



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:01 PM EDT

PDB ID : 9YJ1 / pdb_00009yj1
EMDB ID : EMD-73008
Title : PC94-A.31 Fab in complex with BG505 SOSIP trimer and RM20A3 Fab
Authors : Phulera, S.; Omorodion, O.; Ward, A.B.; Ozorowski, G.
Deposited on : 2025-10-03
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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:

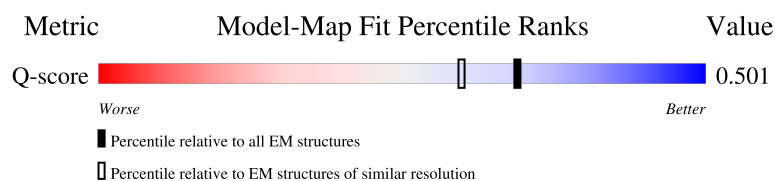
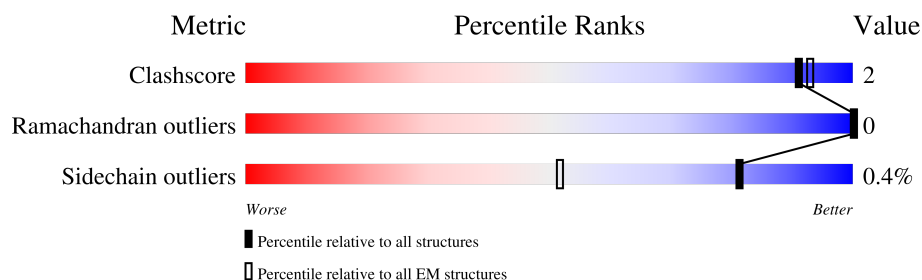
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

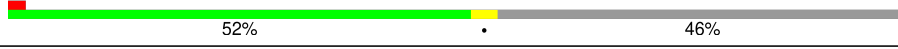
The reported resolution of this entry is 3.10 Å.

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.



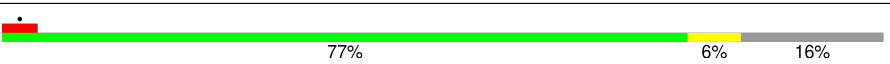
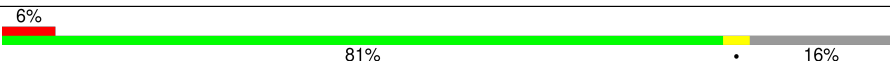
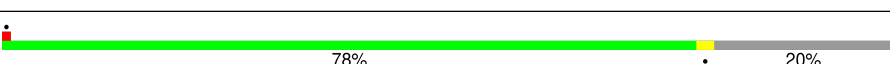
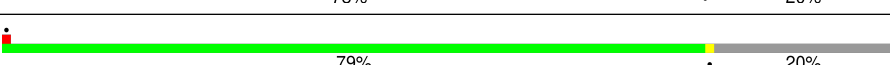
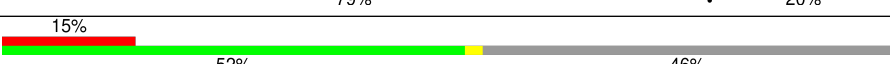
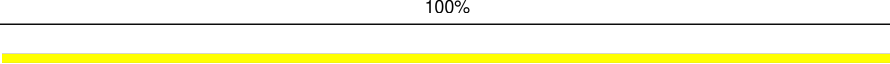
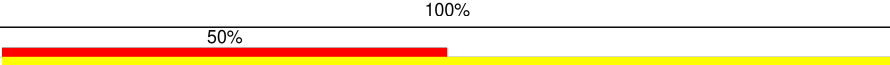
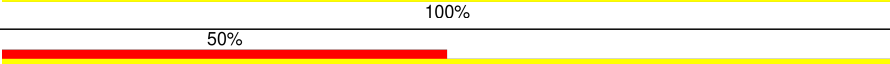
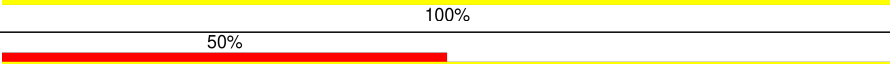
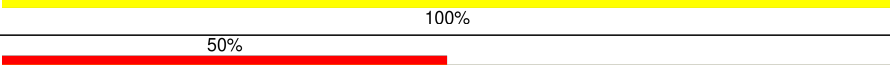
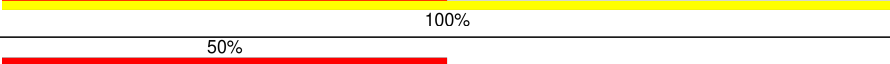
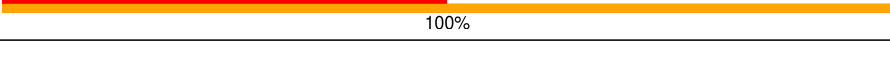
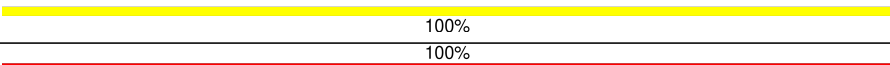
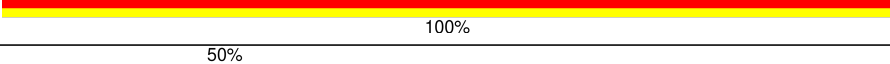
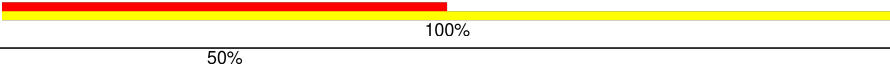
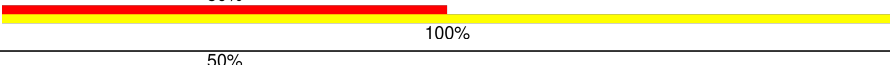
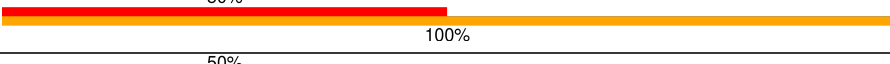
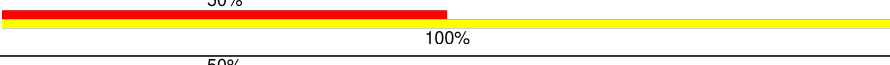
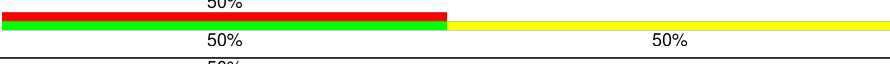
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	I	229	
1	K	229	
1	Q	229	
2	M	215	

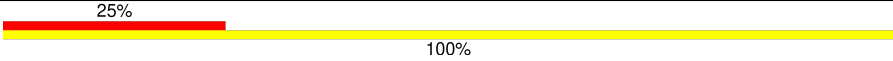
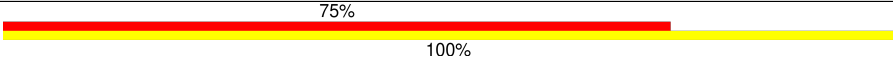
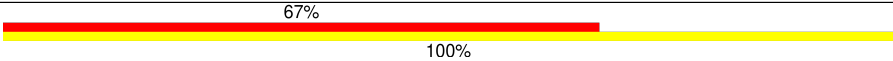
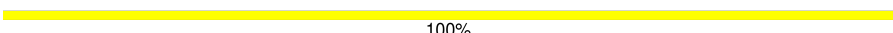
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Mol	Chain	Length	Quality of chain
2	O	215	
2	S	215	
3	A	516	
3	C	516	
3	E	516	
4	B	153	
4	D	153	
4	F	153	
5	H	234	
6	L	214	
7	G	2	
7	J	2	
7	R	2	
7	T	2	
7	U	2	
7	V	2	
7	W	2	
7	X	2	
7	a	2	
7	b	2	
7	c	2	
7	d	2	
7	e	2	
7	h	2	
7	i	2	

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Mol	Chain	Length	Quality of chain
8	N	4	
8	Y	4	
8	f	4	
9	P	4	
10	Z	3	
11	g	11	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21625 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 RM20A3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
1	Q	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
1	I	123	Total	C	N	O	S	0	0
			934	590	160	179	5		

- Molecule 2 is a protein called RM20A3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
2	S	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
2	M	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

- Molecule 3 is a protein called BG505 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3422	2153	604	637	28		
3	E	435	Total	C	N	O	S	0	0
			3435	2161	608	638	28		
3	A	435	Total	C	N	O	S	0	0
			3432	2158	606	640	28		

- Molecule 4 is a protein called BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	122	Total	C	N	O	S	0	0
			973	614	168	185	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	122	Total	C	N	O	S	0	0
			973	614	168	185	6		
4	B	122	Total	C	N	O	S	0	0
			973	614	168	185	6		

- Molecule 5 is a protein called PC94-A.31 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	127	Total	C	N	O	S	0	0
			1007	639	177	187	4		

- Molecule 6 is a protein called PC94-A.31 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			825	521	139	160	5		

- Molecule 7 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
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	J	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 8 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.



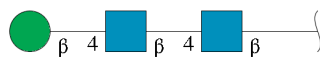
Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	4	Total	C	N	O	0	0
			50	28	2	20		
8	Y	4	Total	C	N	O	0	0
			50	28	2	20		
8	f	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



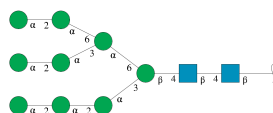
Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 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.



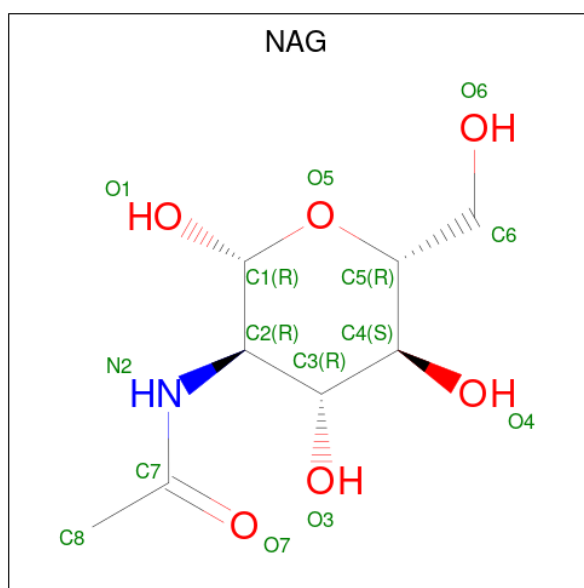
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	g	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

Chain O:

Chain S:

6% 50% 49%

VAL ALA TRP LYS ALA ASP SER SER PRO VAL LYS ALA GLY VAL GLU THR THR THR PRO PRO SER LYS GLN SER ASN ASN GLY TYR TYR ALA ALA ALA SER SER TYR LEU LEU LEU THR PRO GLU GLN TRP SER LYS SER HIS ARG SER TYR SER CYS GLN VAL THR THR HIS GLU GLY SER THR VAL GLU LYS THR

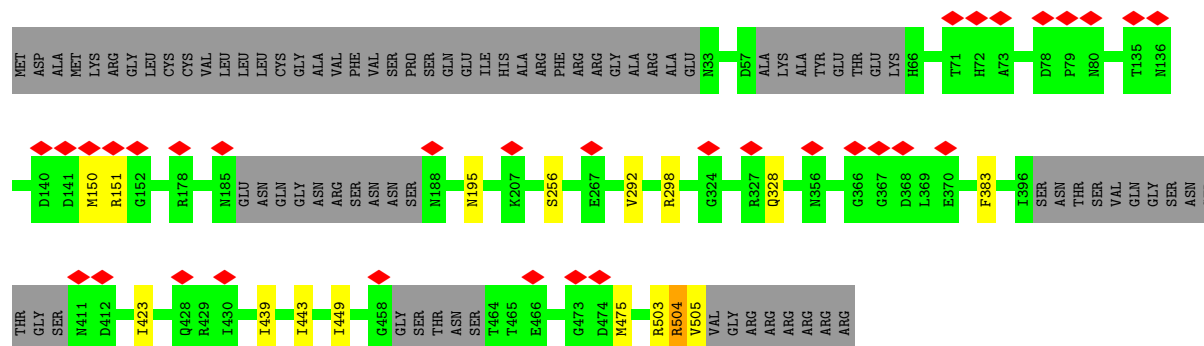
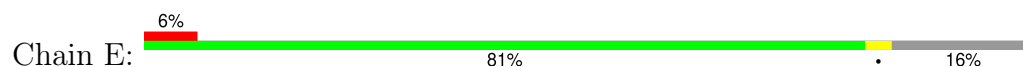
Chain M:

Chain C:

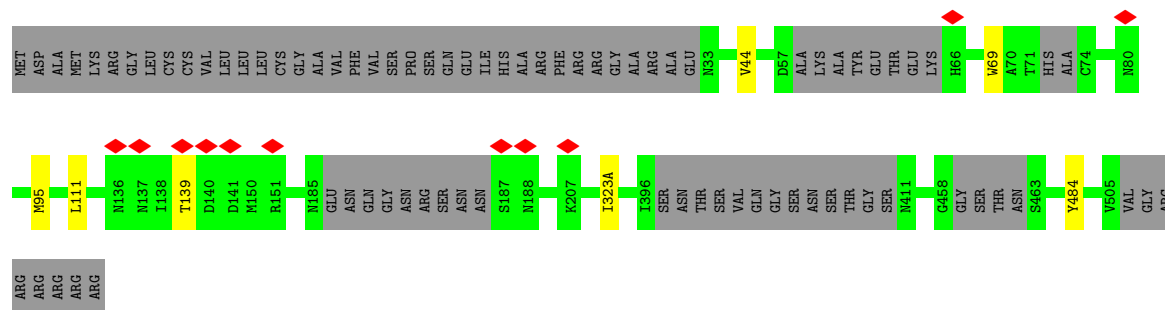
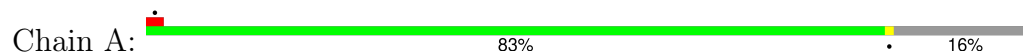
Position	Amino Acid	Conservation (%)
1	MET	100
2	ASP	100
3	ALA	100
4	MET	100
5	LYS	100
6	ARG	100
7	GLY	100
8	LEU	100
9	CYS	100
10	CYS	100
11	VAL	100
12	LEU	100
13	LEU	100
14	CYS	100
15	GLY	100
16	ALA	100
17	VAL	100
18	PHE	100
19	GLN	100
20	ASN	100
21	SER	100
22	PRO	100
23	SER	100
24	SER	100
25	GLN	100
26	GLU	100
27	ILE	100
28	HIS	100
29	ALA	100
30	ARG	100
31	PHE	100
32	ARG	100
33	ARG	100
34	GLY	100
35	ALA	100
36	ARG	100
37	ALA	100
38	GLU	100
39	ALA	100
40	GLU	100
41	ASP	100
42	ASP	100
43	ASP	100
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45	ASP	100
46	ASP	100
47	ASP	100
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99	ASP	100
100	ASP	100



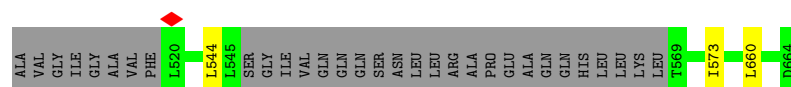
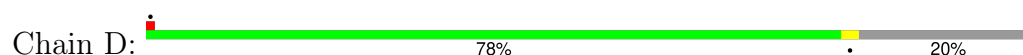
• Molecule 3: BG505 SOSIP gp120



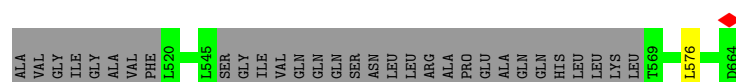
• Molecule 3: BG505 SOSIP gp120



• Molecule 4: BG505 SOSIP gp41

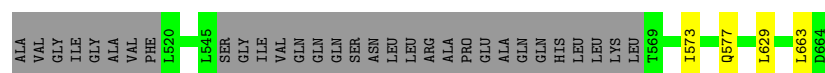


• Molecule 4: BG505 SOSIP gp41



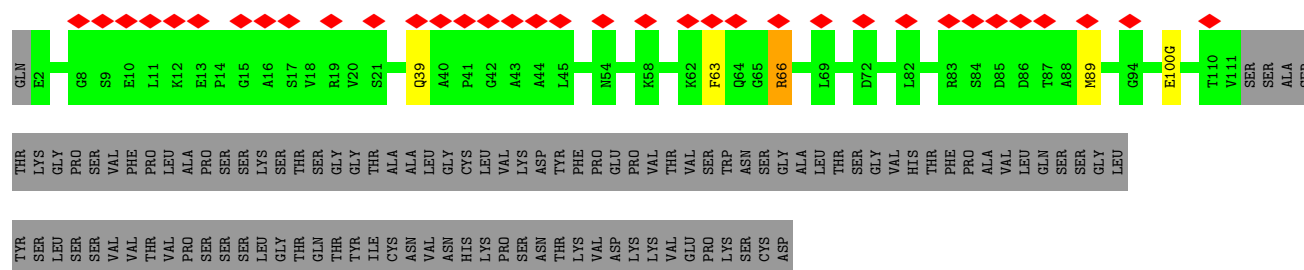
• Molecule 4: BG505 SOSIP gp41

Chain B:  77% 20%



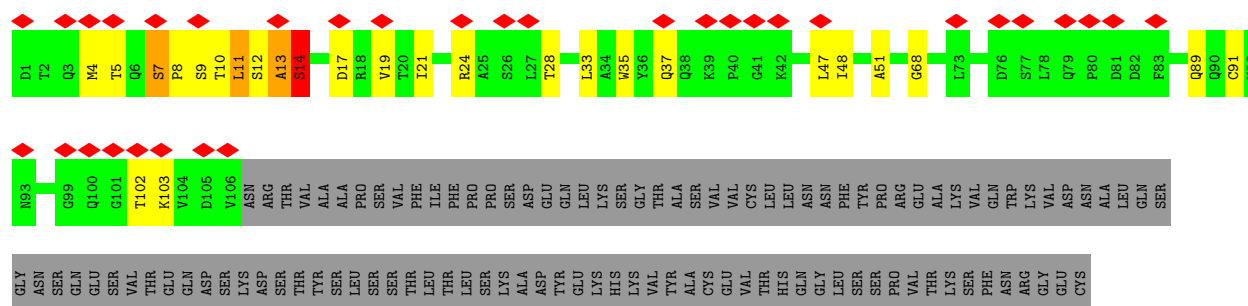
- Molecule 5: PC94-A.31 Fab heavy chain

Chain H:  15% 52% 46%

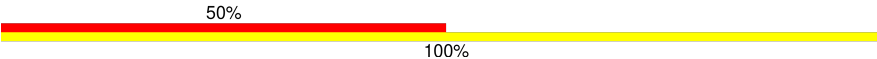


- Molecule 6: PC94-A.31 light chain

Chain L:  15% 37% 10% 50%

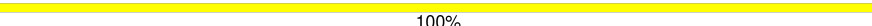


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 100%



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

Chain J:  100%



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



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



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



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



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



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



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



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



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



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



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



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



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

Chain i: 



- 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

Chain N: 



- 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

Chain Y: 



- 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

Chain f: 



- Molecule 9: 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 P: 



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 



- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain g:

100%

MAG1
MAG2
BR43
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10
MAN11

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.126	Depositor
Minimum map value	-0.561	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	413.56, 413.56, 413.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0339, 1.0339, 1.0339	Depositor

5 Model quality

5.1 Standard geometry

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

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	I	0.25	0/954	0.59	0/1288
1	K	0.25	0/963	0.60	0/1300
1	Q	0.22	0/963	0.57	0/1300
2	M	0.24	0/830	0.65	0/1129
2	O	0.25	0/830	0.66	0/1129
2	S	0.23	0/830	0.62	0/1129
3	A	0.25	0/3501	0.60	0/4750
3	C	0.25	0/3491	0.63	2/4737 (0.0%)
3	E	0.24	0/3506	0.60	0/4759
4	B	0.29	0/990	0.62	2/1343 (0.1%)
4	D	0.24	0/990	0.49	0/1343
4	F	0.24	0/990	0.51	0/1343
5	H	0.31	0/1033	0.74	0/1405
6	L	0.44	0/847	0.94	4/1153 (0.3%)
All	All	0.26	0/20718	0.63	8/28108 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	2
3	C	0	4
3	E	0	3
5	H	0	1
6	L	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	7	SER	N-CA-C	7.81	122.81	112.35
6	L	14	SER	CA-C-N	-7.27	111.13	122.69
6	L	14	SER	C-N-CA	-7.27	111.13	122.69
4	B	663	LEU	CA-C-N	6.53	133.45	121.70
4	B	663	LEU	C-N-CA	6.53	133.45	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	151	ARG	Sidechain
3	C	327	ARG	Sidechain
3	C	503	ARG	Sidechain
3	C	504	ARG	Sidechain
3	E	151	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	I	934	0	906	3	0
1	K	943	0	915	4	0
1	Q	943	0	915	3	0
2	M	811	0	767	3	0
2	O	811	0	767	2	0
2	S	811	0	767	1	0
3	A	3432	0	3374	5	0
3	C	3422	0	3366	17	0
3	E	3435	0	3377	6	0
4	B	973	0	949	3	0
4	D	973	0	949	3	0
4	F	973	0	949	1	0
5	H	1007	0	973	3	0
6	L	825	0	786	16	0
7	G	28	0	25	0	0
7	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	1	0
7	X	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	1	0
7	e	28	0	25	0	0
7	h	28	0	25	0	0
7	i	28	0	25	0	0
8	N	50	0	43	0	0
8	Y	50	0	43	0	0
8	f	50	0	43	0	0
9	P	50	0	43	0	0
10	Z	39	0	34	0	0
11	g	127	0	106	0	0
12	A	154	0	143	1	0
12	B	42	0	39	0	0
12	C	140	0	130	0	0
12	D	28	0	26	0	0
12	E	140	0	130	0	0
12	F	42	0	39	0	0
All	All	21625	0	20954	66	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 2.

