



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 07:12 AM EDT

PDB ID : 7LL1
EMDB ID : EMD-23411
Title : Cryo-EM structure of BG505 DS-SOSIP in complex with glycan276-dependent broadly neutralizing antibody VRC40.01 Fab
Authors : Manne, K.; Acharya, P.
Deposited on : 2021-02-03
Resolution : 3.73 Å (reported)
Based on initial models : 7L79, 6CDI

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:

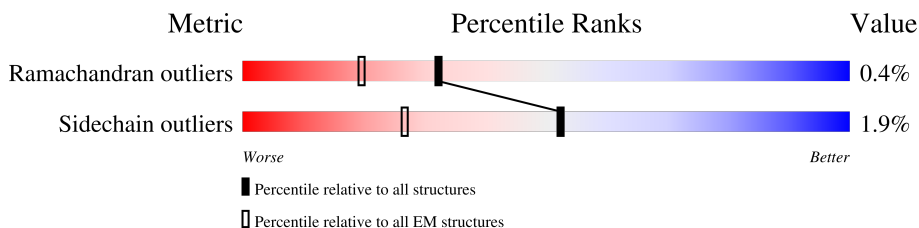
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 3.73 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)
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	473	<div> <div>19%</div> <div>90%</div> <div>5%</div> </div>
1	C	473	<div> <div>19%</div> <div>90%</div> <div>5%</div> </div>
1	G	473	<div> <div>19%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
2	B	153	<div> <div>32%</div> <div>96%</div> <div>.</div> </div>
2	D	153	<div> <div>31%</div> <div>96%</div> <div>.</div> <div>.</div> </div>
2	I	153	<div> <div>33%</div> <div>97%</div> <div>.</div> <div>.</div> </div>
3	E	229	<div> <div>45%</div> <div>96%</div> <div>.</div> </div>
3	H	229	<div> <div>45%</div> <div>96%</div> <div>.</div> </div>
3	J	229	<div> <div>45%</div> <div>97%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	214	57% 96%
4	K	214	58% 96%
4	L	214	59% 95% 5%
5	M	3	67% 100%
5	N	3	67% 100%
5	O	3	67% 100%
5	P	3	67% 100%
5	R	3	67% 100%
5	S	3	67% 100%
5	T	3	67% 100%
5	U	3	100%
5	V	3	100%
5	W	3	67% 100%
5	X	3	100%
5	Y	3	100%
5	Z	3	67% 100%
5	b	3	67% 100%
5	c	3	67% 100%
5	d	3	67% 100%
5	e	3	100%
5	f	3	100%
5	g	3	67% 100%
5	h	3	100%
5	i	3	67% 100%
5	j	3	67% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	l	3	<div><div>67%</div><div>100%</div></div>
5	m	3	<div><div>67%</div><div>100%</div></div>
5	n	3	<div><div>67%</div><div>100%</div></div>
5	o	3	<div><div>100%</div><div>100%</div></div>
5	p	3	<div><div>100%</div><div>100%</div></div>
6	Q	6	<div><div>17%</div><div>100%</div></div>
6	a	6	<div><div>100%</div><div>100%</div></div>
6	k	6	<div><div>100%</div><div>100%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25773 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	449	Total	C	N	O	S	0	0
			3533	2215	626	662	30		
1	C	449	Total	C	N	O	S	0	0
			3533	2215	626	662	30		
1	G	449	Total	C	N	O	S	0	0
			3533	2215	626	662	30		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
G	201	CYS	ILE	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	433	CYS	ALA	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	153	Total	C	N	O	S	0	0
			1205	762	211	226	6		
2	D	153	Total	C	N	O	S	0	0
			1205	762	211	226	6		
2	I	153	Total	C	N	O	S	0	0
			1205	762	211	226	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S7
D	605	CYS	THR	conflict	UNP Q2N0S7
I	605	CYS	THR	conflict	UNP Q2N0S7

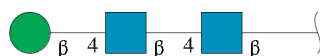
- Molecule 3 is a protein called VRC40.01 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	229	Total	C	N	O	S	0	0
			1729	1102	297	324	6		
3	E	229	Total	C	N	O	S	0	0
			1729	1102	297	324	6		
3	J	229	Total	C	N	O	S	0	0
			1729	1102	297	324	6		

- Molecule 4 is a protein called VRC40.01 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	214	Total	C	N	O	S	0	0
			1659	1036	286	330	7		
4	F	214	Total	C	N	O	S	0	0
			1659	1036	286	330	7		
4	K	214	Total	C	N	O	S	0	0
			1659	1036	286	330	7		

- Molecule 5 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
5	M	3	Total	C	N	O		0	0
			39	22	2	15			
5	N	3	Total	C	N	O		0	0
			39	22	2	15			
5	O	3	Total	C	N	O		0	0
			39	22	2	15			
5	P	3	Total	C	N	O		0	0
			39	22	2	15			

Continued on next page...

Continued from previous page...

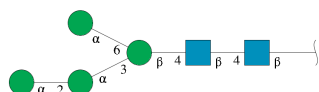
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	3	Total	C	N	O	0	0
			39	22	2	15		
5	S	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	U	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	b	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	3	Total	C	N	O	0	0
			39	22	2	15		
5	d	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		
5	f	3	Total	C	N	O	0	0
			39	22	2	15		
5	g	3	Total	C	N	O	0	0
			39	22	2	15		
5	h	3	Total	C	N	O	0	0
			39	22	2	15		
5	i	3	Total	C	N	O	0	0
			39	22	2	15		
5	j	3	Total	C	N	O	0	0
			39	22	2	15		
5	l	3	Total	C	N	O	0	0
			39	22	2	15		
5	m	3	Total	C	N	O	0	0
			39	22	2	15		
5	n	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

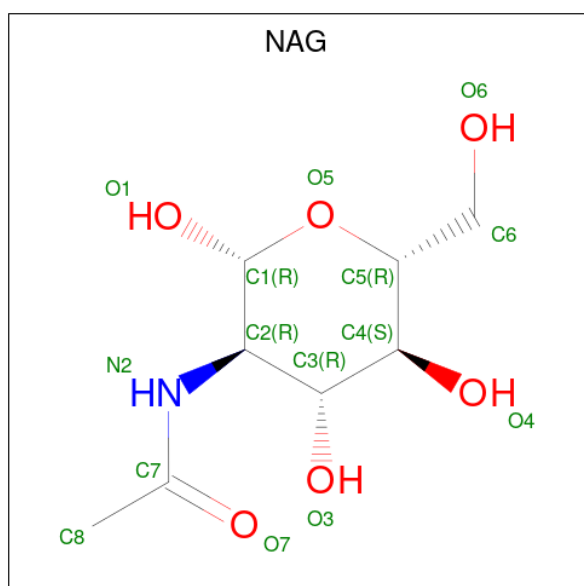
Mol	Chain	Residues	Atoms				AltConf	Trace
5	o	3	Total	C	N	O	0	0
			39	22	2	15		
5	p	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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
6	Q	6	Total	C	N	O	0	0
			72	40	2	30		
6	a	6	Total	C	N	O	0	0
			72	40	2	30		
6	k	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

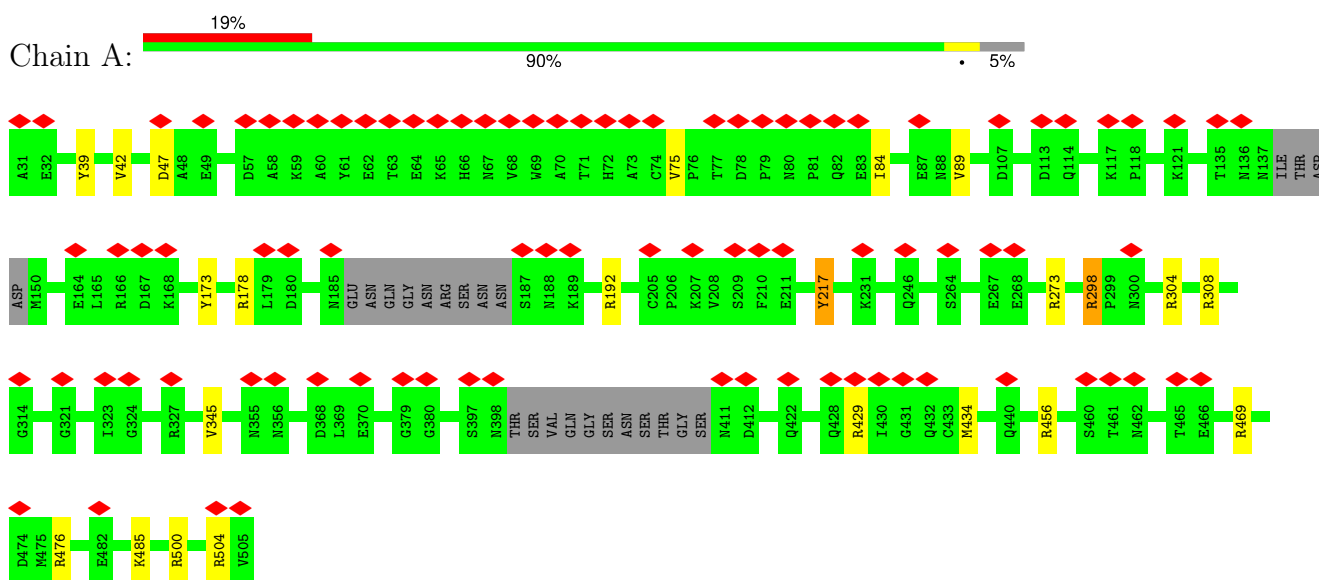


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	G	1	Total	C	N	O	0
			14	8	1	5	
7	G	1	Total	C	N	O	0
			14	8	1	5	
7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

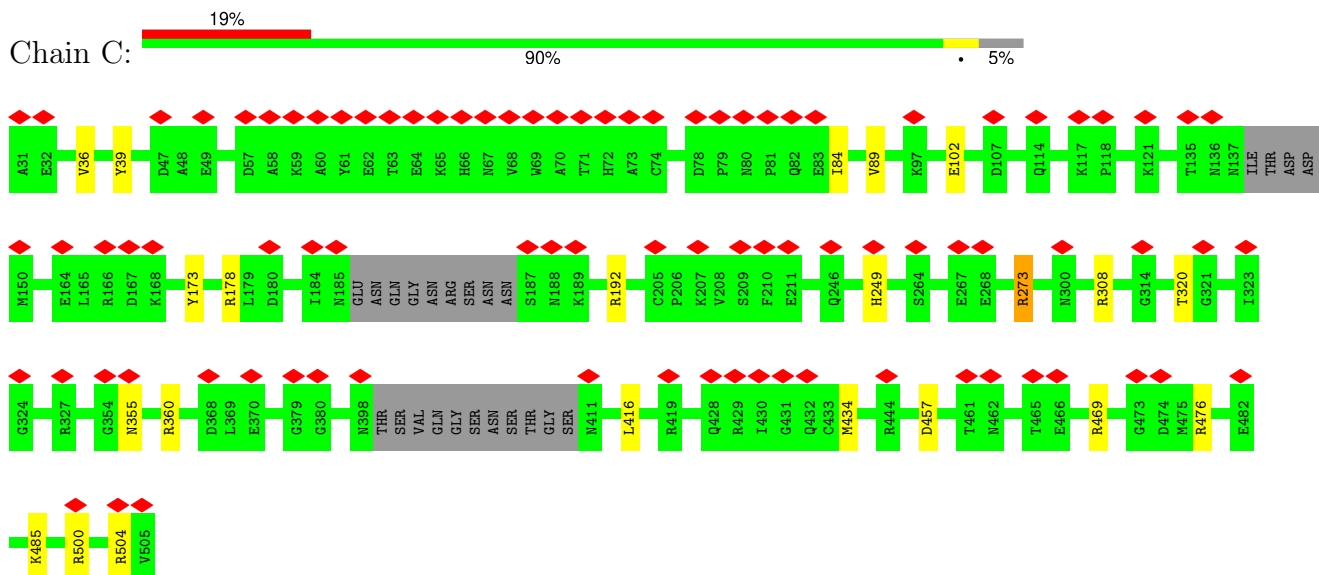
3 Residue-property plots

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

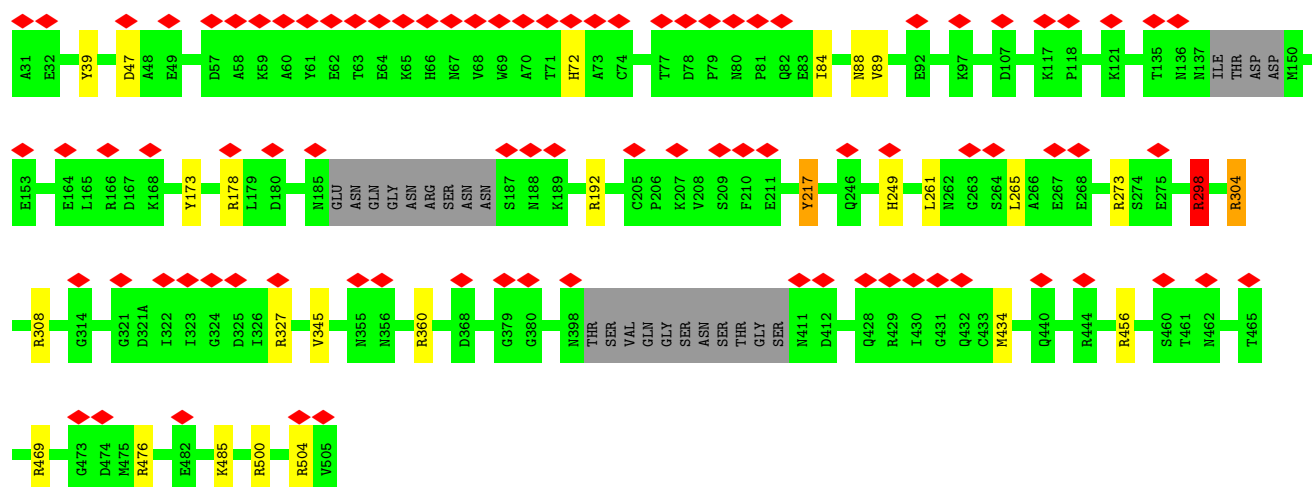


• Molecule 1: Envelope glycoprotein gp120



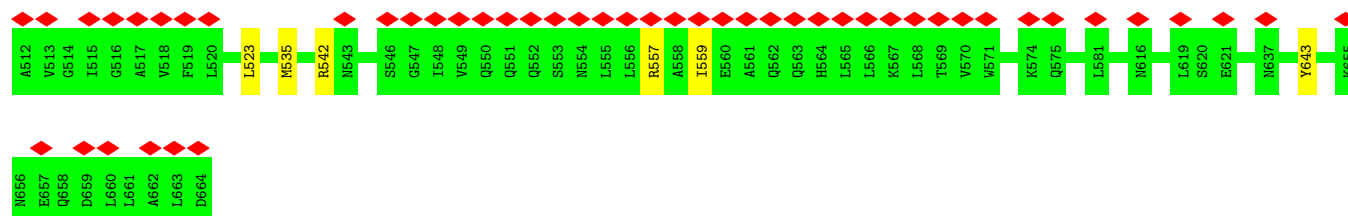
• Molecule 1: Envelope glycoprotein gp120

Chain G: 19% 89% 5% 5%



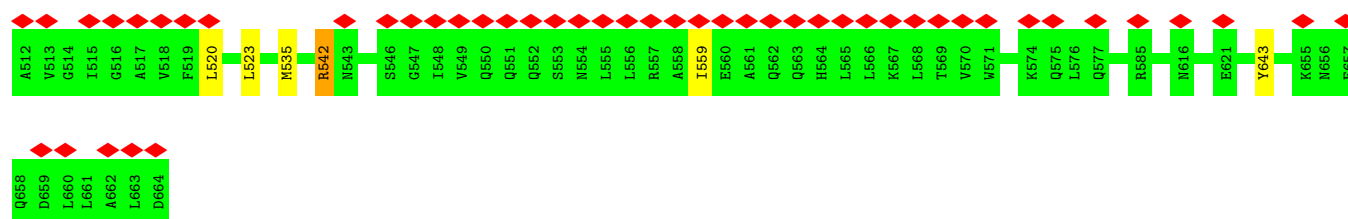
• Molecule 2: Envelope glycoprotein gp41

Chain B: 32% 96%



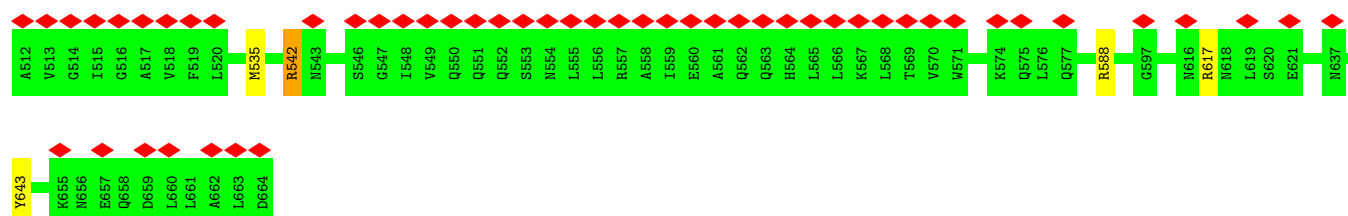
• Molecule 2: Envelope glycoprotein gp41

Chain D: 31% 96%

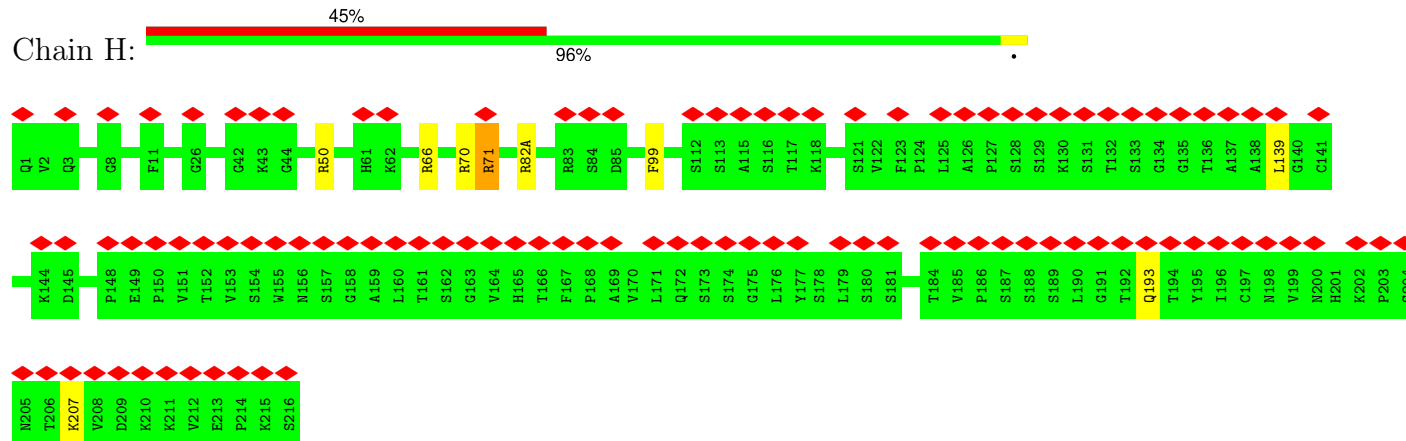


• Molecule 2: Envelope glycoprotein gp41

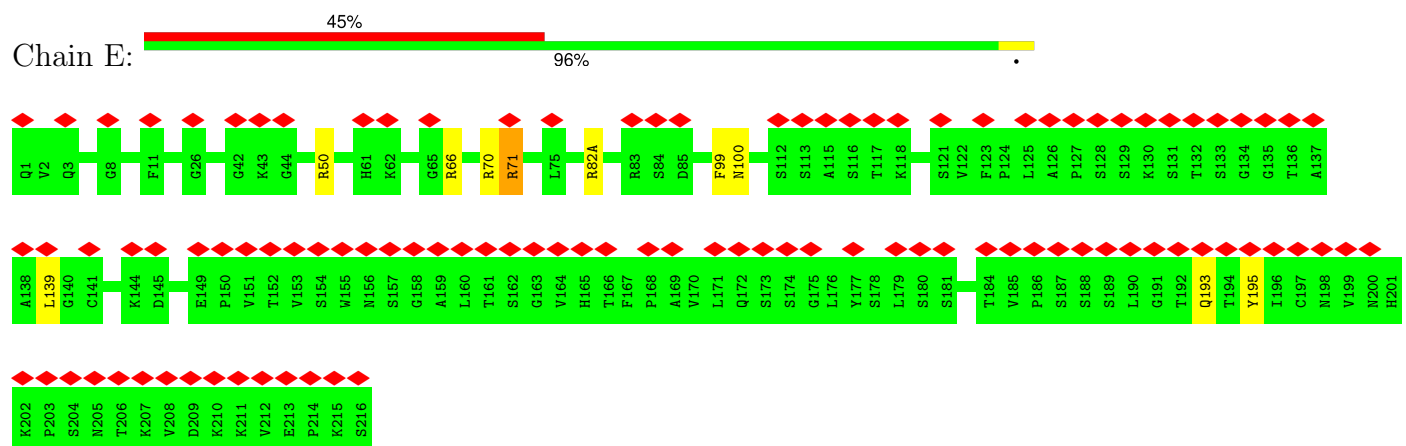
Chain I: 33% 97%



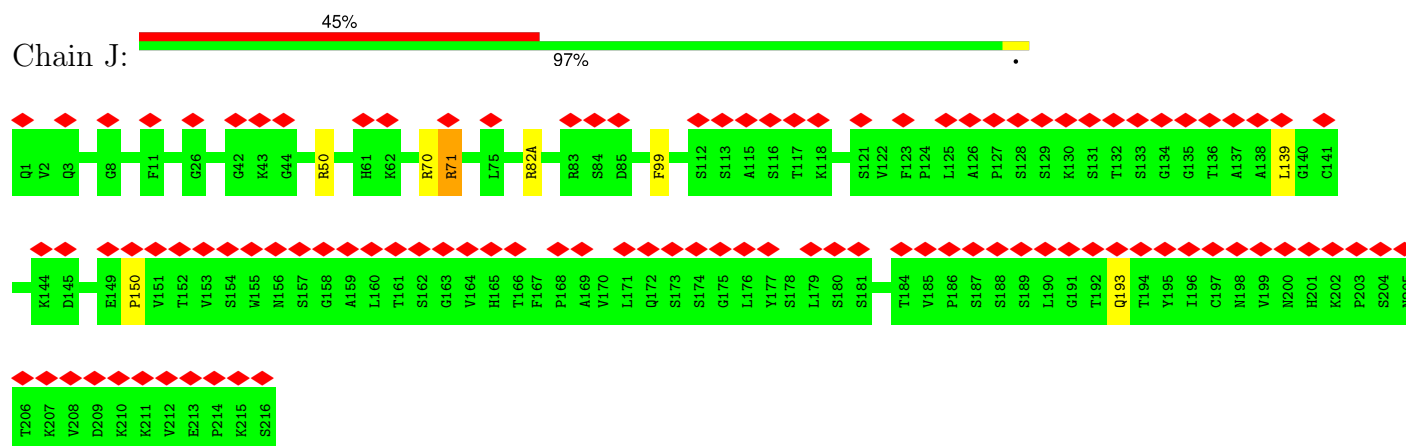
- Molecule 3: VRC40.01 Fab Heavy chain



- Molecule 3: VRC40.01 Fab Heavy chain

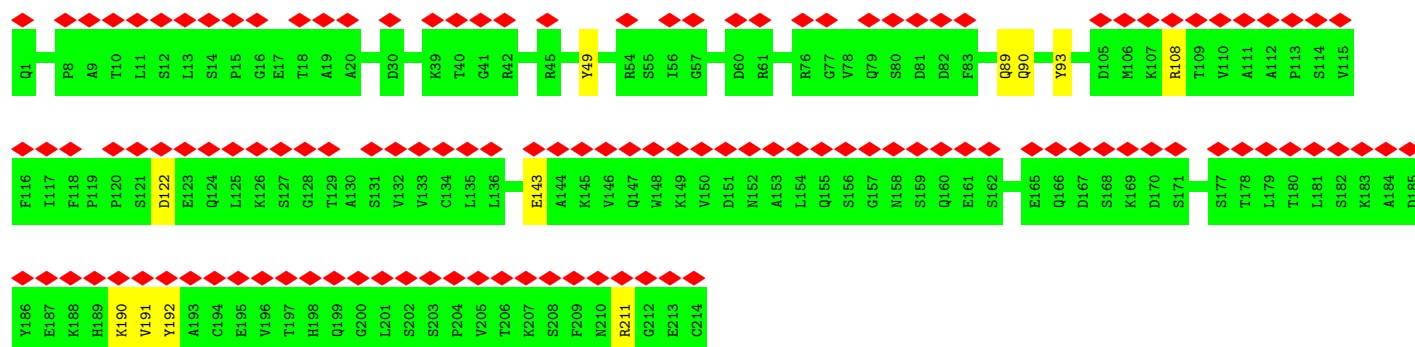


- Molecule 3: VRC40.01 Fab Heavy chain



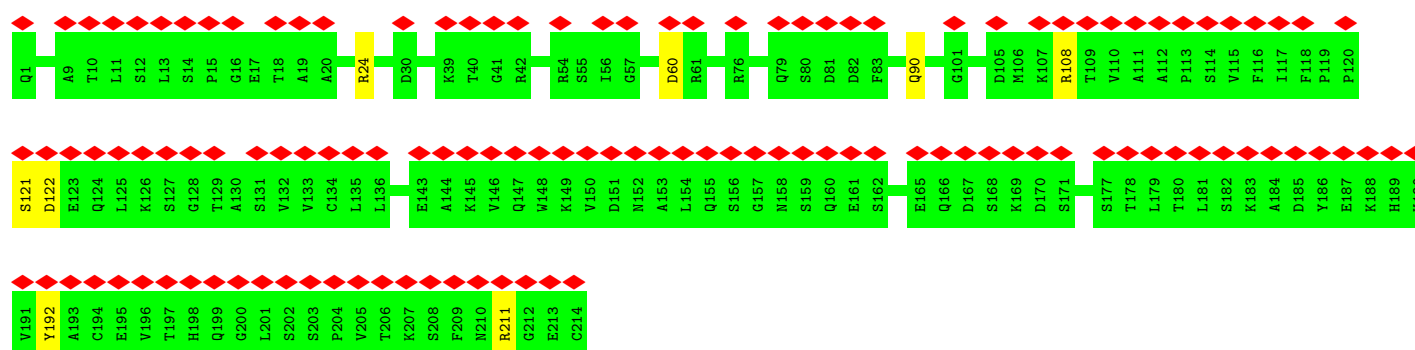
- Molecule 4: VRC40.01 Fab Light chain





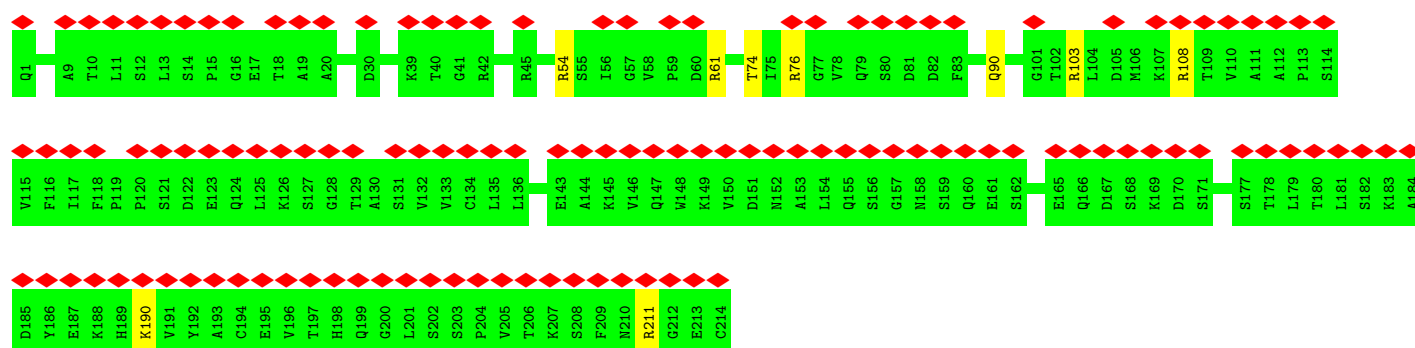
• Molecule 4: VRC40.01 Fab Light chain

Chain F: 57% 96%



• Molecule 4: VRC40.01 Fab Light chain

Chain K: 58% 96%



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

Chain M: 67% 100%



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

Chain N: 



