



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:56 PM UTC

PDB ID : 9BGE / pdb_00009bge
EMDB ID : EMD-44510
Title : Cryo-EM structure of mAb8-24 bound to 426c.WITO.TM.SOSIP
Authors : Hurlburt, N.K.; Pancera, M.
Deposited on : 2024-04-18
Resolution : 4.20 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:

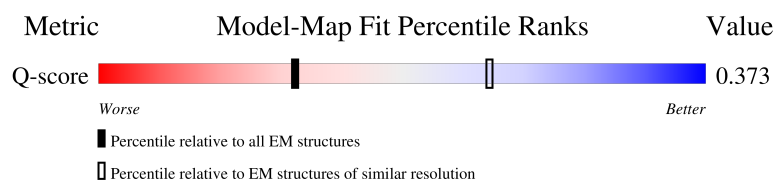
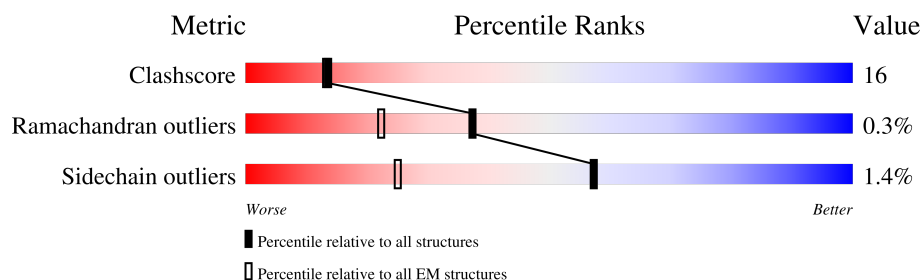
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.20 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.



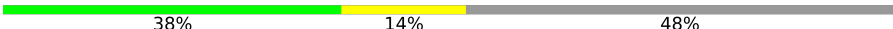
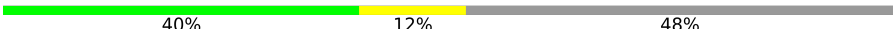
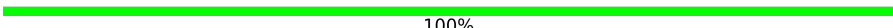
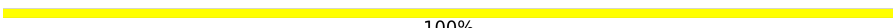
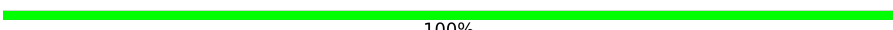
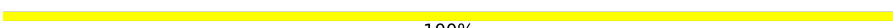
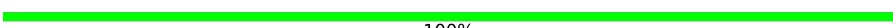
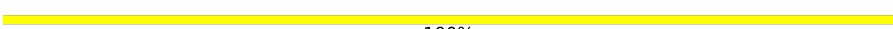
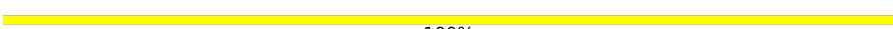
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	619	
1	B	619	
1	C	619	
2	D	233	

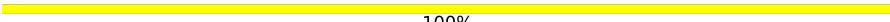
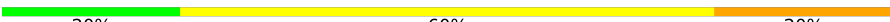
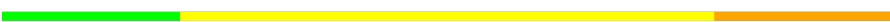
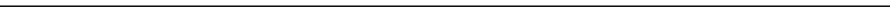
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Mol	Chain	Length	Quality of chain
2	F	233	
2	H	233	
3	E	200	
3	G	200	
3	L	200	
4	I	2	
4	M	2	
4	O	2	
4	Q	2	
4	S	2	
4	T	2	
4	U	2	
4	X	2	
4	Z	2	
4	b	2	
4	d	2	
4	e	2	
4	f	2	
4	i	2	
4	k	2	
4	m	2	
4	o	2	
4	p	2	
5	J	5	
5	K	5	

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Mol	Chain	Length	Quality of chain
5	V	5	 100%
5	W	5	 20% 60% 20%
5	g	5	 100%
5	h	5	 20% 60% 20%
6	N	5	 100%
6	R	5	 40% 60%
6	Y	5	 100%
6	c	5	 40% 60%
6	j	5	 100%
6	n	5	 40% 60%
7	P	4	 50% 50%
7	a	4	 50% 50%
7	l	4	 50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 39918 atoms, of which 19731 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 426c.WITO.TM.SOSIP.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	562	Total	C	H	N	O	S	0	0
			8782	2786	4363	772	826	35		
1	C	562	Total	C	H	N	O	S	0	0
			8782	2786	4363	772	826	35		
1	A	562	Total	C	H	N	O	S	0	0
			8782	2786	4363	772	826	35		

- Molecule 2 is a protein called Fv domain of heavy chain of mAb 8-24.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	119	Total	C	H	N	O	S	0	0
			1850	604	896	170	175	5		
2	F	119	Total	C	H	N	O	S	0	0
			1850	604	896	170	175	5		
2	H	119	Total	C	H	N	O	S	0	0
			1850	604	896	170	175	5		

- Molecule 3 is a protein called Fv domain of light chain of mAb 8-24.

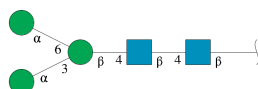
Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	104	Total	C	H	N	O	S	0	0
			1579	506	783	127	160	3		
3	G	104	Total	C	H	N	O	S	0	0
			1579	506	783	127	160	3		
3	L	104	Total	C	H	N	O	S	0	0
			1579	506	783	127	160	3		

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



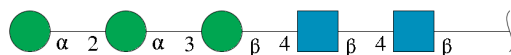
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	M	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	O	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	S	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	T	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	U	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	X	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	Z	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	b	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	d	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	e	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	f	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	i	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	k	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	m	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	o	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	p	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 5 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
5	J	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	K	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	V	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	W	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	g	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	h	5	Total	C	H	N	O	0	0
			118	34	57	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



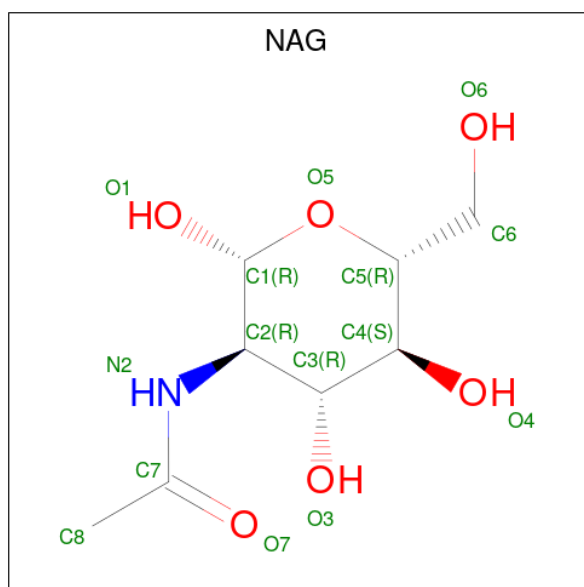
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
6	R	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
6	Y	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
6	c	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
6	j	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
6	n	5	Total	C	H	N	O	0	0
			118	34	57	2	25		

- Molecule 7 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
7	P	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	a	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	l	4	Total	C	H	N	O	0	0
			97	28	47	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	B	1	Total 28	C 8	H 14	N 1	O 5	0
8	C	1	Total 28	C 8	H 14	N 1	O 5	0

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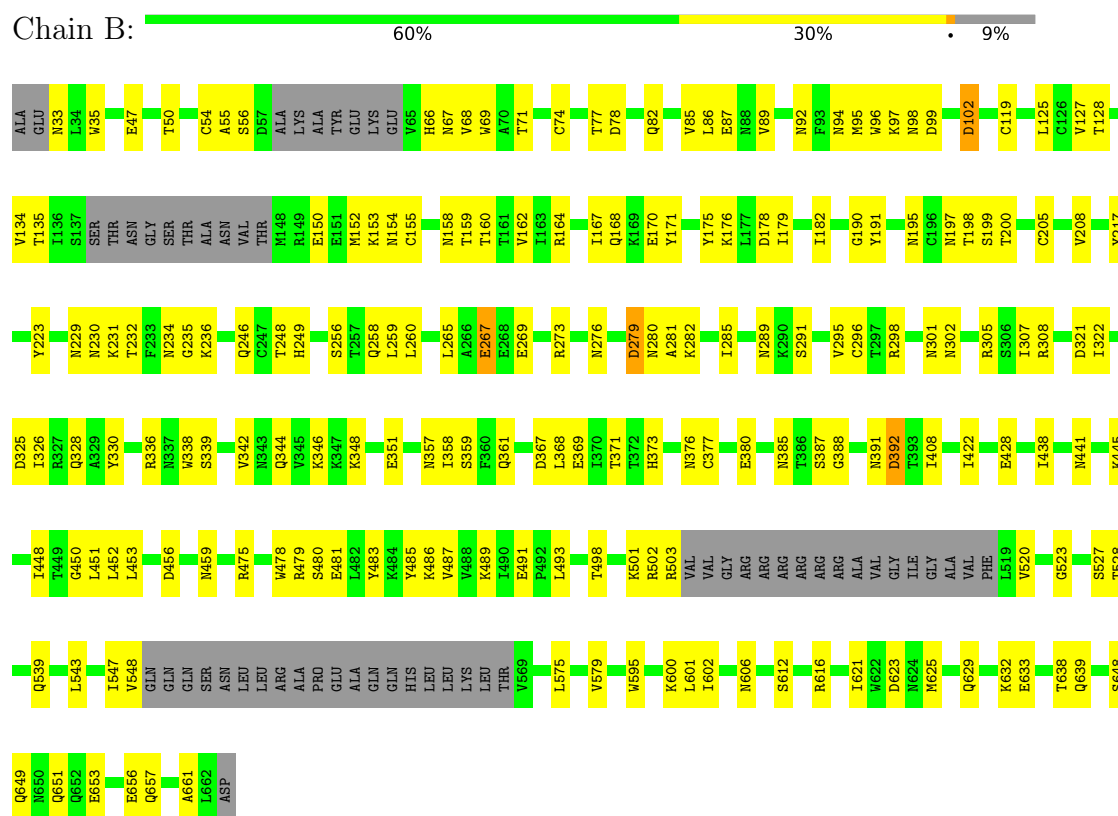
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Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	A	1	Total	C	H	N	O	0
			28	8	14	1	5	

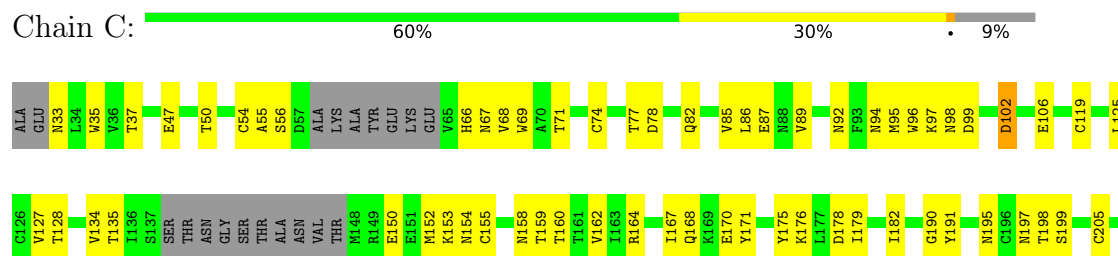
3 Residue-property plots [i](#)

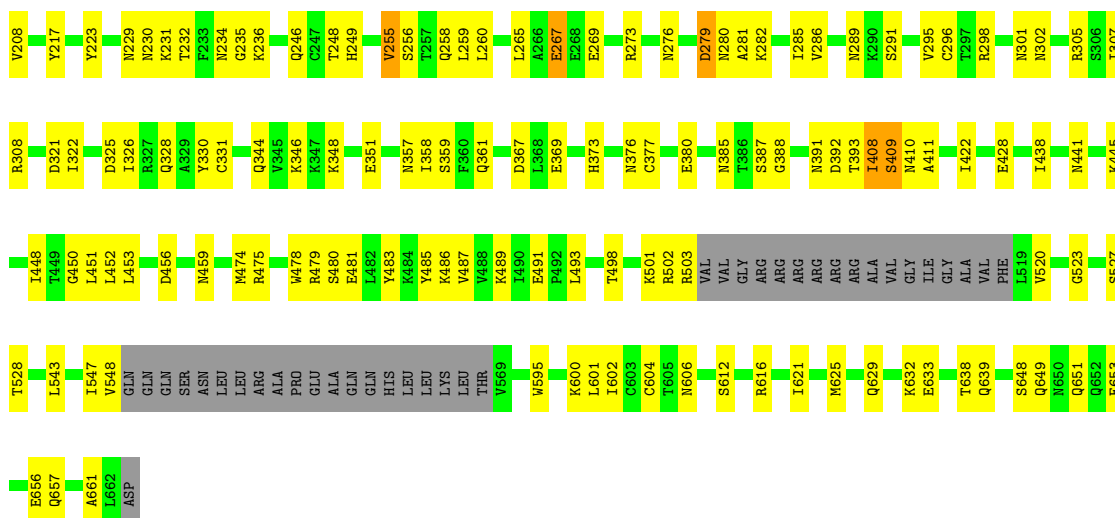
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 426c.WITO.TM.SOSIP



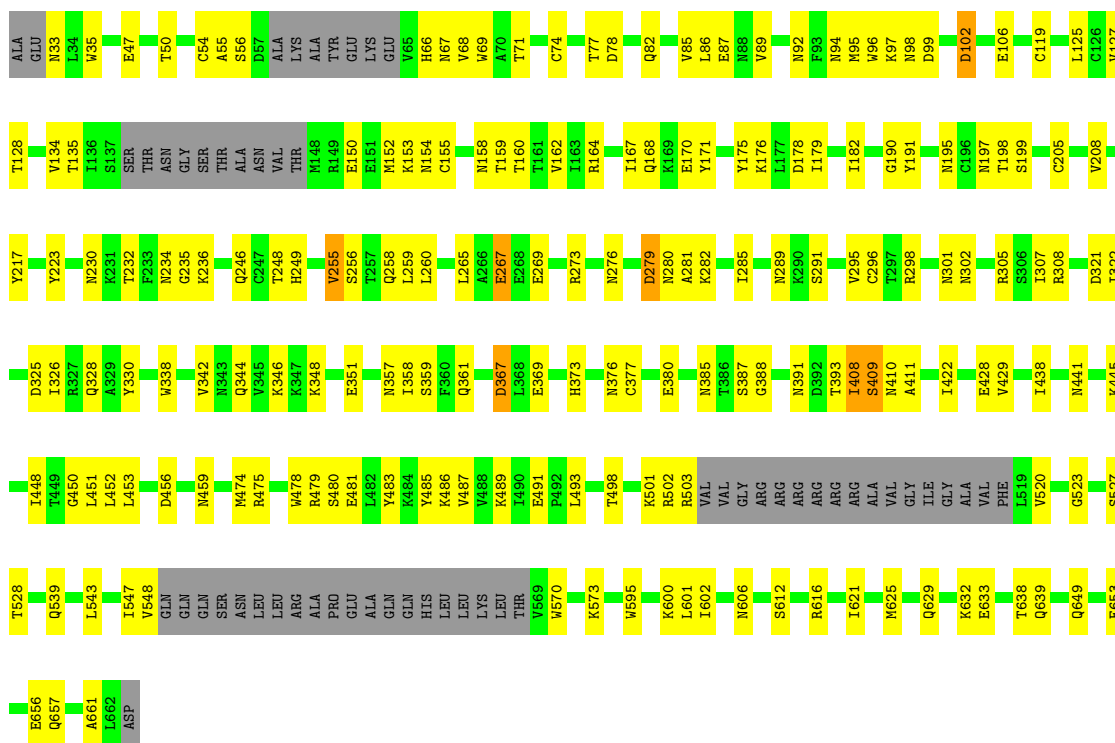
• Molecule 1: 426c.WITO.TM.SOSIP





• Molecule 1: 426c.WITO.TM.SOSIP

Chain A: 61% 29% 9%

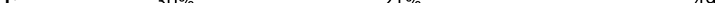


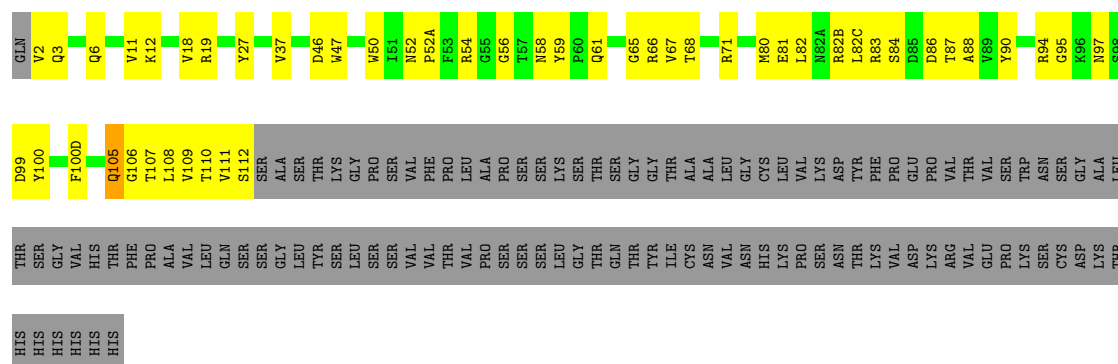
• Molecule 2: Fv domain of heavy chain of mAb 8-24

Chain D: 30% 21% 49%



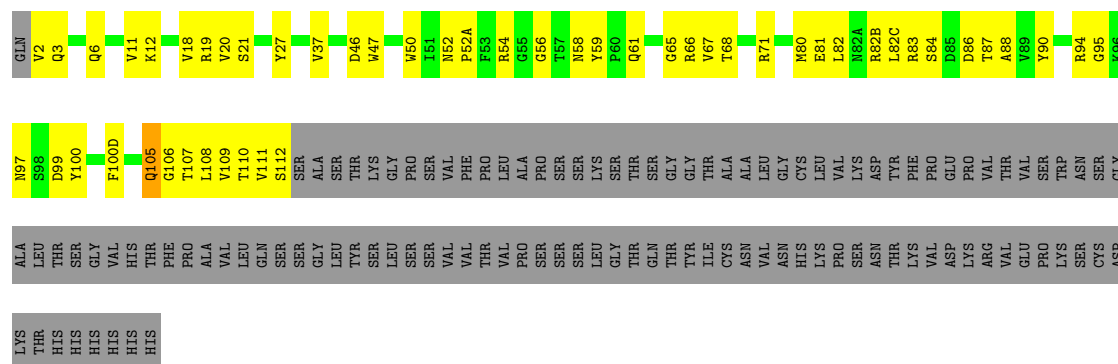
- Molecule 2: Fv domain of heavy chain of mAb 8-24

Chain F:  30% 21% 49%

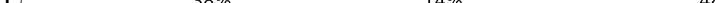


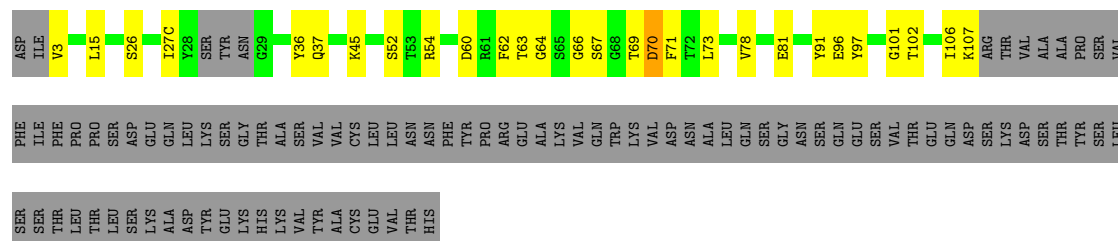
- Molecule 2: Fv domain of heavy chain of mAb 8-24

Chain H: 



- Molecule 3: Fv domain of light chain of mAb 8-24

Chain E:  38% 14% 48%



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

Chain Q:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  100%



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

Chain U:  50% 50%



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

Chain X:  100%



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

Chain Z:  50% 50%



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

Chain b:  50% 50%

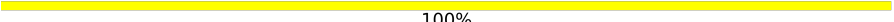


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50%

MAG1
MAG2

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

Chain e:  100%

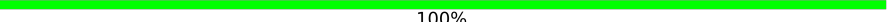
MAG1
MAG2

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

Chain f:  50% 50%

MAG1
MAG2

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

Chain i:  100%

MAG1
MAG2

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

Chain k:  50% 50%

MAG1
MAG2

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

Chain m:  50% 50%

MAG1
MAG2

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

Chain o:  50% 50%



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

Chain p: 100%



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

Chain J: 100%



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

Chain K: 20% 60% 20%



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

Chain V: 100%



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

Chain W: 20% 60% 20%



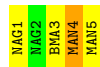
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%



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

Chain h:



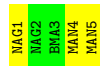
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain R:



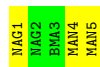
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



- Molecule 6: alpha-D-mannopyranose-(1-2)-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 c:



- Molecule 6: alpha-D-mannopyranose-(1-2)-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 j:  100%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 6: alpha-D-mannopyranose-(1-2)-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 n:  40% 60%

