



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:47 PM EST

PDB ID : 7LLK
EMDB ID : EMD-23424
Title : Cryo-EM structure of Q23.17_DS-SOSIP in complex with Glycan276-Dependent Broadly Neutralizing Antibody 179NC75 Fab
Authors : Manne, K.; Acharya, P.
Deposited on : 2021-02-04
Resolution : 4.80 Å(reported)
Based on initial model : 6VKN

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

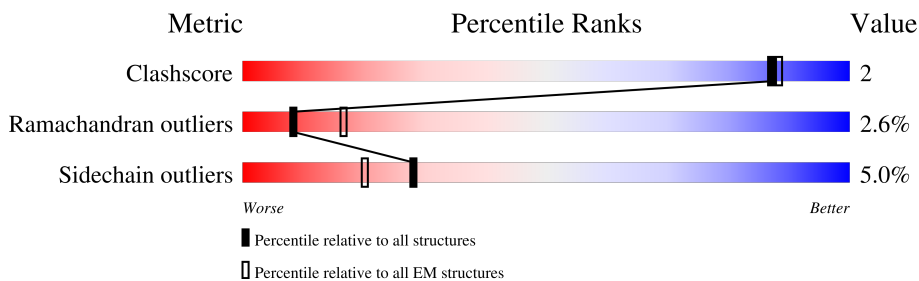
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	474	
1	E	474	
1	I	474	
2	B	153	
2	F	153	
2	J	153	
3	C	238	
3	G	238	

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Mol	Chain	Length	Quality of chain
3	K	238	
4	D	215	
4	H	215	
4	L	215	
5	M	2	
5	V	2	
5	f	2	
5	q	2	
6	N	3	
6	O	3	
6	P	3	
6	Q	3	
6	R	3	
6	T	3	
6	U	3	
6	W	3	
6	Y	3	
6	Z	3	
6	a	3	
6	b	3	
6	d	3	
6	e	3	
6	g	3	
6	j	3	
6	k	3	

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Mol	Chain	Length	Quality of chain
6	l	3	100%
6	m	3	100%
6	o	3	100%
6	p	3	100%
6	r	3	67%
7	S	4	75%
7	X	4	100%
7	c	4	75%
7	h	4	100%
7	n	4	75%
7	s	4	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 40248 atoms, of which 19893 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	
			Total	C	H	N	O			S
1	E	440	6894	2187	3417	615	647	28	0	0
1	A	440	6894	2187	3417	615	647	28	0	0
1	I	440	6894	2187	3417	615	647	28	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	31	ALA	-	expression tag	UNP O55774
E	201	CYS	ILE	conflict	UNP O55774
E	219	ALA	THR	conflict	UNP O55774
E	334	SER	THR	conflict	UNP O55774
E	433	CYS	ALA	conflict	UNP O55774
E	490	LYS	GLU	conflict	UNP O55774
E	501	CYS	ALA	conflict	UNP O55774
E	509	ARG	-	expression tag	UNP O55774
E	510	ARG	-	expression tag	UNP O55774
E	511	ARG	-	expression tag	UNP O55774
E	512	ARG	-	expression tag	UNP O55774
E	513	ARG	-	expression tag	UNP O55774
A	31	ALA	-	expression tag	UNP O55774
A	201	CYS	ILE	conflict	UNP O55774
A	219	ALA	THR	conflict	UNP O55774
A	334	SER	THR	conflict	UNP O55774
A	433	CYS	ALA	conflict	UNP O55774
A	490	LYS	GLU	conflict	UNP O55774
A	501	CYS	ALA	conflict	UNP O55774
A	509	ARG	-	expression tag	UNP O55774
A	510	ARG	-	expression tag	UNP O55774
A	511	ARG	-	expression tag	UNP O55774
A	512	ARG	-	expression tag	UNP O55774
A	513	ARG	-	expression tag	UNP O55774

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Chain	Residue	Modelled	Actual	Comment	Reference
I	31	ALA	-	expression tag	UNP O55774
I	201	CYS	ILE	conflict	UNP O55774
I	219	ALA	THR	conflict	UNP O55774
I	334	SER	THR	conflict	UNP O55774
I	433	CYS	ALA	conflict	UNP O55774
I	490	LYS	GLU	conflict	UNP O55774
I	501	CYS	ALA	conflict	UNP O55774
I	509	ARG	-	expression tag	UNP O55774
I	510	ARG	-	expression tag	UNP O55774
I	511	ARG	-	expression tag	UNP O55774
I	512	ARG	-	expression tag	UNP O55774
I	513	ARG	-	expression tag	UNP O55774

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	F	126	Total	C	H	N	O	S	0	0
			2005	642	998	170	190	5		
2	B	126	Total	C	H	N	O	S	0	0
			2005	642	998	170	190	5		
2	J	126	Total	C	H	N	O	S	0	0
			2005	642	998	170	190	5		

- Molecule 3 is a protein called 179NC75 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	G	131	Total	C	H	N	O	S	0	0
			2100	668	1051	189	187	5		
3	C	131	Total	C	H	N	O	S	0	0
			2100	668	1051	189	187	5		
3	K	131	Total	C	H	N	O	S	0	0
			2100	668	1051	189	187	5		

- Molecule 4 is a protein called 179NC75 Fab Light chain.

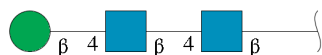
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	H	102	Total	C	H	N	O	S	0	0
			1525	484	743	136	159	3		
4	D	102	Total	C	H	N	O	S	0	0
			1525	484	743	136	159	3		
4	L	102	Total	C	H	N	O	S	0	0
			1525	484	743	136	159	3		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	2	28	16	2	10	0	0
5	V	2	55	16	27	2	10	0
5	f	2	55	16	27	2	10	0
5	q	2	55	16	27	2	10	0

- Molecule 6 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
			Total	C	N	O		
6	N	3	39	22	2	15	0	0
6	O	3	76	22	37	2	15	0
6	P	3	76	22	37	2	15	0
6	Q	3	76	22	37	2	15	0
6	R	3	76	22	37	2	15	0
6	T	3	76	22	37	2	15	0
6	U	3	76	22	37	2	15	0
6	W	3	76	22	37	2	15	0
6	Y	3	76	22	37	2	15	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	a	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	b	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	d	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	e	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	g	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	j	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	k	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	l	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	m	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	o	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	p	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
6	r	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



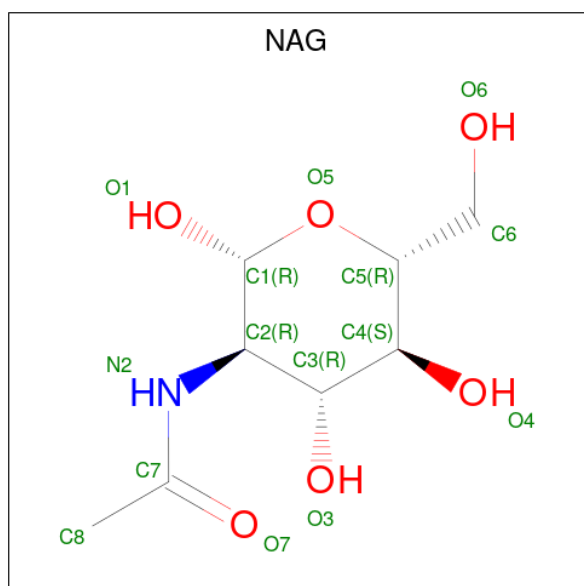
Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	X	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	c	4	Total	C	H	N	O	0	0
			97	28	47	2	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	n	4	Total	C	H	N	O	0	0
			97	28	47	2	20		
7	s	4	Total	C	H	N	O	0	0
			97	28	47	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
8	E	1	Total	C	H	N	O	0
			84	24	42	3	15	
8	E	1	Total	C	H	N	O	0
			84	24	42	3	15	
8	E	1	Total	C	H	N	O	0
			84	24	42	3	15	
8	A	1	Total	C	H	N	O	0
			98	32	42	4	20	
8	A	1	Total	C	H	N	O	0
			98	32	42	4	20	
8	A	1	Total	C	H	N	O	0
			98	32	42	4	20	
8	A	1	Total	C	H	N	O	0
			98	32	42	4	20	
8	I	1	Total	C	H	N	O	0
			84	24	42	3	15	

