



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 04:12 PM EDT

PDB ID : 9NC3 / pdb_00009nc3
EMDB ID : EMD-49240
Title : AMC008 v4.2 SOSIP Env trimer in complex with b12 and 3BC315 Fabs
Authors : Cui, J.; Du, J.; Lin, Z.; Pallesen, J.
Deposited on : 2025-02-14
Resolution : 3.74 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

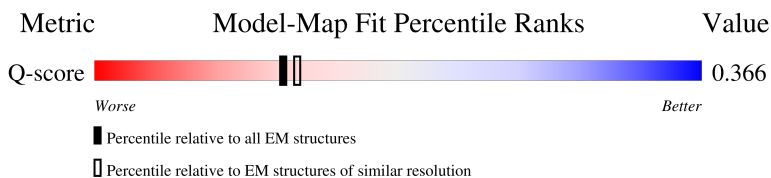
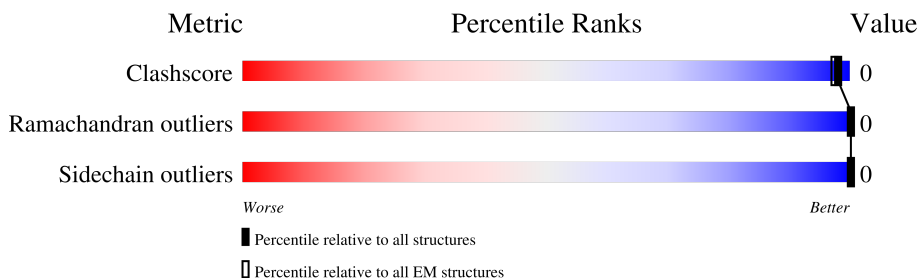
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 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	10346 (3.24 - 4.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	
1	C	488	
1	E	488	
2	B	154	

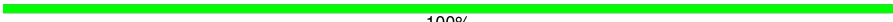
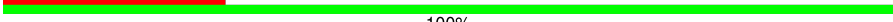
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Mol	Chain	Length	Quality of chain
2	D	154	
2	F	154	
3	G	232	
3	K	232	
3	O	232	
4	H	216	
4	L	216	
4	P	216	
5	I	230	
5	M	230	
5	Q	230	
6	J	215	
6	N	215	
6	R	215	
7	S	2	
7	T	2	
7	V	2	
7	W	2	
7	X	2	
7	a	2	
7	c	2	
7	e	2	
7	g	2	
7	i	2	
7	l	2	

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Mol	Chain	Length	Quality of chain
7	m	2	 100%
8	U	6	 33% 100%
9	Y	5	 40% 60%
10	Z	3	 67% 100%
10	d	3	 33% 67% 33%
10	j	3	 67% 100%
10	q	3	 33% 67% 33%
11	b	8	 25% 100%
12	f	4	 25% 50% 50%
12	n	4	 50% 25% 75%
12	o	4	 50% 75% 25%
13	h	4	 50% 100%
13	p	4	 25% 50% 50%
14	k	3	 33% 67%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 28821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3559	2232	621	679	27		
1	C	450	Total	C	N	O	S	0	0
			3559	2232	621	679	27		
1	E	450	Total	C	N	O	S	0	0
			3559	2232	621	679	27		

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	S	0	0
			972	618	167	179	8		
2	D	123	Total	C	N	O	S	0	0
			993	630	171	185	7		
2	F	119	Total	C	N	O	S	0	0
			950	605	163	174	8		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	514	THR	ALA	conflict	UNP Q1AII4
B	543	ASN	GLN	conflict	UNP Q1AII4
B	559	PRO	ILE	conflict	UNP Q1AII4
B	605	CYS	THR	conflict	UNP Q1AII4
B	607	SER	ALA	conflict	UNP Q1AII4
B	612	THR	ALA	conflict	UNP Q1AII4
B	646	LEU	ILE	conflict	UNP Q1AII4
B	659	LEU	GLU	conflict	UNP Q1AII4
D	514	THR	ALA	conflict	UNP Q1AII4
D	543	ASN	GLN	conflict	UNP Q1AII4
D	559	PRO	ILE	conflict	UNP Q1AII4
D	605	CYS	THR	conflict	UNP Q1AII4
D	607	SER	ALA	conflict	UNP Q1AII4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	612	THR	ALA	conflict	UNP Q1AII4
D	646	LEU	ILE	conflict	UNP Q1AII4
D	659	LEU	GLU	conflict	UNP Q1AII4
F	514	THR	ALA	conflict	UNP Q1AII4
F	543	ASN	GLN	conflict	UNP Q1AII4
F	559	PRO	ILE	conflict	UNP Q1AII4
F	605	CYS	THR	conflict	UNP Q1AII4
F	607	SER	ALA	conflict	UNP Q1AII4
F	612	THR	ALA	conflict	UNP Q1AII4
F	646	LEU	ILE	conflict	UNP Q1AII4
F	659	LEU	GLU	conflict	UNP Q1AII4

- Molecule 3 is a protein called 3BC315 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	223	Total	C	N	O	S	0	0
			1699	1084	288	318	9		
3	K	126	Total	C	N	O	S	0	0
			991	633	172	179	7		
3	O	126	Total	C	N	O	S	0	0
			992	635	172	178	7		

- Molecule 4 is a protein called 3BC315 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	210	Total	C	N	O	S	0	0
			1573	989	263	316	5		
4	L	109	Total	C	N	O	S	0	0
			808	507	135	163	3		
4	P	107	Total	C	N	O	S	0	0
			796	499	133	161	3		

- Molecule 5 is a protein called b12 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	230	Total	C	N	O	S	0	0
			1753	1108	297	340	8		
5	M	127	Total	C	N	O	S	0	0
			1013	642	175	191	5		
5	Q	125	Total	C	N	O	S	0	0
			998	634	172	187	5		

- Molecule 6 is a protein called b12 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	215	Total	C	N	O	S	0	0
			1668	1036	297	330	5		
6	N	106	Total	C	N	O	S	0	0
			816	508	148	158	2		
6	R	105	Total	C	N	O	S	0	0
			807	503	147	155	2		

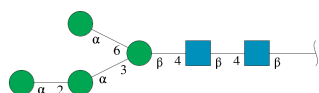
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	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	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		
7	a	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	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		

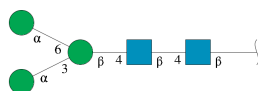
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



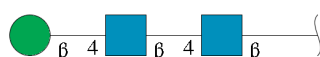
Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



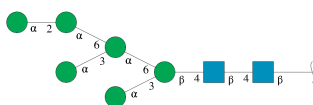
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	5	Total	C	N	O	0	0
			61	34	2	25		

- 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		
10	d	3	Total	C	N	O	0	0
			39	22	2	15		
10	j	3	Total	C	N	O	0	0
			39	22	2	15		
10	q	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-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[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
11	b	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 12 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.



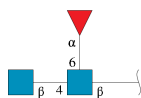
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	4	Total	C	N	O	0	0
			50	28	2	20		
12	n	4	Total	C	N	O	0	0
			50	28	2	20		
12	o	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 13 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.



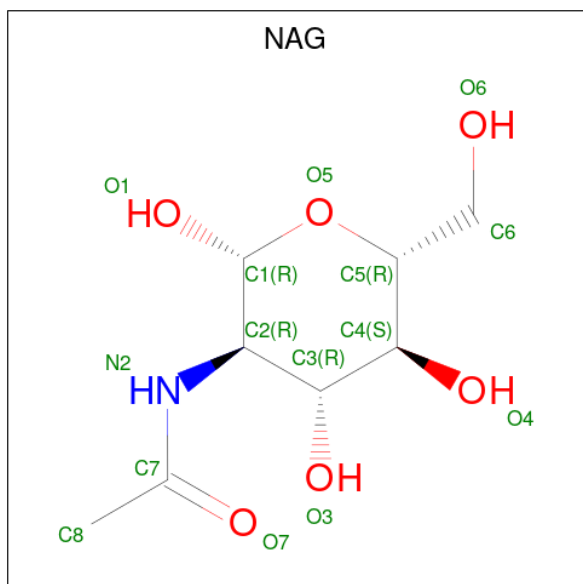
Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	4	Total	C	N	O	0	0
			50	28	2	20		
13	p	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	k	3	Total	C	N	O	0	0
			38	22	2	14		

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



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

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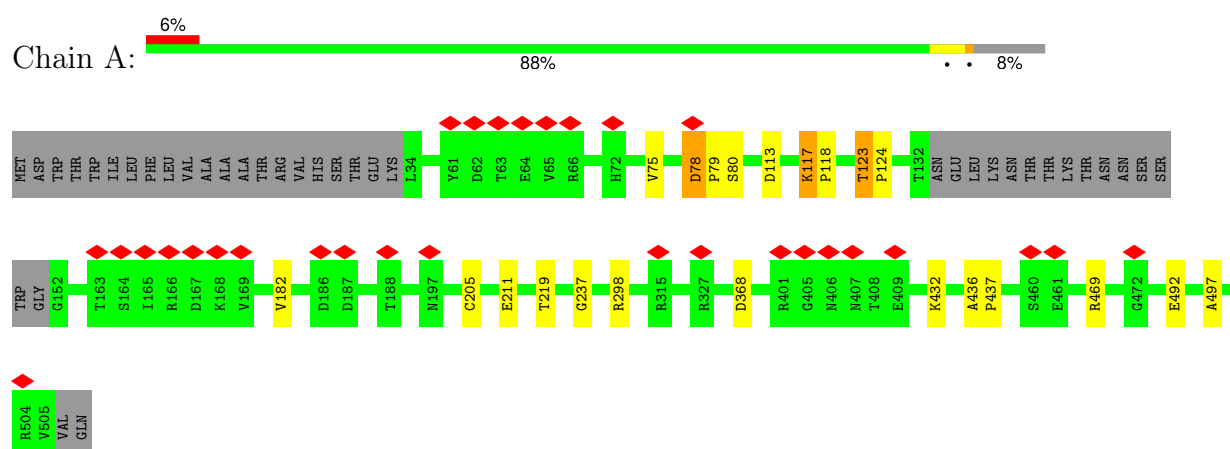
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Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total	C	N	O	0
			14	8	1	5	
15	E	1	Total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

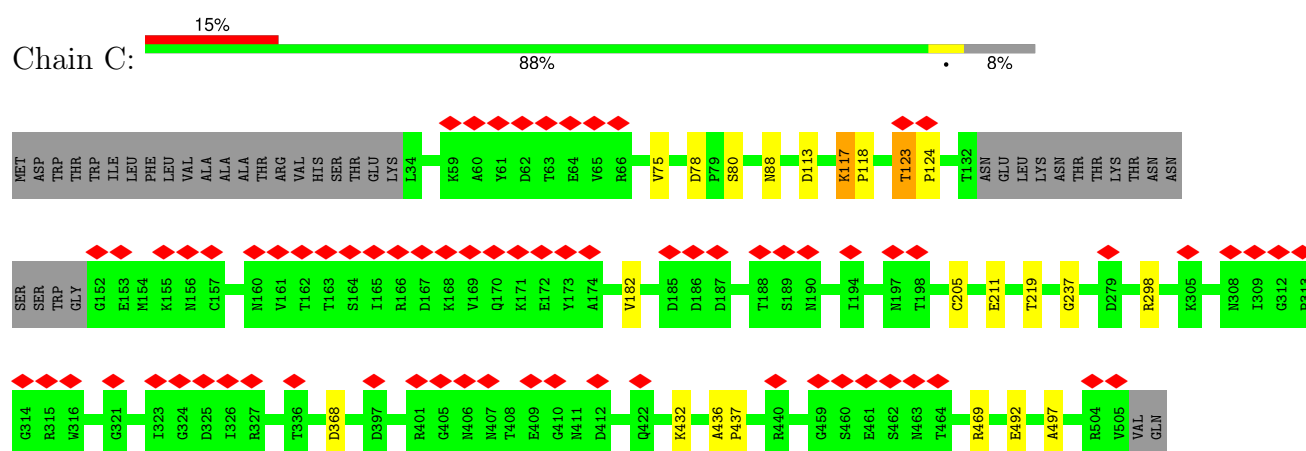
3 Residue-property plots

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

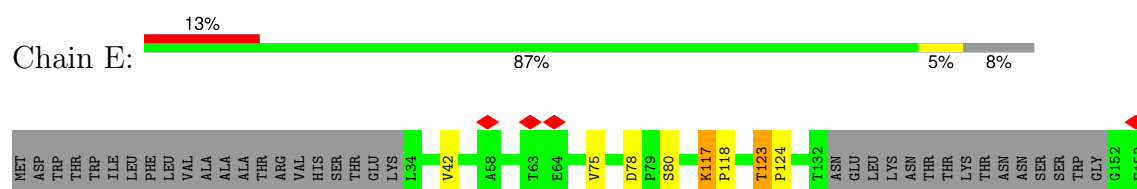
• Molecule 1: Envelope glycoprotein gp120

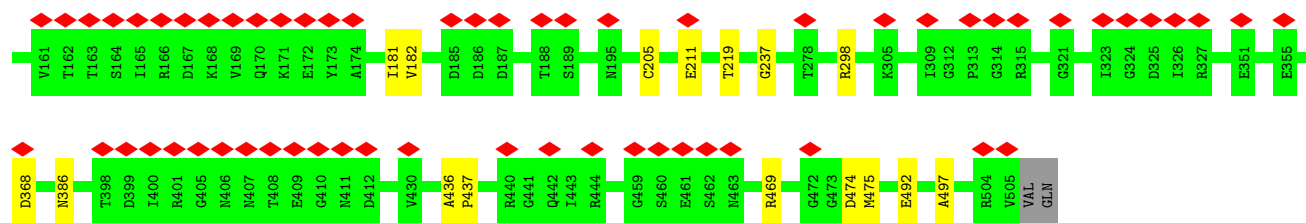


• Molecule 1: Envelope glycoprotein gp120

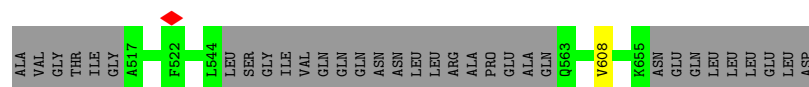
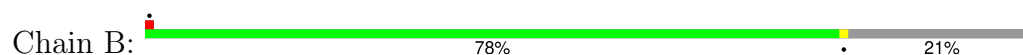


• Molecule 1: Envelope glycoprotein gp120

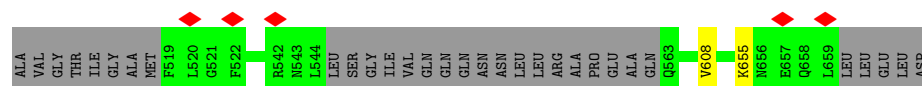
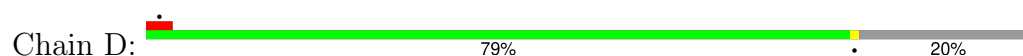




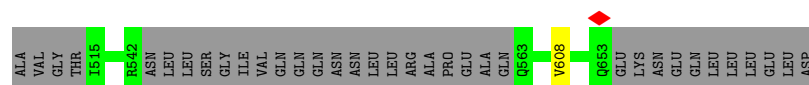
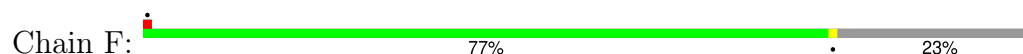
• Molecule 2: Envelope glycoprotein gp41



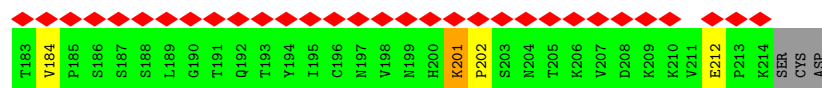
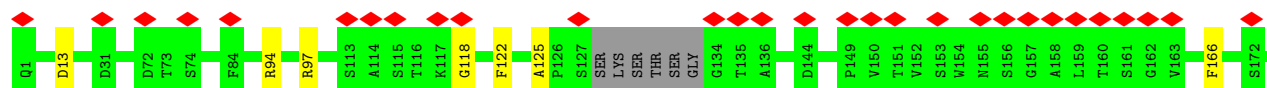
• Molecule 2: Envelope glycoprotein gp41



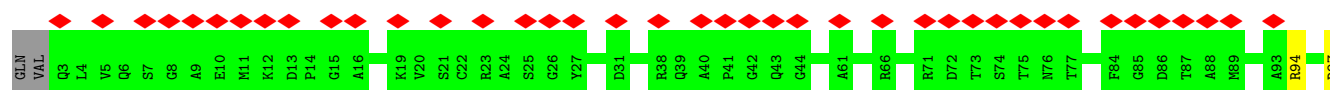
• Molecule 2: Envelope glycoprotein gp41

