



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:18 AM UTC

PDB ID : 6CRQ / pdb_00006crq
EMDB ID : EMD-7568
Title : Glutaraldehyde-treated BG505 SOSIP.664 Env in complex with PGV04 Fab
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2018-03-19
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:

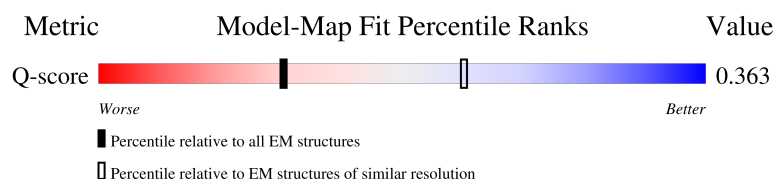
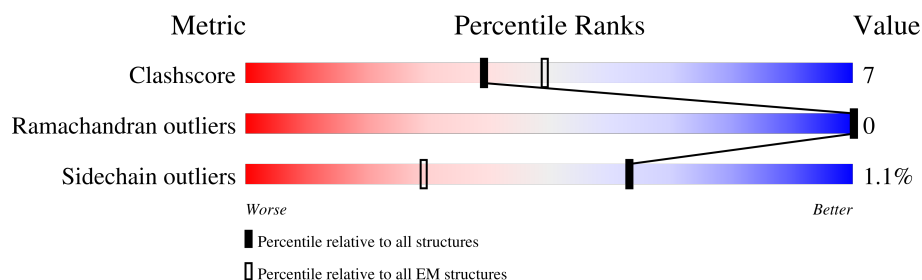
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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	480	21% 84% 9% 6%
1	B	480	24% 82% 10% 6%
1	F	480	21% 85% 8% 6%
2	C	153	28% 69% 10% 20%

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Mol	Chain	Length	Quality of chain
2	G	153	
2	H	153	
3	D	228	
3	I	228	
3	J	228	
4	E	208	
4	K	208	
4	L	208	
5	M	4	
5	Y	4	
5	k	4	
6	N	2	
6	P	2	
6	Q	2	
6	R	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Z	2	
6	b	2	
6	c	2	
6	d	2	
6	f	2	

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Mol	Chain	Length	Quality of chain
6	g	2	50% 50%
6	h	2	100% 100%
6	i	2	50% 50%
6	j	2	100% 100%
6	l	2	100% 100%
6	n	2	50% 100%
6	o	2	50% 100%
6	p	2	50% 50%
6	r	2	100% 50%
6	s	2	50% 100%
6	t	2	100% 100%
6	u	2	50% 50%
6	v	2	100% 100%
7	O	4	75% 25%
7	a	4	25% 100%
7	m	4	25% 50% 25%
8	S	3	100% 67% 33%
8	e	3	67% 67% 33%
8	q	3	67% 33% 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	M	2	-	-	X	-
6	NAG	d	1	-	-	X	-
6	NAG	i	1	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3537	2223	625	661	28		
1	B	450	Total	C	N	O	S	0	0
			3537	2223	625	661	28		
1	F	450	Total	C	N	O	S	0	0
			3537	2223	625	661	28		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	ASN	conflict	UNP Q2N0S5
A	332	ASN	THR	conflict	UNP Q2N0S5
A	501	CYS	ALA	conflict	UNP Q2N0S5
A	509	ARG	-	expression tag	UNP Q2N0S5
A	510	ARG	-	expression tag	UNP Q2N0S5
A	511	ARG	-	expression tag	UNP Q2N0S5
A	512	ARG	-	expression tag	UNP Q2N0S5
A	513	ARG	-	expression tag	UNP Q2N0S5
B	137	ALA	ASN	conflict	UNP Q2N0S5
B	332	ASN	THR	conflict	UNP Q2N0S5
B	501	CYS	ALA	conflict	UNP Q2N0S5
B	509	ARG	-	expression tag	UNP Q2N0S5
B	510	ARG	-	expression tag	UNP Q2N0S5
B	511	ARG	-	expression tag	UNP Q2N0S5
B	512	ARG	-	expression tag	UNP Q2N0S5
B	513	ARG	-	expression tag	UNP Q2N0S5
F	137	ALA	ASN	conflict	UNP Q2N0S5
F	332	ASN	THR	conflict	UNP Q2N0S5
F	501	CYS	ALA	conflict	UNP Q2N0S5
F	509	ARG	-	expression tag	UNP Q2N0S5
F	510	ARG	-	expression tag	UNP Q2N0S5
F	511	ARG	-	expression tag	UNP Q2N0S5
F	512	ARG	-	expression tag	UNP Q2N0S5
F	513	ARG	-	expression tag	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	122	Total	C	N	O	S	0	0
			967	609	168	184	6		
2	G	122	Total	C	N	O	S	0	0
			967	609	168	184	6		
2	H	122	Total	C	N	O	S	0	0
			967	609	168	184	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	559	PRO	ILE	conflict	UNP Q2N0S7
C	605	CYS	THR	conflict	UNP Q2N0S7
G	559	PRO	ILE	conflict	UNP Q2N0S7
G	605	CYS	THR	conflict	UNP Q2N0S7
H	559	PRO	ILE	conflict	UNP Q2N0S7
H	605	CYS	THR	conflict	UNP Q2N0S7

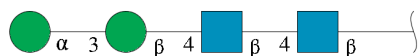
- Molecule 3 is a protein called PGV04 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
3	I	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
3	J	125	Total	C	N	O	S	0	0
			994	632	179	180	3		

- Molecule 4 is a protein called PGV04 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
4	K	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
4	L	100	Total	C	N	O	S	0	0
			784	500	131	149	4		

- Molecule 5 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
5	M	4	Total	C	N	O	0	0
			50	28	2	20		
5	Y	4	Total	C	N	O	0	0
			50	28	2	20		
5	k	4	Total	C	N	O	0	0
			50	28	2	20		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	d	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		
6	i	2	Total	C	N	O	0	0
			28	16	2	10		
6	j	2	Total	C	N	O	0	0
			28	16	2	10		
6	l	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	o	2	Total	C	N	O	0	0
			28	16	2	10		
6	p	2	Total	C	N	O	0	0
			28	16	2	10		
6	r	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		
6	t	2	Total	C	N	O	0	0
			28	16	2	10		
6	u	2	Total	C	N	O	0	0
			28	16	2	10		
6	v	2	Total	C	N	O	0	0
			28	16	2	10		

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



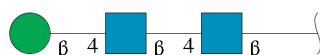
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	4	Total	C	N	O	0	0
			50	28	2	20		

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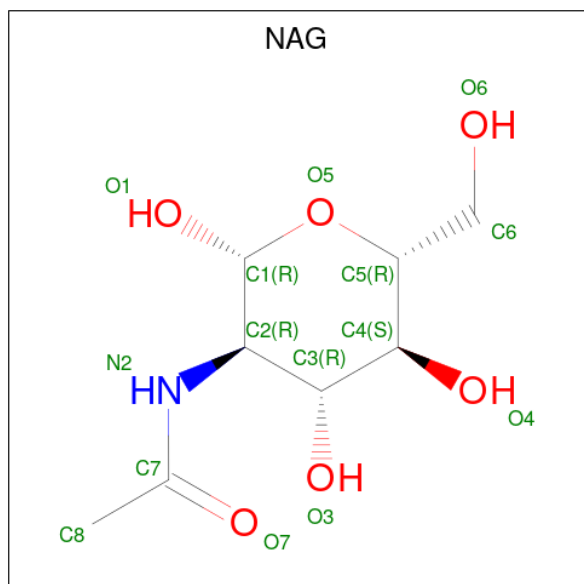
Mol	Chain	Residues	Atoms				AltConf	Trace
7	a	4	Total	C	N	O	0	0
			50	28	2	20		
7	m	4	Total	C	N	O	0	0
			50	28	2	20		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	3	Total	C	N	O	0	0
			39	22	2	15		
8	e	3	Total	C	N	O	0	0
			39	22	2	15		
8	q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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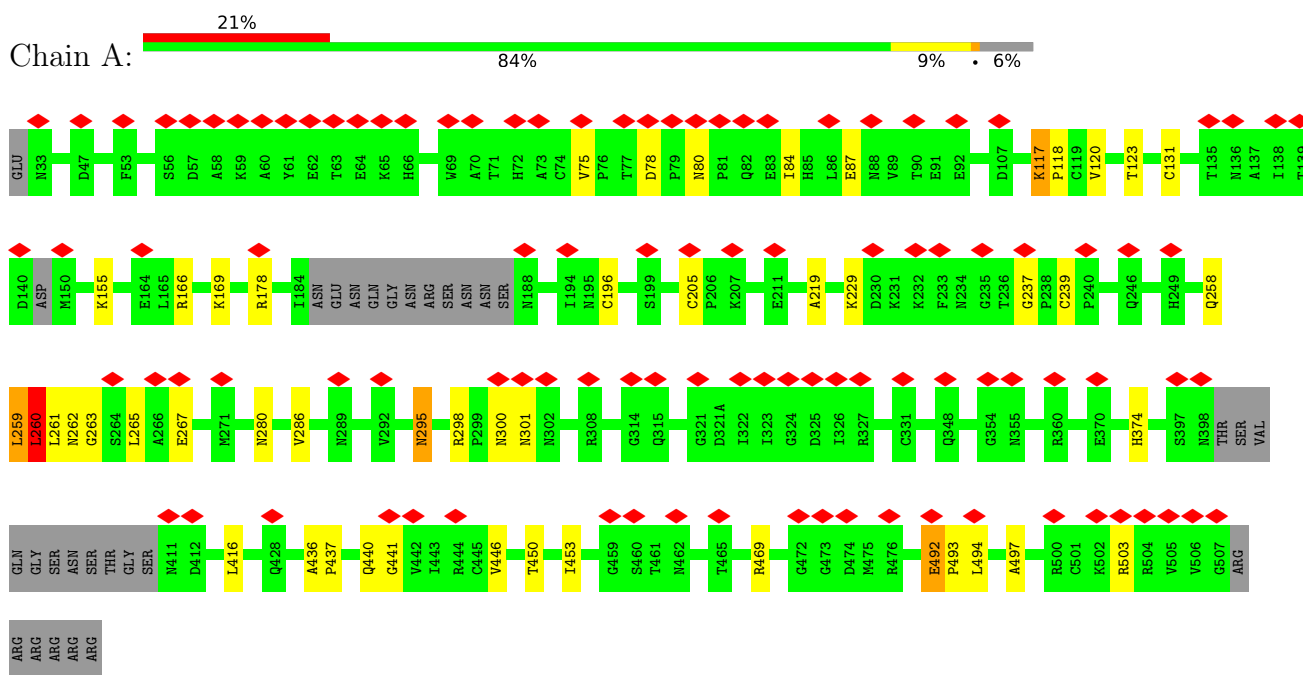
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Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	G	1	Total	C	N	O	0
			14	8	1	5	
9	G	1	Total	C	N	O	0
			14	8	1	5	
9	G	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	

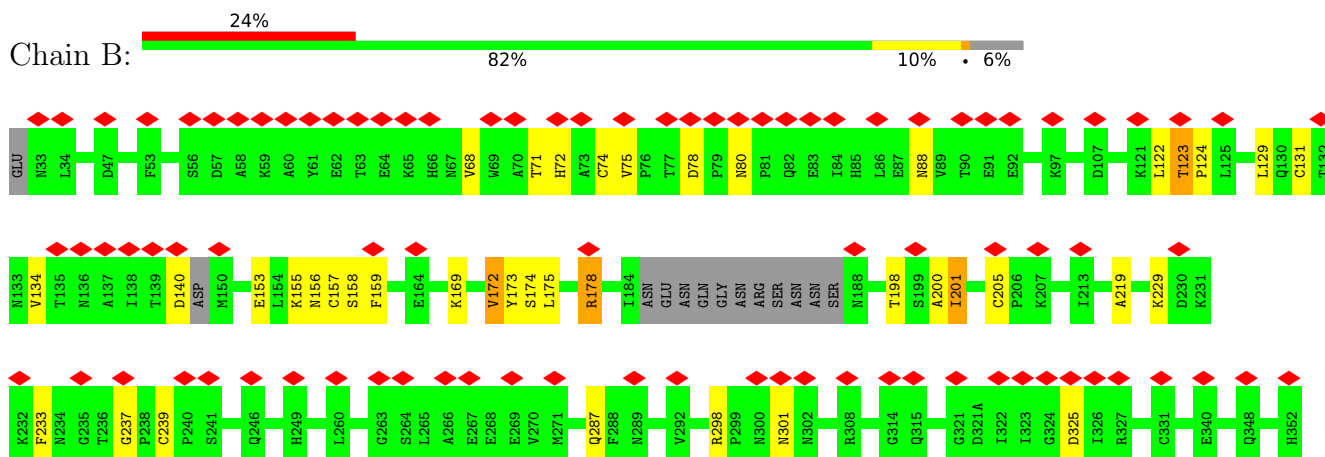
3 Residue-property plots

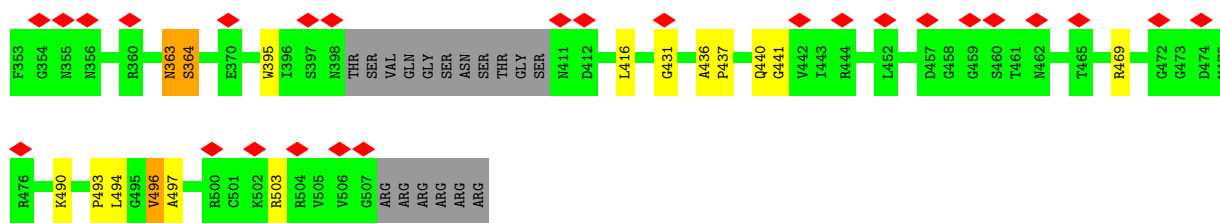
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Envelope glycoprotein gp160

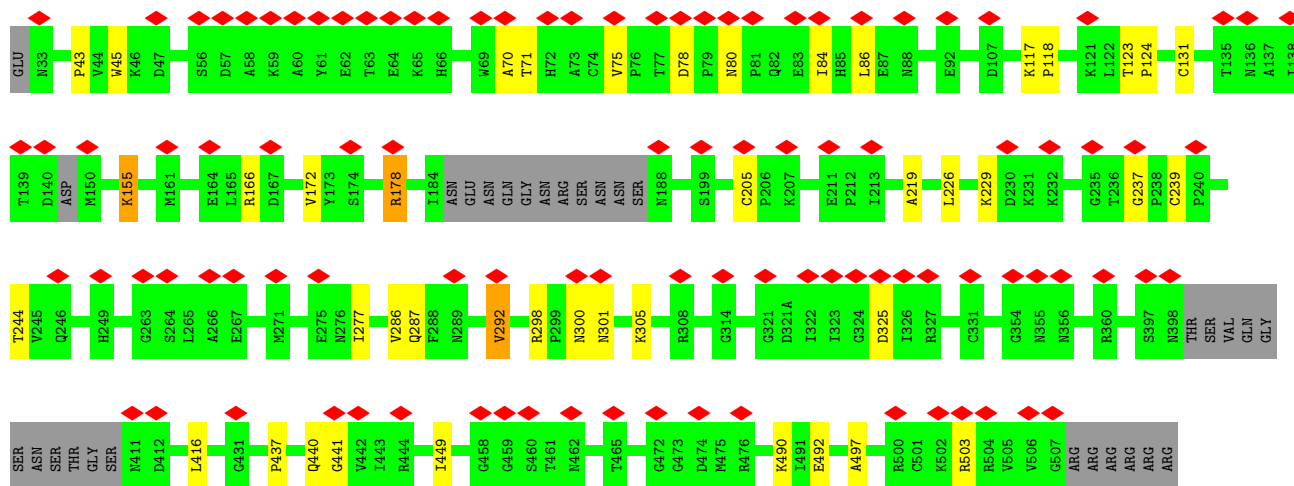
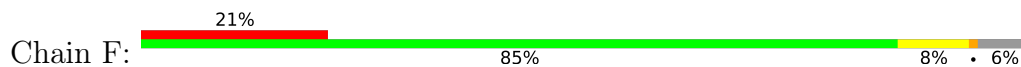


• Molecule 1: Envelope glycoprotein gp160

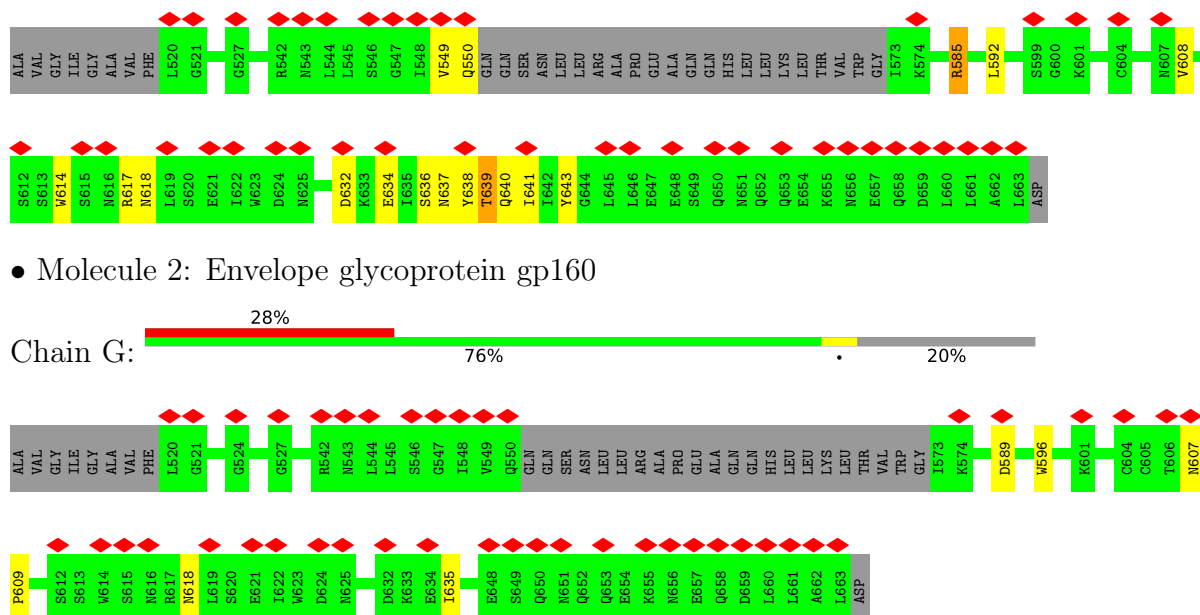




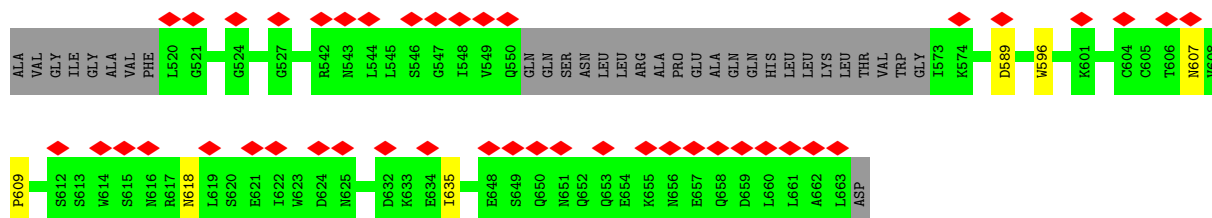
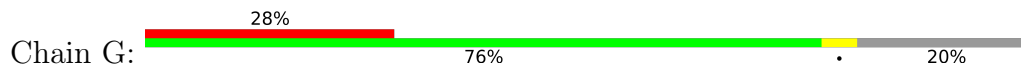
• Molecule 1: Envelope glycoprotein gp160



• Molecule 2: Envelope glycoprotein gp160



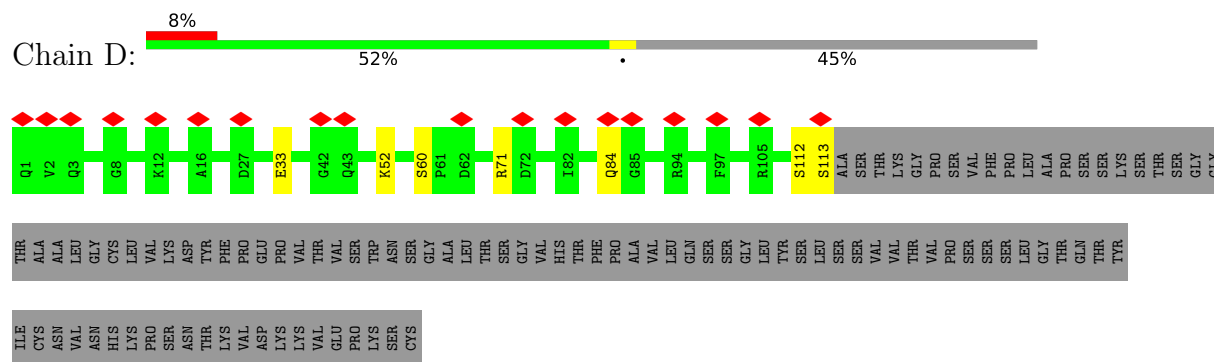
• Molecule 2: Envelope glycoprotein gp160



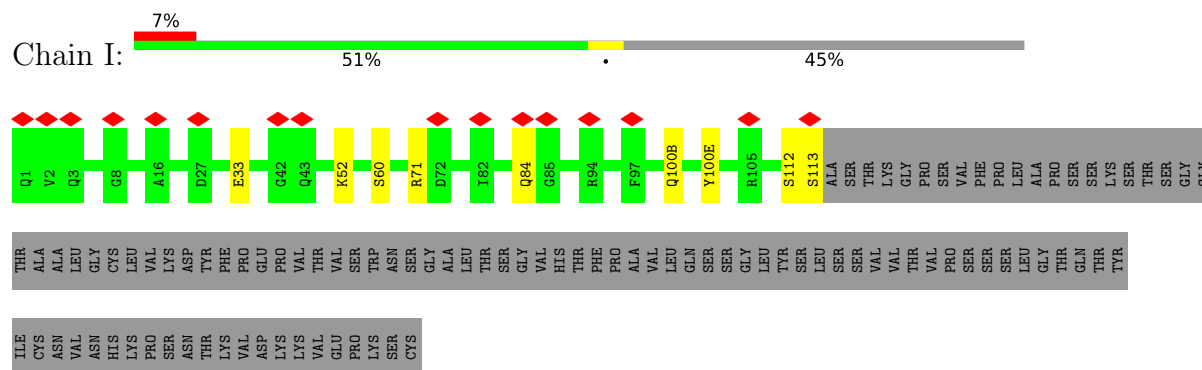
• Molecule 2: Envelope glycoprotein gp160



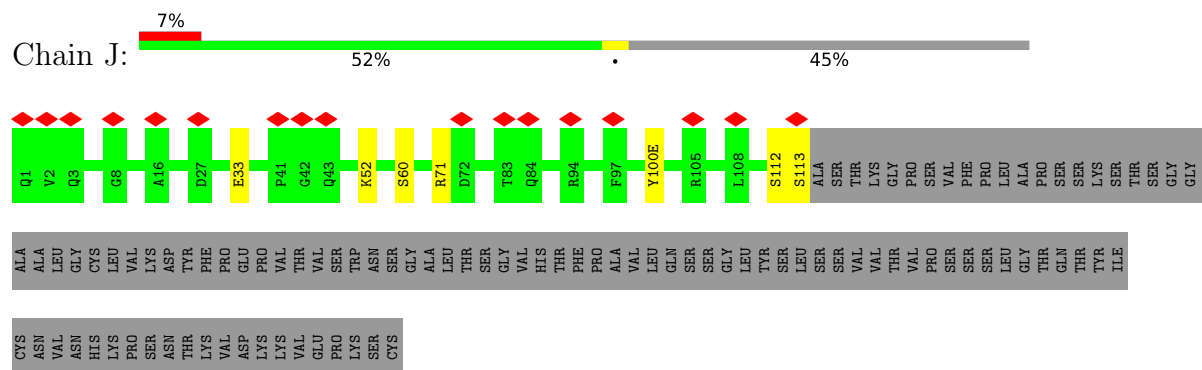
• Molecule 3: PGV04 VH



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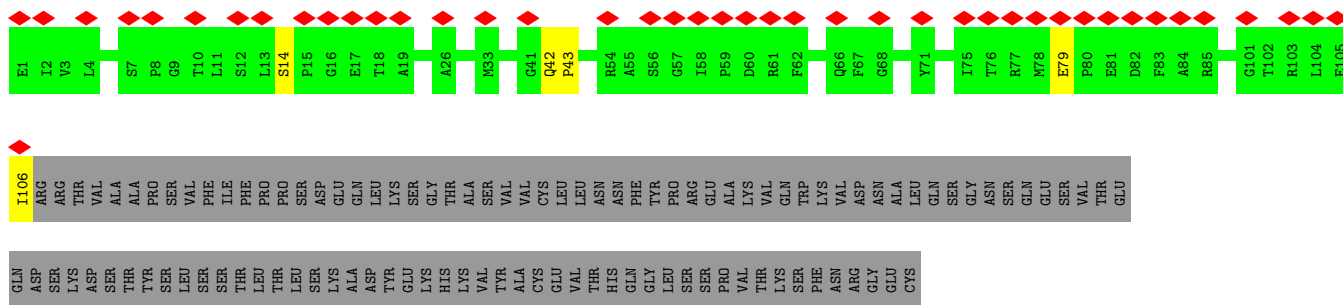


• Molecule 3: PGV04 VH

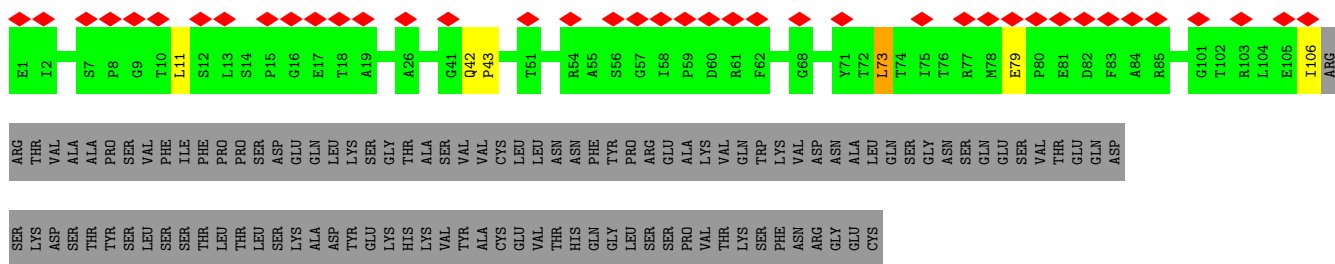


• Molecule 4: PGV04 VL

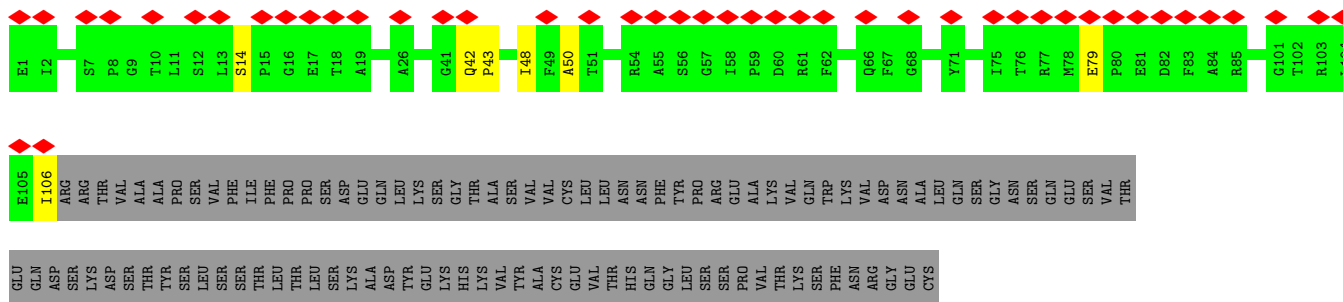
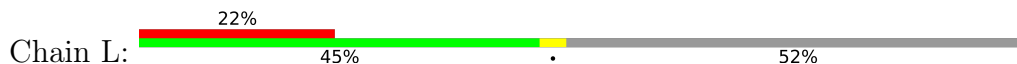




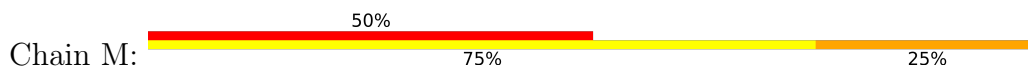
• Molecule 4: PGV04 VL



• Molecule 4: PGV04 VL



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



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





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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



- Molecule 7: 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 O:  75% 25%

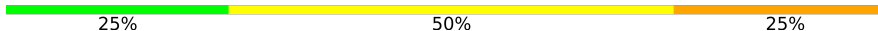


- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  25% 100%



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

Chain m:  25% 50% 25%



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

Chain S:  100% 67% 33%



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

Chain e:  67% 67% 33%



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

Chain q:  33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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, BMA, NAG

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	0.74	2/3610 (0.1%)	1.11	40/4900 (0.8%)
1	B	0.71	0/3610	1.08	36/4900 (0.7%)
1	F	0.72	1/3610 (0.0%)	1.08	32/4900 (0.7%)
2	C	0.70	0/982	0.84	2/1330 (0.2%)
2	G	0.73	0/982	0.84	0/1330
2	H	0.71	0/982	0.98	5/1330 (0.4%)
3	D	0.71	0/1020	0.95	2/1383 (0.1%)
3	I	0.71	0/1020	0.94	2/1383 (0.1%)
3	J	0.71	0/1020	0.92	2/1383 (0.1%)
4	E	0.70	0/804	1.09	8/1087 (0.7%)
4	K	0.68	0/804	1.12	6/1087 (0.6%)
4	L	0.70	0/804	1.11	9/1087 (0.8%)
All	All	0.72	3/19248 (0.0%)	1.04	144/26100 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	ASN	C-N	7.04	1.44	1.33
1	F	300	ASN	C-N	7.02	1.44	1.33
1	A	87	GLU	C-N	-5.92	1.25	1.33

