



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 06:48 PM EDT

PDB ID : 9BEW
EMDB ID : EMD-44484
Title : Cryo-EM structure of the HIV-1 BG505 IDL Env trimer in complex with 3BNC117 and 10-1074 Fabs
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2024-04-16
Resolution : 3.30 Å(reported)
Based on initial model : 5V8M

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

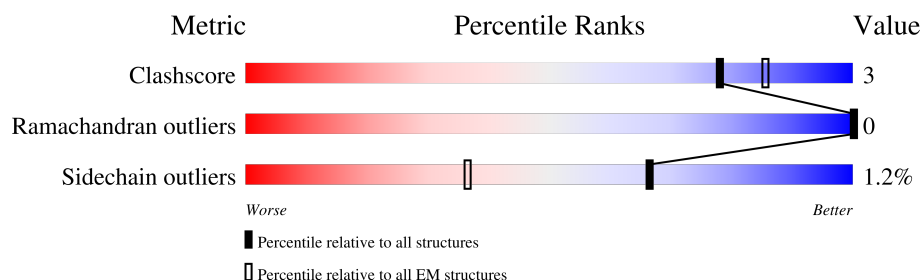
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



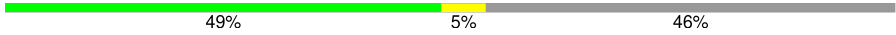







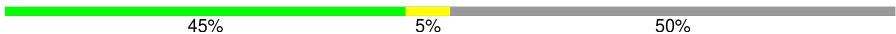





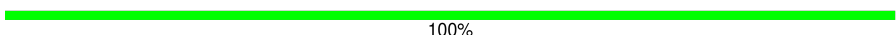
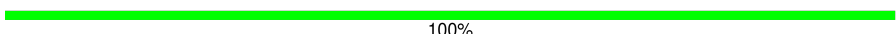
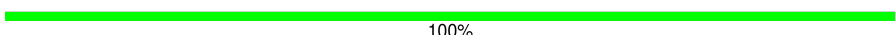
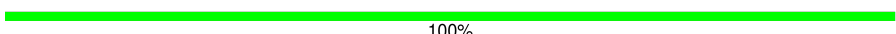
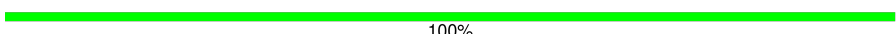
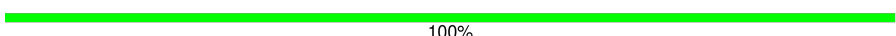
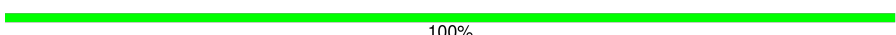
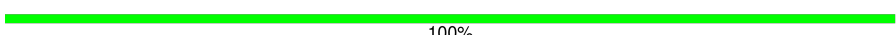



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	483	
1	G	483	
1	M	483	
2	B	153	
2	E	153	
2	N	153	
3	C	226	
3	F	226	







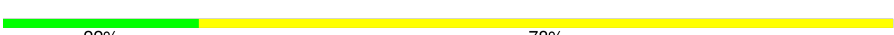
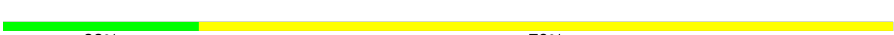

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Mol	Chain	Length	Quality of chain
3	O	226	
4	D	206	
4	I	206	
4	P	206	
5	H	235	
5	J	235	
5	Q	235	
6	K	214	
6	L	214	
6	R	214	
7	S	2	
7	T	2	
7	U	2	
7	Y	2	
7	a	2	
7	b	2	
7	c	2	
7	g	2	
7	i	2	
7	j	2	
7	k	2	
7	o	2	
8	V	6	
8	d	6	
8	l	6	

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Mol	Chain	Length	Quality of chain
9	W	5	 60%40%
9	e	5	 60%40%
9	m	5	 60%40%
10	X	4	 75%25%
10	f	4	 75%25%
10	n	4	 75%25%
11	Z	9	 22%78%
11	h	9	 22%78%
11	p	9	 22%78%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MAN	Z	6	X	-	-	-
11	MAN	h	6	X	-	-	-
11	MAN	p	6	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26100 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	G	445	Total	C	N	O	S	0	0
			3481	2188	617	647	29		
1	A	445	Total	C	N	O	S	0	0
			3481	2188	617	647	29		
1	M	445	Total	C	N	O	S	0	0
			3481	2188	617	647	29		

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1008	636	177	190	5		
2	E	126	Total	C	N	O	S	0	0
			1008	636	177	190	5		
2	N	126	Total	C	N	O	S	0	0
			1008	636	177	190	5		

- Molecule 3 is a protein called 3BNC117 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	F	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	O	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 4 is a protein called 3BNC117 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			767	483	135	146	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	96	Total	C	N	O	S	0	0
			767	483	135	146	3		
4	P	96	Total	C	N	O	S	0	0
			767	483	135	146	3		

- Molecule 5 is a protein called 10-1074 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	J	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	Q	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 6 is a protein called 10-1074 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	108	Total	C	N	O	S	0	0
			836	524	153	156	3		
6	K	108	Total	C	N	O	S	0	0
			836	524	153	156	3		
6	R	108	Total	C	N	O	S	0	0
			836	524	153	156	3		

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



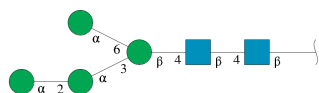
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		

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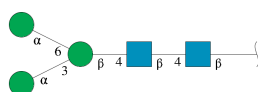
Mol	Chain	Residues	Atoms				AltConf	Trace
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	k	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	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	V	6	Total	C	N	O	0	0
			72	40	2	30		
8	d	6	Total	C	N	O	0	0
			72	40	2	30		
8	l	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.



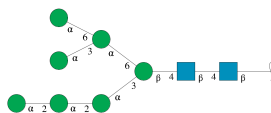
Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	5	Total	C	N	O	0	0
			61	34	2	25		
9	e	5	Total	C	N	O	0	0
			61	34	2	25		
9	m	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 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
10	X	4	Total	C	N	O	0	0
			50	28	2	20		
10	f	4	Total	C	N	O	0	0
			50	28	2	20		
10	n	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[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	Z	9	Total	C	N	O	0	0
			105	58	2	45		
11	h	9	Total	C	N	O	0	0
			105	58	2	45		
11	p	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

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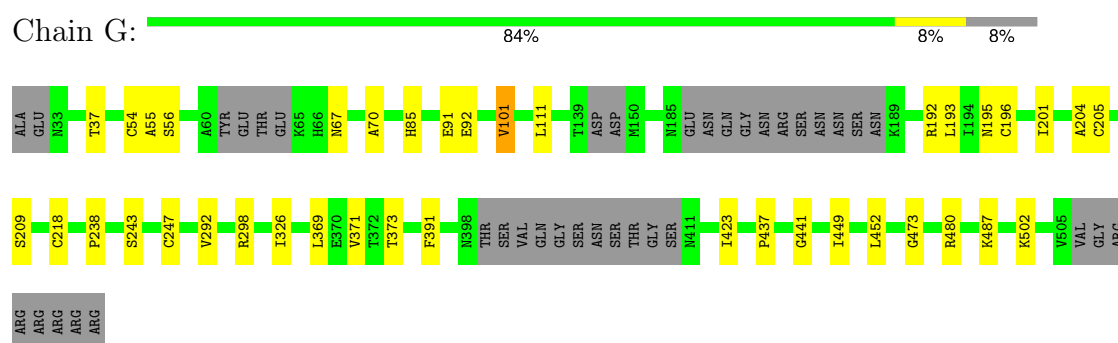
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Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			14	8	1	5	
12	N	1	Total	C	N	O	0
			14	8	1	5	
12	N	1	Total	C	N	O	0
			14	8	1	5	
12	P	1	Total	C	N	O	0
			14	8	1	5	

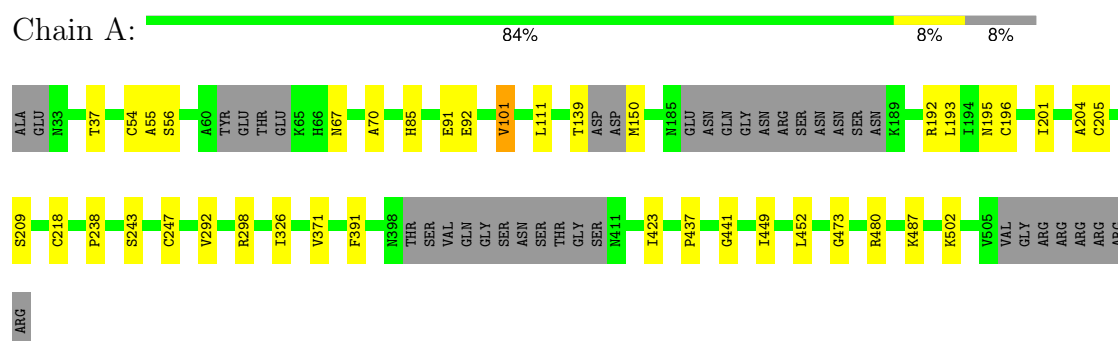
3 Residue-property plots

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.

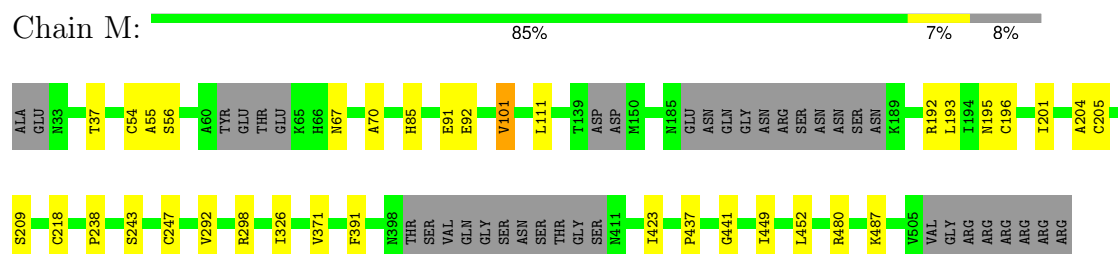
• Molecule 1: Envelope glycoprotein gp120



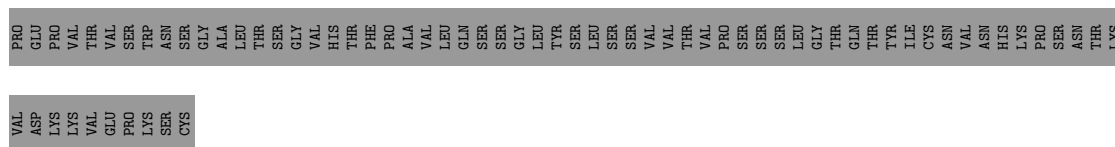
• Molecule 1: Envelope glycoprotein gp120



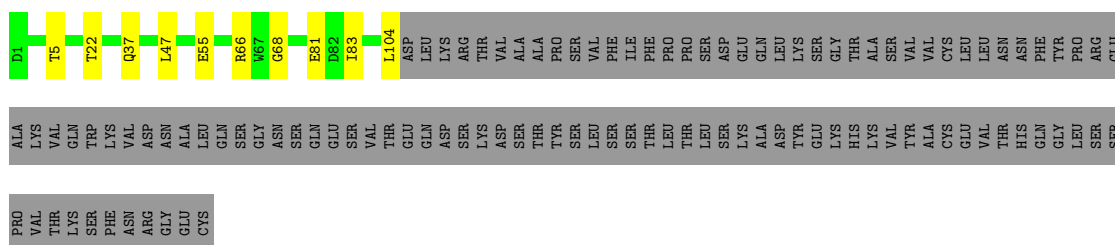
• Molecule 1: Envelope glycoprotein gp120



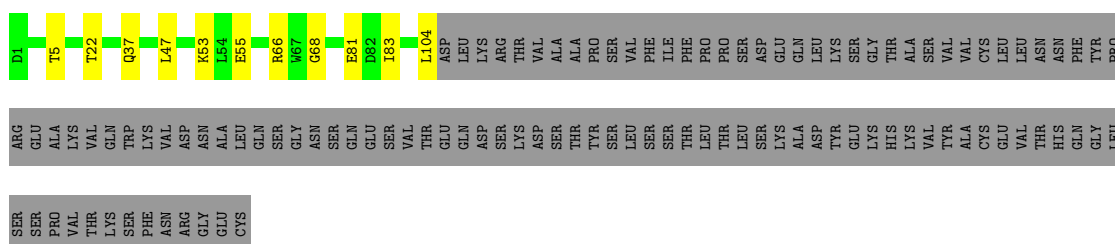
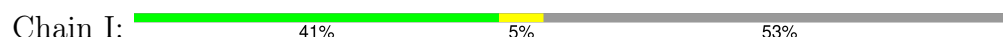
• Molecule 2: Envelope glycoprotein gp41



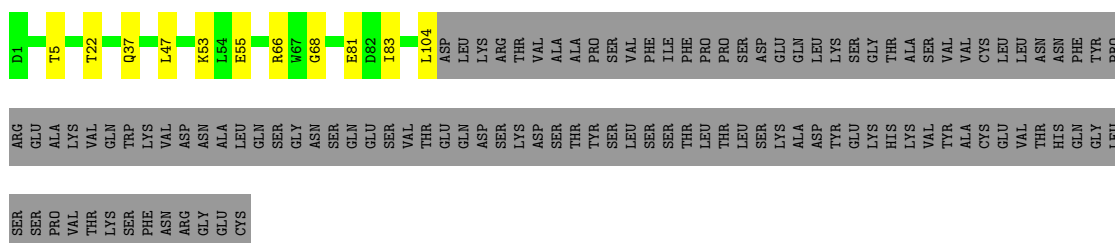
- Molecule 4: 3BNC117 light chain



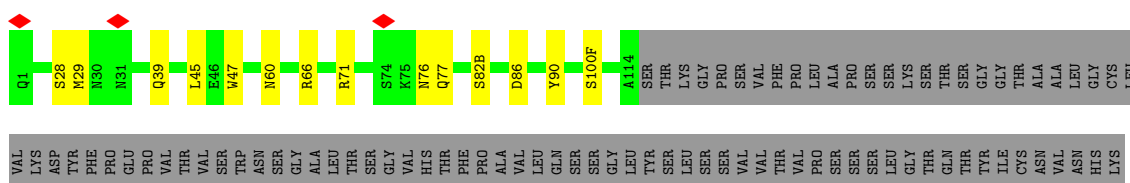
- Molecule 4: 3BNC117 light chain



- Molecule 4: 3BNC117 light chain



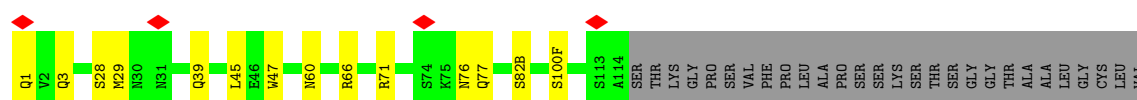
- Molecule 5: 10-1074 heavy chain



PRO
SER
ASP
THR
LYS
VAL
ASP
LYS
ARG
VAL
GLU
PRO
LYS
SER
CYS

• Molecule 5: 10-1074 heavy chain

Chain J: 

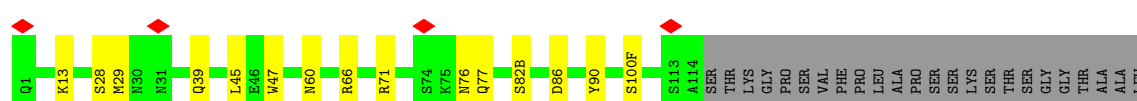

Q1 V2 Q3 S28 N29 N30 N31 Q39 L45 E46 W47 N60 R66 R71 S74 K75 N76 Q77 S82B S100F S113 A114

LYS ASP TYR PHE GLU PRO VAL THR VAL TRP ASN SER GLY ALA LEU THR SER GLY HIS THR PHE PRO VAL ALA LEU GLN SER SER GLY TYR SER LEU SER SER VAL PHE THR VAL PRO LEU ALA SER SER LEU SER THR GLN THR SER ILE GLY THR ASN VAL ASN HIS LYS PRO

SER ASN THR LYS VAL ASP LYS ARG VAL PRO LYS SER CYS

• Molecule 5: 10-1074 heavy chain

Chain Q: 

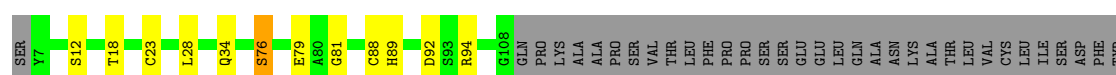

Q1 K13 S28 N29 N31 Q39 L45 E46 W47 N60 R66 R71 S74 K75 N76 Q77 S82B D86 Y90 S100F S113 A114

GLY CYS LEU VAL LYS ASP TYR PHE PRO VAL THR VAL TRP ASN SER GLY ALA LEU THR SER PHE PRO VAL ALA LEU GLN SER SER GLY TYR SER LEU SER SER VAL PHE THR VAL PRO LEU SER SER LEU SER THR GLN THR TYR ILE CYS ASN VAL

ASN HIS LYS PRO ASN THR LYS VAL ASP LYS ARG VAL GLU PRO LYS SER CYS

• Molecule 6: 10-1074 light chain

Chain L: 

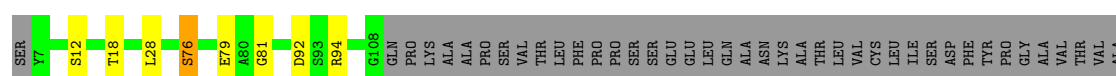

SER Y7 S12 T18 C23 L28 Q34 S76 E79 A80 G81 C88 H89 D92 S93 R94 G108

PRO GLY ALA VAL THR VAL ALA TRP LYS ALA ASP SER SER PRO VAL LYS ALA GLY VAL GLU THR THR THR PRO LYS SER GLN THR LYS

THR VAL GLU LYS THR VAL ALA PRO THR THR GLU CYS SER

• Molecule 6: 10-1074 light chain

Chain K: 


SER Y7 S12 T18 L28 S76 E79 A80 G81 D92 S93 R94 G108

THR LYS ASP LYS SER PRO VAL LYS VAL GLU THR THR THR PRO LYS SER GLN THR LYS

PRO
THR
GLU
CYS
SER

- Molecule 6: 10-1074 light chain

Chain R:  46% 50%

SER Y7 S12 T18 L28 Q34 S76 E79 A80 G81 H89 D92 S93 R94 G108 GLN PRO LYS ALA ALA PRO SER VAL THR PHE LEU PRO SER SER SER GLU LEU LEU GLN ALA ASN LYS THR LEU VAL CYS ILE SER ASP PHE TYR PRO GLY ALA VAL THR VAL THR LYS ASP SER PRO VAL LYS ALA GLY VAL GLU THR THR PRO SER LYS GLN SER ASN ASN LYS TYR ALA SER THR TYR LEU SER LEU THR PRO GLU GLN TRP LYS SER HIS ARG SER TYR SER CYS GLN VAL THR HIS GLY SER THR VAL GLU

LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

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

Chain S:  100%

NAG1
NAG2

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

Chain T:  100%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain Y:  100%

NAG1
NAG2

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

Chain a:  100%



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

Chain b:  100%



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

Chain c:  100%



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

Chain g:  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 j:  100%



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

Chain k:  100%



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

Chain o:  100%

MAG1
MAG2

- 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 V:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- 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 d:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- 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 l:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- 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

Chain W:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

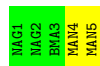
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

- 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

Chain m:  60% 40%



- Molecule 10: 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 X:  75% 25%



- Molecule 10: 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 f:  75% 25%



- Molecule 10: 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 n:  75% 25%



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

Chain Z:  22% 78%




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

Chain h:  22% 78%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[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 p:  22% 78%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.90	Depositor
Minimum defocus (nm)	160	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.086	Depositor
Minimum map value	-1.774	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	385.82718, 385.82718, 385.82718	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/3552	0.45	0/4820
1	G	0.26	0/3552	0.45	0/4820
1	M	0.26	0/3552	0.45	0/4820
2	B	0.22	0/1026	0.39	0/1390
2	E	0.22	0/1026	0.39	0/1390
2	N	0.22	0/1026	0.39	0/1390
3	C	0.24	0/1017	0.42	0/1386
3	F	0.24	0/1017	0.42	0/1386
3	O	0.24	0/1017	0.42	0/1386
4	D	0.25	0/784	0.47	0/1064
4	I	0.25	0/784	0.47	0/1064
4	P	0.26	0/784	0.47	0/1064
5	H	0.25	0/1066	0.47	0/1451
5	J	0.25	0/1066	0.47	0/1451
5	Q	0.25	0/1066	0.47	0/1451
6	K	0.25	0/858	0.47	0/1166
6	L	0.25	0/858	0.47	0/1166
6	R	0.25	0/858	0.47	0/1166
All	All	0.25	0/24909	0.45	0/33831