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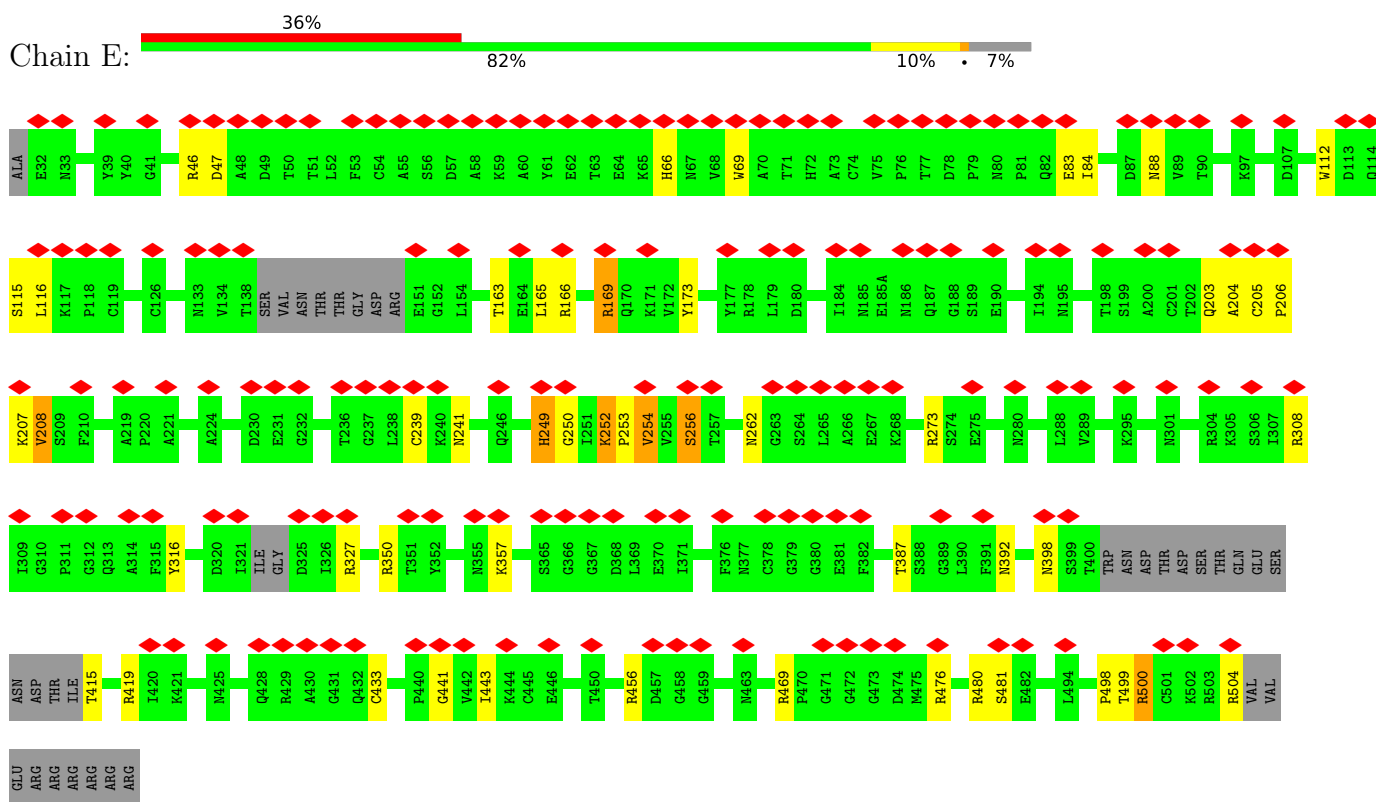
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
8	I	1	Total	C	H	N	O	0
			84	24	42	3	15	
8	I	1	Total	C	H	N	O	0
			84	24	42	3	15	

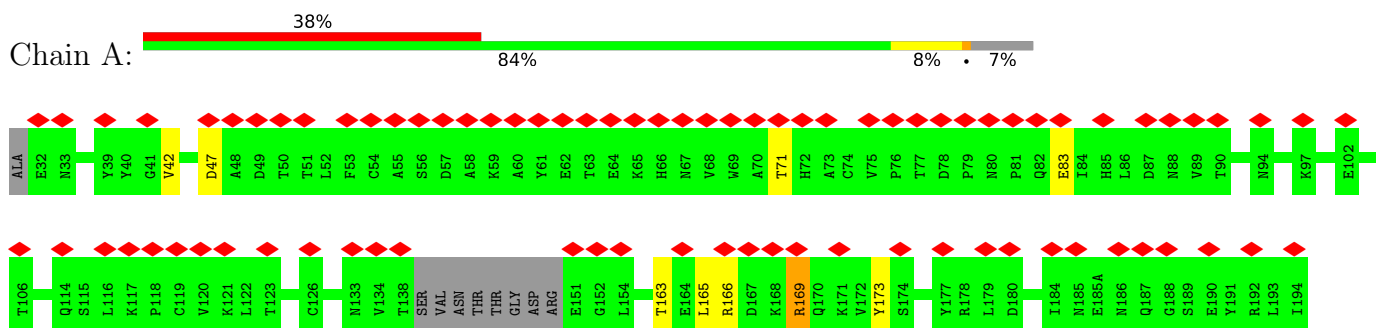
3 Residue-property plots

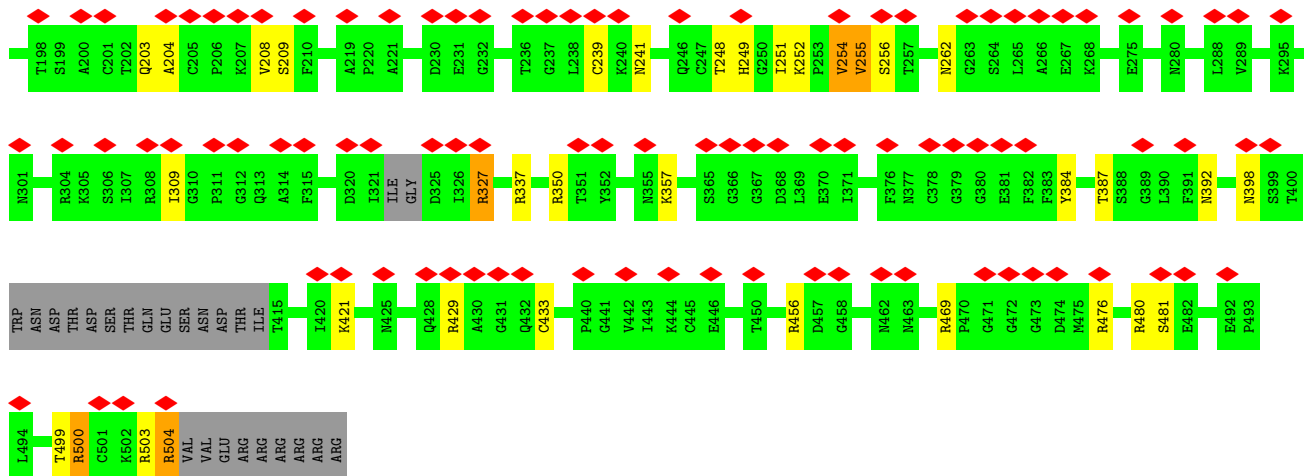
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Envelope glycoprotein gp120

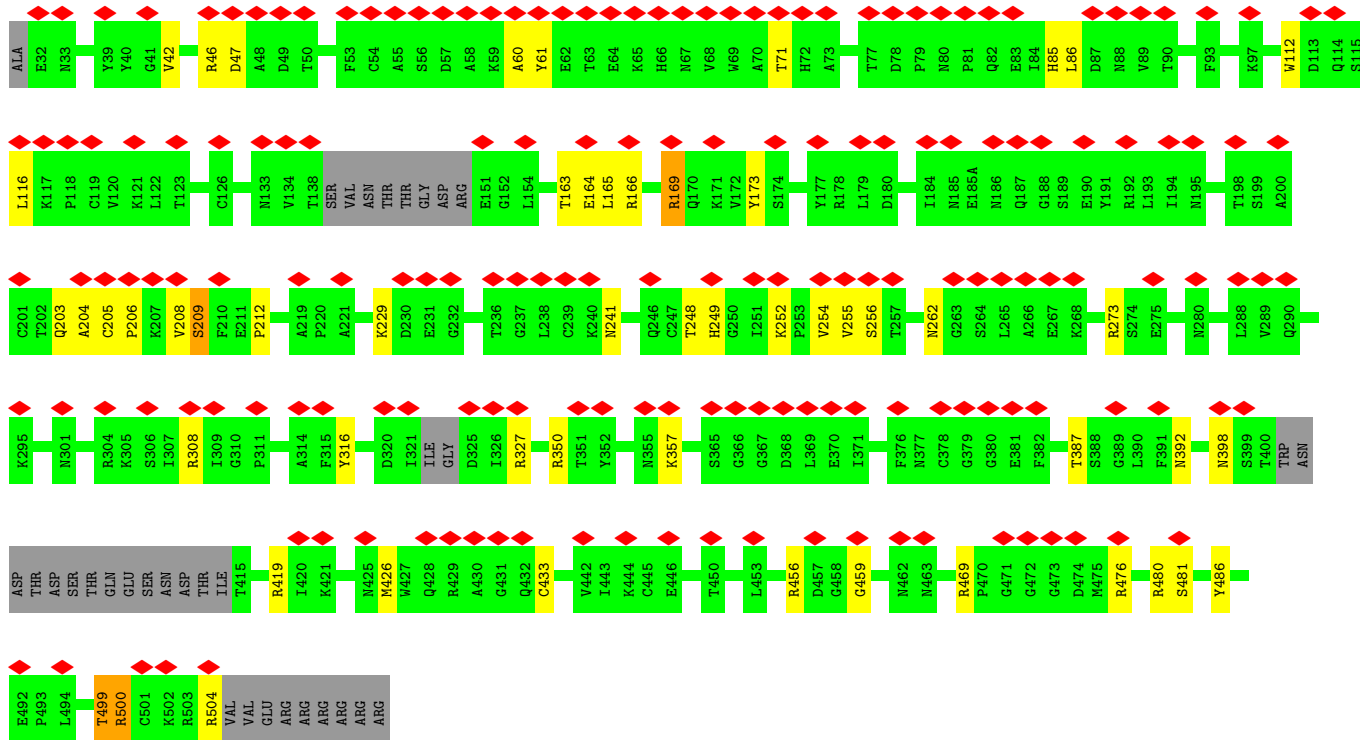
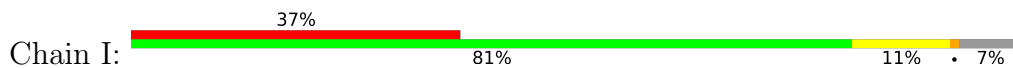


- Molecule 1: Envelope glycoprotein gp120

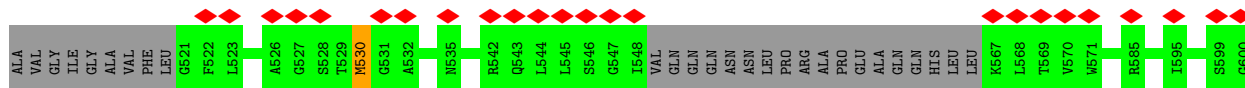
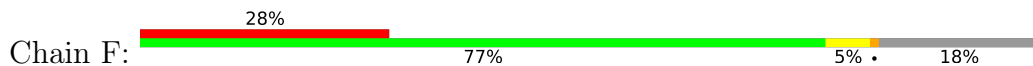