The worst 5 of 66 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:L:10:THR:HA	6:L:103:LYS:O	1.91	0.71
3:C:204:ALA:HB2	3:C:434:MET:HE2	1.82	0.60
6:L:33:LEU:HB3	6:L:51:ALA:HB2	1.84	0.59
6:L:89:GLN:HE22	6:L:91:CYS:HB3	1.66	0.59
1:K:87:THR:HG23	1:K:110:THR:HA	1.87	0.56

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	I	121/229 (53%)	118 (98%)	3 (2%)	0	100	100
1	K	122/229 (53%)	117 (96%)	5 (4%)	0	100	100
1	Q	122/229 (53%)	119 (98%)	3 (2%)	0	100	100
2	M	107/215 (50%)	100 (94%)	7 (6%)	0	100	100
2	O	107/215 (50%)	102 (95%)	5 (5%)	0	100	100
2	S	107/215 (50%)	102 (95%)	5 (5%)	0	100	100
3	A	423/516 (82%)	410 (97%)	13 (3%)	0	100	100
3	C	421/516 (82%)	405 (96%)	16 (4%)	0	100	100
3	E	425/516 (82%)	407 (96%)	18 (4%)	0	100	100
4	B	118/153 (77%)	116 (98%)	2 (2%)	0	100	100
4	D	118/153 (77%)	116 (98%)	2 (2%)	0	100	100
4	F	118/153 (77%)	115 (98%)	3 (2%)	0	100	100
5	H	125/234 (53%)	114 (91%)	11 (9%)	0	100	100
6	L	104/214 (49%)	93 (89%)	11 (11%)	0	100	100
All	All	2538/3787 (67%)	2434 (96%)	104 (4%)	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	I	100/192 (52%)	100 (100%)	0	100	100
1	K	101/192 (53%)	101 (100%)	0	100	100
1	Q	101/192 (53%)	101 (100%)	0	100	100
2	M	89/180 (49%)	89 (100%)	0	100	100
2	O	89/180 (49%)	89 (100%)	0	100	100
2	S	89/180 (49%)	89 (100%)	0	100	100
3	A	391/456 (86%)	391 (100%)	0	100	100
3	C	390/456 (86%)	386 (99%)	4 (1%)	68	79
3	E	390/456 (86%)	388 (100%)	2 (0%)	81	85
4	B	105/129 (81%)	105 (100%)	0	100	100
4	D	105/129 (81%)	105 (100%)	0	100	100
4	F	105/129 (81%)	105 (100%)	0	100	100
5	H	107/200 (54%)	107 (100%)	0	100	100
6	L	91/188 (48%)	87 (96%)	4 (4%)	25	56
All	All	2253/3259 (69%)	2243 (100%)	10 (0%)	81	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	L	7	SER
6	L	11	LEU
6	L	14	SER
3	C	504	ARG
3	E	504	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	85	HIS
3	E	432	GLN
6	L	89	GLN
3	E	425	ASN
2	M	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	1	7,3	14,14,15	0.66	0	17,19,21	1.87	4 (23%)
7	NAG	G	2	7	14,14,15	0.76	1 (7%)	17,19,21	1.27	1 (5%)
7	NAG	J	1	7,3	14,14,15	0.67	0	17,19,21	1.26	2 (11%)
7	NAG	J	2	7	14,14,15	0.68	0	17,19,21	0.86	1 (5%)
8	NAG	N	1	3,8	14,14,15	0.71	0	17,19,21	1.53	2 (11%)
8	NAG	N	2	8	14,14,15	0.72	0	17,19,21	1.16	0
8	BMA	N	3	8	11,11,12	0.79	0	15,15,17	1.19	1 (6%)
8	MAN	N	4	8	11,11,12	0.67	0	15,15,17	1.33	1 (6%)
9	NAG	P	1	3,9	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
9	NAG	P	2	9	14,14,15	0.70	0	17,19,21	1.11	2 (11%)
9	BMA	P	3	9	11,11,12	0.84	0	15,15,17	1.22	1 (6%)
9	MAN	P	4	9	11,11,12	0.67	0	15,15,17	1.41	1 (6%)
7	NAG	R	1	7,3	14,14,15	0.65	0	17,19,21	0.92	1 (5%)
7	NAG	R	2	7	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
7	NAG	T	1	7,3	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
7	NAG	T	2	7	14,14,15	0.86	1 (7%)	17,19,21	1.92	2 (11%)
7	NAG	U	1	7,3	14,14,15	0.68	0	17,19,21	1.53	2 (11%)
7	NAG	U	2	7	14,14,15	0.70	0	17,19,21	1.86	3 (17%)
7	NAG	V	1	4,7	14,14,15	0.83	1 (7%)	17,19,21	1.09	1 (5%)
7	NAG	V	2	7	14,14,15	0.69	0	17,19,21	0.95	1 (5%)
7	NAG	W	1	7,3	14,14,15	0.69	0	17,19,21	1.16	2 (11%)
7	NAG	W	2	7	14,14,15	0.70	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	X	1	7,3	14,14,15	0.66	0	17,19,21	1.16	1 (5%)
7	NAG	X	2	7	14,14,15	0.70	0	17,19,21	1.09	1 (5%)
8	NAG	Y	1	3,8	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
8	NAG	Y	2	8	14,14,15	0.74	0	17,19,21	0.94	2 (11%)
8	BMA	Y	3	8	11,11,12	0.81	0	15,15,17	1.27	1 (6%)
8	MAN	Y	4	8	11,11,12	0.70	0	15,15,17	1.25	1 (6%)
10	NAG	Z	1	3,10	14,14,15	0.70	0	17,19,21	1.04	1 (5%)
10	NAG	Z	2	10	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
10	BMA	Z	3	10	11,11,12	0.83	0	15,15,17	1.29	1 (6%)
7	NAG	a	1	7,3	14,14,15	0.66	0	17,19,21	1.10	2 (11%)
7	NAG	a	2	7	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
7	NAG	b	1	7,3	14,14,15	0.68	0	17,19,21	1.49	1 (5%)
7	NAG	b	2	7	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
7	NAG	c	1	7,3	14,14,15	0.69	0	17,19,21	1.11	1 (5%)
7	NAG	c	2	7	14,14,15	0.70	0	17,19,21	1.32	2 (11%)
7	NAG	d	1	7,3	14,14,15	0.69	0	17,19,21	1.59	4 (23%)
7	NAG	d	2	7	14,14,15	0.82	1 (7%)	17,19,21	3.12	5 (29%)
7	NAG	e	1	7,3	14,14,15	0.68	0	17,19,21	0.82	2 (11%)
7	NAG	e	2	7	14,14,15	0.69	0	17,19,21	1.09	1 (5%)
8	NAG	f	1	3,8	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
8	NAG	f	2	8	14,14,15	0.70	0	17,19,21	0.84	0
8	BMA	f	3	8	11,11,12	0.80	0	15,15,17	1.56	3 (20%)
8	MAN	f	4	8	11,11,12	0.73	0	15,15,17	1.24	1 (6%)
11	NAG	g	1	3,11	14,14,15	0.73	0	17,19,21	1.04	2 (11%)
11	MAN	g	10	11	11,11,12	0.72	0	15,15,17	1.19	1 (6%)
11	MAN	g	11	11	11,11,12	0.81	0	15,15,17	1.05	1 (6%)
11	NAG	g	2	11	14,14,15	0.70	0	17,19,21	1.33	2 (11%)
11	BMA	g	3	11	11,11,12	0.84	0	15,15,17	1.20	1 (6%)
11	MAN	g	4	11	11,11,12	0.68	0	15,15,17	1.50	1 (6%)
11	MAN	g	5	11	11,11,12	0.68	0	15,15,17	1.39	1 (6%)
11	MAN	g	6	11	11,11,12	0.81	0	15,15,17	1.15	1 (6%)
11	MAN	g	7	11	11,11,12	0.66	0	15,15,17	1.73	1 (6%)
11	MAN	g	8	11	11,11,12	0.67	0	15,15,17	1.40	1 (6%)
11	MAN	g	9	11	11,11,12	0.71	0	15,15,17	1.36	1 (6%)
7	NAG	h	1	7,3	14,14,15	0.70	0	17,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	h	2	7	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
7	NAG	i	1	7,3	14,14,15	0.77	0	17,19,21	0.99	1 (5%)
7	NAG	i	2	7	14,14,15	0.80	1 (7%)	17,19,21	1.38	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	NAG	J	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
8	NAG	N	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	BMA	N	3	8	-	1/2/19/22	0/1/1/1
8	MAN	N	4	8	-	2/2/19/22	0/1/1/1
9	NAG	P	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	P	2	9	-	0/6/23/26	0/1/1/1
9	BMA	P	3	9	-	0/2/19/22	0/1/1/1
9	MAN	P	4	9	-	2/2/19/22	0/1/1/1
7	NAG	R	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
7	NAG	T	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	1/6/23/26	0/1/1/1
7	NAG	U	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	3/6/23/26	0/1/1/1
7	NAG	V	1	4,7	-	1/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	NAG	W	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
8	NAG	Y	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	2/2/19/22	0/1/1/1
10	NAG	Z	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
7	NAG	a	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	1/6/23/26	0/1/1/1
7	NAG	b	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	NAG	c	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	3/6/23/26	0/1/1/1
7	NAG	d	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	1/6/23/26	0/1/1/1
7	NAG	e	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	e	2	7	-	1/6/23/26	0/1/1/1
8	NAG	f	1	3,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	BMA	f	3	8	-	1/2/19/22	0/1/1/1
8	MAN	f	4	8	-	2/2/19/22	0/1/1/1
11	NAG	g	1	3,11	-	0/6/23/26	0/1/1/1
11	MAN	g	10	11	-	2/2/19/22	0/1/1/1
11	MAN	g	11	11	-	0/2/19/22	0/1/1/1
11	NAG	g	2	11	-	2/6/23/26	0/1/1/1
11	BMA	g	3	11	-	0/2/19/22	0/1/1/1
11	MAN	g	4	11	-	2/2/19/22	0/1/1/1
11	MAN	g	5	11	-	2/2/19/22	0/1/1/1
11	MAN	g	6	11	-	1/2/19/22	0/1/1/1
11	MAN	g	7	11	-	0/2/19/22	0/1/1/1
11	MAN	g	8	11	-	2/2/19/22	0/1/1/1
11	MAN	g	9	11	-	2/2/19/22	0/1/1/1
7	NAG	h	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	1/6/23/26	0/1/1/1
7	NAG	i	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	2	NAG	C1-C2	2.43	1.55	1.52
7	V	1	NAG	C1-C2	2.33	1.55	1.52
7	T	2	NAG	C1-C2	2.23	1.55	1.52
7	G	2	NAG	C1-C2	2.13	1.55	1.52
7	i	2	NAG	C1-C2	2.13	1.55	1.52

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	2	NAG	C2-N2-C7	10.48	136.94	122.90
7	T	2	NAG	C2-N2-C7	6.05	131.00	122.90
11	g	7	MAN	C1-O5-C5	5.87	120.06	112.19
7	U	2	NAG	C2-N2-C7	5.79	130.66	122.90
11	g	4	MAN	C1-O5-C5	4.97	118.85	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

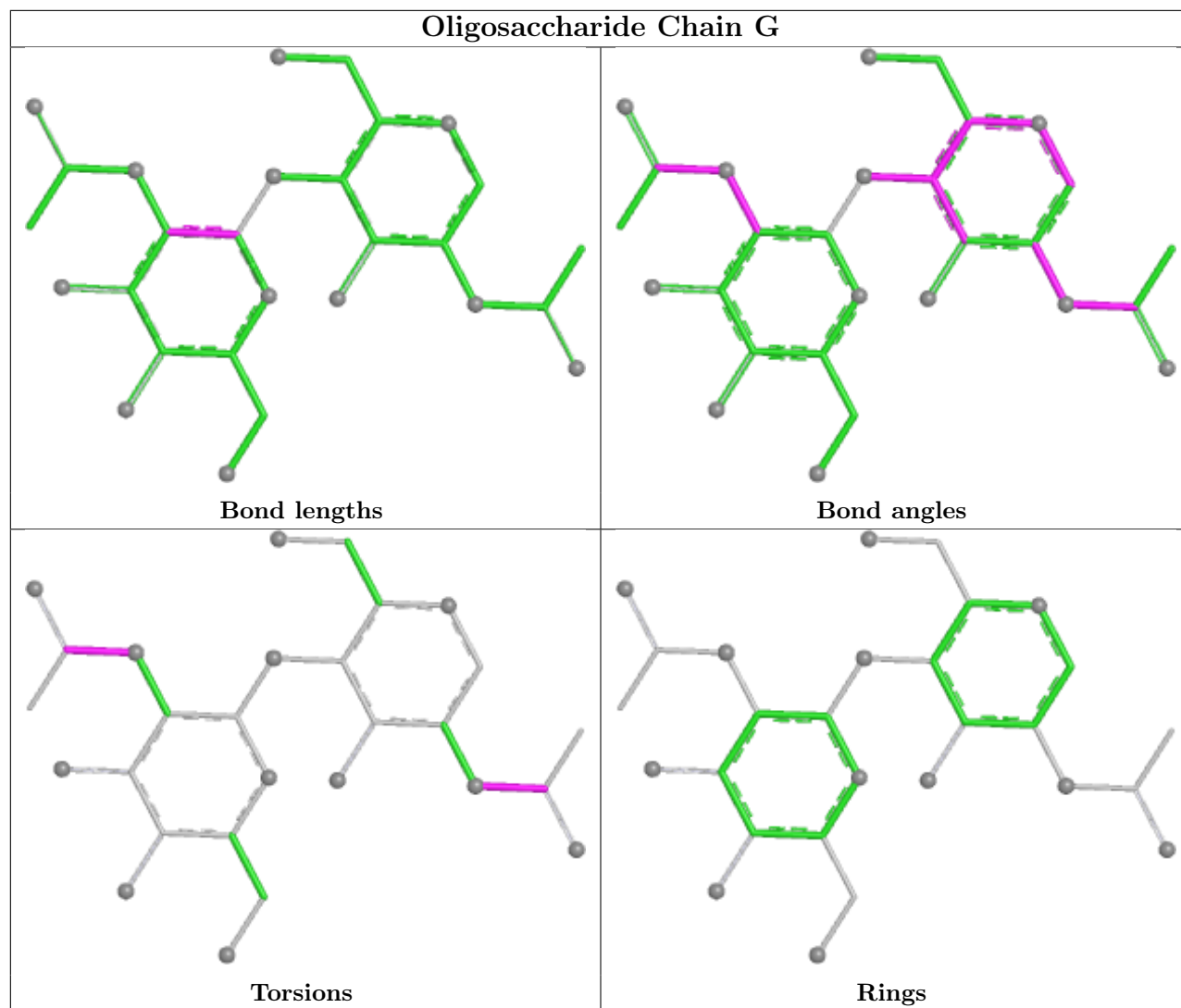
Mol	Chain	Res	Type	Atoms
7	d	2	NAG	C1-C2-N2-C7
8	N	4	MAN	O5-C5-C6-O6
11	g	5	MAN	O5-C5-C6-O6
8	Y	4	MAN	O5-C5-C6-O6
11	g	9	MAN	O5-C5-C6-O6

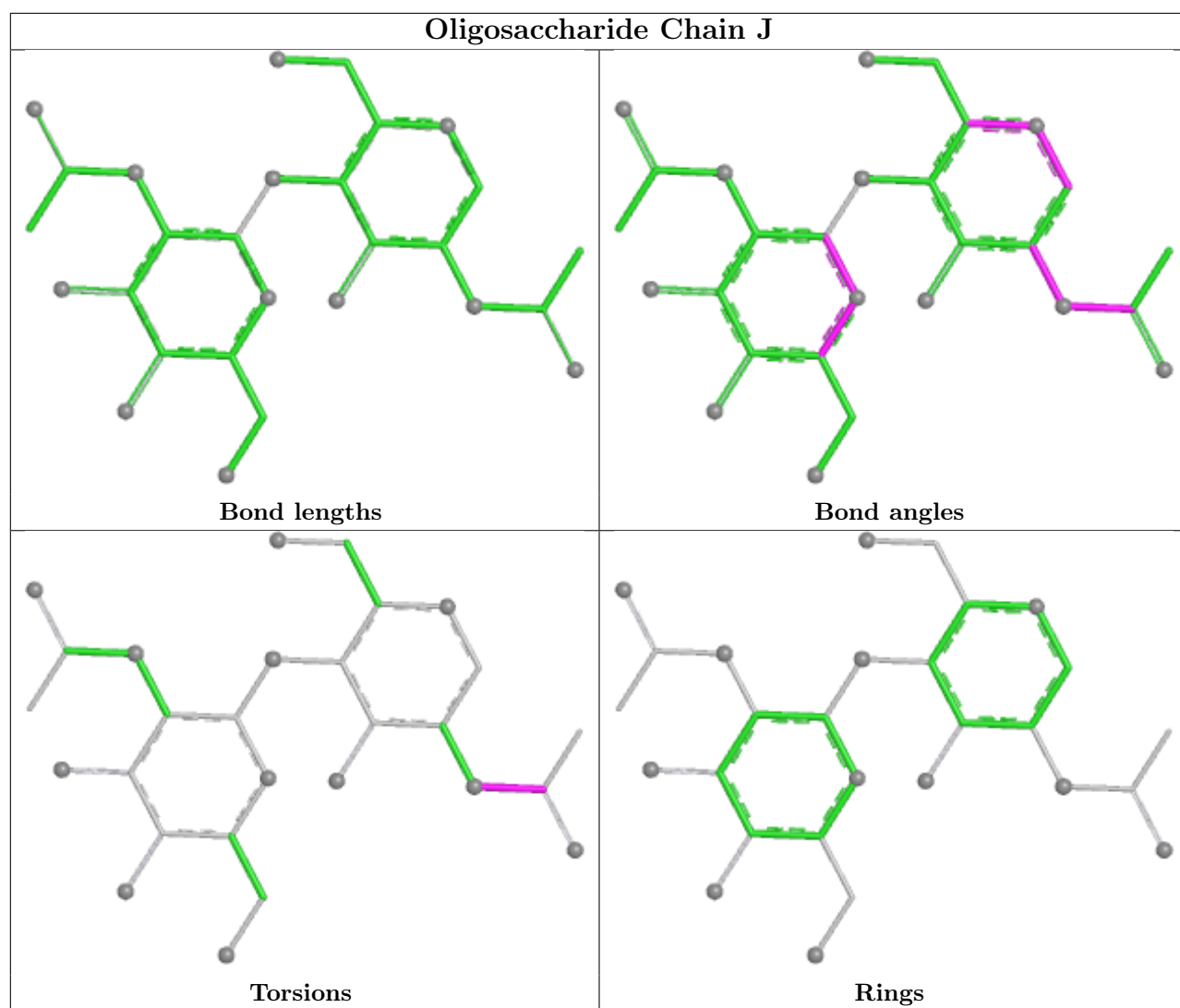
There are no ring outliers.

