



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:04 PM UTC

PDB ID : 7SQ1 / pdb_00007sq1
EMDB ID : EMD-25376
Title : BG505.MD39TS Env trimer in complex with Fab from antibody C05
Authors : Moore, A.; Du, J.; Xu, Z.; Walker, S.; Kulp, D.W.; Pallesen, J.
Deposited on : 2021-11-04
Resolution : 3.80 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:

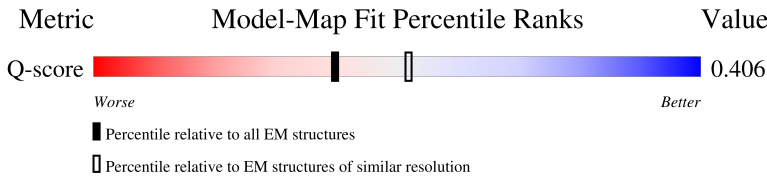
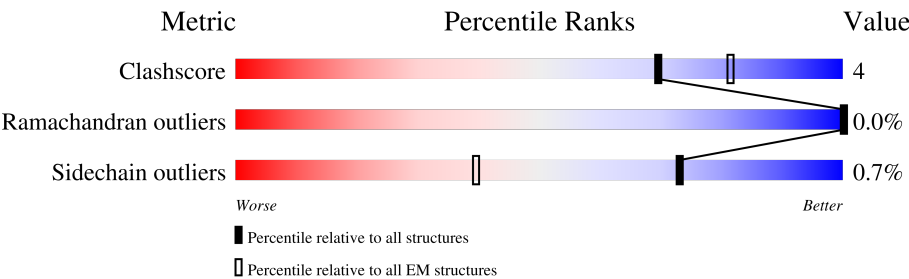
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.80 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	10198 (3.30 - 4.30)

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	B	153	
1	D	153	
1	F	153	
2	C	472	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	472	
2	G	472	
3	I	111	
3	L	111	
4	A	122	
4	H	122	
5	J	2	
5	K	2	
5	M	2	
5	N	2	
5	P	2	
5	Q	2	
5	R	2	
5	S	2	
5	T	2	
5	W	2	
5	X	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	
5	d	2	
5	e	2	
5	h	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	i	2	
5	j	2	
6	O	2	
7	U	3	
7	f	3	
7	g	3	
8	V	4	

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	c	1	-	-	X	-
5	NAG	h	2	-	-	X	-
9	NAG	E	601	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18340 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	121	Total	C	N	O	S	0	0
			969	611	168	184	6		
1	D	121	Total	C	N	O	S	0	0
			969	611	168	184	6		
1	F	121	Total	C	N	O	S	0	0
			969	611	168	184	6		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	PRO	ALA	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	519	SER	PHE	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	561	PRO	ALA	conflict	UNP Q2N0S6
D	568	ASP	LEU	conflict	UNP Q2N0S6
D	570	HIS	VAL	conflict	UNP Q2N0S6
D	585	HIS	ARG	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
F	519	SER	PHE	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	PRO	ALA	conflict	UNP Q2N0S6
F	568	ASP	LEU	conflict	UNP Q2N0S6
F	570	HIS	VAL	conflict	UNP Q2N0S6
F	585	HIS	ARG	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	440	Total	C	N	O	S	0	0
			3467	2182	609	649	27		
2	E	446	Total	C	N	O	S	0	0
			3512	2208	617	660	27		
2	G	444	Total	C	N	O	S	0	0
			3497	2198	614	658	27		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	106	GLU	THR	conflict	UNP Q2N0S6
C	271	ILE	MET	conflict	UNP Q2N0S6
C	288	LEU	PHE	conflict	UNP Q2N0S6
C	304	VAL	ARG	conflict	UNP Q2N0S6
C	319	TYR	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	363	GLN	ASN	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
E	106	GLU	THR	conflict	UNP Q2N0S6
E	271	ILE	MET	conflict	UNP Q2N0S6
E	288	LEU	PHE	conflict	UNP Q2N0S6
E	304	VAL	ARG	conflict	UNP Q2N0S6
E	319	TYR	ALA	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	363	GLN	ASN	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
G	106	GLU	THR	conflict	UNP Q2N0S6
G	271	ILE	MET	conflict	UNP Q2N0S6
G	288	LEU	PHE	conflict	UNP Q2N0S6
G	304	VAL	ARG	conflict	UNP Q2N0S6
G	319	TYR	ALA	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	363	GLN	ASN	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 3 is a protein called C05 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			845	532	142	166	5		
3	I	111	Total	C	N	O	S	0	0
			845	532	142	166	5		

- Molecule 4 is a protein called C05 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	121	Total	C	N	O	S	0	0
			958	602	165	185	6		
4	A	121	Total	C	N	O	S	0	0
			958	602	165	185	6		

- Molecule 5 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
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

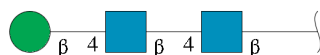
Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
6	O	2	Total	C	O	0	0
			22	12	10		

- Molecule 7 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
7	U	3	Total	C	N	O	0	0
			39	22	2	15		
7	f	3	Total	C	N	O	0	0
			39	22	2	15		
7	g	3	Total	C	N	O	0	0
			39	22	2	15		

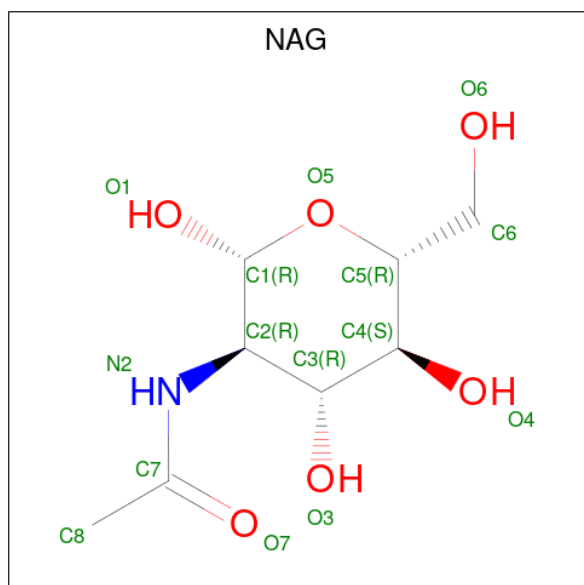
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose.

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
8	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
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	B	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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

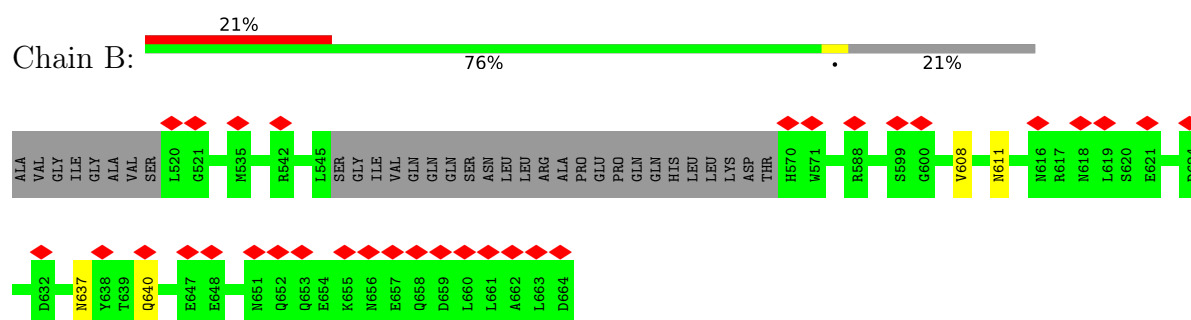
Continued from previous page...

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

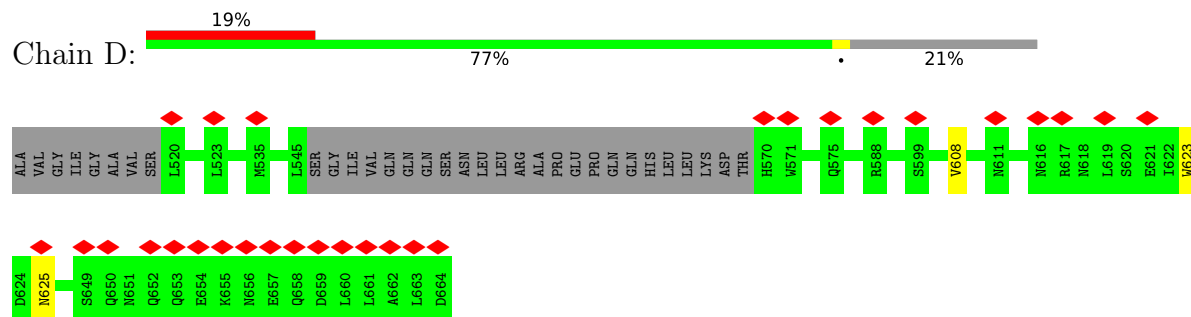
3 Residue-property plots [i](#)

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.

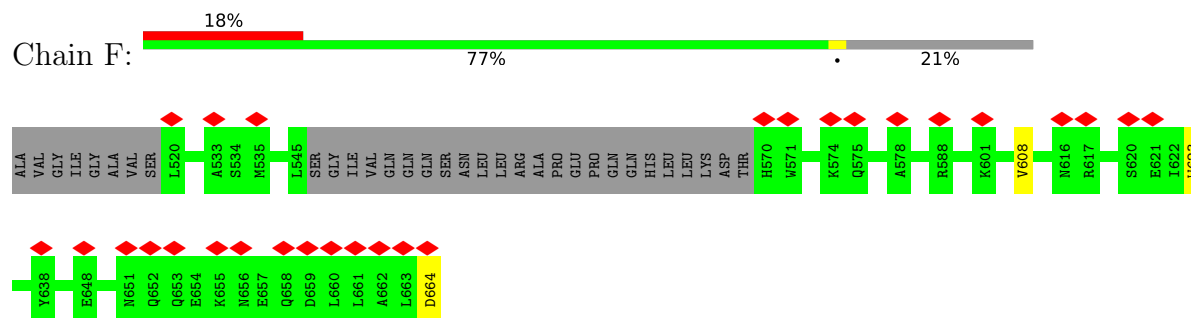
- Molecule 1: Transmembrane protein gp41



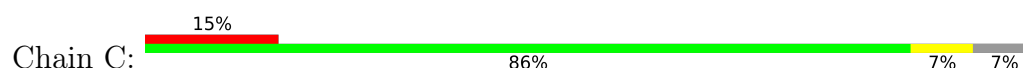
- Molecule 1: Transmembrane protein gp41

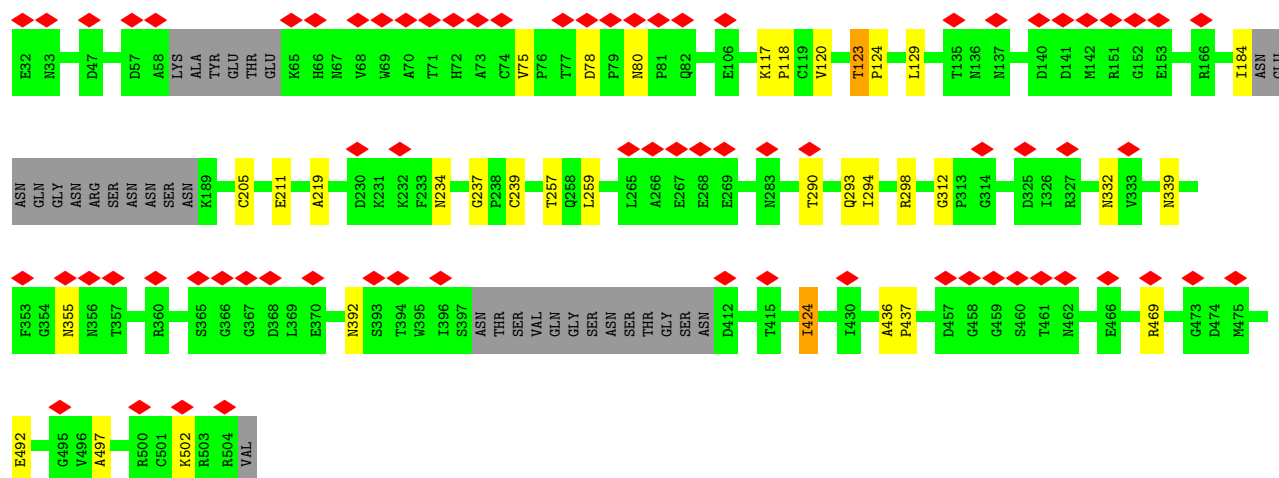


- Molecule 1: Transmembrane protein gp41

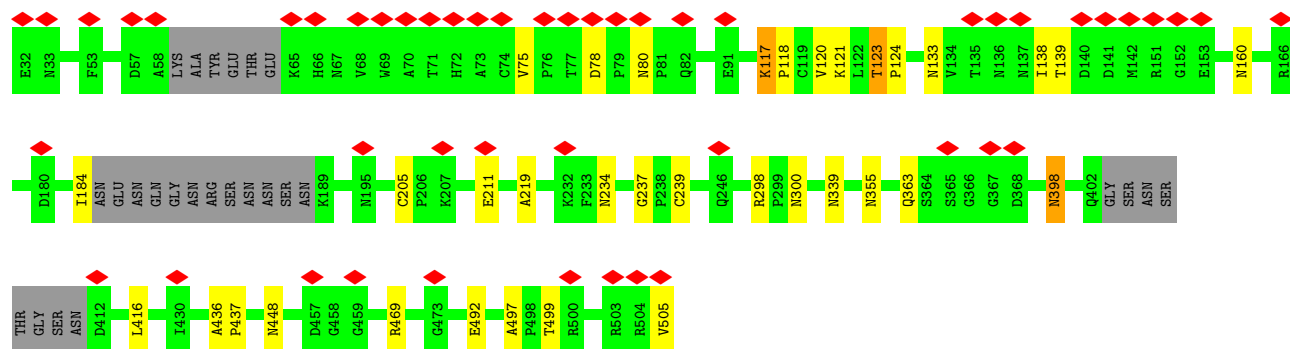
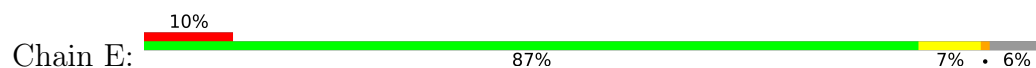


- Molecule 2: Envelope glycoprotein gp160

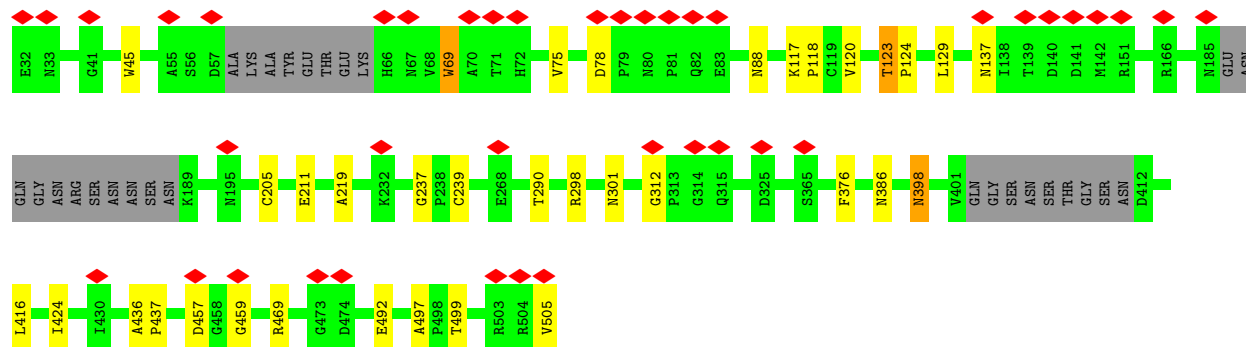
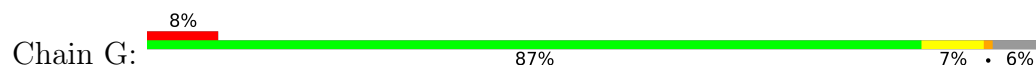




- Molecule 2: Envelope glycoprotein gp160



- Molecule 2: Envelope glycoprotein gp160

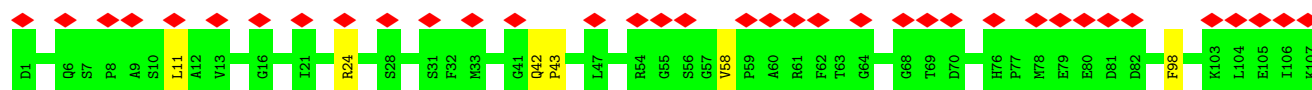
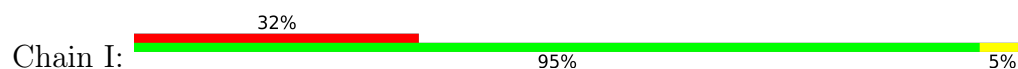


- Molecule 3: C05 Fab Light chain

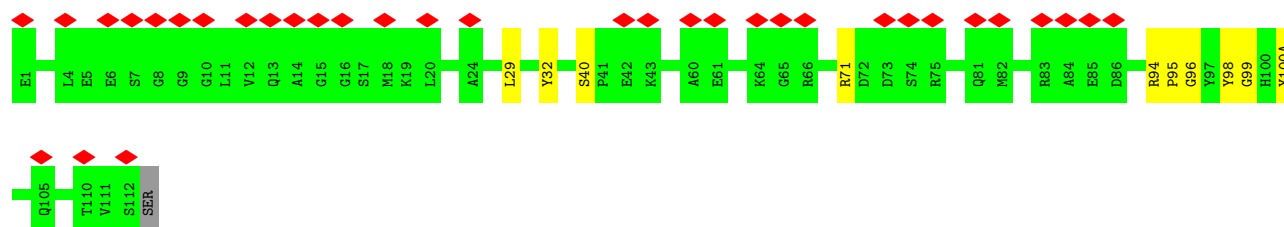




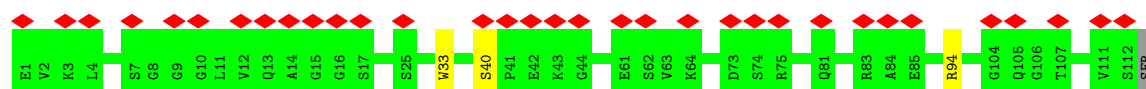
- Molecule 3: C05 Fab Light chain



- Molecule 4: C05 Fab heavy chain



- Molecule 4: C05 Fab heavy chain



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



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



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



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



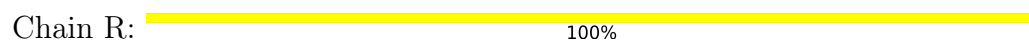
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose



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



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



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



- Molecule 8: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121929	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 ($e^-/\text{\AA}^2$)	60.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	430.08, 430.08, 430.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	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	B	0.61	0/988	0.70	2/1339 (0.1%)
1	D	0.60	0/988	0.68	2/1339 (0.1%)
1	F	0.62	0/988	0.67	2/1339 (0.1%)
2	C	0.63	0/3539	1.01	35/4805 (0.7%)
2	E	0.64	0/3584	1.03	38/4866 (0.8%)
2	G	0.63	0/3569	1.00	38/4847 (0.8%)
3	I	0.62	0/866	1.05	9/1172 (0.8%)
3	L	0.60	0/866	1.03	8/1172 (0.7%)
4	A	0.68	0/982	0.93	4/1328 (0.3%)
4	H	0.66	0/982	0.93	5/1328 (0.4%)
All	All	0.63	0/17352	0.96	143/23535 (0.6%)

There are no bond length outliers.

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	497	ALA	CA-C-N	8.93	129.16	119.87
2	C	497	ALA	C-N-CA	8.93	129.16	119.87
2	E	497	ALA	CA-C-N	8.73	128.95	119.87
2	E	497	ALA	C-N-CA	8.73	128.95	119.87
4	H	94	ARG	CA-C-N	8.56	128.21	119.56
4	H	94	ARG	C-N-CA	8.56	128.21	119.56
2	G	497	ALA	CA-C-N	8.55	128.76	119.87
2	G	497	ALA	C-N-CA	8.55	128.76	119.87
4	A	94	ARG	CA-C-N	8.30	129.10	119.47
4	A	94	ARG	C-N-CA	8.30	129.10	119.47
3	L	42	GLN	CA-C-N	8.05	125.45	119.66
3	L	42	GLN	C-N-CA	8.05	125.45	119.66
3	I	42	GLN	CA-C-N	7.92	125.36	119.66
3	I	42	GLN	C-N-CA	7.92	125.36	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	436	ALA	CA-C-N	7.66	125.18	119.66
2	E	436	ALA	C-N-CA	7.66	125.18	119.66
2	C	492	GLU	CA-C-N	7.63	127.27	119.56
2	C	492	GLU	C-N-CA	7.63	127.27	119.56
2	G	492	GLU	CA-C-N	7.54	127.17	119.56
2	G	492	GLU	C-N-CA	7.54	127.17	119.56
2	G	298	ARG	CA-C-N	7.52	127.16	119.56
2	G	298	ARG	C-N-CA	7.52	127.16	119.56
2	E	298	ARG	CA-C-N	7.35	127.98	120.04
2	E	298	ARG	C-N-CA	7.35	127.98	120.04
2	C	298	ARG	CA-C-N	7.30	127.92	120.04
2	C	298	ARG	C-N-CA	7.30	127.92	120.04
2	E	492	GLU	CA-C-N	7.25	126.88	119.56
2	E	492	GLU	C-N-CA	7.25	126.88	119.56
2	G	219	ALA	CA-C-N	7.14	127.10	120.03
2	G	219	ALA	C-N-CA	7.14	127.10	120.03
2	G	205	CYS	CA-C-N	7.05	126.68	119.56
2	G	205	CYS	C-N-CA	7.05	126.68	119.56
2	E	205	CYS	CA-C-N	7.01	126.64	119.56
2	E	205	CYS	C-N-CA	7.01	126.64	119.56
2	E	219	ALA	CA-C-N	6.95	126.92	120.03
2	E	219	ALA	C-N-CA	6.95	126.92	120.03
2	C	219	ALA	CA-C-N	6.92	126.88	120.03
2	C	219	ALA	C-N-CA	6.92	126.88	120.03
2	E	239	CYS	CA-C-N	6.91	126.89	119.28
2	E	239	CYS	C-N-CA	6.91	126.89	119.28
2	C	239	CYS	CA-C-N	6.78	126.74	119.28
2	C	239	CYS	C-N-CA	6.78	126.74	119.28
3	I	58	VAL	CA-C-N	6.77	126.75	119.78
3	I	58	VAL	C-N-CA	6.77	126.75	119.78
3	I	24	ARG	CA-C-N	6.73	126.69	119.76
3	I	24	ARG	C-N-CA	6.73	126.69	119.76
2	C	205	CYS	CA-C-N	6.63	126.25	119.56
2	C	205	CYS	C-N-CA	6.63	126.25	119.56
2	E	237	GLY	CA-C-N	6.61	126.57	119.76
2	E	237	GLY	C-N-CA	6.61	126.57	119.76
2	G	239	CYS	CA-C-N	6.55	126.25	119.56
2	G	239	CYS	C-N-CA	6.55	126.25	119.56
2	C	237	GLY	CA-C-N	6.47	126.43	119.76
2	C	237	GLY	C-N-CA	6.47	126.43	119.76
2	E	117	LYS	CA-C-N	6.22	125.84	119.56
2	E	117	LYS	C-N-CA	6.22	125.84	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	58	VAL	CA-C-N	6.09	126.01	119.85
3	L	58	VAL	C-N-CA	6.09	126.01	119.85
2	C	436	ALA	CA-C-N	6.02	123.99	119.66
2	C	436	ALA	C-N-CA	6.02	123.99	119.66
2	C	78	ASP	CA-C-N	6.01	125.69	119.56
2	C	78	ASP	C-N-CA	6.01	125.69	119.56
2	G	237	GLY	CA-C-N	6.00	125.76	119.76
2	G	237	GLY	C-N-CA	6.00	125.76	119.76
2	G	211	GLU	CA-C-N	5.93	125.87	119.76
2	G	211	GLU	C-N-CA	5.93	125.87	119.76
2	C	211	GLU	CA-C-N	5.92	125.86	119.76
2	C	211	GLU	C-N-CA	5.92	125.86	119.76
2	C	123	THR	CA-C-N	5.91	125.59	119.56
2	C	123	THR	C-N-CA	5.91	125.59	119.56
2	E	211	GLU	CA-C-N	5.89	125.83	119.76
2	E	211	GLU	C-N-CA	5.89	125.83	119.76
2	C	75	VAL	CA-C-N	5.89	125.85	119.78
2	C	75	VAL	C-N-CA	5.89	125.85	119.78
2	C	120	VAL	N-CA-C	5.88	116.66	109.30
2	G	312	GLY	CA-C-N	5.87	125.42	119.19
2	G	312	GLY	C-N-CA	5.87	125.42	119.19
2	E	416	LEU	CA-C-N	5.87	125.78	119.85
2	E	416	LEU	C-N-CA	5.87	125.78	119.85
3	L	43	PRO	CA-C-N	5.87	125.83	119.78
3	L	43	PRO	C-N-CA	5.87	125.83	119.78
2	G	436	ALA	CA-C-N	5.87	123.89	119.66
2	G	436	ALA	C-N-CA	5.87	123.89	119.66
2	E	78	ASP	CA-C-N	5.86	125.53	119.56
2	E	78	ASP	C-N-CA	5.86	125.53	119.56
3	I	43	PRO	CA-C-N	5.83	125.78	119.78
3	I	43	PRO	C-N-CA	5.83	125.78	119.78
2	E	123	THR	CA-C-N	5.81	125.48	119.56
2	E	123	THR	C-N-CA	5.81	125.48	119.56
2	G	376	PHE	CA-CB-CG	5.76	119.56	113.80
2	E	437	PRO	CA-C-N	5.70	125.61	119.85
2	E	437	PRO	C-N-CA	5.70	125.61	119.85
1	B	608	VAL	CA-C-N	5.70	125.60	119.85
1	B	608	VAL	C-N-CA	5.70	125.60	119.85
2	E	469	ARG	CA-C-N	5.64	125.57	119.76
2	E	469	ARG	C-N-CA	5.64	125.57	119.76
2	G	459	GLY	N-CA-C	-5.64	107.48	115.43
2	G	123	THR	CA-C-N	5.64	125.31	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	123	THR	C-N-CA	5.64	125.31	119.56
3	L	24	ARG	CA-C-N	5.58	125.51	119.76
3	L	24	ARG	C-N-CA	5.58	125.51	119.76
2	C	312	GLY	CA-C-N	5.57	125.10	119.19
2	C	312	GLY	C-N-CA	5.57	125.10	119.19
2	C	437	PRO	CA-C-N	5.55	125.45	119.85
2	C	437	PRO	C-N-CA	5.55	125.45	119.85
2	G	120	VAL	N-CA-C	5.55	116.23	109.30
2	E	120	VAL	N-CA-C	5.46	116.13	109.30
1	D	608	VAL	CA-C-N	5.46	125.36	119.85
1	D	608	VAL	C-N-CA	5.46	125.36	119.85
2	E	139	THR	N-CA-C	-5.43	106.70	113.38
2	G	416	LEU	CA-C-N	5.38	125.29	119.85
2	G	416	LEU	C-N-CA	5.38	125.29	119.85
2	G	78	ASP	CA-C-N	5.38	125.05	119.56
2	G	78	ASP	C-N-CA	5.38	125.05	119.56
3	I	98	PHE	CA-CB-CG	5.38	119.18	113.80
2	G	290	THR	CA-C-N	5.37	125.83	120.14
2	G	290	THR	C-N-CA	5.37	125.83	120.14
2	C	80	ASN	CA-C-N	5.37	125.29	119.76
2	C	80	ASN	C-N-CA	5.37	125.29	119.76
2	E	138	ILE	N-CA-C	5.26	115.42	107.75
2	E	75	VAL	CA-C-N	5.22	125.14	119.76
2	E	75	VAL	C-N-CA	5.22	125.14	119.76
2	E	80	ASN	CA-C-N	5.19	125.10	119.76
2	E	80	ASN	C-N-CA	5.19	125.10	119.76
2	G	469	ARG	CA-C-N	5.19	125.10	119.76
2	G	469	ARG	C-N-CA	5.19	125.10	119.76
2	C	290	THR	CA-C-N	5.18	125.64	120.14
2	C	290	THR	C-N-CA	5.18	125.64	120.14
2	G	75	VAL	CA-C-N	5.18	125.10	119.76
2	G	75	VAL	C-N-CA	5.18	125.10	119.76
2	G	69	TRP	N-CA-C	5.18	117.22	110.53
4	H	99	GLY	N-CA-C	-5.15	108.51	115.36
4	H	40	SER	CA-C-N	5.12	124.78	119.56
4	H	40	SER	C-N-CA	5.12	124.78	119.56
4	A	40	SER	CA-C-N	5.10	124.76	119.56
4	A	40	SER	C-N-CA	5.10	124.76	119.56
2	C	469	ARG	CA-C-N	5.09	125.00	119.76
2	C	469	ARG	C-N-CA	5.09	125.00	119.76
1	F	608	VAL	CA-C-N	5.06	124.96	119.85
1	F	608	VAL	C-N-CA	5.06	124.96	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	300	ASN	N-CA-C	5.05	119.07	113.01
2	G	437	PRO	CA-C-N	5.02	124.92	119.85
2	G	437	PRO	C-N-CA	5.02	124.92	119.85