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain P:  50% 50%

NAG1
NAG2
BMA3
MAN4

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

Chain a:  50% 50%

NAG1
NAG2
BMA3
MAN4

- Molecule 7: 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:  50% 50%

NAG1
NAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	23004	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.554	Depositor
Minimum map value	-1.259	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	430.848, 430.848, 430.848	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/4506	0.33	0/6116
1	B	0.21	0/4506	0.33	0/6116
1	C	0.22	0/4506	0.33	0/6116
2	D	0.25	0/983	0.36	0/1336
2	F	0.25	0/983	0.36	0/1336
2	H	0.25	0/983	0.36	0/1336
3	E	0.19	0/811	0.34	0/1096
3	G	0.19	0/811	0.34	0/1096
3	L	0.19	0/811	0.34	0/1096
All	All	0.22	0/18900	0.33	0/25644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4419	4363	4360	161	0
1	B	4419	4363	4360	166	0
1	C	4419	4363	4360	166	0
2	D	954	896	892	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	954	896	892	33	0
2	H	954	896	892	33	0
3	E	796	783	781	22	0
3	G	796	783	781	19	0
3	L	796	783	781	21	0
4	I	28	27	25	1	0
4	M	28	27	25	0	0
4	O	28	27	25	2	0
4	Q	28	27	25	1	0
4	S	28	27	25	2	0
4	T	28	27	25	2	0
4	U	28	27	25	1	0
4	X	28	27	25	0	0
4	Z	28	27	25	3	0
4	b	28	27	25	0	0
4	d	28	27	25	2	0
4	e	28	27	25	3	0
4	f	28	27	25	1	0
4	i	28	27	25	0	0
4	k	28	27	25	3	0
4	m	28	27	25	0	0
4	o	28	27	25	2	0
4	p	28	27	25	3	0
5	J	61	57	52	2	0
5	K	61	57	52	3	0
5	V	61	57	52	3	0
5	W	61	57	52	3	0
5	g	61	57	52	2	0
5	h	61	57	52	3	0
6	N	61	57	52	4	0
6	R	61	57	52	1	0
6	Y	61	57	52	3	0
6	c	61	57	52	1	0
6	j	61	57	52	4	0
6	n	61	57	52	1	0
7	P	50	47	43	1	0
7	a	50	47	43	1	0
7	l	50	47	43	1	0
8	A	98	98	91	5	0
8	B	98	98	91	5	0
8	C	98	98	91	6	0
All	All	20187	19731	19575	636	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 16.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG23	1:A:135:THR:HG23	1.56	0.88
1:B:369:GLU:OE2	2:D:54:ARG:NH1	2.08	0.87
1:C:134:VAL:HG23	1:C:135:THR:HG23	1.56	0.87
1:C:369:GLU:OE2	2:F:54:ARG:NH1	2.08	0.86
2:H:54:ARG:NH1	1:A:369:GLU:OE2	2.08	0.86
1:B:279:ASP:OD1	3:E:91:TYR:OH	1.93	0.86
1:C:279:ASP:OD1	3:G:91:TYR:OH	1.93	0.86
1:B:638:THR:OG1	1:B:639:GLN:OE1	1.94	0.86
1:B:134:VAL:HG23	1:B:135:THR:HG23	1.55	0.85
1:B:87:GLU:OE2	4:I:1:NAG:N2	2.10	0.85
1:A:87:GLU:OE2	4:f:1:NAG:N2	2.10	0.84
1:C:87:GLU:OE2	4:U:1:NAG:N2	2.10	0.84
1:C:638:THR:OG1	1:C:639:GLN:OE1	1.94	0.84
1:A:638:THR:OG1	1:A:639:GLN:OE1	1.94	0.83
3:L:91:TYR:OH	1:A:279:ASP:OD1	1.94	0.82
1:C:282:LYS:NZ	2:F:99:ASP:O	2.11	0.82
3:L:81:GLU:N	3:L:81:GLU:OE1	2.14	0.80
1:C:481:GLU:OE1	1:C:481:GLU:N	2.15	0.80
1:A:154:ASN:ND2	5:g:1:NAG:O5	2.15	0.80
3:L:3:VAL:O	3:L:26:SER:OG	2.00	0.79
1:B:282:LYS:NZ	2:D:99:ASP:O	2.12	0.79
1:B:481:GLU:N	1:B:481:GLU:OE1	2.15	0.79
1:C:47:GLU:N	1:C:47:GLU:OE1	2.15	0.79
2:D:100(D):PHE:N	3:E:36:TYR:OH	2.16	0.79
1:B:154:ASN:ND2	5:J:1:NAG:O5	2.15	0.79
3:G:3:VAL:O	3:G:26:SER:OG	2.00	0.79
3:E:81:GLU:N	3:E:81:GLU:OE1	2.14	0.79
1:A:481:GLU:N	1:A:481:GLU:OE1	2.15	0.79
2:F:100(D):PHE:N	3:G:36:TYR:OH	2.16	0.78
1:A:47:GLU:N	1:A:47:GLU:OE1	2.16	0.78
4:p:1:NAG:O3	4:p:2:NAG:O5	2.00	0.78
1:B:47:GLU:OE1	1:B:47:GLU:N	2.15	0.78
1:B:170:GLU:OE1	1:B:171:TYR:N	2.17	0.78
2:H:100(D):PHE:N	3:L:36:TYR:OH	2.16	0.78
1:C:154:ASN:ND2	5:V:1:NAG:O5	2.15	0.78
1:A:230:ASN:ND2	4:o:1:NAG:O7	2.17	0.78
3:G:81:GLU:N	3:G:81:GLU:OE1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLU:OE1	1:A:171:TYR:N	2.17	0.78
1:C:170:GLU:OE1	1:C:171:TYR:N	2.16	0.78
3:E:3:VAL:O	3:E:26:SER:OG	2.00	0.77
1:B:230:ASN:ND2	4:S:1:NAG:O7	2.18	0.77
4:e:1:NAG:O3	4:e:2:NAG:O5	2.03	0.77
2:H:19:ARG:NE	5:h:4:MAN:O6	2.16	0.77
1:C:230:ASN:ND2	4:d:1:NAG:O7	2.17	0.77
1:A:639:GLN:OE1	1:A:639:GLN:N	2.17	0.77
2:H:99:ASP:O	1:A:282:LYS:NZ	2.12	0.77
2:D:19:ARG:NE	5:K:4:MAN:O6	2.17	0.76
2:F:19:ARG:NE	5:W:4:MAN:O6	2.17	0.76
1:B:639:GLN:OE1	1:B:639:GLN:N	2.17	0.76
5:g:1:NAG:O3	5:g:2:NAG:O5	2.04	0.76
1:C:639:GLN:OE1	1:C:639:GLN:N	2.17	0.76
1:A:182:ILE:HG23	1:A:191:TYR:N	2.01	0.76
5:J:1:NAG:O3	5:J:2:NAG:O5	2.03	0.76
5:V:1:NAG:O3	5:V:2:NAG:O5	2.04	0.76
1:B:298:ARG:NH1	1:B:302:ASN:OD1	2.19	0.75
1:A:280:ASN:OD1	1:A:281:ALA:N	2.19	0.75
1:C:182:ILE:HG23	1:C:191:TYR:N	2.01	0.75
1:B:280:ASN:OD1	1:B:281:ALA:N	2.20	0.74
1:A:298:ARG:NH1	1:A:302:ASN:OD1	2.20	0.74
1:B:182:ILE:HG23	1:B:191:TYR:N	2.02	0.74
1:C:280:ASN:OD1	1:C:281:ALA:N	2.20	0.74
1:A:256:SER:OG	1:A:259:LEU:O	2.05	0.74
1:B:168:GLN:OE1	1:B:168:GLN:N	2.20	0.74
1:B:328:GLN:N	1:B:328:GLN:OE1	2.18	0.74
1:C:134:VAL:O	1:C:135:THR:OG1	2.05	0.74
1:A:249:HIS:ND1	1:A:485:TYR:OH	2.21	0.74
4:T:1:NAG:O3	4:T:2:NAG:O5	2.03	0.74
1:B:256:SER:OG	1:B:259:LEU:O	2.06	0.74
1:A:168:GLN:N	1:A:168:GLN:OE1	2.20	0.74
1:C:168:GLN:N	1:C:168:GLN:OE1	2.21	0.74
1:C:249:HIS:ND1	1:C:485:TYR:OH	2.20	0.73
1:B:249:HIS:ND1	1:B:485:TYR:OH	2.21	0.73
1:C:298:ARG:NH1	1:C:302:ASN:OD1	2.21	0.73
1:A:95:MET:HE2	1:A:483:TYR:HB3	1.70	0.73
1:C:328:GLN:N	1:C:328:GLN:OE1	2.20	0.72
1:A:328:GLN:N	1:A:328:GLN:OE1	2.21	0.72
1:B:98:ASN:OD1	1:B:99:ASP:N	2.23	0.72
1:B:95:MET:HE2	1:B:483:TYR:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:MET:HE2	1:C:483:TYR:HB3	1.70	0.72
1:B:258:GLN:C	1:B:259:LEU:HD22	2.15	0.72
2:D:37:VAL:HG13	2:D:46:ASP:O	1.90	0.72
2:D:94:ARG:NH1	2:D:95:GLY:O	2.23	0.72
1:A:134:VAL:O	1:A:135:THR:OG1	2.05	0.71
1:C:256:SER:OG	1:C:259:LEU:O	2.06	0.71
1:C:197:ASN:O	1:A:308:ARG:NH2	2.23	0.71
1:A:150:GLU:OE1	1:A:176:LYS:NZ	2.24	0.71
1:C:258:GLN:C	1:C:259:LEU:HD22	2.15	0.71
1:A:98:ASN:OD1	1:A:99:ASP:N	2.24	0.71
2:F:94:ARG:NH1	2:F:95:GLY:O	2.23	0.71
1:B:267:GLU:N	1:B:267:GLU:OE1	2.24	0.71
1:B:95:MET:HE3	1:B:273:ARG:HD3	1.73	0.70
2:H:94:ARG:NH1	2:H:95:GLY:O	2.24	0.70
1:B:308:ARG:NH2	1:A:197:ASN:O	2.24	0.70
1:C:98:ASN:OD1	1:C:99:ASP:N	2.24	0.70
1:A:267:GLU:OE1	1:A:267:GLU:N	2.25	0.70
1:C:321:ASP:OD1	1:C:322:ILE:N	2.25	0.69
1:A:95:MET:HE3	1:A:273:ARG:HD3	1.74	0.69
1:A:258:GLN:C	1:A:259:LEU:HD22	2.17	0.69
1:B:321:ASP:OD1	1:B:322:ILE:N	2.26	0.69
1:B:197:ASN:O	1:C:308:ARG:NH2	2.24	0.69
1:B:633:GLU:OE1	1:B:633:GLU:N	2.25	0.69
1:C:95:MET:HE3	1:C:273:ARG:HD3	1.74	0.69
1:C:267:GLU:N	1:C:267:GLU:OE1	2.24	0.69
1:A:259:LEU:HD23	1:A:373:HIS:CG	2.28	0.69
1:A:321:ASP:OD1	1:A:322:ILE:N	2.25	0.69
1:B:67:ASN:O	1:B:71:THR:OG1	2.07	0.68
2:H:37:VAL:HG13	2:H:46:ASP:O	1.93	0.68
1:C:629:GLN:N	1:C:629:GLN:OE1	2.25	0.68
1:A:629:GLN:N	1:A:629:GLN:OE1	2.26	0.68
1:B:600:LYS:C	1:B:601:LEU:HD22	2.19	0.68
1:C:502:ARG:O	1:C:606:ASN:ND2	2.27	0.68
1:C:633:GLU:N	1:C:633:GLU:OE1	2.24	0.68
1:C:600:LYS:C	1:C:601:LEU:HD22	2.19	0.68
1:B:134:VAL:O	1:B:135:THR:OG1	2.05	0.67
6:j:1:NAG:O7	6:j:1:NAG:O3	2.12	0.67
1:B:259:LEU:HD23	1:B:373:HIS:CG	2.29	0.67
1:A:600:LYS:C	1:A:601:LEU:HD22	2.19	0.67
1:B:102:ASP:OD1	1:B:102:ASP:N	2.28	0.67
1:C:102:ASP:OD1	1:C:102:ASP:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD23	1:C:373:HIS:CG	2.30	0.67
1:C:346:LYS:NZ	1:C:358:ILE:O	2.24	0.67
1:A:629:GLN:O	1:A:632:LYS:NZ	2.20	0.67
6:Y:1:NAG:O7	6:Y:1:NAG:O3	2.13	0.67
1:B:502:ARG:O	1:B:606:ASN:ND2	2.27	0.67
1:A:633:GLU:OE1	1:A:633:GLU:N	2.24	0.67
1:B:441:ASN:OD1	8:B:706:NAG:N2	2.28	0.66
1:A:502:ARG:O	1:A:606:ASN:ND2	2.28	0.66
2:D:46:ASP:OD1	2:D:47:TRP:N	2.28	0.66
1:C:441:ASN:OD1	8:C:706:NAG:N2	2.27	0.66
1:B:232:THR:O	4:S:1:NAG:O6	2.08	0.66
1:C:78:ASP:OD2	1:C:246:GLN:NE2	2.29	0.65
2:H:58:ASN:OD1	2:H:59:TYR:N	2.29	0.65
1:B:178:ASP:OD2	1:B:422:ILE:N	2.30	0.65
2:F:37:VAL:HG13	2:F:46:ASP:O	1.96	0.65
1:C:428:GLU:N	1:C:428:GLU:OE1	2.29	0.65
3:L:97:TYR:OH	1:A:459:ASN:N	2.29	0.65
1:A:178:ASP:OD2	1:A:422:ILE:N	2.30	0.65
1:A:441:ASN:OD1	8:A:706:NAG:N2	2.29	0.64
1:B:78:ASP:OD2	1:B:246:GLN:NE2	2.30	0.64
1:B:150:GLU:OE1	1:B:176:LYS:NZ	2.22	0.64
6:N:1:NAG:O7	6:N:1:NAG:O3	2.13	0.64
1:A:87:GLU:O	1:A:89:VAL:HG23	1.97	0.64
1:C:459:ASN:N	3:G:97:TYR:OH	2.30	0.64
1:B:301:ASN:ND2	8:B:705:NAG:O7	2.31	0.64
1:C:87:GLU:O	1:C:89:VAL:HG23	1.98	0.64
2:D:105:GLN:OE1	2:D:106:GLY:N	2.30	0.64
1:C:629:GLN:O	1:C:632:LYS:NZ	2.20	0.64
1:A:78:ASP:OD2	1:A:246:GLN:NE2	2.29	0.63
1:B:346:LYS:NZ	1:B:358:ILE:O	2.25	0.63
1:C:178:ASP:OD2	1:C:422:ILE:N	2.30	0.63
1:A:205:CYS:O	1:A:208:VAL:HG22	1.99	0.63
4:p:1:NAG:O3	4:p:2:NAG:O6	2.13	0.63
1:A:301:ASN:ND2	8:A:705:NAG:O7	2.31	0.63
1:C:260:LEU:HD21	1:C:452:LEU:CD2	2.29	0.63
1:A:102:ASP:N	1:A:102:ASP:OD1	2.28	0.63
1:B:428:GLU:OE1	1:B:428:GLU:N	2.31	0.63
1:C:232:THR:O	4:d:1:NAG:O6	2.10	0.63
1:C:330:TYR:OH	7:a:1:NAG:N2	2.32	0.63
1:C:301:ASN:ND2	8:C:705:NAG:O7	2.31	0.62
3:E:37:GLN:O	3:E:45:LYS:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:O	1:B:89:VAL:HG23	1.98	0.62
1:C:205:CYS:O	1:C:208:VAL:HG22	1.99	0.62
3:G:37:GLN:O	3:G:45:LYS:N	2.29	0.62
1:A:428:GLU:N	1:A:428:GLU:OE1	2.33	0.62
2:F:105:GLN:OE1	2:F:106:GLY:N	2.32	0.62
1:C:67:ASN:O	1:C:71:THR:OG1	2.07	0.62
2:D:86:ASP:OD1	2:D:87:THR:N	2.32	0.62
1:B:380:GLU:HG2	1:B:438:ILE:HD12	1.81	0.62
1:B:459:ASN:N	3:E:97:TYR:OH	2.30	0.62
2:H:105:GLN:OE1	2:H:106:GLY:N	2.33	0.62
1:C:182:ILE:HG23	1:C:191:TYR:CA	2.30	0.62
1:A:182:ILE:HG23	1:A:191:TYR:CA	2.30	0.62
1:A:265:LEU:HD11	1:A:291:SER:H	1.65	0.62
1:A:380:GLU:HG2	1:A:438:ILE:HD12	1.82	0.61
1:B:629:GLN:O	1:B:632:LYS:NZ	2.30	0.61
1:C:380:GLU:HG2	1:C:438:ILE:HD12	1.81	0.61
1:C:409:SER:OG	1:C:411:ALA:N	2.32	0.61
3:E:54:ARG:NH2	3:E:63:THR:OG1	2.34	0.61
1:A:260:LEU:HD21	1:A:452:LEU:CD2	2.31	0.61
3:L:54:ARG:NH2	3:L:63:THR:OG1	2.34	0.61
1:A:35:TRP:N	1:A:498:THR:O	2.33	0.61
1:A:67:ASN:O	1:A:71:THR:OG1	2.07	0.61
1:A:232:THR:O	4:o:1:NAG:O6	2.08	0.61
1:B:205:CYS:O	1:B:208:VAL:HG22	2.00	0.61
1:B:260:LEU:HD21	1:B:452:LEU:CD2	2.30	0.61
1:C:265:LEU:HD11	1:C:291:SER:H	1.65	0.61
2:D:97:ASN:OD1	2:D:100:TYR:N	2.31	0.61
1:A:289:ASN:ND2	4:k:1:NAG:O7	2.34	0.61
1:B:35:TRP:N	1:B:498:THR:O	2.33	0.61
1:B:66:HIS:O	1:B:66:HIS:ND1	2.33	0.61
1:C:249:HIS:CE1	1:C:485:TYR:HH	2.19	0.61
2:D:18:VAL:HG12	2:D:82(C):LEU:HD21	1.83	0.61
3:G:54:ARG:NH2	3:G:63:THR:OG1	2.33	0.61
1:B:265:LEU:HD11	1:B:291:SER:H	1.65	0.61
1:B:289:ASN:ND2	4:O:1:NAG:O7	2.34	0.61
1:C:35:TRP:N	1:C:498:THR:O	2.33	0.61
1:C:289:ASN:ND2	4:Z:1:NAG:O7	2.34	0.61
2:H:46:ASP:OD1	2:H:47:TRP:N	2.34	0.61
1:A:249:HIS:CE1	1:A:485:TYR:HH	2.19	0.61
1:A:445:LYS:HB3	6:j:2:NAG:H81	1.83	0.61
2:H:61:GLN:NE2	1:A:456:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:ASP:OD1	2:H:87:THR:N	2.34	0.60
1:B:388:GLY:HA2	4:T:1:NAG:H81	1.81	0.60
1:B:445:LYS:HB3	6:N:2:NAG:H81	1.83	0.60
1:B:491:GLU:N	1:B:491:GLU:OE1	2.35	0.60
1:C:491:GLU:OE1	1:C:491:GLU:N	2.35	0.60
1:B:629:GLN:OE1	1:B:629:GLN:N	2.34	0.60
2:F:86:ASP:OD1	2:F:87:THR:N	2.34	0.60
1:B:182:ILE:HG23	1:B:191:TYR:CA	2.32	0.60
1:C:66:HIS:ND1	1:C:66:HIS:O	2.35	0.60
1:B:330:TYR:OH	7:P:1:NAG:N2	2.32	0.60
1:C:445:LYS:HB3	6:Y:2:NAG:H81	1.83	0.60
1:A:409:SER:OG	1:A:411:ALA:N	2.32	0.60
1:B:376:ASN:OD1	1:B:377:CYS:N	2.35	0.59
1:A:66:HIS:O	1:A:66:HIS:ND1	2.35	0.59
1:C:94:ASN:OD1	1:C:97:LYS:N	2.34	0.59
1:B:229:ASN:O	1:B:231:LYS:NZ	2.22	0.59
3:G:54:ARG:NH2	3:G:62:PHE:O	2.34	0.59
2:F:58:ASN:OD1	2:F:59:TYR:N	2.35	0.59
1:A:330:TYR:OH	7:I:1:NAG:N2	2.33	0.58
2:D:58:ASN:OD1	2:D:59:TYR:N	2.35	0.58
2:F:18:VAL:HG12	2:F:82(C):LEU:HD21	1.84	0.58
1:A:612:SER:OG	8:A:703:NAG:N2	2.36	0.58
2:H:18:VAL:HG12	2:H:82(C):LEU:HD21	1.85	0.58
2:H:65:GLY:O	2:H:82(B):ARG:NH2	2.37	0.58
3:E:54:ARG:NH2	3:E:62:PHE:O	2.35	0.58
1:A:376:ASN:OD1	1:A:377:CYS:N	2.35	0.58
1:C:150:GLU:OE1	1:C:176:LYS:NZ	2.28	0.58
1:C:612:SER:OG	8:C:703:NAG:N2	2.36	0.58
3:L:37:GLN:O	3:L:45:LYS:N	2.29	0.58
1:B:150:GLU:OE2	1:B:153:LYS:NZ	2.36	0.58
1:C:33:ASN:OD1	1:C:35:TRP:NE1	2.37	0.58
1:A:388:GLY:HA2	4:p:1:NAG:H81	1.85	0.58
1:A:195:ASN:ND2	1:A:199:SER:O	2.36	0.57
1:A:154:ASN:OD1	1:A:155:CYS:N	2.37	0.57
1:B:456:ASP:OD2	2:D:61:GLN:NE2	2.37	0.57
1:A:491:GLU:OE1	1:A:491:GLU:N	2.36	0.57
1:B:154:ASN:OD1	1:B:155:CYS:N	2.37	0.57
1:C:376:ASN:OD1	1:C:377:CYS:N	2.36	0.57
1:C:456:ASP:OD2	2:F:61:GLN:NE2	2.37	0.57
3:L:54:ARG:NH2	3:L:62:PHE:O	2.35	0.57
2:H:97:ASN:OD1	2:H:100:TYR:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:OD1	1:B:35:TRP:NE1	2.38	0.57
2:H:88:ALA:O	2:H:108:LEU:HD12	2.05	0.57
2:H:19:ARG:HE	5:h:4:MAN:HO6	1.52	0.57
2:F:88:ALA:O	2:F:108:LEU:HD12	2.05	0.56
1:A:96:TRP:O	1:A:479:ARG:NH1	2.39	0.56
1:B:344:GLN:OE1	4:O:1:NAG:O4	2.24	0.56
1:B:452:LEU:C	1:B:453:LEU:HD22	2.31	0.56
1:A:94:ASN:OD1	1:A:97:LYS:N	2.35	0.56
1:A:452:LEU:C	1:A:453:LEU:HD22	2.31	0.56
1:B:85:VAL:C	1:B:86:LEU:HD22	2.31	0.56
1:C:154:ASN:OD1	1:C:155:CYS:N	2.39	0.56
2:D:19:ARG:HE	5:K:4:MAN:HO6	1.53	0.56
2:H:11:VAL:HG22	2:H:110:THR:CG2	2.36	0.56
1:B:520:VAL:HG23	1:B:520:VAL:O	2.06	0.56
1:A:346:LYS:NZ	1:A:358:ILE:O	2.23	0.56
1:B:96:TRP:O	1:B:479:ARG:NH1	2.39	0.56
1:A:150:GLU:OE2	1:A:153:LYS:NZ	2.35	0.56
1:C:96:TRP:O	1:C:479:ARG:NH1	2.39	0.56
2:H:58:ASN:ND2	1:A:456:ASP:O	2.36	0.56
1:C:85:VAL:C	1:C:86:LEU:HD22	2.31	0.56
1:C:385:ASN:ND2	6:c:1:NAG:O7	2.39	0.56
1:A:520:VAL:HG23	1:A:520:VAL:O	2.06	0.56
1:C:171:TYR:O	1:C:305:ARG:NH1	2.38	0.55
1:C:520:VAL:O	1:C:520:VAL:HG23	2.06	0.55
1:B:456:ASP:O	2:D:58:ASN:ND2	2.38	0.55
1:A:171:TYR:O	1:A:305:ARG:NH1	2.37	0.55
1:C:452:LEU:C	1:C:453:LEU:HD22	2.31	0.55
2:D:88:ALA:O	2:D:108:LEU:HD12	2.05	0.55
1:C:388:GLY:HA2	4:e:1:NAG:H81	1.88	0.55
1:C:456:ASP:O	2:F:58:ASN:ND2	2.36	0.55
1:C:269:GLU:OE2	1:C:348:LYS:NZ	2.40	0.55
1:B:385:ASN:ND2	6:R:1:NAG:O7	2.40	0.55
1:C:344:GLN:OE1	4:Z:1:NAG:O4	2.25	0.55
2:D:3:GLN:N	2:D:3:GLN:OE1	2.40	0.55
2:F:46:ASP:OD1	2:F:47:TRP:N	2.39	0.55
1:A:85:VAL:C	1:A:86:LEU:HD22	2.31	0.55
4:e:1:NAG:HO3	4:e:2:NAG:HO6	1.46	0.55
1:A:385:ASN:ND2	6:n:1:NAG:O7	2.40	0.54
2:F:11:VAL:HG22	2:F:110:THR:CG2	2.37	0.54
2:D:11:VAL:HG22	2:D:110:THR:CG2	2.38	0.54
1:C:234:ASN:OD1	1:C:236:LYS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:OE2	1:A:348:LYS:NZ	2.40	0.54
1:B:269:GLU:OE2	1:B:348:LYS:NZ	2.40	0.54
1:A:344:GLN:OE1	4:k:1:NAG:O4	2.25	0.54
1:C:95:MET:HE2	1:C:483:TYR:CB	2.37	0.54
3:E:106:ILE:HG22	3:E:107:LYS:H	1.73	0.54
2:H:12:LYS:O	2:H:112:SER:N	2.35	0.54
2:F:3:GLN:OE1	2:F:3:GLN:N	2.40	0.54
2:F:65:GLY:O	2:F:82(B):ARG:NH2	2.41	0.54
1:B:195:ASN:ND2	1:B:199:SER:O	2.36	0.53
1:C:68:VAL:HG13	1:C:69:TRP:N	2.23	0.53
1:B:246:GLN:OE1	1:B:246:GLN:N	2.32	0.53
2:H:3:GLN:OE1	2:H:3:GLN:N	2.40	0.53
2:D:65:GLY:O	2:D:82(B):ARG:NH2	2.40	0.53
1:C:159:THR:O	1:C:167:ILE:HG23	2.09	0.53
1:B:68:VAL:HG13	1:B:69:TRP:N	2.23	0.53
1:B:612:SER:OG	8:B:703:NAG:N2	2.36	0.53
1:A:33:ASN:OD1	1:A:35:TRP:NE1	2.41	0.53
1:C:119:CYS:SG	1:C:205:CYS:N	2.81	0.53
1:A:68:VAL:HG13	1:A:69:TRP:N	2.23	0.53
1:B:249:HIS:CE1	1:B:485:TYR:HH	2.22	0.52
1:B:279:ASP:OD1	1:B:279:ASP:N	2.42	0.52
2:D:6:GLN:OE1	2:D:107:THR:N	2.42	0.52
1:B:171:TYR:O	1:B:305:ARG:NH1	2.40	0.52
1:B:182:ILE:HD13	1:B:190:GLY:HA3	1.92	0.52
1:B:94:ASN:OD1	1:B:97:LYS:N	2.37	0.52
1:C:195:ASN:ND2	1:C:199:SER:O	2.37	0.52
1:A:159:THR:O	1:A:167:ILE:HG23	2.09	0.52
1:B:276:ASN:ND2	1:B:279:ASP:OD1	2.42	0.52
6:Y:2:NAG:O3	6:Y:3:BMA:O5	2.27	0.52
1:B:625:MET:HE3	1:B:629:GLN:HB2	1.91	0.52
3:L:54:ARG:NH2	3:L:60:ASP:O	2.42	0.52
1:B:92:ASN:O	1:B:486:LYS:NZ	2.40	0.52
1:A:452:LEU:O	1:A:453:LEU:HD22	2.10	0.52
1:B:95:MET:HE2	1:B:483:TYR:CB	2.38	0.52
3:G:106:ILE:HG22	3:G:107:LYS:H	1.73	0.52
1:C:380:GLU:CG	1:C:438:ILE:HD12	2.41	0.51
1:C:217:TYR:N	1:C:248:THR:OG1	2.36	0.51
1:A:95:MET:HE2	1:A:483:TYR:CB	2.38	0.51
1:B:158:ASN:H	8:B:707:NAG:H81	1.75	0.51
1:B:217:TYR:N	1:B:248:THR:OG1	2.35	0.51
1:B:616:ARG:HB2	1:B:621:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106:ILE:HG22	3:L:107:LYS:H	1.74	0.51
1:B:159:THR:O	1:B:167:ILE:HG23	2.10	0.51
1:C:150:GLU:OE2	1:C:153:LYS:NZ	2.39	0.51
1:C:448:ILE:HD12	1:C:448:ILE:N	2.26	0.51
1:A:657:GLN:O	1:A:661:ALA:N	2.43	0.51
1:A:448:ILE:N	1:A:448:ILE:HD12	2.26	0.51
1:C:279:ASP:OD1	1:C:279:ASP:N	2.43	0.51
3:E:54:ARG:NH2	3:E:60:ASP:O	2.44	0.51
1:A:182:ILE:HD13	1:A:190:GLY:HA3	1.93	0.51
1:A:119:CYS:SG	1:A:205:CYS:N	2.82	0.51
1:C:657:GLN:O	1:C:661:ALA:N	2.44	0.51
1:A:92:ASN:O	1:A:486:LYS:NZ	2.41	0.51
1:B:448:ILE:N	1:B:448:ILE:HD12	2.26	0.50
3:E:37:GLN:N	3:E:45:LYS:O	2.43	0.50
1:B:170:GLU:HG2	1:B:307:ILE:HD13	1.93	0.50
1:B:387:SER:O	1:B:391:ASN:ND2	2.43	0.50
1:C:276:ASN:ND2	1:C:279:ASP:OD1	2.43	0.50
3:G:54:ARG:NH2	3:G:60:ASP:O	2.43	0.50
1:B:392:ASP:N	1:B:392:ASP:OD1	2.45	0.50
1:C:152:MET:HE3	1:C:175:TYR:CG	2.47	0.50
1:C:170:GLU:HG2	1:C:307:ILE:HD13	1.93	0.50
1:A:276:ASN:ND2	1:A:279:ASP:OD1	2.44	0.50
1:B:452:LEU:O	1:B:453:LEU:HD22	2.11	0.50
1:B:656:GLU:OE1	1:B:657:GLN:N	2.45	0.50
2:F:6:GLN:OE1	2:F:107:THR:N	2.45	0.50
3:L:52:SER:OG	3:L:64:GLY:O	2.26	0.50
2:H:6:GLN:OE1	2:H:107:THR:N	2.44	0.50
1:B:380:GLU:CG	1:B:438:ILE:HD12	2.41	0.50
1:A:170:GLU:HG2	1:A:307:ILE:HD13	1.93	0.50
1:A:217:TYR:N	1:A:248:THR:OG1	2.35	0.50
1:B:78:ASP:OD2	1:B:82:GLN:NE2	2.43	0.50
1:C:182:ILE:HD13	1:C:190:GLY:HA3	1.94	0.50
1:C:656:GLU:OE1	1:C:657:GLN:N	2.45	0.50
1:B:119:CYS:SG	1:B:205:CYS:N	2.84	0.50
1:B:152:MET:HE3	1:B:175:TYR:CG	2.47	0.50
2:F:80:MET:SD	2:F:81:GLU:N	2.85	0.50
1:A:152:MET:HE3	1:A:175:TYR:CG	2.47	0.50
1:B:657:GLN:O	1:B:661:ALA:N	2.45	0.49
2:F:19:ARG:HE	5:W:4:MAN:HO6	1.57	0.49
1:A:234:ASN:OD1	1:A:236:LYS:N	2.39	0.49
1:B:602:ILE:HD12	1:A:657:GLN:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:O	1:C:453:LEU:HD22	2.12	0.49
1:A:387:SER:O	1:A:391:ASN:ND2	2.42	0.49
1:A:656:GLU:OE1	1:A:657:GLN:N	2.45	0.49
3:G:70:ASP:N	3:G:70:ASP:OD1	2.44	0.49
1:A:67:ASN:OD1	1:A:68:VAL:N	2.41	0.49
1:A:246:GLN:OE1	1:A:246:GLN:N	2.32	0.49
1:A:380:GLU:CG	1:A:438:ILE:HD12	2.41	0.49
1:C:158:ASN:H	8:C:707:NAG:H81	1.77	0.49
2:H:80:MET:SD	2:H:81:GLU:N	2.85	0.49
3:L:73:LEU:C	3:L:73:LEU:HD23	2.38	0.49
1:C:657:GLN:CB	1:A:602:ILE:HD12	2.43	0.48
3:L:101:GLY:O	3:L:102:THR:OG1	2.28	0.48
1:A:158:ASN:H	8:A:707:NAG:H81	1.78	0.48
1:B:234:ASN:OD1	1:B:236:LYS:N	2.40	0.48
2:D:12:LYS:O	2:D:112:SER:N	2.35	0.48
1:A:616:ARG:HB2	1:A:621:ILE:HD11	1.95	0.48
1:B:625:MET:HE3	1:B:629:GLN:CB	2.43	0.48
1:C:92:ASN:O	1:C:486:LYS:NZ	2.44	0.48
1:B:657:GLN:CB	1:C:602:ILE:HD12	2.43	0.48
3:G:73:LEU:C	3:G:73:LEU:HD23	2.37	0.48
1:C:260:LEU:HD23	1:C:450:GLY:C	2.38	0.48
2:F:66:ARG:O	2:F:82:LEU:HD12	2.13	0.48
1:A:162:VAL:O	1:A:164:ARG:NH2	2.45	0.48
1:A:260:LEU:HD23	1:A:450:GLY:C	2.39	0.48
1:A:279:ASP:OD1	1:A:279:ASP:N	2.43	0.48
1:C:543:LEU:C	1:C:543:LEU:HD12	2.39	0.48
1:C:616:ARG:HB2	1:C:621:ILE:HD11	1.96	0.48
1:A:543:LEU:C	1:A:543:LEU:HD12	2.39	0.48
1:B:162:VAL:O	1:B:164:ARG:NH2	2.47	0.48
1:C:162:VAL:O	1:C:164:ARG:NH2	2.47	0.48
1:C:527:SER:OG	1:C:528:THR:N	2.47	0.48
3:G:37:GLN:N	3:G:45:LYS:O	2.41	0.48
2:F:12:LYS:O	2:F:112:SER:N	2.35	0.48
1:B:197:ASN:ND2	5:K:1:NAG:O7	2.47	0.47
1:B:543:LEU:HD12	1:B:543:LEU:C	2.39	0.47
3:E:73:LEU:C	3:E:73:LEU:HD23	2.38	0.47
2:H:66:ARG:O	2:H:82:LEU:HD12	2.14	0.47
1:A:197:ASN:ND2	5:h:1:NAG:O7	2.47	0.47
1:B:260:LEU:HD23	1:B:450:GLY:C	2.38	0.47
1:B:528:THR:HG21	1:B:623:ASP:O	2.15	0.47
1:B:359:SER:OG	1:B:361:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ASN:OD1	2:D:56:GLY:N	2.48	0.47
3:E:101:GLY:O	3:E:102:THR:OG1	2.27	0.47
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.97	0.47
3:E:70:ASP:OD1	3:E:70:ASP:N	2.47	0.47
1:B:67:ASN:OD1	1:B:68:VAL:N	2.41	0.47
1:B:451:LEU:HD23	1:B:451:LEU:N	2.30	0.47
1:C:259:LEU:C	1:C:260:LEU:HD22	2.40	0.47
2:D:80:MET:SD	2:D:81:GLU:N	2.88	0.47
1:C:159:THR:OG1	1:C:160:THR:N	2.48	0.46
1:C:255:VAL:HG23	1:C:474:MET:HE1	1.97	0.46
1:C:451:LEU:N	1:C:451:LEU:HD23	2.30	0.46
2:D:66:ARG:O	2:D:82:LEU:HD12	2.14	0.46
3:E:106:ILE:HG22	3:E:107:LYS:N	2.30	0.46
1:C:387:SER:O	1:C:391:ASN:ND2	2.43	0.46
3:E:66:GLY:HA3	3:E:71:PHE:HA	1.98	0.46
1:B:657:GLN:HB2	1:C:602:ILE:HD12	1.97	0.46
3:L:106:ILE:HG22	3:L:107:LYS:N	2.30	0.46
6:N:2:NAG:O3	6:N:3:BMA:O5	2.26	0.46
1:B:602:ILE:HD12	1:A:657:GLN:HB2	1.97	0.46
1:A:258:GLN:O	1:A:259:LEU:HD22	2.15	0.46
1:A:527:SER:OG	1:A:528:THR:N	2.48	0.46
1:B:259:LEU:C	1:B:260:LEU:HD22	2.41	0.46
3:L:15:LEU:HA	3:L:78:VAL:HG23	1.97	0.46
1:A:78:ASP:OD2	1:A:82:GLN:NE2	2.43	0.46
1:C:78:ASP:OD2	1:C:82:GLN:NE2	2.43	0.46
1:A:475:ARG:HA	1:A:478:TRP:CE3	2.51	0.46
2:F:52:ASN:OD1	2:F:56:GLY:N	2.49	0.46
1:C:197:ASN:ND2	5:W:1:NAG:O7	2.48	0.46
1:C:475:ARG:HA	1:C:478:TRP:CE3	2.51	0.46
3:E:15:LEU:HA	3:E:78:VAL:HG23	1.98	0.46
3:G:66:GLY:HA3	3:G:71:PHE:HA	1.98	0.46
1:A:56:SER:O	1:A:77:THR:N	2.49	0.46
1:C:179:ILE:HD11	1:C:191:TYR:CG	2.51	0.46
1:C:182:ILE:HG23	1:C:190:GLY:C	2.41	0.46
1:C:359:SER:OG	1:C:361:GLN:NE2	2.47	0.46
1:C:657:GLN:HB2	1:A:602:ILE:HD12	1.96	0.46
1:A:451:LEU:N	1:A:451:LEU:HD23	2.30	0.46
1:C:54:CYS:SG	1:C:55:ALA:N	2.88	0.46
3:L:37:GLN:N	3:L:45:LYS:O	2.42	0.46
3:G:106:ILE:HG22	3:G:107:LYS:N	2.30	0.45
1:A:159:THR:OG1	1:A:160:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HG23	1:A:190:GLY:C	2.41	0.45
1:B:475:ARG:HA	1:B:478:TRP:CE3	2.50	0.45
1:C:67:ASN:OD1	1:C:68:VAL:N	2.41	0.45
1:C:229:ASN:O	1:C:231:LYS:NZ	2.22	0.45
1:A:259:LEU:C	1:A:260:LEU:HD22	2.40	0.45
1:B:182:ILE:HG23	1:B:190:GLY:C	2.41	0.45
3:L:54:ARG:NE	3:L:62:PHE:O	2.49	0.45
1:A:409:SER:OG	1:A:410:ASN:N	2.50	0.45
1:B:339:SER:HB2	1:B:408:ILE:HD11	1.99	0.45
1:C:273:ARG:HG3	1:C:285:ILE:HG23	1.98	0.45
2:F:97:ASN:OD1	2:F:100:TYR:N	2.32	0.45
2:H:81:GLU:OE2	2:H:82:LEU:N	2.49	0.45
1:A:273:ARG:HG3	1:A:285:ILE:HG23	1.99	0.45
1:B:527:SER:OG	1:B:528:THR:N	2.49	0.45
1:C:595:TRP:HA	1:C:649:GLN:HG3	1.98	0.45
1:B:602:ILE:HD11	1:A:653:GLU:HG3	1.98	0.45
1:B:653:GLU:HG3	1:C:602:ILE:HD11	1.99	0.45
1:C:68:VAL:HG13	1:C:69:TRP:CD2	2.52	0.45
2:F:81:GLU:OE2	2:F:82:LEU:N	2.50	0.45
3:G:15:LEU:HA	3:G:78:VAL:HG23	1.99	0.45
1:A:195:ASN:O	1:A:198:THR:N	2.44	0.45
1:A:255:VAL:HG23	1:A:474:MET:HE1	1.98	0.45
1:B:159:THR:OG1	1:B:160:THR:N	2.50	0.45
2:H:90:TYR:HE1	2:H:109:VAL:HG12	1.82	0.45
1:A:249:HIS:CG	1:A:485:TYR:HH	2.31	0.45
1:A:54:CYS:SG	1:A:55:ALA:N	2.90	0.45
1:C:653:GLU:HG3	1:A:602:ILE:HD11	1.98	0.44
1:A:625:MET:SD	1:A:629:GLN:HB2	2.57	0.44
1:B:54:CYS:SG	1:B:55:ALA:N	2.91	0.44
1:C:326:ILE:HD12	1:C:326:ILE:N	2.32	0.44
1:B:501:LYS:NZ	1:B:503:ARG:O	2.49	0.44
2:D:52(A):PRO:O	2:D:71:ARG:NE	2.50	0.44
1:C:325:ASP:C	1:C:326:ILE:HD12	2.43	0.44
1:C:258:GLN:O	1:C:259:LEU:HD22	2.16	0.44
1:B:273:ARG:HG3	1:B:285:ILE:HG23	1.98	0.44
1:B:326:ILE:N	1:B:326:ILE:HD12	2.32	0.44
2:D:81:GLU:OE2	2:D:82:LEU:N	2.50	0.44
2:D:90:TYR:HE1	2:D:109:VAL:HG12	1.83	0.44
2:H:52(A):PRO:O	2:H:71:ARG:NE	2.51	0.44
1:B:56:SER:O	1:B:77:THR:N	2.51	0.44
1:B:260:LEU:HD23	1:B:451:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ASN:OD1	2:H:56:GLY:N	2.50	0.44
1:C:249:HIS:CG	1:C:485:TYR:HH	2.31	0.44
1:C:409:SER:OG	1:C:410:ASN:N	2.49	0.44
2:F:52(A):PRO:O	2:F:71:ARG:NE	2.50	0.44
1:B:249:HIS:CG	1:B:485:TYR:HH	2.31	0.43
1:C:56:SER:O	1:C:77:THR:N	2.50	0.43
1:C:648:SER:O	1:C:651:GLN:NE2	2.49	0.43
6:j:2:NAG:O3	6:j:3:BMA:O5	2.27	0.43
1:C:195:ASN:O	1:C:198:THR:N	2.45	0.43
1:C:547:ILE:HG13	1:C:548:VAL:HG22	2.00	0.43
1:C:625:MET:SD	1:C:629:GLN:HB2	2.58	0.43
2:D:83:ARG:O	2:D:84:SER:C	2.61	0.43
3:L:70:ASP:OD1	3:L:70:ASP:N	2.51	0.43
1:B:195:ASN:O	1:B:199:SER:N	2.44	0.43
1:B:258:GLN:O	1:B:259:LEU:HD22	2.18	0.43
1:A:359:SER:OG	1:A:361:GLN:NE2	2.49	0.43
1:B:357:ASN:OD1	8:B:701:NAG:C2	2.66	0.43
1:B:595:TRP:HA	1:B:649:GLN:HG3	2.00	0.43
2:F:90:TYR:HE1	2:F:109:VAL:HG12	1.82	0.43
1:A:68:VAL:HG13	1:A:69:TRP:CD2	2.53	0.43
1:B:68:VAL:HG13	1:B:69:TRP:CD2	2.53	0.43
1:B:125:LEU:N	1:B:125:LEU:HD12	2.34	0.43
1:A:325:ASP:C	1:A:326:ILE:HD12	2.43	0.43
1:A:326:ILE:HD12	1:A:326:ILE:N	2.33	0.43
1:B:325:ASP:C	1:B:326:ILE:HD12	2.43	0.43
1:B:338:TRP:NE1	1:B:342:VAL:HG21	2.33	0.43
1:C:127:VAL:HG22	1:C:128:THR:N	2.33	0.43
3:E:54:ARG:NE	3:E:62:PHE:O	2.50	0.43
1:C:246:GLN:OE1	1:C:246:GLN:N	2.32	0.43
1:C:260:LEU:HD23	1:C:451:LEU:HA	2.01	0.43
2:F:83:ARG:O	2:F:84:SER:C	2.61	0.43
1:B:167:ILE:N	1:B:167:ILE:HD12	2.34	0.43
1:B:179:ILE:HD11	1:B:191:TYR:CG	2.54	0.43
1:C:357:ASN:OD1	8:C:701:NAG:C2	2.66	0.43
1:C:125:LEU:O	1:C:127:VAL:N	2.52	0.43
2:F:12:LYS:O	2:F:111:VAL:HA	2.19	0.43
1:A:95:MET:SD	1:A:96:TRP:CD2	3.12	0.43
2:H:2:VAL:HG13	2:H:27:TYR:CE1	2.55	0.42
1:A:348:LYS:O	1:A:351:GLU:HB3	2.19	0.42
1:B:127:VAL:HG22	1:B:128:THR:N	2.34	0.42
1:C:348:LYS:O	1:C:351:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD23	1:A:451:LEU:HA	2.00	0.42
1:A:357:ASN:OD1	8:A:701:NAG:C2	2.67	0.42
2:H:83:ARG:O	2:H:84:SER:C	2.61	0.42
1:A:179:ILE:HD11	1:A:191:TYR:CG	2.55	0.42
1:B:95:MET:SD	1:B:96:TRP:CD2	3.12	0.42
1:C:50:THR:HG21	1:C:487:VAL:HG11	2.01	0.42
1:C:167:ILE:HD12	1:C:167:ILE:N	2.34	0.42
1:C:322:ILE:HD13	1:C:326:ILE:HG13	2.01	0.42
1:A:86:LEU:HD11	1:A:523:GLY:HA2	2.01	0.42
1:A:501:LYS:NZ	1:A:503:ARG:O	2.51	0.42
1:B:195:ASN:O	1:B:198:THR:N	2.44	0.42
1:B:539:GLN:OE1	1:B:539:GLN:N	2.43	0.42
1:C:95:MET:SD	1:C:96:TRP:CD2	3.12	0.42
2:D:12:LYS:O	2:D:111:VAL:HA	2.19	0.42
2:D:47:TRP:CE3	3:E:96:GLU:HB3	2.55	0.42
2:H:67:VAL:HG12	2:H:68:THR:N	2.34	0.42
1:A:367:ASP:OD1	1:A:367:ASP:N	2.52	0.42
1:B:348:LYS:O	1:B:351:GLU:HB3	2.19	0.42
1:A:125:LEU:HD12	1:A:125:LEU:N	2.33	0.42
1:A:127:VAL:HG22	1:A:128:THR:N	2.34	0.42
1:A:452:LEU:N	1:A:452:LEU:HD22	2.35	0.42
1:B:152:MET:HE3	1:B:175:TYR:CD2	2.55	0.42
1:C:125:LEU:N	1:C:125:LEU:HD12	2.33	0.42
2:F:67:VAL:HG12	2:F:68:THR:N	2.35	0.42
1:A:167:ILE:HD12	1:A:167:ILE:N	2.34	0.42
1:A:234:ASN:OD1	1:A:235:GLY:N	2.53	0.42
1:A:408:ILE:HG13	1:A:409:SER:H	1.85	0.42
1:C:408:ILE:HG13	1:C:409:SER:H	1.85	0.42
2:F:2:VAL:HG13	2:F:27:TYR:CE1	2.55	0.42
2:F:50:TRP:C	2:F:50:TRP:CE3	2.98	0.42
1:A:595:TRP:HA	1:A:649:GLN:HG3	2.00	0.42
1:B:616:ARG:CB	1:B:621:ILE:HD11	2.50	0.42
1:C:86:LEU:HD11	1:C:523:GLY:HA2	2.01	0.42
1:A:493:LEU:N	1:A:493:LEU:HD22	2.35	0.42
1:B:373:HIS:CD2	1:B:373:HIS:C	2.98	0.42
1:C:68:VAL:HG13	1:C:69:TRP:H	1.85	0.42
1:C:102:ASP:O	1:C:106:GLU:OE1	2.38	0.42
2:F:47:TRP:CE3	3:G:96:GLU:HB3	2.55	0.42
1:B:322:ILE:HD13	1:B:326:ILE:HG13	2.02	0.41
6:j:1:NAG:HO3	6:j:1:NAG:C7	2.27	0.41
1:B:629:GLN:N	1:B:629:GLN:CD	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:TRP:CE3	2:D:50:TRP:C	2.99	0.41
1:B:368:LEU:O	1:B:371:THR:OG1	2.38	0.41
1:B:452:LEU:N	1:B:452:LEU:HD22	2.35	0.41
1:B:68:VAL:HG13	1:B:69:TRP:H	1.85	0.41
1:B:493:LEU:N	1:B:493:LEU:HD22	2.35	0.41
1:C:223:TYR:CE2	1:C:489:LYS:HB3	2.56	0.41
1:A:152:MET:HE3	1:A:175:TYR:CD2	2.55	0.41
1:A:547:ILE:HG13	1:A:548:VAL:HG22	2.02	0.41
1:B:547:ILE:HG13	1:B:548:VAL:HG22	2.02	0.41
1:C:273:ARG:HG3	1:C:285:ILE:CG2	2.51	0.41
3:E:67:SER:O	3:E:69:THR:N	2.54	0.41
2:H:12:LYS:O	2:H:111:VAL:HA	2.20	0.41
1:B:134:VAL:C	1:B:135:THR:HG23	2.45	0.41
1:B:367:ASP:OD1	1:B:367:ASP:N	2.54	0.41
1:C:134:VAL:C	1:C:135:THR:HG23	2.46	0.41
1:C:152:MET:HE3	1:C:175:TYR:CD2	2.56	0.41
1:C:452:LEU:N	1:C:452:LEU:HD22	2.35	0.41
1:C:501:LYS:NZ	1:C:503:ARG:O	2.51	0.41
2:D:2:VAL:HG13	2:D:27:TYR:CE1	2.55	0.41
3:E:52:SER:OG	3:E:64:GLY:O	2.24	0.41
3:G:67:SER:O	3:G:69:THR:N	2.54	0.41
1:A:134:VAL:C	1:A:135:THR:HG23	2.45	0.41
1:C:373:HIS:CD2	1:C:373:HIS:C	2.98	0.41
1:C:493:LEU:N	1:C:493:LEU:HD22	2.35	0.41
1:B:50:THR:HG21	1:B:487:VAL:HG11	2.02	0.41
1:B:336:ARG:HG3	4:Q:1:NAG:H81	2.02	0.41
1:C:392:ASP:OD1	1:C:392:ASP:N	2.53	0.41
1:C:410:ASN:HD22	8:C:702:NAG:C7	2.33	0.41
3:E:63:THR:HG22	3:E:64:GLY:N	2.36	0.41
2:H:50:TRP:CE3	2:H:50:TRP:C	2.99	0.41
1:A:373:HIS:CD2	1:A:373:HIS:C	2.99	0.41
1:B:86:LEU:HD11	1:B:523:GLY:HA2	2.02	0.41
1:B:199:SER:OG	1:B:200:THR:N	2.54	0.41
1:B:648:SER:O	1:B:651:GLN:NE2	2.49	0.41
1:C:37:THR:HG23	1:C:604:CYS:HA	2.03	0.41
1:C:234:ASN:OD1	1:C:235:GLY:N	2.53	0.41
1:C:286:VAL:O	1:C:286:VAL:HG13	2.21	0.41
2:D:67:VAL:HG12	2:D:68:THR:N	2.36	0.41
3:L:67:SER:O	3:L:69:THR:N	2.54	0.41
1:A:125:LEU:O	1:A:127:VAL:N	2.53	0.41
1:A:223:TYR:CE2	1:A:489:LYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HG3	1:A:285:ILE:CG2	2.51	0.41
1:A:338:TRP:NE1	1:A:342:VAL:HG21	2.36	0.41
1:A:429:VAL:HG12	1:A:429:VAL:O	2.21	0.41
1:A:539:GLN:OE1	1:A:539:GLN:N	2.42	0.41
3:G:54:ARG:NE	3:G:62:PHE:O	2.50	0.41
1:A:68:VAL:HG13	1:A:69:TRP:H	1.85	0.41
1:B:234:ASN:OD1	1:B:235:GLY:N	2.54	0.40
3:L:63:THR:HG22	3:L:64:GLY:N	2.36	0.40
1:C:150:GLU:CD	1:C:176:LYS:HZ2	2.20	0.40
1:C:296:CYS:HA	1:C:331:CYS:HA	2.04	0.40
1:A:102:ASP:O	1:A:106:GLU:OE1	2.39	0.40
1:B:66:HIS:O	1:B:66:HIS:CG	2.75	0.40
1:B:295:VAL:HG12	1:B:296:CYS:N	2.36	0.40
1:C:289:ASN:ND2	4:Z:1:NAG:C7	2.85	0.40
1:A:295:VAL:HG12	1:A:296:CYS:N	2.36	0.40
1:A:570:TRP:HA	1:A:573:LYS:HE2	2.04	0.40
1:B:223:TYR:CE2	1:B:489:LYS:HB3	2.55	0.40
1:C:295:VAL:HG12	1:C:296:CYS:N	2.37	0.40
1:C:481:GLU:N	1:C:481:GLU:CD	2.79	0.40
1:A:289:ASN:ND2	4:k:1:NAG:C7	2.84	0.40
6:N:1:NAG:HO3	6:N:1:NAG:C7	2.24	0.40
1:B:575:LEU:O	1:B:579:VAL:HG23	2.22	0.40
2:H:20:VAL:HG22	2:H:21:SER:N	2.37	0.40
1:A:50:THR:HG21	1:A:487:VAL:HG11	2.03	0.40
5:V:2:NAG:O7	5:V:2:NAG:O3	2.37	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	552/619 (89%)	501 (91%)	50 (9%)	1 (0%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	552/619 (89%)	502 (91%)	49 (9%)	1 (0%)	43	77
1	C	552/619 (89%)	503 (91%)	48 (9%)	1 (0%)	43	77
2	D	117/233 (50%)	110 (94%)	7 (6%)	0	100	100
2	F	117/233 (50%)	109 (93%)	8 (7%)	0	100	100
2	H	117/233 (50%)	110 (94%)	7 (6%)	0	100	100
3	E	100/200 (50%)	85 (85%)	14 (14%)	1 (1%)	12	47
3	G	100/200 (50%)	87 (87%)	12 (12%)	1 (1%)	12	47
3	L	100/200 (50%)	85 (85%)	14 (14%)	1 (1%)	12	47
All	All	2307/3156 (73%)	2092 (91%)	209 (9%)	6 (0%)	37	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27(C)	ILE
3	G	27(C)	ILE
3	L	27(C)	ILE
1	B	74	CYS
1	C	74	CYS
1	A	74	CYS