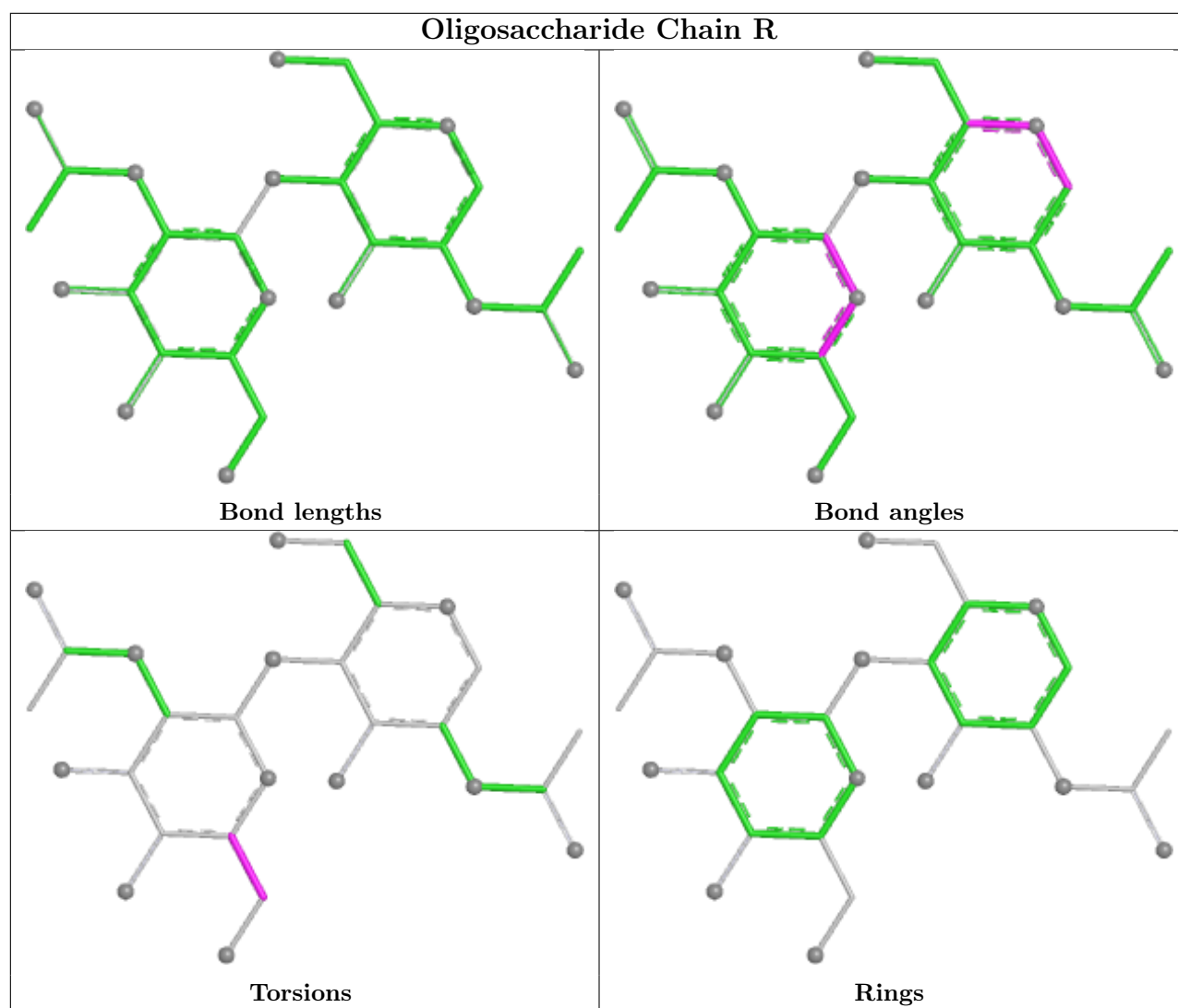
4 monomers are involved in 2 short contacts:

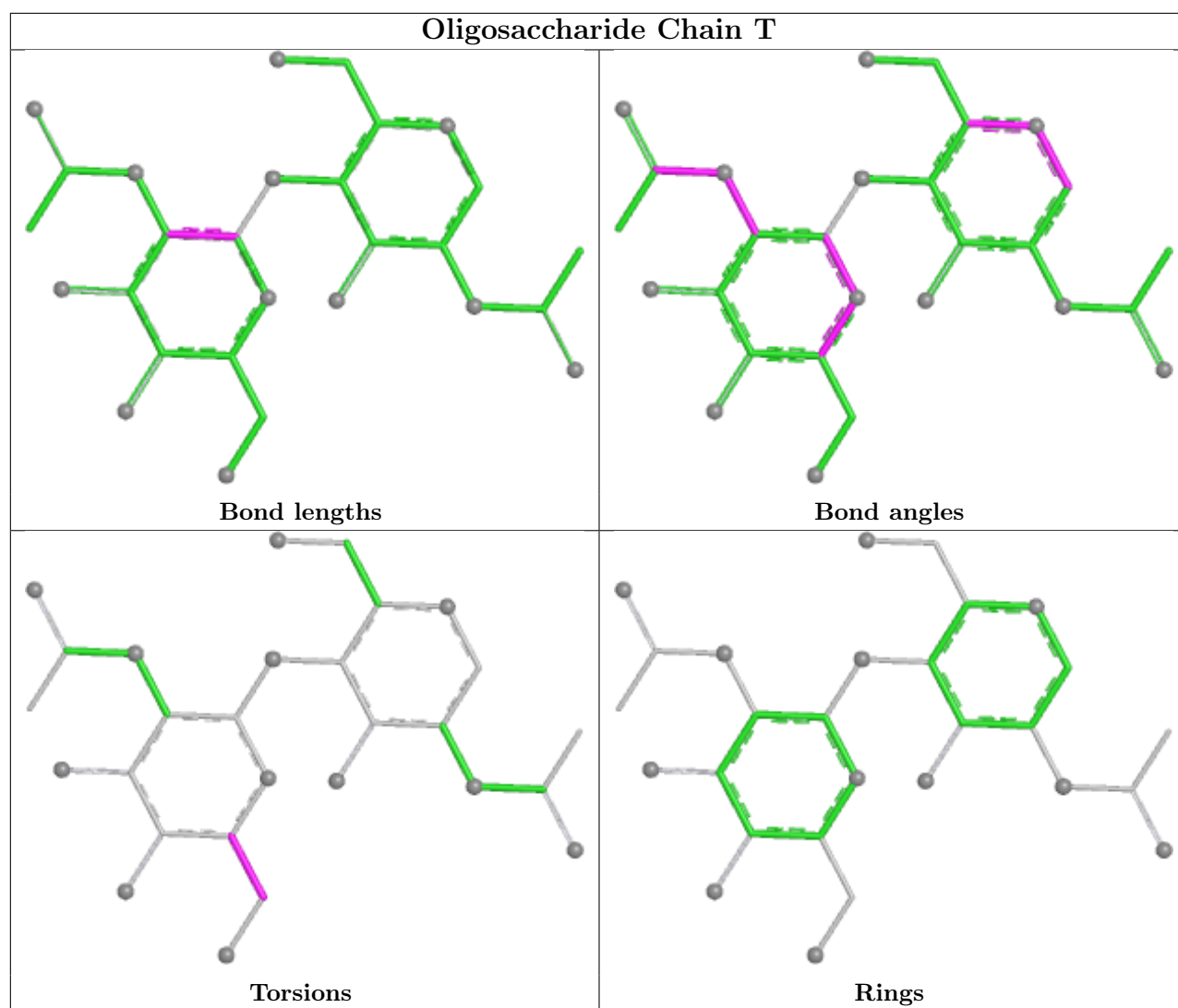
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	W	2	NAG	1	0
7	d	2	NAG	1	0
7	d	1	NAG	1	0
7	W	1	NAG	1	0

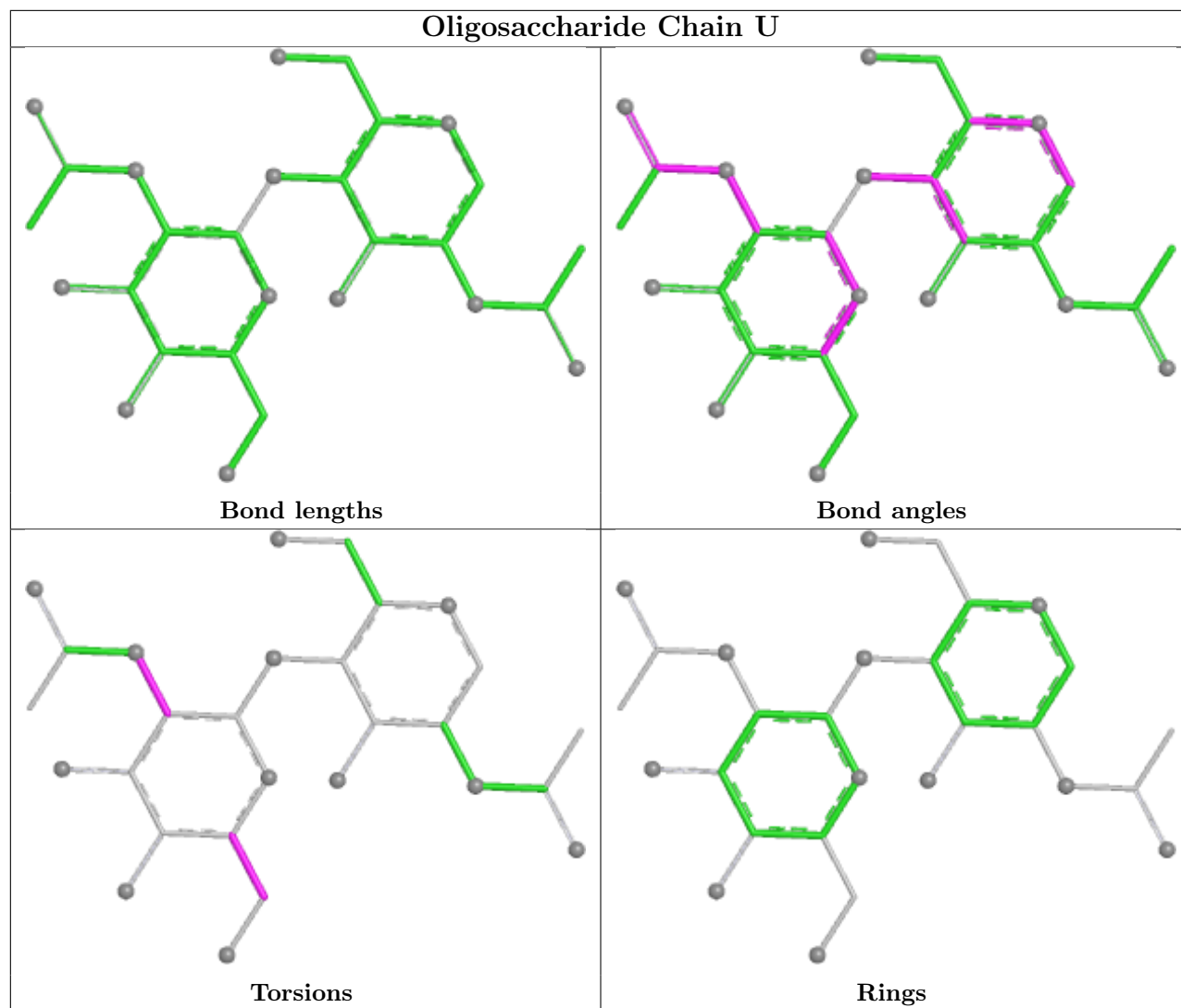
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