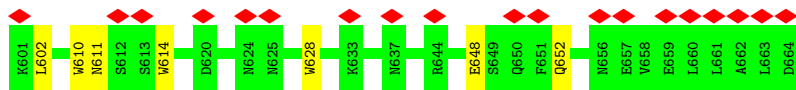


• Molecule 1: Envelope glycoprotein gp120

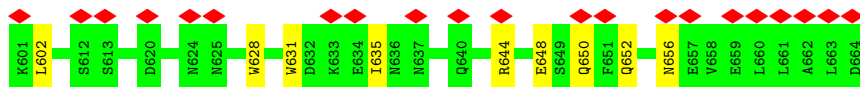
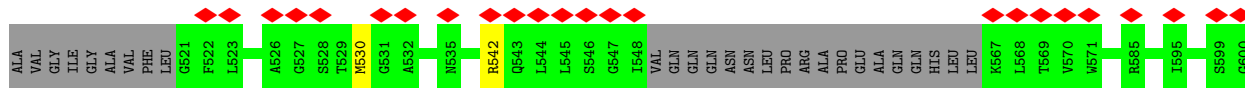
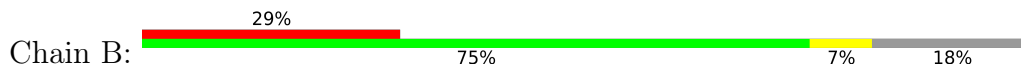


• Molecule 2: Envelope glycoprotein gp41

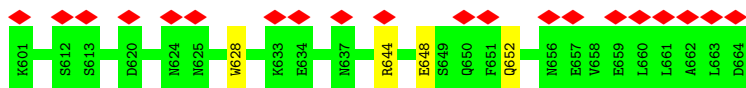
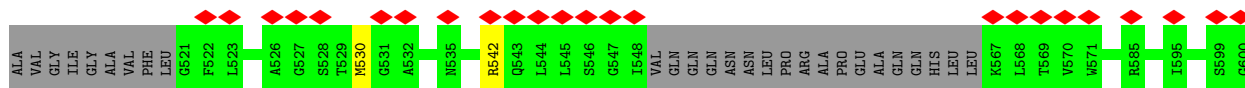
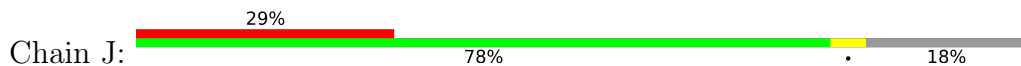




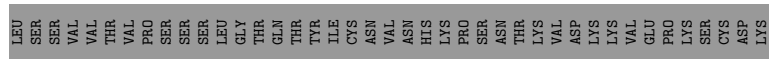
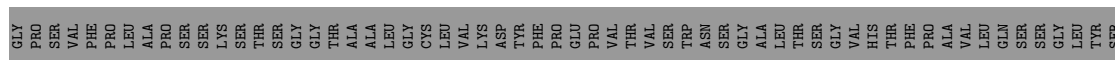
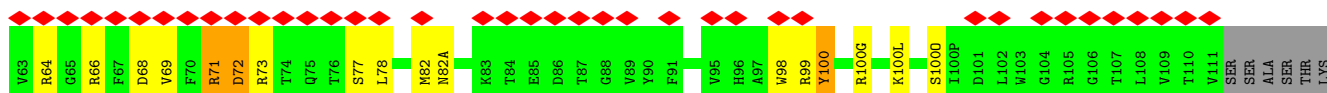
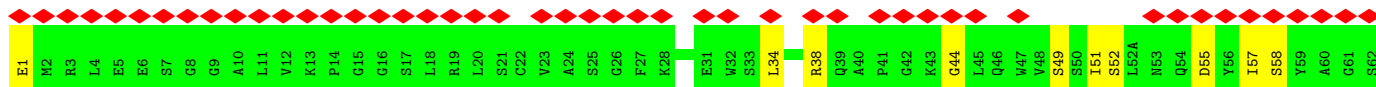
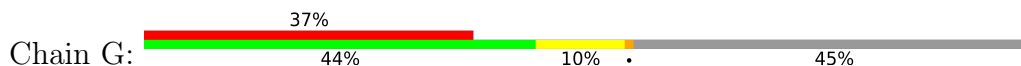
• Molecule 2: Envelope glycoprotein gp41



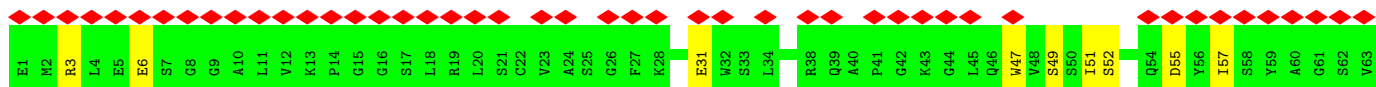
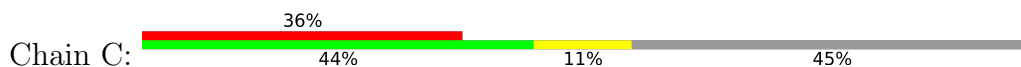
• Molecule 2: Envelope glycoprotein gp41

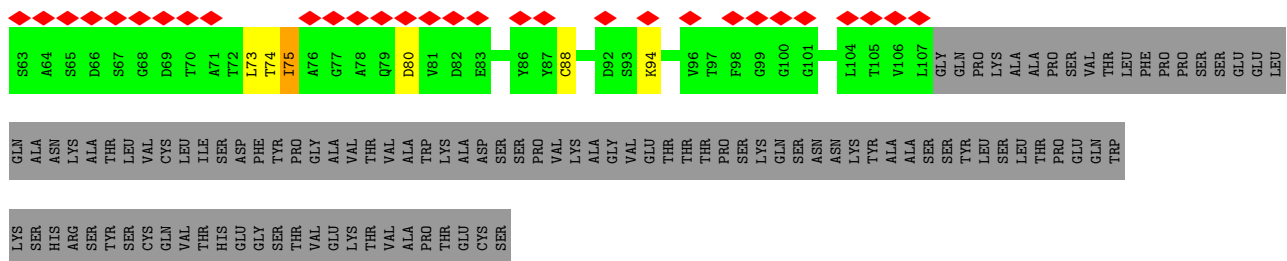


• Molecule 3: 179NC75 Fab Heavy chain

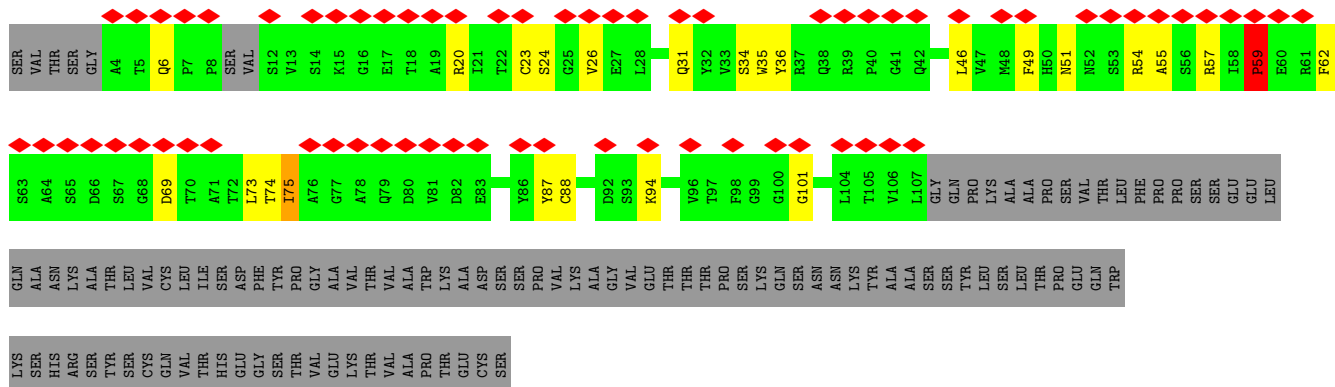
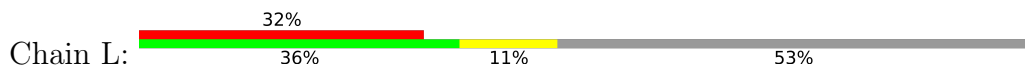


• Molecule 3: 179NC75 Fab Heavy chain





• Molecule 4: 179NC75 Fab Light chain



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



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



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



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

Chain q:  100%
100%



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

Chain N:  100%
67% 33%



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

Chain O:  100%
100%



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

Chain P:  100%
100%



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

Chain Q:  100%
100%



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

Chain R:  100%
100%



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



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Chain a:  100%
100%



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

Chain b:  100%
100%



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

Chain d:  100%
100%



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

Chain e:  100%
100%



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

Chain g:  100%
100%



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

Chain j:  100%
100%



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

Chain k:  100%
100%



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

Chain l:  100%
100%



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

Chain m:  100%
100%



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

Chain o:  100%
100%



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

Chain p:  100%
100%

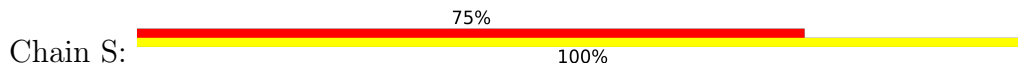


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  67%
100%



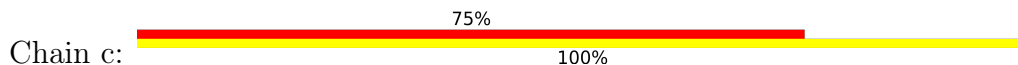
- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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



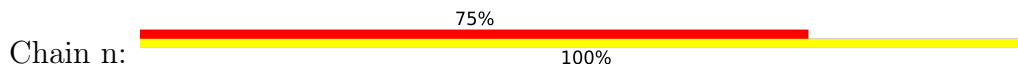
- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