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	B	969	0	933	1	0
1	D	969	0	933	2	0
1	F	969	0	934	2	0
2	C	3467	0	3411	16	0
2	E	3512	0	3453	13	0
2	G	3497	0	3433	15	0
3	I	845	0	817	2	0
3	L	845	0	817	1	0
4	A	958	0	907	0	0
4	H	958	0	907	6	0
5	J	28	0	25	0	0
5	K	28	0	25	3	0
5	M	28	0	25	4	0
5	N	28	0	24	5	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	3	0
5	S	28	0	25	2	0
5	T	28	0	25	1	0
5	W	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	4	0
5	Z	28	0	25	0	0
5	a	28	0	25	2	0
5	b	28	0	25	0	0
5	c	28	0	25	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	d	28	0	25	0	0
5	e	28	0	25	4	0
5	h	28	0	25	8	0
5	i	28	0	25	0	0
5	j	28	0	25	1	0
6	O	22	0	19	4	0
7	U	39	0	34	1	0
7	f	39	0	34	1	0
7	g	39	0	34	3	0
8	V	50	0	41	3	0
9	B	56	0	52	0	0
9	C	140	0	130	14	0
9	D	56	0	52	0	0
9	E	126	0	115	14	0
9	F	42	0	39	0	0
9	G	154	0	143	1	0
All	All	18340	0	17762	129	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 4.

All (129) 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)
9:E:608:NAG:C6	8:V:1:NAG:C6	1.75	1.61
5:N:2:NAG:O4	6:O:1:BMA:C1	1.66	1.42
5:h:1:NAG:H61	5:h:2:NAG:C1	1.54	1.35
9:E:601:NAG:H83	9:E:601:NAG:O3	1.20	1.32
5:c:1:NAG:O3	5:c:1:NAG:H83	1.21	1.30
5:h:1:NAG:H61	5:h:2:NAG:O5	1.24	1.30
5:c:1:NAG:C3	5:c:1:NAG:C8	2.17	1.18
5:h:1:NAG:C6	5:h:2:NAG:O5	1.92	1.16
9:E:601:NAG:C3	9:E:601:NAG:C8	2.17	1.15
9:E:601:NAG:C8	9:E:601:NAG:H3	1.74	1.11
5:c:1:NAG:C8	5:c:1:NAG:H3	1.74	1.10
9:E:601:NAG:H3	9:E:601:NAG:H82	1.12	1.07
9:E:608:NAG:C6	8:V:1:NAG:C5	2.31	1.07
5:c:1:NAG:H3	5:c:1:NAG:H82	1.12	1.06
9:E:601:NAG:O3	9:E:601:NAG:C8	2.07	1.02
9:E:609:NAG:C3	9:E:609:NAG:O7	2.08	1.02
5:c:1:NAG:O3	5:c:1:NAG:C8	2.07	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:601:NAG:H83	9:E:601:NAG:C3	1.86	0.97
5:c:1:NAG:H83	5:c:1:NAG:C3	1.86	0.97
5:R:1:NAG:H62	5:R:2:NAG:N2	1.82	0.95
5:h:1:NAG:C6	5:h:2:NAG:C1	2.26	0.93
5:c:1:NAG:C3	5:c:1:NAG:H82	1.92	0.92
9:E:609:NAG:O7	9:E:609:NAG:O3	1.89	0.91
2:G:398:ASN:OD1	2:G:398:ASN:O	1.90	0.89
5:Y:1:NAG:C3	5:Y:1:NAG:O7	2.21	0.88
5:M:2:NAG:O7	5:M:2:NAG:C3	2.22	0.88
9:E:608:NAG:C6	8:V:1:NAG:H5	2.02	0.88
9:E:601:NAG:H83	9:E:601:NAG:HO3	1.38	0.86
9:C:601:NAG:C3	9:C:601:NAG:O7	2.22	0.85
5:Y:1:NAG:O7	5:Y:1:NAG:O3	1.95	0.85
9:E:609:NAG:O7	9:E:609:NAG:H3	1.76	0.84
7:g:2:NAG:C3	7:g:2:NAG:O7	2.25	0.84
5:N:2:NAG:C4	6:O:1:BMA:C1	2.56	0.83
5:K:1:NAG:O7	5:K:1:NAG:C3	2.28	0.81
2:E:398:ASN:O	2:E:398:ASN:OD1	2.02	0.78
9:C:601:NAG:O7	9:C:601:NAG:O3	2.01	0.78
5:M:2:NAG:O7	5:M:2:NAG:O3	2.02	0.78
9:C:607:NAG:C3	9:C:607:NAG:O7	2.31	0.77
5:h:2:NAG:C3	5:h:2:NAG:O7	2.32	0.77
9:C:602:NAG:O7	9:C:602:NAG:C3	2.34	0.76
5:e:2:NAG:O7	5:e:2:NAG:C3	2.33	0.75
5:h:2:NAG:O7	5:h:2:NAG:H3	1.87	0.74
2:G:505:VAL:HG12	2:G:505:VAL:OXT	1.87	0.73
2:G:398:ASN:OD1	2:G:398:ASN:C	2.32	0.73
7:g:2:NAG:O7	7:g:2:NAG:O3	2.07	0.72
5:M:2:NAG:O7	5:M:2:NAG:H3	1.90	0.71
5:h:1:NAG:O6	5:h:2:NAG:O5	2.09	0.71
2:E:505:VAL:OXT	2:E:505:VAL:HG12	1.89	0.70
9:C:601:NAG:O7	9:C:601:NAG:H3	1.91	0.70
5:K:1:NAG:O7	5:K:1:NAG:O3	2.11	0.68
9:C:607:NAG:O7	9:C:607:NAG:O3	2.12	0.67
7:g:2:NAG:O7	7:g:2:NAG:H3	1.94	0.67
9:C:602:NAG:O7	9:C:602:NAG:H3	1.94	0.67
5:Y:1:NAG:O7	5:Y:1:NAG:H3	1.94	0.66
5:K:1:NAG:O7	5:K:1:NAG:H3	1.95	0.65
2:E:398:ASN:OD1	2:E:398:ASN:C	2.38	0.65
5:e:2:NAG:O7	5:e:2:NAG:H3	1.99	0.62
9:C:607:NAG:O7	9:C:607:NAG:H3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ILE:O	2:C:184:ILE:HG22	2.02	0.60
5:e:2:NAG:O7	5:e:2:NAG:O3	2.21	0.59
5:R:1:NAG:H62	5:R:2:NAG:C7	2.32	0.59
9:C:610:NAG:H62	5:N:1:NAG:H62	1.84	0.58
2:C:339:ASN:C	2:C:339:ASN:OD1	2.47	0.58
4:H:32:TYR:HE2	4:H:95:PRO:HD2	1.69	0.57
2:G:386:ASN:O	2:G:386:ASN:OD1	2.21	0.57
5:h:2:NAG:O7	5:h:2:NAG:O3	2.24	0.56
5:R:1:NAG:H62	5:R:2:NAG:HN2	1.66	0.56
2:G:45:TRP:C	2:G:45:TRP:CD1	2.84	0.56
3:I:11:LEU:HD23	3:I:11:LEU:N	2.20	0.55
9:C:602:NAG:O7	9:C:602:NAG:O3	2.25	0.54
5:Y:1:NAG:O3	5:Y:1:NAG:C7	2.56	0.53
4:H:32:TYR:OH	4:H:96:GLY:N	2.40	0.53
2:G:505:VAL:OXT	2:G:505:VAL:CG1	2.57	0.52
9:E:609:NAG:O3	9:E:609:NAG:C7	2.55	0.52
5:e:1:NAG:H62	5:e:2:NAG:HN2	1.75	0.50
2:C:424:ILE:HD13	2:C:424:ILE:N	2.26	0.50
1:F:623:TRP:NE1	2:G:499:THR:OG1	2.44	0.50
3:I:11:LEU:HD23	3:I:11:LEU:H	1.77	0.50
2:C:129:LEU:O	2:C:129:LEU:HG	2.12	0.49
2:E:117:LYS:N	2:E:118:PRO:CD	2.76	0.48
2:E:355:ASN:HD22	4:H:32:TYR:HE1	1.62	0.48
2:G:386:ASN:OD1	2:G:386:ASN:C	2.57	0.48
1:B:640:GLN:OE1	1:B:640:GLN:N	2.29	0.48
2:C:294:ILE:HA	9:C:606:NAG:O7	2.14	0.48
1:D:623:TRP:NE1	2:E:499:THR:OG1	2.45	0.47
4:H:32:TYR:CE2	4:H:95:PRO:HD2	2.48	0.47
2:C:332:ASN:C	9:C:606:NAG:H81	2.40	0.47
1:D:625:ASN:OD1	1:D:625:ASN:O	2.34	0.46
7:U:2:NAG:H4	7:U:3:BMA:H2	1.47	0.46
5:j:1:NAG:H3	5:j:1:NAG:H82	1.11	0.46
2:G:123:THR:N	2:G:124:PRO:CD	2.79	0.46
2:C:123:THR:N	2:C:124:PRO:CD	2.79	0.46
5:S:1:NAG:H61	5:S:2:NAG:N2	2.30	0.46
2:G:69:TRP:CE3	2:G:69:TRP:HA	2.51	0.45
2:G:457:ASP:OD1	2:G:457:ASP:C	2.57	0.45
2:E:339:ASN:OD1	2:E:339:ASN:C	2.59	0.45
2:E:121:LYS:N	2:E:121:LYS:HD2	2.31	0.45
2:E:234:ASN:OD1	2:E:234:ASN:C	2.59	0.45
5:T:1:NAG:H62	5:T:2:NAG:N2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:LEU:N	3:L:11:LEU:HD23	2.33	0.44
5:S:1:NAG:H61	5:S:2:NAG:HN2	1.82	0.44
2:C:184:ILE:O	2:C:184:ILE:CG2	2.65	0.43
2:C:117:LYS:N	2:C:118:PRO:HD2	2.33	0.43
7:f:2:NAG:H4	7:f:3:BMA:H2	1.47	0.43
2:E:123:THR:N	2:E:124:PRO:CD	2.81	0.43
5:a:1:NAG:H61	5:a:2:NAG:N2	2.32	0.43
9:G:606:NAG:H3	9:G:606:NAG:H82	1.09	0.43
2:C:424:ILE:HD13	2:C:424:ILE:H	1.84	0.43
2:G:117:LYS:N	2:G:118:PRO:CD	2.81	0.43
2:G:117:LYS:N	2:G:118:PRO:HD2	2.33	0.43
2:C:234:ASN:OD1	2:C:234:ASN:C	2.61	0.43
5:N:2:NAG:H4	6:O:1:BMA:C1	2.44	0.43
2:C:293:GLN:O	9:C:606:NAG:O7	2.37	0.42
2:C:117:LYS:N	2:C:118:PRO:CD	2.82	0.42
2:E:184:ILE:O	2:E:184:ILE:HG22	2.20	0.42
2:E:505:VAL:OXT	2:E:505:VAL:CG1	2.60	0.42
5:N:2:NAG:O4	6:O:1:BMA:O5	2.29	0.41
2:C:502:LYS:NZ	1:F:664:ASP:O	2.53	0.41
4:H:100(A):TYR:CD2	4:H:100(A):TYR:C	2.98	0.41
5:c:1:NAG:H62	5:c:2:NAG:N2	2.34	0.41
2:C:339:ASN:OD1	2:C:339:ASN:O	2.39	0.41
2:G:129:LEU:O	2:G:129:LEU:HG	2.21	0.41
4:H:29:LEU:O	4:H:71:ARG:NH2	2.54	0.41
9:C:605:NAG:O6	9:C:605:NAG:O4	2.39	0.41
5:a:1:NAG:H61	5:a:2:NAG:HN2	1.85	0.40
2:E:363:GLN:OE1	2:E:363:GLN:N	2.41	0.40
2:C:257:THR:C	2:C:259:LEU:H	2.29	0.40
2:G:424:ILE:HD12	2:G:424:ILE:C	2.46	0.40
5:M:1:NAG:H61	5:M:2:NAG:HN2	1.85	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	B	117/153 (76%)	117 (100%)	0	0	100	100
1	D	117/153 (76%)	116 (99%)	1 (1%)	0	100	100
1	F	117/153 (76%)	117 (100%)	0	0	100	100
2	C	432/472 (92%)	428 (99%)	4 (1%)	0	100	100
2	E	438/472 (93%)	432 (99%)	6 (1%)	0	100	100
2	G	436/472 (92%)	430 (99%)	6 (1%)	0	100	100
3	I	109/111 (98%)	107 (98%)	2 (2%)	0	100	100
3	L	109/111 (98%)	107 (98%)	2 (2%)	0	100	100
4	A	119/122 (98%)	116 (98%)	2 (2%)	1 (1%)	16	48
4	H	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
All	All	2113/2341 (90%)	2087 (99%)	25 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	33	TRP

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	B	104/130 (80%)	102 (98%)	2 (2%)	50	66
1	D	104/130 (80%)	104 (100%)	0	100	100
1	F	104/130 (80%)	104 (100%)	0	100	100
2	C	394/422 (93%)	391 (99%)	3 (1%)	73	76
2	E	400/422 (95%)	396 (99%)	4 (1%)	68	74
2	G	399/422 (94%)	395 (99%)	4 (1%)	68	74
3	I	93/93 (100%)	93 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	93/93 (100%)	93 (100%)	0	100	100
4	A	101/102 (99%)	101 (100%)	0	100	100
4	H	101/102 (99%)	100 (99%)	1 (1%)	68	74
All	All	1893/2046 (92%)	1879 (99%)	14 (1%)	73	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	611	ASN
1	B	637	ASN
2	C	355	ASN
2	C	392	ASN
2	C	424	ILE
2	E	133	ASN
2	E	160	ASN
2	E	398	ASN
2	E	448	ASN
4	H	98	TYR
2	G	88	ASN
2	G	137	ASN
2	G	301	ASN
2	G	398	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	195	ASN
2	C	422	GLN
1	D	570	HIS
2	E	374	HIS
2	E	422	GLN
2	E	432	GLN
3	L	37	GLN
1	F	575	GLN
4	A	35	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

57 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	J	1	5,2	14,14,15	0.28	0	17,19,21	0.71	0
5	NAG	J	2	5	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
5	NAG	K	1	5,2	14,14,15	0.27	0	17,19,21	0.79	0
5	NAG	K	2	5	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
5	NAG	M	1	5,2	14,14,15	0.31	0	17,19,21	0.84	0
5	NAG	M	2	5	14,14,15	0.30	0	17,19,21	0.74	0
5	NAG	N	1	5,2	14,14,15	1.22	1 (7%)	17,19,21	1.26	3 (17%)
5	NAG	N	2	5	14,14,15	0.28	0	17,19,21	0.60	0
6	BMA	O	1	6	11,11,12	0.23	0	15,15,17	0.75	0
6	MAN	O	2	6	11,11,12	0.26	0	15,15,17	0.62	0
5	NAG	P	1	5,2	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	P	2	5	14,14,15	0.27	0	17,19,21	0.69	0
5	NAG	Q	1	5,2	14,14,15	0.29	0	17,19,21	0.81	0
5	NAG	Q	2	5	14,14,15	0.29	0	17,19,21	0.84	0
5	NAG	R	1	5,2	14,14,15	0.27	0	17,19,21	0.66	0
5	NAG	R	2	5	14,14,15	0.28	0	17,19,21	0.70	0
5	NAG	S	1	5,2	14,14,15	0.30	0	17,19,21	0.53	0
5	NAG	S	2	5	14,14,15	0.27	0	17,19,21	0.66	0
5	NAG	T	1	5,2	14,14,15	0.25	0	17,19,21	0.64	0
5	NAG	T	2	5	14,14,15	0.28	0	17,19,21	0.62	0
7	NAG	U	1	7,2	14,14,15	0.45	0	17,19,21	0.70	0
7	NAG	U	2	7	14,14,15	0.30	0	17,19,21	0.69	0
7	BMA	U	3	7	11,11,12	0.25	0	15,15,17	0.79	0
8	NAG	V	1	8,2	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
8	NAG	V	2	8	14,14,15	0.26	0	17,19,21	0.58	0
8	BMA	V	3	8	11,11,12	0.49	0	15,15,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	V	4	8	11,11,12	0.23	0	15,15,17	0.73	0
5	NAG	W	1	5,2	14,14,15	0.29	0	17,19,21	0.59	0
5	NAG	W	2	5	14,14,15	0.27	0	17,19,21	0.71	0
5	NAG	X	1	5,2	14,14,15	0.28	0	17,19,21	0.73	0
5	NAG	X	2	5	14,14,15	0.27	0	17,19,21	0.64	0
5	NAG	Y	1	5,2	14,14,15	0.34	0	17,19,21	1.15	1 (5%)
5	NAG	Y	2	5	14,14,15	0.37	0	17,19,21	0.87	1 (5%)
5	NAG	Z	1	5,2	14,14,15	0.28	0	17,19,21	0.82	0
5	NAG	Z	2	5	14,14,15	0.27	0	17,19,21	0.65	0
5	NAG	a	1	5,2	14,14,15	0.27	0	17,19,21	0.65	0
5	NAG	a	2	5	14,14,15	0.25	0	17,19,21	0.63	0
5	NAG	b	1	5,2	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	b	2	5	14,14,15	0.27	0	17,19,21	0.68	0
5	NAG	c	1	5,2	14,14,15	0.41	0	17,19,21	0.76	0
5	NAG	c	2	5	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
5	NAG	d	1	5,2	14,14,15	0.27	0	17,19,21	0.63	0
5	NAG	d	2	5	14,14,15	0.26	0	17,19,21	0.64	0
5	NAG	e	1	5,2	14,14,15	0.28	0	17,19,21	0.68	0
5	NAG	e	2	5	14,14,15	0.28	0	17,19,21	0.65	0
7	NAG	f	1	7,2	14,14,15	0.40	0	17,19,21	0.70	0
7	NAG	f	2	7	14,14,15	0.33	0	17,19,21	0.75	0
7	BMA	f	3	7	11,11,12	0.27	0	15,15,17	0.76	0
7	NAG	g	1	7,2	14,14,15	0.41	0	17,19,21	0.66	0
7	NAG	g	2	7	14,14,15	0.28	0	17,19,21	0.63	0
7	BMA	g	3	7	11,11,12	0.23	0	15,15,17	0.75	0
5	NAG	h	1	5,2	14,14,15	0.41	0	17,19,21	0.75	0
5	NAG	h	2	5	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
5	NAG	i	1	5,2	14,14,15	0.27	0	17,19,21	0.80	0
5	NAG	i	2	5	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
5	NAG	j	1	5,2	14,14,15	0.26	0	17,19,21	0.83	0
5	NAG	j	2	5	14,14,15	0.28	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	5,2	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	d	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
5	NAG	e	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
7	NAG	f	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	BMA	f	3	7	-	0/2/19/22	0/1/1/1
7	NAG	g	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	1/6/23/26	0/1/1/1
7	BMA	g	3	7	-	0/2/19/22	0/1/1/1
5	NAG	h	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	1/6/23/26	0/1/1/1
5	NAG	i	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
5	NAG	j	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1	NAG	C1-C2	4.48	1.58	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2	NAG	O5-C5-C6	6.52	120.36	107.66
5	J	2	NAG	O5-C5-C6	6.52	120.35	107.66
5	i	2	NAG	O5-C5-C6	6.51	120.34	107.66
5	K	2	NAG	O5-C5-C6	6.50	120.31	107.66
5	h	2	NAG	O5-C5-C6	6.50	120.31	107.66
5	N	1	NAG	O5-C1-C2	-3.41	106.02	111.29
5	K	2	NAG	C4-C3-C2	2.74	115.04	111.02
5	i	2	NAG	C4-C3-C2	2.72	115.01	111.02
5	c	2	NAG	C4-C3-C2	2.72	115.00	111.02
5	h	2	NAG	C4-C3-C2	2.70	114.98	111.02
5	J	2	NAG	C4-C3-C2	2.70	114.98	111.02
5	N	1	NAG	C1-O5-C5	2.62	115.70	112.19
5	c	2	NAG	O3-C3-C4	2.46	116.18	110.38
5	i	2	NAG	O3-C3-C4	2.46	116.17	110.38
5	K	2	NAG	O3-C3-C4	2.46	116.17	110.38
5	h	2	NAG	O3-C3-C4	2.46	116.17	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	NAG	O3-C3-C4	2.45	116.16	110.38
5	N	1	NAG	C4-C3-C2	-2.37	107.55	111.02
5	Y	2	NAG	C1-O5-C5	2.21	115.14	112.19
5	Y	1	NAG	O5-C1-C2	-2.12	108.01	111.29
8	V	1	NAG	C1-O5-C5	2.09	114.99	112.19
5	c	2	NAG	O4-C4-C5	2.06	114.40	109.32
5	K	2	NAG	O4-C4-C5	2.06	114.39	109.32
5	J	2	NAG	O4-C4-C5	2.04	114.35	109.32
5	i	2	NAG	O4-C4-C5	2.03	114.32	109.32
8	V	3	BMA	O3-C3-C4	2.02	115.15	110.38
5	h	2	NAG	O4-C4-C5	2.02	114.29	109.32

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C3-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
5	R	2	NAG	C3-C2-N2-C7
5	Y	1	NAG	C3-C2-N2-C7
5	c	1	NAG	C3-C2-N2-C7
5	e	2	NAG	C3-C2-N2-C7
5	h	2	NAG	C3-C2-N2-C7
5	j	1	NAG	C3-C2-N2-C7
7	g	2	NAG	C3-C2-N2-C7
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	X	2	NAG	O7-C7-N2-C2
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	c	2	NAG	C8-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
5	i	2	NAG	C8-C7-N2-C2
5	i	2	NAG	O7-C7-N2-C2
5	j	1	NAG	C8-C7-N2-C2
5	j	1	NAG	O7-C7-N2-C2
5	j	2	NAG	C8-C7-N2-C2
5	j	2	NAG	O7-C7-N2-C2
7	f	2	NAG	C8-C7-N2-C2
7	f	2	NAG	O7-C7-N2-C2
8	V	2	NAG	C8-C7-N2-C2
8	V	2	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
8	V	3	BMA	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6

There are no ring outliers.

