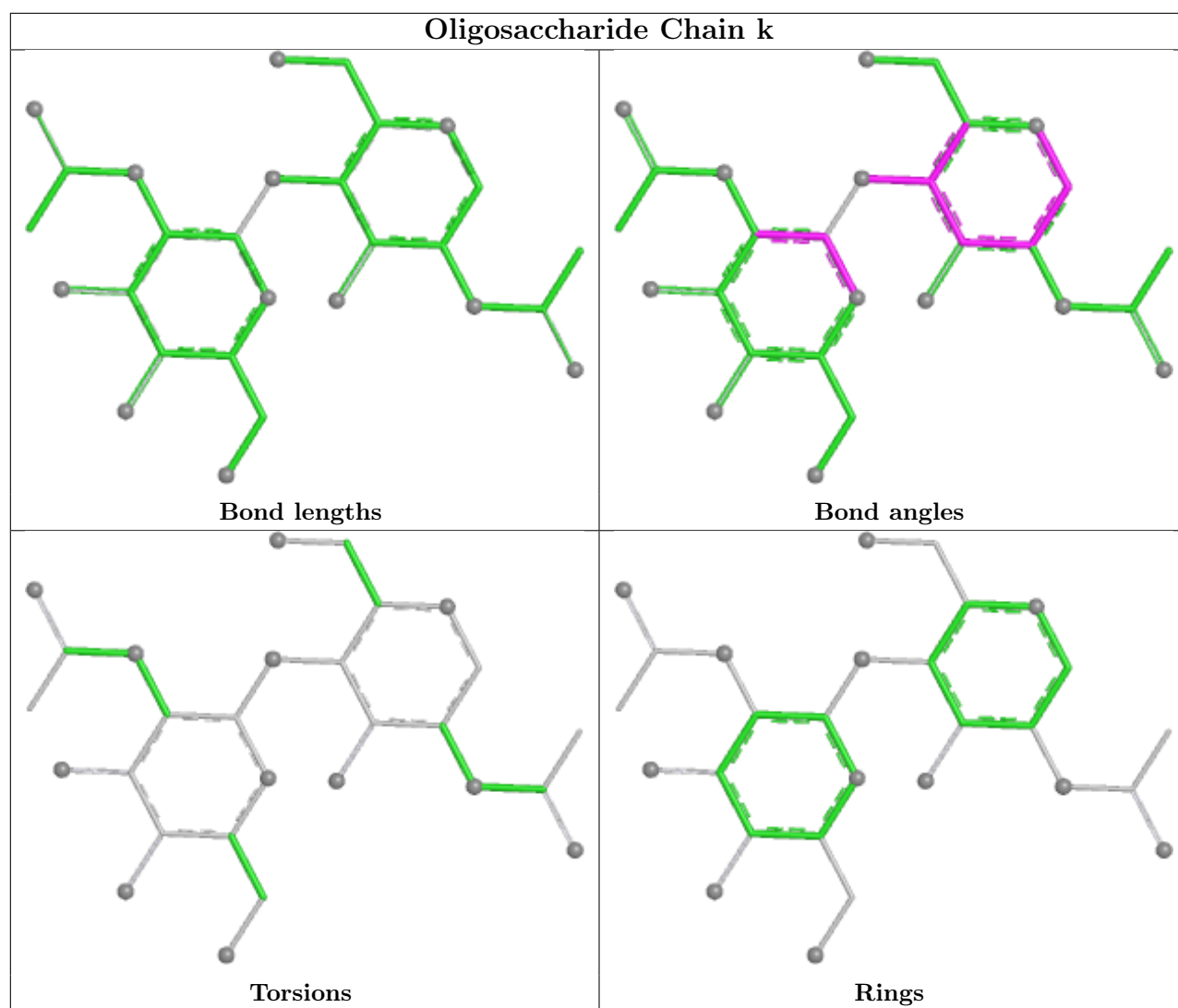


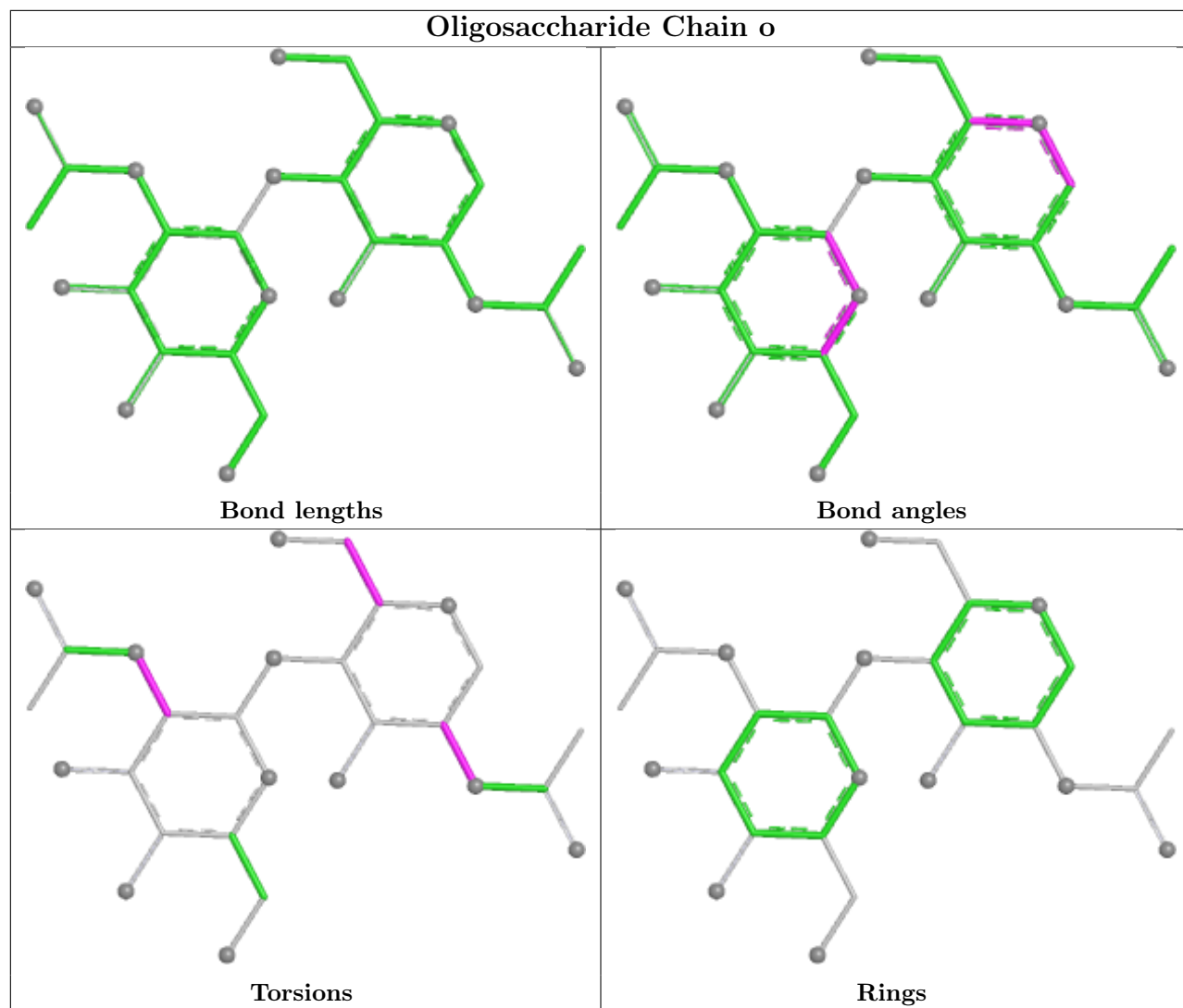


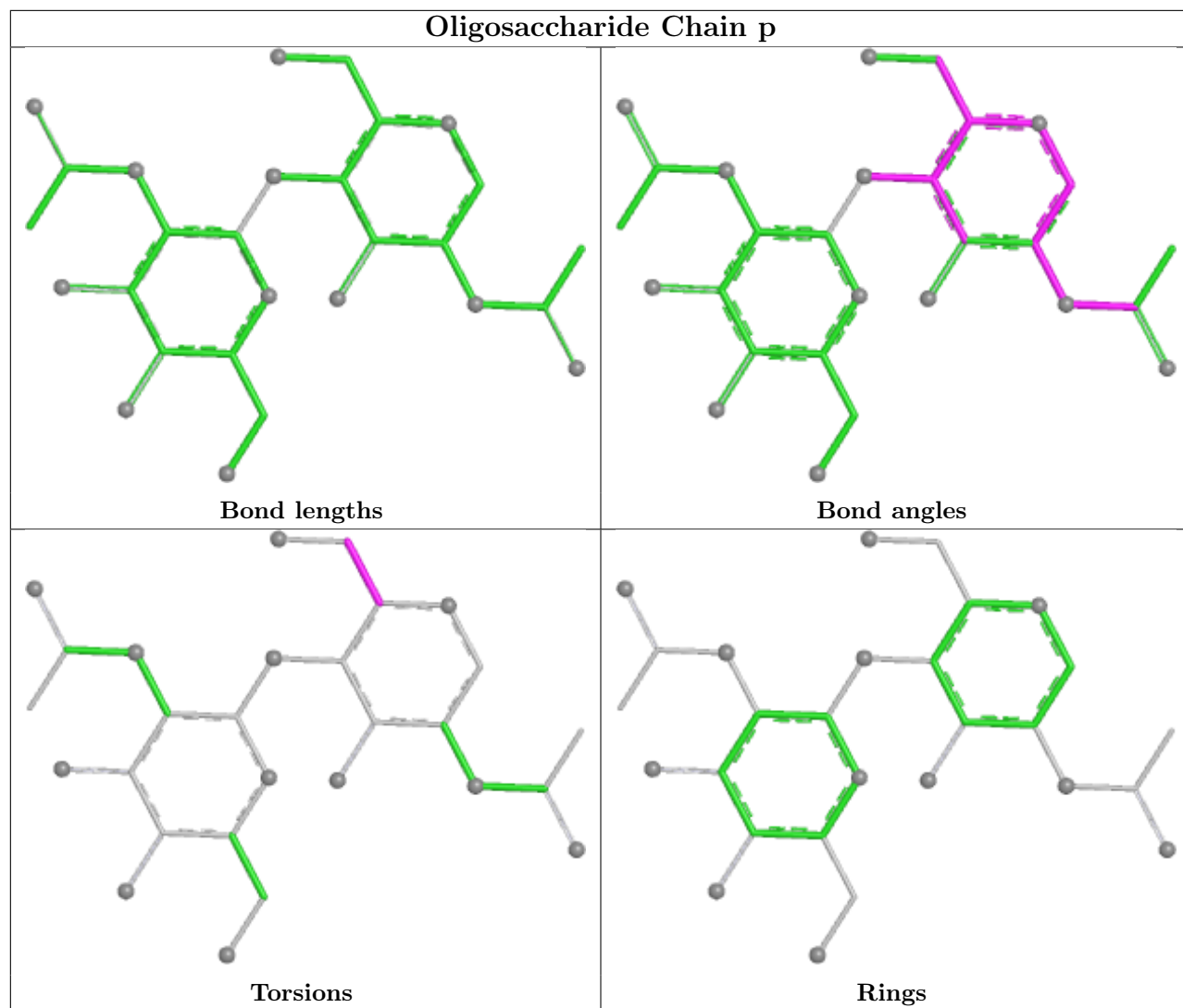


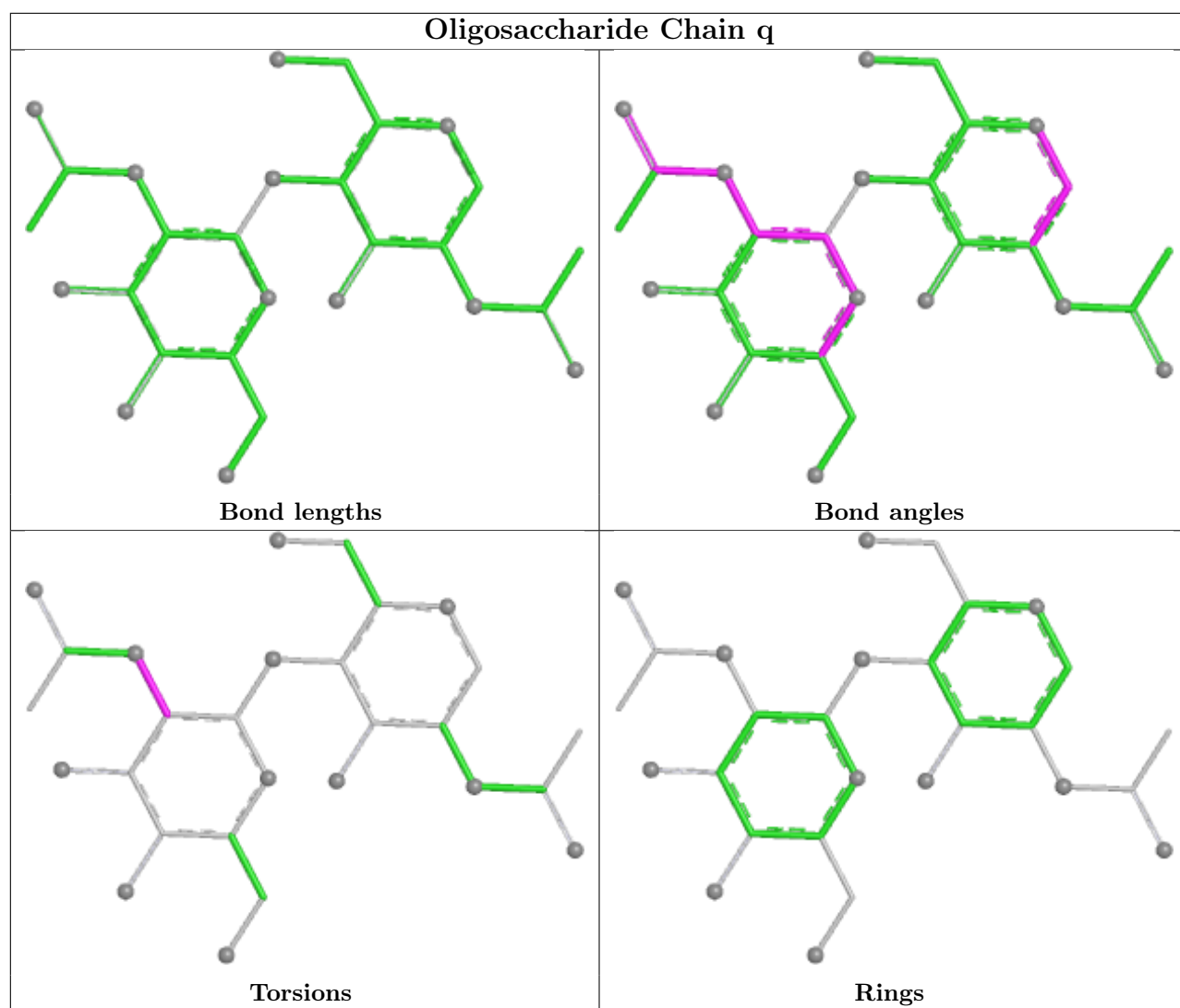