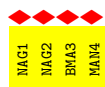
- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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 7: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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	2.335	Depositor
Minimum map value	-0.723	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	1.05	Depositor
Map size (Å)	320.2083, 320.2083, 320.2083	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.000651, 1.000651, 1.000651	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	0.67	0/3551	1.09	14/4819 (0.3%)
1	E	0.67	0/3551	1.09	13/4819 (0.3%)
1	I	0.67	0/3551	1.09	14/4819 (0.3%)
2	B	0.62	0/1025	1.05	2/1390 (0.1%)
2	F	0.62	0/1025	1.06	0/1390
2	J	0.61	0/1025	1.08	2/1390 (0.1%)
3	C	0.73	0/1073	1.26	9/1450 (0.6%)
3	G	0.74	0/1073	1.27	7/1450 (0.5%)
3	K	0.73	0/1073	1.24	5/1450 (0.3%)
4	D	0.68	0/798	1.11	2/1084 (0.2%)
4	H	0.70	0/798	1.13	3/1084 (0.3%)
4	L	0.72	0/798	1.14	5/1084 (0.5%)
All	All	0.68	0/19341	1.12	76/26229 (0.3%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	ARG	NE-CZ-NH2	8.64	124.62	120.30
3	G	71	ARG	NE-CZ-NH1	8.60	124.60	120.30
3	G	99	ARG	NE-CZ-NH1	8.03	124.31	120.30
3	C	71	ARG	NE-CZ-NH1	8.02	124.31	120.30
3	C	94	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	I	480	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	I	469	ARG	NE-CZ-NH2	7.43	124.02	120.30
3	G	64	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	476	ARG	NE-CZ-NH1	7.27	123.93	120.30
3	C	99	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	476	ARG	NE-CZ-NH1	7.15	123.87	120.30
3	G	38	ARG	NE-CZ-NH1	7.06	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	99	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	456	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	469	ARG	NE-CZ-NH2	6.83	123.71	120.30
4	D	54	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	469	ARG	NE-CZ-NH2	6.72	123.66	120.30
3	C	64	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	I	499	THR	CA-CB-CG2	6.68	121.75	112.40
1	I	46	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	I	476	ARG	NE-CZ-NH1	6.65	123.63	120.30
4	H	57	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	476	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	480	ARG	NE-CZ-NH1	6.56	123.58	120.30
4	H	54	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	327	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	350	ARG	NE-CZ-NH1	6.51	123.55	120.30
3	C	73	ARG	NE-CZ-NH1	6.49	123.54	120.30
3	K	73	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	I	456	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	I	350	ARG	NE-CZ-NH1	6.39	123.49	120.30
4	D	57	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	I	419	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	480	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	273	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	E	350	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	J	542	ARG	NE-CZ-NH1	6.26	123.43	120.30
3	K	100(F)	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	503	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	456	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	G	73	ARG	NE-CZ-NH1	5.97	123.29	120.30
3	K	71	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	I	169	ARG	NE-CZ-NH2	5.81	123.20	120.30
3	G	100(G)	ARG	NE-CZ-NH1	5.80	123.20	120.30
4	L	23	CYS	CA-CB-SG	5.75	124.35	114.00
4	L	54	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	L	57	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	337	ARG	NE-CZ-NH2	5.62	123.11	120.30
3	C	66	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	E	169	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	E	88	ASN	CB-CA-C	-5.54	99.32	110.40
1	A	429	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	I	476	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	J	644	ARG	NE-CZ-NH2	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	308	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	500	ARG	NE-CZ-NH2	5.40	123.00	120.30
3	C	3	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	I	166	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	542	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	K	38	ARG	NE-CZ-NH1	5.34	122.97	120.30
4	L	59	PRO	CA-N-CD	-5.34	104.03	111.50
2	B	644	ARG	NE-CZ-NH2	5.32	122.96	120.30
4	H	20	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	I	273	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	504	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	E	166	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	169	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	E	419	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	500	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	I	500	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	166	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	G	66	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	L	20	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	308	ARG	NE-CZ-NH2	5.07	122.83	120.30
3	C	47	TRP	CB-CG-CD2	5.06	133.18	126.60
3	C	100(G)	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3477	3417	3415	13	0
1	E	3477	3417	3415	15	0
1	I	3477	3417	3415	19	0
2	B	1007	998	996	5	0
2	F	1007	998	996	3	0
2	J	1007	998	996	3	0
3	C	1049	1051	1051	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1049	1051	1051	3	0
3	K	1049	1051	1051	2	0
4	D	782	743	741	7	0
4	H	782	743	741	6	0
4	L	782	743	741	8	0
5	M	28	0	25	0	0
5	V	28	27	25	0	0
5	f	28	27	25	0	0
5	q	28	27	25	0	0
6	N	39	0	34	0	0
6	O	39	37	34	0	0
6	P	39	37	34	0	0
6	Q	39	37	34	0	0
6	R	39	37	34	0	0
6	T	39	37	34	2	0
6	U	39	37	34	0	0
6	W	39	37	34	0	0
6	Y	39	37	34	0	0
6	Z	39	37	34	0	0
6	a	39	37	34	0	0
6	b	39	37	34	0	0
6	d	39	37	34	0	0
6	e	39	37	34	0	0
6	g	39	37	34	0	0
6	j	39	37	34	0	0
6	k	39	37	34	0	0
6	l	39	37	34	0	0
6	m	39	37	34	0	0
6	o	39	37	34	0	0
6	p	39	37	34	0	0
6	r	39	37	34	0	0
7	S	50	47	43	0	0
7	X	50	47	43	0	0
7	c	50	47	43	0	0
7	h	50	47	43	0	0
7	n	50	47	43	0	0
7	s	50	47	43	0	0
8	A	56	42	52	0	0
8	E	42	42	39	0	0
8	I	42	42	39	0	0
All	All	20355	19893	19845	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 2.

All (80) 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:I:204:ALA:HB1	1:I:208:VAL:HG21	1.37	1.05
1:I:212:PRO:HG3	1:I:254:VAL:HG22	1.46	0.97
1:I:205:CYS:O	1:I:208:VAL:HG22	1.89	0.72
1:A:163:THR:HG23	1:A:165:LEU:H	1.63	0.64
1:A:252:LYS:HB2	1:A:254:VAL:HG22	1.78	0.64
1:A:254:VAL:O	1:A:255:VAL:HG13	2.01	0.59
1:I:163:THR:HG23	1:I:165:LEU:H	1.68	0.59
1:I:204:ALA:HB1	1:I:208:VAL:CG2	2.22	0.59
1:I:499:THR:HG22	1:I:500:ARG:H	1.69	0.57
1:I:212:PRO:HG3	1:I:254:VAL:CG2	2.28	0.55
1:E:163:THR:HG23	1:E:165:LEU:H	1.73	0.53
1:E:254:VAL:HG12	1:E:254:VAL:O	2.09	0.52
1:A:254:VAL:HG12	1:A:256:SER:H	1.74	0.51
1:E:206:PRO:HD3	1:E:316:TYR:CE1	2.45	0.51
4:D:73:LEU:HD12	4:D:73:LEU:H	1.76	0.51
1:I:42:VAL:HG11	2:J:628:TRP:CZ2	2.45	0.51
1:E:239:CYS:SG	1:E:241:ASN:O	2.69	0.51
4:L:73:LEU:HD12	4:L:73:LEU:H	1.75	0.51
4:D:55:ALA:HB3	4:D:62:PHE:CZ	2.47	0.50
1:E:252:LYS:HB2	1:E:254:VAL:HG23	1.94	0.49
1:I:255:VAL:HB	1:I:426:MET:CE	2.42	0.49
3:C:94:ARG:HD3	3:C:95:VAL:H	1.78	0.49
1:A:254:VAL:O	1:A:255:VAL:HG22	2.13	0.48
1:I:212:PRO:CG	1:I:254:VAL:HG22	2.32	0.48
1:I:116:LEU:CD2	1:I:204:ALA:HB2	2.44	0.48
1:E:69:TRP:CH2	1:E:253:PRO:HB2	2.49	0.48
1:E:115:SER:HB2	1:E:208:VAL:HG11	1.96	0.48
4:H:37:ARG:HA	4:H:86:TYR:CD2	2.49	0.47
1:I:248:THR:HB	1:I:486:TYR:CZ	2.49	0.47
3:G:100(O):SER:HB3	4:H:49:PHE:CZ	2.49	0.47
4:L:35:TRP:HA	4:L:88:CYS:HA	1.97	0.47
1:A:252:LYS:C	1:A:254:VAL:N	2.64	0.47
4:D:35:TRP:HA	4:D:88:CYS:HA	1.96	0.47
1:I:116:LEU:HD23	1:I:204:ALA:HB2	1.97	0.46
1:A:239:CYS:SG	1:A:241:ASN:O	2.73	0.46
4:H:36:TYR:CD2	4:H:46:LEU:HA	2.51	0.46
4:D:36:TYR:CD2	4:D:46:LEU:HA	2.51	0.46
1:A:248:THR:HG21	1:A:251:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:THR:HB	1:I:486:TYR:CE2	2.50	0.46
1:I:42:VAL:HG21	2:J:628:TRP:CE3	2.51	0.46
4:L:36:TYR:CD2	4:L:46:LEU:HA	2.51	0.46
4:D:35:TRP:HB3	4:D:88:CYS:SG	2.55	0.46
1:E:441:GLY:CA	6:T:1:NAG:H81	2.45	0.45
2:J:530:MET:SD	2:J:628:TRP:CD2	3.10	0.45
1:I:229:LYS:HB3	1:I:241:ASN:HD22	1.81	0.45
1:I:499:THR:CG2	1:I:500:ARG:H	2.29	0.45
1:E:498:PRO:HD3	2:F:610:TRP:CH2	2.52	0.44
1:E:116:LEU:CD2	1:E:204:ALA:HB2	2.47	0.44
2:F:530:MET:SD	2:F:628:TRP:CD2	3.11	0.44
4:L:87:TYR:CD2	4:L:101:GLY:HA3	2.53	0.43
3:K:55:ASP:HB3	3:K:56:TYR:CE2	2.54	0.43
2:B:650:GLN:H	2:B:650:GLN:CD	2.22	0.43
1:E:499:THR:HG22	1:E:500:ARG:H	1.82	0.43
4:L:35:TRP:HB3	4:L:88:CYS:SG	2.58	0.43
4:H:35:TRP:C	4:H:36:TYR:CD1	2.92	0.43
1:A:499:THR:HG22	1:A:500:ARG:H	1.83	0.43
1:I:208:VAL:O	1:I:209:SER:C	2.56	0.43
4:H:73:LEU:HD12	4:H:73:LEU:H	1.83	0.43
1:A:204:ALA:HB1	1:A:208:VAL:CG2	2.49	0.43
3:C:100(O):SER:HB3	4:D:49:PHE:CZ	2.54	0.43
3:G:34:LEU:HD22	3:G:69:VAL:HG13	2.01	0.42
4:L:35:TRP:C	4:L:36:TYR:CD1	2.93	0.42
3:C:72:ASP:CB	3:C:77:SER:HB2	2.49	0.42
1:A:384:TYR:CE1	1:A:421:LYS:HE3	2.54	0.42
3:C:72:ASP:HB3	3:C:77:SER:HB2	2.00	0.42
3:K:100(O):SER:HB3	4:L:49:PHE:CZ	2.55	0.42
1:A:42:VAL:HG21	2:B:628:TRP:CZ3	2.55	0.41
4:L:55:ALA:HB3	4:L:62:PHE:CZ	2.55	0.41
1:E:441:GLY:HA2	6:T:1:NAG:H81	2.02	0.41
1:I:206:PRO:HD3	1:I:316:TYR:CE1	2.55	0.41
4:D:35:TRP:CG	4:D:73:LEU:HG	2.56	0.41
1:E:205:CYS:C	1:E:207:LYS:N	2.71	0.41
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.56	0.41
1:E:254:VAL:HG12	1:E:256:SER:HB2	2.03	0.41
4:H:55:ALA:HB3	4:H:62:PHE:CZ	2.55	0.41
1:E:249:HIS:O	1:E:250:GLY:C	2.59	0.41
3:G:72:ASP:HB3	3:G:77:SER:HB2	2.03	0.40
2:F:611:ASN:HB3	2:F:614:TRP:CE2	2.56	0.40
1:A:42:VAL:HG21	2:B:628:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:MET:SD	2:B:628:TRP:CD2	3.14	0.40