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	496/544 (91%)	487 (98%)	9 (2%)	51	66
1	B	496/544 (91%)	491 (99%)	5 (1%)	68	75
1	C	496/544 (91%)	487 (98%)	9 (2%)	51	66
2	D	100/201 (50%)	99 (99%)	1 (1%)	68	75
2	F	100/201 (50%)	99 (99%)	1 (1%)	68	75
2	H	100/201 (50%)	99 (99%)	1 (1%)	68	75
3	E	89/177 (50%)	88 (99%)	1 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	89/177 (50%)	88 (99%)	1 (1%)	65	73
3	L	89/177 (50%)	88 (99%)	1 (1%)	65	73
All	All	2055/2766 (74%)	2026 (99%)	29 (1%)	57	70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	ASP
1	B	267	GLU
1	B	279	ASP
1	B	392	ASP
1	B	480	SER
1	C	102	ASP
1	C	255	VAL
1	C	267	GLU
1	C	279	ASP
1	C	367	ASP
1	C	393	THR
1	C	408	ILE
1	C	409	SER
1	C	480	SER
2	D	105	GLN
3	E	70	ASP
2	F	105	GLN
3	G	70	ASP
2	H	105	GLN
3	L	70	ASP
1	A	102	ASP
1	A	255	VAL
1	A	267	GLU
1	A	279	ASP
1	A	367	ASP
1	A	393	THR
1	A	408	ILE
1	A	409	SER
1	A	480	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	HIS
1	C	72	HIS
1	C	355	HIS
1	C	361	GLN
2	D	101	GLN
3	E	37	GLN
2	F	101	GLN
3	G	37	GLN
2	H	101	GLN
3	L	37	GLN
1	A	72	HIS
1	A	355	HIS
1	A	361	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

108 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	$\# Z > 2$
4	NAG	I	1	4,1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	I	2	4	14,14,15	0.17	0	17,19,21	0.51	0
5	NAG	J	1	5	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	J	2	5	14,14,15	0.22	0	17,19,21	0.69	0
5	BMA	J	3	5	11,11,12	0.58	0	15,15,17	1.26	1 (6%)
5	MAN	J	4	5	11,11,12	0.50	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	J	5	5	11,11,12	0.59	0	15,15,17	1.08	2 (13%)
5	NAG	K	1	1,5	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	K	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	BMA	K	3	5	11,11,12	0.62	0	15,15,17	1.26	3 (20%)
5	MAN	K	4	5	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
5	MAN	K	5	5	11,11,12	0.55	0	15,15,17	0.98	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.38	0	17,19,21	0.43	0
4	NAG	M	2	4	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	N	1	1,6	14,14,15	0.20	0	17,19,21	0.39	0
6	NAG	N	2	6	14,14,15	0.26	0	17,19,21	0.39	0
6	BMA	N	3	6	11,11,12	0.47	0	15,15,17	0.81	0
6	MAN	N	4	6	11,11,12	0.63	0	15,15,17	1.19	2 (13%)
6	MAN	N	5	6	11,11,12	0.66	0	15,15,17	0.79	1 (6%)
4	NAG	O	1	4,1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	O	2	4	14,14,15	0.19	0	17,19,21	0.49	0
7	NAG	P	1	7,1	14,14,15	0.54	0	17,19,21	0.58	0
7	NAG	P	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	BMA	P	3	7	11,11,12	0.46	0	15,15,17	0.70	0
7	MAN	P	4	7	11,11,12	0.56	0	15,15,17	0.93	2 (13%)
4	NAG	Q	1	4,1	14,14,15	0.62	1 (7%)	17,19,21	0.51	0
4	NAG	Q	2	4	14,14,15	0.19	0	17,19,21	0.48	0
6	NAG	R	1	1,6	14,14,15	0.43	0	17,19,21	0.39	0
6	NAG	R	2	6	14,14,15	0.20	0	17,19,21	0.50	0
6	BMA	R	3	6	11,11,12	0.47	0	15,15,17	0.72	0
6	MAN	R	4	6	11,11,12	0.52	0	15,15,17	0.88	1 (6%)
6	MAN	R	5	6	11,11,12	0.66	0	15,15,17	1.19	2 (13%)
4	NAG	S	1	4,1	14,14,15	0.46	0	17,19,21	0.45	0
4	NAG	S	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	T	1	4	14,14,15	0.23	0	17,19,21	0.38	0
4	NAG	T	2	4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	U	1	4,1	14,14,15	0.22	0	17,19,21	0.53	0
4	NAG	U	2	4	14,14,15	0.18	0	17,19,21	0.50	0
5	NAG	V	1	5	14,14,15	0.34	0	17,19,21	0.44	0
5	NAG	V	2	5	14,14,15	0.15	0	17,19,21	0.71	0
5	BMA	V	3	5	11,11,12	0.60	0	15,15,17	1.27	1 (6%)
5	MAN	V	4	5	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
5	MAN	V	5	5	11,11,12	0.59	0	15,15,17	1.09	2 (13%)
5	NAG	W	1	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	W	2	5	14,14,15	0.25	0	17,19,21	0.41	0
5	BMA	W	3	5	11,11,12	0.63	0	15,15,17	1.27	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	W	4	5	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
5	MAN	W	5	5	11,11,12	0.55	0	15,15,17	0.99	2 (13%)
4	NAG	X	1	4,1	14,14,15	0.38	0	17,19,21	0.43	0
4	NAG	X	2	4	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	Y	1	1,6	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	Y	2	6	14,14,15	0.27	0	17,19,21	0.39	0
6	BMA	Y	3	6	11,11,12	0.46	0	15,15,17	0.80	0
6	MAN	Y	4	6	11,11,12	0.64	0	15,15,17	1.20	2 (13%)
6	MAN	Y	5	6	11,11,12	0.66	0	15,15,17	0.79	1 (6%)
4	NAG	Z	1	4,1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	Z	2	4	14,14,15	0.20	0	17,19,21	0.49	0
7	NAG	a	1	7,1	14,14,15	0.53	0	17,19,21	0.57	0
7	NAG	a	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	BMA	a	3	7	11,11,12	0.46	0	15,15,17	0.71	0
7	MAN	a	4	7	11,11,12	0.56	0	15,15,17	0.93	2 (13%)
4	NAG	b	1	4,1	14,14,15	0.61	1 (7%)	17,19,21	0.50	0
4	NAG	b	2	4	14,14,15	0.19	0	17,19,21	0.48	0
6	NAG	c	1	1,6	14,14,15	0.42	0	17,19,21	0.40	0
6	NAG	c	2	6	14,14,15	0.20	0	17,19,21	0.50	0
6	BMA	c	3	6	11,11,12	0.47	0	15,15,17	0.72	0
6	MAN	c	4	6	11,11,12	0.52	0	15,15,17	0.88	1 (6%)
6	MAN	c	5	6	11,11,12	0.66	0	15,15,17	1.19	2 (13%)
4	NAG	d	1	4,1	14,14,15	0.47	0	17,19,21	0.45	0
4	NAG	d	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	e	1	4	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	e	2	4	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	f	1	4,1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	f	2	4	14,14,15	0.17	0	17,19,21	0.51	0
5	NAG	g	1	5	14,14,15	0.35	0	17,19,21	0.44	0
5	NAG	g	2	5	14,14,15	0.20	0	17,19,21	0.69	0
5	BMA	g	3	5	11,11,12	0.59	0	15,15,17	1.26	1 (6%)
5	MAN	g	4	5	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
5	MAN	g	5	5	11,11,12	0.59	0	15,15,17	1.09	2 (13%)
5	NAG	h	1	1,5	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	h	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	BMA	h	3	5	11,11,12	0.62	0	15,15,17	1.28	3 (20%)
5	MAN	h	4	5	11,11,12	0.62	0	15,15,17	1.16	2 (13%)
5	MAN	h	5	5	11,11,12	0.55	0	15,15,17	0.99	2 (13%)
4	NAG	i	1	4,1	14,14,15	0.38	0	17,19,21	0.43	0
4	NAG	i	2	4	14,14,15	0.21	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	j	1	1,6	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	j	2	6	14,14,15	0.27	0	17,19,21	0.40	0
6	BMA	j	3	6	11,11,12	0.47	0	15,15,17	0.80	0
6	MAN	j	4	6	11,11,12	0.63	0	15,15,17	1.20	2 (13%)
6	MAN	j	5	6	11,11,12	0.66	0	15,15,17	0.79	1 (6%)
4	NAG	k	1	4,1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	k	2	4	14,14,15	0.19	0	17,19,21	0.49	0
7	NAG	l	1	7,1	14,14,15	0.52	0	17,19,21	0.57	0
7	NAG	l	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	BMA	l	3	7	11,11,12	0.47	0	15,15,17	0.71	0
7	MAN	l	4	7	11,11,12	0.56	0	15,15,17	0.93	2 (13%)
4	NAG	m	1	4,1	14,14,15	0.62	1 (7%)	17,19,21	0.50	0
4	NAG	m	2	4	14,14,15	0.19	0	17,19,21	0.48	0
6	NAG	n	1	1,6	14,14,15	0.43	0	17,19,21	0.39	0
6	NAG	n	2	6	14,14,15	0.20	0	17,19,21	0.50	0
6	BMA	n	3	6	11,11,12	0.46	0	15,15,17	0.72	0
6	MAN	n	4	6	11,11,12	0.52	0	15,15,17	0.87	1 (6%)
6	MAN	n	5	6	11,11,12	0.65	0	15,15,17	1.19	2 (13%)
4	NAG	o	1	4,1	14,14,15	0.48	0	17,19,21	0.45	0
4	NAG	o	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	p	1	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	p	2	4	14,14,15	0.23	0	17,19,21	0.55	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
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5	-	1/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	5	6	-	1/2/19/22	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
7	NAG	a	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	BMA	a	3	7	-	2/2/19/22	0/1/1/1
7	MAN	a	4	7	-	1/2/19/22	0/1/1/1
4	NAG	b	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	c	2	6	-	0/6/23/26	0/1/1/1
6	BMA	c	3	6	-	2/2/19/22	0/1/1/1
6	MAN	c	4	6	-	2/2/19/22	0/1/1/1
6	MAN	c	5	6	-	2/2/19/22	0/1/1/1
4	NAG	d	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	4	-	4/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
5	NAG	g	1	5	-	1/6/23/26	0/1/1/1
5	NAG	g	2	5	-	3/6/23/26	0/1/1/1
5	BMA	g	3	5	-	0/2/19/22	0/1/1/1
5	MAN	g	4	5	-	0/2/19/22	0/1/1/1
5	MAN	g	5	5	-	1/2/19/22	0/1/1/1
5	NAG	h	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
5	BMA	h	3	5	-	2/2/19/22	0/1/1/1
5	MAN	h	4	5	-	2/2/19/22	0/1/1/1
5	MAN	h	5	5	-	1/2/19/22	0/1/1/1
4	NAG	i	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
6	NAG	j	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	BMA	j	3	6	-	2/2/19/22	0/1/1/1
6	MAN	j	4	6	-	2/2/19/22	0/1/1/1
6	MAN	j	5	6	-	1/2/19/22	0/1/1/1
4	NAG	k	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	2/6/23/26	0/1/1/1
7	NAG	l	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	l	2	7	-	2/6/23/26	0/1/1/1
7	BMA	l	3	7	-	2/2/19/22	0/1/1/1
7	MAN	l	4	7	-	1/2/19/22	0/1/1/1
4	NAG	m	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
6	NAG	n	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
6	BMA	n	3	6	-	2/2/19/22	0/1/1/1
6	MAN	n	4	6	-	2/2/19/22	0/1/1/1
6	MAN	n	5	6	-	2/2/19/22	0/1/1/1
4	NAG	o	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	o	2	4	-	0/6/23/26	0/1/1/1
4	NAG	p	1	4	-	4/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	1	NAG	O5-C1	-2.18	1.40	1.43
4	b	1	NAG	O5-C1	-2.15	1.40	1.43
4	m	1	NAG	O5-C1	-2.15	1.40	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	3	BMA	C1-O5-C5	3.75	117.22	112.19
5	g	3	BMA	C1-O5-C5	3.73	117.18	112.19
5	J	3	BMA	C1-O5-C5	3.72	117.18	112.19
6	n	5	MAN	C1-O5-C5	3.45	116.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	5	MAN	C1-O5-C5	3.44	116.80	112.19
6	c	5	MAN	C1-O5-C5	3.43	116.79	112.19
5	W	4	MAN	C1-O5-C5	3.38	116.72	112.19
5	K	4	MAN	C1-O5-C5	3.34	116.66	112.19
5	h	4	MAN	C1-O5-C5	3.33	116.65	112.19
6	Y	4	MAN	O2-C2-C3	-3.02	103.90	110.15
6	j	4	MAN	O2-C2-C3	-3.01	103.91	110.15
6	N	4	MAN	O2-C2-C3	-3.01	103.92	110.15
5	g	5	MAN	C1-O5-C5	2.97	116.17	112.19
5	V	5	MAN	C1-O5-C5	2.95	116.14	112.19
5	J	5	MAN	C1-O5-C5	2.92	116.09	112.19
6	j	4	MAN	C1-O5-C5	2.63	115.70	112.19
6	Y	4	MAN	C1-O5-C5	2.61	115.68	112.19
6	N	4	MAN	C1-O5-C5	2.61	115.68	112.19
5	h	5	MAN	C1-O5-C5	2.52	115.56	112.19
5	W	5	MAN	C1-O5-C5	2.51	115.55	112.19
5	h	3	BMA	C1-O5-C5	2.51	115.55	112.19
5	K	5	MAN	C1-O5-C5	2.49	115.53	112.19
5	W	3	BMA	C1-O5-C5	2.49	115.53	112.19
5	K	3	BMA	C1-O5-C5	2.46	115.48	112.19
6	c	5	MAN	O2-C2-C3	-2.32	105.34	110.15
6	n	5	MAN	O2-C2-C3	-2.32	105.35	110.15
6	R	5	MAN	O2-C2-C3	-2.31	105.37	110.15
7	a	4	MAN	C1-O5-C5	2.24	115.19	112.19
7	P	4	MAN	C1-O5-C5	2.22	115.16	112.19
5	J	5	MAN	O2-C2-C3	-2.21	105.57	110.15
5	V	5	MAN	O2-C2-C3	-2.21	105.57	110.15
5	g	5	MAN	O2-C2-C3	-2.21	105.57	110.15
7	l	4	MAN	C1-O5-C5	2.21	115.15	112.19
5	W	4	MAN	O2-C2-C3	-2.14	105.71	110.15
5	h	4	MAN	O2-C2-C3	-2.13	105.73	110.15
5	K	4	MAN	O2-C2-C3	-2.13	105.74	110.15
5	h	3	BMA	C3-C4-C5	-2.11	106.40	110.23
5	W	3	BMA	C3-C4-C5	-2.10	106.43	110.23
6	c	4	MAN	C1-O5-C5	2.09	114.99	112.19
7	a	4	MAN	O2-C2-C3	-2.08	105.83	110.15
7	l	4	MAN	O2-C2-C3	-2.08	105.84	110.15
7	P	4	MAN	O2-C2-C3	-2.08	105.84	110.15
5	K	3	BMA	C3-C4-C5	-2.08	106.46	110.23
5	K	5	MAN	O2-C2-C3	-2.08	105.85	110.15
5	W	5	MAN	O2-C2-C3	-2.07	105.86	110.15
5	h	5	MAN	O2-C2-C3	-2.07	105.86	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	4	MAN	C1-O5-C5	2.07	114.96	112.19
5	g	4	MAN	O2-C2-C3	-2.06	105.87	110.15
5	V	4	MAN	O2-C2-C3	-2.06	105.89	110.15
5	J	4	MAN	O2-C2-C3	-2.05	105.90	110.15
6	n	4	MAN	C1-O5-C5	2.05	114.93	112.19
6	N	5	MAN	O2-C2-C3	-2.02	105.97	110.15
6	j	5	MAN	O2-C2-C3	-2.02	105.97	110.15
5	K	3	BMA	O2-C2-C3	-2.02	105.97	110.15
6	Y	5	MAN	O2-C2-C3	-2.02	105.97	110.15
5	h	3	BMA	O2-C2-C3	-2.01	105.98	110.15
5	W	3	BMA	O2-C2-C3	-2.01	106.00	110.15

There are no chirality outliers.

All (181) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	1	NAG	C1-C2-N2-C7
4	T	1	NAG	C1-C2-N2-C7
4	d	1	NAG	C1-C2-N2-C7
4	e	1	NAG	C1-C2-N2-C7
4	o	1	NAG	C1-C2-N2-C7
4	p	1	NAG	C1-C2-N2-C7
4	Q	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	k	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	p	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	c	1	NAG	C4-C5-C6-O6
6	n	1	NAG	C4-C5-C6-O6
6	c	3	BMA	O5-C5-C6-O6
6	j	4	MAN	O5-C5-C6-O6
6	n	3	BMA	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	j	3	BMA	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	Y	4	MAN	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	h	3	BMA	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
6	R	5	MAN	O5-C5-C6-O6
6	c	4	MAN	O5-C5-C6-O6
6	n	4	MAN	O5-C5-C6-O6
6	c	5	MAN	O5-C5-C6-O6
4	k	2	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
6	n	5	MAN	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	p	1	NAG	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	j	3	BMA	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	N	4	MAN	C4-C5-C6-O6
6	j	4	MAN	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
6	R	4	MAN	C4-C5-C6-O6
6	Y	4	MAN	C4-C5-C6-O6
6	c	4	MAN	C4-C5-C6-O6
6	n	4	MAN	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
4	p	2	NAG	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	h	3	BMA	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
6	n	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
5	V	5	MAN	O5-C5-C6-O6
7	a	4	MAN	O5-C5-C6-O6
7	l	4	MAN	O5-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
5	h	5	MAN	O5-C5-C6-O6
7	P	4	MAN	O5-C5-C6-O6
5	g	5	MAN	O5-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6
6	j	5	MAN	O5-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	c	3	BMA	C4-C5-C6-O6
6	Y	5	MAN	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	n	3	BMA	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	P	1	NAG	C4-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
5	h	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	d	1	NAG	C3-C2-N2-C7
4	o	1	NAG	C3-C2-N2-C7
4	p	1	NAG	C3-C2-N2-C7
4	O	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
6	n	5	MAN	C4-C5-C6-O6
4	o	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
5	K	4	MAN	O5-C5-C6-O6
6	c	5	MAN	C4-C5-C6-O6
6	R	5	MAN	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
6	N	1	NAG	C1-C2-N2-C7
6	Y	1	NAG	C1-C2-N2-C7
6	j	1	NAG	C1-C2-N2-C7
5	W	4	MAN	O5-C5-C6-O6
5	h	4	MAN	O5-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6
5	h	4	MAN	C4-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
7	l	3	BMA	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	a	3	BMA	C4-C5-C6-O6
6	j	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C3-C2-N2-C7
6	Y	1	NAG	C3-C2-N2-C7
6	j	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	f	2	NAG	C4-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
4	m	1	NAG	C4-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
7	l	3	BMA	O5-C5-C6-O6
4	O	1	NAG	C1-C2-N2-C7
4	Z	1	NAG	C1-C2-N2-C7
4	k	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
5	V	1	NAG	C1-C2-N2-C7
5	g	1	NAG	C1-C2-N2-C7
6	R	1	NAG	C1-C2-N2-C7
6	c	1	NAG	C1-C2-N2-C7
6	n	1	NAG	C1-C2-N2-C7
7	a	3	BMA	O5-C5-C6-O6
4	e	1	NAG	C3-C2-N2-C7
5	J	2	NAG	C3-C2-N2-C7
5	V	2	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6

There are no ring outliers.