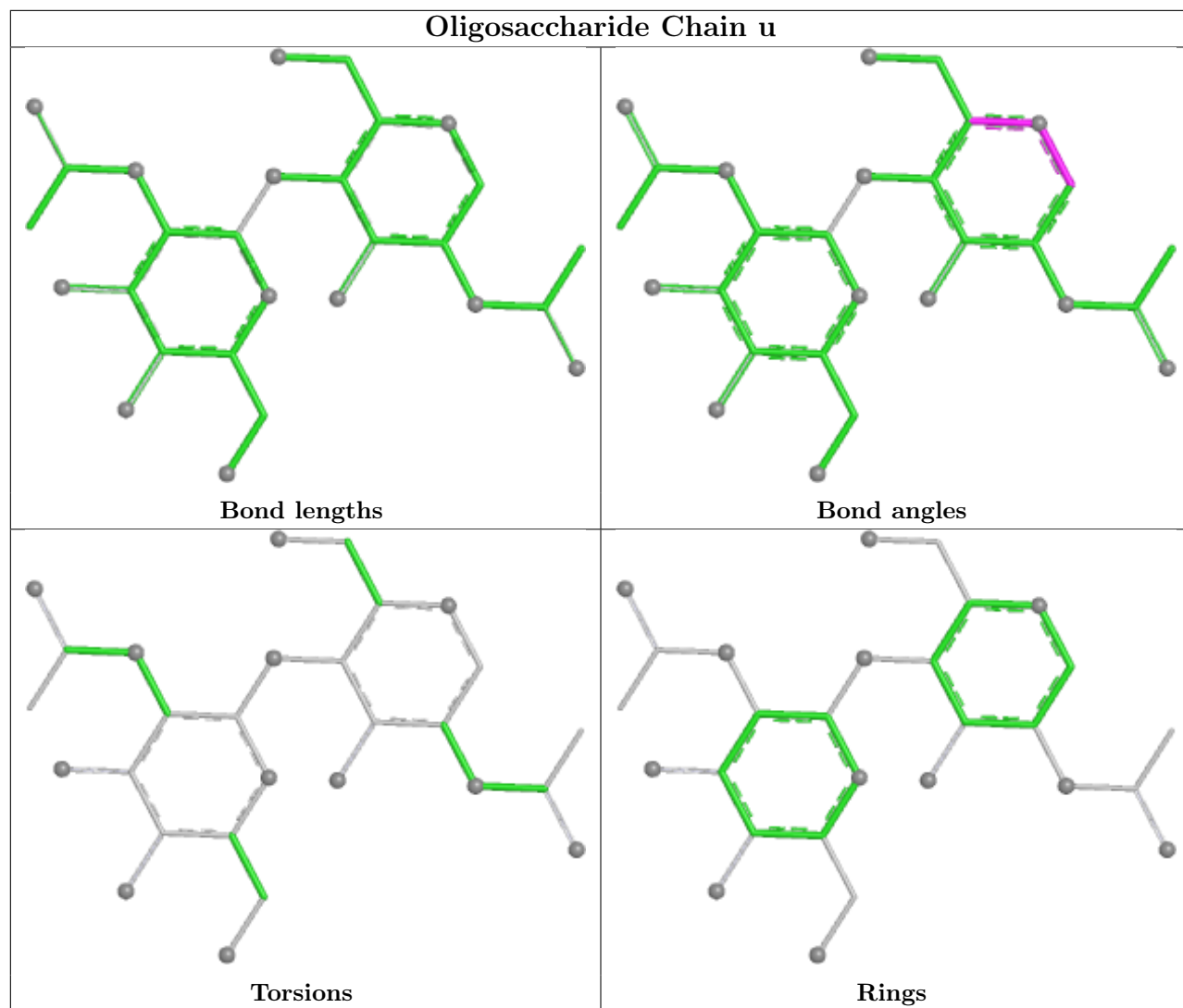


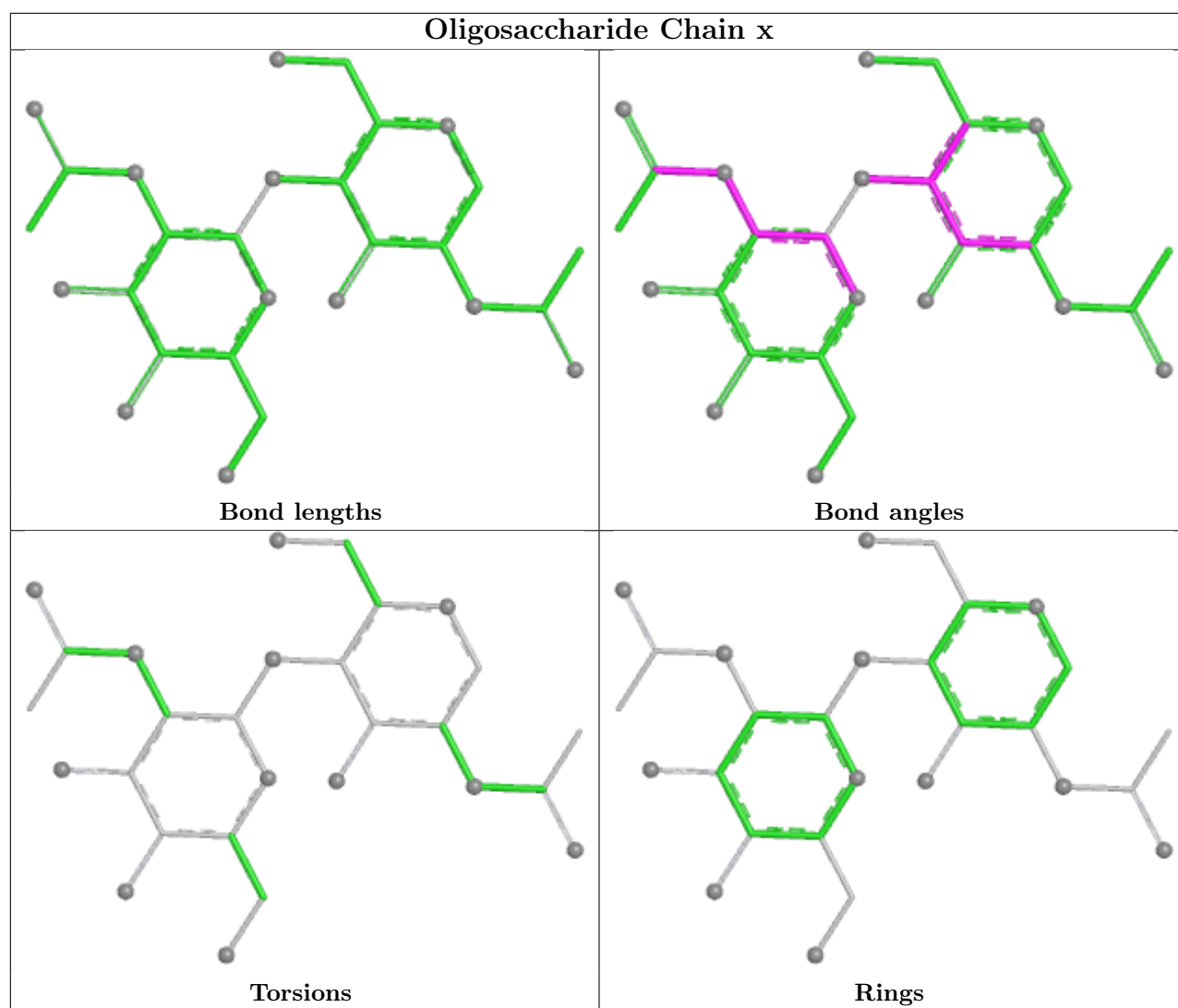


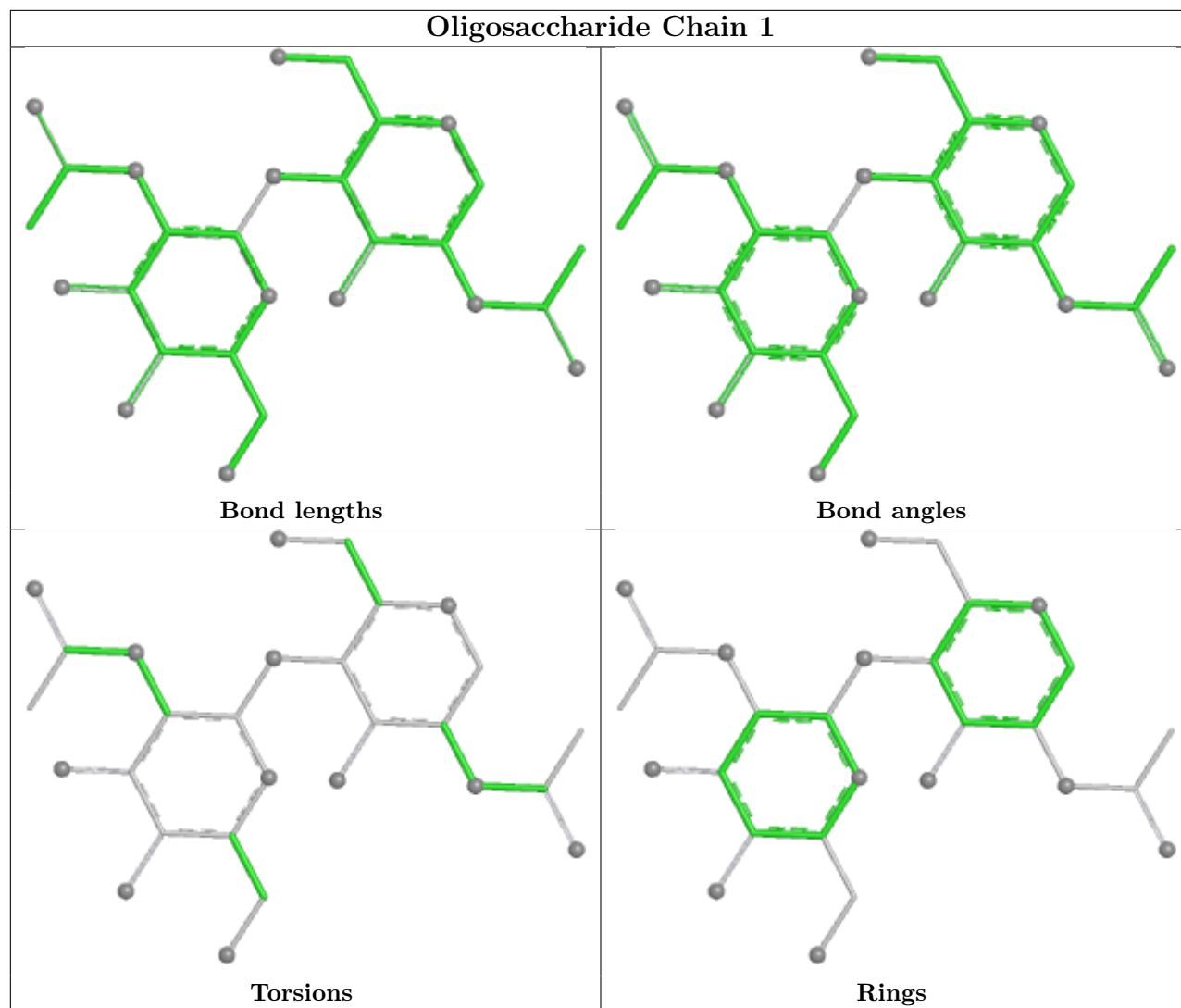