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	3481	0	3422	21	0
1	G	3481	0	3422	22	0
1	M	3481	0	3422	19	0
2	B	1008	0	990	7	0
2	E	1008	0	990	7	0
2	N	1008	0	990	6	0
3	C	985	0	919	9	0
3	F	985	0	919	8	0
3	O	985	0	919	6	0
4	D	767	0	748	5	0
4	I	767	0	748	6	0
4	P	767	0	748	6	0
5	H	1041	0	1005	6	0
5	J	1041	0	1005	6	0
5	Q	1041	0	1005	7	0
6	K	836	0	797	4	0
6	L	836	0	797	6	0
6	R	836	0	797	5	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	Y	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	g	28	0	25	0	0
7	i	28	0	25	0	0
7	j	28	0	25	0	0
7	k	28	0	25	0	0
7	o	28	0	25	0	0
8	V	72	0	61	0	0
8	d	72	0	61	0	0
8	l	72	0	61	0	0
9	W	61	0	52	0	0
9	e	61	0	52	0	0
9	m	61	0	52	0	0
10	X	50	0	43	0	0
10	f	50	0	43	0	0
10	n	50	0	43	0	0
11	Z	105	0	87	0	0
11	h	105	0	87	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	p	105	0	87	0	0
12	A	140	0	130	0	0
12	B	28	0	26	0	0
12	D	14	0	13	0	0
12	E	28	0	26	0	0
12	G	140	0	130	0	0
12	I	14	0	13	0	0
12	M	140	0	130	0	0
12	N	28	0	26	0	0
12	P	14	0	13	0	0
All	All	26100	0	25179	137	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 3.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:HB3	1:A:437:PRO:HD3	1.77	0.66
1:G:204:ALA:HB3	1:G:437:PRO:HD3	1.77	0.66
1:M:204:ALA:HB3	1:M:437:PRO:HD3	1.77	0.65
5:J:39:GLN:HB2	5:J:45:LEU:HD13	1.81	0.62
5:Q:39:GLN:HB2	5:Q:45:LEU:HD13	1.81	0.62
1:G:218:CYS:HA	1:G:247:CYS:HB3	1.81	0.62
1:A:218:CYS:HA	1:A:247:CYS:HB3	1.81	0.62
5:H:39:GLN:HB2	5:H:45:LEU:HD13	1.81	0.61
1:M:218:CYS:HA	1:M:247:CYS:HB3	1.81	0.61
4:P:83:ILE:HG23	4:P:104:LEU:HB2	1.83	0.60
4:I:83:ILE:HG23	4:I:104:LEU:HB2	1.83	0.59
4:D:83:ILE:HG23	4:D:104:LEU:HB2	1.83	0.59
1:G:54:CYS:SG	1:G:55:ALA:N	2.79	0.56
2:E:627:THR:HG22	2:E:630:GLN:HE21	1.70	0.56
2:N:627:THR:HG22	2:N:630:GLN:HE21	1.70	0.56
1:A:54:CYS:SG	1:A:55:ALA:N	2.79	0.56
2:B:627:THR:HG22	2:B:630:GLN:HE21	1.70	0.55
2:B:591:GLN:NE2	2:N:541:ALA:O	2.40	0.55
2:E:541:ALA:O	2:N:591:GLN:NE2	2.40	0.55
1:M:54:CYS:SG	1:M:55:ALA:N	2.79	0.55
5:J:47:TRP:O	5:J:60:ASN:ND2	2.40	0.55
5:Q:47:TRP:O	5:Q:60:ASN:ND2	2.40	0.54
2:B:541:ALA:O	2:E:591:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:NH2	3:C:86:ASP:OD2	2.42	0.53
3:F:66:ARG:NH2	3:F:86:ASP:OD2	2.42	0.53
1:G:101:VAL:HG21	1:G:480:ARG:HD2	1.91	0.53
3:F:28:ASN:ND2	3:F:31:ASP:OD1	2.42	0.53
5:H:47:TRP:O	5:H:60:ASN:ND2	2.40	0.53
1:M:101:VAL:HG21	1:M:480:ARG:HD2	1.91	0.53
3:C:28:ASN:ND2	3:C:31:ASP:OD1	2.42	0.53
3:O:28:ASN:ND2	3:O:31:ASP:OD1	2.42	0.53
2:E:539:VAL:O	2:E:543:ASN:ND2	2.43	0.52
2:B:539:VAL:O	2:B:543:ASN:ND2	2.43	0.52
1:A:101:VAL:HG21	1:A:480:ARG:HD2	1.91	0.52
2:N:539:VAL:O	2:N:543:ASN:ND2	2.43	0.52
3:O:66:ARG:NH2	3:O:86:ASP:OD2	2.42	0.52
1:M:67:ASN:HA	1:M:209:SER:H	1.74	0.52
1:A:67:ASN:HA	1:A:209:SER:H	1.74	0.51
3:F:96:ARG:NH2	4:I:55:GLU:OE2	2.42	0.51
5:H:28:SER:OG	5:H:29:MET:N	2.43	0.51
5:J:28:SER:OG	5:J:29:MET:N	2.43	0.51
1:G:67:ASN:HA	1:G:209:SER:H	1.74	0.51
1:M:37:THR:HG22	2:N:605:ALA:HA	1.93	0.51
1:G:91:GLU:OE2	1:G:487:LYS:NZ	2.44	0.50
1:A:91:GLU:OE2	1:A:487:LYS:NZ	2.44	0.50
1:A:37:THR:HG22	2:E:605:ALA:HA	1.94	0.49
1:M:91:GLU:OE2	1:M:487:LYS:NZ	2.44	0.49
5:Q:28:SER:OG	5:Q:29:MET:N	2.43	0.49
3:O:96:ARG:NH2	4:P:55:GLU:OE2	2.45	0.49
1:G:326:ILE:HG12	6:L:94:ARG:HD3	1.95	0.49
5:J:66:ARG:NH2	5:J:82(B):SER:OG	2.46	0.49
3:C:96:ARG:NH2	4:D:55:GLU:OE2	2.46	0.48
5:H:66:ARG:NH2	5:H:82(B):SER:OG	2.46	0.48
1:G:37:THR:HG22	2:B:605:ALA:HA	1.95	0.48
6:L:28:LEU:N	6:L:92:ASP:OD1	2.45	0.48
1:A:326:ILE:HG12	6:K:94:ARG:HD3	1.95	0.48
6:K:18:THR:HG22	6:K:76:SER:HA	1.96	0.48
1:M:326:ILE:HG12	6:R:94:ARG:HD3	1.95	0.48
5:Q:66:ARG:NH2	5:Q:82(B):SER:OG	2.46	0.48
6:R:18:THR:HG22	6:R:76:SER:HA	1.96	0.48
6:L:18:THR:HG22	6:L:76:SER:HA	1.96	0.48
1:A:192:ARG:NH1	1:A:195:ASN:O	2.38	0.48
1:M:298:ARG:NH2	1:M:441:GLY:O	2.48	0.47
1:A:298:ARG:NH2	1:A:441:GLY:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:37:GLN:HB2	4:P:47:LEU:HD11	1.97	0.46
1:G:92:GLU:HA	1:G:238:PRO:HA	1.98	0.46
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.97	0.46
1:G:298:ARG:NH2	1:G:441:GLY:O	2.48	0.46
1:A:92:GLU:HA	1:A:238:PRO:HA	1.98	0.46
5:Q:76:ASN:O	5:Q:77:GLN:NE2	2.49	0.46
1:M:92:GLU:HA	1:M:238:PRO:HA	1.97	0.46
5:J:76:ASN:O	5:J:77:GLN:NE2	2.49	0.46
5:H:76:ASN:O	5:H:77:GLN:NE2	2.49	0.46
6:K:28:LEU:N	6:K:92:ASP:OD1	2.45	0.46
1:A:70:ALA:H	1:A:111:LEU:HD13	1.82	0.45
4:I:37:GLN:HB2	4:I:47:LEU:HD11	1.97	0.45
1:G:371:VAL:HG11	3:C:54:THR:HB	1.98	0.45
4:P:53:LYS:HE3	4:P:53:LYS:HB2	1.84	0.45
1:M:192:ARG:NH1	1:M:195:ASN:O	2.38	0.45
1:G:70:ALA:H	1:G:111:LEU:HD13	1.81	0.45
1:M:70:ALA:H	1:M:111:LEU:HD13	1.82	0.45
1:G:502:LYS:NZ	2:B:607:ASN:OD1	2.42	0.45
4:I:66:ARG:NH2	4:I:68:GLY:O	2.50	0.44
1:G:473:GLY:HA3	3:C:54:THR:HG21	2.00	0.44
1:A:292:VAL:HB	1:A:449:ILE:HB	2.00	0.44
3:F:39:GLN:HB3	3:F:45:LEU:HD23	2.00	0.44
1:G:292:VAL:HB	1:G:449:ILE:HB	2.00	0.43
5:Q:13:LYS:HA	5:Q:13:LYS:HD2	1.83	0.43
3:F:47:TRP:HZ2	3:F:50:TRP:HD1	1.66	0.43
3:O:39:GLN:HB3	3:O:45:LEU:HD23	2.00	0.43
1:A:85:HIS:HA	1:A:243:SER:HB2	2.01	0.43
6:K:79:GLU:HG3	6:K:81:GLY:H	1.84	0.43
6:R:79:GLU:HG3	6:R:81:GLY:H	1.83	0.43
3:C:39:GLN:HB3	3:C:45:LEU:HD23	2.00	0.42
1:M:67:ASN:N	1:M:67:ASN:OD1	2.52	0.42
1:M:292:VAL:HB	1:M:449:ILE:HB	2.00	0.42
3:O:47:TRP:HZ2	3:O:50:TRP:HD1	1.66	0.42
3:C:47:TRP:HZ2	3:C:50:TRP:HD1	1.66	0.42
1:G:192:ARG:NH1	1:G:195:ASN:O	2.38	0.42
1:M:201:ILE:HD13	1:M:423:ILE:HD13	2.01	0.42
1:G:85:HIS:HA	1:G:243:SER:HB2	2.01	0.42
6:L:79:GLU:HG3	6:L:81:GLY:H	1.83	0.42
1:A:371:VAL:HG11	3:F:54:THR:HB	2.01	0.42
1:M:371:VAL:HG11	3:O:54:THR:HB	2.01	0.42
5:Q:86:ASP:OD2	5:Q:90:TYR:OH	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:28:LEU:N	6:R:92:ASP:OD1	2.45	0.42
4:D:83:ILE:HA	4:D:104:LEU:HD12	2.02	0.42
1:A:502:LYS:NZ	2:E:607:ASN:OD1	2.42	0.42
4:I:53:LYS:HB2	4:I:53:LYS:HE3	1.84	0.42
4:I:83:ILE:HA	4:I:104:LEU:HD12	2.02	0.42
4:D:66:ARG:NH2	4:D:68:GLY:O	2.50	0.42
1:M:85:HIS:HA	1:M:243:SER:HB2	2.01	0.42
1:G:67:ASN:N	1:G:67:ASN:OD1	2.52	0.41
2:B:647:GLU:O	2:B:651:ASN:ND2	2.53	0.41
1:A:201:ILE:HD13	1:A:423:ILE:HD13	2.01	0.41
3:C:2:VAL:HG22	3:C:27:TYR:HB3	2.03	0.41
5:H:86:ASP:OD2	5:H:90:TYR:OH	2.38	0.41
1:A:391:PHE:HE1	1:A:452:LEU:HD13	1.86	0.41
2:E:647:GLU:O	2:E:651:ASN:ND2	2.53	0.41
1:M:193:LEU:HB2	1:M:196:CYS:SG	2.61	0.41
1:G:201:ILE:HD13	1:G:423:ILE:HD13	2.01	0.41
1:G:369:LEU:O	1:G:373:THR:OG1	2.39	0.41
2:N:647:GLU:O	2:N:651:ASN:ND2	2.53	0.41
4:P:66:ARG:NH2	4:P:68:GLY:O	2.50	0.41
1:A:473:GLY:HA3	3:F:54:THR:HG21	2.02	0.41
6:R:34:GLN:HB2	6:R:89:HIS:HB3	2.03	0.41
1:G:193:LEU:HB2	1:G:196:CYS:SG	2.61	0.40
1:G:391:PHE:HE1	1:G:452:LEU:HD13	1.86	0.40
1:A:139:THR:OG1	1:A:150:MET:SD	2.80	0.40
1:A:193:LEU:HB2	1:A:196:CYS:SG	2.61	0.40
6:L:23:CYS:HB3	6:L:88:CYS:HB2	1.96	0.40
3:F:2:VAL:HG22	3:F:27:TYR:HB3	2.03	0.40
5:J:1:GLN:OE1	5:J:3:GLN:NE2	2.54	0.40
1:M:391:PHE:HE1	1:M:452:LEU:HD13	1.86	0.40
4:P:83:ILE:HA	4:P:104:LEU:HD12	2.02	0.40
6:L:34:GLN:HB2	6:L:89:HIS:HB3	2.03	0.40
3:C:101:ASP:N	3:C:101:ASP:OD1	2.55	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	435/483 (90%)	415 (95%)	20 (5%)	0	100	100
1	G	435/483 (90%)	415 (95%)	20 (5%)	0	100	100
1	M	435/483 (90%)	415 (95%)	20 (5%)	0	100	100
2	B	122/153 (80%)	120 (98%)	2 (2%)	0	100	100
2	E	122/153 (80%)	120 (98%)	2 (2%)	0	100	100
2	N	122/153 (80%)	120 (98%)	2 (2%)	0	100	100
3	C	119/226 (53%)	118 (99%)	1 (1%)	0	100	100
3	F	119/226 (53%)	118 (99%)	1 (1%)	0	100	100
3	O	119/226 (53%)	118 (99%)	1 (1%)	0	100	100
4	D	94/206 (46%)	87 (93%)	7 (7%)	0	100	100
4	I	94/206 (46%)	87 (93%)	7 (7%)	0	100	100
4	P	94/206 (46%)	87 (93%)	7 (7%)	0	100	100
5	H	131/235 (56%)	128 (98%)	3 (2%)	0	100	100
5	J	131/235 (56%)	128 (98%)	3 (2%)	0	100	100
5	Q	131/235 (56%)	128 (98%)	3 (2%)	0	100	100
6	K	106/214 (50%)	102 (96%)	4 (4%)	0	100	100
6	L	106/214 (50%)	102 (96%)	4 (4%)	0	100	100
6	R	106/214 (50%)	102 (96%)	4 (4%)	0	100	100
All	All	3021/4551 (66%)	2910 (96%)	111 (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	A	393/427 (92%)	390 (99%)	3 (1%)	79	87
1	G	393/427 (92%)	390 (99%)	3 (1%)	79	87
1	M	393/427 (92%)	390 (99%)	3 (1%)	79	87
2	B	108/128 (84%)	108 (100%)	0	100	100
2	E	108/128 (84%)	108 (100%)	0	100	100
2	N	108/128 (84%)	108 (100%)	0	100	100
3	C	102/193 (53%)	101 (99%)	1 (1%)	73	84
3	F	102/193 (53%)	101 (99%)	1 (1%)	73	84
3	O	102/193 (53%)	101 (99%)	1 (1%)	73	84
4	D	84/183 (46%)	81 (96%)	3 (4%)	30	57
4	I	84/183 (46%)	81 (96%)	3 (4%)	30	57
4	P	84/183 (46%)	81 (96%)	3 (4%)	30	57
5	H	116/205 (57%)	114 (98%)	2 (2%)	56	74
5	J	116/205 (57%)	114 (98%)	2 (2%)	56	74
5	Q	116/205 (57%)	114 (98%)	2 (2%)	56	74
6	K	86/178 (48%)	84 (98%)	2 (2%)	45	68
6	L	86/178 (48%)	84 (98%)	2 (2%)	45	68
6	R	86/178 (48%)	84 (98%)	2 (2%)	45	68
All	All	2667/3942 (68%)	2634 (99%)	33 (1%)	66	80

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	56	SER
1	G	101	VAL
1	G	205	CYS
3	C	71	ARG
4	D	5	THR
4	D	22	THR
4	D	81	GLU
5	H	71	ARG
5	H	100(F)	SER
6	L	12	SER
6	L	76	SER
1	A	56	SER
1	A	101	VAL
1	A	205	CYS

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Mol	Chain	Res	Type
3	F	71	ARG
4	I	5	THR
4	I	22	THR
4	I	81	GLU
5	J	71	ARG
5	J	100(F)	SER
6	K	12	SER
6	K	76	SER
1	M	56	SER
1	M	101	VAL
1	M	205	CYS
3	O	71	ARG
4	P	5	THR
4	P	22	THR
4	P	81	GLU
5	Q	71	ARG
5	Q	100(F)	SER
6	R	12	SER
6	R	76	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	315	GLN
1	G	328	GLN
1	G	411	ASN
2	B	590	GLN
2	B	630	GLN
3	C	62	GLN
4	D	69	GLN
5	H	1	GLN
5	H	3	GLN
5	H	31	ASN
5	H	39	GLN
1	A	315	GLN
1	A	328	GLN
1	A	411	ASN
2	E	590	GLN
2	E	630	GLN
3	F	62	GLN
4	I	69	GLN
5	J	1	GLN

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Mol	Chain	Res	Type
5	J	3	GLN
5	J	31	ASN
5	J	39	GLN
1	M	315	GLN
1	M	328	GLN
1	M	411	ASN
2	N	590	GLN
2	N	630	GLN
3	O	62	GLN
4	P	69	GLN
5	Q	1	GLN
5	Q	3	GLN
5	Q	31	ASN
5	Q	39	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 ⓘ

96 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	0.25	0	17,19,21	0.48	0
7	NAG	S	2	7	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	T	1	1,7	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	T	2	7	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	U	1	1,7	14,14,15	0.34	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	U	2	7	14,14,15	0.24	0	17,19,21	0.48	0
8	NAG	V	1	1,8	14,14,15	0.28	0	17,19,21	0.50	0
8	NAG	V	2	8	14,14,15	0.22	0	17,19,21	0.47	0
8	BMA	V	3	8	11,11,12	0.64	0	15,15,17	0.77	0
8	MAN	V	4	8	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
8	MAN	V	5	8	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
8	MAN	V	6	8	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
9	NAG	W	1	1,9	14,14,15	0.26	0	17,19,21	0.52	0
9	NAG	W	2	9	14,14,15	0.21	0	17,19,21	0.47	0
9	BMA	W	3	9	11,11,12	0.65	0	15,15,17	0.79	0
9	MAN	W	4	9	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
9	MAN	W	5	9	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
10	NAG	X	1	1,10	14,14,15	0.31	0	17,19,21	0.59	0
10	NAG	X	2	10	14,14,15	0.23	0	17,19,21	0.50	0
10	BMA	X	3	10	11,11,12	0.63	0	15,15,17	0.78	0
10	MAN	X	4	10	11,11,12	0.74	0	15,15,17	1.05	2 (13%)
7	NAG	Y	1	1,7	14,14,15	0.28	0	17,19,21	0.53	0
7	NAG	Y	2	7	14,14,15	0.23	0	17,19,21	0.47	0
11	NAG	Z	1	1,11	14,14,15	0.22	0	17,19,21	0.48	0
11	NAG	Z	2	11	14,14,15	0.65	0	17,19,21	2.11	2 (11%)
11	BMA	Z	3	11	11,11,12	0.62	0	15,15,17	0.75	0
11	MAN	Z	4	11	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
11	MAN	Z	5	11	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
11	MAN	Z	6	11	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
11	MAN	Z	7	11	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
11	MAN	Z	8	11	11,11,12	0.71	0	15,15,17	1.06	2 (13%)
11	MAN	Z	9	11	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
7	NAG	a	1	1,7	14,14,15	0.28	0	17,19,21	0.48	0
7	NAG	a	2	7	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	b	1	1,7	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	b	2	7	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	c	1	1,7	14,14,15	0.35	0	17,19,21	0.51	0
7	NAG	c	2	7	14,14,15	0.25	0	17,19,21	0.46	0
8	NAG	d	1	1,8	14,14,15	0.28	0	17,19,21	0.50	0
8	NAG	d	2	8	14,14,15	0.23	0	17,19,21	0.47	0
8	BMA	d	3	8	11,11,12	0.65	0	15,15,17	0.78	0
8	MAN	d	4	8	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
8	MAN	d	5	8	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
8	MAN	d	6	8	11,11,12	0.73	0	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	e	1	1,9	14,14,15	0.26	0	17,19,21	0.53	0
9	NAG	e	2	9	14,14,15	0.21	0	17,19,21	0.47	0
9	BMA	e	3	9	11,11,12	0.65	0	15,15,17	0.78	0
9	MAN	e	4	9	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
9	MAN	e	5	9	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
10	NAG	f	1	1,10	14,14,15	0.32	0	17,19,21	0.60	0
10	NAG	f	2	10	14,14,15	0.25	0	17,19,21	0.48	0
10	BMA	f	3	10	11,11,12	0.64	0	15,15,17	0.79	0
10	MAN	f	4	10	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
7	NAG	g	1	1,7	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	g	2	7	14,14,15	0.25	0	17,19,21	0.46	0
11	NAG	h	1	1,11	14,14,15	0.20	0	17,19,21	0.48	0
11	NAG	h	2	11	14,14,15	0.66	0	17,19,21	2.11	2 (11%)
11	BMA	h	3	11	11,11,12	0.63	0	15,15,17	0.75	0
11	MAN	h	4	11	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
11	MAN	h	5	11	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
11	MAN	h	6	11	11,11,12	0.67	0	15,15,17	1.03	2 (13%)
11	MAN	h	7	11	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
11	MAN	h	8	11	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
11	MAN	h	9	11	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
7	NAG	i	1	1,7	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	i	2	7	14,14,15	0.23	0	17,19,21	0.48	0
7	NAG	j	1	1,7	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	j	2	7	14,14,15	0.23	0	17,19,21	0.45	0
7	NAG	k	1	1,7	14,14,15	0.35	0	17,19,21	0.50	0
7	NAG	k	2	7	14,14,15	0.25	0	17,19,21	0.46	0
8	NAG	l	1	1,8	14,14,15	0.28	0	17,19,21	0.50	0
8	NAG	l	2	8	14,14,15	0.22	0	17,19,21	0.47	0
8	BMA	l	3	8	11,11,12	0.64	0	15,15,17	0.78	0
8	MAN	l	4	8	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
8	MAN	l	5	8	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
8	MAN	l	6	8	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
9	NAG	m	1	1,9	14,14,15	0.25	0	17,19,21	0.53	0
9	NAG	m	2	9	14,14,15	0.22	0	17,19,21	0.47	0
9	BMA	m	3	9	11,11,12	0.64	0	15,15,17	0.78	0
9	MAN	m	4	9	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
9	MAN	m	5	9	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
10	NAG	n	1	1,10	14,14,15	0.32	0	17,19,21	0.59	0
10	NAG	n	2	10	14,14,15	0.24	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	n	3	10	11,11,12	0.64	0	15,15,17	0.78	0
10	MAN	n	4	10	11,11,12	0.74	0	15,15,17	1.06	2 (13%)
7	NAG	o	1	1,7	14,14,15	0.26	0	17,19,21	0.53	0
7	NAG	o	2	7	14,14,15	0.24	0	17,19,21	0.46	0
11	NAG	p	1	1,11	14,14,15	0.22	0	17,19,21	0.48	0
11	NAG	p	2	11	14,14,15	0.65	0	17,19,21	2.11	2 (11%)
11	BMA	p	3	11	11,11,12	0.64	0	15,15,17	0.75	0
11	MAN	p	4	11	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
11	MAN	p	5	11	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
11	MAN	p	6	11	11,11,12	0.66	0	15,15,17	1.04	2 (13%)
11	MAN	p	7	11	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
11	MAN	p	8	11	11,11,12	0.71	0	15,15,17	1.06	2 (13%)
11	MAN	p	9	11	11,11,12	0.72	0	15,15,17	1.03	2 (13%)

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
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	NAG	T	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	NAG	U	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
8	NAG	V	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	V	2	8	-	0/6/23/26	0/1/1/1
8	BMA	V	3	8	-	0/2/19/22	0/1/1/1
8	MAN	V	4	8	-	0/2/19/22	0/1/1/1
8	MAN	V	5	8	-	1/2/19/22	0/1/1/1
8	MAN	V	6	8	-	0/2/19/22	0/1/1/1
9	NAG	W	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	BMA	W	3	9	-	0/2/19/22	0/1/1/1
9	MAN	W	4	9	-	0/2/19/22	0/1/1/1
9	MAN	W	5	9	-	0/2/19/22	0/1/1/1
10	NAG	X	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	X	2	10	-	0/6/23/26	0/1/1/1
10	BMA	X	3	10	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	h	6	11	1/1/4/5	1/2/19/22	0/1/1/1
11	MAN	h	7	11	-	0/2/19/22	0/1/1/1
11	MAN	h	8	11	-	0/2/19/22	0/1/1/1
11	MAN	h	9	11	-	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	-	0/6/23/26	0/1/1/1
7	NAG	j	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	NAG	k	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	k	2	7	-	0/6/23/26	0/1/1/1
8	NAG	l	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
8	BMA	l	3	8	-	0/2/19/22	0/1/1/1
8	MAN	l	4	8	-	0/2/19/22	0/1/1/1
8	MAN	l	5	8	-	1/2/19/22	0/1/1/1
8	MAN	l	6	8	-	0/2/19/22	0/1/1/1
9	NAG	m	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	m	2	9	-	0/6/23/26	0/1/1/1
9	BMA	m	3	9	-	0/2/19/22	0/1/1/1
9	MAN	m	4	9	-	0/2/19/22	0/1/1/1
9	MAN	m	5	9	-	0/2/19/22	0/1/1/1
10	NAG	n	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	n	2	10	-	0/6/23/26	0/1/1/1
10	BMA	n	3	10	-	0/2/19/22	0/1/1/1
10	MAN	n	4	10	-	0/2/19/22	0/1/1/1
7	NAG	o	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	2/6/23/26	0/1/1/1
11	NAG	p	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	p	2	11	-	6/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	1/2/19/22	0/1/1/1
11	MAN	p	5	11	-	0/2/19/22	0/1/1/1
11	MAN	p	6	11	1/1/4/5	1/2/19/22	0/1/1/1
11	MAN	p	7	11	-	0/2/19/22	0/1/1/1
11	MAN	p	8	11	-	0/2/19/22	0/1/1/1
11	MAN	p	9	11	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	p	2	NAG	C2-N2-C7	7.36	132.77	122.90
11	h	2	NAG	C2-N2-C7	7.34	132.74	122.90
11	Z	2	NAG	C2-N2-C7	7.31	132.70	122.90
11	Z	2	NAG	C1-C2-N2	3.59	116.09	110.43
11	p	2	NAG	C1-C2-N2	3.58	116.07	110.43
11	h	2	NAG	C1-C2-N2	3.57	116.06	110.43
8	d	4	MAN	C1-O5-C5	2.74	115.86	112.19
11	h	8	MAN	C1-O5-C5	2.73	115.84	112.19
8	l	4	MAN	C1-O5-C5	2.72	115.83	112.19
11	Z	4	MAN	C1-O5-C5	2.72	115.83	112.19
11	Z	8	MAN	C1-O5-C5	2.72	115.83	112.19
11	p	8	MAN	C1-O5-C5	2.71	115.81	112.19
8	V	4	MAN	C1-O5-C5	2.71	115.81	112.19
11	p	4	MAN	C1-O5-C5	2.70	115.81	112.19
9	e	4	MAN	C1-O5-C5	2.70	115.81	112.19
10	n	4	MAN	C1-O5-C5	2.70	115.80	112.19
8	l	6	MAN	C1-O5-C5	2.69	115.80	112.19
9	e	5	MAN	C1-O5-C5	2.69	115.79	112.19
9	m	5	MAN	C1-O5-C5	2.69	115.79	112.19
8	V	6	MAN	C1-O5-C5	2.68	115.78	112.19
9	W	4	MAN	C1-O5-C5	2.68	115.77	112.19
9	W	5	MAN	C1-O5-C5	2.67	115.77	112.19
10	f	4	MAN	C1-O5-C5	2.67	115.77	112.19
8	d	6	MAN	C1-O5-C5	2.66	115.76	112.19
11	h	4	MAN	C1-O5-C5	2.66	115.75	112.19
8	d	5	MAN	C1-O5-C5	2.66	115.75	112.19
9	m	4	MAN	C1-O5-C5	2.65	115.74	112.19
10	X	4	MAN	C1-O5-C5	2.65	115.74	112.19
11	p	6	MAN	C1-O5-C5	2.65	115.74	112.19
8	V	5	MAN	C1-O5-C5	2.65	115.73	112.19
11	Z	9	MAN	C1-O5-C5	2.64	115.73	112.19
11	p	9	MAN	C1-O5-C5	2.63	115.71	112.19
8	l	5	MAN	C1-O5-C5	2.63	115.71	112.19
11	h	6	MAN	C1-O5-C5	2.63	115.71	112.19
11	Z	6	MAN	C1-O5-C5	2.63	115.71	112.19
11	h	9	MAN	C1-O5-C5	2.61	115.69	112.19
11	h	7	MAN	C1-O5-C5	2.60	115.67	112.19
11	Z	7	MAN	C1-O5-C5	2.58	115.65	112.19
11	p	7	MAN	C1-O5-C5	2.58	115.65	112.19
11	h	5	MAN	C1-O5-C5	2.57	115.64	112.19
11	Z	5	MAN	C1-O5-C5	2.55	115.61	112.19
11	p	5	MAN	C1-O5-C5	2.54	115.59	112.19
11	h	4	MAN	O2-C2-C3	-2.34	105.30	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	p	4	MAN	O2-C2-C3	-2.33	105.33	110.15
11	Z	4	MAN	O2-C2-C3	-2.31	105.36	110.15
11	p	7	MAN	O2-C2-C3	-2.26	105.47	110.15
11	h	7	MAN	O2-C2-C3	-2.26	105.48	110.15
11	Z	7	MAN	O2-C2-C3	-2.25	105.50	110.15
11	Z	9	MAN	O2-C2-C3	-2.23	105.53	110.15
11	p	9	MAN	O2-C2-C3	-2.22	105.56	110.15
11	Z	8	MAN	O2-C2-C3	-2.22	105.56	110.15
11	p	8	MAN	O2-C2-C3	-2.21	105.57	110.15
11	h	9	MAN	O2-C2-C3	-2.21	105.58	110.15
8	V	4	MAN	O2-C2-C3	-2.20	105.59	110.15
11	p	6	MAN	O2-C2-C3	-2.20	105.59	110.15
8	l	4	MAN	O2-C2-C3	-2.20	105.60	110.15
11	h	8	MAN	O2-C2-C3	-2.20	105.60	110.15
11	Z	6	MAN	O2-C2-C3	-2.19	105.61	110.15
8	d	4	MAN	O2-C2-C3	-2.19	105.61	110.15
9	e	5	MAN	O2-C2-C3	-2.19	105.62	110.15
9	m	4	MAN	O2-C2-C3	-2.18	105.63	110.15
9	e	4	MAN	O2-C2-C3	-2.18	105.64	110.15
9	m	5	MAN	O2-C2-C3	-2.18	105.64	110.15
9	W	4	MAN	O2-C2-C3	-2.18	105.65	110.15
11	h	6	MAN	O2-C2-C3	-2.18	105.65	110.15
8	d	6	MAN	O2-C2-C3	-2.17	105.65	110.15
9	W	5	MAN	O2-C2-C3	-2.17	105.65	110.15
8	l	6	MAN	O2-C2-C3	-2.17	105.66	110.15
8	l	5	MAN	O2-C2-C3	-2.17	105.66	110.15
10	X	4	MAN	O2-C2-C3	-2.16	105.67	110.15
10	n	4	MAN	O2-C2-C3	-2.16	105.68	110.15
8	d	5	MAN	O2-C2-C3	-2.16	105.69	110.15
10	f	4	MAN	O2-C2-C3	-2.15	105.69	110.15
8	V	6	MAN	O2-C2-C3	-2.15	105.69	110.15
8	V	5	MAN	O2-C2-C3	-2.13	105.73	110.15
11	h	5	MAN	O2-C2-C3	-2.10	105.80	110.15
11	Z	5	MAN	O2-C2-C3	-2.10	105.81	110.15
11	p	5	MAN	O2-C2-C3	-2.10	105.81	110.15