There are no symmetry-related clashes.

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	432/474 (91%)	371 (86%)	55 (13%)	6 (1%)	11	46
1	E	432/474 (91%)	368 (85%)	60 (14%)	4 (1%)	17	56
1	I	432/474 (91%)	359 (83%)	65 (15%)	8 (2%)	8	40
2	B	122/153 (80%)	111 (91%)	10 (8%)	1 (1%)	19	59
2	F	122/153 (80%)	114 (93%)	7 (6%)	1 (1%)	19	59
2	J	122/153 (80%)	114 (93%)	8 (7%)	0	100	100
3	C	129/238 (54%)	101 (78%)	21 (16%)	7 (5%)	2	21
3	G	129/238 (54%)	103 (80%)	19 (15%)	7 (5%)	2	21
3	K	129/238 (54%)	100 (78%)	20 (16%)	9 (7%)	1	16
4	D	98/215 (46%)	84 (86%)	9 (9%)	5 (5%)	2	22
4	H	98/215 (46%)	79 (81%)	14 (14%)	5 (5%)	2	22
4	L	98/215 (46%)	83 (85%)	7 (7%)	8 (8%)	1	13
All	All	2343/3240 (72%)	1987 (85%)	295 (13%)	61 (3%)	8	34

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	256	SER
4	H	24	SER
4	H	59	PRO

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Mol	Chain	Res	Type
1	A	209	SER
1	A	255	VAL
4	D	26	VAL
4	D	59	PRO
4	D	94	LYS
1	I	256	SER
4	L	59	PRO
4	L	94	LYS
1	E	481	SER
3	G	78	LEU
3	G	100	TYR
3	G	100(L)	LYS
4	H	94	LYS
3	C	78	LEU
3	C	100(L)	LYS
4	D	24	SER
1	I	459	GLY
1	I	481	SER
3	K	55	ASP
3	K	72	ASP
4	L	24	SER
4	L	69	ASP
1	E	66	HIS
2	F	602	LEU
3	G	49	SER
4	H	69	ASP
2	B	602	LEU
3	C	100	TYR
3	C	100(F)	ARG
1	I	252	LYS
3	K	52(A)	LEU
3	K	100	TYR
3	G	72	ASP
1	A	254	VAL
1	A	481	SER
3	C	49	SER
3	C	55	ASP
1	I	209	SER
3	K	31	GLU
3	K	100(F)	ARG
4	L	51	ASN
4	L	75	ILE

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Mol	Chain	Res	Type
1	A	71	THR
3	C	31	GLU
4	D	75	ILE
1	I	60	ALA
1	I	61	TYR
1	I	71	THR
3	K	49	SER
3	K	78	LEU
4	L	26	VAL
4	L	31	GLN
3	G	55	ASP
4	H	75	ILE
3	K	100(L)	LYS
1	E	254	VAL
3	G	44	GLY
1	A	309	ILE

5.3.2 Protein sidechains [i](#)

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	392/423 (93%)	378 (96%)	14 (4%)	35 59
1	E	392/423 (93%)	372 (95%)	20 (5%)	24 50
1	I	392/423 (93%)	375 (96%)	17 (4%)	29 54
2	B	109/130 (84%)	106 (97%)	3 (3%)	43 65
2	F	109/130 (84%)	106 (97%)	3 (3%)	43 65
2	J	109/130 (84%)	107 (98%)	2 (2%)	59 77
3	C	113/206 (55%)	104 (92%)	9 (8%)	12 37
3	G	113/206 (55%)	102 (90%)	11 (10%)	8 29
3	K	113/206 (55%)	103 (91%)	10 (9%)	10 33
4	D	86/183 (47%)	79 (92%)	7 (8%)	11 37
4	H	86/183 (47%)	82 (95%)	4 (5%)	26 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	86/183 (47%)	81 (94%)	5 (6%)	20	47
All	All	2100/2826 (74%)	1995 (95%)	105 (5%)	28	50

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	47	ASP
1	E	83	GLU
1	E	84	ILE
1	E	112	TRP
1	E	169	ARG
1	E	173	TYR
1	E	203	GLN
1	E	208	VAL
1	E	249	HIS
1	E	252	LYS
1	E	262	ASN
1	E	327	ARG
1	E	357	LYS
1	E	387	THR
1	E	392	ASN
1	E	398	ASN
1	E	415	THR
1	E	433	CYS
1	E	443	ILE
1	E	504	ARG
2	F	530	MET
2	F	648	GLU
2	F	652	GLN
3	G	1	GLU
3	G	51	ILE
3	G	52	SER
3	G	57	ILE
3	G	58	SER
3	G	68	ASP
3	G	71	ARG
3	G	82	MET
3	G	82(A)	ASN
3	G	98	TRP
3	G	100	TYR
4	H	31	GLN
4	H	59	PRO

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Mol	Chain	Res	Type
4	H	75	ILE
4	H	80	ASP
1	A	47	ASP
1	A	83	GLU
1	A	169	ARG
1	A	173	TYR
1	A	203	GLN
1	A	249	HIS
1	A	262	ASN
1	A	327	ARG
1	A	357	LYS
1	A	387	THR
1	A	392	ASN
1	A	398	ASN
1	A	433	CYS
1	A	504	ARG
2	B	648	GLU
2	B	652	GLN
2	B	656	ASN
3	C	6	GLU
3	C	51	ILE
3	C	52	SER
3	C	57	ILE
3	C	68	ASP
3	C	71	ARG
3	C	82	MET
3	C	82(A)	ASN
3	C	94	ARG
4	D	31	GLN
4	D	32	TYR
4	D	34	SER
4	D	59	PRO
4	D	74	THR
4	D	75	ILE
4	D	80	ASP
1	I	47	ASP
1	I	85	HIS
1	I	86	LEU
1	I	112	TRP
1	I	164	GLU
1	I	169	ARG
1	I	173	TYR

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Mol	Chain	Res	Type
1	I	203	GLN
1	I	249	HIS
1	I	262	ASN
1	I	327	ARG
1	I	357	LYS
1	I	387	THR
1	I	392	ASN
1	I	398	ASN
1	I	433	CYS
1	I	504	ARG
2	J	648	GLU
2	J	652	GLN
3	K	51	ILE
3	K	52	SER
3	K	57	ILE
3	K	58	SER
3	K	68	ASP
3	K	77	SER
3	K	82	MET
3	K	82(A)	ASN
3	K	98	TRP
3	K	100(B)	ASP
4	L	6	GLN
4	L	34	SER
4	L	59	PRO
4	L	74	THR
4	L	75	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	203	GLN
1	E	241	ASN
1	A	241	ASN
1	I	203	GLN
1	I	241	ASN
1	I	302	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