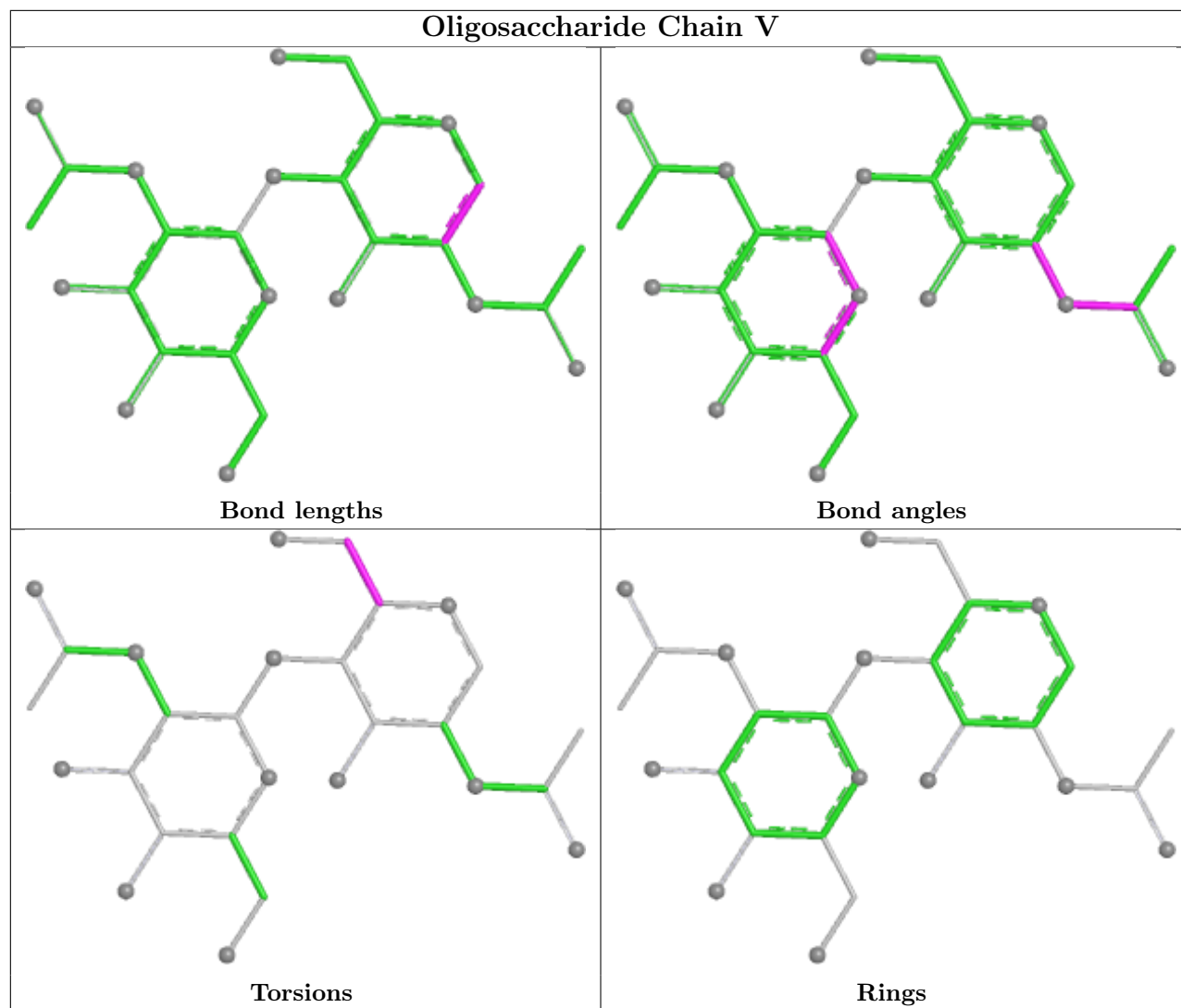


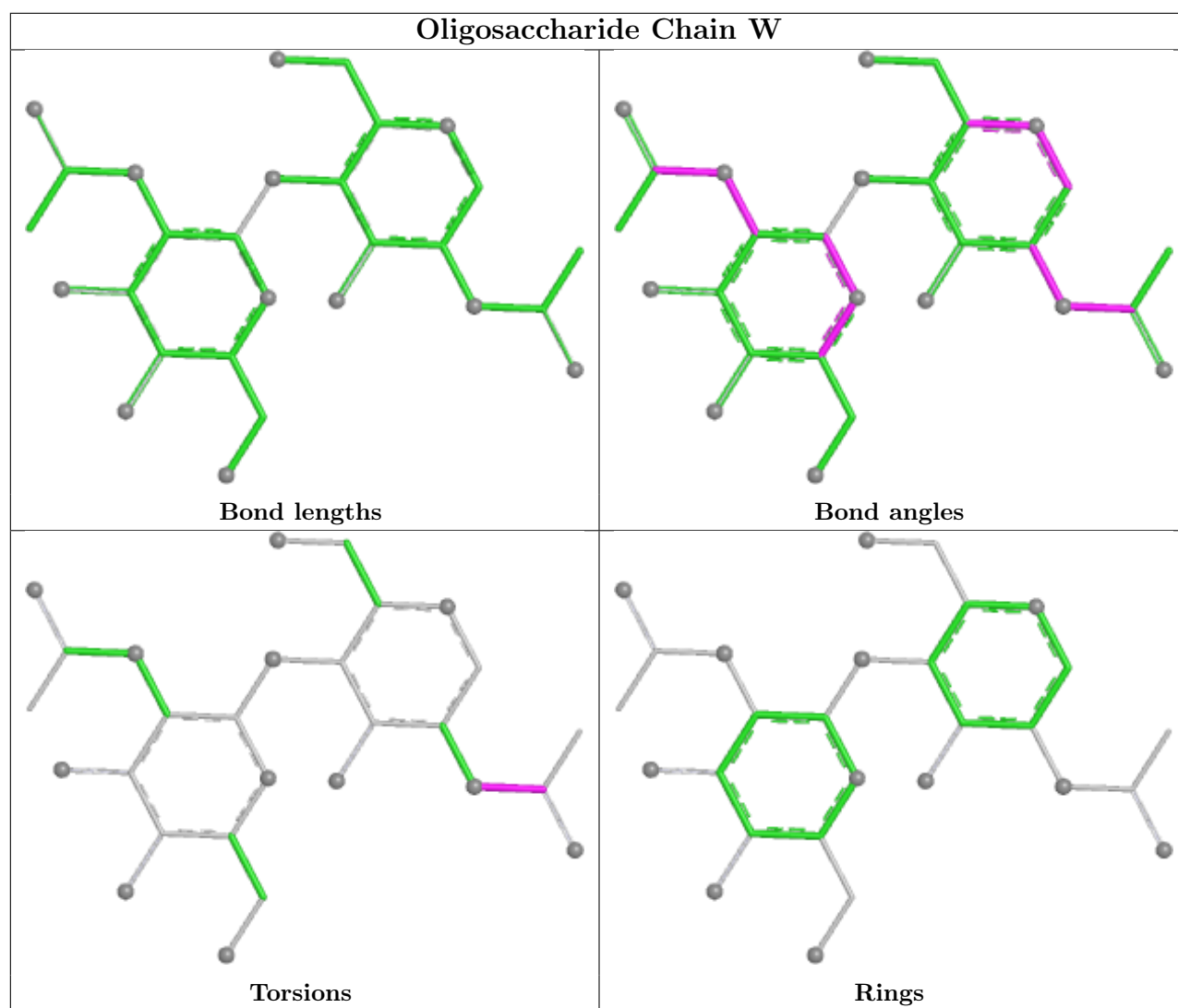


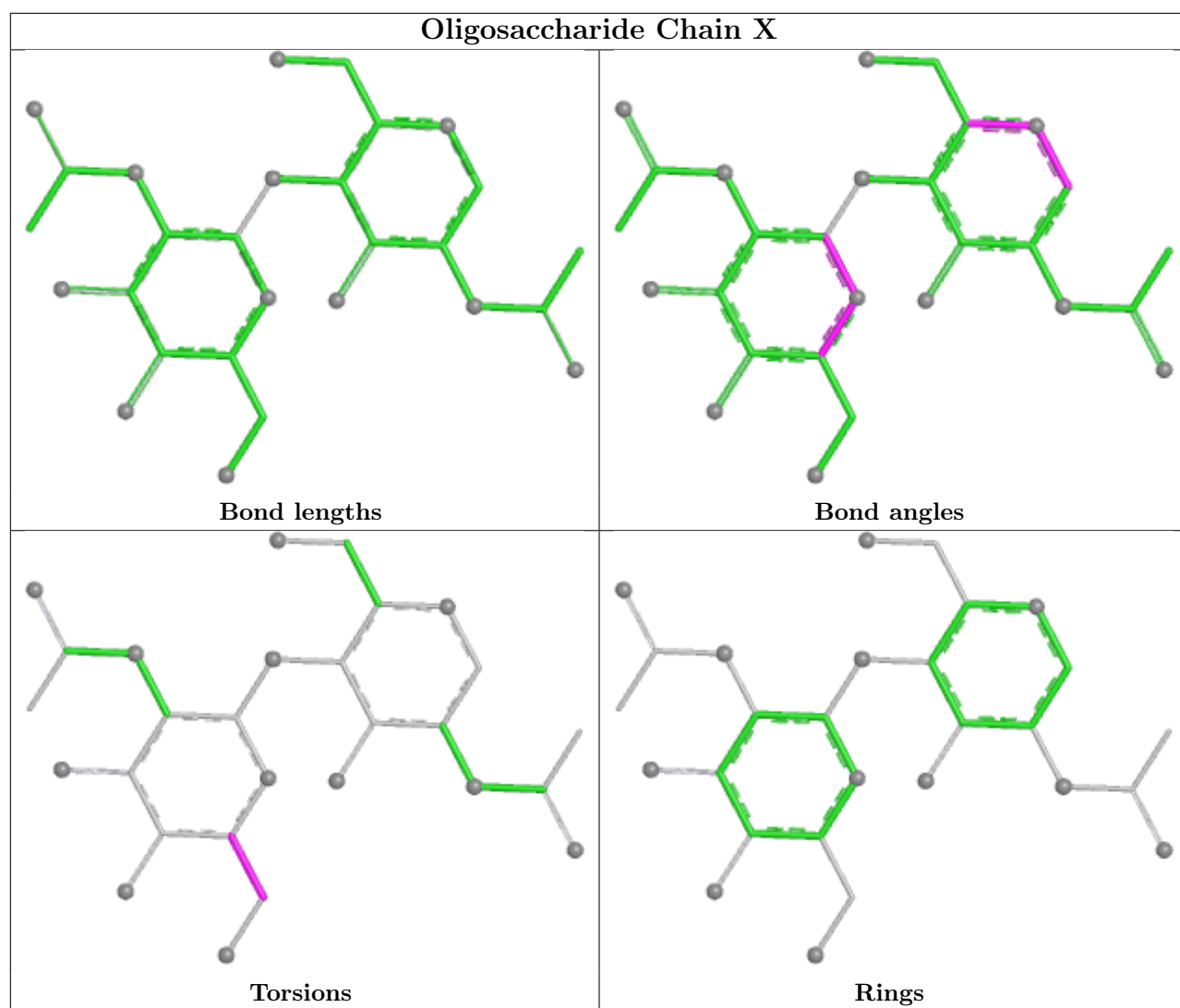


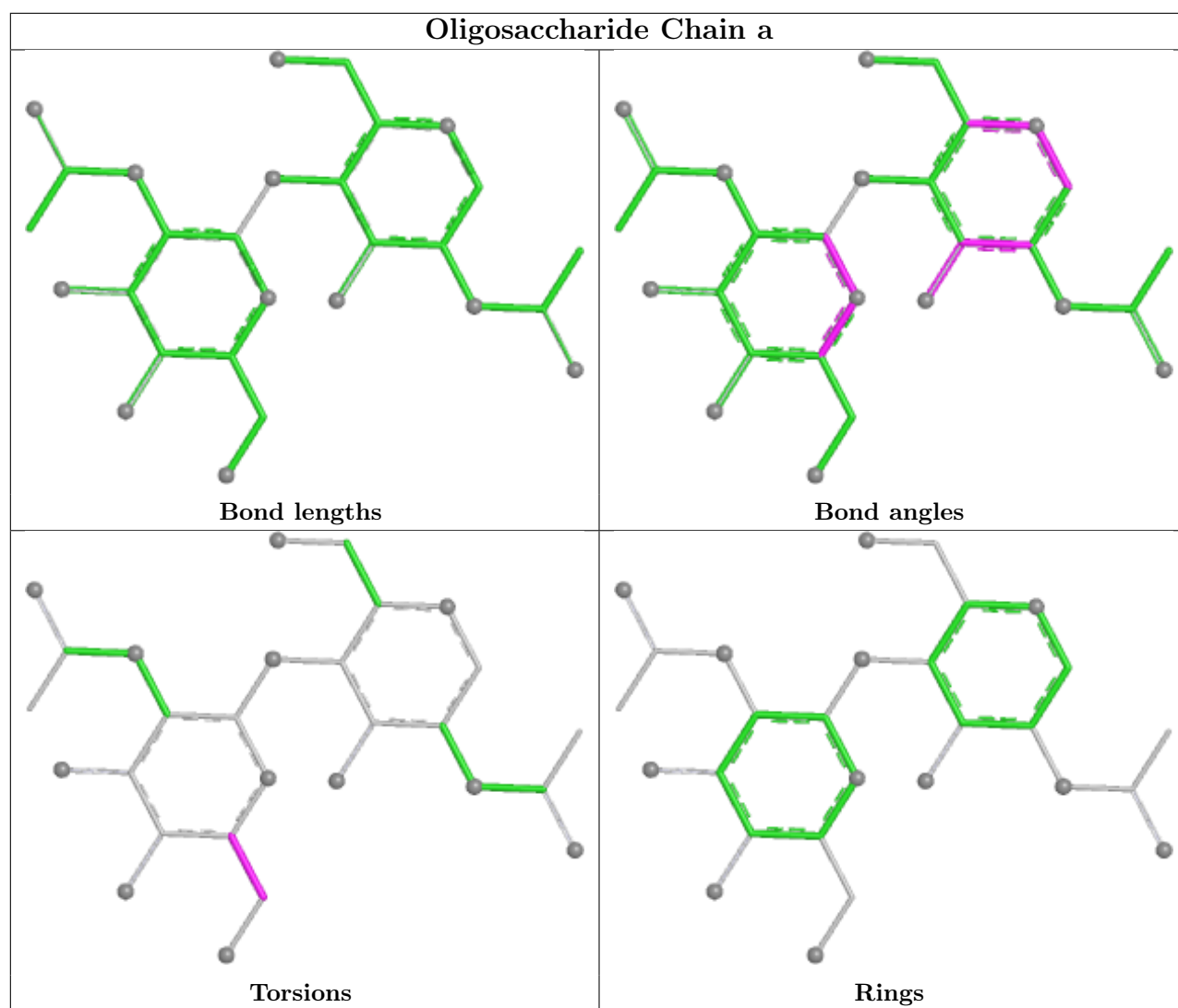


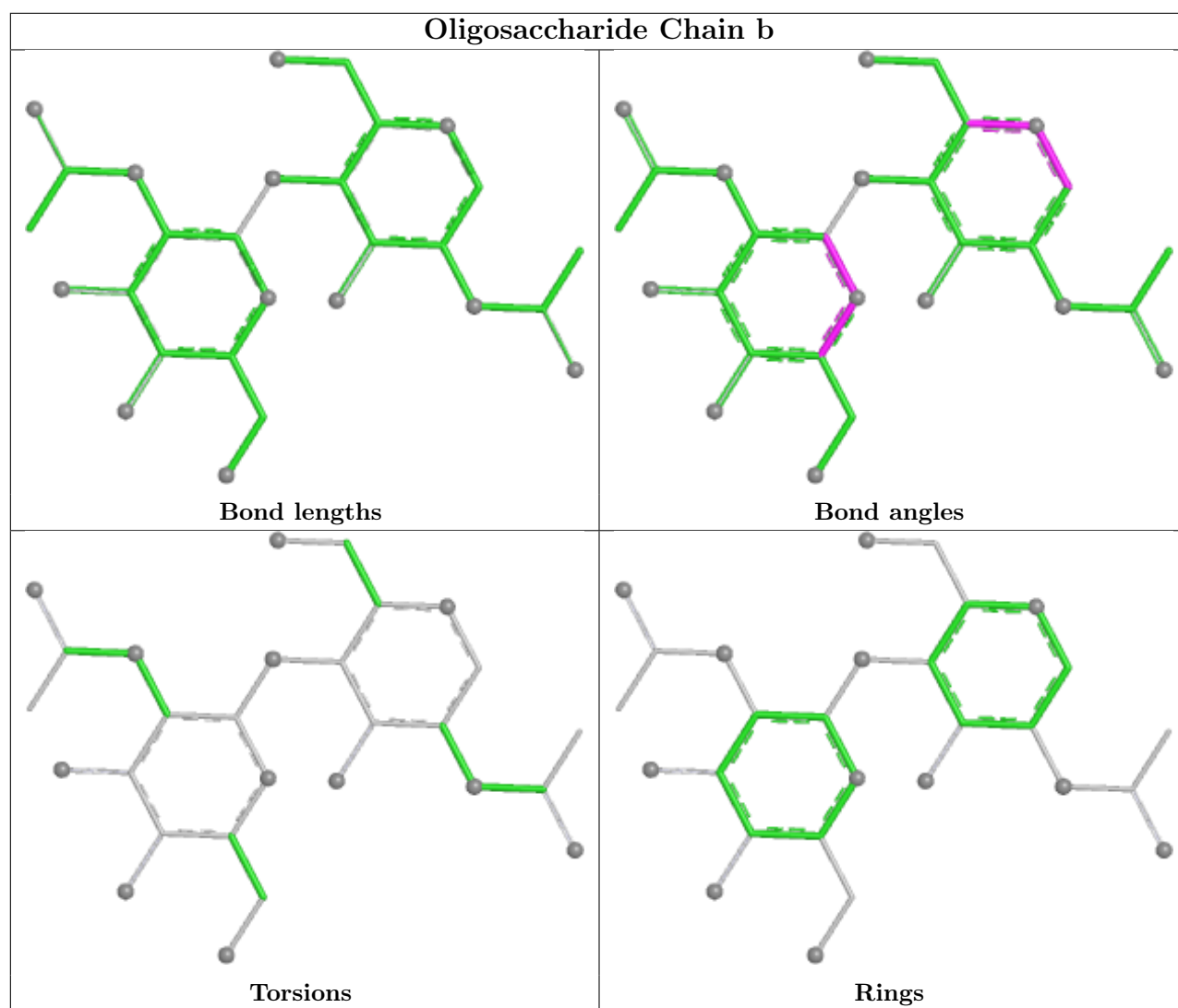


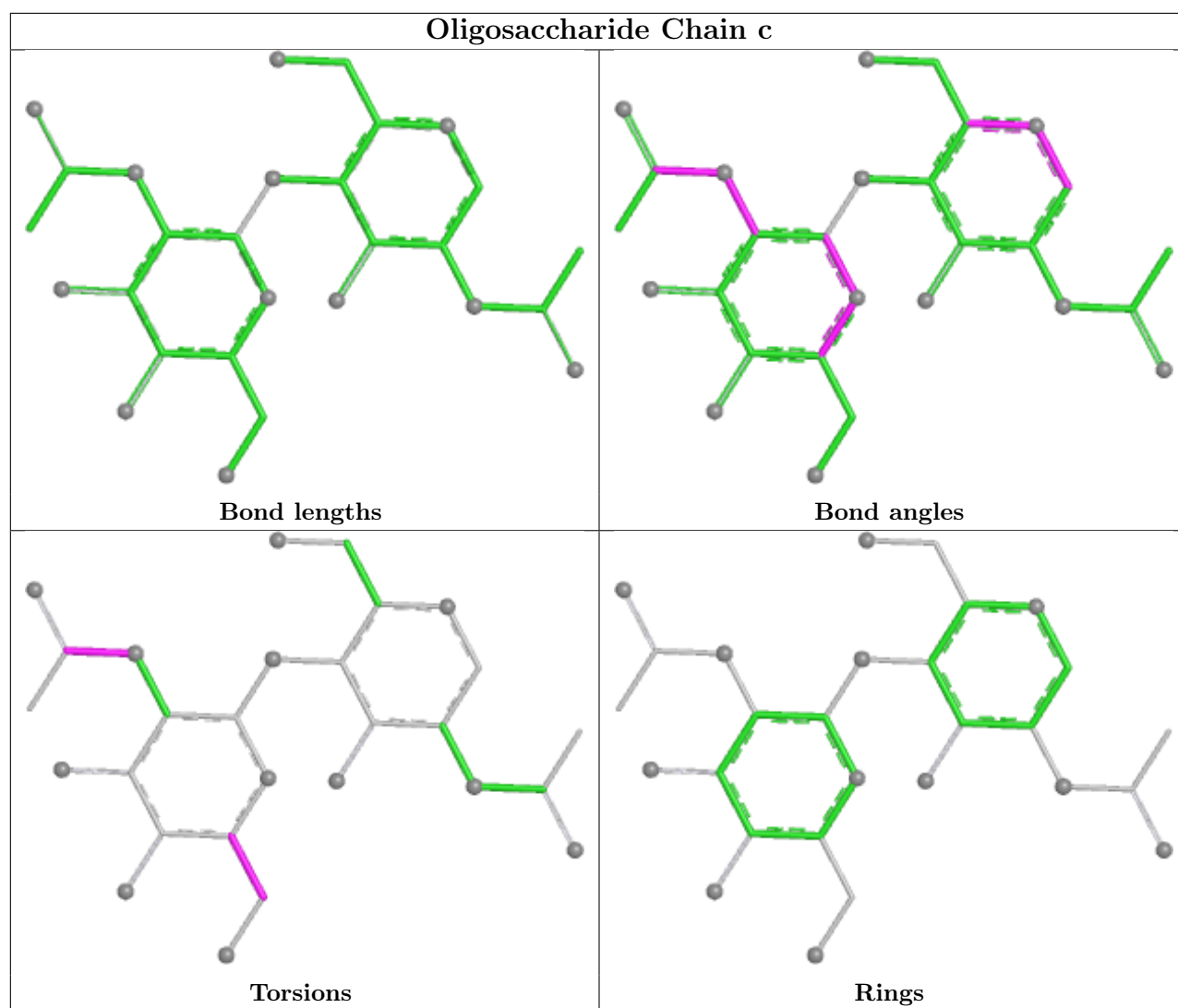


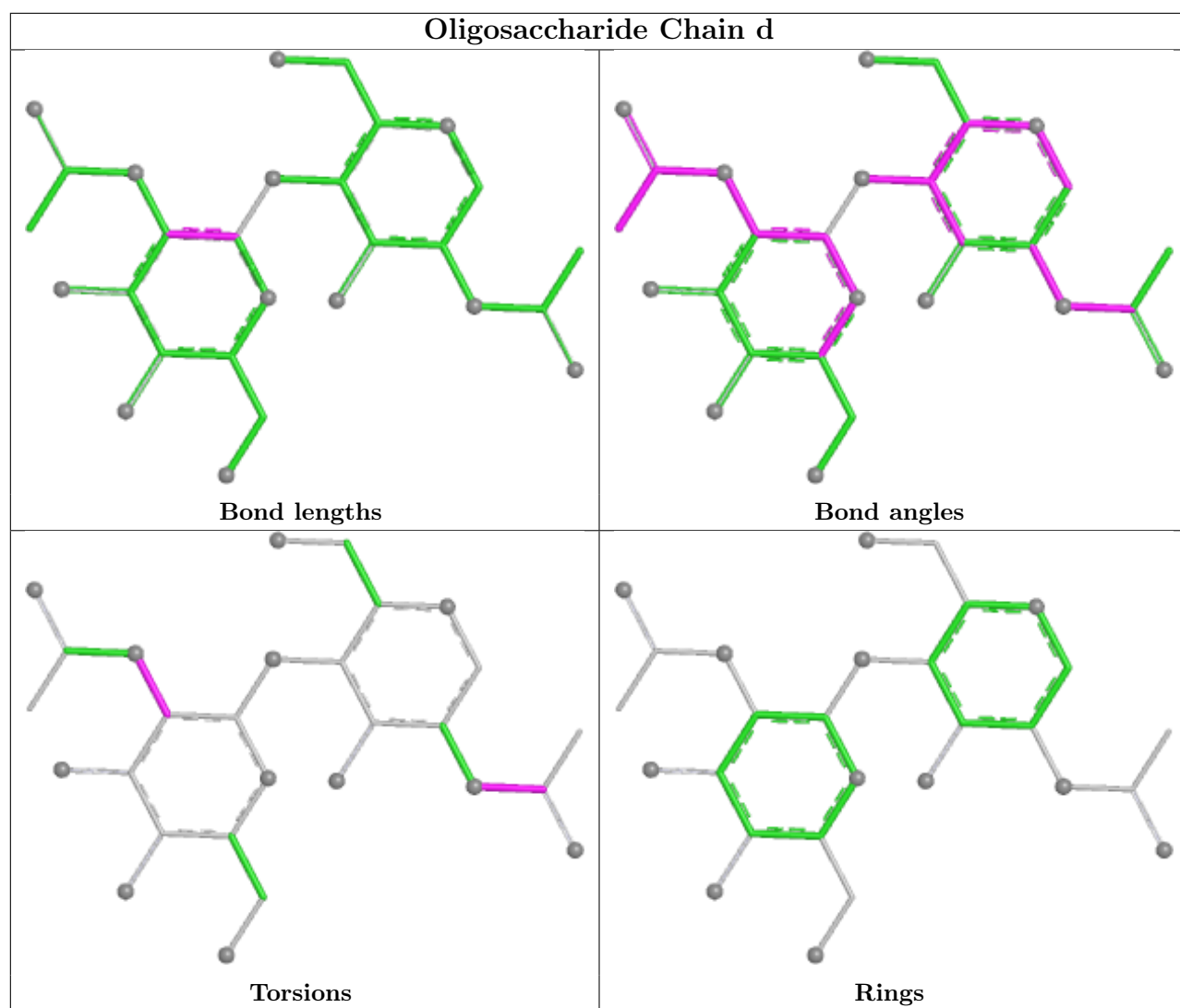