43 monomers are involved in 59 short contacts:

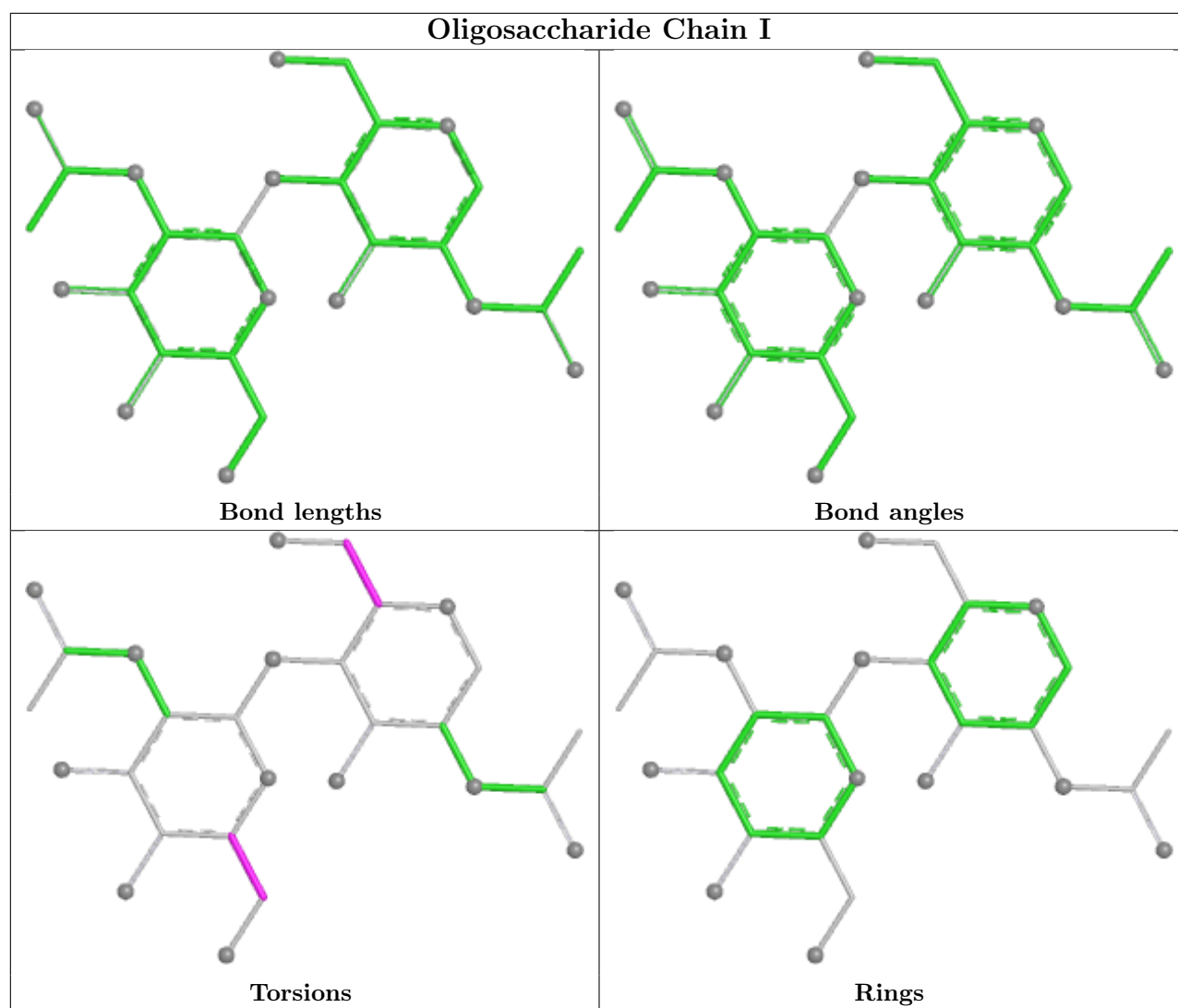
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	l	1	NAG	1	0
5	J	2	NAG	1	0
5	W	4	MAN	2	0
5	J	1	NAG	2	0
6	N	1	NAG	2	0
4	f	1	NAG	1	0
4	k	1	NAG	3	0
4	U	1	NAG	1	0

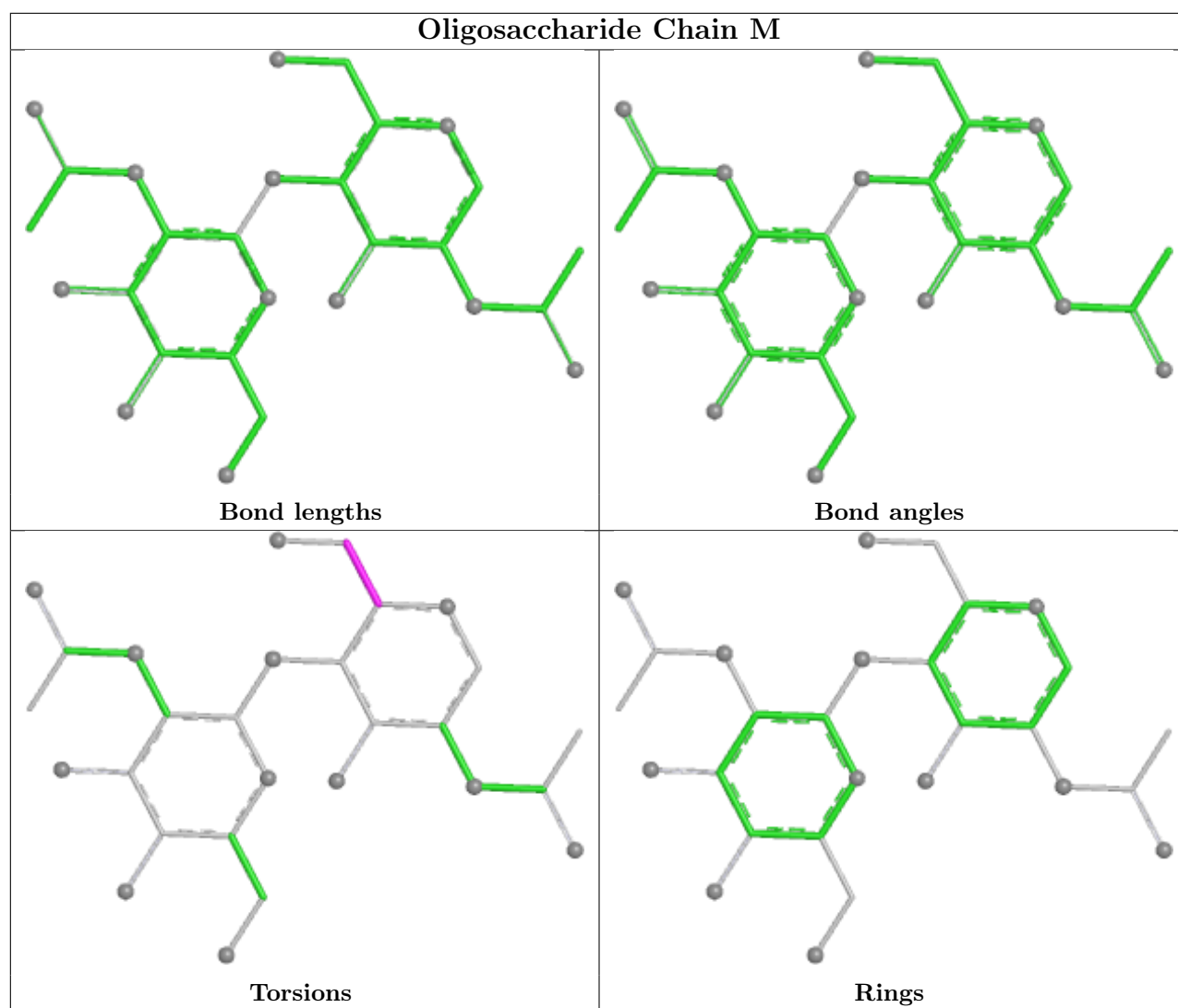
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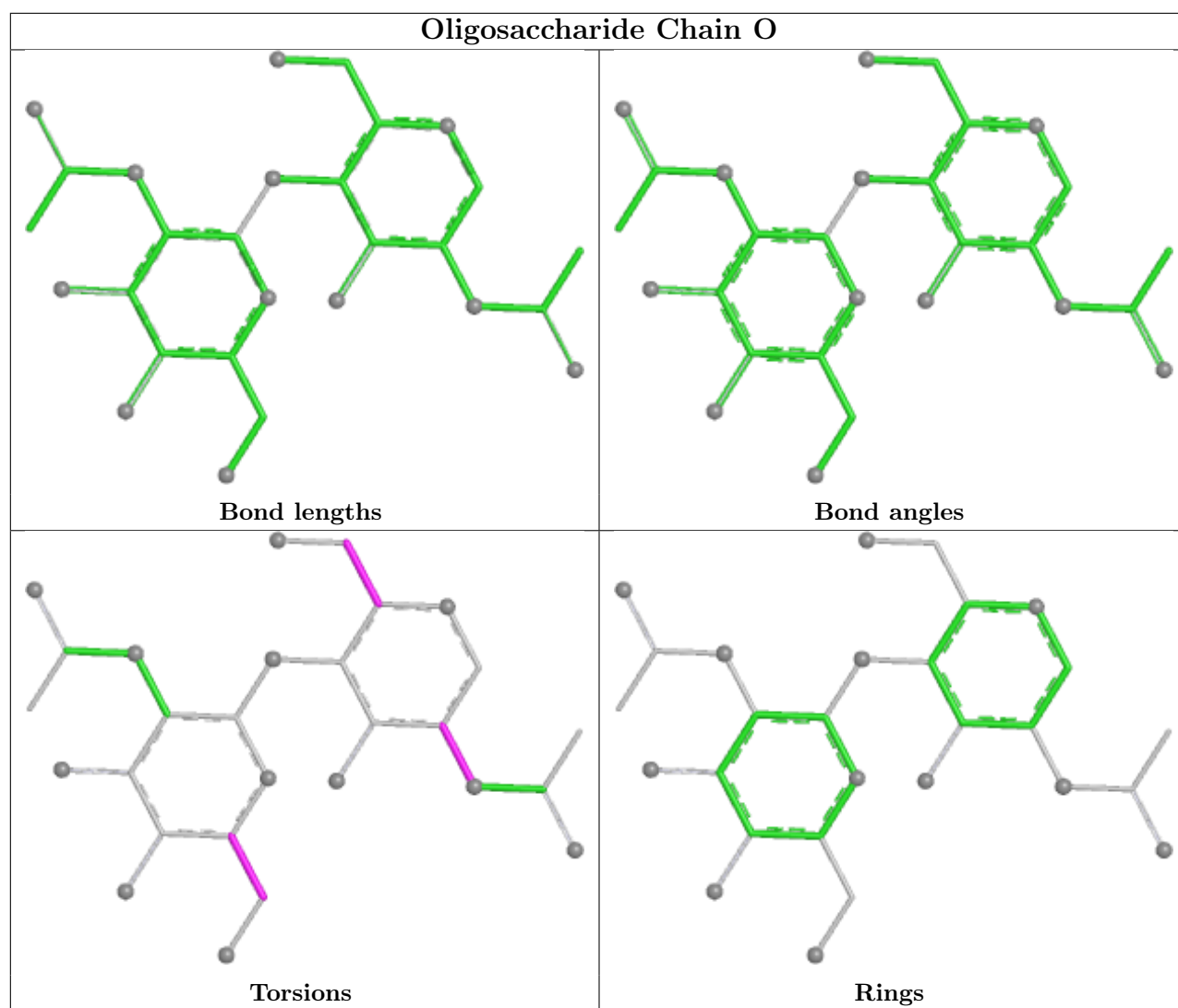
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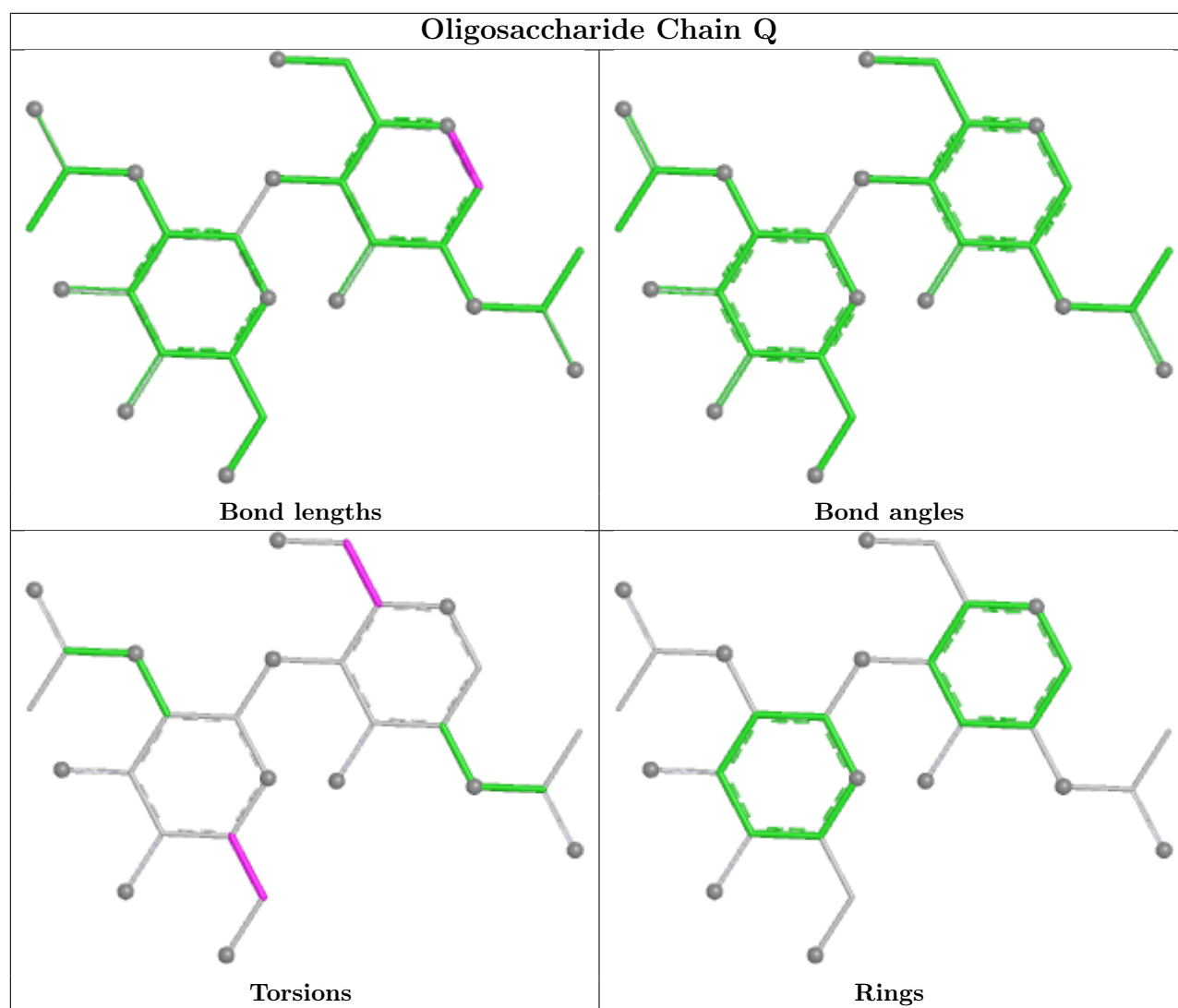
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	p	1	NAG	3	0
4	e	1	NAG	3	0
7	P	1	NAG	1	0
4	O	1	NAG	2	0
4	I	1	NAG	1	0
5	V	2	NAG	2	0
5	W	1	NAG	1	0
6	c	1	NAG	1	0
4	d	1	NAG	2	0
6	Y	3	BMA	1	0
4	p	2	NAG	2	0
4	e	2	NAG	2	0
4	T	1	NAG	2	0
4	S	1	NAG	2	0
4	T	2	NAG	1	0
6	j	1	NAG	2	0
5	h	1	NAG	1	0
6	Y	2	NAG	2	0
6	Y	1	NAG	1	0
4	o	1	NAG	2	0
7	a	1	NAG	1	0
4	Q	1	NAG	1	0
6	j	3	BMA	1	0
5	g	1	NAG	2	0
5	V	1	NAG	2	0
6	j	2	NAG	2	0
6	N	2	NAG	2	0
6	N	3	BMA	1	0
4	Z	1	NAG	3	0
6	n	1	NAG	1	0
5	K	1	NAG	1	0
5	h	4	MAN	2	0
5	g	2	NAG	1	0
6	R	1	NAG	1	0
5	K	4	MAN	2	0

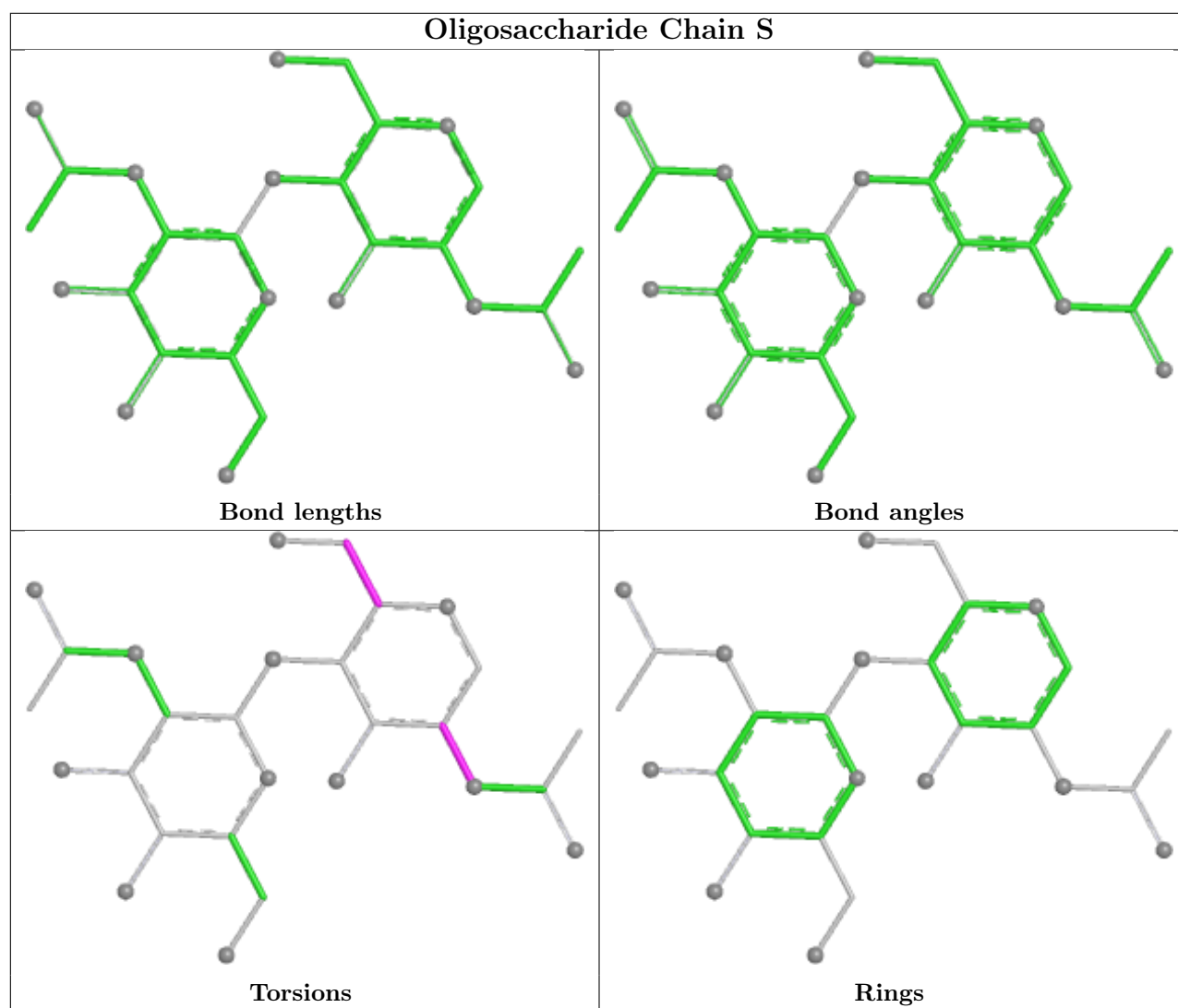
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