28 monomers are involved in 53 short contacts:

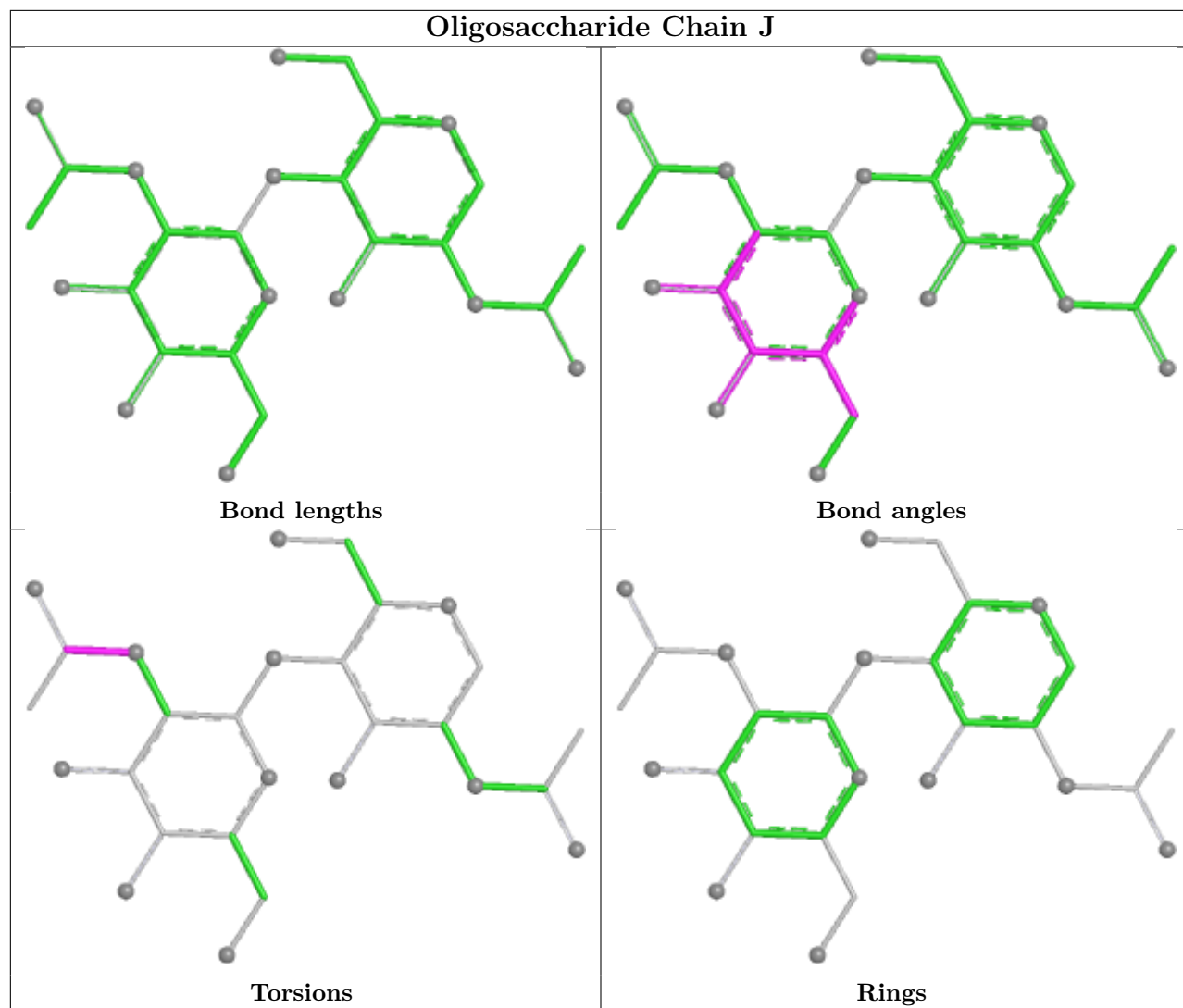
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	2	NAG	2	0
5	Y	1	NAG	4	0
5	S	2	NAG	2	0
6	O	1	BMA	4	0

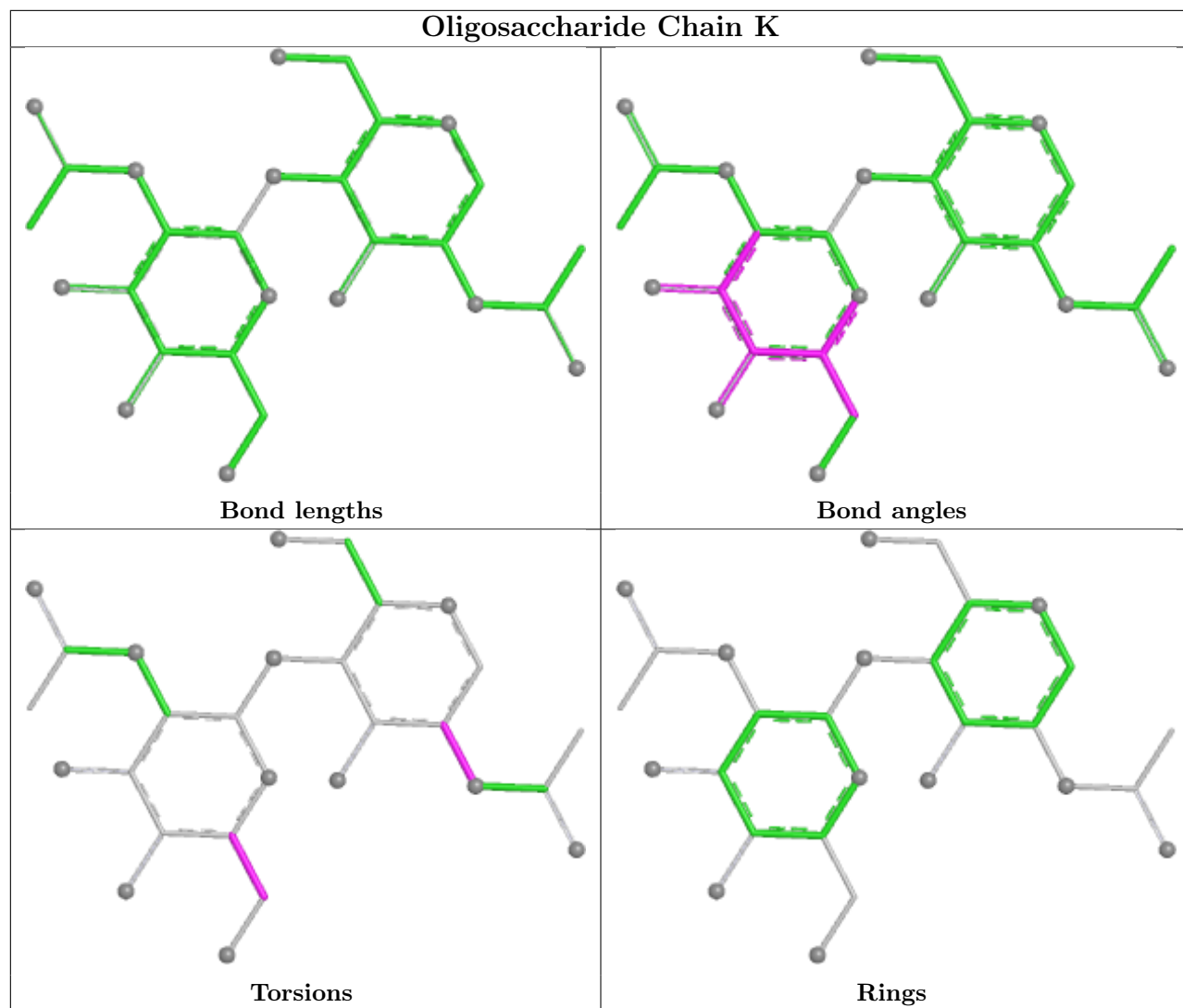
Continued on next page...

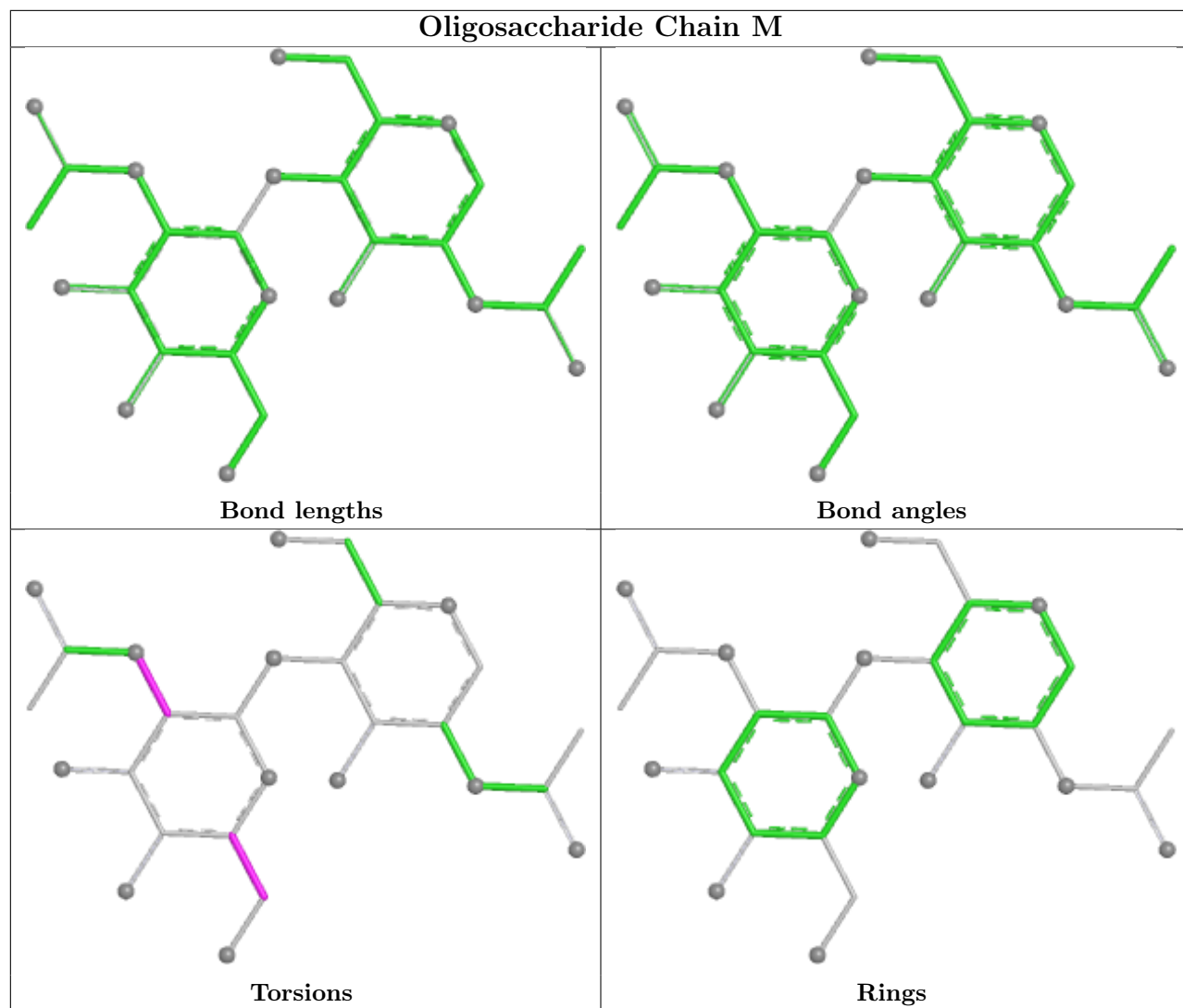
Continued from previous page...

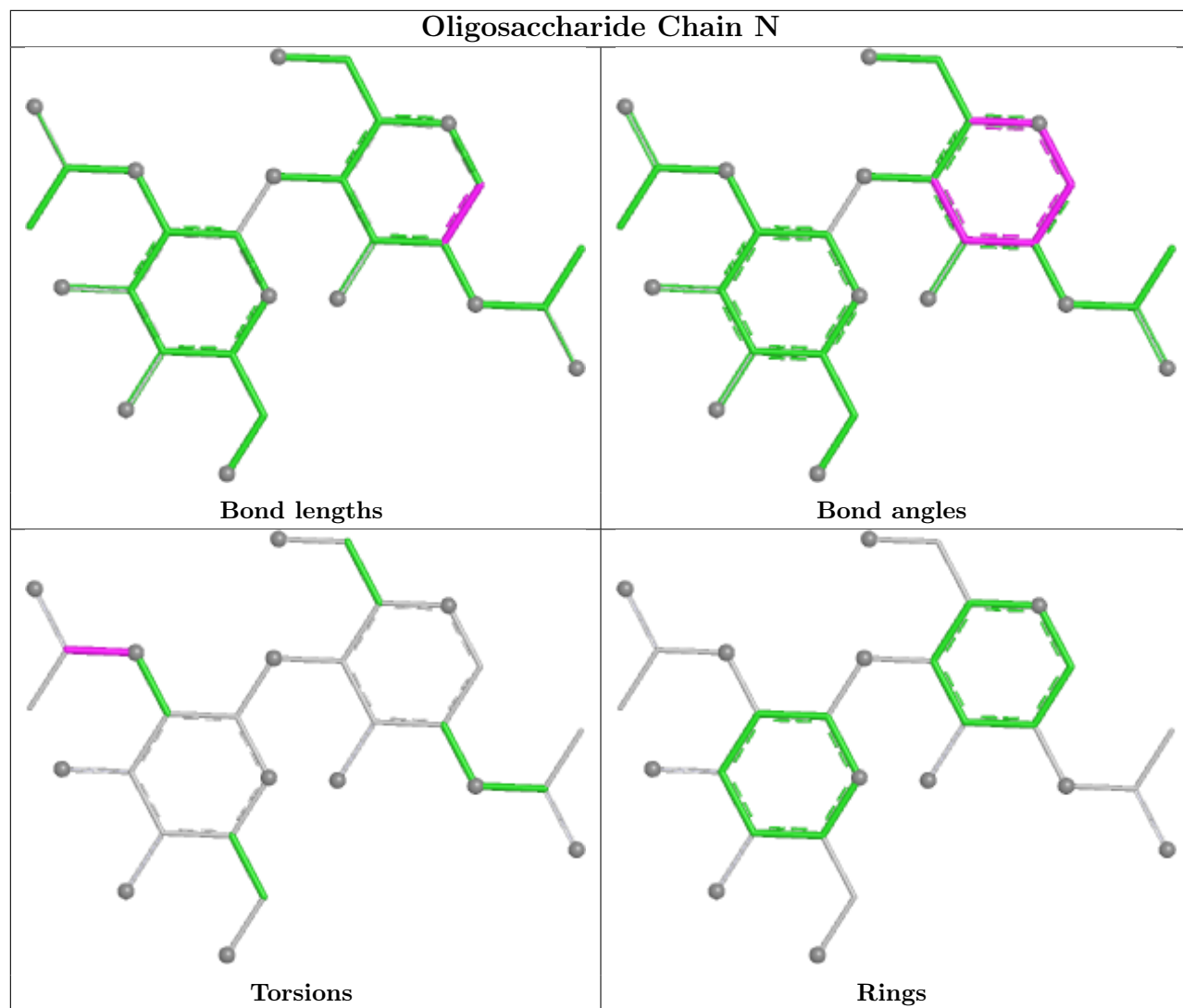
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	3	BMA	1	0
8	V	1	NAG	3	0
5	T	2	NAG	1	0
5	c	1	NAG	8	0
5	S	1	NAG	2	0
5	T	1	NAG	1	0
5	R	2	NAG	3	0
7	U	2	NAG	1	0
5	R	1	NAG	3	0
5	N	1	NAG	1	0
5	e	1	NAG	1	0
7	f	3	BMA	1	0
5	e	2	NAG	4	0
5	j	1	NAG	1	0
5	N	2	NAG	4	0
5	h	1	NAG	5	0
5	h	2	NAG	8	0
5	a	1	NAG	2	0
5	M	2	NAG	4	0
5	K	1	NAG	3	0
5	M	1	NAG	1	0
7	f	2	NAG	1	0
7	g	2	NAG	3	0
5	c	2	NAG	1	0

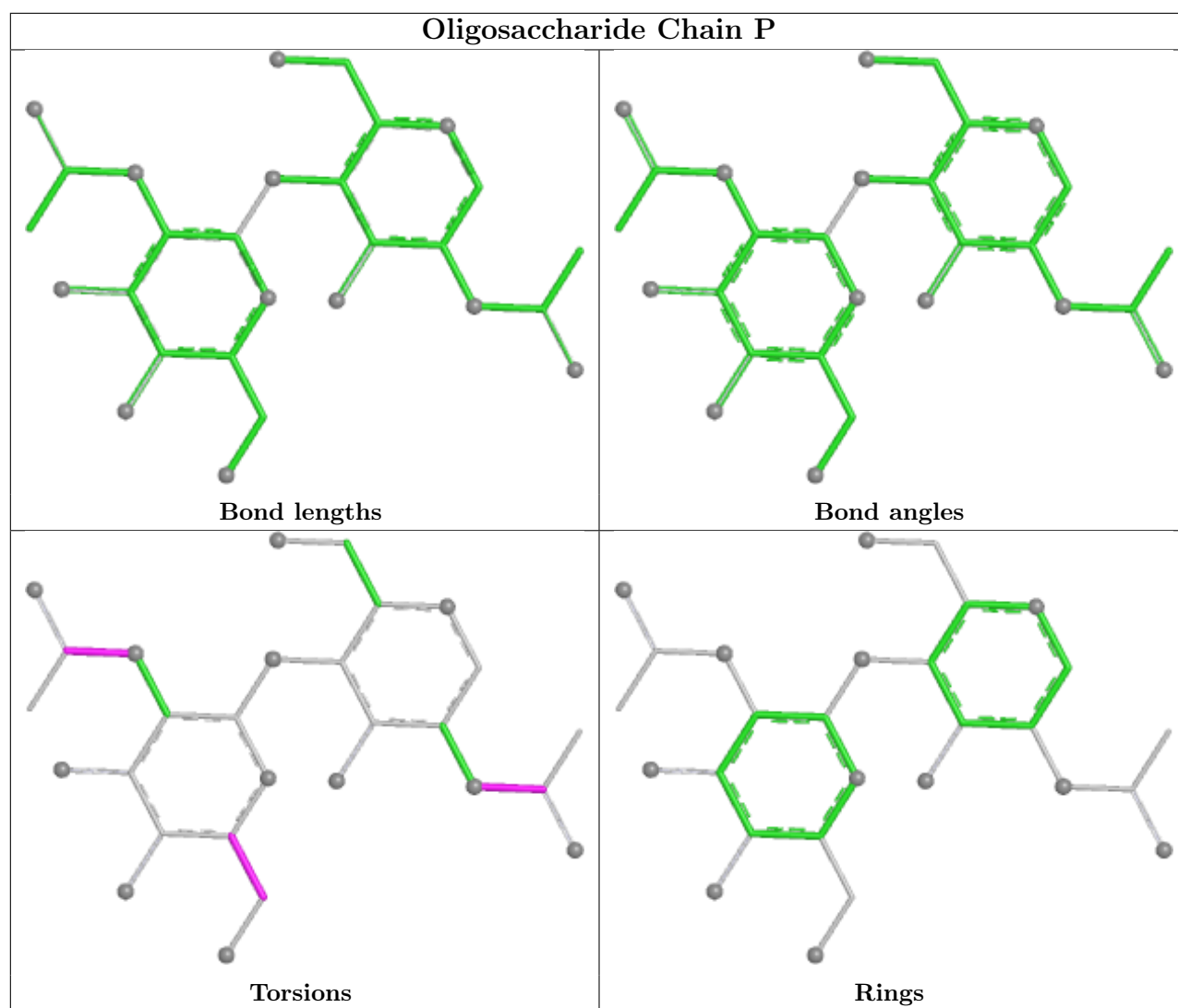
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