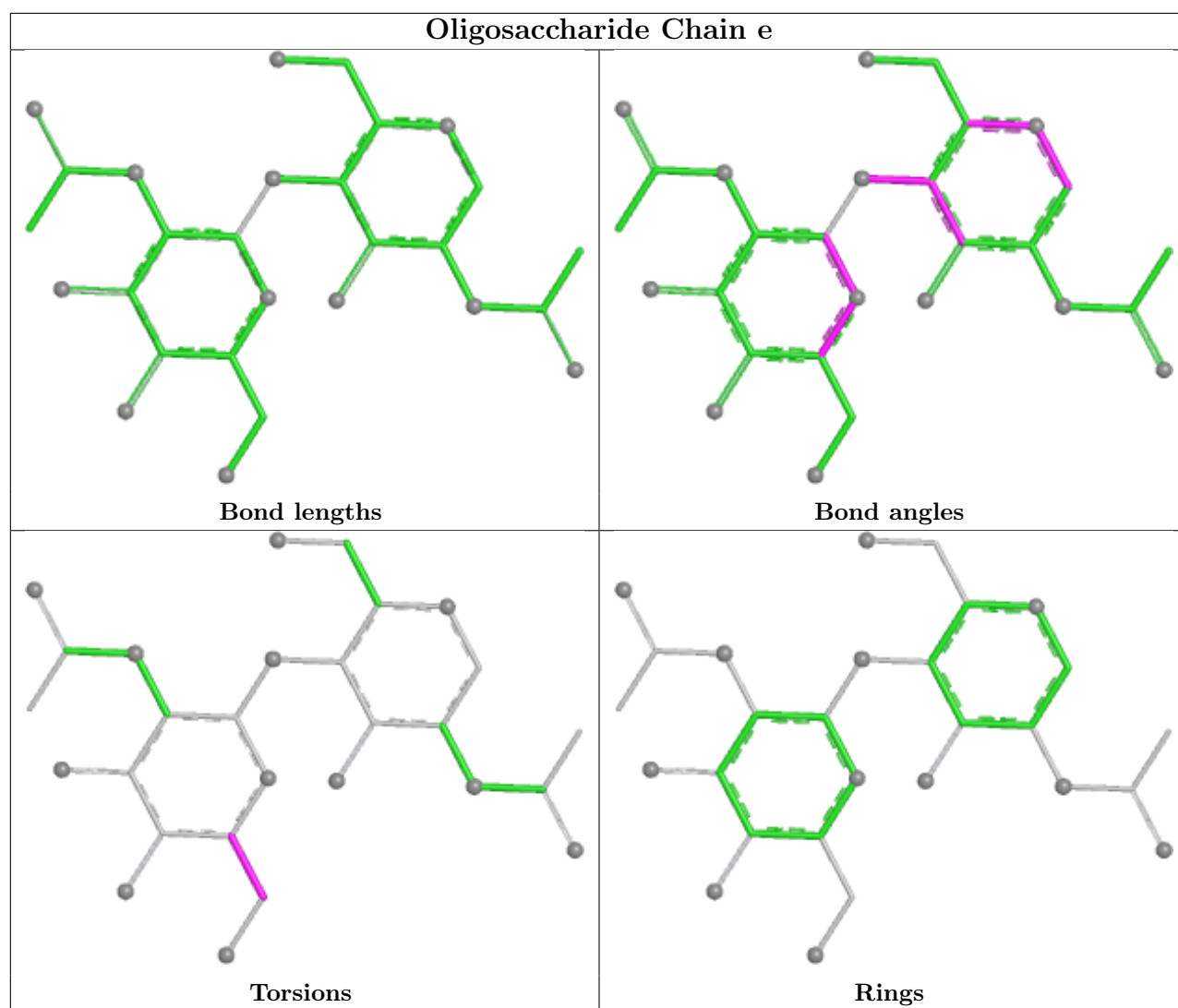


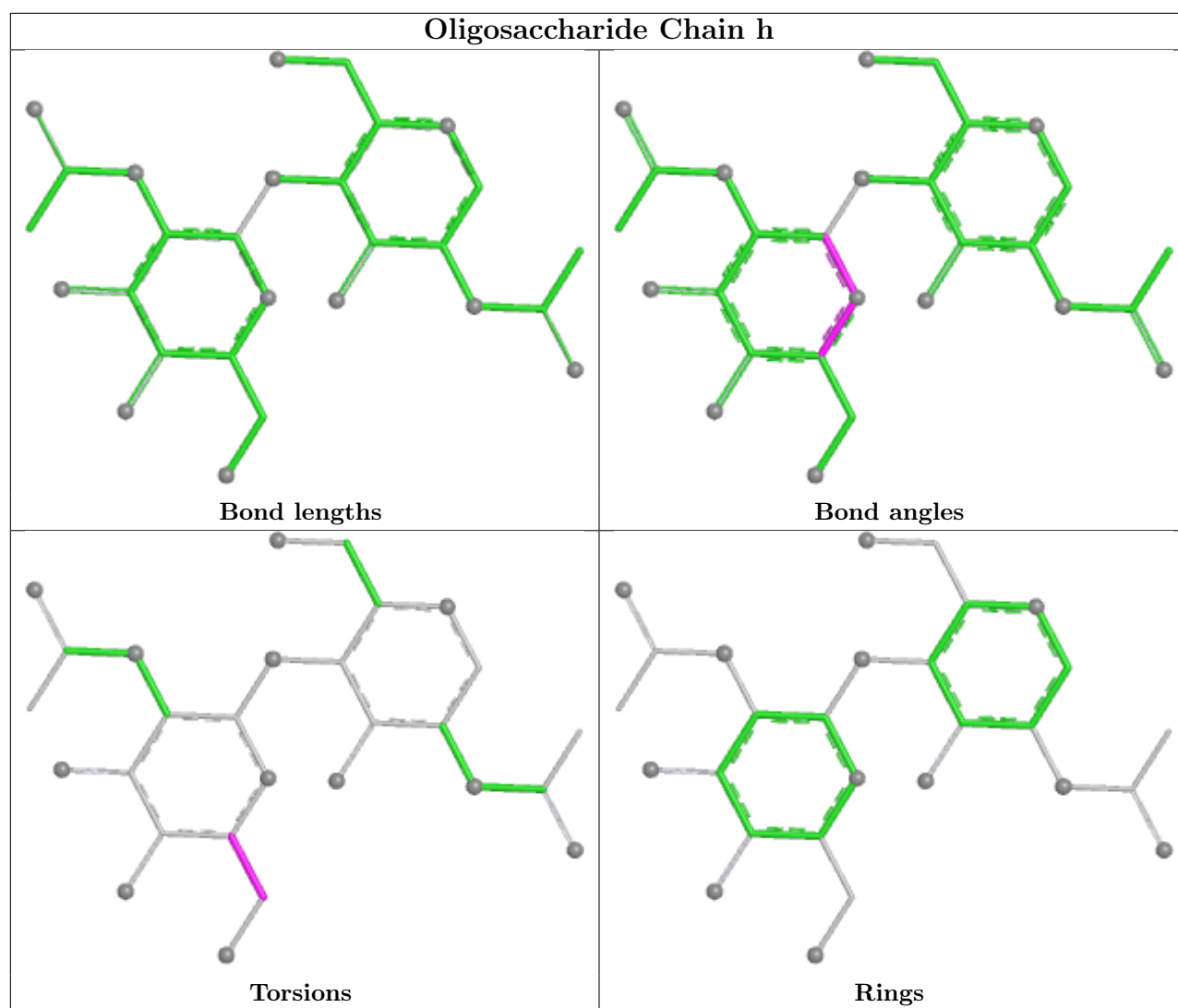


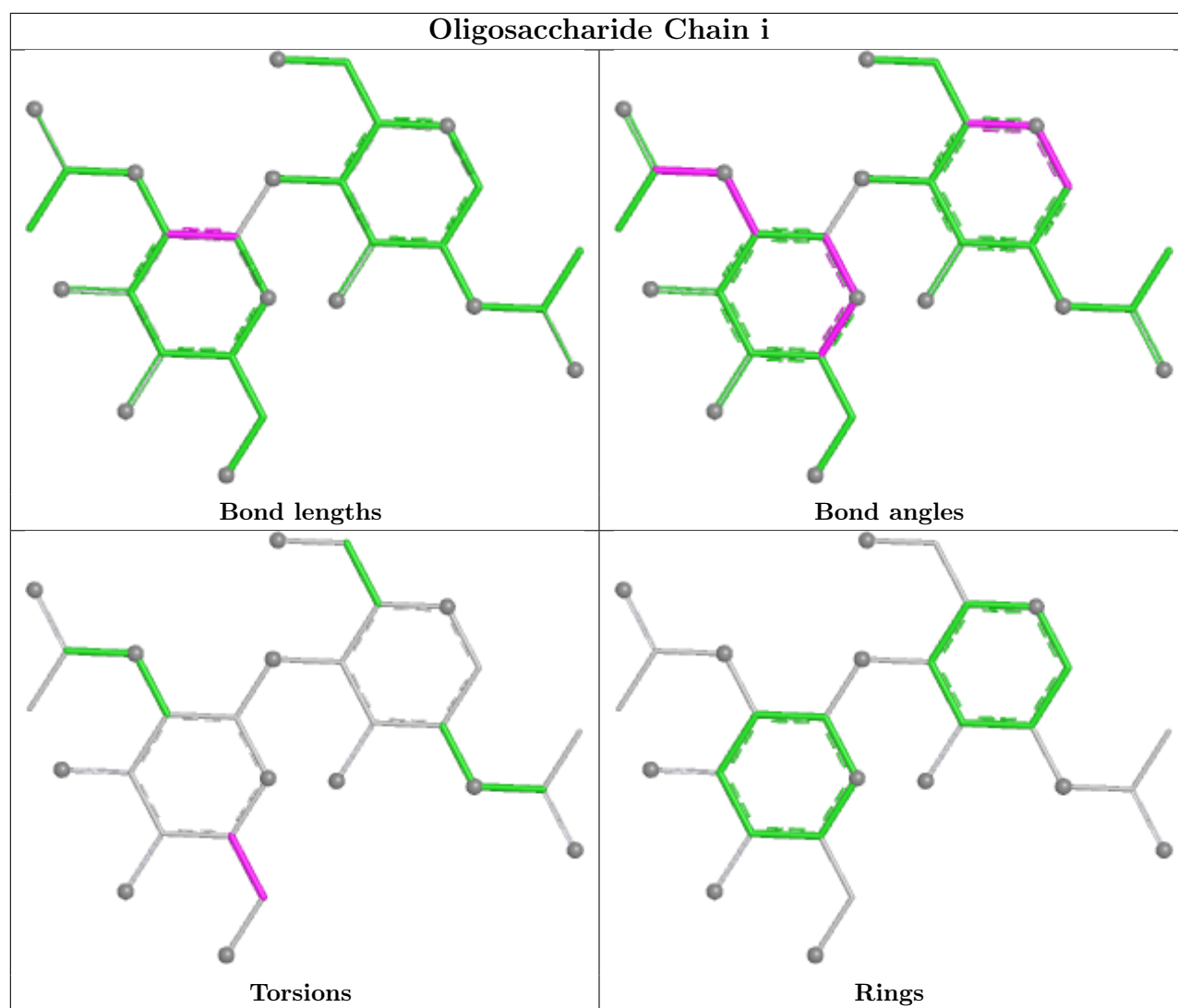


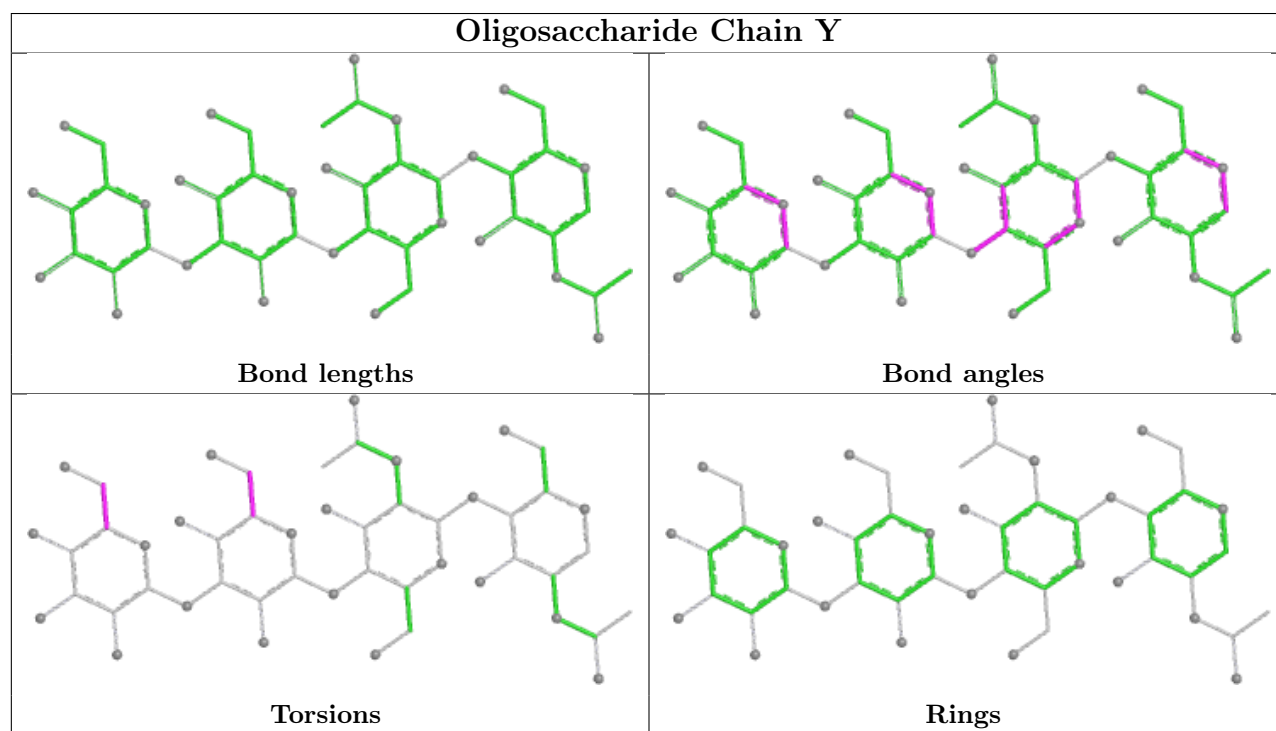
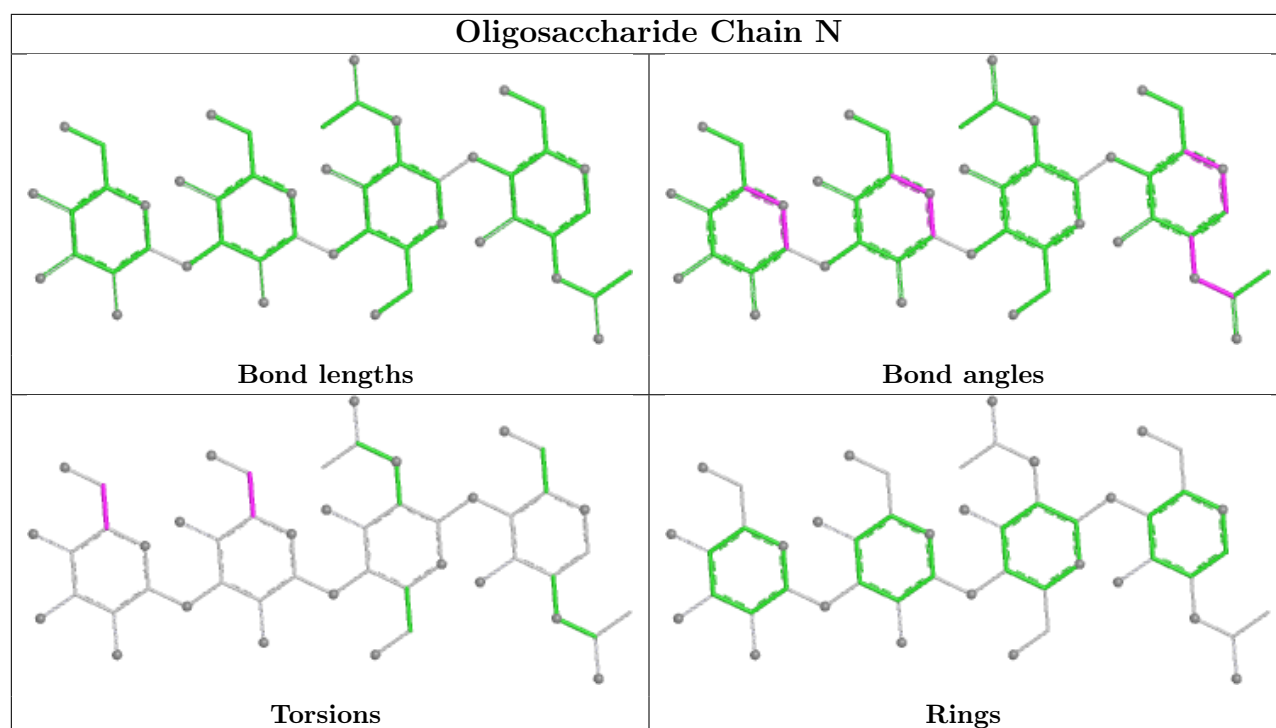


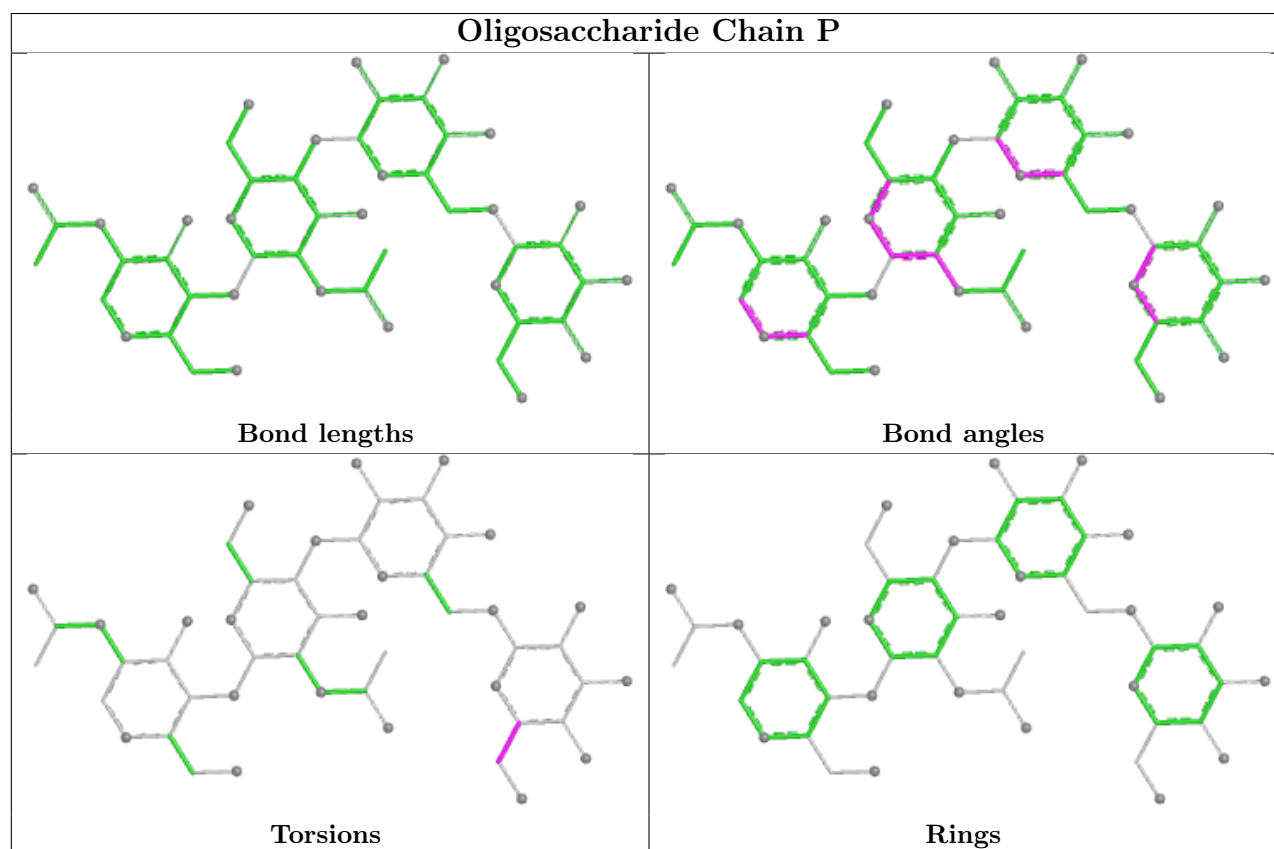
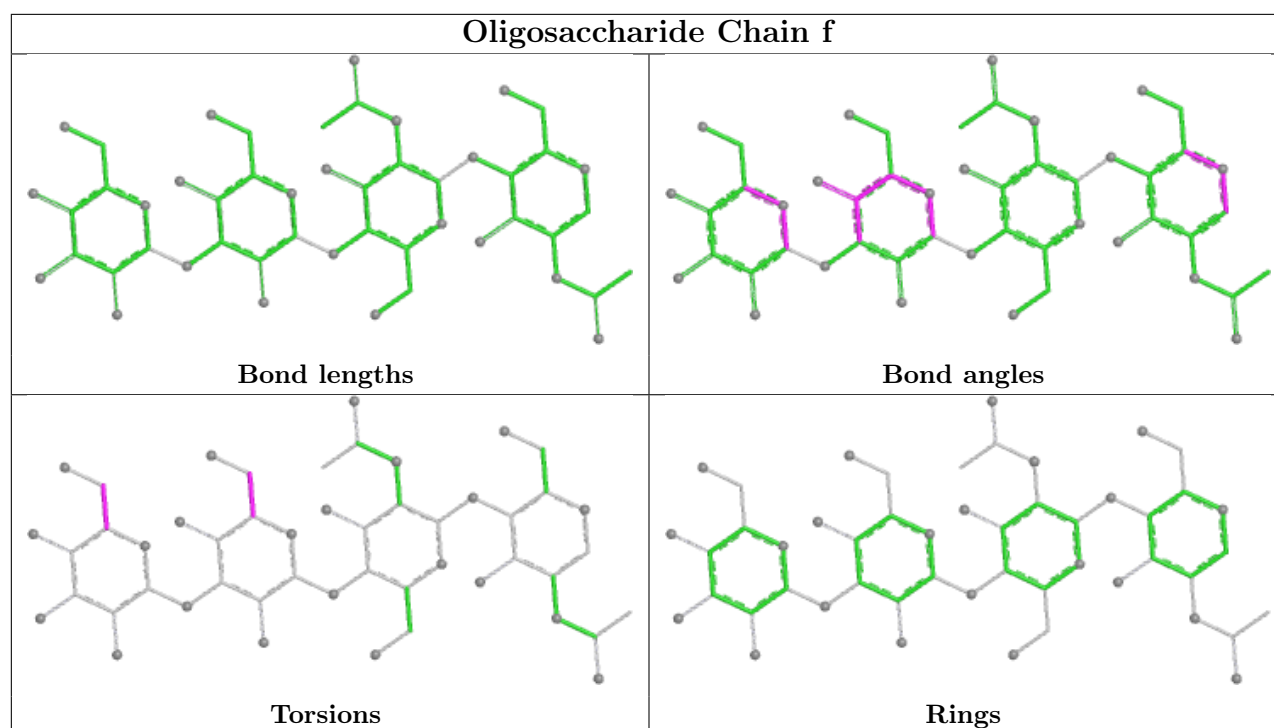