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	Z	6	MAN	C1
11	h	6	MAN	C1
11	p	6	MAN	C1

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	V	1	NAG	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
11	Z	2	NAG	O5-C5-C6-O6
11	h	2	NAG	O5-C5-C6-O6
11	p	2	NAG	O5-C5-C6-O6
7	Y	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
11	Z	2	NAG	C4-C5-C6-O6
10	X	1	NAG	O5-C5-C6-O6
10	f	1	NAG	O5-C5-C6-O6
10	n	1	NAG	O5-C5-C6-O6
11	h	2	NAG	C4-C5-C6-O6
11	p	2	NAG	C4-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
8	l	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
7	k	1	NAG	C4-C5-C6-O6
10	X	1	NAG	C4-C5-C6-O6
10	f	1	NAG	C4-C5-C6-O6
10	n	1	NAG	C4-C5-C6-O6
7	Y	2	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
11	Z	2	NAG	C8-C7-N2-C2
11	Z	2	NAG	O7-C7-N2-C2
11	h	2	NAG	C8-C7-N2-C2
11	h	2	NAG	O7-C7-N2-C2
11	p	2	NAG	C8-C7-N2-C2
11	p	2	NAG	O7-C7-N2-C2
7	U	1	NAG	O5-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
7	k	1	NAG	O5-C5-C6-O6

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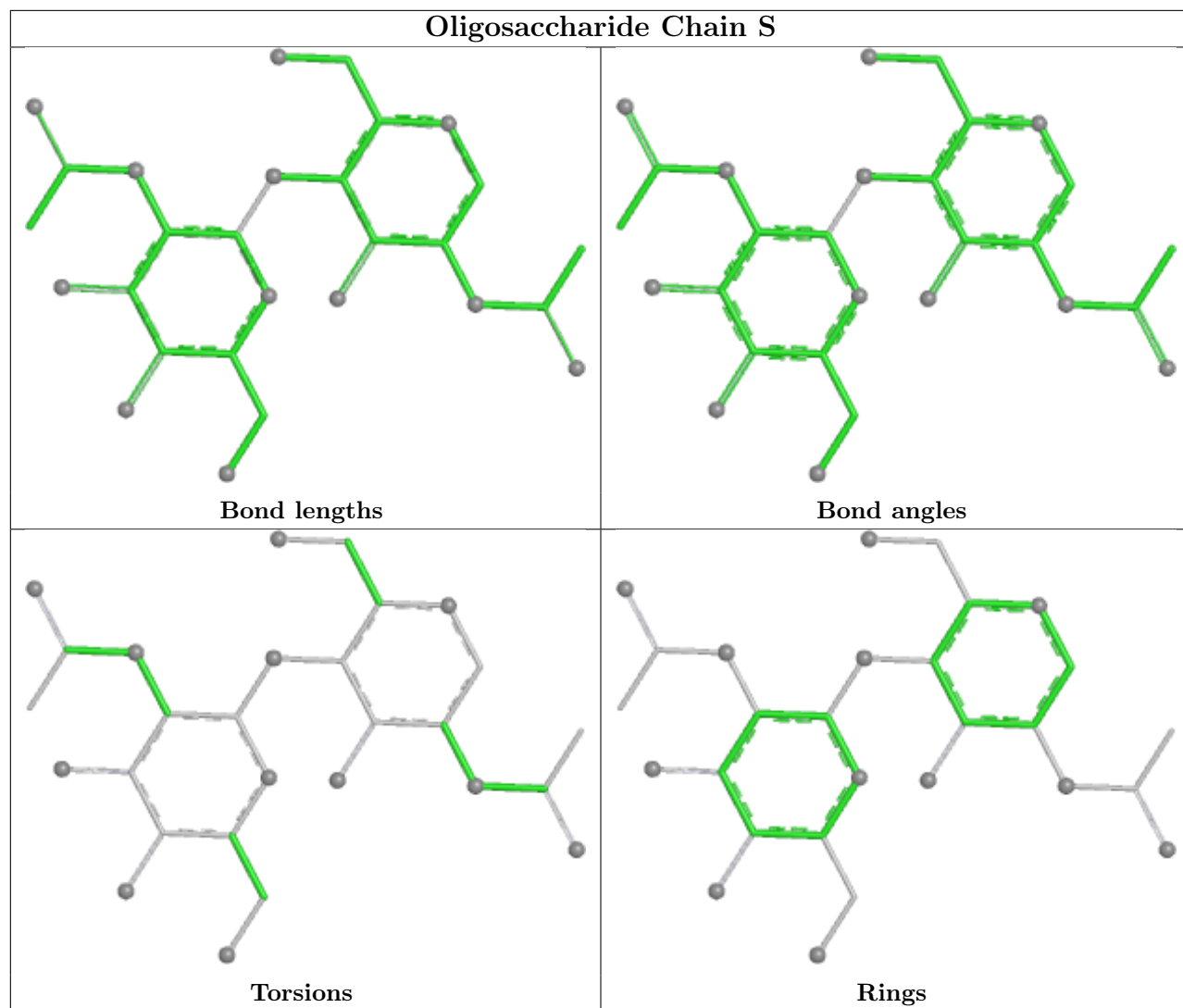
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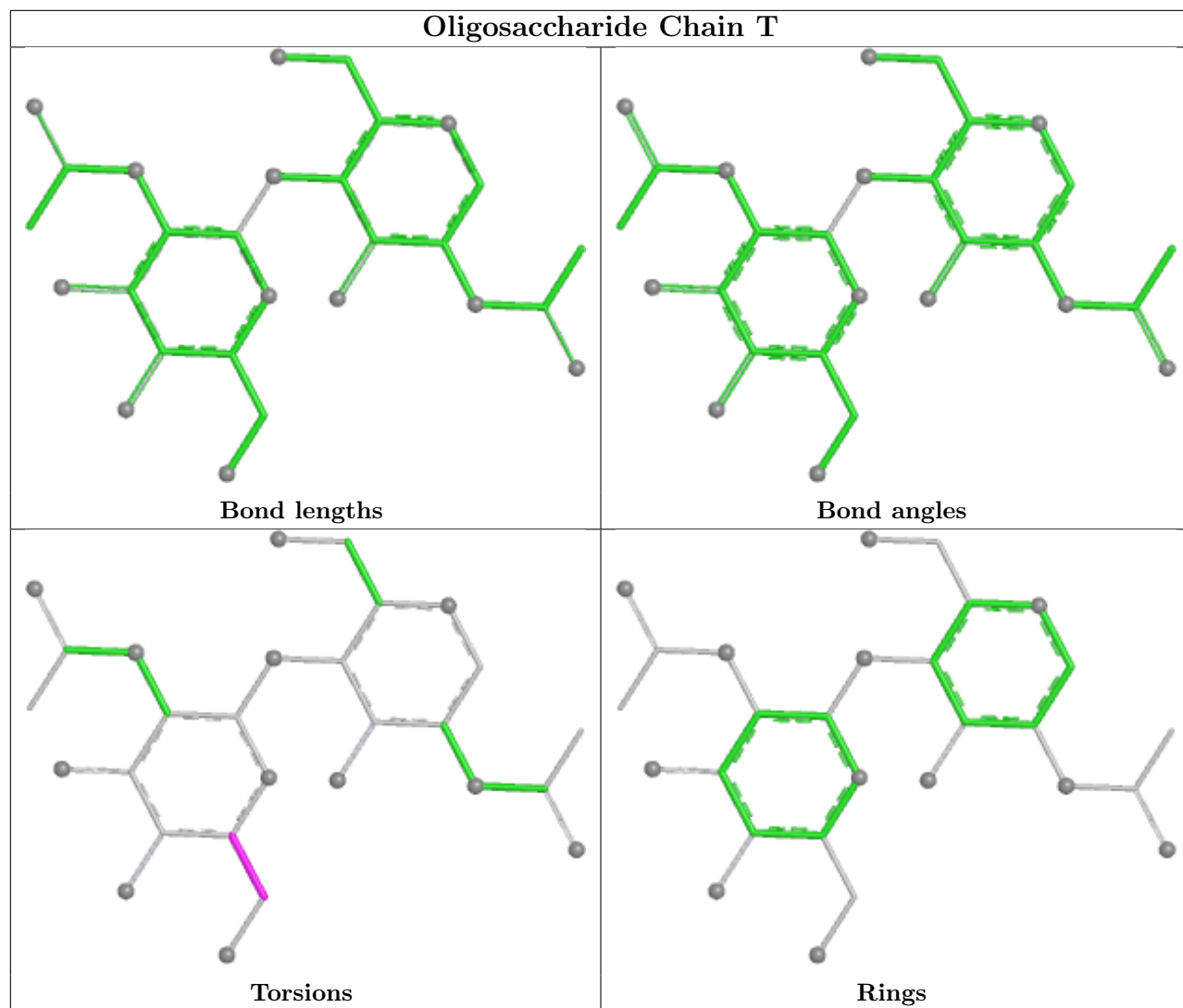
Mol	Chain	Res	Type	Atoms
7	Y	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
9	e	1	NAG	C4-C5-C6-O6
9	m	1	NAG	C4-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	e	1	NAG	O5-C5-C6-O6
9	m	1	NAG	O5-C5-C6-O6
11	Z	4	MAN	O5-C5-C6-O6
11	h	4	MAN	O5-C5-C6-O6
11	p	4	MAN	O5-C5-C6-O6
8	d	5	MAN	O5-C5-C6-O6
8	V	5	MAN	O5-C5-C6-O6
8	l	5	MAN	O5-C5-C6-O6
11	p	6	MAN	O5-C5-C6-O6
11	Z	6	MAN	O5-C5-C6-O6
11	h	6	MAN	O5-C5-C6-O6
11	Z	2	NAG	C3-C2-N2-C7
11	h	2	NAG	C3-C2-N2-C7
11	p	2	NAG	C3-C2-N2-C7
11	Z	2	NAG	C1-C2-N2-C7
11	h	2	NAG	C1-C2-N2-C7
11	p	2	NAG	C1-C2-N2-C7

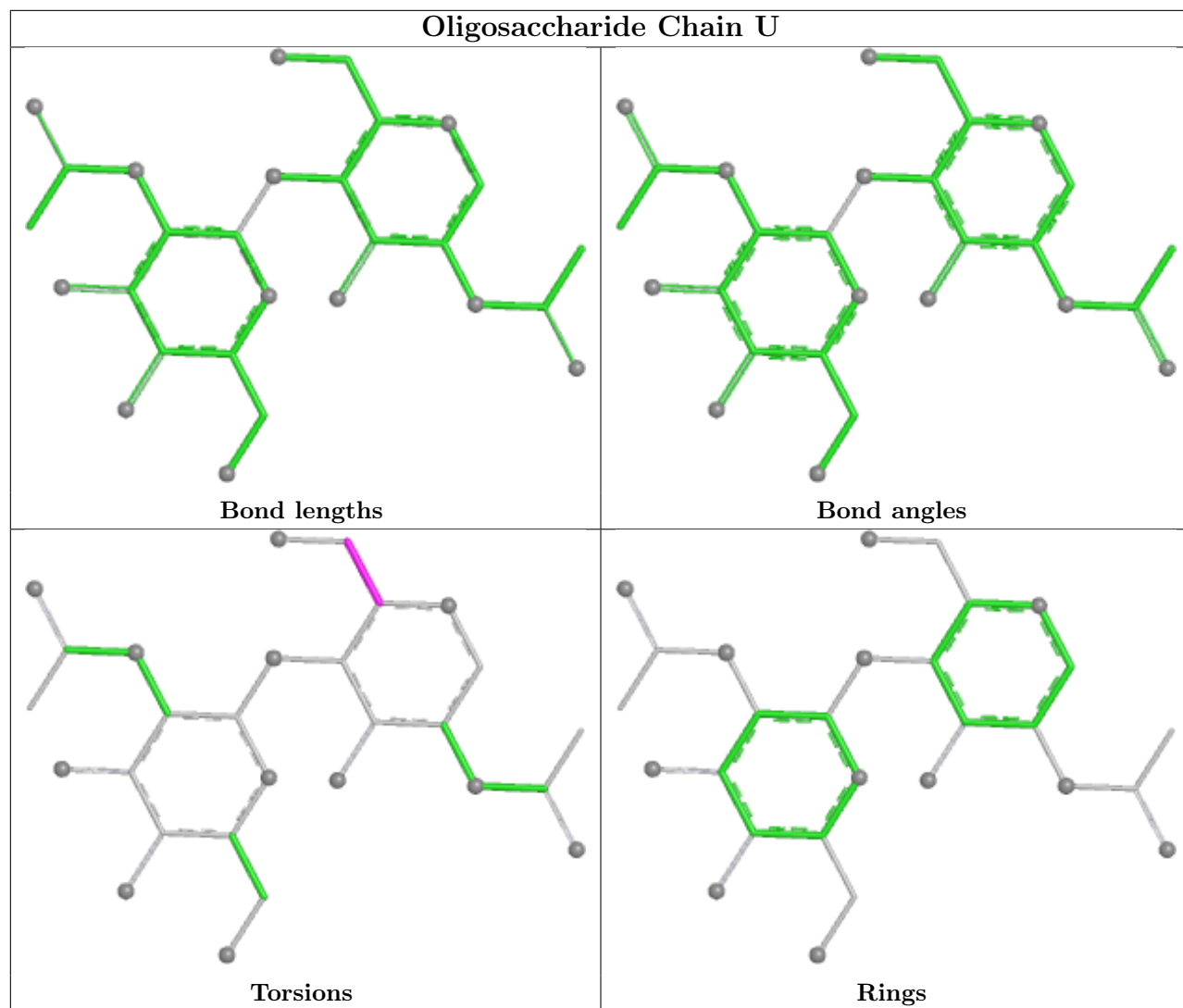
There are no ring outliers.

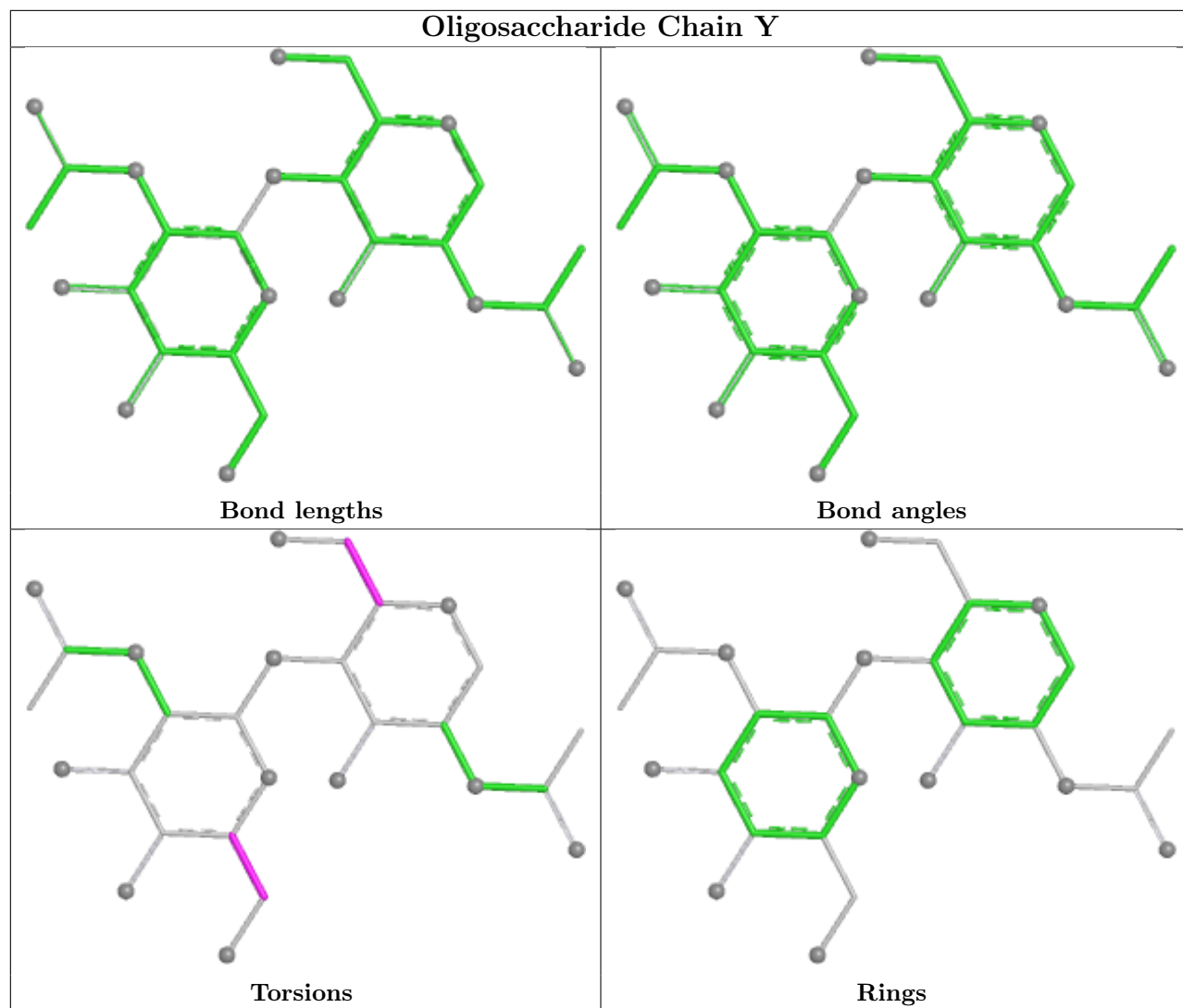
No monomer is involved in short contacts.

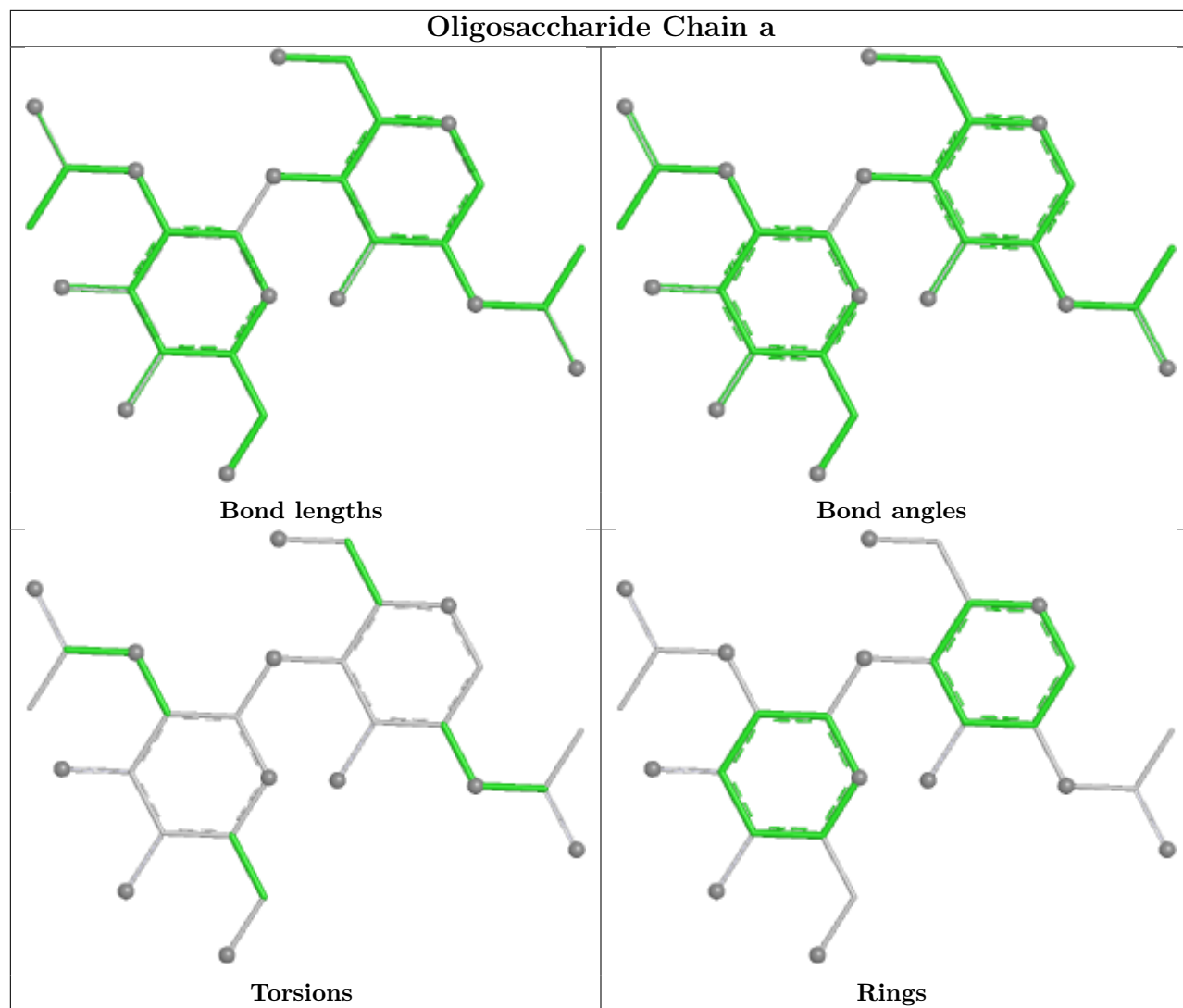
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