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	VAL	N-CA-C	10.24	121.07	110.72
1	B	298	ARG	CA-C-N	9.93	130.04	120.31
1	B	298	ARG	C-N-CA	9.93	130.04	120.31
1	F	298	ARG	CA-C-N	9.44	129.56	120.31
1	F	298	ARG	C-N-CA	9.44	129.56	120.31
1	A	298	ARG	CA-C-N	9.41	129.54	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ARG	C-N-CA	9.41	129.54	120.31
2	H	525	ALA	N-CA-C	8.82	120.89	111.28
1	A	295	ASN	CA-CB-CG	8.59	121.19	112.60
2	H	637	ASN	N-CA-C	8.30	120.33	111.28
4	L	42	GLN	CA-C-N	8.12	125.51	119.66
4	L	42	GLN	C-N-CA	8.12	125.51	119.66
4	E	42	GLN	CA-C-N	7.87	125.33	119.66
4	E	42	GLN	C-N-CA	7.87	125.33	119.66
1	B	78	ASP	CA-C-N	7.66	127.83	119.87
1	B	78	ASP	C-N-CA	7.66	127.83	119.87
1	A	78	ASP	CA-C-N	7.61	127.78	119.87
1	A	78	ASP	C-N-CA	7.61	127.78	119.87
1	A	239	CYS	CA-C-N	7.52	127.23	119.56
1	A	239	CYS	C-N-CA	7.52	127.23	119.56
4	K	42	GLN	CA-C-N	7.47	125.04	119.66
4	K	42	GLN	C-N-CA	7.47	125.04	119.66
1	A	205	CYS	CA-C-N	7.39	127.10	119.56
1	A	205	CYS	C-N-CA	7.39	127.10	119.56
1	F	205	CYS	CA-C-N	7.24	126.94	119.56
1	F	205	CYS	C-N-CA	7.24	126.94	119.56
1	B	239	CYS	CA-C-N	7.04	127.02	119.28
1	B	239	CYS	C-N-CA	7.04	127.02	119.28
1	F	78	ASP	CA-C-N	6.93	127.08	119.87
1	F	78	ASP	C-N-CA	6.93	127.08	119.87
1	B	72	HIS	N-CA-C	-6.92	103.74	111.28
2	H	636	SER	N-CA-C	6.90	118.80	111.28
4	L	79	GLU	CA-C-N	6.81	126.51	119.56
4	L	79	GLU	C-N-CA	6.81	126.51	119.56
1	A	219	ALA	CA-C-N	6.78	126.76	119.78
1	A	219	ALA	C-N-CA	6.78	126.76	119.78
1	F	239	CYS	CA-C-N	6.78	126.41	119.56
1	F	239	CYS	C-N-CA	6.78	126.41	119.56
1	B	80	ASN	CA-C-N	6.75	126.71	120.03
1	B	80	ASN	C-N-CA	6.75	126.71	120.03
1	B	219	ALA	CA-C-N	6.74	126.72	119.78
1	B	219	ALA	C-N-CA	6.74	126.72	119.78
4	K	79	GLU	CA-C-N	6.71	126.41	119.56
4	K	79	GLU	C-N-CA	6.71	126.41	119.56
1	A	117	LYS	CA-C-N	6.70	126.84	119.87
1	A	117	LYS	C-N-CA	6.70	126.84	119.87
1	F	292	VAL	N-CA-C	-6.67	98.14	107.80
4	E	79	GLU	CA-C-N	6.61	126.30	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	79	GLU	C-N-CA	6.61	126.30	119.56
1	B	205	CYS	CA-C-N	6.56	126.19	119.56
1	B	205	CYS	C-N-CA	6.56	126.19	119.56
1	F	219	ALA	CA-C-N	6.55	126.52	119.78
1	F	219	ALA	C-N-CA	6.55	126.52	119.78
1	A	286	VAL	N-CA-C	6.42	117.20	110.72
3	D	60	SER	CA-C-N	6.42	126.11	119.56
3	D	60	SER	C-N-CA	6.42	126.11	119.56
1	A	437	PRO	N-CA-C	-6.33	103.81	110.58
1	A	416	LEU	CA-C-N	6.31	126.28	119.78
1	A	416	LEU	C-N-CA	6.31	126.28	119.78
1	F	437	PRO	N-CA-C	-6.30	103.84	110.58
1	A	436	ALA	CA-C-N	6.28	124.18	119.66
1	A	436	ALA	C-N-CA	6.28	124.18	119.66
1	A	80	ASN	CA-C-N	6.21	126.12	119.85
1	A	80	ASN	C-N-CA	6.21	126.12	119.85
1	A	84	ILE	N-CA-C	6.14	116.77	108.17
1	F	492	GLU	CA-C-N	6.11	127.52	120.98
1	F	492	GLU	C-N-CA	6.11	127.52	120.98
1	B	441	GLY	N-CA-C	6.08	122.32	115.08
1	B	497	ALA	CA-C-N	6.06	125.97	119.85
1	B	497	ALA	C-N-CA	6.06	125.97	119.85
1	B	123	THR	CA-C-N	6.01	125.69	119.56
1	B	123	THR	C-N-CA	6.01	125.69	119.56
3	I	60	SER	CA-C-N	6.00	125.68	119.56
3	I	60	SER	C-N-CA	6.00	125.68	119.56
3	J	60	SER	CA-C-N	5.97	125.65	119.56
3	J	60	SER	C-N-CA	5.97	125.65	119.56
1	F	80	ASN	CA-C-N	5.95	125.86	119.85
1	F	80	ASN	C-N-CA	5.95	125.86	119.85
4	K	43	PRO	CA-C-N	5.92	125.90	120.03
4	K	43	PRO	C-N-CA	5.92	125.90	120.03
1	F	286	VAL	N-CA-C	5.92	116.70	110.72
1	F	305	LYS	CA-C-N	-5.89	114.93	122.77
1	F	305	LYS	C-N-CA	-5.89	114.93	122.77
1	B	364	SER	N-CA-C	5.89	118.36	110.35
1	B	436	ALA	CA-C-N	5.80	123.83	119.66
1	B	436	ALA	C-N-CA	5.80	123.83	119.66
1	B	68	VAL	N-CA-C	5.79	116.52	110.62
4	E	43	PRO	CA-C-N	5.71	125.68	120.03
4	E	43	PRO	C-N-CA	5.71	125.68	120.03
1	B	416	LEU	CA-C-N	5.61	125.56	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	LEU	C-N-CA	5.61	125.56	119.78
4	L	43	PRO	CA-C-N	5.61	125.51	119.85
4	L	43	PRO	C-N-CA	5.61	125.51	119.85
1	A	75	VAL	CA-C-N	5.60	125.55	119.78
1	A	75	VAL	C-N-CA	5.60	125.55	119.78
1	F	416	LEU	CA-C-N	5.57	125.52	119.78
1	F	416	LEU	C-N-CA	5.57	125.52	119.78
1	F	305	LYS	O-C-N	5.53	130.42	123.23
1	F	497	ALA	CA-C-N	5.53	125.29	119.76
1	F	497	ALA	C-N-CA	5.53	125.29	119.76
1	B	437	PRO	N-CA-C	-5.50	104.69	110.58
1	B	75	VAL	CA-C-N	5.49	125.44	119.78
1	B	75	VAL	C-N-CA	5.49	125.44	119.78
1	A	497	ALA	CA-C-N	5.42	125.18	119.76
1	A	497	ALA	C-N-CA	5.42	125.18	119.76
1	A	441	GLY	N-CA-C	5.40	122.23	115.21
4	L	48	ILE	N-CA-C	5.39	115.65	108.11
1	B	153	GLU	N-CA-C	5.37	117.22	111.36
1	B	469	ARG	CA-C-N	5.37	125.31	119.78
1	B	469	ARG	C-N-CA	5.37	125.31	119.78
1	F	440	GLN	N-CA-C	5.37	117.92	109.39
1	F	131	CYS	N-CA-C	5.34	116.26	108.14
1	A	123	THR	CA-C-N	5.33	125.00	119.56
1	A	123	THR	C-N-CA	5.33	125.00	119.56
1	A	440	GLN	N-CA-C	5.31	117.84	109.39
1	F	75	VAL	CA-C-N	5.27	125.21	119.78
1	F	75	VAL	C-N-CA	5.27	125.21	119.78
1	F	441	GLY	N-CA-C	5.27	122.06	115.21
4	E	14	SER	CA-C-N	5.26	125.27	119.90
4	E	14	SER	C-N-CA	5.26	125.27	119.90
1	B	131	CYS	N-CA-C	5.25	116.13	108.14
2	C	608	VAL	CA-C-N	5.24	125.14	119.85
2	C	608	VAL	C-N-CA	5.24	125.14	119.85
1	F	237	GLY	CA-C-N	5.23	125.48	119.83
1	F	237	GLY	C-N-CA	5.23	125.48	119.83
1	B	237	GLY	CA-C-N	5.22	125.47	119.83
1	B	237	GLY	C-N-CA	5.22	125.47	119.83
1	A	295	ASN	CB-CG-ND2	5.21	124.21	116.40
1	A	237	GLY	CA-C-N	5.19	125.44	119.83
1	A	237	GLY	C-N-CA	5.19	125.44	119.83
2	H	608	VAL	CA-C-N	5.18	125.08	119.85
2	H	608	VAL	C-N-CA	5.18	125.08	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	172	VAL	N-CA-C	5.12	116.58	111.00
1	A	260	LEU	N-CA-C	-5.11	102.30	109.96
1	A	469	ARG	CA-C-N	5.10	125.03	119.78
1	A	469	ARG	C-N-CA	5.10	125.03	119.78
4	L	14	SER	CA-C-N	5.09	125.10	119.90
4	L	14	SER	C-N-CA	5.09	125.10	119.90
1	A	492	GLU	CA-C-N	5.08	124.69	119.05
1	A	492	GLU	C-N-CA	5.08	124.69	119.05
1	B	440	GLN	N-CA-C	5.08	117.47	109.39
1	B	157	CYS	N-CA-C	5.05	117.13	108.90
1	A	131	CYS	N-CA-C	5.03	115.78	108.14
1	A	267	GLU	N-CA-C	5.02	116.75	111.28

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	3537	0	3484	61	0
1	B	3537	0	3488	47	0
1	F	3537	0	3484	59	0
2	C	967	0	952	19	0
2	G	967	0	952	7	0
2	H	967	0	952	48	0
3	D	994	0	964	4	0
3	I	994	0	964	5	0
3	J	994	0	964	6	0
4	E	784	0	771	1	0
4	K	784	0	771	6	0
4	L	784	0	771	3	0
5	M	50	0	41	8	0
5	Y	50	0	41	0	0
5	k	50	0	41	0	0
6	N	28	0	25	0	0
6	P	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	28	0	25	0	0
6	R	28	0	25	3	0
6	T	28	0	25	4	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	1	0
6	X	28	0	25	0	0
6	Z	28	0	25	0	0
6	b	28	0	25	0	0
6	c	28	0	25	1	0
6	d	28	0	25	8	0
6	f	28	0	25	1	0
6	g	28	0	25	2	0
6	h	28	0	25	0	0
6	i	28	0	25	11	0
6	j	28	0	25	0	0
6	l	28	0	25	0	0
6	n	28	0	25	0	0
6	o	28	0	25	0	0
6	p	28	0	25	3	0
6	r	28	0	25	0	0
6	s	28	0	25	0	0
6	t	28	0	25	0	0
6	u	28	0	25	7	0
6	v	28	0	25	0	0
7	O	50	0	41	4	0
7	a	50	0	41	0	0
7	m	50	0	41	4	0
8	S	39	0	33	0	0
8	e	39	0	33	0	0
8	q	39	0	33	4	0
9	A	42	0	39	4	0
9	B	42	0	39	1	0
9	C	42	0	39	1	0
9	F	42	0	39	4	0
9	G	42	0	39	1	0
9	H	42	0	39	3	0
All	All	20271	0	19771	285	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 7.

All (285) 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)
6:i:1:NAG:O3	6:i:1:NAG:H83	1.26	1.30
6:d:1:NAG:O3	6:d:1:NAG:H83	1.16	1.25
1:A:259:LEU:CD2	1:A:374:HIS:CD2	2.23	1.20
1:F:244:THR:CG2	2:H:523:LEU:HD13	1.75	1.15
6:d:1:NAG:O3	6:d:1:NAG:C8	1.97	1.13
1:F:244:THR:HG21	2:H:523:LEU:HD13	1.20	1.10
1:A:259:LEU:HD23	1:A:374:HIS:CE1	1.87	1.09
1:A:259:LEU:HD21	1:A:374:HIS:CG	1.87	1.09
1:A:494:LEU:HD11	2:C:592:LEU:HD23	1.24	1.09
1:A:155:LYS:CE	1:A:178:ARG:CZ	2.30	1.09
6:d:1:NAG:C8	6:d:1:NAG:C3	2.30	1.07
6:i:1:NAG:C8	6:i:1:NAG:C3	2.34	1.06
1:F:244:THR:CB	2:H:523:LEU:HD13	1.87	1.04
1:B:155:LYS:O	1:B:175:LEU:HD23	1.58	1.04
1:A:155:LYS:HE2	1:A:178:ARG:NH2	1.73	1.03
1:A:259:LEU:HD22	1:A:374:HIS:CD2	1.93	1.03
4:K:73:LEU:HD12	4:K:73:LEU:O	1.57	1.03
6:d:1:NAG:H82	6:d:1:NAG:H3	1.35	1.03
1:F:43:PRO:HB2	2:H:526:ALA:HB2	1.37	1.02
1:A:259:LEU:CD2	1:A:374:HIS:CG	2.43	1.02
6:i:1:NAG:H82	6:i:1:NAG:H3	1.42	1.01
1:A:155:LYS:HE2	1:A:178:ARG:CZ	1.90	1.00
1:A:259:LEU:HD23	1:A:374:HIS:NE2	1.76	0.99
6:i:1:NAG:O3	6:i:1:NAG:C8	2.11	0.98
1:F:84:ILE:HG21	2:H:523:LEU:HB2	1.48	0.96
1:A:446:VAL:HG11	5:M:2:NAG:H81	1.48	0.96
6:i:1:NAG:H83	6:i:1:NAG:HO3	1.31	0.95
1:F:155:LYS:NZ	1:F:178:ARG:HH12	1.63	0.95
1:A:155:LYS:CE	1:A:178:ARG:NH1	2.30	0.94
9:A:807:NAG:O7	9:A:807:NAG:C3	2.12	0.94
1:F:244:THR:CB	2:H:523:LEU:CD1	2.46	0.94
1:A:494:LEU:HD11	2:C:592:LEU:CD2	1.99	0.93
9:A:807:NAG:O7	9:A:807:NAG:O3	1.87	0.92
7:m:2:NAG:O3	7:m:2:NAG:O7	1.86	0.92
7:O:2:NAG:O7	7:O:2:NAG:O3	1.87	0.92
7:m:2:NAG:O7	7:m:2:NAG:C3	2.12	0.92
9:F:807:NAG:O7	9:F:807:NAG:O3	1.87	0.91
1:F:84:ILE:HG12	2:H:522:PHE:O	1.68	0.91
1:F:244:THR:OG1	2:H:523:LEU:HD12	1.71	0.91
1:B:123:THR:CG2	1:B:124:PRO:HD3	2.01	0.91
8:q:1:NAG:O7	8:q:1:NAG:C3	2.18	0.91
6:d:1:NAG:C8	6:d:1:NAG:H3	1.97	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:2:NAG:O7	7:O:2:NAG:C3	2.15	0.90
1:A:155:LYS:HE3	1:A:178:ARG:CZ	2.03	0.88
8:q:1:NAG:O7	8:q:1:NAG:O3	1.90	0.88
9:F:807:NAG:O7	9:F:807:NAG:C3	2.16	0.88
6:u:2:NAG:O7	6:u:2:NAG:C3	2.21	0.88
4:K:73:LEU:HD12	4:K:73:LEU:C	1.99	0.88
6:T:1:NAG:O7	6:T:1:NAG:C3	2.21	0.88
6:i:2:NAG:O7	6:i:2:NAG:O3	1.92	0.88
1:A:155:LYS:HE3	1:A:178:ARG:NH1	1.89	0.87
6:T:1:NAG:O7	6:T:1:NAG:O3	1.91	0.87
1:F:70:ALA:O	1:F:71:THR:OG1	1.92	0.86
6:i:2:NAG:O7	6:i:2:NAG:C3	2.21	0.86
6:u:2:NAG:O7	6:u:2:NAG:O3	1.92	0.85
2:H:527:GLY:O	2:H:627:THR:HG22	1.75	0.85
1:A:259:LEU:CD2	1:A:374:HIS:NE2	2.37	0.83
1:B:123:THR:HG22	1:B:124:PRO:HD3	1.60	0.83
1:B:155:LYS:O	1:B:175:LEU:CD2	2.27	0.81
6:i:1:NAG:C8	6:i:1:NAG:H3	2.02	0.81
1:A:446:VAL:CG1	5:M:2:NAG:H81	2.11	0.81
6:i:1:NAG:H83	6:i:1:NAG:C3	2.01	0.81
1:A:259:LEU:CD2	1:A:374:HIS:CE1	2.62	0.80
1:F:244:THR:OG1	2:H:523:LEU:CD1	2.29	0.80
1:A:258:GLN:C	1:A:259:LEU:HD13	2.08	0.79
2:C:614:TRP:CD1	2:C:638:TYR:CE2	2.71	0.79
1:A:446:VAL:CG1	5:M:2:NAG:C8	2.61	0.78
2:H:528:SER:HA	6:u:1:NAG:H81	1.64	0.77
1:F:155:LYS:HZ1	1:F:178:ARG:HH12	1.33	0.77
7:m:2:NAG:O7	7:m:2:NAG:H3	1.85	0.76
1:B:156:ASN:HA	1:B:175:LEU:HD23	1.67	0.76
6:p:2:NAG:O7	6:p:2:NAG:C3	2.33	0.76
1:F:84:ILE:HB	1:F:244:THR:HG1	1.49	0.76
1:B:158:SER:HB3	1:B:173:TYR:CD1	2.21	0.76
1:B:178:ARG:HG3	1:B:178:ARG:HH11	1.50	0.76
9:A:807:NAG:O7	9:A:807:NAG:H3	1.84	0.75
1:B:71:THR:OG1	1:B:74:CYS:HB3	1.85	0.75
9:H:703:NAG:O7	9:H:703:NAG:C3	2.34	0.75
1:F:84:ILE:CG1	2:H:522:PHE:O	2.33	0.75
1:F:292:VAL:HB	1:F:449:ILE:HB	1.69	0.75
6:R:2:NAG:C3	6:R:2:NAG:O7	2.33	0.74
1:B:198:THR:HB	1:B:431:GLY:O	1.87	0.74
7:O:2:NAG:O7	7:O:2:NAG:H3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:LYS:HZ2	1:F:178:ARG:HH12	1.35	0.73
1:A:260:LEU:C	1:A:261:LEU:HD23	2.12	0.73
1:F:84:ILE:HG21	2:H:523:LEU:CB	2.18	0.73
1:A:155:LYS:NZ	1:A:178:ARG:NH1	2.36	0.73
1:F:43:PRO:HB2	2:H:526:ALA:CB	2.15	0.72
9:F:807:NAG:O7	9:F:807:NAG:H3	1.88	0.72
1:A:260:LEU:N	1:A:260:LEU:HD23	2.06	0.71
1:F:84:ILE:CG2	2:H:523:LEU:HB2	2.19	0.71
2:H:522:PHE:CD2	2:H:543:ASN:HB3	2.24	0.71
1:A:155:LYS:NZ	1:A:178:ARG:HH12	1.89	0.71
1:F:86:LEU:HD11	1:F:244:THR:HG23	1.72	0.71
1:B:178:ARG:HG3	1:B:178:ARG:NH1	2.03	0.71
4:K:73:LEU:C	4:K:73:LEU:CD1	2.63	0.71
1:F:86:LEU:HD23	2:H:523:LEU:O	1.91	0.71
2:H:528:SER:HB2	6:u:1:NAG:O7	1.91	0.70
1:A:259:LEU:HD13	1:A:259:LEU:N	2.06	0.70
2:C:639:THR:HG22	2:C:643:TYR:CE2	2.26	0.70
1:A:259:LEU:HD22	1:A:259:LEU:H	1.56	0.69
1:A:446:VAL:HG11	5:M:2:NAG:C8	2.18	0.69
1:F:244:THR:HB	2:H:523:LEU:CD1	2.22	0.69
9:H:703:NAG:O7	9:H:703:NAG:O3	2.10	0.69
6:T:1:NAG:O7	6:T:1:NAG:H3	1.94	0.68
8:q:1:NAG:O7	8:q:1:NAG:H3	1.92	0.68
6:p:2:NAG:O7	6:p:2:NAG:O3	2.11	0.68
6:R:2:NAG:O7	6:R:2:NAG:O3	2.11	0.68
6:u:2:NAG:O7	6:u:2:NAG:H3	1.94	0.67
1:F:226:LEU:CD2	1:F:244:THR:HG22	2.24	0.67
2:H:635:ILE:O	2:H:639:THR:HG23	1.95	0.67
1:B:175:LEU:HD11	6:g:1:NAG:C8	2.24	0.67
1:F:229:LYS:HE3	1:F:229:LYS:HA	1.77	0.67
6:i:2:NAG:O7	6:i:2:NAG:H3	1.93	0.66
1:A:261:LEU:O	1:A:262:ASN:HB2	1.95	0.66
1:B:233:PHE:HA	9:B:818:NAG:H81	1.76	0.65
1:B:123:THR:HG23	1:B:124:PRO:HD3	1.75	0.65
1:A:229:LYS:HE3	1:A:229:LYS:HA	1.79	0.65
1:B:172:VAL:HG12	1:B:174:SER:OG	1.97	0.65
1:F:43:PRO:O	2:H:526:ALA:CB	2.45	0.64
1:F:43:PRO:HG2	2:H:526:ALA:HA	1.79	0.64
2:C:639:THR:CG2	2:C:643:TYR:CZ	2.80	0.64
2:H:527:GLY:O	2:H:627:THR:CG2	2.45	0.64
1:F:244:THR:HG21	2:H:523:LEU:CD1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LYS:HE3	1:B:229:LYS:HA	1.81	0.63
1:B:493:PRO:HG2	2:G:589:ASP:OD2	1.99	0.63
2:C:617:ARG:HE	2:C:634:GLU:CD	2.07	0.62
1:A:494:LEU:CD1	2:C:592:LEU:HD23	2.14	0.62
1:F:43:PRO:CG	2:H:526:ALA:HA	2.28	0.62
1:F:86:LEU:HD21	2:H:523:LEU:HB3	1.80	0.62
1:A:503:ARG:O	1:A:503:ARG:HG2	2.00	0.62
1:F:84:ILE:HB	1:F:244:THR:OG1	2.00	0.62
1:B:129:LEU:HD22	1:B:159:PHE:CD2	2.36	0.61
2:H:522:PHE:CE2	2:H:543:ASN:HB3	2.35	0.61
2:H:585:ARG:HH11	2:H:585:ARG:CG	2.14	0.60
1:A:259:LEU:HB2	1:A:261:LEU:HD21	1.84	0.60
1:B:156:ASN:HA	1:B:175:LEU:CD2	2.32	0.60
3:J:33:GLU:OE2	3:J:52:LYS:NZ	2.35	0.60
6:R:2:NAG:O7	6:R:2:NAG:H3	2.02	0.60
1:A:263:GLY:N	1:A:450:THR:HG21	2.16	0.60
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.15	0.59
3:I:84:GLN:N	3:I:84:GLN:OE1	2.35	0.59
1:A:259:LEU:CD2	1:A:374:HIS:ND1	2.64	0.59
1:F:503:ARG:O	1:F:503:ARG:HG2	2.02	0.59
6:W:1:NAG:H61	6:W:2:NAG:H82	1.85	0.59
2:H:522:PHE:CD2	2:H:543:ASN:CB	2.85	0.59
1:B:287:GLN:HG3	1:B:287:GLN:O	2.02	0.58
6:p:2:NAG:O7	6:p:2:NAG:H3	2.02	0.58
7:m:2:NAG:O3	7:m:2:NAG:C7	2.51	0.58
1:A:229:LYS:HE3	1:A:229:LYS:CA	2.33	0.57
1:A:259:LEU:HD21	1:A:374:HIS:ND1	2.18	0.57
3:D:84:GLN:N	3:D:84:GLN:OE1	2.35	0.57
1:A:263:GLY:H	1:A:450:THR:HG21	1.69	0.57
1:F:155:LYS:HZ2	1:F:178:ARG:NH1	2.02	0.57
1:B:493:PRO:CG	2:G:589:ASP:OD2	2.53	0.56
2:H:522:PHE:O	2:H:523:LEU:HB2	2.04	0.56
1:A:155:LYS:HZ1	1:A:178:ARG:HH12	1.50	0.56
1:F:43:PRO:O	2:H:526:ALA:HB1	2.05	0.56
1:F:229:LYS:HE3	1:F:229:LYS:CA	2.34	0.56
4:K:106:ILE:HG23	4:K:106:ILE:O	2.06	0.56
1:F:84:ILE:CB	1:F:244:THR:OG1	2.53	0.56
1:B:229:LYS:HE3	1:B:229:LYS:CA	2.34	0.56
1:F:287:GLN:O	1:F:287:GLN:HG3	2.05	0.55
1:B:496:VAL:HG23	2:G:635:ILE:HD12	1.87	0.55
6:d:1:NAG:C3	6:d:1:NAG:H82	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:CD1	2:C:592:LEU:CD2	2.79	0.54
1:F:43:PRO:O	2:H:526:ALA:HB2	2.08	0.54
7:O:2:NAG:O3	7:O:2:NAG:C7	2.54	0.54
9:A:807:NAG:O3	9:A:807:NAG:C7	2.56	0.54
2:C:549:VAL:O	2:C:550:GLN:C	2.50	0.54
1:B:158:SER:CB	1:B:173:TYR:CD1	2.91	0.53
8:q:1:NAG:O3	8:q:1:NAG:C7	2.55	0.53
1:F:178:ARG:HH11	1:F:178:ARG:CG	2.21	0.53
3:D:33:GLU:OE2	3:D:52:LYS:NZ	2.41	0.53
1:A:259:LEU:HD22	1:A:259:LEU:N	2.22	0.53
2:C:614:TRP:CD1	2:C:638:TYR:CD2	2.96	0.53
2:C:639:THR:CG2	2:C:643:TYR:CE2	2.92	0.53
9:H:703:NAG:O7	9:H:703:NAG:H3	2.07	0.53
6:c:1:NAG:HN2	6:d:1:NAG:C7	2.21	0.53
1:F:155:LYS:NZ	1:F:178:ARG:NH1	2.46	0.53
1:A:155:LYS:CE	1:A:178:ARG:NH2	2.51	0.53
1:F:178:ARG:HH11	1:F:178:ARG:HB2	1.74	0.53
2:C:639:THR:HG22	2:C:643:TYR:CZ	2.44	0.53
1:F:229:LYS:HA	1:F:229:LYS:CE	2.38	0.52
2:C:614:TRP:HA	2:C:638:TYR:CZ	2.44	0.52
1:B:229:LYS:HA	1:B:229:LYS:CE	2.38	0.52
1:F:86:LEU:CD2	2:H:523:LEU:O	2.57	0.52
1:B:175:LEU:HD11	6:g:1:NAG:H82	1.92	0.52
2:H:522:PHE:CD1	2:H:523:LEU:HG	2.44	0.52
2:C:632:ASP:O	2:C:636:SER:HB3	2.10	0.52
1:B:134:VAL:HG22	1:B:156:ASN:HB2	1.92	0.52
1:B:155:LYS:C	1:B:175:LEU:HD23	2.31	0.52
1:A:260:LEU:O	1:A:261:LEU:HD23	2.10	0.51
3:J:112:SER:O	3:J:113:SER:C	2.53	0.51
2:C:640:GLN:HG2	2:C:641:ILE:N	2.26	0.51
3:I:33:GLU:OE2	3:I:52:LYS:NZ	2.43	0.51
1:F:84:ILE:HG21	1:F:244:THR:OG1	2.11	0.51
6:u:2:NAG:O3	6:u:2:NAG:C7	2.58	0.51
1:A:229:LYS:HA	1:A:229:LYS:CE	2.39	0.50
1:A:446:VAL:HG12	5:M:2:NAG:C7	2.42	0.50
2:C:637:ASN:H	9:C:701:NAG:H82	1.75	0.50
6:d:1:NAG:H83	6:d:1:NAG:C3	2.05	0.50
1:F:86:LEU:HD11	1:F:244:THR:CG2	2.39	0.50
1:F:226:LEU:HD23	1:F:244:THR:HG22	1.94	0.50
2:H:585:ARG:HH11	2:H:585:ARG:HG3	1.75	0.50
4:E:106:ILE:HG23	4:E:106:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:HB	2:H:523:LEU:HD13	1.81	0.49
1:B:140:ASP:OD1	1:B:140:ASP:O	2.30	0.49
2:H:606:THR:OG1	2:H:607:ASN:N	2.45	0.49
1:F:277:ILE:HG22	1:F:277:ILE:O	2.13	0.49
3:J:100(E):TYR:OH	4:L:50:ALA:N	2.35	0.49
6:i:2:NAG:O3	6:i:2:NAG:C7	2.58	0.49
3:J:71:ARG:HD2	3:J:71:ARG:C	2.37	0.49
3:I:71:ARG:HD2	3:I:71:ARG:C	2.38	0.48
3:D:71:ARG:HD2	3:D:71:ARG:C	2.39	0.48
9:F:807:NAG:O3	9:F:807:NAG:C7	2.54	0.48
3:I:112:SER:O	3:I:113:SER:C	2.57	0.47
1:A:280:ASN:C	1:A:280:ASN:OD1	2.57	0.47
1:B:158:SER:HA	1:B:173:TYR:HA	1.97	0.47
3:D:112:SER:O	3:D:113:SER:C	2.57	0.47
2:C:639:THR:HG23	2:C:643:TYR:CZ	2.49	0.47
1:F:84:ILE:CG2	1:F:244:THR:OG1	2.63	0.46
2:H:522:PHE:CD1	2:H:522:PHE:C	2.91	0.46
1:B:123:THR:HG23	1:B:124:PRO:CD	2.43	0.46
1:B:503:ARG:HG2	1:B:503:ARG:O	2.15	0.46
2:H:522:PHE:CD1	2:H:523:LEU:N	2.84	0.46
2:H:585:ARG:CG	2:H:585:ARG:NH1	2.73	0.46
1:A:196:CYS:SG	1:A:196:CYS:O	2.73	0.46
1:B:494:LEU:HD21	2:G:596:TRP:HZ3	1.80	0.46
1:B:155:LYS:C	1:B:175:LEU:CD2	2.89	0.46
1:F:178:ARG:NH1	1:F:178:ARG:HG3	2.29	0.46
1:A:263:GLY:H	1:A:450:THR:CG2	2.30	0.45
1:F:490:LYS:O	1:F:490:LYS:HG3	2.16	0.45
6:T:1:NAG:O3	6:T:1:NAG:C7	2.62	0.45
1:A:117:LYS:N	1:A:118:PRO:CD	2.80	0.45
4:K:11:LEU:N	4:K:11:LEU:HD23	2.32	0.45
1:A:446:VAL:HG12	5:M:2:NAG:O7	2.16	0.45
2:C:614:TRP:HD1	2:C:638:TYR:CE2	2.27	0.45
2:G:609:PRO:HB2	9:G:703:NAG:O7	2.17	0.45
3:I:100(B):GLN:O	3:I:100(E):TYR:CE2	2.69	0.45
1:A:260:LEU:HD21	1:A:453:ILE:HG13	1.99	0.45
1:B:129:LEU:CD2	1:B:159:PHE:CD2	2.99	0.45
1:B:363:ASN:CG	1:B:364:SER:N	2.73	0.45
1:A:446:VAL:HG12	5:M:2:NAG:C8	2.45	0.45
1:B:496:VAL:HG23	2:G:635:ILE:CD1	2.47	0.44
1:F:45:TRP:CD1	1:F:45:TRP:C	2.96	0.44
1:A:258:GLN:CB	1:A:259:LEU:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LEU:CD1	1:F:244:THR:HG23	2.44	0.44
2:H:522:PHE:HD1	2:H:523:LEU:N	2.16	0.43
1:F:123:THR:N	1:F:124:PRO:CD	2.81	0.43
2:H:611:ASN:HB3	2:H:614:TRP:CD2	2.53	0.43
1:A:261:LEU:HD23	1:A:261:LEU:N	2.33	0.43
1:B:395:TRP:N	1:B:395:TRP:CD1	2.85	0.43
6:f:1:NAG:H82	6:f:1:NAG:H3	1.12	0.43
1:A:492:GLU:HA	1:A:493:PRO:HD2	1.89	0.43
1:F:178:ARG:HH11	1:F:178:ARG:CB	2.32	0.43
1:A:261:LEU:O	1:A:262:ASN:CB	2.64	0.42
2:G:607:ASN:OD1	2:G:607:ASN:C	2.62	0.42
3:J:71:ARG:HD2	3:J:71:ARG:O	2.19	0.42
1:B:325:ASP:OD1	1:B:325:ASP:C	2.62	0.42
2:C:585:ARG:HG3	2:C:585:ARG:HH11	1.84	0.42
1:F:43:PRO:HB2	2:H:526:ALA:CA	2.49	0.42
1:F:277:ILE:O	1:F:277:ILE:CG2	2.67	0.42
2:H:638:TYR:HB3	2:H:641:ILE:HD12	2.01	0.42
2:H:611:ASN:HB3	2:H:614:TRP:CE3	2.54	0.42
1:A:166:ARG:NH2	1:B:169:LYS:HZ1	2.18	0.42
1:B:123:THR:CG2	1:B:124:PRO:CD	2.87	0.42
1:B:122:LEU:HB2	1:B:201:ILE:O	2.20	0.42
1:B:123:THR:HB	1:B:200:ALA:HB1	2.01	0.42
4:K:11:LEU:HD23	4:K:11:LEU:H	1.85	0.42
2:H:528:SER:CB	6:u:1:NAG:O7	2.64	0.42
2:H:522:PHE:CE1	2:H:523:LEU:HG	2.55	0.42
1:A:169:LYS:NZ	1:F:166:ARG:HH12	2.18	0.41
1:A:120:VAL:O	1:A:120:VAL:HG22	2.19	0.41
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.81	0.41
1:B:490:LYS:O	1:B:490:LYS:HG3	2.20	0.41
3:J:100(E):TYR:OH	4:L:50:ALA:HB2	2.20	0.41
1:A:166:ARG:NH2	1:B:169:LYS:NZ	2.68	0.41
1:B:363:ASN:OD1	1:B:364:SER:N	2.53	0.41
1:A:261:LEU:HB2	5:M:1:NAG:H82	2.03	0.41
2:H:638:TYR:CD1	2:H:638:TYR:N	2.89	0.41
1:B:172:VAL:CG1	1:B:174:SER:OG	2.66	0.40
4:L:106:ILE:O	4:L:106:ILE:HG23	2.21	0.40
1:F:325:ASP:OD1	1:F:325:ASP:C	2.64	0.40
1:F:117:LYS:N	1:F:118:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/480 (92%)	430 (97%)	12 (3%)	0	100	100
1	B	442/480 (92%)	434 (98%)	8 (2%)	0	100	100
1	F	442/480 (92%)	427 (97%)	15 (3%)	0	100	100
2	C	118/153 (77%)	117 (99%)	1 (1%)	0	100	100
2	G	118/153 (77%)	117 (99%)	1 (1%)	0	100	100
2	H	118/153 (77%)	115 (98%)	3 (2%)	0	100	100
3	D	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
3	I	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
3	J	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
4	E	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
4	K	98/208 (47%)	96 (98%)	2 (2%)	0	100	100
4	L	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
All	All	2343/3207 (73%)	2290 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	400/427 (94%)	395 (99%)	5 (1%)	61	71
1	B	400/427 (94%)	394 (98%)	6 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	400/427 (94%)	397 (99%)	3 (1%)	73	77
2	C	105/129 (81%)	102 (97%)	3 (3%)	37	58
2	G	105/129 (81%)	104 (99%)	1 (1%)	68	75
2	H	105/129 (81%)	102 (97%)	3 (3%)	37	58
3	D	104/193 (54%)	104 (100%)	0	100	100
3	I	104/193 (54%)	104 (100%)	0	100	100
3	J	104/193 (54%)	104 (100%)	0	100	100
4	E	85/182 (47%)	85 (100%)	0	100	100
4	K	85/182 (47%)	84 (99%)	1 (1%)	63	73
4	L	85/182 (47%)	85 (100%)	0	100	100
All	All	2082/2793 (74%)	2060 (99%)	22 (1%)	63	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	260	LEU
1	A	265	LEU
1	A	295	ASN
1	A	301	ASN
2	C	585	ARG
2	C	618	ASN
2	C	639	THR
1	B	88	ASN
1	B	178	ARG
1	B	201	ILE
1	B	301	ASN
1	B	363	ASN
1	B	496	VAL
2	G	618	ASN
4	K	73	LEU
1	F	155	LYS
1	F	178	ARG
1	F	301	ASN
2	H	585	ARG
2	H	618	ASN
2	H	638	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	GLN
2	C	590	GLN
2	C	616	ASN
3	D	1	GLN
3	D	6	GLN
3	D	35(A)	HIS
3	D	79	HIS
4	E	37	GLN
3	I	1	GLN
4	K	37	GLN
4	K	66	GLN
3	J	6	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](#)