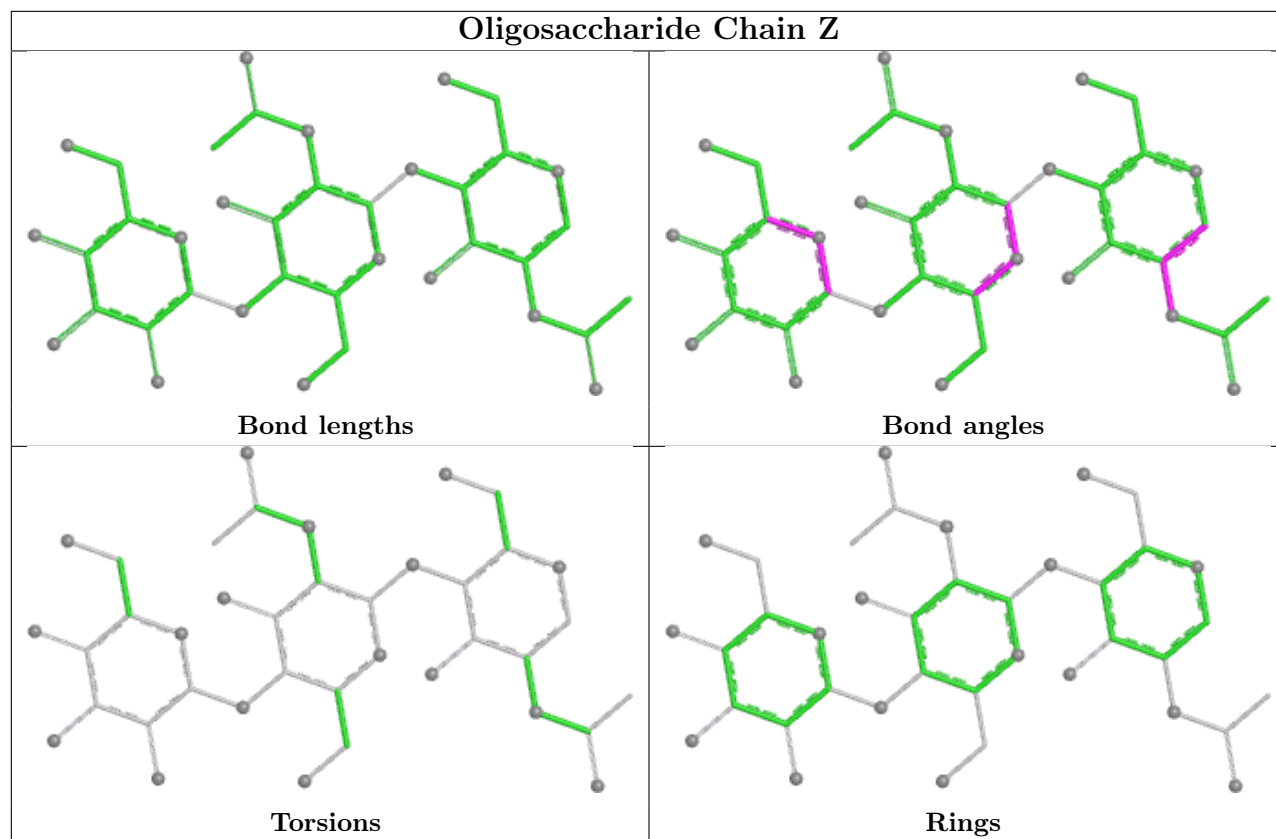


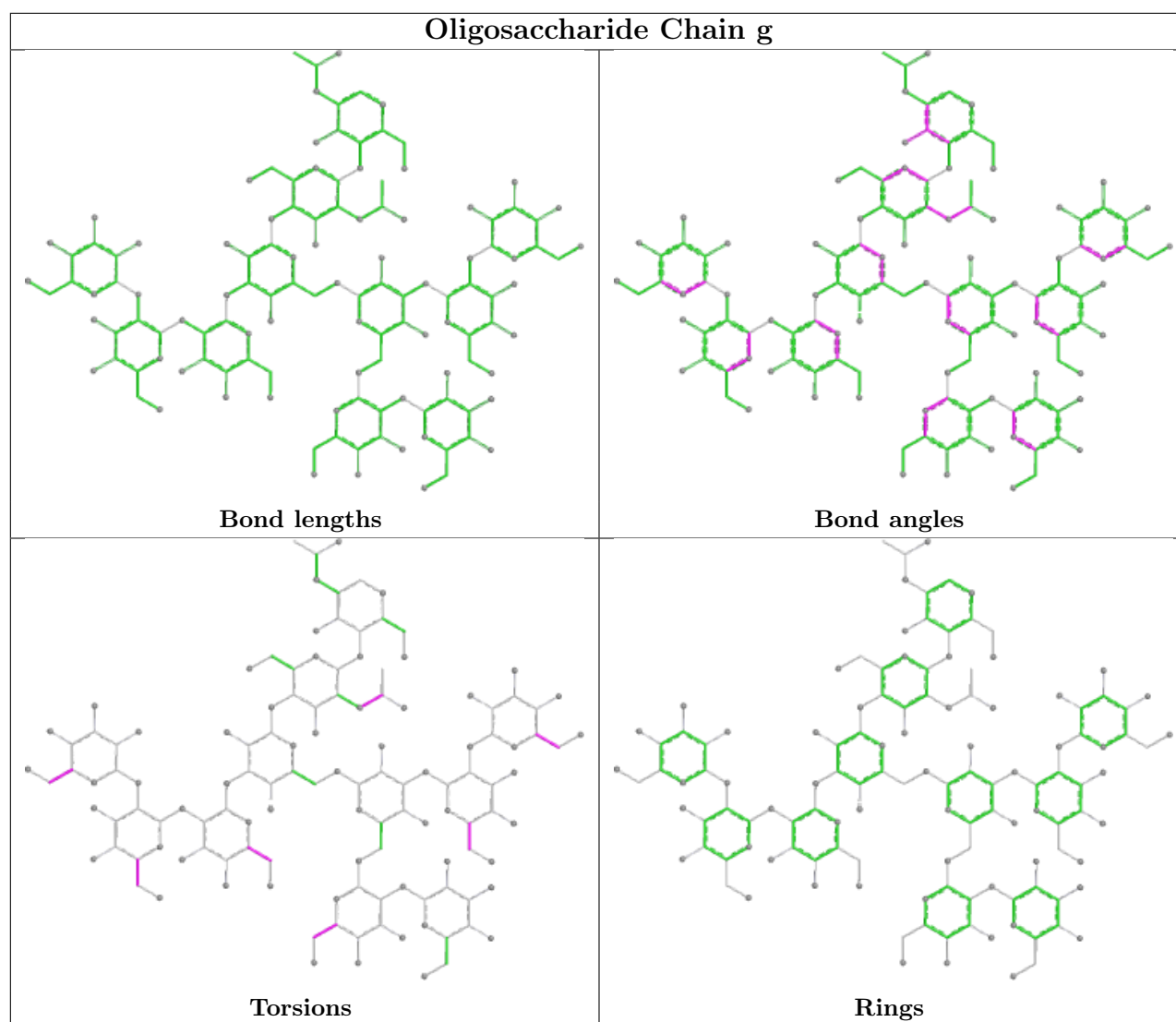












5.6 Ligand geometry [i](#)

39 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	$\# Z > 2$
12	NAG	C	603	3	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
12	NAG	C	610	3	14,14,15	0.69	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	E	608	3	14,14,15	0.68	0	17,19,21	1.45	2 (11%)
12	NAG	F	701	4	14,14,15	0.72	0	17,19,21	1.19	1 (5%)
12	NAG	C	605	3	14,14,15	0.73	0	17,19,21	1.51	1 (5%)
12	NAG	E	607	3	14,14,15	0.71	0	17,19,21	1.30	2 (11%)
12	NAG	A	608	3	14,14,15	0.65	0	17,19,21	1.31	2 (11%)
12	NAG	A	603	3	14,14,15	0.70	0	17,19,21	1.24	1 (5%)
12	NAG	B	702	4	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
12	NAG	E	602	3	14,14,15	0.70	0	17,19,21	1.49	2 (11%)
12	NAG	D	702	4	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
12	NAG	A	605	3	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
12	NAG	C	604	3	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
12	NAG	E	606	3	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
12	NAG	A	601	3	14,14,15	0.69	0	17,19,21	1.17	1 (5%)
12	NAG	C	608	3	14,14,15	0.66	0	17,19,21	1.63	3 (17%)
12	NAG	F	703	4	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
12	NAG	E	604	3	14,14,15	0.67	0	17,19,21	1.05	1 (5%)
12	NAG	E	609	3	14,14,15	0.72	0	17,19,21	1.45	2 (11%)
12	NAG	A	610	3	14,14,15	0.65	0	17,19,21	1.11	2 (11%)
12	NAG	A	607	3	14,14,15	0.72	0	17,19,21	1.23	1 (5%)
12	NAG	C	601	3	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
12	NAG	A	606	3	14,14,15	0.71	0	17,19,21	1.05	2 (11%)
12	NAG	E	601	3	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
12	NAG	C	607	3	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
12	NAG	D	701	4	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
12	NAG	C	606	3	14,14,15	0.71	0	17,19,21	0.80	0
12	NAG	E	605	3	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
12	NAG	C	609	3	14,14,15	0.69	0	17,19,21	1.37	2 (11%)
12	NAG	E	610	3	14,14,15	0.67	0	17,19,21	1.29	2 (11%)
12	NAG	A	602	3	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
12	NAG	A	611	3	14,14,15	0.68	0	17,19,21	1.23	1 (5%)
12	NAG	F	702	4	14,14,15	0.66	0	17,19,21	1.24	2 (11%)
12	NAG	A	604	3	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
12	NAG	E	603	3	14,14,15	0.69	0	17,19,21	1.08	1 (5%)
12	NAG	B	701	4	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
12	NAG	C	602	3	14,14,15	0.68	0	17,19,21	1.54	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	B	703	4	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
12	NAG	A	609	3	14,14,15	0.71	0	17,19,21	1.22	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
12	NAG	C	603	3	-	1/6/23/26	0/1/1/1
12	NAG	C	610	3	-	0/6/23/26	0/1/1/1
12	NAG	E	608	3	-	3/6/23/26	0/1/1/1
12	NAG	F	701	4	-	1/6/23/26	0/1/1/1
12	NAG	C	605	3	-	1/6/23/26	0/1/1/1
12	NAG	E	607	3	-	1/6/23/26	0/1/1/1
12	NAG	A	608	3	-	2/6/23/26	0/1/1/1
12	NAG	A	603	3	-	1/6/23/26	0/1/1/1
12	NAG	B	702	4	-	0/6/23/26	0/1/1/1
12	NAG	E	602	3	-	1/6/23/26	0/1/1/1
12	NAG	D	702	4	-	1/6/23/26	0/1/1/1
12	NAG	A	605	3	-	1/6/23/26	0/1/1/1
12	NAG	C	604	3	-	1/6/23/26	0/1/1/1
12	NAG	E	606	3	-	0/6/23/26	0/1/1/1
12	NAG	A	601	3	-	1/6/23/26	0/1/1/1
12	NAG	C	608	3	-	3/6/23/26	0/1/1/1
12	NAG	F	703	4	-	0/6/23/26	0/1/1/1
12	NAG	E	604	3	-	1/6/23/26	0/1/1/1
12	NAG	E	609	3	-	3/6/23/26	0/1/1/1
12	NAG	A	610	3	-	0/6/23/26	0/1/1/1
12	NAG	A	607	3	-	1/6/23/26	0/1/1/1
12	NAG	C	601	3	-	1/6/23/26	0/1/1/1
12	NAG	A	606	3	-	1/6/23/26	0/1/1/1
12	NAG	E	601	3	-	0/6/23/26	0/1/1/1
12	NAG	C	607	3	-	1/6/23/26	0/1/1/1
12	NAG	D	701	4	-	1/6/23/26	0/1/1/1
12	NAG	C	606	3	-	0/6/23/26	0/1/1/1
12	NAG	E	605	3	-	1/6/23/26	0/1/1/1
12	NAG	C	609	3	-	3/6/23/26	0/1/1/1
12	NAG	E	610	3	-	3/6/23/26	0/1/1/1
12	NAG	A	602	3	-	1/6/23/26	0/1/1/1
12	NAG	A	611	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	F	702	4	-	2/6/23/26	0/1/1/1
12	NAG	A	604	3	-	1/6/23/26	0/1/1/1
12	NAG	E	603	3	-	1/6/23/26	0/1/1/1
12	NAG	B	701	4	-	1/6/23/26	0/1/1/1
12	NAG	C	602	3	-	1/6/23/26	0/1/1/1
12	NAG	B	703	4	-	0/6/23/26	0/1/1/1
12	NAG	A	609	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	608	NAG	C1-O5-C5	4.45	118.15	112.19
12	C	605	NAG	C1-O5-C5	4.34	118.00	112.19
12	A	608	NAG	C2-N2-C7	4.19	128.51	122.90
12	C	602	NAG	C1-O5-C5	4.14	117.73	112.19
12	E	602	NAG	C1-O5-C5	4.07	117.64	112.19

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	608	NAG	C8-C7-N2-C2
12	C	608	NAG	O7-C7-N2-C2
12	C	609	NAG	C8-C7-N2-C2
12	C	609	NAG	O7-C7-N2-C2
12	E	608	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	607	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

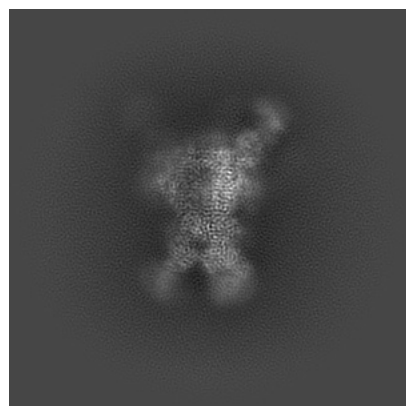
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73008. These allow visual inspection of the internal detail of the map and identification of artifacts.

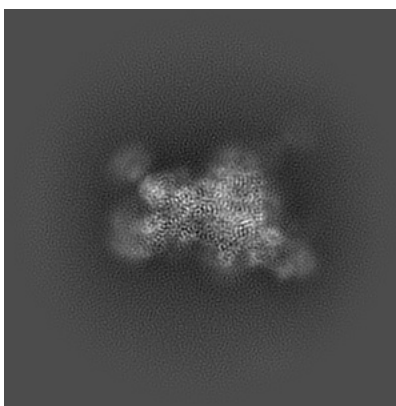
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

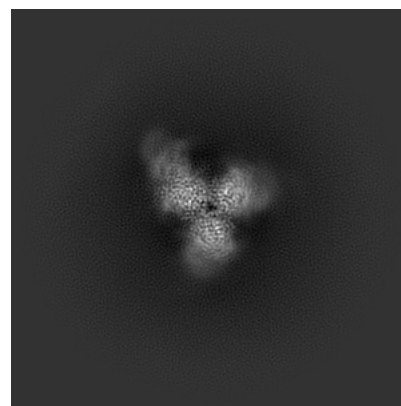
6.1.1 Primary map



X

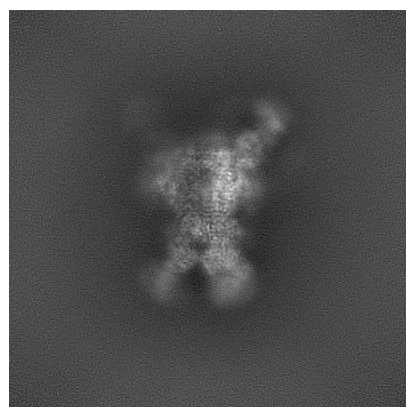


Y

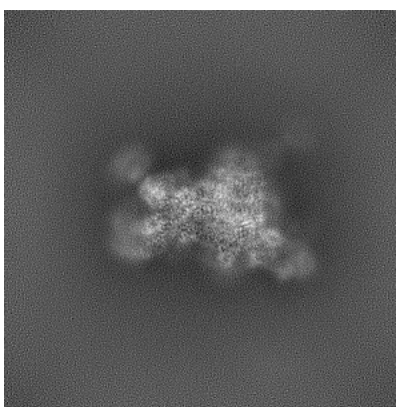


Z

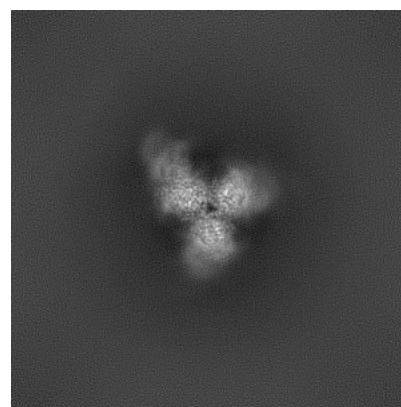
6.1.2 Raw map



X



Y

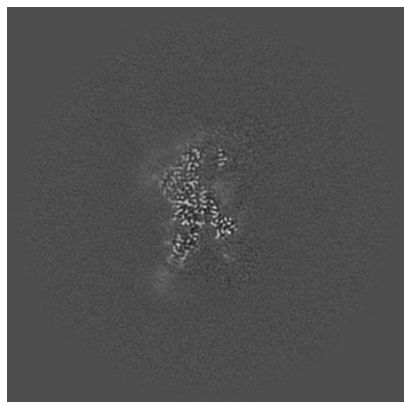


Z

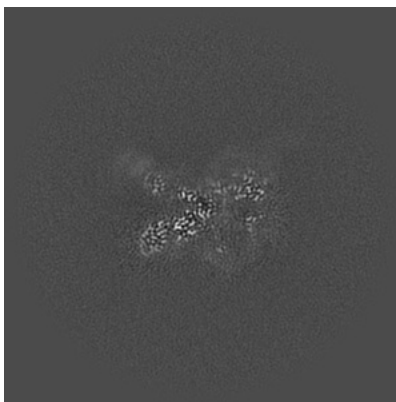
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