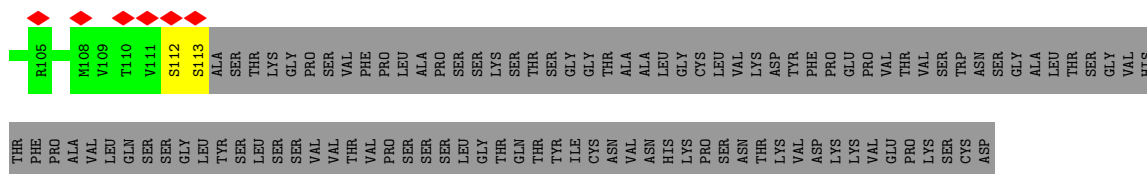


• Molecule 3: 3BC315 Fab heavy chain

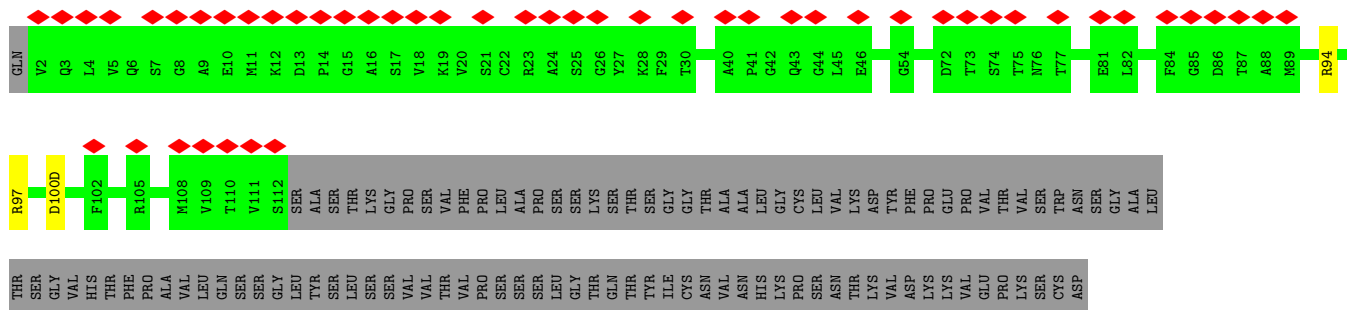


• Molecule 3: 3BC315 Fab heavy chain





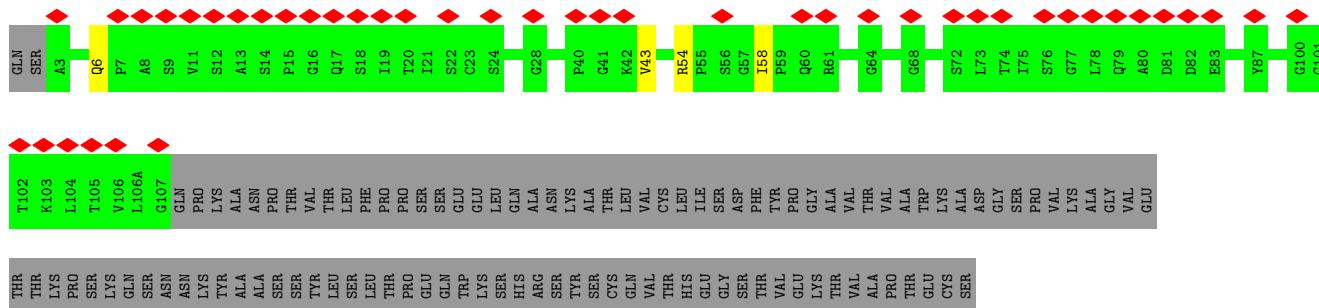
- Molecule 3: 3BC315 Fab heavy chain



- Molecule 4: 3BC315 Fab light chain

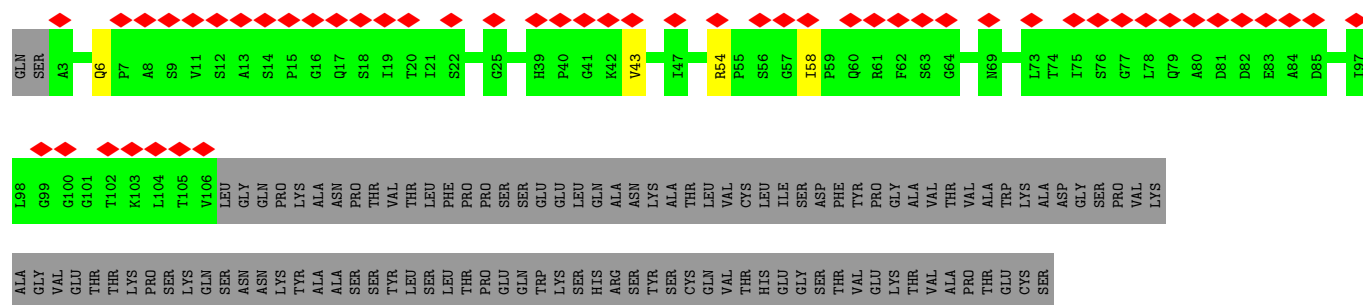


- Molecule 4: 3BC315 Fab light chain

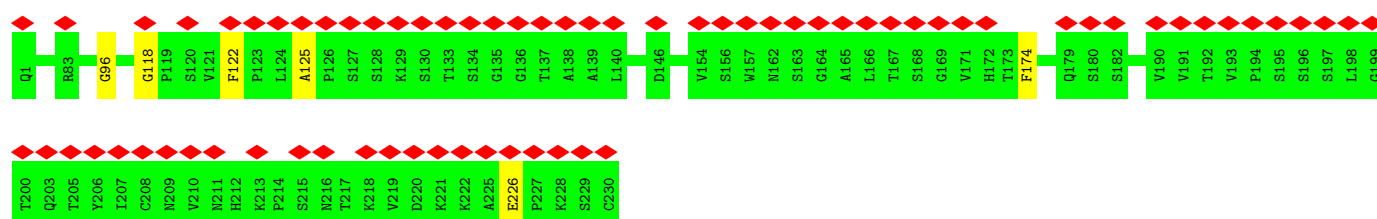


- Molecule 4: 3BC315 Fab light chain

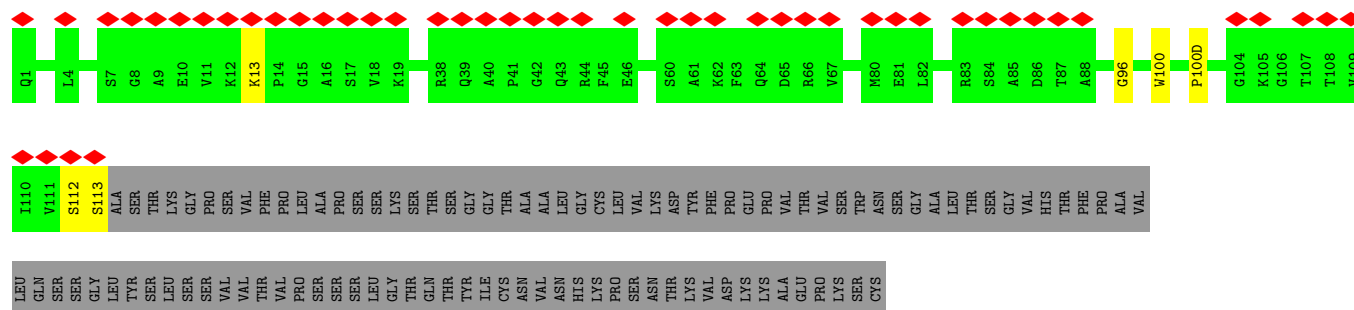




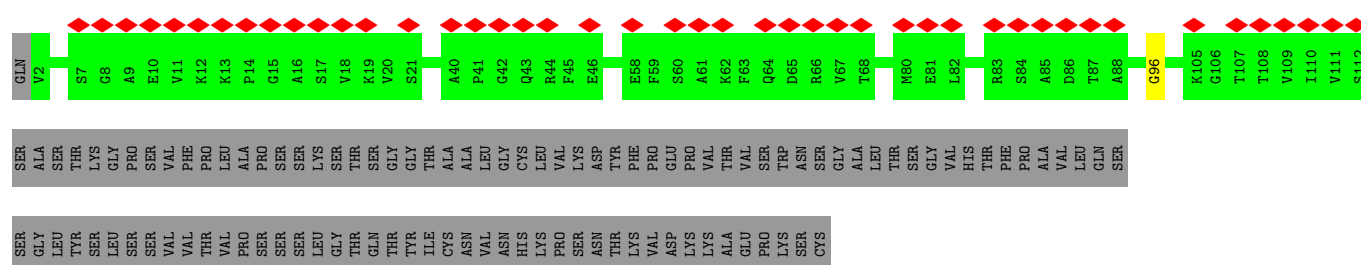
• Molecule 5: b12 Fab heavy chain



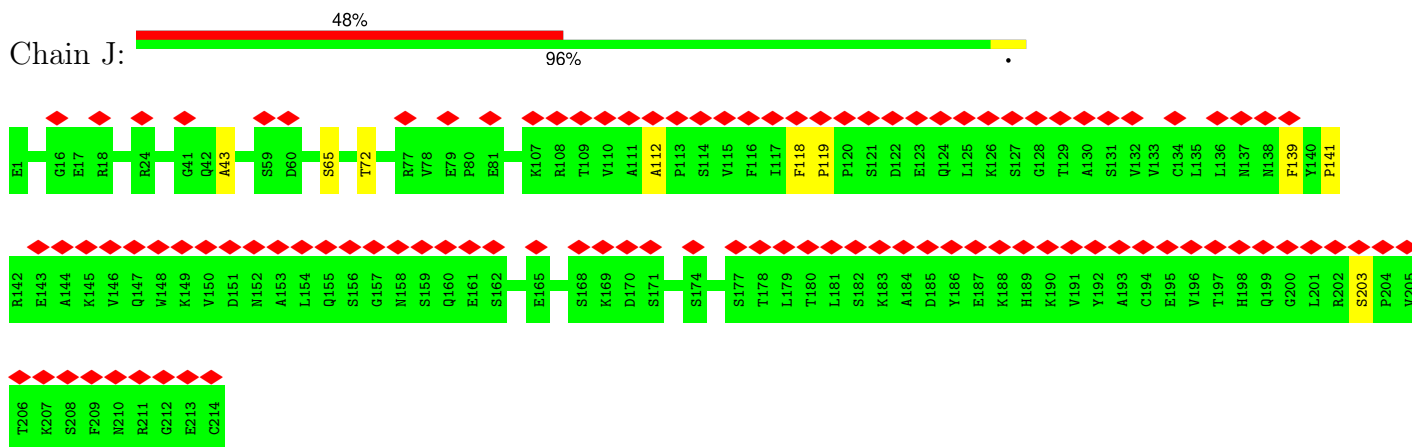
• Molecule 5: b12 Fab heavy chain



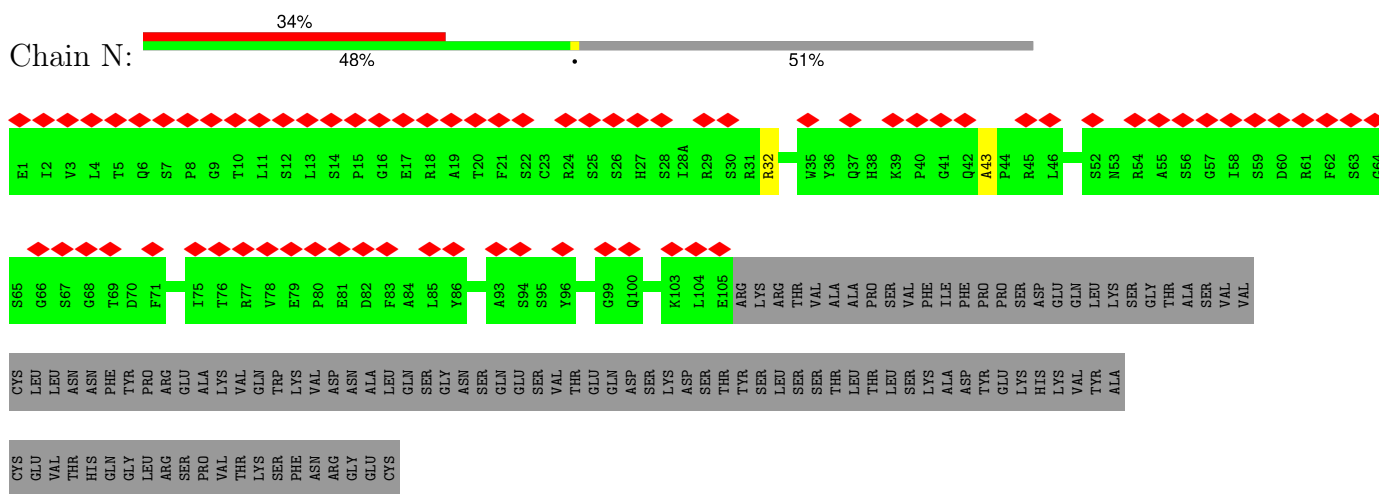
• Molecule 5: b12 Fab heavy chain



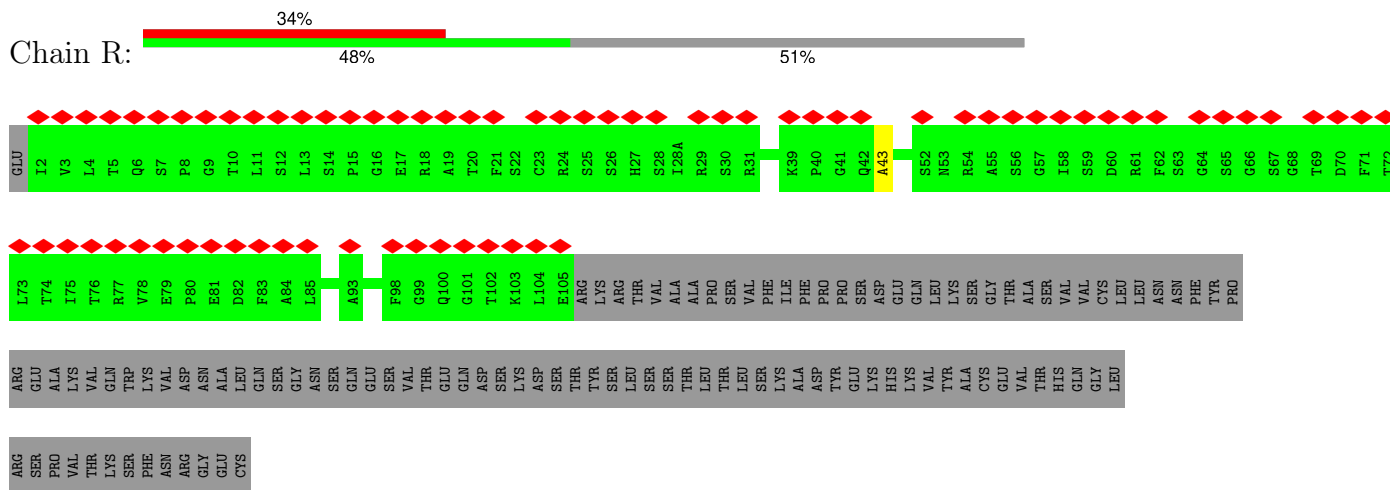
• Molecule 6: b12 Fab light chain



- Molecule 6: b12 Fab light chain



- Molecule 6: b12 Fab light chain



- 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 T:  100%



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

Chain V:  50% 100%



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

Chain W:  50% 100%



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

Chain X:  50% 100%



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

Chain a:  50% 50%

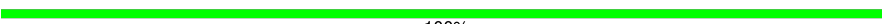


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50% 100%



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

Chain e:  100%



- 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 i:  100%



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

Chain l:  100%



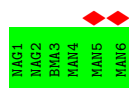
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%

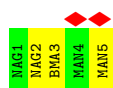


- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 100%



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

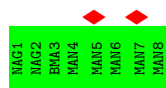


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(

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



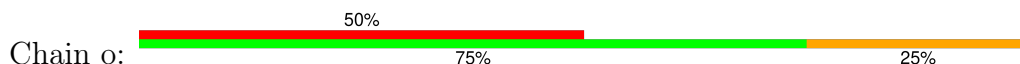
- Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.937	Depositor
Minimum map value	-0.760	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	421.6, 421.6, 421.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3632	0.95	34/4939 (0.7%)
1	C	0.62	0/3632	0.95	34/4939 (0.7%)
1	E	0.62	0/3632	0.94	37/4939 (0.7%)
2	B	0.59	0/991	0.66	2/1342 (0.1%)
2	D	0.60	0/1012	0.64	2/1371 (0.1%)
2	F	0.61	0/969	0.65	2/1313 (0.2%)
3	G	0.57	0/1745	0.99	20/2374 (0.8%)
3	K	0.57	0/1019	0.91	4/1379 (0.3%)
3	O	0.58	0/1020	0.92	4/1381 (0.3%)
4	H	0.59	0/1611	1.00	18/2196 (0.8%)
4	L	0.57	0/825	0.98	8/1120 (0.7%)
4	P	0.57	0/813	0.97	8/1104 (0.7%)
5	I	0.61	0/1801	0.96	12/2455 (0.5%)
5	M	0.60	0/1042	0.89	4/1416 (0.3%)
5	Q	0.59	0/1027	0.85	2/1396 (0.1%)
6	J	0.62	0/1704	0.92	10/2306 (0.4%)
6	N	0.61	0/835	0.90	2/1130 (0.2%)
6	R	0.59	0/826	0.92	2/1118 (0.2%)
All	All	0.60	0/28136	0.92	205/38218 (0.5%)

There are no bond length outliers.

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ALA	CA-C-N	8.30	125.72	119.66
1	A	436	ALA	C-N-CA	8.30	125.72	119.66
1	C	436	ALA	CA-C-N	7.96	125.39	119.66
1	C	436	ALA	C-N-CA	7.96	125.39	119.66
1	A	492	GLU	CA-C-N	7.83	127.47	119.56
1	A	492	GLU	C-N-CA	7.83	127.47	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	CYS	CA-C-N	7.79	127.50	119.56
1	C	205	CYS	C-N-CA	7.79	127.50	119.56
1	C	492	GLU	CA-C-N	7.72	127.36	119.56
1	C	492	GLU	C-N-CA	7.72	127.36	119.56
1	E	492	GLU	CA-C-N	7.70	127.41	119.56
1	E	492	GLU	C-N-CA	7.70	127.41	119.56
1	E	436	ALA	CA-C-N	7.63	125.23	119.66
1	E	436	ALA	C-N-CA	7.63	125.23	119.66
3	K	94	ARG	CA-C-N	7.42	127.42	119.78
3	K	94	ARG	C-N-CA	7.42	127.42	119.78
1	A	205	CYS	CA-C-N	7.35	127.06	119.56
1	A	205	CYS	C-N-CA	7.35	127.06	119.56
3	O	94	ARG	CA-C-N	7.24	127.17	119.85
3	O	94	ARG	C-N-CA	7.24	127.17	119.85
1	C	219	THR	CA-C-N	7.23	127.19	120.03
1	C	219	THR	C-N-CA	7.23	127.19	120.03
4	P	54	ARG	CA-C-N	7.15	127.15	119.78
4	P	54	ARG	C-N-CA	7.15	127.15	119.78
1	C	237	GLY	CA-C-N	7.14	127.11	119.76
1	C	237	GLY	C-N-CA	7.14	127.11	119.76
5	Q	96	GLY	CA-C-N	7.13	127.05	119.85
5	Q	96	GLY	C-N-CA	7.13	127.05	119.85
5	I	118	GLY	CA-C-N	7.10	127.02	119.85
5	I	118	GLY	C-N-CA	7.10	127.02	119.85
1	A	237	GLY	CA-C-N	7.07	126.99	119.85
1	A	237	GLY	C-N-CA	7.07	126.99	119.85
1	E	205	CYS	CA-C-N	7.04	126.74	119.56
1	E	205	CYS	C-N-CA	7.04	126.74	119.56
5	I	96	GLY	CA-C-N	6.97	126.89	119.85
5	I	96	GLY	C-N-CA	6.97	126.89	119.85
1	E	219	THR	CA-C-N	6.88	126.84	120.03
1	E	219	THR	C-N-CA	6.88	126.84	120.03
1	A	219	THR	CA-C-N	6.82	126.78	120.03
1	A	219	THR	C-N-CA	6.82	126.78	120.03
4	L	54	ARG	CA-C-N	6.80	126.77	120.03
4	L	54	ARG	C-N-CA	6.80	126.77	120.03
6	J	112	ALA	CA-C-N	6.78	126.95	120.31
6	J	112	ALA	C-N-CA	6.78	126.95	120.31
1	C	368	ASP	CA-C-N	6.68	127.22	119.47
1	C	368	ASP	C-N-CA	6.68	127.22	119.47
1	E	298	ARG	CA-C-N	6.67	126.36	119.56
1	E	298	ARG	C-N-CA	6.67	126.36	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	237	GLY	CA-C-N	6.66	126.42	119.76
1	E	237	GLY	C-N-CA	6.66	126.42	119.76
1	E	368	ASP	CA-C-N	6.65	126.59	119.28
1	E	368	ASP	C-N-CA	6.65	126.59	119.28
4	H	118	PHE	CA-C-N	6.62	127.20	120.38
4	H	118	PHE	C-N-CA	6.62	127.20	120.38
1	C	298	ARG	CA-C-N	6.55	126.24	119.56
1	C	298	ARG	C-N-CA	6.55	126.24	119.56
1	A	298	ARG	CA-C-N	6.51	126.20	119.56
1	A	298	ARG	C-N-CA	6.51	126.20	119.56
5	M	96	GLY	CA-C-N	6.50	126.42	119.85
5	M	96	GLY	C-N-CA	6.50	126.42	119.85
6	N	43	ALA	CA-C-N	6.48	126.45	119.78
6	N	43	ALA	C-N-CA	6.48	126.45	119.78
3	G	118	GLY	CA-C-N	6.47	126.38	119.85
3	G	118	GLY	C-N-CA	6.47	126.38	119.85
4	H	112	ASN	CA-C-N	6.46	126.37	119.85
4	H	112	ASN	C-N-CA	6.46	126.37	119.85
3	G	212	GLU	CA-C-N	6.39	126.34	119.76
3	G	212	GLU	C-N-CA	6.39	126.34	119.76
4	H	54	ARG	CA-C-N	6.37	126.55	120.31
4	H	54	ARG	C-N-CA	6.37	126.55	120.31
1	C	78	ASP	CA-C-N	6.33	125.95	119.56
1	C	78	ASP	C-N-CA	6.33	125.95	119.56
3	G	94	ARG	CA-C-N	6.31	126.22	119.85
3	G	94	ARG	C-N-CA	6.31	126.22	119.85
1	A	211	GLU	CA-C-N	6.28	126.23	119.76
1	A	211	GLU	C-N-CA	6.28	126.23	119.76
6	J	118	PHE	CA-C-N	6.27	126.84	120.38
6	J	118	PHE	C-N-CA	6.27	126.84	120.38
4	L	58	ILE	CA-C-N	6.26	126.23	119.78
4	L	58	ILE	C-N-CA	6.26	126.23	119.78
4	H	58	ILE	CA-C-N	6.26	126.22	119.78
4	H	58	ILE	C-N-CA	6.26	126.22	119.78
1	A	368	ASP	CA-C-N	6.25	126.15	119.28
1	A	368	ASP	C-N-CA	6.25	126.15	119.28
3	G	125	ALA	CA-C-N	6.22	126.13	119.85
3	G	125	ALA	C-N-CA	6.22	126.13	119.85
1	E	469	ARG	CA-C-N	6.20	126.11	119.85
1	E	469	ARG	C-N-CA	6.20	126.11	119.85
4	H	119	PRO	CA-C-N	6.07	126.03	119.78
4	H	119	PRO	C-N-CA	6.07	126.03	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LYS	CA-C-N	6.05	125.67	119.56
1	A	117	LYS	C-N-CA	6.05	125.67	119.56
4	L	43	VAL	CA-C-N	6.05	126.01	119.78
4	L	43	VAL	C-N-CA	6.05	126.01	119.78
6	R	43	ALA	CA-C-N	6.01	125.92	119.85
6	R	43	ALA	C-N-CA	6.01	125.92	119.85
1	A	469	ARG	CA-C-N	5.98	125.89	119.85
1	A	469	ARG	C-N-CA	5.98	125.89	119.85
2	F	608	VAL	CA-C-N	5.96	125.92	119.78
2	F	608	VAL	C-N-CA	5.96	125.92	119.78
1	A	75	VAL	CA-C-N	5.92	125.88	119.78
1	A	75	VAL	C-N-CA	5.92	125.88	119.78
3	O	97	ARG	CA-C-N	5.92	125.83	119.85
3	O	97	ARG	C-N-CA	5.92	125.83	119.85
1	C	75	VAL	CA-C-N	5.92	125.87	119.78
1	C	75	VAL	C-N-CA	5.92	125.87	119.78
5	I	226	GLU	CA-C-N	5.91	125.92	119.90
5	I	226	GLU	C-N-CA	5.91	125.92	119.90
1	E	182	VAL	CA-C-N	5.87	125.78	119.85
1	E	182	VAL	C-N-CA	5.87	125.78	119.85
1	C	117	LYS	CA-C-N	5.87	125.54	119.56
1	C	117	LYS	C-N-CA	5.87	125.54	119.56
4	P	43	VAL	CA-C-N	5.84	125.75	119.85
4	P	43	VAL	C-N-CA	5.84	125.75	119.85
5	I	174	PHE	CA-C-N	5.82	125.77	119.78
5	I	174	PHE	C-N-CA	5.82	125.77	119.78
4	H	43	VAL	CA-C-N	5.82	125.77	119.78
4	H	43	VAL	C-N-CA	5.82	125.77	119.78
5	I	122	PHE	CA-C-N	5.81	125.74	119.76
5	I	122	PHE	C-N-CA	5.81	125.74	119.76
2	B	608	VAL	CA-C-N	5.79	125.69	119.85
2	B	608	VAL	C-N-CA	5.79	125.69	119.85
3	G	166	PHE	CA-C-N	5.78	125.72	119.76
3	G	166	PHE	C-N-CA	5.78	125.72	119.76
1	E	80	SER	CA-C-N	5.73	125.64	119.85
1	E	80	SER	C-N-CA	5.73	125.64	119.85
1	C	469	ARG	CA-C-N	5.72	125.63	119.85
1	C	469	ARG	C-N-CA	5.72	125.63	119.85
6	J	43	ALA	CA-C-N	5.72	125.62	119.85
6	J	43	ALA	C-N-CA	5.72	125.62	119.85
1	A	182	VAL	CA-C-N	5.70	125.63	119.76
1	A	182	VAL	C-N-CA	5.70	125.63	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	SER	CA-C-N	5.67	125.58	119.85
1	C	80	SER	C-N-CA	5.67	125.58	119.85
3	G	122	PHE	CA-C-N	5.67	125.58	119.85
3	G	122	PHE	C-N-CA	5.67	125.58	119.85
3	G	184	VAL	CA-C-N	5.66	125.59	119.76
3	G	184	VAL	C-N-CA	5.66	125.59	119.76
4	P	6	GLN	CA-C-N	5.59	125.52	119.76
4	P	6	GLN	C-N-CA	5.59	125.52	119.76
1	C	123	THR	CA-C-N	5.59	125.26	119.56
1	C	123	THR	C-N-CA	5.59	125.26	119.56
4	P	58	ILE	CA-C-N	5.59	125.54	119.78
4	P	58	ILE	C-N-CA	5.59	125.54	119.78
3	K	97	ARG	CA-C-N	5.54	125.48	119.78
3	K	97	ARG	C-N-CA	5.54	125.48	119.78
1	C	437	PRO	CA-C-N	5.53	125.29	119.76
1	C	437	PRO	C-N-CA	5.53	125.29	119.76
1	A	437	PRO	CA-C-N	5.50	125.40	119.85
1	A	437	PRO	C-N-CA	5.50	125.40	119.85
1	E	117	LYS	CA-C-N	5.48	125.15	119.56
1	E	117	LYS	C-N-CA	5.48	125.15	119.56
1	E	437	PRO	CA-C-N	5.47	125.38	119.85
1	E	437	PRO	C-N-CA	5.47	125.38	119.85
1	E	497	ALA	CA-C-N	5.44	125.20	119.76
1	E	497	ALA	C-N-CA	5.44	125.20	119.76
1	A	497	ALA	CA-C-N	5.44	125.20	119.76
1	A	497	ALA	C-N-CA	5.44	125.20	119.76
1	E	75	VAL	CA-C-N	5.43	125.44	119.90
1	E	75	VAL	C-N-CA	5.43	125.44	119.90
1	E	211	GLU	CA-C-N	5.43	125.19	119.76
1	E	211	GLU	C-N-CA	5.43	125.19	119.76
1	E	123	THR	CA-C-N	5.41	125.08	119.56
1	E	123	THR	C-N-CA	5.41	125.08	119.56
1	C	497	ALA	CA-C-N	5.41	125.17	119.76
1	C	497	ALA	C-N-CA	5.41	125.17	119.76
1	E	78	ASP	CA-C-N	5.39	125.73	119.47
1	E	78	ASP	C-N-CA	5.39	125.73	119.47
2	D	608	VAL	CA-C-N	5.39	125.29	119.85
2	D	608	VAL	C-N-CA	5.39	125.29	119.85
4	L	6	GLN	CA-C-N	5.36	125.27	119.85
4	L	6	GLN	C-N-CA	5.36	125.27	119.85
4	H	108	GLN	CA-C-N	5.33	125.25	119.76
4	H	108	GLN	C-N-CA	5.33	125.25	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	13	ASP	CA-C-N	5.29	125.21	119.76
3	G	13	ASP	C-N-CA	5.29	125.21	119.76
1	C	182	VAL	CA-C-N	5.28	125.20	119.76
1	C	182	VAL	C-N-CA	5.28	125.20	119.76
1	E	42	VAL	CA-C-N	5.28	126.44	119.84
1	E	42	VAL	C-N-CA	5.28	126.44	119.84
5	I	125	ALA	CA-C-N	5.27	125.19	119.76
5	I	125	ALA	C-N-CA	5.27	125.19	119.76
3	G	97	ARG	CA-C-N	5.24	125.18	119.78
3	G	97	ARG	C-N-CA	5.24	125.18	119.78
6	J	203	SER	CA-C-N	5.23	125.17	119.78
6	J	203	SER	C-N-CA	5.23	125.17	119.78
1	A	80	SER	CA-C-N	5.20	125.10	119.85
1	A	80	SER	C-N-CA	5.20	125.10	119.85
5	M	13	LYS	CA-C-N	5.17	125.17	119.90
5	M	13	LYS	C-N-CA	5.17	125.17	119.90
1	C	211	GLU	CA-C-N	5.11	124.87	119.76
1	C	211	GLU	C-N-CA	5.11	124.87	119.76
1	A	78	ASP	CA-C-N	5.09	124.58	119.19
1	A	78	ASP	C-N-CA	5.09	124.58	119.19
4	H	182	THR	CA-C-N	5.09	125.37	119.47
4	H	182	THR	C-N-CA	5.09	125.37	119.47
1	A	123	THR	CA-C-N	5.08	124.74	119.56
1	A	123	THR	C-N-CA	5.08	124.74	119.56
6	J	119	PRO	CA-C-N	5.08	124.99	119.76
6	J	119	PRO	C-N-CA	5.08	124.99	119.76
4	H	14	SER	CA-C-N	5.03	124.94	119.76
4	H	14	SER	C-N-CA	5.03	124.94	119.76
3	G	201	LYS	CA-C-N	5.03	124.81	119.28
3	G	201	LYS	C-N-CA	5.03	124.81	119.28
1	E	181	ILE	N-CA-C	5.02	115.08	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3559	0	3477	4	0
1	C	3559	0	3480	4	0
1	E	3559	0	3481	4	0
2	B	972	0	959	0	0
2	D	993	0	976	1	0
2	F	950	0	937	0	0
3	G	1699	0	1665	1	0
3	K	991	0	950	1	0
3	O	992	0	954	1	0
4	H	1573	0	1541	1	0
4	L	808	0	789	0	0
4	P	796	0	775	0	0
5	I	1753	0	1694	0	0
5	M	1013	0	955	3	0
5	Q	998	0	939	0	0
6	J	1668	0	1621	2	0
6	N	816	0	789	1	0
6	R	807	0	780	0	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	a	28	0	25	0	0
7	c	28	0	25	0	0
7	e	28	0	25	0	0
7	g	28	0	25	0	0
7	i	28	0	25	0	0
7	l	28	0	25	0	0
7	m	28	0	25	0	0
8	U	72	0	61	0	0
9	Y	61	0	52	1	0
10	Z	39	0	34	0	0
10	d	39	0	34	0	0
10	j	39	0	34	0	0
10	q	39	0	34	0	0
11	b	94	0	79	0	0
12	f	50	0	43	0	0
12	n	50	0	43	1	0
12	o	50	0	43	1	0
13	h	50	0	43	0	0
13	p	50	0	43	2	0
14	k	38	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	98	0	91	0	0
15	C	98	0	91	0	0
15	E	112	0	104	0	0
All	All	28821	0	27925	25	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 0.