87 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	M	1	1,5	14,14,15	0.77	0	17,19,21	0.98	0
5	NAG	M	2	5	14,14,15	0.84	0	17,19,21	1.08	1 (5%)
5	BMA	M	3	5	11,11,12	1.84	1 (9%)	15,15,17	0.88	1 (6%)
5	MAN	M	4	5	11,11,12	1.83	2 (18%)	15,15,17	0.78	0
6	NAG	N	1	1,6	14,14,15	0.80	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	2	6	14,14,15	0.89	0	17,19,21	0.89	1 (5%)
7	NAG	O	1	1,7	14,14,15	0.82	0	17,19,21	1.02	1 (5%)
7	NAG	O	2	7	14,14,15	0.89	1 (7%)	17,19,21	0.92	1 (5%)
7	BMA	O	3	7	11,11,12	1.94	3 (27%)	15,15,17	0.93	0
7	MAN	O	4	7	11,11,12	1.85	2 (18%)	15,15,17	0.89	1 (6%)
6	NAG	P	1	1,6	14,14,15	0.80	1 (7%)	17,19,21	1.06	1 (5%)
6	NAG	P	2	6	14,14,15	0.83	0	17,19,21	0.90	1 (5%)
6	NAG	Q	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	0.90	1 (5%)
6	NAG	Q	2	6	14,14,15	0.81	0	17,19,21	0.84	1 (5%)
6	NAG	R	1	1,6	14,14,15	0.86	1 (7%)	17,19,21	1.52	2 (11%)
6	NAG	R	2	6	14,14,15	0.88	0	17,19,21	1.04	1 (5%)
8	NAG	S	1	1,8	14,14,15	0.94	0	17,19,21	0.89	0
8	NAG	S	2	8	14,14,15	0.84	0	17,19,21	0.82	0
8	BMA	S	3	8	11,11,12	1.85	2 (18%)	15,15,17	0.80	0
6	NAG	T	1	1,6	14,14,15	0.71	0	17,19,21	1.05	0
6	NAG	T	2	6	14,14,15	0.79	0	17,19,21	0.82	1 (5%)
6	NAG	U	1	1,6	14,14,15	0.83	1 (7%)	17,19,21	1.14	2 (11%)
6	NAG	U	2	6	14,14,15	0.89	1 (7%)	17,19,21	0.94	1 (5%)
6	NAG	V	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.28	2 (11%)
6	NAG	V	2	6	14,14,15	0.83	0	17,19,21	0.81	1 (5%)
6	NAG	W	1	1,6	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
6	NAG	W	2	6	14,14,15	0.90	0	17,19,21	0.76	0
6	NAG	X	1	1,6	14,14,15	0.82	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	X	2	6	14,14,15	0.84	0	17,19,21	0.89	1 (5%)
5	NAG	Y	1	1,5	14,14,15	0.71	0	17,19,21	0.90	0
5	NAG	Y	2	5	14,14,15	0.79	0	17,19,21	1.10	1 (5%)
5	BMA	Y	3	5	11,11,12	1.85	1 (9%)	15,15,17	0.87	1 (6%)
5	MAN	Y	4	5	11,11,12	1.82	2 (18%)	15,15,17	0.79	0
6	NAG	Z	1	1,6	14,14,15	0.82	1 (7%)	17,19,21	1.02	0
6	NAG	Z	2	6	14,14,15	0.89	0	17,19,21	0.89	1 (5%)
7	NAG	a	1	1,7	14,14,15	0.79	0	17,19,21	0.94	1 (5%)
7	NAG	a	2	7	14,14,15	0.80	0	17,19,21	0.97	1 (5%)
7	BMA	a	3	7	11,11,12	1.98	4 (36%)	15,15,17	1.05	1 (6%)
7	MAN	a	4	7	11,11,12	1.85	2 (18%)	15,15,17	0.90	0
6	NAG	b	1	1,6	14,14,15	0.75	0	17,19,21	0.95	1 (5%)
6	NAG	b	2	6	14,14,15	0.81	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	c	1	1,6	14,14,15	1.05	1 (7%)	17,19,21	1.18	2 (11%)
6	NAG	c	2	6	14,14,15	0.84	0	17,19,21	0.90	1 (5%)
6	NAG	d	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.46	4 (23%)
6	NAG	d	2	6	14,14,15	1.00	0	17,19,21	1.09	2 (11%)
8	NAG	e	1	1,8	14,14,15	0.95	0	17,19,21	0.89	0
8	NAG	e	2	8	14,14,15	0.83	0	17,19,21	0.82	0
8	BMA	e	3	8	11,11,12	1.84	2 (18%)	15,15,17	0.81	0
6	NAG	f	1	1,6	14,14,15	0.69	0	17,19,21	0.91	0
6	NAG	f	2	6	14,14,15	0.78	0	17,19,21	0.89	1 (5%)
6	NAG	g	1	1,6	14,14,15	0.83	1 (7%)	17,19,21	0.98	0
6	NAG	g	2	6	14,14,15	0.84	1 (7%)	17,19,21	0.97	1 (5%)
6	NAG	h	1	1,6	14,14,15	0.84	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	h	2	6	14,14,15	0.86	0	17,19,21	0.80	1 (5%)
6	NAG	i	1	1,6	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
6	NAG	i	2	6	14,14,15	0.96	0	17,19,21	0.73	0
6	NAG	j	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	1.07	1 (5%)
6	NAG	j	2	6	14,14,15	0.83	0	17,19,21	0.90	1 (5%)
5	NAG	k	1	1,5	14,14,15	0.77	0	17,19,21	0.97	0
5	NAG	k	2	5	14,14,15	0.84	0	17,19,21	1.05	1 (5%)
5	BMA	k	3	5	11,11,12	1.85	1 (9%)	15,15,17	0.88	1 (6%)
5	MAN	k	4	5	11,11,12	1.85	2 (18%)	15,15,17	0.79	0
6	NAG	l	1	1,6	14,14,15	0.79	1 (7%)	17,19,21	1.11	2 (11%)
6	NAG	l	2	6	14,14,15	0.89	0	17,19,21	0.88	1 (5%)
7	NAG	m	1	1,7	14,14,15	0.85	0	17,19,21	0.92	0
7	NAG	m	2	7	14,14,15	0.91	1 (7%)	17,19,21	1.09	1 (5%)
7	BMA	m	3	7	11,11,12	1.98	4 (36%)	15,15,17	1.08	1 (6%)
7	MAN	m	4	7	11,11,12	1.88	3 (27%)	15,15,17	0.90	0
6	NAG	n	1	1,6	14,14,15	0.75	1 (7%)	17,19,21	0.95	0
6	NAG	n	2	6	14,14,15	0.84	0	17,19,21	0.86	1 (5%)
6	NAG	o	1	1,6	14,14,15	0.96	1 (7%)	17,19,21	1.09	1 (5%)
6	NAG	o	2	6	14,14,15	0.81	0	17,19,21	0.85	1 (5%)
6	NAG	p	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.54	3 (17%)
6	NAG	p	2	6	14,14,15	0.88	0	17,19,21	0.99	1 (5%)
8	NAG	q	1	1,8	14,14,15	0.92	0	17,19,21	0.90	0
8	NAG	q	2	8	14,14,15	0.81	0	17,19,21	0.83	0
8	BMA	q	3	8	11,11,12	1.84	2 (18%)	15,15,17	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	r	1	1,6	14,14,15	0.63	0	17,19,21	0.96	0
6	NAG	r	2	6	14,14,15	0.80	0	17,19,21	0.85	1 (5%)
6	NAG	s	1	1,6	14,14,15	0.81	1 (7%)	17,19,21	0.95	0
6	NAG	s	2	6	14,14,15	0.85	1 (7%)	17,19,21	0.95	1 (5%)
6	NAG	t	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.29	2 (11%)
6	NAG	t	2	6	14,14,15	0.83	0	17,19,21	0.80	1 (5%)
6	NAG	u	1	1,6	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
6	NAG	u	2	6	14,14,15	0.92	0	17,19,21	0.72	0
6	NAG	v	1	1,6	14,14,15	0.88	1 (7%)	17,19,21	1.03	1 (5%)
6	NAG	v	2	6	14,14,15	0.79	0	17,19,21	0.91	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	3/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	1/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	BMA	a	3	7	-	2/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
6	NAG	b	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	3/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
8	NAG	e	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	2/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	g	2	6	-	2/6/23/26	0/1/1/1
6	NAG	h	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	3/6/23/26	0/1/1/1
6	NAG	i	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	i	2	6	-	2/6/23/26	0/1/1/1
6	NAG	j	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	3/6/23/26	0/1/1/1
5	NAG	k	1	1,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
5	BMA	k	3	5	-	1/2/19/22	0/1/1/1
5	MAN	k	4	5	-	1/2/19/22	0/1/1/1
6	NAG	l	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1
7	NAG	m	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	m	2	7	-	1/6/23/26	0/1/1/1
7	BMA	m	3	7	-	2/2/19/22	0/1/1/1
7	MAN	m	4	7	-	0/2/19/22	0/1/1/1
6	NAG	n	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	n	2	6	-	1/6/23/26	0/1/1/1
6	NAG	o	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	o	2	6	-	3/6/23/26	0/1/1/1
6	NAG	p	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	p	2	6	-	2/6/23/26	0/1/1/1
8	NAG	q	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	q	3	8	-	1/2/19/22	0/1/1/1
6	NAG	r	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	r	2	6	-	2/6/23/26	0/1/1/1
6	NAG	s	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
6	NAG	t	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	t	2	6	-	1/6/23/26	0/1/1/1
6	NAG	u	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	u	2	6	-	2/6/23/26	0/1/1/1
6	NAG	v	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	v	2	6	-	3/6/23/26	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	4	MAN	O2-C2	-4.31	1.34	1.43
5	k	3	BMA	O2-C2	-4.29	1.34	1.43
7	m	4	MAN	O2-C2	-4.28	1.34	1.43
5	Y	3	BMA	O2-C2	-4.27	1.34	1.43
7	a	4	MAN	O2-C2	-4.26	1.34	1.43
5	M	3	BMA	O2-C2	-4.26	1.34	1.43
7	a	3	BMA	O2-C2	-4.24	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	m	3	BMA	O2-C2	-4.23	1.34	1.43
8	S	3	BMA	O2-C2	-4.21	1.34	1.43
5	k	4	MAN	O2-C2	-4.20	1.34	1.43
8	e	3	BMA	O2-C2	-4.20	1.34	1.43
8	q	3	BMA	O2-C2	-4.19	1.34	1.43
7	O	3	BMA	O2-C2	-4.17	1.34	1.43
5	M	4	MAN	O2-C2	-4.15	1.34	1.43
5	Y	4	MAN	O2-C2	-4.14	1.34	1.43
7	O	3	BMA	C2-C3	-2.82	1.48	1.52
7	m	3	BMA	C2-C3	-2.80	1.48	1.52
7	a	3	BMA	C2-C3	-2.75	1.48	1.52
6	c	1	NAG	C3-C2	-2.69	1.46	1.52
7	a	4	MAN	C2-C3	-2.64	1.48	1.52
7	O	4	MAN	C2-C3	-2.53	1.48	1.52
7	m	4	MAN	C2-C3	-2.49	1.48	1.52
6	o	1	NAG	C3-C2	-2.46	1.47	1.52
6	Q	1	NAG	C3-C2	-2.44	1.47	1.52
5	k	4	MAN	C2-C3	-2.38	1.48	1.52
6	g	1	NAG	C3-C2	-2.37	1.47	1.52
5	M	4	MAN	C2-C3	-2.36	1.48	1.52
5	Y	4	MAN	C2-C3	-2.32	1.48	1.52
6	s	1	NAG	C3-C2	-2.32	1.47	1.52
8	q	3	BMA	C2-C3	-2.31	1.48	1.52
8	e	3	BMA	C2-C3	-2.30	1.49	1.52
8	S	3	BMA	C2-C3	-2.28	1.49	1.52
6	P	1	NAG	C3-C2	-2.25	1.47	1.52
6	R	1	NAG	C3-C2	-2.24	1.47	1.52
7	a	3	BMA	C6-C5	2.24	1.59	1.51
6	j	1	NAG	C3-C2	-2.23	1.47	1.52
7	m	4	MAN	O5-C1	2.21	1.47	1.43
6	p	1	NAG	C3-C2	-2.19	1.47	1.52
6	X	1	NAG	C3-C2	-2.18	1.47	1.52
6	d	1	NAG	C3-C2	-2.18	1.48	1.52
7	m	3	BMA	C6-C5	2.17	1.59	1.51
6	U	2	NAG	C3-C2	-2.16	1.48	1.52
7	m	2	NAG	C3-C2	-2.14	1.48	1.52
6	v	1	NAG	C3-C2	-2.13	1.48	1.52
6	s	2	NAG	C3-C2	-2.10	1.48	1.52
6	U	1	NAG	C3-C2	-2.10	1.48	1.52
6	t	1	NAG	C3-C2	-2.07	1.48	1.52
7	m	3	BMA	O5-C1	2.07	1.47	1.43
6	g	2	NAG	C3-C2	-2.05	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	NAG	C3-C2	-2.05	1.48	1.52
7	O	3	BMA	C6-C5	2.04	1.58	1.51
7	O	2	NAG	C3-C2	-2.04	1.48	1.52
6	l	1	NAG	C3-C2	-2.04	1.48	1.52
6	n	1	NAG	C3-C2	-2.03	1.48	1.52
6	h	1	NAG	C3-C2	-2.03	1.48	1.52
6	Z	1	NAG	C3-C2	-2.02	1.48	1.52
7	a	3	BMA	O5-C1	2.01	1.47	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	p	1	NAG	O4-C4-C3	3.90	119.58	110.38
6	R	1	NAG	O4-C4-C3	3.83	119.41	110.38
6	p	1	NAG	C4-C3-C2	-3.35	106.11	111.02
6	R	1	NAG	C4-C3-C2	-3.31	106.17	111.02
6	o	1	NAG	C1-C2-N2	-3.25	105.31	110.43
6	i	1	NAG	C4-C3-C2	-3.21	106.31	111.02
6	u	1	NAG	C4-C3-C2	-3.12	106.45	111.02
6	d	1	NAG	C8-C7-N2	3.03	121.14	116.12
6	V	1	NAG	C4-C3-C2	-3.02	106.59	111.02
6	t	1	NAG	C4-C3-C2	-3.01	106.61	111.02
6	v	1	NAG	C1-C2-N2	-3.00	105.71	110.43
6	c	1	NAG	C1-C2-N2	-2.89	105.88	110.43
6	d	2	NAG	C4-C3-C2	-2.81	106.90	111.02
6	c	1	NAG	C4-C3-C2	-2.79	106.93	111.02
6	g	2	NAG	C4-C3-C2	-2.74	107.00	111.02
6	j	1	NAG	C1-C2-N2	-2.73	106.14	110.43
6	d	1	NAG	O4-C4-C3	2.72	116.78	110.38
6	h	1	NAG	C4-C3-C2	-2.71	107.04	111.02
5	Y	2	NAG	C4-C3-C2	-2.70	107.07	111.02
6	s	2	NAG	C4-C3-C2	-2.69	107.08	111.02
6	t	1	NAG	C2-N2-C7	-2.68	119.31	122.90
6	V	1	NAG	C2-N2-C7	-2.66	119.33	122.90
5	M	2	NAG	C4-C3-C2	-2.61	107.19	111.02
6	v	2	NAG	C4-C3-C2	-2.55	107.28	111.02
6	f	2	NAG	C4-C3-C2	-2.54	107.30	111.02
5	k	2	NAG	C4-C3-C2	-2.53	107.31	111.02
6	U	2	NAG	C4-C3-C2	-2.52	107.32	111.02
6	j	2	NAG	C4-C3-C2	-2.52	107.33	111.02
6	X	2	NAG	C4-C3-C2	-2.50	107.35	111.02
6	R	2	NAG	C4-C3-C2	-2.47	107.39	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	m	3	BMA	O6-C6-C5	2.46	119.70	111.33
6	U	1	NAG	O5-C5-C6	-2.45	102.89	107.66
6	P	2	NAG	C4-C3-C2	-2.44	107.45	111.02
5	k	3	BMA	C2-C3-C4	-2.43	106.58	110.86
5	M	3	BMA	C2-C3-C4	-2.43	106.59	110.86
6	N	2	NAG	C4-C3-C2	-2.40	107.50	111.02
7	a	3	BMA	O6-C6-C5	2.39	119.49	111.33
6	T	2	NAG	C4-C3-C2	-2.39	107.52	111.02
5	Y	3	BMA	C2-C3-C4	-2.39	106.66	110.86
6	r	2	NAG	C4-C3-C2	-2.38	107.53	111.02
6	Z	2	NAG	C4-C3-C2	-2.38	107.53	111.02
6	l	2	NAG	C4-C3-C2	-2.36	107.56	111.02
6	n	2	NAG	C4-C3-C2	-2.34	107.59	111.02
6	c	2	NAG	C4-C3-C2	-2.34	107.59	111.02
6	p	2	NAG	C4-C3-C2	-2.30	107.64	111.02
6	o	2	NAG	C4-C3-C2	-2.27	107.70	111.02
6	Q	2	NAG	C4-C3-C2	-2.26	107.70	111.02
6	b	2	NAG	C4-C3-C2	-2.25	107.72	111.02
6	X	1	NAG	C1-C2-N2	-2.23	106.92	110.43
6	d	1	NAG	C4-C3-C2	-2.20	107.80	111.02
7	a	1	NAG	C1-C2-N2	-2.16	107.03	110.43
6	P	1	NAG	O4-C4-C3	-2.16	105.29	110.38
7	m	2	NAG	C4-C3-C2	-2.16	107.86	111.02
7	a	2	NAG	C4-C3-C2	-2.15	107.86	111.02
6	U	1	NAG	C4-C3-C2	-2.14	107.89	111.02
6	V	2	NAG	C4-C3-C2	-2.13	107.89	111.02
6	h	2	NAG	C4-C3-C2	-2.13	107.90	111.02
6	l	1	NAG	C4-C3-C2	-2.12	107.90	111.02
6	W	1	NAG	C4-C3-C2	-2.12	107.91	111.02
6	t	2	NAG	C4-C3-C2	-2.12	107.91	111.02
6	b	1	NAG	C1-C2-N2	-2.10	107.13	110.43
6	N	1	NAG	C4-C3-C2	-2.09	107.95	111.02
6	l	1	NAG	C1-C2-N2	-2.07	107.17	110.43
7	O	1	NAG	C1-C2-N2	-2.05	107.20	110.43
6	d	2	NAG	C6-C5-C4	-2.04	108.00	113.02
6	Q	1	NAG	C1-C2-N2	-2.04	107.22	110.43
6	W	1	NAG	O5-C5-C6	-2.03	103.71	107.66
7	O	2	NAG	C4-C3-C2	-2.02	108.05	111.02
6	d	1	NAG	O7-C7-N2	-2.02	118.41	121.98
6	p	1	NAG	C1-C2-N2	-2.02	107.25	110.43
7	O	4	MAN	C2-C3-C4	-2.01	107.32	110.86

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	2	NAG	C3-C2-N2-C7
6	T	1	NAG	C3-C2-N2-C7
6	d	1	NAG	C3-C2-N2-C7
6	f	1	NAG	C3-C2-N2-C7
6	i	1	NAG	C3-C2-N2-C7
6	i	2	NAG	C3-C2-N2-C7
6	p	2	NAG	C3-C2-N2-C7
6	r	1	NAG	C3-C2-N2-C7
6	u	2	NAG	C3-C2-N2-C7
7	O	2	NAG	C3-C2-N2-C7
7	m	2	NAG	C3-C2-N2-C7
8	q	1	NAG	C3-C2-N2-C7
7	O	3	BMA	O5-C5-C6-O6
7	a	3	BMA	O5-C5-C6-O6
6	g	2	NAG	C4-C5-C6-O6
7	m	3	BMA	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
7	a	3	BMA	C4-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
7	m	3	BMA	C4-C5-C6-O6
7	O	3	BMA	C4-C5-C6-O6
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	k	1	NAG	C8-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	k	2	NAG	C8-C7-N2-C2
5	k	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	P	2	NAG	C8-C7-N2-C2
6	P	2	NAG	O7-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	X	2	NAG	C8-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
6	Z	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	Z	2	NAG	O7-C7-N2-C2
6	b	2	NAG	C8-C7-N2-C2
6	b	2	NAG	O7-C7-N2-C2
6	c	1	NAG	C8-C7-N2-C2
6	c	1	NAG	O7-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2
6	c	2	NAG	O7-C7-N2-C2
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	d	2	NAG	C8-C7-N2-C2
6	d	2	NAG	O7-C7-N2-C2
6	f	1	NAG	C8-C7-N2-C2
6	f	1	NAG	O7-C7-N2-C2
6	f	2	NAG	C8-C7-N2-C2
6	f	2	NAG	O7-C7-N2-C2
6	h	2	NAG	C8-C7-N2-C2
6	h	2	NAG	O7-C7-N2-C2
6	i	1	NAG	C8-C7-N2-C2
6	i	1	NAG	O7-C7-N2-C2
6	j	1	NAG	C8-C7-N2-C2
6	j	1	NAG	O7-C7-N2-C2
6	j	2	NAG	C8-C7-N2-C2
6	j	2	NAG	O7-C7-N2-C2
6	l	2	NAG	C8-C7-N2-C2
6	l	2	NAG	O7-C7-N2-C2
6	o	2	NAG	C8-C7-N2-C2
6	o	2	NAG	O7-C7-N2-C2
6	r	1	NAG	C8-C7-N2-C2
6	r	1	NAG	O7-C7-N2-C2
6	r	2	NAG	C8-C7-N2-C2
6	r	2	NAG	O7-C7-N2-C2
6	s	1	NAG	C8-C7-N2-C2
6	s	1	NAG	O7-C7-N2-C2
6	s	2	NAG	C8-C7-N2-C2
6	s	2	NAG	O7-C7-N2-C2
6	u	1	NAG	C8-C7-N2-C2
6	u	1	NAG	O7-C7-N2-C2
6	v	1	NAG	C8-C7-N2-C2
6	v	1	NAG	O7-C7-N2-C2
6	v	2	NAG	C8-C7-N2-C2
6	v	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	O	1	NAG	O7-C7-N2-C2
7	m	1	NAG	C8-C7-N2-C2
7	m	1	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
6	V	2	NAG	O5-C5-C6-O6
6	t	2	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
6	u	2	NAG	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	k	4	MAN	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	i	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	b	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	o	2	NAG	O5-C5-C6-O6
6	p	2	NAG	O5-C5-C6-O6
6	v	2	NAG	O5-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
8	q	3	BMA	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
8	e	3	BMA	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 60 short contacts:

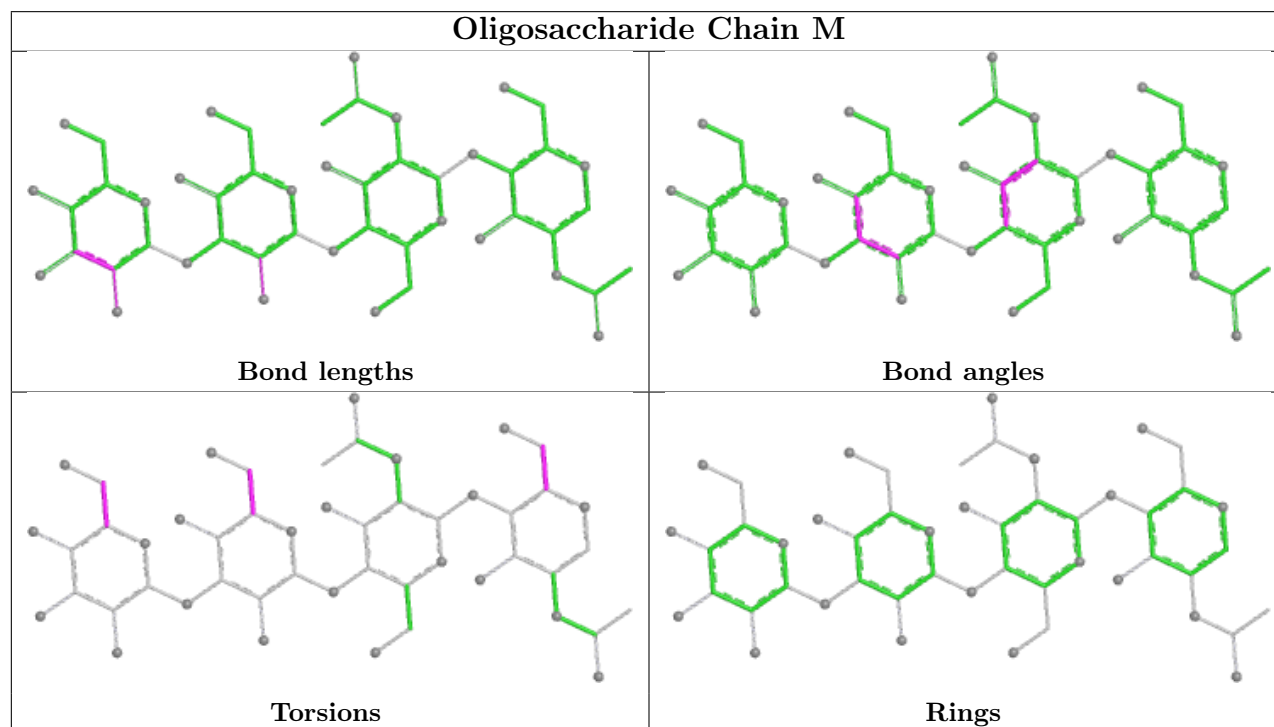
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	c	1	NAG	1	0
6	R	2	NAG	3	0
6	i	2	NAG	4	0

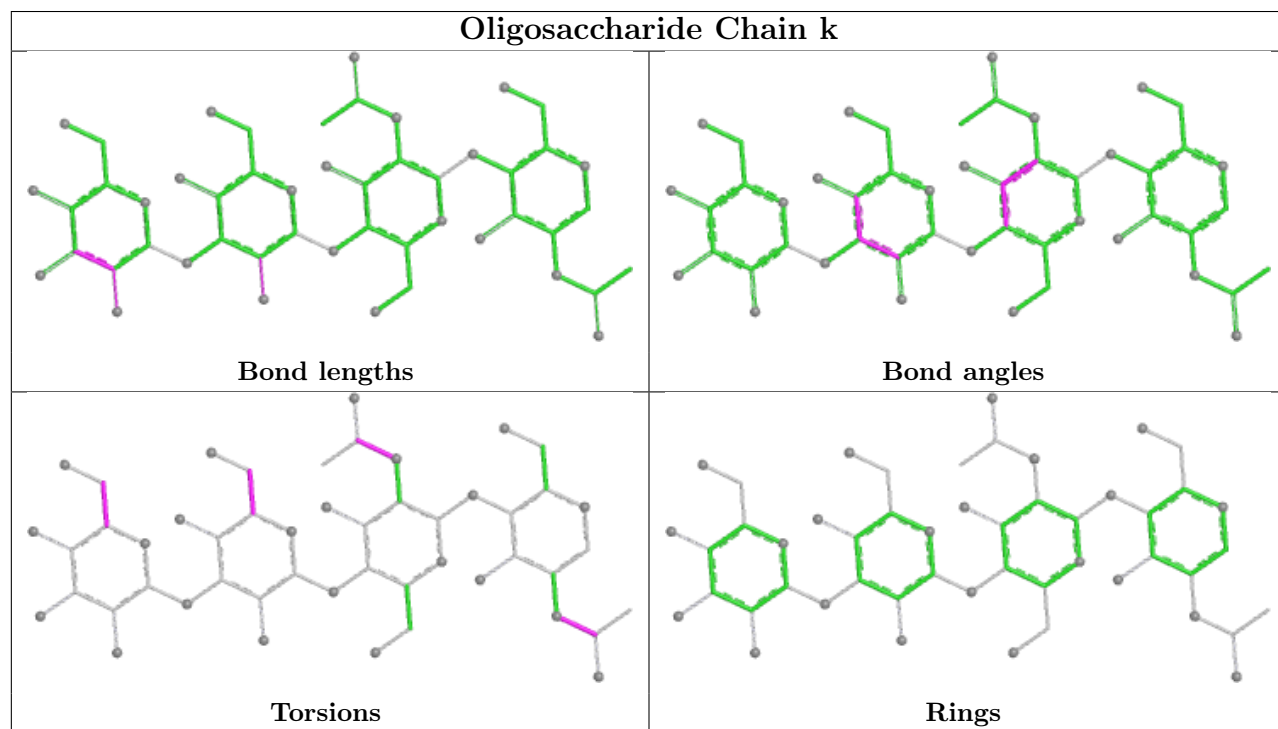
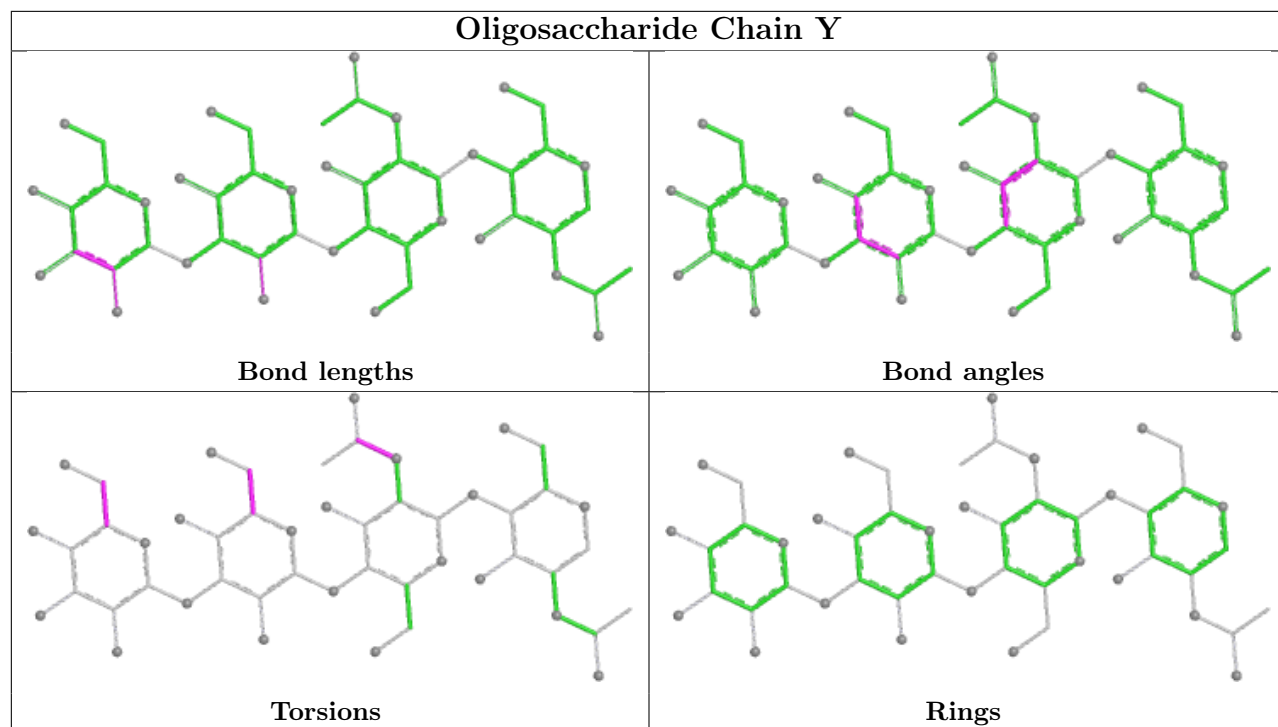
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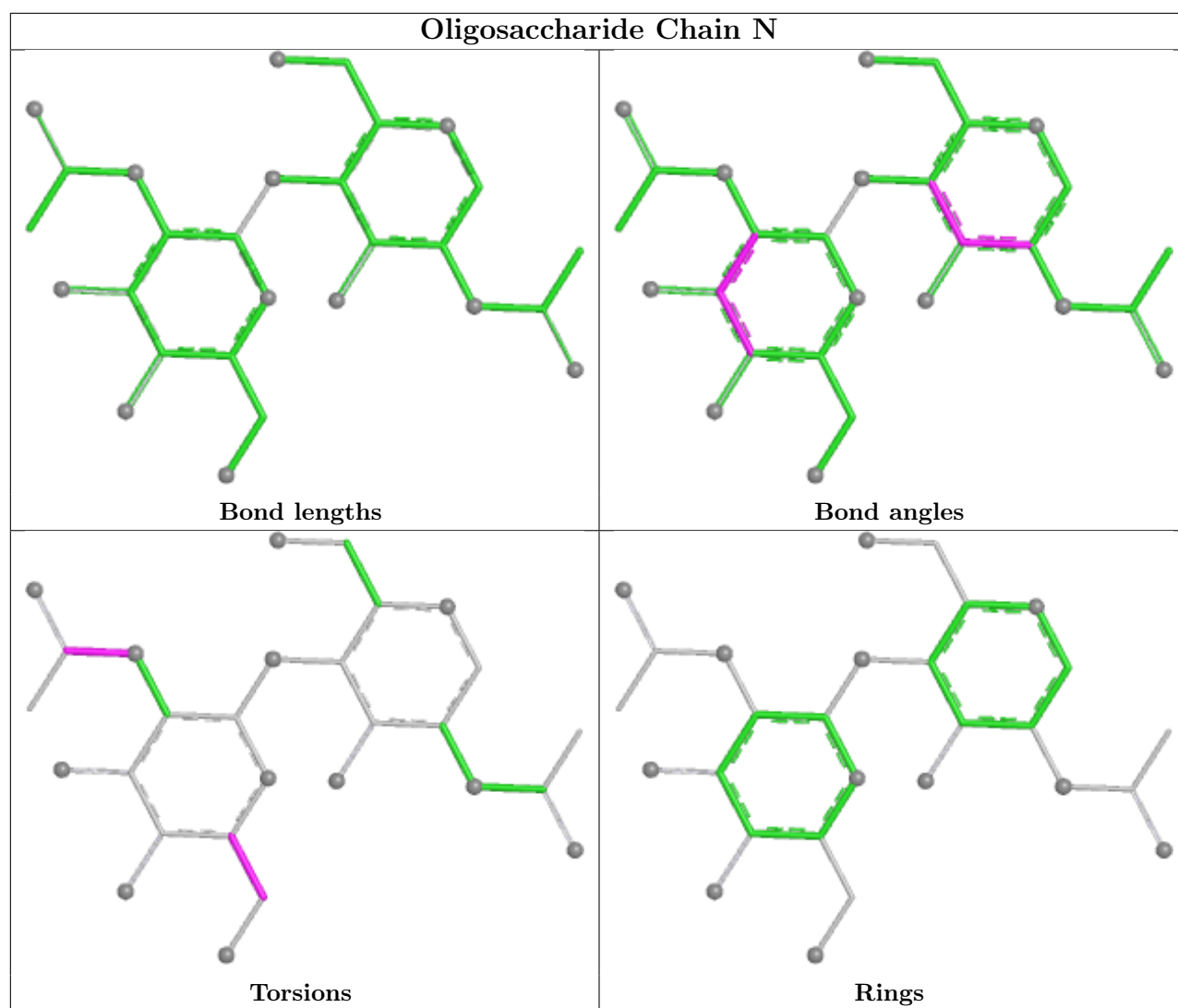
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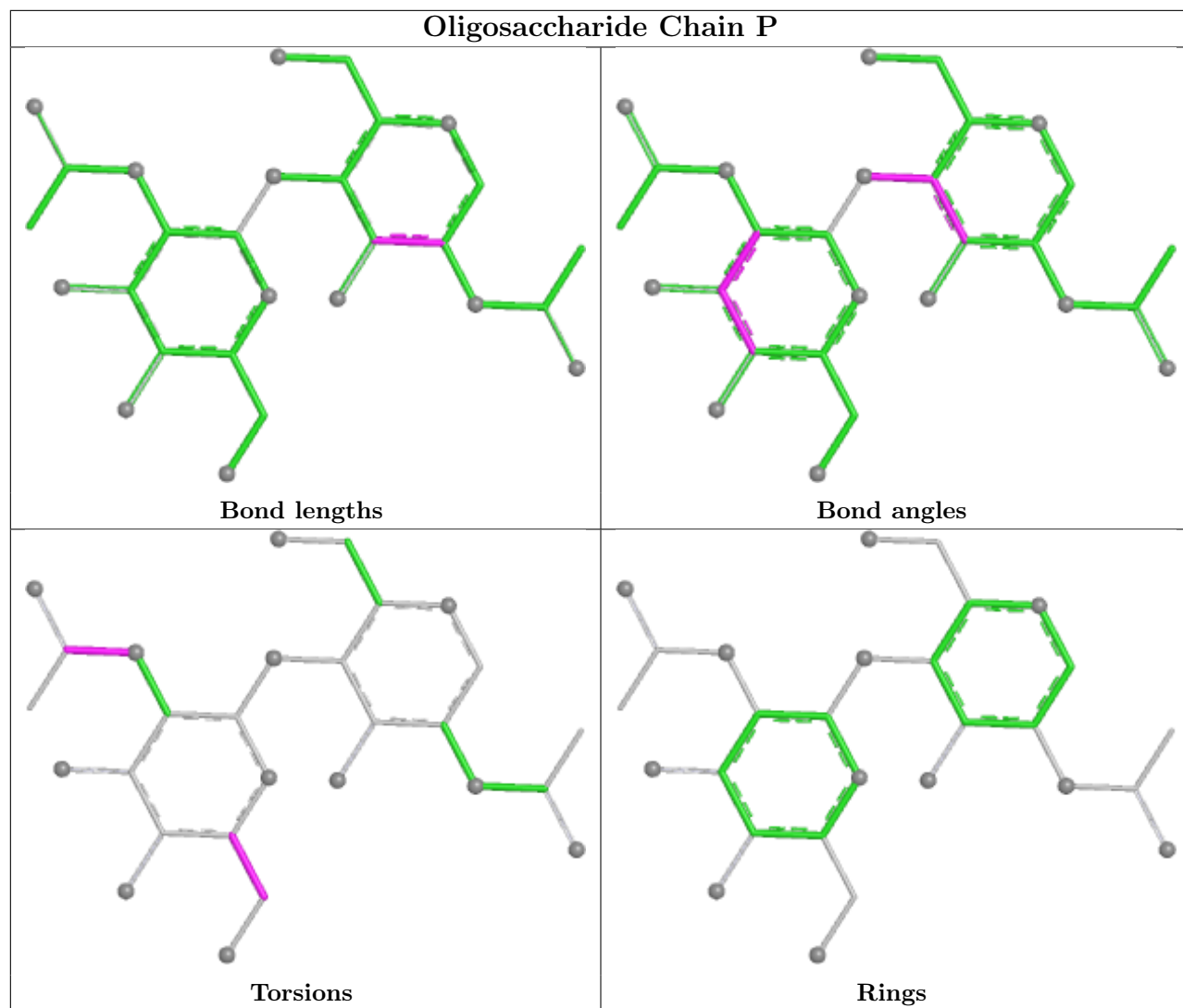
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	2	NAG	4	0
6	W	1	NAG	1	0
6	f	1	NAG	1	0
6	T	1	NAG	4	0
6	p	2	NAG	3	0
6	g	1	NAG	2	0
6	d	1	NAG	8	0
5	M	2	NAG	7	0
6	i	1	NAG	7	0
5	M	1	NAG	1	0
8	q	1	NAG	4	0
6	u	2	NAG	4	0
6	W	2	NAG	1	0
6	u	1	NAG	3	0
7	m	2	NAG	4	0