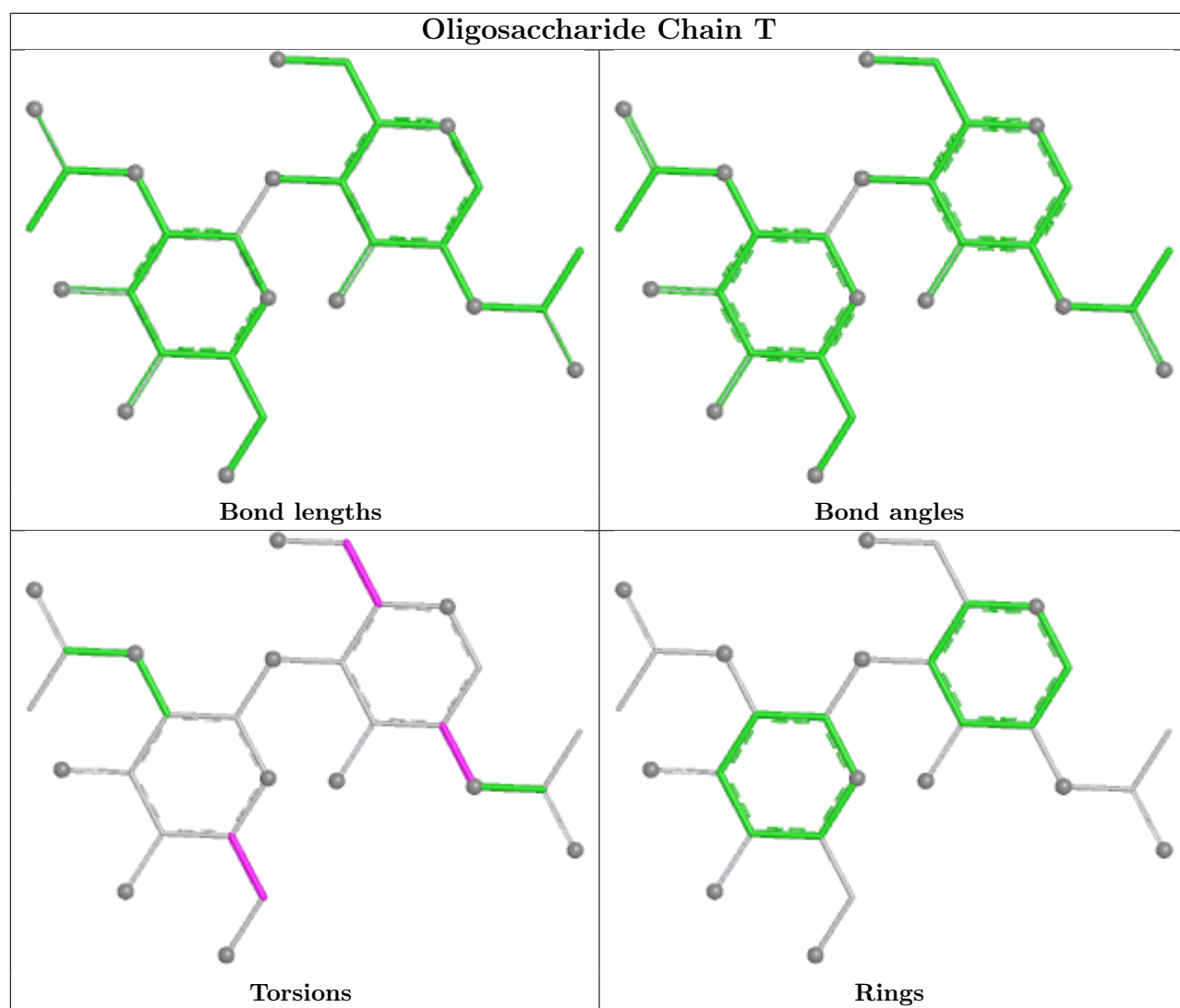


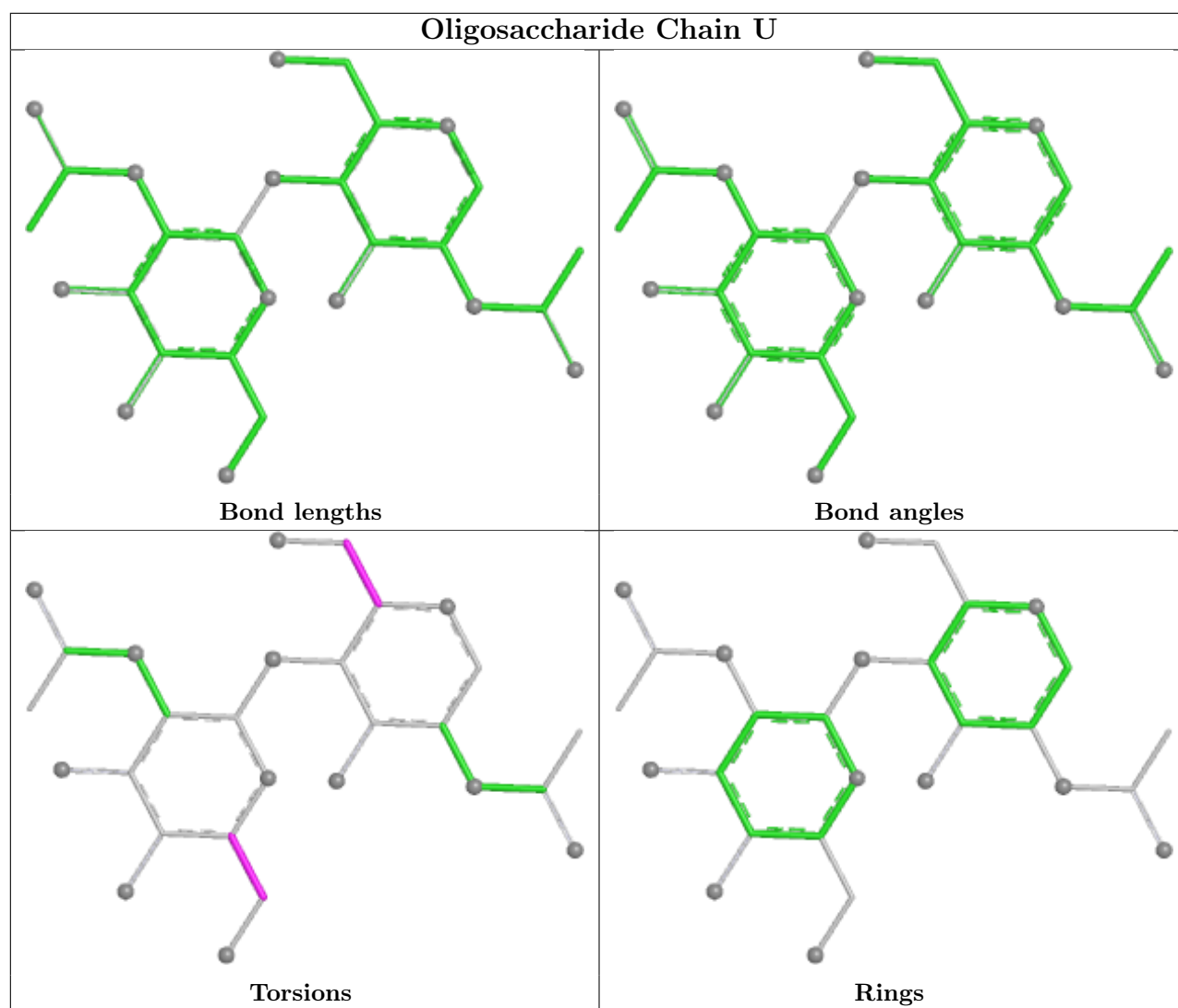


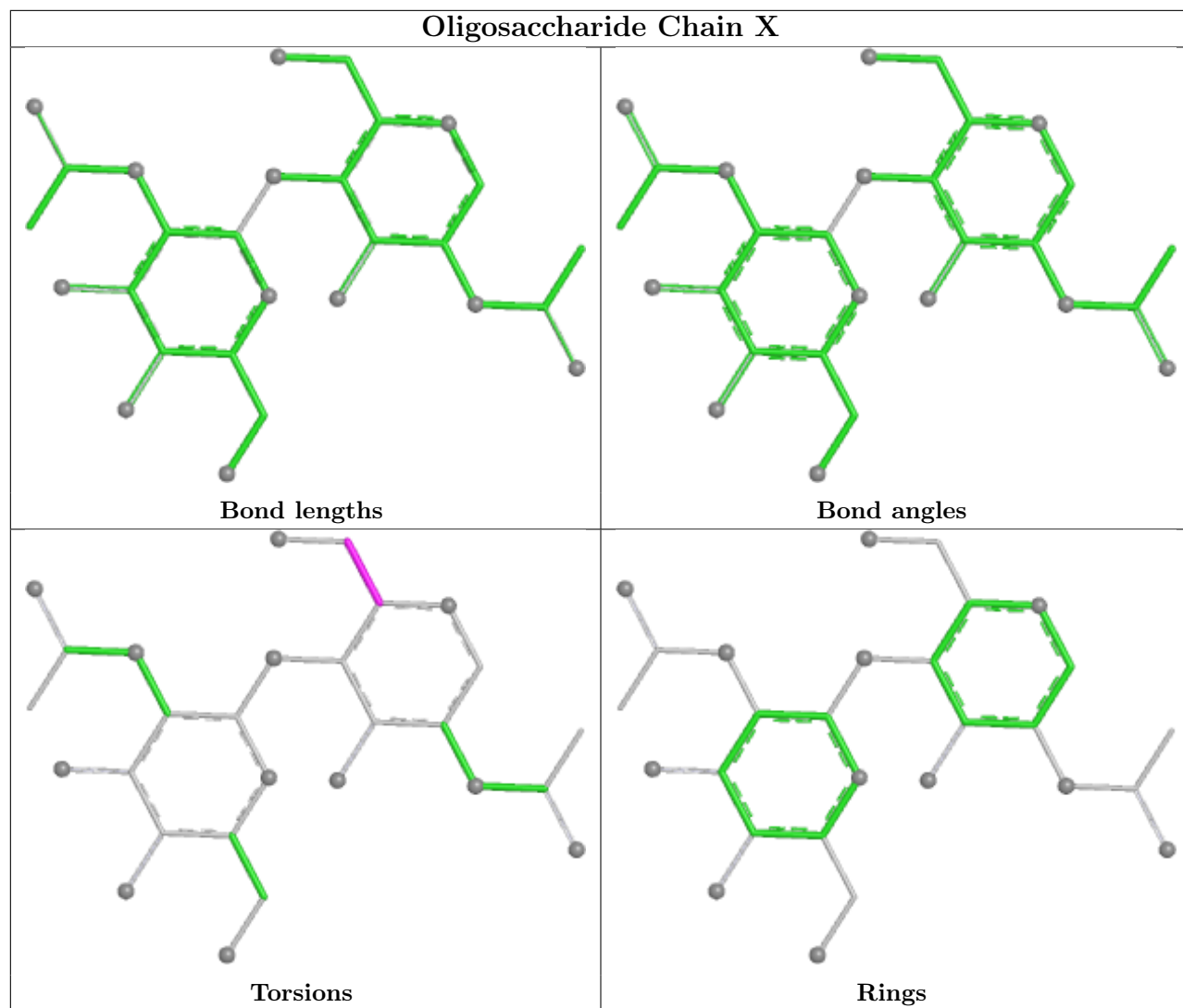


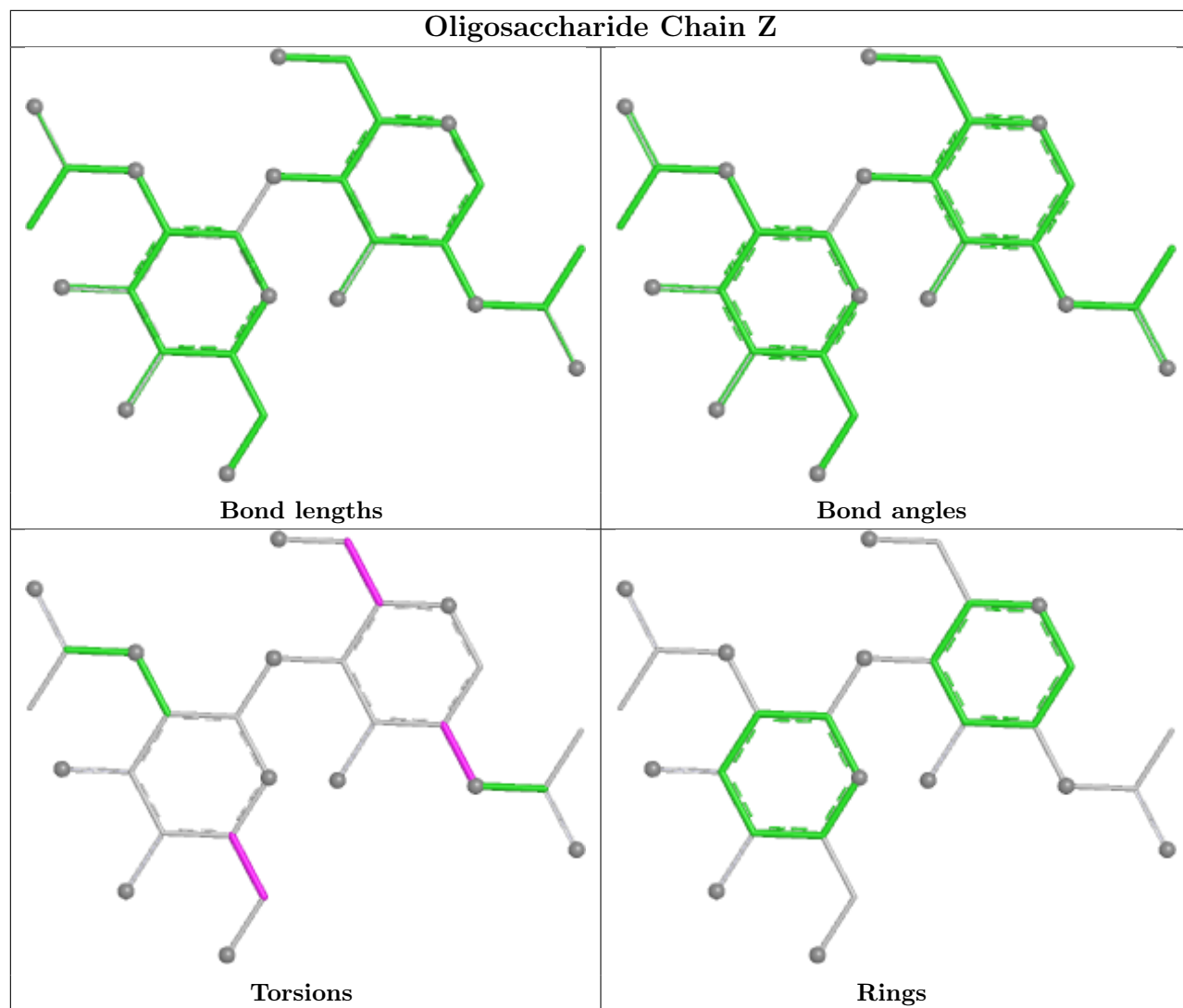


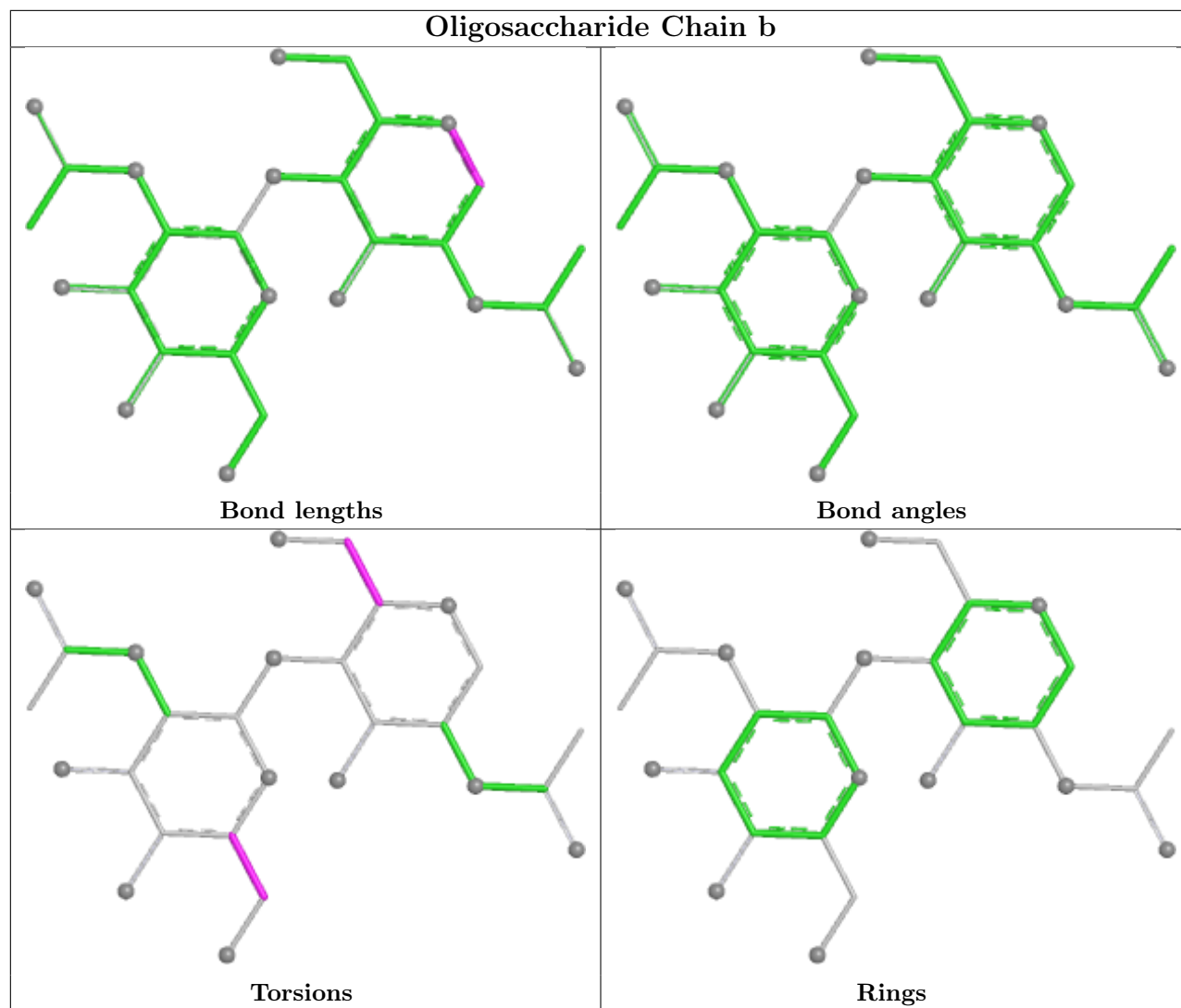


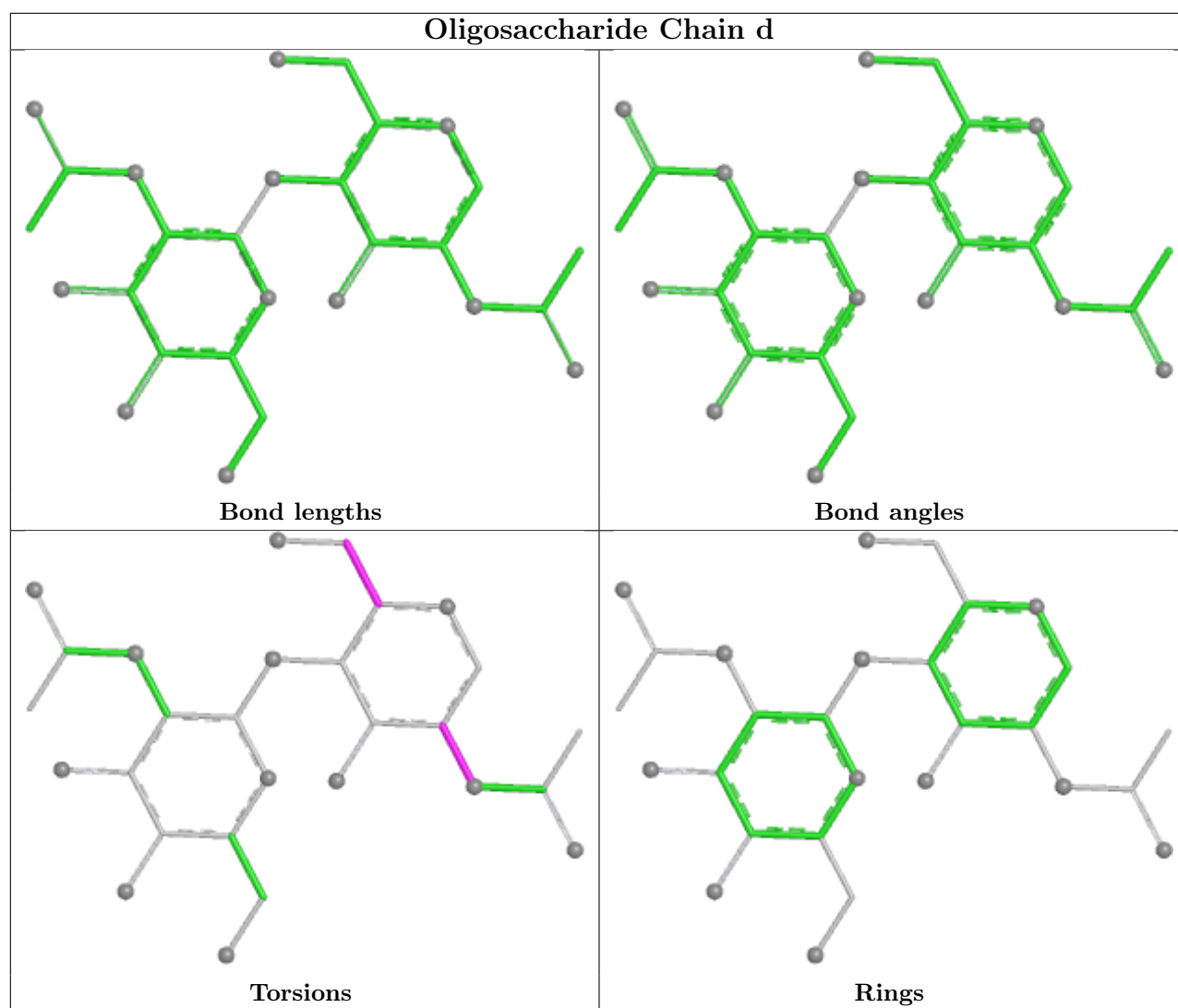


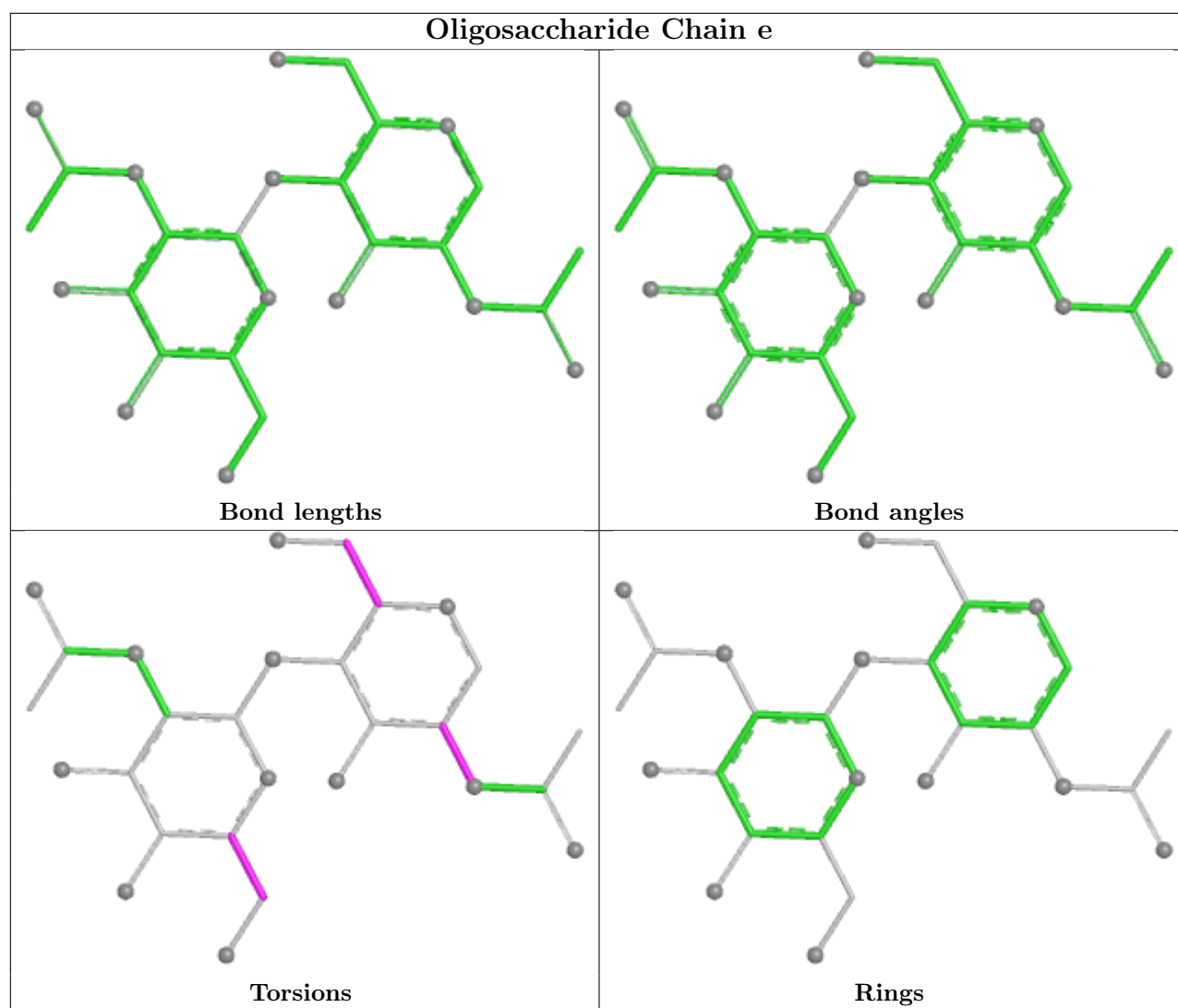


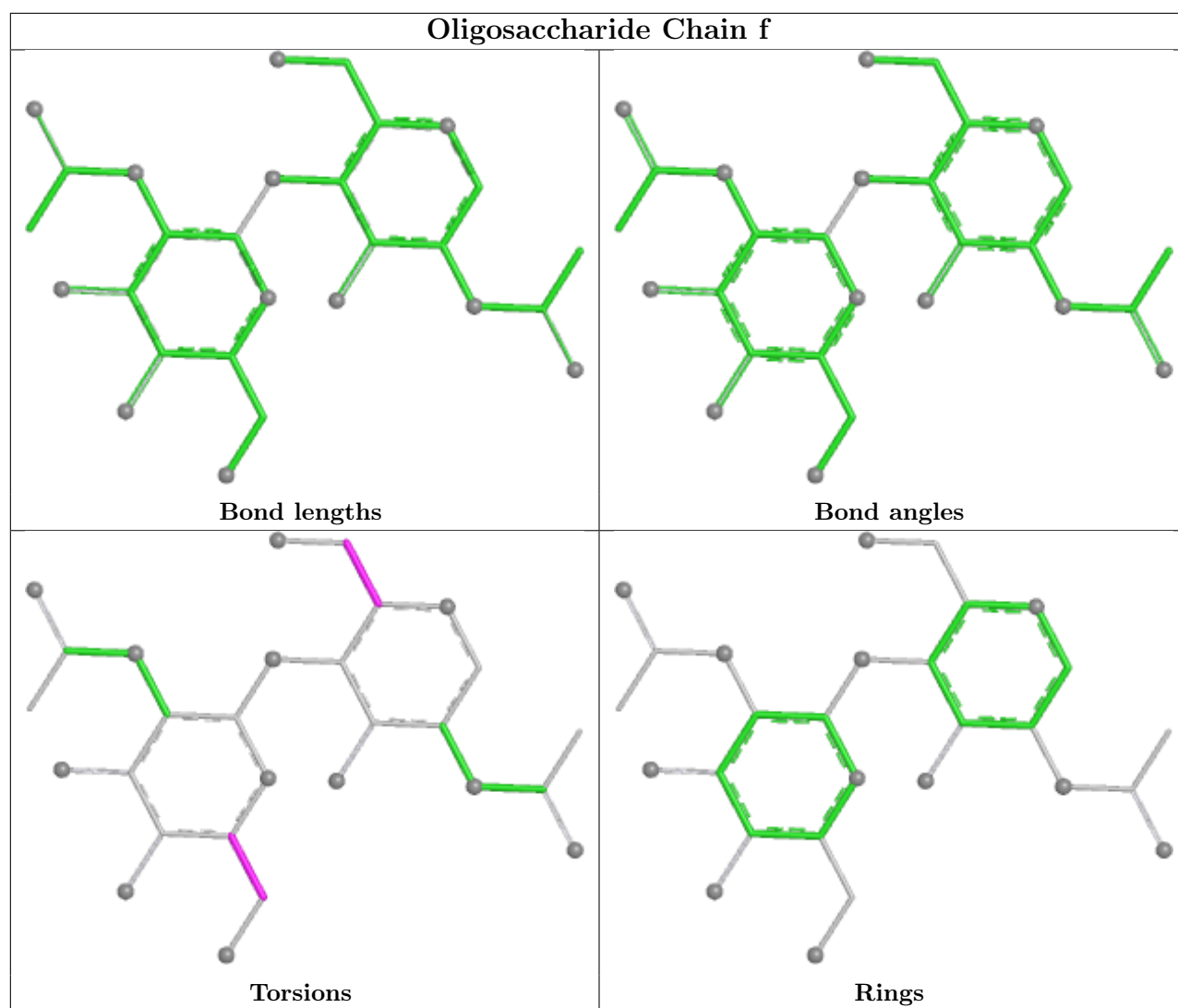


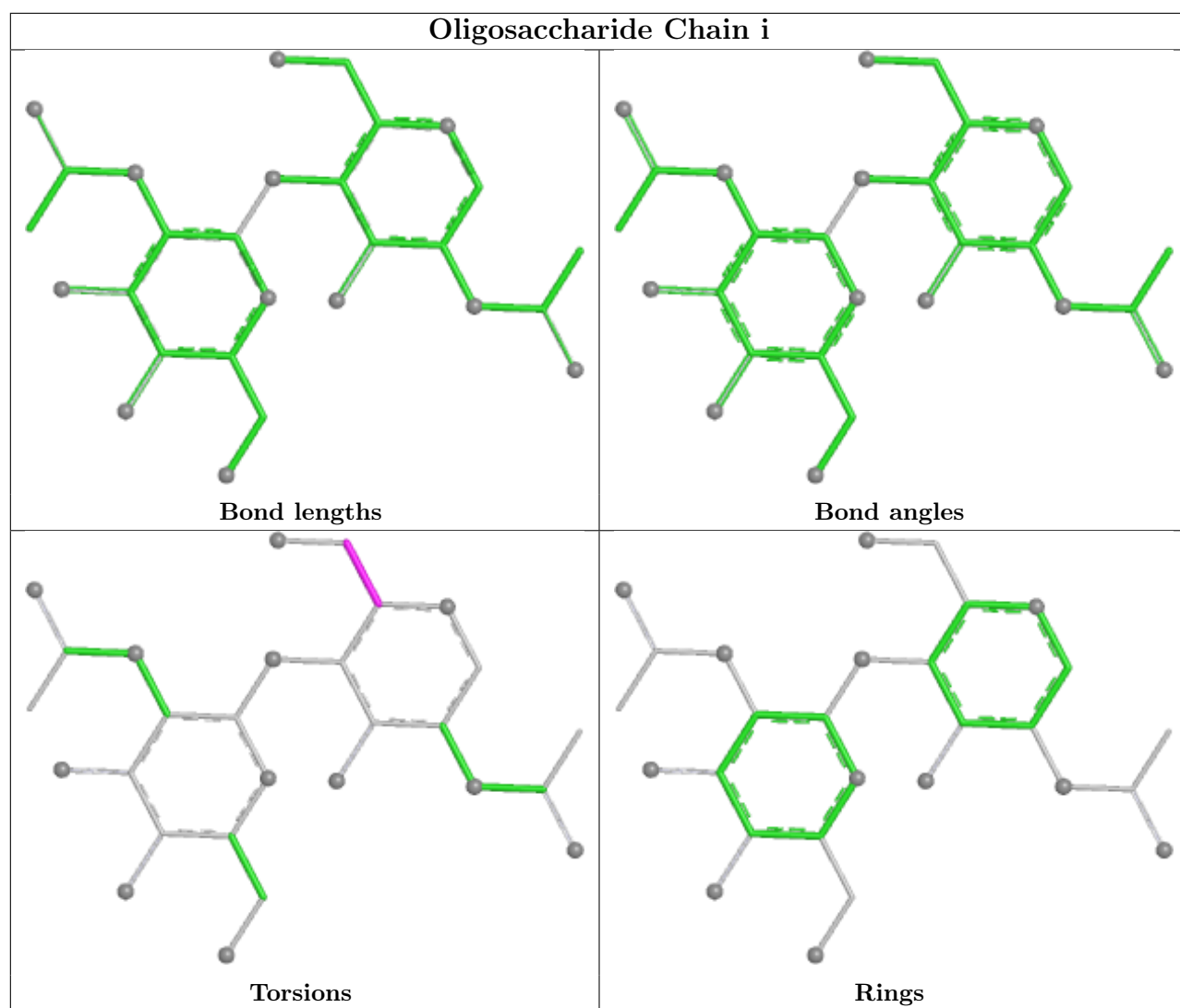


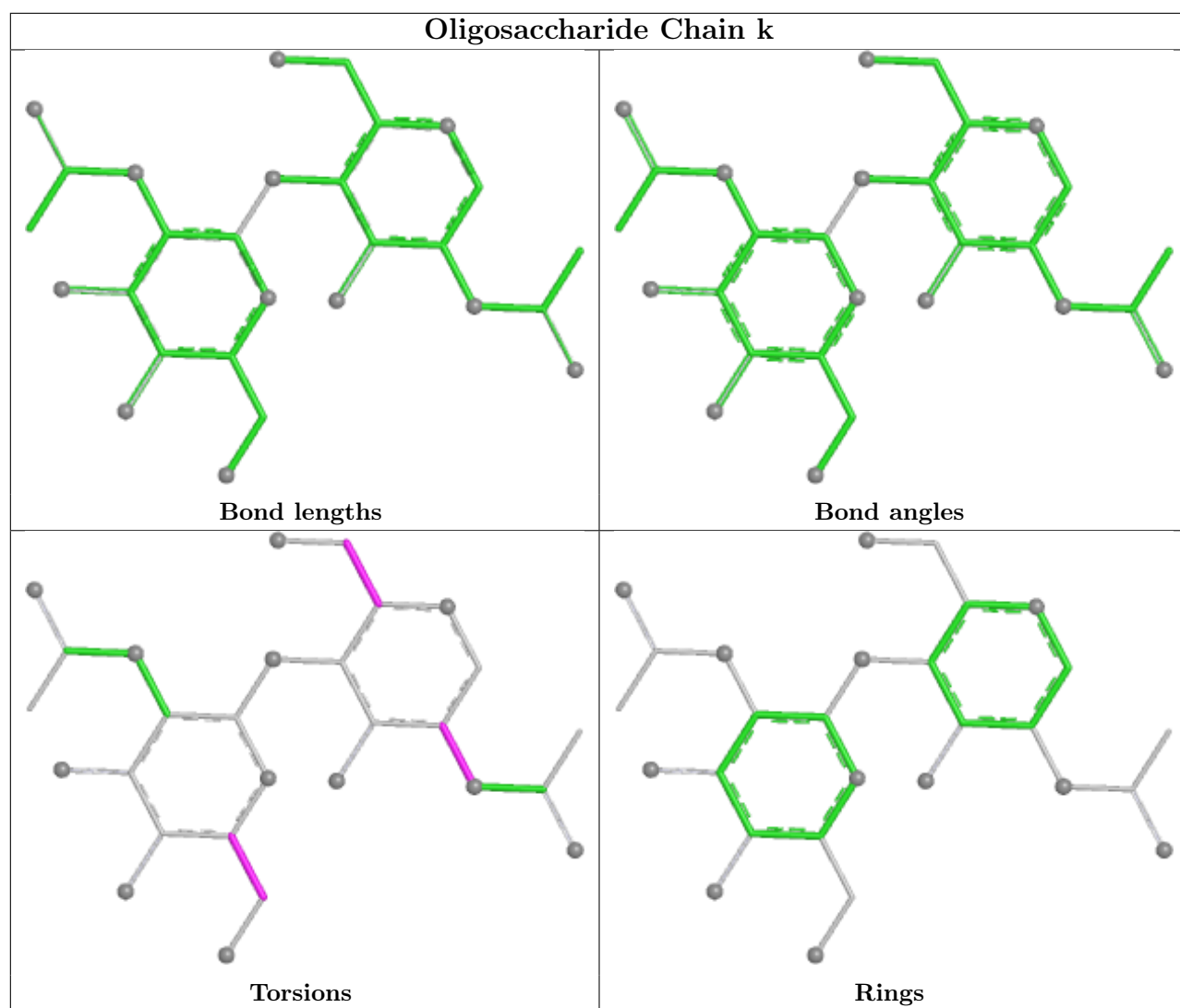