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

Chain O: 



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

Chain P: 



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

Chain R: 



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

Chain S: 



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

Chain T: 



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



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



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



- Molecule 6: 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



- Molecule 6: 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



- Molecule 6: 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

ido-2-deoxy-beta-D-glucopyranose

Chain k:

100%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	489824	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 ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.568	Depositor
Minimum map value	-0.892	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	1.35	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/3606	1.03	14/4893 (0.3%)
1	C	0.61	0/3606	1.03	11/4893 (0.2%)
1	G	0.61	0/3606	1.04	16/4893 (0.3%)
2	B	0.59	0/1225	1.03	2/1662 (0.1%)
2	D	0.59	0/1225	1.01	2/1662 (0.1%)
2	I	0.58	0/1225	1.01	4/1662 (0.2%)
3	E	0.63	0/1773	0.99	4/2416 (0.2%)
3	H	0.64	0/1773	1.00	4/2416 (0.2%)
3	J	0.63	0/1773	0.97	3/2416 (0.1%)
4	F	0.66	0/1695	1.01	2/2301 (0.1%)
4	K	0.67	0/1695	1.02	5/2301 (0.2%)
4	L	0.67	0/1695	1.00	1/2301 (0.0%)
All	All	0.62	0/24897	1.02	68/33816 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
1	G	0	4
2	D	0	1
2	I	0	1
3	E	0	3
3	H	0	3
3	J	0	3
4	F	0	1
4	L	0	3
All	All	0	23

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	VAL	CA-CB-CG1	13.11	130.56	110.90
1	A	89	VAL	CA-CB-CG1	12.67	129.91	110.90
1	G	89	VAL	CA-CB-CG1	12.08	129.03	110.90
1	C	469	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	G	84	ILE	CA-CB-CG1	8.74	127.61	111.00
1	G	469	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	469	ARG	NE-CZ-NH1	8.07	124.33	120.30
4	F	211	ARG	NE-CZ-NH1	7.75	124.18	120.30
4	L	211	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	84	ILE	CA-CB-CG1	7.23	124.73	111.00
1	A	273	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	84	ILE	CA-CB-CG1	7.02	124.34	111.00
3	E	70	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	G	273	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	192	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	G	476	ARG	NE-CZ-NH2	6.56	123.58	120.30
3	H	70	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	C	308	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	500	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	G	500	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	G	217	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	476	ARG	NE-CZ-NH2	6.33	123.47	120.30
3	H	82(A)	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	G	456	ARG	NE-CZ-NH1	6.22	123.41	120.30
4	K	76	ARG	NE-CZ-NH2	6.22	123.41	120.30
2	I	542	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	360	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	B	542	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	D	542	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	308	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	273	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	504	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	217	TYR	CB-CG-CD1	-6.05	117.37	121.00
3	H	207	LYS	CA-CB-CG	5.95	126.50	113.40
1	C	476	ARG	NE-CZ-NH2	5.94	123.27	120.30
3	J	70	ARG	NE-CZ-NH2	5.94	123.27	120.30
3	H	71	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	178	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	G	178	ARG	NE-CZ-NH1	5.89	123.24	120.30
3	J	82(A)	ARG	NE-CZ-NH2	5.88	123.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	211	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	192	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	G	504	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	E	82(A)	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	178	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	G	298	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	G	192	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	G	308	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	327	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	I	643	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	504	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	G	304	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	E	71	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	D	643	TYR	CB-CG-CD2	-5.33	117.80	121.00
4	K	103	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	E	66	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	B	643	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	I	588	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	I	617	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	F	24	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	456	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	429	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	360	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	500	ARG	NE-CZ-NH1	5.11	122.85	120.30
4	K	54	ARG	NE-CZ-NH1	5.10	122.85	120.30
4	K	61	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	304	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	J	71	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	TYR	Sidechain
1	A	298	ARG	Sidechain
1	A	39	TYR	Sidechain
1	C	39	TYR	Sidechain
2	D	542	ARG	Sidechain
3	E	195	TYR	Sidechain
3	E	50	ARG	Sidechain
3	E	71	ARG	Sidechain
4	F	192	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	G	217	TYR	Sidechain
1	G	298	ARG	Sidechain
1	G	304	ARG	Sidechain
1	G	39	TYR	Sidechain
3	H	50	ARG	Sidechain
3	H	66	ARG	Sidechain
3	H	71	ARG	Sidechain
2	I	542	ARG	Sidechain
3	J	150	PRO	Peptide
3	J	50	ARG	Sidechain
3	J	71	ARG	Sidechain
4	L	192	TYR	Sidechain
4	L	49	TYR	Sidechain
4	L	93	TYR	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	441/473 (93%)	413 (94%)	27 (6%)	1 (0%)	44	72
1	C	441/473 (93%)	412 (93%)	27 (6%)	2 (0%)	25	57
1	G	441/473 (93%)	407 (92%)	32 (7%)	2 (0%)	25	57
2	B	151/153 (99%)	137 (91%)	11 (7%)	3 (2%)	6	34
2	D	151/153 (99%)	139 (92%)	10 (7%)	2 (1%)	10	40
2	I	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
3	E	227/229 (99%)	214 (94%)	12 (5%)	1 (0%)	30	62
3	H	227/229 (99%)	214 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	227/229 (99%)	210 (92%)	17 (8%)	0	100	100
4	F	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
4	K	212/214 (99%)	191 (90%)	21 (10%)	0	100	100
4	L	212/214 (99%)	196 (92%)	15 (7%)	1 (0%)	25	57
All	All	3093/3207 (96%)	2871 (93%)	210 (7%)	12 (0%)	32	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	559	ILE
1	G	249	HIS
3	E	100	ASN
2	B	523	LEU
1	C	249	HIS
2	D	523	LEU
4	L	143	GLU
2	B	557	ARG
1	C	355	ASN
2	D	559	ILE
1	G	88	ASN
1	A	75	VAL

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	401/422 (95%)	394 (98%)	7 (2%)	56	73
1	C	401/422 (95%)	392 (98%)	9 (2%)	47	66
1	G	401/422 (95%)	392 (98%)	9 (2%)	47	66
2	B	129/129 (100%)	128 (99%)	1 (1%)	79	85
2	D	129/129 (100%)	127 (98%)	2 (2%)	58	74
2	I	129/129 (100%)	128 (99%)	1 (1%)	79	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	195/195 (100%)	192 (98%)	3 (2%)	60	75
3	H	195/195 (100%)	192 (98%)	3 (2%)	60	75
3	J	195/195 (100%)	192 (98%)	3 (2%)	60	75
4	F	186/186 (100%)	181 (97%)	5 (3%)	40	61
4	K	186/186 (100%)	182 (98%)	4 (2%)	47	66
4	L	186/186 (100%)	180 (97%)	6 (3%)	34	57
All	All	2733/2796 (98%)	2680 (98%)	53 (2%)	52	70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	47	ASP
1	A	173	TYR
1	A	298	ARG
1	A	345	VAL
1	A	434	MET
1	A	485	LYS
2	B	535	MET
1	C	36	VAL
1	C	102	GLU
1	C	173	TYR
1	C	273	ARG
1	C	320	THR
1	C	416	LEU
1	C	434	MET
1	C	457	ASP
1	C	485	LYS
2	D	520	LEU
2	D	535	MET
1	G	47	ASP
1	G	72	HIS
1	G	173	TYR
1	G	261	LEU
1	G	265	LEU
1	G	298	ARG
1	G	345	VAL
1	G	434	MET
1	G	485	LYS
2	I	535	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	99	PHE
3	H	139	LEU
3	H	193	GLN
4	L	89	GLN
4	L	90	GLN
4	L	108	ARG
4	L	122	ASP
4	L	190	LYS
4	L	191	VAL
3	E	99	PHE
3	E	139	LEU
3	E	193	GLN
4	F	60	ASP
4	F	90	GLN
4	F	108	ARG
4	F	121	SER
4	F	122	ASP
3	J	99	PHE
3	J	139	LEU
3	J	193	GLN
4	K	74	THR
4	K	90	GLN
4	K	108	ARG
4	K	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	650	GLN
2	I	562	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 ⓘ

99 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	1	5,1	14,14,15	1.15	1 (7%)	17,19,21	0.97	0
5	NAG	M	2	5	14,14,15	1.32	2 (14%)	17,19,21	0.82	0
5	BMA	M	3	5	11,11,12	1.22	1 (9%)	15,15,17	0.65	0
5	NAG	N	1	5,1	14,14,15	1.29	2 (14%)	17,19,21	1.08	1 (5%)
5	NAG	N	2	5	14,14,15	1.29	2 (14%)	17,19,21	0.77	0
5	BMA	N	3	5	11,11,12	1.38	2 (18%)	15,15,17	1.16	1 (6%)
5	NAG	O	1	5,1	14,14,15	1.09	1 (7%)	17,19,21	0.85	0
5	NAG	O	2	5	14,14,15	1.20	1 (7%)	17,19,21	0.74	0
5	BMA	O	3	5	11,11,12	1.33	2 (18%)	15,15,17	0.87	1 (6%)
5	NAG	P	1	5,1	14,14,15	1.27	2 (14%)	17,19,21	0.98	2 (11%)
5	NAG	P	2	5	14,14,15	1.27	2 (14%)	17,19,21	1.61	3 (17%)
5	BMA	P	3	5	11,11,12	1.29	2 (18%)	15,15,17	1.21	2 (13%)
6	NAG	Q	1	1,6	14,14,15	1.01	0	17,19,21	0.95	1 (5%)
6	NAG	Q	2	6	14,14,15	1.11	2 (14%)	17,19,21	1.03	1 (5%)
6	BMA	Q	3	6	11,11,12	1.20	2 (18%)	15,15,17	0.74	0
6	MAN	Q	4	6	11,11,12	1.28	2 (18%)	15,15,17	1.39	3 (20%)
6	MAN	Q	5	6	11,11,12	0.99	1 (9%)	15,15,17	1.26	2 (13%)
6	MAN	Q	6	6	11,11,12	1.06	1 (9%)	15,15,17	0.94	1 (6%)
5	NAG	R	1	5,1	14,14,15	1.20	2 (14%)	17,19,21	1.06	1 (5%)
5	NAG	R	2	5	14,14,15	1.31	2 (14%)	17,19,21	0.94	1 (5%)
5	BMA	R	3	5	11,11,12	1.22	1 (9%)	15,15,17	1.23	2 (13%)
5	NAG	S	1	5,1	14,14,15	1.12	2 (14%)	17,19,21	0.81	0
5	NAG	S	2	5	14,14,15	1.26	2 (14%)	17,19,21	1.10	1 (5%)
5	BMA	S	3	5	11,11,12	1.24	1 (9%)	15,15,17	1.40	3 (20%)
5	NAG	T	1	5,1	14,14,15	1.14	1 (7%)	17,19,21	1.35	2 (11%)
5	NAG	T	2	5	14,14,15	1.33	2 (14%)	17,19,21	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	T	3	5	11,11,12	1.22	2 (18%)	15,15,17	0.94	1 (6%)
5	NAG	U	1	5,1	14,14,15	1.27	2 (14%)	17,19,21	0.99	2 (11%)
5	NAG	U	2	5	14,14,15	1.38	3 (21%)	17,19,21	1.16	1 (5%)
5	BMA	U	3	5	11,11,12	1.33	2 (18%)	15,15,17	0.56	0
5	NAG	V	1	5,1	14,14,15	1.21	2 (14%)	17,19,21	1.41	2 (11%)
5	NAG	V	2	5	14,14,15	1.62	3 (21%)	17,19,21	1.21	1 (5%)
5	BMA	V	3	5	11,11,12	1.32	2 (18%)	15,15,17	1.39	1 (6%)
5	NAG	W	1	5,1	14,14,15	1.10	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	W	2	5	14,14,15	1.30	1 (7%)	17,19,21	0.96	1 (5%)
5	BMA	W	3	5	11,11,12	1.33	2 (18%)	15,15,17	0.83	1 (6%)
5	NAG	X	1	5,1	14,14,15	1.30	2 (14%)	17,19,21	1.17	1 (5%)
5	NAG	X	2	5	14,14,15	1.35	2 (14%)	17,19,21	0.70	0
5	BMA	X	3	5	11,11,12	1.37	2 (18%)	15,15,17	0.94	1 (6%)
5	NAG	Y	1	5,1	14,14,15	1.19	1 (7%)	17,19,21	0.70	1 (5%)
5	NAG	Y	2	5	14,14,15	1.32	2 (14%)	17,19,21	0.68	0
5	BMA	Y	3	5	11,11,12	1.29	2 (18%)	15,15,17	0.85	1 (6%)
5	NAG	Z	1	5,1	14,14,15	1.25	2 (14%)	17,19,21	0.94	1 (5%)
5	NAG	Z	2	5	14,14,15	1.19	2 (14%)	17,19,21	1.80	2 (11%)
5	BMA	Z	3	5	11,11,12	1.31	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	a	1	1,6	14,14,15	1.03	0	17,19,21	0.91	1 (5%)
6	NAG	a	2	6	14,14,15	1.13	2 (14%)	17,19,21	1.12	1 (5%)
6	BMA	a	3	6	11,11,12	1.16	2 (18%)	15,15,17	0.83	0
6	MAN	a	4	6	11,11,12	1.32	2 (18%)	15,15,17	1.28	3 (20%)
6	MAN	a	5	6	11,11,12	0.98	1 (9%)	15,15,17	1.23	3 (20%)
6	MAN	a	6	6	11,11,12	1.07	2 (18%)	15,15,17	0.95	0
5	NAG	b	1	5,1	14,14,15	1.22	2 (14%)	17,19,21	2.00	3 (17%)
5	NAG	b	2	5	14,14,15	1.38	3 (21%)	17,19,21	0.88	1 (5%)
5	BMA	b	3	5	11,11,12	1.28	1 (9%)	15,15,17	0.99	1 (6%)
5	NAG	c	1	5,1	14,14,15	1.17	2 (14%)	17,19,21	0.78	0
5	NAG	c	2	5	14,14,15	1.15	0	17,19,21	1.00	1 (5%)
5	BMA	c	3	5	11,11,12	1.22	1 (9%)	15,15,17	1.57	1 (6%)
5	NAG	d	1	5,1	14,14,15	1.22	2 (14%)	17,19,21	1.24	1 (5%)
5	NAG	d	2	5	14,14,15	1.38	2 (14%)	17,19,21	0.90	1 (5%)
5	BMA	d	3	5	11,11,12	1.37	2 (18%)	15,15,17	0.80	1 (6%)
5	NAG	e	1	5,1	14,14,15	1.31	2 (14%)	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	e	2	5	14,14,15	1.45	4 (28%)	17,19,21	1.16	1 (5%)
5	BMA	e	3	5	11,11,12	1.34	2 (18%)	15,15,17	0.65	0
5	NAG	f	1	5,1	14,14,15	1.17	2 (14%)	17,19,21	1.31	2 (11%)
5	NAG	f	2	5	14,14,15	1.57	3 (21%)	17,19,21	1.21	2 (11%)
5	BMA	f	3	5	11,11,12	1.34	2 (18%)	15,15,17	1.01	1 (6%)
5	NAG	g	1	5,1	14,14,15	1.10	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	g	2	5	14,14,15	1.32	2 (14%)	17,19,21	0.88	1 (5%)
5	BMA	g	3	5	11,11,12	1.34	2 (18%)	15,15,17	0.86	1 (6%)
5	NAG	h	1	5,1	14,14,15	1.31	2 (14%)	17,19,21	1.12	1 (5%)
5	NAG	h	2	5	14,14,15	1.29	2 (14%)	17,19,21	0.86	1 (5%)
5	BMA	h	3	5	11,11,12	1.38	2 (18%)	15,15,17	0.90	1 (6%)
5	NAG	i	1	5,1	14,14,15	1.12	1 (7%)	17,19,21	0.68	0
5	NAG	i	2	5	14,14,15	1.22	2 (14%)	17,19,21	0.79	0
5	BMA	i	3	5	11,11,12	1.28	2 (18%)	15,15,17	0.94	1 (6%)
5	NAG	j	1	5,1	14,14,15	1.18	2 (14%)	17,19,21	0.87	0
5	NAG	j	2	5	14,14,15	1.25	2 (14%)	17,19,21	1.38	1 (5%)
5	BMA	j	3	5	11,11,12	1.29	2 (18%)	15,15,17	1.01	1 (6%)
6	NAG	k	1	1,6	14,14,15	1.09	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	k	2	6	14,14,15	1.21	2 (14%)	17,19,21	1.12	1 (5%)
6	BMA	k	3	6	11,11,12	1.28	2 (18%)	15,15,17	0.76	0
6	MAN	k	4	6	11,11,12	1.30	2 (18%)	15,15,17	1.35	3 (20%)
6	MAN	k	5	6	11,11,12	0.97	1 (9%)	15,15,17	1.29	2 (13%)
6	MAN	k	6	6	11,11,12	1.07	1 (9%)	15,15,17	0.99	0
5	NAG	l	1	5,1	14,14,15	1.19	1 (7%)	17,19,21	1.29	3 (17%)
5	NAG	l	2	5	14,14,15	1.31	3 (21%)	17,19,21	0.89	1 (5%)
5	BMA	l	3	5	11,11,12	1.37	2 (18%)	15,15,17	0.98	1 (6%)
5	NAG	m	1	5,1	14,14,15	1.26	2 (14%)	17,19,21	1.07	2 (11%)
5	NAG	m	2	5	14,14,15	1.29	2 (14%)	17,19,21	1.38	3 (17%)
5	BMA	m	3	5	11,11,12	1.20	1 (9%)	15,15,17	1.49	2 (13%)
5	NAG	n	1	5,1	14,14,15	1.25	2 (14%)	17,19,21	1.34	2 (11%)
5	NAG	n	2	5	14,14,15	1.33	3 (21%)	17,19,21	0.77	0
5	BMA	n	3	5	11,11,12	1.28	2 (18%)	15,15,17	0.65	0
5	NAG	o	1	5,1	14,14,15	1.33	2 (14%)	17,19,21	1.01	2 (11%)
5	NAG	o	2	5	14,14,15	1.46	4 (28%)	17,19,21	1.14	1 (5%)
5	BMA	o	3	5	11,11,12	1.38	2 (18%)	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	p	1	5,1	14,14,15	1.18	2 (14%)	17,19,21	1.44	1 (5%)
5	NAG	p	2	5	14,14,15	1.37	2 (14%)	17,19,21	1.06	1 (5%)
5	BMA	p	3	5	11,11,12	1.34	2 (18%)	15,15,17	1.37	1 (6%)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	2	NAG	C1-C2	3.42	1.57	1.52
5	V	2	NAG	C1-C2	3.41	1.57	1.52
5	P	1	NAG	O5-C5	3.04	1.49	1.43
5	X	3	BMA	O5-C5	2.97	1.49	1.43
6	a	4	MAN	O2-C2	2.92	1.49	1.43
5	V	2	NAG	O5-C1	2.88	1.48	1.43
6	k	4	MAN	O2-C2	2.87	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	1	NAG	O5-C5	2.86	1.49	1.43
5	T	2	NAG	O5-C5	2.86	1.49	1.43
5	l	3	BMA	O5-C5	2.85	1.49	1.43
6	Q	4	MAN	O2-C2	2.83	1.49	1.43
5	N	3	BMA	O5-C5	2.82	1.48	1.43
5	j	3	BMA	O5-C5	2.82	1.48	1.43
5	h	3	BMA	O5-C5	2.79	1.48	1.43
5	g	3	BMA	O5-C5	2.79	1.48	1.43
5	p	3	BMA	O5-C5	2.76	1.48	1.43
5	p	2	NAG	O5-C5	2.76	1.48	1.43
5	P	3	BMA	O5-C5	2.75	1.48	1.43
5	O	3	BMA	O5-C5	2.74	1.48	1.43
5	W	3	BMA	O5-C5	2.74	1.48	1.43
5	f	3	BMA	O5-C5	2.73	1.48	1.43
5	V	2	NAG	O5-C5	2.72	1.48	1.43
5	d	3	BMA	O5-C5	2.72	1.48	1.43
6	k	3	BMA	O5-C5	2.72	1.48	1.43
5	b	3	BMA	O5-C5	2.71	1.48	1.43
5	X	2	NAG	O5-C5	2.71	1.48	1.43
5	Z	3	BMA	O5-C5	2.70	1.48	1.43
5	n	2	NAG	O5-C5	2.70	1.48	1.43
5	e	1	NAG	O4-C4	2.70	1.49	1.43
5	c	1	NAG	O5-C5	2.69	1.48	1.43
5	U	1	NAG	O4-C4	2.69	1.49	1.43
5	b	2	NAG	O5-C5	2.68	1.48	1.43
5	f	2	NAG	O5-C1	2.67	1.48	1.43
5	d	2	NAG	O5-C5	2.67	1.48	1.43
5	c	3	BMA	O5-C5	2.66	1.48	1.43
5	o	2	NAG	O5-C5	2.65	1.48	1.43
5	g	2	NAG	O5-C5	2.65	1.48	1.43
5	i	3	BMA	O5-C5	2.65	1.48	1.43
5	e	2	NAG	O5-C5	2.64	1.48	1.43
5	o	1	NAG	O5-C5	2.64	1.48	1.43
5	Y	3	BMA	O5-C5	2.64	1.48	1.43
5	V	3	BMA	O5-C5	2.63	1.48	1.43
5	W	2	NAG	O5-C5	2.62	1.48	1.43
5	o	3	BMA	O5-C5	2.62	1.48	1.43
5	n	3	BMA	O5-C5	2.62	1.48	1.43
5	N	1	NAG	C1-C2	2.61	1.55	1.52
5	M	2	NAG	O5-C5	2.61	1.48	1.43
5	X	1	NAG	C1-C2	2.61	1.55	1.52
5	j	2	NAG	O5-C5	2.61	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	l	2	NAG	O5-C5	2.61	1.48	1.43
5	e	3	BMA	O5-C5	2.61	1.48	1.43
5	o	1	NAG	O4-C4	2.60	1.49	1.43
5	U	3	BMA	O5-C5	2.59	1.48	1.43
5	h	1	NAG	C1-C2	2.59	1.55	1.52
5	V	1	NAG	O4-C4	2.58	1.49	1.43
5	Y	2	NAG	O5-C5	2.58	1.48	1.43
5	o	2	NAG	O4-C4	2.56	1.49	1.43
5	j	1	NAG	O5-C5	2.56	1.48	1.43
5	R	2	NAG	O5-C5	2.56	1.48	1.43
5	h	1	NAG	O5-C5	2.54	1.48	1.43
5	Y	1	NAG	O5-C5	2.54	1.48	1.43
5	l	1	NAG	O5-C5	2.54	1.48	1.43
6	k	2	NAG	O4-C4	2.52	1.49	1.43
5	n	1	NAG	O5-C5	2.52	1.48	1.43
5	U	2	NAG	O4-C4	2.51	1.49	1.43
5	f	1	NAG	O4-C4	2.51	1.49	1.43
5	X	1	NAG	O5-C5	2.50	1.48	1.43
5	S	1	NAG	O5-C5	2.49	1.48	1.43
6	k	3	BMA	O3-C3	2.48	1.49	1.43
5	f	2	NAG	O5-C5	2.48	1.48	1.43
5	d	2	NAG	O4-C4	2.48	1.49	1.43
5	Z	1	NAG	O4-C4	2.48	1.49	1.43
5	N	2	NAG	O5-C5	2.48	1.48	1.43
6	Q	3	BMA	O5-C5	2.48	1.48	1.43
5	R	1	NAG	O5-C5	2.48	1.48	1.43
5	m	1	NAG	O4-C4	2.47	1.49	1.43
5	T	3	BMA	O5-C5	2.46	1.48	1.43
5	N	1	NAG	O5-C5	2.46	1.48	1.43
6	a	4	MAN	O5-C5	2.46	1.48	1.43
5	h	2	NAG	O5-C5	2.45	1.48	1.43
6	Q	3	BMA	O3-C3	2.45	1.49	1.43
5	d	3	BMA	O5-C1	2.45	1.47	1.43
5	P	1	NAG	O4-C4	2.43	1.49	1.43
5	j	1	NAG	O4-C4	2.43	1.49	1.43
5	X	3	BMA	O5-C1	2.42	1.47	1.43
5	R	3	BMA	O5-C5	2.42	1.48	1.43
6	a	3	BMA	O3-C3	2.42	1.48	1.43
5	h	3	BMA	O5-C1	2.41	1.47	1.43
6	Q	5	MAN	O5-C5	2.40	1.48	1.43
5	e	2	NAG	C1-C2	2.40	1.55	1.52
5	P	2	NAG	O4-C4	2.40	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	2	NAG	O5-C1	2.40	1.47	1.43
5	P	2	NAG	O5-C5	2.40	1.48	1.43
5	Z	2	NAG	O5-C5	2.38	1.48	1.43
5	N	3	BMA	O5-C1	2.38	1.47	1.43
6	k	4	MAN	O5-C5	2.38	1.48	1.43
5	S	2	NAG	O5-C5	2.36	1.48	1.43
5	U	2	NAG	O5-C5	2.36	1.48	1.43
5	e	1	NAG	O5-C5	2.36	1.48	1.43
6	a	3	BMA	O5-C5	2.36	1.48	1.43
5	T	1	NAG	O5-C5	2.35	1.48	1.43
5	Z	1	NAG	O5-C5	2.35	1.48	1.43
5	U	3	BMA	O5-C1	2.35	1.47	1.43
5	m	2	NAG	O5-C5	2.35	1.48	1.43
5	M	3	BMA	O5-C5	2.34	1.48	1.43
6	a	5	MAN	O5-C5	2.34	1.48	1.43
5	V	1	NAG	O5-C5	2.34	1.48	1.43
5	S	3	BMA	O5-C5	2.33	1.48	1.43
6	k	2	NAG	O5-C5	2.33	1.48	1.43
5	M	1	NAG	O5-C5	2.33	1.48	1.43
5	V	3	BMA	O5-C1	2.32	1.47	1.43
6	Q	4	MAN	O5-C5	2.32	1.48	1.43
5	O	2	NAG	O5-C5	2.32	1.48	1.43
5	b	1	NAG	O5-C5	2.32	1.47	1.43
5	W	3	BMA	O5-C1	2.31	1.47	1.43
5	o	3	BMA	O5-C1	2.31	1.47	1.43
5	d	1	NAG	O4-C4	2.30	1.48	1.43
5	e	2	NAG	O4-C4	2.30	1.48	1.43
5	m	3	BMA	O5-C5	2.30	1.47	1.43
5	e	3	BMA	O5-C1	2.29	1.47	1.43
5	U	2	NAG	C1-C2	2.29	1.55	1.52
5	p	1	NAG	O5-C5	2.29	1.47	1.43
5	f	3	BMA	O5-C1	2.29	1.47	1.43
5	d	1	NAG	O5-C5	2.29	1.47	1.43
5	g	3	BMA	O5-C1	2.28	1.47	1.43
5	b	2	NAG	O5-C1	2.28	1.47	1.43
6	Q	2	NAG	O4-C4	2.28	1.48	1.43
5	W	1	NAG	O5-C5	2.27	1.47	1.43
6	k	5	MAN	O5-C5	2.26	1.47	1.43
6	a	2	NAG	O4-C4	2.25	1.48	1.43
5	n	3	BMA	O5-C1	2.24	1.47	1.43
5	p	1	NAG	O4-C4	2.23	1.48	1.43
5	Z	3	BMA	O5-C1	2.23	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	p	2	NAG	O4-C4	2.22	1.48	1.43
5	j	2	NAG	O4-C4	2.22	1.48	1.43
5	Z	2	NAG	O4-C4	2.22	1.48	1.43
5	R	2	NAG	O5-C1	2.21	1.47	1.43
5	n	2	NAG	O4-C4	2.21	1.48	1.43
5	g	1	NAG	O5-C5	2.21	1.47	1.43
5	n	1	NAG	O4-C4	2.20	1.48	1.43
5	b	2	NAG	O4-C4	2.20	1.48	1.43
5	o	2	NAG	C1-C2	2.19	1.55	1.52
5	h	2	NAG	O4-C4	2.19	1.48	1.43
5	i	3	BMA	O5-C1	2.19	1.47	1.43
5	Y	2	NAG	O4-C4	2.19	1.48	1.43
5	T	3	BMA	O5-C1	2.19	1.47	1.43
5	i	1	NAG	O5-C5	2.19	1.47	1.43
5	O	1	NAG	O5-C5	2.19	1.47	1.43
5	U	1	NAG	O5-C5	2.18	1.47	1.43
5	i	2	NAG	O5-C5	2.18	1.47	1.43
6	Q	6	MAN	O5-C5	2.17	1.47	1.43
5	N	2	NAG	O4-C4	2.16	1.48	1.43
5	l	3	BMA	O5-C1	2.16	1.47	1.43
5	f	1	NAG	O5-C5	2.16	1.47	1.43
5	O	3	BMA	O5-C1	2.16	1.47	1.43
5	M	2	NAG	O4-C4	2.15	1.48	1.43
5	Y	3	BMA	O5-C1	2.15	1.47	1.43
5	e	2	NAG	O5-C1	2.14	1.47	1.43
6	a	6	MAN	O5-C5	2.12	1.47	1.43
5	X	2	NAG	O4-C4	2.11	1.48	1.43
5	b	1	NAG	O4-C4	2.11	1.48	1.43
5	c	1	NAG	O4-C4	2.10	1.48	1.43
5	o	2	NAG	O5-C1	2.10	1.47	1.43
5	j	3	BMA	O5-C1	2.09	1.47	1.43
6	k	6	MAN	O5-C5	2.09	1.47	1.43
5	S	2	NAG	C1-C2	2.09	1.55	1.52
5	p	3	BMA	O5-C1	2.07	1.47	1.43
6	Q	2	NAG	O5-C5	2.07	1.47	1.43
5	n	2	NAG	O5-C1	2.07	1.47	1.43
5	P	3	BMA	O5-C1	2.06	1.47	1.43
5	R	1	NAG	O4-C4	2.05	1.48	1.43
5	i	2	NAG	O4-C4	2.05	1.48	1.43
5	S	1	NAG	O4-C4	2.04	1.48	1.43
6	k	1	NAG	O5-C5	2.03	1.47	1.43
5	l	2	NAG	O5-C1	2.02	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	2	NAG	O4-C4	2.01	1.47	1.43
5	g	2	NAG	O4-C4	2.01	1.47	1.43
6	a	2	NAG	O5-C5	2.01	1.47	1.43
6	a	6	MAN	O5-C1	2.00	1.47	1.43
5	l	2	NAG	O4-C4	2.00	1.47	1.43