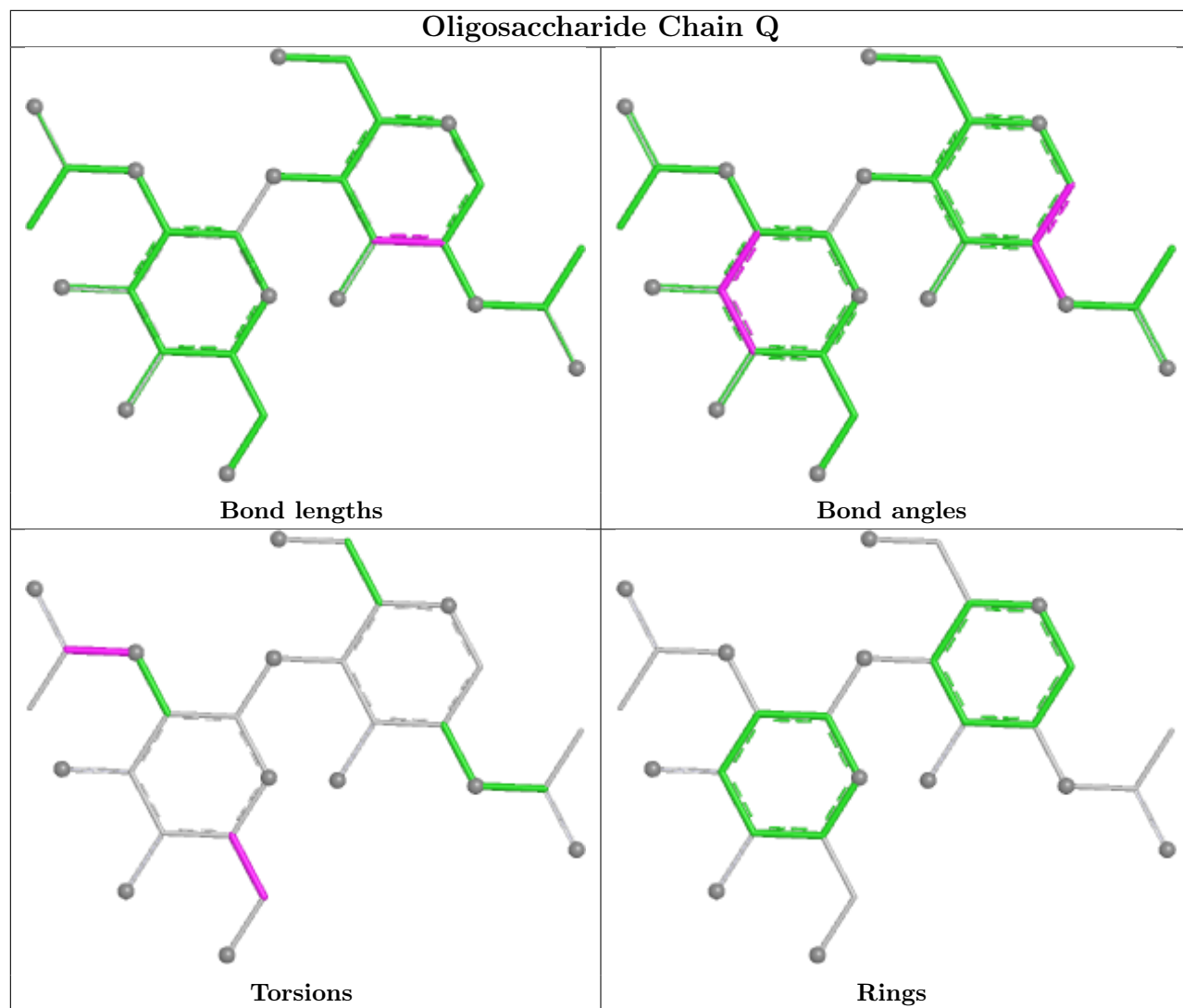
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