All (25) 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)
3:K:112:SER:O	3:K:113:SER:C	2.49	0.56
1:E:386:ASN:OD1	1:E:386:ASN:C	2.53	0.51
12:o:2:NAG:H82	13:p:3:BMA:H2	1.94	0.50
1:A:123:THR:N	1:A:124:PRO:CD	2.75	0.50
1:E:123:THR:N	1:E:124:PRO:CD	2.74	0.49
2:D:655:LYS:NZ	3:O:100(D):ASP:OD2	2.45	0.49
5:M:100(D):PRO:O	6:N:32:ARG:NH2	2.46	0.48
1:C:113:ASP:OD1	1:C:432:LYS:NZ	2.47	0.47
1:C:123:THR:N	1:C:124:PRO:CD	2.78	0.47
1:A:113:ASP:OD1	1:A:432:LYS:NZ	2.47	0.47
5:M:100:TRP:N	13:p:1:NAG:O7	2.48	0.47
1:C:117:LYS:N	1:C:118:PRO:CD	2.78	0.47
5:M:112:SER:O	5:M:113:SER:C	2.57	0.46
1:E:117:LYS:N	1:E:118:PRO:CD	2.80	0.46
3:G:201:LYS:N	3:G:202:PRO:CD	2.79	0.46
6:J:139:PHE:CE2	6:J:141:PRO:O	2.69	0.46
6:J:65:SER:OG	6:J:72:THR:OG1	2.36	0.43
1:A:117:LYS:N	1:A:118:PRO:CD	2.82	0.42
9:Y:3:BMA:H62	9:Y:5:MAN:H2	1.78	0.42
1:A:78:ASP:N	1:A:79:PRO:CD	2.83	0.41
1:E:474:ASP:OD1	1:E:475:MET:N	2.54	0.41
4:H:93:ASN:HA	4:H:94:TYR:HA	1.89	0.40
14:k:1:NAG:H62	14:k:3:FUC:O2	2.21	0.40
12:n:3:BMA:O2	12:n:4:MAN:H2	2.21	0.40
1:C:88:ASN:N	1:C:88:ASN:OD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/488 (91%)	441 (99%)	5 (1%)	0	100	100
1	C	446/488 (91%)	444 (100%)	2 (0%)	0	100	100
1	E	446/488 (91%)	441 (99%)	5 (1%)	0	100	100
2	B	117/154 (76%)	116 (99%)	1 (1%)	0	100	100
2	D	119/154 (77%)	119 (100%)	0	0	100	100
2	F	115/154 (75%)	115 (100%)	0	0	100	100
3	G	219/232 (94%)	218 (100%)	1 (0%)	0	100	100
3	K	124/232 (53%)	124 (100%)	0	0	100	100
3	O	124/232 (53%)	123 (99%)	1 (1%)	0	100	100
4	H	208/216 (96%)	204 (98%)	4 (2%)	0	100	100
4	L	107/216 (50%)	106 (99%)	1 (1%)	0	100	100
4	P	105/216 (49%)	102 (97%)	3 (3%)	0	100	100
5	I	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
5	M	125/230 (54%)	125 (100%)	0	0	100	100
5	Q	123/230 (54%)	123 (100%)	0	0	100	100
6	J	213/215 (99%)	212 (100%)	1 (0%)	0	100	100
6	N	104/215 (48%)	103 (99%)	1 (1%)	0	100	100
6	R	103/215 (48%)	102 (99%)	1 (1%)	0	100	100
All	All	3472/4605 (75%)	3444 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/441 (92%)	407 (100%)	0	100	100
1	C	407/441 (92%)	407 (100%)	0	100	100
1	E	407/441 (92%)	407 (100%)	0	100	100
2	B	105/132 (80%)	105 (100%)	0	100	100
2	D	108/132 (82%)	108 (100%)	0	100	100
2	F	102/132 (77%)	102 (100%)	0	100	100
3	G	188/196 (96%)	188 (100%)	0	100	100
3	K	104/196 (53%)	104 (100%)	0	100	100
3	O	104/196 (53%)	104 (100%)	0	100	100
4	H	176/182 (97%)	176 (100%)	0	100	100
4	L	89/182 (49%)	89 (100%)	0	100	100
4	P	88/182 (48%)	88 (100%)	0	100	100
5	I	195/195 (100%)	195 (100%)	0	100	100
5	M	107/195 (55%)	107 (100%)	0	100	100
5	Q	105/195 (54%)	105 (100%)	0	100	100
6	J	187/187 (100%)	187 (100%)	0	100	100
6	N	89/187 (48%)	89 (100%)	0	100	100
6	R	88/187 (47%)	88 (100%)	0	100	100
All	All	3056/3999 (76%)	3056 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	A	328	GLN
1	A	330	HIS
1	A	352	GLN
1	A	363	GLN
1	A	442	GLN
2	B	563	GLN
1	C	92	ASN
1	C	229	ASN

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Mol	Chain	Res	Type
1	C	246	GLN
1	C	352	GLN
2	D	564	HIS
1	E	92	ASN
1	E	190	ASN
1	E	308	ASN
1	E	352	GLN
1	E	363	GLN
2	F	567	GLN
2	F	624	ASN
4	H	195	GLN
5	I	211	ASN
3	K	3	GLN
3	K	76	ASN
4	P	37	GLN
4	P	60	GLN
6	R	49	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

78 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	S	1	1,7	14,14,15	0.35	0	17,19,21	0.69	0
7	NAG	S	2	7	14,14,15	0.37	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	1	1,7	14,14,15	0.38	0	17,19,21	0.47	0
7	NAG	T	2	7	14,14,15	0.37	0	17,19,21	0.46	0
8	NAG	U	1	1,8	14,14,15	0.40	0	17,19,21	0.69	0
8	NAG	U	2	8	14,14,15	0.38	0	17,19,21	0.65	0
8	BMA	U	3	8	11,11,12	0.26	0	15,15,17	0.54	0
8	MAN	U	4	8	11,11,12	0.27	0	15,15,17	0.53	0
8	MAN	U	5	8	11,11,12	0.33	0	15,15,17	0.57	0
8	MAN	U	6	8	11,11,12	0.29	0	15,15,17	0.49	0
7	NAG	V	1	1,7	14,14,15	0.37	0	17,19,21	0.58	0
7	NAG	V	2	7	14,14,15	0.37	0	17,19,21	0.44	0
7	NAG	W	1	1,7	14,14,15	0.39	0	17,19,21	0.79	0
7	NAG	W	2	7	14,14,15	0.37	0	17,19,21	0.57	0
7	NAG	X	1	1,7	14,14,15	0.39	0	17,19,21	0.42	0
7	NAG	X	2	7	14,14,15	0.37	0	17,19,21	0.51	0
9	NAG	Y	1	1,9	14,14,15	0.38	0	17,19,21	0.60	0
9	NAG	Y	2	9	14,14,15	0.34	0	17,19,21	1.92	2 (11%)
9	BMA	Y	3	9	11,11,12	0.27	0	15,15,17	0.51	0
9	MAN	Y	4	9	11,11,12	0.29	0	15,15,17	0.50	0
9	MAN	Y	5	9	11,11,12	0.27	0	15,15,17	0.50	0
10	NAG	Z	1	1,10	14,14,15	0.38	0	17,19,21	0.76	0
10	NAG	Z	2	10	14,14,15	0.36	0	17,19,21	0.65	0
10	BMA	Z	3	10	11,11,12	0.26	0	15,15,17	0.51	0
7	NAG	a	1	1,7	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
7	NAG	a	2	7	14,14,15	0.39	0	17,19,21	0.49	0
11	NAG	b	1	1,11	14,14,15	0.43	0	17,19,21	0.63	0
11	NAG	b	2	11	14,14,15	0.37	0	17,19,21	0.62	0
11	BMA	b	3	11	11,11,12	0.31	0	15,15,17	0.53	0
11	MAN	b	4	11	11,11,12	0.35	0	15,15,17	0.44	0
11	MAN	b	5	11	11,11,12	0.27	0	15,15,17	0.65	0
11	MAN	b	6	11	11,11,12	0.40	0	15,15,17	0.46	0
11	MAN	b	7	11	11,11,12	0.32	0	15,15,17	0.46	0
11	MAN	b	8	11	11,11,12	0.29	0	15,15,17	0.54	0
7	NAG	c	1	7,2	14,14,15	0.39	0	17,19,21	0.62	0
7	NAG	c	2	7	14,14,15	0.36	0	17,19,21	0.46	0
10	NAG	d	1	1,10	14,14,15	0.39	0	17,19,21	2.04	2 (11%)
10	NAG	d	2	10	14,14,15	0.38	0	17,19,21	0.71	0
10	BMA	d	3	10	11,11,12	0.31	0	15,15,17	0.48	0
7	NAG	e	1	1,7	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	e	2	7	14,14,15	0.38	0	17,19,21	0.42	0
12	NAG	f	1	1,12	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
12	NAG	f	2	12	14,14,15	0.38	0	17,19,21	0.66	0
12	BMA	f	3	12	11,11,12	0.26	0	15,15,17	0.69	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	f	4	12	11,11,12	0.26	0	15,15,17	0.51	0
7	NAG	g	1	1,7	14,14,15	0.37	0	17,19,21	0.59	0
7	NAG	g	2	7	14,14,15	0.37	0	17,19,21	0.61	0
13	NAG	h	1	1,13	14,14,15	0.39	0	17,19,21	0.61	0
13	NAG	h	2	13	14,14,15	0.39	0	17,19,21	0.47	0
13	BMA	h	3	13	11,11,12	0.30	0	15,15,17	0.45	0
13	MAN	h	4	13	11,11,12	0.33	0	15,15,17	0.50	0
7	NAG	i	1	1,7	14,14,15	0.42	0	17,19,21	0.73	0
7	NAG	i	2	7	14,14,15	0.38	0	17,19,21	0.54	0
10	NAG	j	1	1,10	14,14,15	0.38	0	17,19,21	0.64	0
10	NAG	j	2	10	14,14,15	0.38	0	17,19,21	0.61	0
10	BMA	j	3	10	11,11,12	0.26	0	15,15,17	0.54	0
14	NAG	k	1	2,14	14,14,15	0.38	0	17,19,21	0.76	0
14	NAG	k	2	14	14,14,15	0.37	0	17,19,21	0.42	0
14	FUC	k	3	14	10,10,11	0.31	0	14,14,16	0.60	0
7	NAG	l	1	1,7	14,14,15	0.38	0	17,19,21	0.79	0
7	NAG	l	2	7	14,14,15	0.37	0	17,19,21	0.54	0
7	NAG	m	1	1,7	14,14,15	0.39	0	17,19,21	0.62	0
7	NAG	m	2	7	14,14,15	0.37	0	17,19,21	0.48	0
12	NAG	n	1	1,12	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
12	NAG	n	2	12	14,14,15	0.38	0	17,19,21	0.51	0
12	BMA	n	3	12	11,11,12	0.25	0	15,15,17	0.66	0
12	MAN	n	4	12	11,11,12	0.30	0	15,15,17	0.52	0
12	NAG	o	1	1,12	14,14,15	0.39	0	17,19,21	0.81	0
12	NAG	o	2	12	14,14,15	0.34	0	17,19,21	1.83	1 (5%)
12	BMA	o	3	12	11,11,12	0.29	0	15,15,17	0.55	0
12	MAN	o	4	12	11,11,12	0.30	0	15,15,17	0.54	0
13	NAG	p	1	1,13	14,14,15	0.42	0	17,19,21	0.75	0
13	NAG	p	2	13	14,14,15	0.37	0	17,19,21	0.79	0
13	BMA	p	3	13	11,11,12	0.21	0	15,15,17	0.63	0
13	MAN	p	4	13	11,11,12	0.27	0	15,15,17	0.56	0
10	NAG	q	1	10,2	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
10	NAG	q	2	10	14,14,15	0.37	0	17,19,21	0.57	0
10	BMA	q	3	10	11,11,12	0.27	0	15,15,17	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1
12	MAN	f	4	12	-	1/2/19/22	0/1/1/1
7	NAG	g	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	g	2	7	-	1/6/23/26	0/1/1/1
13	NAG	h	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	h	2	13	-	0/6/23/26	0/1/1/1
13	BMA	h	3	13	-	0/2/19/22	0/1/1/1
13	MAN	h	4	13	-	0/2/19/22	0/1/1/1
7	NAG	i	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	1/6/23/26	0/1/1/1
10	NAG	j	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	j	2	10	-	0/6/23/26	0/1/1/1
10	BMA	j	3	10	-	1/2/19/22	0/1/1/1
14	NAG	k	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	k	2	14	-	0/6/23/26	0/1/1/1
14	FUC	k	3	14	-	-	0/1/1/1
7	NAG	l	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	l	2	7	-	1/6/23/26	0/1/1/1
7	NAG	m	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	m	2	7	-	0/6/23/26	0/1/1/1
12	NAG	n	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	n	2	12	-	0/6/23/26	0/1/1/1
12	BMA	n	3	12	-	0/2/19/22	0/1/1/1
12	MAN	n	4	12	-	1/2/19/22	0/1/1/1
12	NAG	o	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	o	2	12	-	1/6/23/26	0/1/1/1
12	BMA	o	3	12	-	1/2/19/22	0/1/1/1
12	MAN	o	4	12	-	1/2/19/22	0/1/1/1
13	NAG	p	1	1,13	-	0/6/23/26	0/1/1/1
13	NAG	p	2	13	-	0/6/23/26	0/1/1/1
13	BMA	p	3	13	-	1/2/19/22	0/1/1/1
13	MAN	p	4	13	-	0/2/19/22	0/1/1/1
10	NAG	q	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	q	2	10	-	0/6/23/26	0/1/1/1
10	BMA	q	3	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	o	2	NAG	C2-N2-C7	7.09	132.40	122.90
9	Y	2	NAG	C2-N2-C7	6.95	132.21	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	1	NAG	C2-N2-C7	6.04	131.00	122.90
10	d	1	NAG	C1-C2-N2	5.04	118.37	110.43
10	q	1	NAG	C1-C2-N2	2.49	114.36	110.43
9	Y	2	NAG	C1-C2-N2	-2.43	106.60	110.43
7	a	1	NAG	C1-C2-N2	2.26	114.00	110.43
12	n	1	NAG	C1-O5-C5	2.04	114.92	112.19
12	f	3	BMA	C1-O5-C5	2.03	114.90	112.19
12	f	1	NAG	C1-C2-N2	2.01	113.59	110.43

There are no chirality outliers.

All (29) torsion outliers are listed below:

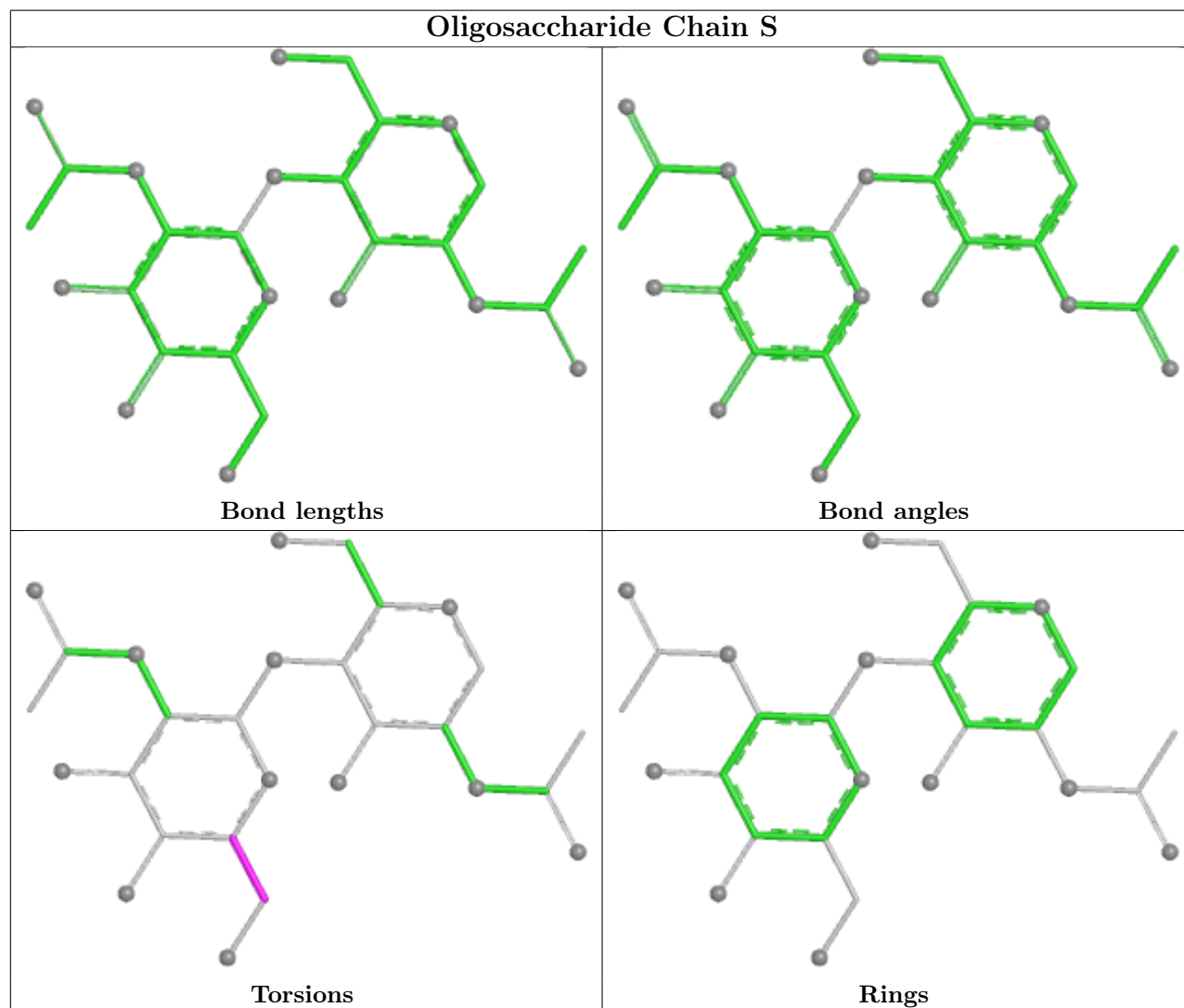
Mol	Chain	Res	Type	Atoms
9	Y	2	NAG	C3-C2-N2-C7
10	d	1	NAG	C1-C2-N2-C7
12	o	2	NAG	C3-C2-N2-C7
10	j	1	NAG	C8-C7-N2-C2
10	j	1	NAG	O7-C7-N2-C2
11	b	2	NAG	C8-C7-N2-C2
11	b	2	NAG	O7-C7-N2-C2
9	Y	3	BMA	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
9	Y	4	MAN	O5-C5-C6-O6
10	d	3	BMA	O5-C5-C6-O6
10	j	3	BMA	O5-C5-C6-O6
11	b	5	MAN	O5-C5-C6-O6
11	b	6	MAN	O5-C5-C6-O6
11	b	8	MAN	O5-C5-C6-O6
12	f	4	MAN	O5-C5-C6-O6
12	n	4	MAN	O5-C5-C6-O6
12	o	3	BMA	O5-C5-C6-O6
12	o	4	MAN	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
13	p	3	BMA	O5-C5-C6-O6

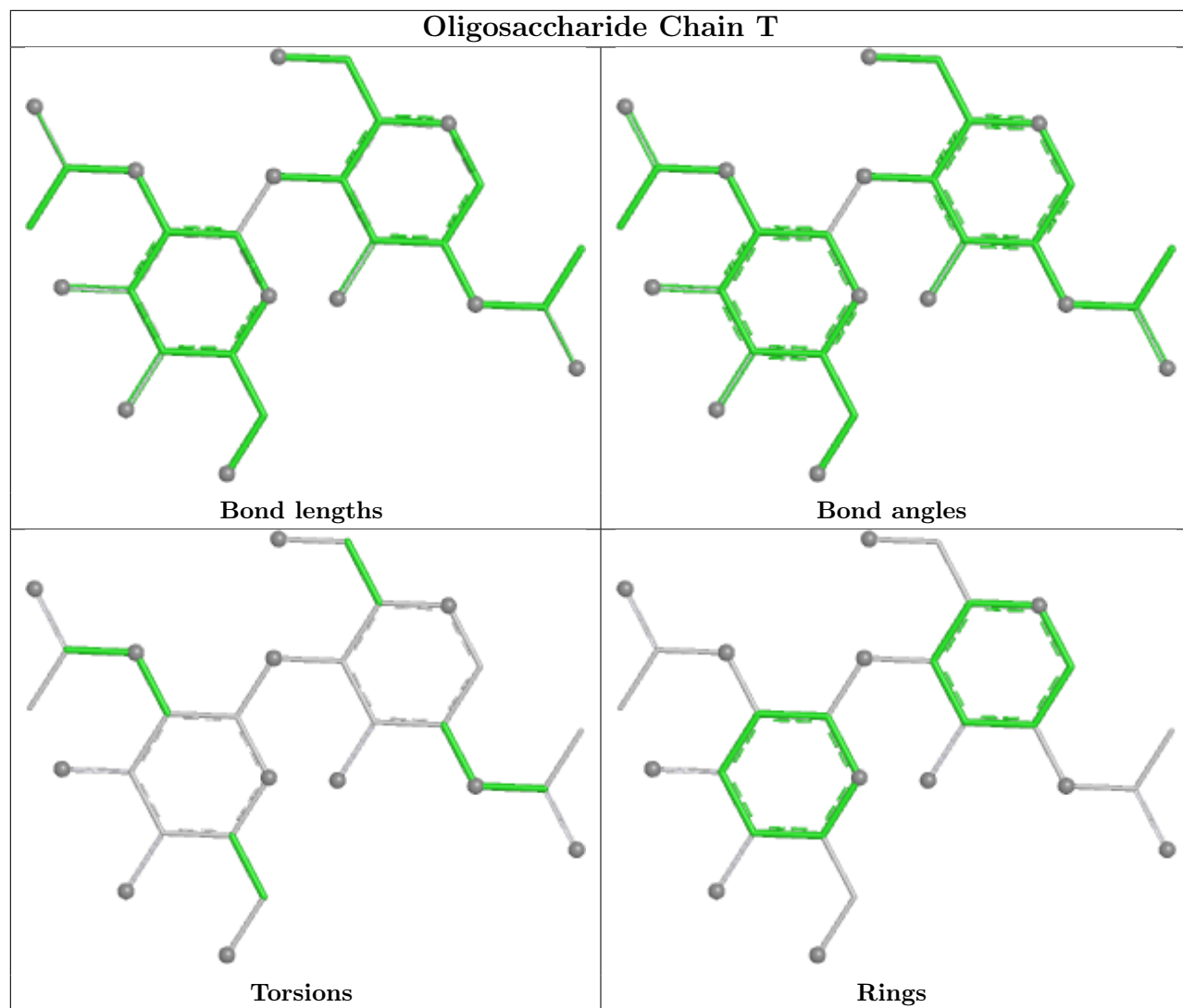
There are no ring outliers.