98 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	1,5	14,14,15	2.49	6 (42%)	17,19,21	4.16	9 (52%)
5	NAG	M	2	5	14,14,15	1.86	3 (21%)	17,19,21	3.24	8 (47%)
6	NAG	N	1	6,1	14,14,15	0.56	0	17,19,21	0.93	0
6	NAG	N	2	6	14,14,15	0.39	0	17,19,21	0.67	1 (5%)
6	BMA	N	3	6	11,11,12	0.25	0	15,15,17	0.67	0
6	NAG	O	1	6,1	14,14,15	1.36	4 (28%)	17,19,21	0.87	1 (5%)
6	NAG	O	2	6	14,14,15	1.50	3 (21%)	17,19,21	0.98	1 (5%)
6	BMA	O	3	6	11,11,12	1.38	2 (18%)	15,15,17	1.09	2 (13%)
6	NAG	P	1	6	14,14,15	0.43	0	17,19,21	1.23	1 (5%)
6	NAG	P	2	6	14,14,15	0.44	0	17,19,21	1.24	3 (17%)
6	BMA	P	3	6	11,11,12	0.29	0	15,15,17	0.91	1 (6%)
6	NAG	Q	1	6,1	14,14,15	1.31	1 (7%)	17,19,21	1.88	4 (23%)
6	NAG	Q	2	6	14,14,15	1.30	2 (14%)	17,19,21	1.40	3 (17%)
6	BMA	Q	3	6	11,11,12	1.30	2 (18%)	15,15,17	1.13	2 (13%)
6	NAG	R	1	6,1	14,14,15	1.25	2 (14%)	17,19,21	1.21	1 (5%)
6	NAG	R	2	6	14,14,15	1.33	4 (28%)	17,19,21	0.86	0
6	BMA	R	3	6	11,11,12	1.26	2 (18%)	15,15,17	0.82	0
7	NAG	S	1	1,7	14,14,15	1.11	2 (14%)	17,19,21	1.34	3 (17%)
7	NAG	S	2	7	14,14,15	1.23	2 (14%)	17,19,21	0.96	1 (5%)
7	BMA	S	3	7	11,11,12	1.24	1 (9%)	15,15,17	1.24	1 (6%)
7	MAN	S	4	7	11,11,12	1.28	2 (18%)	15,15,17	1.15	1 (6%)
6	NAG	T	1	6,1	14,14,15	1.33	2 (14%)	17,19,21	1.50	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	T	2	6	14,14,15	1.41	4 (28%)	17,19,21	0.92	0
6	BMA	T	3	6	11,11,12	1.26	2 (18%)	15,15,17	1.15	1 (6%)
6	NAG	U	1	6,1	14,14,15	1.10	2 (14%)	17,19,21	1.54	5 (29%)
6	NAG	U	2	6	14,14,15	1.44	2 (14%)	17,19,21	0.75	1 (5%)
6	BMA	U	3	6	11,11,12	1.20	2 (18%)	15,15,17	1.07	1 (6%)
5	NAG	V	1	1,5	14,14,15	1.36	3 (21%)	17,19,21	1.37	3 (17%)
5	NAG	V	2	5	14,14,15	1.35	3 (21%)	17,19,21	0.68	0
6	NAG	W	1	6,1	14,14,15	1.11	1 (7%)	17,19,21	0.75	0
6	NAG	W	2	6	14,14,15	1.49	4 (28%)	17,19,21	1.41	2 (11%)
6	BMA	W	3	6	11,11,12	1.05	1 (9%)	15,15,17	1.13	1 (6%)
7	NAG	X	1	7	14,14,15	0.39	0	17,19,21	2.51	6 (35%)
7	NAG	X	2	7	14,14,15	0.51	0	17,19,21	1.87	4 (23%)
7	BMA	X	3	7	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
7	MAN	X	4	7	11,11,12	0.26	0	15,15,17	0.85	1 (6%)
6	NAG	Y	1	6,1	14,14,15	1.31	2 (14%)	17,19,21	0.76	0
6	NAG	Y	2	6	14,14,15	1.68	4 (28%)	17,19,21	1.09	2 (11%)
6	BMA	Y	3	6	11,11,12	1.43	2 (18%)	15,15,17	1.11	1 (6%)
6	NAG	Z	1	6	14,14,15	0.44	0	17,19,21	1.25	2 (11%)
6	NAG	Z	2	6	14,14,15	0.44	0	17,19,21	1.19	3 (17%)
6	BMA	Z	3	6	11,11,12	0.25	0	15,15,17	0.87	1 (6%)
6	NAG	a	1	6,1	14,14,15	1.23	2 (14%)	17,19,21	2.12	3 (17%)
6	NAG	a	2	6	14,14,15	1.32	2 (14%)	17,19,21	1.32	3 (17%)
6	BMA	a	3	6	11,11,12	1.29	2 (18%)	15,15,17	1.27	2 (13%)
6	NAG	b	1	6,1	14,14,15	1.28	2 (14%)	17,19,21	1.19	2 (11%)
6	NAG	b	2	6	14,14,15	1.30	3 (21%)	17,19,21	0.84	0
6	BMA	b	3	6	11,11,12	1.25	2 (18%)	15,15,17	0.79	0
7	NAG	c	1	1,7	14,14,15	1.12	2 (14%)	17,19,21	1.37	3 (17%)
7	NAG	c	2	7	14,14,15	1.37	2 (14%)	17,19,21	1.06	1 (5%)
7	BMA	c	3	7	11,11,12	1.23	1 (9%)	15,15,17	1.28	1 (6%)
7	MAN	c	4	7	11,11,12	1.41	2 (18%)	15,15,17	1.24	1 (6%)
6	NAG	d	1	6,1	14,14,15	1.20	2 (14%)	17,19,21	1.21	2 (11%)
6	NAG	d	2	6	14,14,15	1.38	2 (14%)	17,19,21	0.94	1 (5%)
6	BMA	d	3	6	11,11,12	1.35	2 (18%)	15,15,17	1.29	1 (6%)
6	NAG	e	1	6,1	14,14,15	1.18	2 (14%)	17,19,21	1.48	3 (17%)
6	NAG	e	2	6	14,14,15	1.36	2 (14%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	e	3	6	11,11,12	1.34	2 (18%)	15,15,17	1.04	1 (6%)
5	NAG	f	1	1,5	14,14,15	1.30	2 (14%)	17,19,21	1.45	4 (23%)
5	NAG	f	2	5	14,14,15	1.41	3 (21%)	17,19,21	0.86	0
6	NAG	g	1	6,1	14,14,15	1.13	2 (14%)	17,19,21	0.66	0
6	NAG	g	2	6	14,14,15	1.33	3 (21%)	17,19,21	1.19	3 (17%)
6	BMA	g	3	6	11,11,12	1.18	1 (9%)	15,15,17	0.99	1 (6%)
7	NAG	h	1	7	14,14,15	0.45	0	17,19,21	2.24	6 (35%)
7	NAG	h	2	7	14,14,15	0.52	0	17,19,21	2.15	6 (35%)
7	BMA	h	3	7	11,11,12	0.42	0	15,15,17	0.96	1 (6%)
7	MAN	h	4	7	11,11,12	0.26	0	15,15,17	0.95	1 (6%)
6	NAG	j	1	6,1	14,14,15	1.19	1 (7%)	17,19,21	0.74	0
6	NAG	j	2	6	14,14,15	1.48	3 (21%)	17,19,21	1.23	2 (11%)
6	BMA	j	3	6	11,11,12	1.38	2 (18%)	15,15,17	0.98	2 (13%)
6	NAG	k	1	6	14,14,15	0.45	0	17,19,21	1.12	1 (5%)
6	NAG	k	2	6	14,14,15	0.46	0	17,19,21	1.15	3 (17%)
6	BMA	k	3	6	11,11,12	0.28	0	15,15,17	0.91	1 (6%)
6	NAG	l	1	6,1	14,14,15	1.22	1 (7%)	17,19,21	2.07	4 (23%)
6	NAG	l	2	6	14,14,15	1.28	1 (7%)	17,19,21	1.40	3 (17%)
6	BMA	l	3	6	11,11,12	1.34	2 (18%)	15,15,17	1.22	2 (13%)
6	NAG	m	1	6,1	14,14,15	1.27	2 (14%)	17,19,21	1.36	5 (29%)
6	NAG	m	2	6	14,14,15	1.36	4 (28%)	17,19,21	0.93	0
6	BMA	m	3	6	11,11,12	1.28	2 (18%)	15,15,17	0.83	0
7	NAG	n	1	1,7	14,14,15	1.05	2 (14%)	17,19,21	1.36	3 (17%)
7	NAG	n	2	7	14,14,15	1.38	2 (14%)	17,19,21	0.87	0
7	BMA	n	3	7	11,11,12	1.33	2 (18%)	15,15,17	1.16	1 (6%)
7	MAN	n	4	7	11,11,12	1.33	2 (18%)	15,15,17	1.04	1 (6%)
6	NAG	o	1	6,1	14,14,15	1.25	2 (14%)	17,19,21	1.42	3 (17%)
6	NAG	o	2	6	14,14,15	1.42	4 (28%)	17,19,21	0.88	1 (5%)
6	BMA	o	3	6	11,11,12	1.29	2 (18%)	15,15,17	1.21	2 (13%)
6	NAG	p	1	6,1	14,14,15	1.18	2 (14%)	17,19,21	1.43	3 (17%)
6	NAG	p	2	6	14,14,15	1.42	2 (14%)	17,19,21	0.86	1 (5%)
6	BMA	p	3	6	11,11,12	1.24	2 (18%)	15,15,17	1.03	1 (6%)
5	NAG	q	1	1,5	14,14,15	1.35	2 (14%)	17,19,21	1.47	2 (11%)
5	NAG	q	2	5	14,14,15	1.30	3 (21%)	17,19,21	0.78	0
6	NAG	r	1	6,1	14,14,15	1.00	1 (7%)	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	r	2	6	14,14,15	1.41	4 (28%)	17,19,21	1.58	1 (5%)
6	BMA	r	3	6	11,11,12	1.33	2 (18%)	15,15,17	0.78	0
7	NAG	s	1	7	14,14,15	0.36	0	17,19,21	2.32	6 (35%)
7	NAG	s	2	7	14,14,15	0.48	0	17,19,21	1.61	4 (23%)
7	BMA	s	3	7	11,11,12	0.48	0	15,15,17	0.77	1 (6%)
7	MAN	s	4	7	11,11,12	0.30	0	15,15,17	0.94	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	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	6/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	4/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	1/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1
6	NAG	U	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1