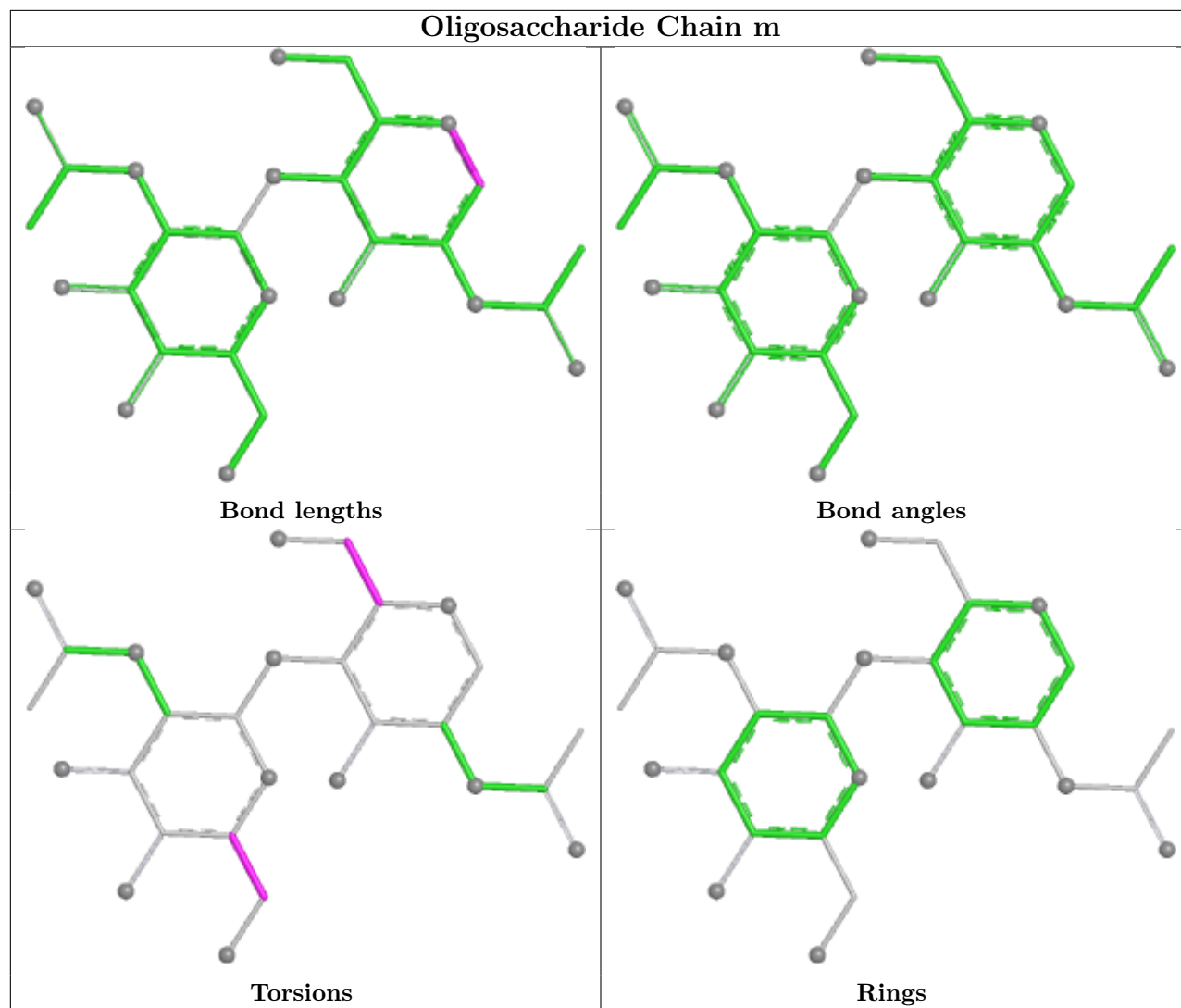


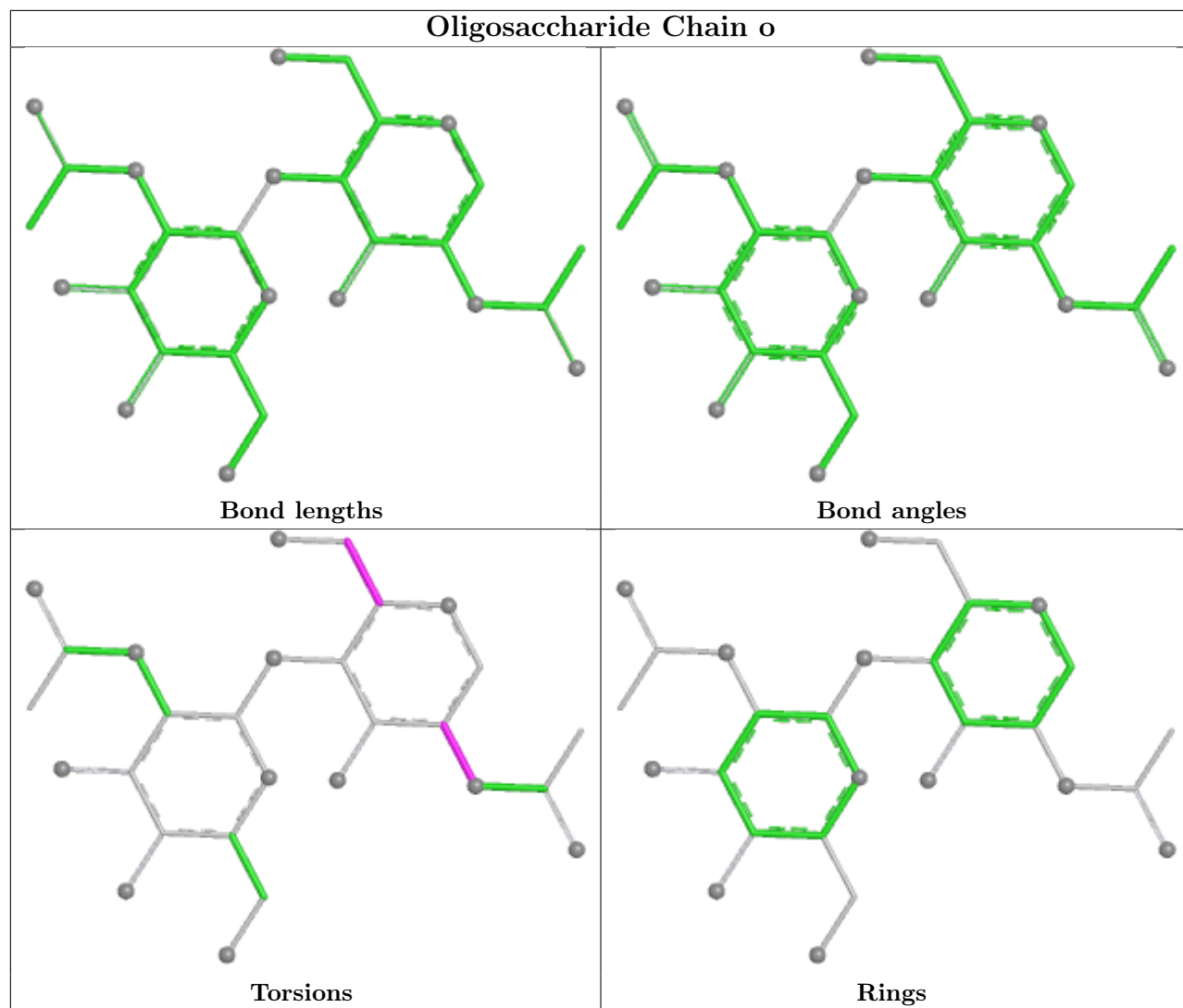


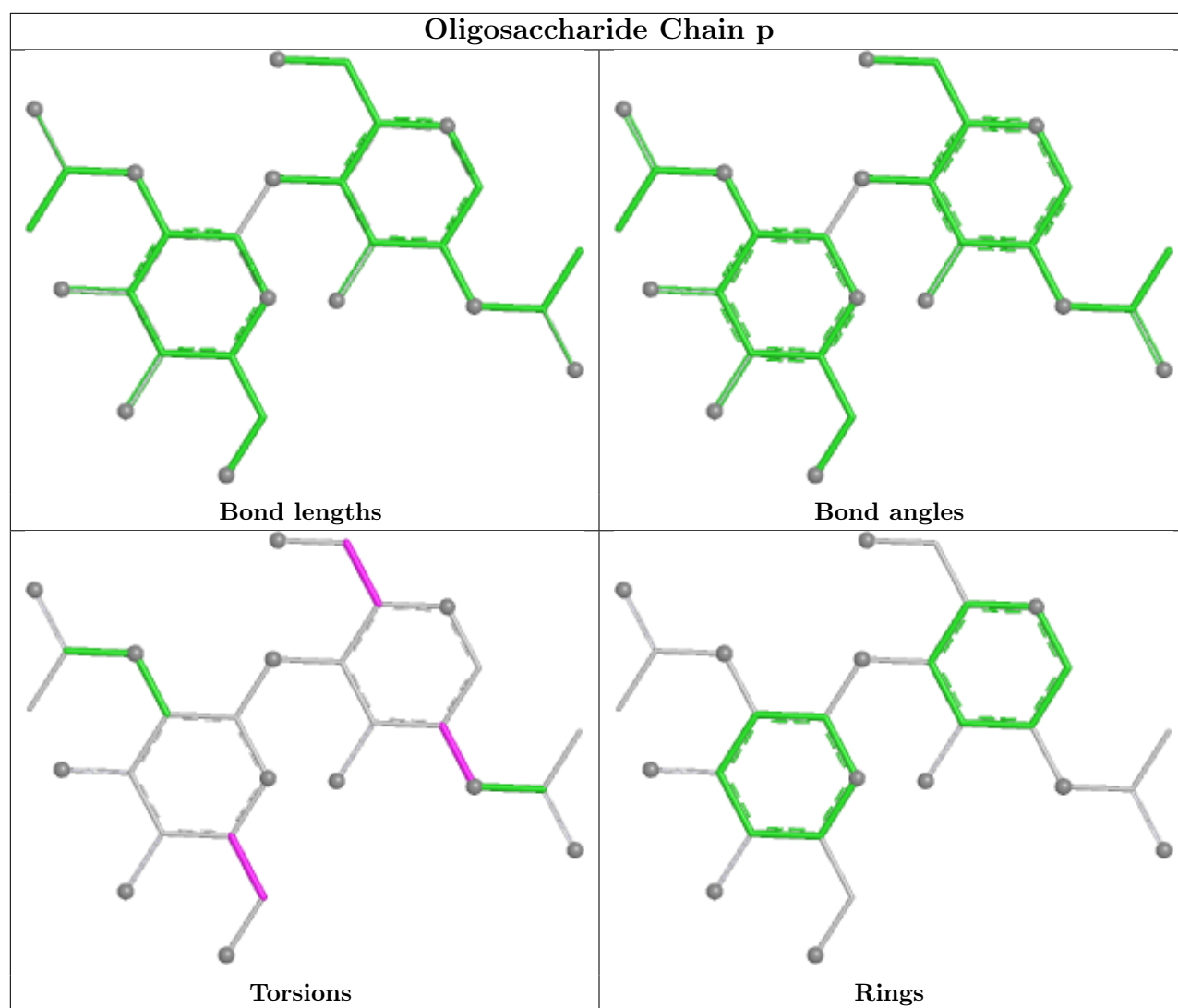


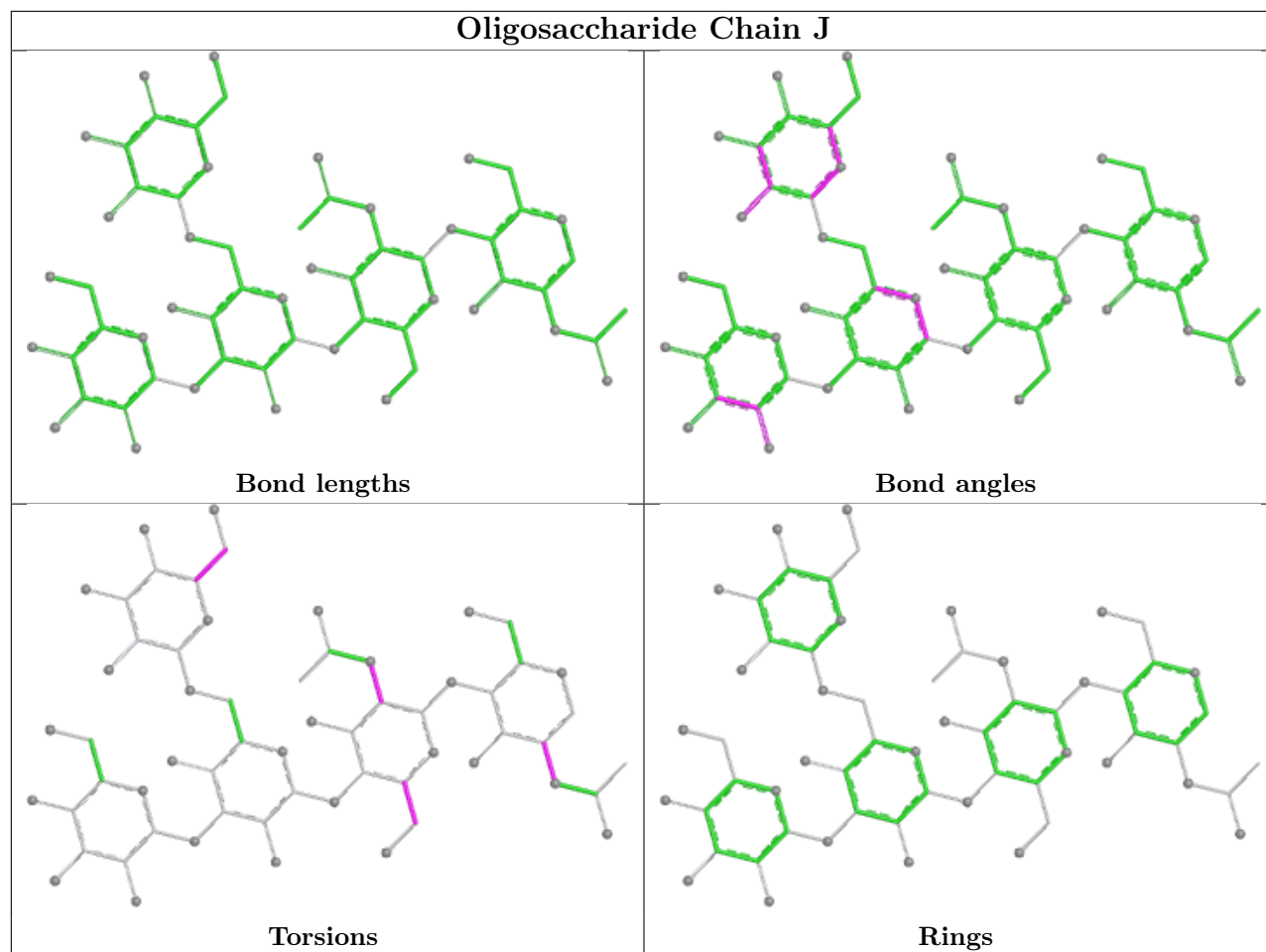


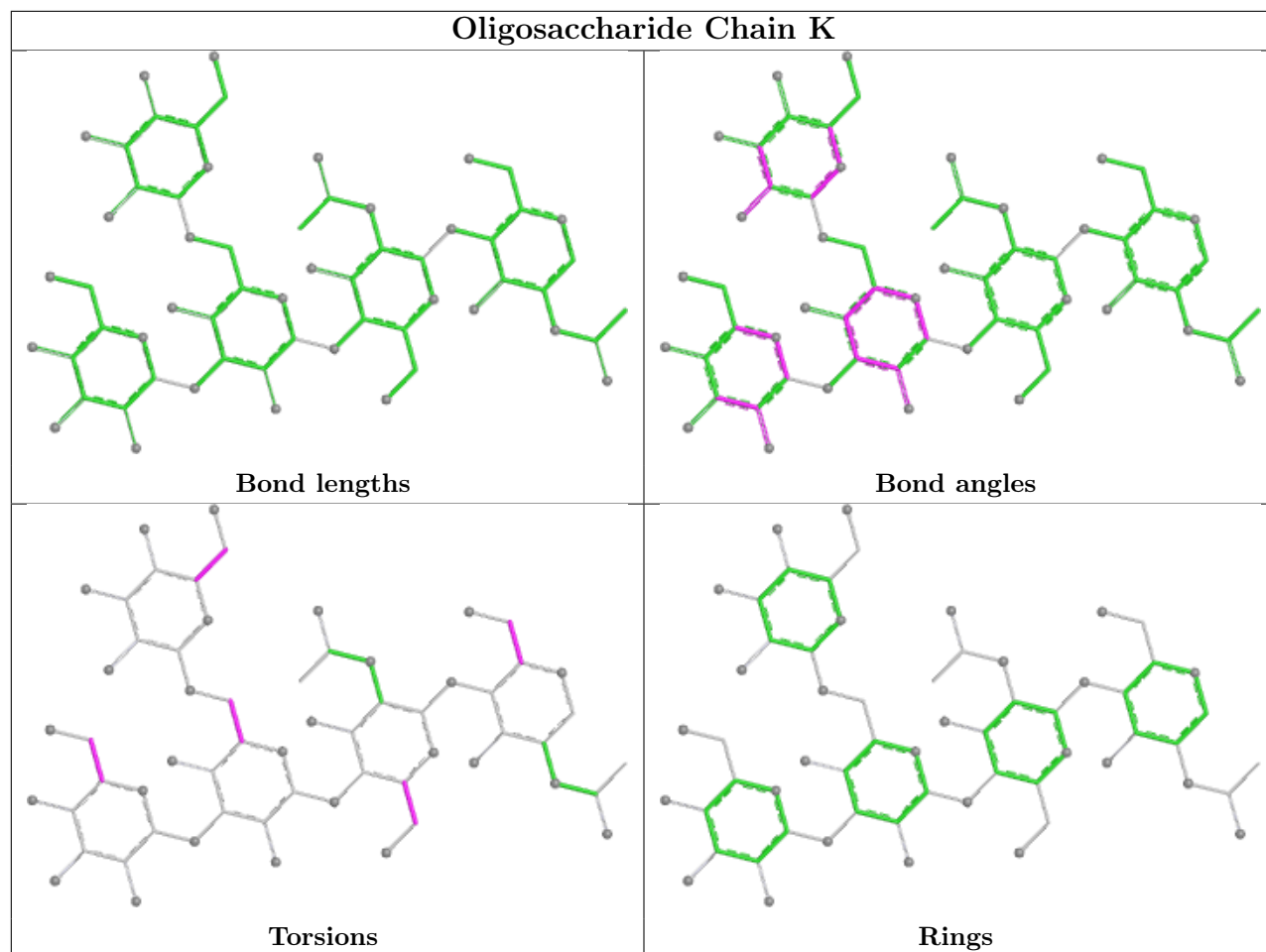


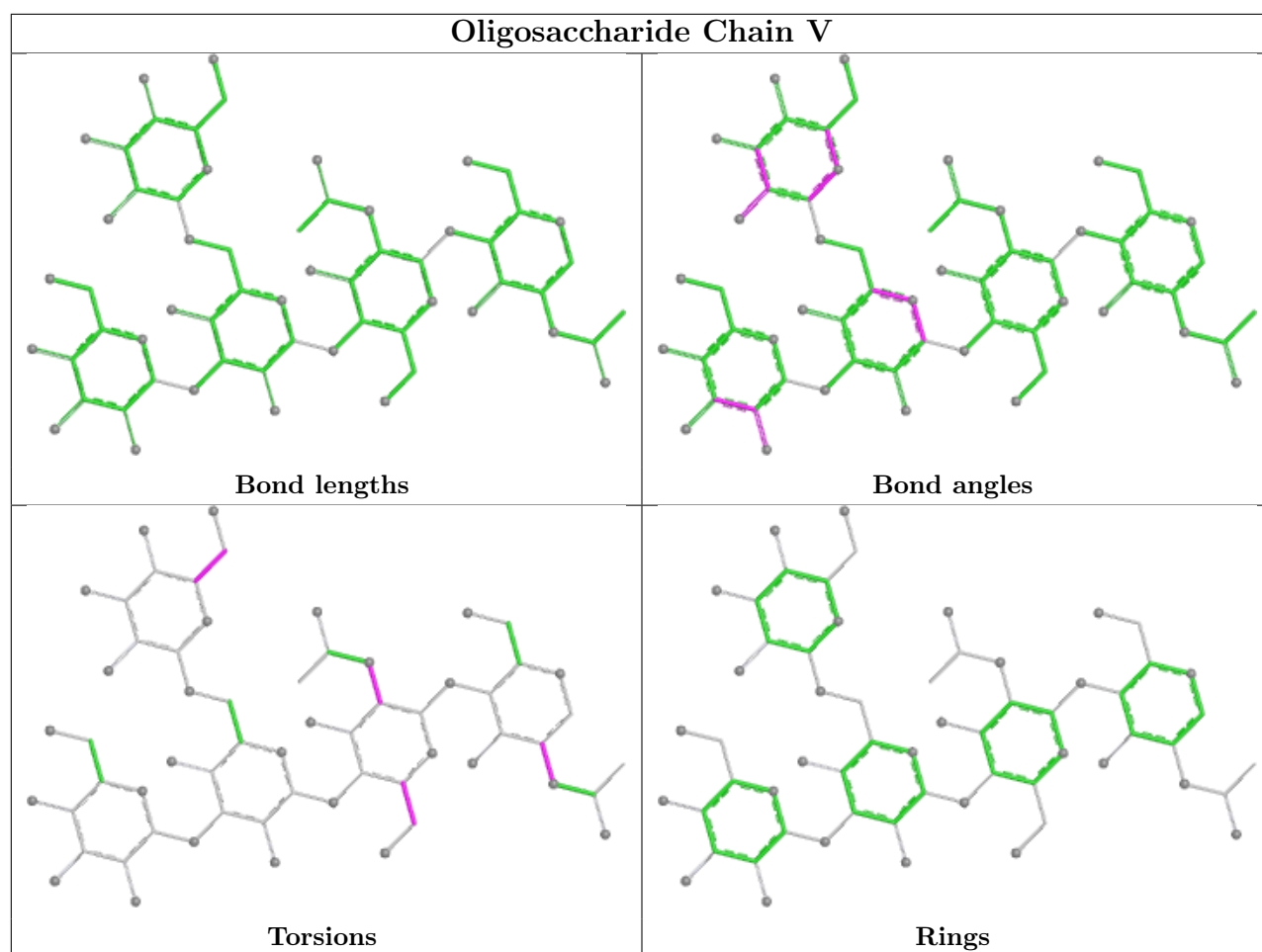


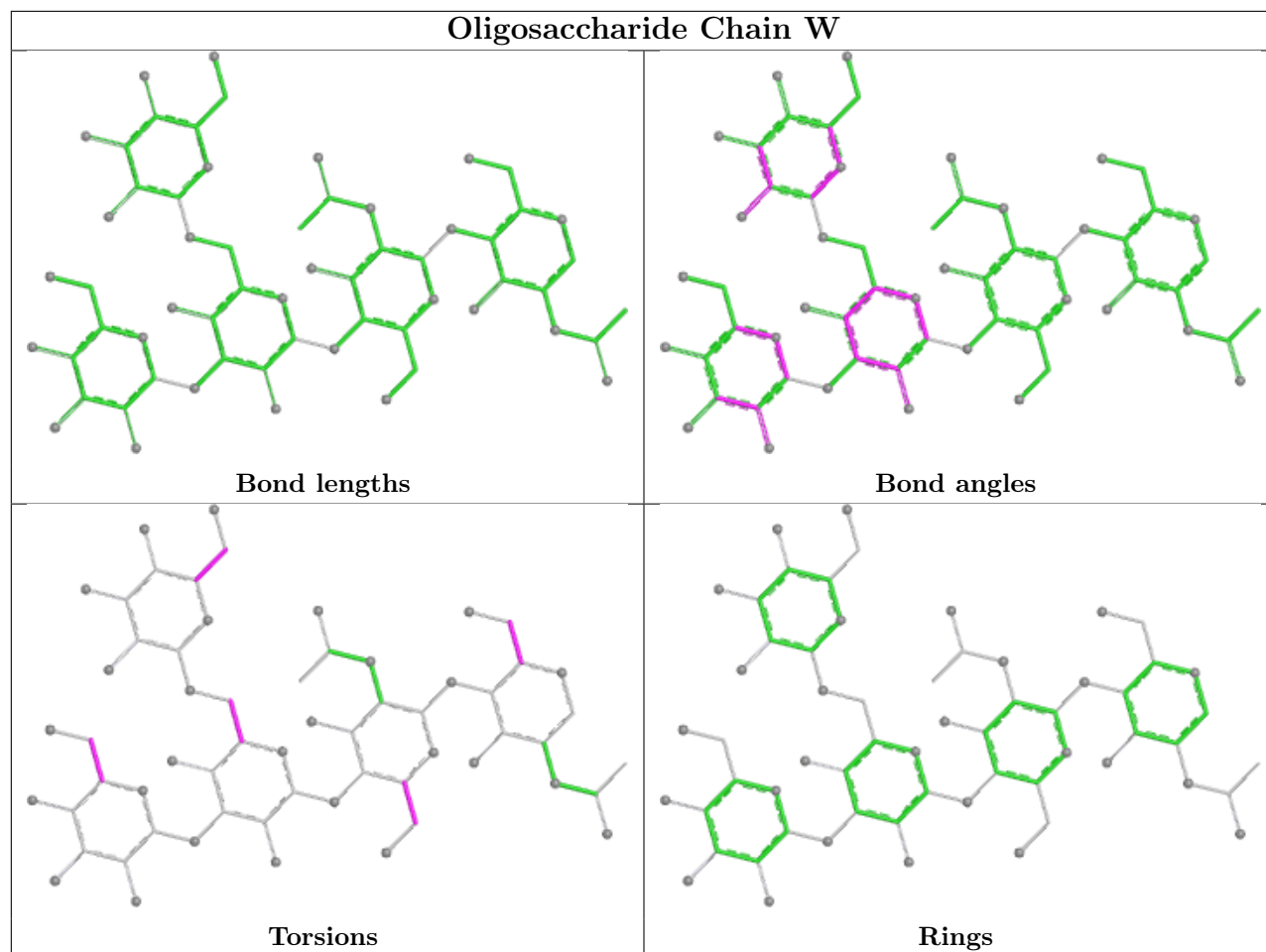


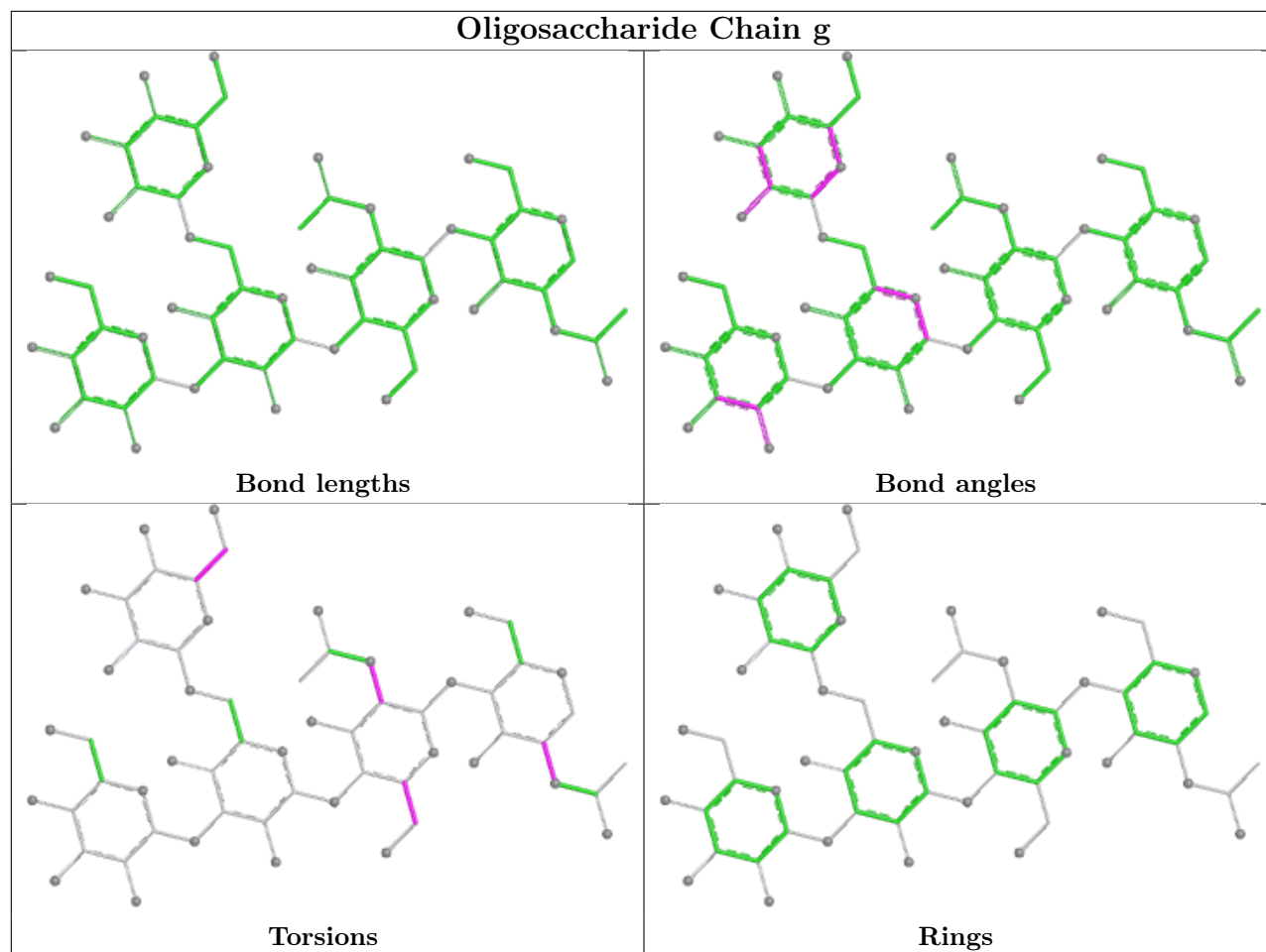


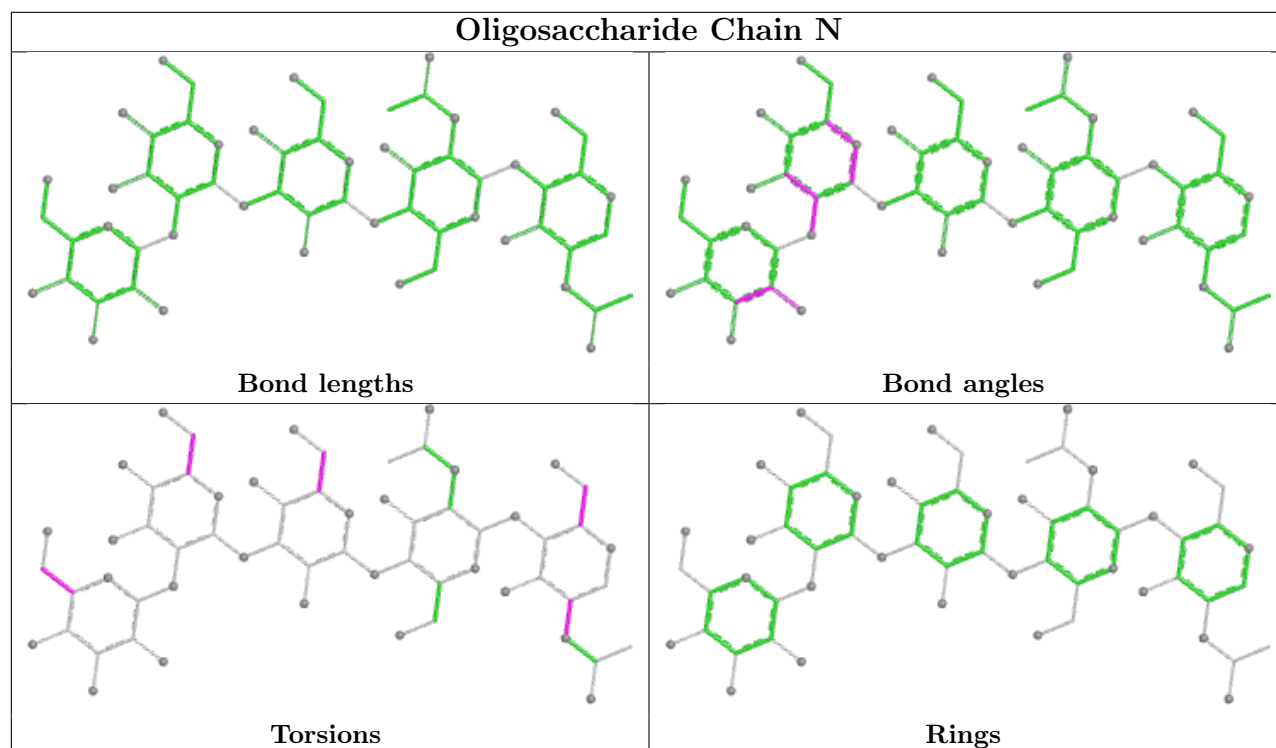
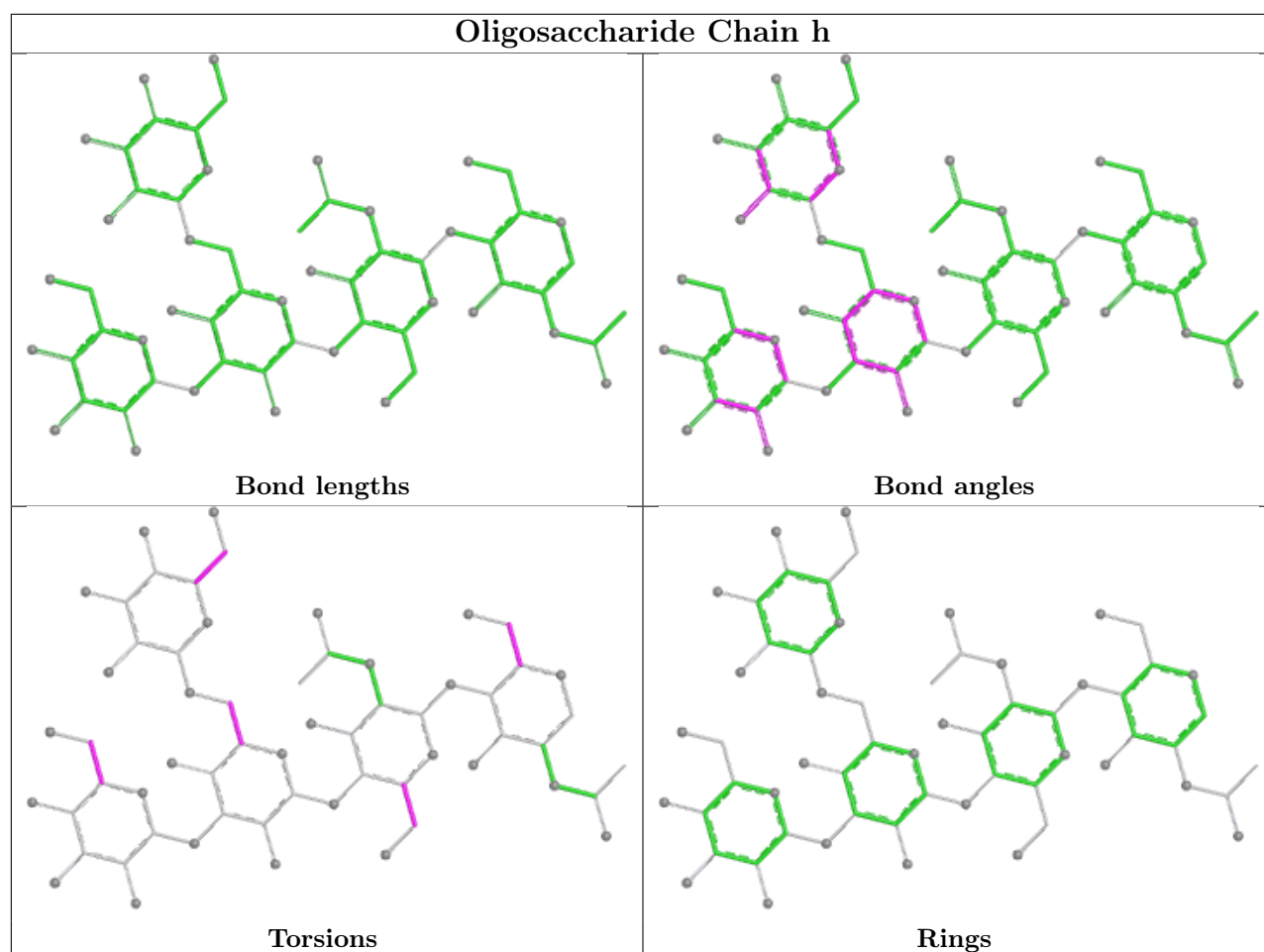