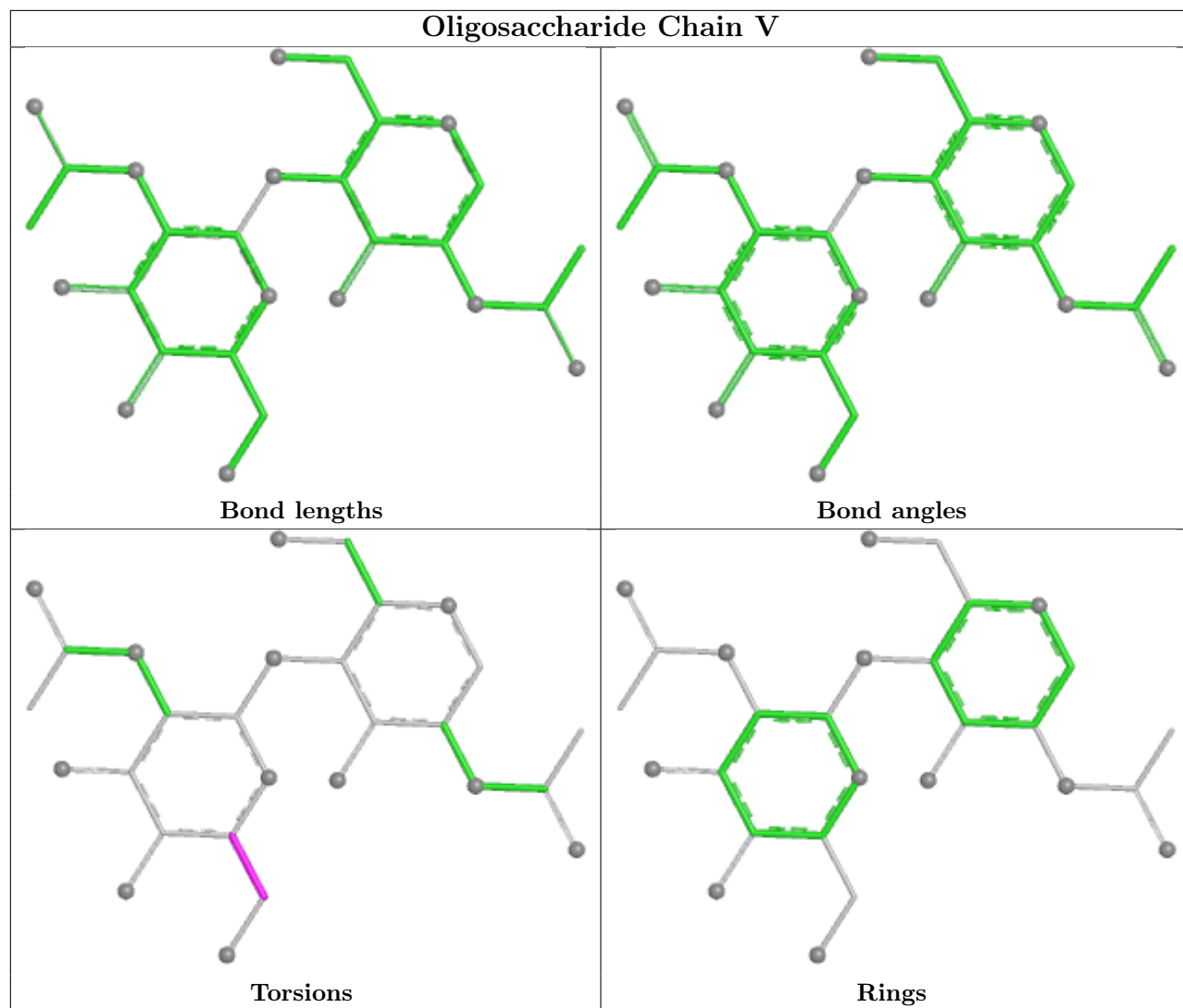
9 monomers are involved in 5 short contacts:

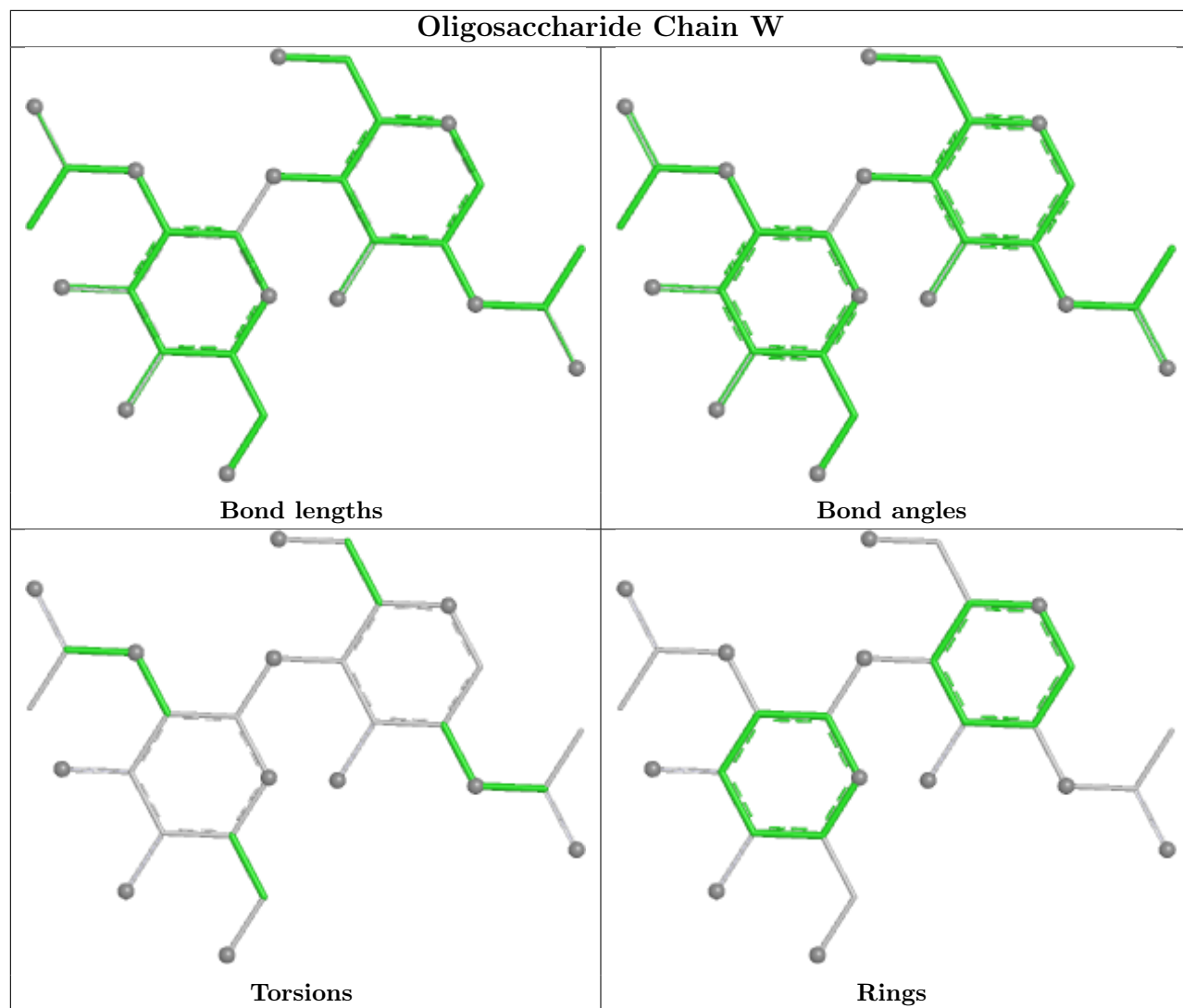
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	k	1	NAG	1	0
14	k	3	FUC	1	0
12	n	4	MAN	1	0
13	p	1	NAG	1	0
9	Y	5	MAN	1	0
12	n	3	BMA	1	0
13	p	3	BMA	1	0
12	o	2	NAG	1	0
9	Y	3	BMA	1	0

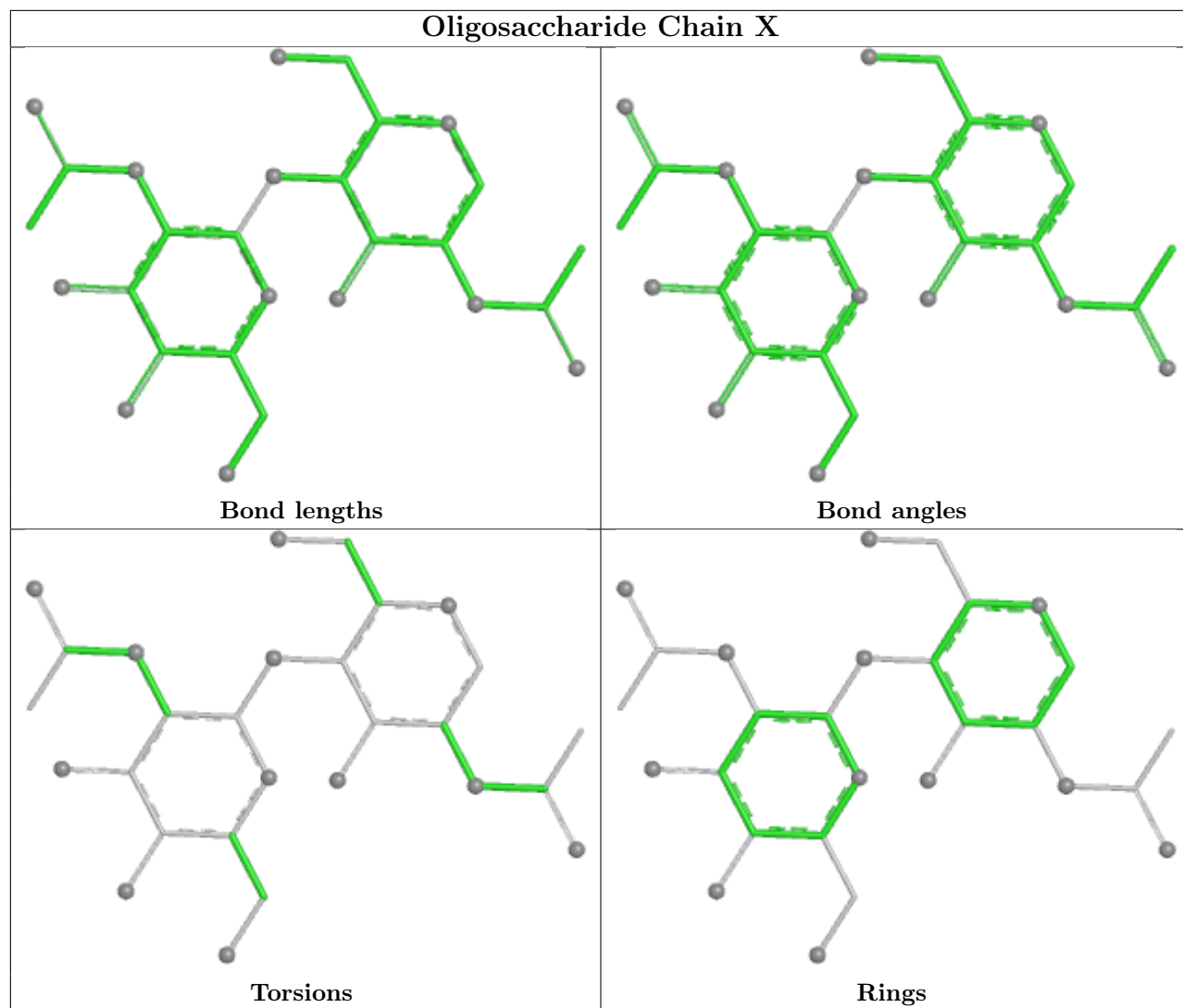
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