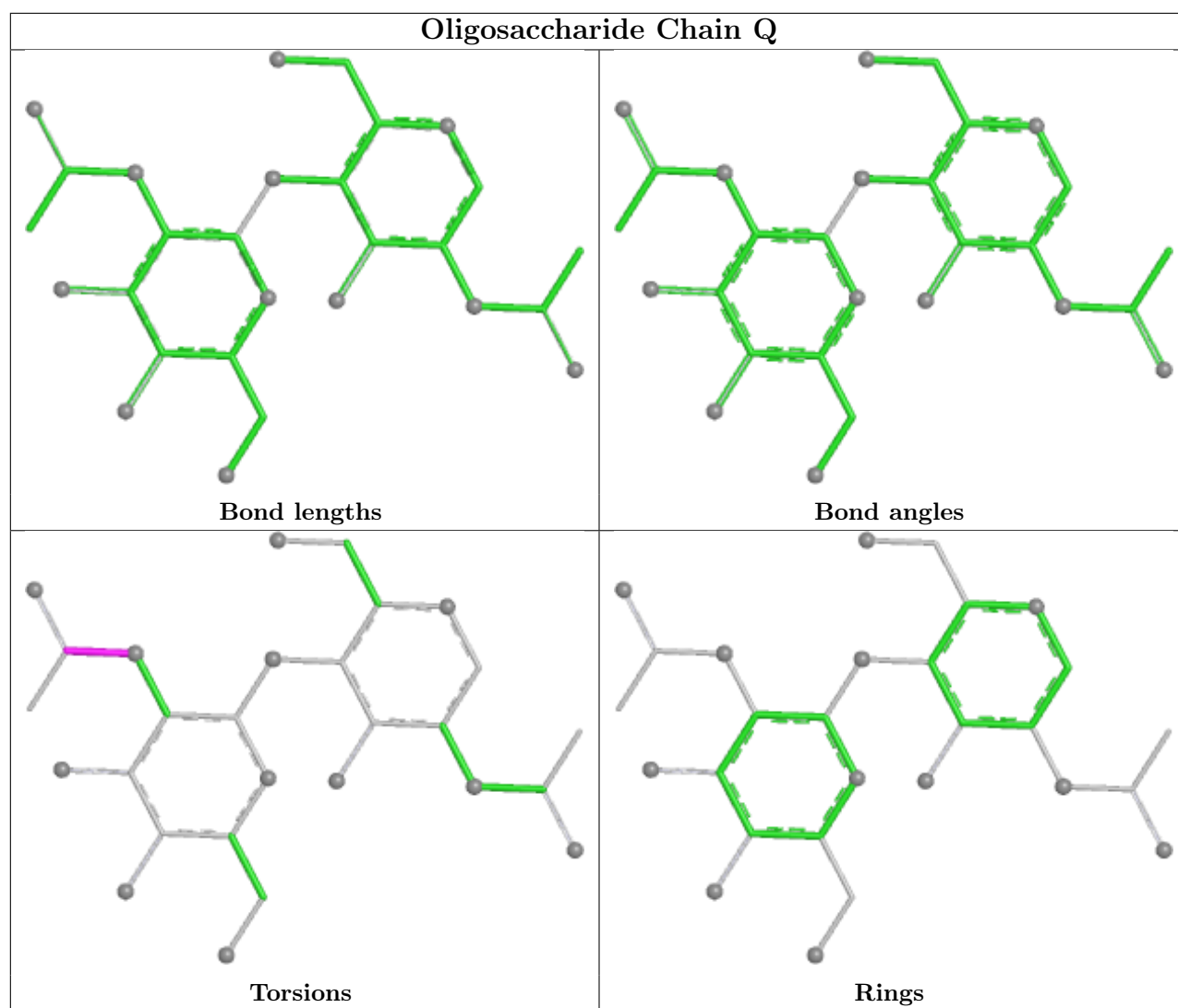


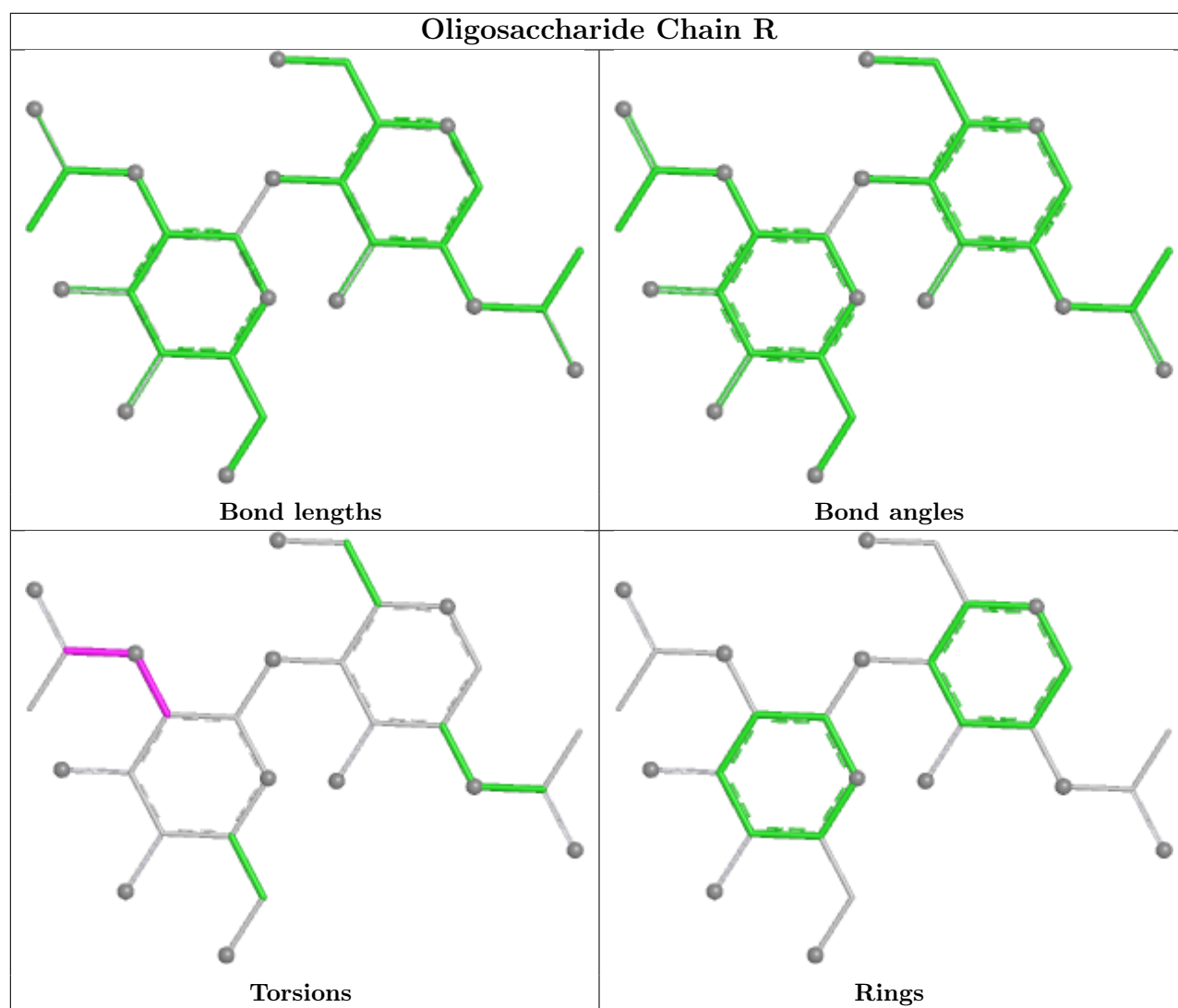


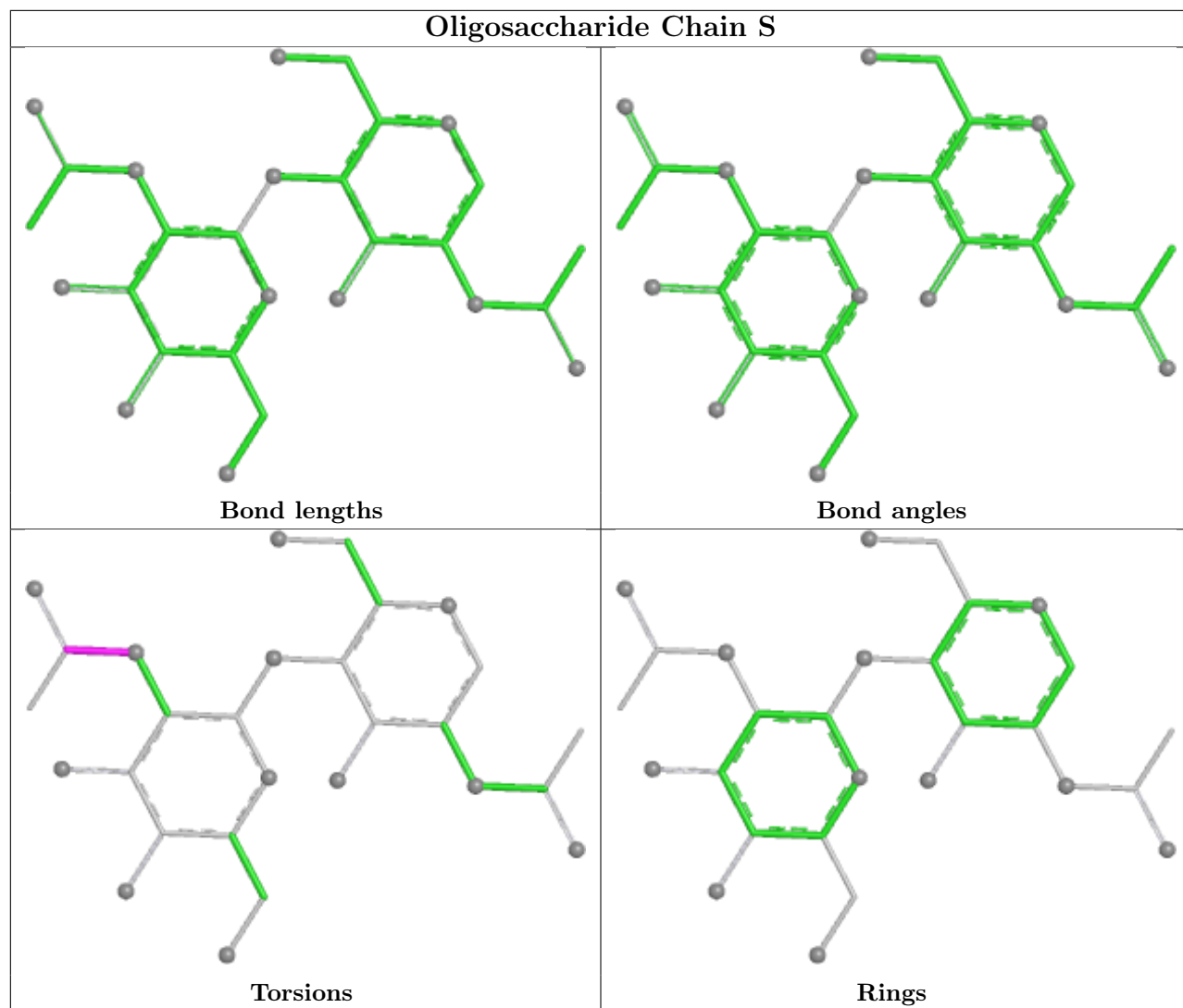


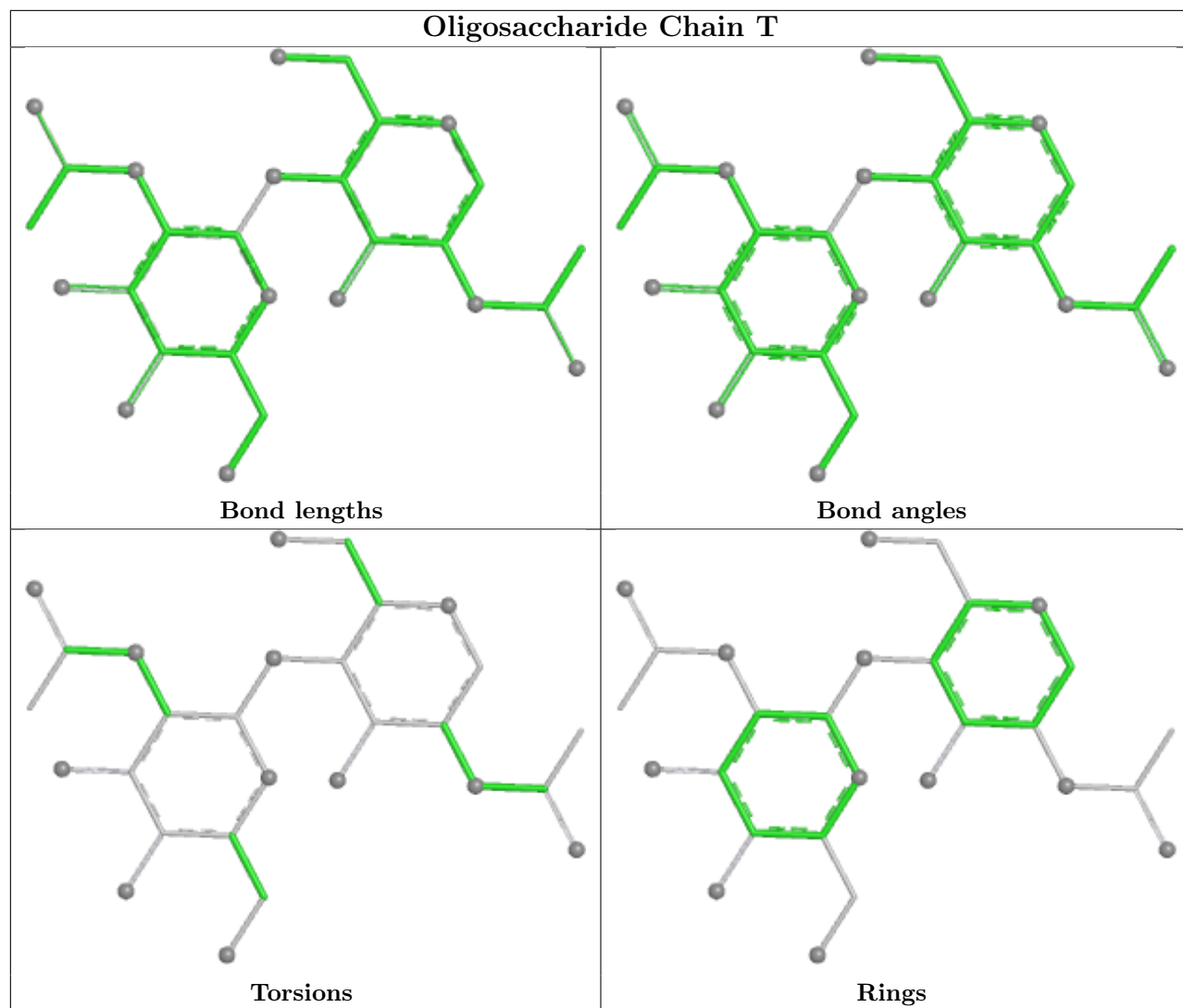


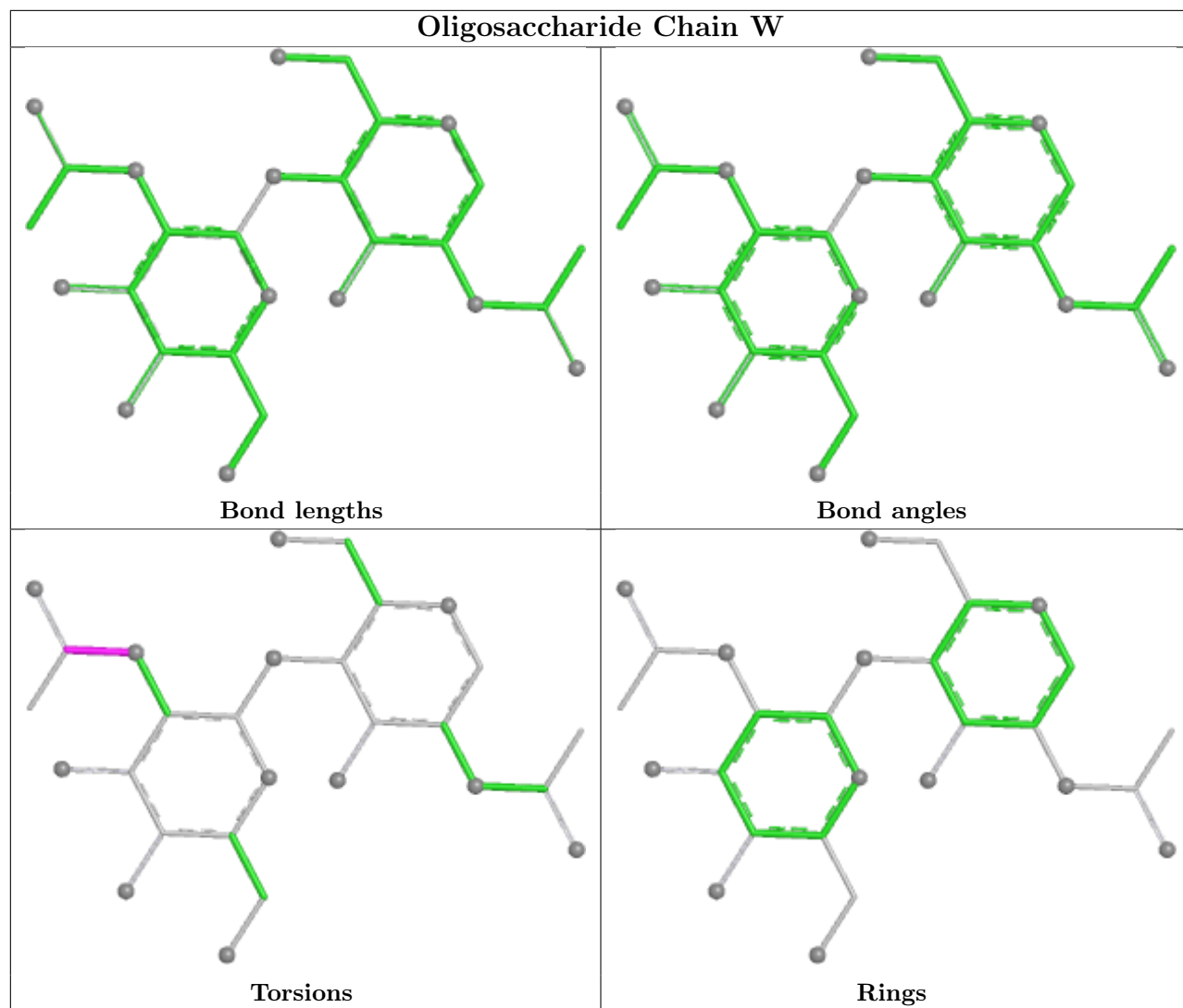


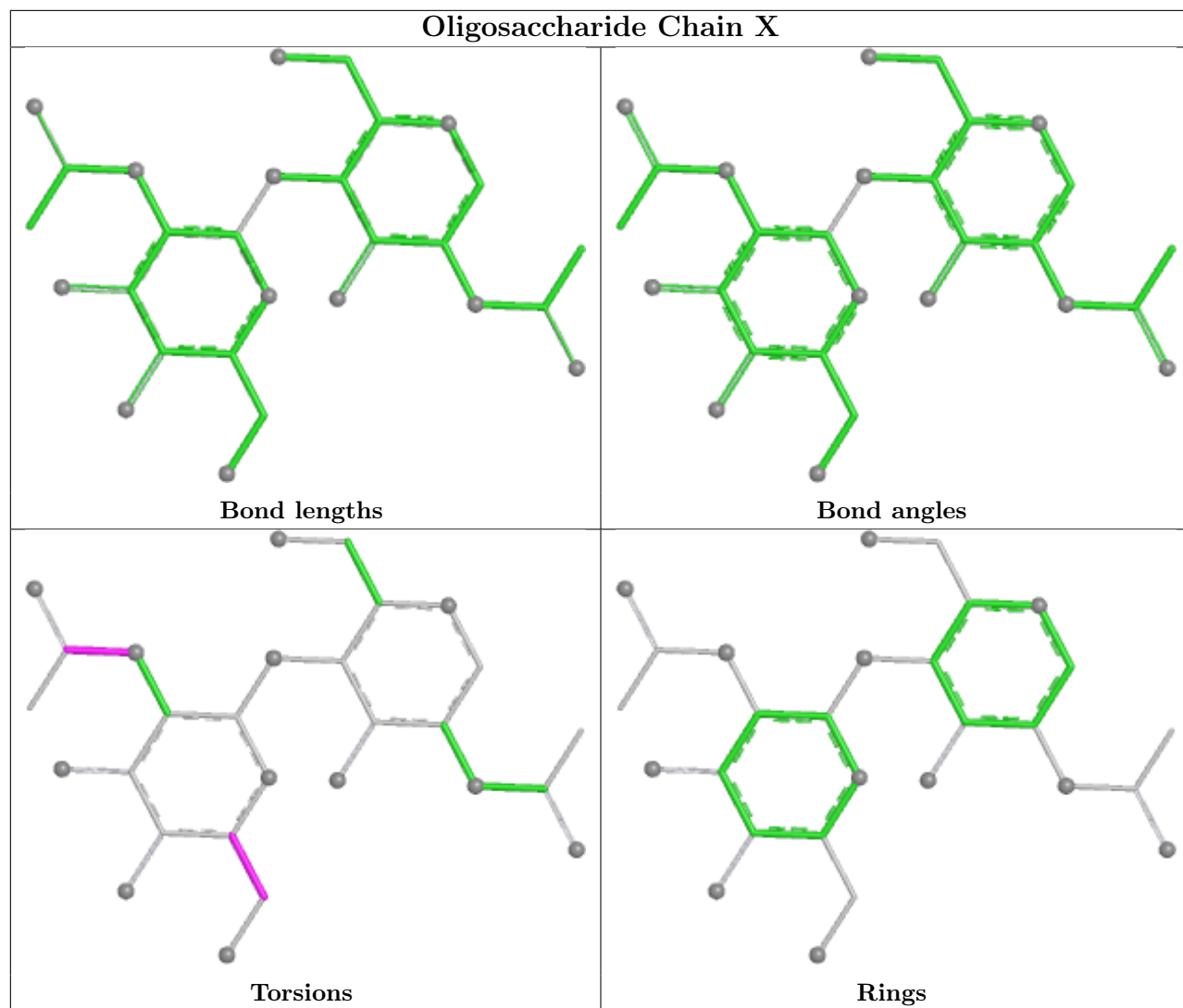


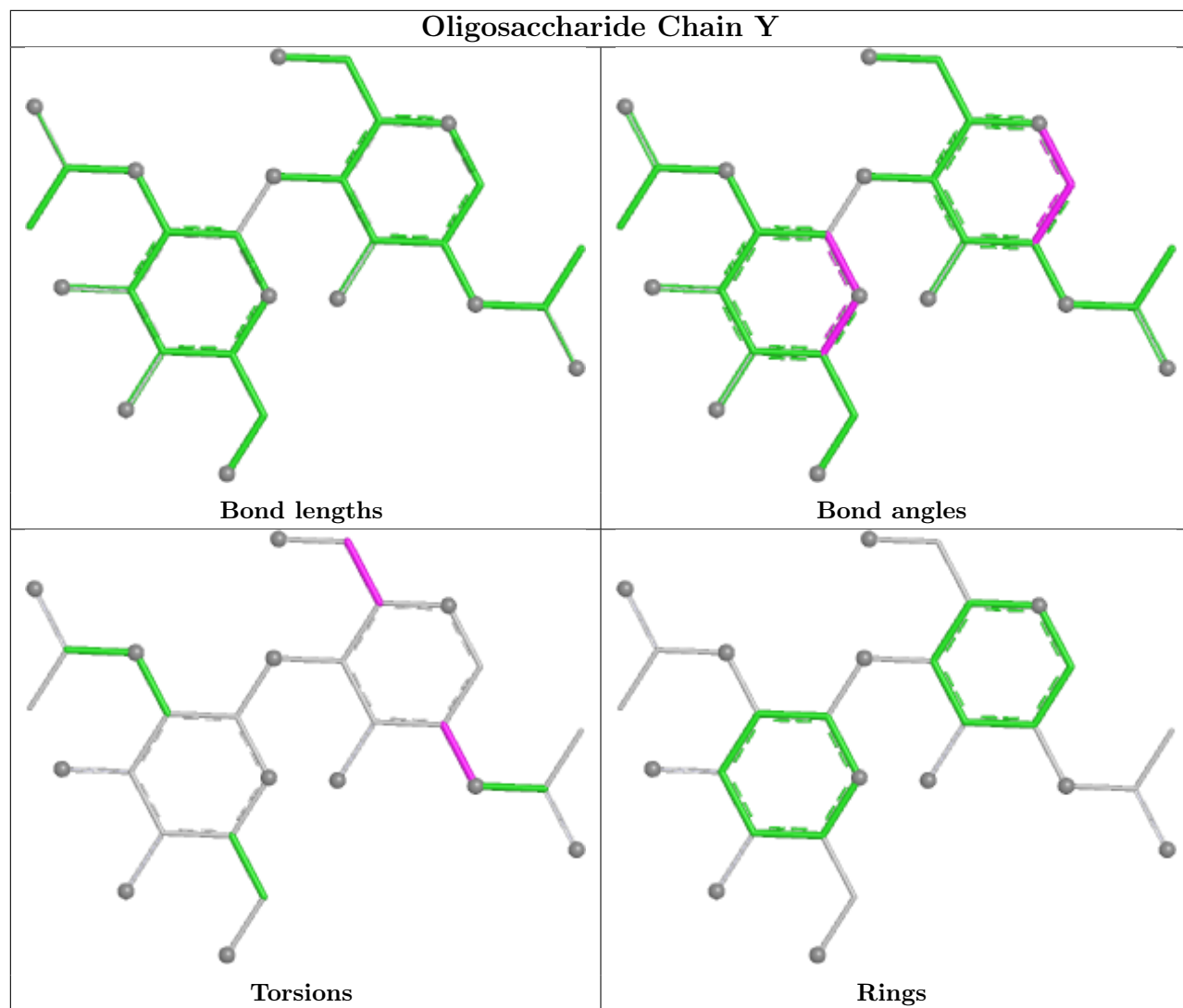