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

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

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	C1-C2	-5.22	1.44	1.52
5	M	2	NAG	C2-N2	-3.88	1.39	1.46
5	M	2	NAG	C1-C2	-3.80	1.46	1.52
5	M	1	NAG	O5-C1	-3.66	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	O5-C5	-3.54	1.36	1.43
5	M	1	NAG	C4-C5	-3.31	1.46	1.53
6	U	2	NAG	O4-C4	3.15	1.50	1.43
6	Y	2	NAG	O4-C4	3.06	1.50	1.43
6	l	3	BMA	O5-C5	3.06	1.49	1.43
6	j	3	BMA	O5-C5	3.02	1.49	1.43
6	r	2	NAG	O4-C4	3.00	1.50	1.43
6	O	2	NAG	O4-C4	2.99	1.50	1.43
5	V	1	NAG	O5-C5	2.98	1.49	1.43
7	n	2	NAG	O4-C4	2.98	1.50	1.43
7	c	2	NAG	O4-C4	2.96	1.50	1.43
6	Y	2	NAG	O5-C5	2.91	1.49	1.43
6	O	3	BMA	O5-C5	2.91	1.49	1.43
6	m	3	BMA	O5-C5	2.90	1.49	1.43
6	j	2	NAG	O5-C5	2.89	1.49	1.43
7	c	4	MAN	O5-C5	2.88	1.49	1.43
6	d	3	BMA	O5-C5	2.87	1.49	1.43
7	c	2	NAG	O5-C5	2.85	1.49	1.43
6	W	2	NAG	O4-C4	2.83	1.49	1.43
6	e	2	NAG	O4-C4	2.83	1.49	1.43
6	o	1	NAG	O4-C4	2.83	1.49	1.43
6	Y	3	BMA	O5-C5	2.82	1.49	1.43
6	Y	3	BMA	O5-C1	2.81	1.48	1.43
5	f	2	NAG	O5-C5	2.81	1.49	1.43
6	Q	1	NAG	O4-C4	2.81	1.49	1.43
6	T	3	BMA	O5-C5	2.78	1.49	1.43
6	b	3	BMA	O5-C5	2.77	1.49	1.43
6	T	1	NAG	O4-C4	2.77	1.49	1.43
5	q	1	NAG	O5-C5	2.75	1.49	1.43
6	g	2	NAG	O4-C4	2.75	1.49	1.43
6	r	3	BMA	O5-C5	2.74	1.49	1.43
6	O	2	NAG	O5-C5	2.73	1.49	1.43
6	p	2	NAG	O4-C4	2.73	1.49	1.43
7	c	4	MAN	O5-C1	2.73	1.48	1.43
6	j	2	NAG	O4-C4	2.72	1.49	1.43
6	b	1	NAG	O5-C5	2.70	1.48	1.43
6	Q	3	BMA	O5-C5	2.70	1.48	1.43
6	a	3	BMA	O5-C5	2.69	1.48	1.43
6	Y	2	NAG	O5-C1	2.68	1.48	1.43
7	n	3	BMA	O5-C5	2.68	1.48	1.43
7	n	4	MAN	O5-C5	2.67	1.48	1.43
6	R	3	BMA	O5-C5	2.67	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	2	NAG	C1-C2	2.66	1.56	1.52
7	S	2	NAG	O4-C4	2.65	1.49	1.43
7	c	3	BMA	O5-C5	2.65	1.48	1.43
7	n	2	NAG	O5-C5	2.64	1.48	1.43
6	g	3	BMA	O5-C5	2.63	1.48	1.43
6	p	2	NAG	O5-C5	2.63	1.48	1.43
7	n	4	MAN	O5-C1	2.62	1.47	1.43
7	S	4	MAN	O5-C5	2.59	1.48	1.43
6	Q	2	NAG	O5-C5	2.58	1.48	1.43
6	m	1	NAG	O5-C5	2.58	1.48	1.43
6	W	2	NAG	O5-C1	2.57	1.47	1.43
5	q	2	NAG	O5-C5	2.57	1.48	1.43
6	l	1	NAG	O4-C4	2.57	1.49	1.43
5	V	2	NAG	C1-C2	2.57	1.56	1.52
6	R	1	NAG	O5-C5	2.56	1.48	1.43
6	e	3	BMA	O5-C1	2.55	1.47	1.43
6	d	2	NAG	O4-C4	2.55	1.49	1.43
5	f	2	NAG	O5-C1	2.54	1.47	1.43
6	a	1	NAG	O4-C4	2.54	1.48	1.43
6	T	1	NAG	O5-C5	2.54	1.48	1.43
6	d	1	NAG	O4-C4	2.52	1.48	1.43
6	j	3	BMA	O5-C1	2.52	1.47	1.43
6	e	2	NAG	O5-C5	2.51	1.48	1.43
6	e	3	BMA	O5-C5	2.51	1.48	1.43
6	o	3	BMA	O5-C5	2.51	1.48	1.43
6	r	3	BMA	O5-C1	2.48	1.47	1.43
6	Y	1	NAG	O5-C5	2.48	1.48	1.43
6	U	2	NAG	O5-C5	2.47	1.48	1.43
6	d	3	BMA	O5-C1	2.47	1.47	1.43
5	f	2	NAG	C1-C2	2.46	1.56	1.52
5	f	1	NAG	O5-C5	2.46	1.48	1.43
7	S	3	BMA	O5-C5	2.45	1.48	1.43
6	p	1	NAG	O4-C4	2.45	1.48	1.43
6	o	2	NAG	O5-C1	2.44	1.47	1.43
6	p	3	BMA	O5-C5	2.44	1.48	1.43
6	l	2	NAG	O5-C5	2.44	1.48	1.43
7	n	3	BMA	O5-C1	2.43	1.47	1.43
5	V	2	NAG	O5-C5	2.42	1.48	1.43
6	a	2	NAG	O5-C5	2.42	1.48	1.43
5	M	1	NAG	C2-N2	-2.41	1.42	1.46
7	S	1	NAG	O5-C5	2.41	1.48	1.43
6	o	2	NAG	O5-C5	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	q	2	NAG	O5-C1	2.39	1.47	1.43
6	Y	2	NAG	C1-C2	2.38	1.55	1.52
6	o	1	NAG	O5-C5	2.37	1.48	1.43
6	j	2	NAG	O5-C1	2.37	1.47	1.43
6	O	3	BMA	O5-C1	2.36	1.47	1.43
7	c	1	NAG	O4-C4	2.36	1.48	1.43
6	p	3	BMA	O5-C1	2.34	1.47	1.43
6	g	2	NAG	O5-C1	2.34	1.47	1.43
6	T	2	NAG	O4-C4	2.34	1.48	1.43
6	m	2	NAG	O5-C5	2.33	1.48	1.43
6	O	1	NAG	O5-C5	2.33	1.48	1.43
7	S	4	MAN	O5-C1	2.32	1.47	1.43
6	o	3	BMA	O5-C1	2.31	1.47	1.43
6	T	2	NAG	O5-C5	2.31	1.48	1.43
6	W	1	NAG	O4-C4	2.30	1.48	1.43
6	U	3	BMA	O5-C5	2.30	1.48	1.43
6	b	2	NAG	O5-C5	2.29	1.48	1.43
6	R	2	NAG	C1-C2	2.27	1.55	1.52
6	Y	1	NAG	O4-C4	2.26	1.48	1.43
6	g	1	NAG	O4-C4	2.26	1.48	1.43
6	b	3	BMA	O5-C1	2.24	1.47	1.43
6	b	1	NAG	O4-C4	2.24	1.48	1.43
5	f	1	NAG	O4-C4	2.24	1.48	1.43
6	l	3	BMA	O5-C1	2.24	1.47	1.43
6	R	1	NAG	O4-C4	2.23	1.48	1.43
7	S	2	NAG	O5-C5	2.23	1.48	1.43
5	q	2	NAG	C1-C2	2.23	1.55	1.52
6	j	1	NAG	C1-C2	2.22	1.55	1.52
6	p	1	NAG	O5-C5	2.21	1.47	1.43
6	m	2	NAG	C1-C2	2.21	1.55	1.52
6	d	2	NAG	O5-C5	2.19	1.47	1.43
6	e	1	NAG	O5-C5	2.19	1.47	1.43
6	O	1	NAG	O5-C1	2.19	1.47	1.43
6	b	2	NAG	O5-C1	2.19	1.47	1.43
6	m	2	NAG	O4-C4	2.19	1.48	1.43
6	R	2	NAG	O5-C1	2.18	1.47	1.43
6	Q	2	NAG	O4-C4	2.18	1.48	1.43
5	M	2	NAG	O5-C1	-2.18	1.40	1.43
6	r	2	NAG	O5-C5	2.18	1.47	1.43
6	b	2	NAG	O4-C4	2.17	1.48	1.43
6	Q	3	BMA	O5-C1	2.17	1.47	1.43
6	T	2	NAG	O5-C1	2.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	1	NAG	O5-C5	2.16	1.47	1.43
6	a	1	NAG	O5-C5	2.16	1.47	1.43
5	V	1	NAG	O4-C4	2.16	1.48	1.43
6	R	2	NAG	O5-C5	2.15	1.47	1.43
6	O	1	NAG	C1-C2	2.15	1.55	1.52
6	r	2	NAG	C1-C2	2.15	1.55	1.52
6	m	2	NAG	O5-C1	2.15	1.47	1.43
6	o	2	NAG	C1-C2	2.15	1.55	1.52
5	V	2	NAG	O5-C1	2.14	1.47	1.43
6	m	1	NAG	O4-C4	2.14	1.48	1.43
6	R	2	NAG	O4-C4	2.13	1.48	1.43
6	a	2	NAG	O4-C4	2.13	1.48	1.43
6	e	1	NAG	O4-C4	2.12	1.48	1.43
6	T	3	BMA	O5-C1	2.12	1.47	1.43
6	W	3	BMA	O5-C5	2.12	1.47	1.43
7	n	1	NAG	O5-C5	2.11	1.47	1.43
6	d	1	NAG	O5-C5	2.11	1.47	1.43
6	g	1	NAG	O5-C5	2.11	1.47	1.43
6	o	2	NAG	O4-C4	2.10	1.47	1.43
5	M	1	NAG	C8-C7	-2.10	1.46	1.50
6	m	3	BMA	O5-C1	2.09	1.47	1.43
6	O	2	NAG	O5-C1	2.08	1.47	1.43
6	U	1	NAG	O4-C4	2.08	1.47	1.43
6	O	1	NAG	O4-C4	2.08	1.47	1.43
6	W	2	NAG	O5-C5	2.08	1.47	1.43
6	g	2	NAG	C1-C2	2.07	1.55	1.52
5	V	1	NAG	O5-C1	2.06	1.47	1.43
6	r	2	NAG	O5-C1	2.06	1.47	1.43
5	q	1	NAG	O4-C4	2.05	1.47	1.43
6	U	3	BMA	O5-C1	2.05	1.47	1.43
7	c	1	NAG	O5-C5	2.04	1.47	1.43
6	a	3	BMA	O5-C1	2.04	1.47	1.43
7	n	1	NAG	O4-C4	2.03	1.47	1.43
7	S	1	NAG	O4-C4	2.03	1.47	1.43
6	r	1	NAG	O5-C5	2.03	1.47	1.43
6	T	2	NAG	C1-C2	2.02	1.55	1.52
6	R	3	BMA	O5-C1	2.01	1.46	1.43