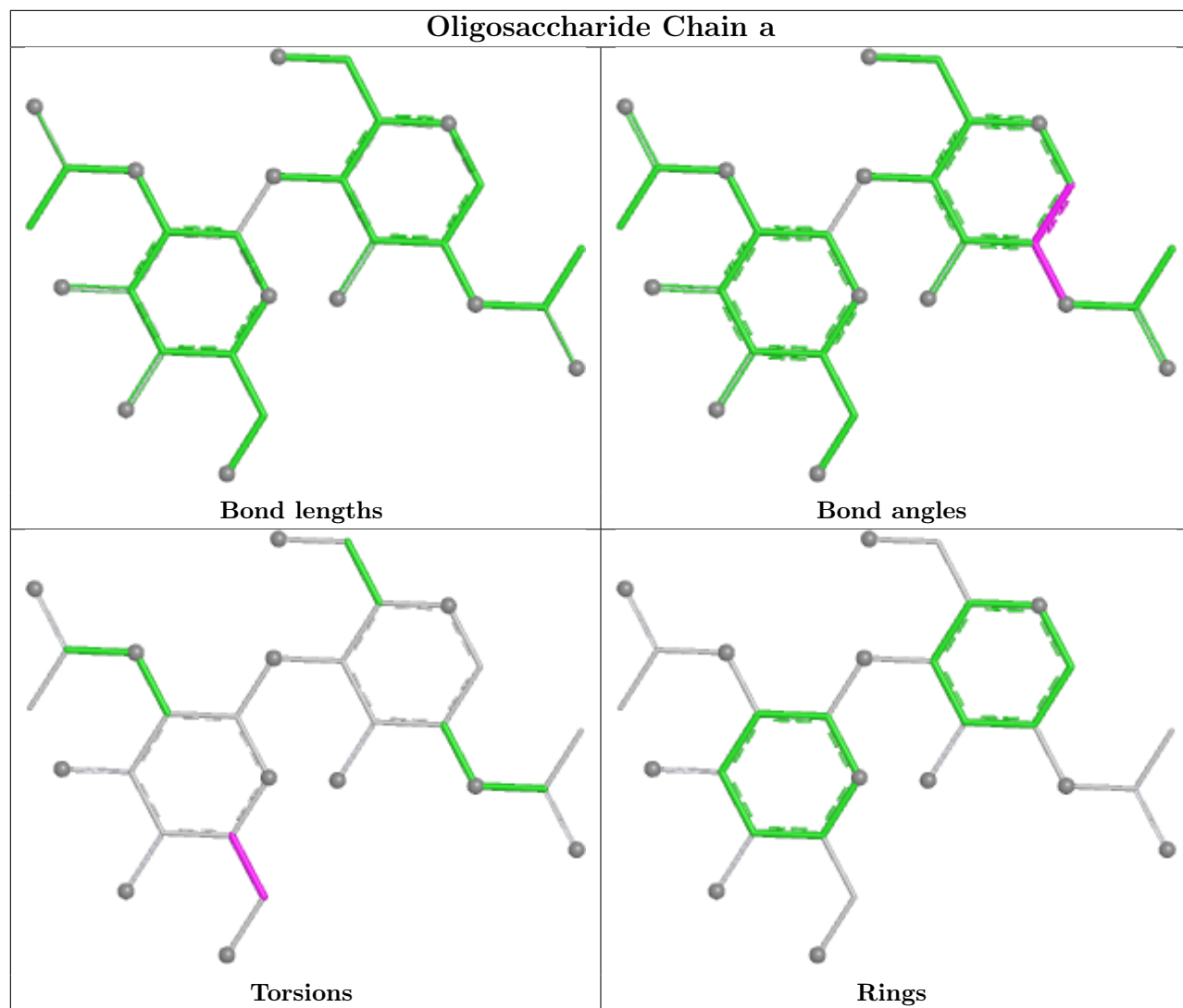


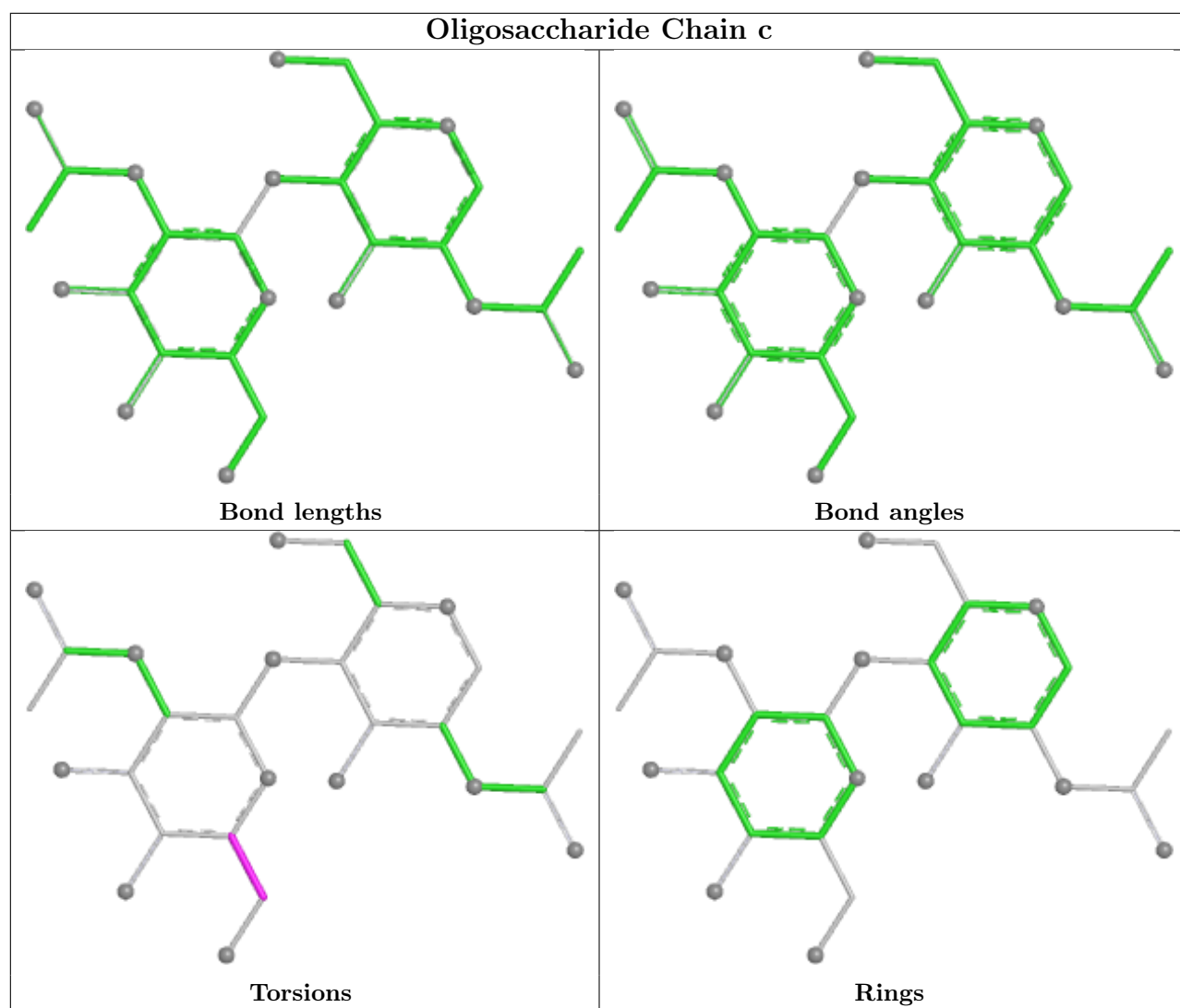


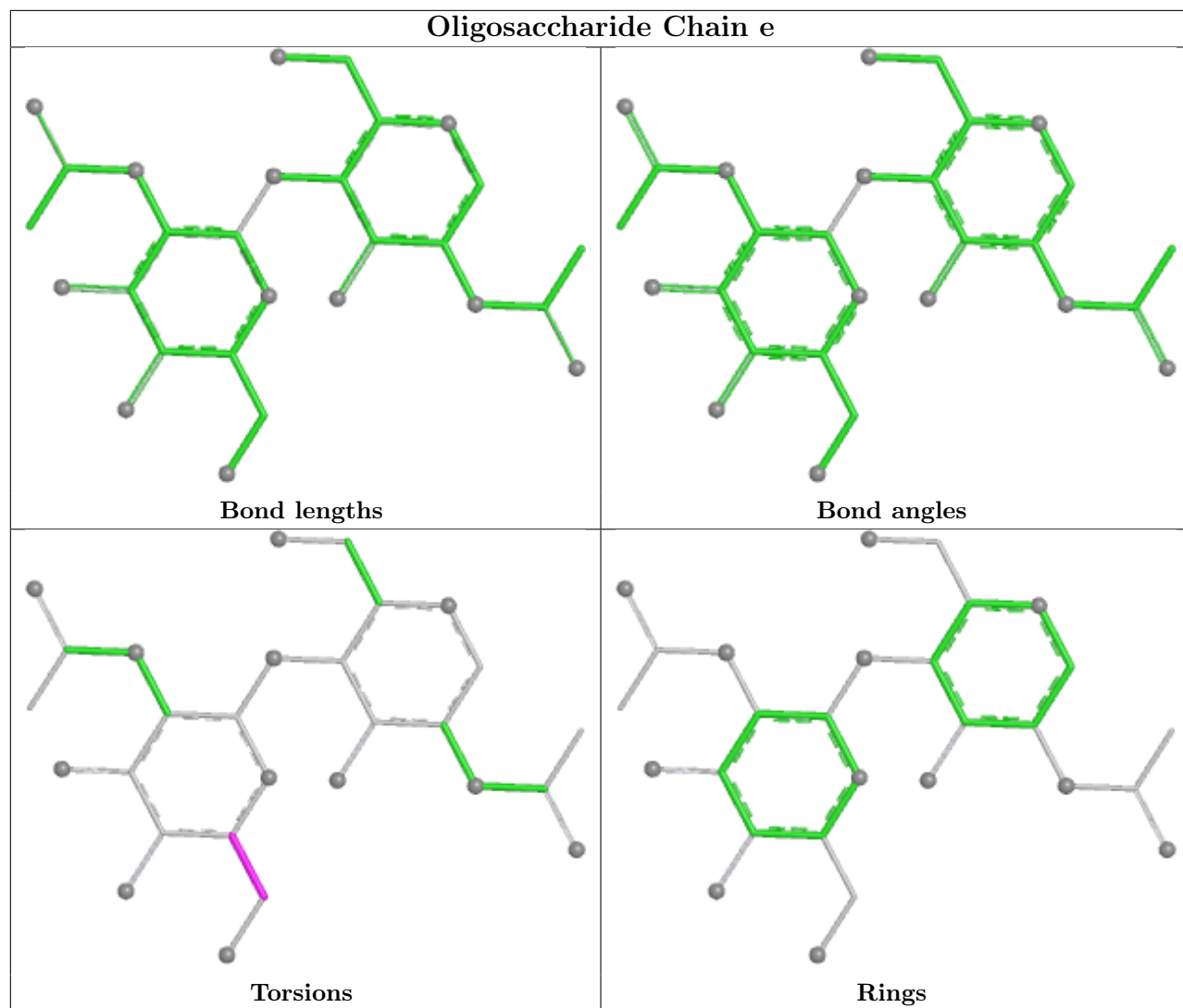


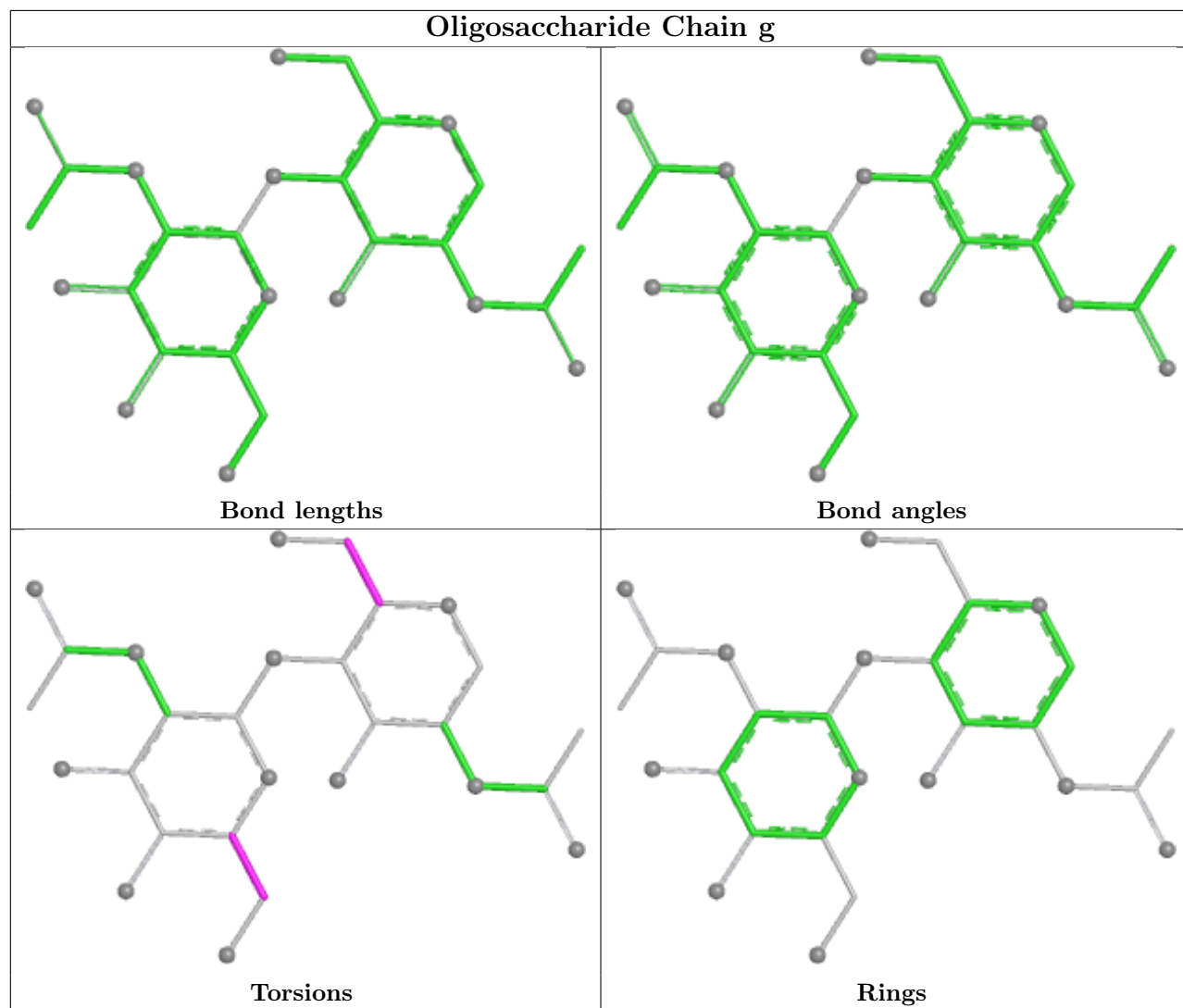


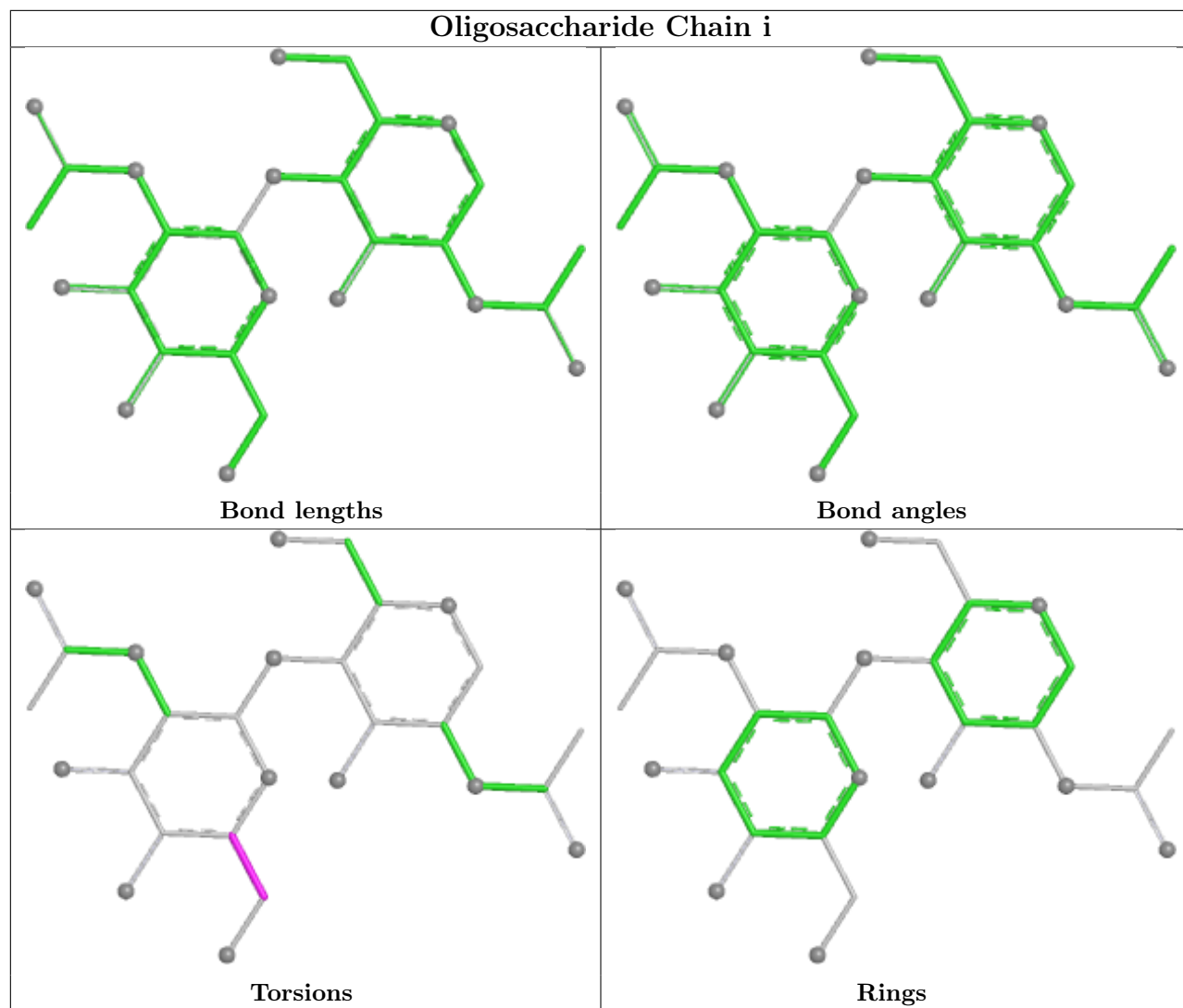


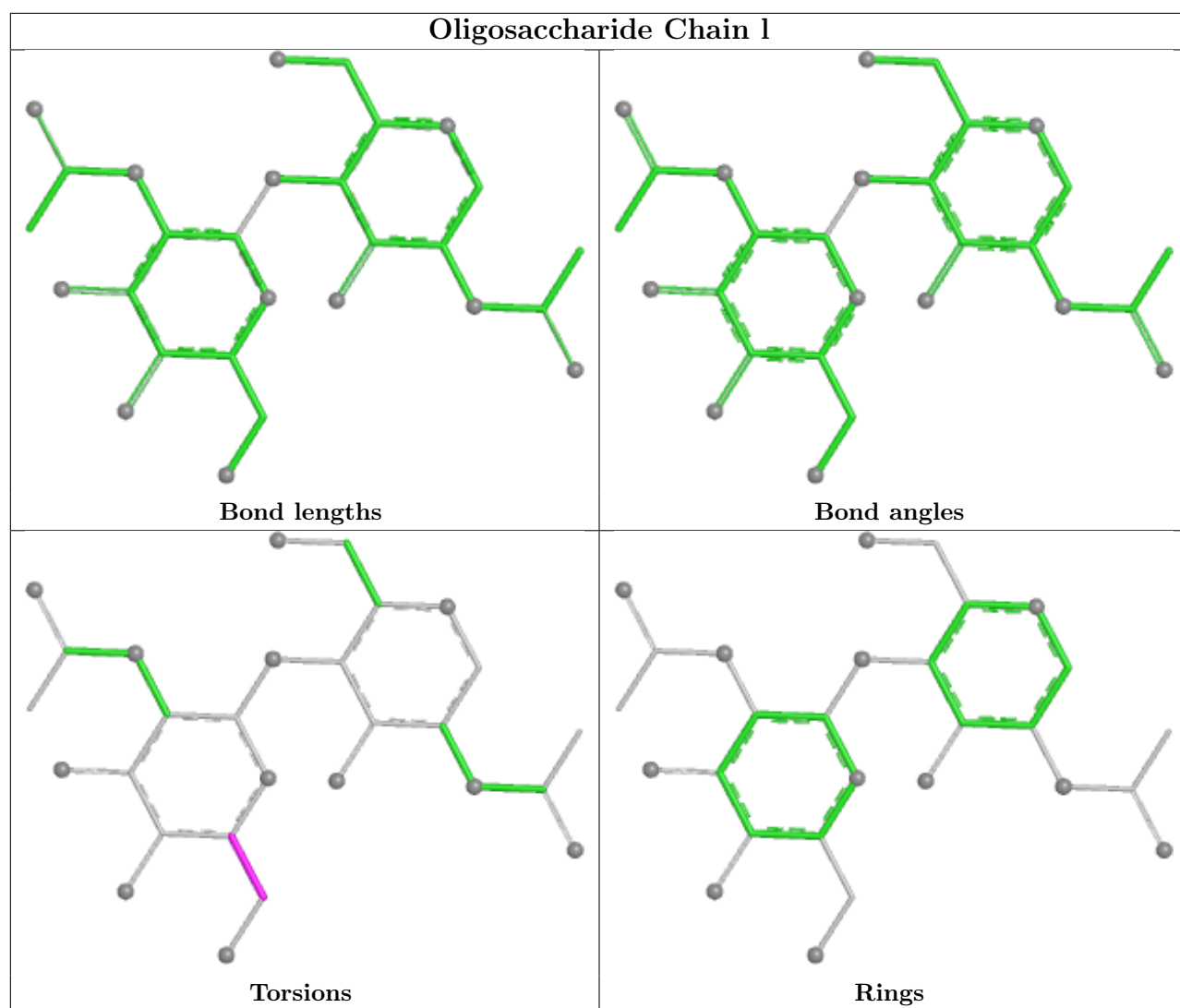


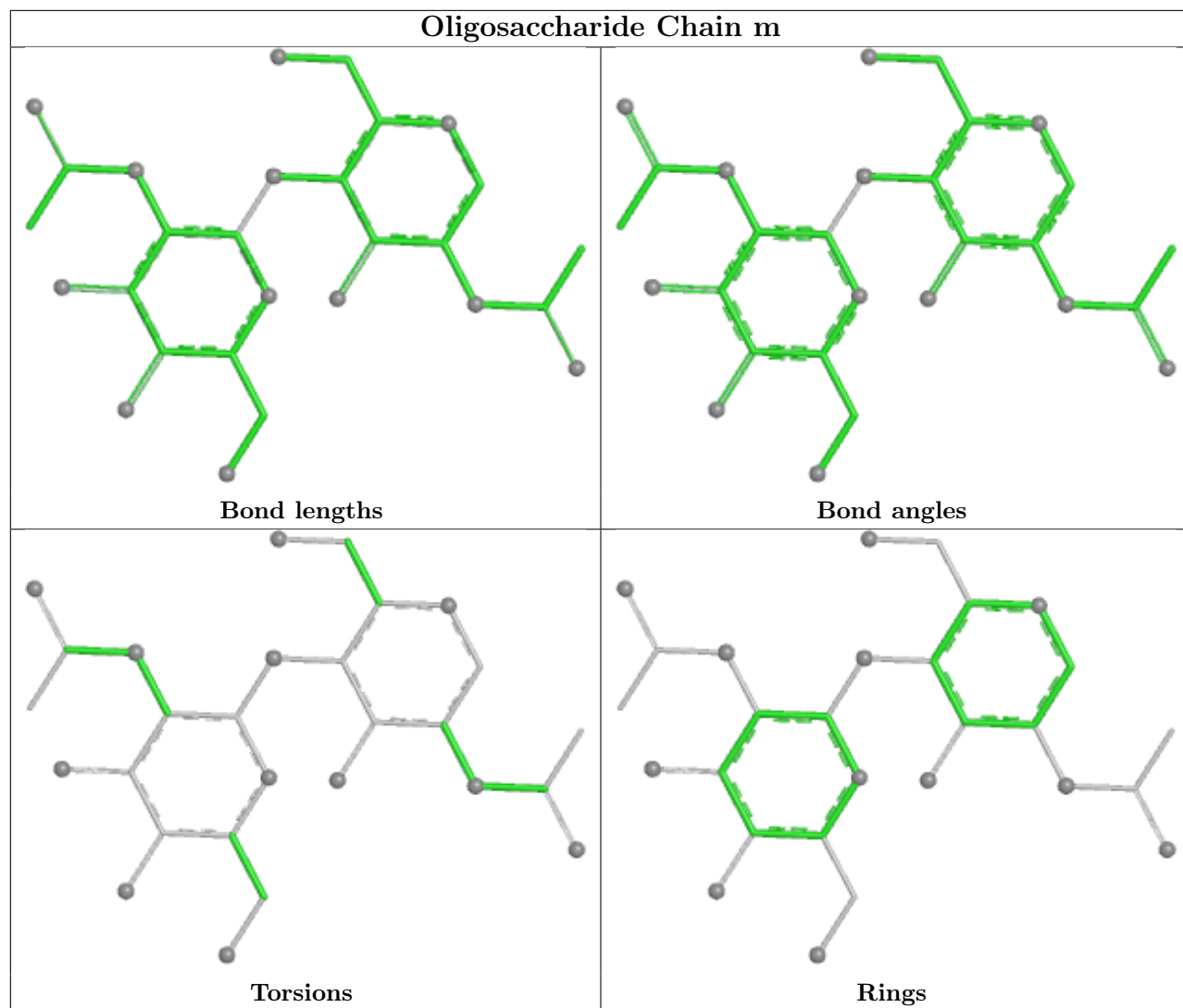


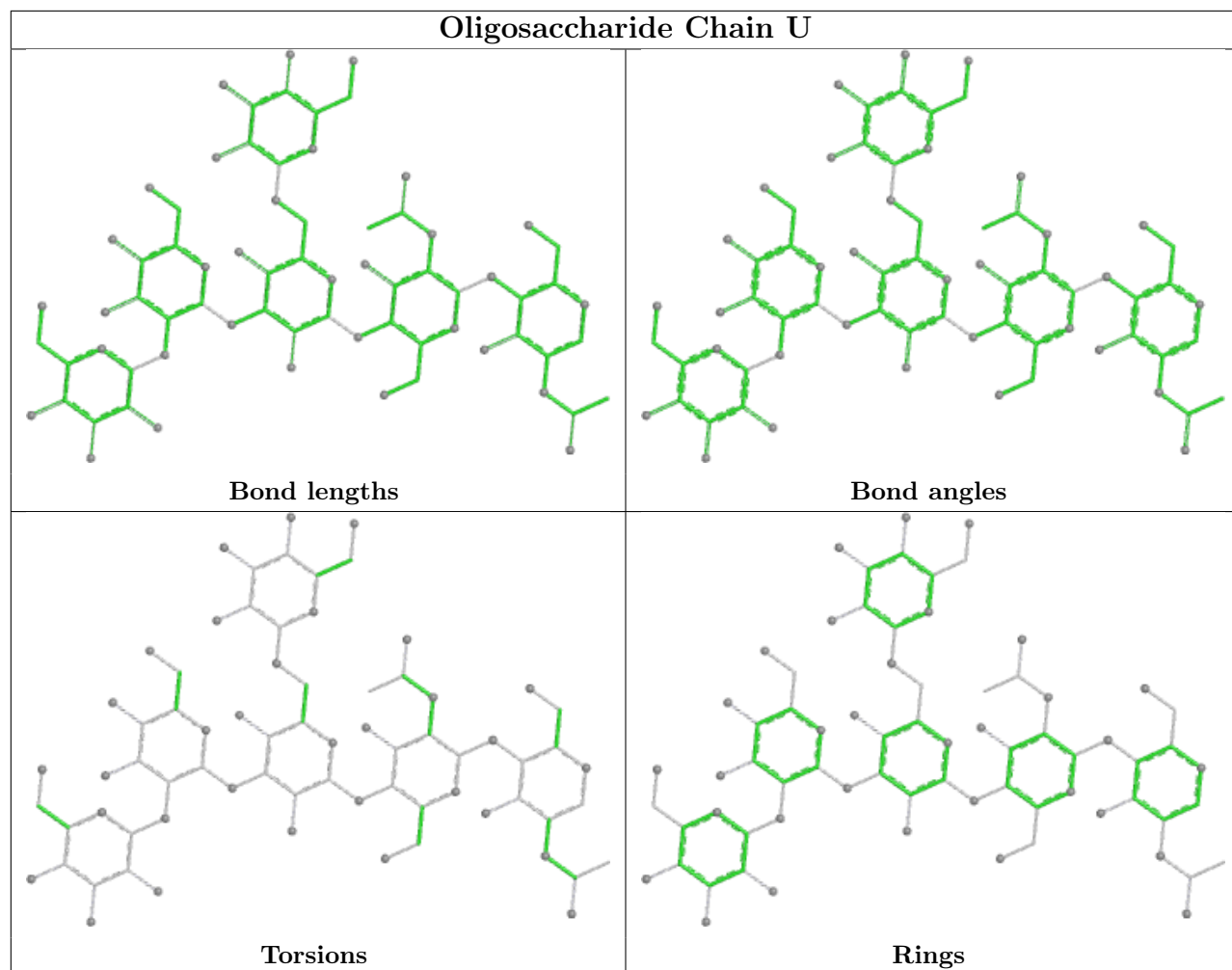




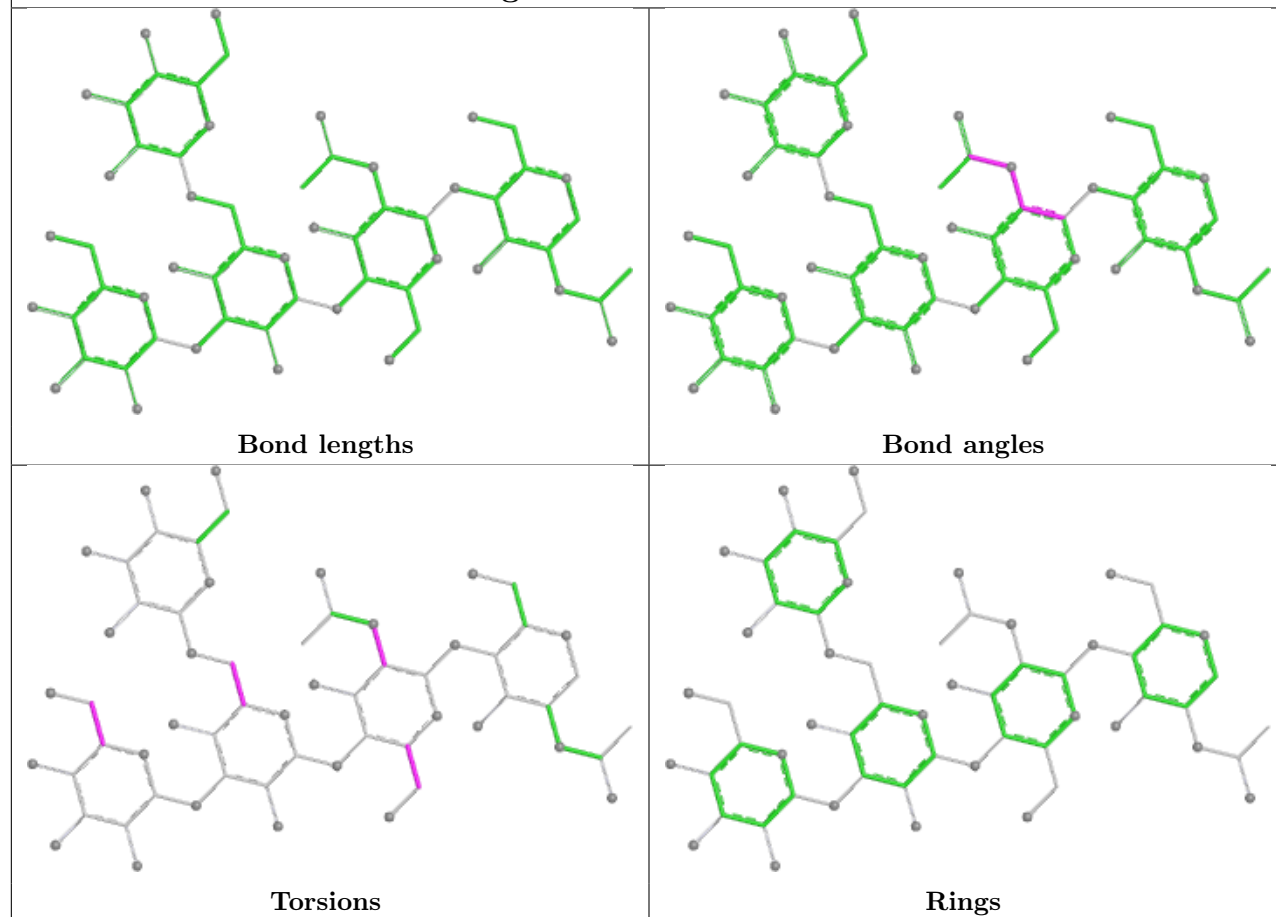




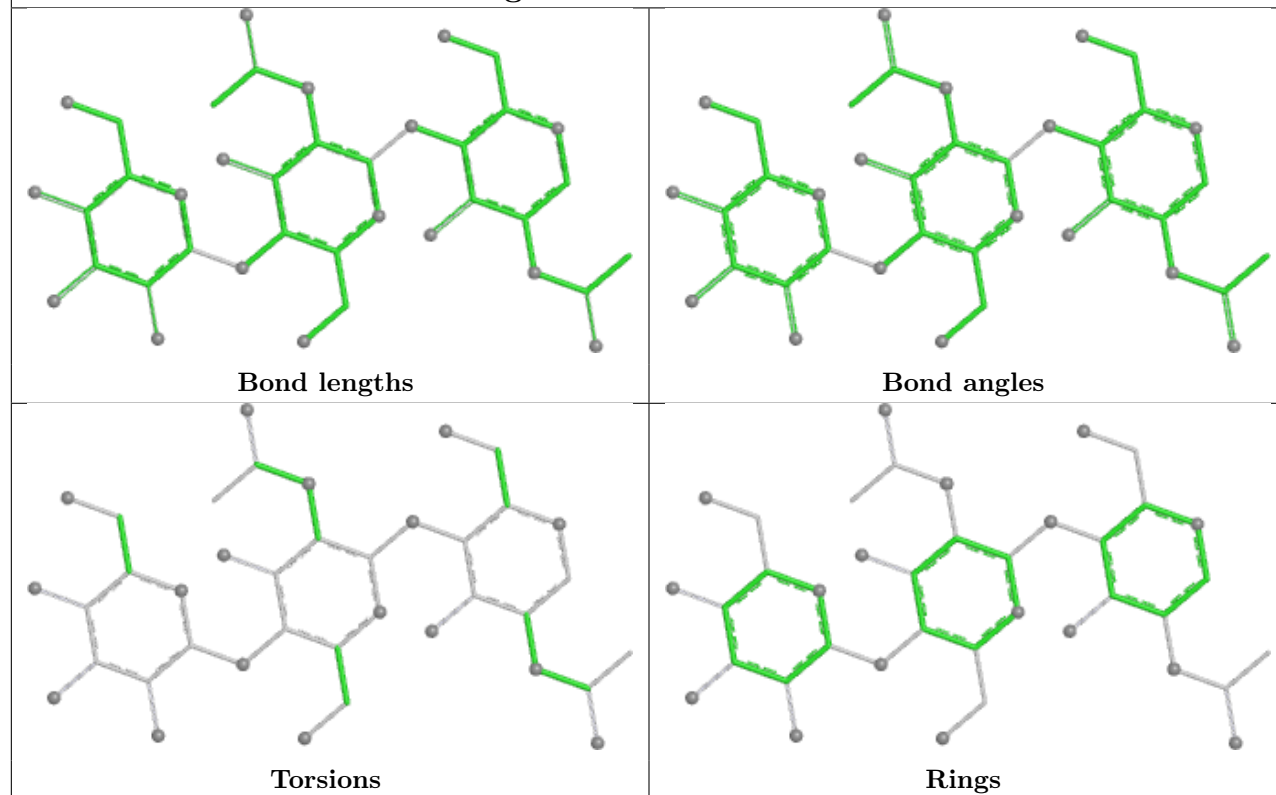


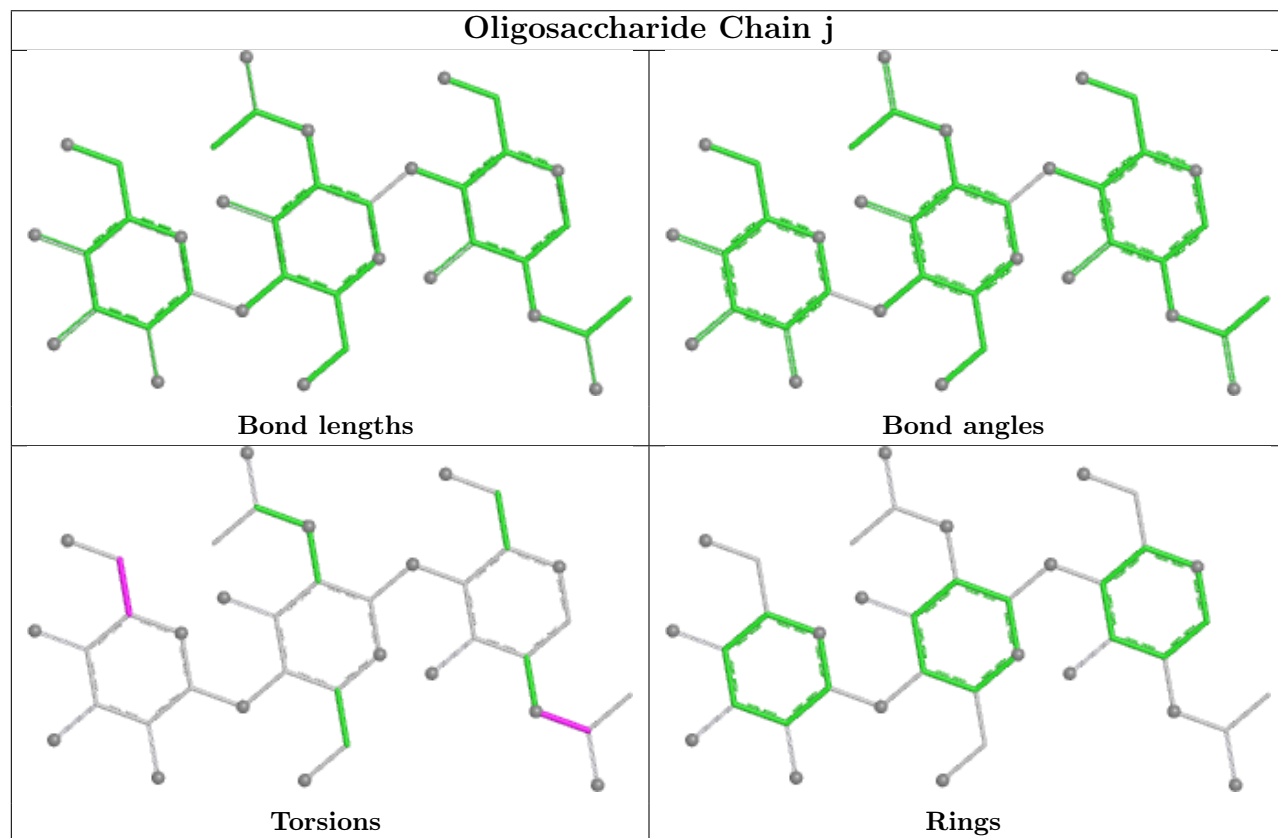
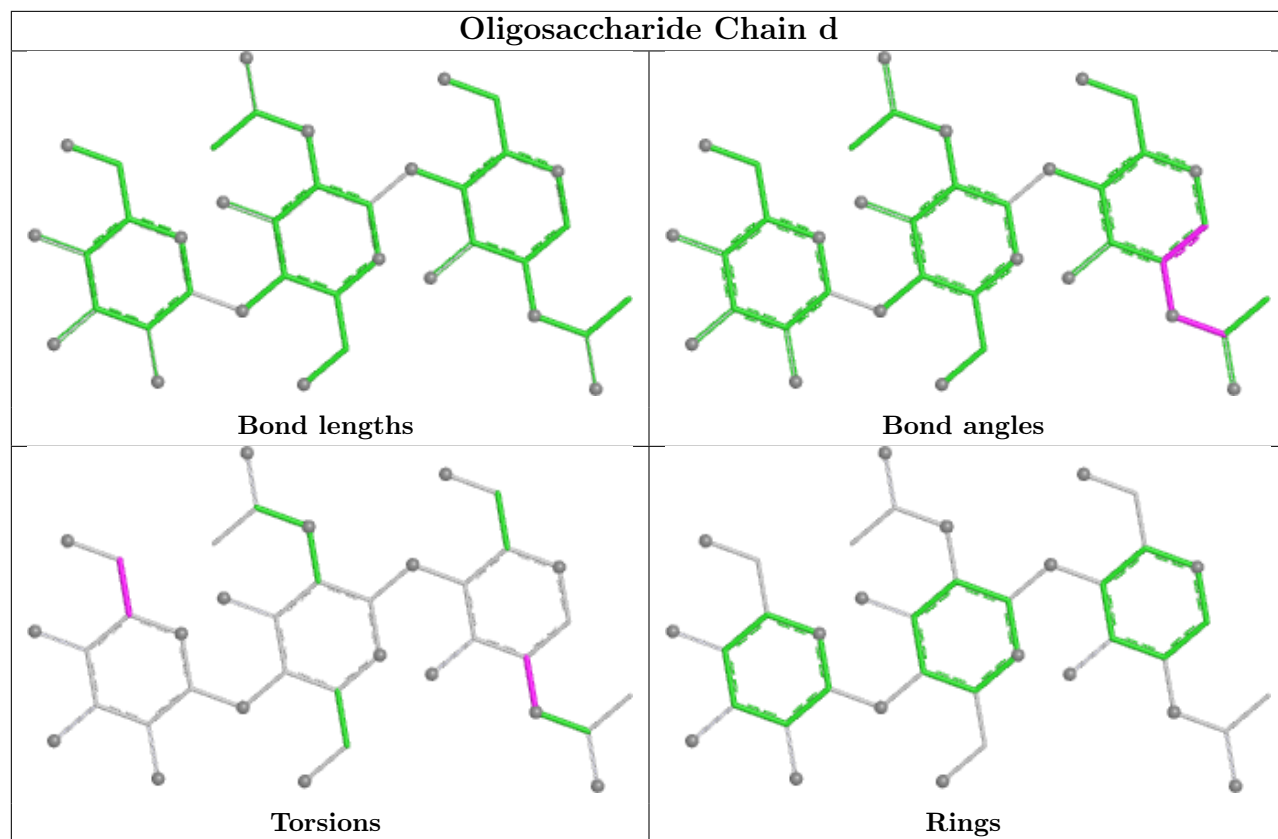