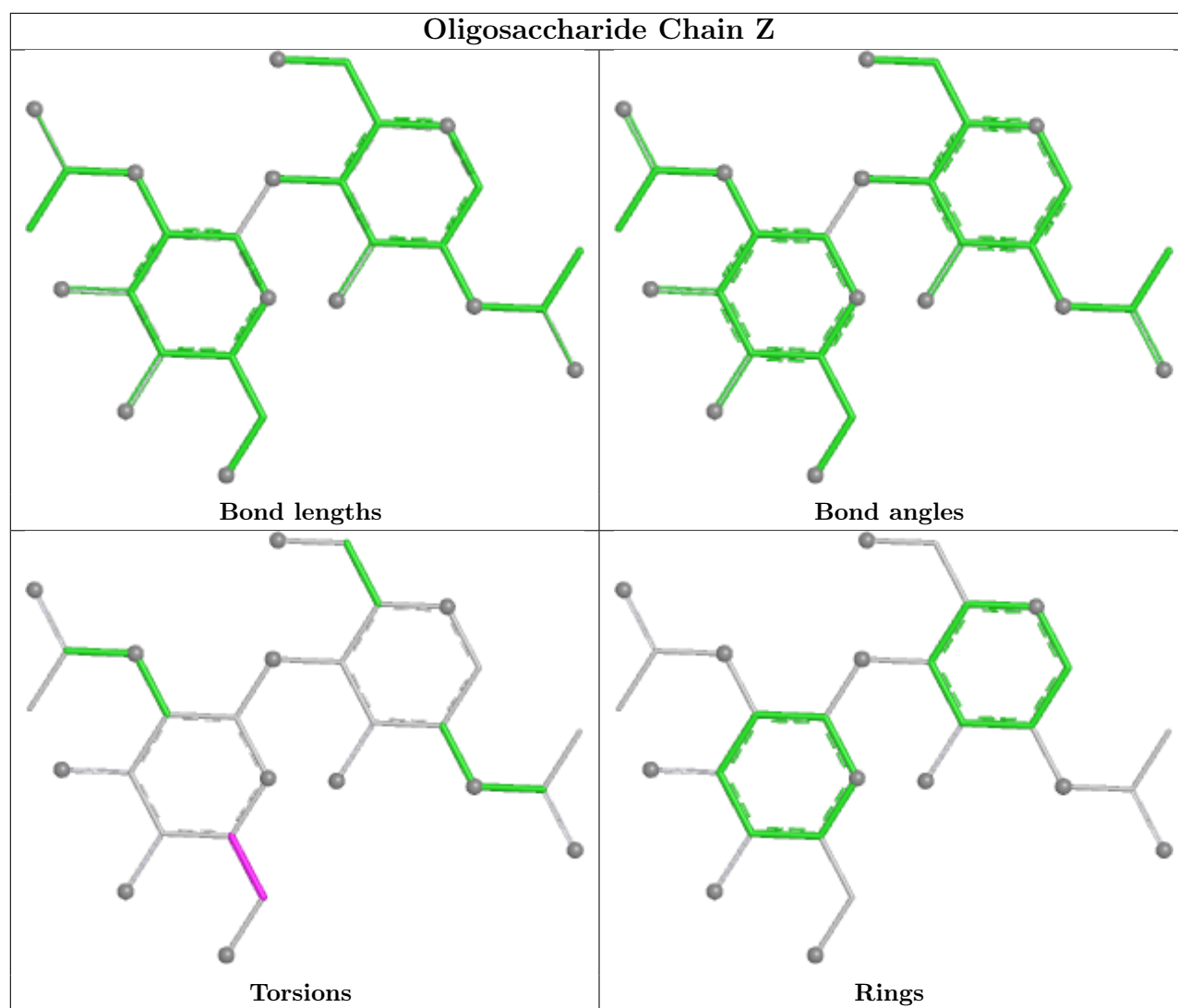


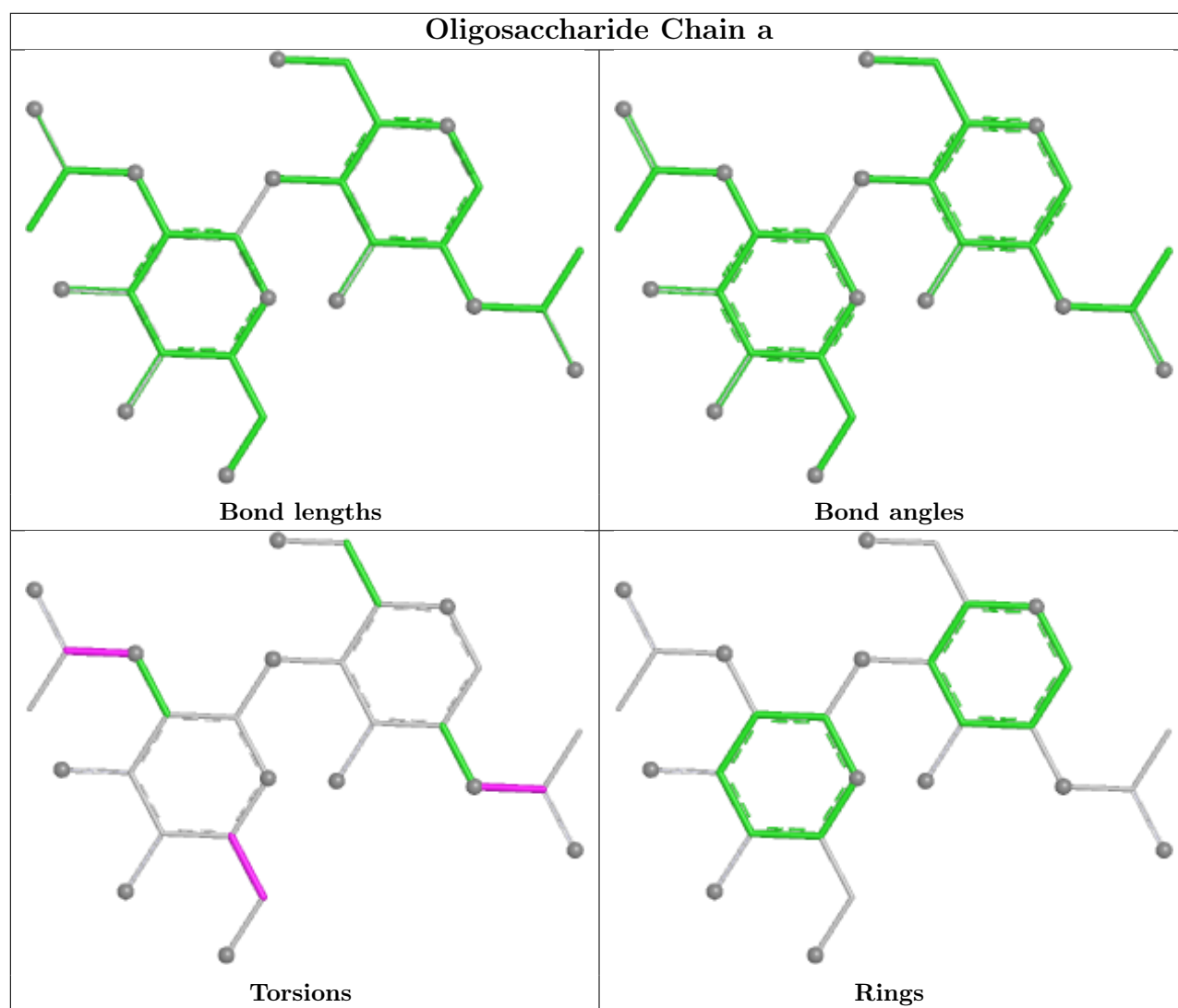


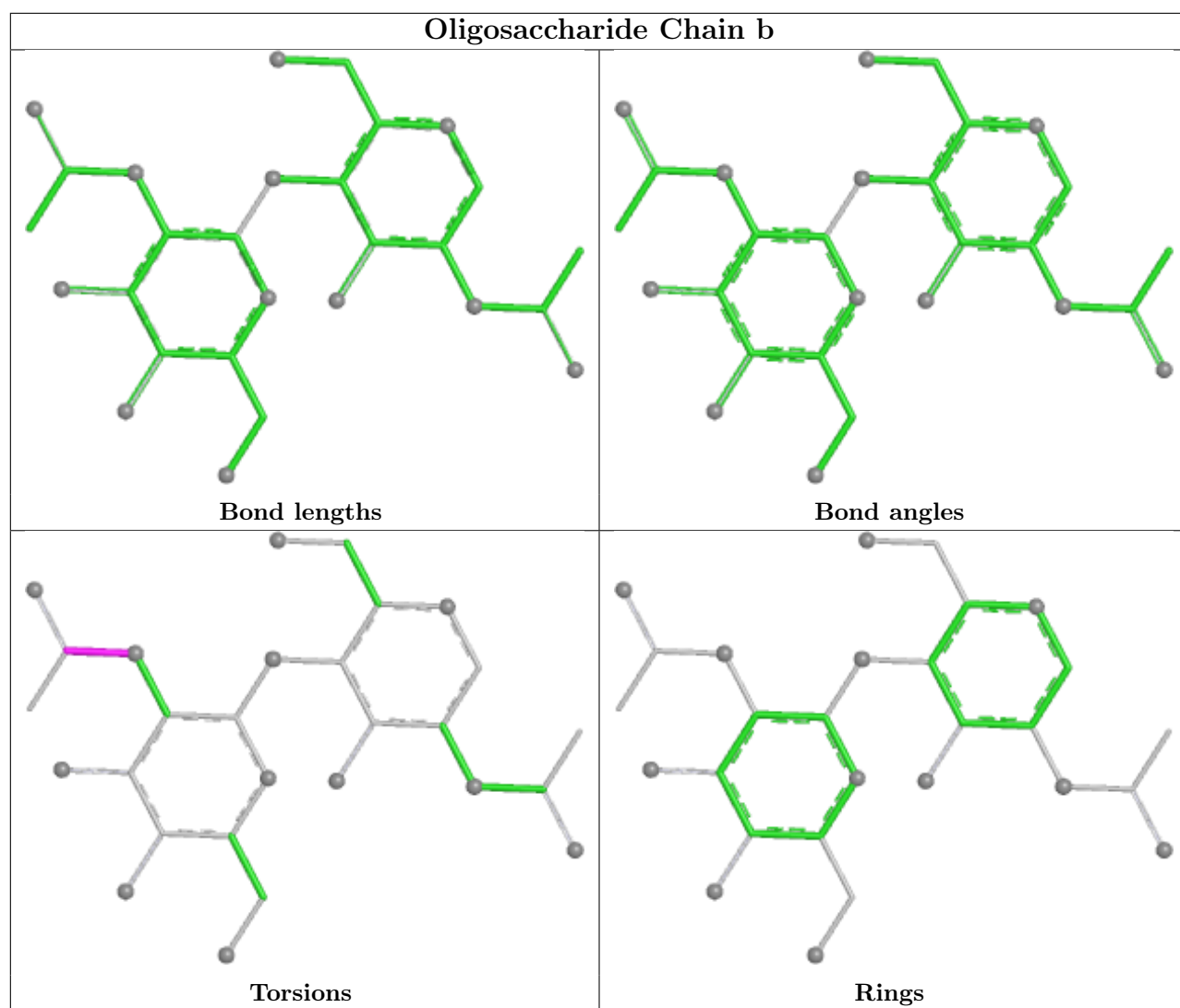


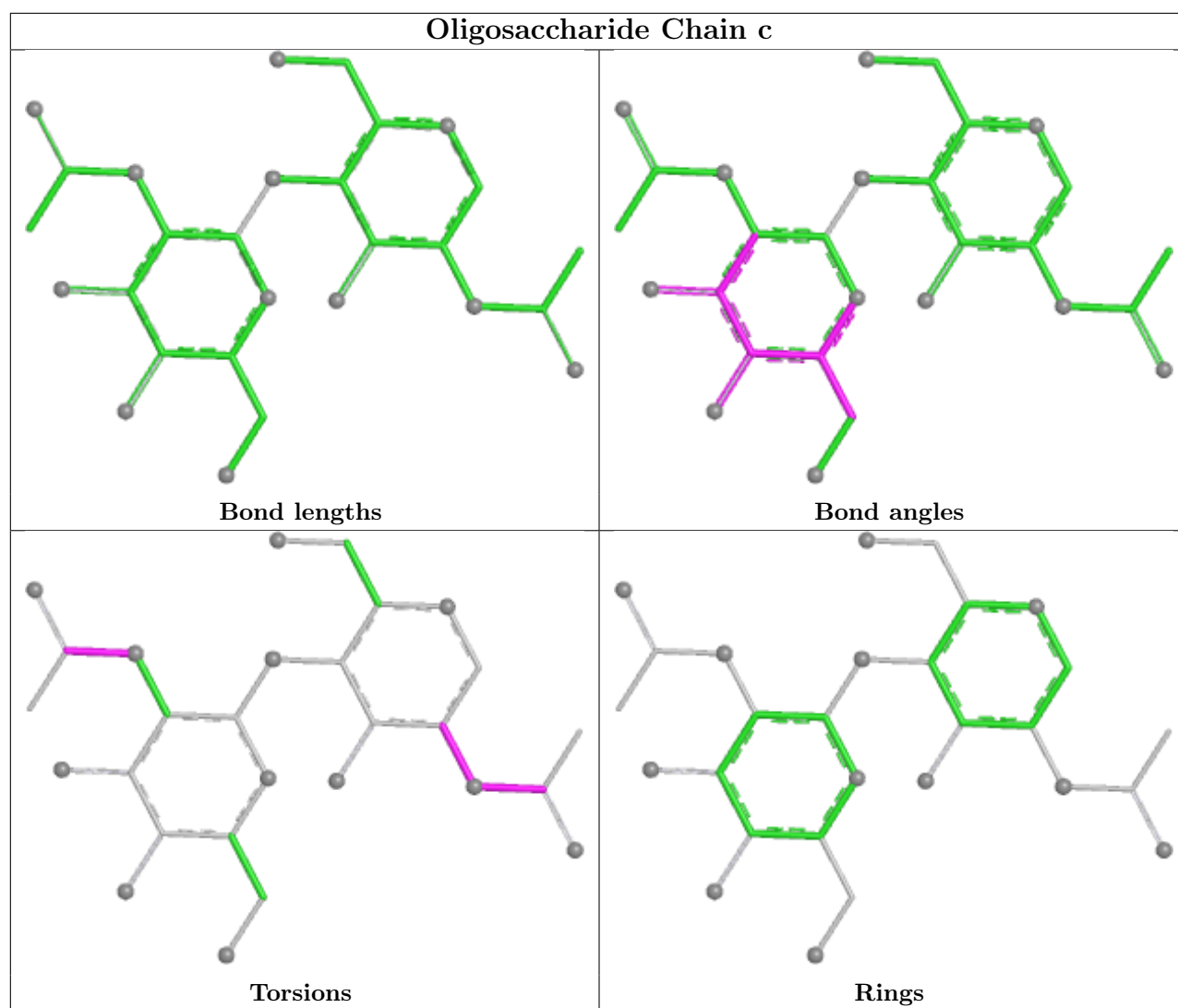


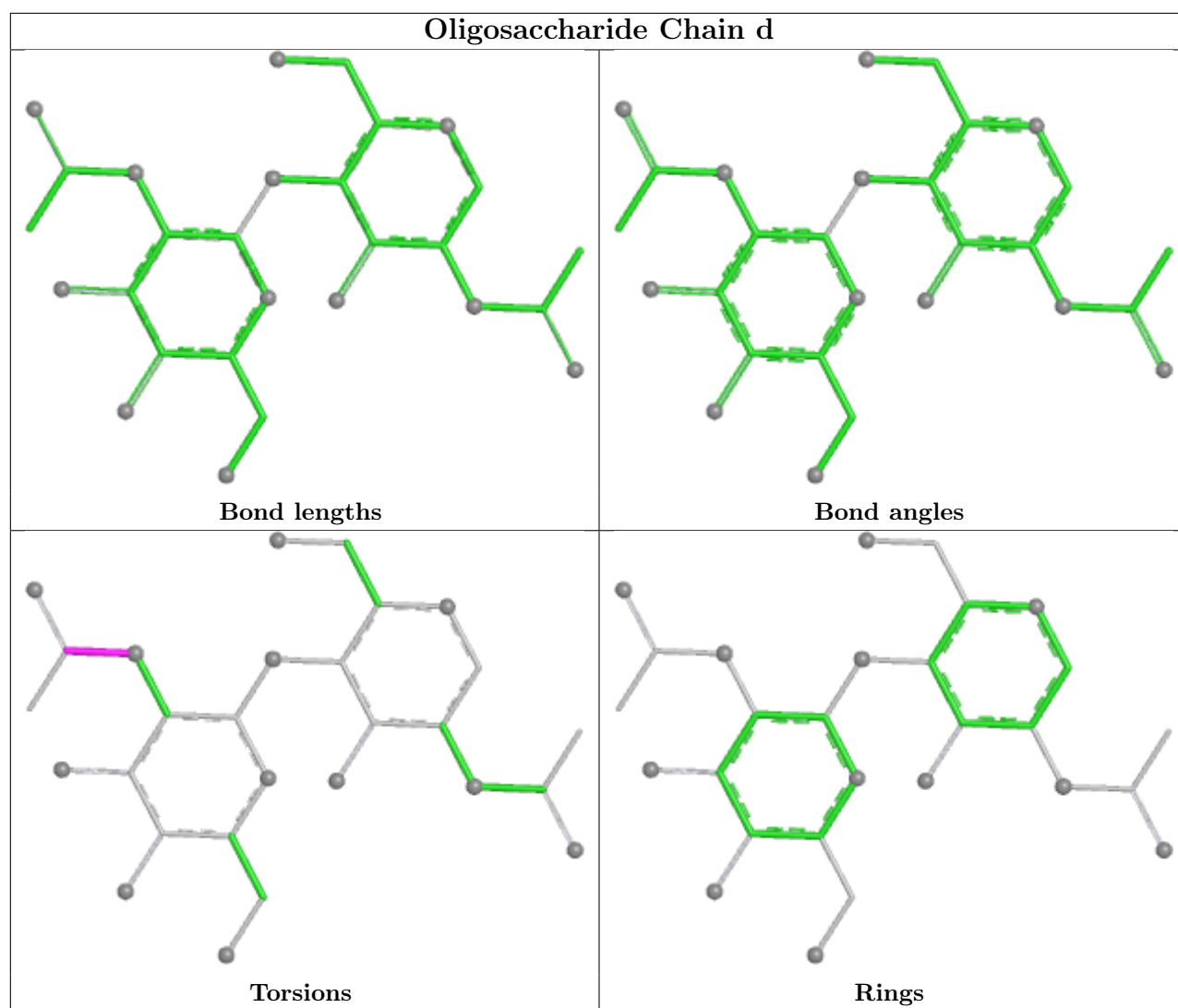


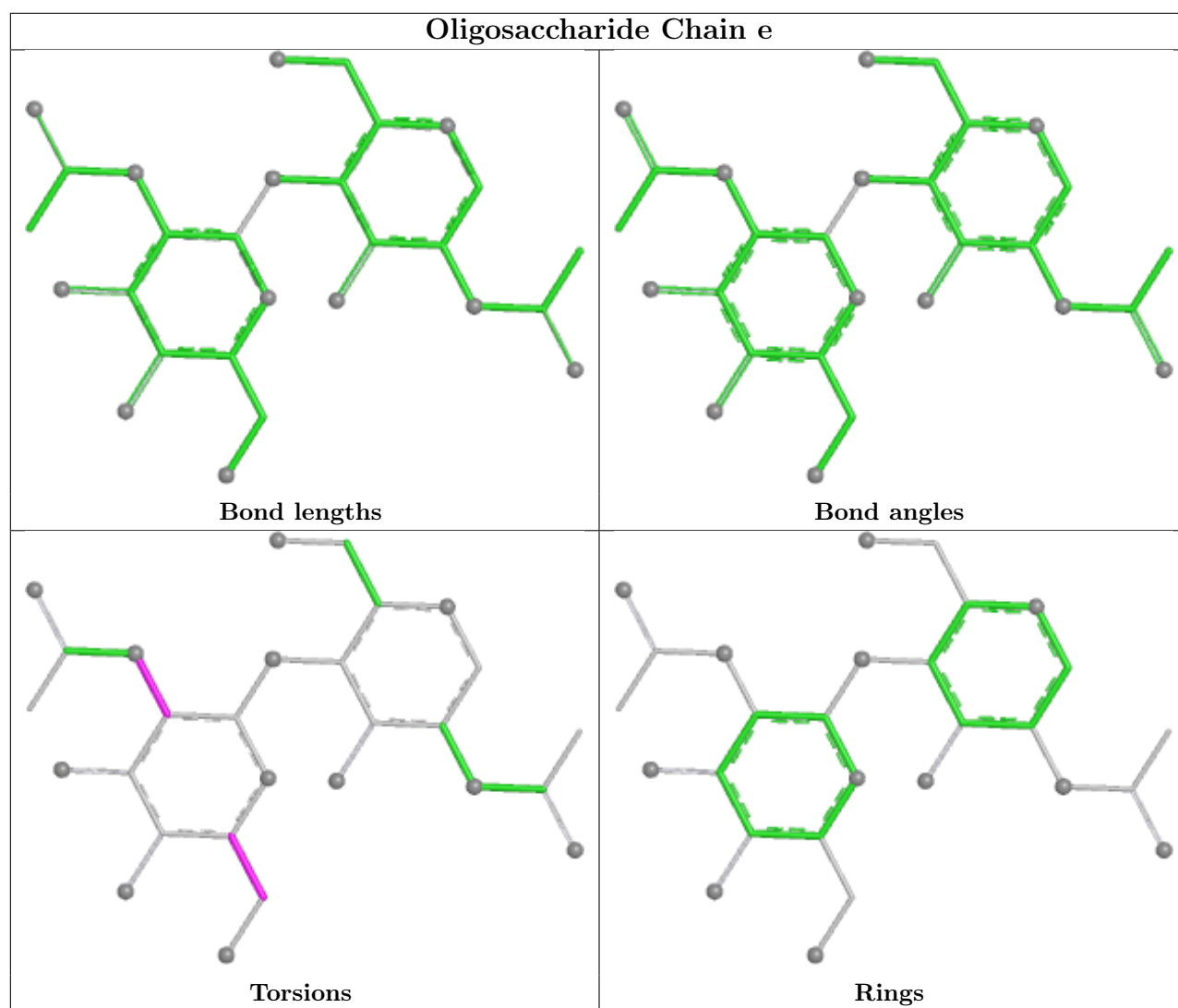