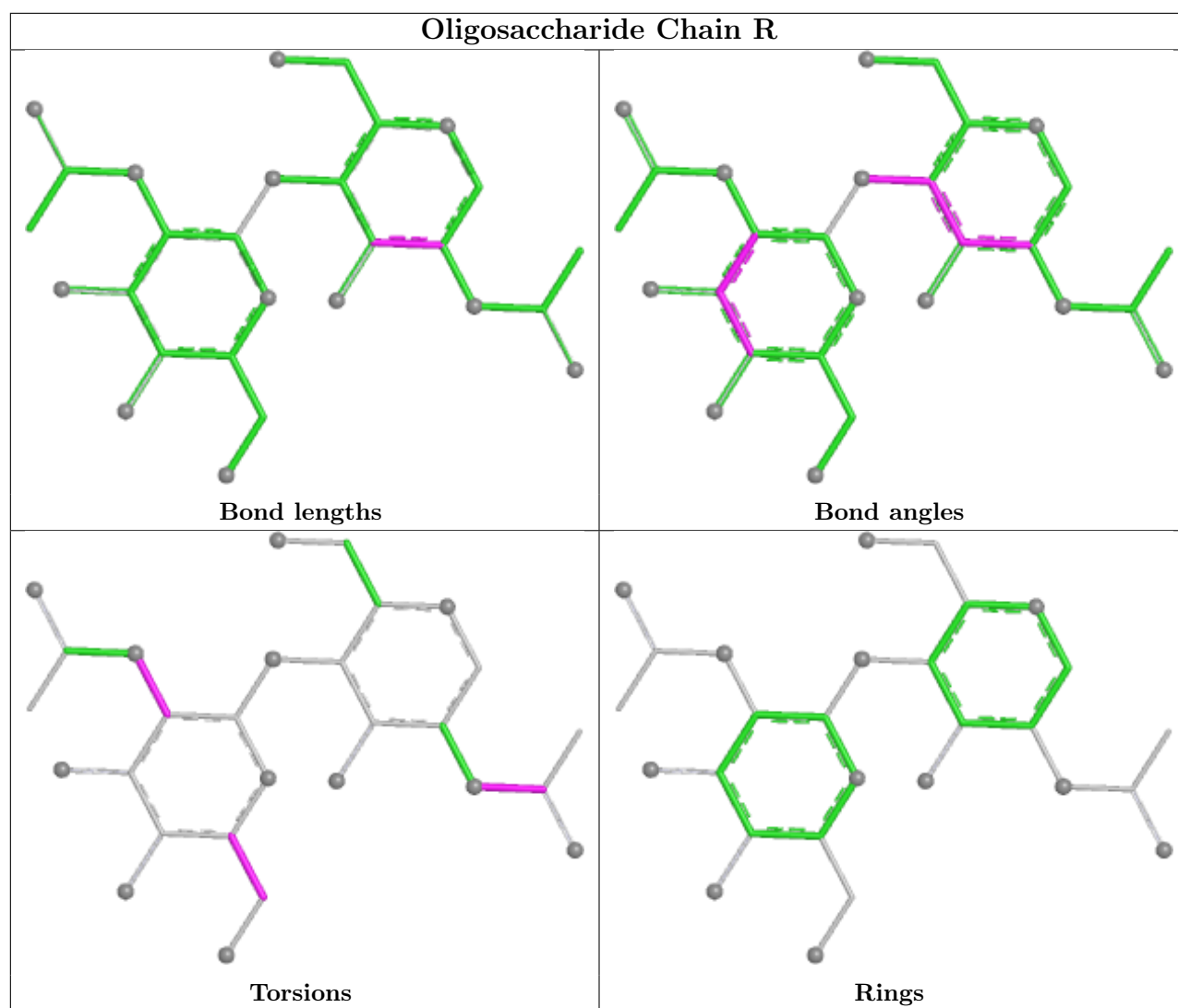


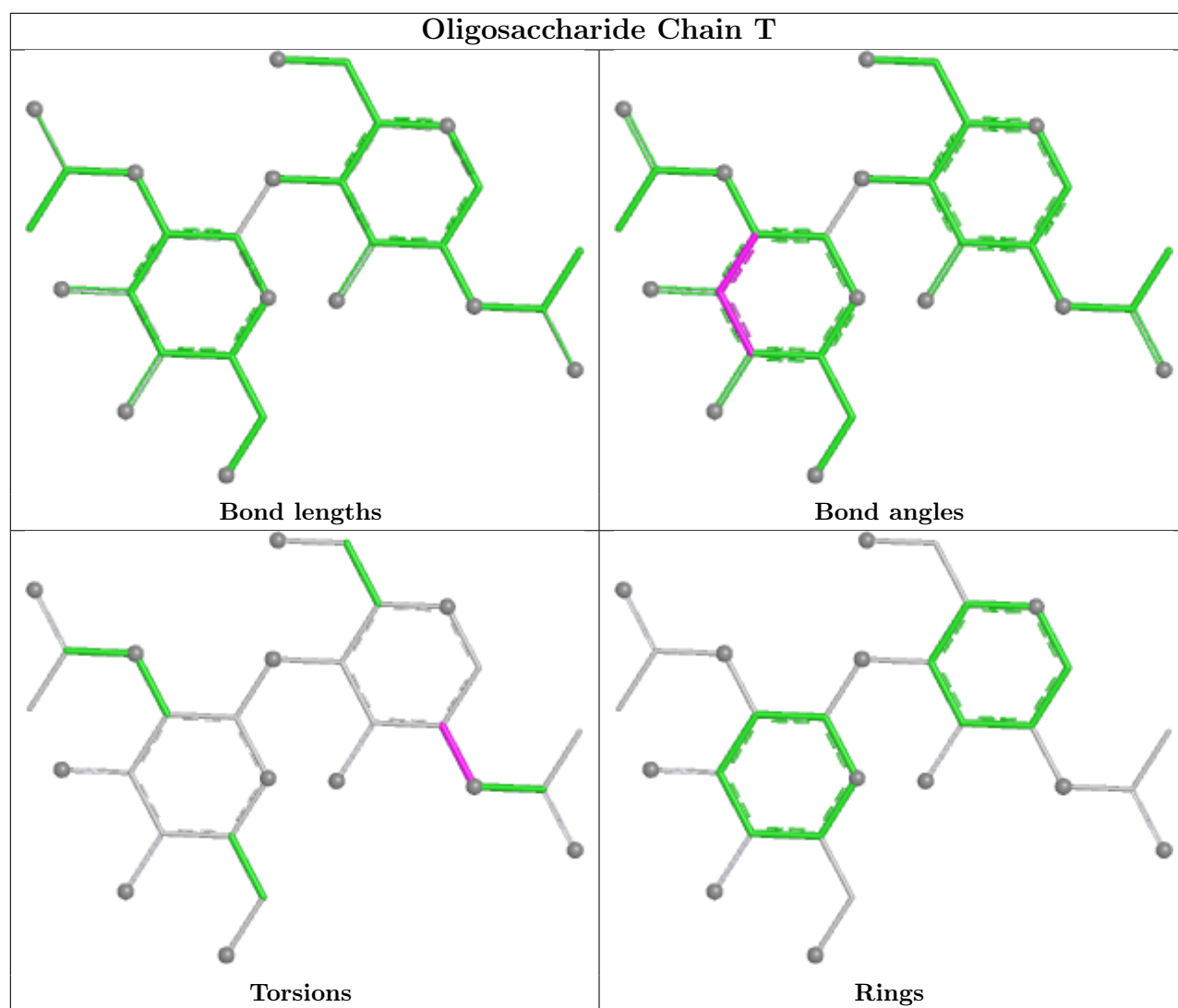


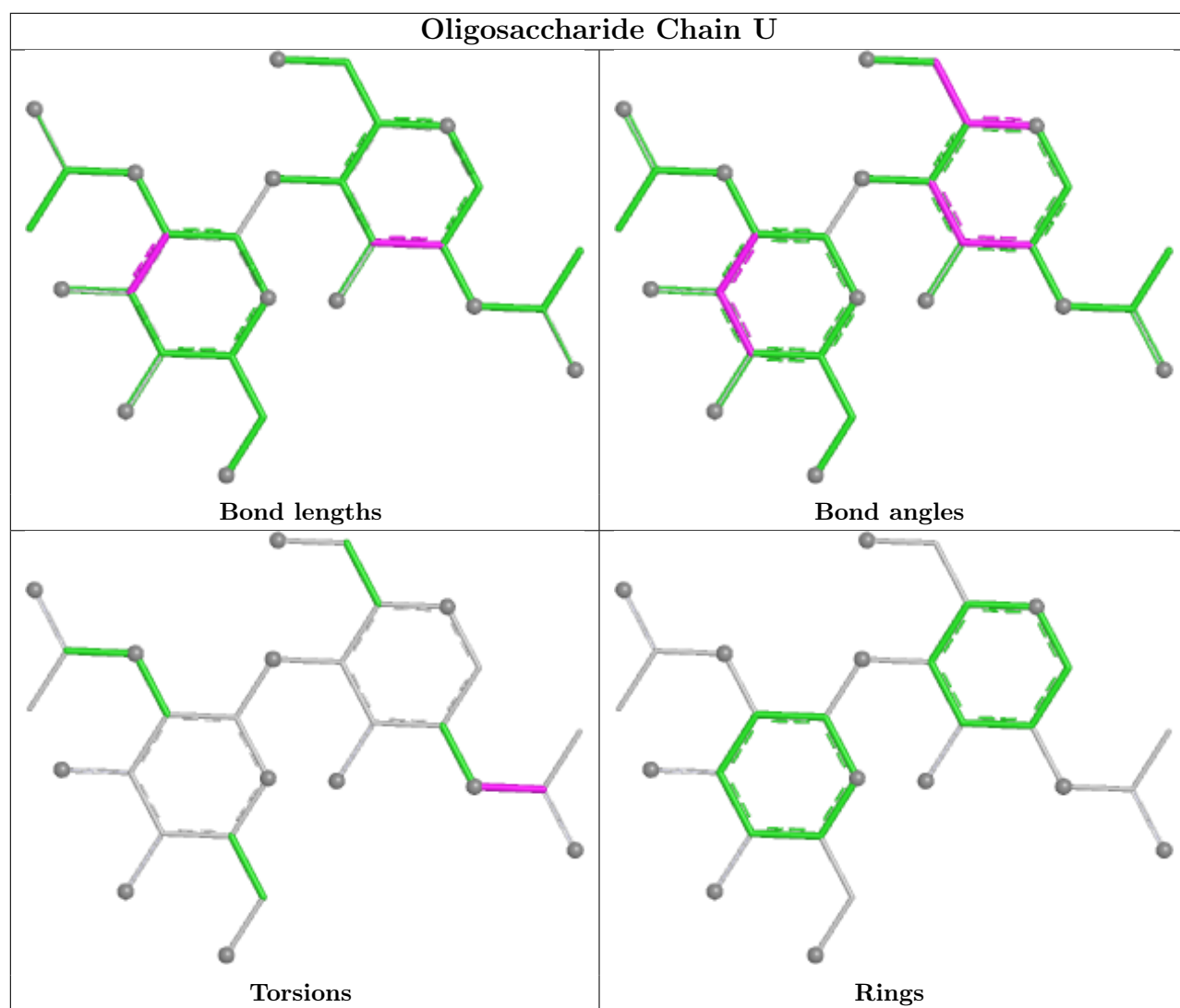


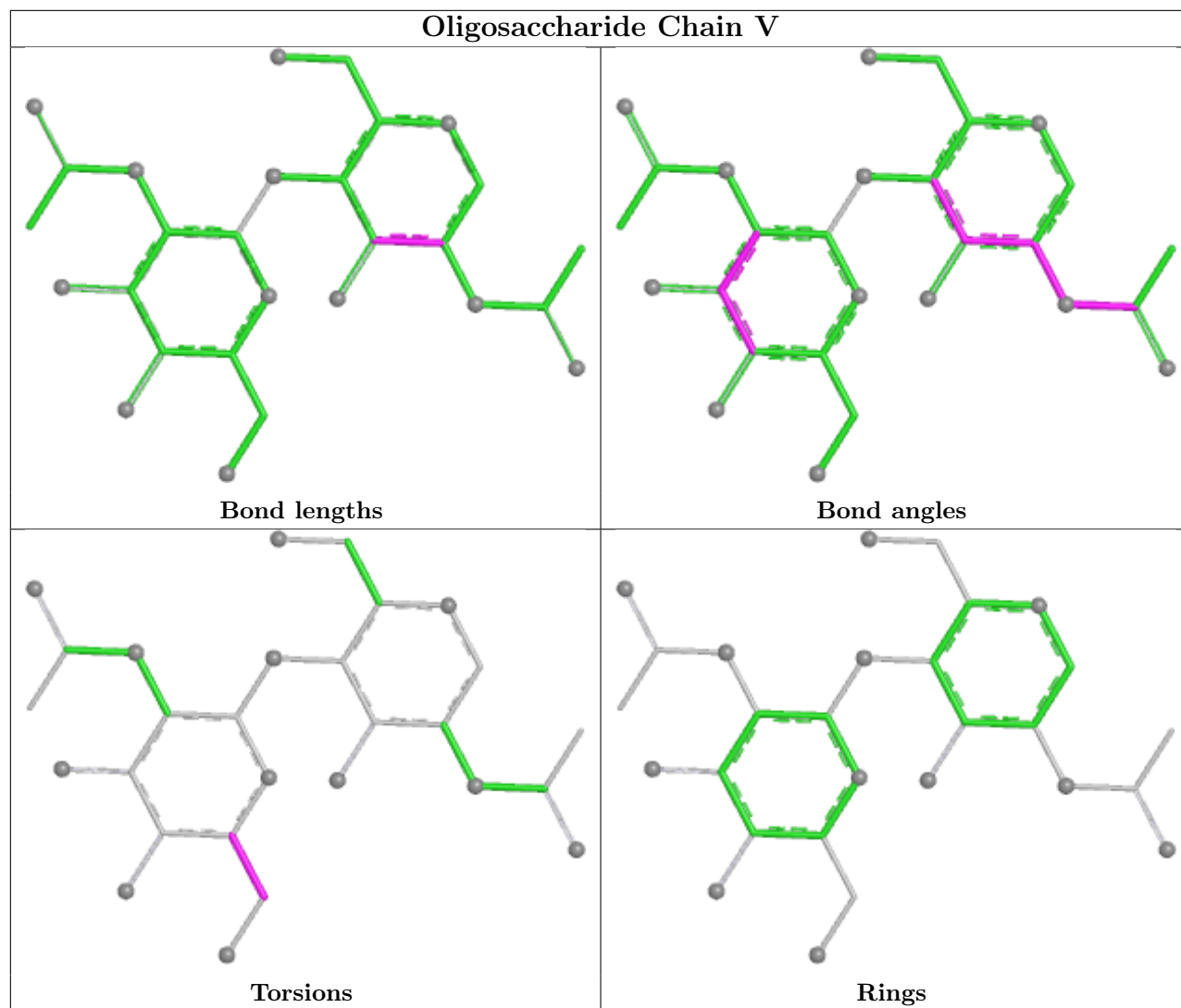


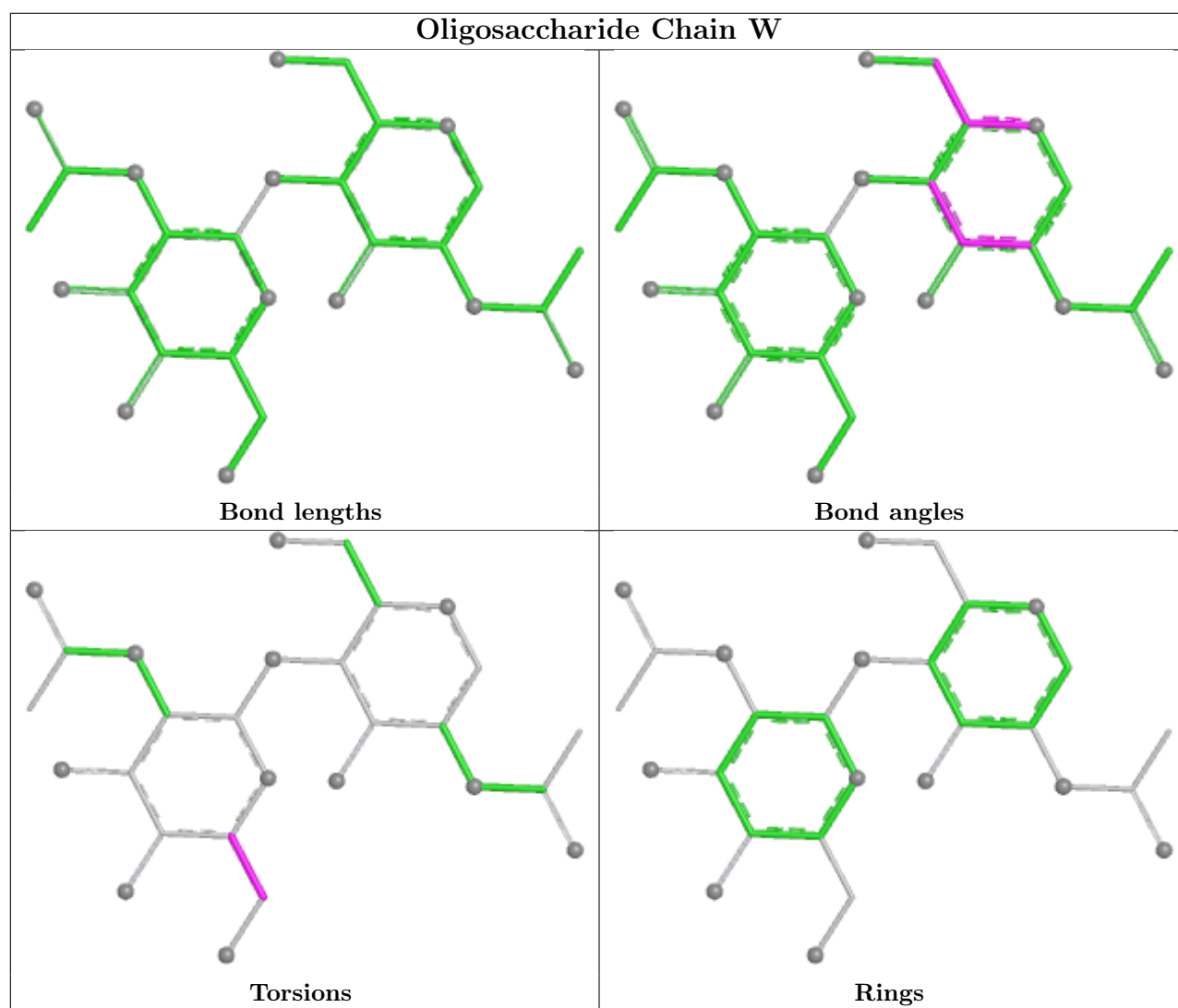


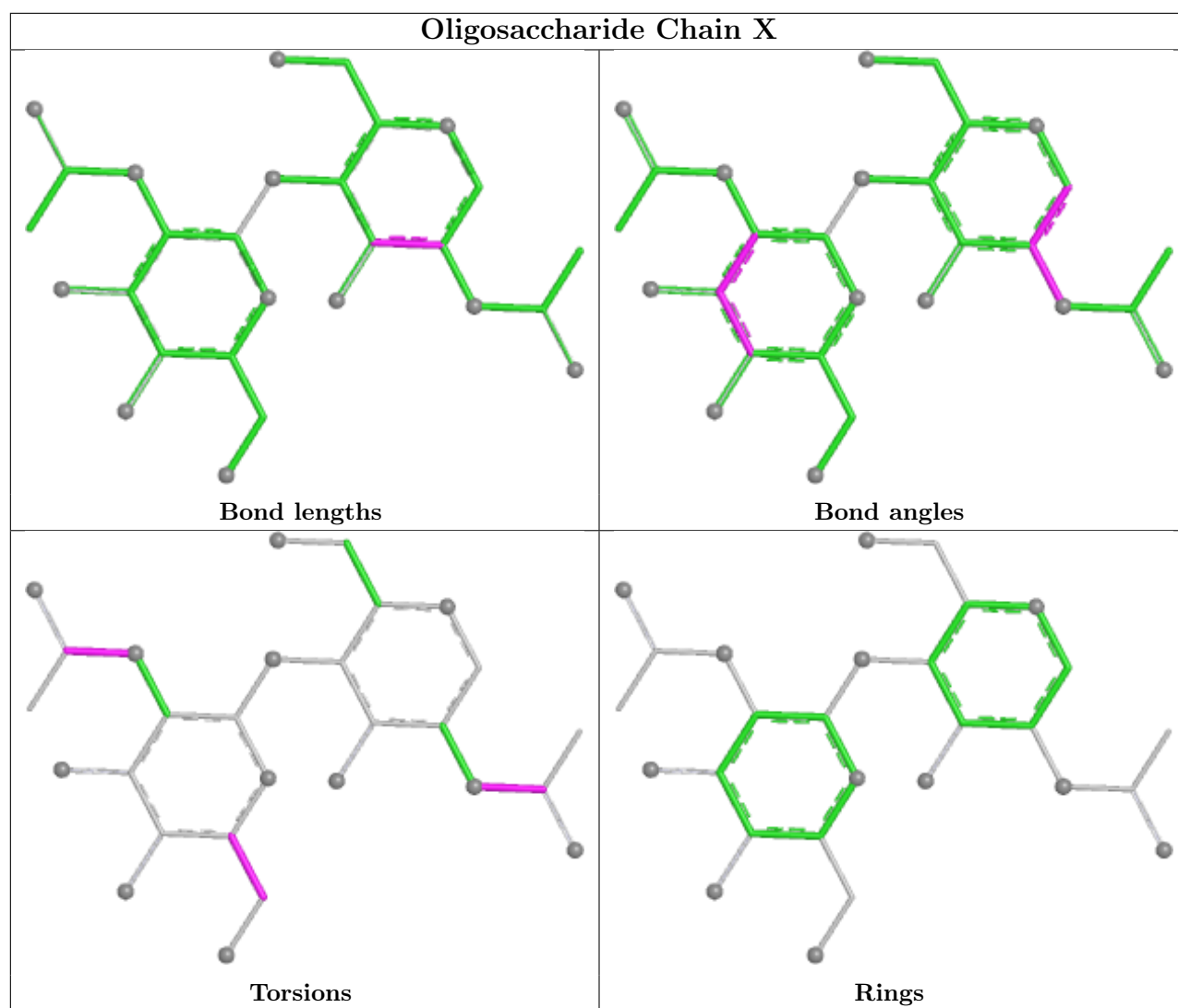


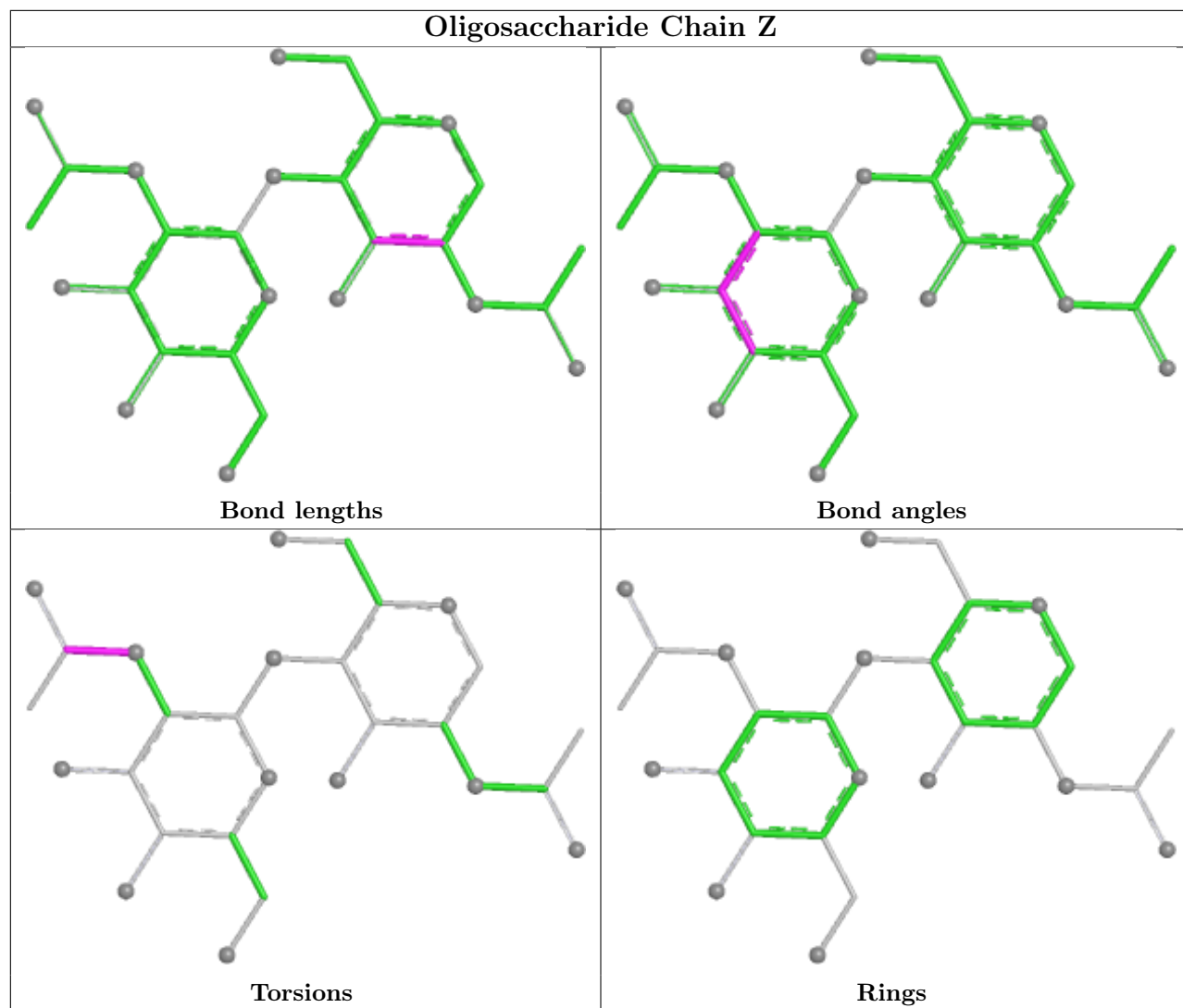


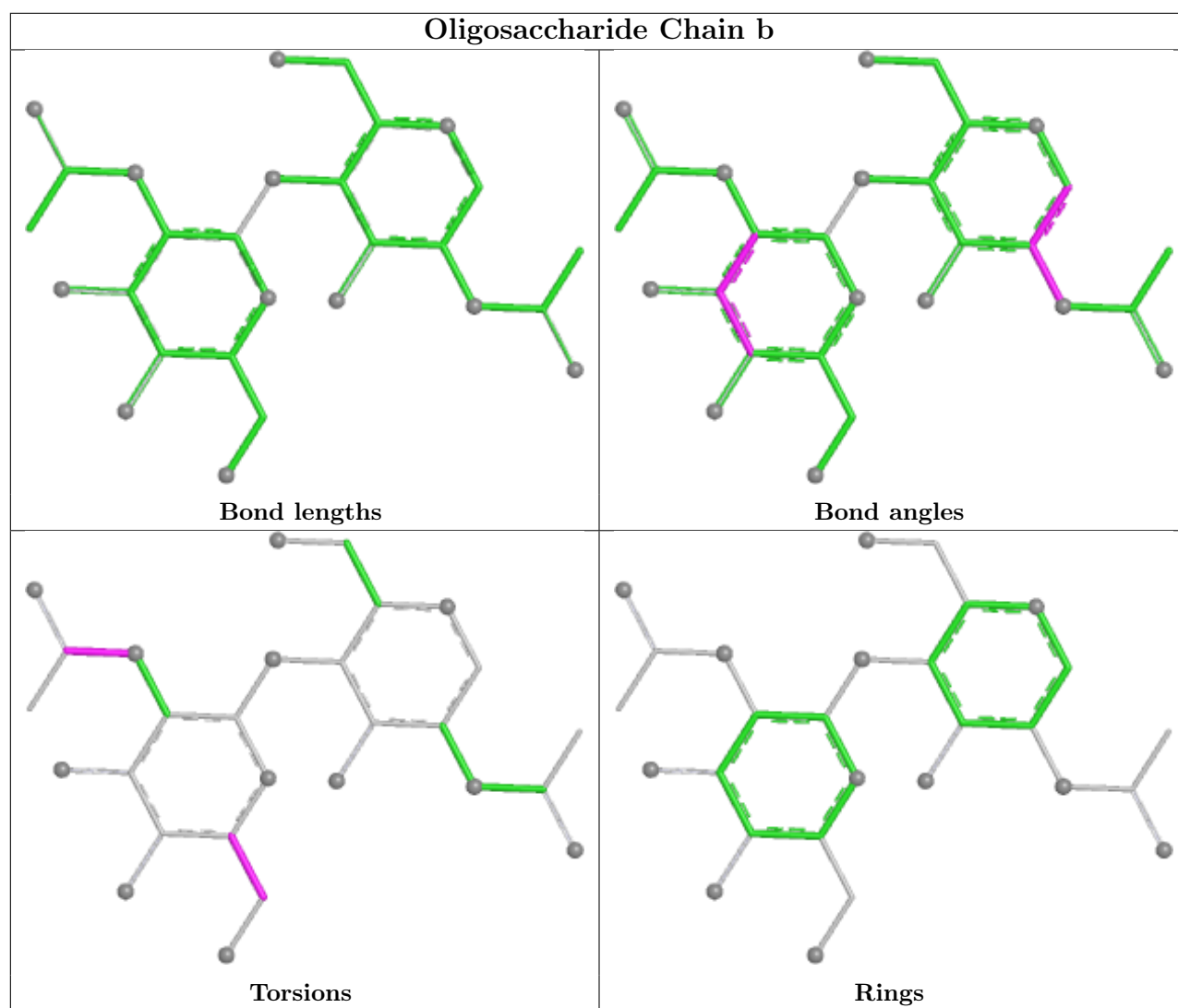


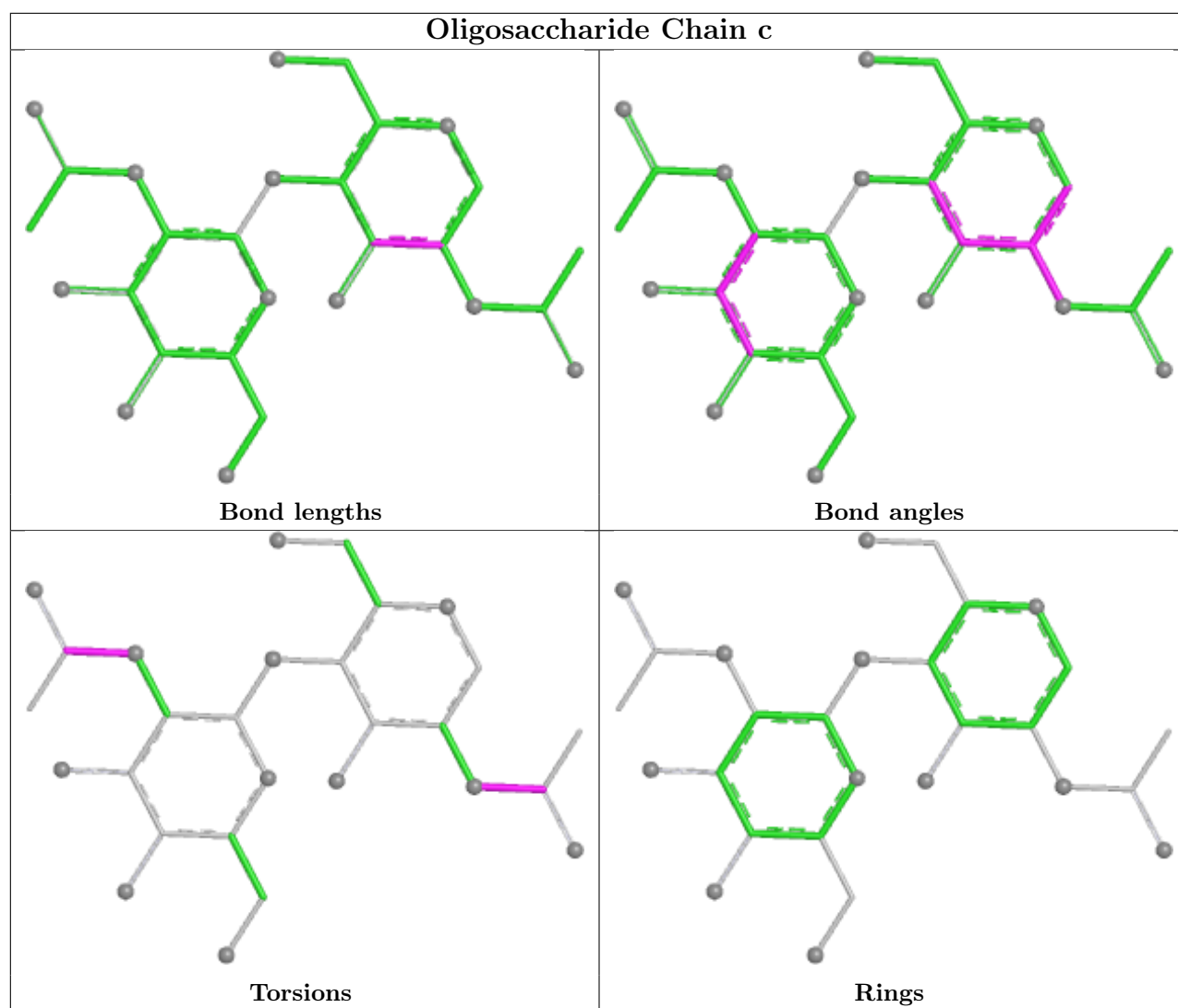


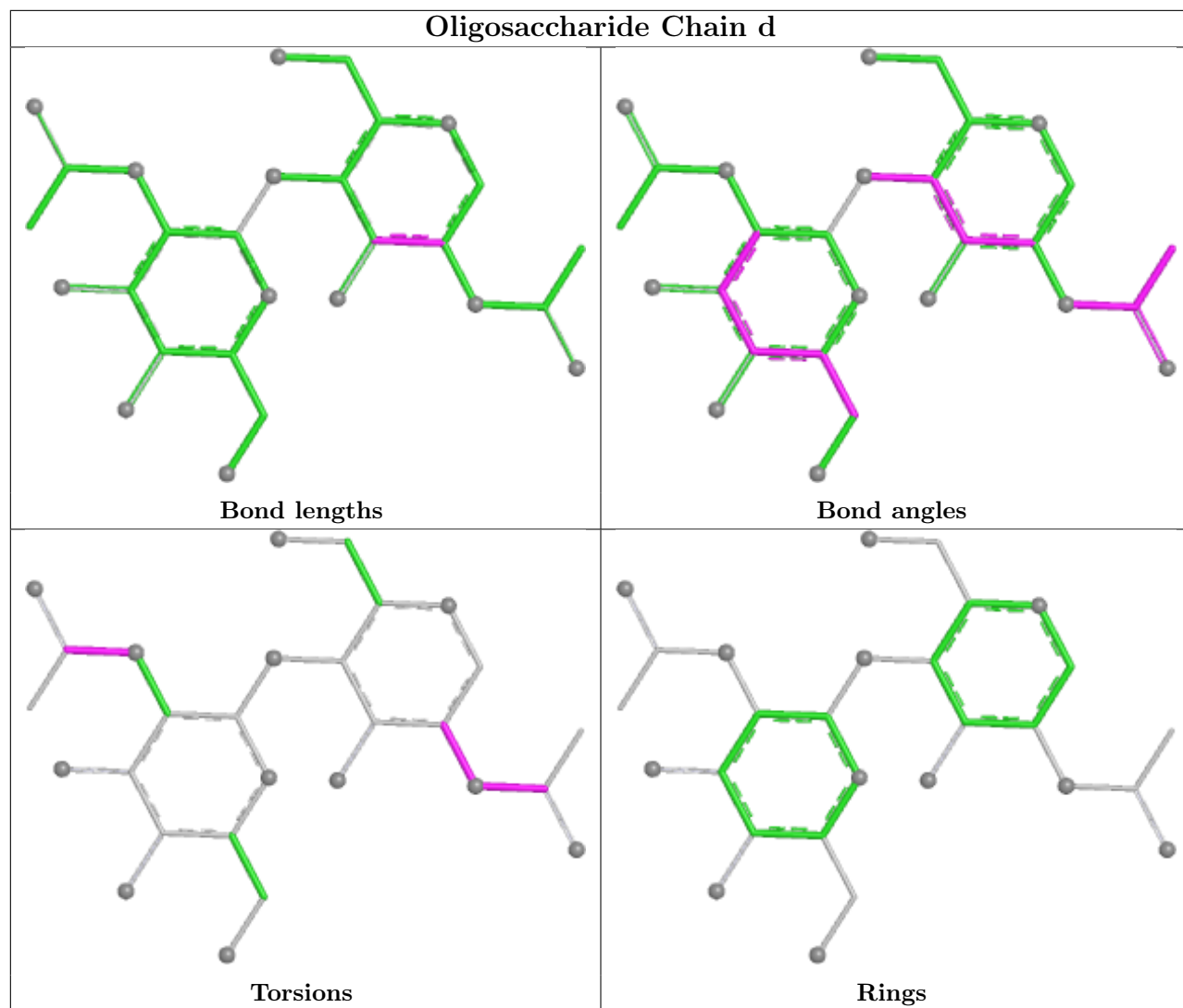


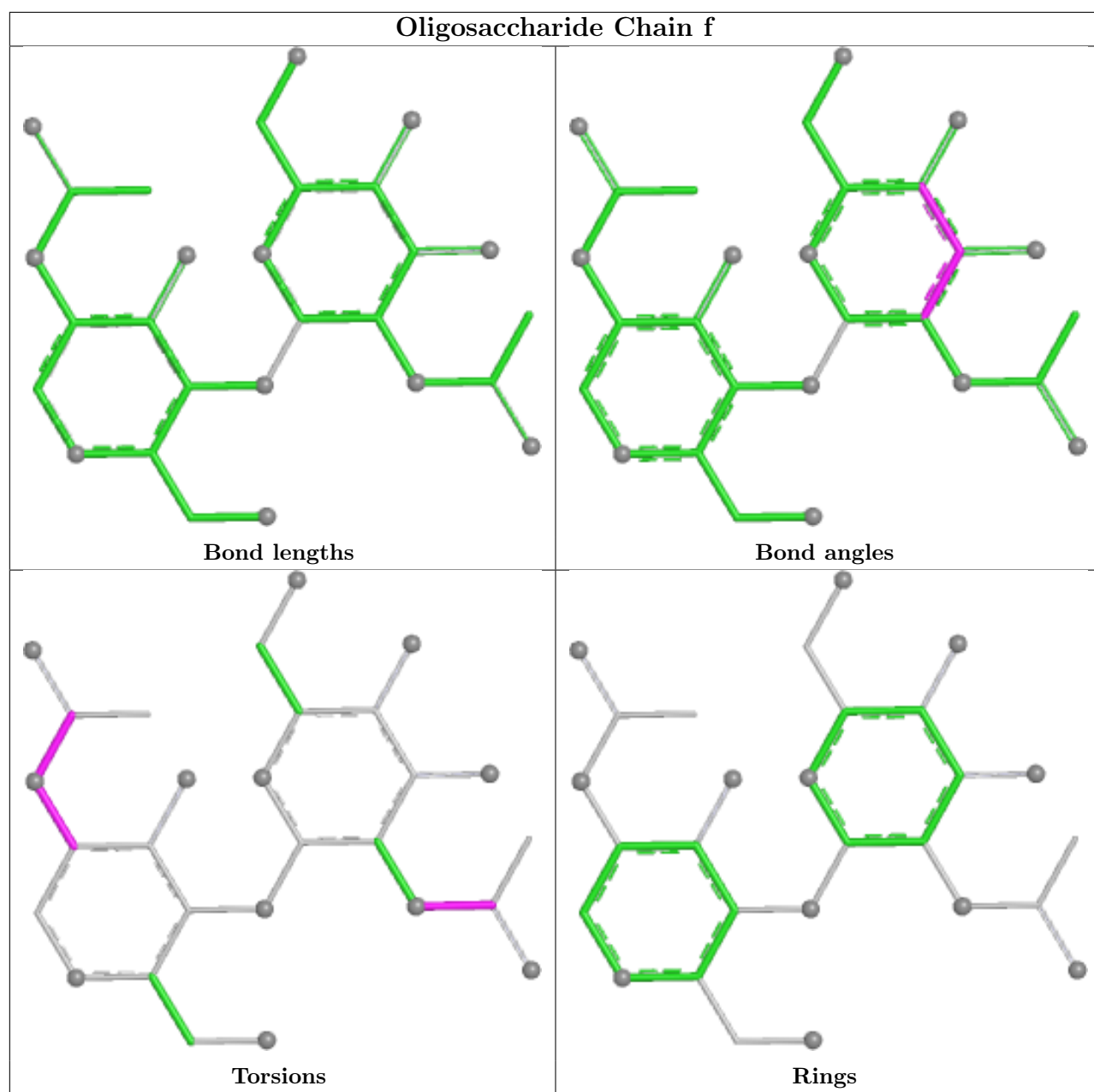


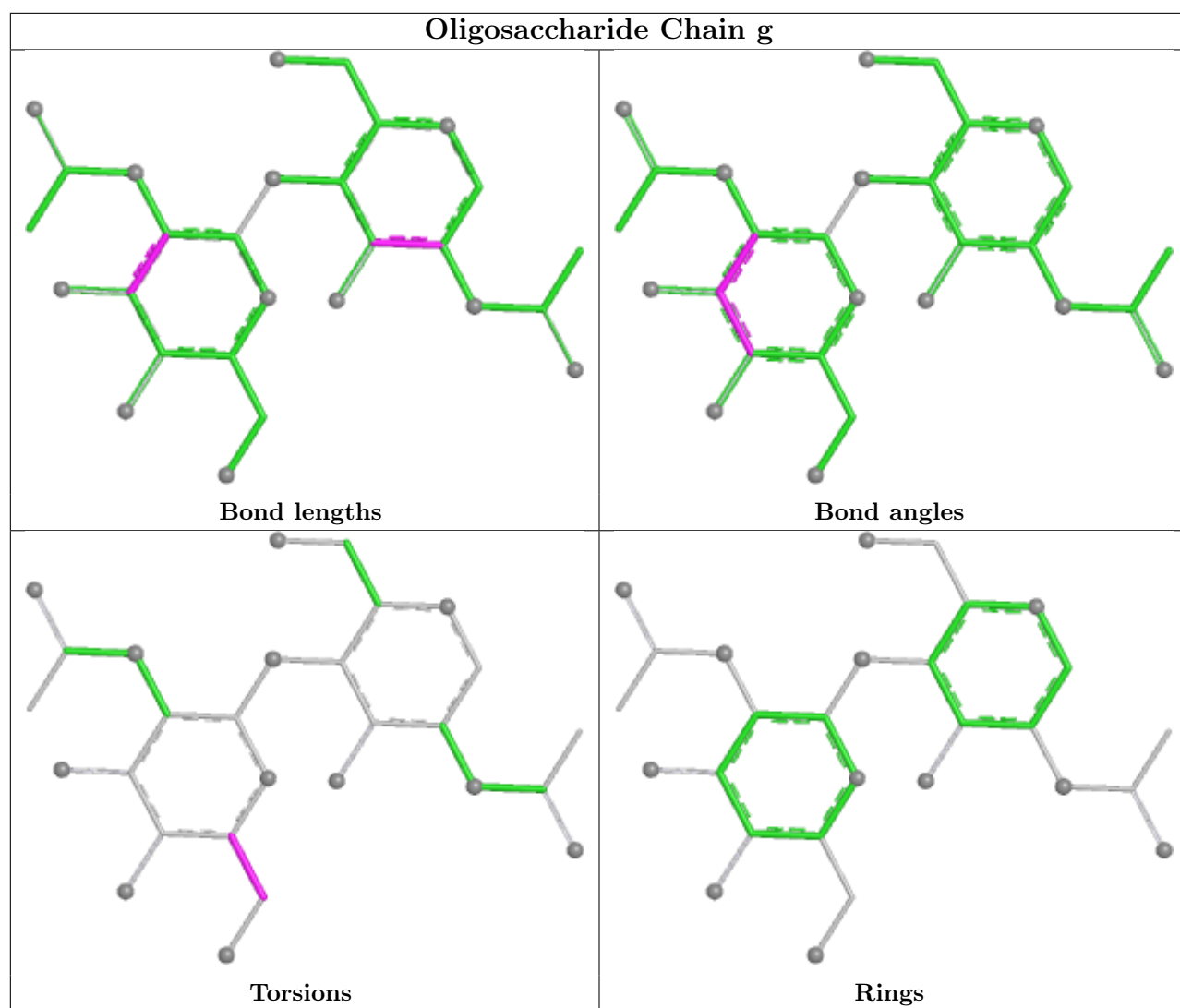


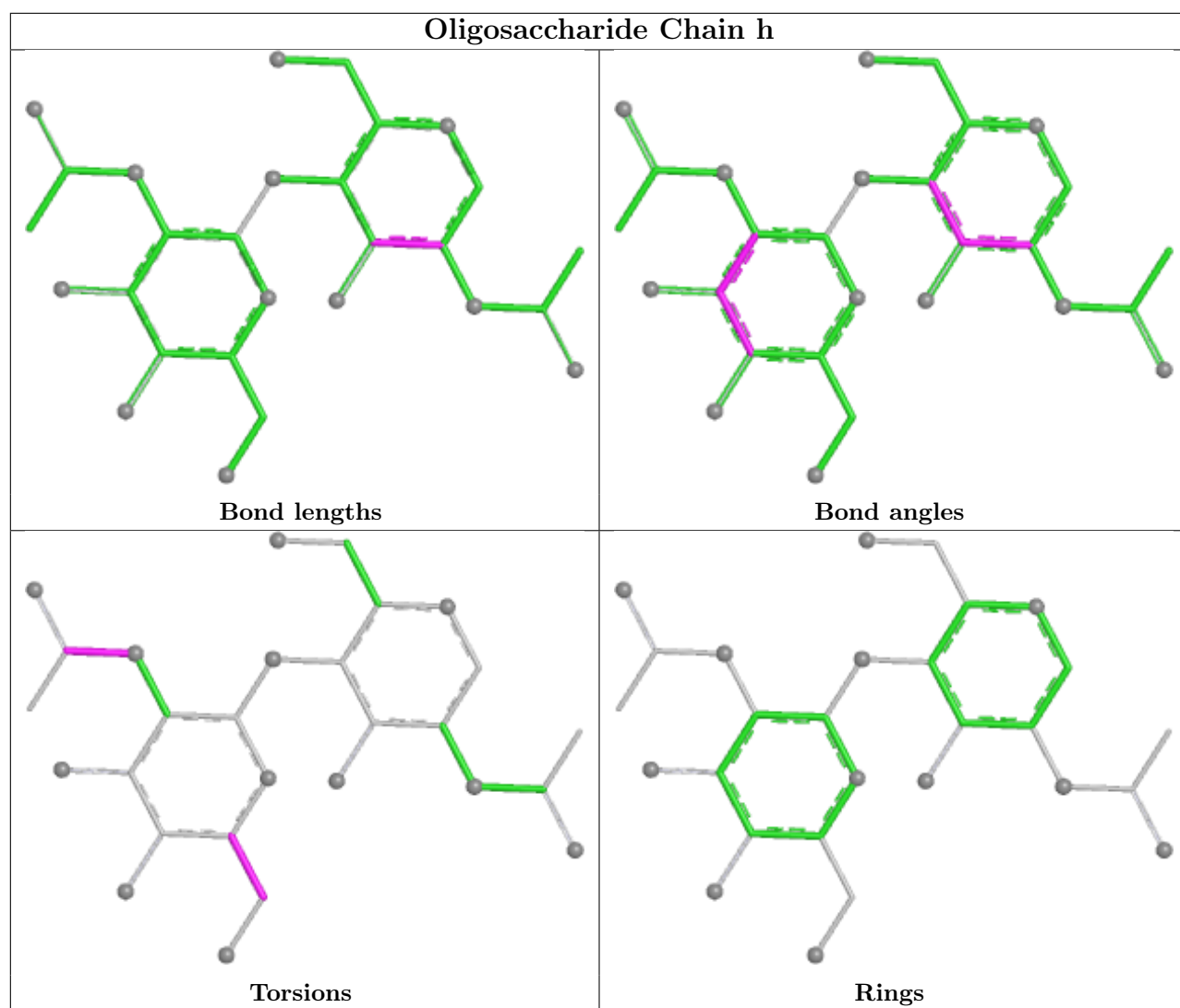