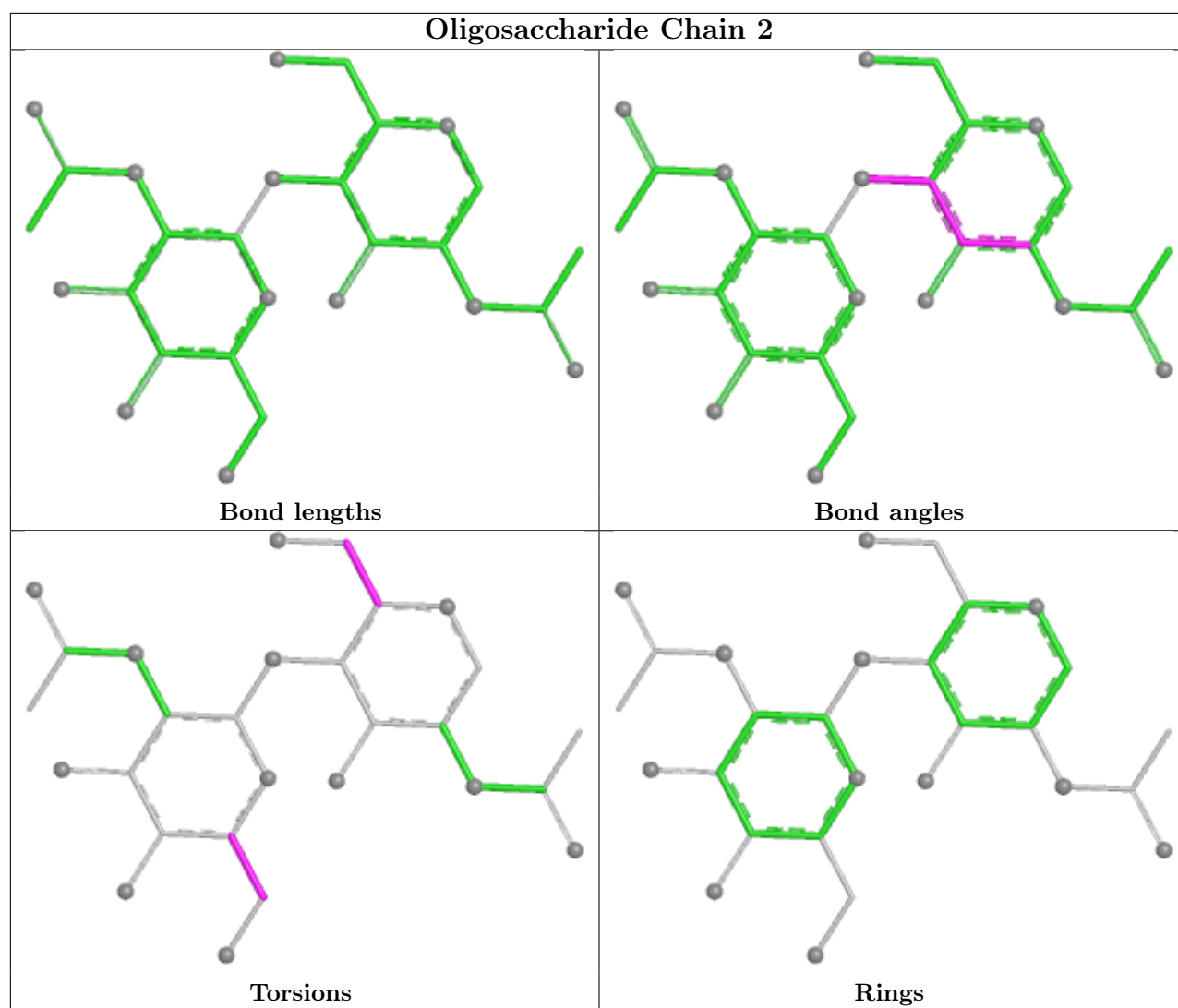


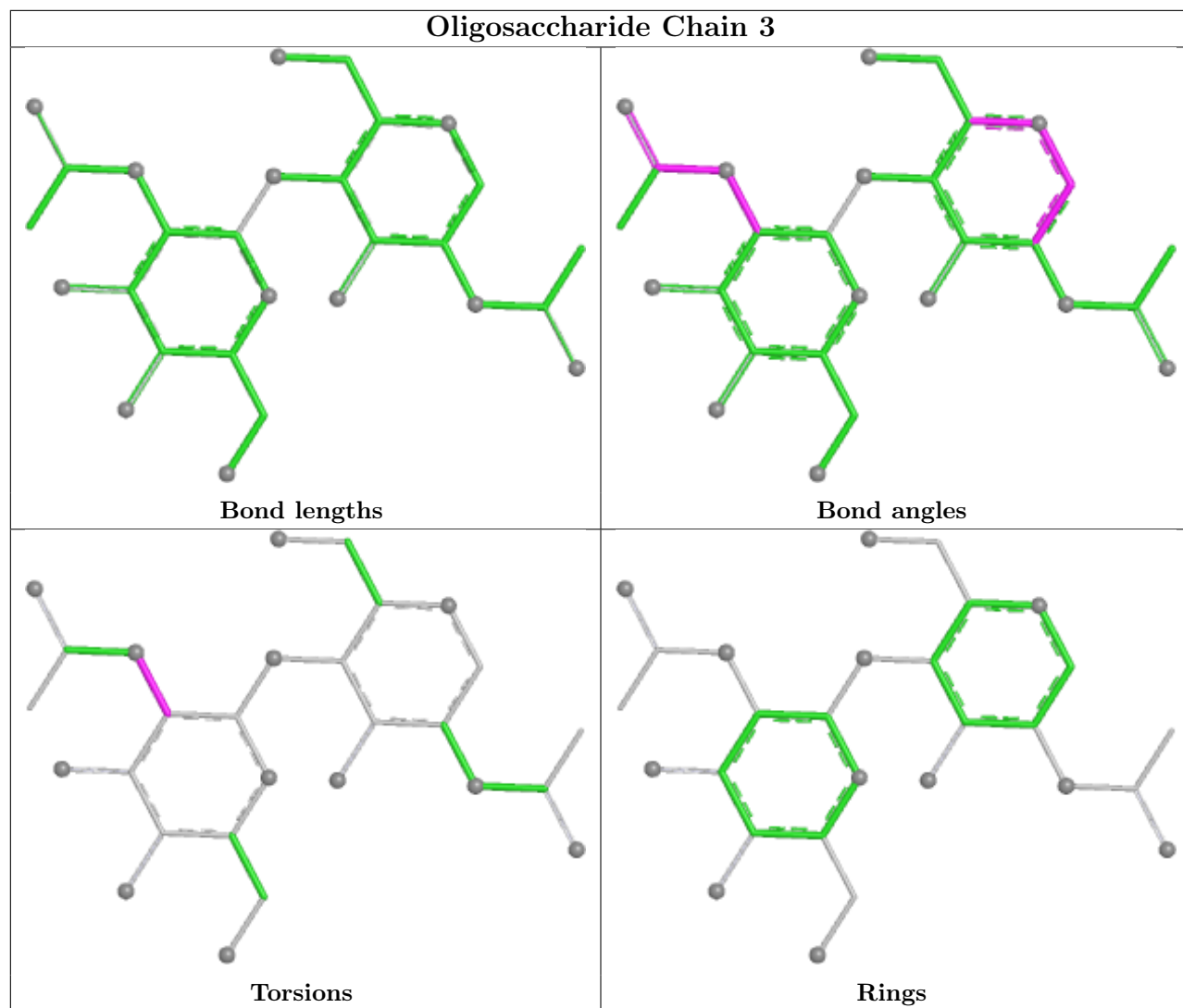


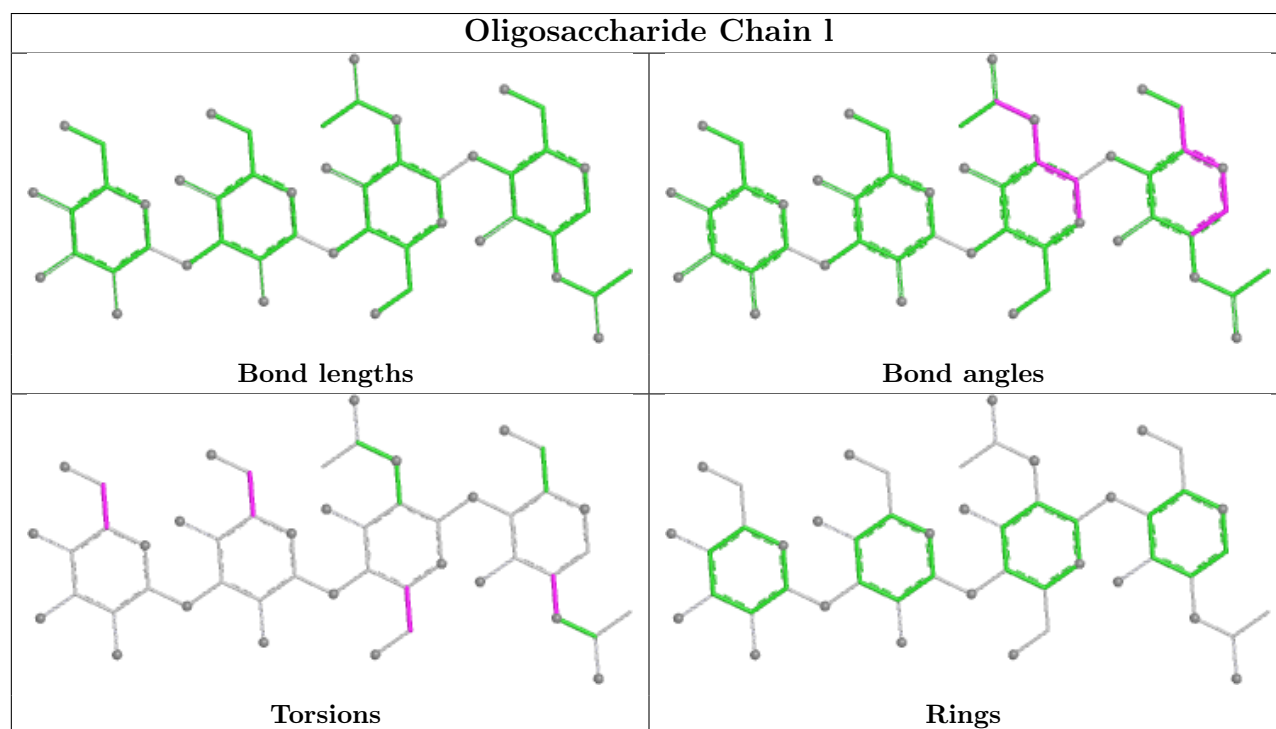
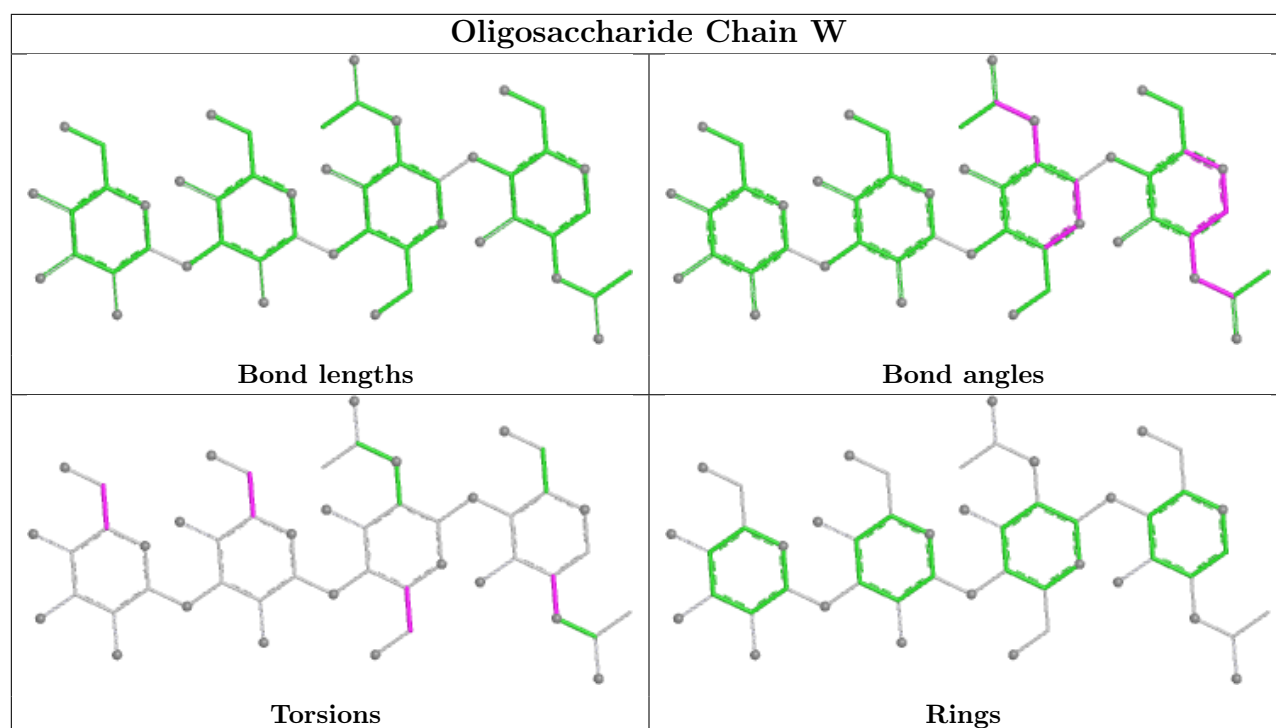