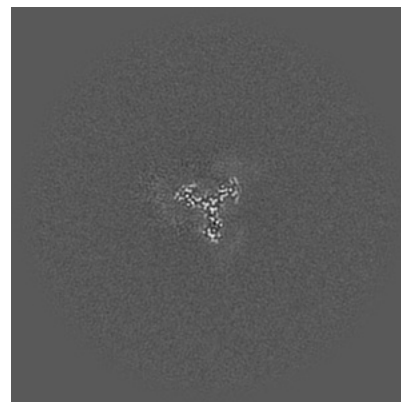
6.2.1 Primary map



X Index: 200

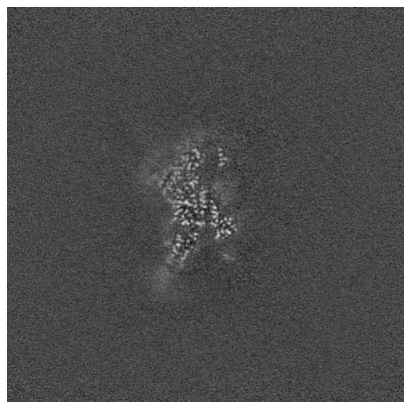


Y Index: 200

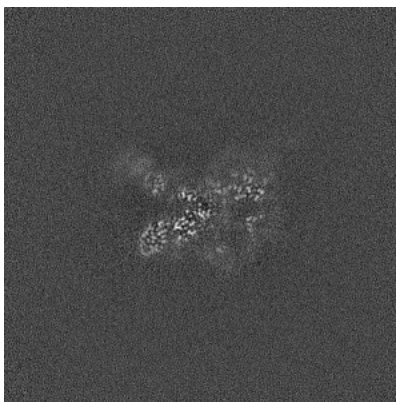


Z Index: 200

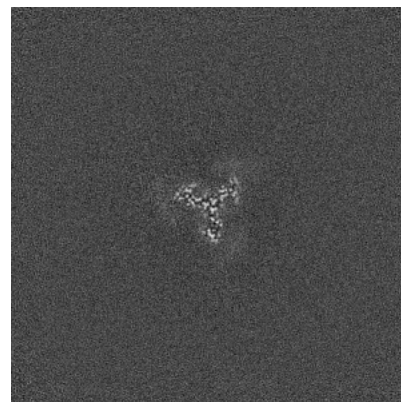
6.2.2 Raw map



X Index: 200



Y Index: 200

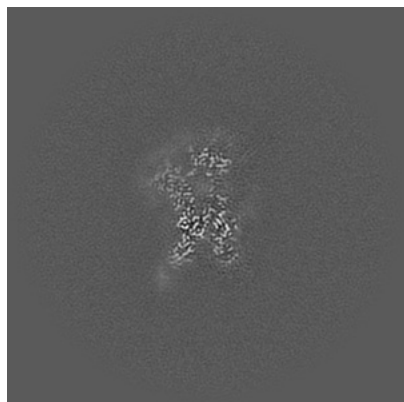


Z Index: 200

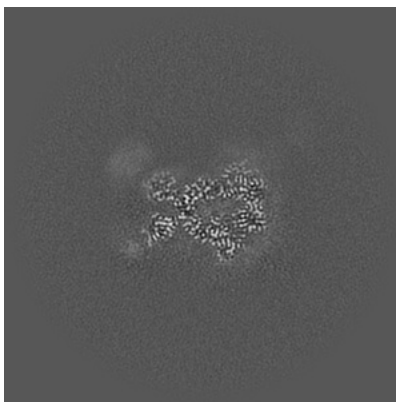
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

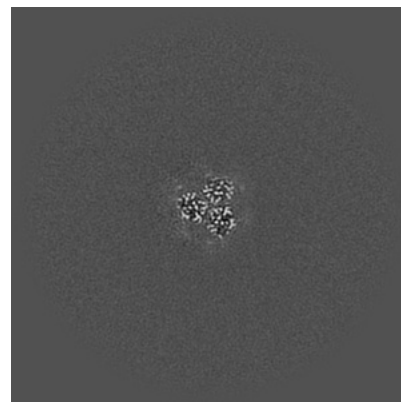
6.3.1 Primary map



X Index: 208

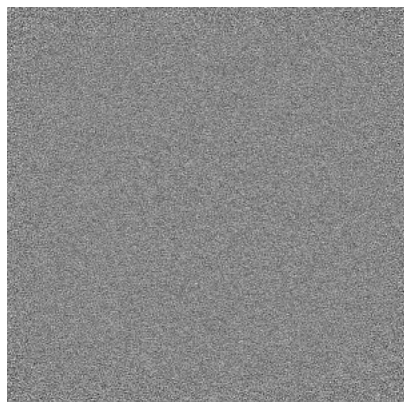


Y Index: 213

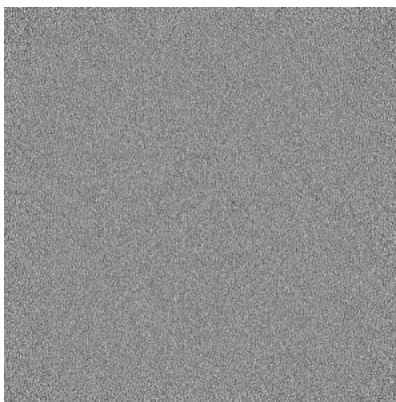


Z Index: 182

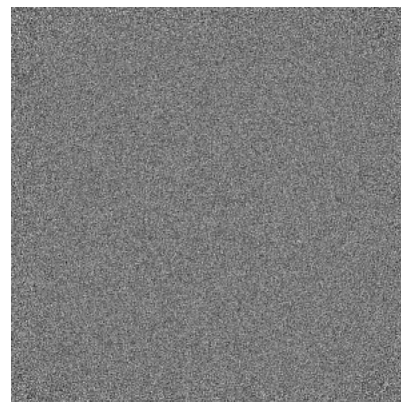
6.3.2 Raw map



X Index: 0



Y Index: 0

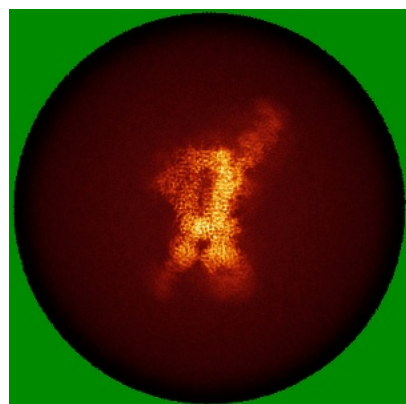


Z Index: 0

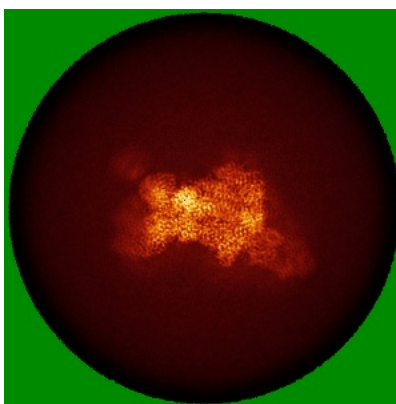
The images above show the largest variance slices of the map in three orthogonal directions.

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

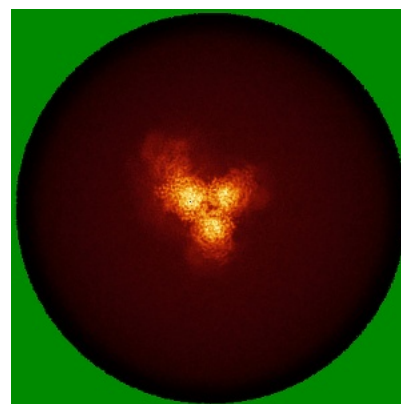
6.4.1 Primary map



X

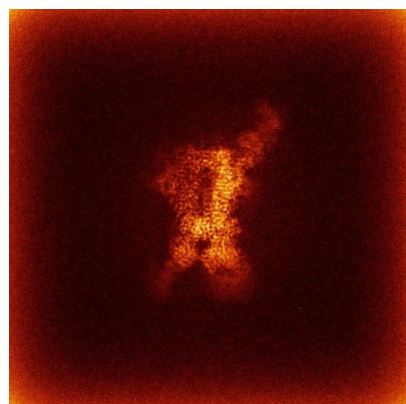


Y

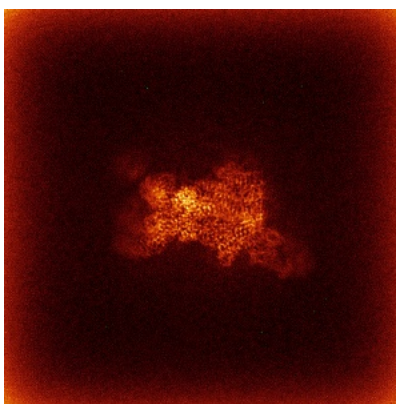


Z

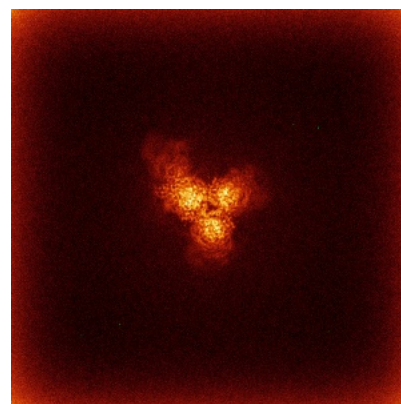
6.4.2 Raw map



X



Y

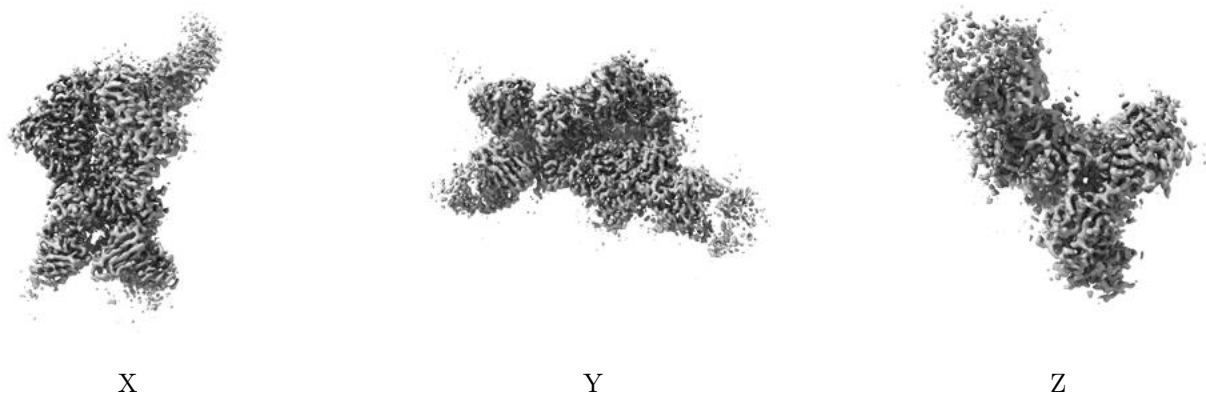


Z

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.

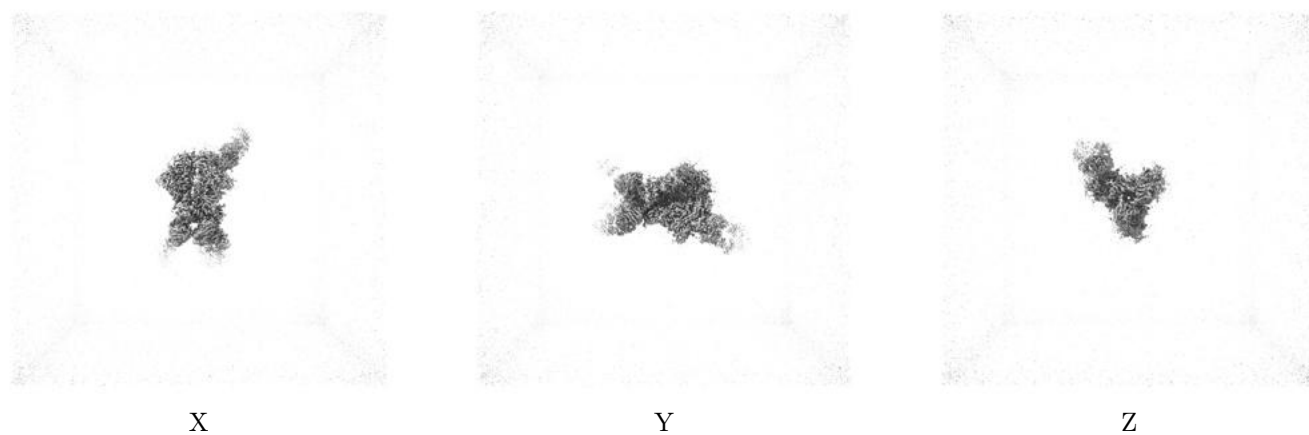
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

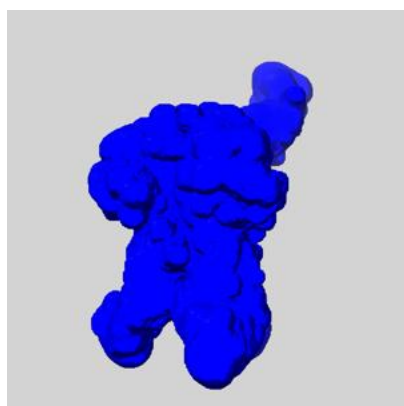
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

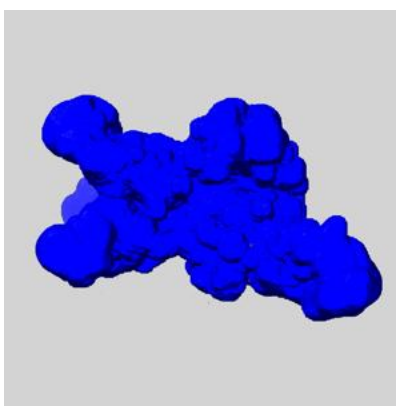
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

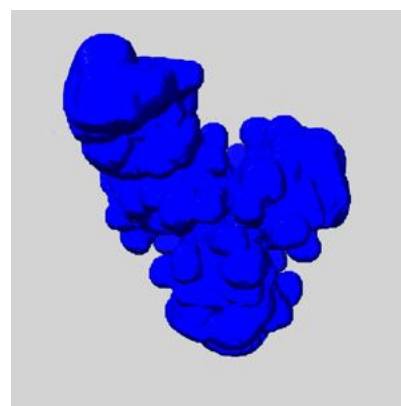
6.6.1 emd_73008_msk_1.map [i](#)



X



Y

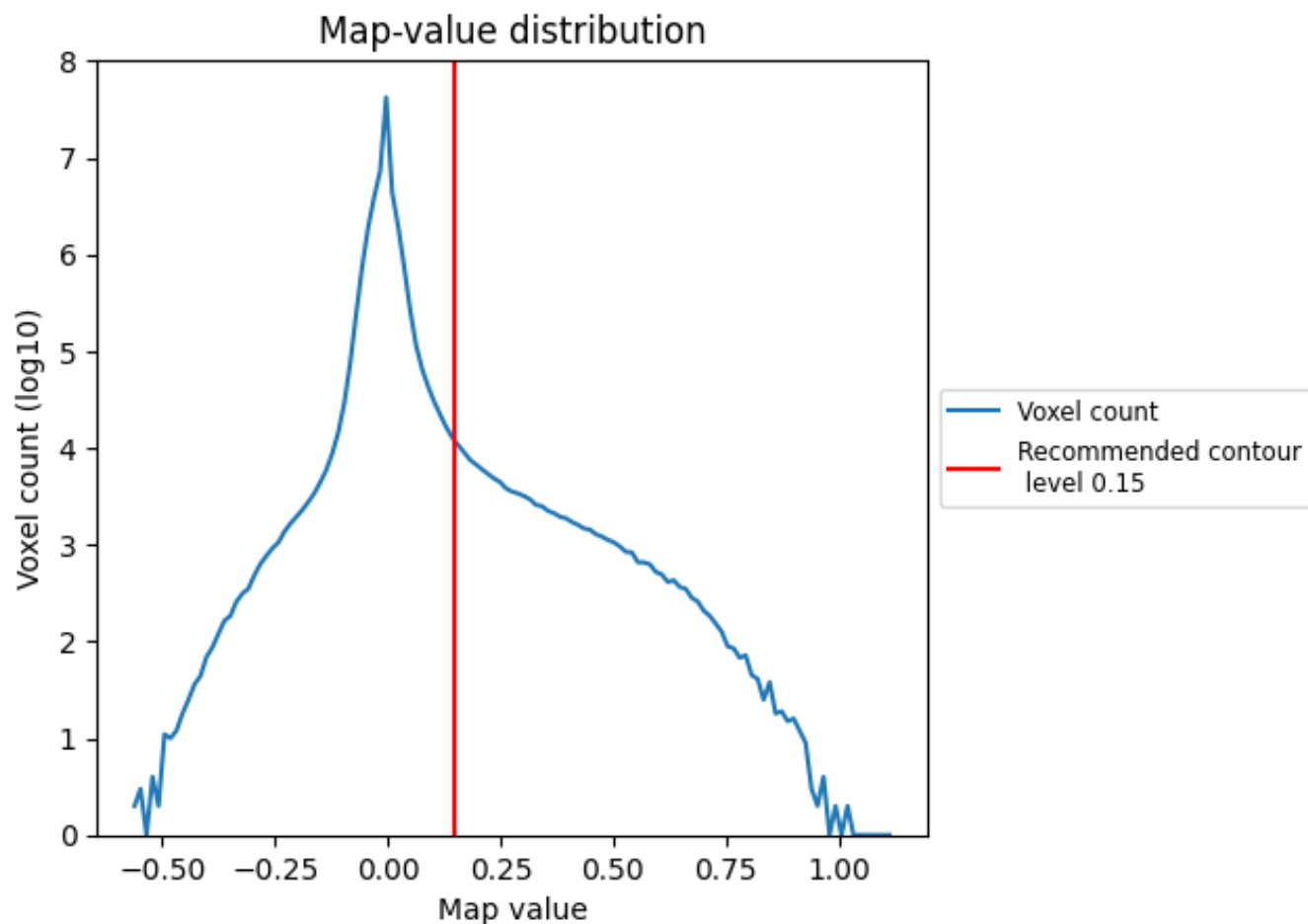


Z

7 Map analysis [i](#)

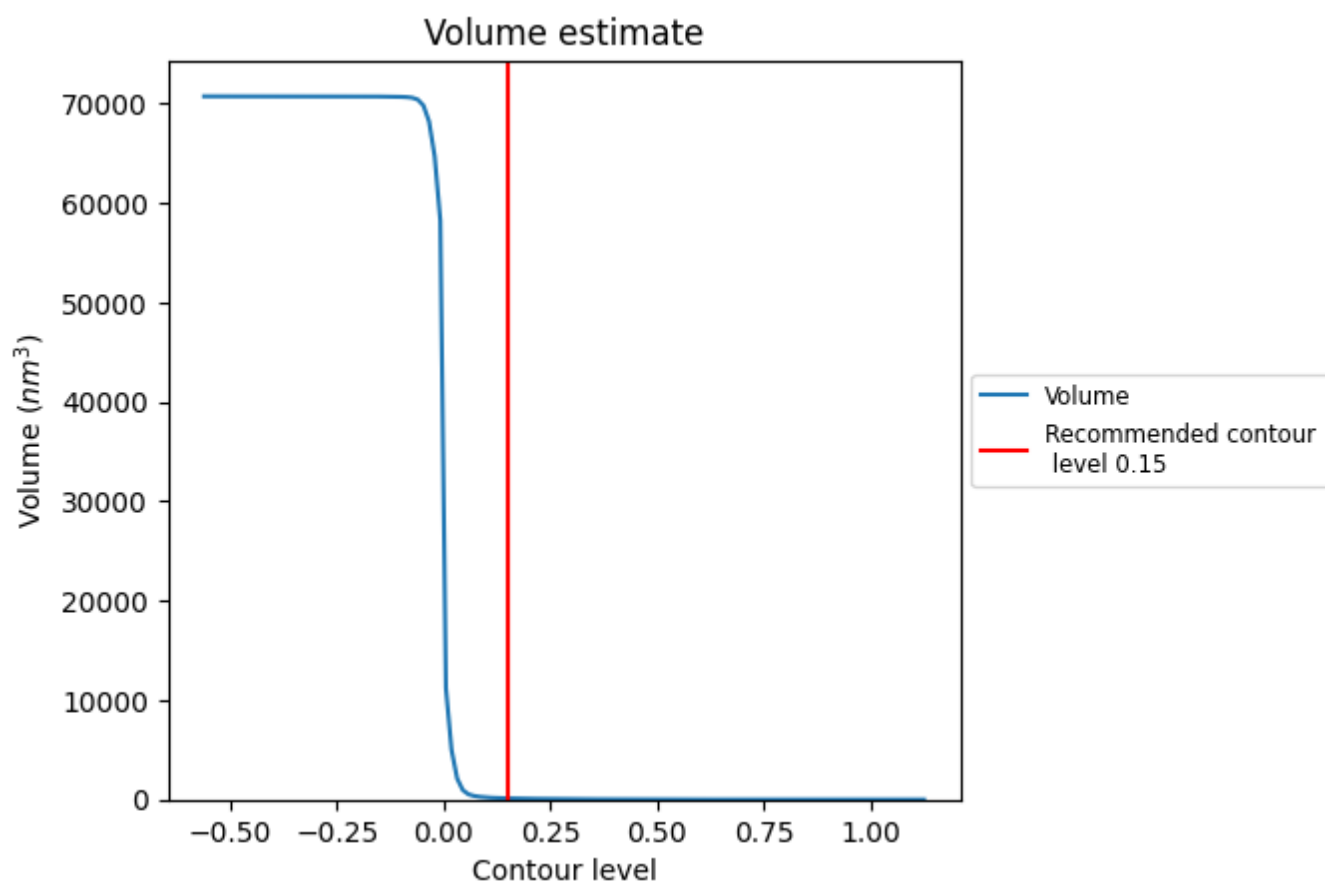
This section contains the results of statistical analysis of the map.