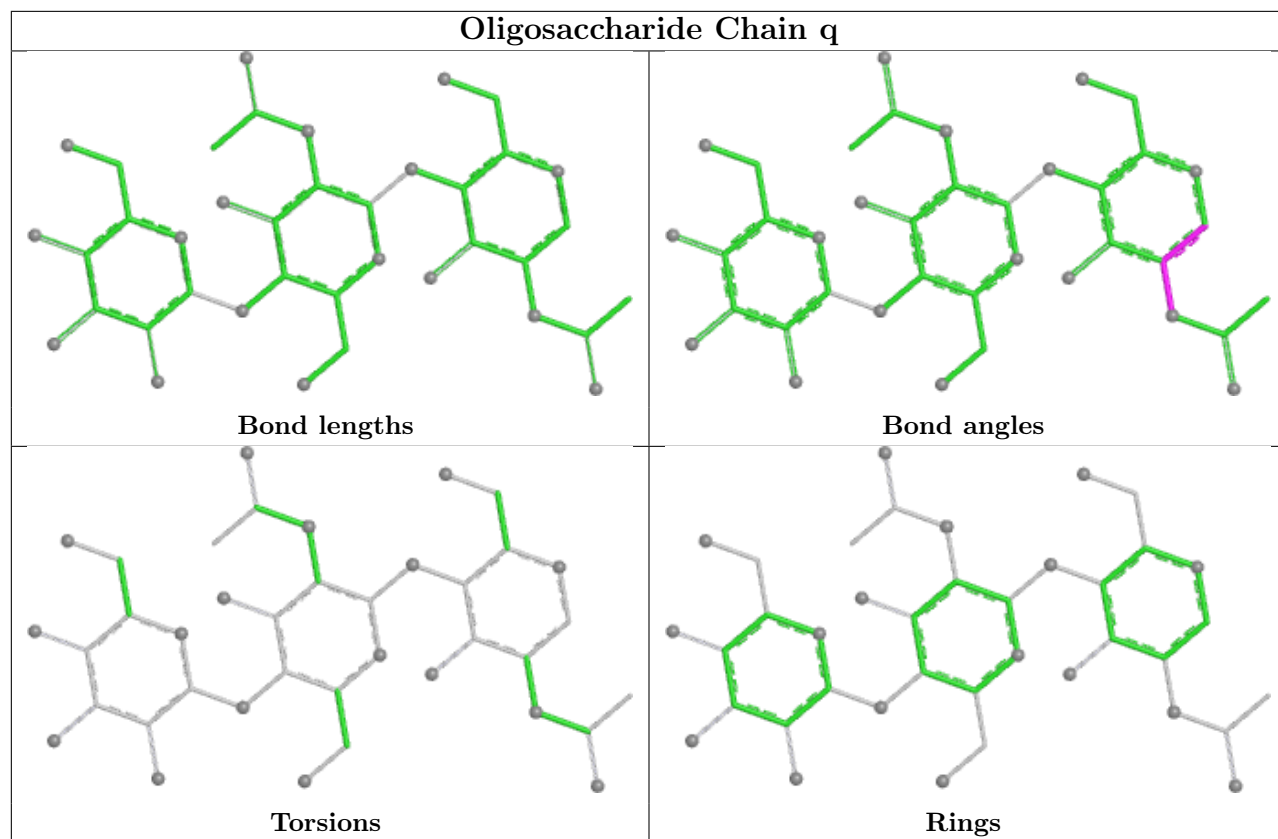
Oligosaccharide Chain Y

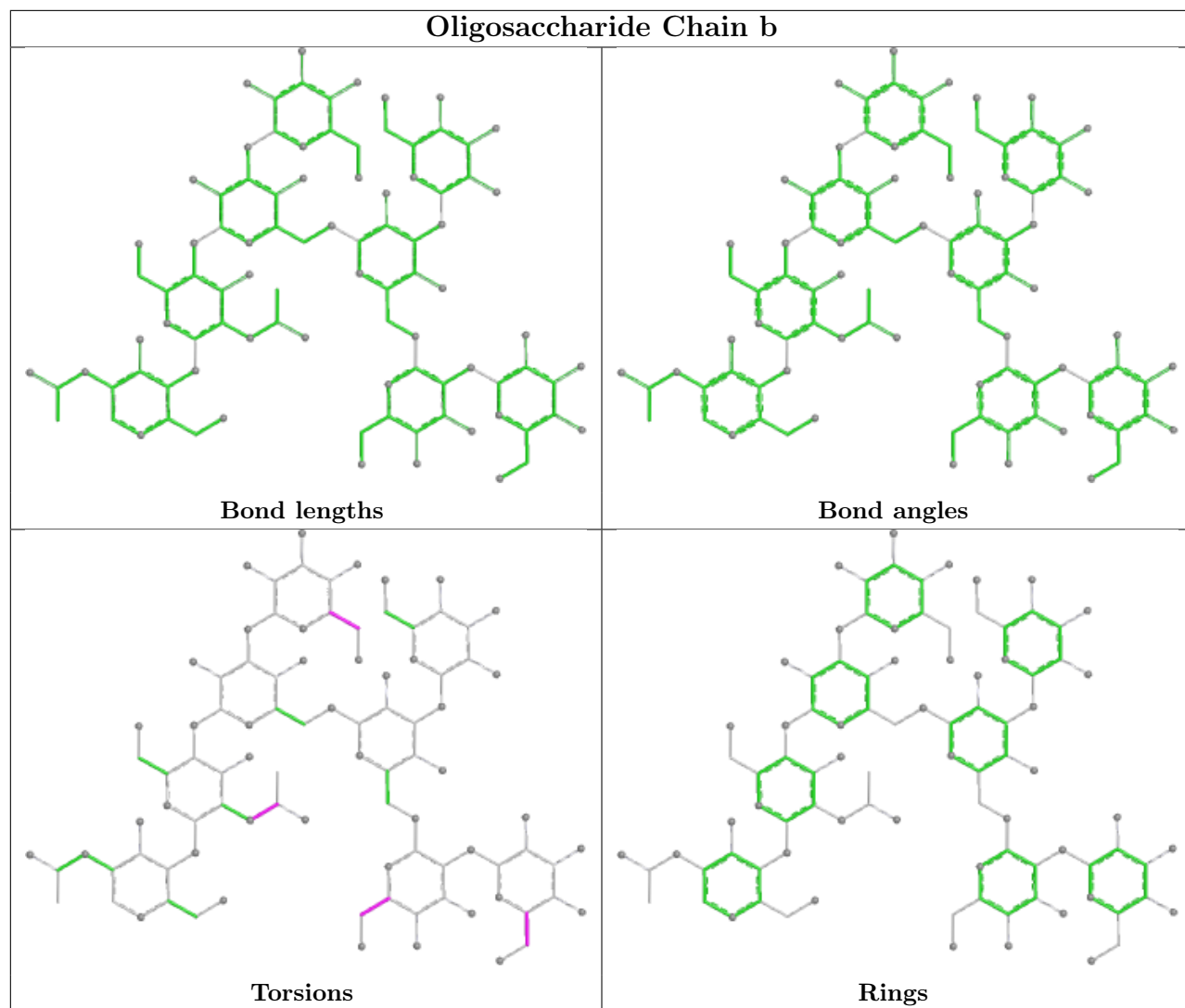


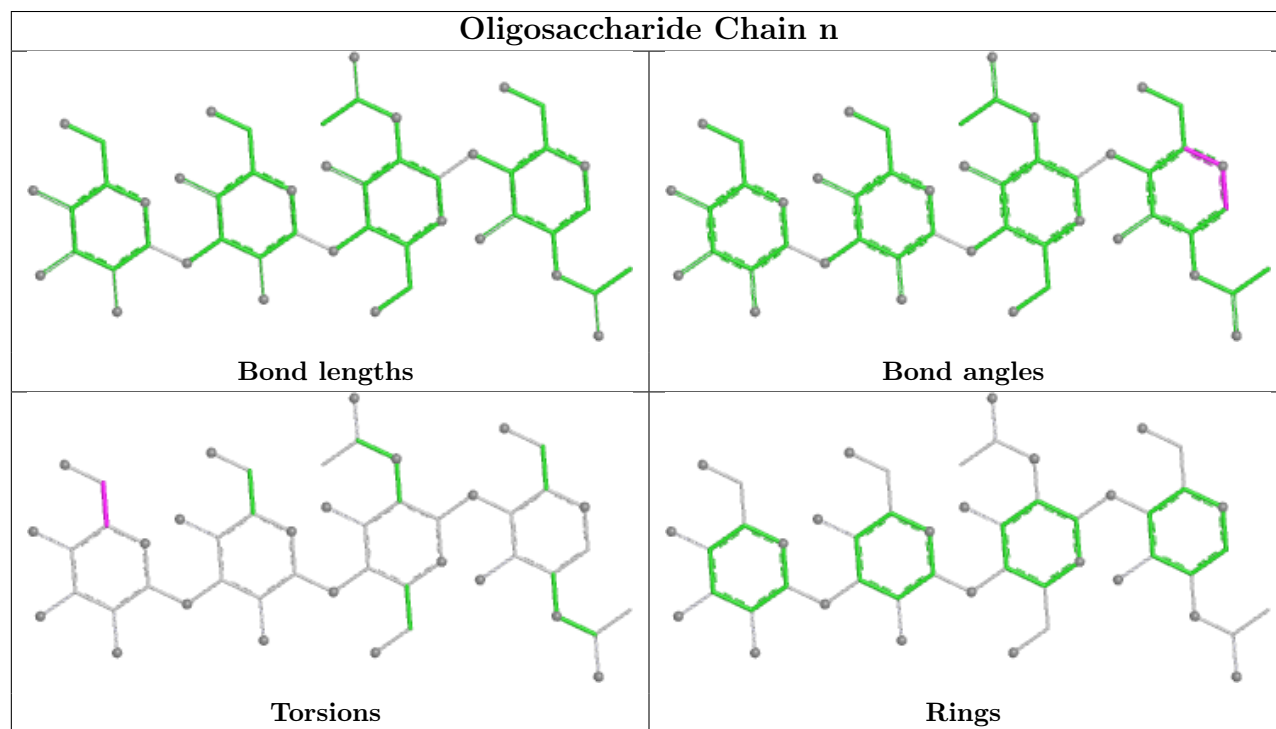
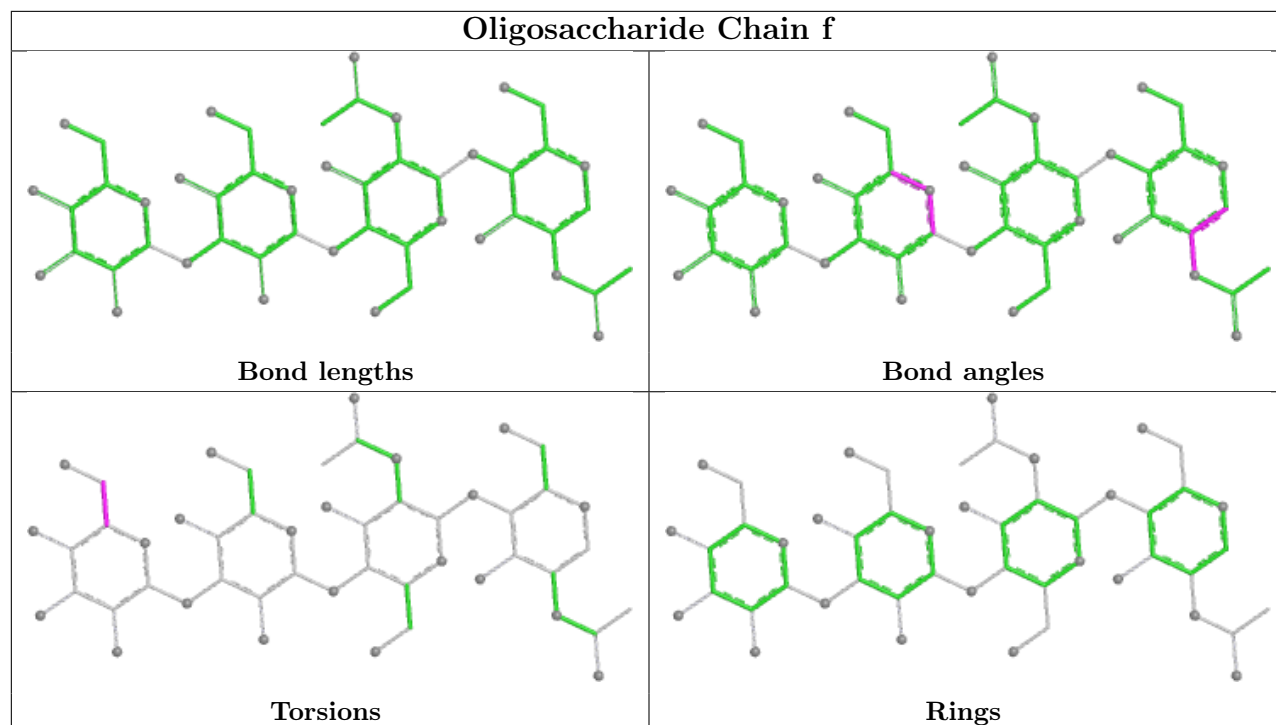
Oligosaccharide Chain Z

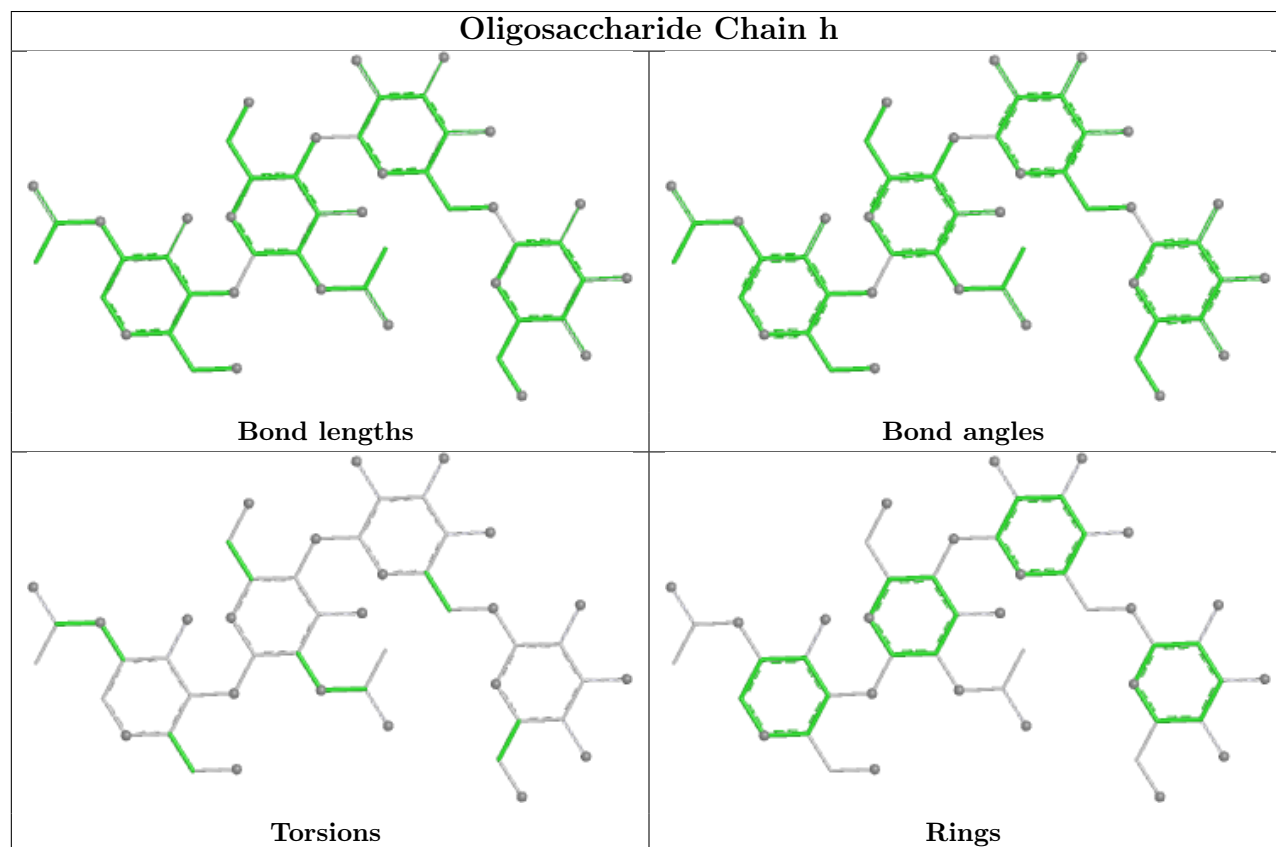
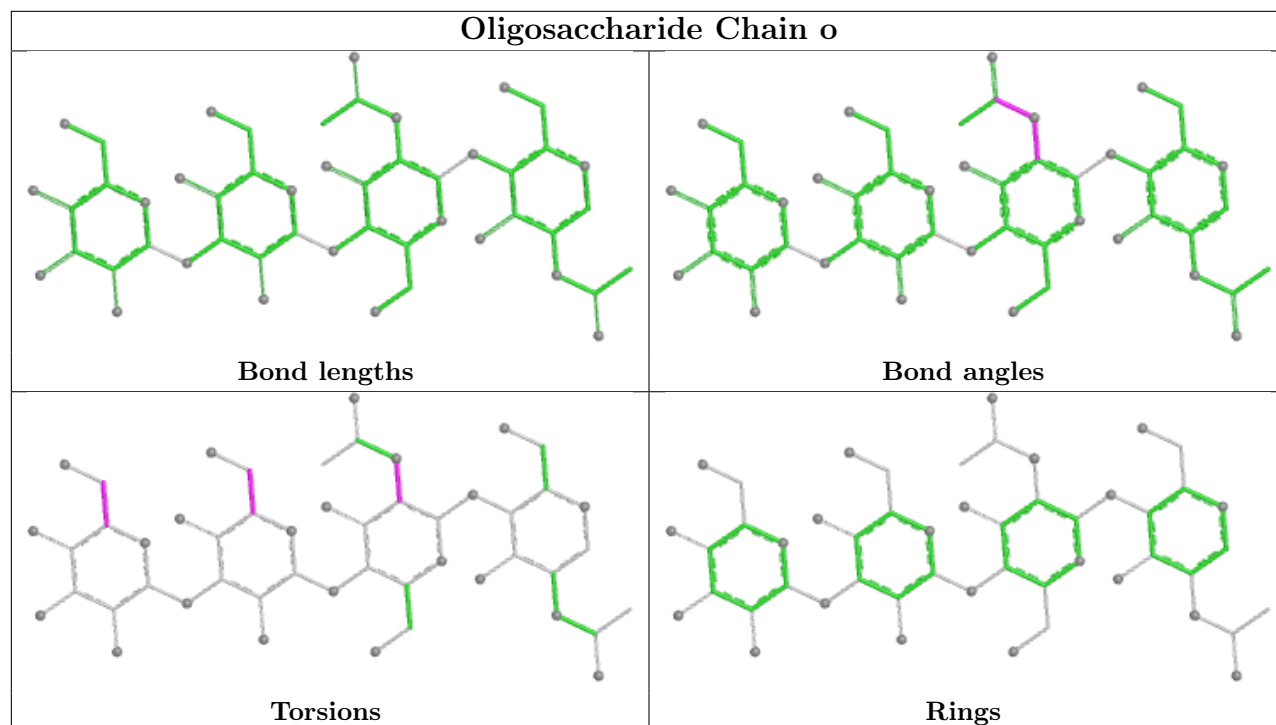