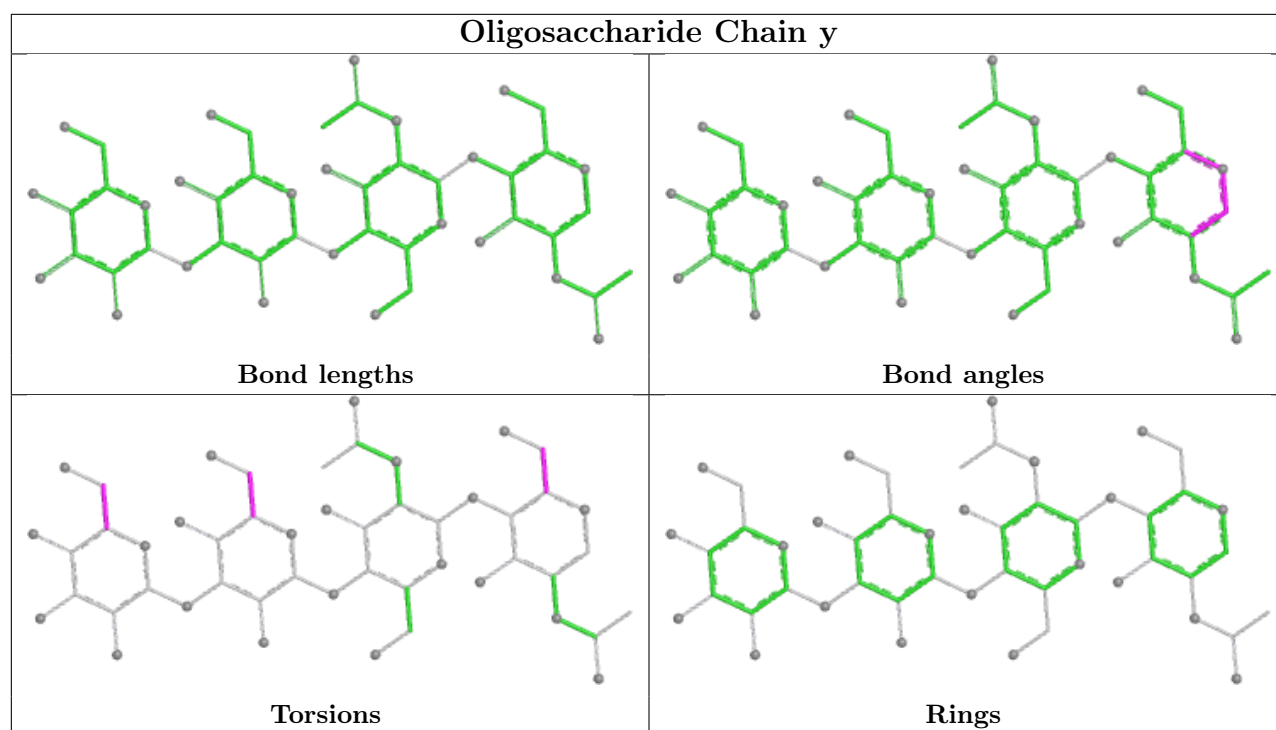


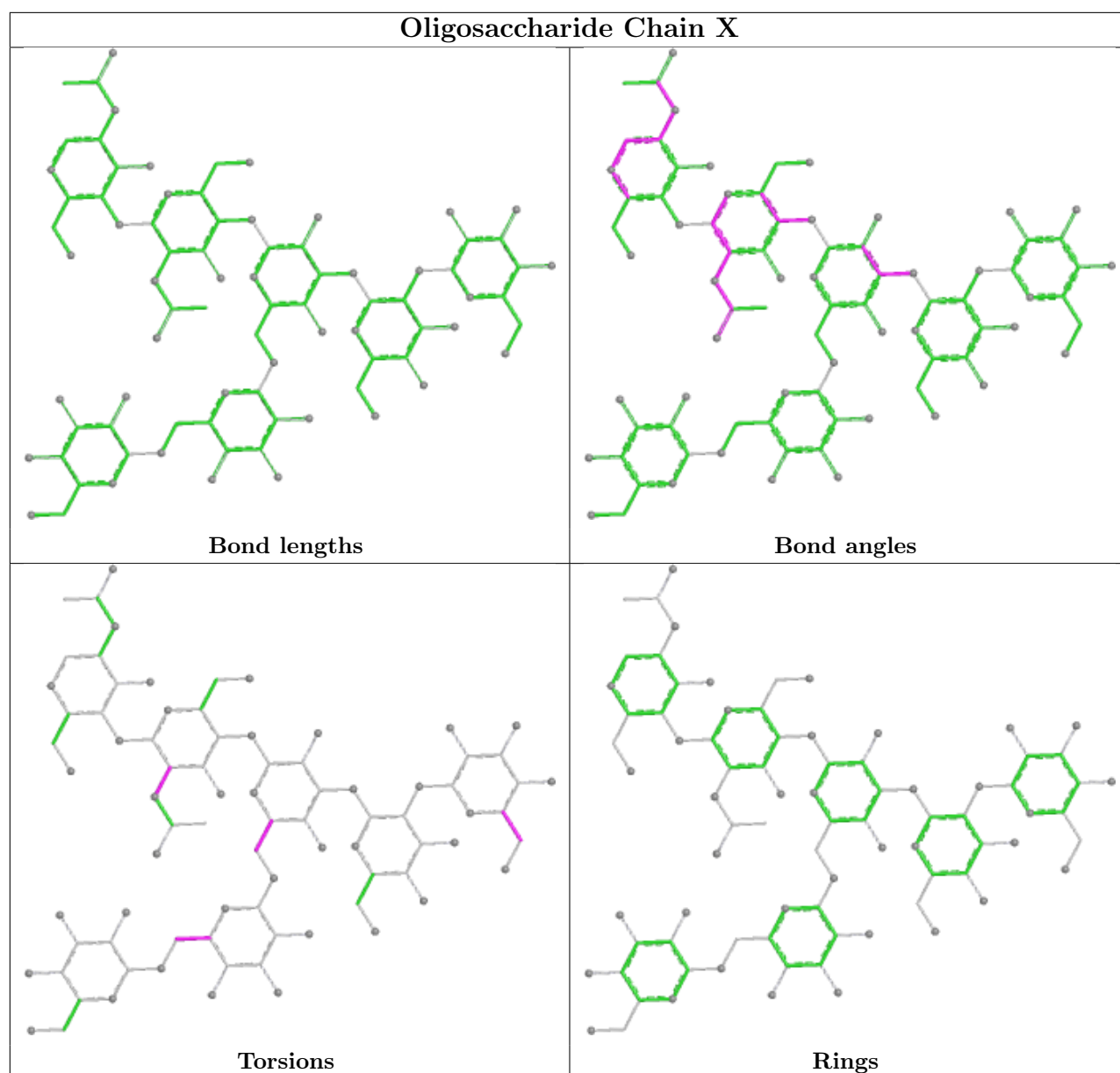


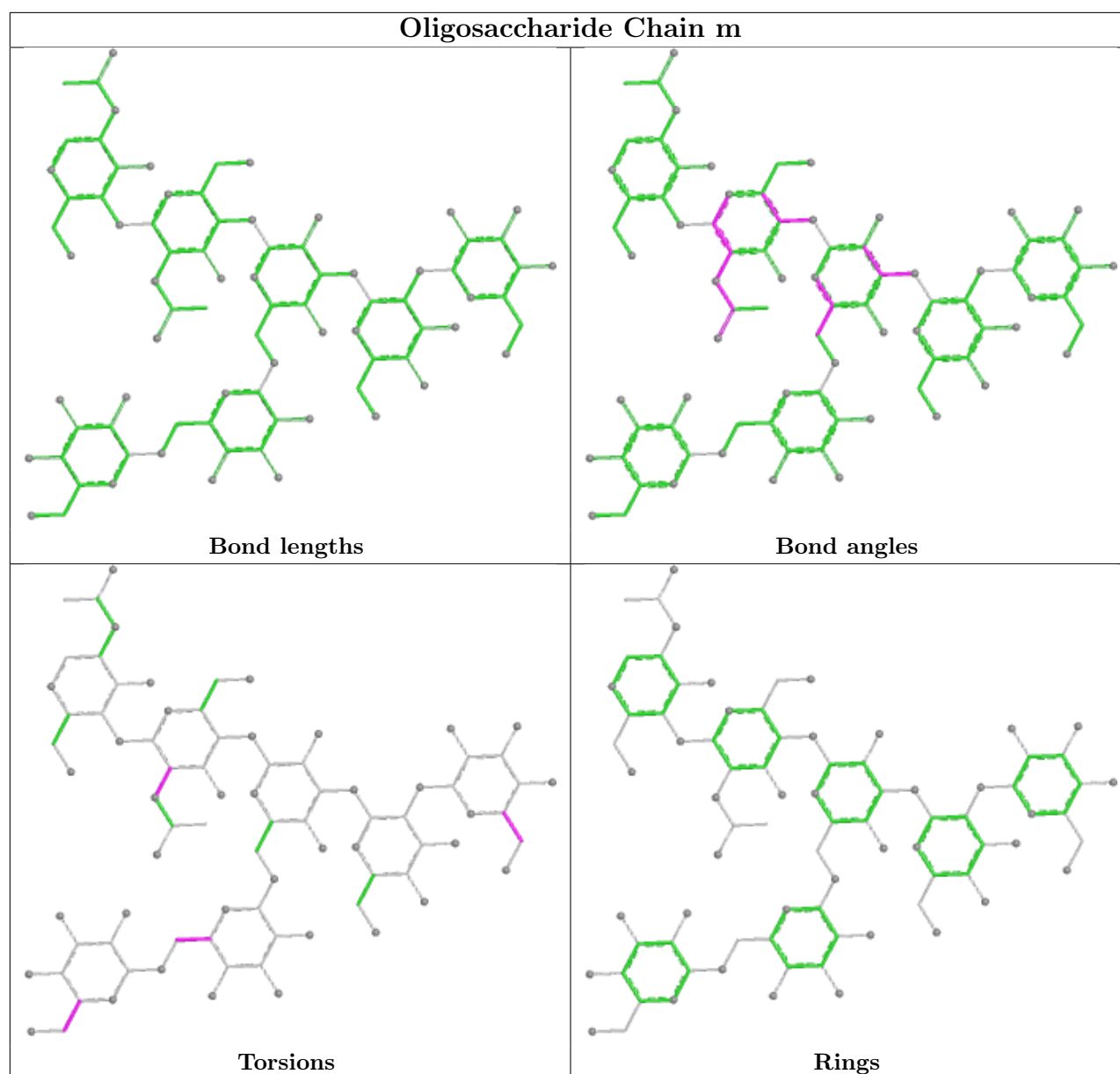


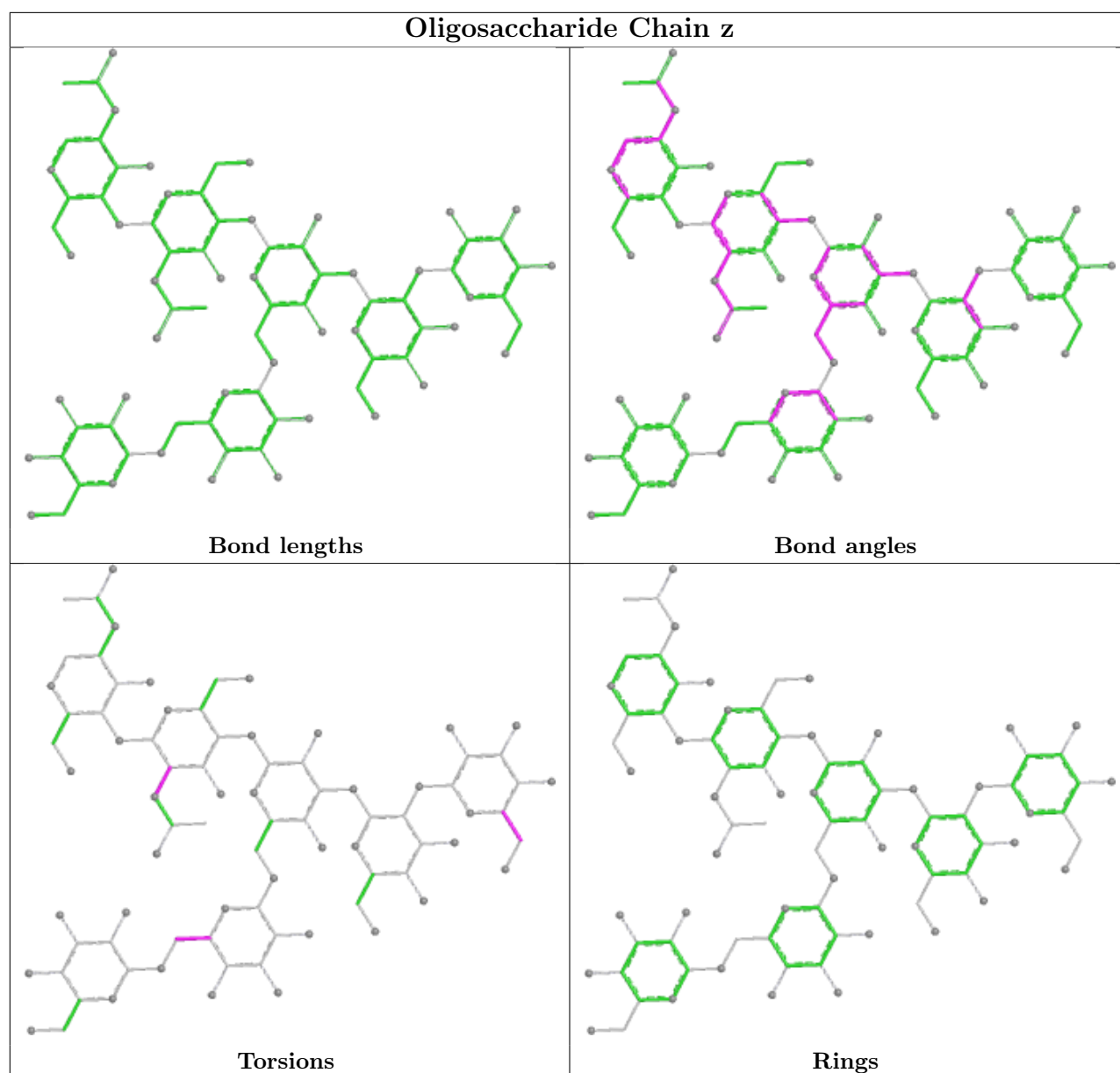


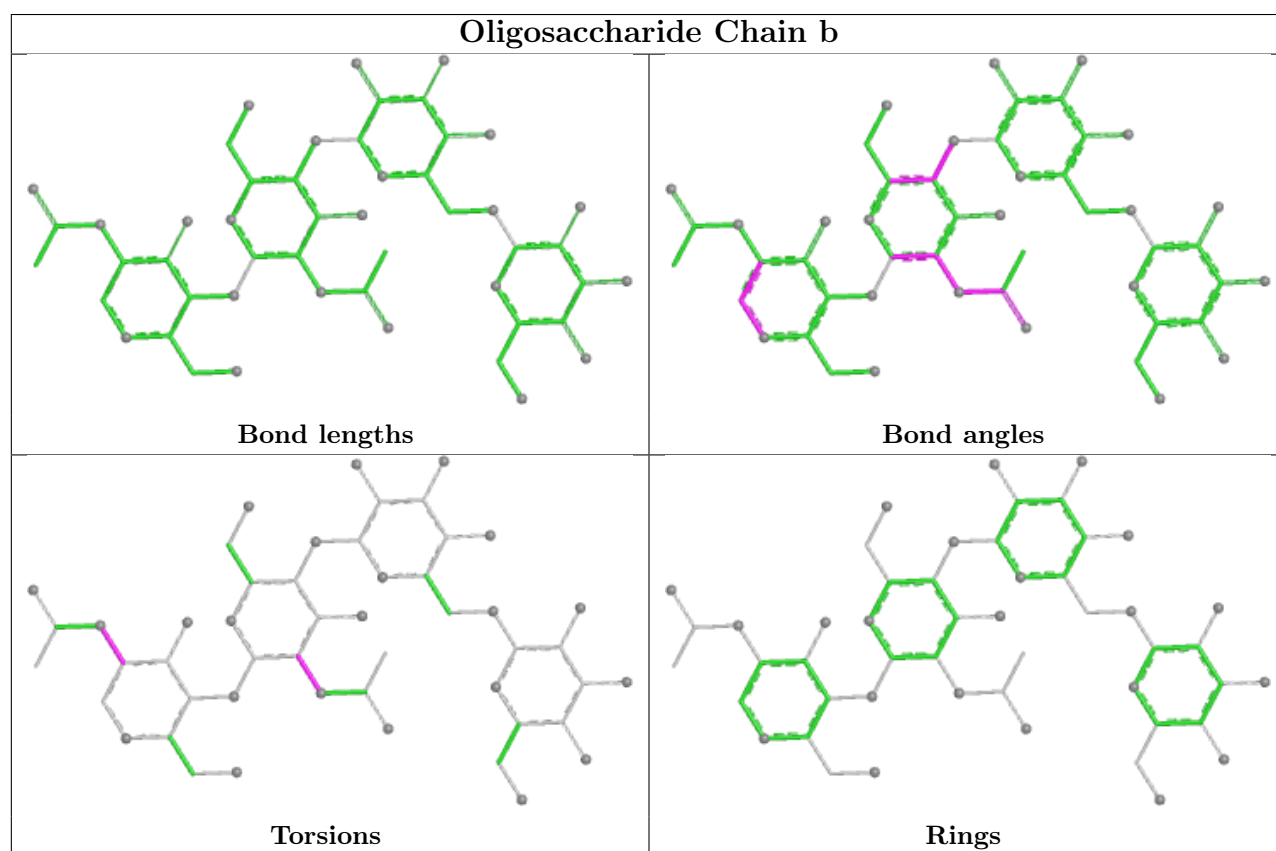
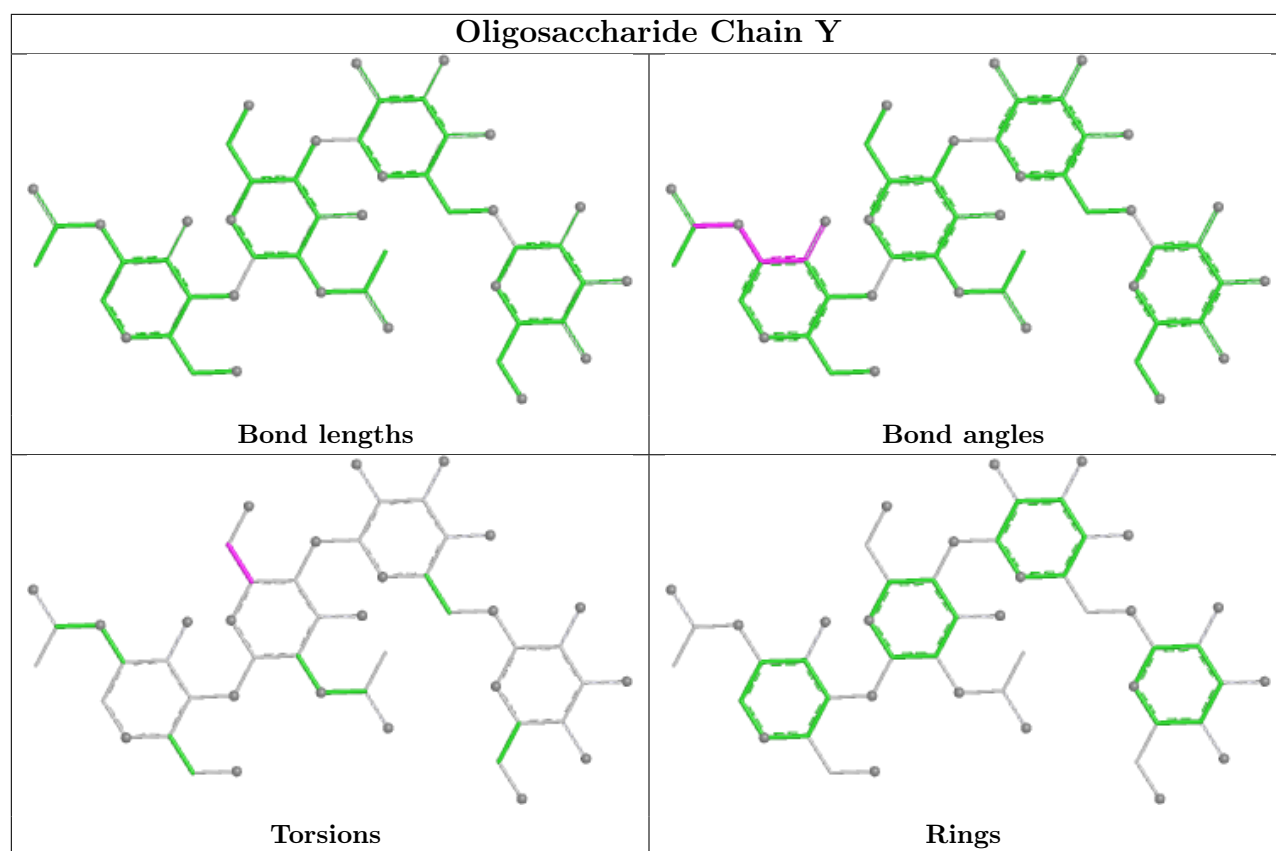