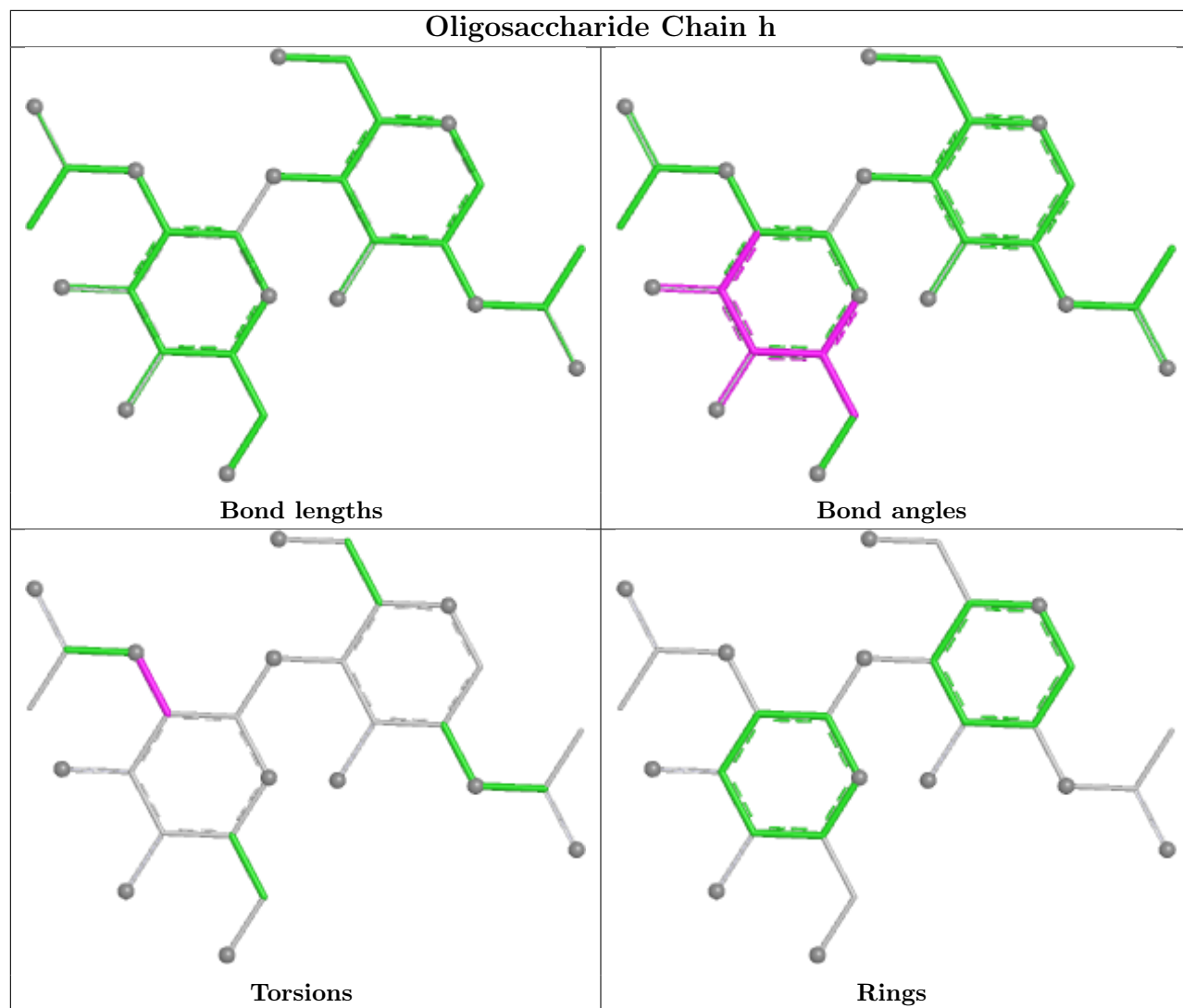


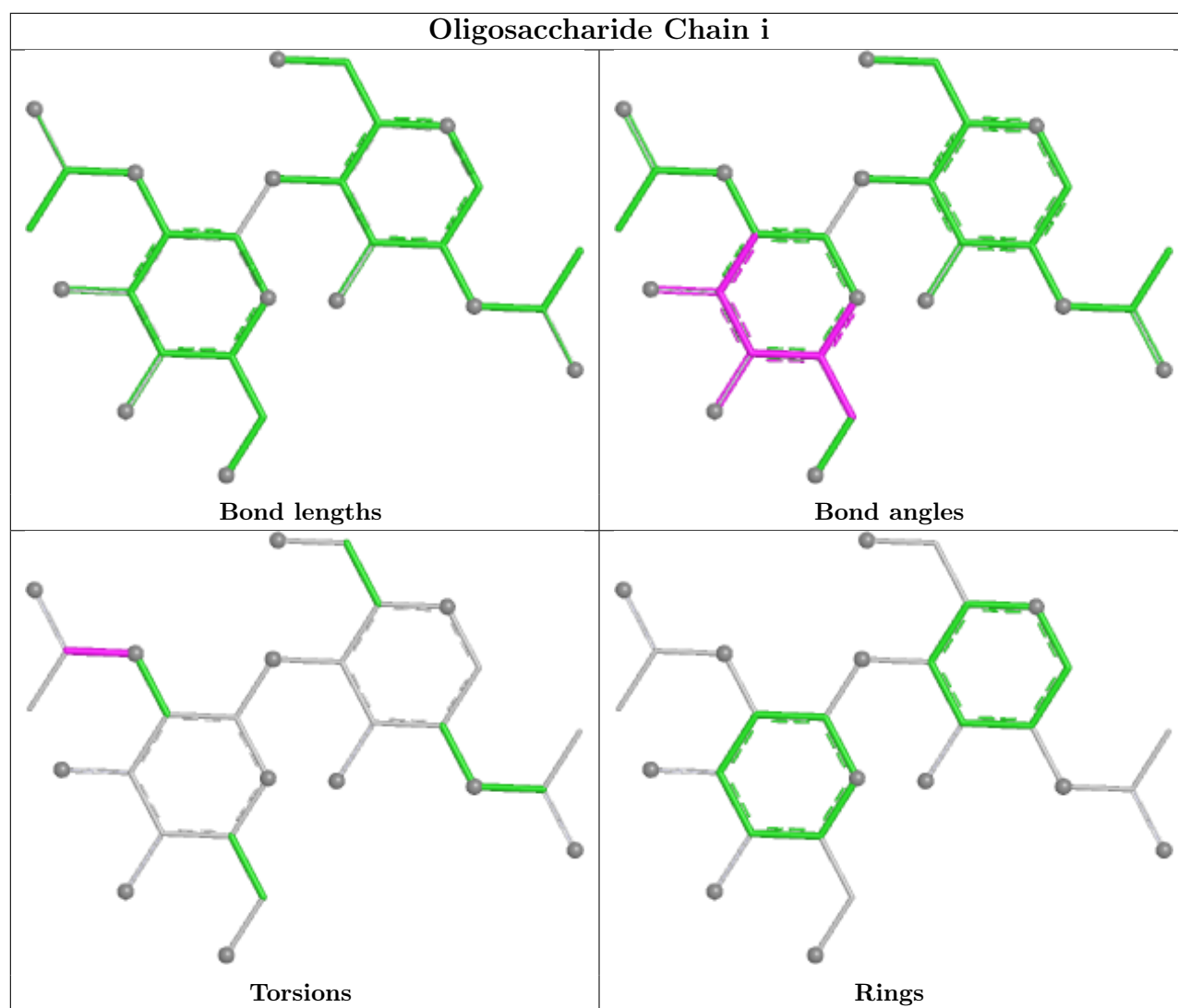


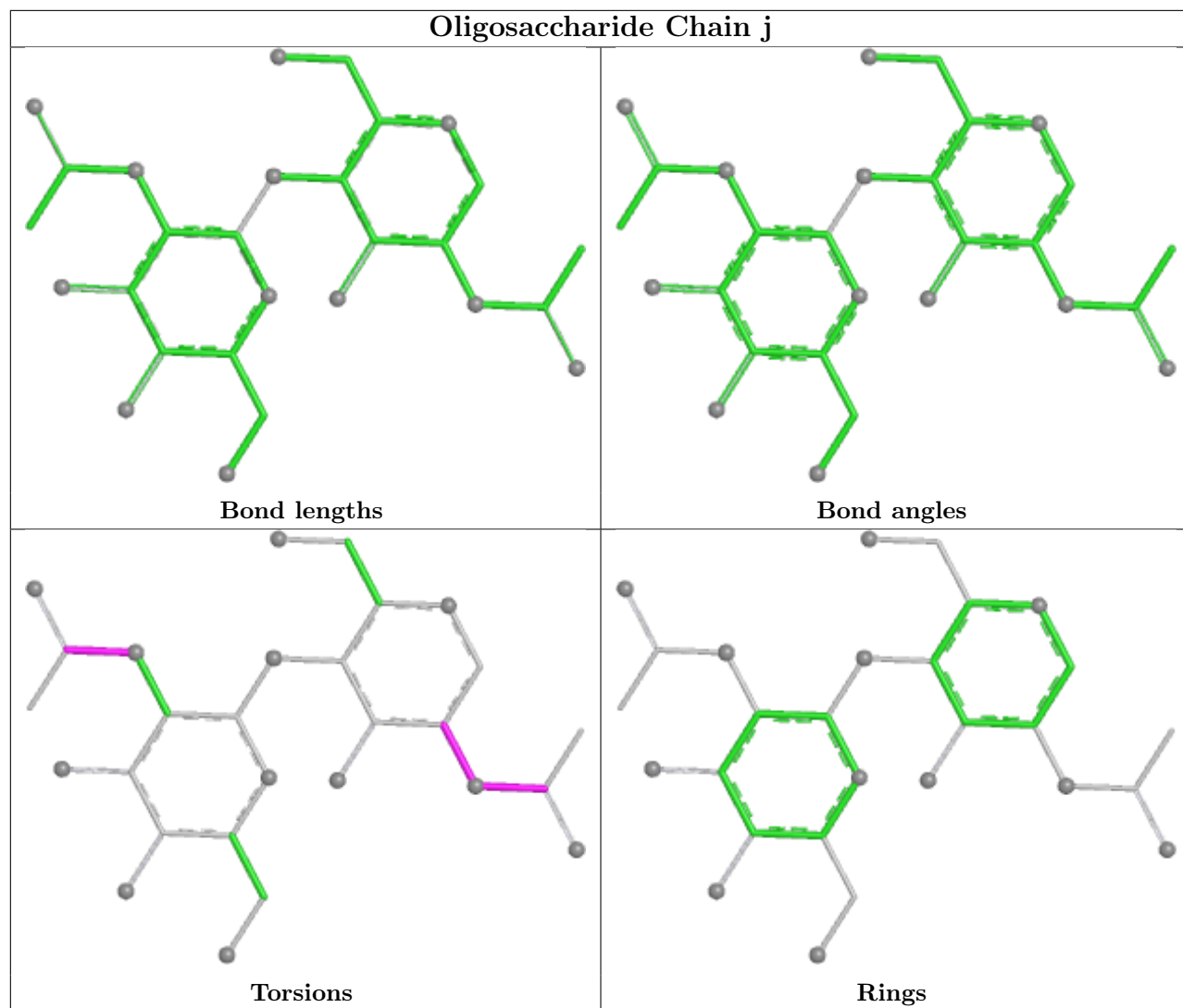


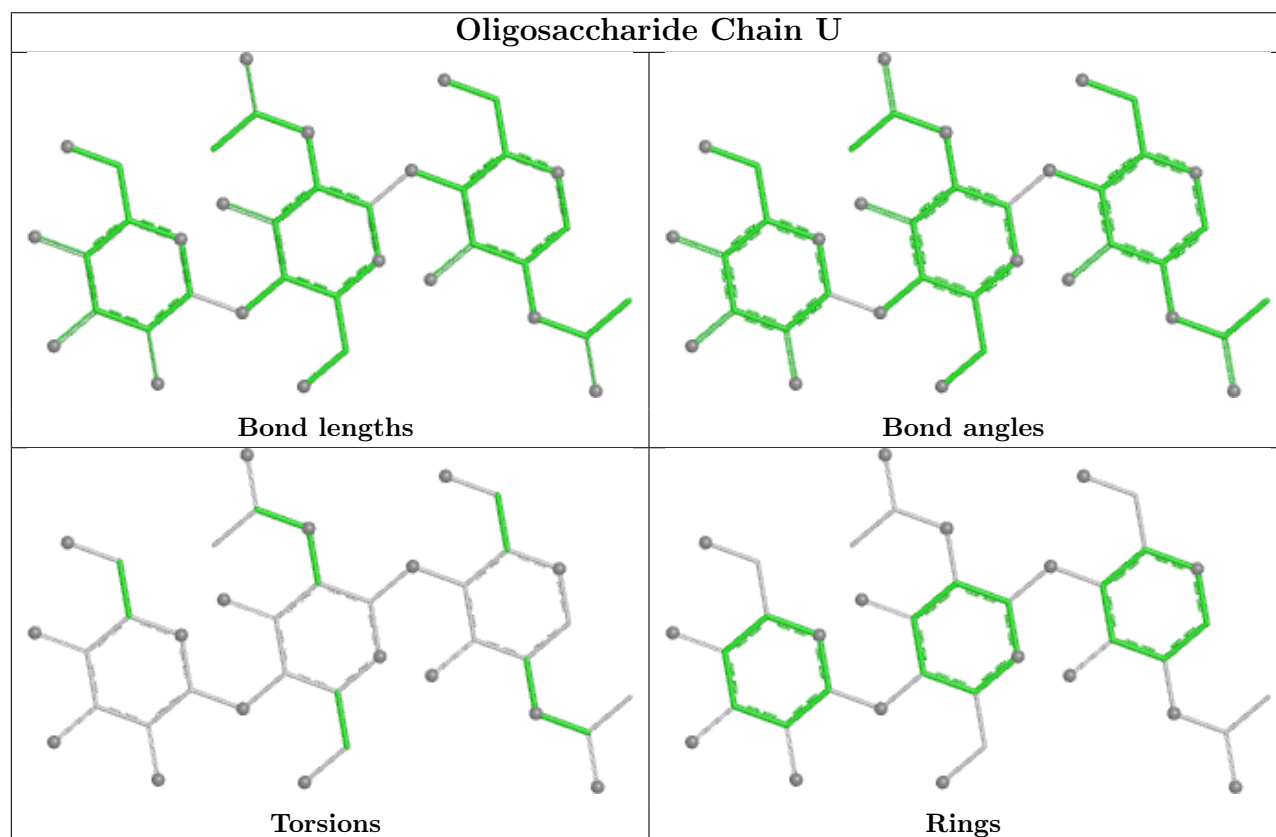
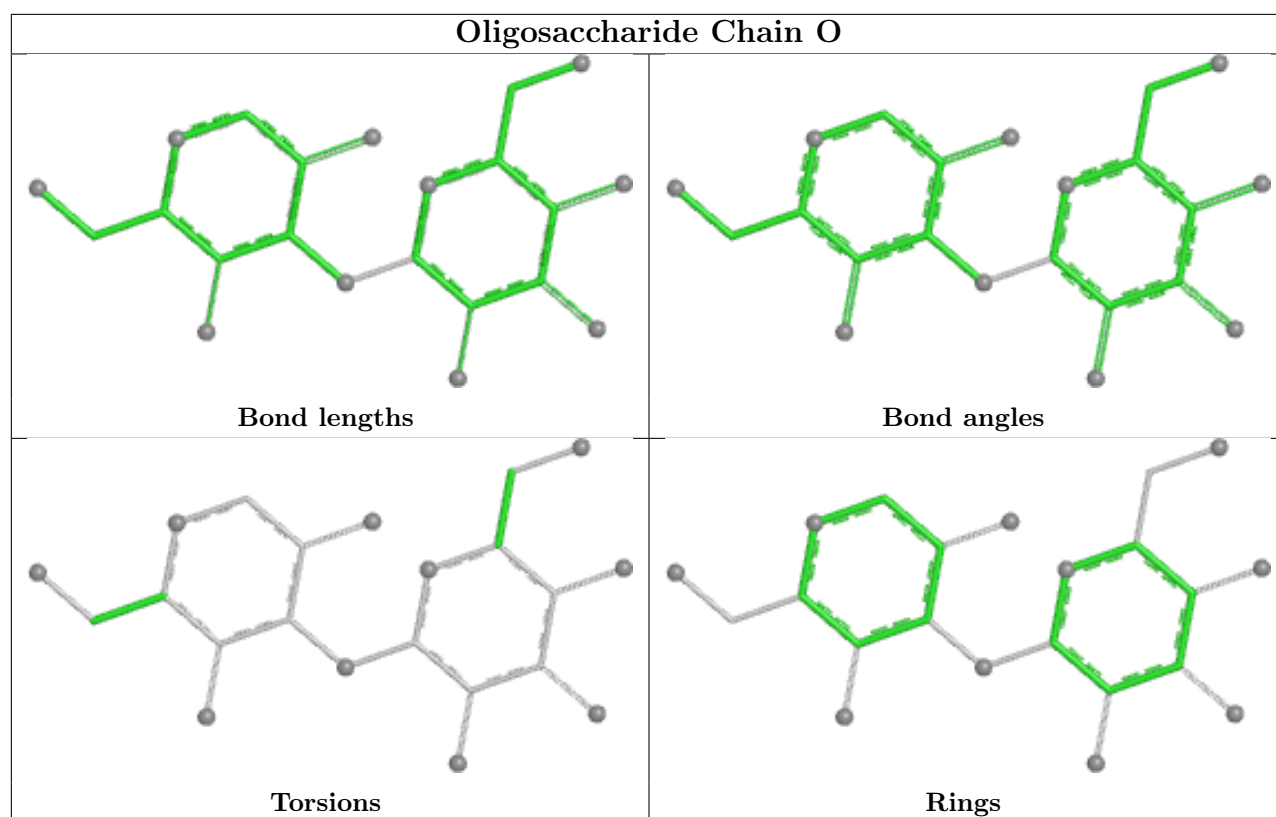


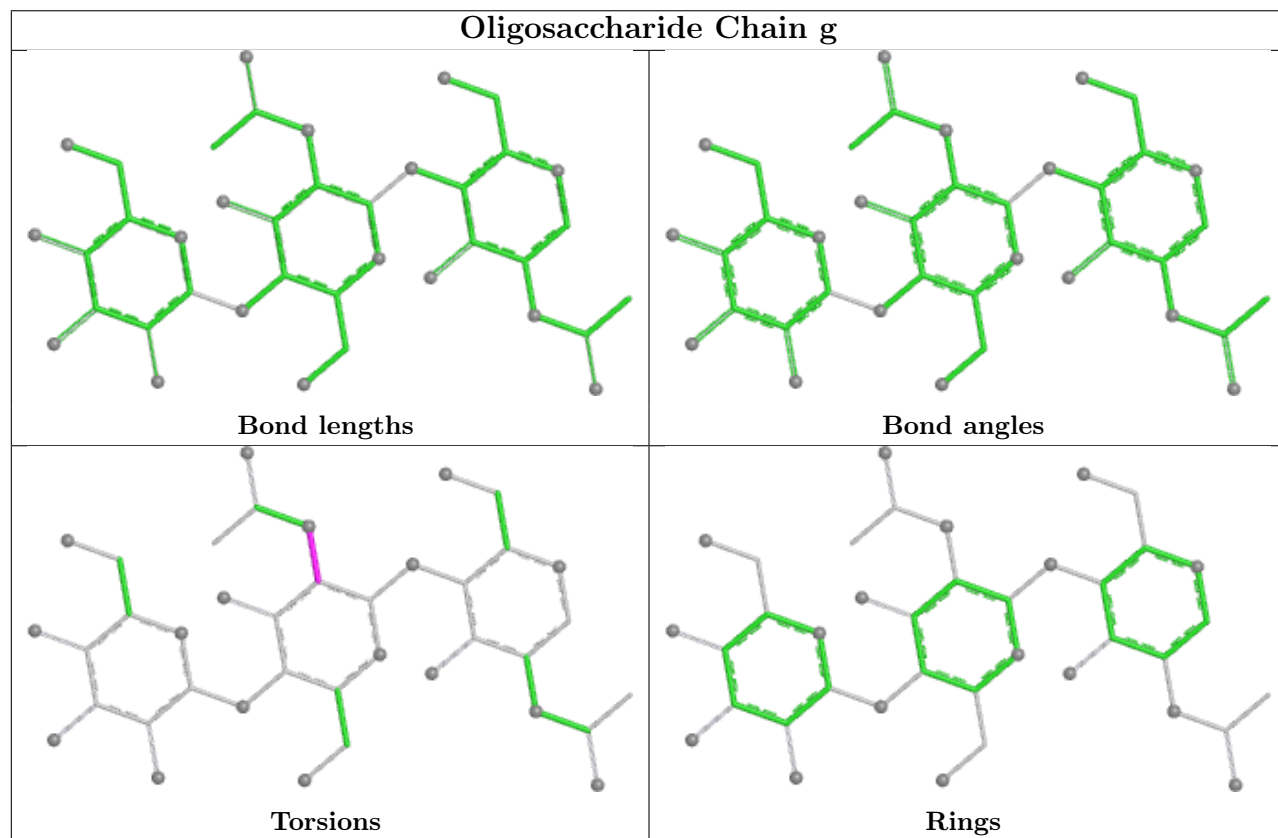
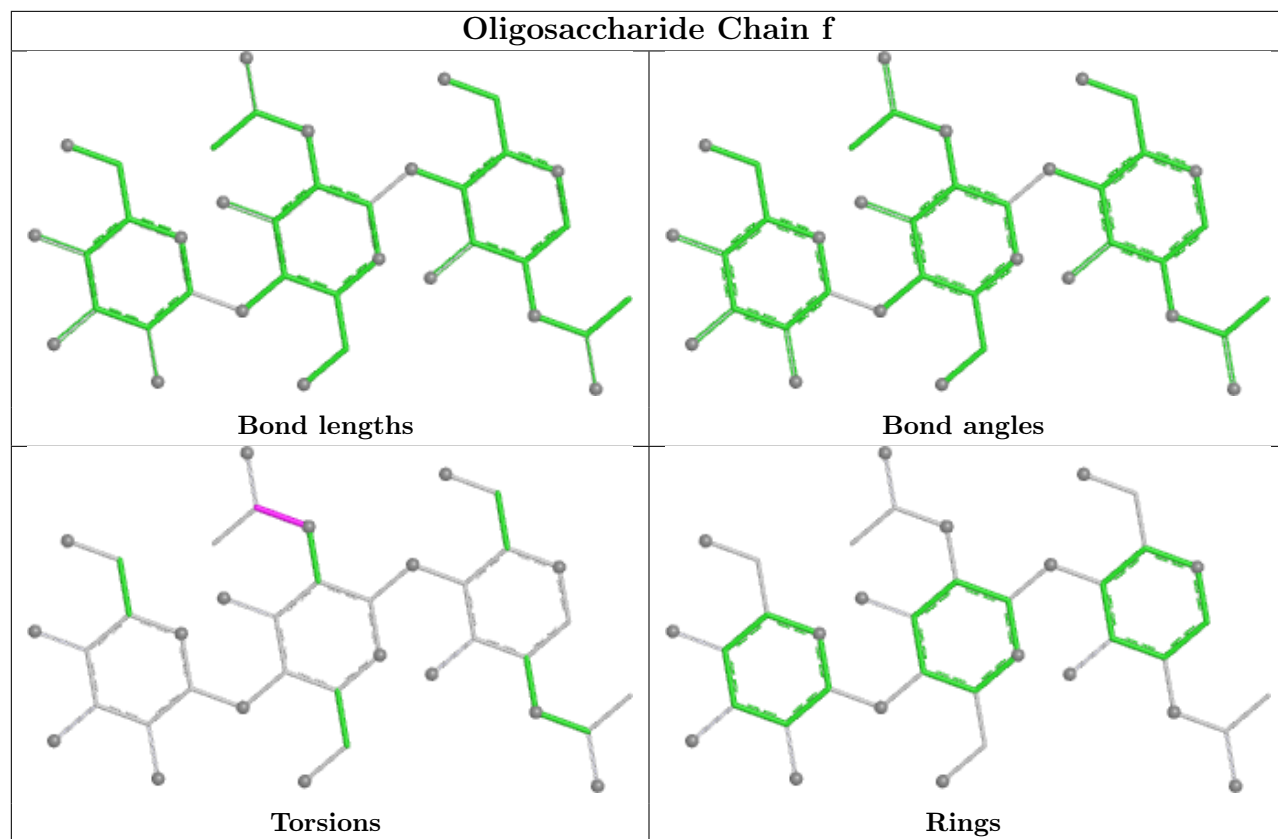