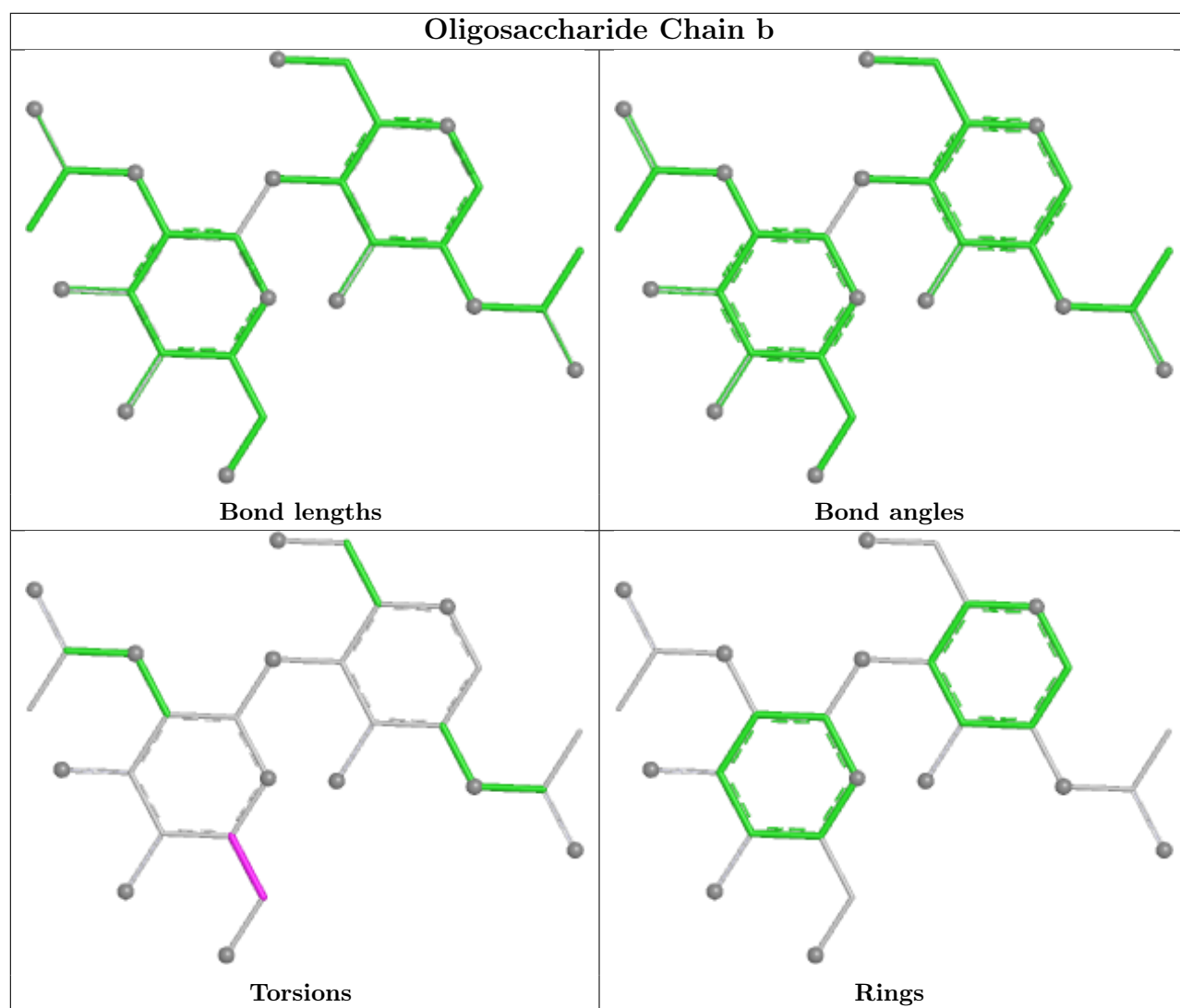


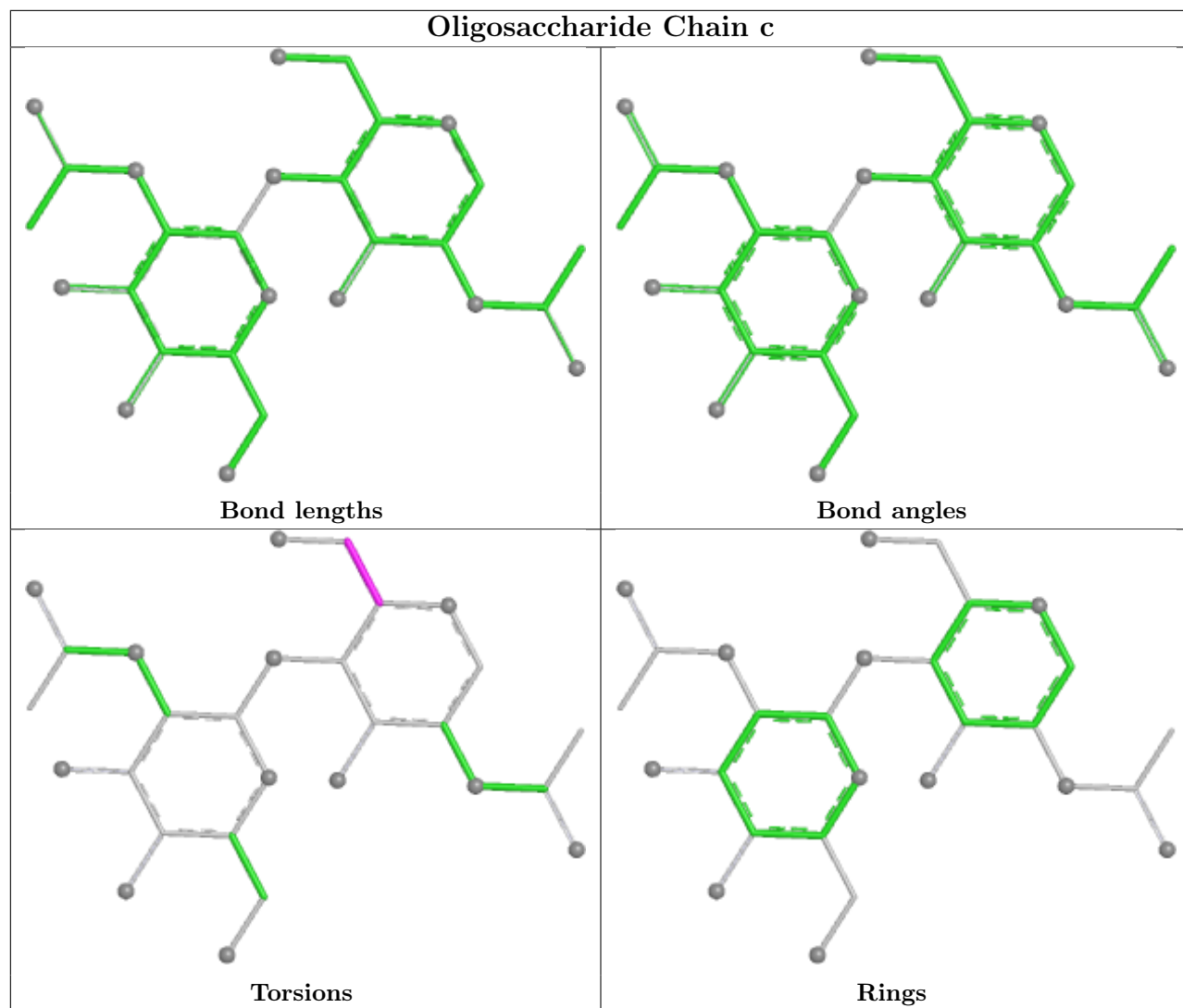


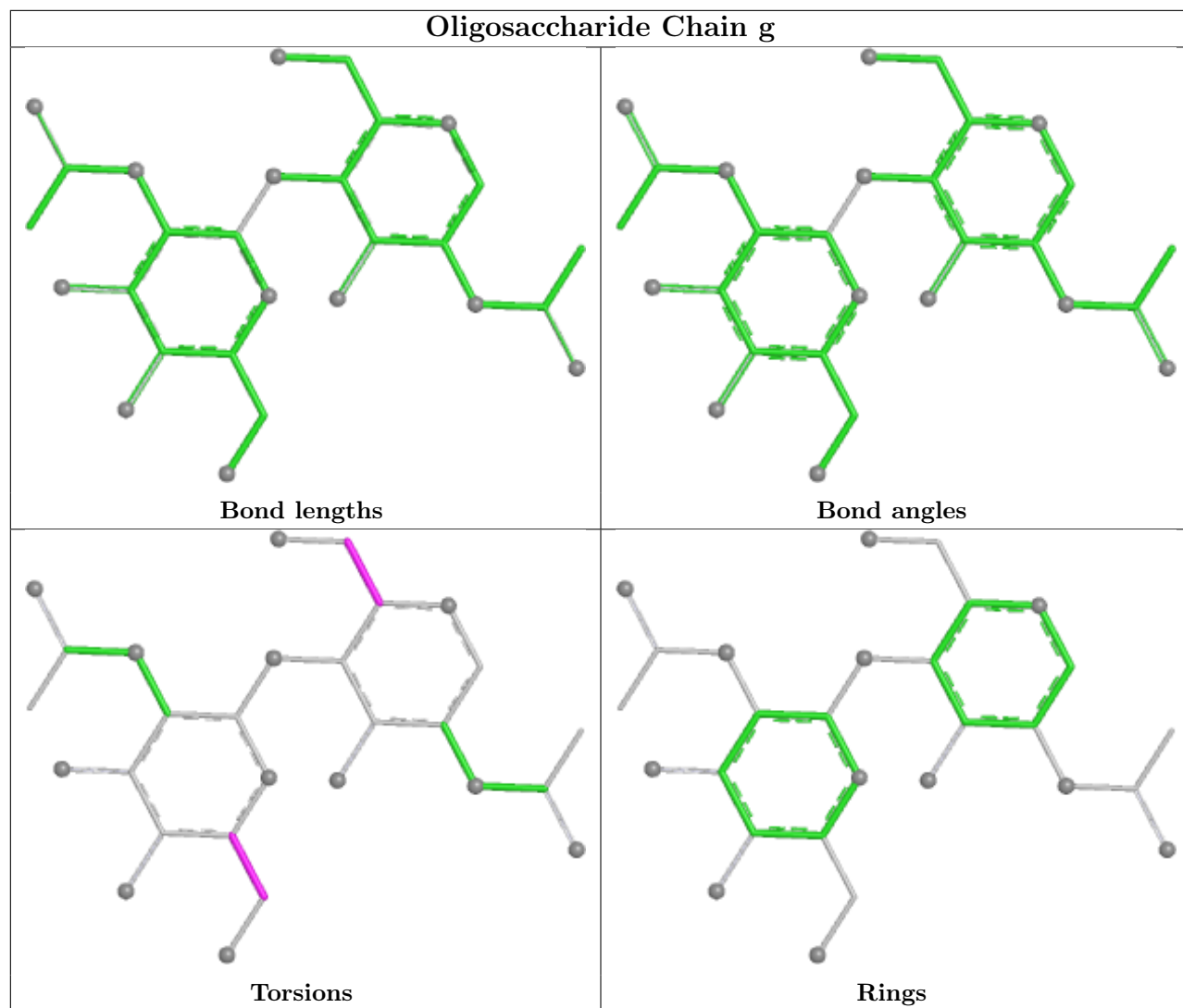


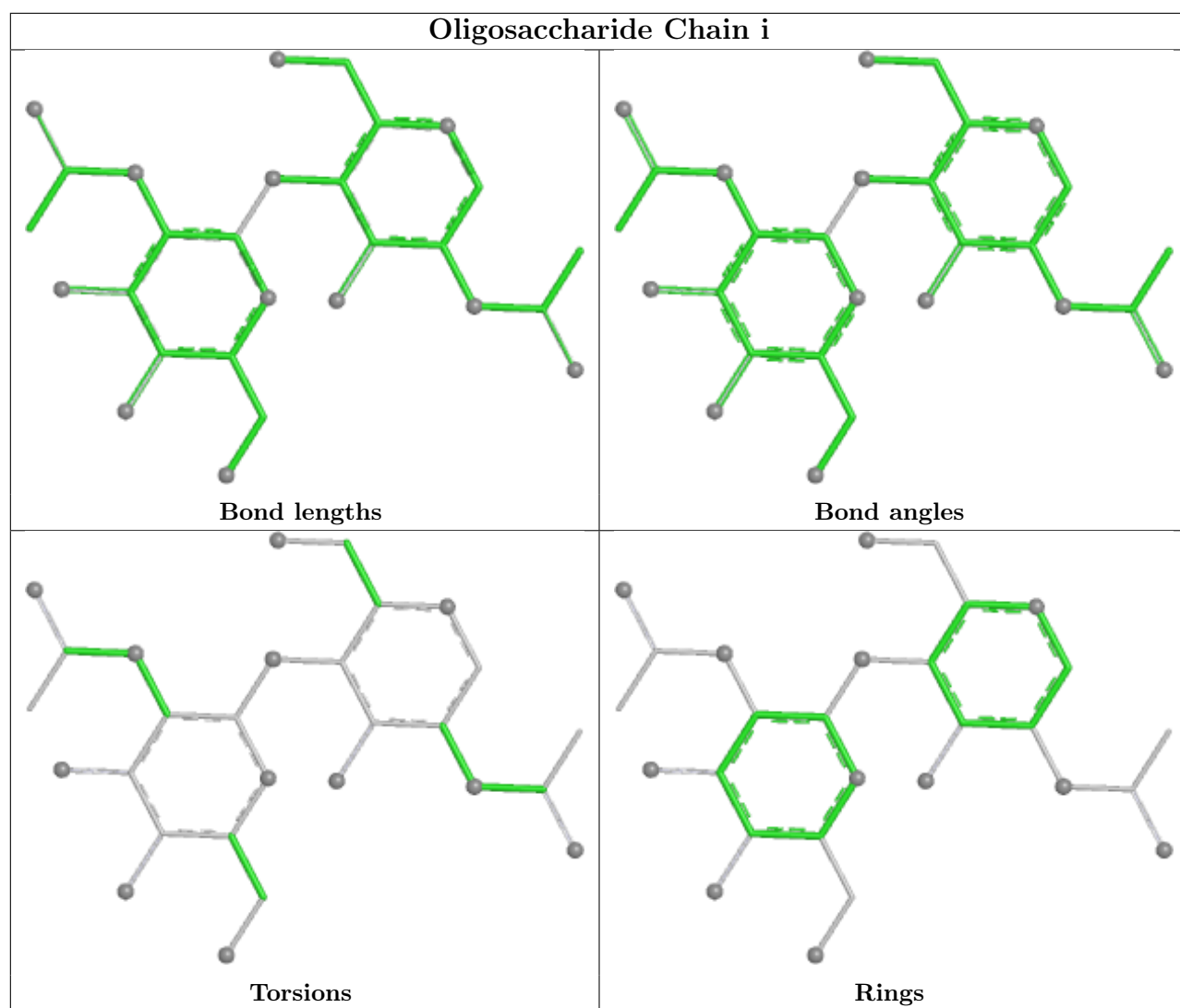


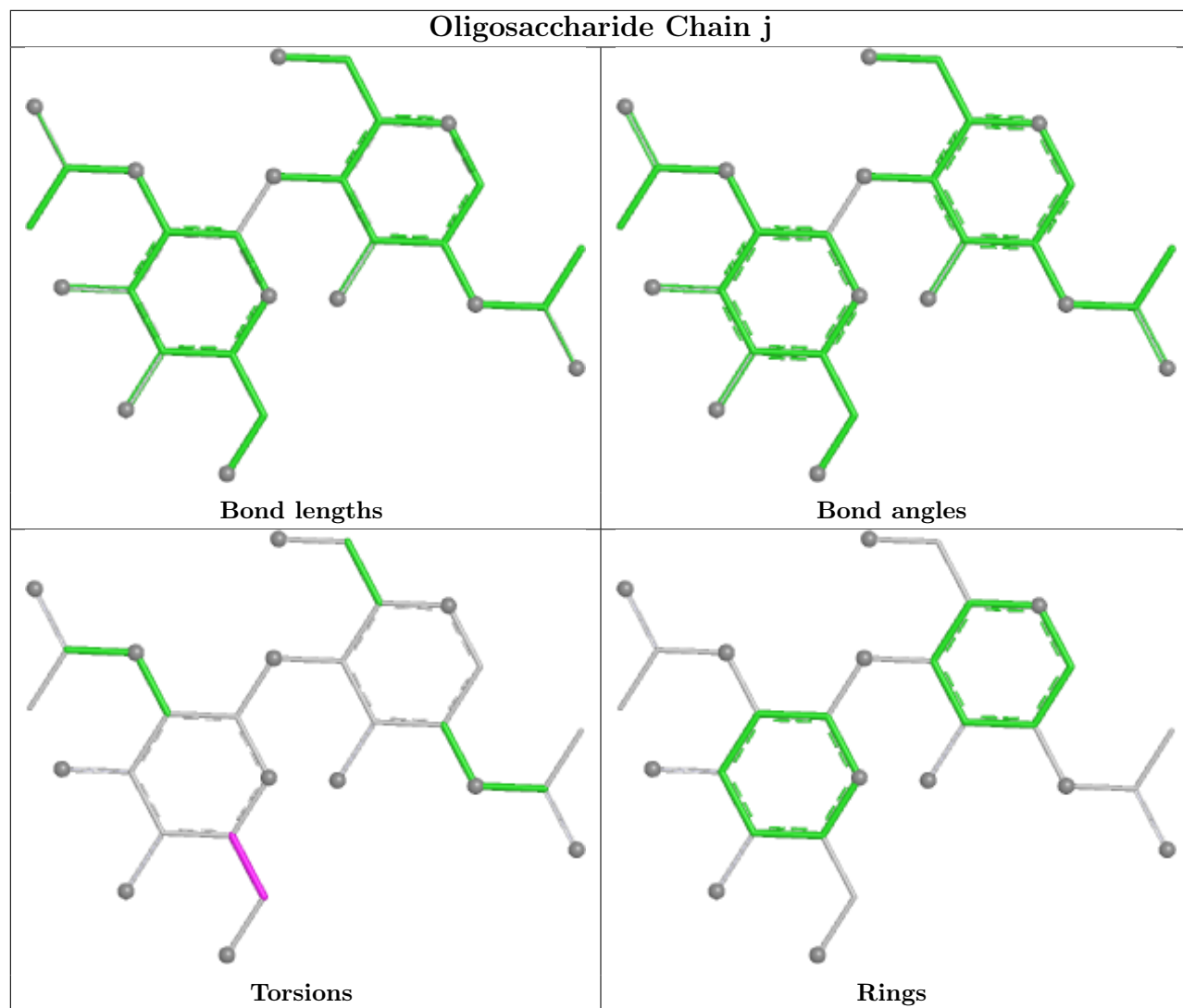


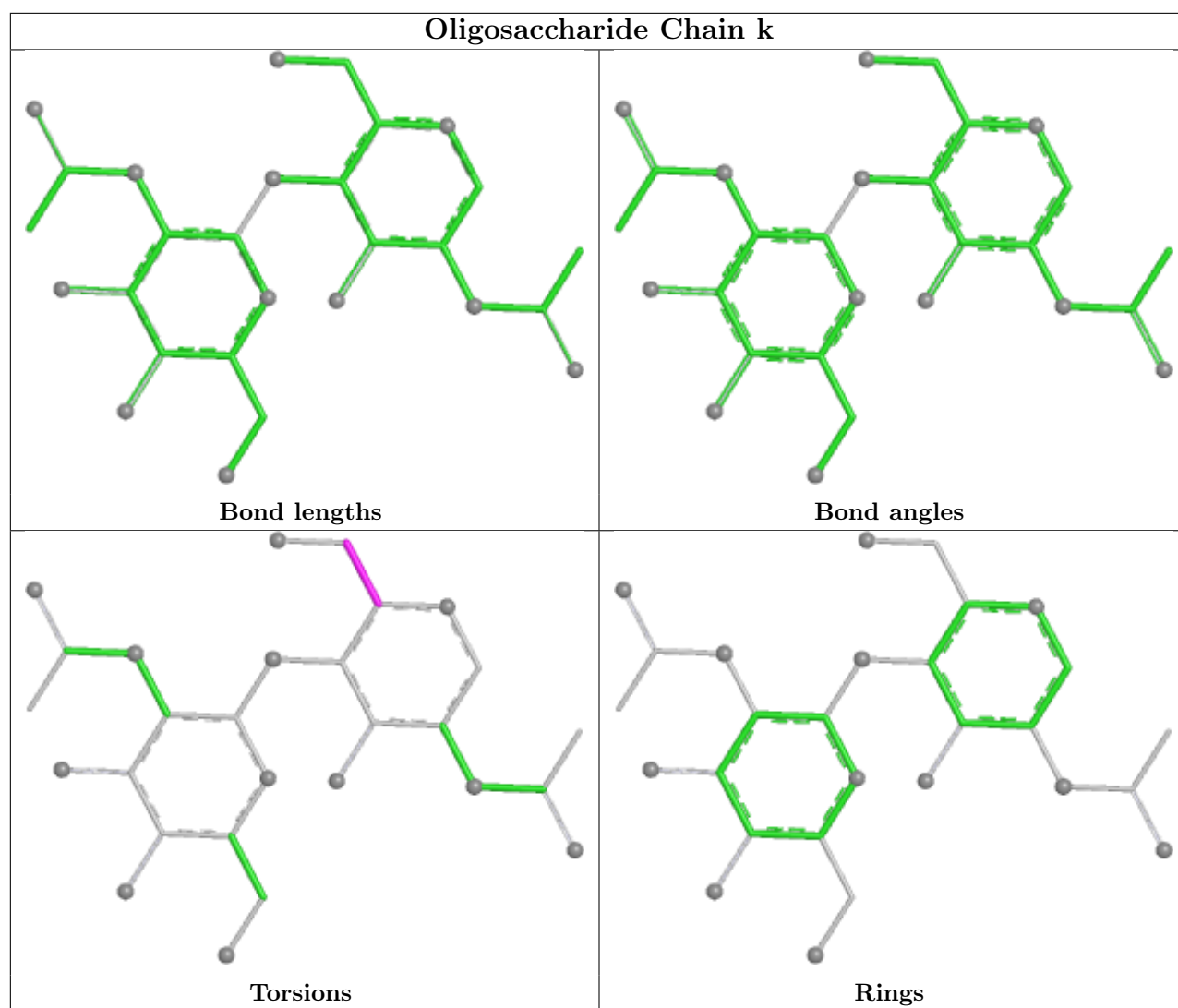


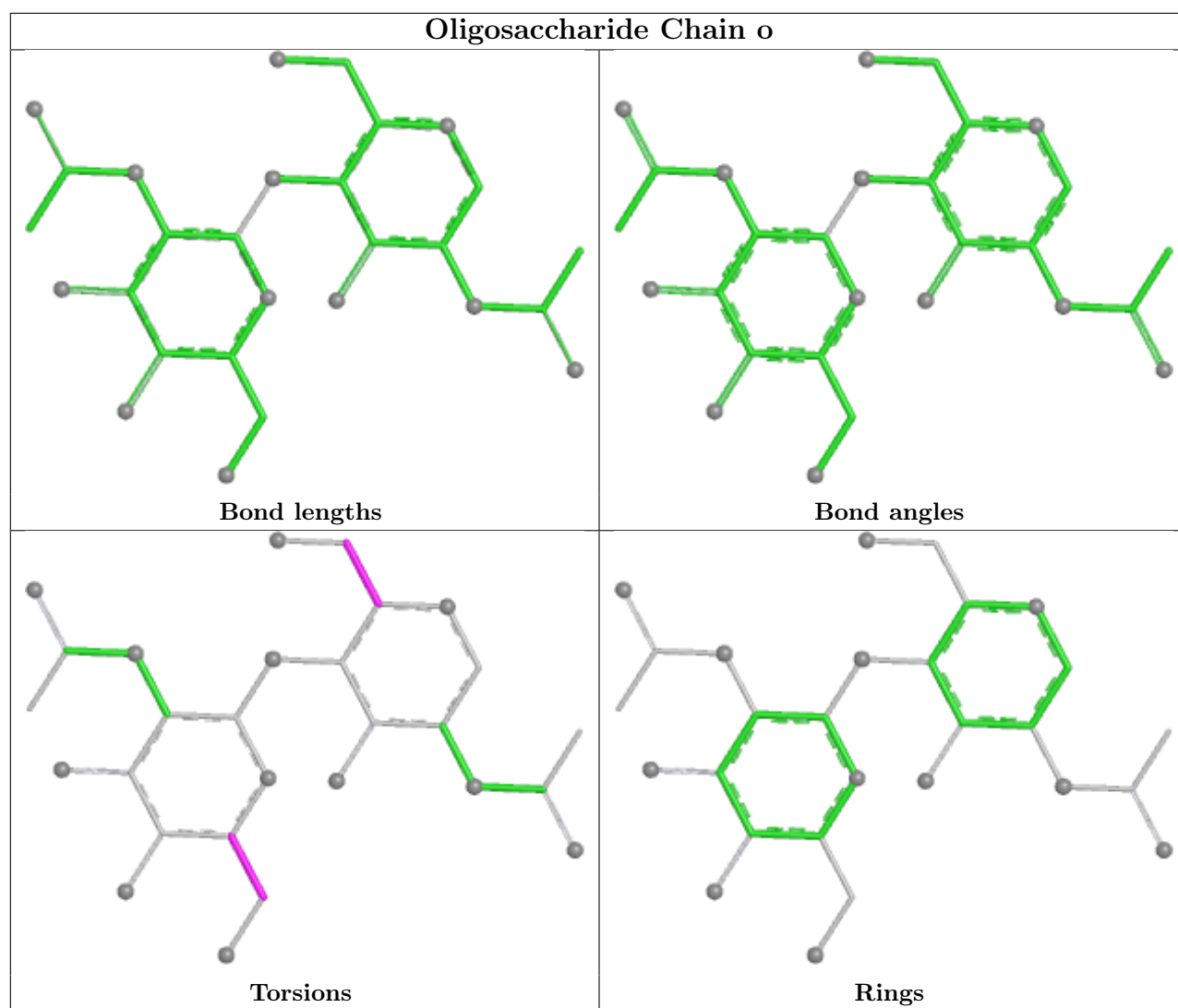


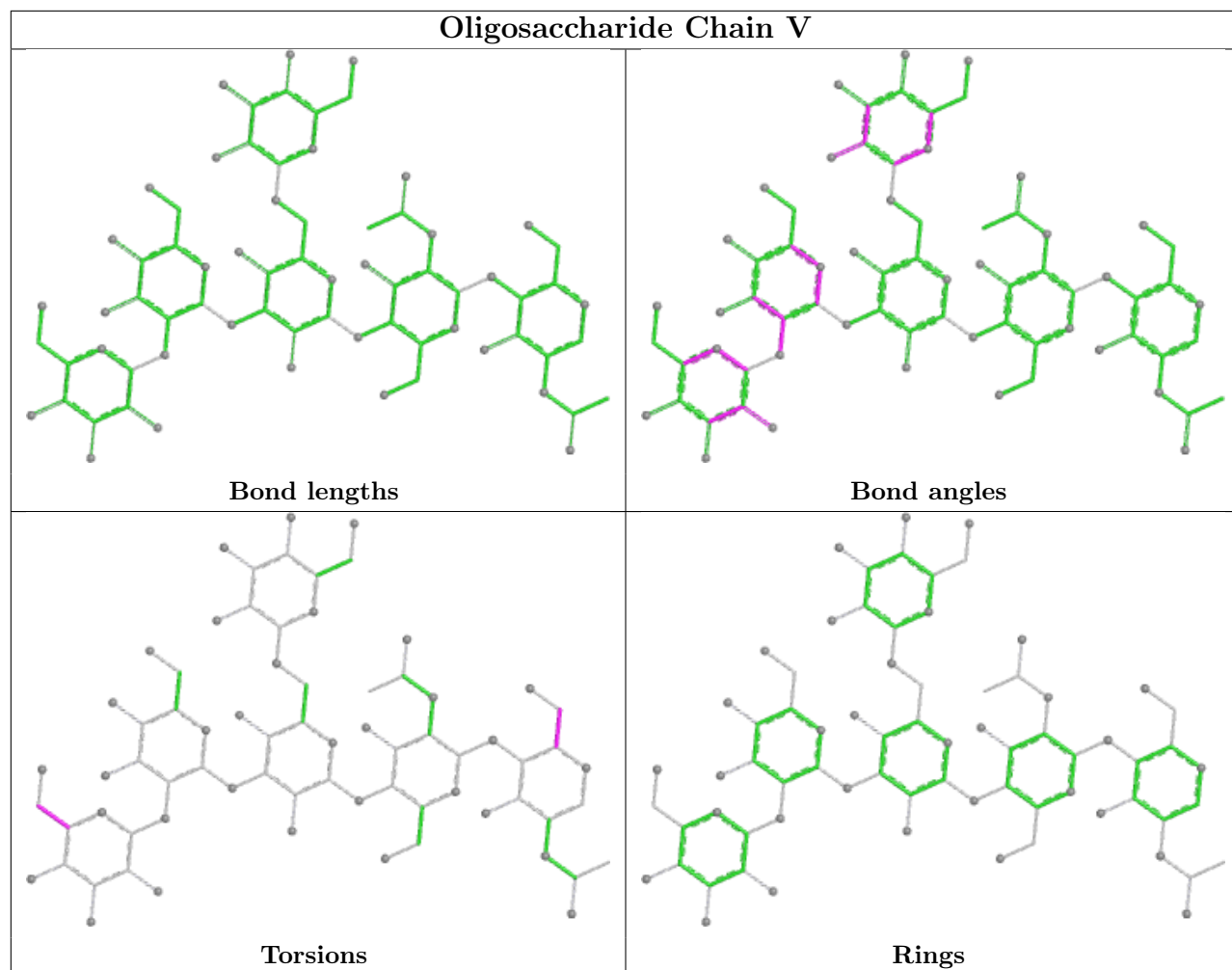


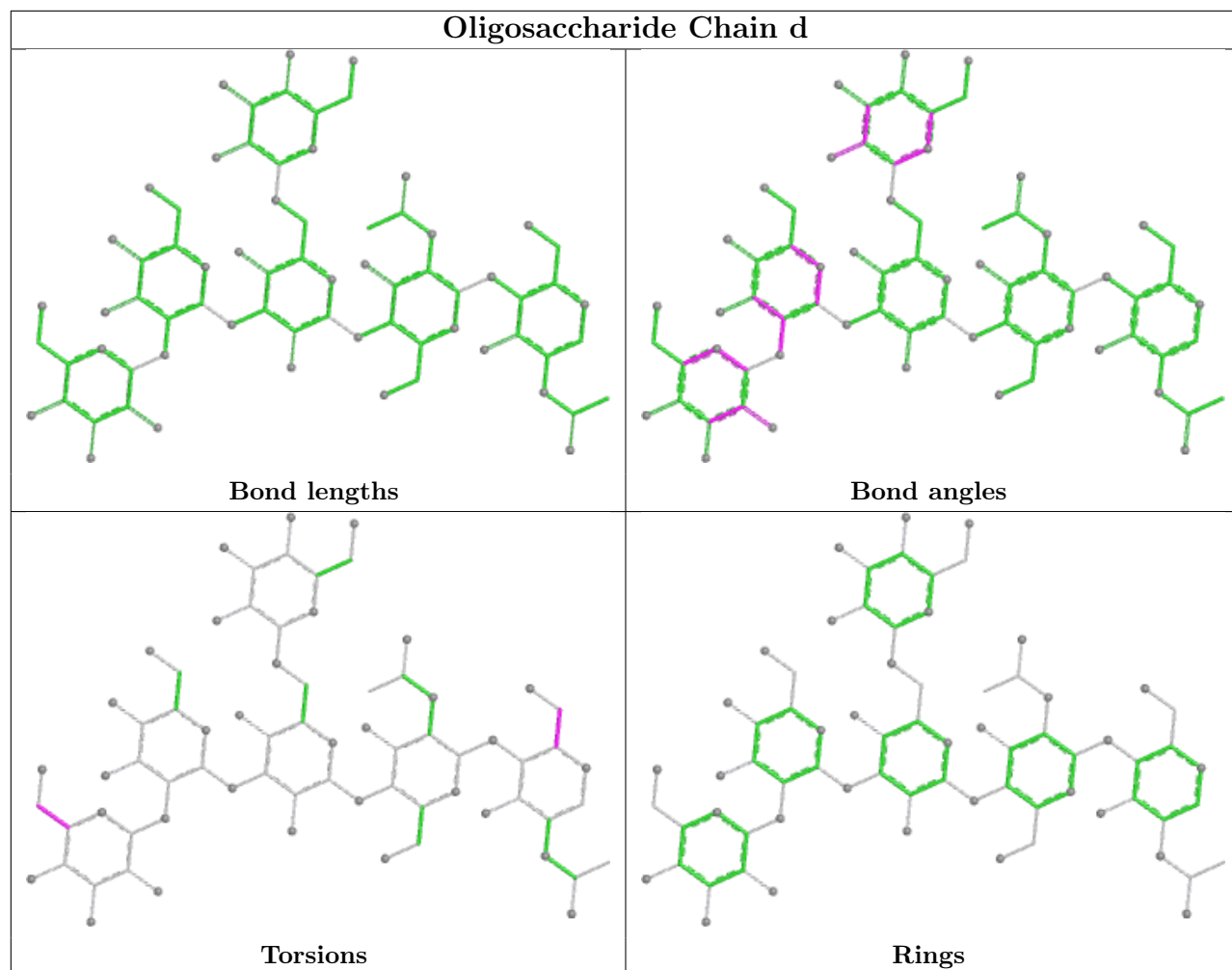


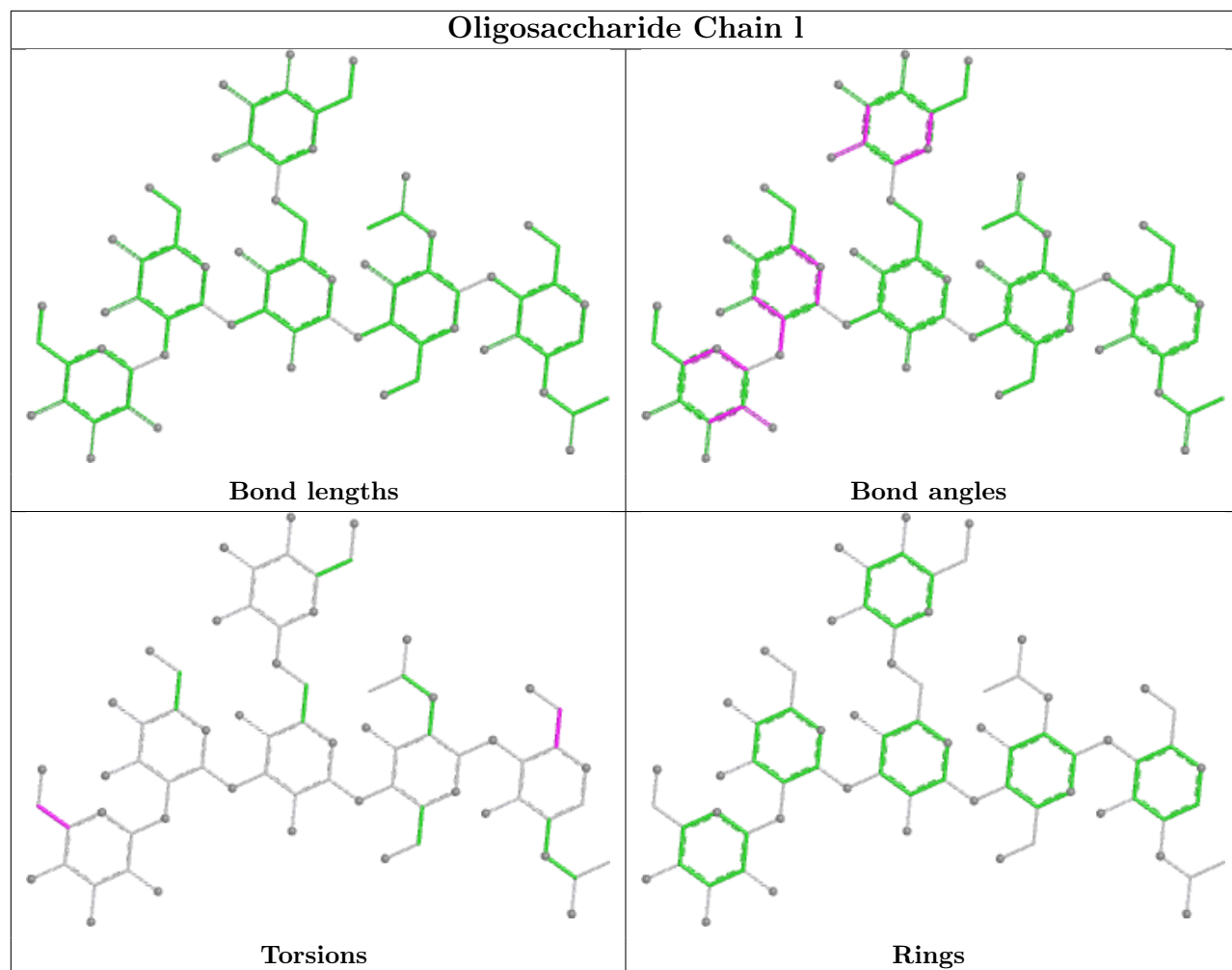


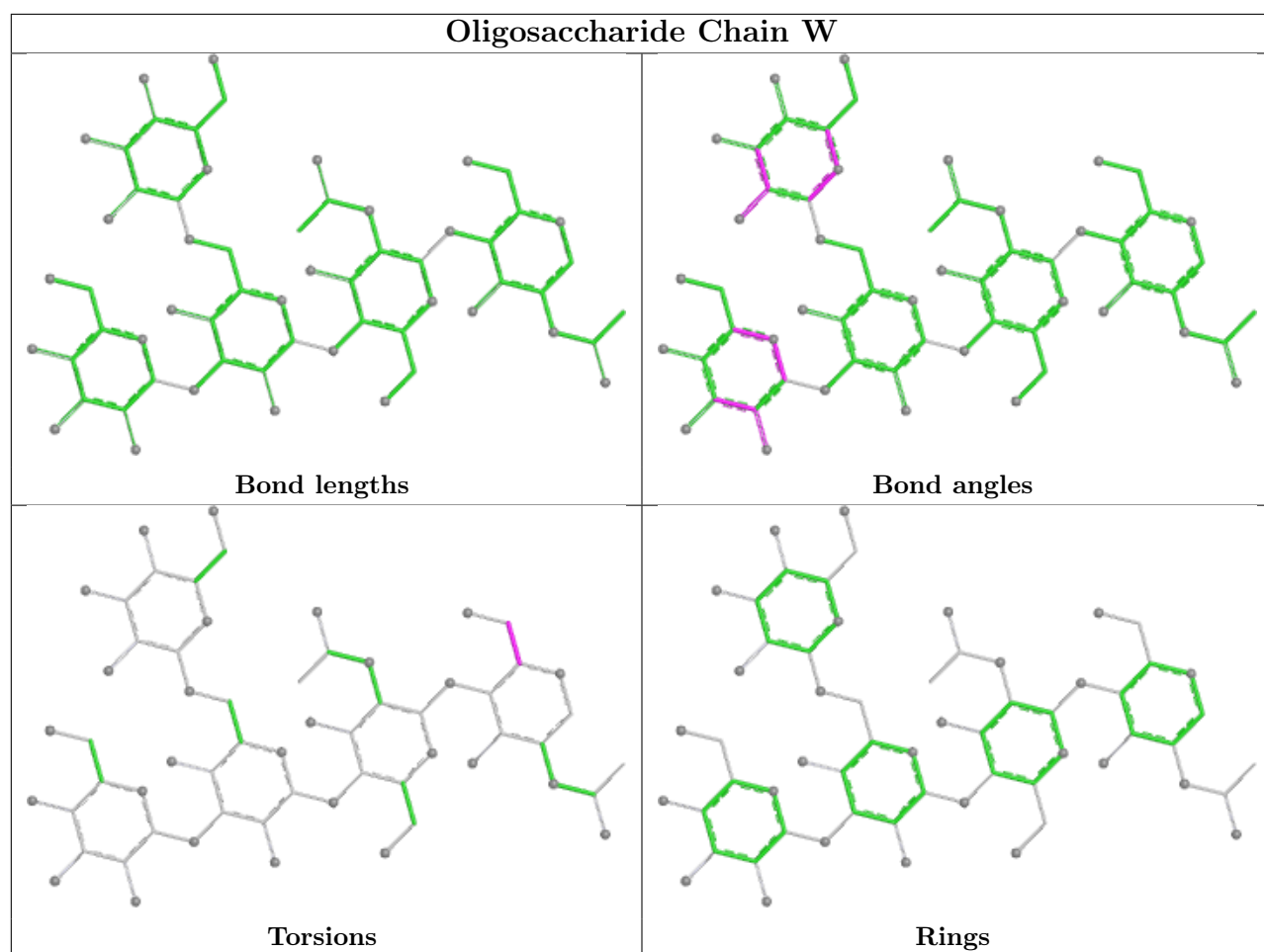


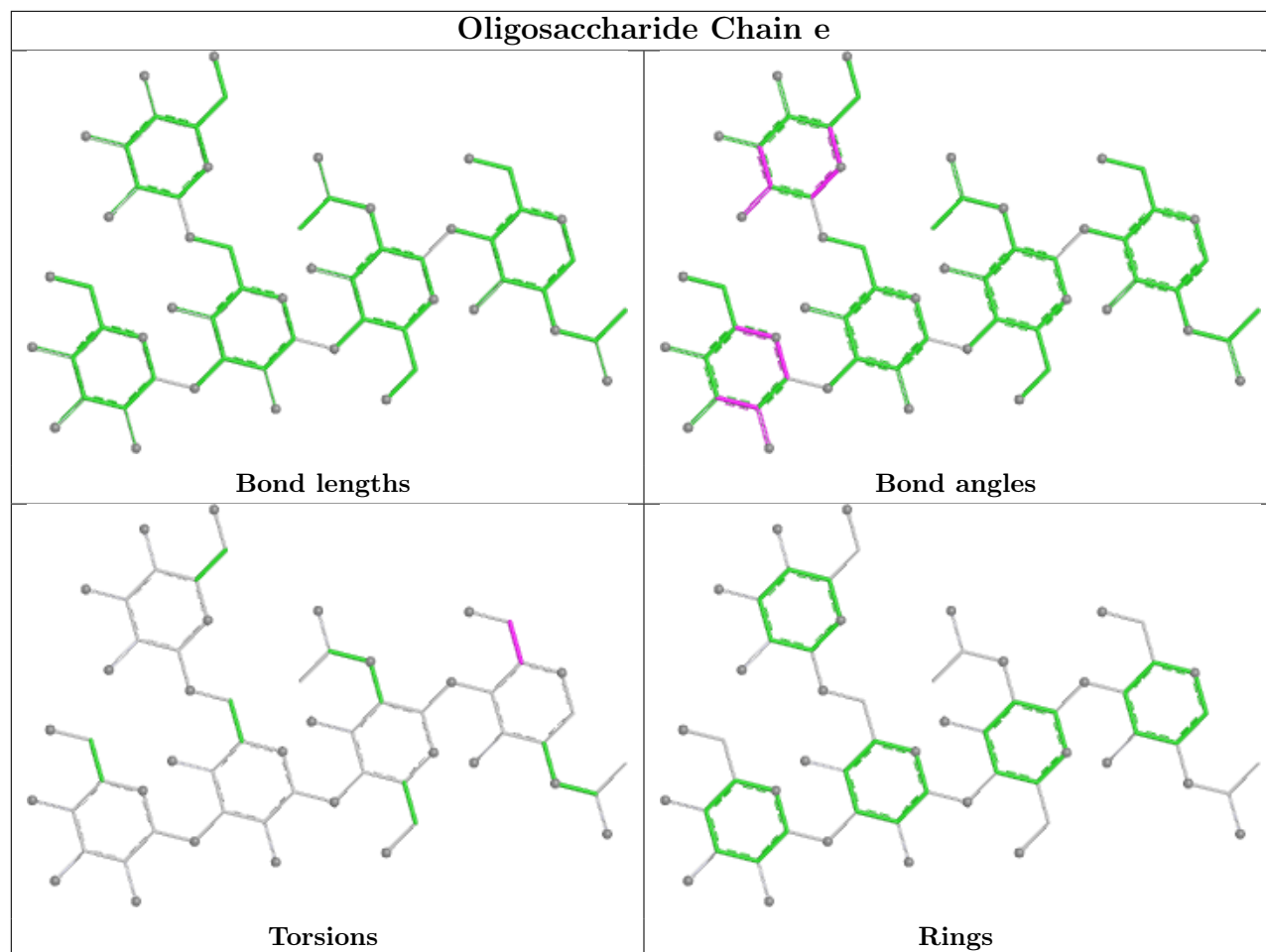


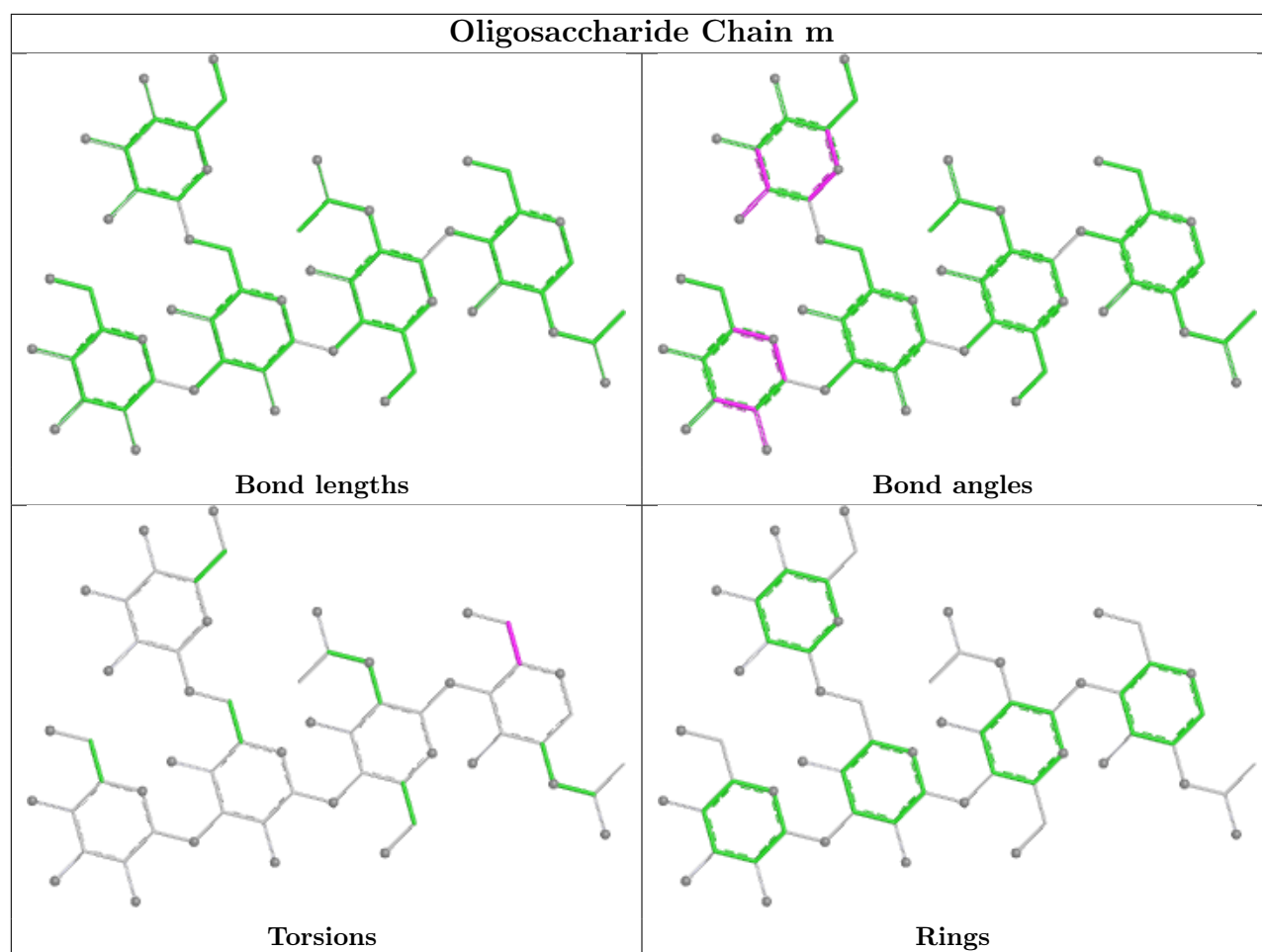


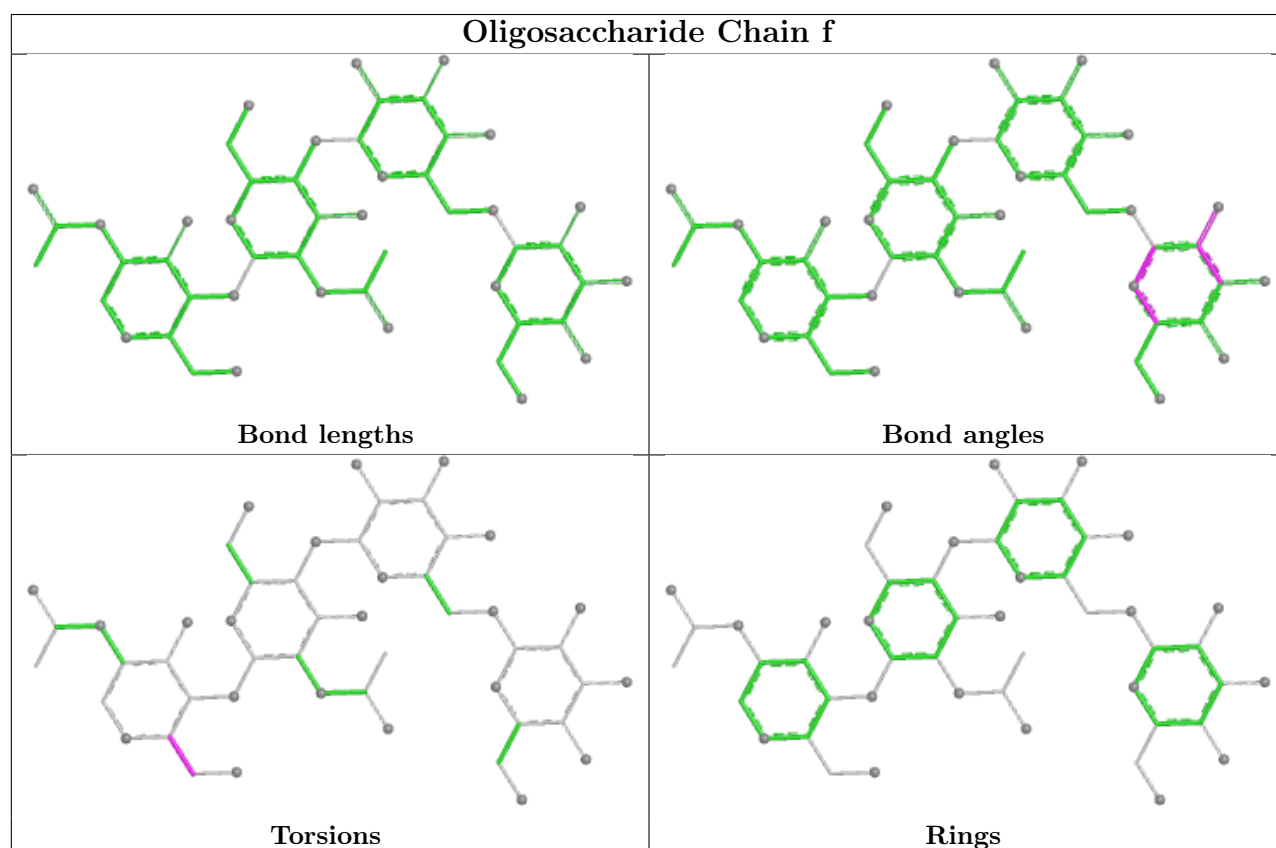
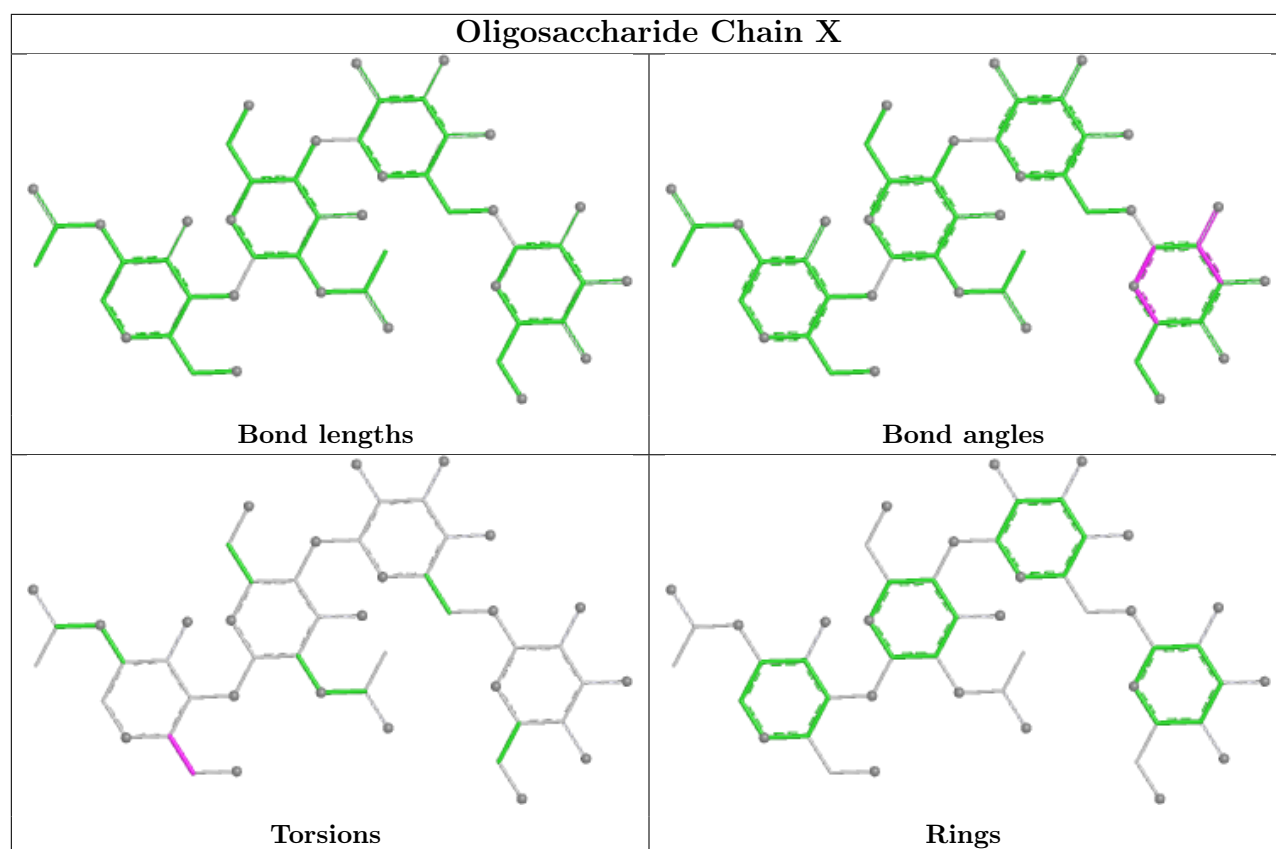


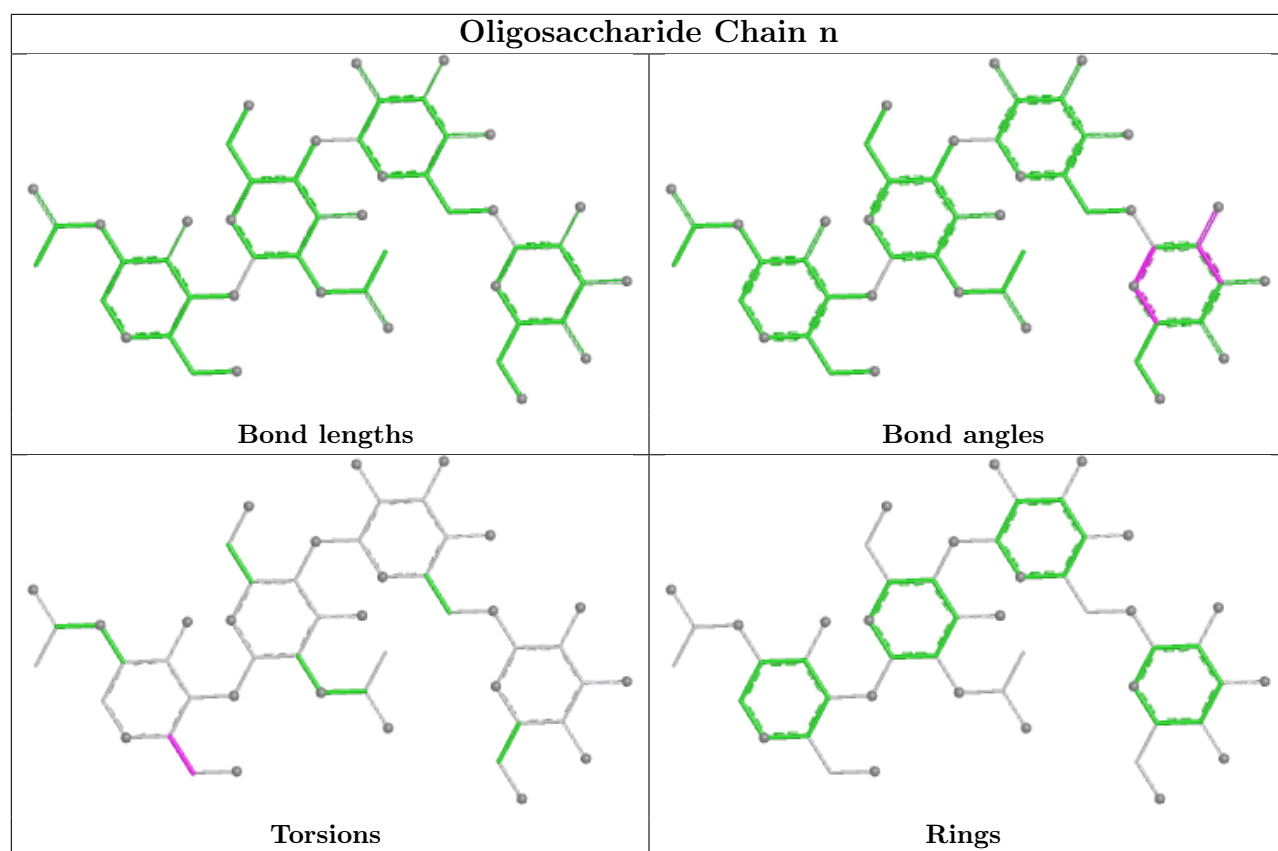


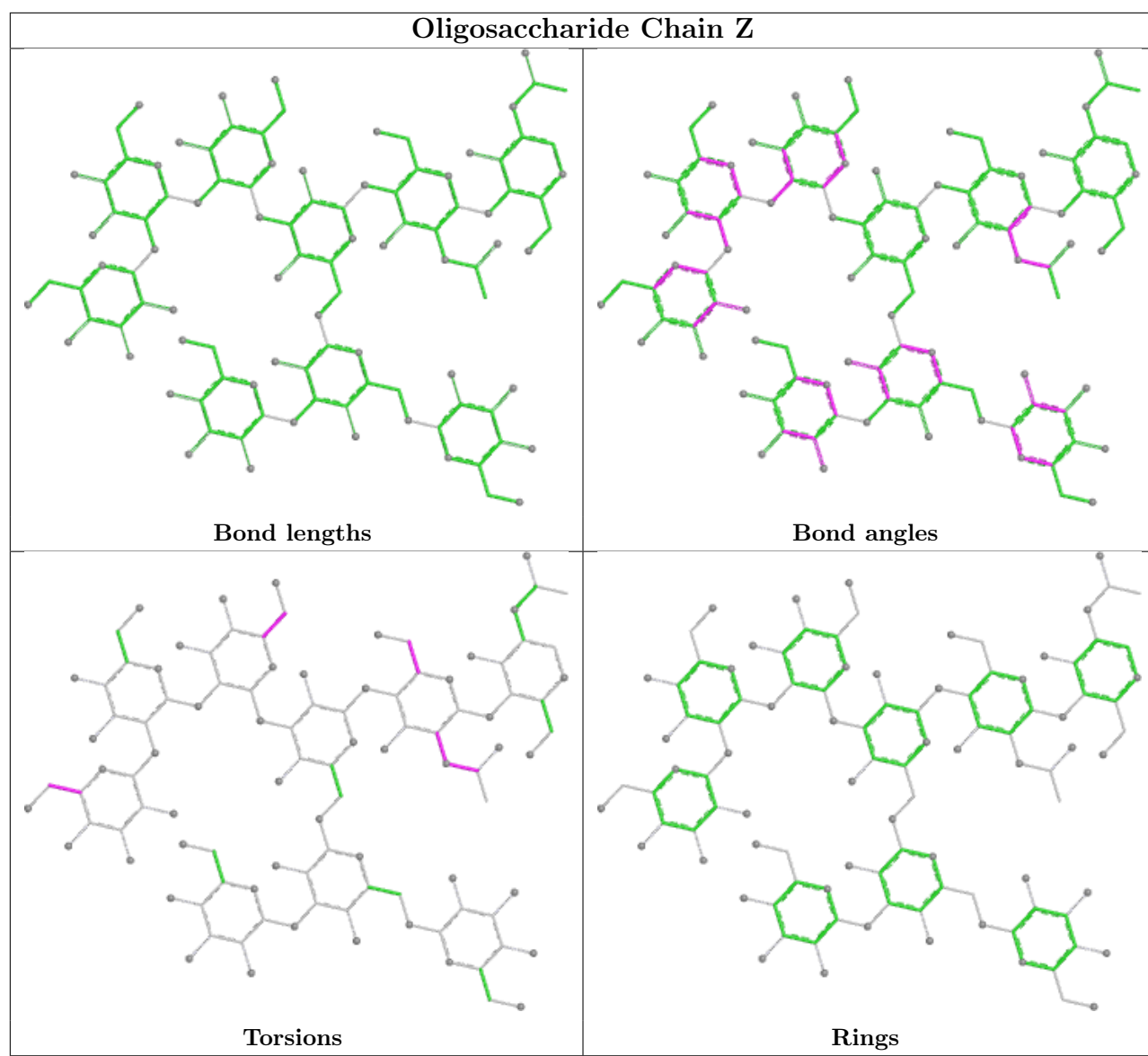


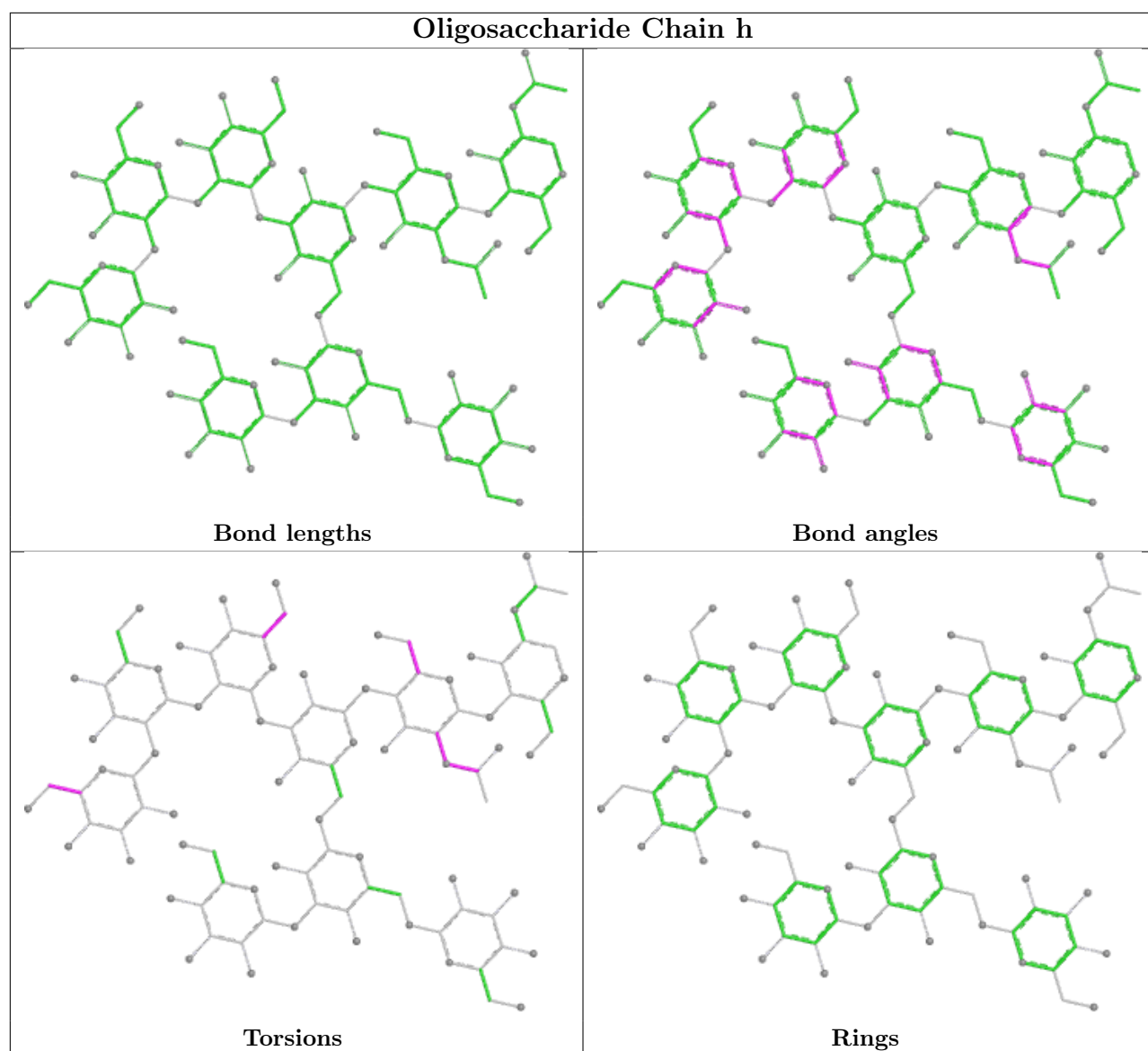


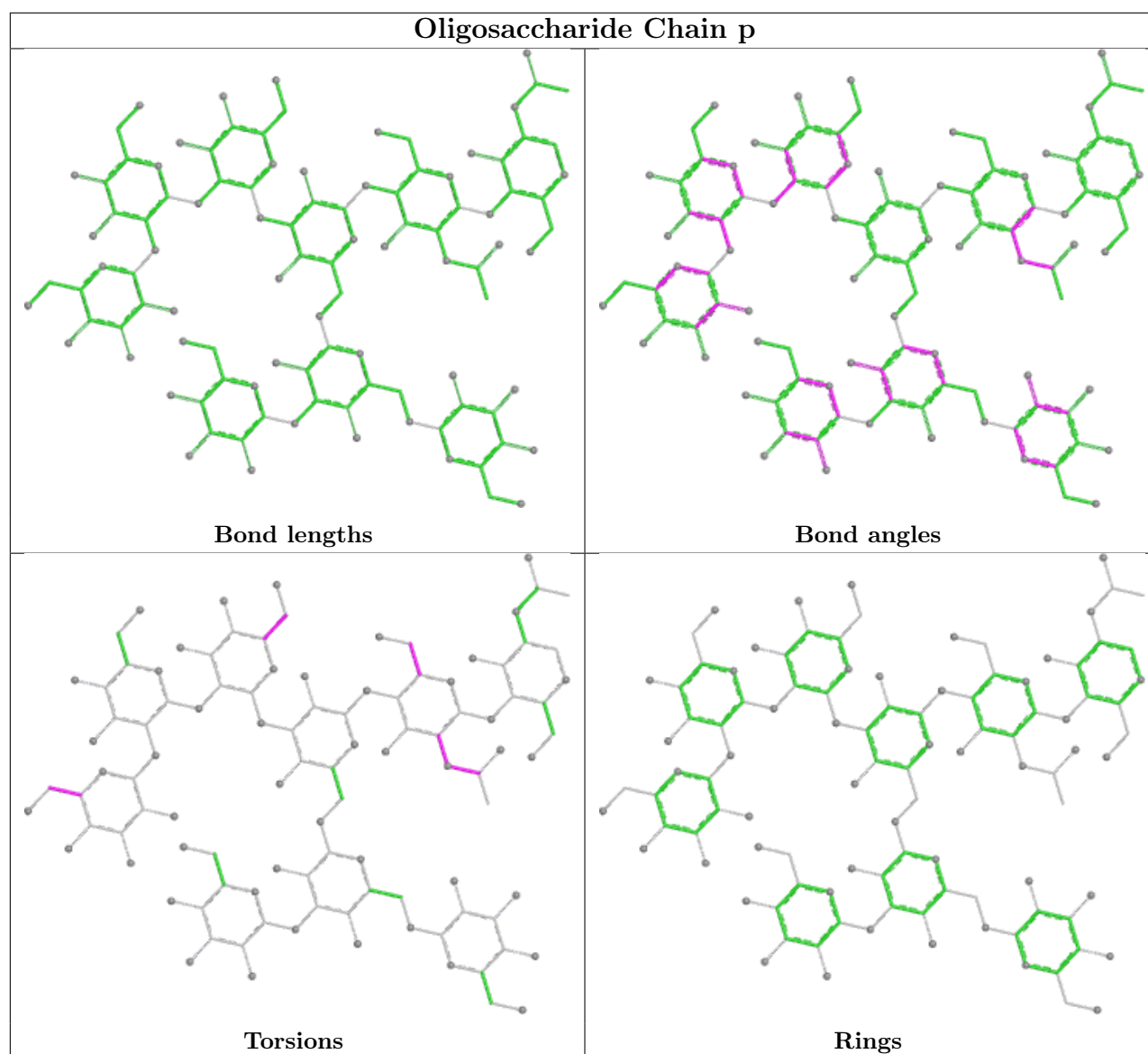












5.6 Ligand geometry [i](#)

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	A	605	1	14,14,15	0.27	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	M	608	1	14,14,15	0.28	0	17,19,21	0.50	0
12	NAG	G	602	1	14,14,15	0.25	0	17,19,21	0.47	0
12	NAG	G	610	1	14,14,15	0.26	0	17,19,21	0.48	0
12	NAG	P	301	4	14,14,15	0.30	0	17,19,21	0.47	0
12	NAG	M	603	1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
12	NAG	G	609	1	14,14,15	0.24	0	17,19,21	0.48	0
12	NAG	A	607	1	14,14,15	0.28	0	17,19,21	0.43	0
12	NAG	M	601	1	14,14,15	0.27	0	17,19,21	0.49	0
12	NAG	M	605	1	14,14,15	0.27	0	17,19,21	0.49	0
12	NAG	G	608	1	14,14,15	0.29	0	17,19,21	0.50	0