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	2	NAG	O5-C1-C2	6.61	121.52	111.29
5	b	1	NAG	C2-N2-C7	5.34	130.05	122.90
5	j	2	NAG	O5-C1-C2	5.21	119.35	111.29
5	P	2	NAG	C4-C3-C2	5.04	118.41	111.02
5	T	2	NAG	C1-O5-C5	5.01	118.91	112.19
5	V	3	BMA	C1-O5-C5	4.89	118.74	112.19
5	p	3	BMA	C1-O5-C5	4.86	118.69	112.19
5	b	1	NAG	C1-C2-N2	4.45	117.44	110.43
5	m	3	BMA	O5-C1-C2	4.44	121.38	110.79
5	c	3	BMA	O5-C1-C2	4.34	121.14	110.79
5	T	1	NAG	C1-O5-C5	4.27	117.91	112.19
5	V	1	NAG	C4-C3-C2	4.13	117.08	111.02
5	p	1	NAG	C4-C3-C2	4.12	117.05	111.02
5	N	3	BMA	C1-O5-C5	3.93	117.45	112.19
5	n	1	NAG	C1-O5-C5	3.88	117.39	112.19
5	f	1	NAG	C4-C3-C2	3.84	116.65	111.02
5	o	2	NAG	C1-O5-C5	3.76	117.23	112.19
5	U	2	NAG	C1-O5-C5	3.75	117.22	112.19
5	S	3	BMA	O5-C1-C2	3.75	119.74	110.79
6	k	1	NAG	C1-O5-C5	3.72	117.17	112.19
5	e	2	NAG	C1-O5-C5	3.69	117.13	112.19
5	b	1	NAG	C1-O5-C5	3.44	116.79	112.19
5	R	2	NAG	C1-O5-C5	3.37	116.70	112.19
5	R	3	BMA	C1-O5-C5	3.36	116.69	112.19
5	m	2	NAG	O5-C1-C2	-3.35	106.10	111.29
5	l	3	BMA	C1-O5-C5	3.33	116.64	112.19
5	d	1	NAG	C1-O5-C5	3.32	116.64	112.19
6	a	2	NAG	C4-C3-C2	3.14	115.62	111.02
5	f	3	BMA	C1-O5-C5	3.12	116.36	112.19
5	l	2	NAG	C1-O5-C5	3.09	116.33	112.19
5	h	3	BMA	C1-O5-C5	3.04	116.26	112.19
6	Q	4	MAN	C1-O5-C5	3.03	116.25	112.19
5	T	3	BMA	C1-O5-C5	3.03	116.24	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	k	2	NAG	C4-C3-C2	3.01	115.42	111.02
5	b	3	BMA	C1-O5-C5	3.00	116.21	112.19
5	j	3	BMA	C1-O5-C5	2.97	116.17	112.19
6	Q	2	NAG	C4-C3-C2	2.94	115.32	111.02
5	b	2	NAG	C1-O5-C5	2.90	116.07	112.19
5	i	3	BMA	C1-O5-C5	2.87	116.04	112.19
6	k	5	MAN	C1-C2-C3	2.87	113.82	109.64
6	a	1	NAG	C1-O5-C5	2.87	116.03	112.19
5	g	3	BMA	C1-O5-C5	2.82	115.97	112.19
5	O	3	BMA	C1-O5-C5	2.81	115.95	112.19
5	l	1	NAG	C1-C2-N2	2.77	114.80	110.43
5	d	2	NAG	C2-N2-C7	2.75	126.59	122.90
5	Z	3	BMA	C1-O5-C5	2.73	115.85	112.19
6	Q	4	MAN	C1-C2-C3	2.73	113.62	109.64
5	P	1	NAG	C1-O5-C5	2.72	115.84	112.19
6	k	4	MAN	C1-C2-C3	2.71	113.59	109.64
6	k	4	MAN	C1-O5-C5	2.69	115.80	112.19
6	a	4	MAN	C1-O5-C5	2.65	115.74	112.19
5	P	3	BMA	C1-O5-C5	2.62	115.70	112.19
5	X	3	BMA	C1-O5-C5	2.62	115.70	112.19
5	l	1	NAG	O5-C1-C2	-2.61	107.26	111.29
5	Z	2	NAG	C4-C3-C2	2.58	114.79	111.02
5	Y	3	BMA	C1-O5-C5	2.58	115.64	112.19
5	S	2	NAG	O5-C1-C2	-2.56	107.33	111.29
6	Q	5	MAN	C3-C4-C5	-2.56	105.60	110.23
6	k	4	MAN	C2-C3-C4	2.54	115.32	110.86
5	m	1	NAG	O5-C1-C2	-2.53	107.38	111.29
5	f	2	NAG	O5-C5-C4	-2.52	104.70	110.83
5	V	2	NAG	O5-C5-C4	-2.52	104.70	110.83
6	Q	4	MAN	C2-C3-C4	2.51	115.27	110.86
5	d	3	BMA	C1-O5-C5	2.49	115.52	112.19
6	Q	1	NAG	C1-O5-C5	2.46	115.49	112.19
5	T	2	NAG	C4-C3-C2	-2.44	107.45	111.02
5	P	1	NAG	O5-C1-C2	-2.43	107.53	111.29
5	m	1	NAG	C1-O5-C5	2.42	115.42	112.19
6	a	4	MAN	C1-C2-C3	2.41	113.16	109.64
5	P	3	BMA	C1-C2-C3	2.41	113.15	109.64
5	V	1	NAG	O5-C1-C2	-2.40	107.57	111.29
5	R	1	NAG	O5-C1-C2	-2.40	107.58	111.29
5	m	2	NAG	C1-O5-C5	2.36	115.35	112.19
5	P	2	NAG	C1-O5-C5	2.34	115.33	112.19
5	P	2	NAG	O4-C4-C3	-2.34	104.86	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	1	NAG	O4-C4-C3	-2.34	104.87	110.38
5	W	3	BMA	C1-O5-C5	2.33	115.31	112.19
5	l	1	NAG	C4-C3-C2	-2.33	107.60	111.02
5	h	2	NAG	O5-C1-C2	-2.33	107.69	111.29
6	a	4	MAN	C2-C3-C4	2.33	114.95	110.86
6	Q	6	MAN	C1-O5-C5	2.31	115.28	112.19
5	U	1	NAG	O5-C1-C2	-2.31	107.72	111.29
6	Q	5	MAN	C1-C2-C3	2.30	113.00	109.64
6	a	5	MAN	C1-C2-C3	2.26	112.94	109.64
6	a	5	MAN	C3-C4-C5	-2.26	106.14	110.23
6	k	5	MAN	C3-C4-C5	-2.25	106.15	110.23
5	R	3	BMA	C1-C2-C3	2.25	112.92	109.64
5	h	1	NAG	O4-C4-C3	-2.24	105.09	110.38
5	e	1	NAG	O4-C4-C3	2.20	115.56	110.38
5	g	1	NAG	O4-C4-C3	-2.19	105.20	110.38
5	m	3	BMA	O2-C2-C1	2.17	114.19	109.22
5	f	1	NAG	O5-C1-C2	-2.16	107.94	111.29
5	Y	1	NAG	C4-C3-C2	-2.14	107.88	111.02
5	N	1	NAG	O4-C4-C3	-2.12	105.37	110.38
5	Z	1	NAG	O5-C1-C2	-2.10	108.05	111.29
5	T	1	NAG	C4-C3-C2	-2.09	107.95	111.02
5	W	1	NAG	O4-C4-C3	-2.09	105.44	110.38
6	a	5	MAN	C1-O5-C5	2.09	114.98	112.19
5	S	3	BMA	O2-C2-C1	2.07	113.95	109.22
5	m	2	NAG	O4-C4-C5	-2.06	104.25	109.32
5	n	1	NAG	C4-C3-C2	-2.03	108.04	111.02
5	p	2	NAG	C1-C2-N2	2.03	113.63	110.43
5	f	2	NAG	C1-O5-C5	2.02	114.90	112.19
5	W	2	NAG	O5-C1-C2	-2.02	108.16	111.29
5	c	2	NAG	O5-C1-C2	-2.02	108.16	111.29
5	o	1	NAG	C1-O5-C5	2.02	114.89	112.19
5	U	1	NAG	C1-O5-C5	2.02	114.89	112.19
5	o	1	NAG	O5-C1-C2	-2.02	108.17	111.29
5	S	3	BMA	C1-O5-C5	2.01	114.89	112.19
5	g	2	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C1-C2-N2-C7
5	R	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	b	1	NAG	C1-C2-N2-C7
5	i	2	NAG	C1-C2-N2-C7
5	l	1	NAG	C1-C2-N2-C7
6	a	3	BMA	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	k	3	BMA	O5-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
6	k	3	BMA	C4-C5-C6-O6
5	i	3	BMA	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
5	Z	2	NAG	C8-C7-N2-C2
5	V	2	NAG	C4-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C8-C7-N2-C2
5	c	2	NAG	C4-C5-C6-O6
5	n	3	BMA	O5-C5-C6-O6
5	Z	2	NAG	O7-C7-N2-C2
5	T	1	NAG	O5-C5-C6-O6
6	Q	6	MAN	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
6	k	6	MAN	O5-C5-C6-O6
5	i	3	BMA	C4-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
6	a	6	MAN	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
6	k	2	NAG	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
5	o	3	BMA	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C1-C2-N2-C7
5	W	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	X	1	NAG	C1-C2-N2-C7
5	Y	2	NAG	C1-C2-N2-C7
5	g	2	NAG	C1-C2-N2-C7
5	h	1	NAG	C1-C2-N2-C7
5	h	2	NAG	C1-C2-N2-C7
5	T	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O7-C7-N2-C2
5	M	1	NAG	C3-C2-N2-C7
5	S	2	NAG	C3-C2-N2-C7
5	V	2	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
5	c	2	NAG	C3-C2-N2-C7
5	f	2	NAG	C3-C2-N2-C7
5	g	1	NAG	C3-C2-N2-C7
5	m	2	NAG	C3-C2-N2-C7
5	V	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	M	2	NAG	C1-C2-N2-C7
5	N	2	NAG	C1-C2-N2-C7
5	S	2	NAG	C1-C2-N2-C7
5	V	2	NAG	C1-C2-N2-C7
5	W	1	NAG	C1-C2-N2-C7
5	X	2	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7
5	c	2	NAG	C1-C2-N2-C7
5	f	2	NAG	C1-C2-N2-C7
5	g	1	NAG	C1-C2-N2-C7
5	m	2	NAG	C1-C2-N2-C7
5	p	2	NAG	C1-C2-N2-C7
5	U	3	BMA	C4-C5-C6-O6
5	M	2	NAG	C3-C2-N2-C7
5	N	1	NAG	C3-C2-N2-C7
5	N	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C3-C2-N2-C7
5	X	1	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7

Continued on next page...

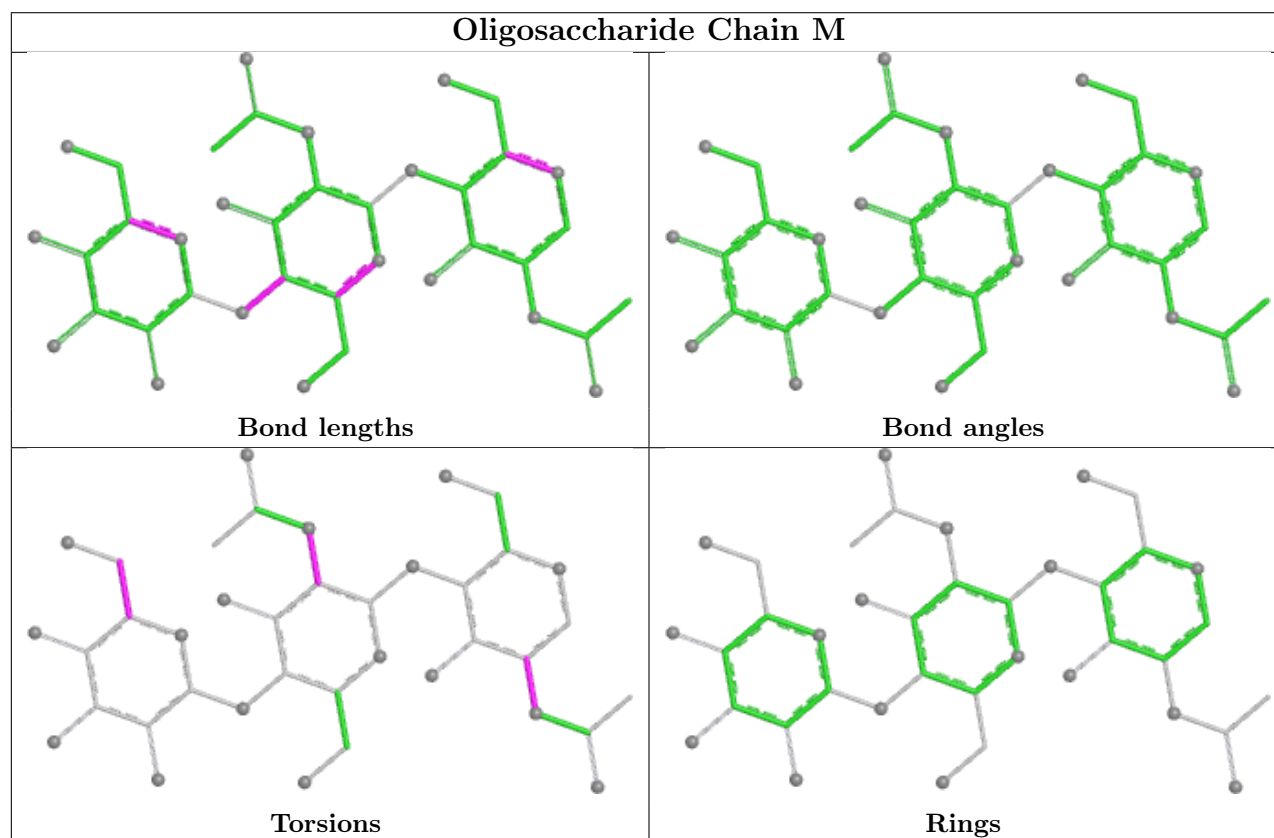
Continued from previous page...

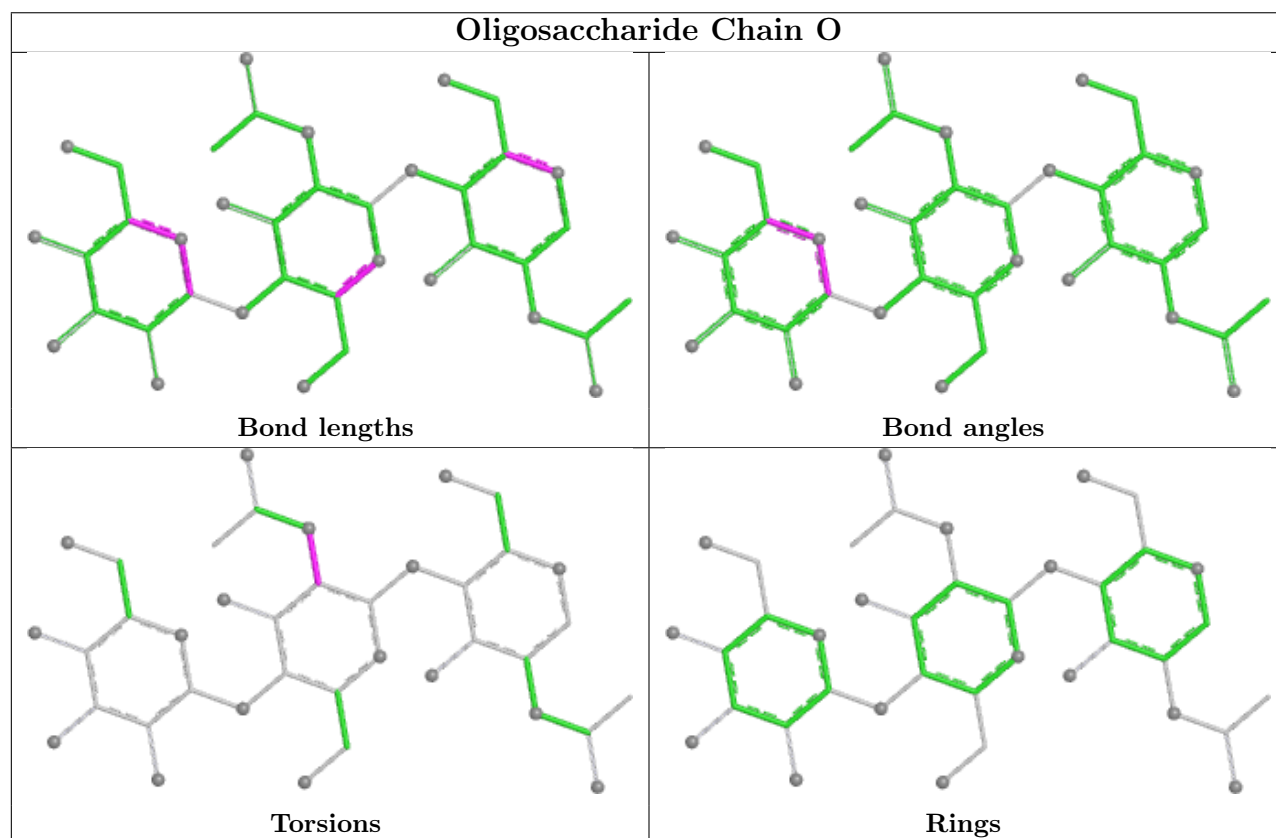
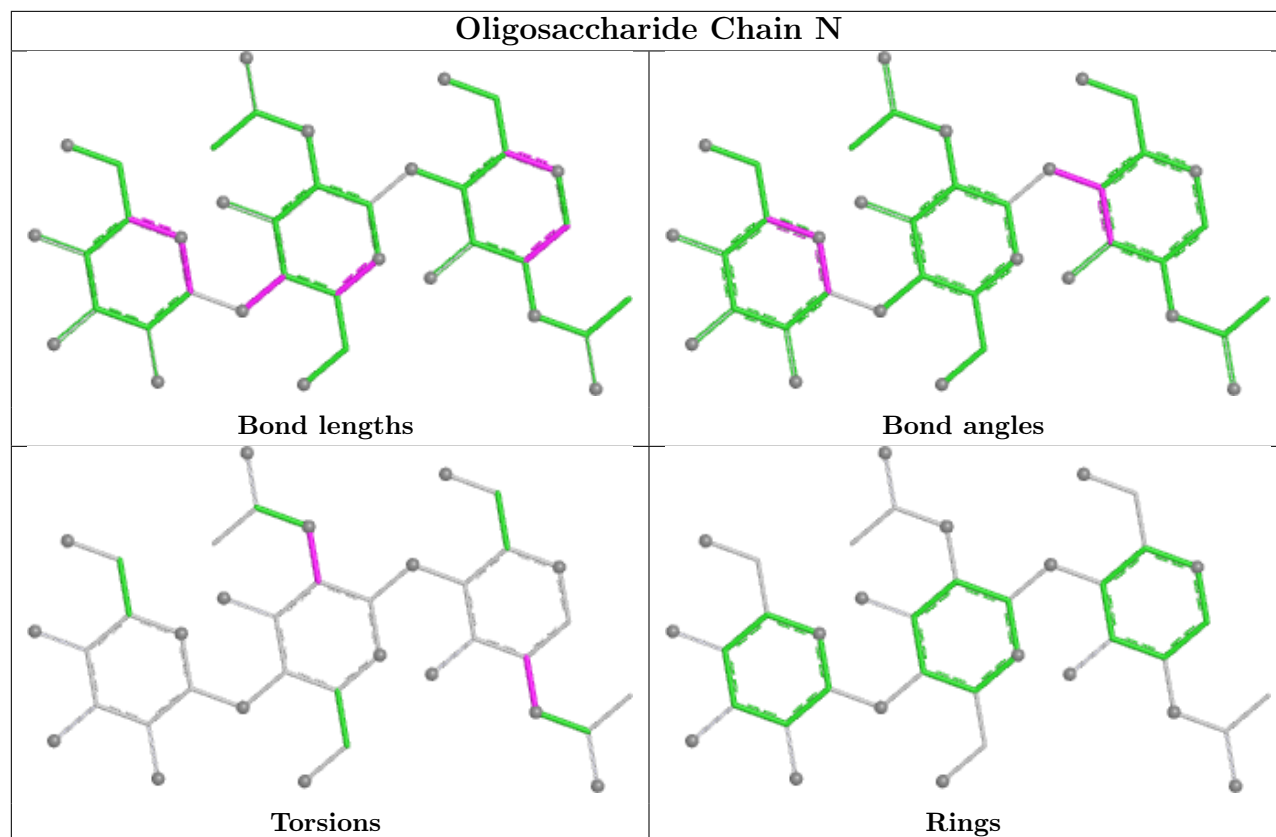
Mol	Chain	Res	Type	Atoms
5	g	2	NAG	C3-C2-N2-C7
5	h	1	NAG	C3-C2-N2-C7
5	h	2	NAG	C3-C2-N2-C7
5	i	2	NAG	C3-C2-N2-C7
5	p	1	NAG	C3-C2-N2-C7
5	p	2	NAG	C3-C2-N2-C7
5	V	3	BMA	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	p	3	BMA	C4-C5-C6-O6