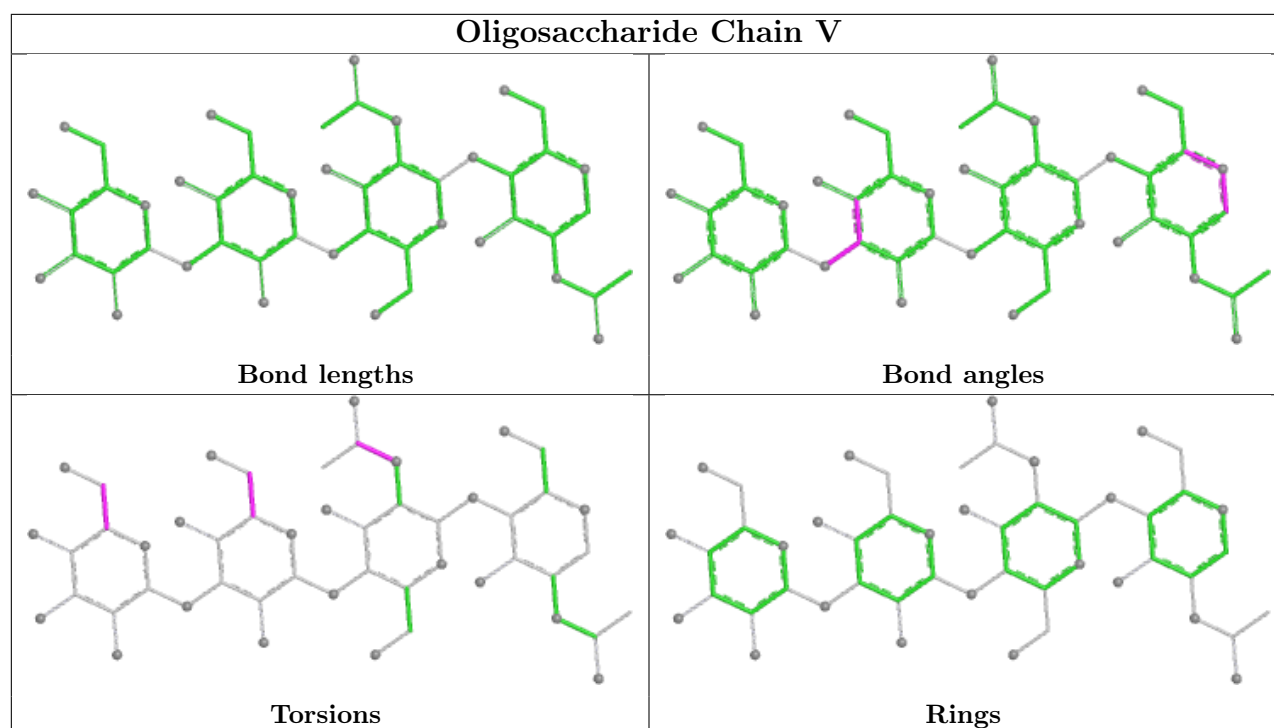












5.6 Ligand geometry [i](#)

41 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	G	601	2	14,14,15	0.28	0	17,19,21	0.71	0
9	NAG	D	704	1	14,14,15	0.26	0	17,19,21	0.75	0
9	NAG	F	701	1	14,14,15	0.27	0	17,19,21	10.38	3 (17%)
9	NAG	E	602	2	14,14,15	0.40	0	17,19,21	0.75	0
9	NAG	C	610	2	14,14,15	0.29	0	17,19,21	0.74	0
9	NAG	C	606	2	14,14,15	0.40	0	17,19,21	0.75	0
9	NAG	G	605	2	14,14,15	0.27	0	17,19,21	0.60	0
9	NAG	G	608	2	14,14,15	0.40	0	17,19,21	0.76	0
9	NAG	E	601	2	14,14,15	0.40	0	17,19,21	0.75	0
9	NAG	D	702	1	14,14,15	0.39	0	17,19,21	0.75	0
9	NAG	G	607	2	14,14,15	0.26	0	17,19,21	0.68	0
9	NAG	E	609	2	14,14,15	0.32	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	G	606	2	14,14,15	0.27	0	17,19,21	0.59	0
9	NAG	E	604	2	14,14,15	0.30	0	17,19,21	0.60	0
9	NAG	C	608	2	14,14,15	0.26	0	17,19,21	0.62	0
9	NAG	B	701	1	14,14,15	1.67	1 (7%)	17,19,21	2.21	3 (17%)
9	NAG	E	606	2	14,14,15	0.27	0	17,19,21	0.62	0
9	NAG	C	605	2	14,14,15	0.41	0	17,19,21	0.75	0
9	NAG	F	702	1	14,14,15	0.27	0	17,19,21	0.73	0
9	NAG	G	602	2	14,14,15	0.42	0	17,19,21	0.78	0
9	NAG	E	603	2	14,14,15	0.31	0	17,19,21	0.64	0
9	NAG	D	703	1	14,14,15	0.28	0	17,19,21	0.70	0
9	NAG	C	603	2	14,14,15	0.26	0	17,19,21	0.76	0
9	NAG	D	701	1	14,14,15	0.28	0	17,19,21	0.70	0
9	NAG	G	604	2	14,14,15	0.40	0	17,19,21	0.75	0
9	NAG	B	703	1	14,14,15	0.41	0	17,19,21	0.75	0
9	NAG	B	704	1	14,14,15	0.28	0	17,19,21	0.71	0
9	NAG	B	702	1	14,14,15	0.41	0	17,19,21	0.76	0
9	NAG	C	601	2	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
9	NAG	C	602	2	14,14,15	0.39	0	17,19,21	0.75	0
9	NAG	G	611	2	14,14,15	0.28	0	17,19,21	0.75	0
9	NAG	C	609	2	14,14,15	0.27	0	17,19,21	0.65	0
9	NAG	C	604	2	14,14,15	0.32	0	17,19,21	0.65	0
9	NAG	E	605	2	14,14,15	0.40	0	17,19,21	0.76	0
9	NAG	E	608	2	14,14,15	0.29	0	17,19,21	0.76	0
9	NAG	E	607	2	14,14,15	0.27	0	17,19,21	0.67	0
9	NAG	G	610	2	14,14,15	0.27	0	17,19,21	10.38	3 (17%)
9	NAG	G	609	2	14,14,15	0.28	0	17,19,21	0.67	0
9	NAG	F	703	1	14,14,15	0.25	0	17,19,21	0.60	0
9	NAG	C	607	2	14,14,15	0.25	0	17,19,21	0.54	0
9	NAG	G	603	2	14,14,15	0.40	0	17,19,21	0.76	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
9	NAG	G	601	2	-	0/6/23/26	0/1/1/1
9	NAG	D	704	1	-	1/6/23/26	0/1/1/1
9	NAG	F	701	1	-	1/6/23/26	0/1/1/1
9	NAG	E	602	2	-	3/6/23/26	0/1/1/1
9	NAG	C	610	2	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	606	2	-	2/6/23/26	0/1/1/1
9	NAG	G	605	2	-	0/6/23/26	0/1/1/1
9	NAG	G	608	2	-	2/6/23/26	0/1/1/1
9	NAG	E	601	2	-	3/6/23/26	0/1/1/1
9	NAG	D	702	1	-	2/6/23/26	0/1/1/1
9	NAG	G	607	2	-	0/6/23/26	0/1/1/1
9	NAG	E	609	2	-	1/6/23/26	0/1/1/1
9	NAG	G	606	2	-	3/6/23/26	0/1/1/1
9	NAG	E	604	2	-	3/6/23/26	0/1/1/1
9	NAG	C	608	2	-	2/6/23/26	0/1/1/1
9	NAG	B	701	1	-	2/6/23/26	0/1/1/1
9	NAG	E	606	2	-	3/6/23/26	0/1/1/1
9	NAG	C	605	2	-	3/6/23/26	0/1/1/1
9	NAG	F	702	1	-	1/6/23/26	0/1/1/1
9	NAG	G	602	2	-	2/6/23/26	0/1/1/1
9	NAG	E	603	2	-	2/6/23/26	0/1/1/1
9	NAG	D	703	1	-	3/6/23/26	0/1/1/1
9	NAG	C	603	2	-	1/6/23/26	0/1/1/1
9	NAG	D	701	1	-	2/6/23/26	0/1/1/1
9	NAG	G	604	2	-	2/6/23/26	0/1/1/1
9	NAG	B	703	1	-	2/6/23/26	0/1/1/1
9	NAG	B	704	1	-	0/6/23/26	0/1/1/1
9	NAG	B	702	1	-	2/6/23/26	0/1/1/1
9	NAG	C	601	2	-	2/6/23/26	0/1/1/1
9	NAG	C	602	2	-	1/6/23/26	0/1/1/1
9	NAG	G	611	2	-	0/6/23/26	0/1/1/1
9	NAG	C	609	2	-	0/6/23/26	0/1/1/1
9	NAG	C	604	2	-	0/6/23/26	0/1/1/1
9	NAG	E	605	2	-	3/6/23/26	0/1/1/1
9	NAG	E	608	2	-	2/6/23/26	0/1/1/1
9	NAG	E	607	2	-	2/6/23/26	0/1/1/1
9	NAG	G	610	2	-	1/6/23/26	0/1/1/1
9	NAG	G	609	2	-	2/6/23/26	0/1/1/1
9	NAG	F	703	1	-	2/6/23/26	0/1/1/1
9	NAG	C	607	2	-	1/6/23/26	0/1/1/1
9	NAG	G	603	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	701	NAG	C1-C2	6.18	1.60	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	610	NAG	C8-C7-N2	26.32	159.76	116.12
9	F	701	NAG	C8-C7-N2	26.31	159.74	116.12
9	F	701	NAG	O7-C7-C8	-23.77	79.72	122.05
9	G	610	NAG	O7-C7-N2	-23.75	80.00	121.98
9	G	610	NAG	O7-C7-C8	-23.75	79.76	122.05
9	F	701	NAG	O7-C7-N2	-23.74	80.02	121.98
9	B	701	NAG	O5-C1-C2	-7.28	100.02	111.29
9	B	701	NAG	C1-O5-C5	4.19	117.80	112.19
9	E	609	NAG	C2-N2-C7	-2.94	118.96	122.90
9	B	701	NAG	C4-C3-C2	-2.46	107.41	111.02
9	E	609	NAG	C1-O5-C5	2.20	115.14	112.19
9	C	601	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	601	NAG	C3-C2-N2-C7
9	C	602	NAG	C3-C2-N2-C7
9	C	607	NAG	C3-C2-N2-C7
9	E	601	NAG	C3-C2-N2-C7
9	E	609	NAG	C3-C2-N2-C7
9	G	606	NAG	C3-C2-N2-C7
9	B	701	NAG	C8-C7-N2-C2
9	B	701	NAG	O7-C7-N2-C2
9	B	702	NAG	C8-C7-N2-C2
9	B	702	NAG	O7-C7-N2-C2
9	B	703	NAG	C8-C7-N2-C2
9	B	703	NAG	O7-C7-N2-C2
9	C	605	NAG	C8-C7-N2-C2
9	C	605	NAG	O7-C7-N2-C2
9	C	606	NAG	C8-C7-N2-C2
9	C	606	NAG	O7-C7-N2-C2
9	C	608	NAG	C8-C7-N2-C2
9	C	608	NAG	O7-C7-N2-C2
9	C	610	NAG	C8-C7-N2-C2
9	C	610	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	701	NAG	C8-C7-N2-C2
9	D	701	NAG	O7-C7-N2-C2
9	D	702	NAG	C8-C7-N2-C2
9	D	702	NAG	O7-C7-N2-C2
9	D	703	NAG	C8-C7-N2-C2
9	D	703	NAG	O7-C7-N2-C2
9	E	601	NAG	C8-C7-N2-C2
9	E	601	NAG	O7-C7-N2-C2
9	E	602	NAG	C8-C7-N2-C2
9	E	602	NAG	O7-C7-N2-C2
9	E	603	NAG	C8-C7-N2-C2
9	E	603	NAG	O7-C7-N2-C2
9	E	604	NAG	C8-C7-N2-C2
9	E	604	NAG	O7-C7-N2-C2
9	E	605	NAG	C8-C7-N2-C2
9	E	605	NAG	O7-C7-N2-C2
9	E	606	NAG	C8-C7-N2-C2
9	E	606	NAG	O7-C7-N2-C2
9	E	607	NAG	C8-C7-N2-C2
9	E	607	NAG	O7-C7-N2-C2
9	E	608	NAG	C8-C7-N2-C2
9	E	608	NAG	O7-C7-N2-C2
9	F	701	NAG	O7-C7-N2-C2
9	F	703	NAG	C8-C7-N2-C2
9	F	703	NAG	O7-C7-N2-C2
9	G	602	NAG	C8-C7-N2-C2
9	G	602	NAG	O7-C7-N2-C2
9	G	604	NAG	C8-C7-N2-C2
9	G	604	NAG	O7-C7-N2-C2
9	G	606	NAG	C8-C7-N2-C2
9	G	606	NAG	O7-C7-N2-C2
9	G	608	NAG	C8-C7-N2-C2
9	G	608	NAG	O7-C7-N2-C2
9	G	609	NAG	C8-C7-N2-C2
9	G	609	NAG	O7-C7-N2-C2
9	G	610	NAG	O7-C7-N2-C2
9	C	601	NAG	O5-C5-C6-O6
9	C	603	NAG	O5-C5-C6-O6
9	C	610	NAG	O5-C5-C6-O6
9	D	703	NAG	O5-C5-C6-O6
9	D	704	NAG	O5-C5-C6-O6
9	E	604	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	E	606	NAG	O5-C5-C6-O6
9	F	702	NAG	O5-C5-C6-O6
9	C	605	NAG	O5-C5-C6-O6
9	E	602	NAG	O5-C5-C6-O6
9	E	605	NAG	O5-C5-C6-O6
9	G	603	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	610	NAG	1	0
9	C	606	NAG	3	0
9	E	601	NAG	7	0
9	E	609	NAG	4	0
9	G	606	NAG	1	0
9	C	605	NAG	1	0
9	C	601	NAG	3	0
9	C	602	NAG	3	0
9	E	608	NAG	3	0
9	C	607	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.

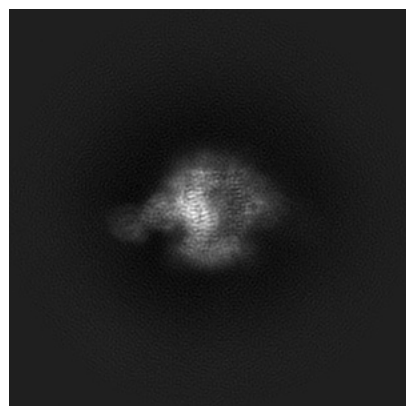
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25376. These allow visual inspection of the internal detail of the map and identification of artifacts.

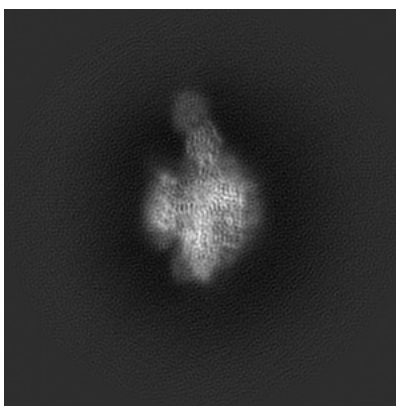
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

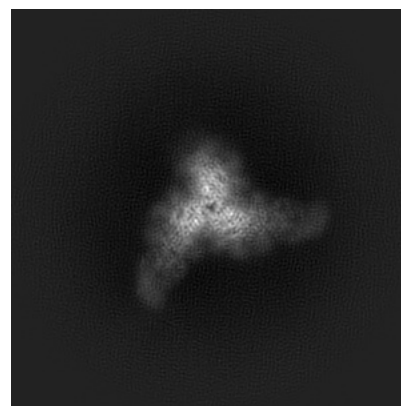
6.1.1 Primary map



X

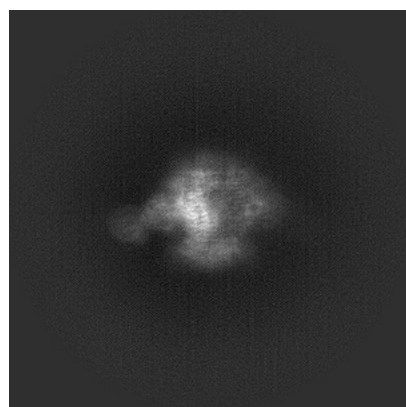


Y

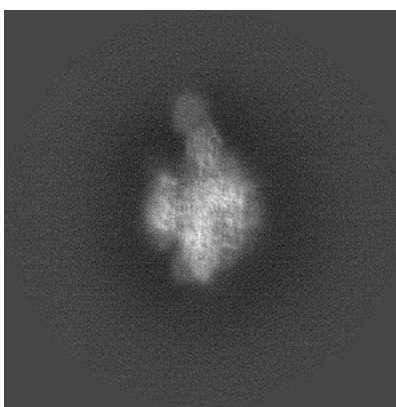


Z

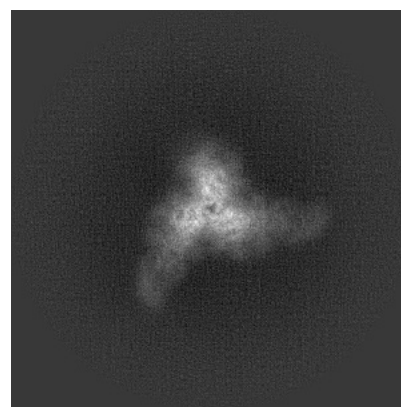
6.1.2 Raw map



X



Y

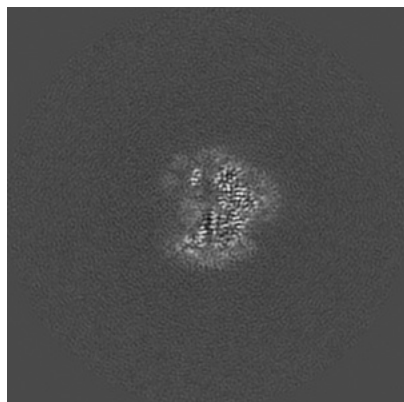


Z

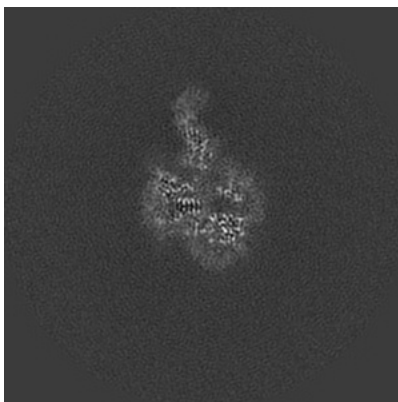
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

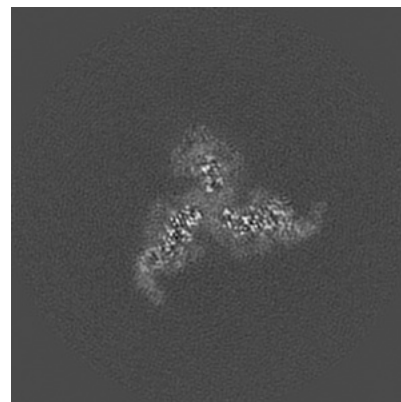
6.2.1 Primary map



X Index: 256

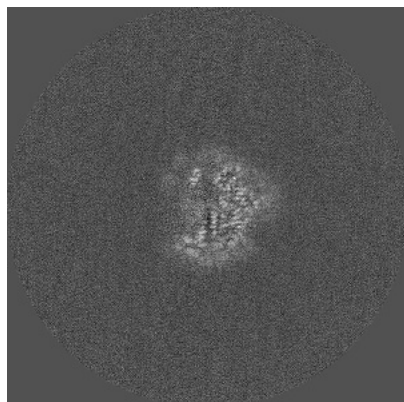


Y Index: 256

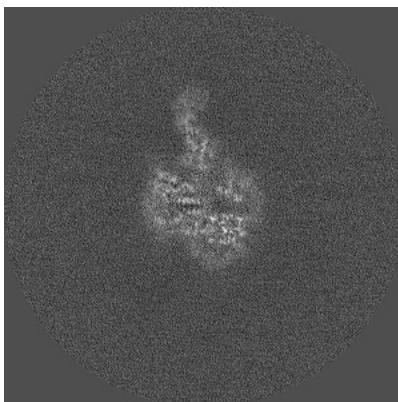


Z Index: 256

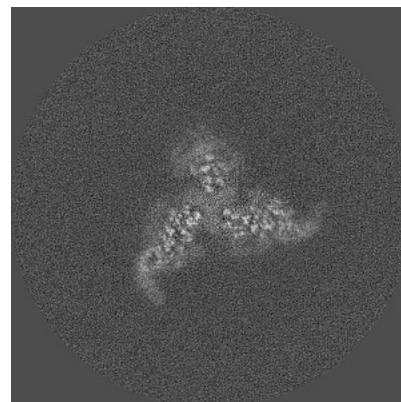
6.2.2 Raw map



X Index: 256



Y Index: 256

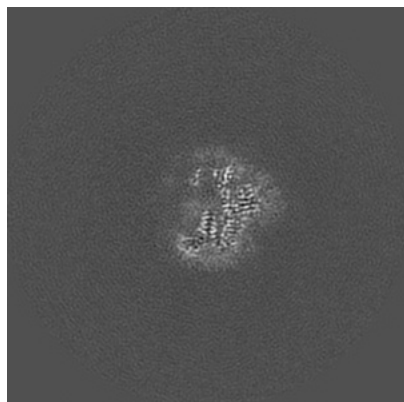


Z Index: 256

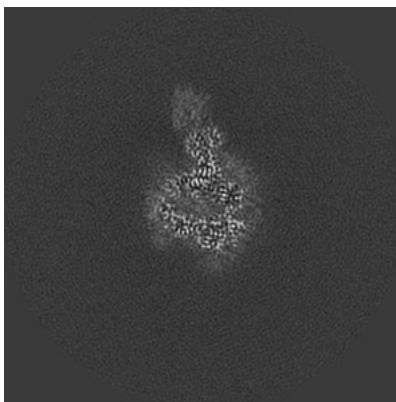
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

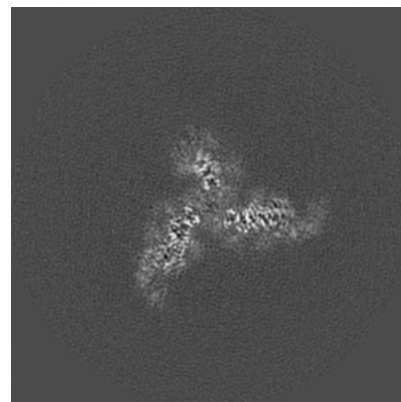
6.3.1 Primary map



X Index: 251

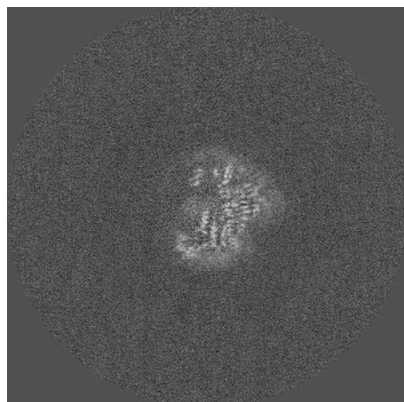


Y Index: 241

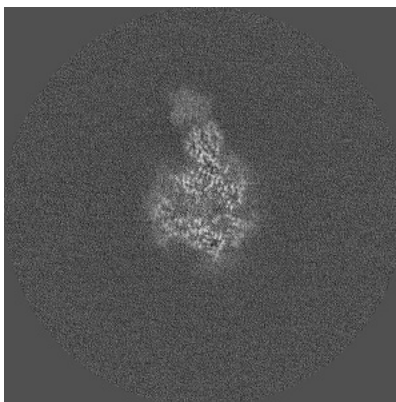


Z Index: 251

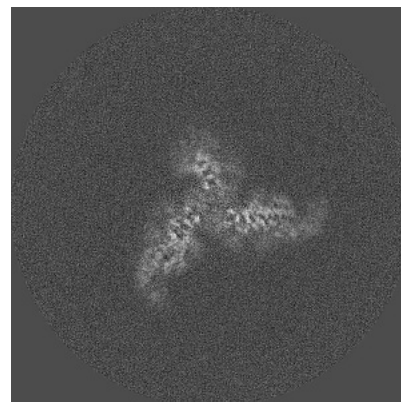
6.3.2 Raw map



X Index: 250



Y Index: 237

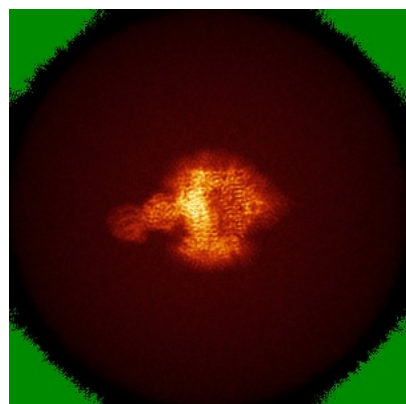


Z Index: 251

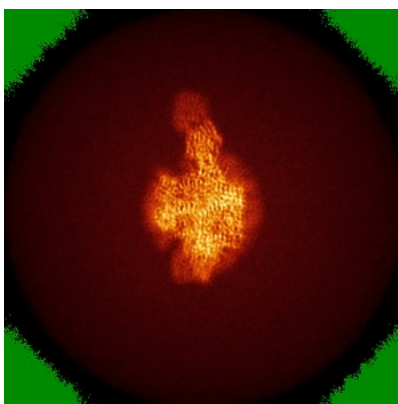
The images above show the largest variance slices of the map in three orthogonal directions.

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

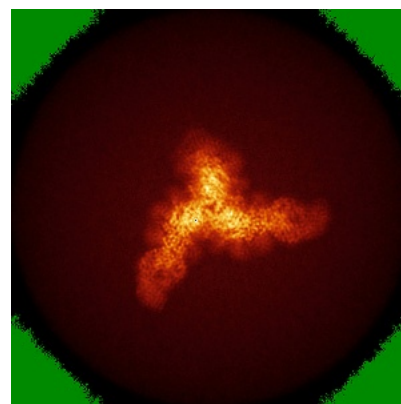
6.4.1 Primary map



X

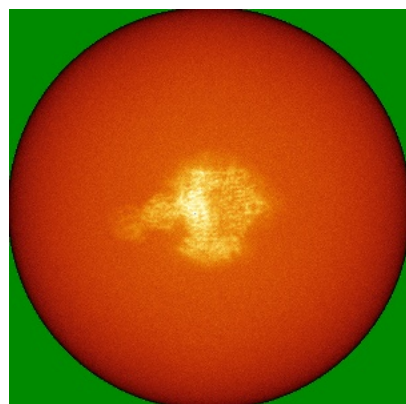


Y

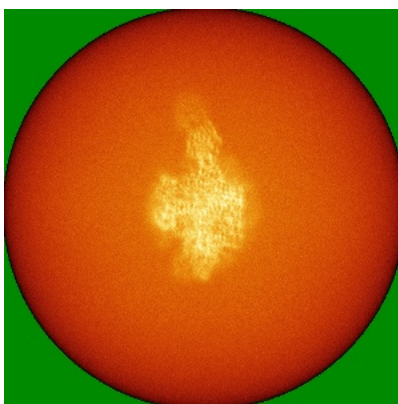


Z

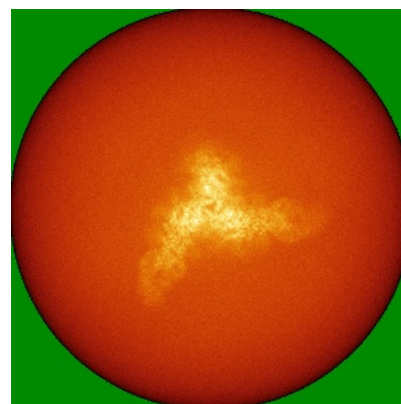
6.4.2 Raw map



X



Y

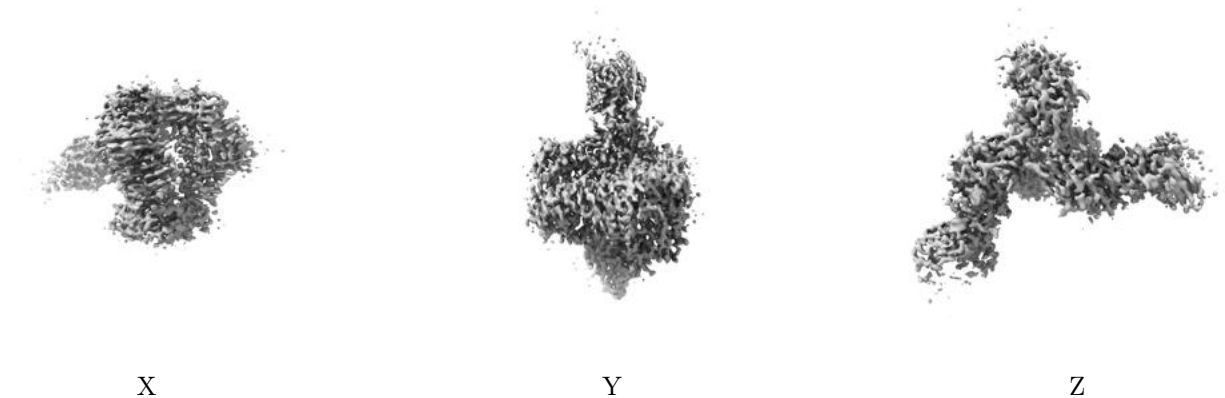


Z

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.