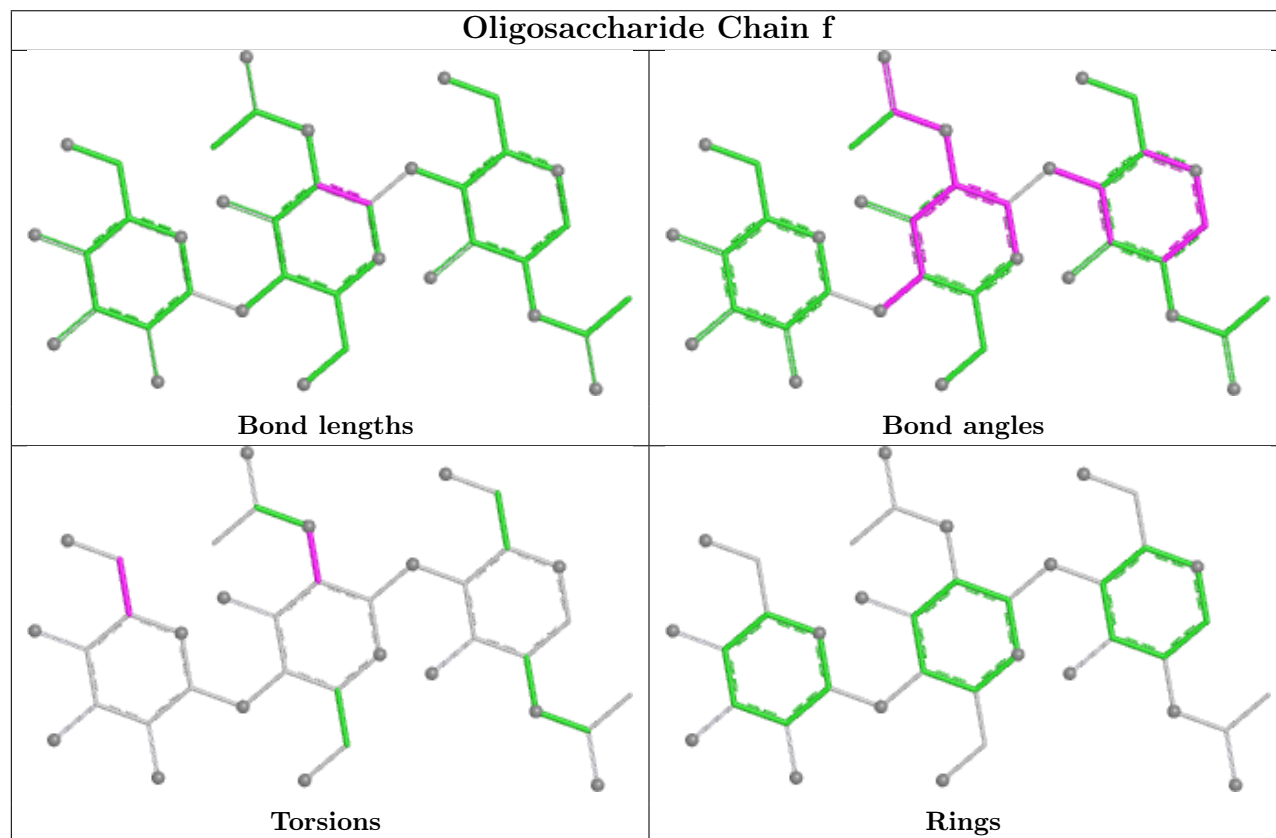
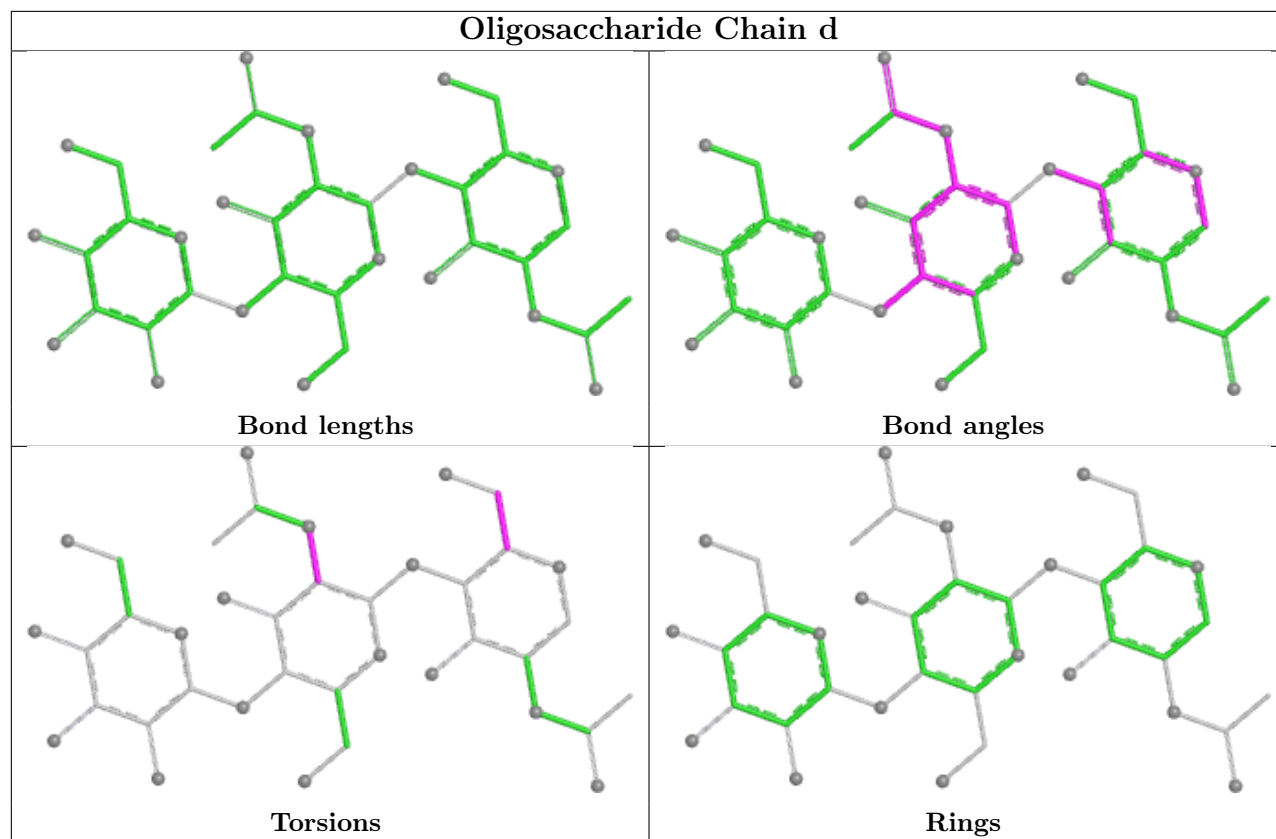


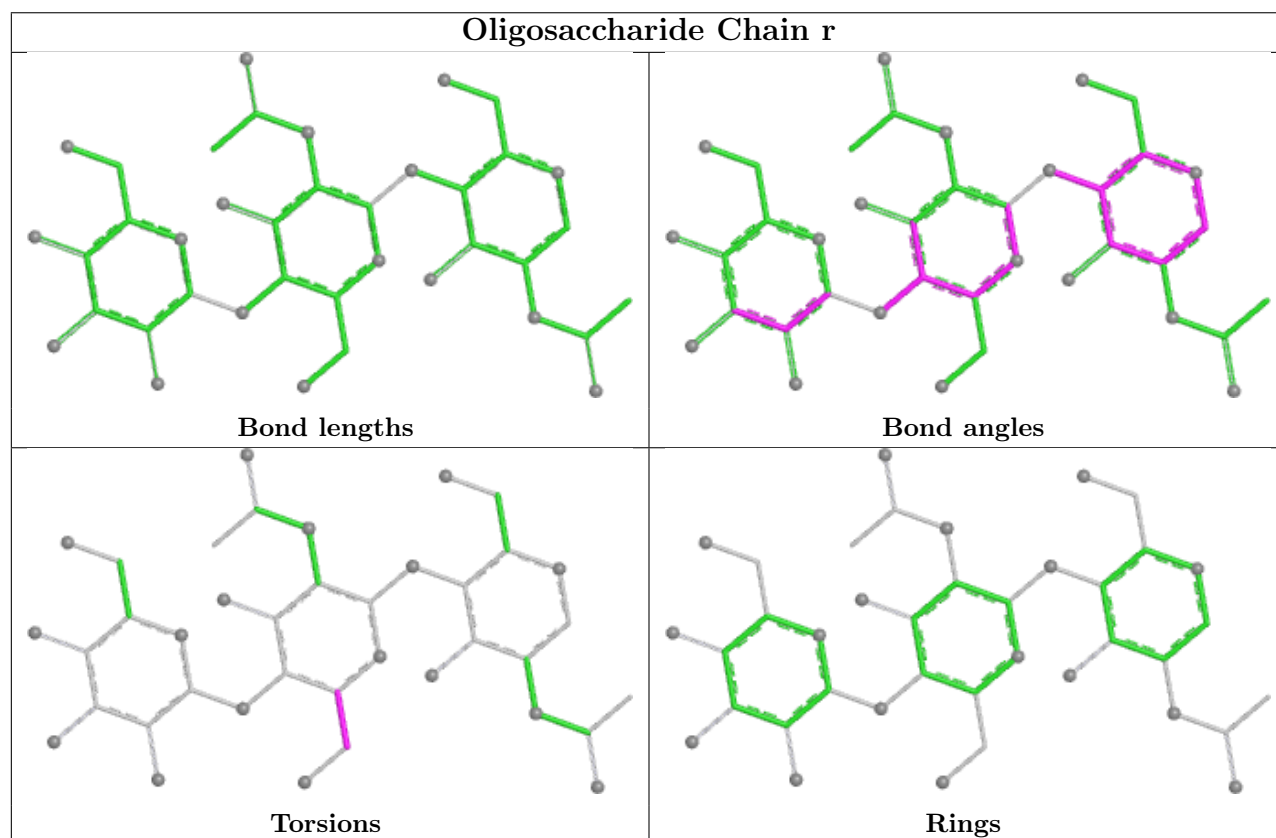
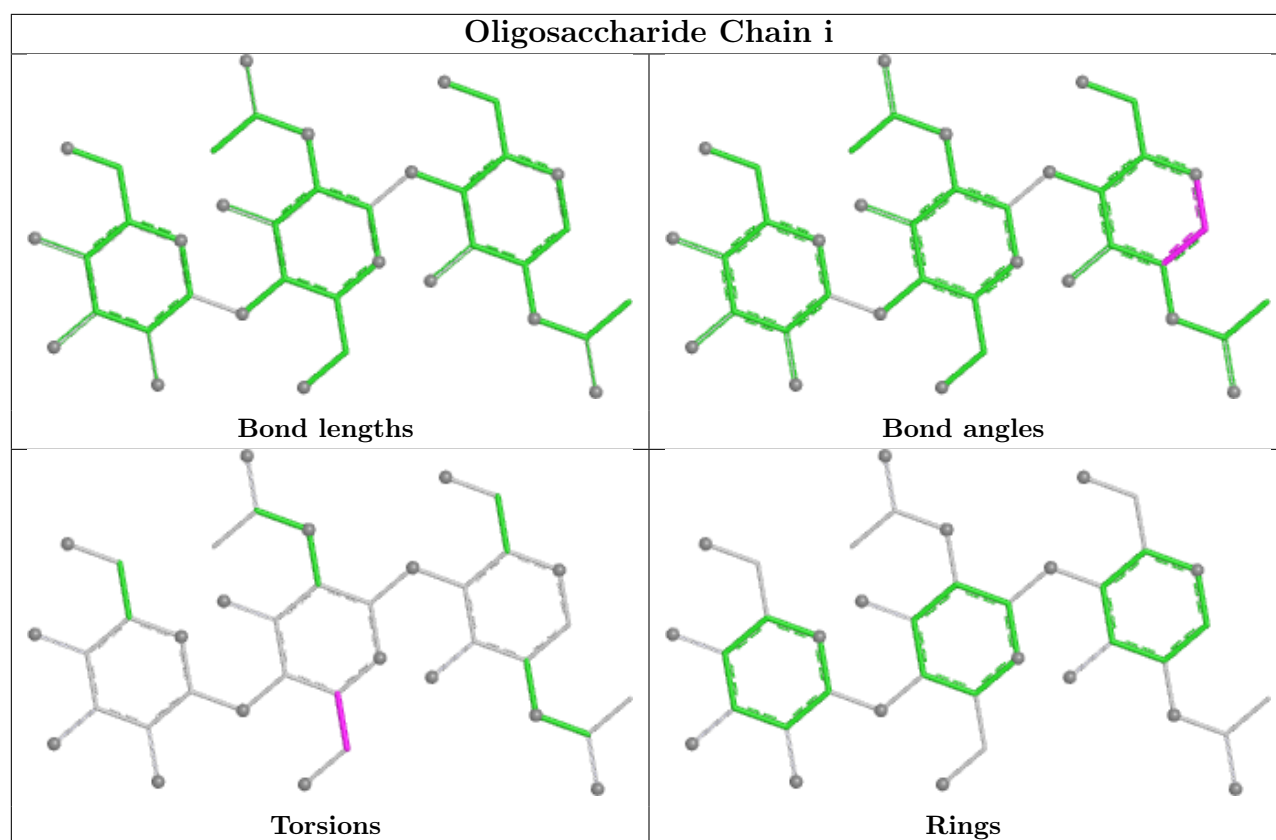