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.

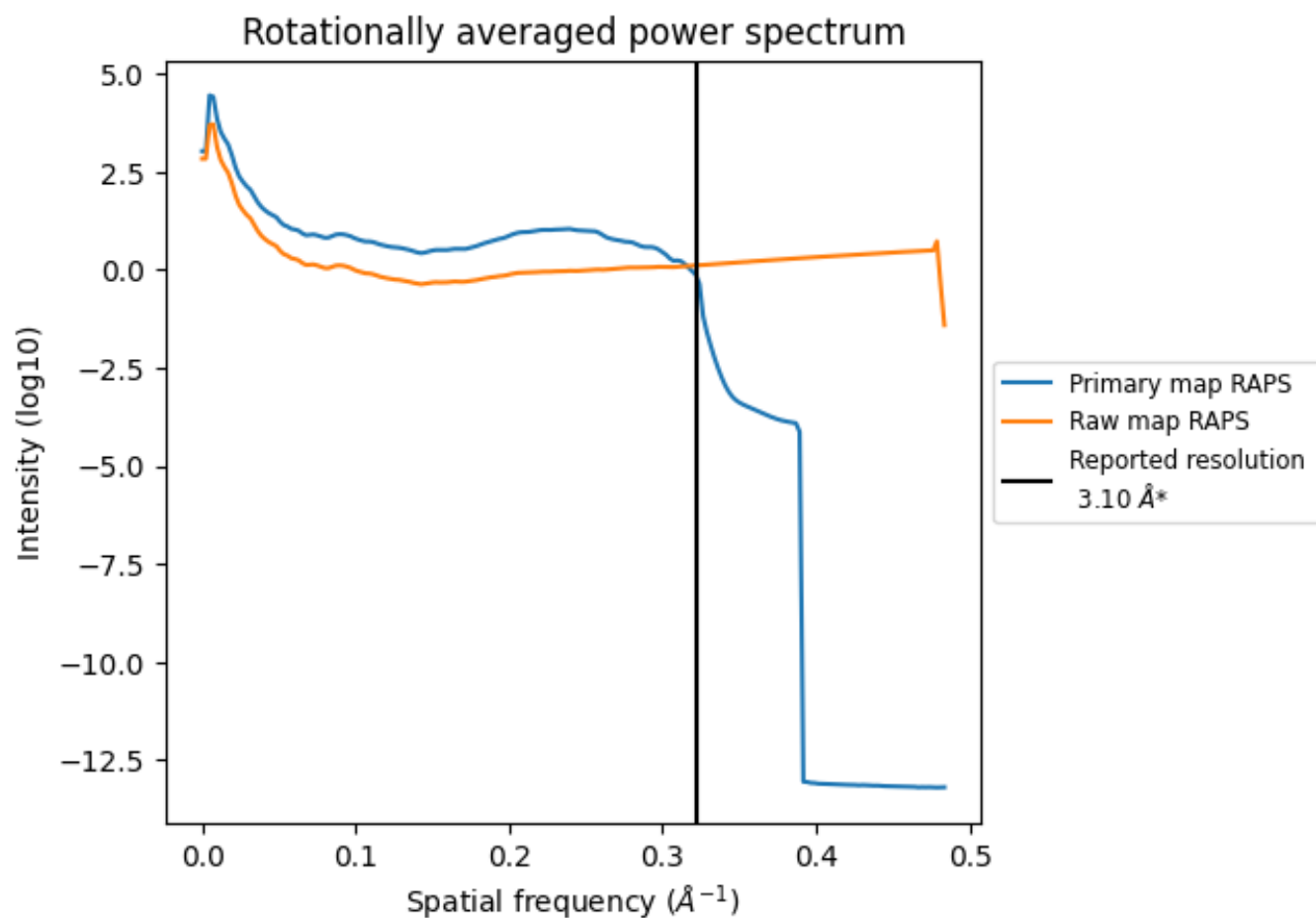
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm³; this corresponds to an approximate mass of 110 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 ⓘ

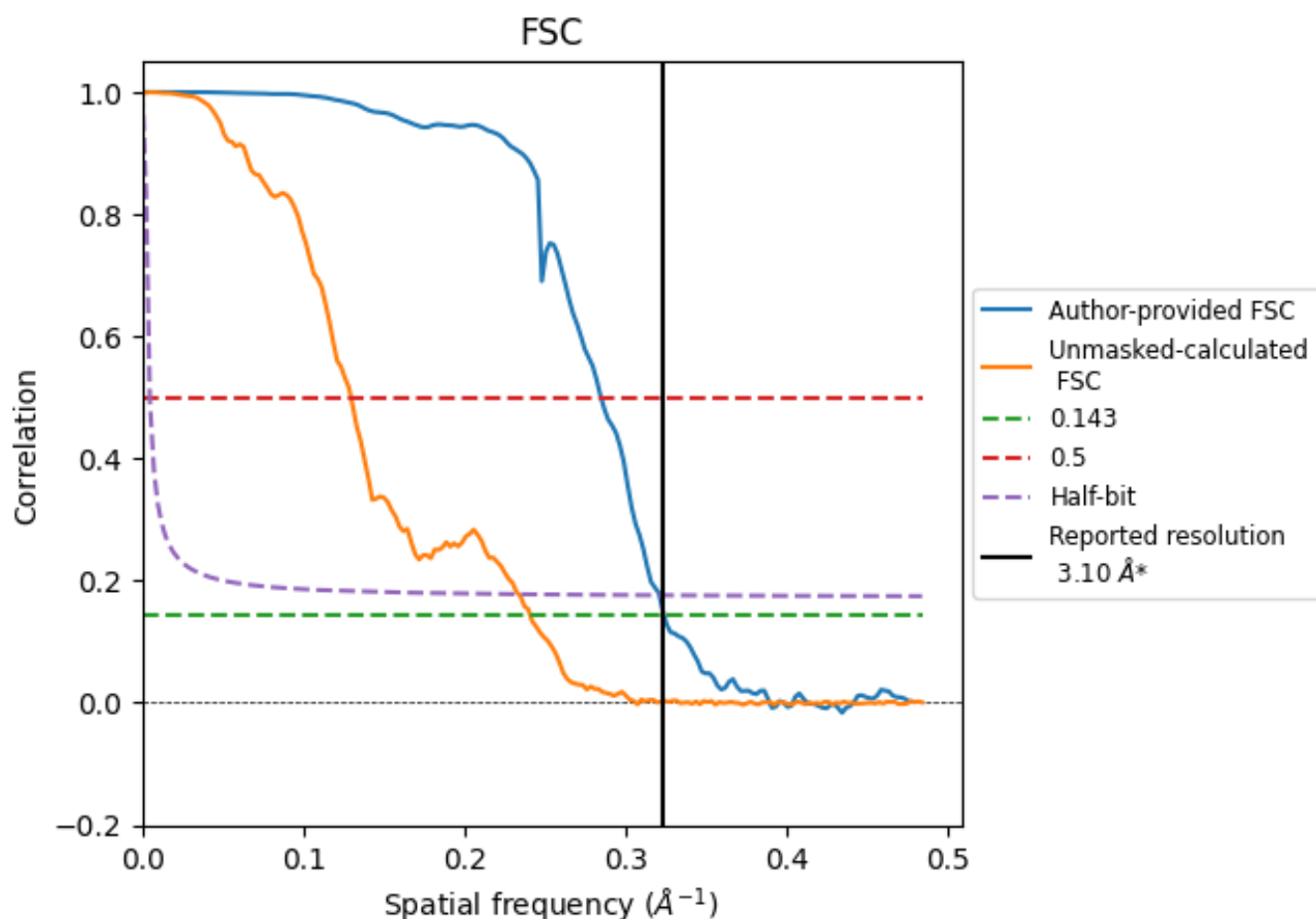


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

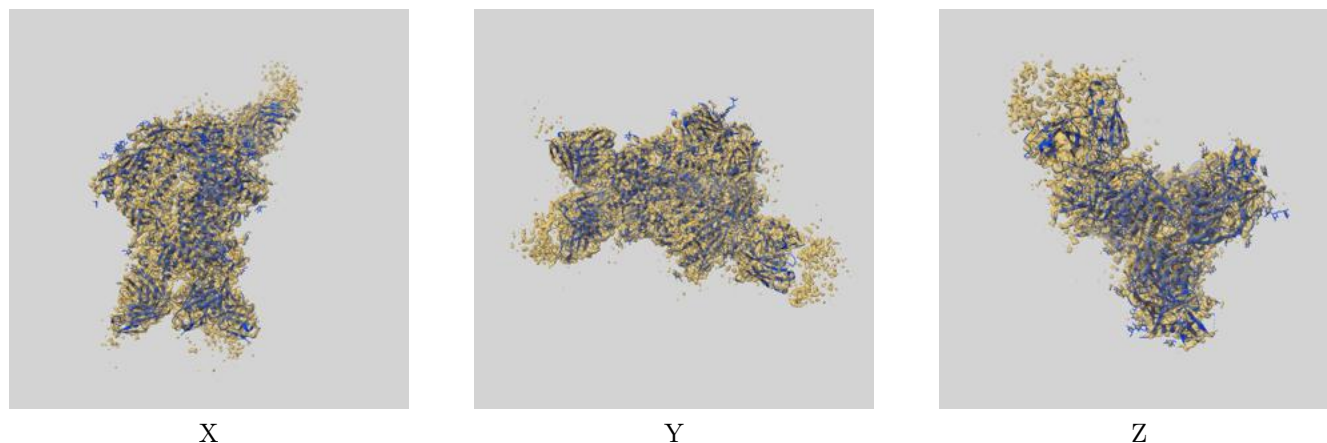
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.51	3.12
Unmasked-calculated*	4.16	7.73	4.28

*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 4.16 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

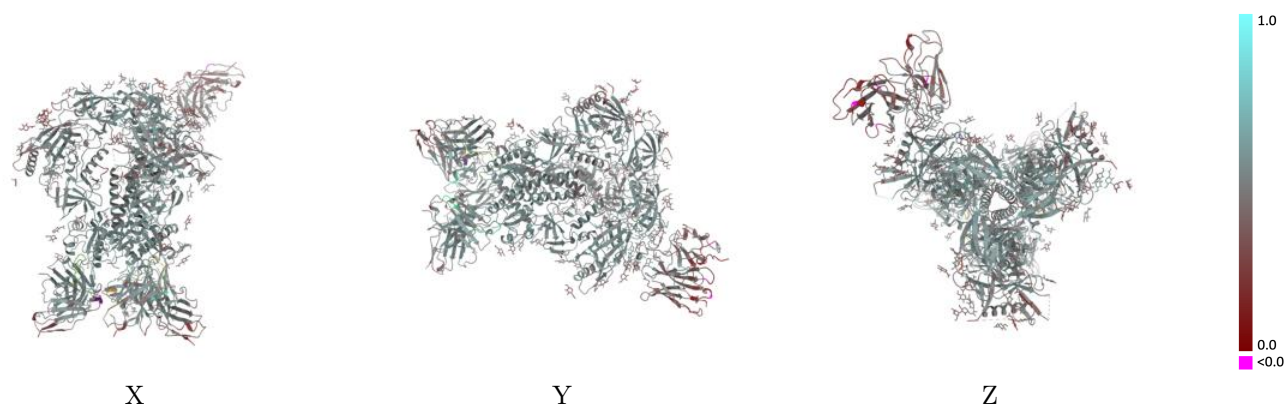
This section contains information regarding the fit between EMDB map EMD-73008 and PDB model 9YJ1. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



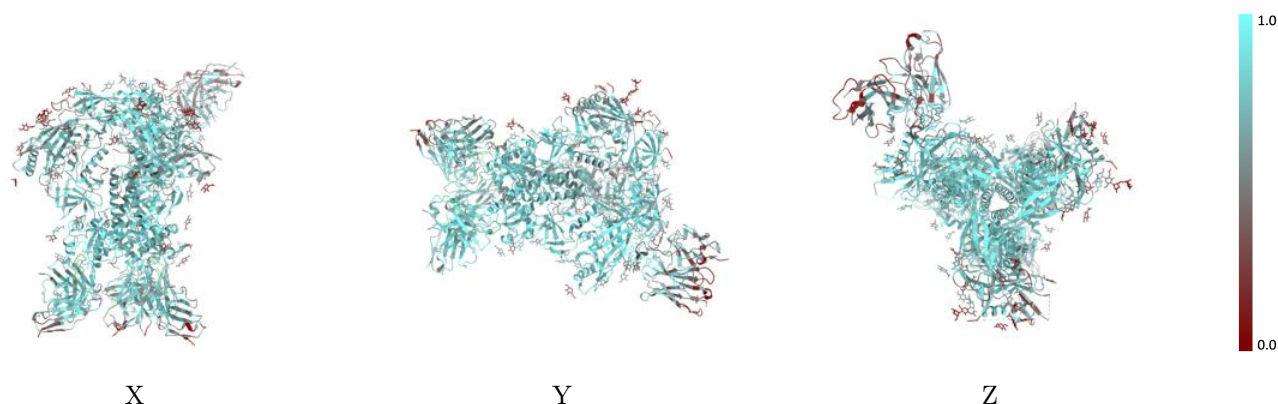
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



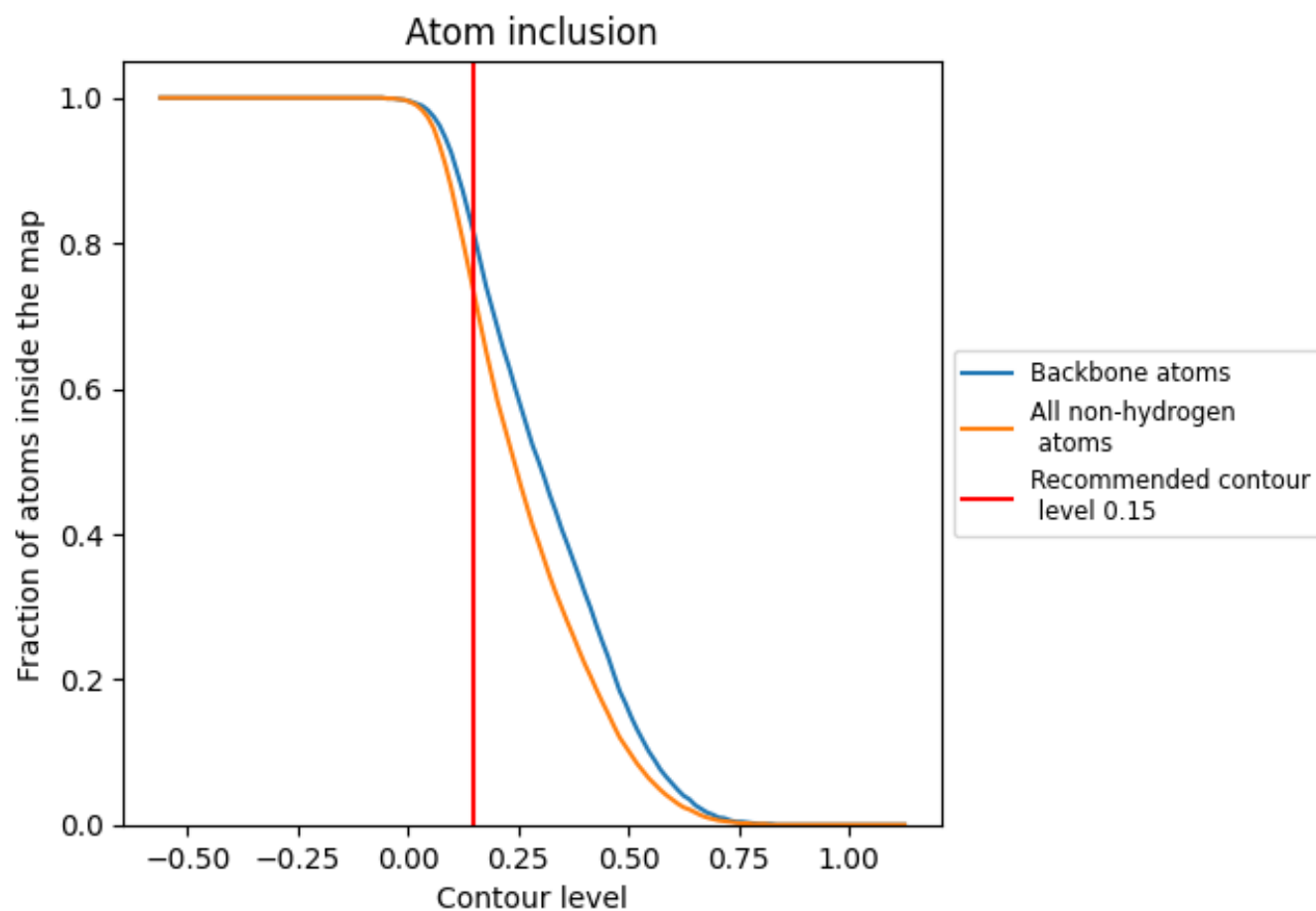
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.5010
A	 0.8000	 0.5320
B	 0.8270	 0.5480
C	 0.7370	 0.5130
D	 0.8120	 0.5370
E	 0.7160	 0.5040
F	 0.8310	 0.5410
G	 0.2500	 0.2950
H	 0.5530	 0.3830
I	 0.8080	 0.5270
J	 0.5710	 0.4560
K	 0.6890	 0.5000
L	 0.5100	 0.3870
M	 0.7970	 0.5120
N	 0.5000	 0.4280
O	 0.6550	 0.4520
P	 0.2600	 0.4270
Q	 0.7770	 0.5190
R	 0.2140	 0.2910
S	 0.6860	 0.4880
T	 0.3570	 0.3790
U	 0.3210	 0.3600
V	 0.4290	 0.4510
W	 0.5000	 0.4140
X	 0.5360	 0.4360
Y	 0.5800	 0.4620
Z	 0.2820	 0.3960
a	 0.1790	 0.2150
b	 0.2500	 0.3790
c	 0.2500	 0.4370
d	 0.5360	 0.3590
e	 0.5710	 0.3770
f	 0.7600	 0.4910
g	 0.7870	 0.5090
h	 0.3930	 0.3430
i	 0.5710	 0.4140