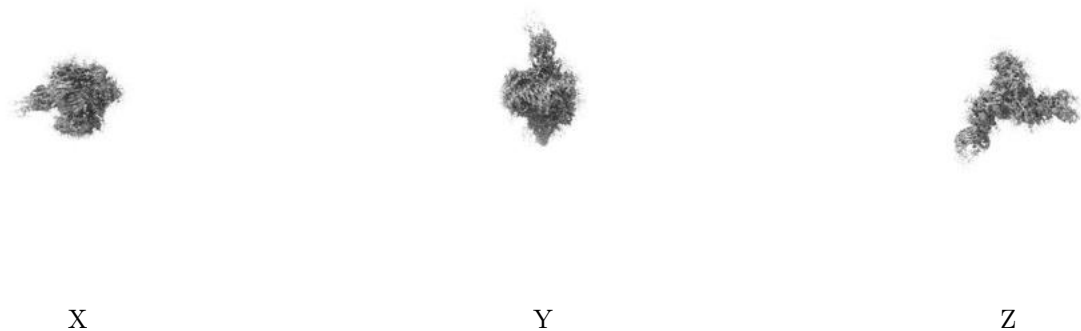
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

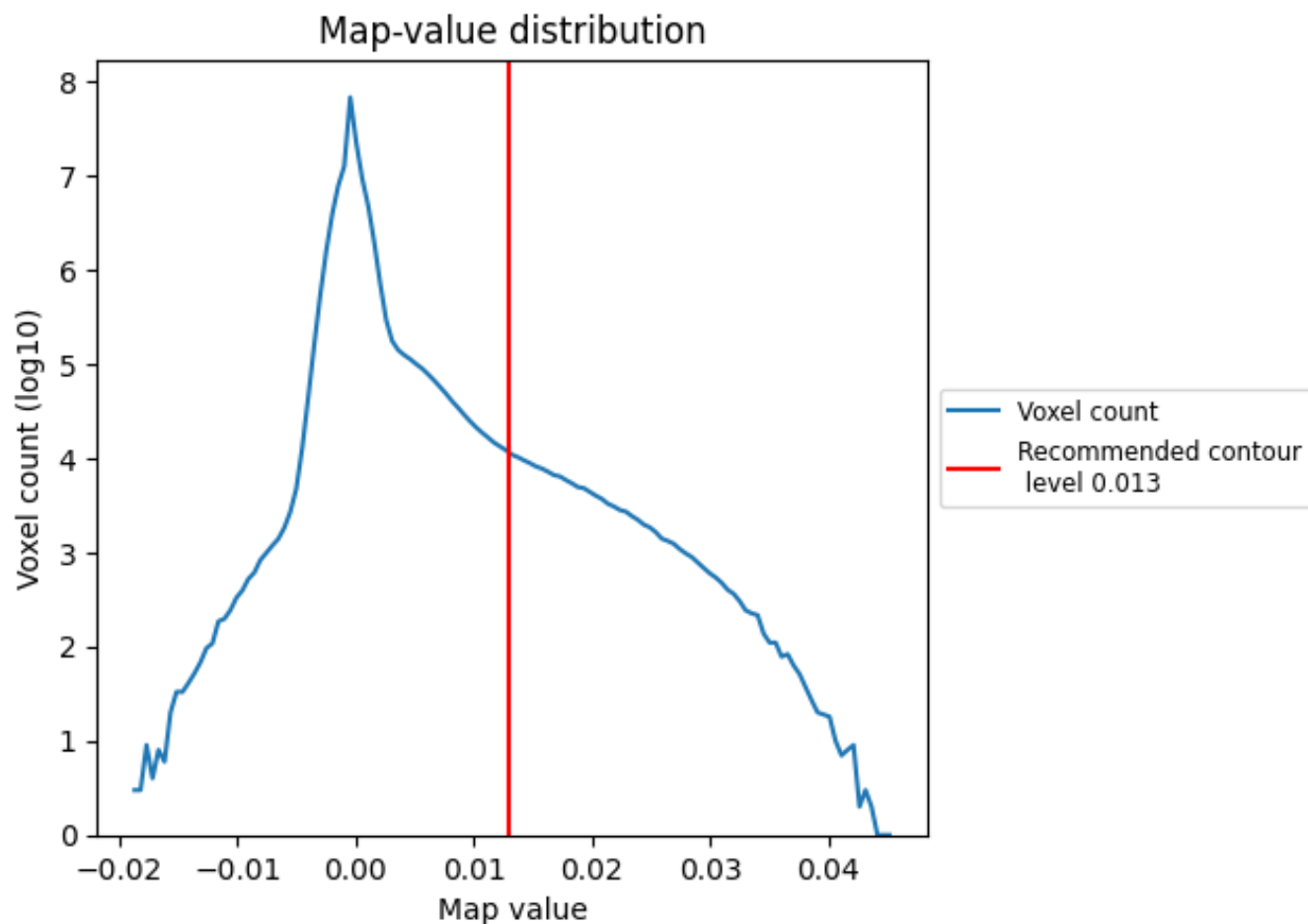
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

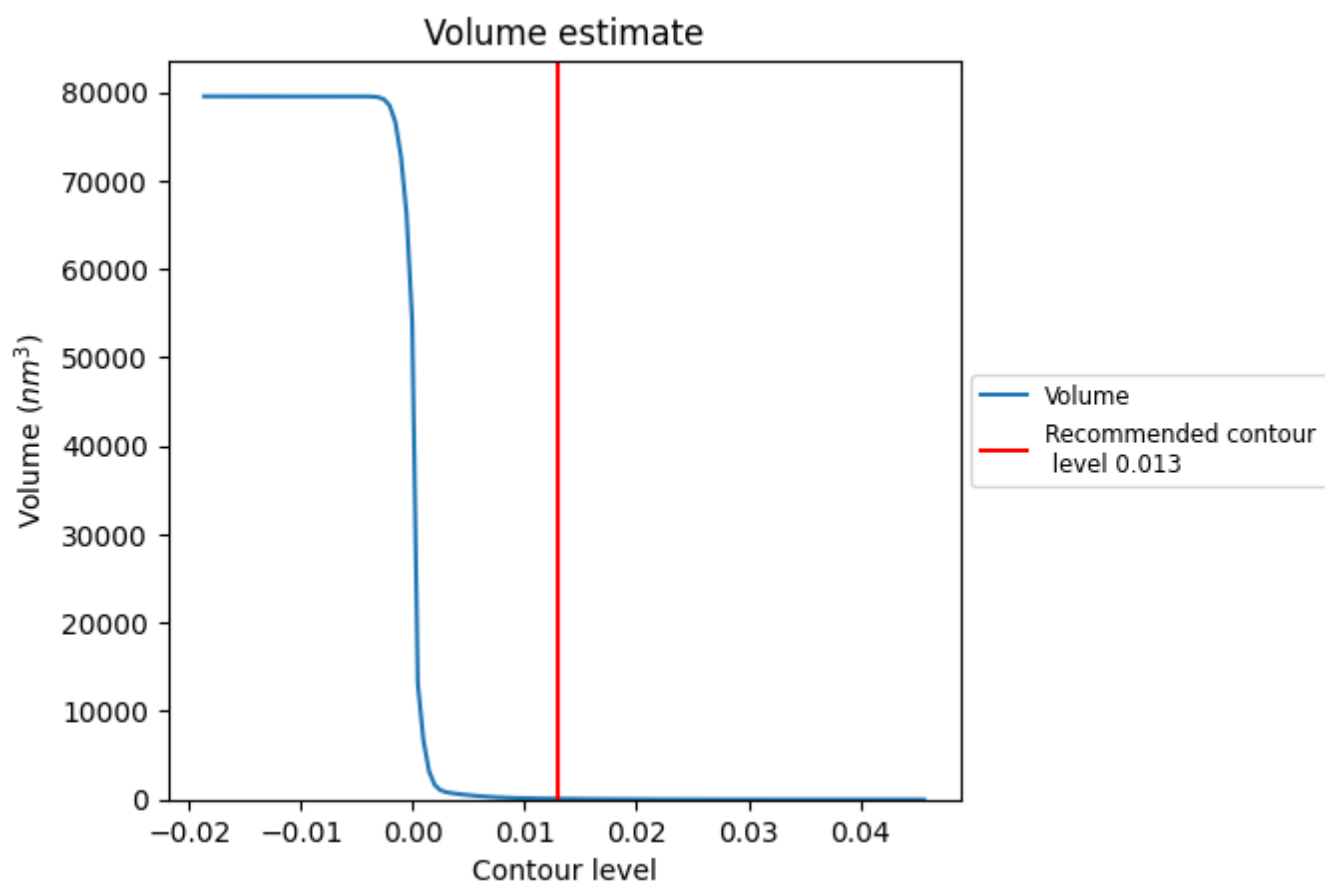
This section contains the results of statistical analysis of the map.

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.

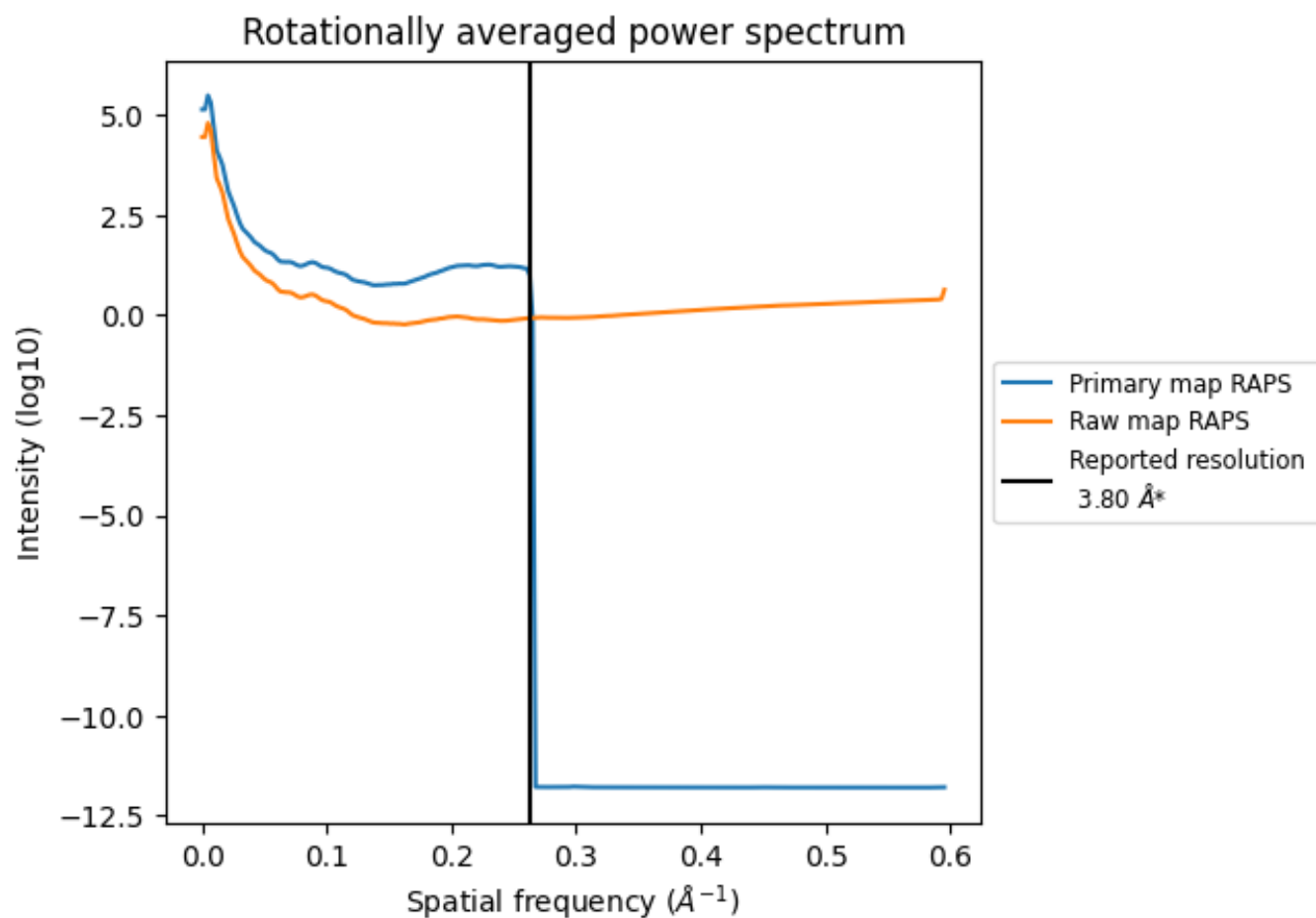
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 80 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 ⓘ

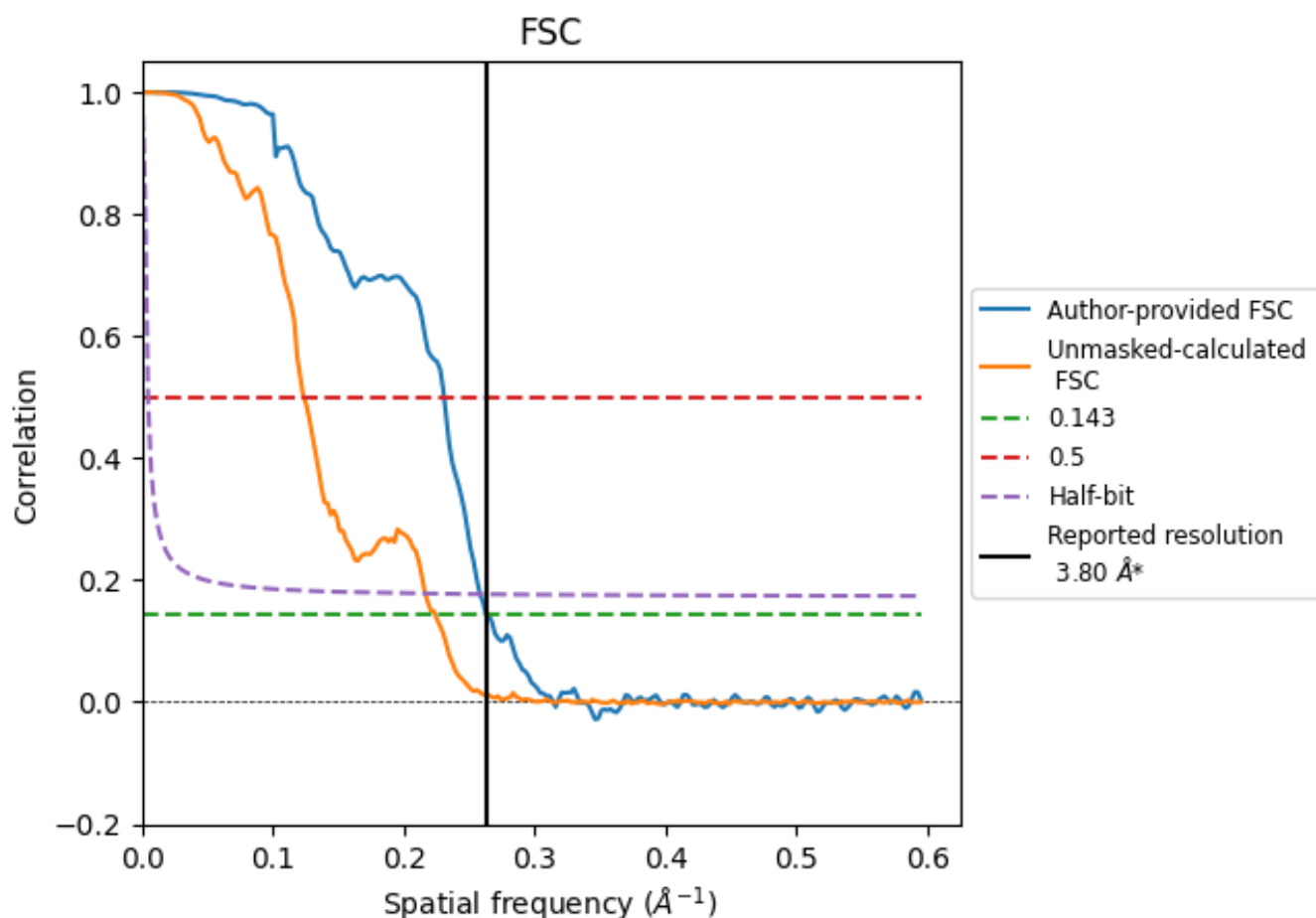


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

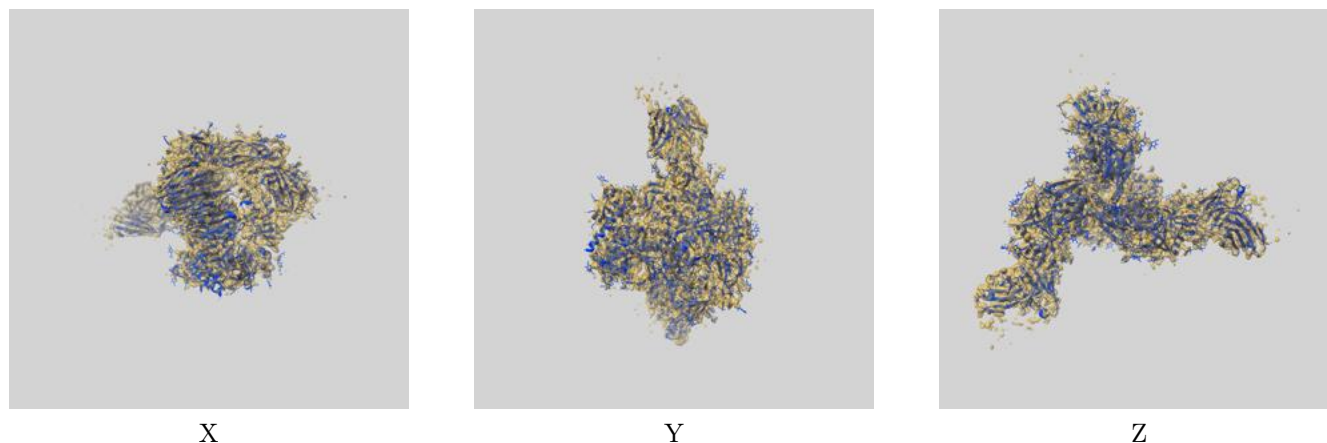
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.33	3.87
Unmasked-calculated*	4.46	8.10	4.62

*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 4.46 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

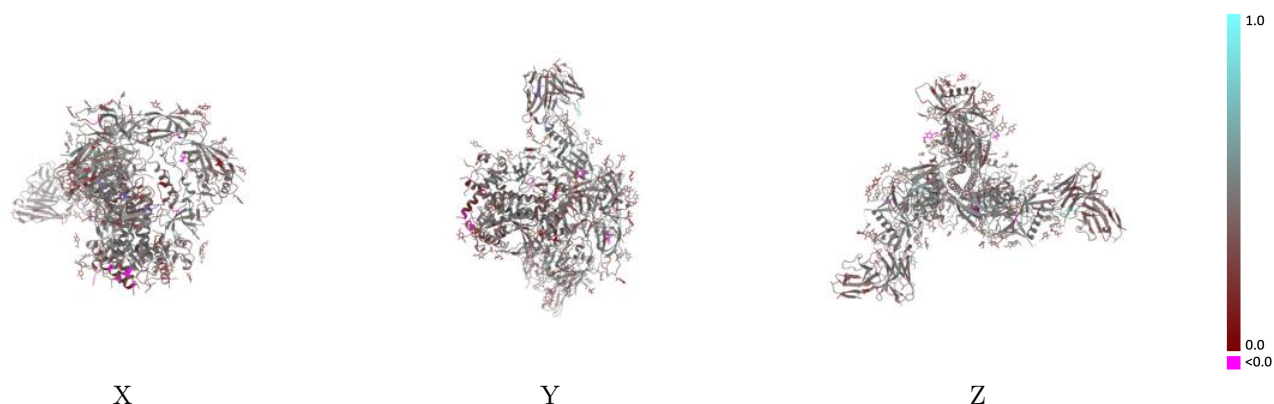
This section contains information regarding the fit between EMDB map EMD-25376 and PDB model 7SQ1. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



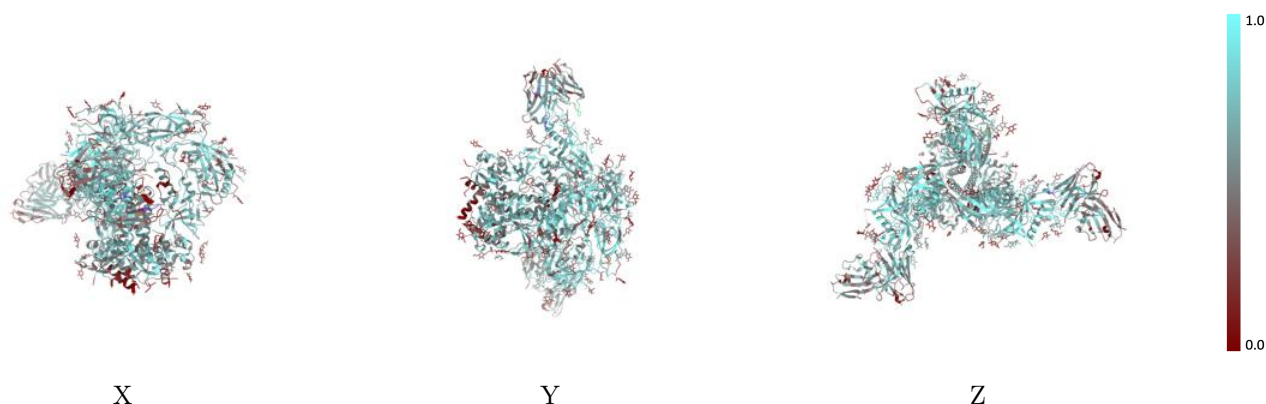
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



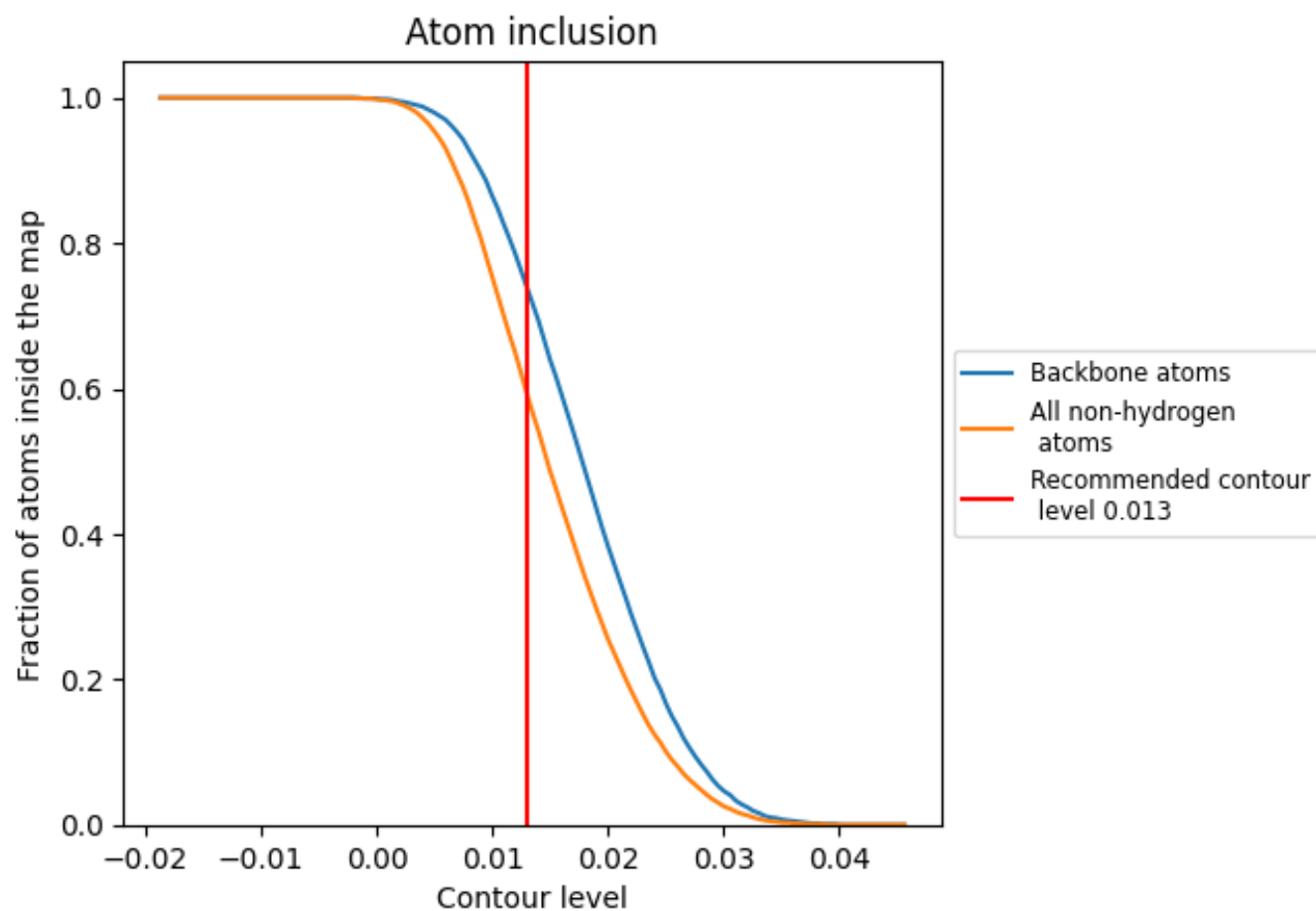
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 59% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5940	 0.4060
A	 0.5500	 0.3900
B	 0.4990	 0.3600
C	 0.6130	 0.4050
D	 0.5050	 0.3720
E	 0.6800	 0.4360
F	 0.5380	 0.3840
G	 0.6710	 0.4360
H	 0.5390	 0.3990
I	 0.4870	 0.3850
J	 0.2860	 0.2450
K	 0.2860	 0.1020
L	 0.5220	 0.3910
M	 0.2500	 0.3330
N	 0.6430	 0.4390
O	 0.1820	 0.1370
P	 0.1790	 0.3200
Q	 0.4290	 0.4020
R	 0.6430	 0.4500
S	 0.4290	 0.3780
T	 0.2860	 0.3250
U	 0.4100	 0.3720
V	 0.4800	 0.3710
W	 0.3570	 0.4130
X	 0.5000	 0.3450
Y	 0.4640	 0.2650
Z	 0.5360	 0.3590
a	 0.1790	 0.3280
b	 0.1070	 0.1340
c	 0.3210	 0.2690
d	 0.4290	 0.4330
e	 0.2860	 0.4100
f	 0.3590	 0.2830
g	 0.5130	 0.3930
h	 0.6430	 0.4000



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.4640	 0.2970
j	 0.1430	 0.2460