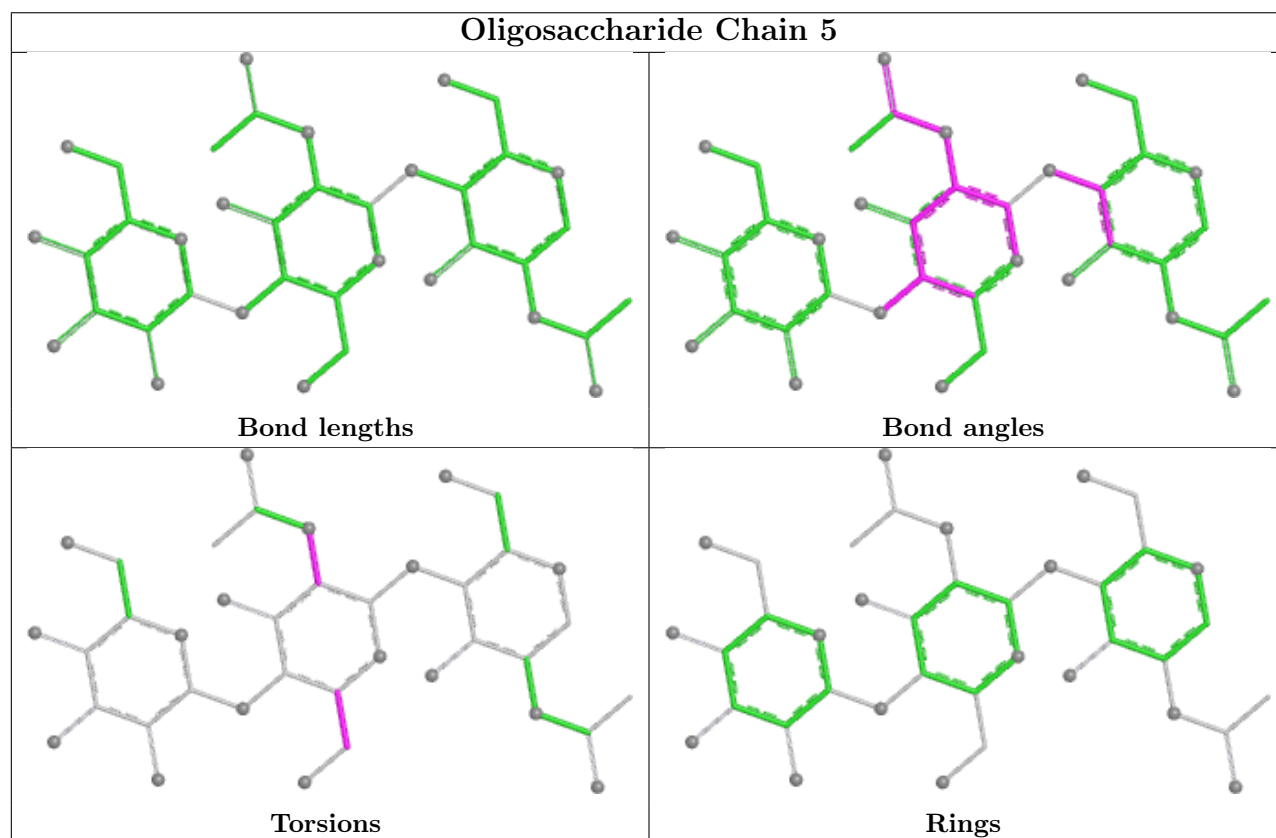
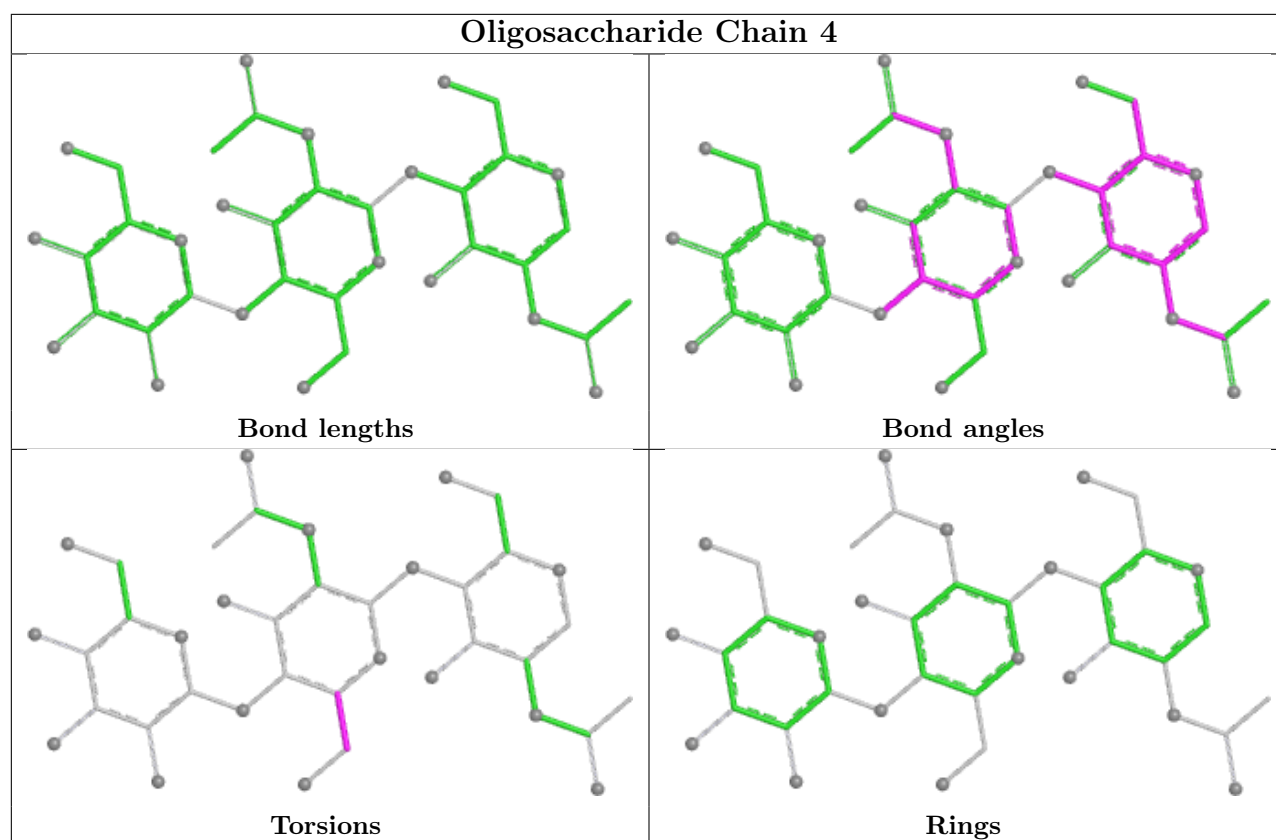


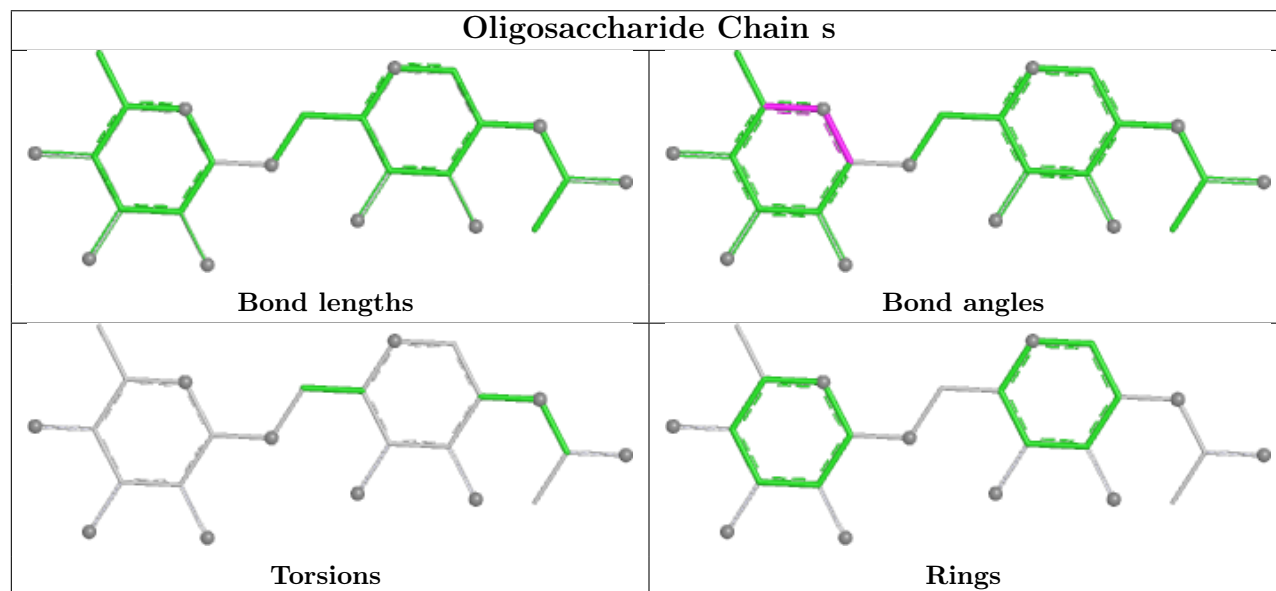
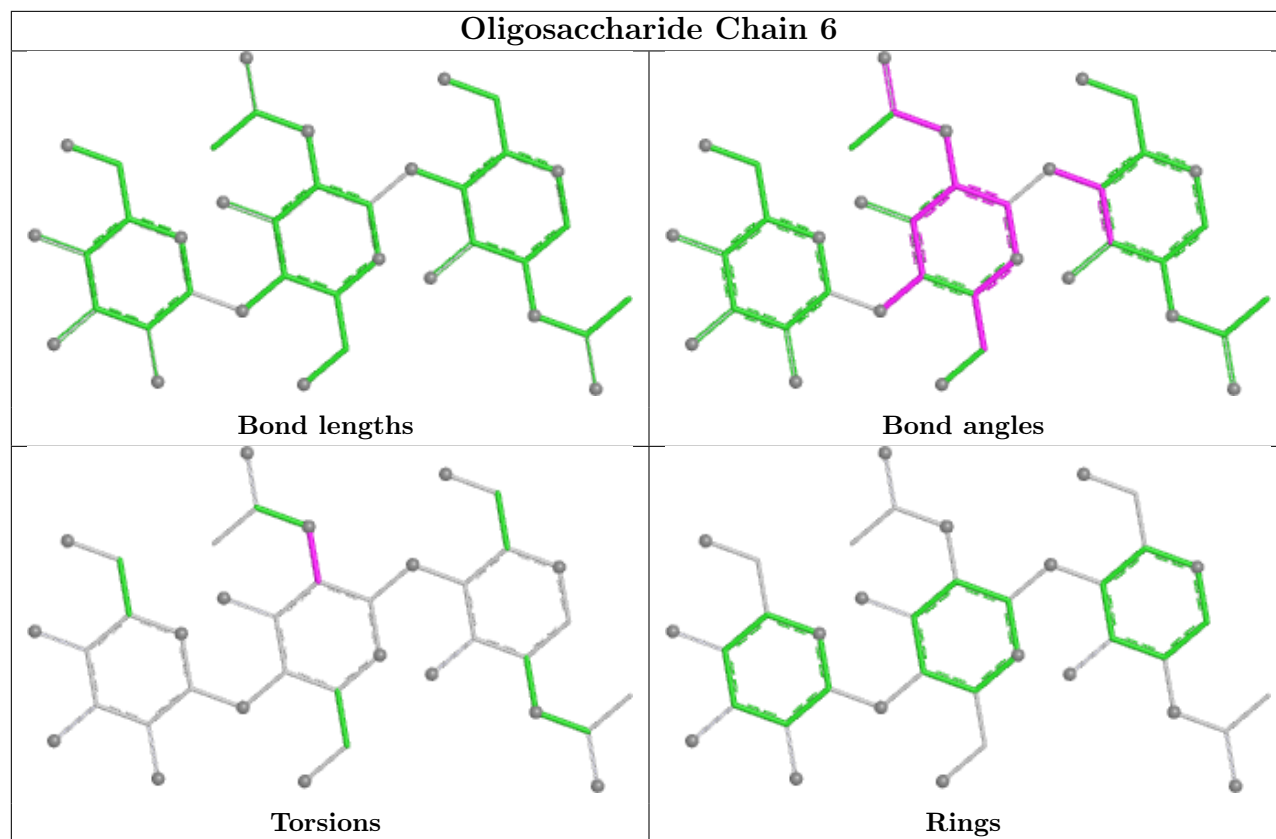


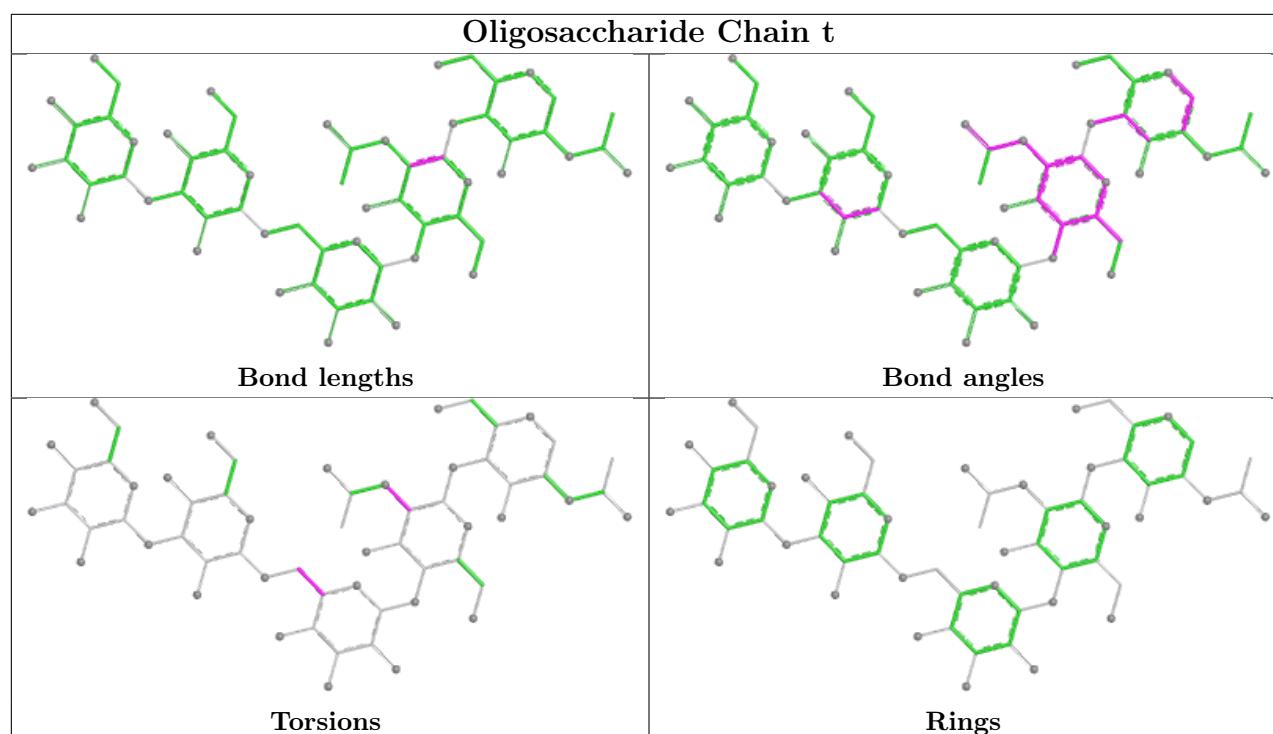












5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	NAG	E	639	2	14,14,15	0.42	0	17,19,21	1.07	1 (5%)
15	NAG	F	646	2	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
15	NAG	D	635	2	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
15	NAG	D	634	2	14,14,15	0.35	0	17,19,21	0.86	0
15	NAG	C	701	1	14,14,15	0.55	0	17,19,21	1.79	3 (17%)
15	NAG	E	635	2	14,14,15	0.34	0	17,19,21	0.84	0
15	NAG	F	639	2	14,14,15	0.35	0	17,19,21	0.85	0
15	NAG	A	701	1	14,14,15	0.41	0	17,19,21	1.60	2 (11%)
15	NAG	F	638	2	14,14,15	0.38	0	17,19,21	0.68	0
15	NAG	F	603	2	14,14,15	0.42	0	17,19,21	1.00	1 (5%)
15	NAG	D	603	2	14,14,15	0.32	0	17,19,21	1.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	E	634	2	14,14,15	0.37	0	17,19,21	0.66	0
15	NAG	B	701	1	14,14,15	0.31	0	17,19,21	1.40	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	E	639	2	-	1/6/23/26	0/1/1/1
15	NAG	F	646	2	-	0/6/23/26	0/1/1/1
15	NAG	D	635	2	-	0/6/23/26	0/1/1/1
15	NAG	D	634	2	-	0/6/23/26	0/1/1/1
15	NAG	C	701	1	-	0/6/23/26	0/1/1/1
15	NAG	E	635	2	-	0/6/23/26	0/1/1/1
15	NAG	F	639	2	-	0/6/23/26	0/1/1/1
15	NAG	A	701	1	-	0/6/23/26	0/1/1/1
15	NAG	F	638	2	-	0/6/23/26	0/1/1/1
15	NAG	F	603	2	-	1/6/23/26	0/1/1/1
15	NAG	D	603	2	-	0/6/23/26	0/1/1/1
15	NAG	E	634	2	-	0/6/23/26	0/1/1/1
15	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	701	NAG	C1-O5-C5	5.34	119.35	112.19
15	A	701	NAG	C1-O5-C5	5.07	118.98	112.19
15	B	701	NAG	C1-O5-C5	4.61	118.37	112.19
15	D	603	NAG	C1-O5-C5	3.29	116.59	112.19
15	E	639	NAG	O4-C4-C5	2.95	116.59	109.32
15	C	701	NAG	C6-C5-C4	-2.46	106.98	113.02
15	C	701	NAG	O5-C1-C2	-2.22	107.86	111.29
15	D	635	NAG	C2-N2-C7	-2.21	119.94	122.90
15	A	701	NAG	C6-C5-C4	-2.20	107.63	113.02
15	F	603	NAG	C4-C3-C2	2.18	114.21	111.02
15	D	603	NAG	C4-C3-C2	-2.16	107.85	111.02
15	D	603	NAG	O5-C1-C2	-2.10	108.04	111.29
15	F	646	NAG	O5-C1-C2	-2.09	108.06	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	F	603	NAG	O5-C5-C6-O6
15	E	639	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	639	NAG	2	0
15	C	701	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

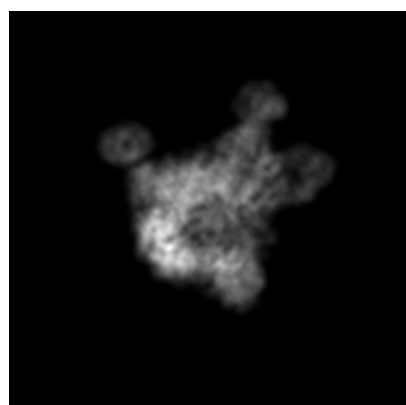
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8693. These allow visual inspection of the internal detail of the map and identification of artifacts.