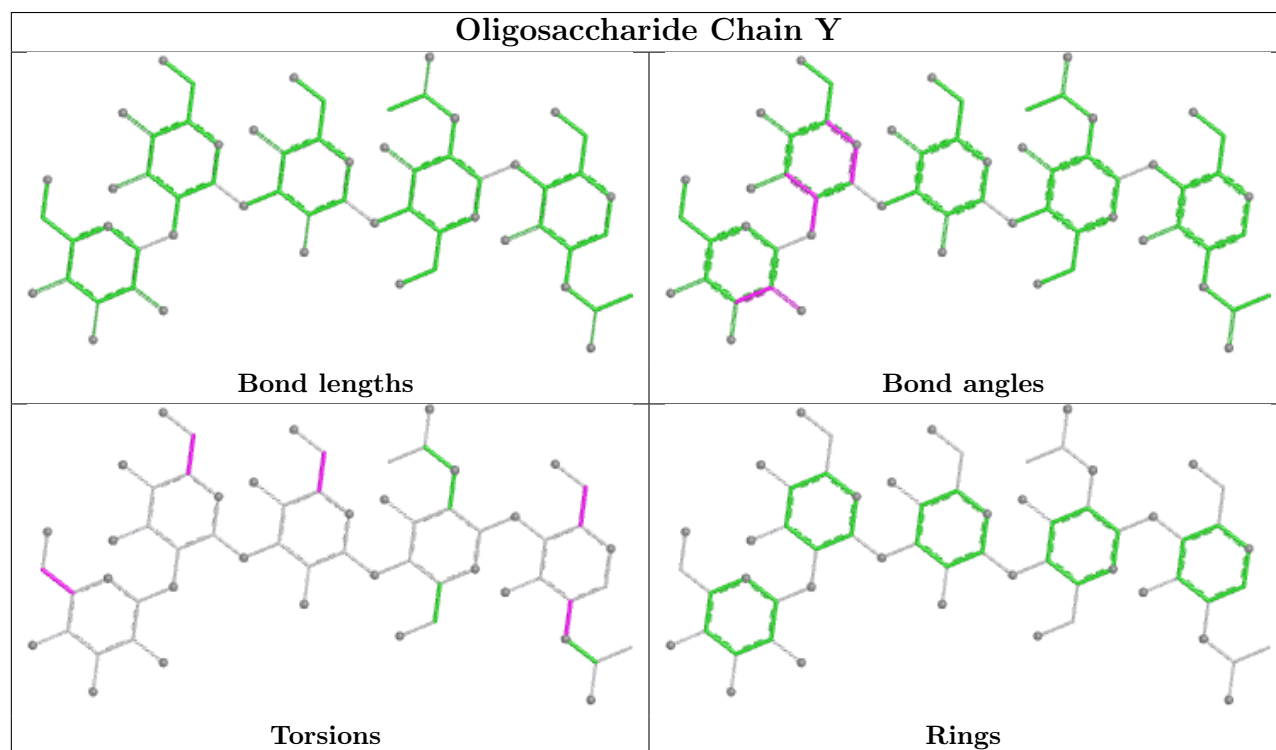
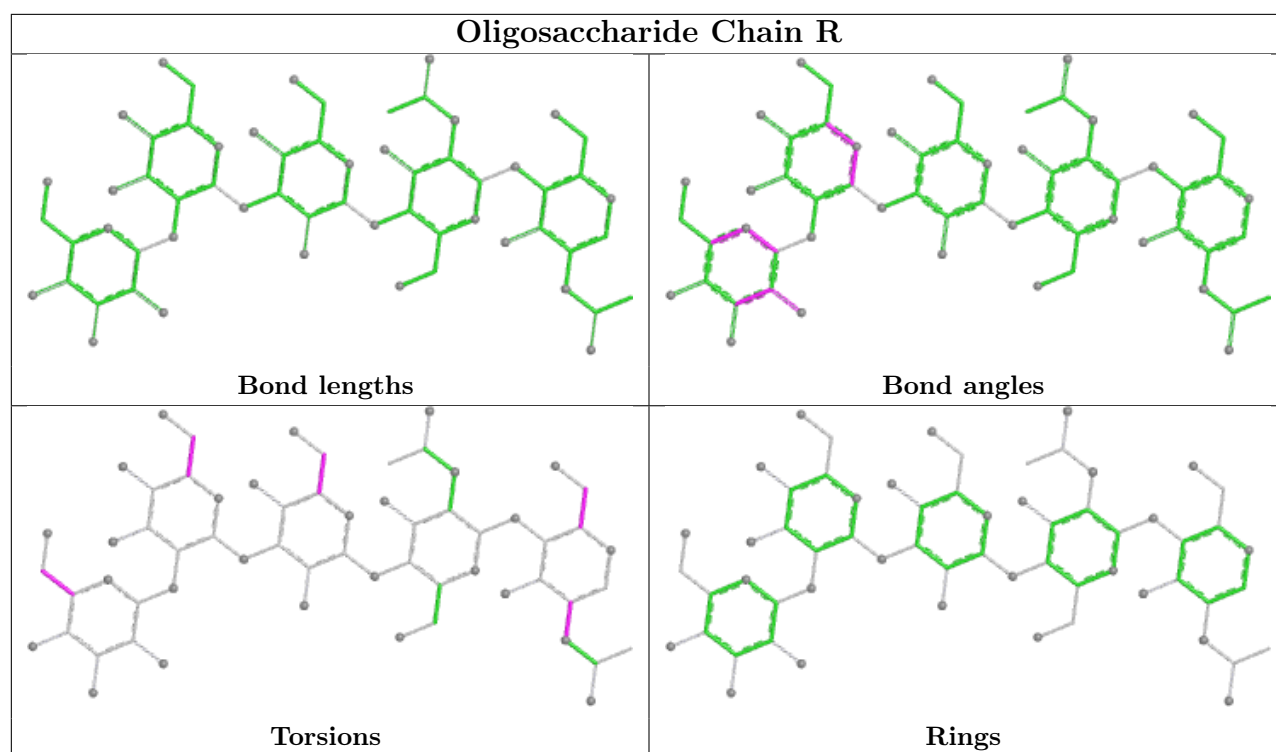


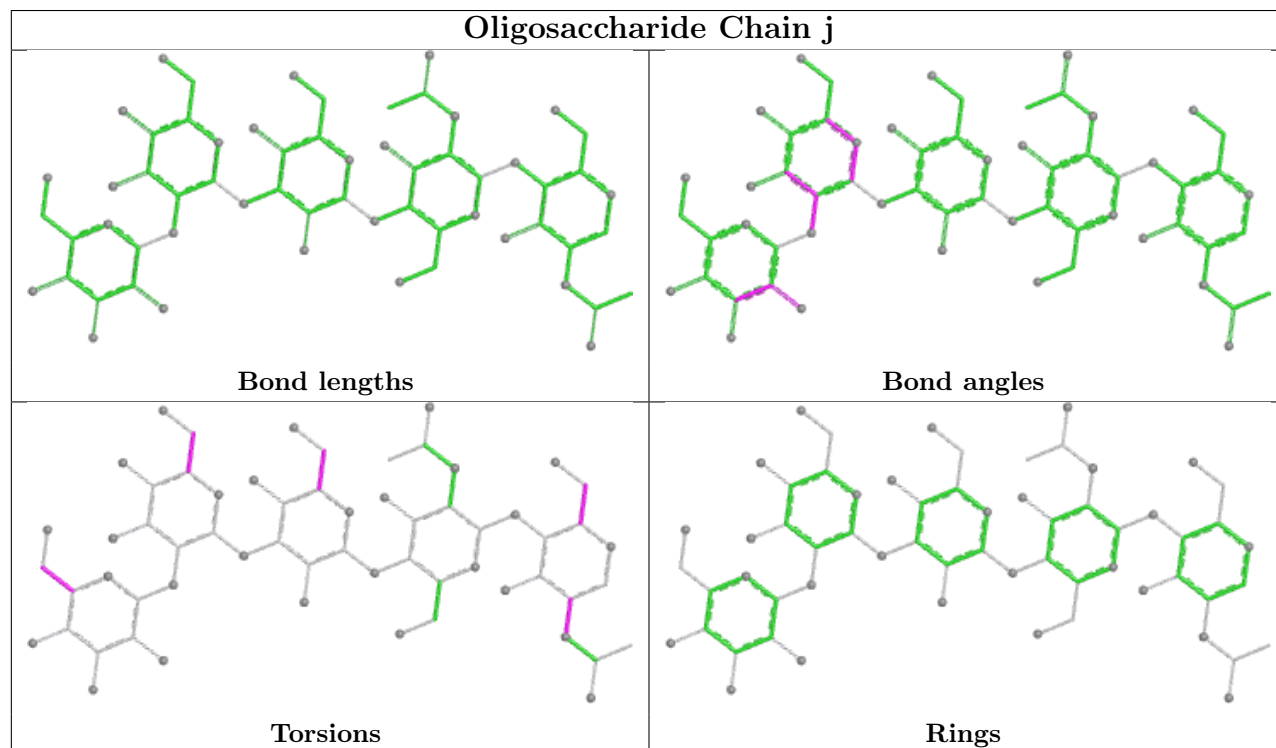
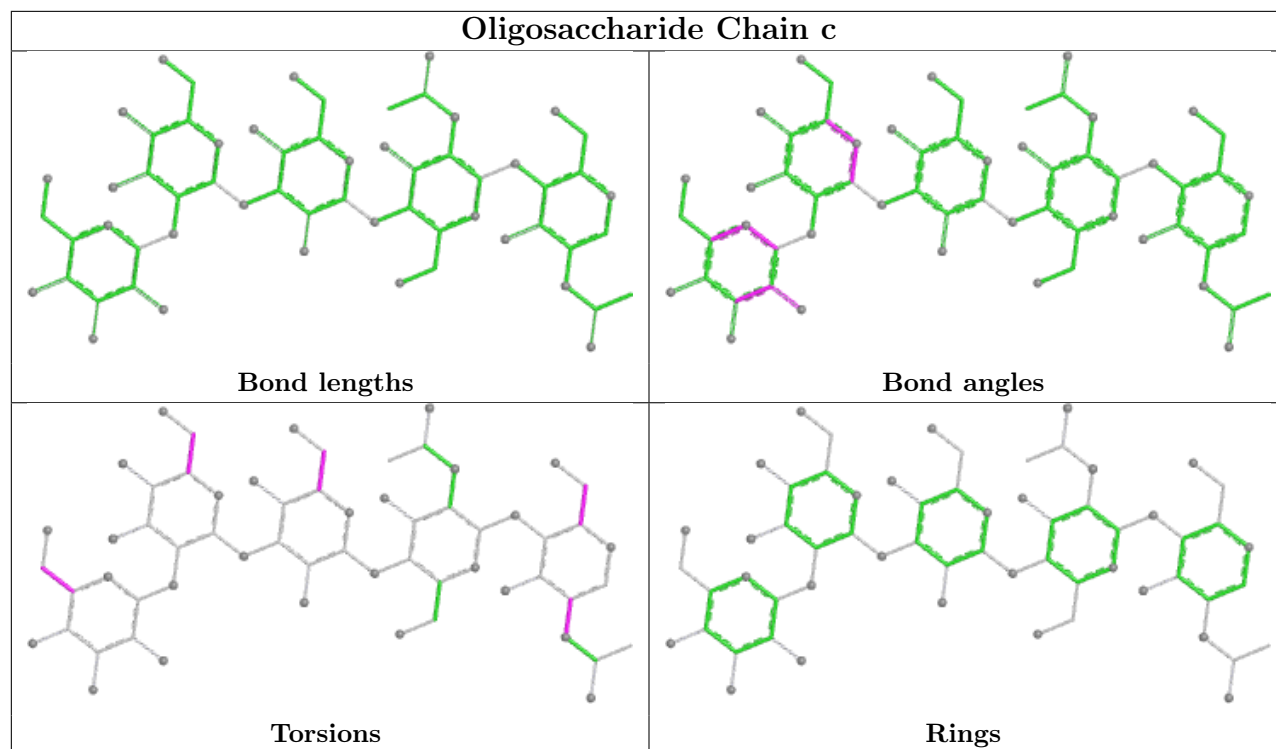


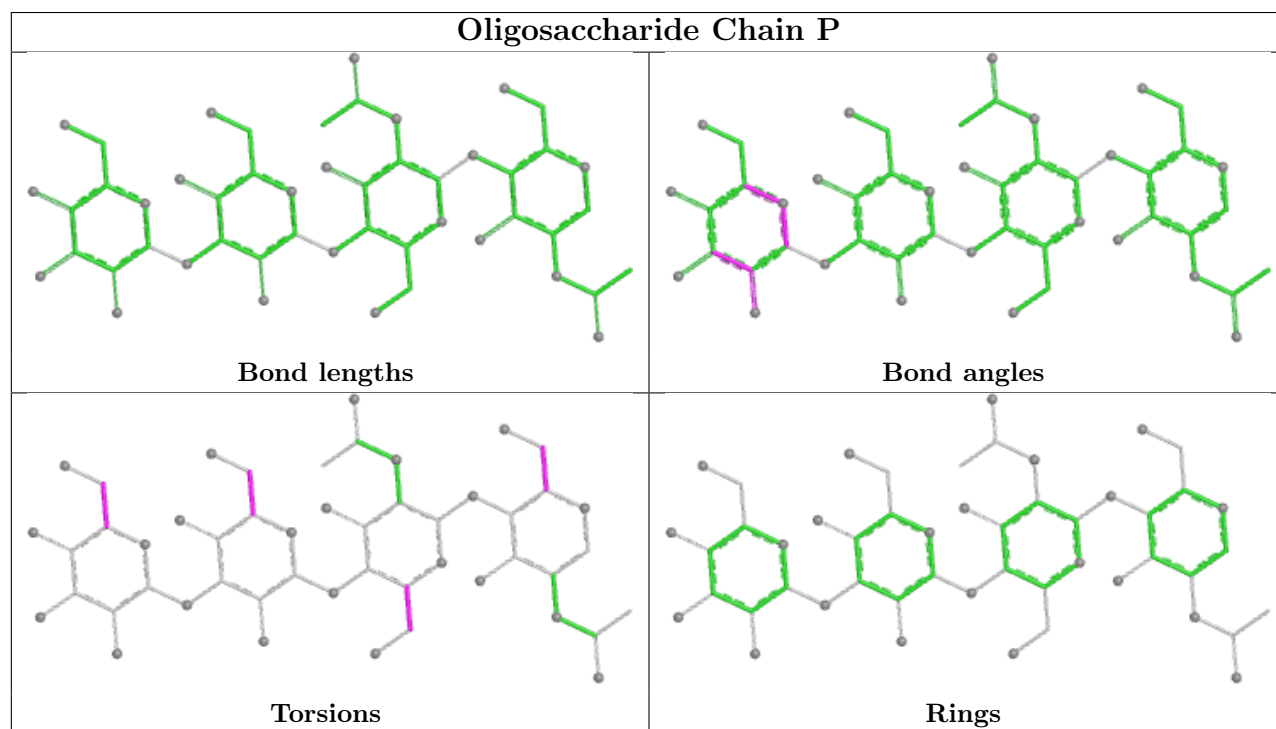
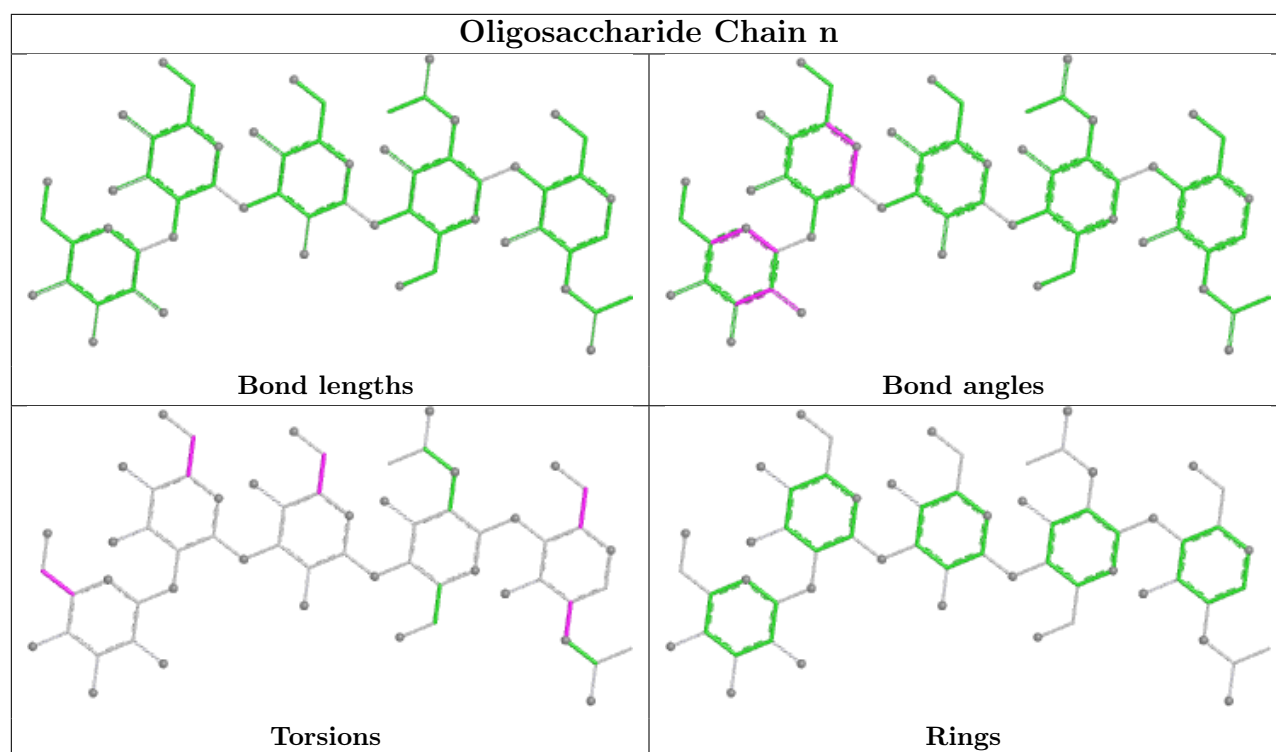


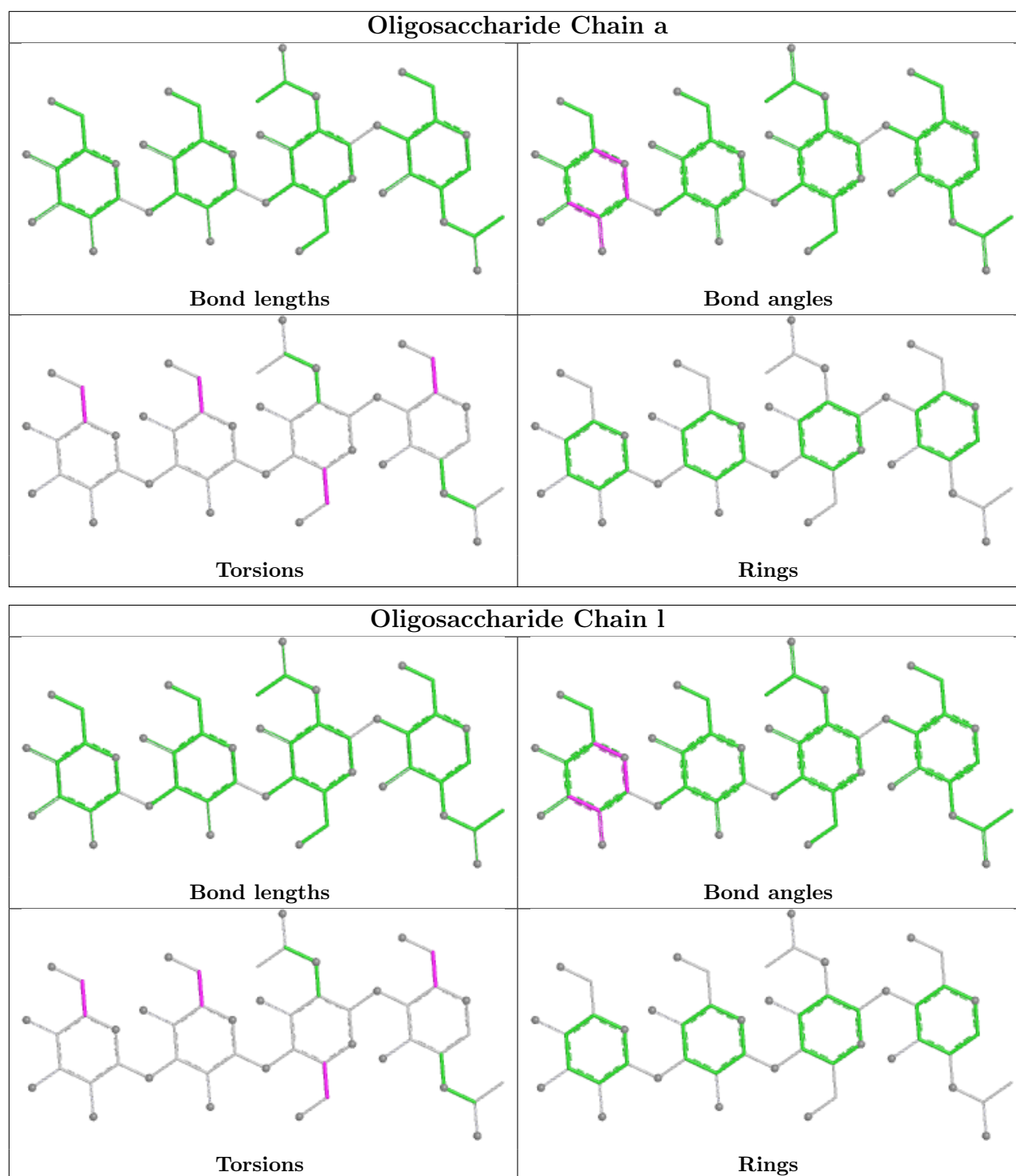












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	706	1	14,14,15	0.34	0	17,19,21	0.59	0
8	NAG	A	705	1	14,14,15	0.28	0	17,19,21	0.52	0
8	NAG	A	703	1	14,14,15	0.20	0	17,19,21	0.50	0
8	NAG	C	706	1	14,14,15	0.34	0	17,19,21	0.59	0
8	NAG	A	707	-	14,14,15	0.23	0	17,19,21	0.47	0
8	NAG	C	702	1	14,14,15	0.32	0	17,19,21	0.43	0
8	NAG	C	703	1	14,14,15	0.20	0	17,19,21	0.49	0
8	NAG	B	701	1	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	C	701	1	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	B	702	1	14,14,15	0.27	0	17,19,21	0.49	0
8	NAG	B	704	1	14,14,15	0.16	0	17,19,21	0.42	0
8	NAG	B	707	-	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	A	704	1	14,14,15	0.16	0	17,19,21	0.43	0
8	NAG	B	706	1	14,14,15	0.33	0	17,19,21	0.58	0
8	NAG	B	705	1	14,14,15	0.27	0	17,19,21	0.51	0
8	NAG	C	705	1	14,14,15	0.28	0	17,19,21	0.52	0
8	NAG	A	702	1	14,14,15	0.32	0	17,19,21	0.43	0
8	NAG	B	703	1	14,14,15	0.20	0	17,19,21	0.50	0
8	NAG	A	701	1	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	C	707	-	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	C	704	1	14,14,15	0.16	0	17,19,21	0.43	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
8	NAG	A	706	1	-	2/6/23/26	0/1/1/1
8	NAG	A	705	1	-	3/6/23/26	0/1/1/1
8	NAG	A	703	1	-	4/6/23/26	0/1/1/1
8	NAG	C	706	1	-	2/6/23/26	0/1/1/1
8	NAG	A	707	-	-	0/6/23/26	0/1/1/1
8	NAG	C	702	1	-	0/6/23/26	0/1/1/1
8	NAG	C	703	1	-	4/6/23/26	0/1/1/1
8	NAG	B	701	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	701	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	1	-	0/6/23/26	0/1/1/1
8	NAG	B	704	1	-	2/6/23/26	0/1/1/1
8	NAG	B	707	-	-	0/6/23/26	0/1/1/1
8	NAG	A	704	1	-	2/6/23/26	0/1/1/1
8	NAG	B	706	1	-	2/6/23/26	0/1/1/1
8	NAG	B	705	1	-	4/6/23/26	0/1/1/1
8	NAG	C	705	1	-	3/6/23/26	0/1/1/1
8	NAG	A	702	1	-	0/6/23/26	0/1/1/1
8	NAG	B	703	1	-	4/6/23/26	0/1/1/1
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1
8	NAG	C	707	-	-	0/6/23/26	0/1/1/1
8	NAG	C	704	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	704	NAG	O5-C5-C6-O6
8	C	703	NAG	O5-C5-C6-O6
8	C	704	NAG	O5-C5-C6-O6
8	A	704	NAG	O5-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	A	703	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	B	703	NAG	C4-C5-C6-O6
8	C	701	NAG	O5-C5-C6-O6
8	A	705	NAG	O5-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	C	705	NAG	O5-C5-C6-O6
8	A	705	NAG	C4-C5-C6-O6
8	B	705	NAG	O5-C5-C6-O6
8	A	706	NAG	O5-C5-C6-O6
8	B	704	NAG	C4-C5-C6-O6
8	C	704	NAG	C4-C5-C6-O6
8	A	704	NAG	C4-C5-C6-O6
8	C	706	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	703	NAG	C4-C5-C6-O6
8	C	705	NAG	C4-C5-C6-O6
8	B	706	NAG	O5-C5-C6-O6
8	B	705	NAG	C4-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	A	703	NAG	C4-C5-C6-O6
8	C	701	NAG	C4-C5-C6-O6
8	A	701	NAG	C4-C5-C6-O6
8	A	706	NAG	C4-C5-C6-O6
8	B	706	NAG	C4-C5-C6-O6
8	C	706	NAG	C4-C5-C6-O6
8	B	703	NAG	C3-C2-N2-C7
8	C	703	NAG	C3-C2-N2-C7
8	A	703	NAG	C3-C2-N2-C7
8	B	703	NAG	C1-C2-N2-C7
8	B	705	NAG	C1-C2-N2-C7
8	C	703	NAG	C1-C2-N2-C7
8	C	705	NAG	C1-C2-N2-C7
8	A	703	NAG	C1-C2-N2-C7
8	A	705	NAG	C1-C2-N2-C7
8	B	705	NAG	C3-C2-N2-C7

There are no ring outliers.

16 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	706	NAG	1	0
8	A	705	NAG	1	0
8	A	703	NAG	1	0
8	C	706	NAG	1	0
8	A	707	NAG	1	0
8	C	702	NAG	1	0
8	C	703	NAG	1	0
8	B	701	NAG	1	0
8	C	701	NAG	1	0
8	B	707	NAG	1	0
8	B	706	NAG	1	0
8	B	705	NAG	1	0
8	C	705	NAG	1	0
8	B	703	NAG	1	0
8	A	701	NAG	1	0
8	C	707	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

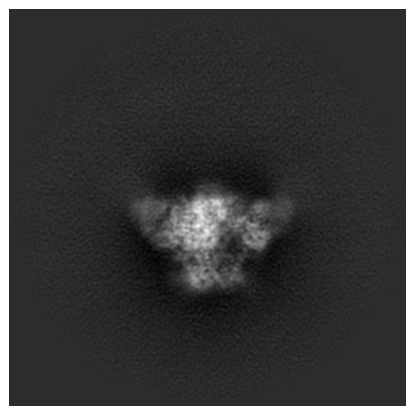
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44510. These allow visual inspection of the internal detail of the map and identification of artifacts.

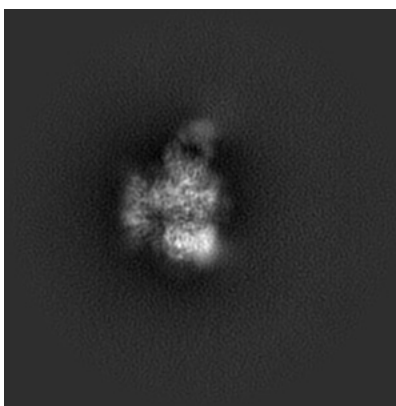
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

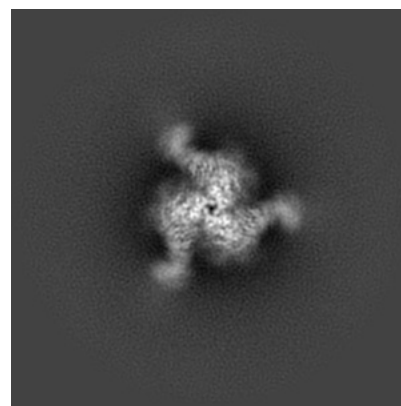
6.1.1 Primary map



X

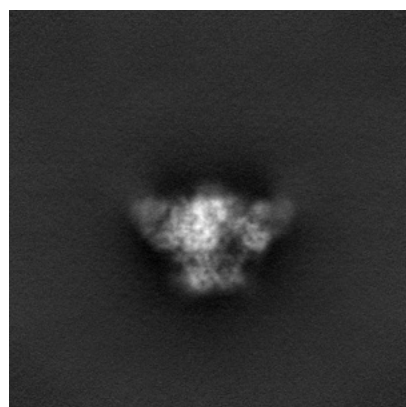


Y

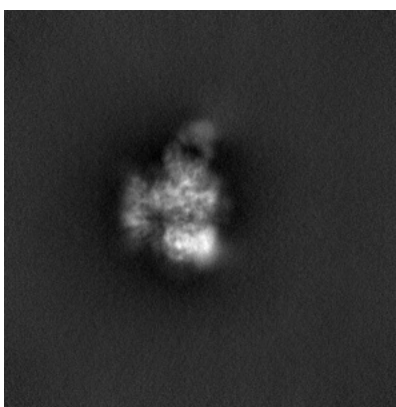


Z

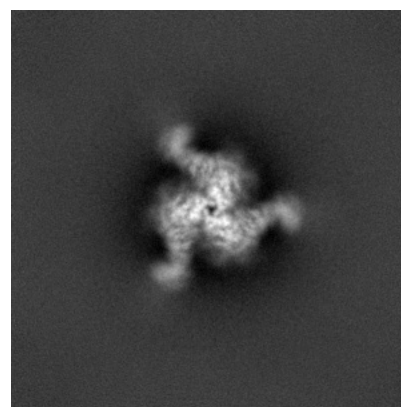
6.1.2 Raw map



X



Y

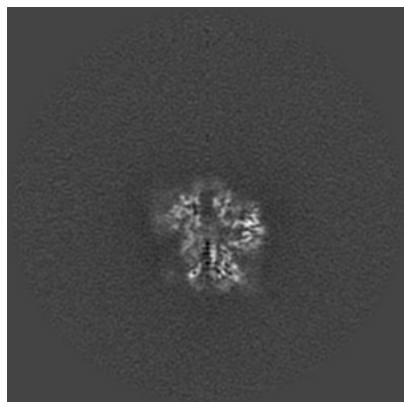


Z

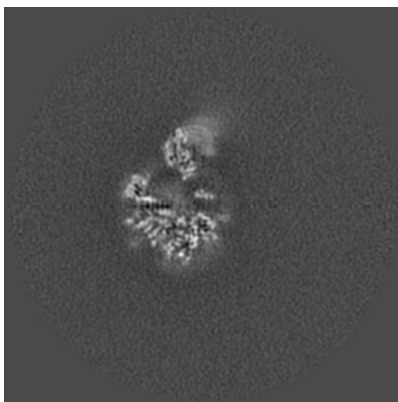
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