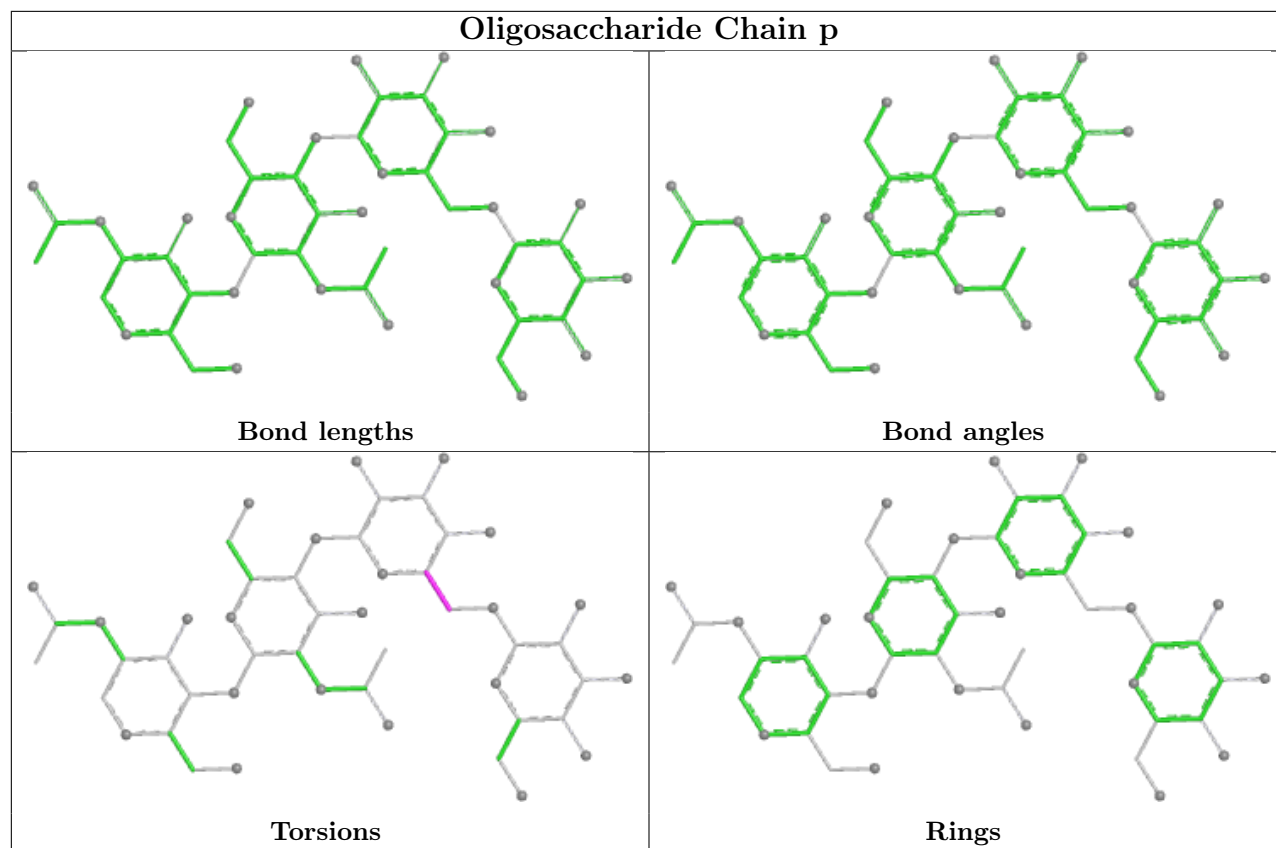


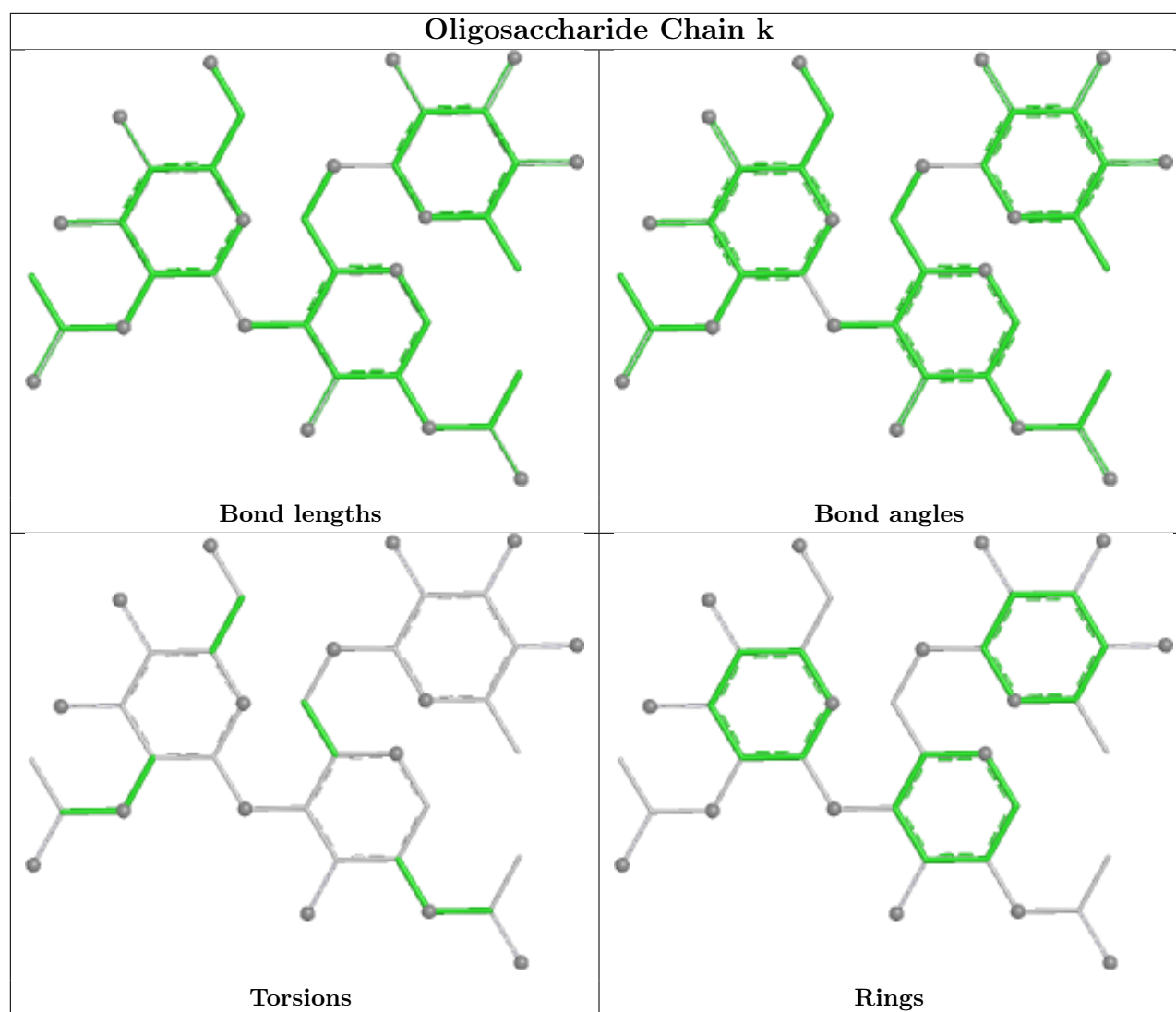












5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	NAG	C	605	1	14,14,15	0.38	0	17,19,21	0.65	0
15	NAG	E	607	1	14,14,15	0.39	0	17,19,21	0.56	0
15	NAG	C	601	1	14,14,15	0.37	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	E	602	1	14,14,15	0.37	0	17,19,21	0.50	0
15	NAG	C	603	1	14,14,15	0.39	0	17,19,21	0.64	0
15	NAG	A	604	1	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
15	NAG	C	607	1	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
15	NAG	C	602	1	14,14,15	0.39	0	17,19,21	0.54	0
15	NAG	E	603	1	14,14,15	0.37	0	17,19,21	0.61	0
15	NAG	A	606	1	14,14,15	0.36	0	17,19,21	0.47	0
15	NAG	A	602	1	14,14,15	0.37	0	17,19,21	0.52	0
15	NAG	A	605	1	14,14,15	0.38	0	17,19,21	0.56	0
15	NAG	E	606	1	14,14,15	0.39	0	17,19,21	0.38	0
15	NAG	C	604	1	14,14,15	0.38	0	17,19,21	0.50	0
15	NAG	E	605	1	14,14,15	0.37	0	17,19,21	0.47	0
15	NAG	A	601	1	14,14,15	0.38	0	17,19,21	0.49	0
15	NAG	E	601	1	14,14,15	0.40	0	17,19,21	0.51	0
15	NAG	E	604	1	14,14,15	0.39	0	17,19,21	0.56	0
15	NAG	E	608	1	14,14,15	0.37	0	17,19,21	0.56	0
15	NAG	C	606	1	14,14,15	0.38	0	17,19,21	0.59	0
15	NAG	A	607	1	14,14,15	0.39	0	17,19,21	0.45	0
15	NAG	A	603	1	14,14,15	0.39	0	17,19,21	0.68	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
15	NAG	C	605	1	-	1/6/23/26	0/1/1/1
15	NAG	E	607	1	-	0/6/23/26	0/1/1/1
15	NAG	C	601	1	-	1/6/23/26	0/1/1/1
15	NAG	E	602	1	-	1/6/23/26	0/1/1/1
15	NAG	C	603	1	-	1/6/23/26	0/1/1/1
15	NAG	A	604	1	-	1/6/23/26	0/1/1/1
15	NAG	C	607	1	-	1/6/23/26	0/1/1/1
15	NAG	C	602	1	-	1/6/23/26	0/1/1/1
15	NAG	E	603	1	-	0/6/23/26	0/1/1/1
15	NAG	A	606	1	-	0/6/23/26	0/1/1/1
15	NAG	A	602	1	-	0/6/23/26	0/1/1/1
15	NAG	A	605	1	-	1/6/23/26	0/1/1/1
15	NAG	E	606	1	-	1/6/23/26	0/1/1/1
15	NAG	C	604	1	-	0/6/23/26	0/1/1/1
15	NAG	E	605	1	-	1/6/23/26	0/1/1/1
15	NAG	A	601	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	E	601	1	-	0/6/23/26	0/1/1/1
15	NAG	E	604	1	-	1/6/23/26	0/1/1/1
15	NAG	E	608	1	-	2/6/23/26	0/1/1/1
15	NAG	C	606	1	-	0/6/23/26	0/1/1/1
15	NAG	A	607	1	-	1/6/23/26	0/1/1/1
15	NAG	A	603	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	604	NAG	C1-O5-C5	2.42	115.43	112.19
15	C	607	NAG	C1-C2-N2	2.11	113.77	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	608	NAG	C8-C7-N2-C2
15	E	608	NAG	O7-C7-N2-C2
15	A	604	NAG	O5-C5-C6-O6
15	C	603	NAG	O5-C5-C6-O6
15	C	605	NAG	O5-C5-C6-O6
15	C	607	NAG	O5-C5-C6-O6
15	A	601	NAG	O5-C5-C6-O6
15	A	605	NAG	O5-C5-C6-O6
15	C	601	NAG	O5-C5-C6-O6
15	C	602	NAG	O5-C5-C6-O6
15	E	604	NAG	O5-C5-C6-O6
15	E	605	NAG	O5-C5-C6-O6
15	A	607	NAG	O5-C5-C6-O6
15	E	602	NAG	O5-C5-C6-O6
15	E	606	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

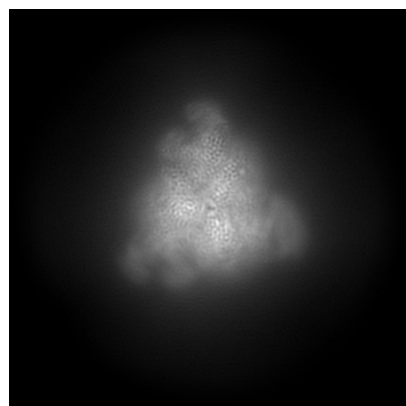
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49240. These allow visual inspection of the internal detail of the map and identification of artifacts.

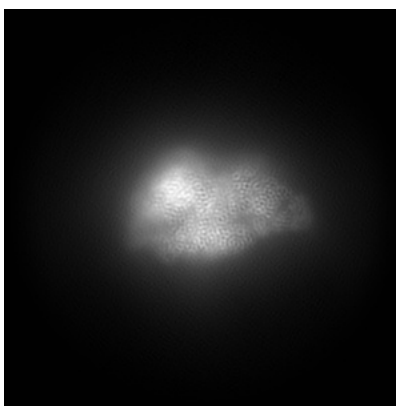
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

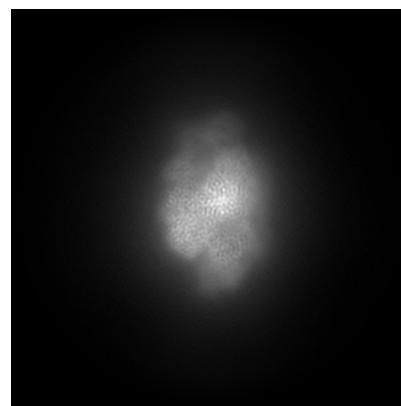
6.1.1 Primary map



X

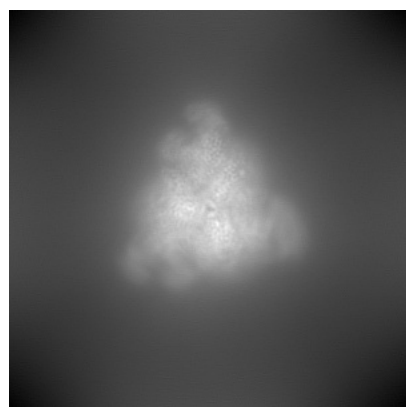


Y

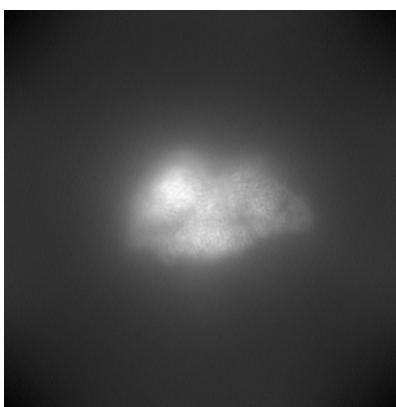


Z

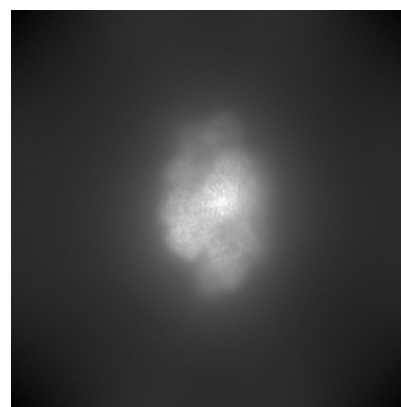
6.1.2 Raw map



X



Y

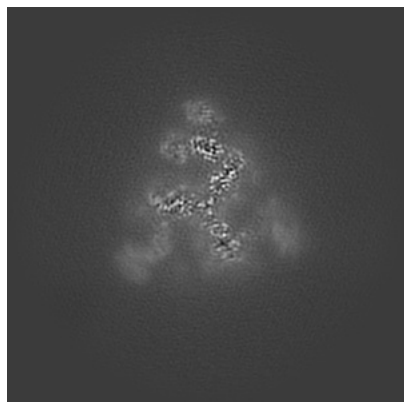


Z

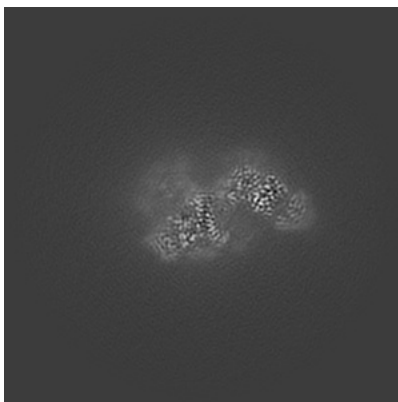
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

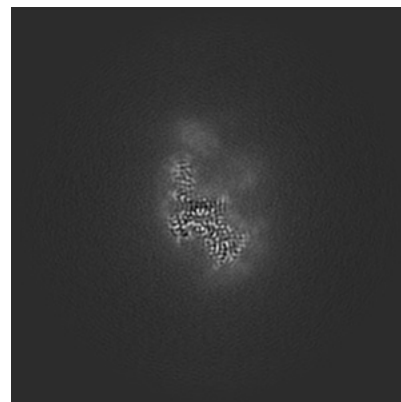
6.2.1 Primary map



X Index: 200

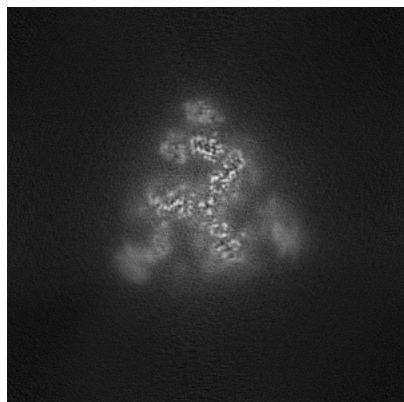


Y Index: 200

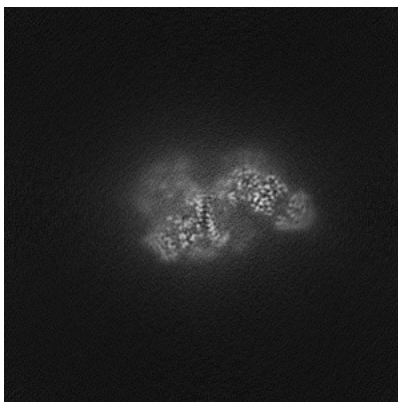


Z Index: 200

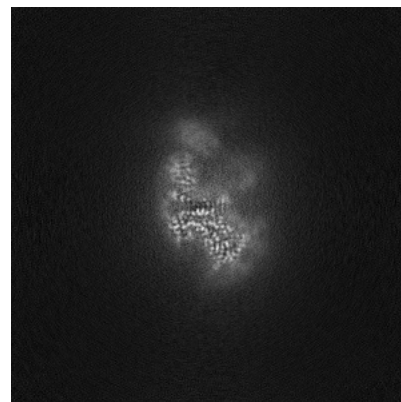
6.2.2 Raw map



X Index: 200



Y Index: 200

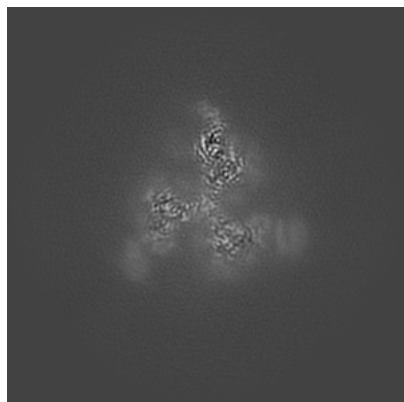


Z Index: 200

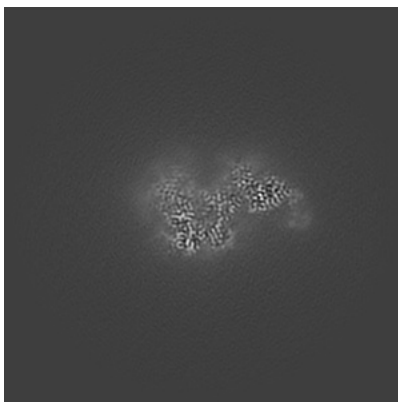
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

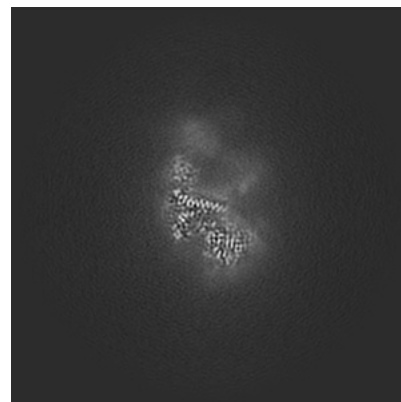
6.3.1 Primary map



X Index: 211

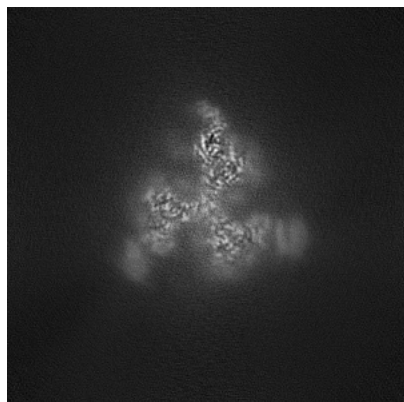


Y Index: 208

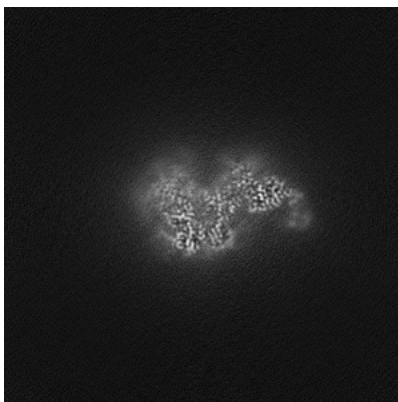


Z Index: 195

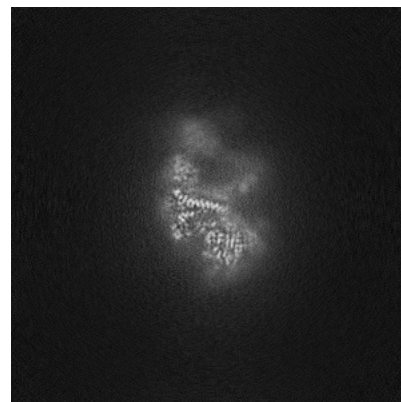
6.3.2 Raw map



X Index: 211



Y Index: 208

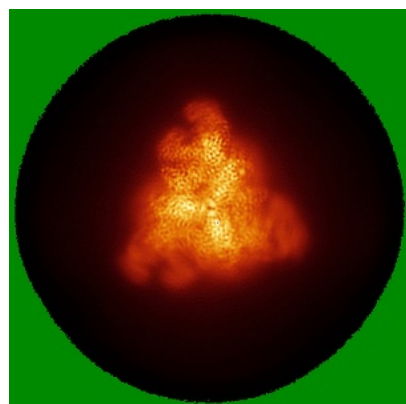


Z Index: 195

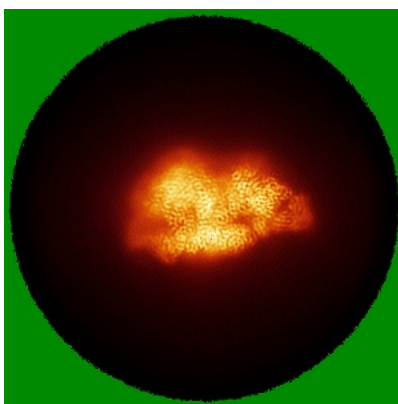
The images above show the largest variance slices of the map in three orthogonal directions.

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

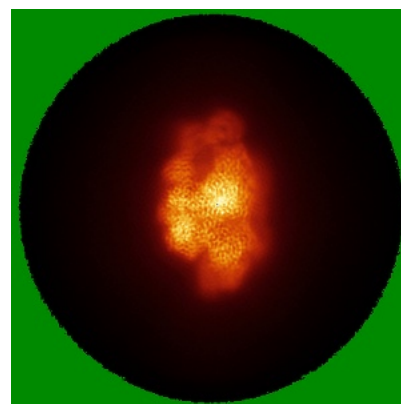
6.4.1 Primary map



X

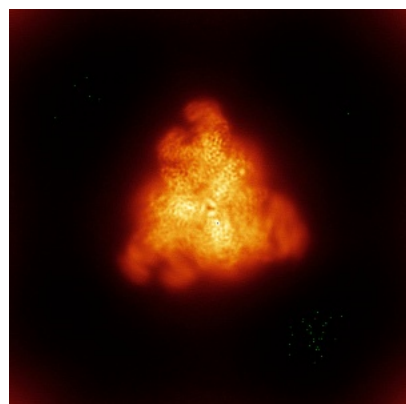


Y

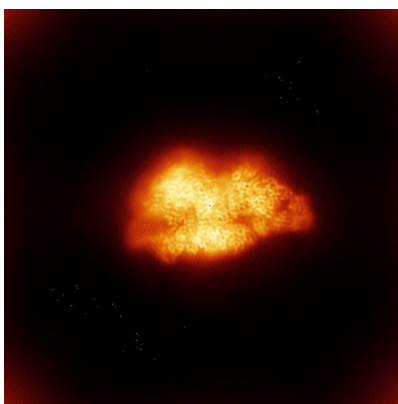


Z

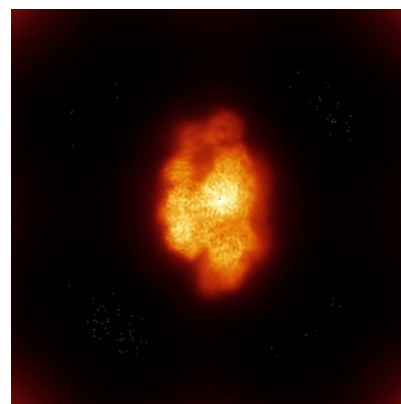
6.4.2 Raw map



X



Y

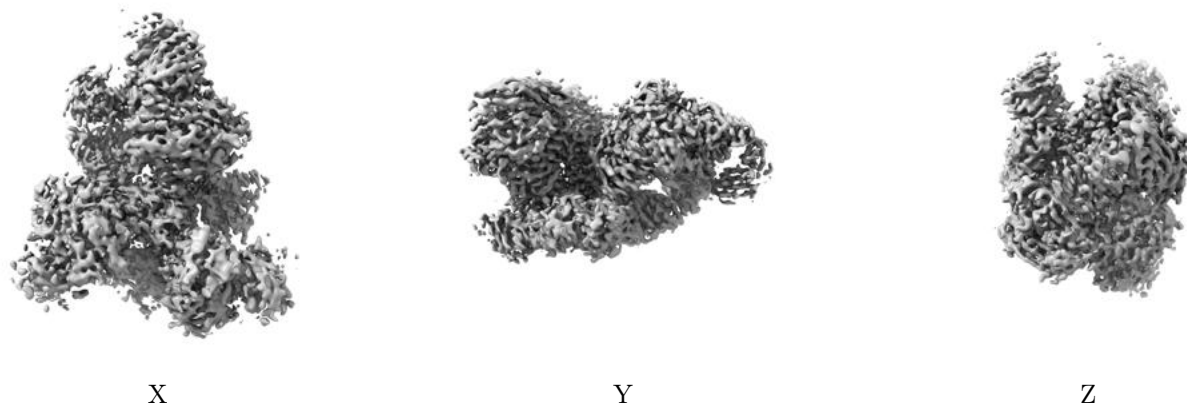


Z

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.