12	NAG	G	605	1	14,14,15	0.27	0	17,19,21	0.48	0
12	NAG	G	601	1	14,14,15	0.26	0	17,19,21	0.50	0
12	NAG	G	604	1	14,14,15	0.24	0	17,19,21	0.47	0
12	NAG	M	606	1	14,14,15	0.29	0	17,19,21	0.49	0
12	NAG	A	610	1	14,14,15	0.26	0	17,19,21	0.49	0
12	NAG	E	701	2	14,14,15	0.26	0	17,19,21	0.49	0
12	NAG	A	609	1	14,14,15	0.23	0	17,19,21	0.48	0
12	NAG	E	702	2	14,14,15	0.29	0	17,19,21	0.48	0
12	NAG	M	610	1	14,14,15	0.26	0	17,19,21	0.48	0
12	NAG	A	608	1	14,14,15	0.30	0	17,19,21	0.50	0
12	NAG	D	301	4	14,14,15	0.29	0	17,19,21	0.47	0
12	NAG	M	609	1	14,14,15	0.24	0	17,19,21	0.48	0
12	NAG	I	301	4	14,14,15	0.30	0	17,19,21	0.47	0
12	NAG	A	602	1	14,14,15	0.24	0	17,19,21	0.47	0
12	NAG	M	607	1	14,14,15	0.28	0	17,19,21	0.44	0
12	NAG	B	702	2	14,14,15	0.29	0	17,19,21	0.49	0
12	NAG	G	606	1	14,14,15	0.29	0	17,19,21	0.50	0
12	NAG	A	603	1	14,14,15	0.45	0	17,19,21	0.83	1 (5%)
12	NAG	N	701	2	14,14,15	0.27	0	17,19,21	0.47	0
12	NAG	N	702	2	14,14,15	0.31	0	17,19,21	0.49	0
12	NAG	G	607	1	14,14,15	0.29	0	17,19,21	0.44	0
12	NAG	B	701	2	14,14,15	0.26	0	17,19,21	0.48	0
12	NAG	G	603	1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
12	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.50	0
12	NAG	A	604	1	14,14,15	0.22	0	17,19,21	0.46	0
12	NAG	M	604	1	14,14,15	0.25	0	17,19,21	0.47	0
12	NAG	A	606	1	14,14,15	0.28	0	17,19,21	0.49	0
12	NAG	M	602	1	14,14,15	0.26	0	17,19,21	0.47	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
12	NAG	A	605	1	-	2/6/23/26	0/1/1/1
12	NAG	M	608	1	-	2/6/23/26	0/1/1/1