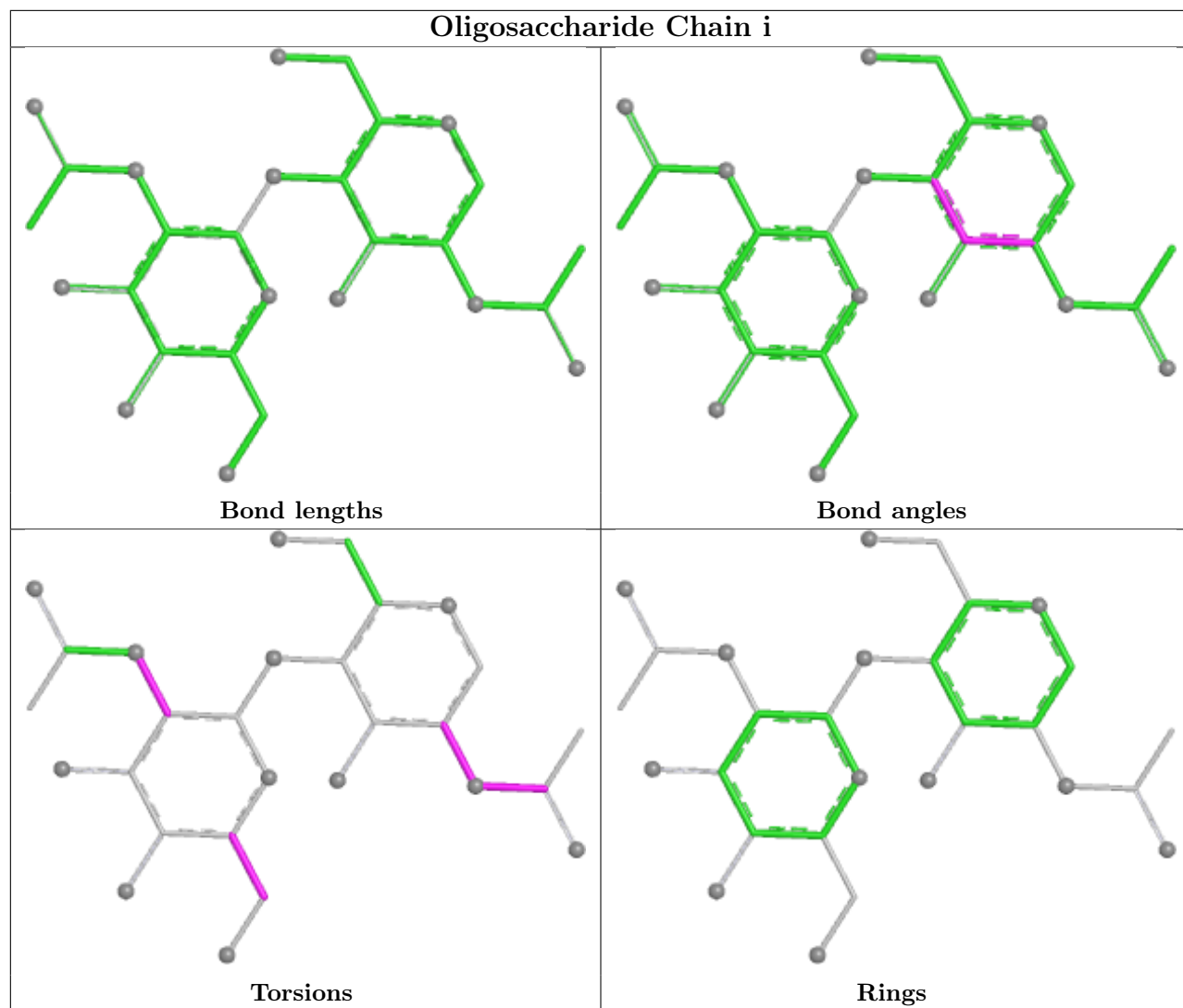


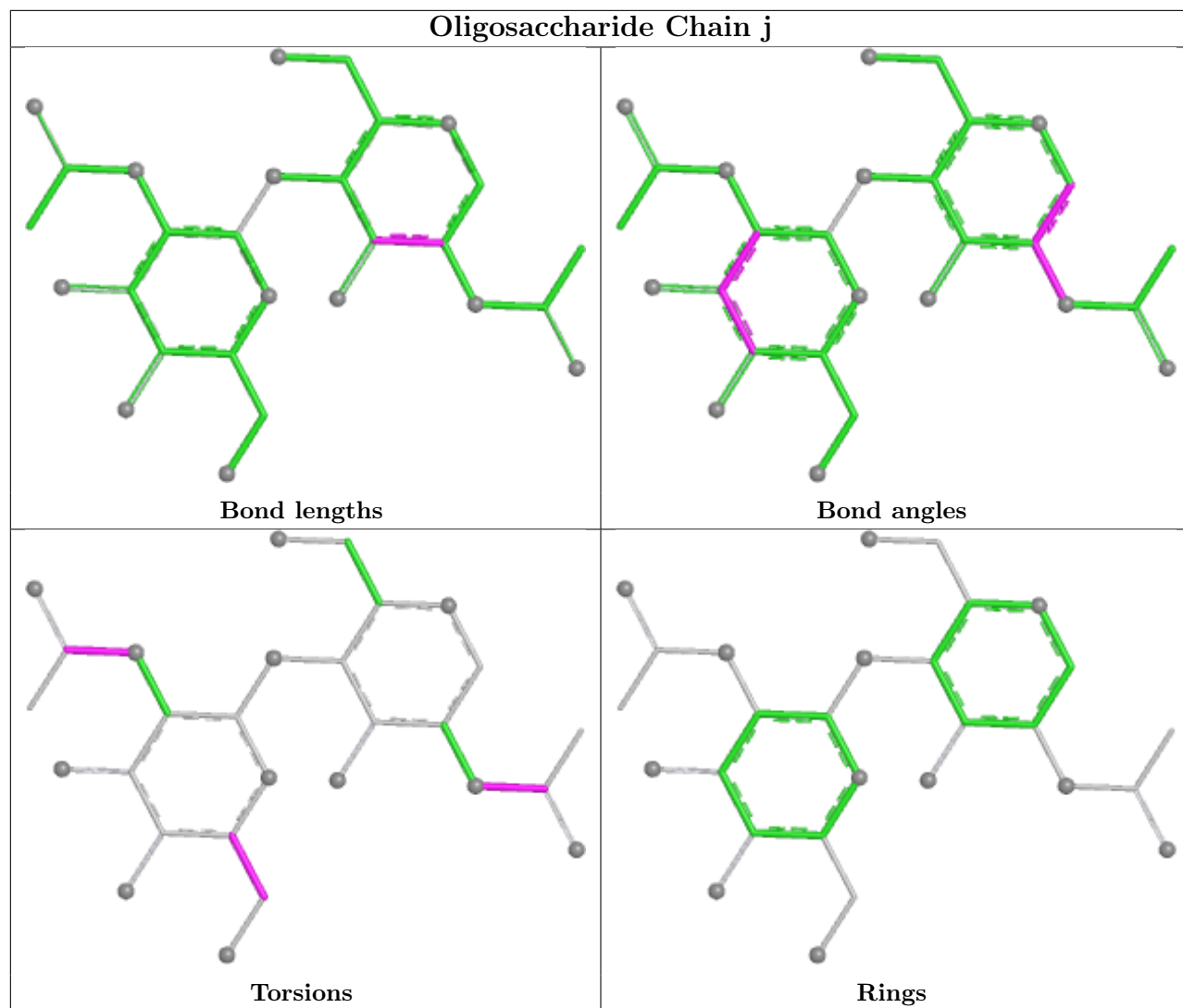


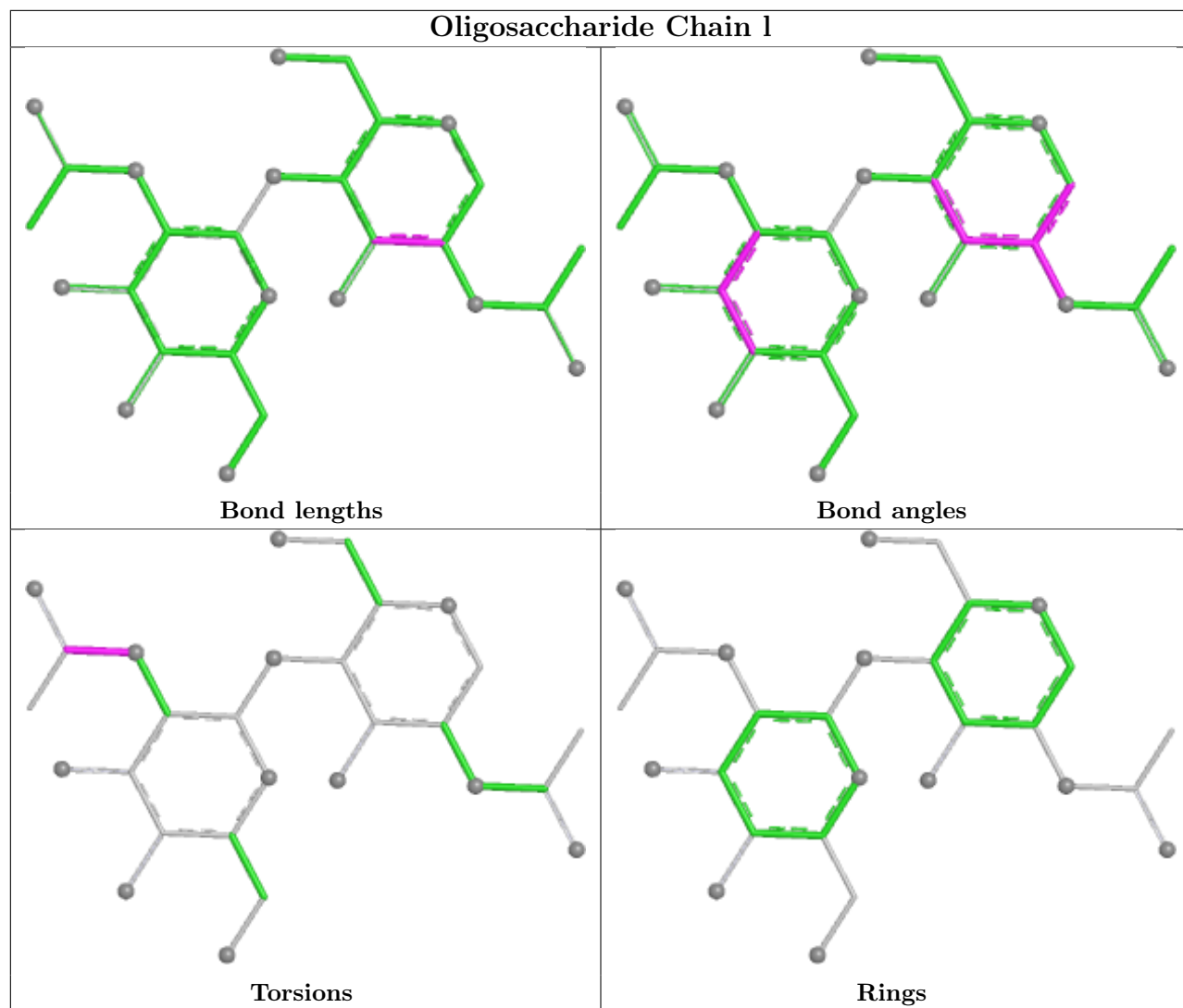


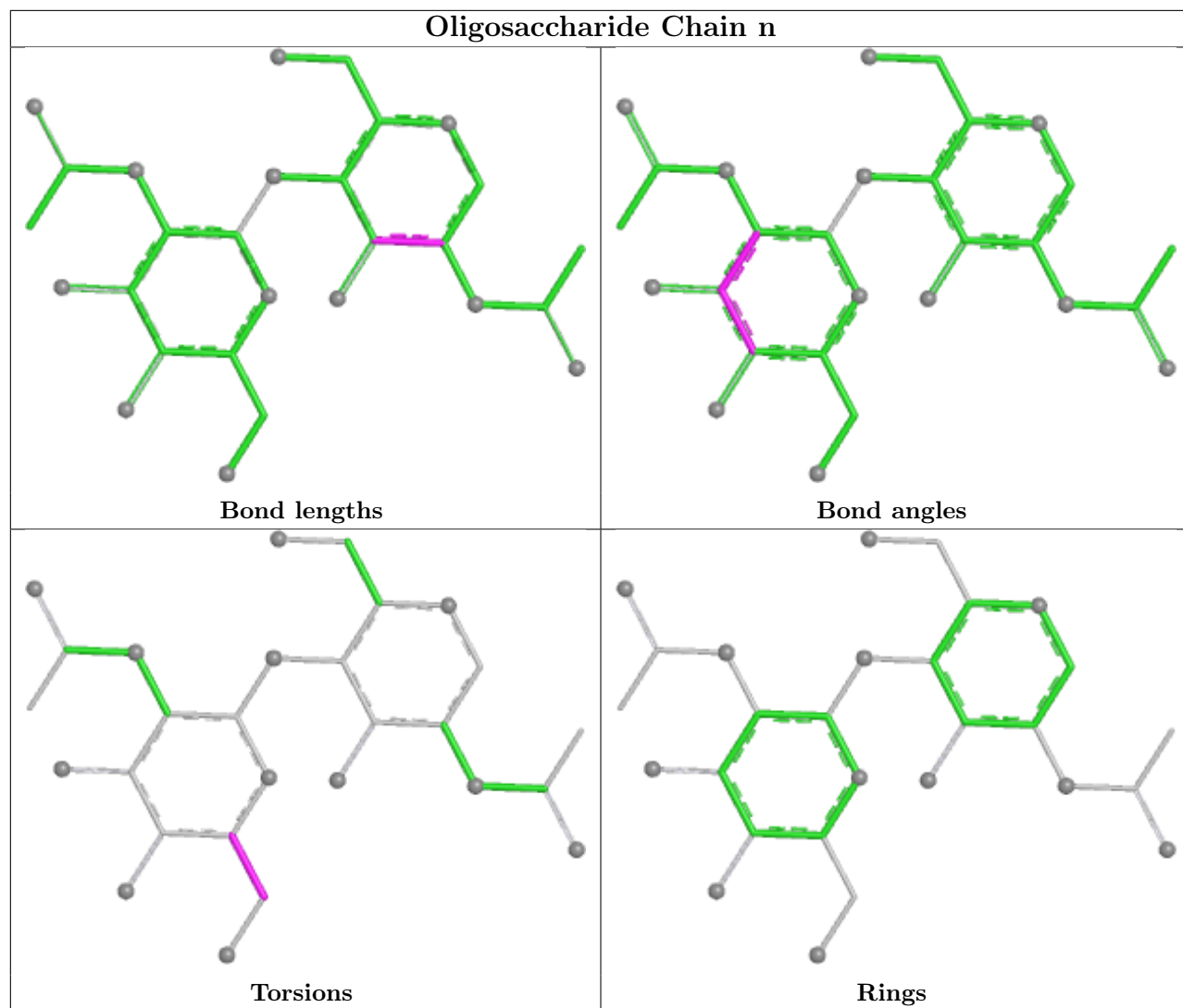


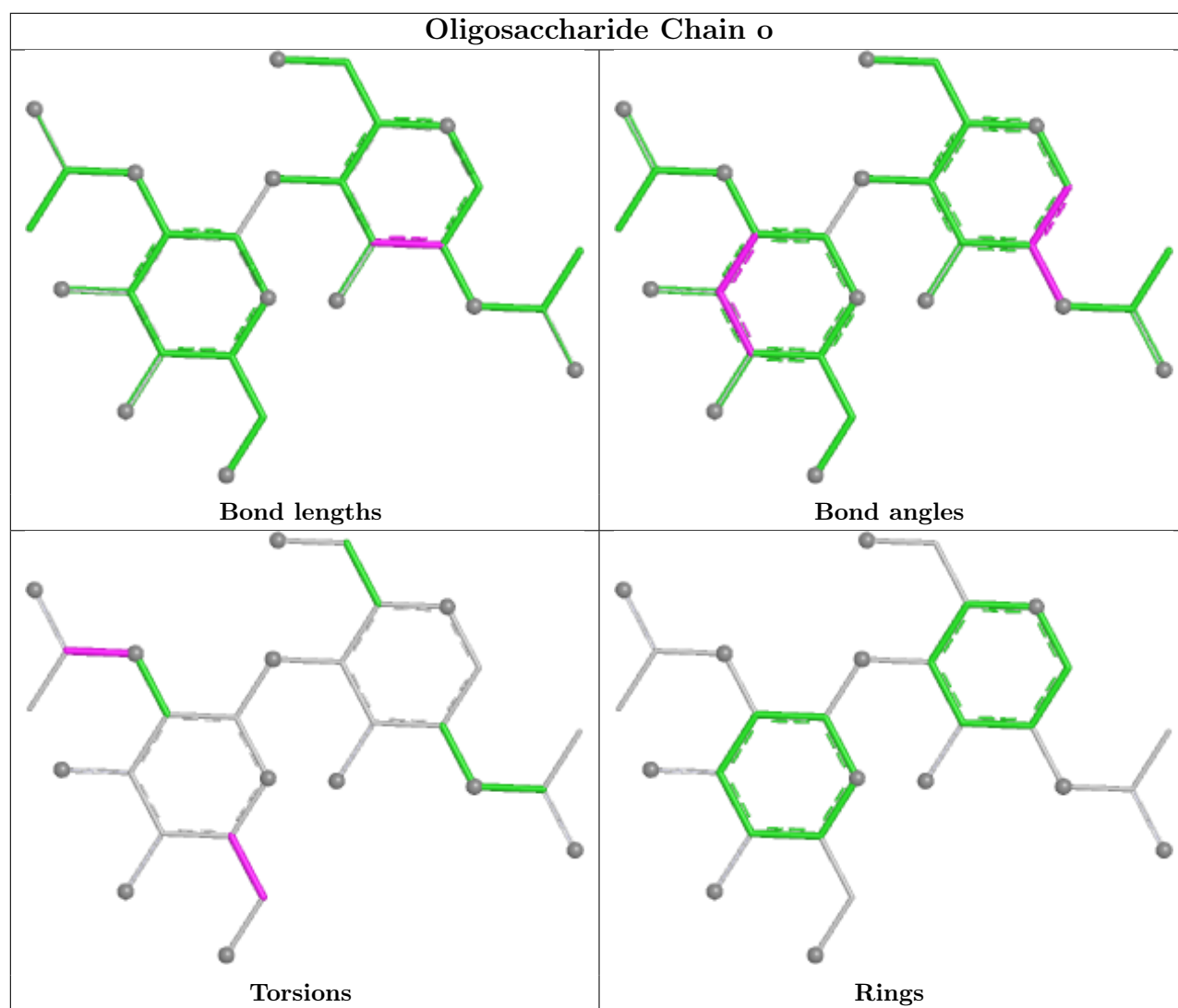


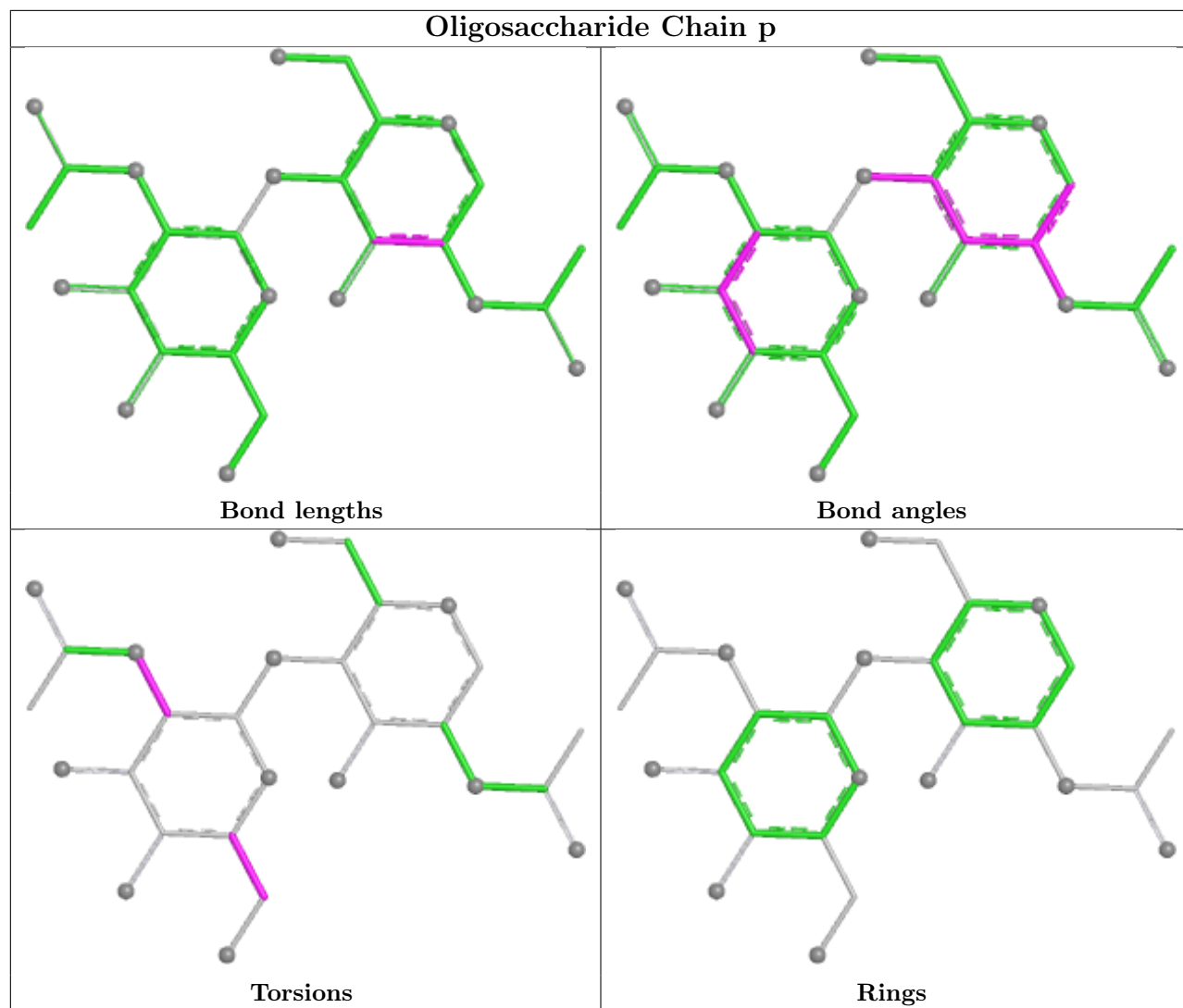


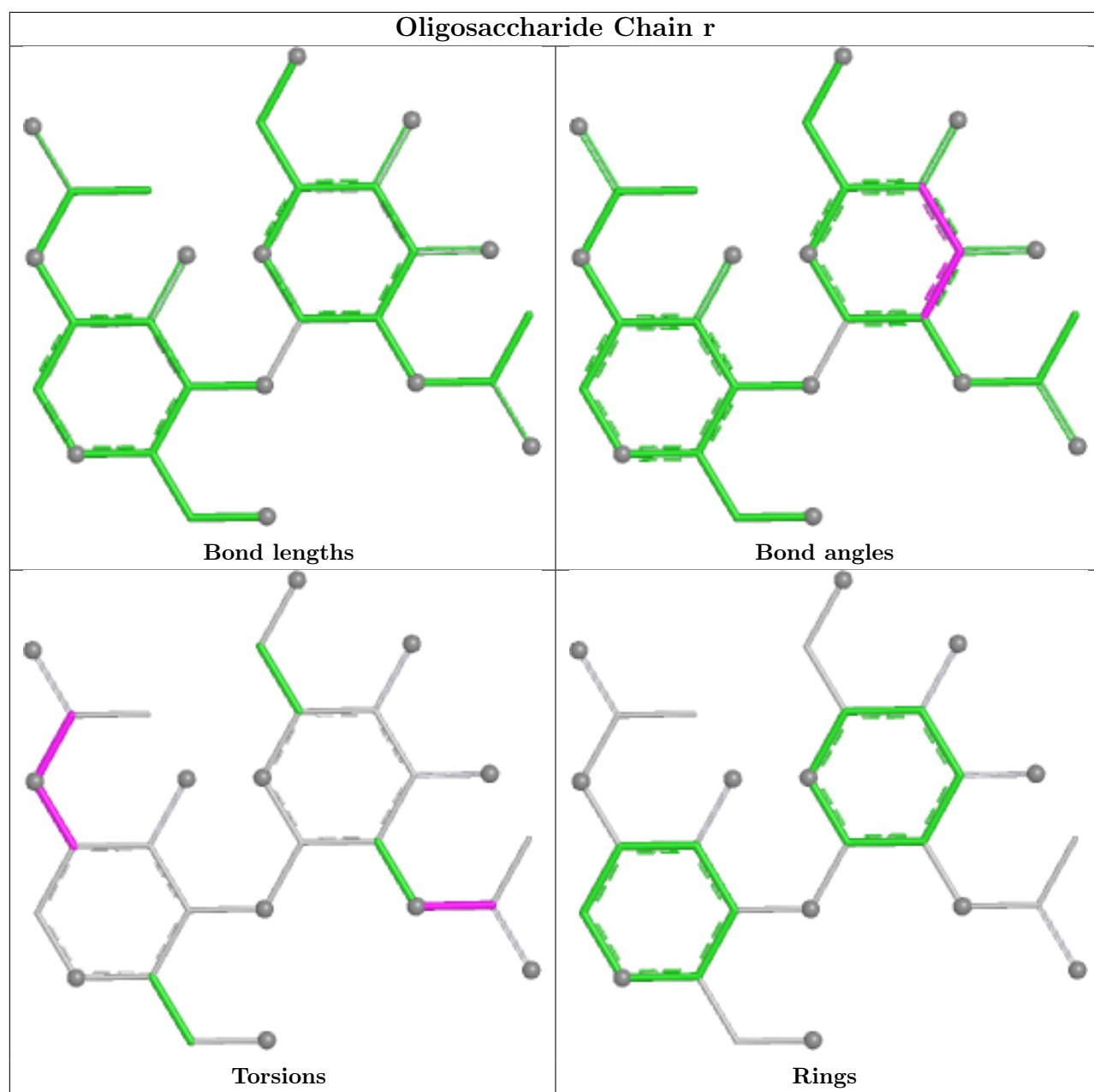


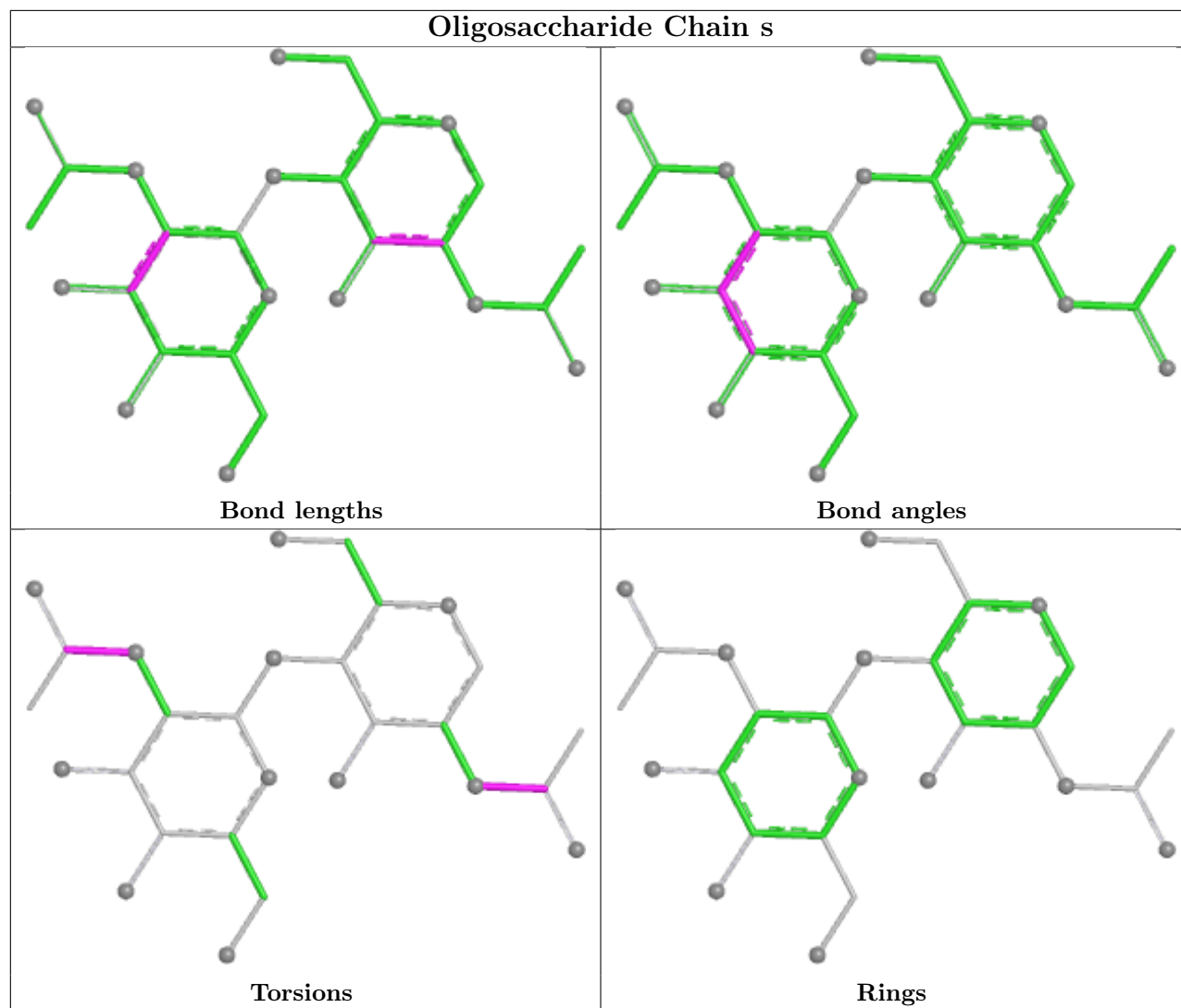


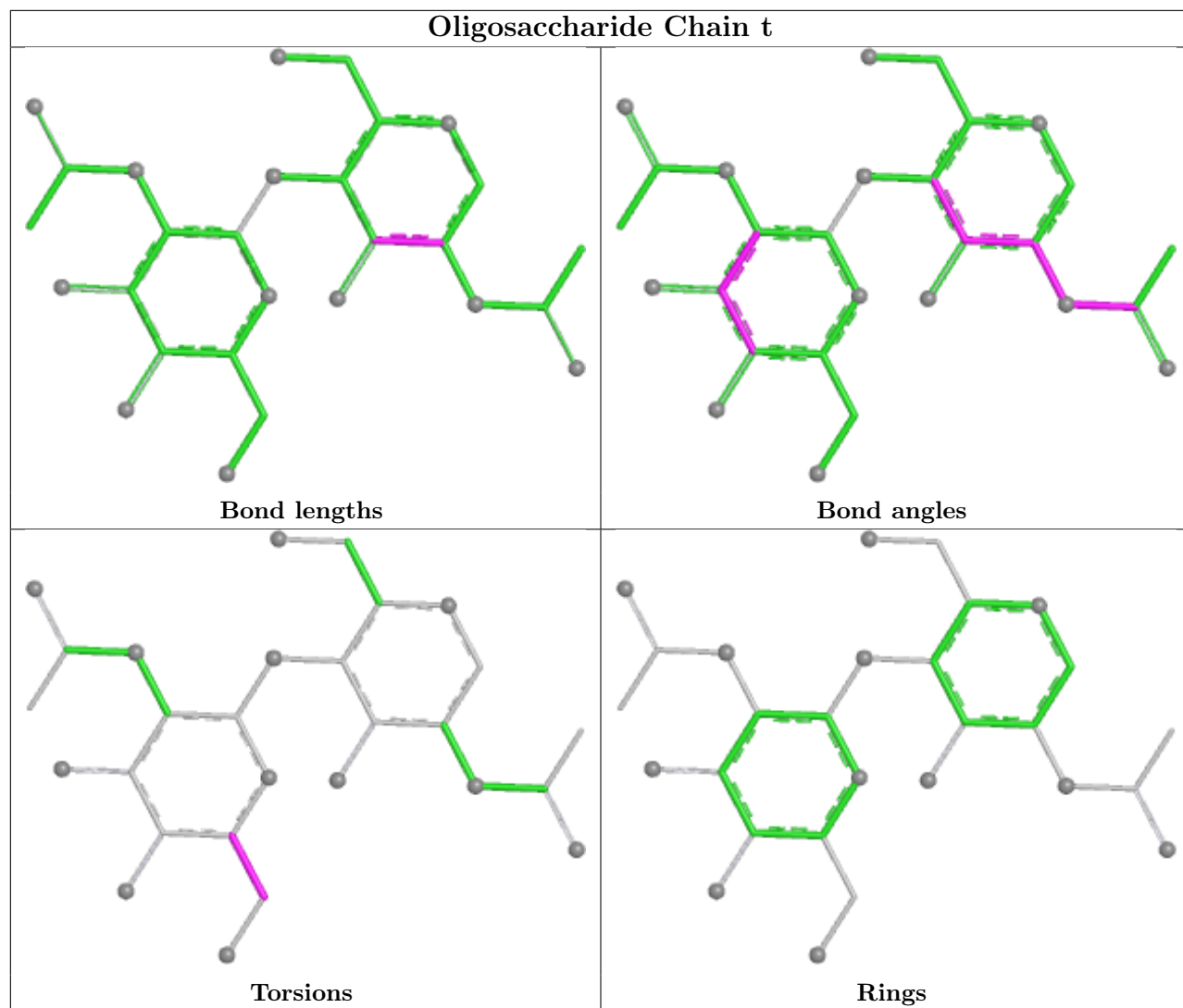


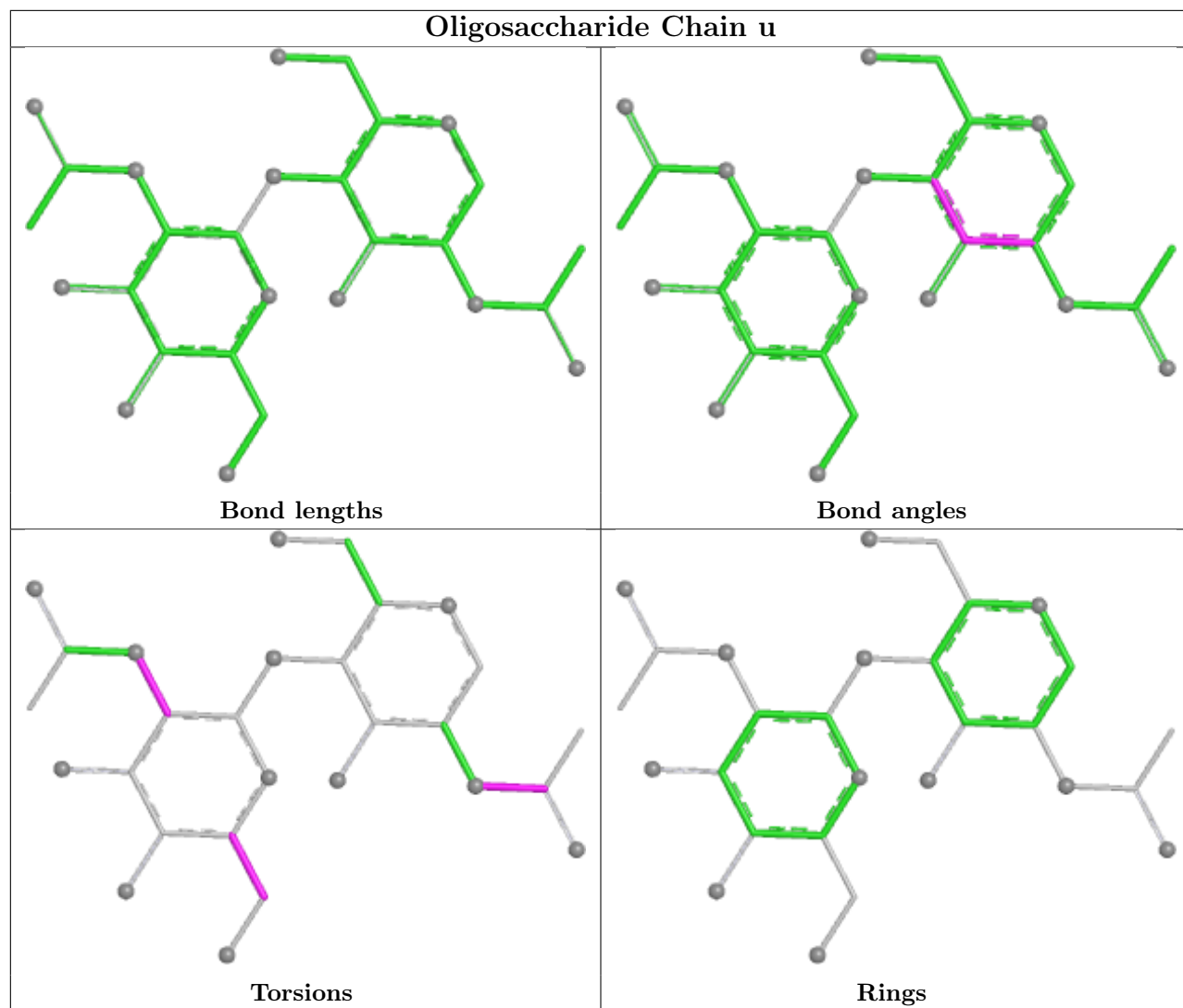


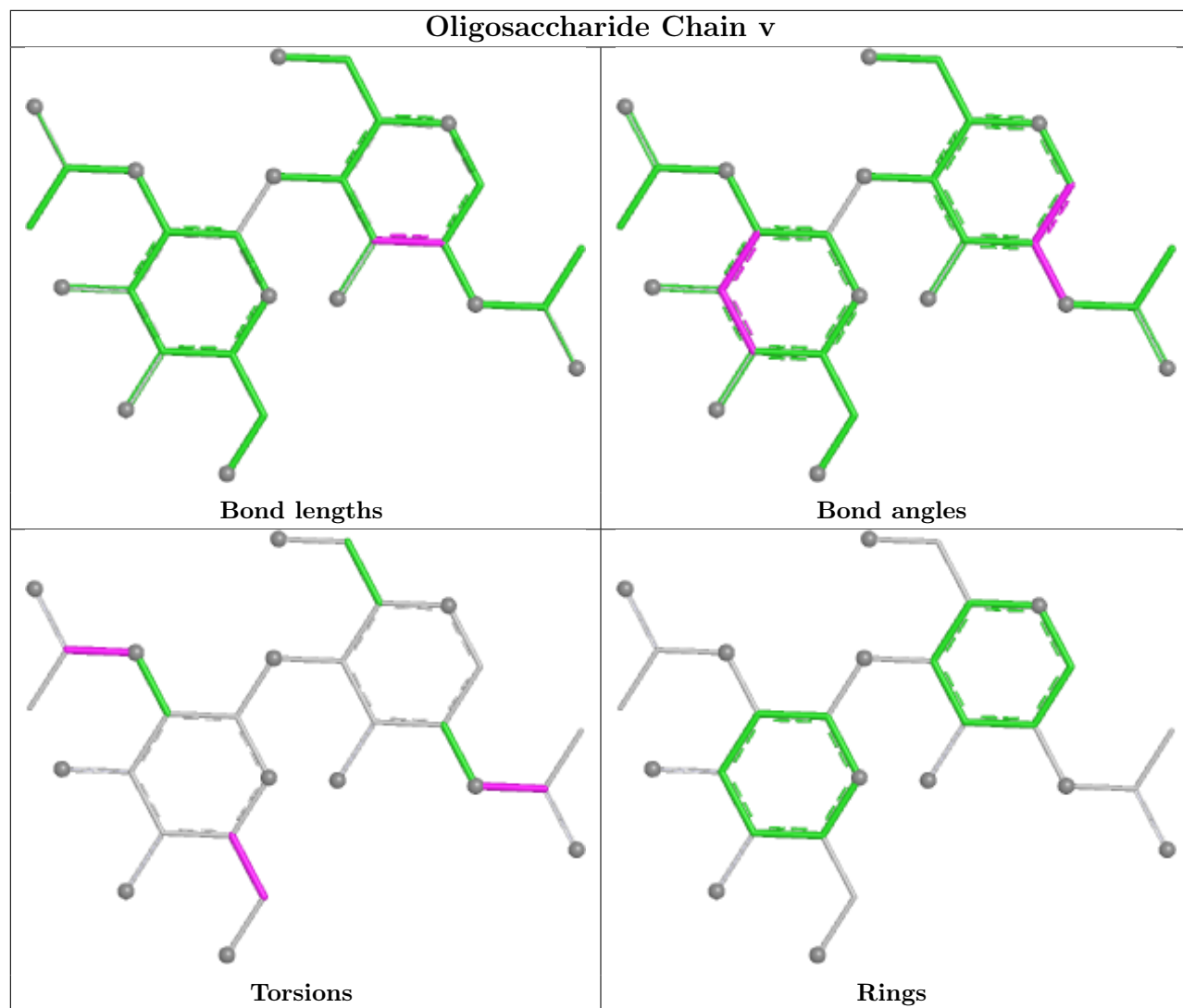


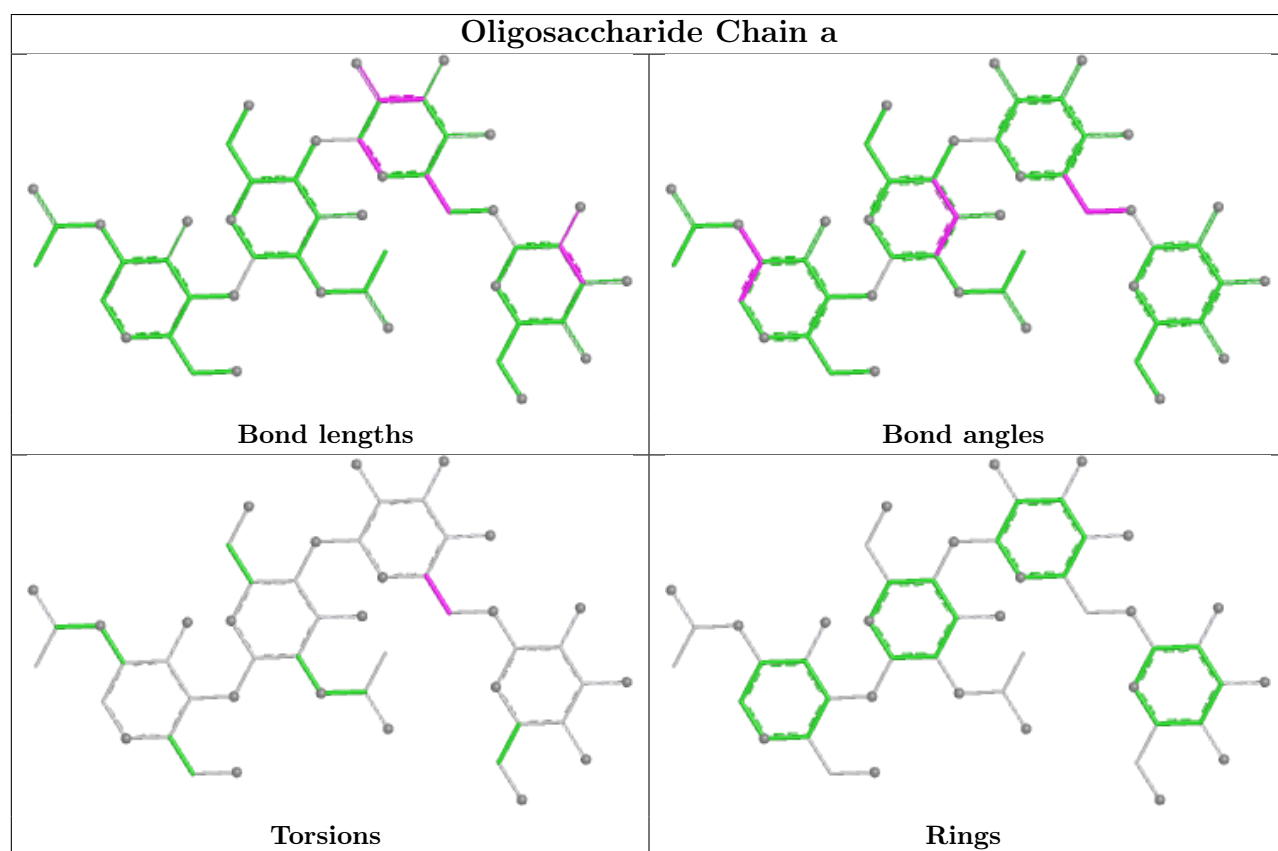
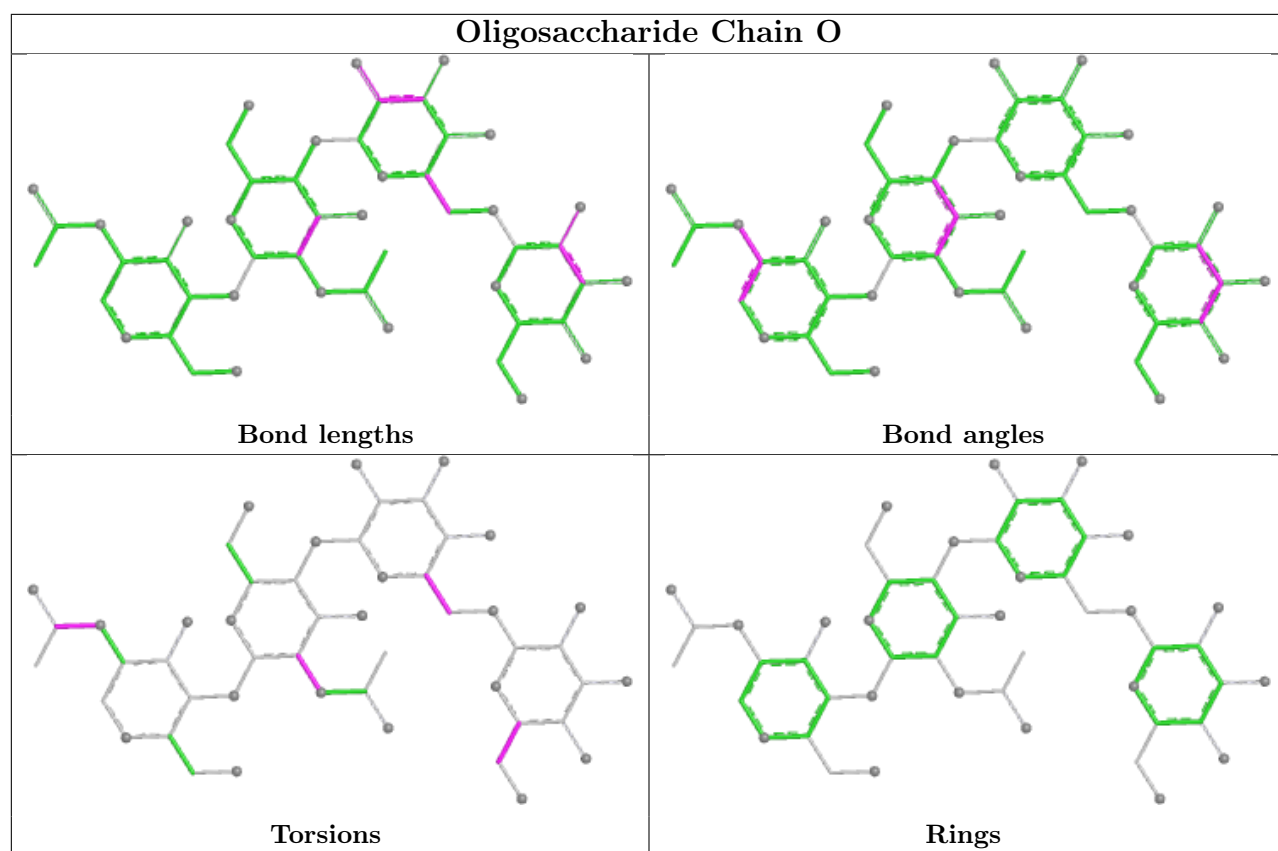