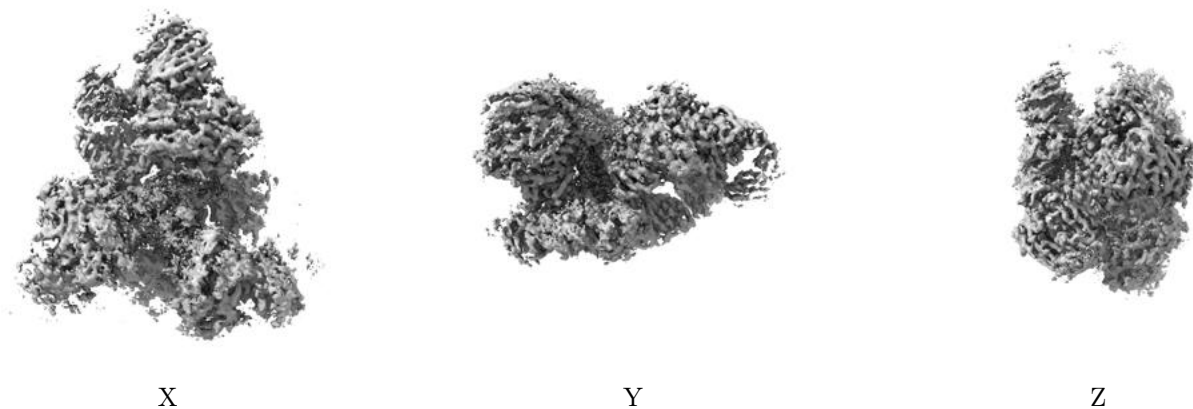
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

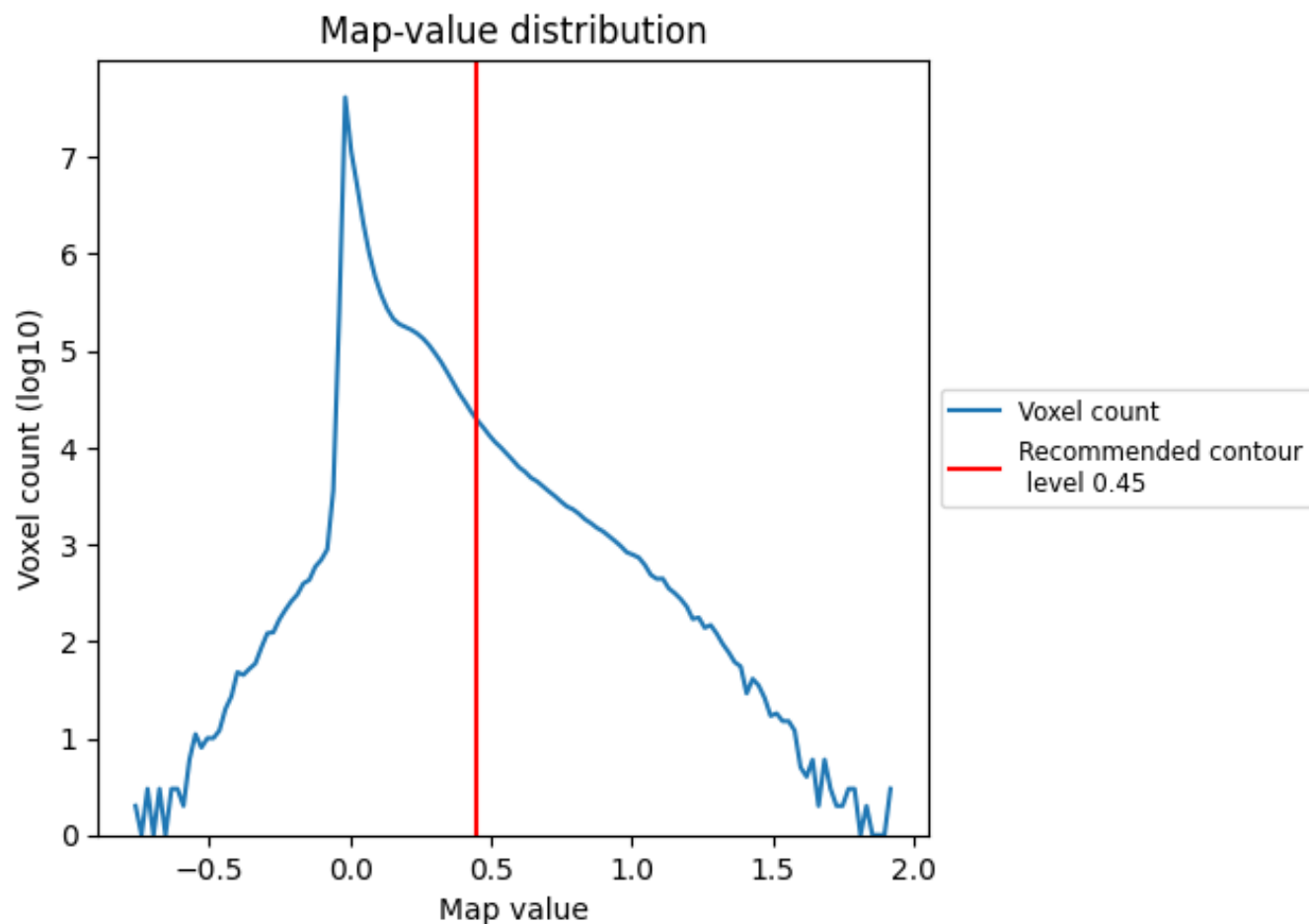
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

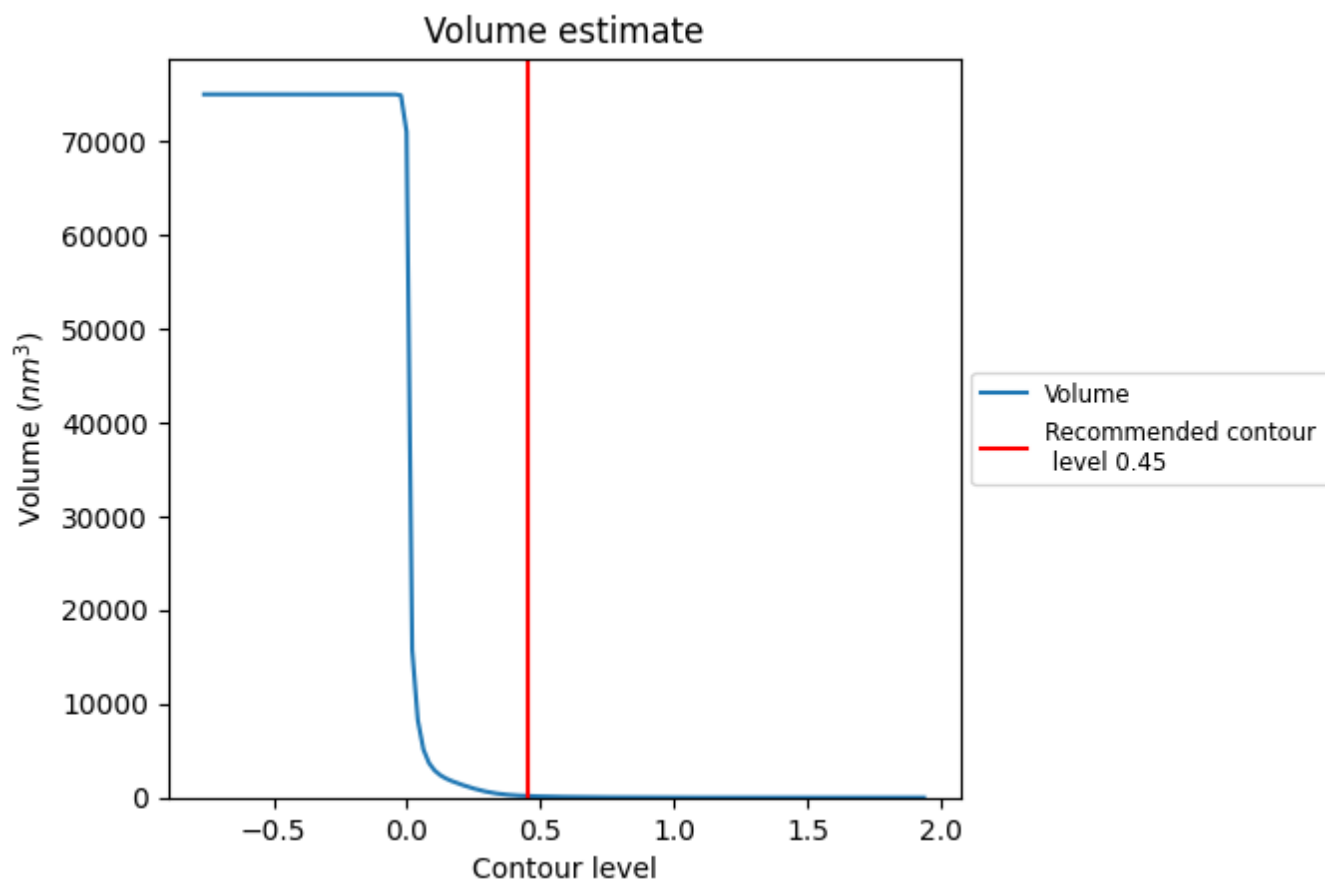
This section contains the results of statistical analysis of the map.

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.

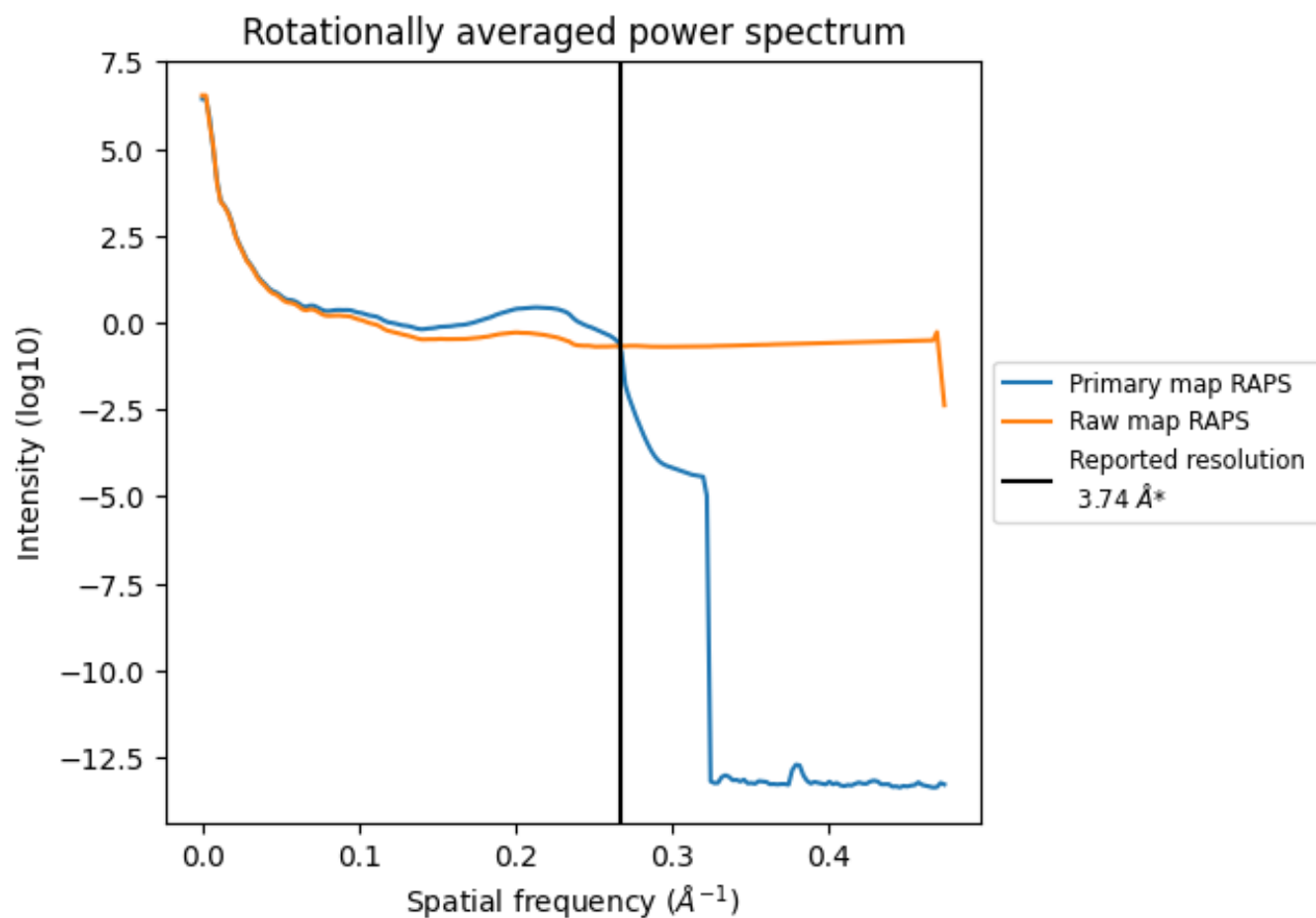
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 153 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 ⓘ

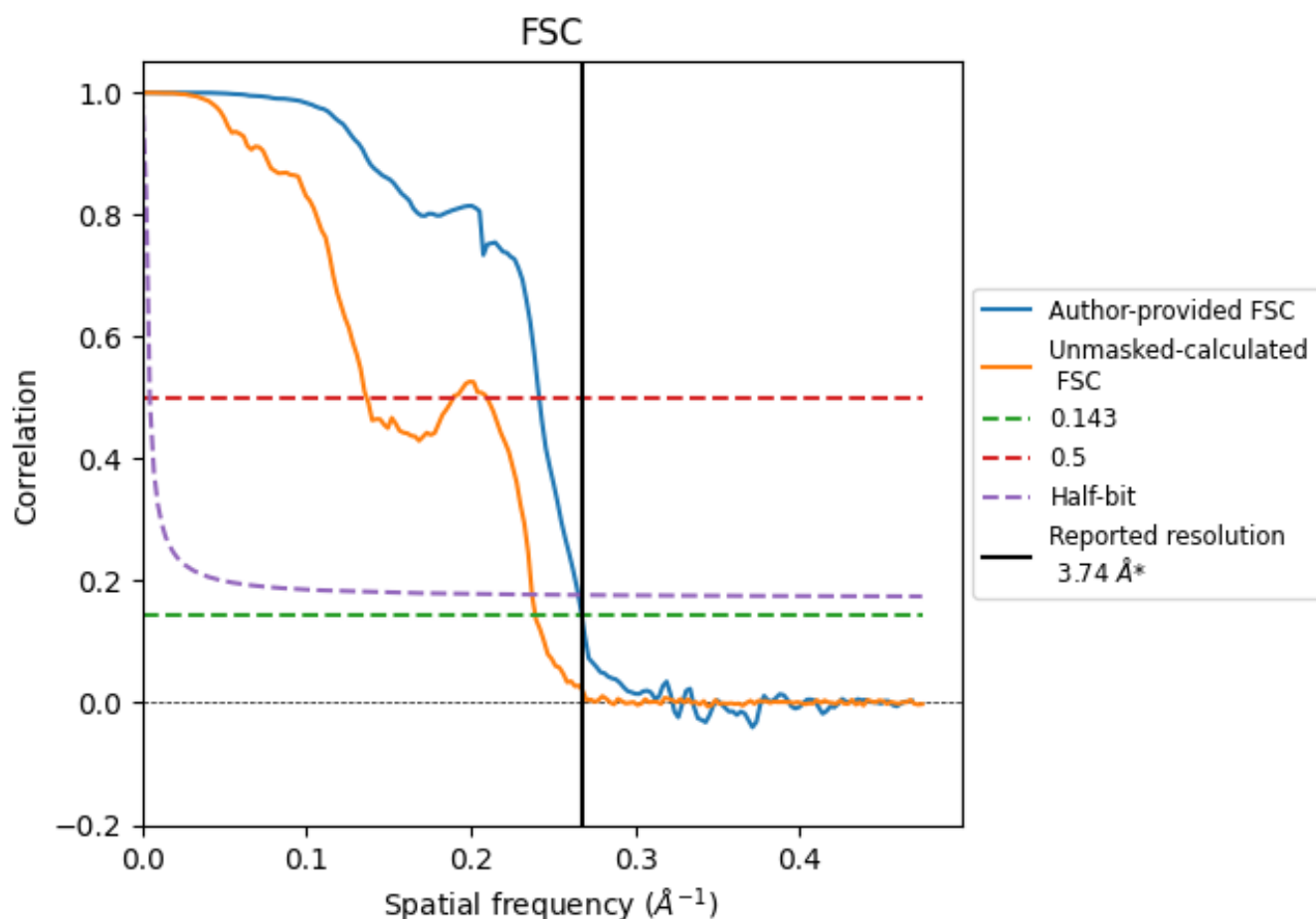


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

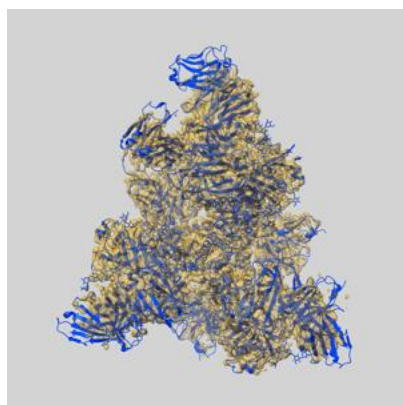
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.74	4.14	3.77
Unmasked-calculated*	4.18	7.33	4.22

*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 4.18 differs from the reported value 3.74 by more than 10 %

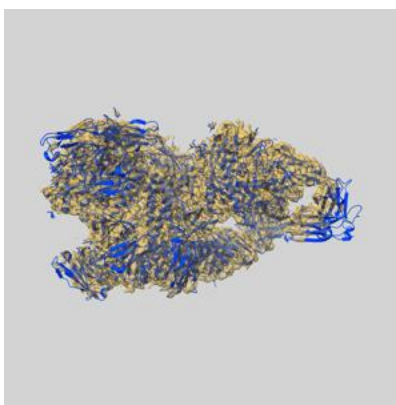
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49240 and PDB model 9NC3. Per-residue inclusion information can be found in section 3 on page 12.

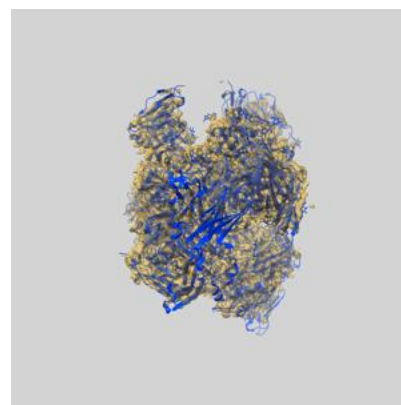
9.1 Map-model overlay [i](#)



X



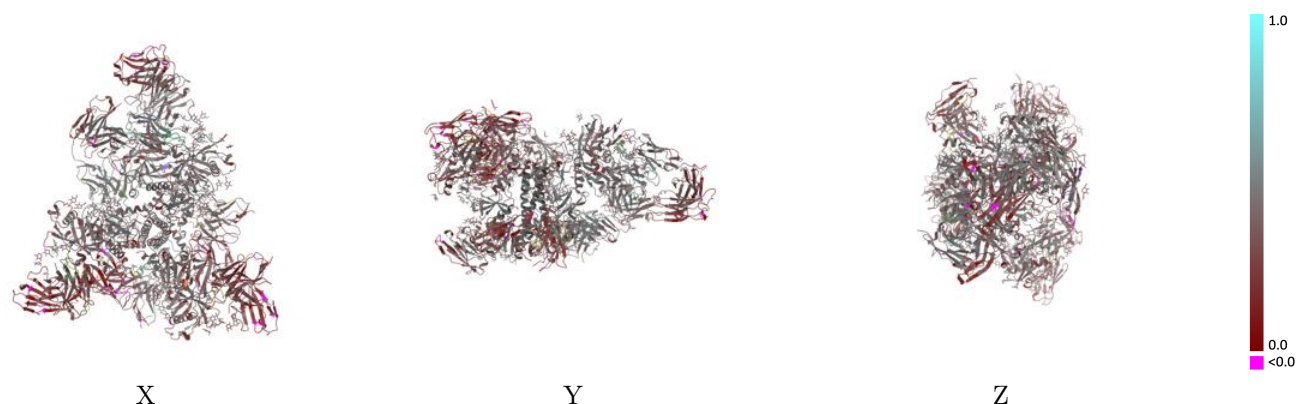
Y



Z

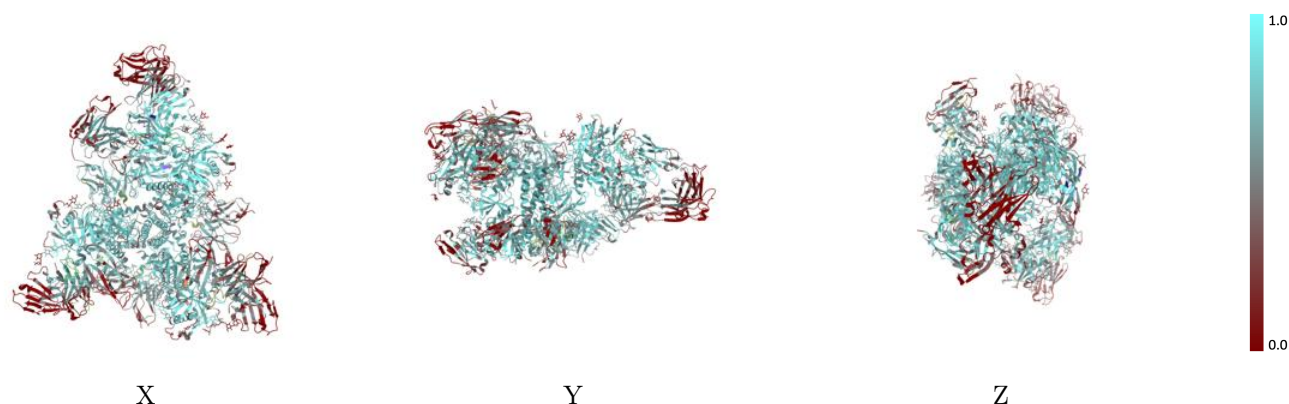
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



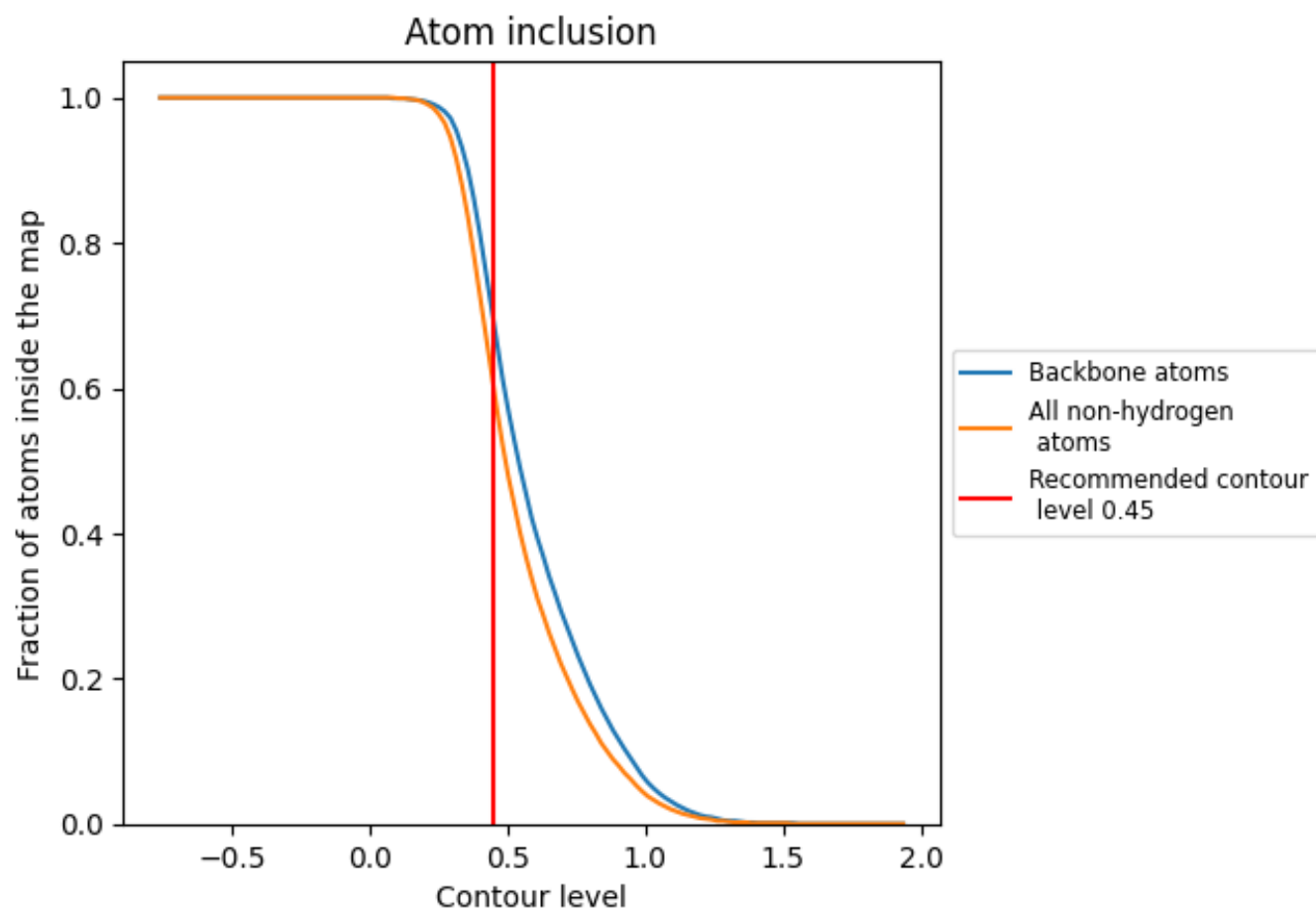
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5990	 0.3660
A	 0.7360	 0.4160
B	 0.7580	 0.4060
C	 0.6740	 0.3630
D	 0.7670	 0.4190
E	 0.6600	 0.3700
F	 0.8230	 0.4240
G	 0.5800	 0.4020
H	 0.6540	 0.4220
I	 0.5810	 0.3950
J	 0.4220	 0.3420
K	 0.5050	 0.3280
L	 0.4920	 0.3210
M	 0.4690	 0.2960
N	 0.2750	 0.2210
O	 0.4820	 0.3350
P	 0.4170	 0.2710
Q	 0.4910	 0.3220
R	 0.2640	 0.2410
S	 0.2860	 0.3540
T	 0.7140	 0.3670
U	 0.5830	 0.4320
V	 0.3930	 0.3950
W	 0.3930	 0.3810
X	 0.4640	 0.4460
Y	 0.5570	 0.4340
Z	 0.4100	 0.3410
a	 0.6070	 0.4030
b	 0.6280	 0.4210
c	 0.3570	 0.4200
d	 0.5380	 0.4610
e	 0.7860	 0.4520
f	 0.6600	 0.4290
g	 0.3210	 0.3620
h	 0.4600	 0.3760



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Chain	Atom inclusion	Q-score
i	 0.8210	 0.4130
j	 0.3330	 0.3400
k	 0.6580	 0.4800
l	 0.5360	 0.4120
m	 0.5710	 0.3770
n	 0.4800	 0.3860
o	 0.3400	 0.3310
p	 0.6400	 0.3780
q	 0.5640	 0.4290