12	NAG	G	602	1	-	2/6/23/26	0/1/1/1
12	NAG	G	610	1	-	2/6/23/26	0/1/1/1
12	NAG	P	301	4	-	1/6/23/26	0/1/1/1
12	NAG	M	603	1	-	3/6/23/26	0/1/1/1
12	NAG	G	609	1	-	0/6/23/26	0/1/1/1
12	NAG	A	607	1	-	1/6/23/26	0/1/1/1
12	NAG	M	601	1	-	2/6/23/26	0/1/1/1
12	NAG	M	605	1	-	2/6/23/26	0/1/1/1
12	NAG	G	608	1	-	2/6/23/26	0/1/1/1
12	NAG	G	605	1	-	2/6/23/26	0/1/1/1
12	NAG	G	601	1	-	2/6/23/26	0/1/1/1
12	NAG	G	604	1	-	0/6/23/26	0/1/1/1
12	NAG	M	606	1	-	2/6/23/26	0/1/1/1
12	NAG	A	610	1	-	2/6/23/26	0/1/1/1
12	NAG	E	701	2	-	0/6/23/26	0/1/1/1
12	NAG	A	609	1	-	0/6/23/26	0/1/1/1
12	NAG	E	702	2	-	2/6/23/26	0/1/1/1
12	NAG	M	610	1	-	2/6/23/26	0/1/1/1
12	NAG	A	608	1	-	2/6/23/26	0/1/1/1
12	NAG	D	301	4	-	1/6/23/26	0/1/1/1
12	NAG	M	609	1	-	0/6/23/26	0/1/1/1
12	NAG	I	301	4	-	1/6/23/26	0/1/1/1
12	NAG	A	602	1	-	2/6/23/26	0/1/1/1
12	NAG	M	607	1	-	1/6/23/26	0/1/1/1
12	NAG	B	702	2	-	2/6/23/26	0/1/1/1
12	NAG	G	606	1	-	2/6/23/26	0/1/1/1
12	NAG	A	603	1	-	3/6/23/26	0/1/1/1
12	NAG	N	701	2	-	0/6/23/26	0/1/1/1
12	NAG	N	702	2	-	2/6/23/26	0/1/1/1
12	NAG	G	607	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	2	-	0/6/23/26	0/1/1/1
12	NAG	G	603	1	-	3/6/23/26	0/1/1/1
12	NAG	A	601	1	-	2/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1
12	NAG	M	604	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	606	1	-	2/6/23/26	0/1/1/1
12	NAG	M	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	603	NAG	C2-N2-C7	2.55	126.32	122.90
12	M	603	NAG	C2-N2-C7	2.54	126.31	122.90
12	G	603	NAG	C2-N2-C7	2.54	126.30	122.90