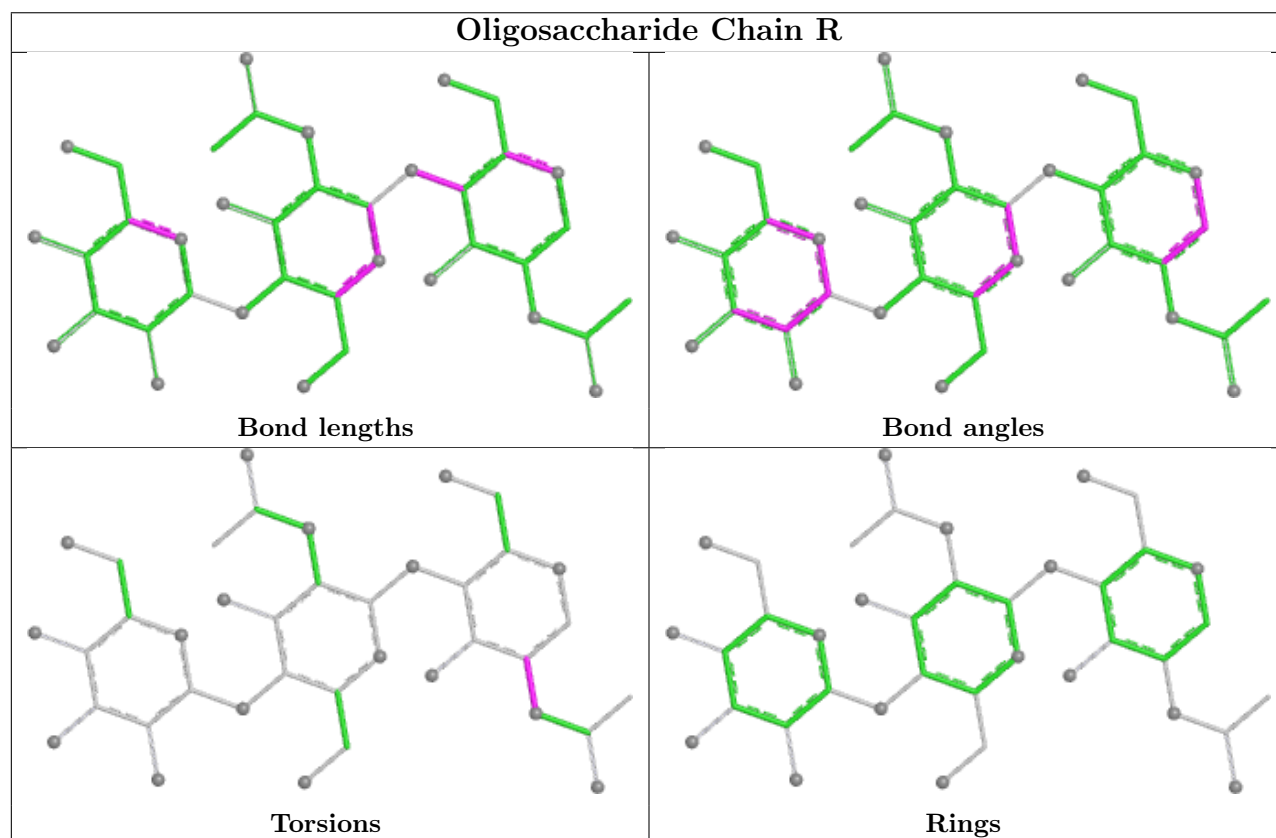
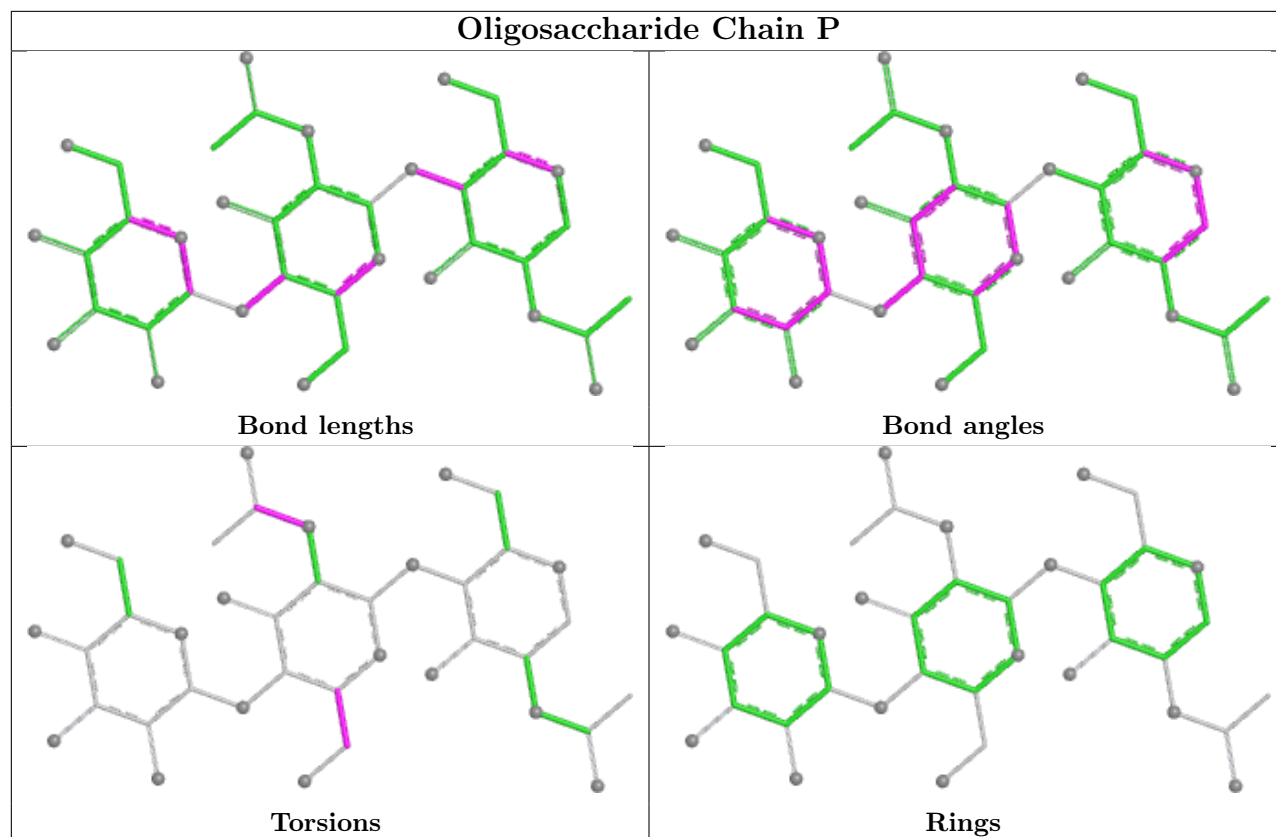
There are no ring outliers.

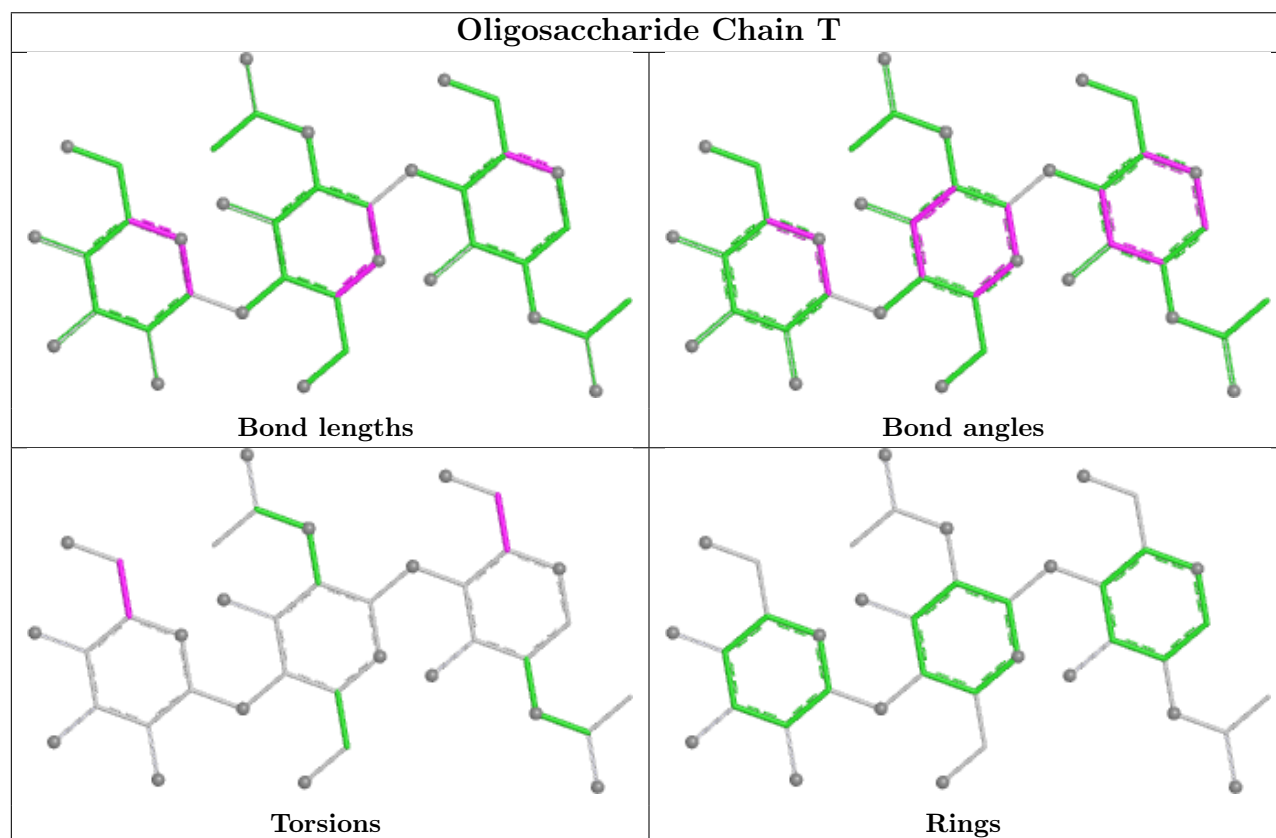
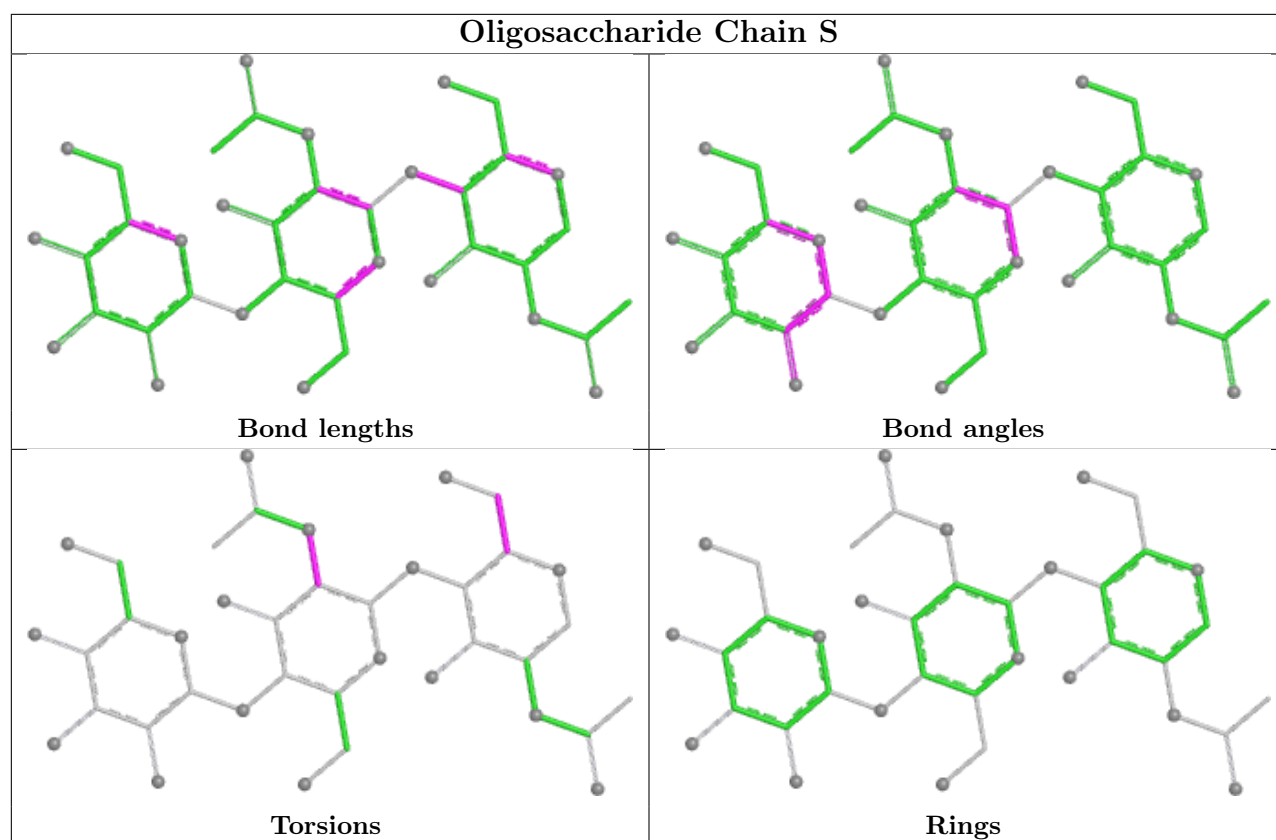
No monomer is involved in short contacts.

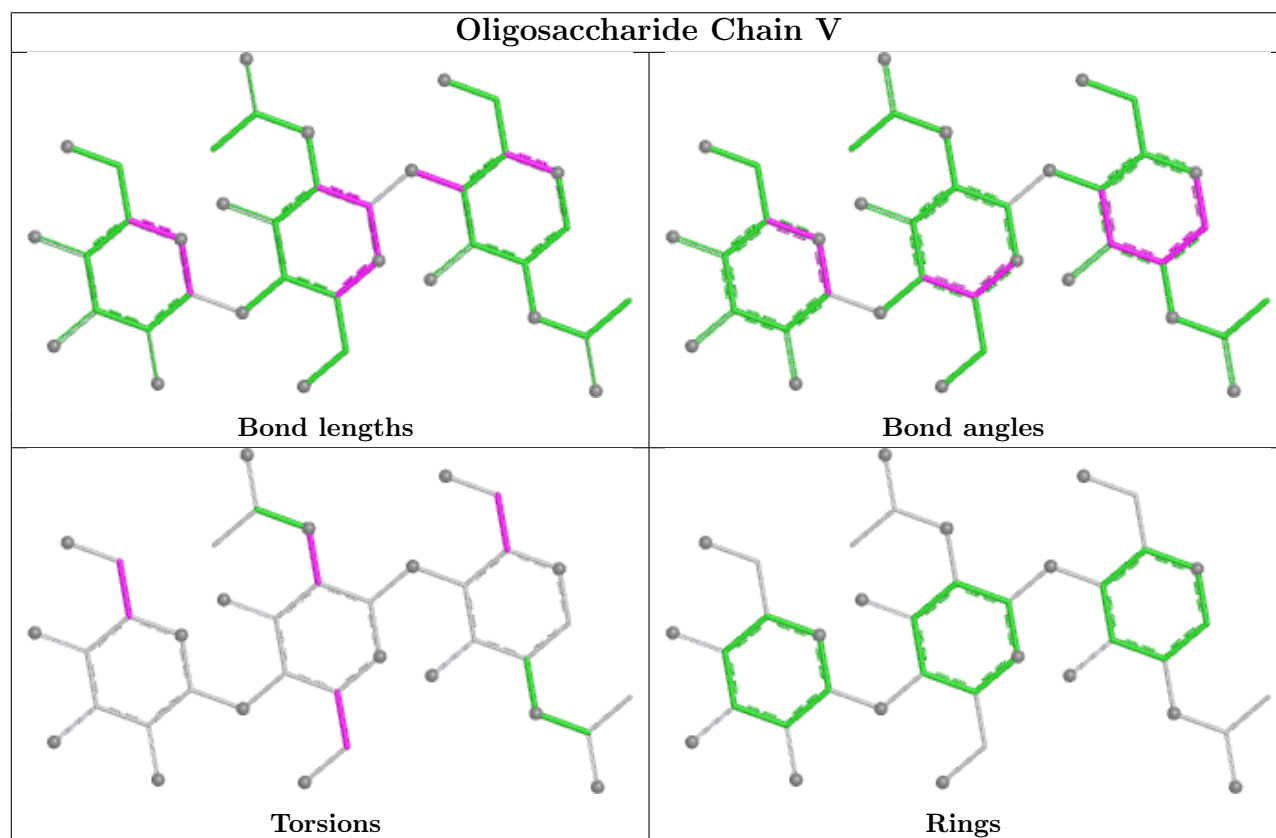
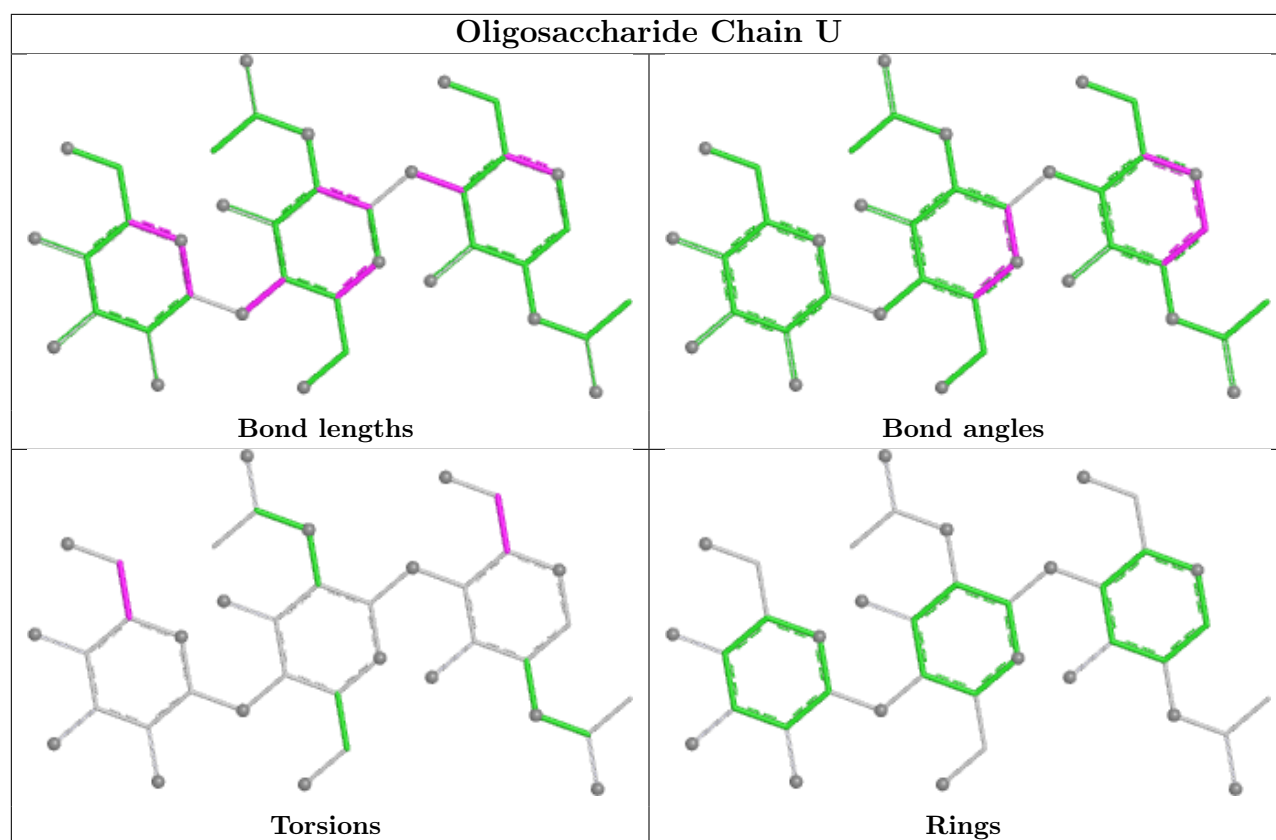
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

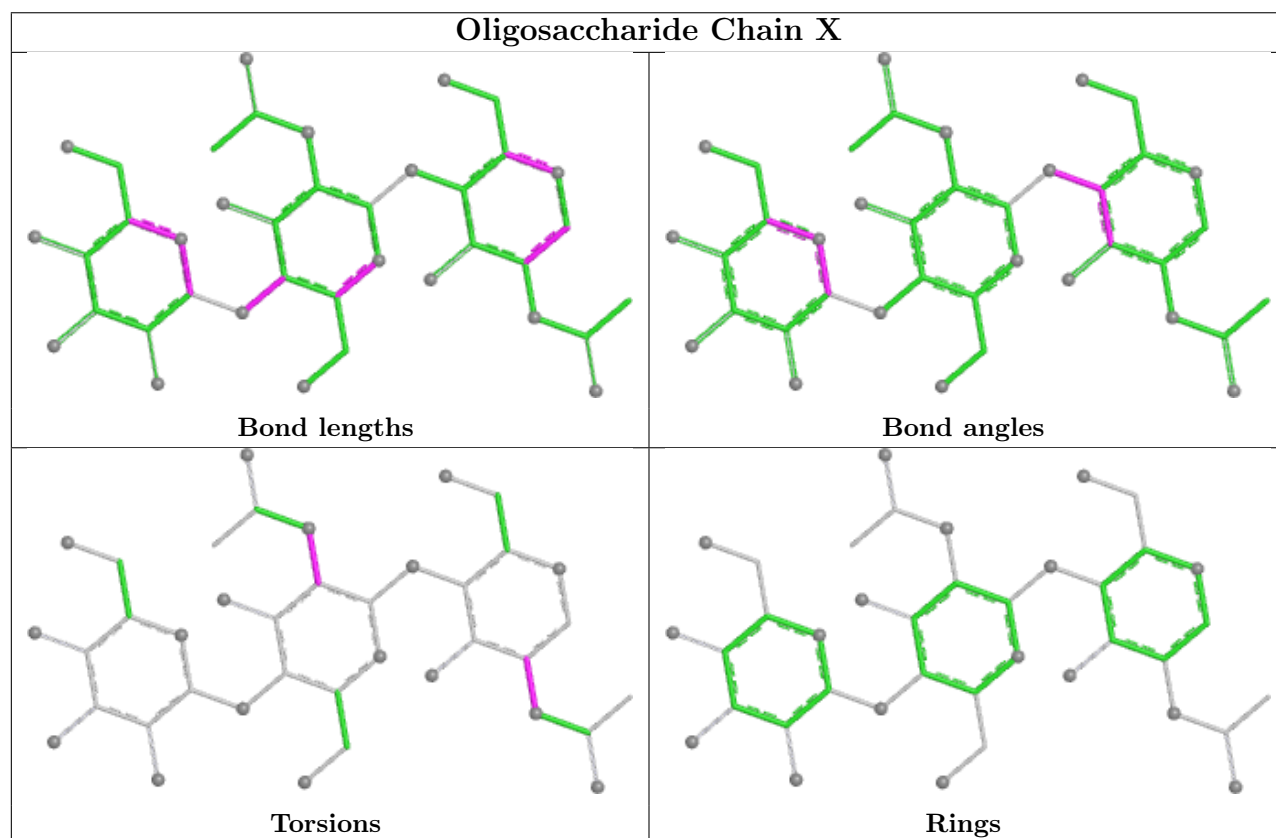
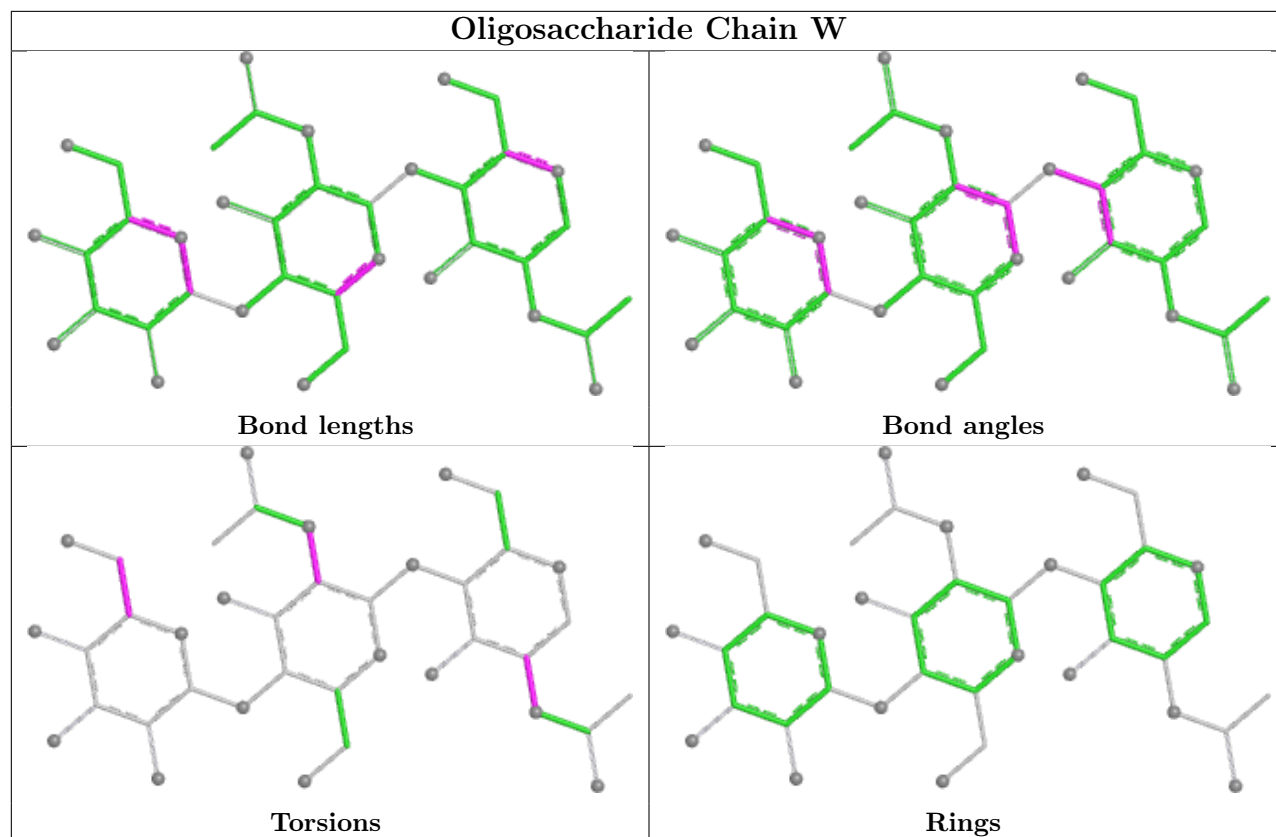