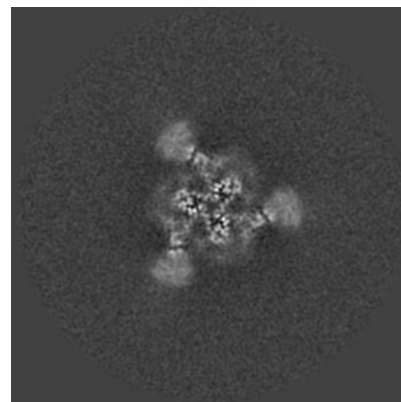
6.2.1 Primary map



X Index: 192

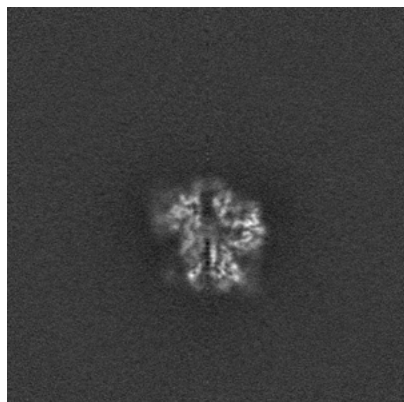


Y Index: 192

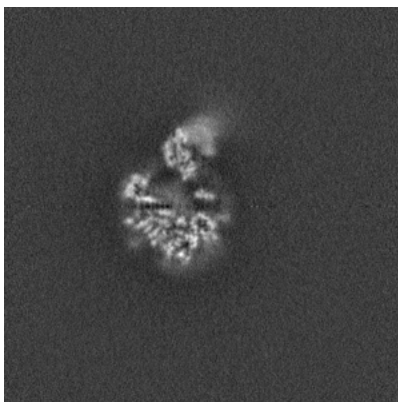


Z Index: 192

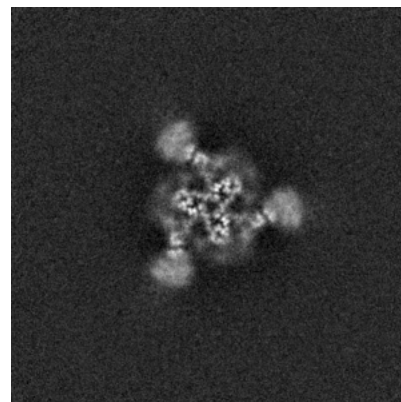
6.2.2 Raw map



X Index: 192



Y Index: 192

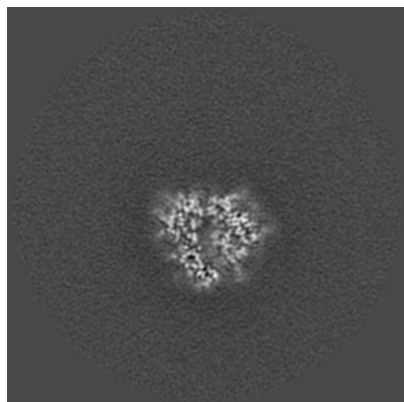


Z Index: 192

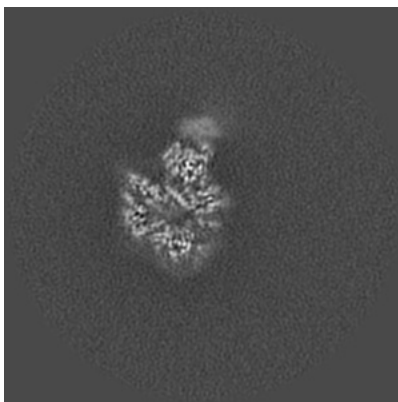
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

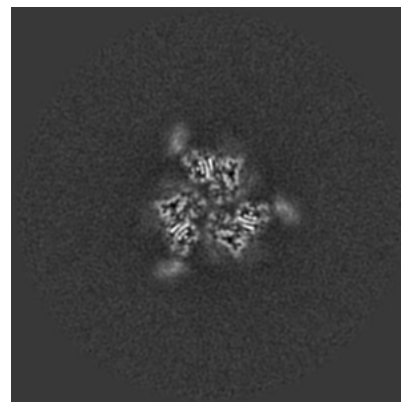
6.3.1 Primary map



X Index: 206

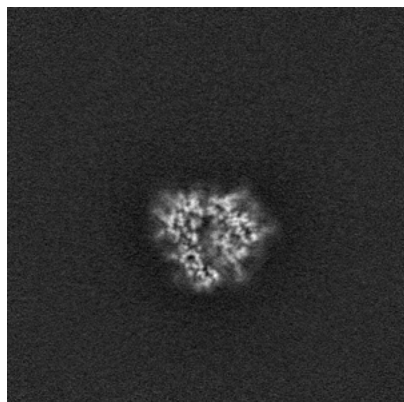


Y Index: 181

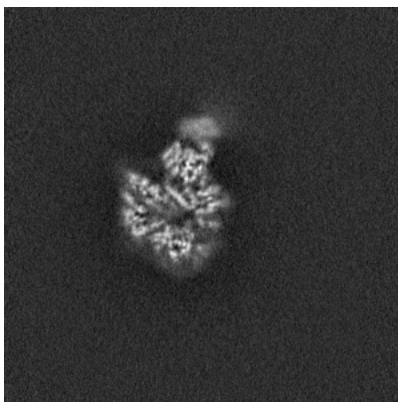


Z Index: 175

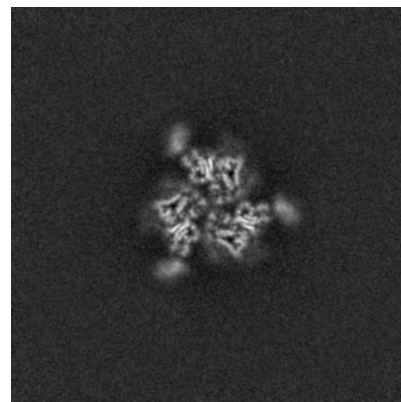
6.3.2 Raw map



X Index: 206



Y Index: 181

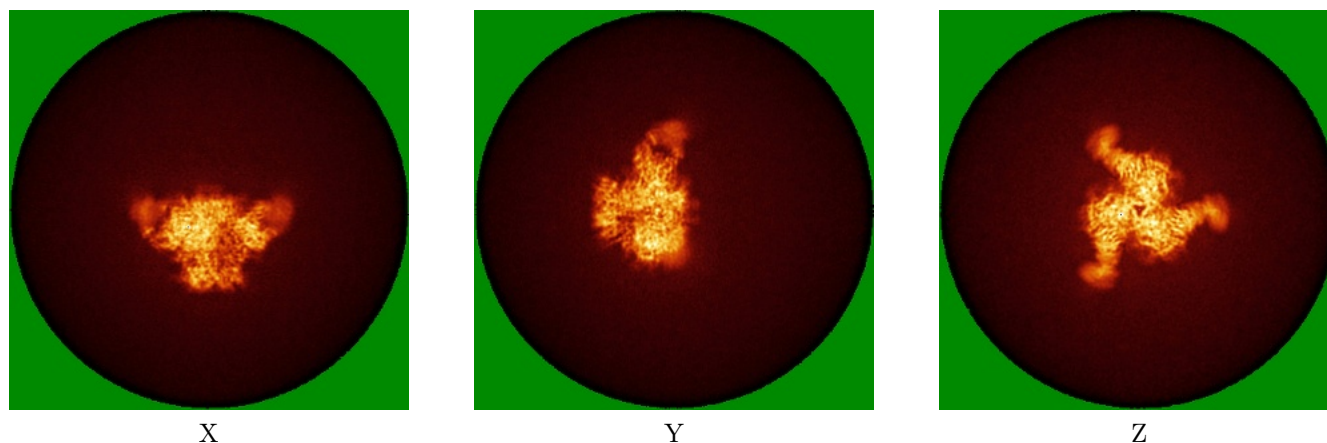


Z Index: 175

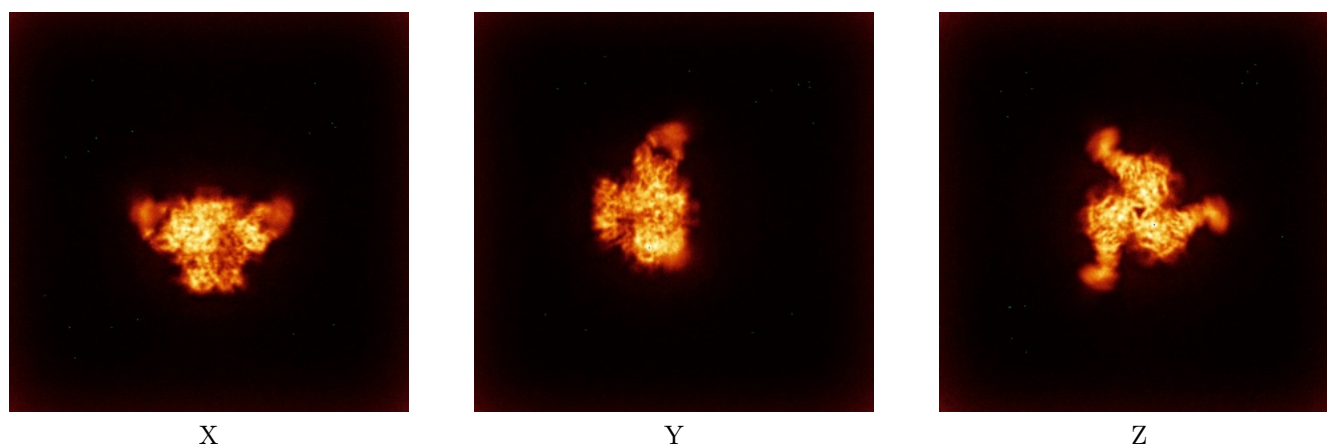
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

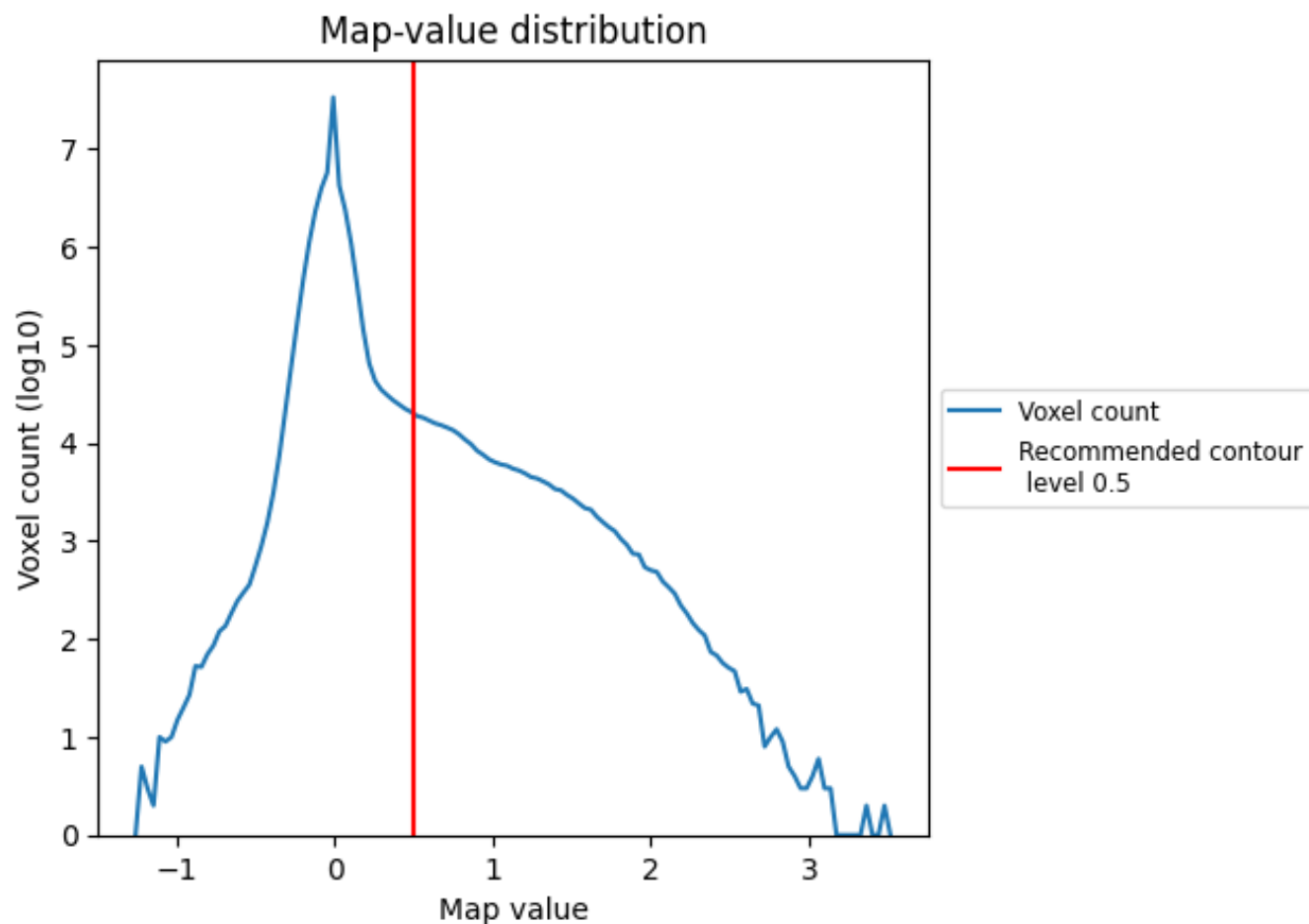
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

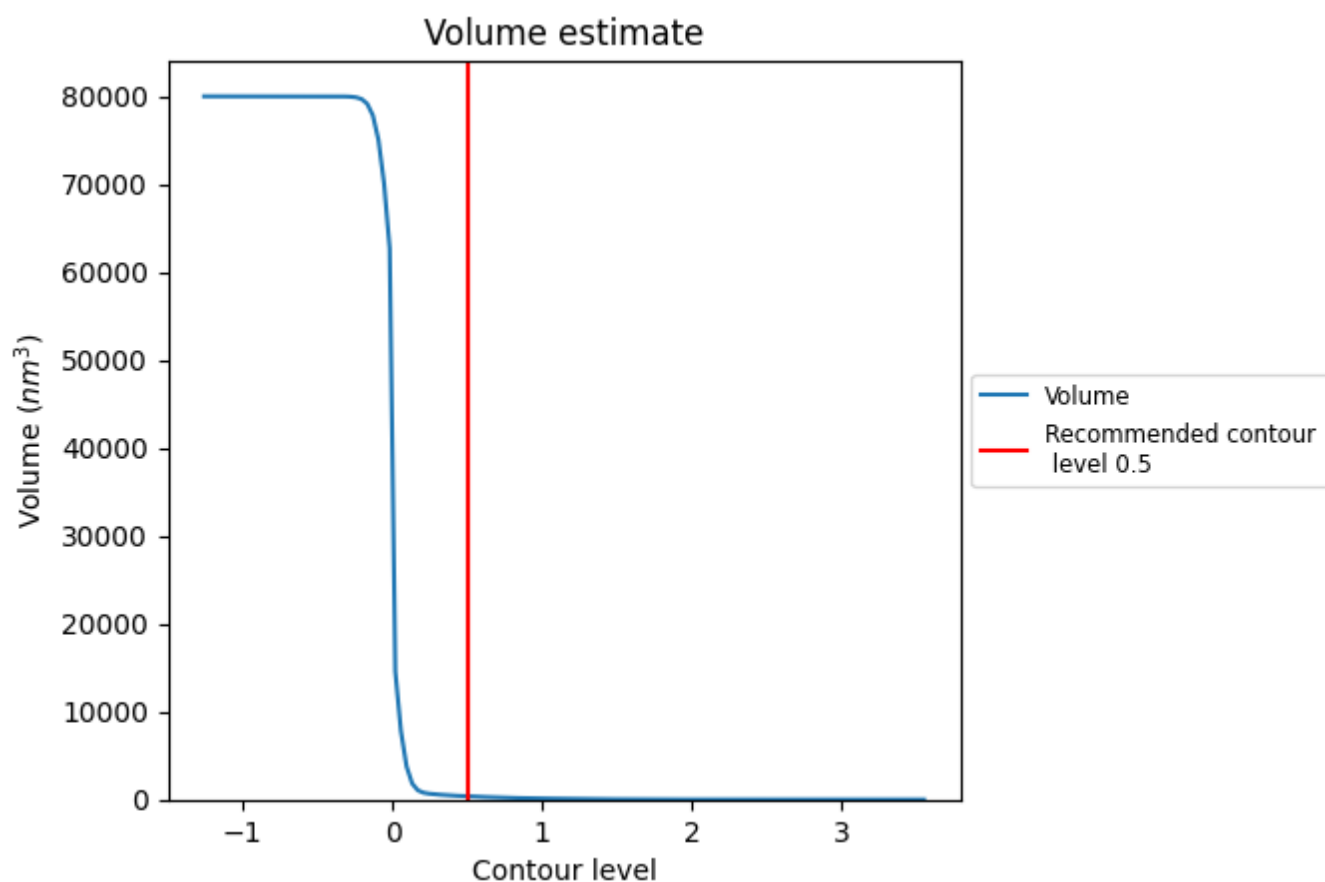
This section contains the results of statistical analysis of the map.

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.

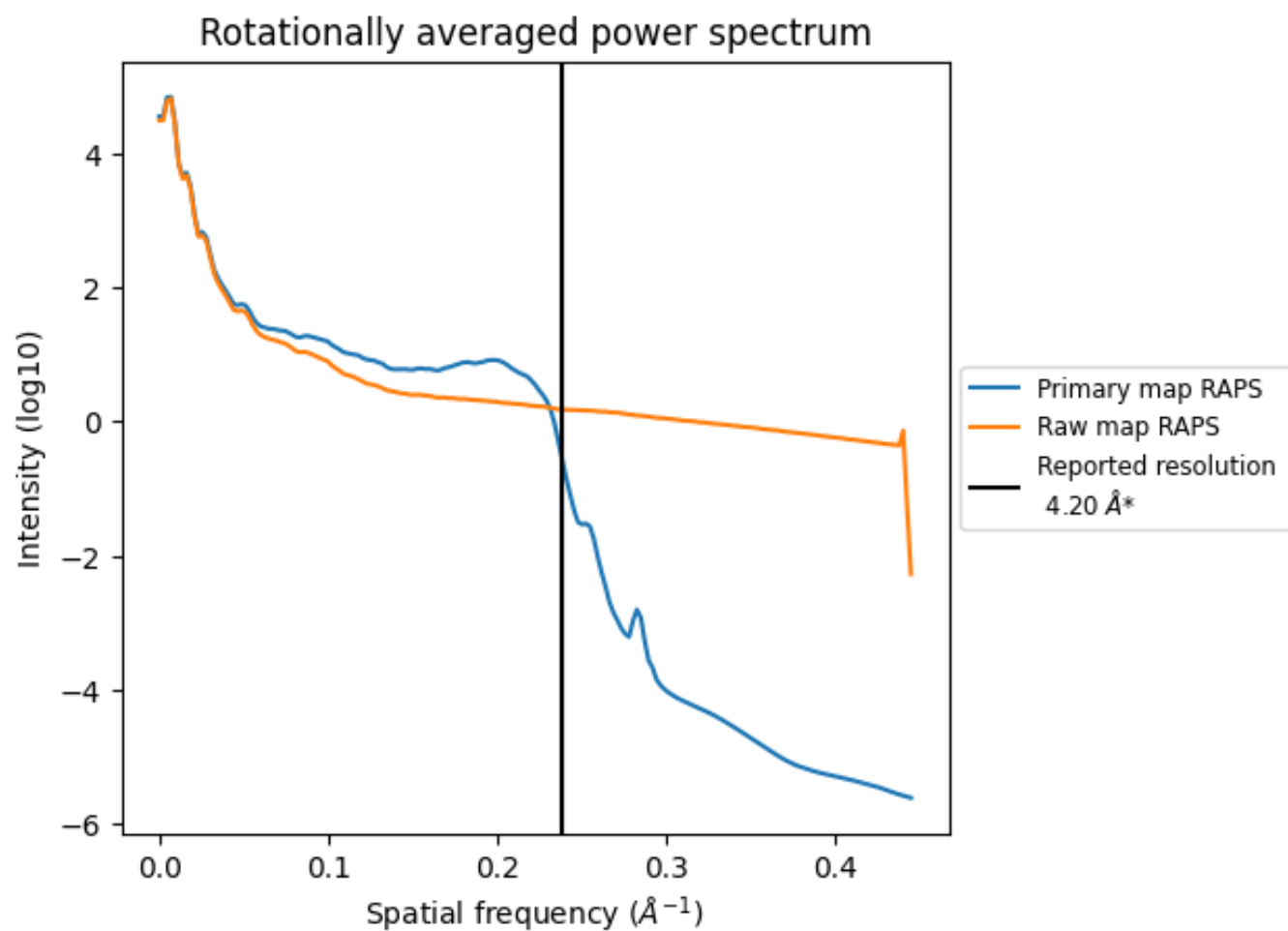
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 373 nm³; this corresponds to an approximate mass of 337 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 ⓘ

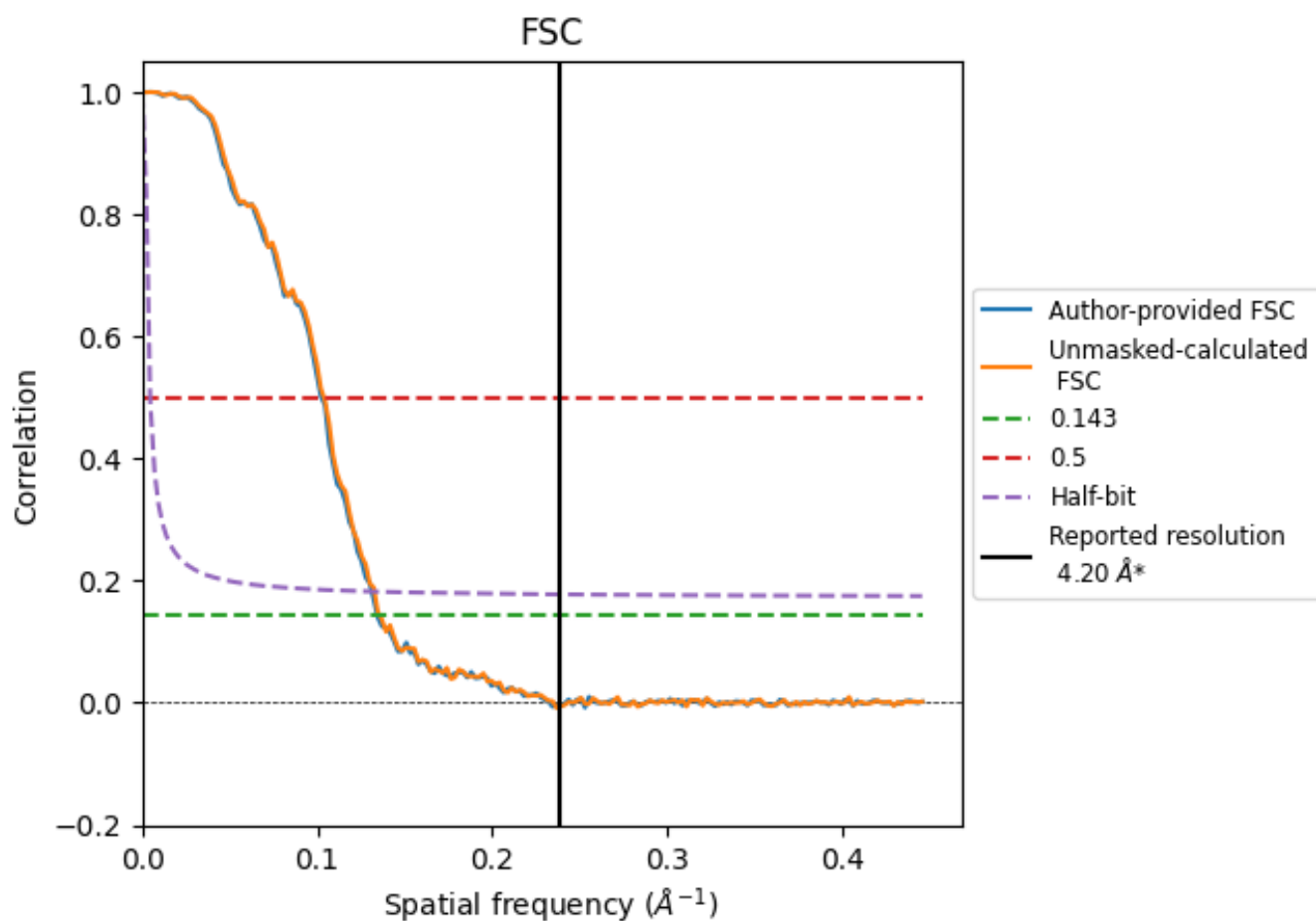


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	7.45	9.78	7.63
Unmasked-calculated*	7.37	9.63	7.54

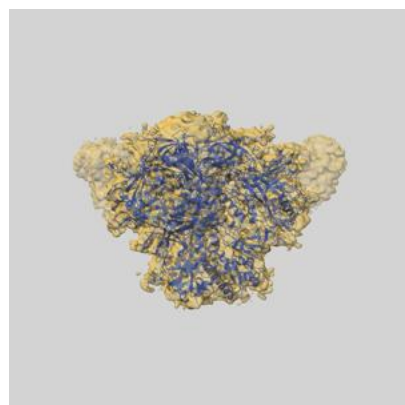
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.45 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.37 differs from the reported value 4.2 by more than 10 %

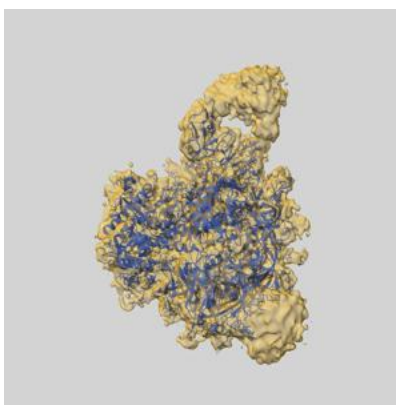
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44510 and PDB model 9BGE. Per-residue inclusion information can be found in section 3 on page 10.

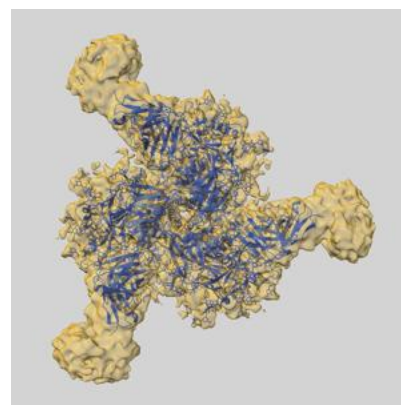
9.1 Map-model overlay [i](#)



X



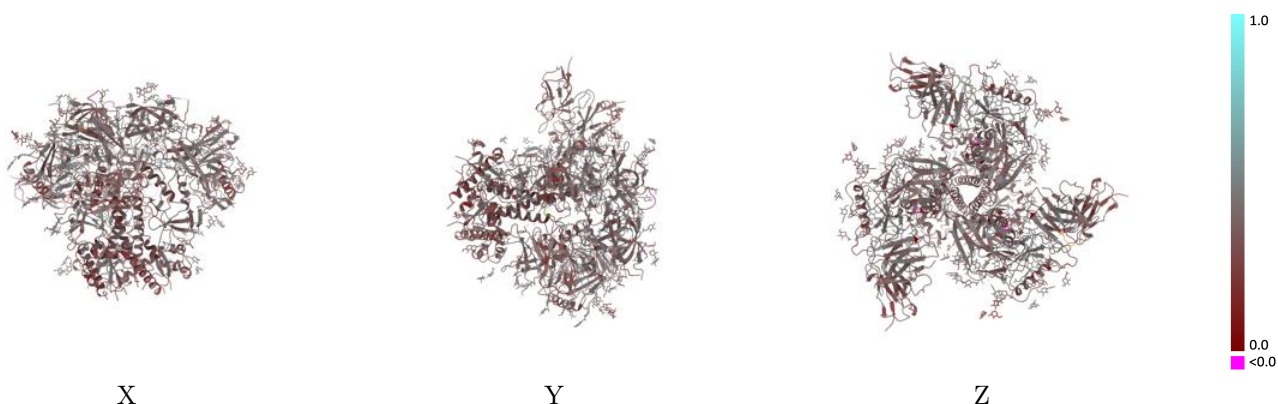
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

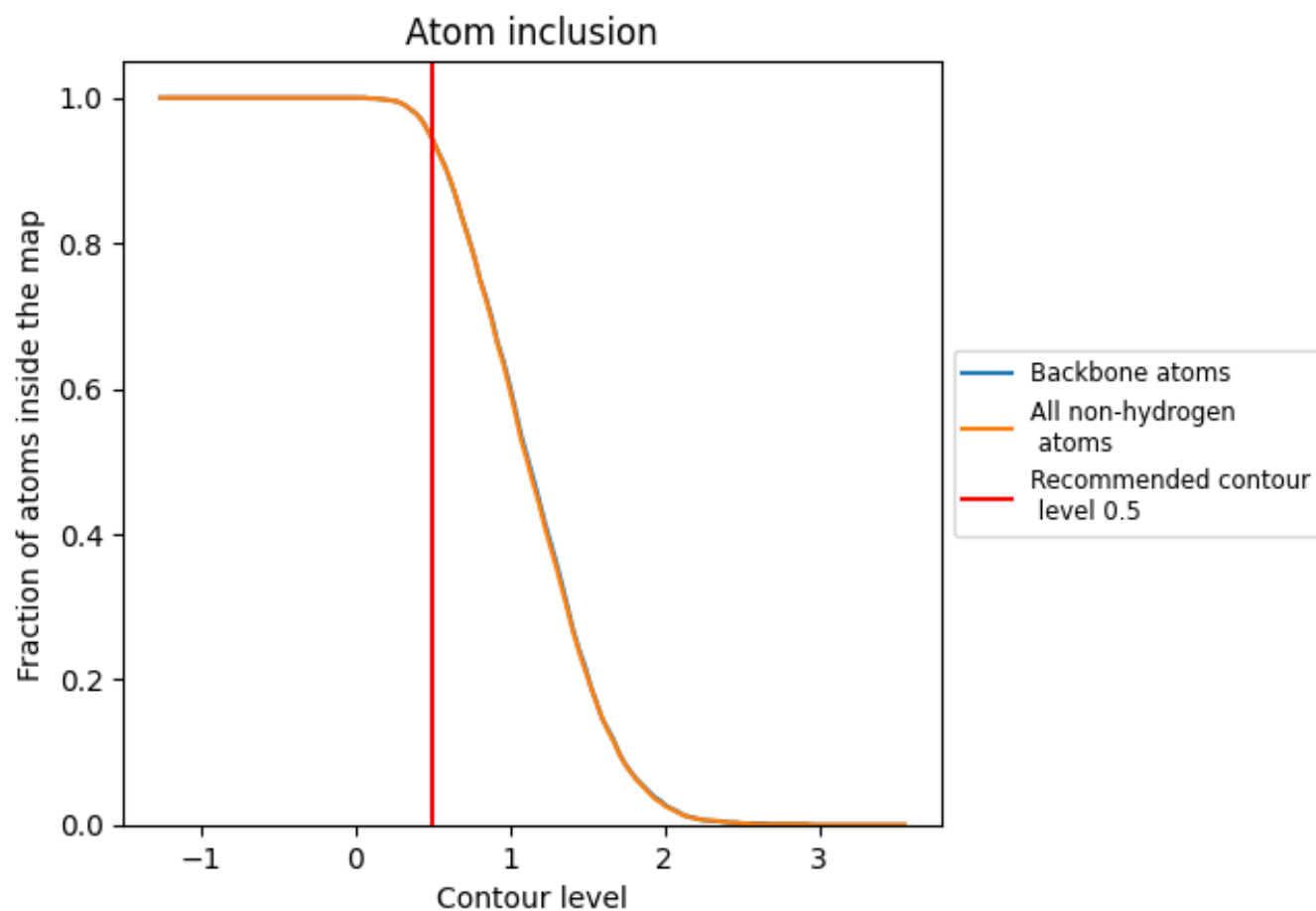


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 94% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.3730
A	 0.9390	 0.3660
B	 0.9380	 0.3680
C	 0.9380	 0.3680
D	 0.9750	 0.4010
E	 0.9670	 0.3490
F	 0.9740	 0.4000
G	 0.9690	 0.3500
H	 0.9740	 0.3990
I	 0.9290	 0.4440
J	 0.9510	 0.4430
K	 0.9340	 0.4320
L	 0.9670	 0.3460
M	 0.9640	 0.4390
N	 0.9180	 0.4410
O	 0.9640	 0.4490
P	 0.8400	 0.3090
Q	 0.8570	 0.3690
R	 0.9510	 0.4130
S	 0.9640	 0.4270
T	 0.9290	 0.3780
U	 0.9290	 0.4470
V	 0.9510	 0.4280
W	 0.9340	 0.4300
X	 0.9290	 0.4280
Y	 0.9180	 0.4380
Z	 0.9640	 0.4700
a	 0.8400	 0.3110
b	 0.8930	 0.3690
c	 0.9340	 0.4150
d	 0.9640	 0.4320
e	 0.9290	 0.3800
f	 0.9290	 0.4330
g	 0.9340	 0.4290
h	 0.9340	 0.4370



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Chain	Atom inclusion	Q-score
i	 0.9640	 0.4210
j	 0.9180	 0.4360
k	 0.9640	 0.4550
l	 0.8400	 0.3190
m	 0.8930	 0.3640
n	 0.9340	 0.4110
o	 0.9640	 0.4270
p	 0.9290	 0.3920