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	O5-C5-C6-O6
12	A	601	NAG	O5-C5-C6-O6
12	M	601	NAG	O5-C5-C6-O6
12	G	605	NAG	O5-C5-C6-O6
12	A	605	NAG	O5-C5-C6-O6
12	M	605	NAG	O5-C5-C6-O6
12	G	608	NAG	O5-C5-C6-O6
12	A	608	NAG	O5-C5-C6-O6
12	M	608	NAG	O5-C5-C6-O6
12	G	608	NAG	C4-C5-C6-O6
12	A	608	NAG	C4-C5-C6-O6
12	M	608	NAG	C4-C5-C6-O6
12	G	601	NAG	C4-C5-C6-O6
12	A	601	NAG	C4-C5-C6-O6
12	M	601	NAG	C4-C5-C6-O6
12	G	602	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	M	602	NAG	O5-C5-C6-O6
12	G	605	NAG	C4-C5-C6-O6
12	A	605	NAG	C4-C5-C6-O6
12	M	605	NAG	C4-C5-C6-O6
12	G	610	NAG	O5-C5-C6-O6
12	A	610	NAG	O5-C5-C6-O6
12	E	702	NAG	O5-C5-C6-O6
12	M	610	NAG	O5-C5-C6-O6
12	N	702	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	B	702	NAG	O5-C5-C6-O6
12	G	602	NAG	C4-C5-C6-O6
12	M	602	NAG	C4-C5-C6-O6
12	A	602	NAG	C4-C5-C6-O6
12	G	610	NAG	C4-C5-C6-O6
12	A	610	NAG	C4-C5-C6-O6
12	E	702	NAG	C4-C5-C6-O6
12	M	610	NAG	C4-C5-C6-O6
12	B	702	NAG	C4-C5-C6-O6
12	N	702	NAG	C4-C5-C6-O6
12	G	606	NAG	C4-C5-C6-O6
12	A	606	NAG	C4-C5-C6-O6
12	M	606	NAG	C4-C5-C6-O6
12	G	607	NAG	O5-C5-C6-O6
12	A	607	NAG	O5-C5-C6-O6
12	M	607	NAG	O5-C5-C6-O6
12	G	603	NAG	O5-C5-C6-O6
12	A	603	NAG	O5-C5-C6-O6
12	M	603	NAG	O5-C5-C6-O6
12	G	606	NAG	O5-C5-C6-O6
12	M	606	NAG	O5-C5-C6-O6
12	A	606	NAG	O5-C5-C6-O6
12	G	603	NAG	C1-C2-N2-C7
12	A	603	NAG	C1-C2-N2-C7
12	M	603	NAG	C1-C2-N2-C7
12	G	603	NAG	C3-C2-N2-C7
12	A	603	NAG	C3-C2-N2-C7
12	M	603	NAG	C3-C2-N2-C7
12	I	301	NAG	O5-C5-C6-O6
12	P	301	NAG	O5-C5-C6-O6
12	D	301	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.

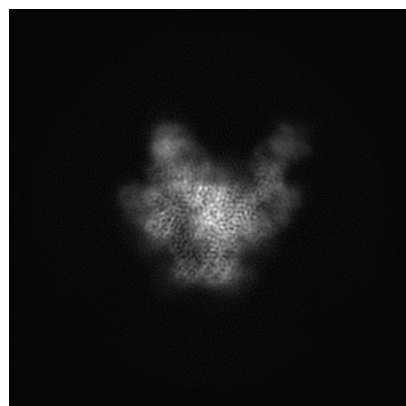
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44484. These allow visual inspection of the internal detail of the map and identification of artifacts.

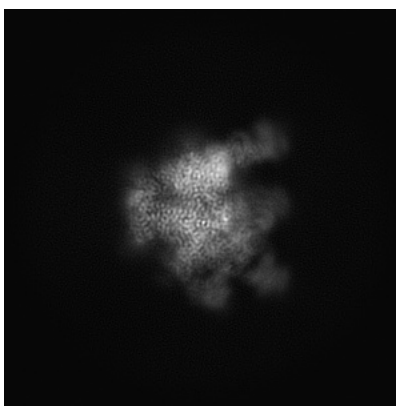
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

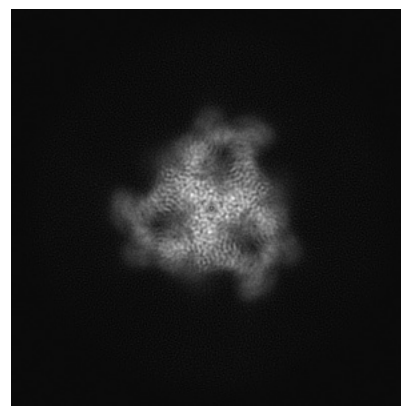
6.1.1 Primary map



X

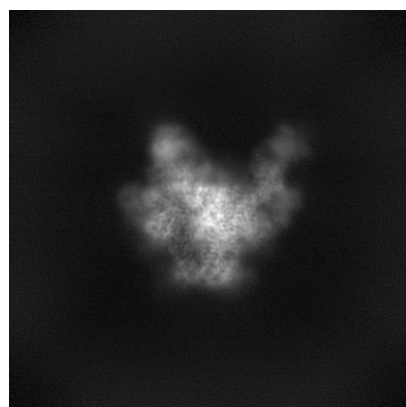


Y

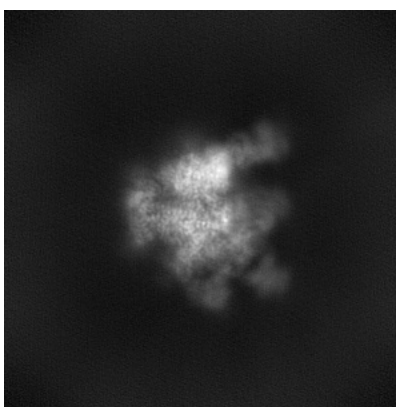


Z

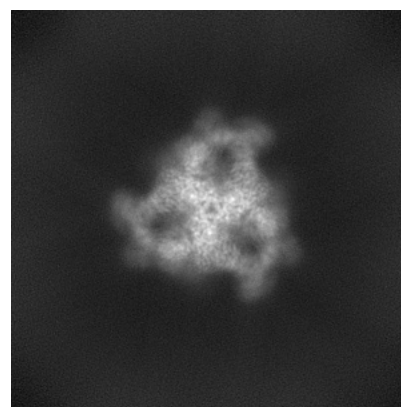
6.1.2 Raw map



X



Y

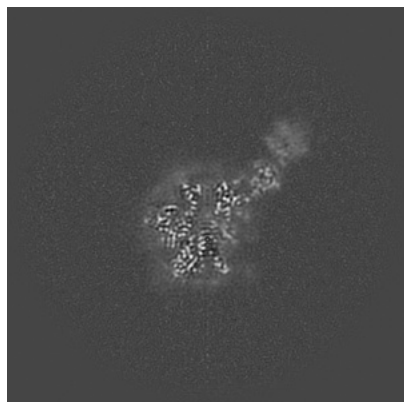


Z

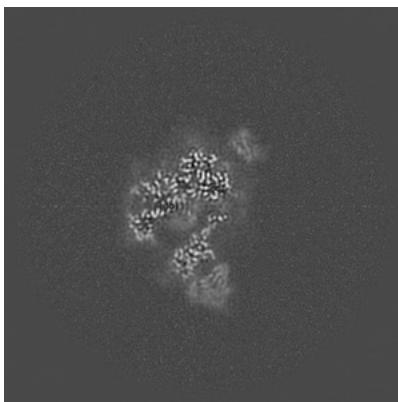
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

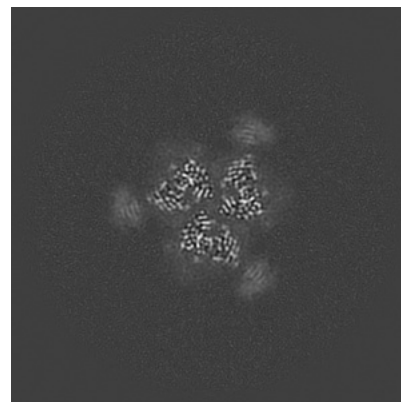
6.2.1 Primary map



X Index: 176

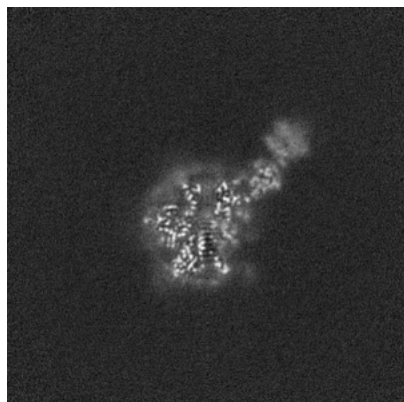


Y Index: 176

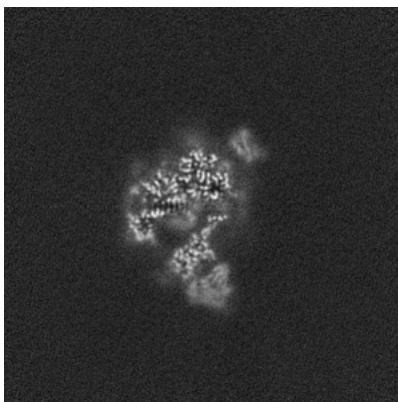


Z Index: 176

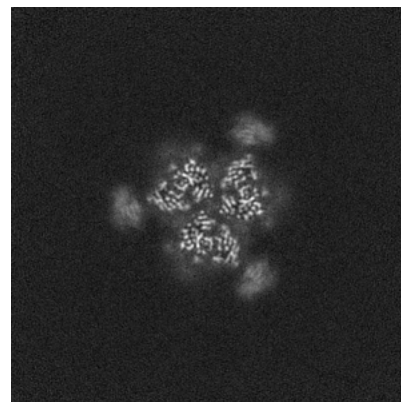
6.2.2 Raw map



X Index: 176



Y Index: 176

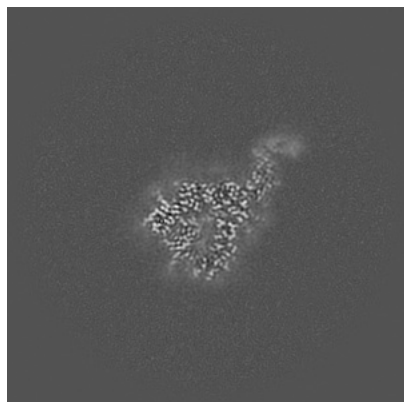


Z Index: 176

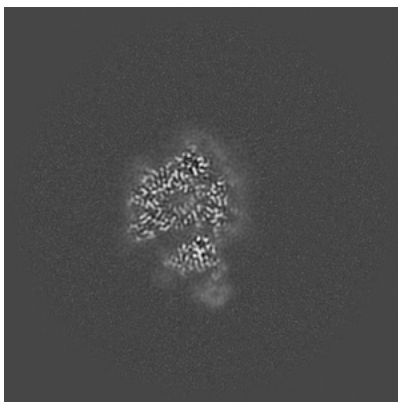
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

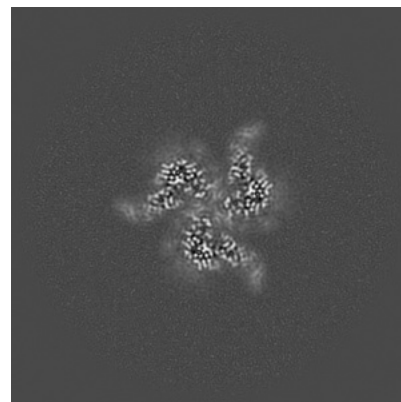
6.3.1 Primary map



X Index: 165

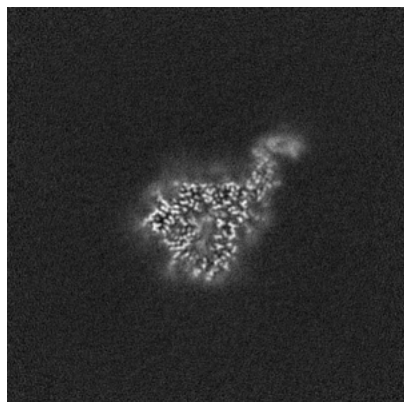


Y Index: 184

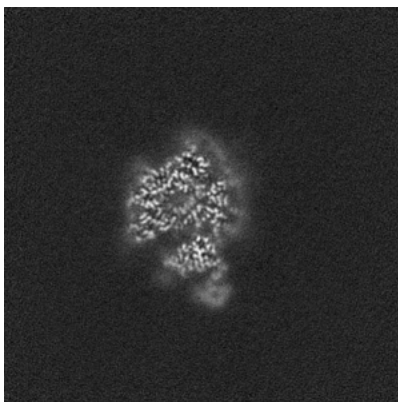


Z Index: 164

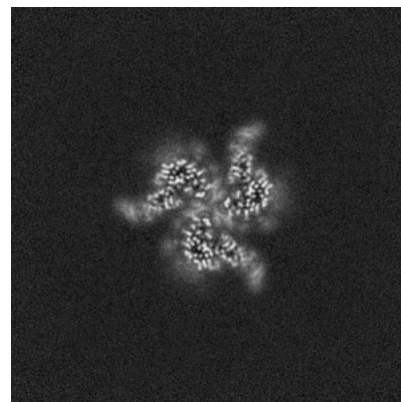
6.3.2 Raw map



X Index: 165



Y Index: 184

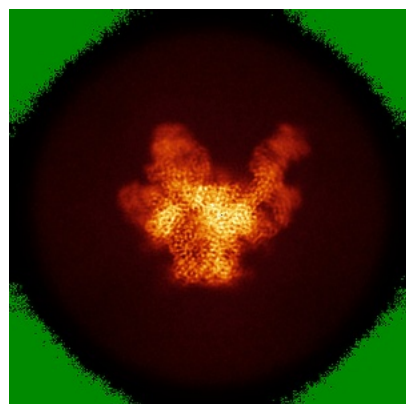


Z Index: 164

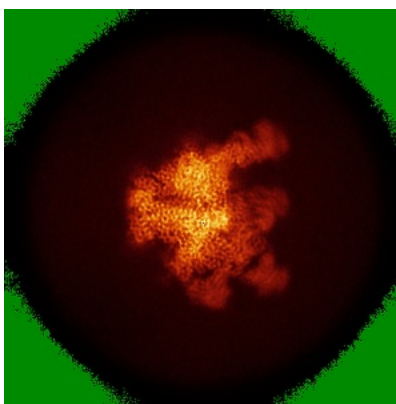
The images above show the largest variance slices of the map in three orthogonal directions.

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

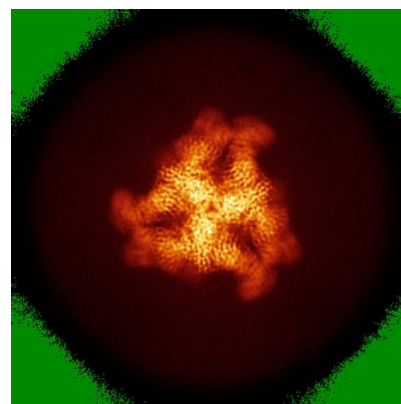
6.4.1 Primary map



X

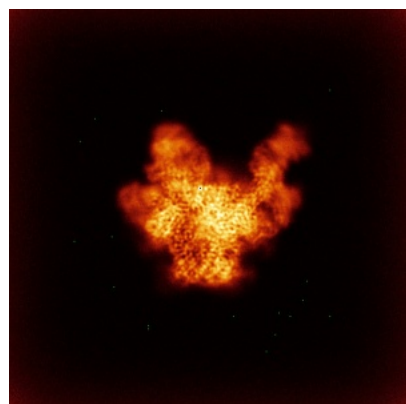


Y

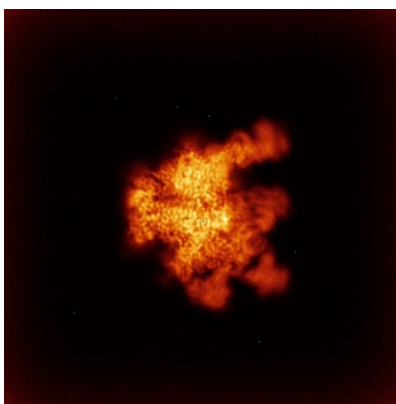


Z

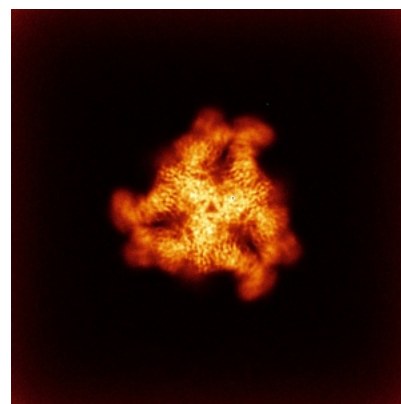
6.4.2 Raw map



X



Y

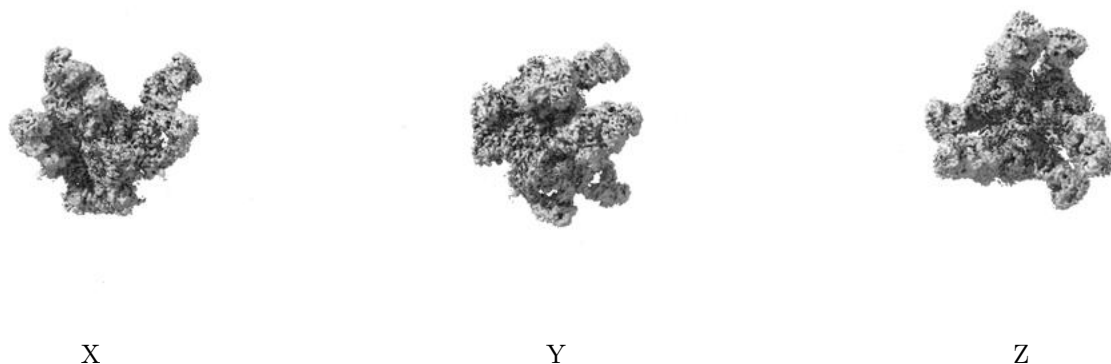


Z

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.

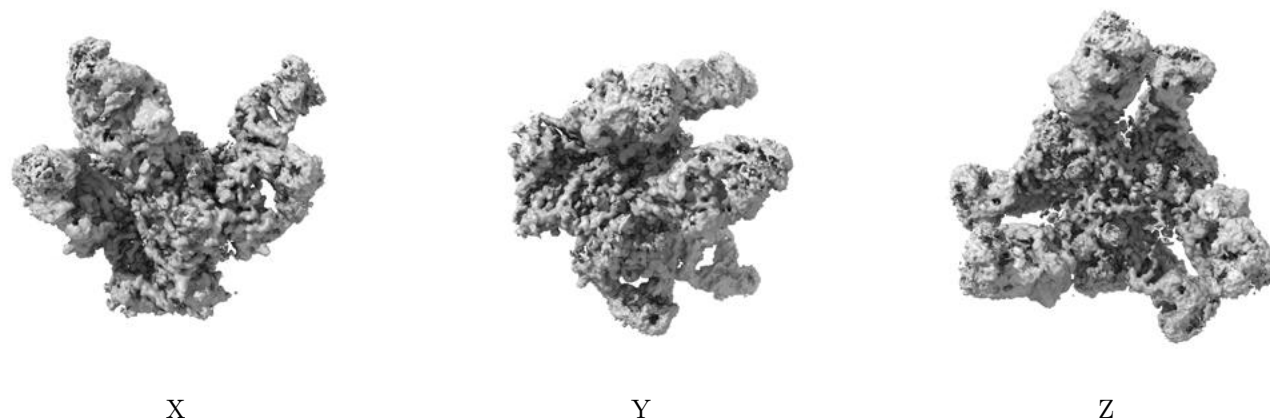
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

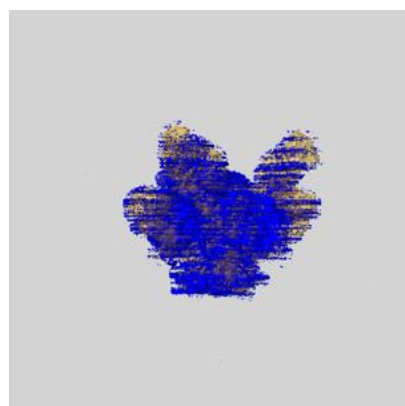
6.6 Mask visualisation [i](#)

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

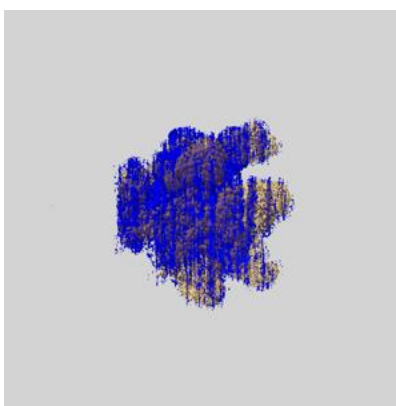
A mask typically either:

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

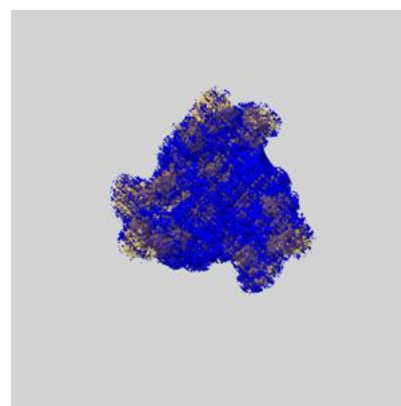
6.6.1 emd_44484_msk_1.map [i](#)