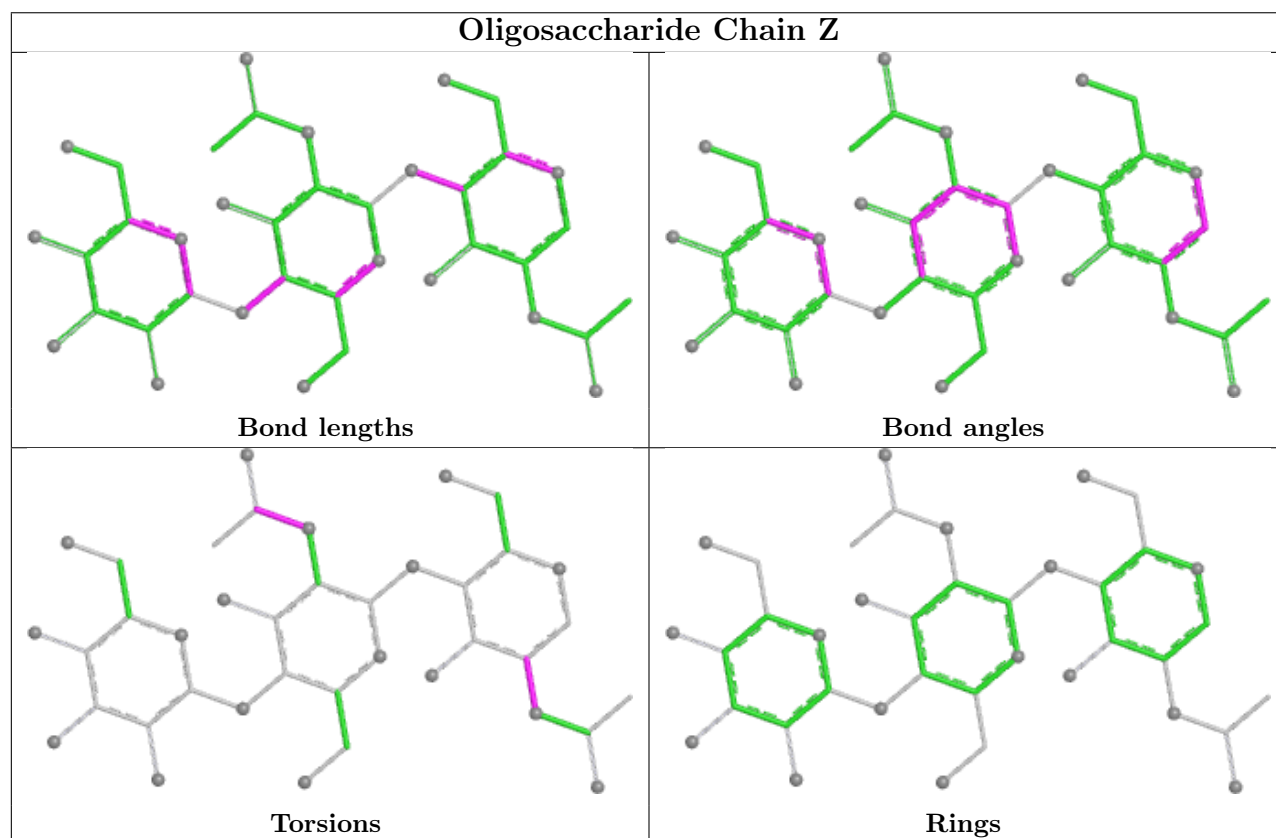
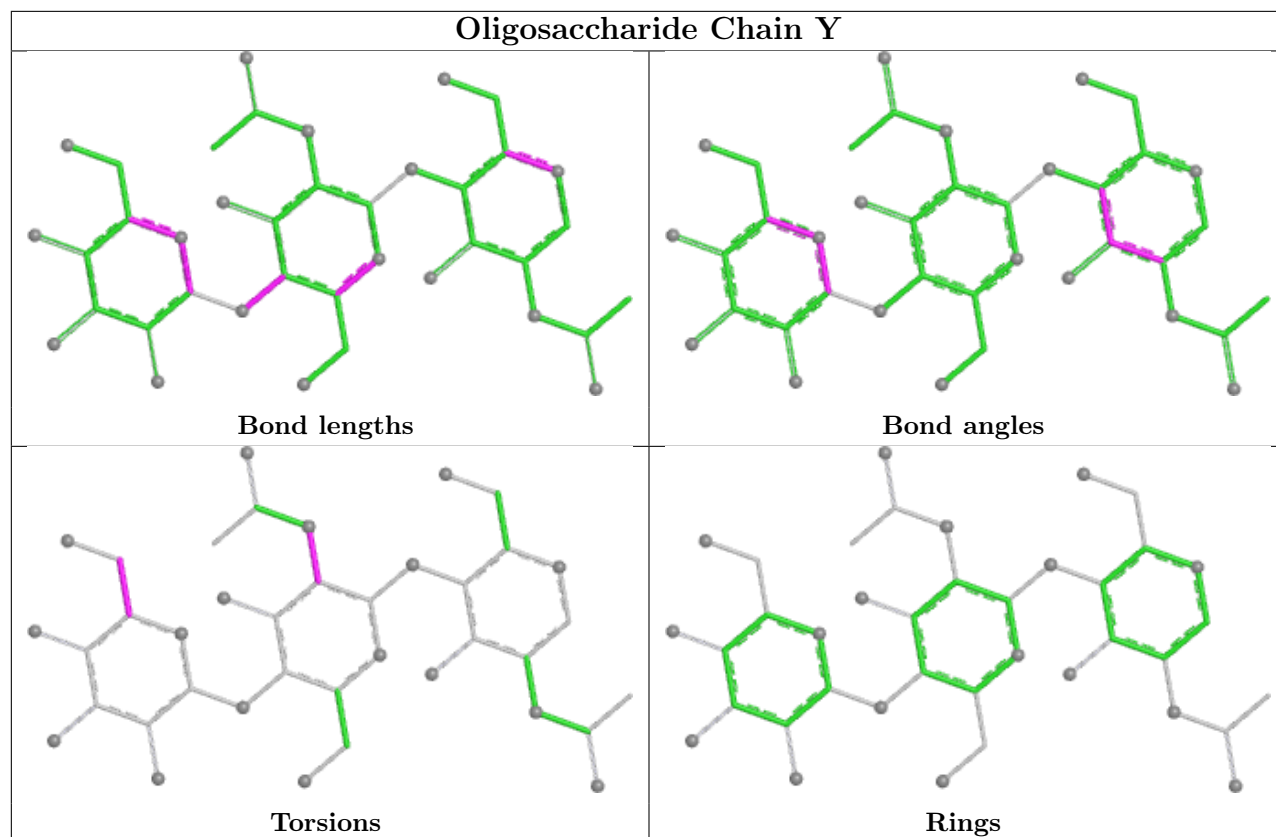


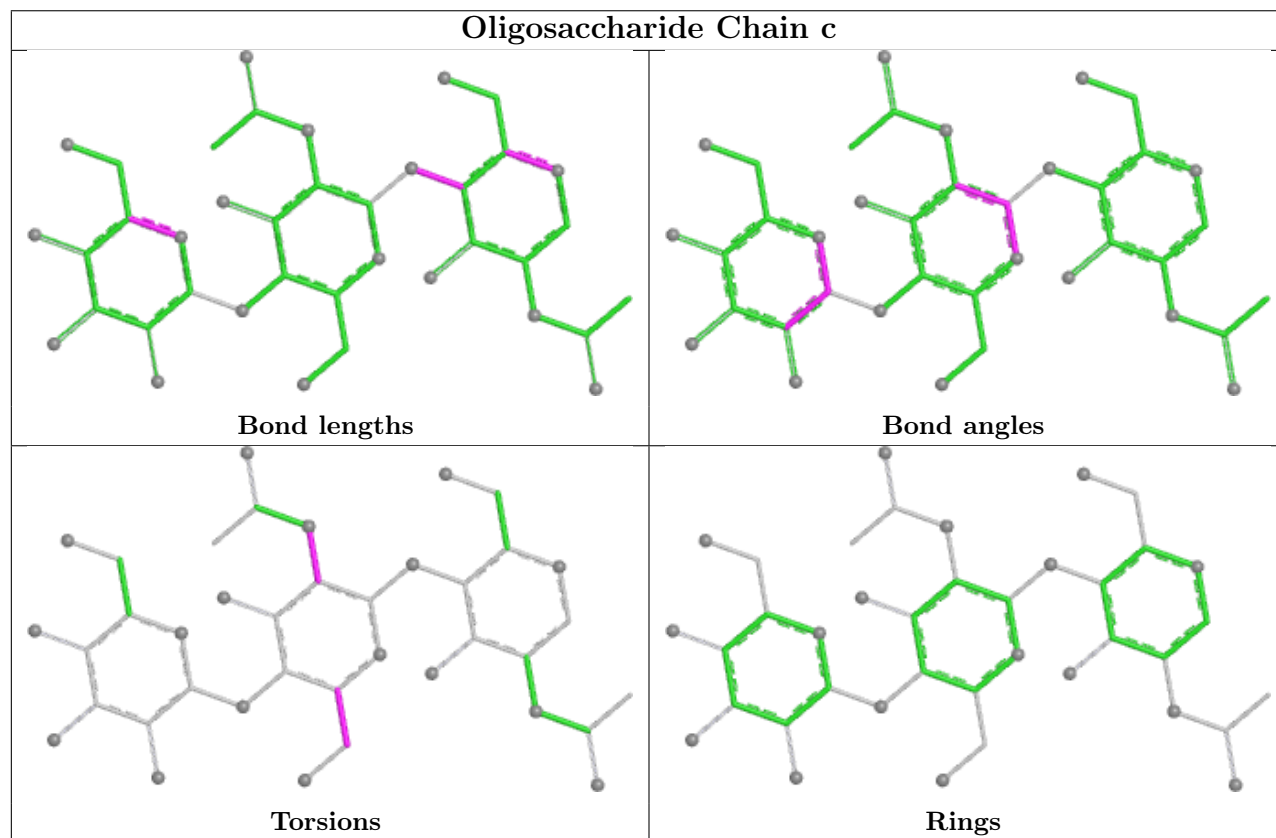
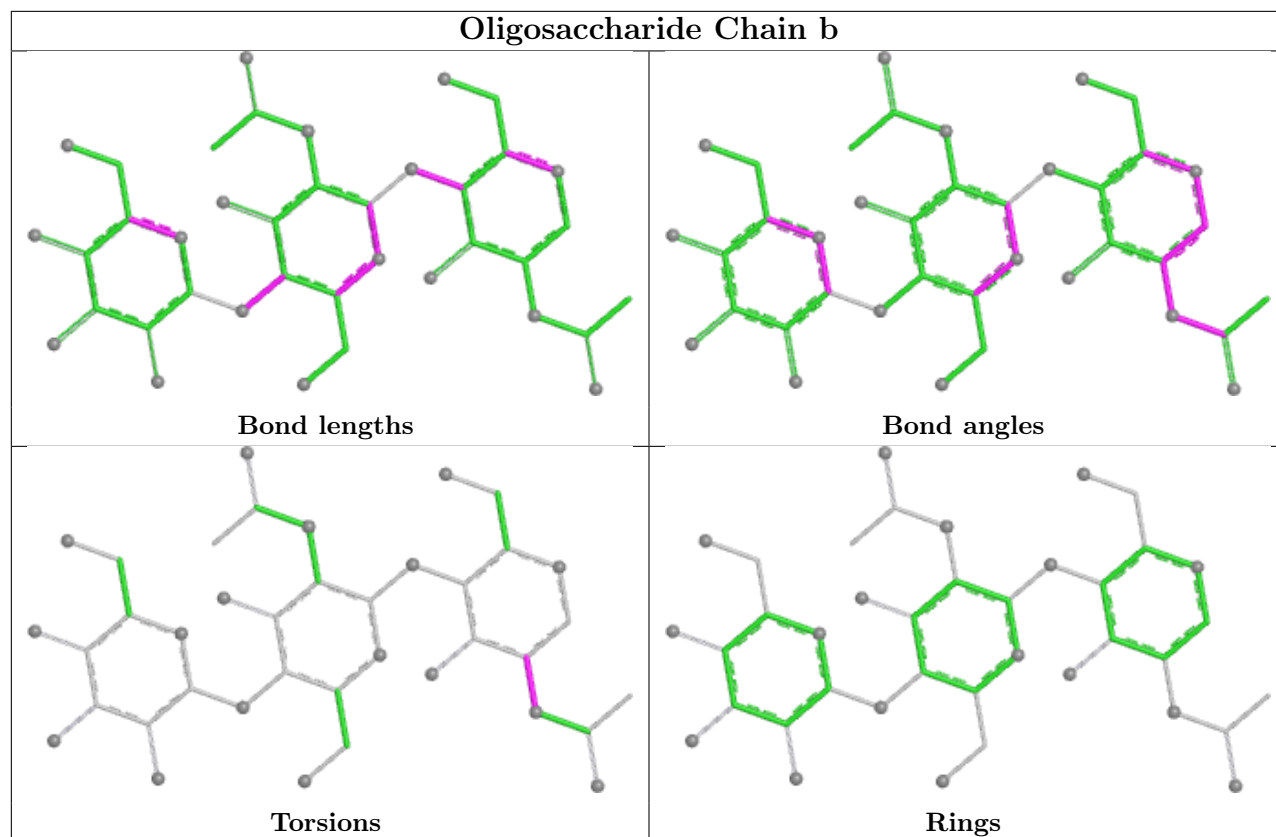


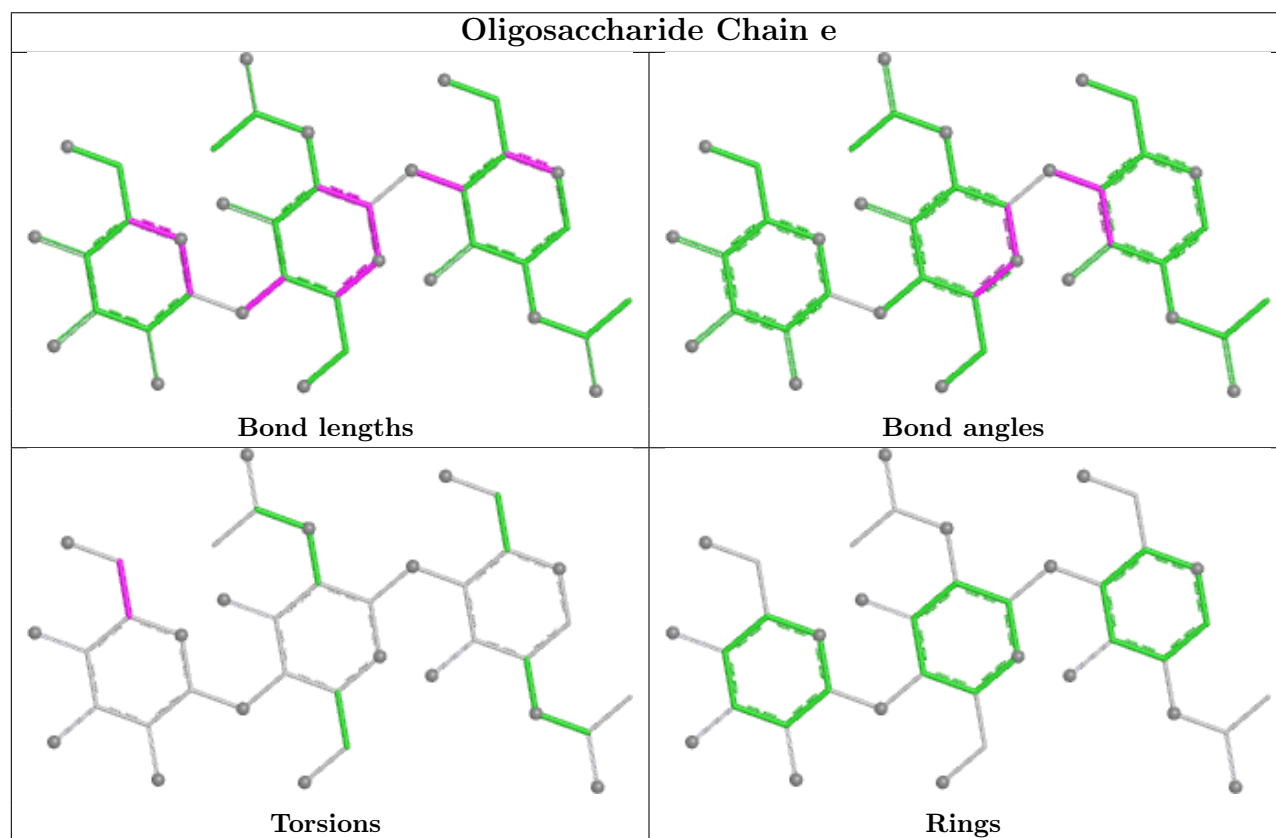
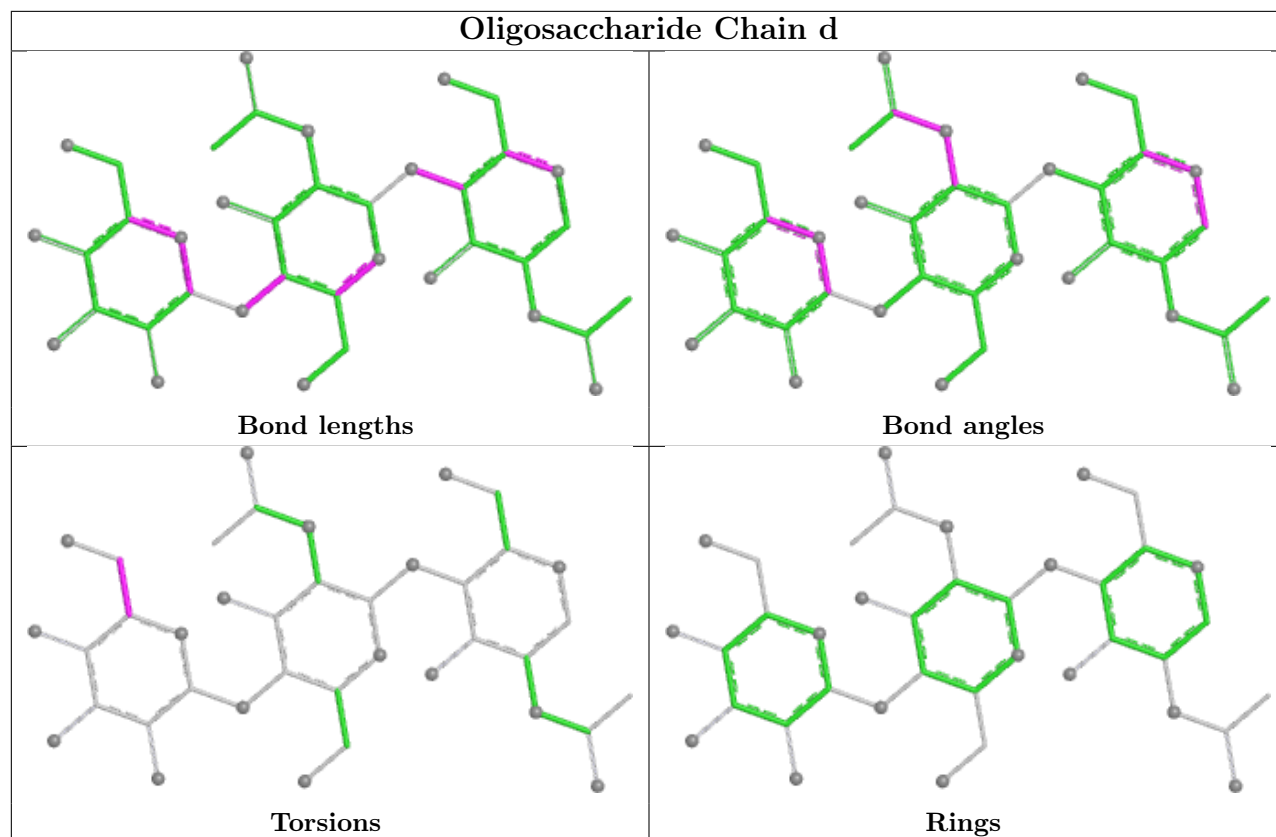


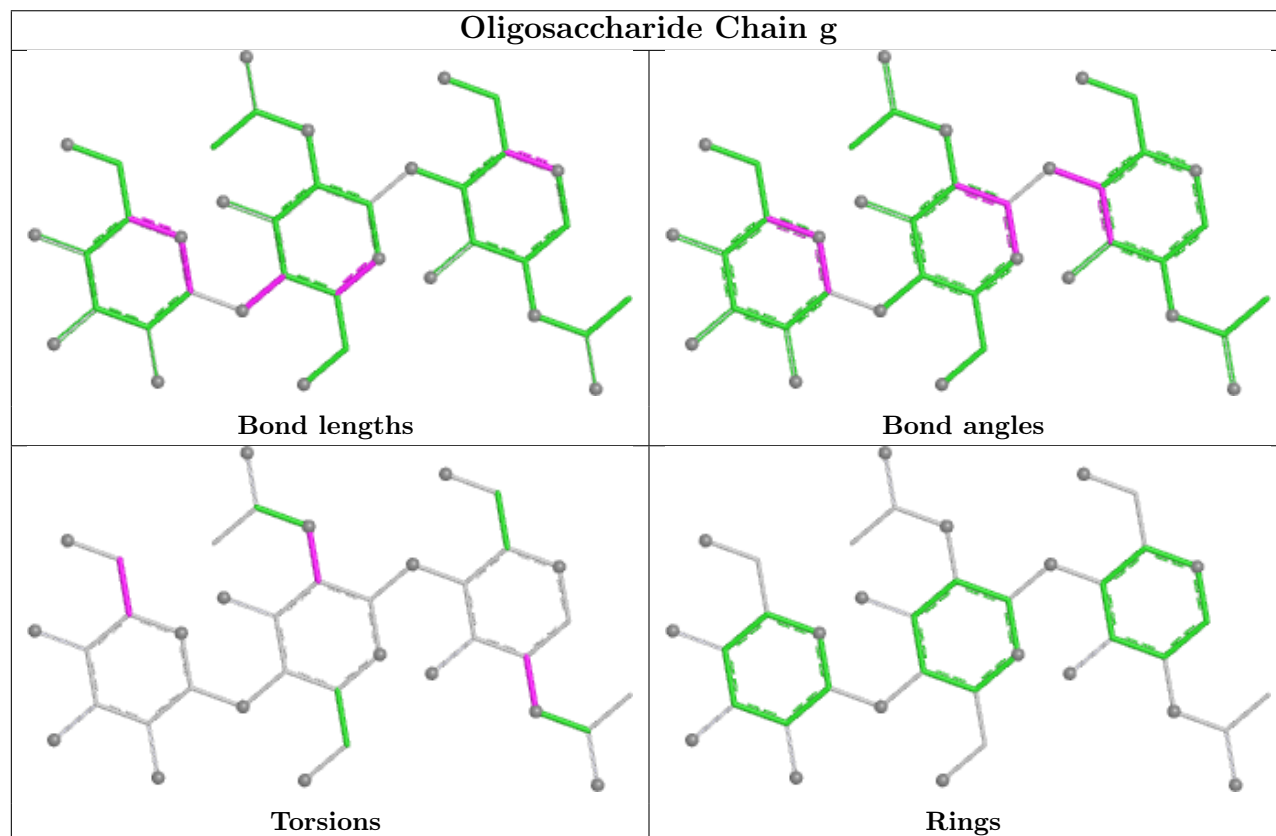
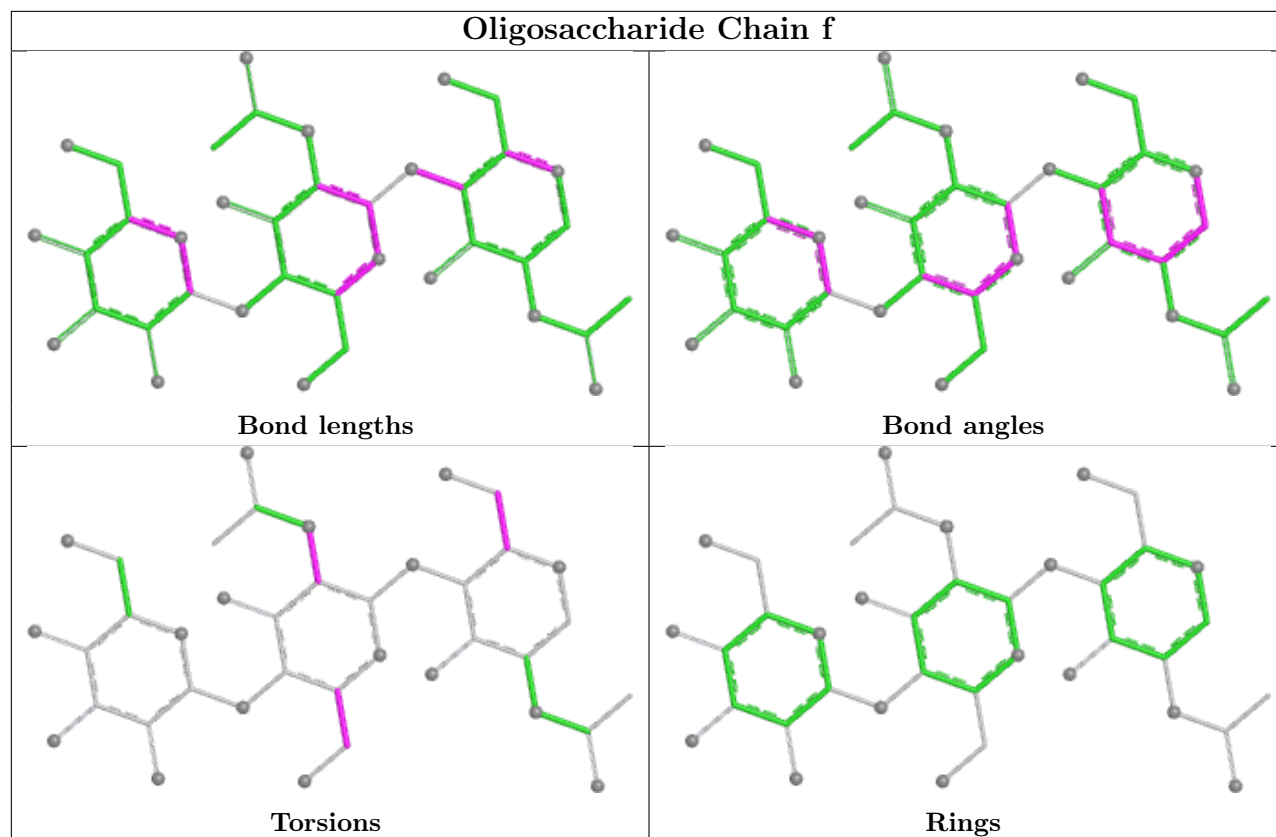