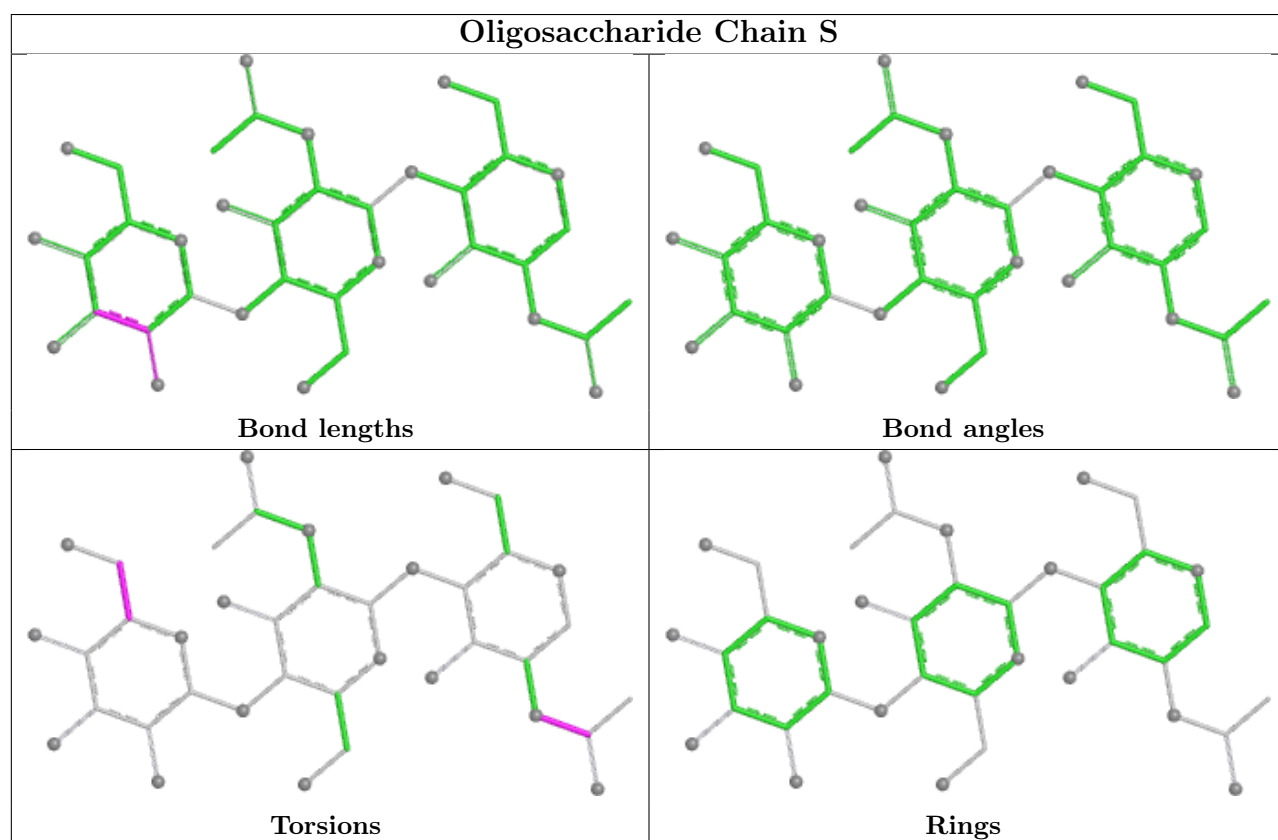
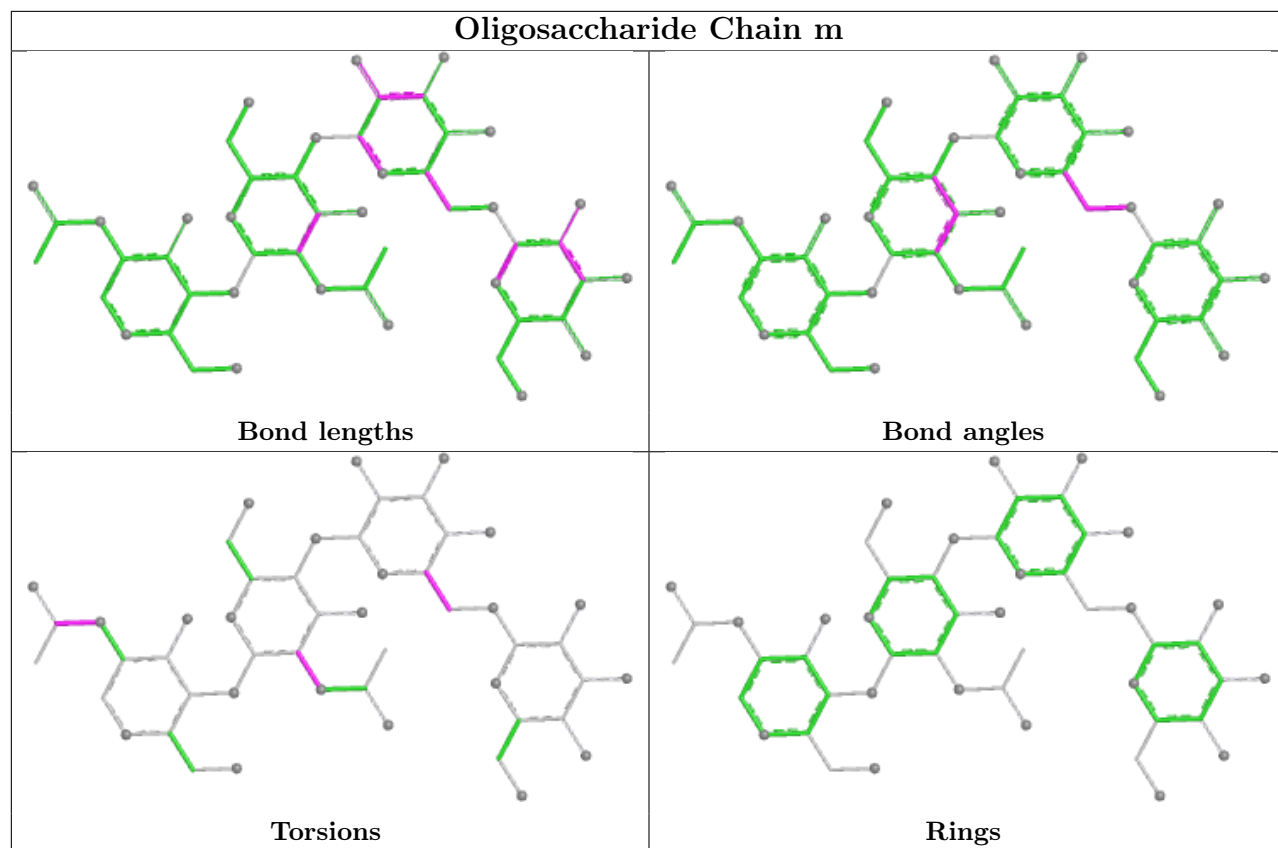


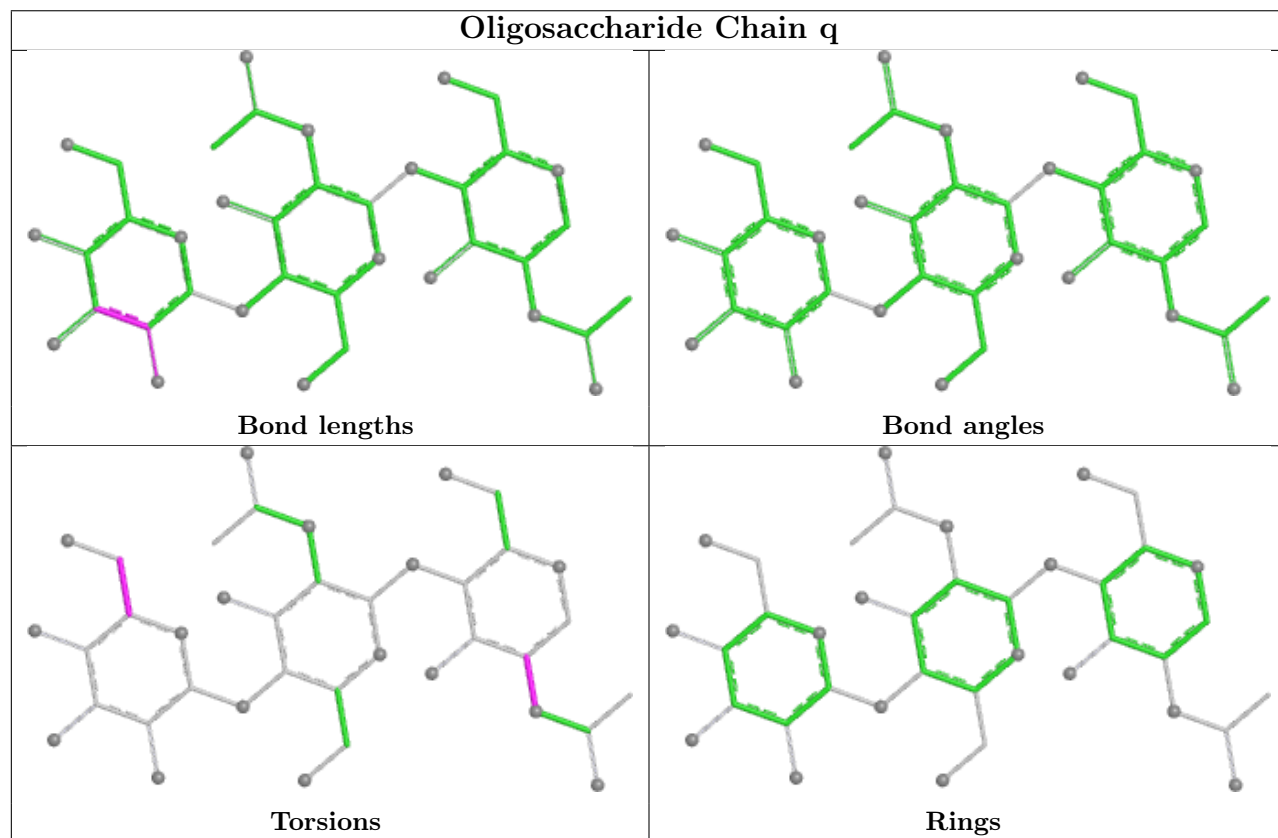
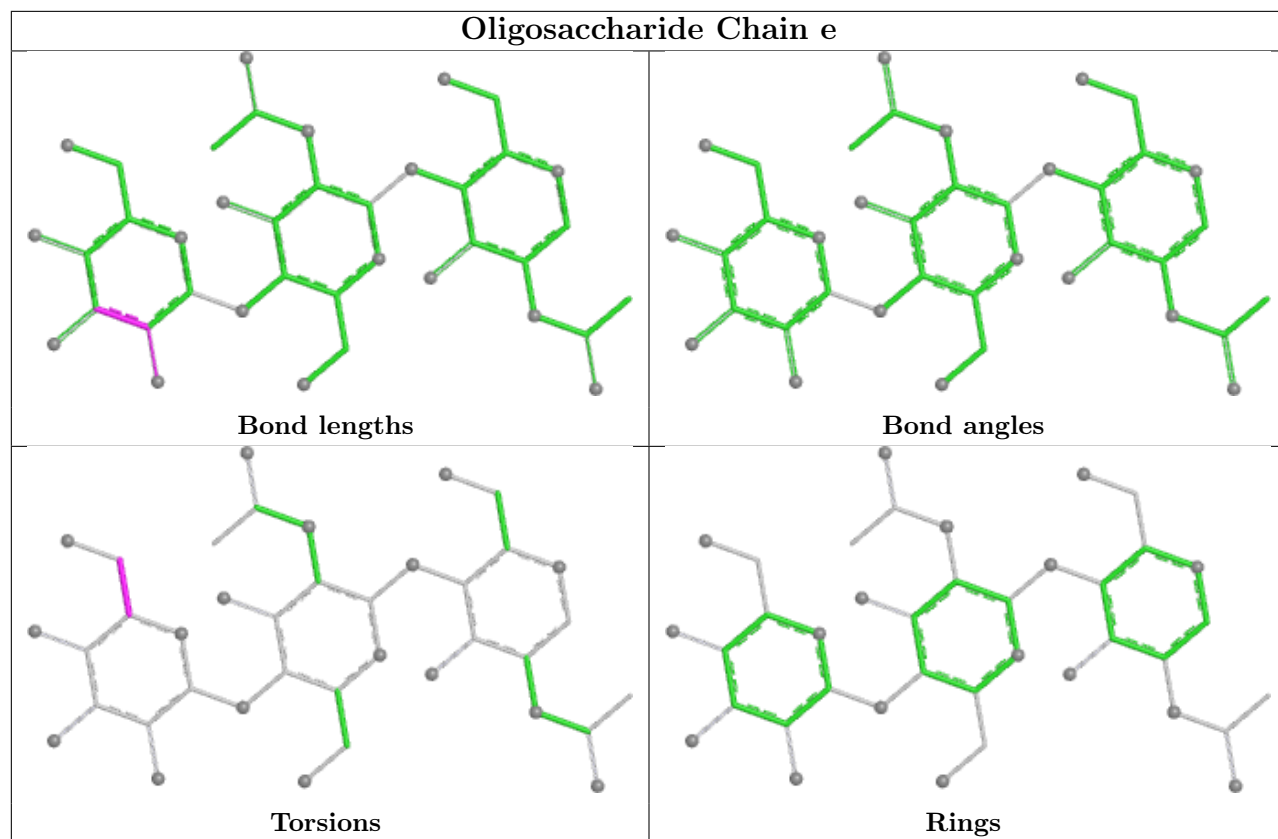












5.6 Ligand geometry

18 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
9	NAG	H	701	2	14,14,15	0.41	0	17,19,21	0.75	0
9	NAG	A	807	1	14,14,15	0.91	1 (7%)	17,19,21	0.97	0
9	NAG	B	818	1	14,14,15	0.87	0	17,19,21	0.89	1 (5%)
9	NAG	G	703	-	14,14,15	0.74	0	17,19,21	1.15	2 (11%)
9	NAG	A	818	1	14,14,15	0.79	0	17,19,21	1.08	1 (5%)
9	NAG	C	701	2	14,14,15	0.77	0	17,19,21	0.96	1 (5%)
9	NAG	G	701	2	14,14,15	0.82	0	17,19,21	0.98	1 (5%)
9	NAG	G	702	2	14,14,15	0.80	1 (7%)	17,19,21	0.91	1 (5%)
9	NAG	C	702	2	14,14,15	0.79	0	17,19,21	0.91	1 (5%)
9	NAG	B	807	1	14,14,15	0.92	1 (7%)	17,19,21	0.85	0
9	NAG	F	807	1	14,14,15	0.91	1 (7%)	17,19,21	0.79	0
9	NAG	H	703	-	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
9	NAG	F	818	1	14,14,15	0.86	0	17,19,21	0.87	1 (5%)
9	NAG	F	832	1	14,14,15	0.82	1 (7%)	17,19,21	0.95	1 (5%)
9	NAG	C	703	2	14,14,15	0.75	0	17,19,21	1.05	1 (5%)
9	NAG	B	832	1	14,14,15	0.80	1 (7%)	17,19,21	0.94	1 (5%)
9	NAG	A	832	1	14,14,15	0.81	1 (7%)	17,19,21	0.92	1 (5%)
9	NAG	H	702	2	14,14,15	0.78	0	17,19,21	0.92	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	H	701	2	-	1/6/23/26	0/1/1/1
9	NAG	A	807	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	818	1	-	3/6/23/26	0/1/1/1
9	NAG	G	703	-	-	2/6/23/26	0/1/1/1
9	NAG	A	818	1	-	0/6/23/26	0/1/1/1
9	NAG	C	701	2	-	2/6/23/26	0/1/1/1
9	NAG	G	701	2	-	0/6/23/26	0/1/1/1
9	NAG	G	702	2	-	2/6/23/26	0/1/1/1
9	NAG	C	702	2	-	3/6/23/26	0/1/1/1
9	NAG	B	807	1	-	3/6/23/26	0/1/1/1
9	NAG	F	807	1	-	2/6/23/26	0/1/1/1
9	NAG	H	703	-	-	1/6/23/26	0/1/1/1
9	NAG	F	818	1	-	2/6/23/26	0/1/1/1
9	NAG	F	832	1	-	2/6/23/26	0/1/1/1
9	NAG	C	703	2	-	1/6/23/26	0/1/1/1
9	NAG	B	832	1	-	2/6/23/26	0/1/1/1
9	NAG	A	832	1	-	2/6/23/26	0/1/1/1
9	NAG	H	702	2	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	832	NAG	C3-C2	-2.10	1.48	1.52
9	A	832	NAG	C3-C2	-2.09	1.48	1.52
9	B	832	NAG	C3-C2	-2.08	1.48	1.52
9	B	807	NAG	C3-C2	-2.07	1.48	1.52
9	G	702	NAG	C3-C2	-2.04	1.48	1.52
9	A	807	NAG	C3-C2	-2.03	1.48	1.52
9	F	807	NAG	C3-C2	-2.02	1.48	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	703	NAG	C4-C3-C2	-2.92	106.74	111.02
9	H	703	NAG	C4-C3-C2	-2.82	106.89	111.02
9	A	818	NAG	C4-C3-C2	-2.74	107.01	111.02
9	C	703	NAG	C4-C3-C2	-2.64	107.15	111.02
9	G	701	NAG	C4-C3-C2	-2.58	107.24	111.02
9	H	702	NAG	C4-C3-C2	-2.48	107.38	111.02
9	C	701	NAG	C4-C3-C2	-2.46	107.42	111.02
9	B	832	NAG	C4-C3-C2	-2.45	107.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	702	NAG	C4-C3-C2	-2.44	107.44	111.02
9	F	832	NAG	C4-C3-C2	-2.43	107.46	111.02
9	G	702	NAG	C4-C3-C2	-2.40	107.49	111.02
9	A	832	NAG	C4-C3-C2	-2.39	107.51	111.02
9	F	818	NAG	C4-C3-C2	-2.19	107.81	111.02
9	B	818	NAG	C4-C3-C2	-2.13	107.90	111.02
9	G	703	NAG	C2-N2-C7	-2.02	120.20	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	807	NAG	C3-C2-N2-C7
9	F	807	NAG	C3-C2-N2-C7
9	H	703	NAG	C3-C2-N2-C7
9	B	818	NAG	C4-C5-C6-O6
9	C	701	NAG	O5-C5-C6-O6
9	B	818	NAG	O5-C5-C6-O6
9	A	832	NAG	C8-C7-N2-C2
9	A	832	NAG	O7-C7-N2-C2
9	C	702	NAG	C8-C7-N2-C2
9	C	702	NAG	O7-C7-N2-C2
9	B	807	NAG	C8-C7-N2-C2
9	B	807	NAG	O7-C7-N2-C2
9	B	832	NAG	C8-C7-N2-C2
9	B	832	NAG	O7-C7-N2-C2
9	G	702	NAG	C8-C7-N2-C2
9	G	702	NAG	O7-C7-N2-C2
9	G	703	NAG	C8-C7-N2-C2
9	G	703	NAG	O7-C7-N2-C2
9	F	818	NAG	C8-C7-N2-C2
9	F	818	NAG	O7-C7-N2-C2
9	F	832	NAG	C8-C7-N2-C2
9	F	832	NAG	O7-C7-N2-C2
9	H	702	NAG	C8-C7-N2-C2
9	H	702	NAG	O7-C7-N2-C2
9	C	702	NAG	O5-C5-C6-O6
9	C	703	NAG	O5-C5-C6-O6
9	H	702	NAG	O5-C5-C6-O6
9	B	807	NAG	O5-C5-C6-O6
9	F	807	NAG	O5-C5-C6-O6
9	C	701	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	818	NAG	C1-C2-N2-C7
9	H	701	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	807	NAG	4	0
9	B	818	NAG	1	0
9	G	703	NAG	1	0
9	C	701	NAG	1	0
9	F	807	NAG	4	0
9	H	703	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

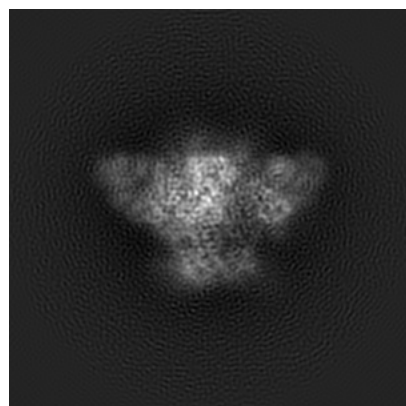
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7568. These allow visual inspection of the internal detail of the map and identification of artifacts.

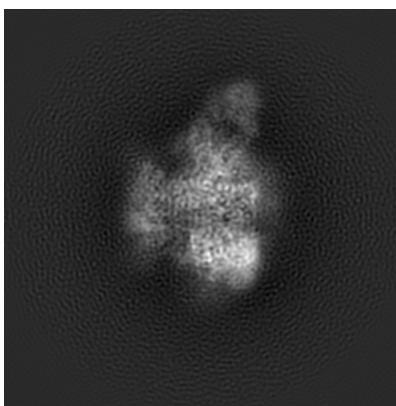
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

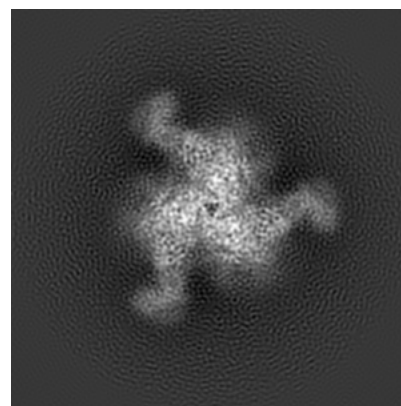
6.1.1 Primary map



X

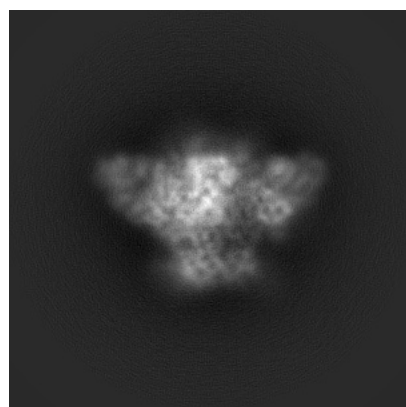


Y

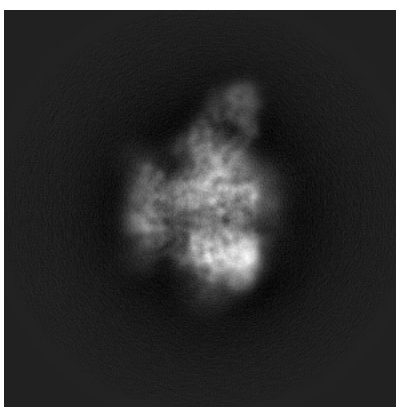


Z

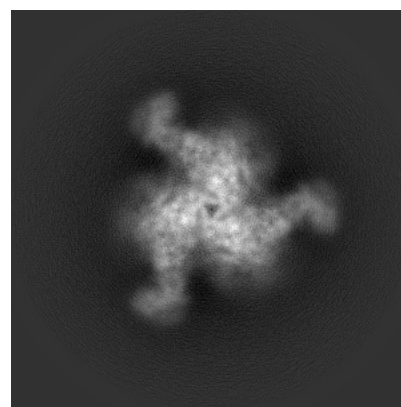
6.1.2 Raw map



X



Y

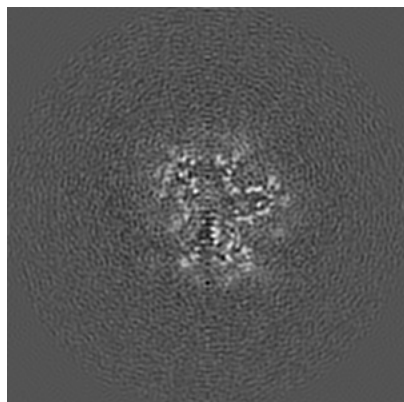


Z

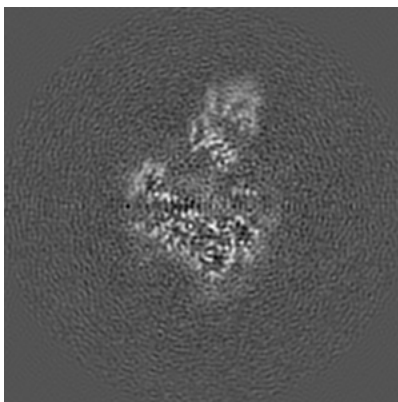
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

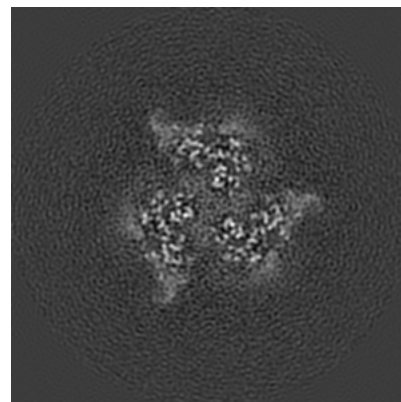
6.2.1 Primary map



X Index: 150

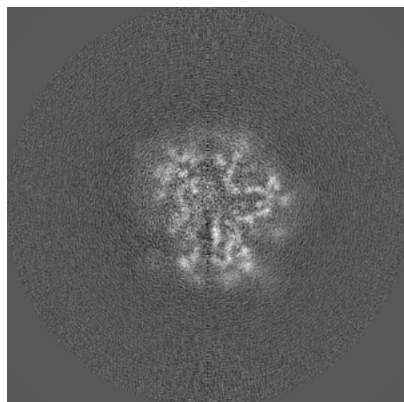


Y Index: 150

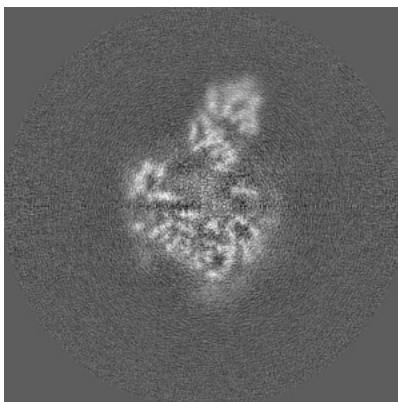


Z Index: 150

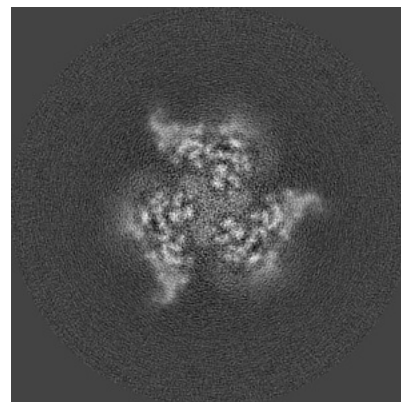
6.2.2 Raw map



X Index: 150



Y Index: 150

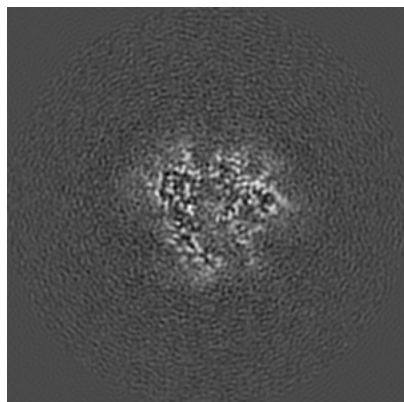


Z Index: 150

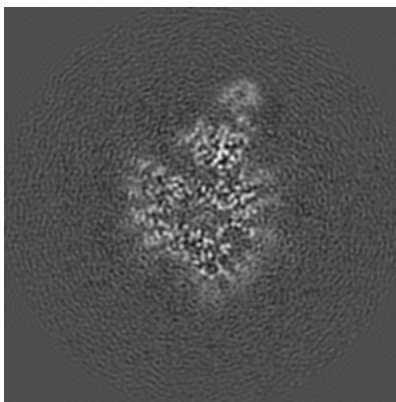
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

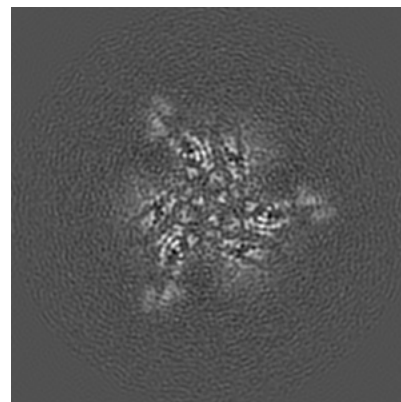
6.3.1 Primary map



X Index: 165

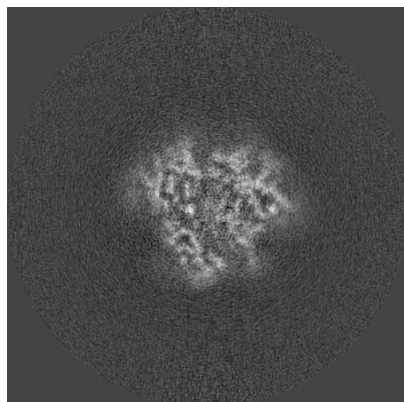


Y Index: 140

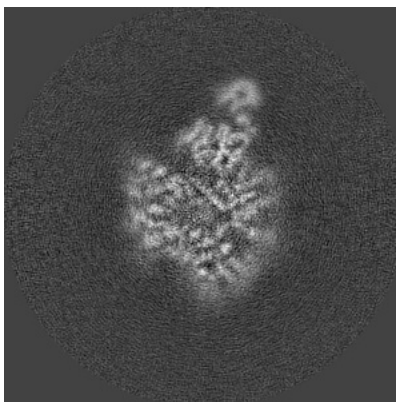


Z Index: 161

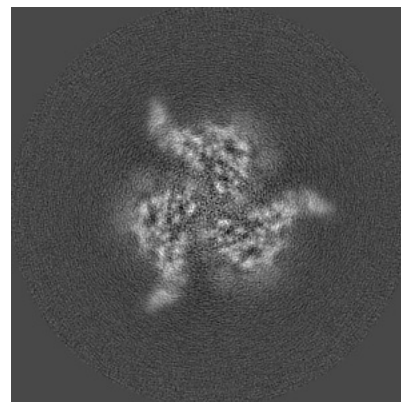
6.3.2 Raw map



X Index: 165



Y Index: 140

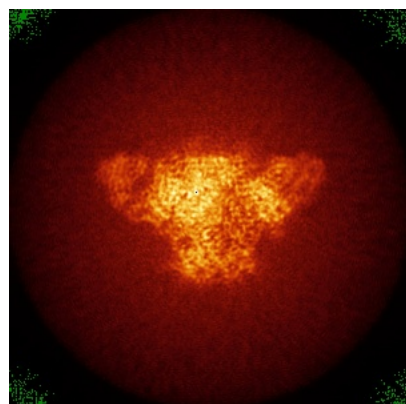


Z Index: 154

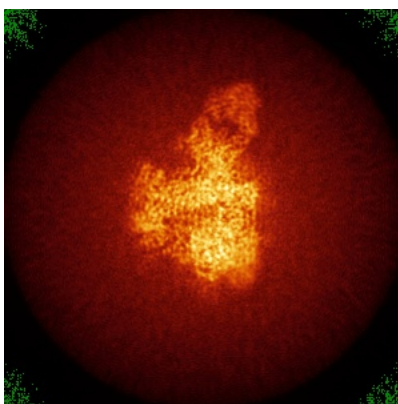
The images above show the largest variance slices of the map in three orthogonal directions.