X



Y

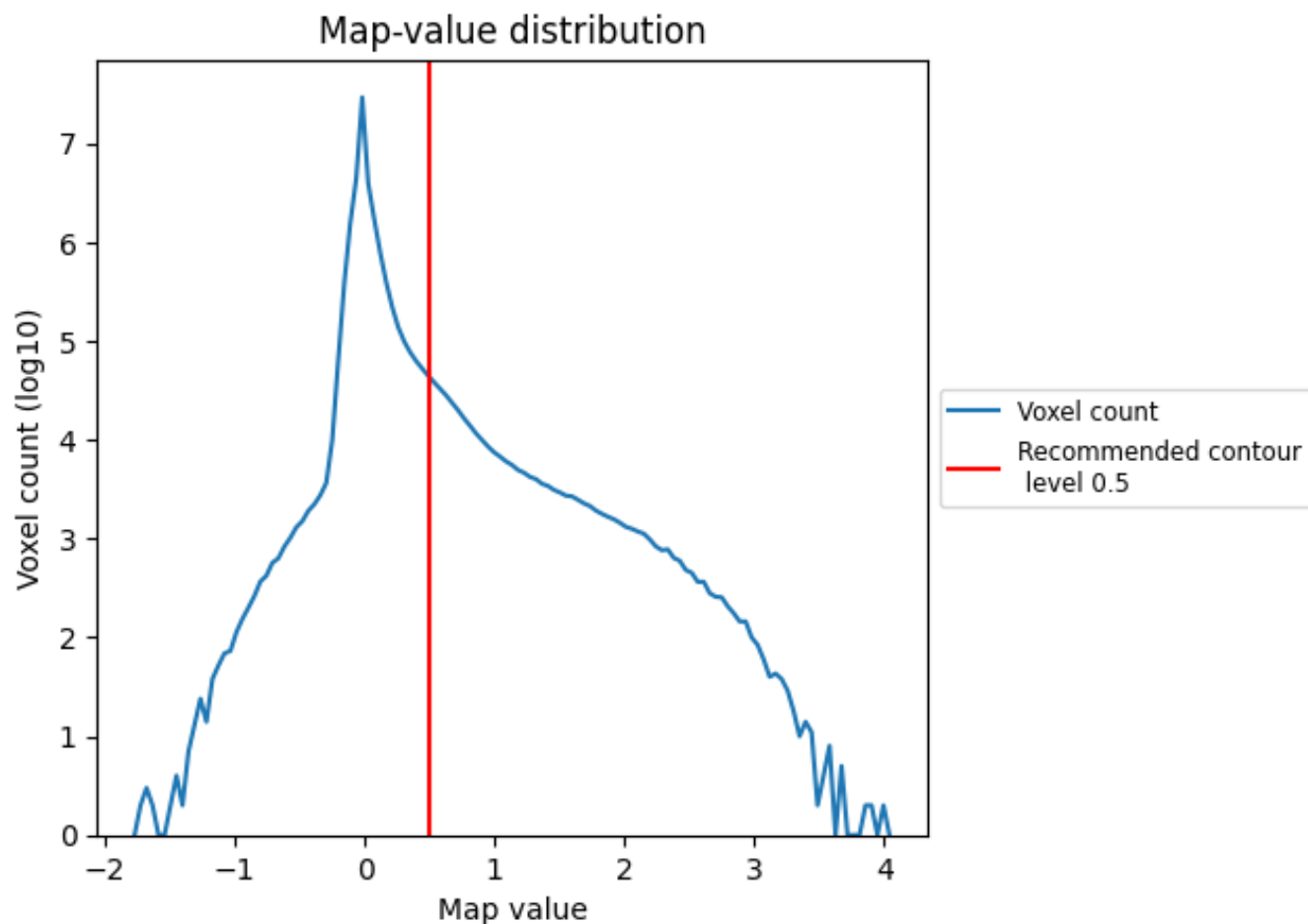


Z

7 Map analysis [i](#)

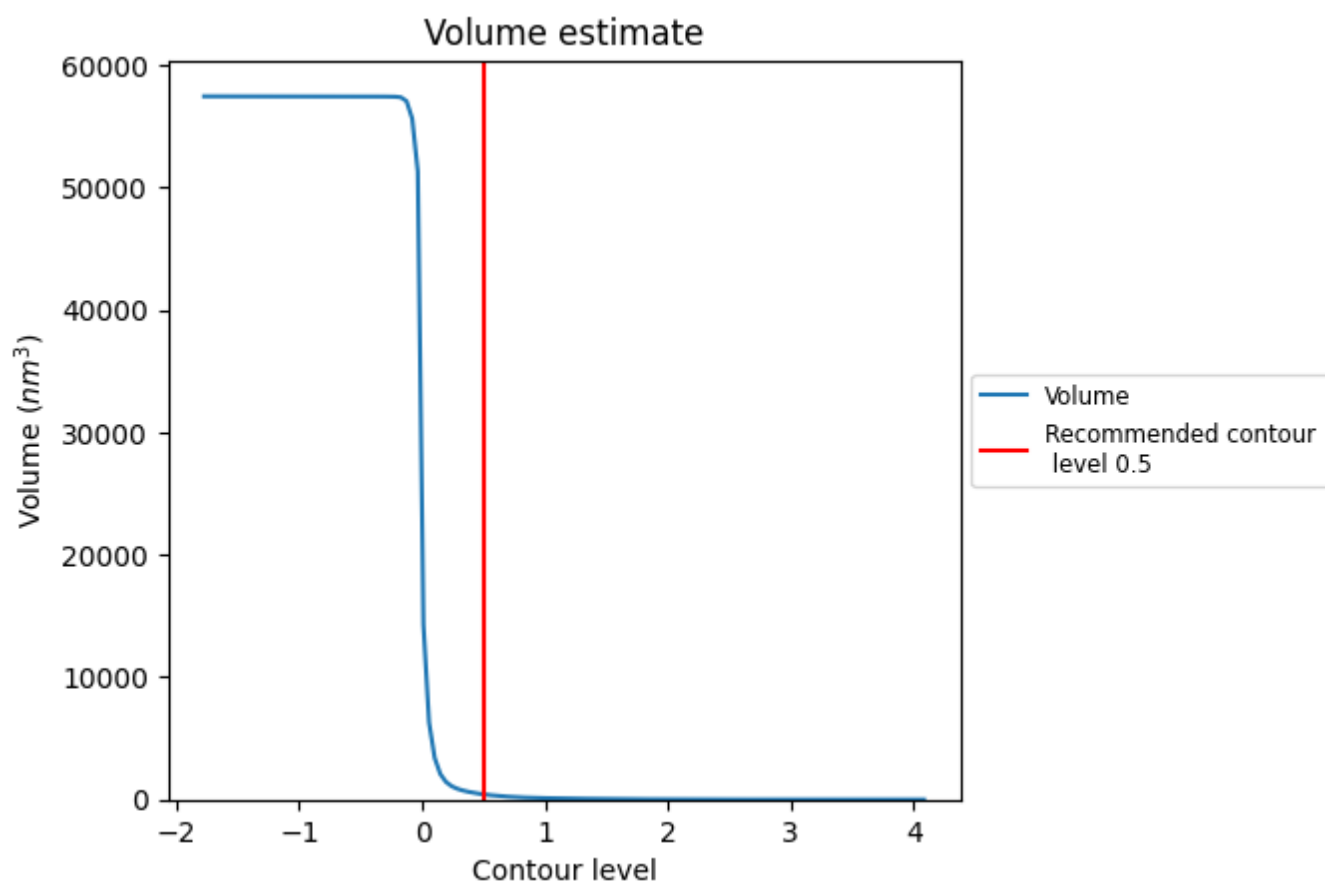
This section contains the results of statistical analysis of the map.

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.

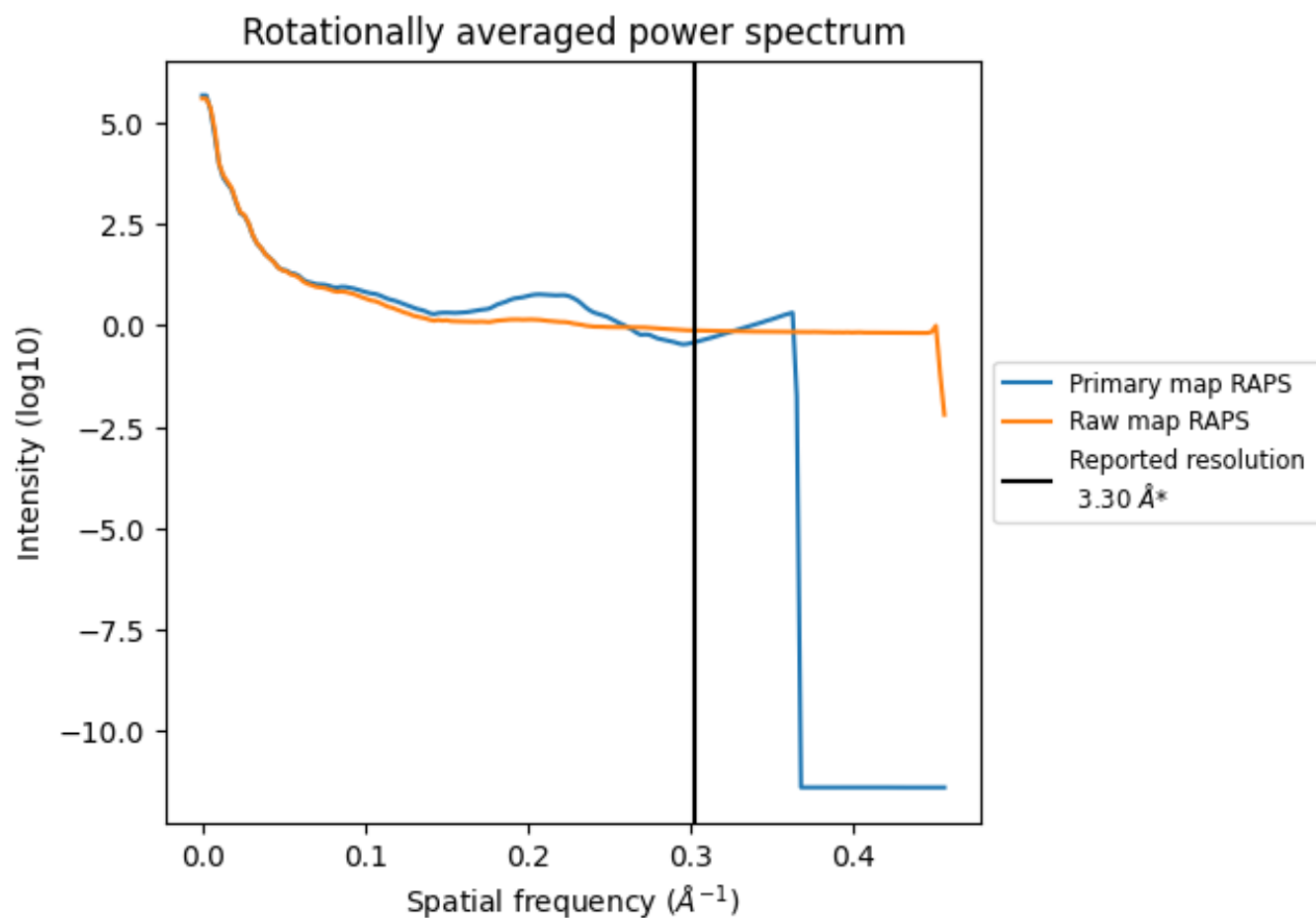
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm³; this corresponds to an approximate mass of 387 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 ⓘ

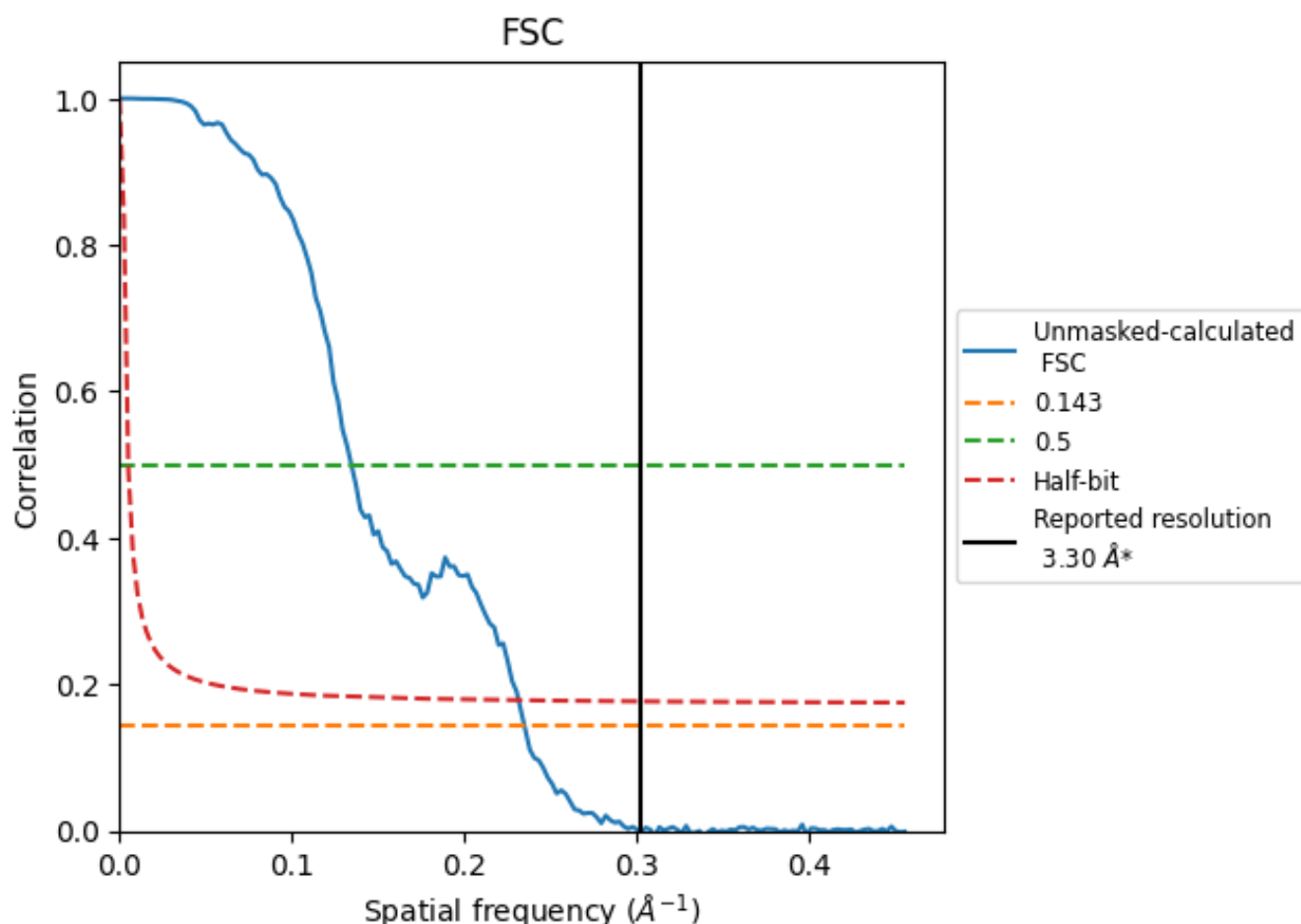


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

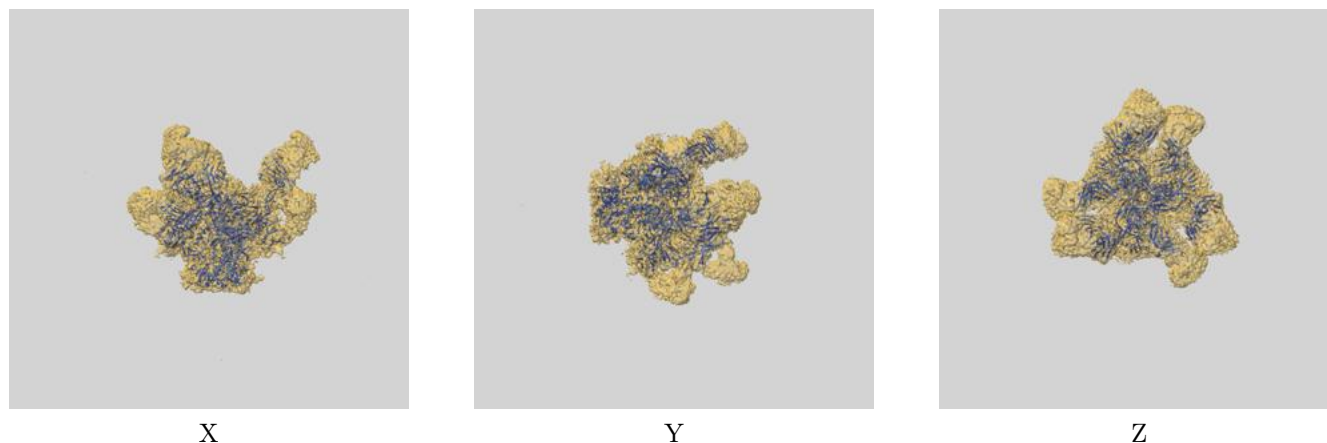
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.43	4.31

*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 4.25 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

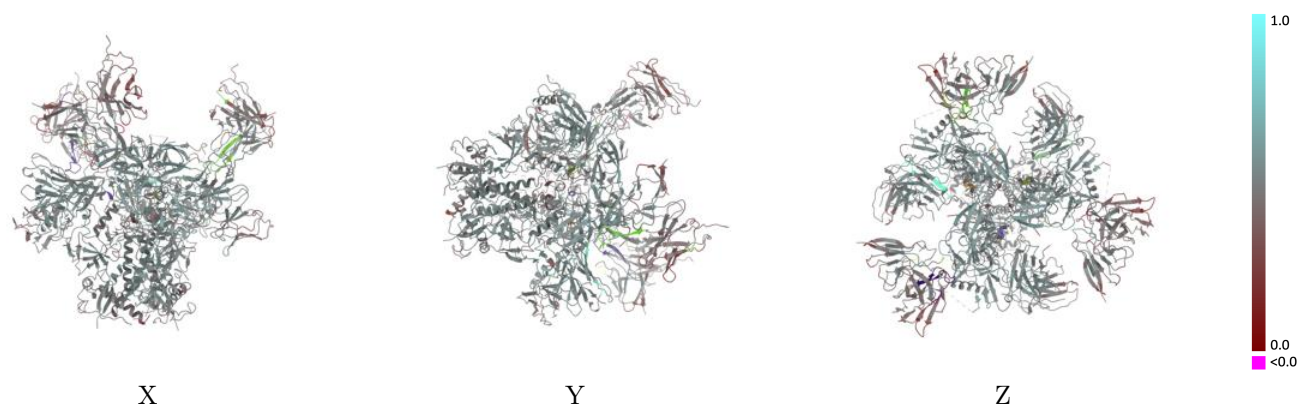
This section contains information regarding the fit between EMDB map EMD-44484 and PDB model 9BEW. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



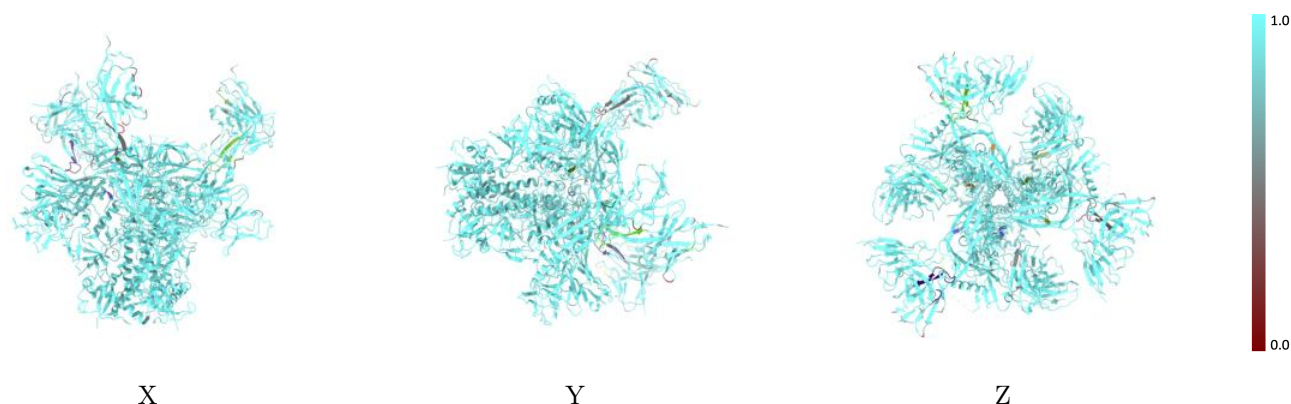
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



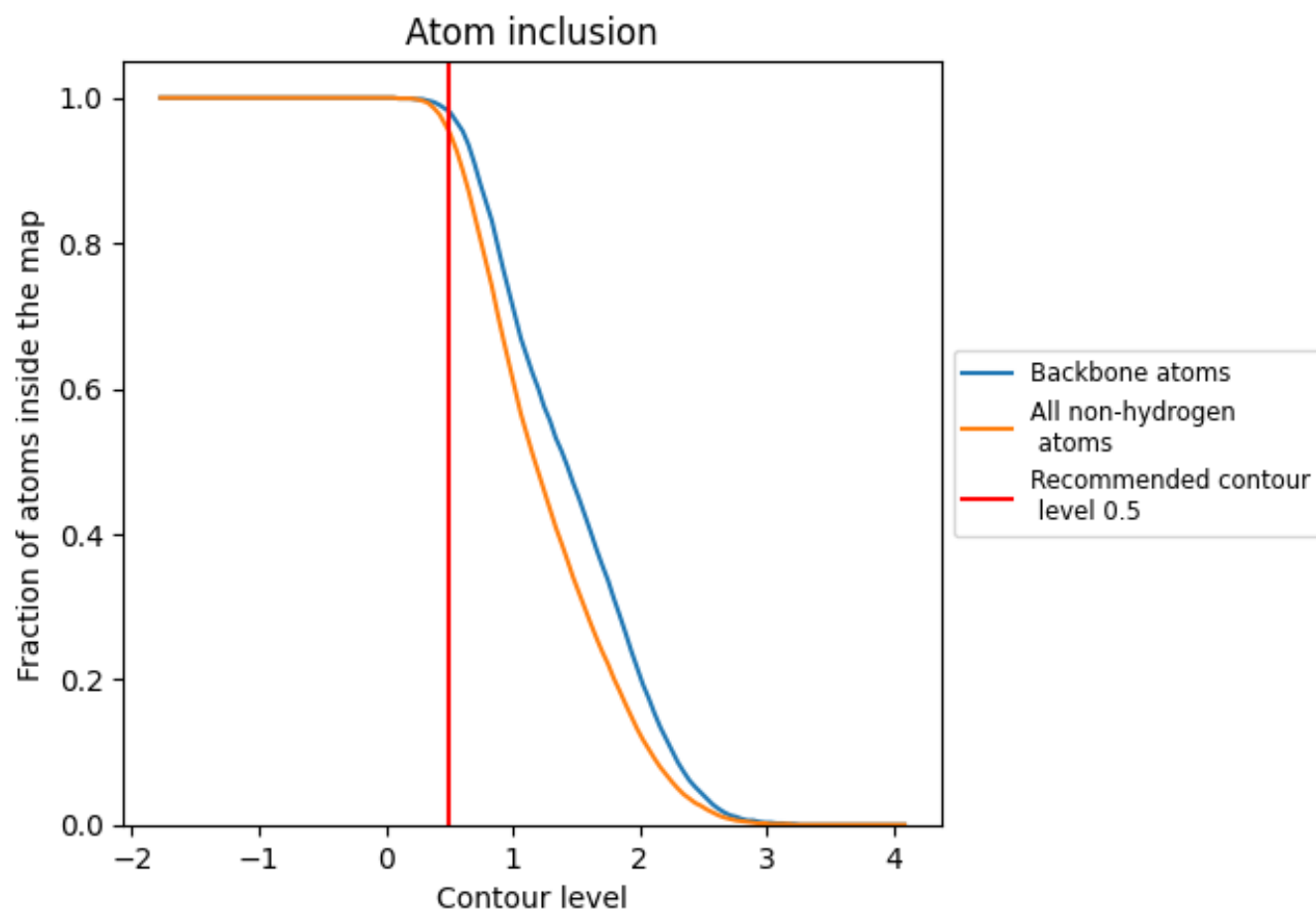
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4880
A	 0.9630	 0.5130
B	 0.9490	 0.4780
C	 0.9700	 0.5170
D	 0.9550	 0.4710
E	 0.9490	 0.4790
F	 0.9670	 0.5170
G	 0.9640	 0.5130
H	 0.9090	 0.4160
I	 0.9590	 0.4710
J	 0.9050	 0.4150
K	 0.9480	 0.4680
L	 0.9470	 0.4680
M	 0.9620	 0.5120
N	 0.9500	 0.4820
O	 0.9680	 0.5160
P	 0.9570	 0.4710
Q	 0.9060	 0.4160
R	 0.9510	 0.4680
S	 0.8930	 0.4930
T	 0.7860	 0.4290
U	 0.9640	 0.4850
V	 0.9720	 0.4990
W	 0.9840	 0.4630
X	 1.0000	 0.5030
Y	 0.9640	 0.5070
Z	 0.9430	 0.5030
a	 0.8930	 0.5150
b	 0.7860	 0.4130
c	 0.9640	 0.4890
d	 0.9720	 0.4980
e	 0.9840	 0.4650
f	 1.0000	 0.5030
g	 0.9640	 0.4930
h	 0.9430	 0.5010



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Chain	Atom inclusion	Q-score
i	 0.9290	 0.5040
j	 0.7860	 0.4180
k	 0.9640	 0.4730
l	 0.9720	 0.4820
m	 0.9840	 0.4670
n	 1.0000	 0.5060
o	 0.9640	 0.5090
p	 0.9430	 0.4960