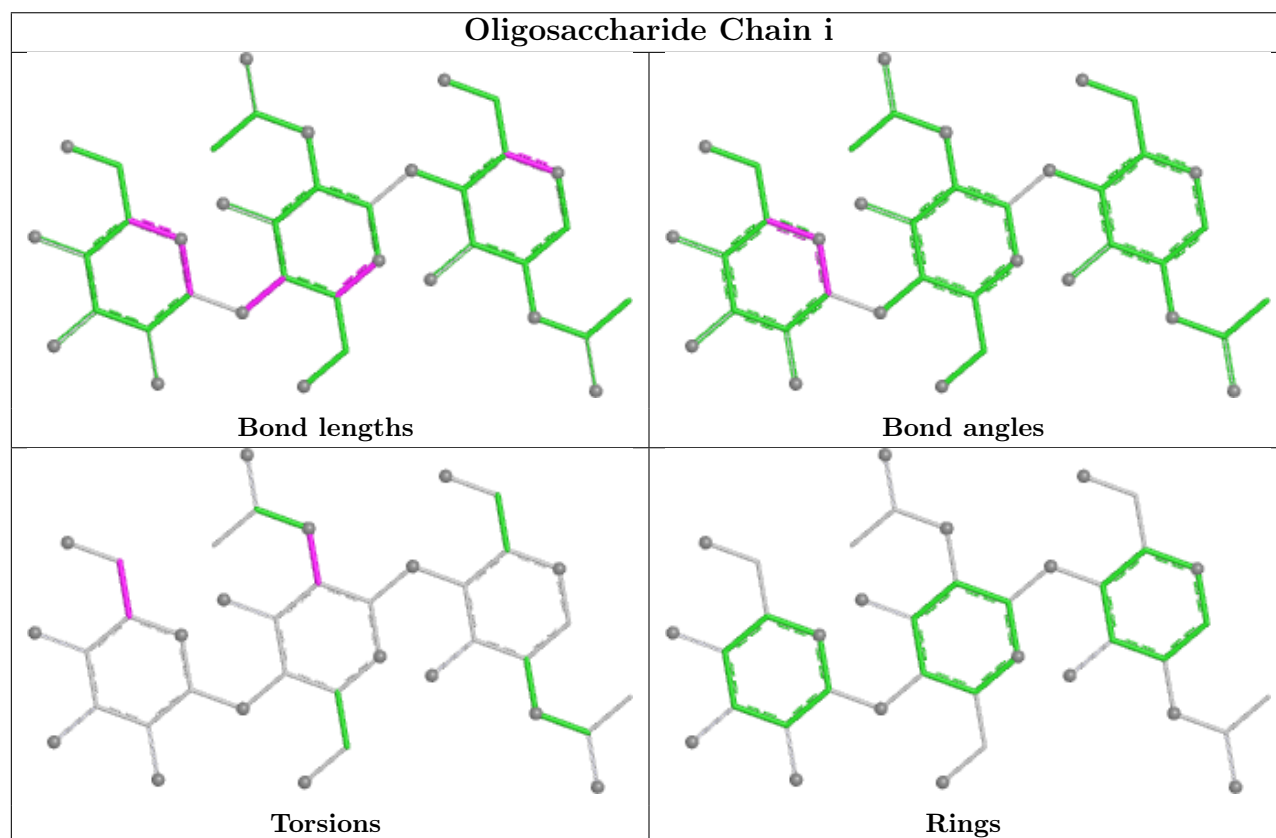
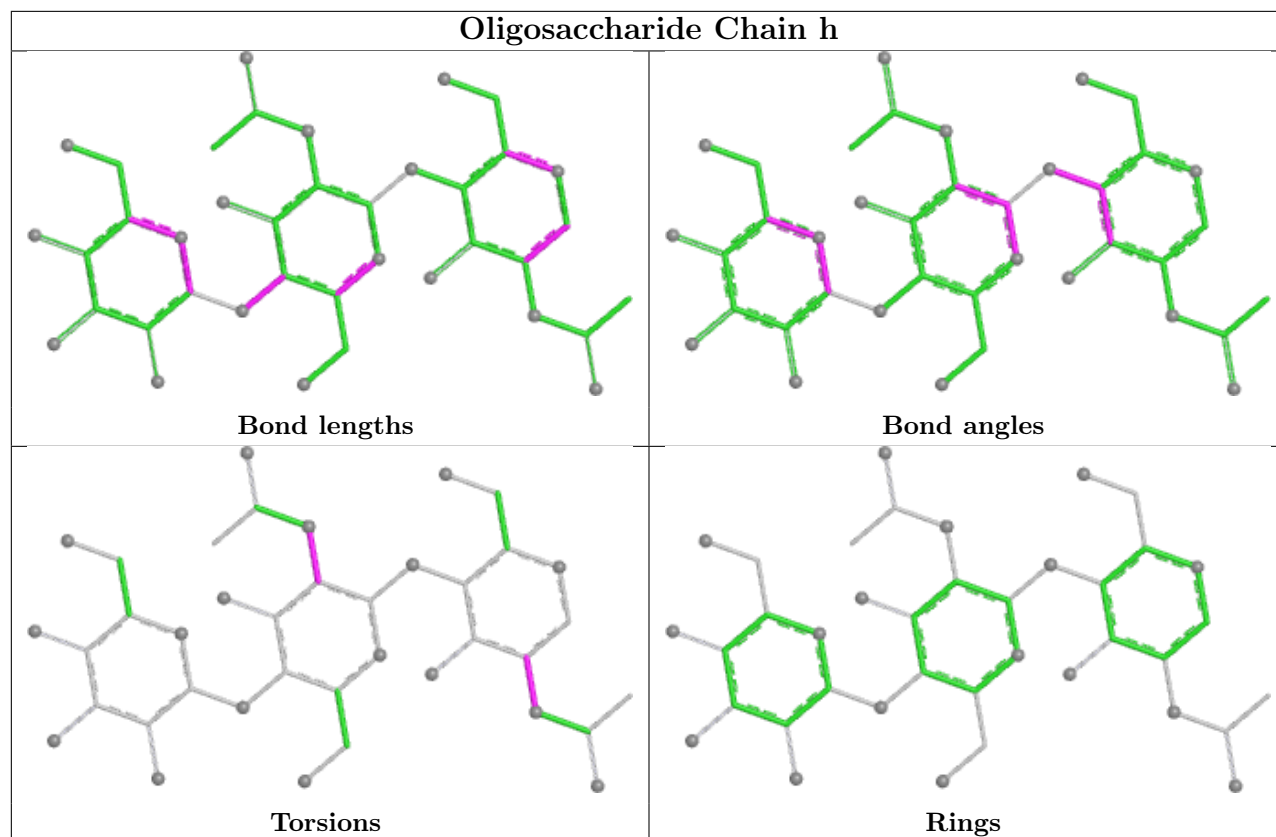


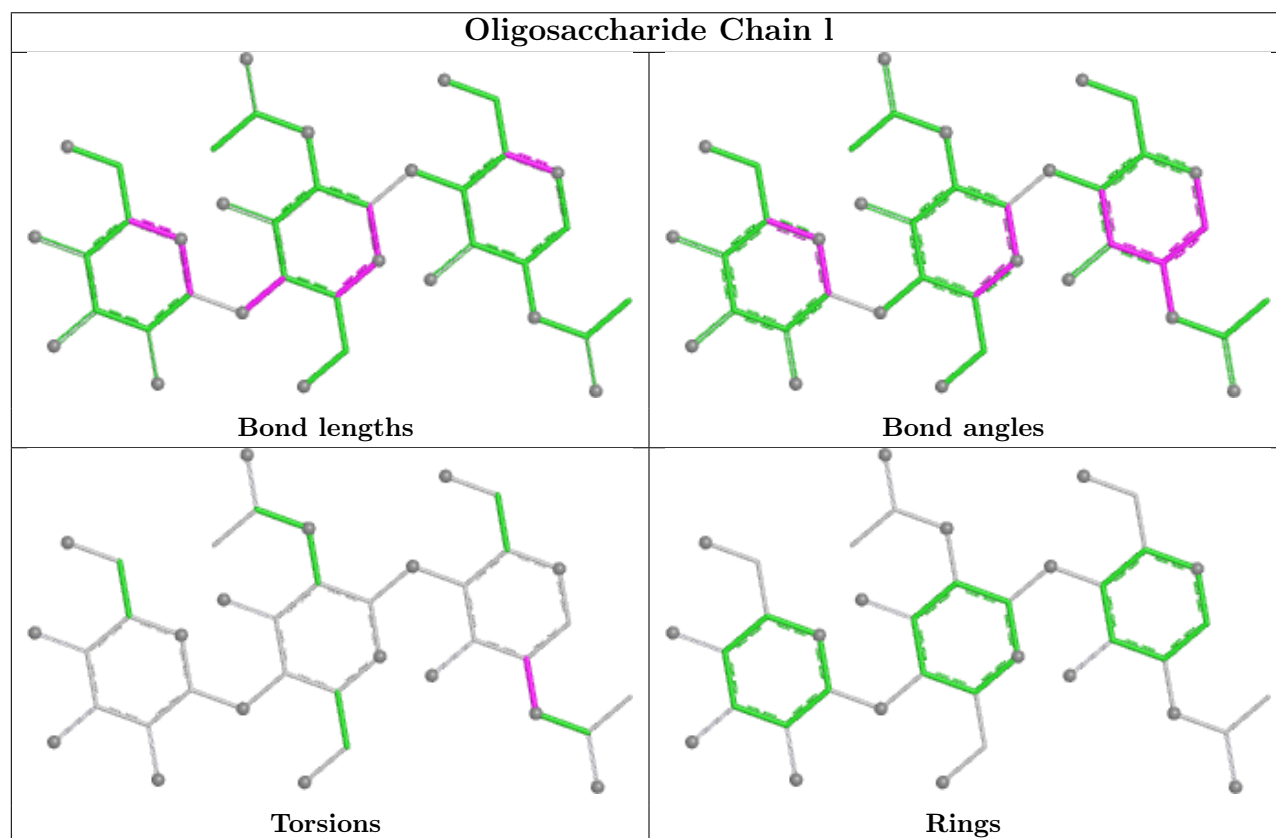
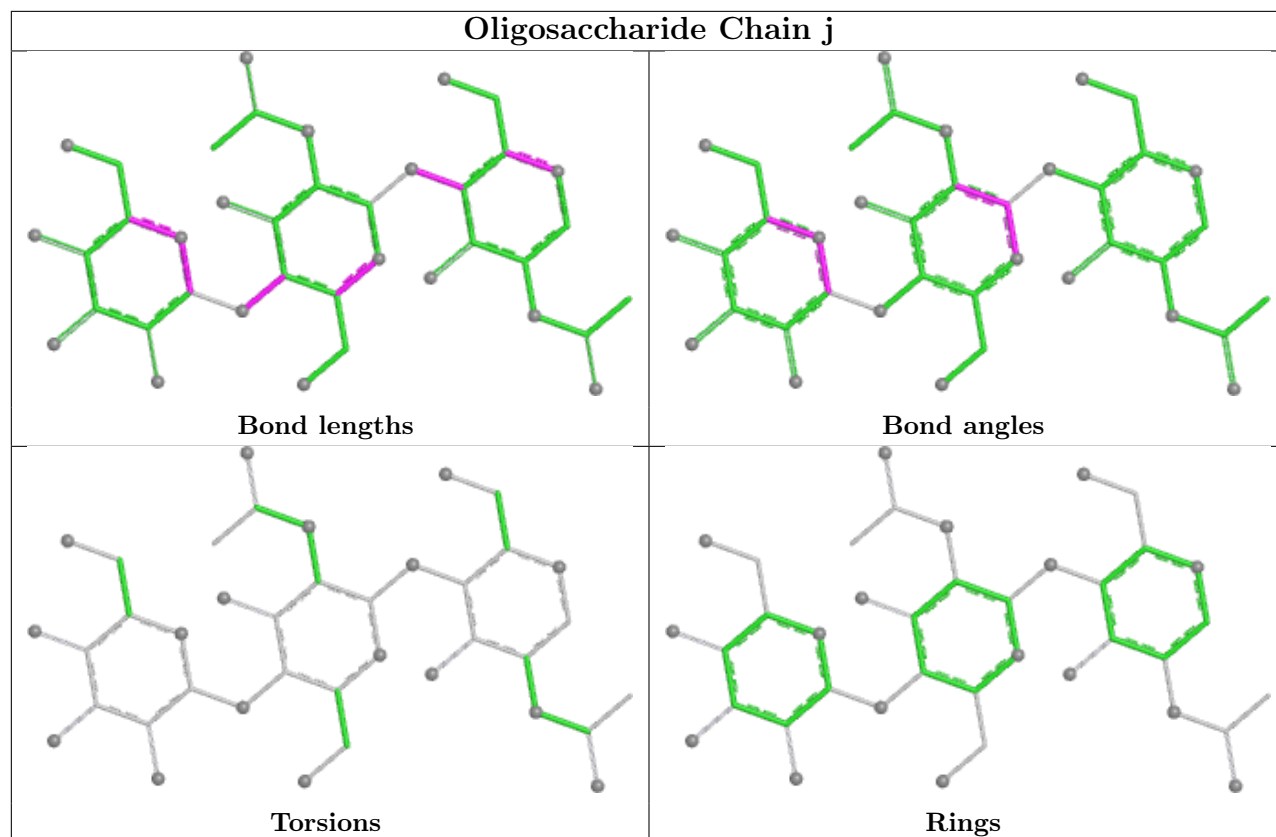


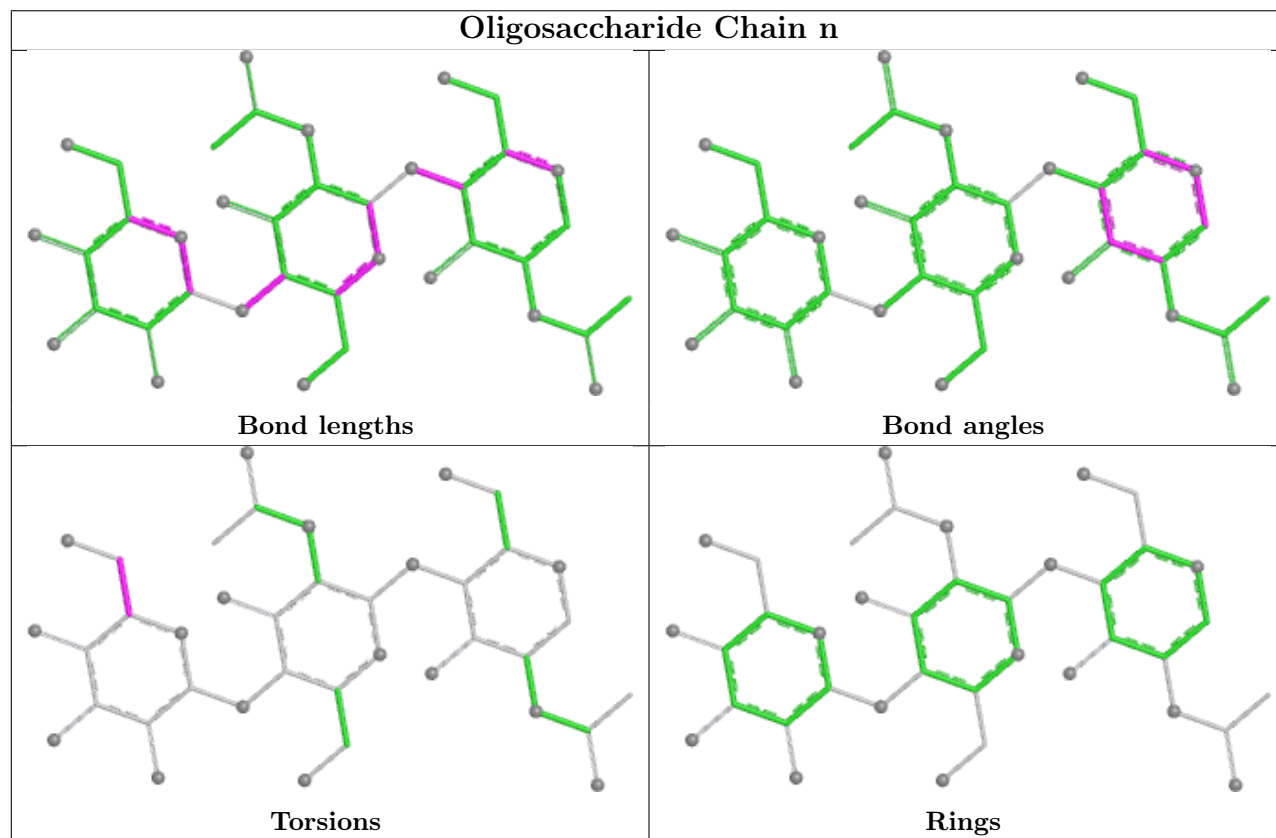
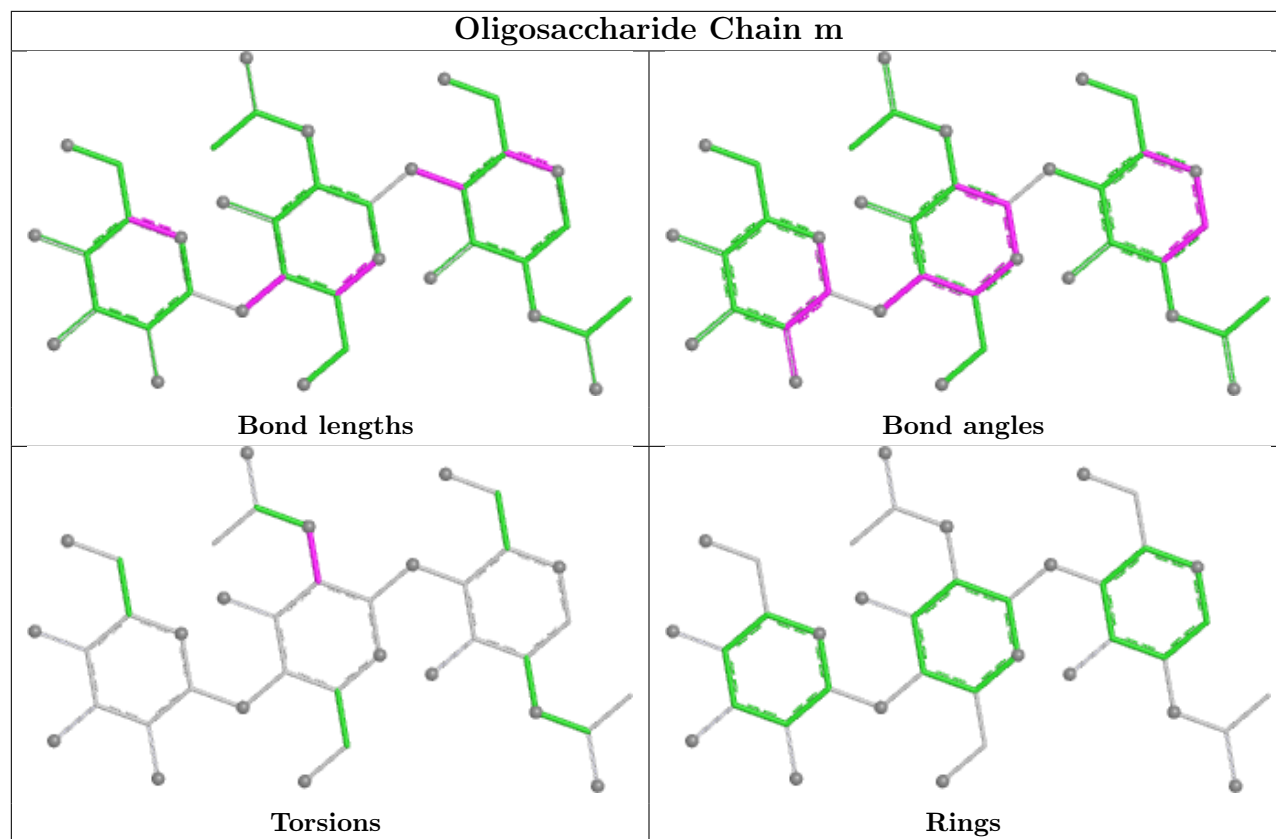


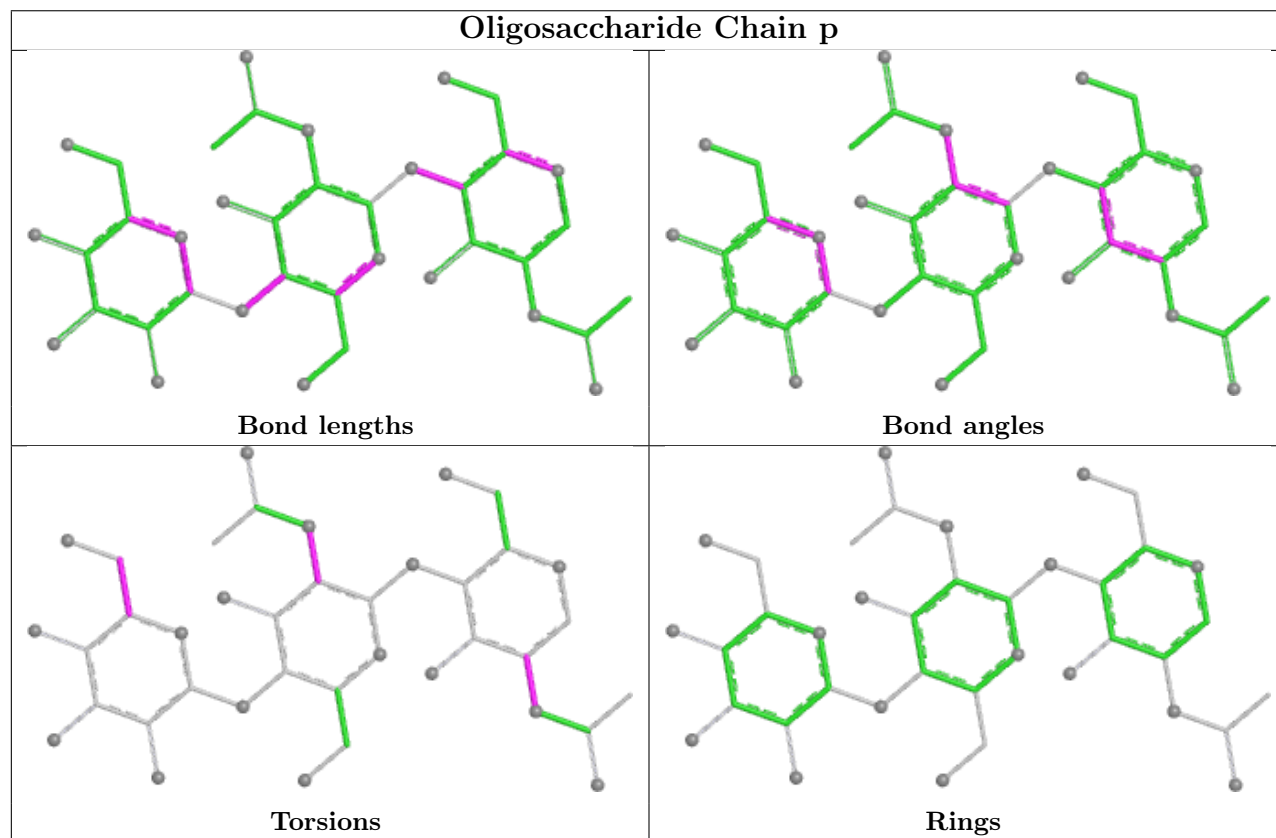
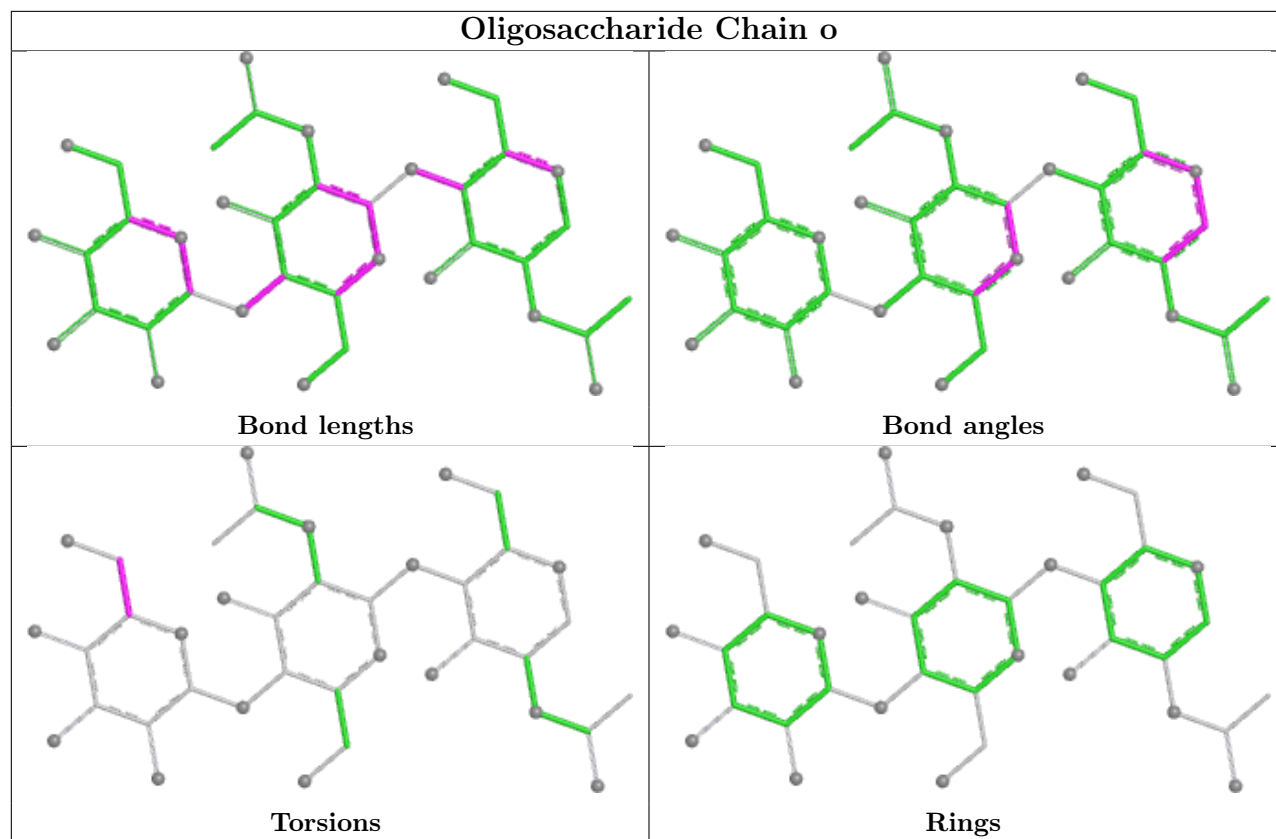