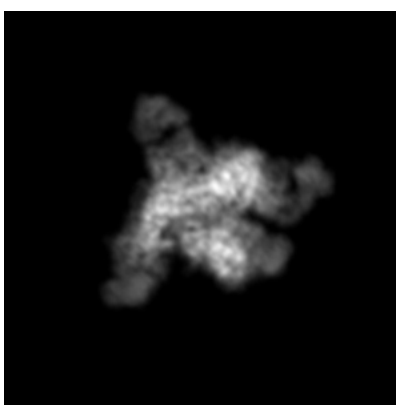
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

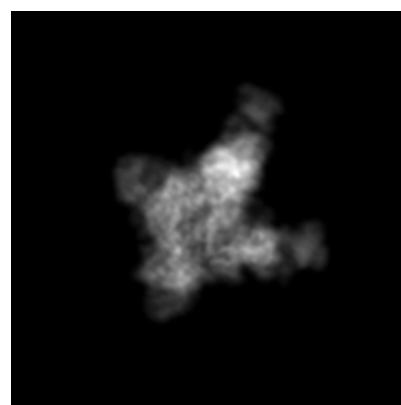
6.1.1 Primary map



X



Y



Z

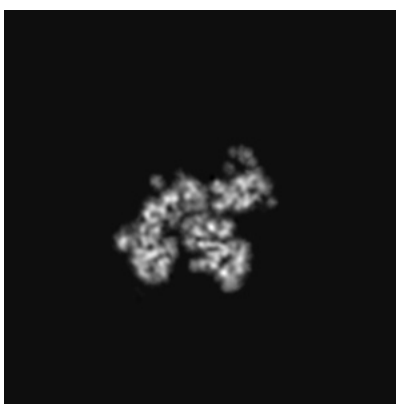
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

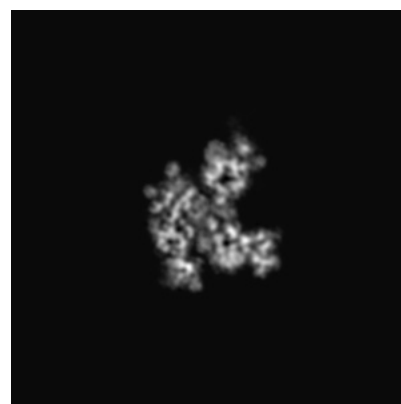
6.2.1 Primary map



X Index: 119



Y Index: 119

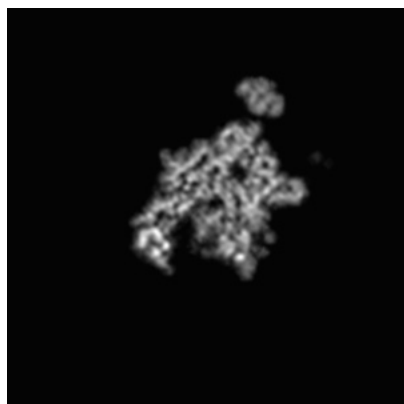


Z Index: 119

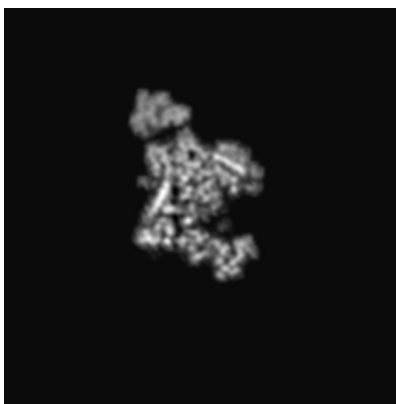
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

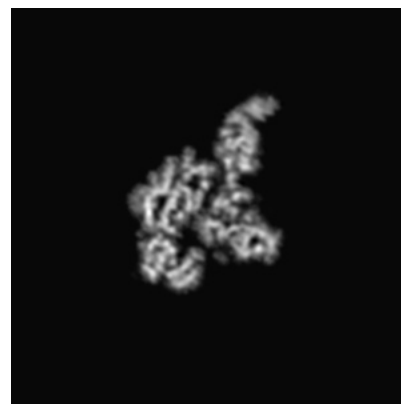
6.3.1 Primary map



X Index: 132



Y Index: 95

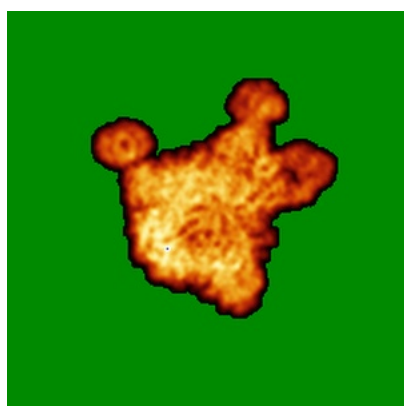


Z Index: 131

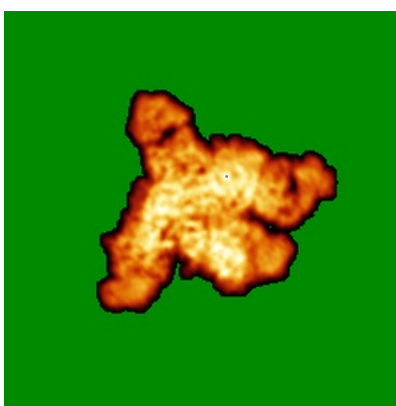
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

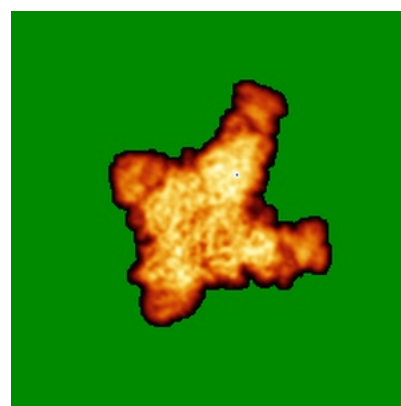
6.4.1 Primary map



X



Y

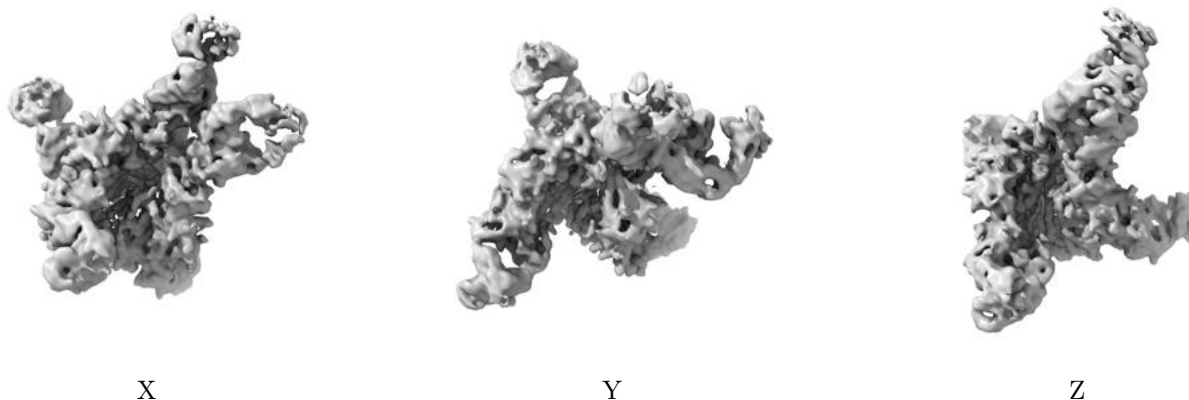


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0342. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

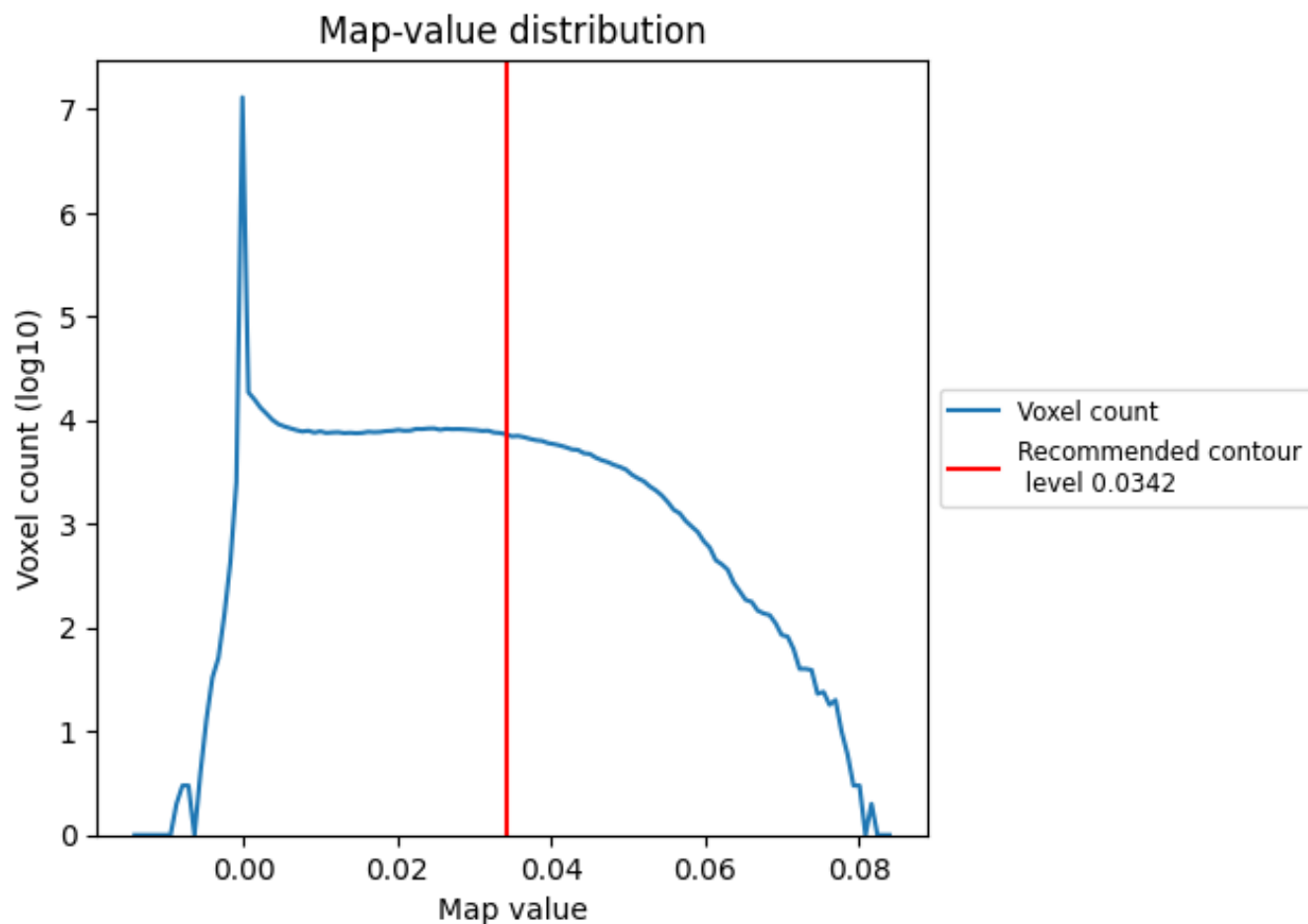
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

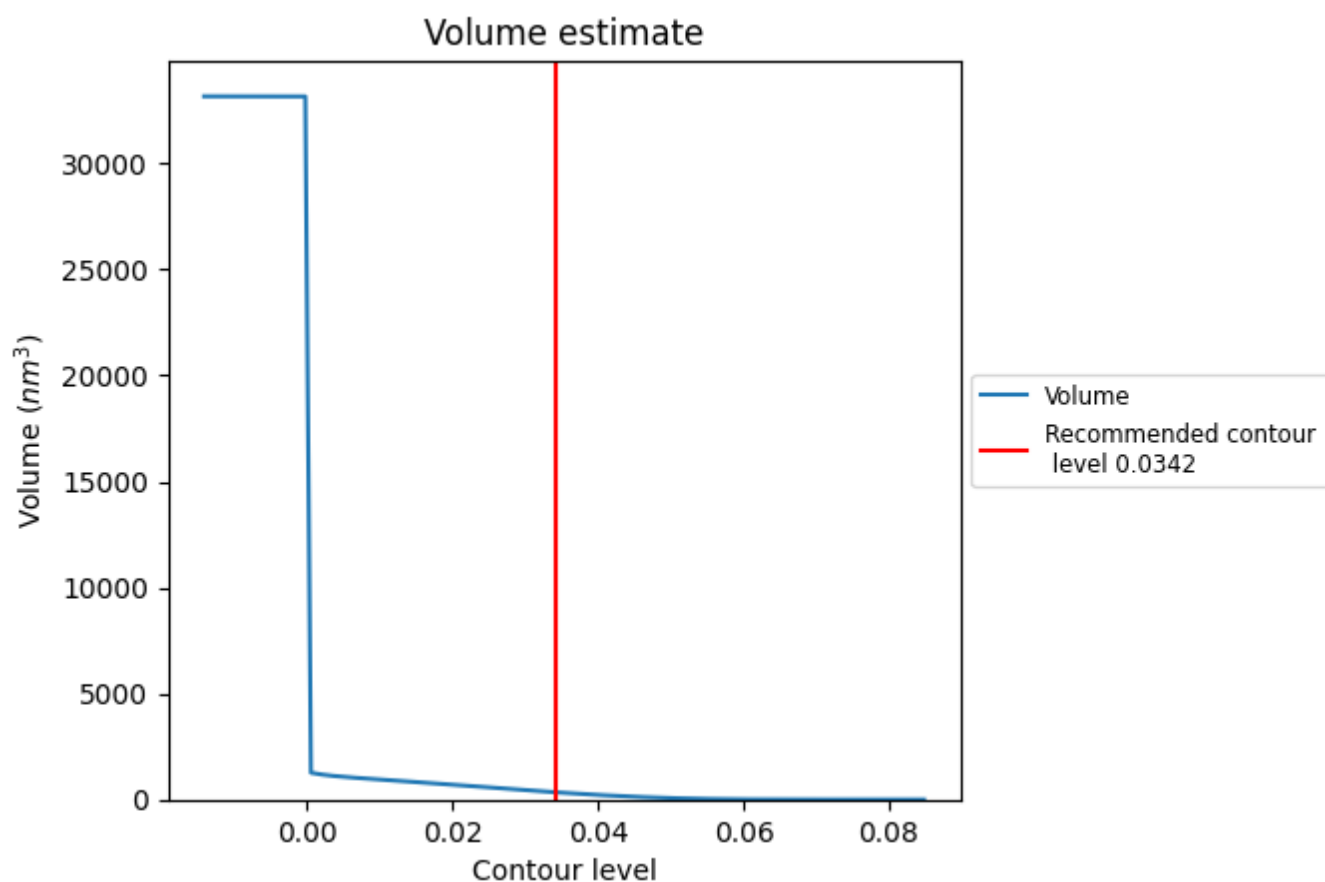
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