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

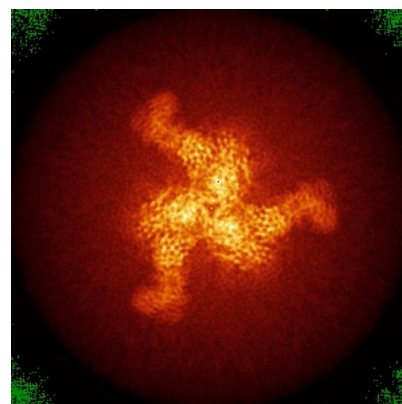
6.4.1 Primary map



X

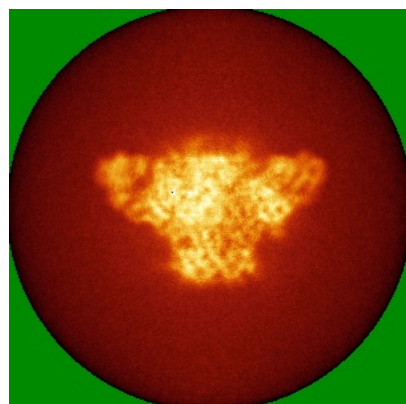


Y

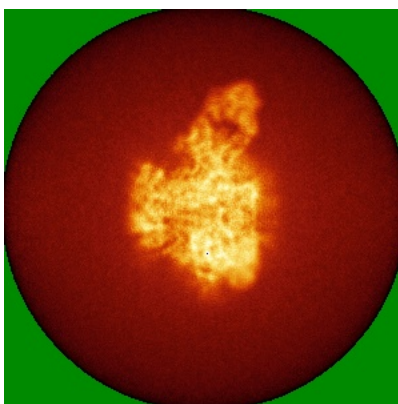


Z

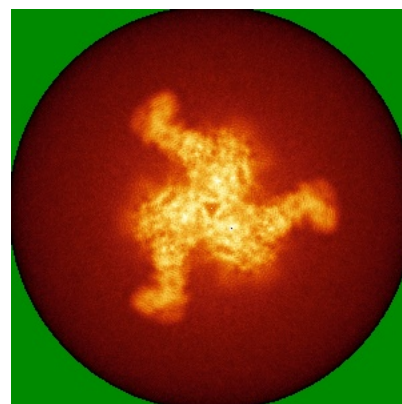
6.4.2 Raw map



X



Y

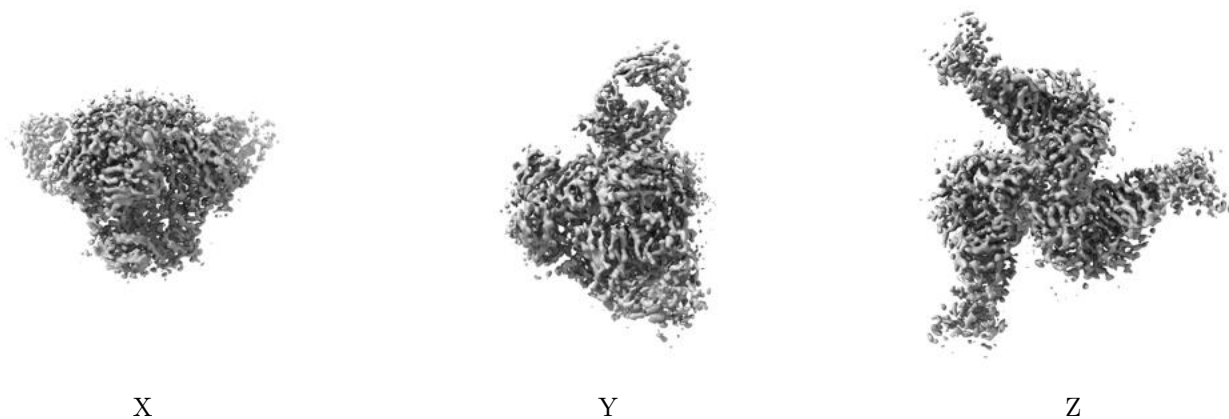


Z

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

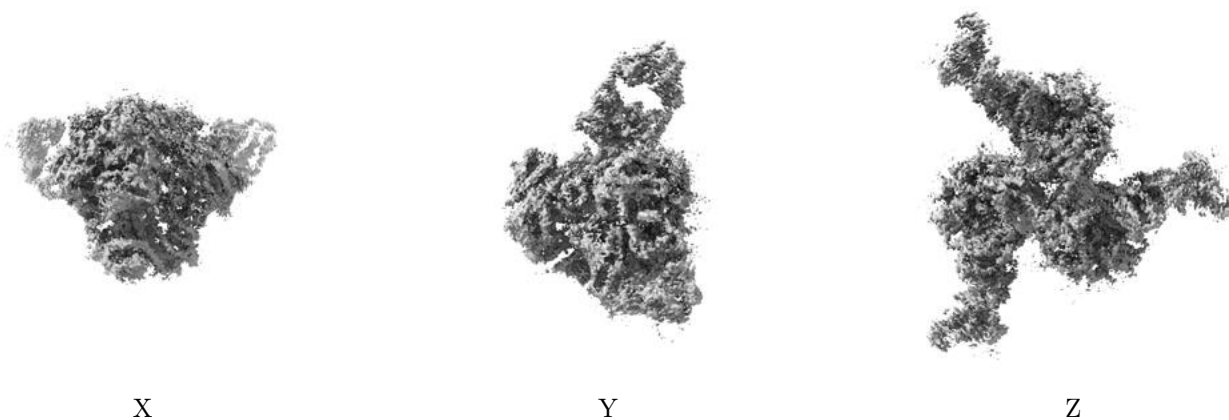
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

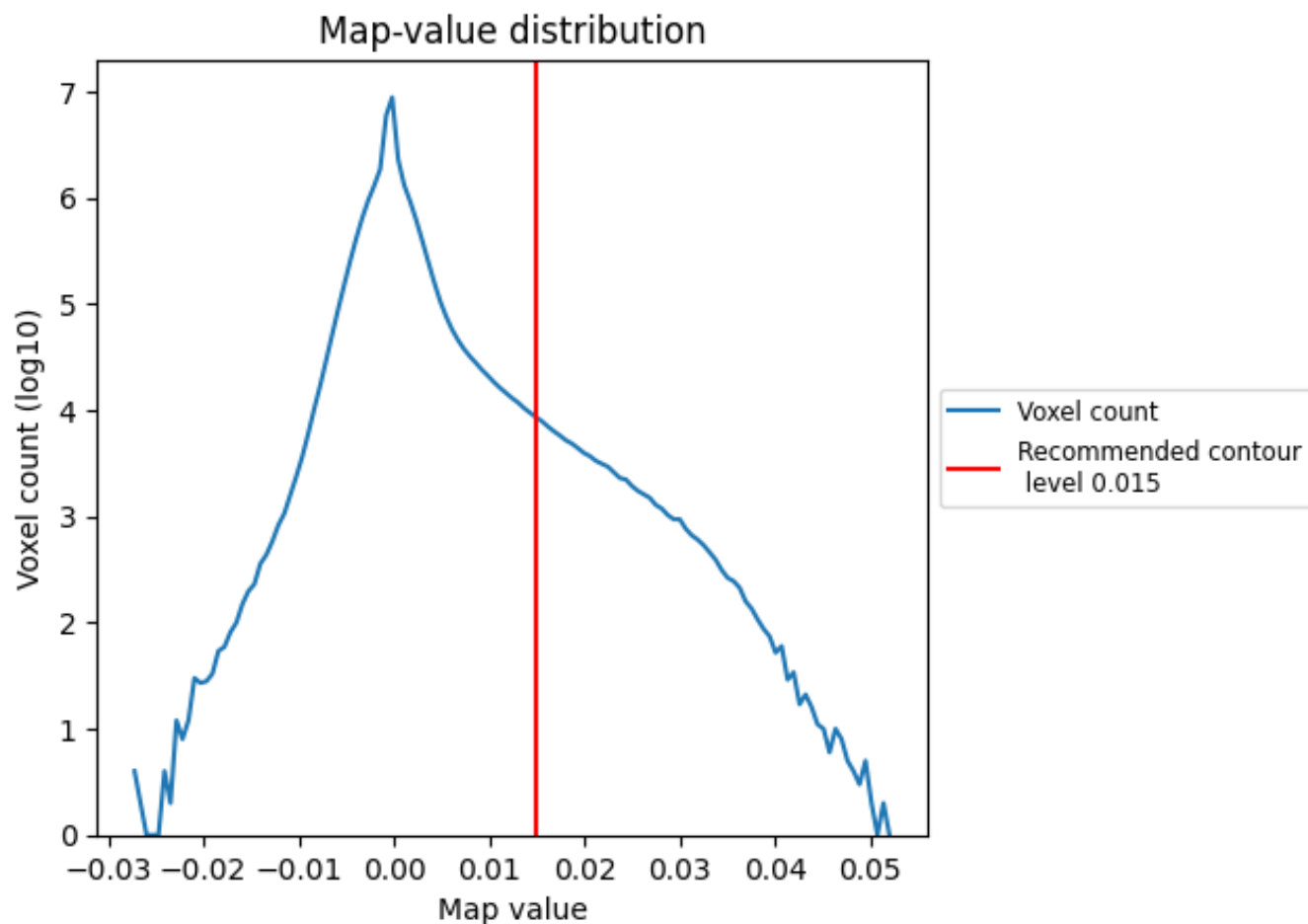
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

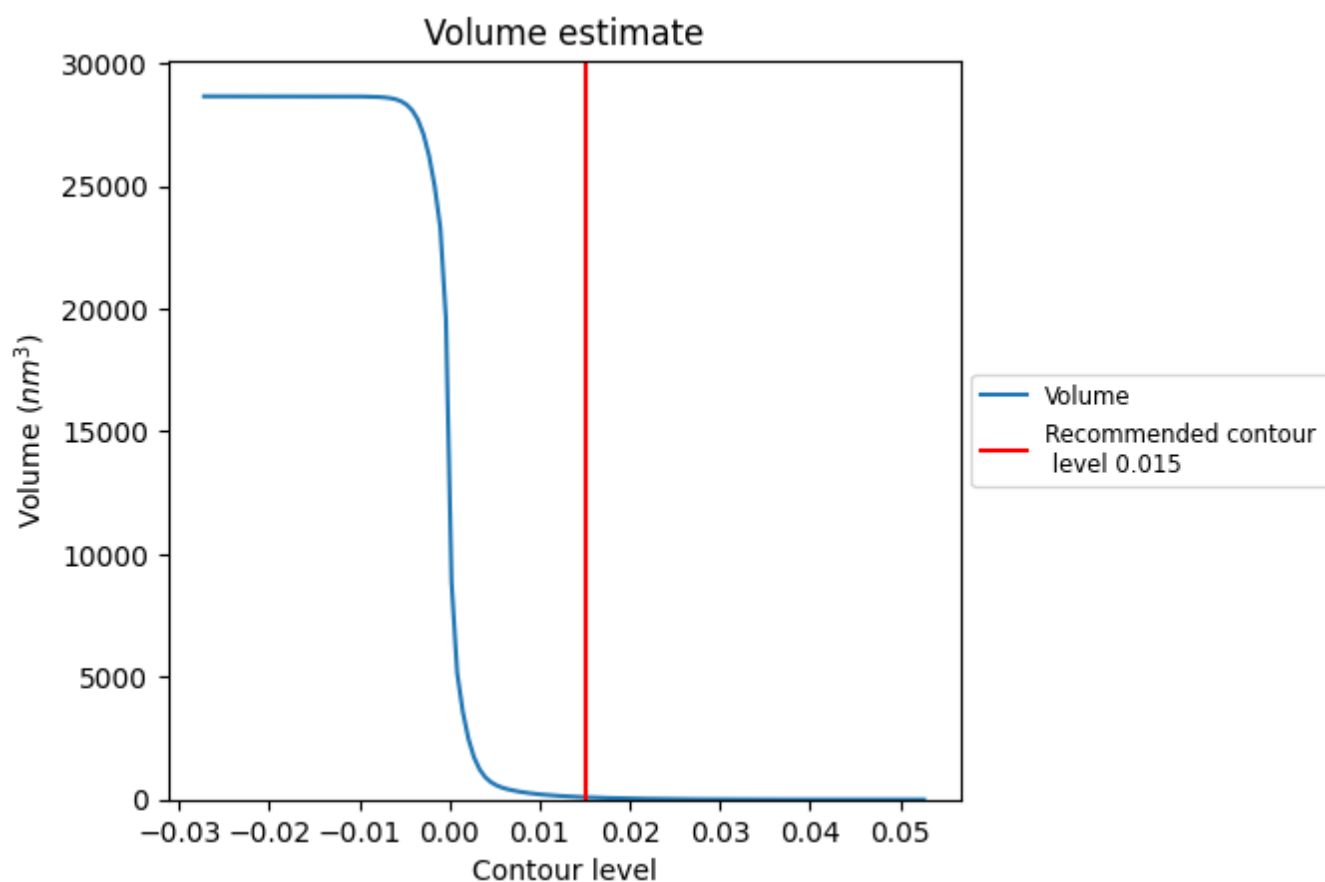
This section contains the results of statistical analysis of the map.

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.

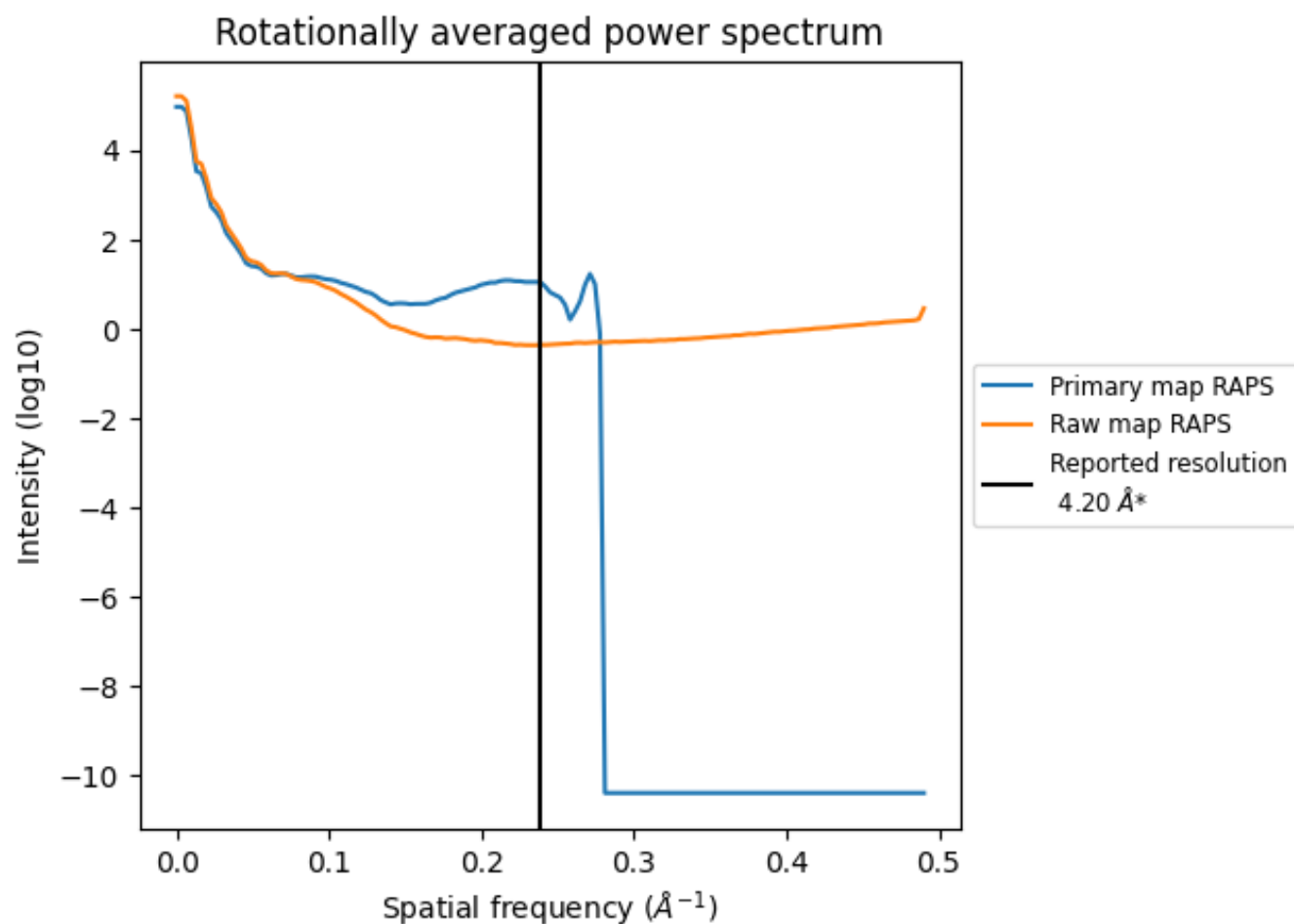
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 86 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 ⓘ

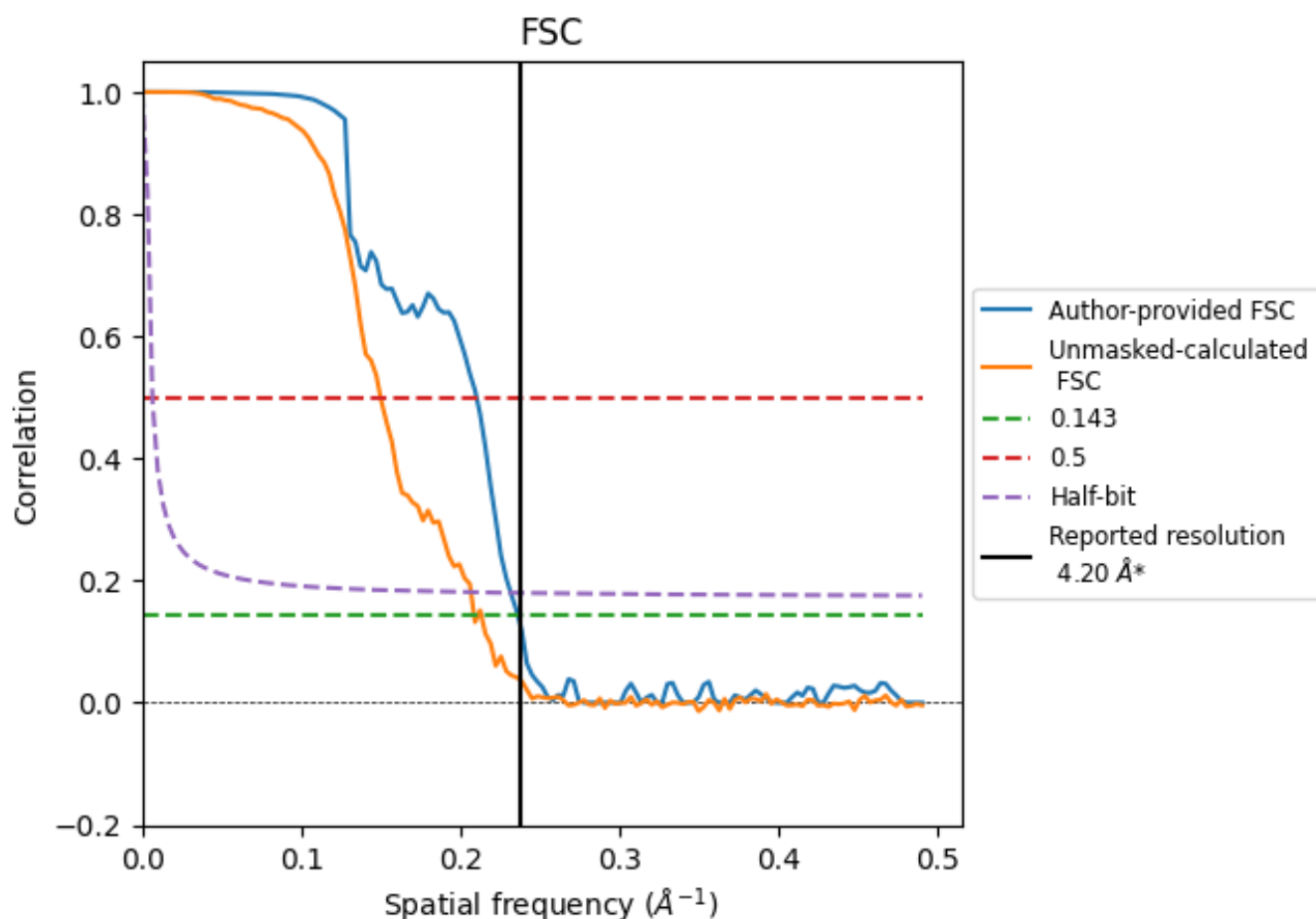


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

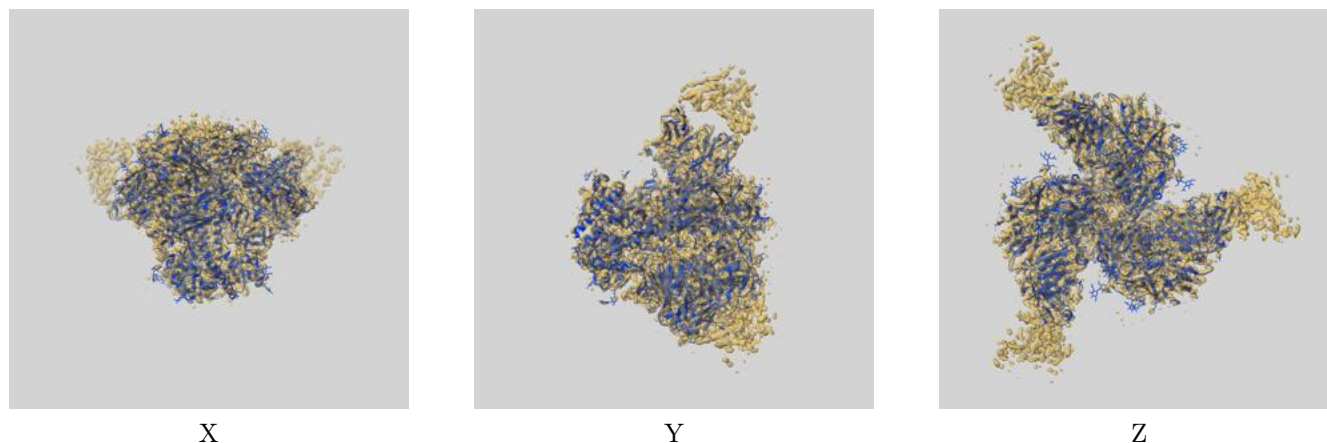
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	4.76	4.32
Unmasked-calculated*	4.79	6.68	4.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.79 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

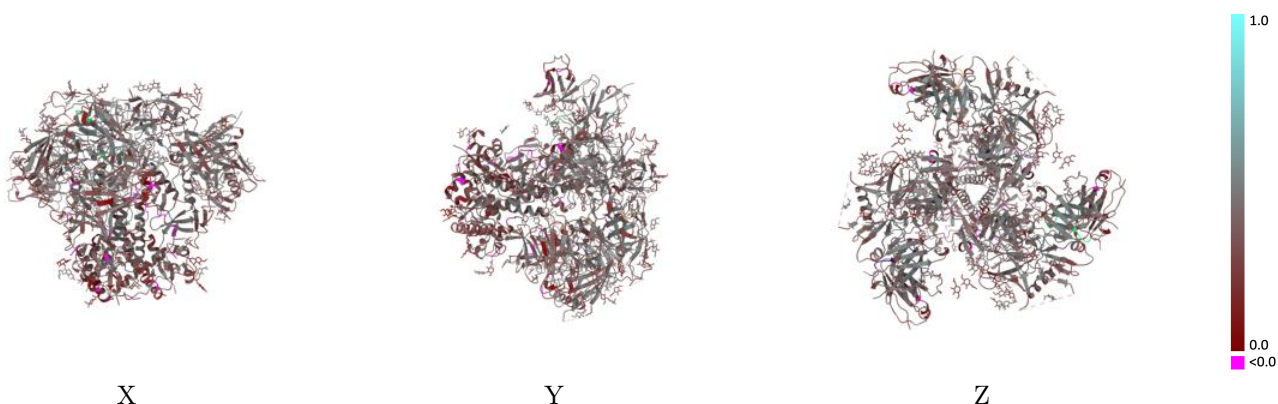
This section contains information regarding the fit between EMDB map EMD-7568 and PDB model 6CRQ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



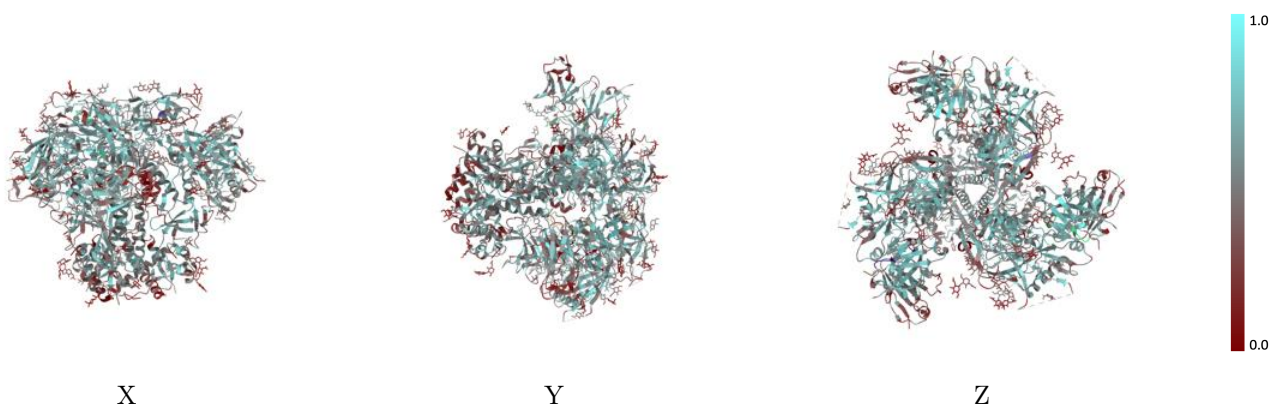
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



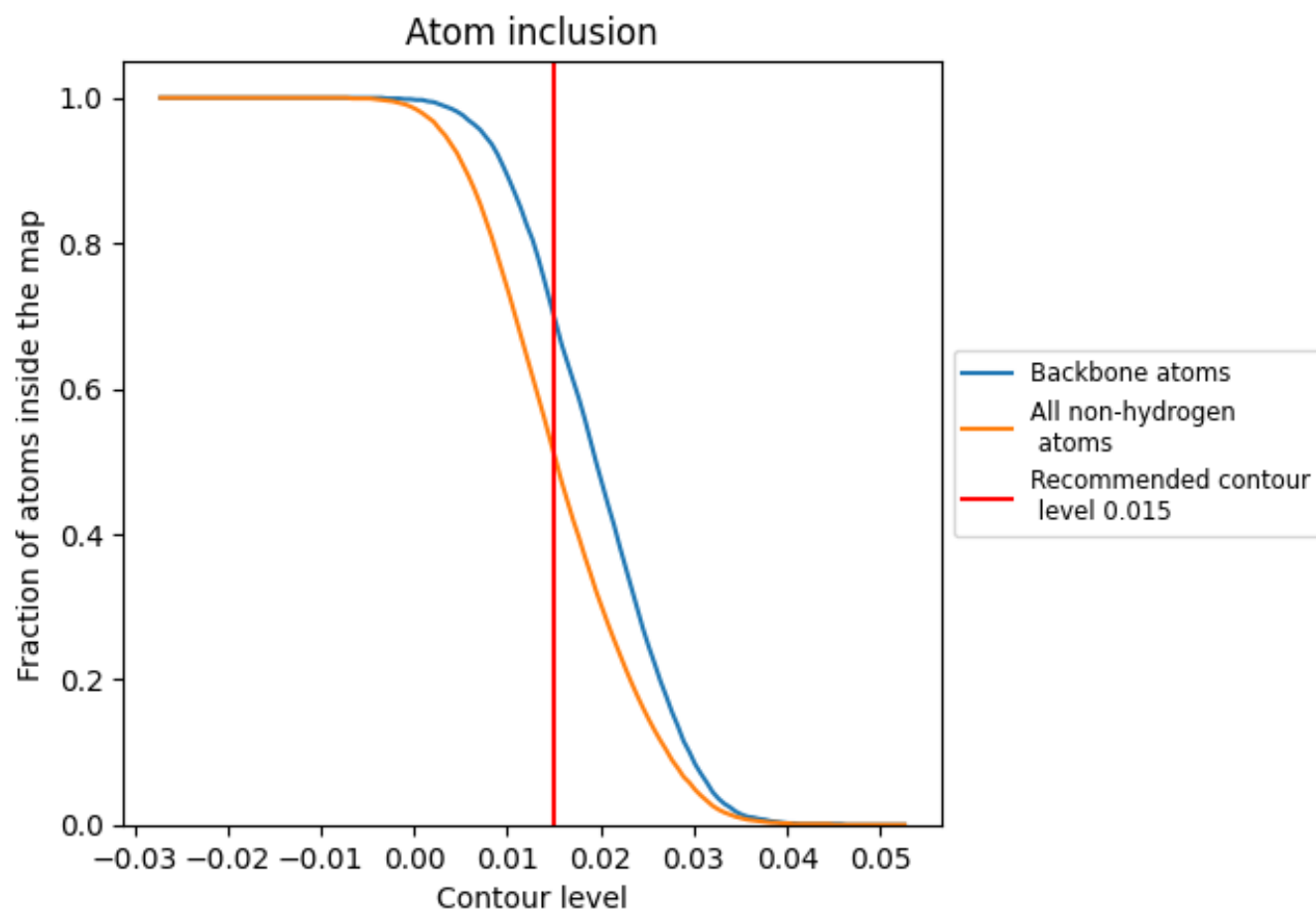
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 51% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5100	 0.3630
A	 0.5410	 0.3800
B	 0.5330	 0.3740
C	 0.4530	 0.3040
D	 0.5930	 0.4130
E	 0.4670	 0.3170
F	 0.5430	 0.3820
G	 0.4390	 0.2960
H	 0.4370	 0.2830
I	 0.5950	 0.4080
J	 0.5880	 0.4150
K	 0.4730	 0.3280
L	 0.4650	 0.3300
M	 0.4000	 0.3800
N	 0.1790	 0.3630
O	 0.5400	 0.3990
P	 0.2140	 0.2740
Q	 0.4290	 0.3240
R	 0.4290	 0.3800
S	 0.2050	 0.3780
T	 0.0710	 0.2990
U	 0.4290	 0.3710
V	 0.1070	 0.2650
W	 0.1070	 0.2630
X	 0.2500	 0.3380
Y	 0.4400	 0.3870
Z	 0.1790	 0.3480
a	 0.5000	 0.3670
b	 0.2500	 0.3440
c	 0.4640	 0.3990
d	 0.4290	 0.3410
e	 0.2310	 0.4000
f	 0.0710	 0.2690
g	 0.4290	 0.4030
h	 0.1430	 0.2360



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Chain	Atom inclusion	Q-score
i	 0.1430	 0.2660
j	 0.1790	 0.3390
k	 0.4200	 0.3890
l	 0.1790	 0.3630
m	 0.5200	 0.3750
n	 0.2500	 0.3010
o	 0.4640	 0.3280
p	 0.4640	 0.3930
q	 0.2310	 0.3830
r	 0.0710	 0.2860
s	 0.4290	 0.3950
t	 0.1070	 0.2460
u	 0.1070	 0.3050
v	 0.2140	 0.3260