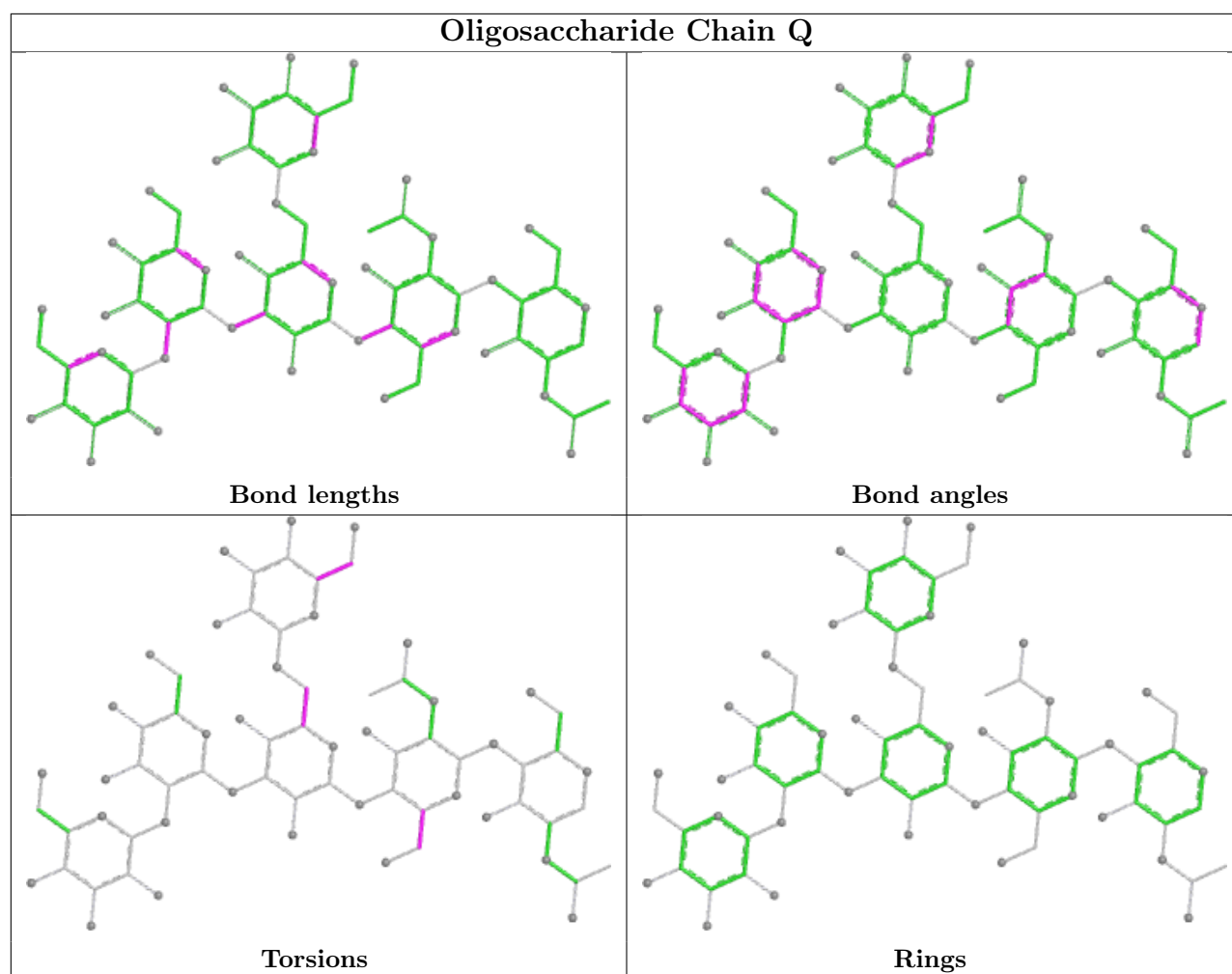


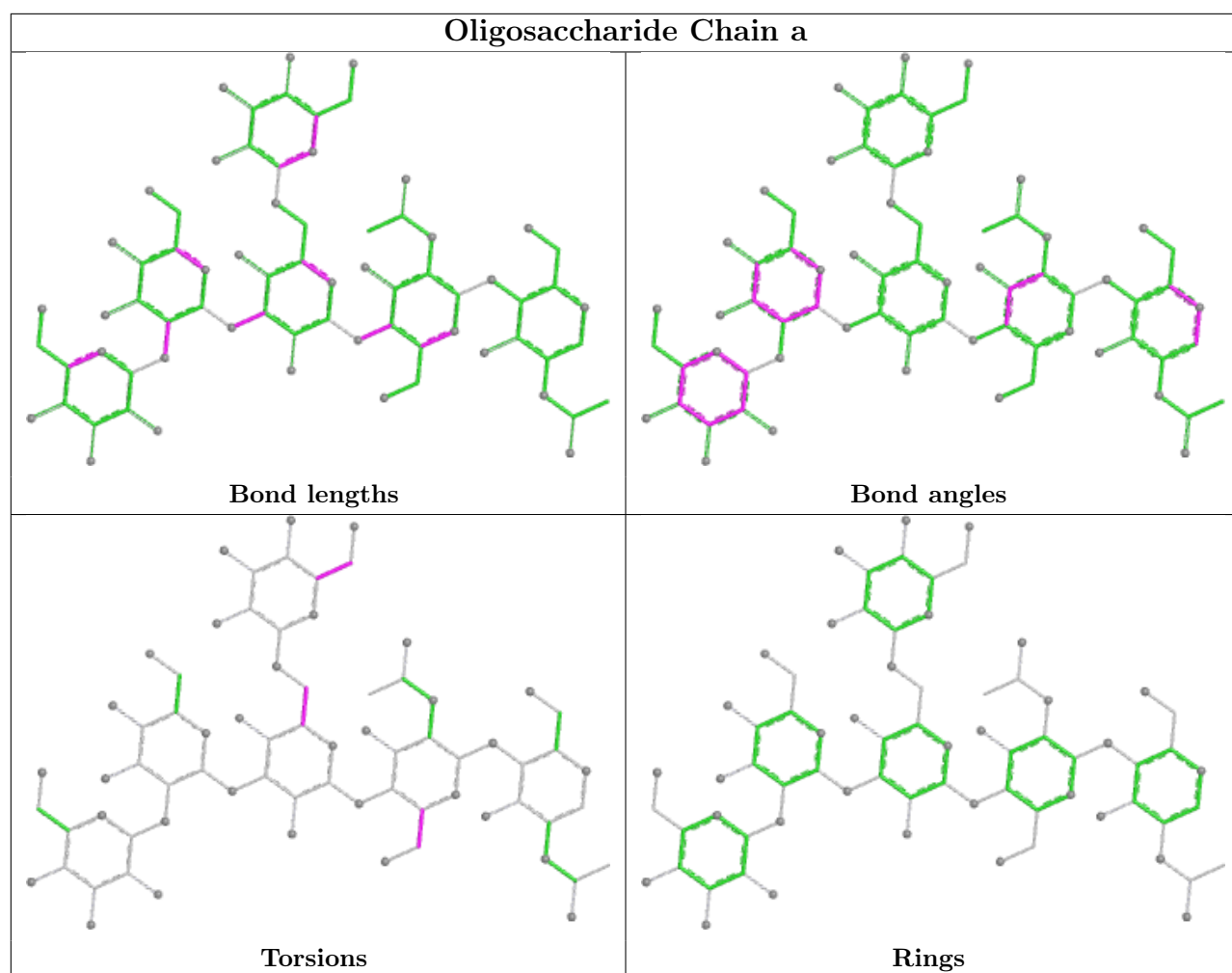


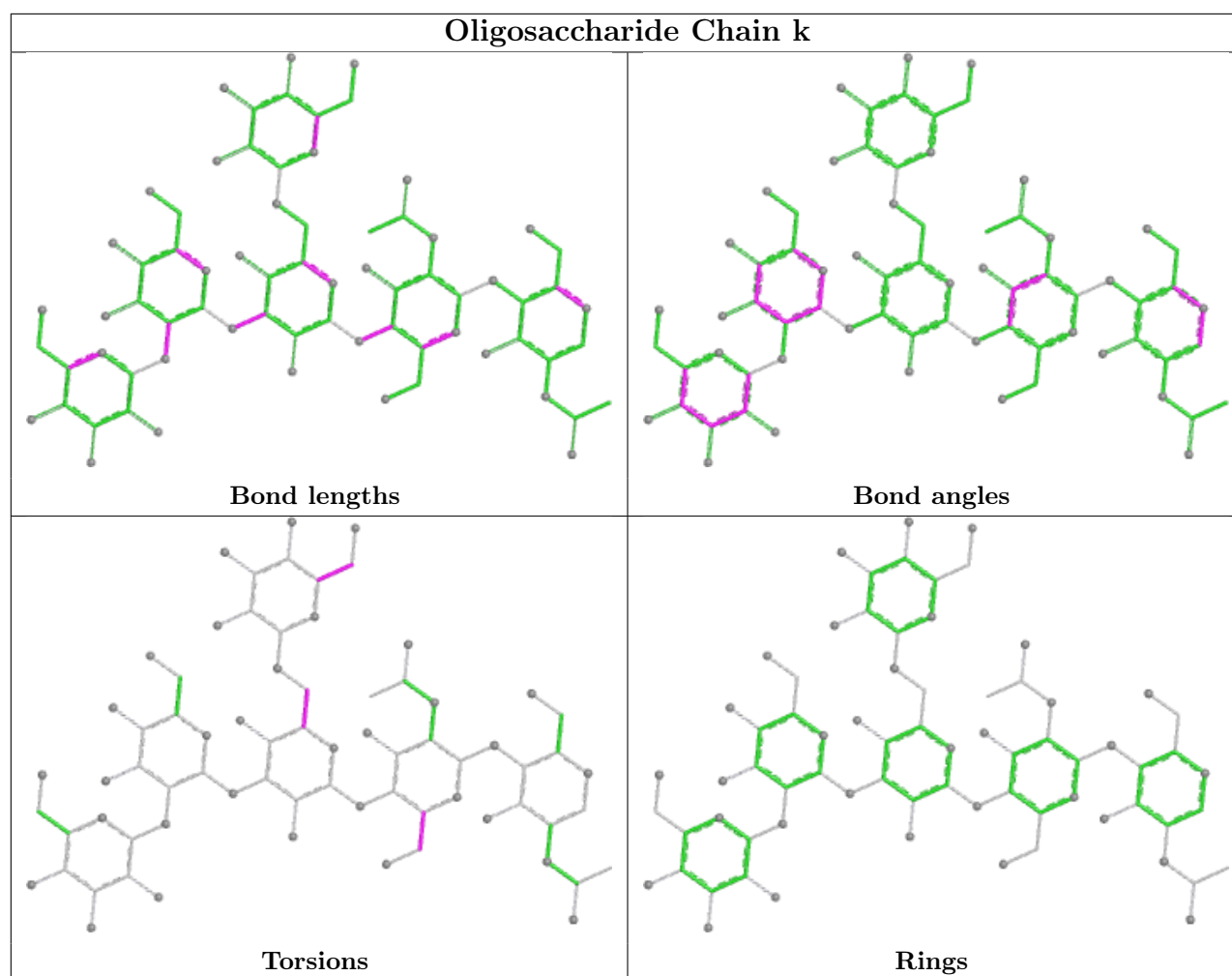












5.6 Ligand geometry [i](#)

9 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
7	NAG	A	603	1	14,14,15	1.18	1 (7%)	17,19,21	0.70	0
7	NAG	C	603	1	14,14,15	1.18	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	A	602	1	14,14,15	1.23	2 (14%)	17,19,21	0.79	0
7	NAG	G	601	1	14,14,15	1.34	2 (14%)	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	602	1	14,14,15	1.25	2 (14%)	17,19,21	0.85	0
7	NAG	A	601	1	14,14,15	1.29	2 (14%)	17,19,21	0.89	1 (5%)
7	NAG	G	603	1	14,14,15	1.22	1 (7%)	17,19,21	0.76	0
7	NAG	G	602	1	14,14,15	1.27	2 (14%)	17,19,21	0.92	0
7	NAG	C	601	1	14,14,15	1.23	2 (14%)	17,19,21	0.84	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	A	603	1	-	0/6/23/26	0/1/1/1
7	NAG	C	603	1	-	2/6/23/26	0/1/1/1
7	NAG	A	602	1	-	0/6/23/26	0/1/1/1
7	NAG	G	601	1	-	0/6/23/26	0/1/1/1
7	NAG	C	602	1	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	NAG	G	603	1	-	1/6/23/26	0/1/1/1
7	NAG	G	602	1	-	1/6/23/26	0/1/1/1
7	NAG	C	601	1	-	1/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	602	NAG	O5-C5	2.79	1.48	1.43
7	C	602	NAG	O5-C5	2.78	1.48	1.43
7	A	602	NAG	O5-C5	2.69	1.48	1.43
7	G	601	NAG	C1-C2	2.68	1.56	1.52
7	G	601	NAG	O5-C5	2.67	1.48	1.43
7	C	603	NAG	O5-C5	2.63	1.48	1.43
7	A	601	NAG	O5-C5	2.62	1.48	1.43
7	G	603	NAG	O5-C5	2.61	1.48	1.43
7	C	601	NAG	O5-C5	2.52	1.48	1.43
7	A	603	NAG	O5-C5	2.52	1.48	1.43
7	A	601	NAG	C1-C2	2.50	1.55	1.52
7	G	602	NAG	C1-C2	2.33	1.55	1.52
7	A	602	NAG	C1-C2	2.31	1.55	1.52
7	C	602	NAG	C1-C2	2.27	1.55	1.52
7	C	601	NAG	C1-C2	2.26	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	601	NAG	C1-O5-C5	3.00	116.20	112.19
7	C	603	NAG	C1-O5-C5	2.93	116.12	112.19
7	A	601	NAG	C1-O5-C5	2.90	116.07	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	603	NAG	C4-C5-C6-O6
7	C	603	NAG	O5-C5-C6-O6
7	G	603	NAG	C1-C2-N2-C7
7	G	602	NAG	C4-C5-C6-O6
7	C	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

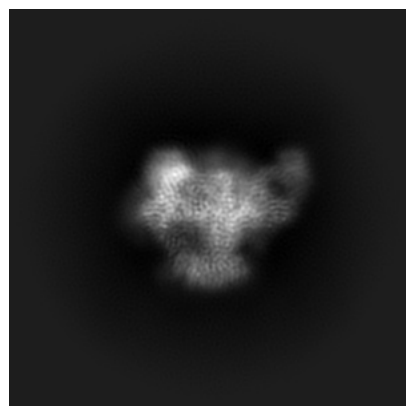
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23411. These allow visual inspection of the internal detail of the map and identification of artifacts.

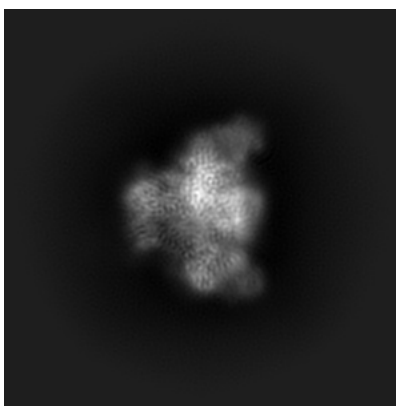
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

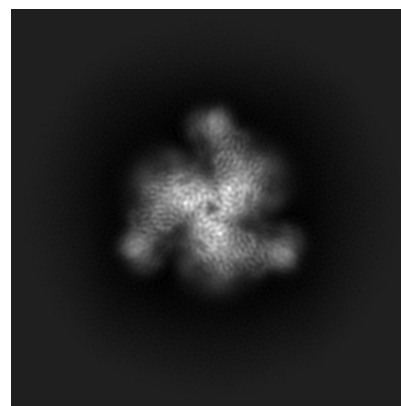
6.1.1 Primary map



X

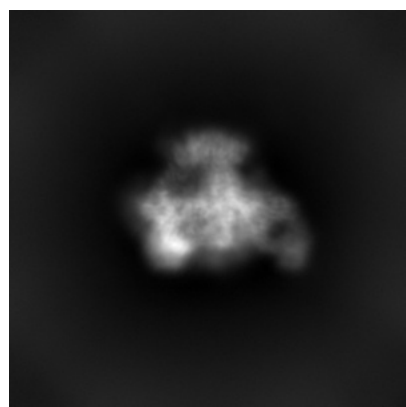


Y

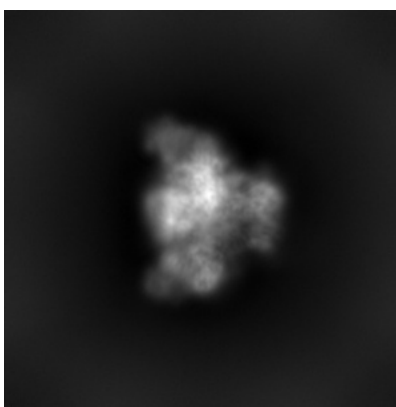


Z

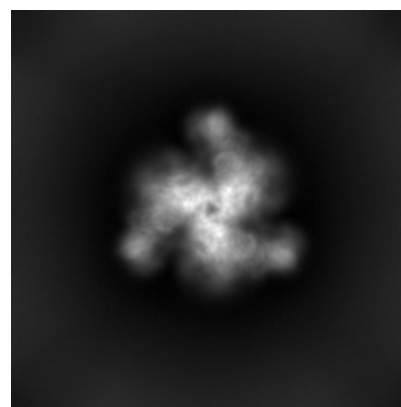
6.1.2 Raw map



X



Y

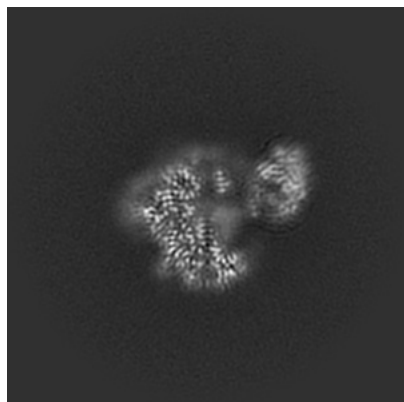


Z

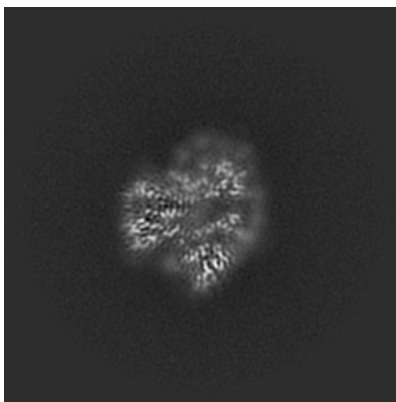
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

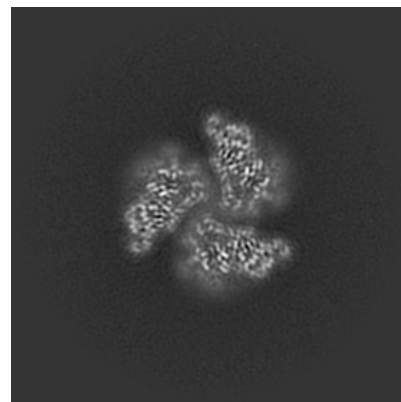
6.2.1 Primary map



X Index: 160

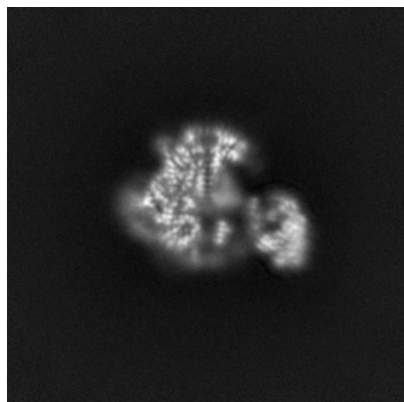


Y Index: 160

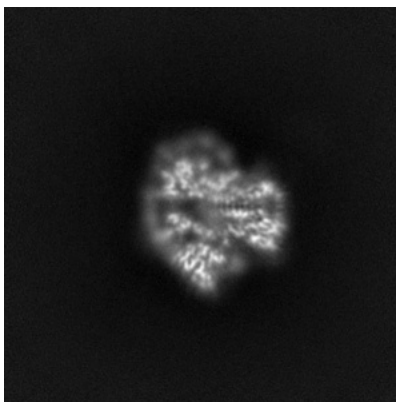


Z Index: 160

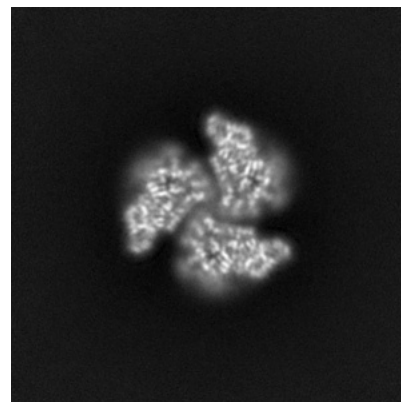
6.2.2 Raw map



X Index: 160



Y Index: 160

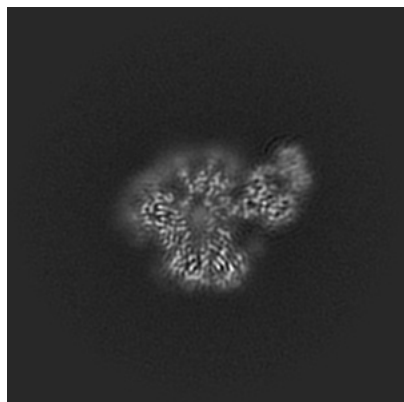


Z Index: 160

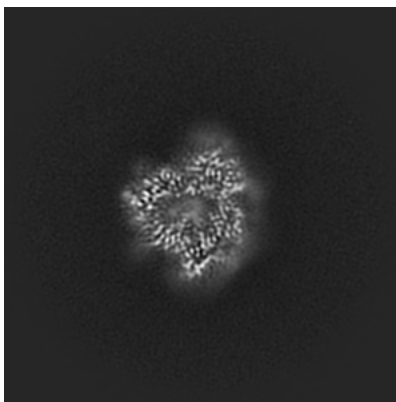
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

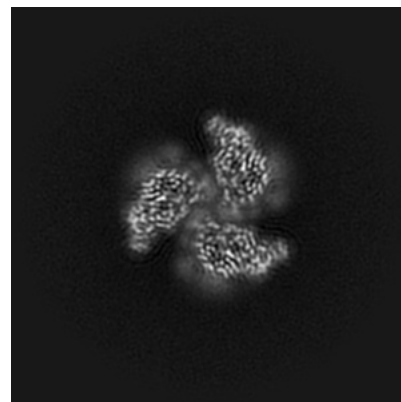
6.3.1 Primary map



X Index: 169

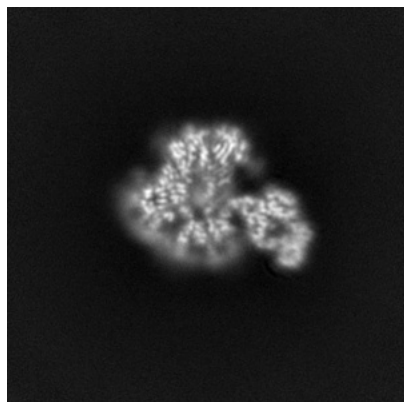


Y Index: 173

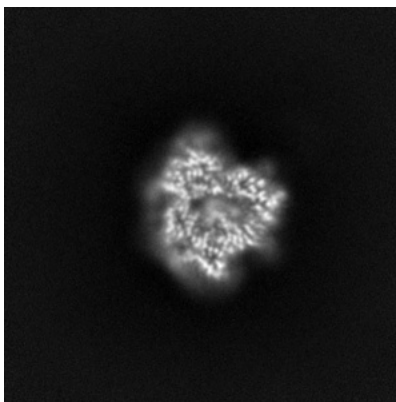


Z Index: 156

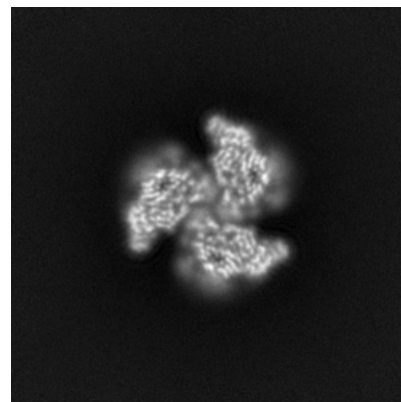
6.3.2 Raw map



X Index: 168



Y Index: 173

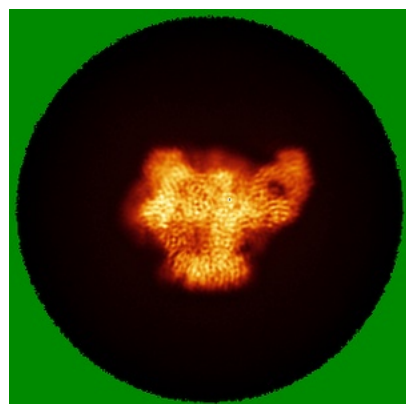


Z Index: 163

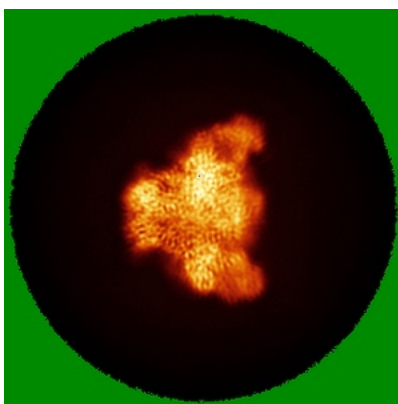
The images above show the largest variance slices of the map in three orthogonal directions.

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

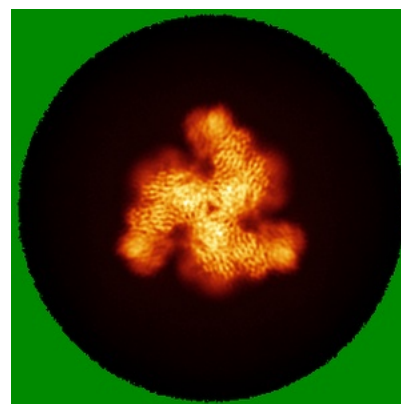
6.4.1 Primary map



X

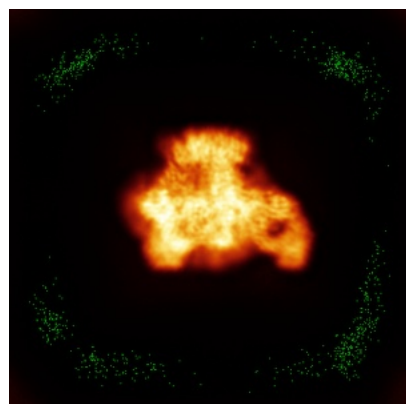


Y

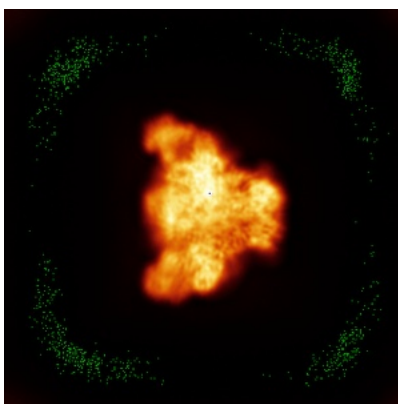


Z

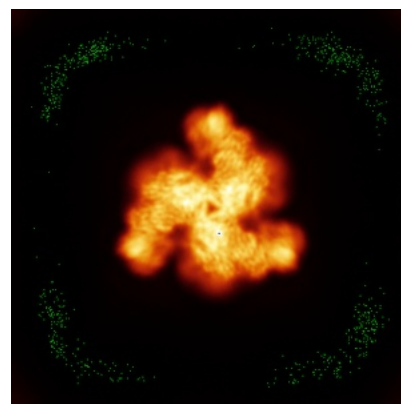
6.4.2 Raw map



X



Y

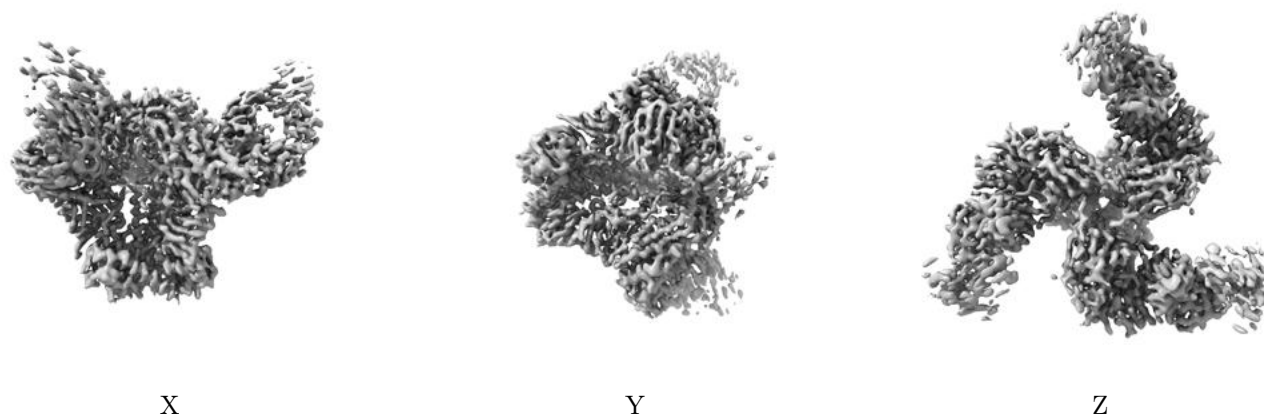


Z

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.