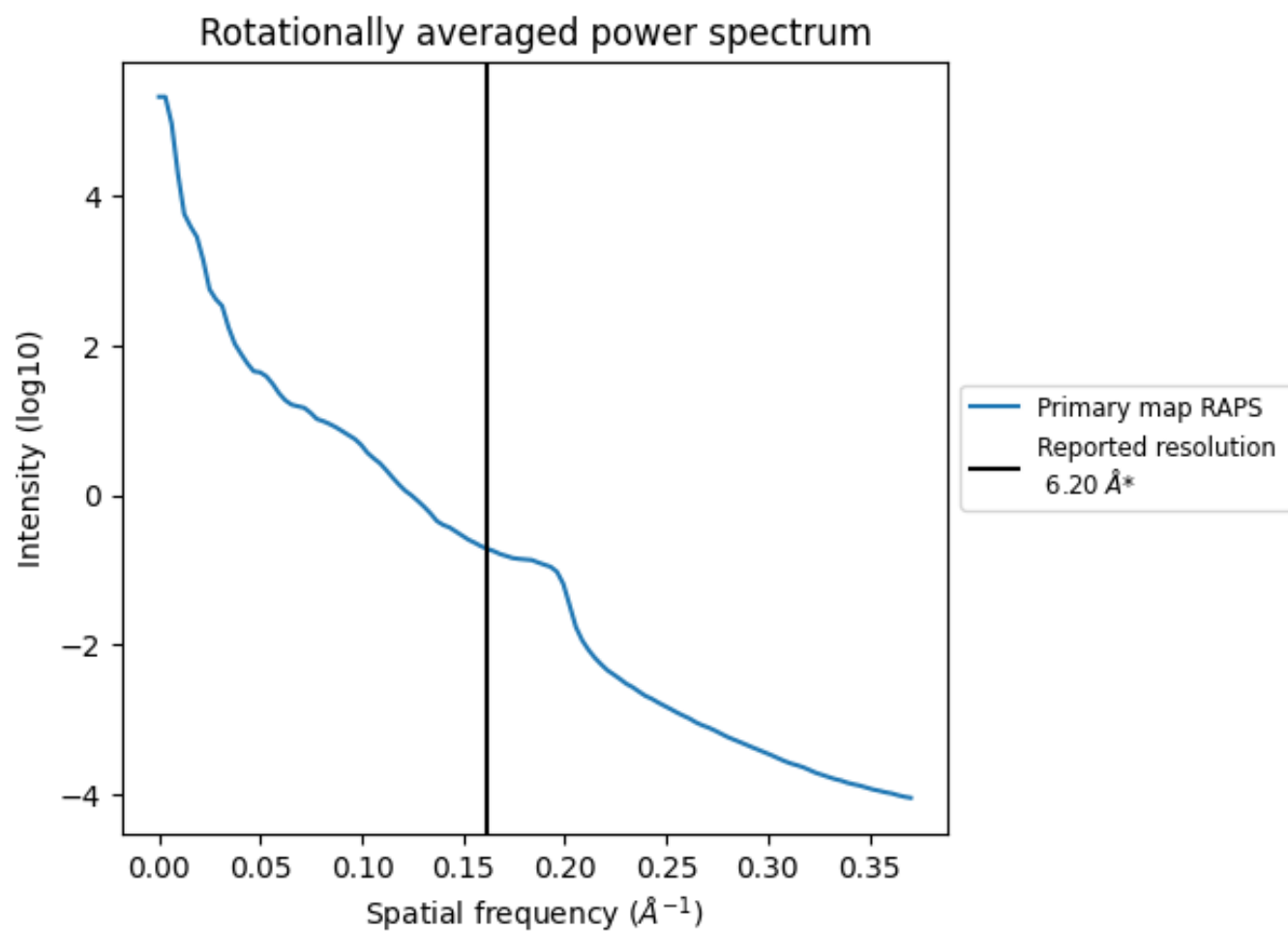
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

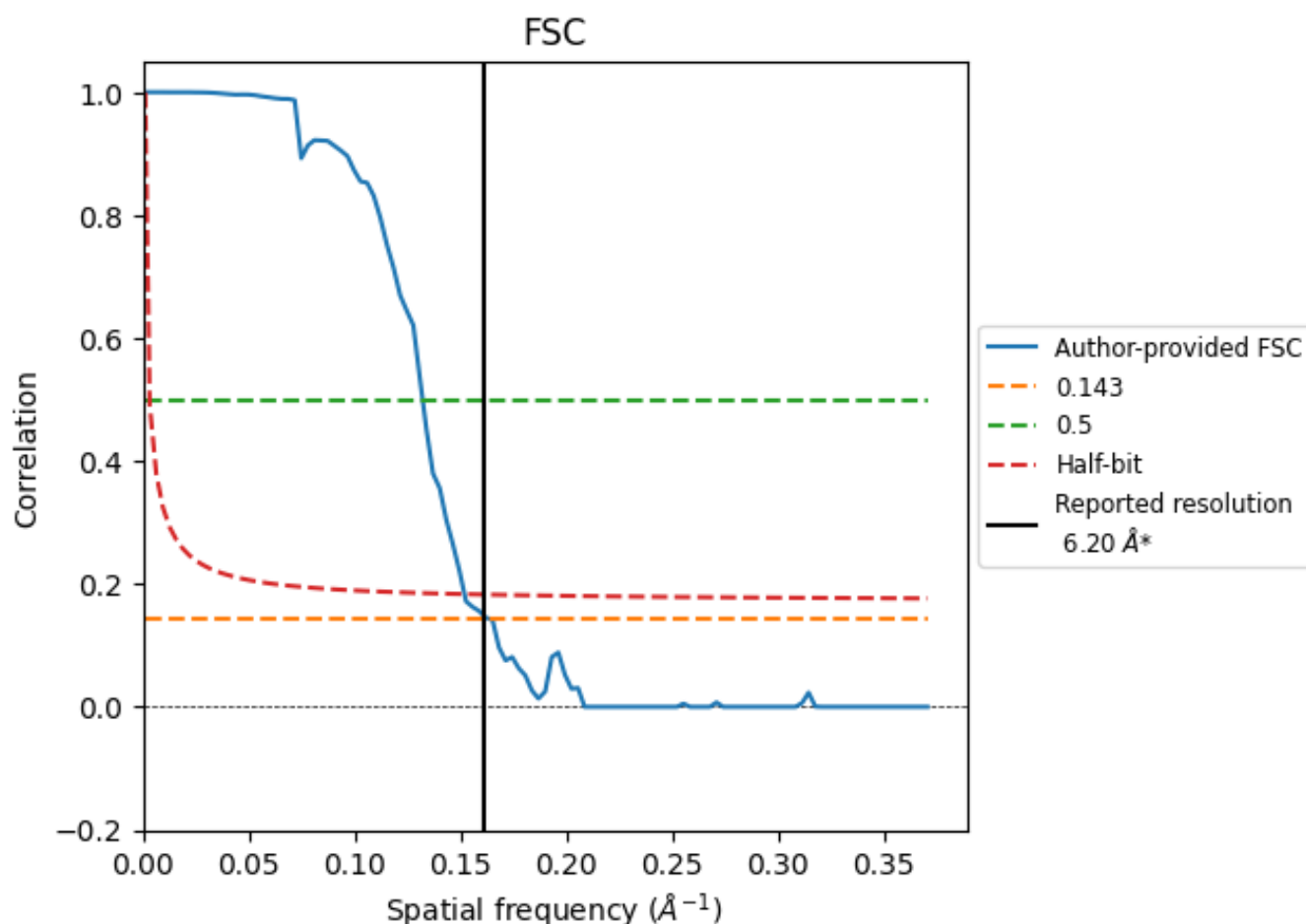


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.11	7.58	6.59
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

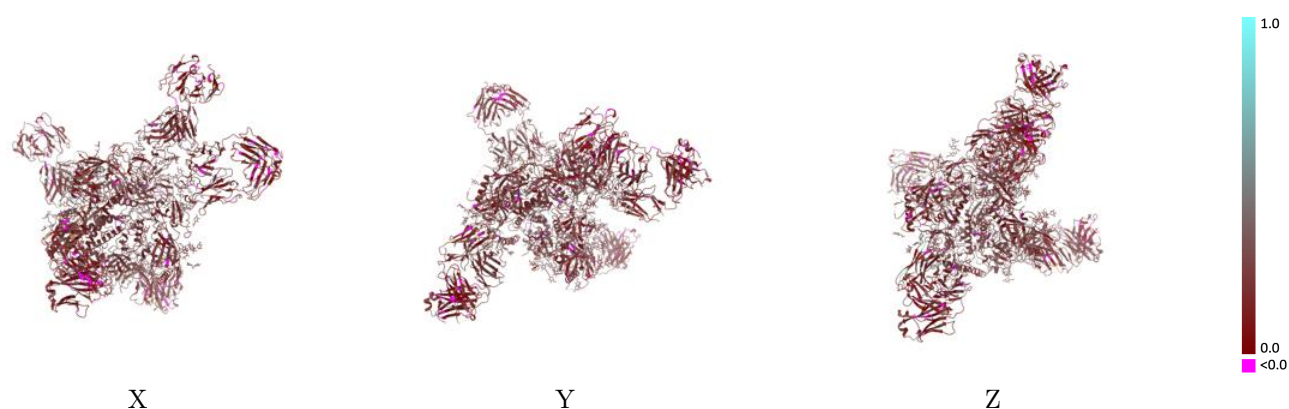
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8693 and PDB model 5VIY. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

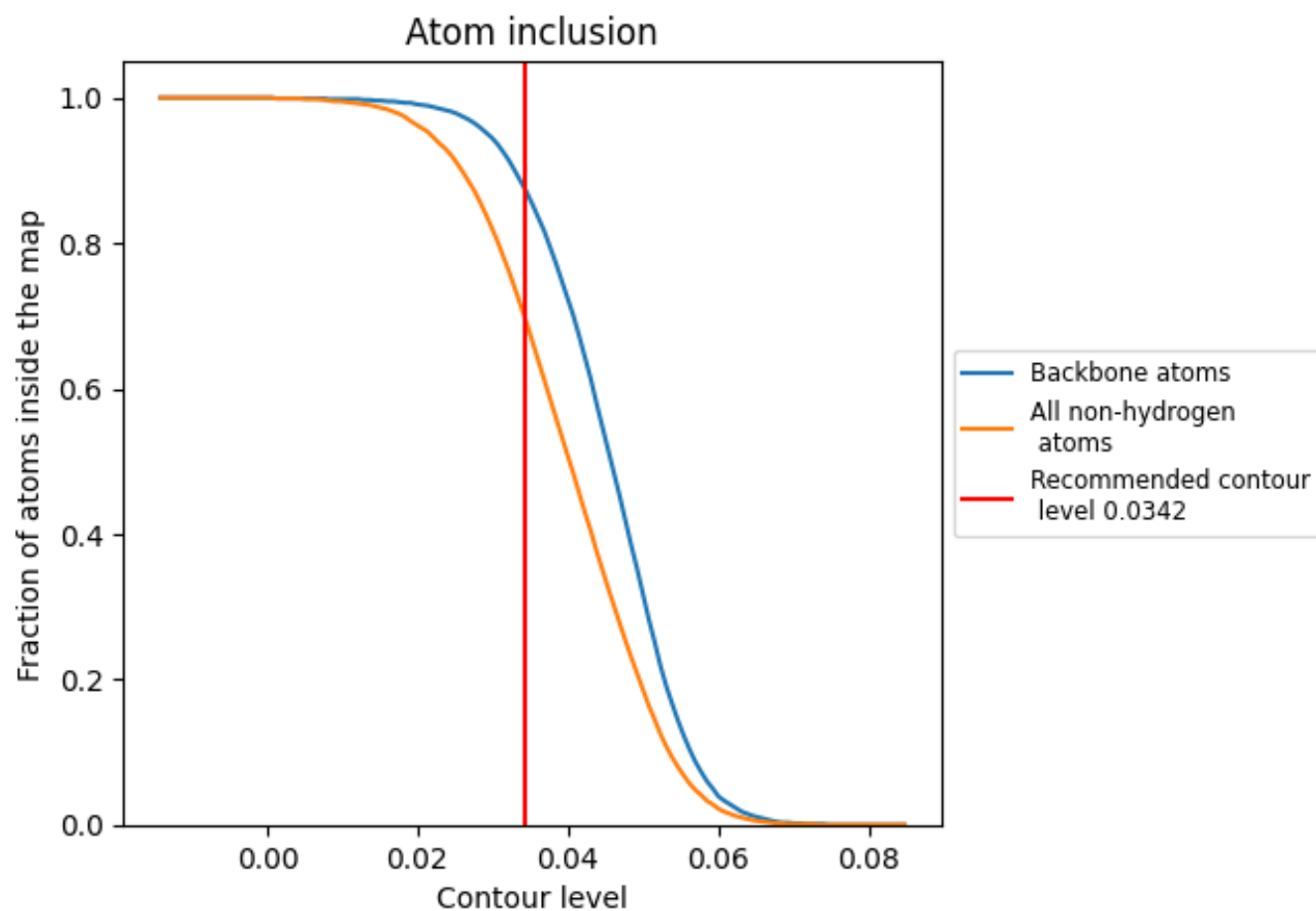


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0342) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.2110
0	 0.6230	 0.2460
1	 0.5360	 0.3170
2	 0.3570	 0.2590
3	 0.6790	 0.3090
4	 0.4100	 0.1790
5	 0.5130	 0.2890
6	 0.4870	 0.3090
7	 0.8360	 0.2980
A	 0.7060	 0.2000
B	 0.6750	 0.1940
C	 0.7260	 0.2170
D	 0.7780	 0.2330
E	 0.7600	 0.2200
F	 0.7660	 0.2360
G	 0.6390	 0.1910
H	 0.6360	 0.1890
I	 0.5760	 0.1800
J	 0.5890	 0.1900
K	 0.7110	 0.1900
L	 0.7350	 0.1930
M	 0.6690	 0.1770
N	 0.7390	 0.2140
O	 0.7060	 0.1890
P	 0.7190	 0.1980
Q	 0.4590	 0.2520
R	 0.5080	 0.2790
S	 0.5410	 0.2430
T	 0.3570	 0.3600
U	 0.7870	 0.3560
V	 0.3930	 0.3390
W	 0.9400	 0.3220
X	 0.4580	 0.3200
Y	 0.8400	 0.2810
Z	 0.5360	 0.2940



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Chain	Atom inclusion	Q-score
a	 0.4290	 0.3130
b	 0.4800	 0.3060
c	 0.6790	 0.2040
d	 0.6150	 0.2520
e	 0.2500	 0.3270
f	 0.4360	 0.3100
g	 0.3930	 0.3630
h	 0.5000	 0.2960
i	 0.5130	 0.3670
j	 0.5000	 0.2970
k	 0.3210	 0.3060
l	 0.9000	 0.2970
m	 0.4820	 0.2860
n	 0.7700	 0.2410
o	 0.4290	 0.3060
p	 0.3570	 0.2320
q	 0.7140	 0.2760
r	 0.4620	 0.1590
s	 0.3330	 0.1670
t	 0.2620	 0.2130
u	 0.3930	 0.3840
v	 0.8030	 0.3540
w	 0.7540	 0.2780
x	 0.3210	 0.3870
y	 0.8200	 0.3260
z	 0.4820	 0.3330