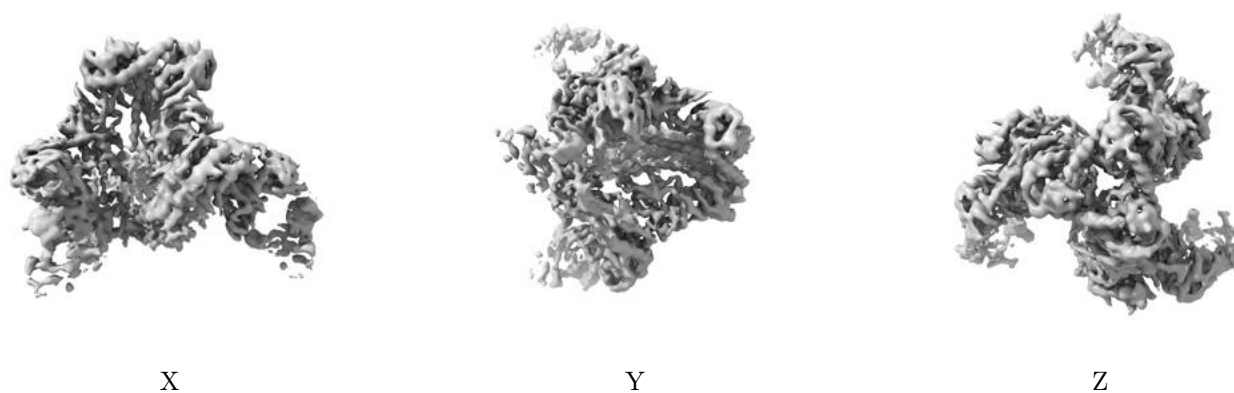
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.35. 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.

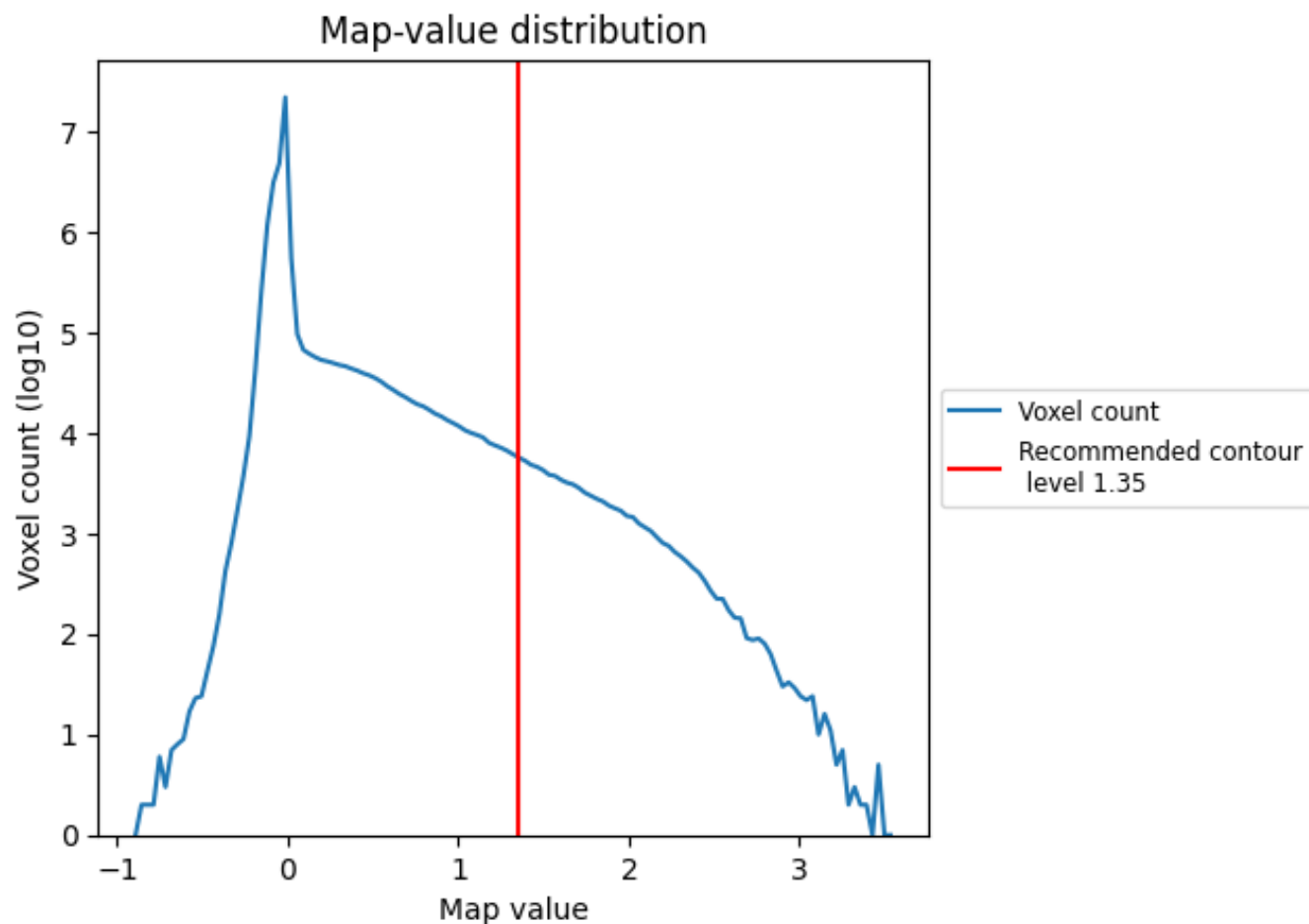
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

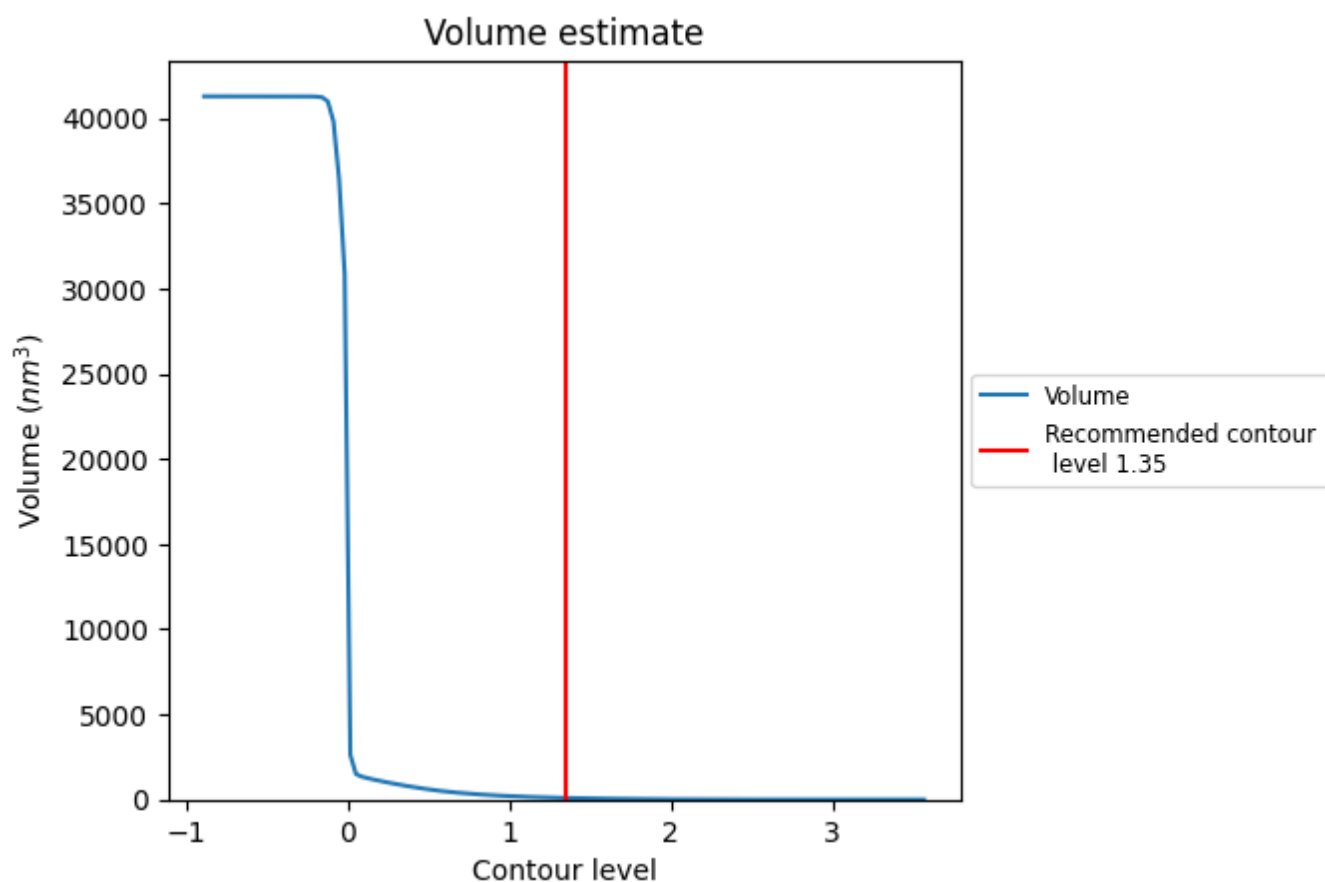
This section contains the results of statistical analysis of the map.

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.

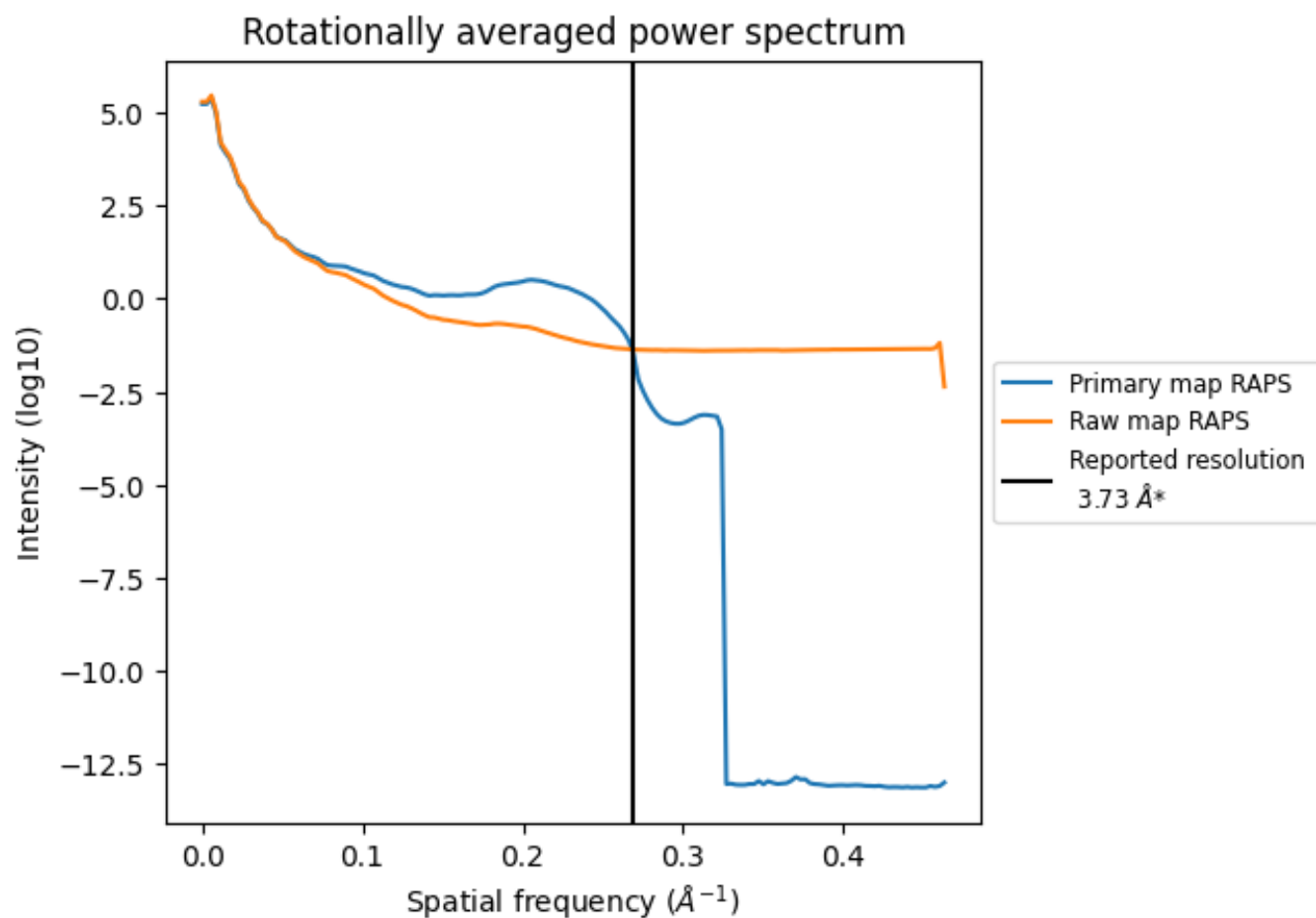
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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 ⓘ

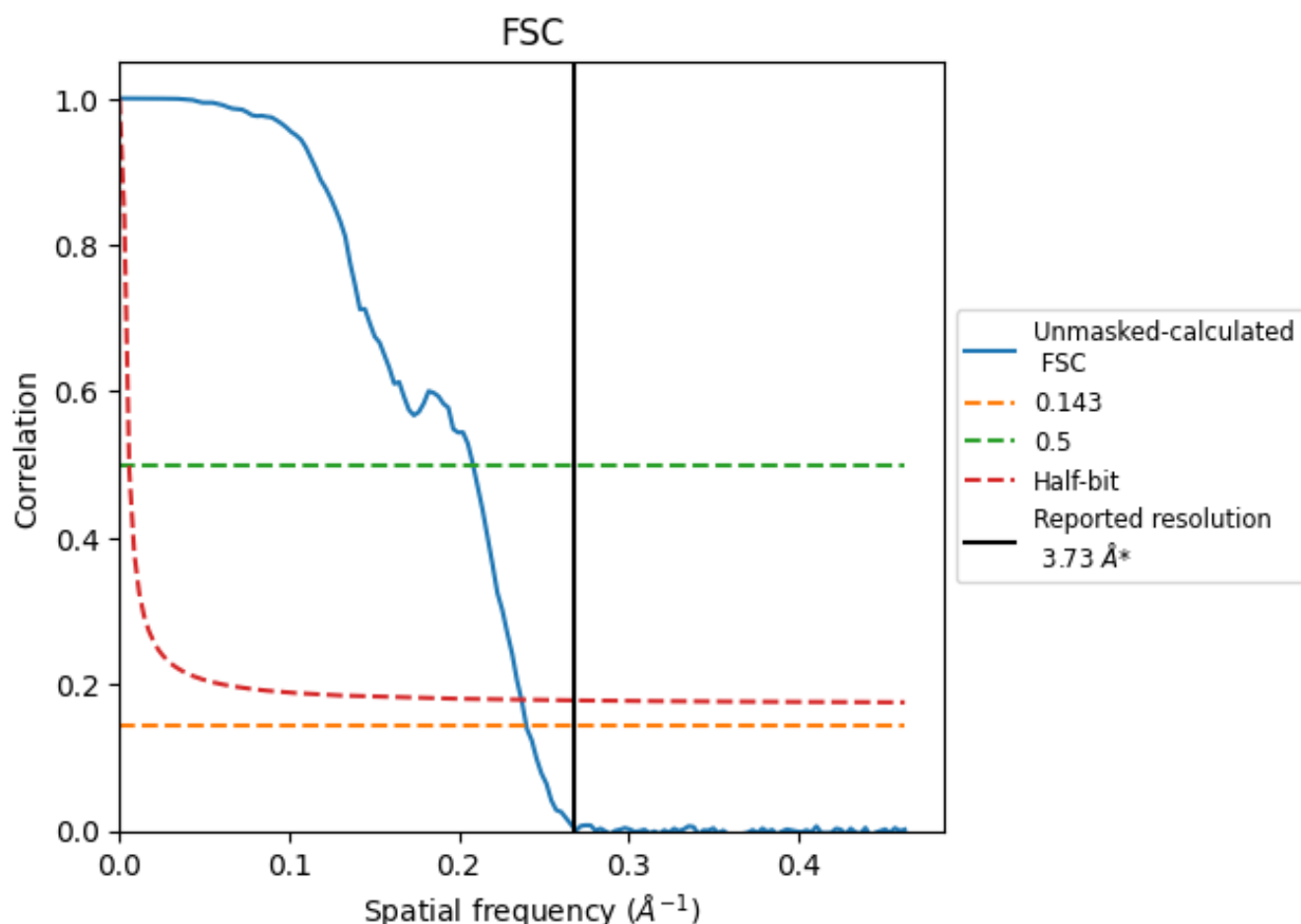


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 \AA^{-1}

8.2 Resolution estimates [i](#)

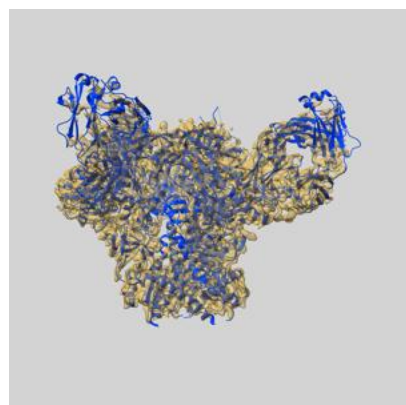
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	4.80	4.22

*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 4.17 differs from the reported value 3.73 by more than 10 %

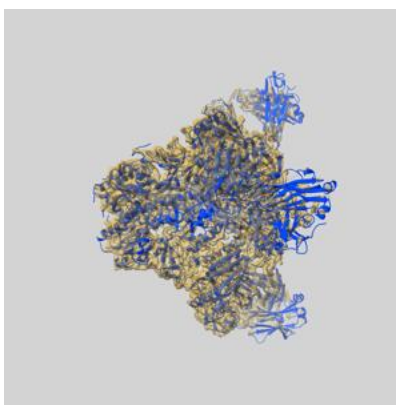
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23411 and PDB model 7LL1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

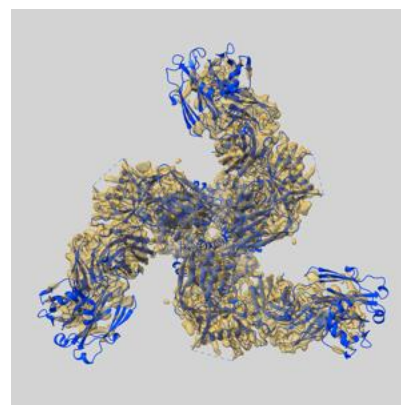
9.1 Map-model overlay [i](#)



X



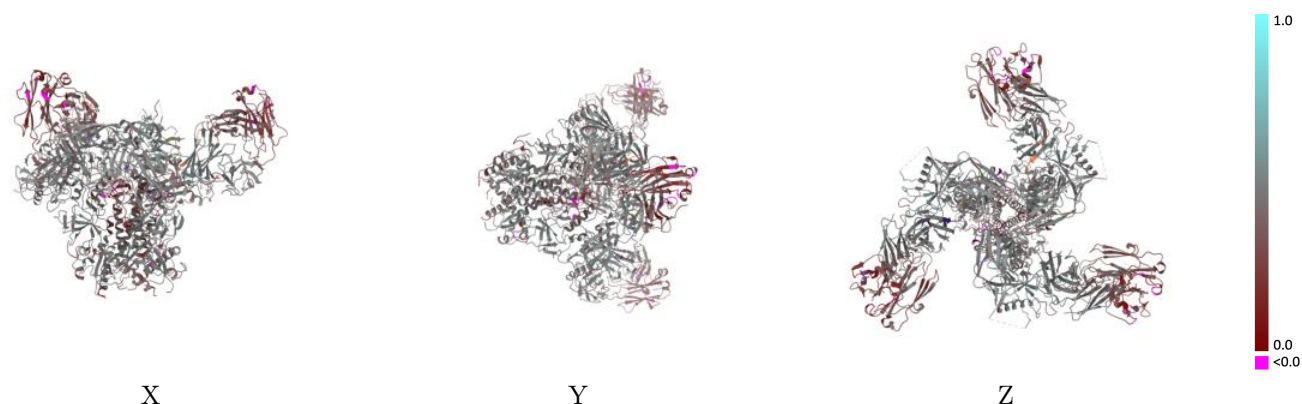
Y



Z

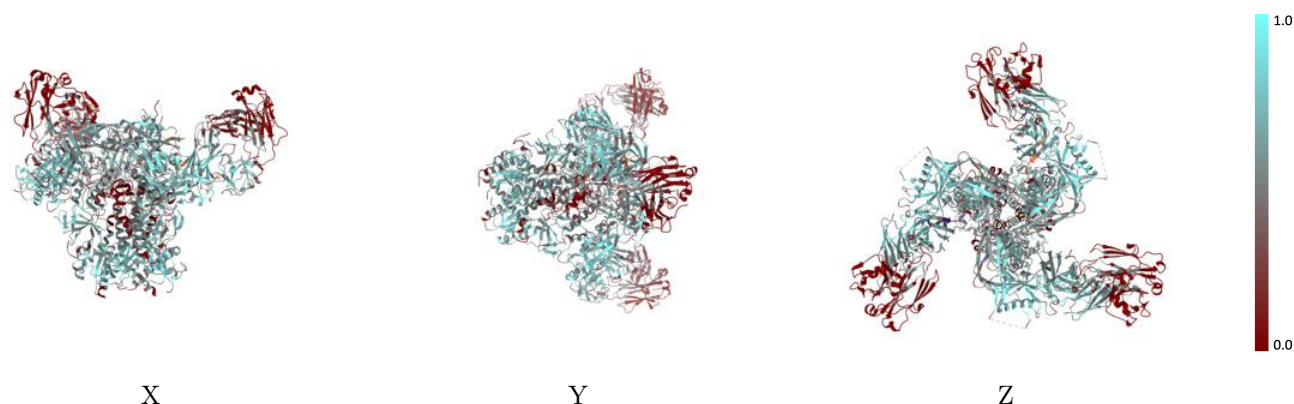
The images above show the 3D surface view of the map at the recommended contour level 1.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



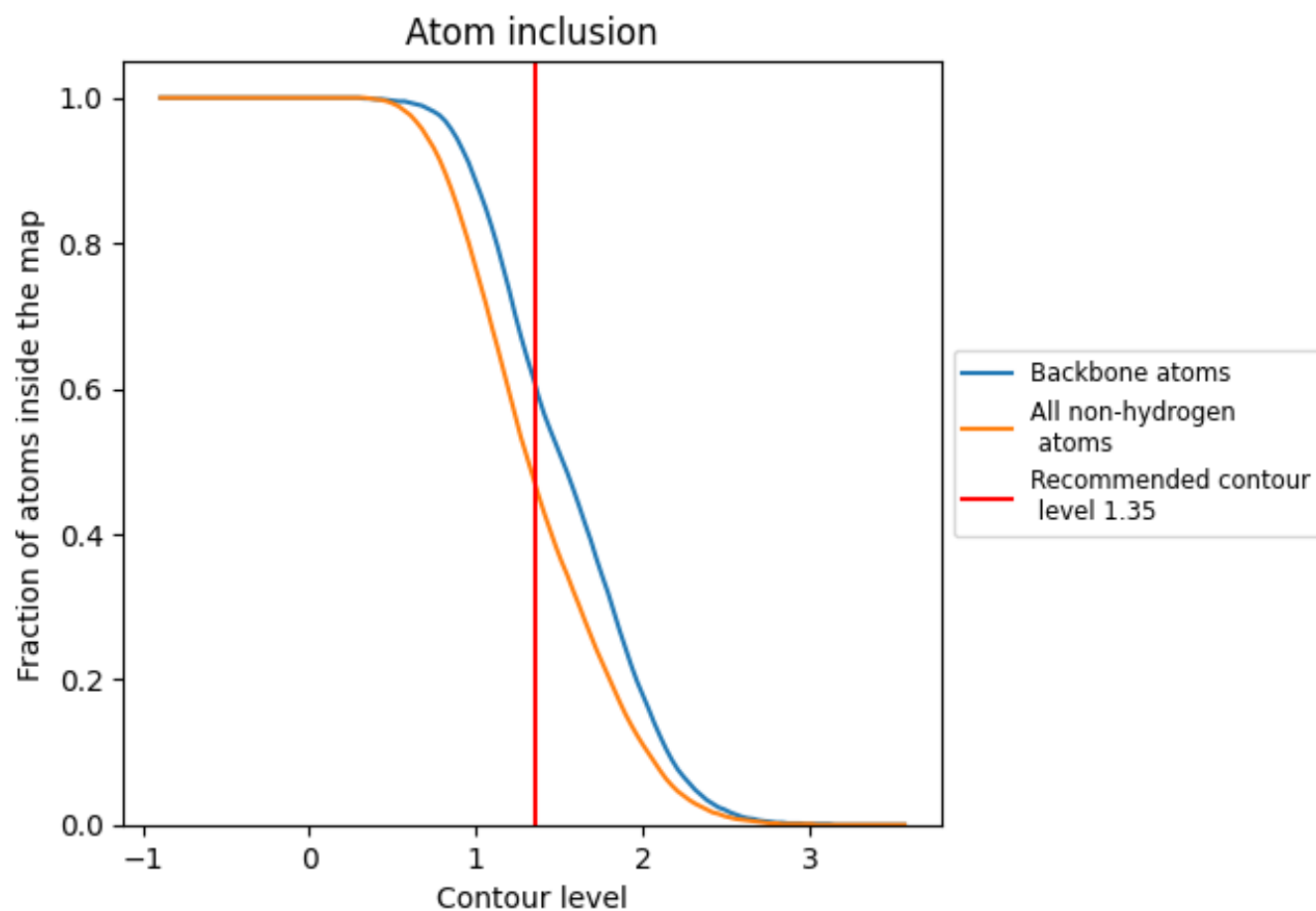
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.35).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 47% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4710	 0.4140
A	 0.5770	 0.4600
B	 0.4890	 0.3840
C	 0.5730	 0.4580
D	 0.4810	 0.3860
E	 0.4110	 0.4080
F	 0.3500	 0.3460
G	 0.5760	 0.4610
H	 0.4170	 0.4040
I	 0.4850	 0.3840
J	 0.4150	 0.4060
K	 0.3500	 0.3490
L	 0.3490	 0.3480
M	 0.2310	 0.4360
N	 0.1540	 0.4380
O	 0.1540	 0.4300
P	 0.3590	 0.3610
Q	 0.5560	 0.4540
R	 0.2310	 0.4440
S	 0.2820	 0.3950
T	 0.3080	 0.3600
U	 0.0510	 0.4160
V	 0.0260	 0.2820
W	 0.2310	 0.4570
X	 0.1280	 0.4390
Y	 0.1280	 0.4320
Z	 0.3080	 0.3310
a	 0.6390	 0.4460
b	 0.2050	 0.4470
c	 0.3330	 0.4470
d	 0.2820	 0.3880
e	 0.0510	 0.4290
f	 0.0260	 0.2840
g	 0.2310	 0.4550
h	 0.1280	 0.4200



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.1540	 0.4150
j	 0.3590	 0.3300
k	 0.6390	 0.4540
l	 0.2310	 0.3850
m	 0.2820	 0.4760
n	 0.2560	 0.3930
o	 0.0510	 0.4270
p	 0.0510	 0.3400