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	C1-C2-N2	-9.28	94.64	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1	NAG	O4-C4-C5	-7.25	91.30	109.30
5	M	2	NAG	C1-C2-N2	-6.80	98.87	110.49
5	M	2	NAG	C2-N2-C7	-6.26	114.00	122.90
5	M	1	NAG	C3-C4-C5	-6.14	99.28	110.24
5	M	1	NAG	O6-C6-C5	-6.12	90.29	111.29
6	r	2	NAG	C1-O5-C5	5.60	119.78	112.19
6	a	1	NAG	C1-O5-C5	5.24	119.29	112.19
6	l	1	NAG	C1-O5-C5	5.23	119.28	112.19
5	M	2	NAG	O5-C5-C6	5.10	115.20	107.20
6	Q	1	NAG	C1-O5-C5	5.00	118.97	112.19
7	X	2	NAG	C1-O5-C5	4.94	118.88	112.19
7	X	1	NAG	C1-C2-N2	4.86	118.78	110.49
7	X	1	NAG	O3-C3-C2	-4.80	99.53	109.47
5	M	2	NAG	O3-C3-C4	-4.74	99.40	110.35
7	h	2	NAG	C2-N2-C7	4.56	129.40	122.90
7	s	1	NAG	O4-C4-C5	-4.44	98.27	109.30
7	X	1	NAG	C2-N2-C7	4.41	129.18	122.90
7	s	1	NAG	C1-C2-N2	4.40	118.01	110.49
6	a	1	NAG	C4-C3-C2	4.37	117.42	111.02
7	h	1	NAG	C2-N2-C7	4.31	129.04	122.90
7	h	1	NAG	C1-C2-N2	4.28	117.80	110.49
7	h	2	NAG	C1-C2-N2	4.27	117.77	110.49
5	M	1	NAG	O5-C5-C6	-4.24	100.56	107.20
7	s	1	NAG	C2-N2-C7	4.18	128.86	122.90
6	W	2	NAG	C1-O5-C5	4.17	117.85	112.19
5	M	1	NAG	C8-C7-N2	-4.16	109.05	116.10
6	l	1	NAG	C4-C3-C2	4.04	116.94	111.02
5	M	1	NAG	O3-C3-C2	-4.01	101.18	109.47
7	X	1	NAG	O4-C4-C5	-3.98	99.41	109.30
6	Q	1	NAG	C4-C3-C2	3.97	116.84	111.02
7	S	4	MAN	C1-O5-C5	3.93	117.52	112.19
5	M	2	NAG	C4-C3-C2	-3.89	105.32	111.02
7	s	2	NAG	C1-O5-C5	3.83	117.38	112.19
7	c	3	BMA	C1-O5-C5	3.77	117.30	112.19
6	a	1	NAG	O4-C4-C3	-3.77	101.64	110.35
7	h	1	NAG	O3-C3-C2	-3.76	101.69	109.47
6	d	3	BMA	C1-O5-C5	3.70	117.20	112.19
7	s	1	NAG	O3-C3-C2	-3.65	101.91	109.47
7	h	1	NAG	O4-C4-C5	-3.63	100.30	109.30
7	n	4	MAN	C1-O5-C5	3.62	117.10	112.19
6	l	1	NAG	O4-C4-C3	-3.56	102.12	110.35
6	W	3	BMA	C1-O5-C5	3.49	116.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	2	NAG	C1-O5-C5	3.45	116.87	112.19
6	j	2	NAG	C1-O5-C5	3.45	116.86	112.19
6	T	1	NAG	C1-C2-N2	-3.41	104.66	110.49
7	c	4	MAN	C1-O5-C5	3.36	116.74	112.19
7	X	2	NAG	O4-C4-C5	-3.31	101.09	109.30
5	M	1	NAG	C1-O5-C5	-3.30	107.72	112.19
7	n	3	BMA	C1-O5-C5	3.27	116.62	112.19
5	q	1	NAG	O4-C4-C3	-3.27	102.80	110.35
6	l	2	NAG	C2-N2-C7	3.22	127.49	122.90
6	e	3	BMA	C1-O5-C5	3.16	116.47	112.19
6	T	3	BMA	C1-O5-C5	3.13	116.44	112.19
5	V	1	NAG	O4-C4-C3	-3.12	103.14	110.35
6	p	1	NAG	C4-C3-C2	3.05	115.49	111.02
7	c	1	NAG	O4-C4-C5	-3.03	101.78	109.30
7	S	3	BMA	C1-O5-C5	3.02	116.28	112.19
6	l	3	BMA	C1-O5-C5	2.98	116.23	112.19
6	U	1	NAG	C1-O5-C5	-2.97	108.16	112.19
6	o	1	NAG	C4-C3-C2	2.97	115.38	111.02
6	Q	3	BMA	C1-O5-C5	2.94	116.17	112.19
6	P	3	BMA	C1-O5-C5	2.93	116.17	112.19
6	g	2	NAG	C1-O5-C5	2.92	116.14	112.19
5	f	1	NAG	O4-C4-C3	-2.90	103.66	110.35
6	U	3	BMA	C1-O5-C5	2.89	116.10	112.19
6	a	3	BMA	C1-C2-C3	2.88	113.21	109.67
6	a	3	BMA	C1-O5-C5	2.88	116.09	112.19
6	k	3	BMA	C1-O5-C5	2.87	116.09	112.19
6	p	3	BMA	C1-O5-C5	2.87	116.09	112.19
5	M	1	NAG	O7-C7-C8	2.87	127.39	122.06
7	X	1	NAG	C1-O5-C5	2.84	116.05	112.19
7	h	3	BMA	C1-O5-C5	2.84	116.04	112.19
6	W	2	NAG	O4-C4-C3	2.80	116.83	110.35
6	g	2	NAG	O4-C4-C3	2.80	116.82	110.35
7	S	1	NAG	O4-C4-C3	-2.79	103.90	110.35
6	Q	1	NAG	O4-C4-C3	-2.79	103.91	110.35
6	Z	3	BMA	C1-O5-C5	2.79	115.97	112.19
7	S	1	NAG	C4-C3-C2	2.78	115.09	111.02
7	h	2	NAG	O4-C4-C5	-2.78	102.40	109.30
7	n	1	NAG	C4-C3-C2	2.77	115.08	111.02
6	Q	2	NAG	O5-C1-C2	-2.76	106.93	111.29
7	n	1	NAG	O4-C4-C5	-2.74	102.49	109.30
6	Q	2	NAG	C2-N2-C7	2.73	126.79	122.90
7	s	1	NAG	C1-O5-C5	2.73	115.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	NAG	C1-O5-C5	-2.67	108.58	112.19
7	s	4	MAN	C1-O5-C5	2.66	115.80	112.19
6	U	1	NAG	C4-C3-C2	2.66	114.91	111.02
6	a	2	NAG	O5-C1-C2	-2.64	107.12	111.29
6	o	1	NAG	C1-C2-N2	-2.64	105.98	110.49
5	q	1	NAG	C3-C4-C5	2.60	114.88	110.24
6	d	1	NAG	C1-C2-N2	-2.60	106.05	110.49
6	p	1	NAG	O4-C4-C3	-2.59	104.35	110.35
6	o	3	BMA	C1-O5-C5	2.58	115.69	112.19
6	T	1	NAG	C2-N2-C7	2.58	126.57	122.90
5	f	1	NAG	C4-C3-C2	2.56	114.76	111.02
7	h	1	NAG	C1-O5-C5	2.55	115.65	112.19
7	S	1	NAG	O4-C4-C5	-2.55	102.97	109.30
6	e	1	NAG	C4-C3-C2	2.53	114.73	111.02
6	T	1	NAG	C4-C3-C2	2.53	114.73	111.02
7	X	4	MAN	C1-O5-C5	2.53	115.62	112.19
7	h	1	NAG	O7-C7-N2	2.52	126.58	121.95
6	a	2	NAG	C1-C2-N2	2.50	114.76	110.49
7	n	1	NAG	O4-C4-C3	-2.50	104.57	110.35
6	g	3	BMA	C1-O5-C5	2.50	115.57	112.19
6	Q	2	NAG	C1-C2-N2	2.49	114.74	110.49
6	U	1	NAG	O4-C4-C5	-2.48	103.13	109.30
6	l	2	NAG	C1-C2-N2	2.45	114.67	110.49
7	h	4	MAN	C1-O5-C5	2.44	115.49	112.19
6	Y	3	BMA	O5-C5-C6	2.43	111.01	107.20
6	a	2	NAG	C2-N2-C7	2.42	126.34	122.90
6	e	1	NAG	O4-C4-C5	-2.41	103.32	109.30
6	O	3	BMA	C1-C2-C3	2.40	112.62	109.67
7	h	2	NAG	O7-C7-N2	2.39	126.34	121.95
6	P	1	NAG	C4-C3-C2	-2.38	107.52	111.02
7	s	1	NAG	O7-C7-N2	2.38	126.32	121.95
7	c	1	NAG	O4-C4-C3	-2.38	104.86	110.35
6	r	1	NAG	C4-C3-C2	-2.38	107.54	111.02
6	o	3	BMA	C1-C2-C3	2.37	112.58	109.67
7	s	2	NAG	O4-C4-C5	-2.35	103.45	109.30
6	o	1	NAG	C2-N2-C7	2.34	126.24	122.90
6	Y	2	NAG	C1-O5-C5	2.34	115.36	112.19
6	d	1	NAG	C2-N2-C7	2.32	126.21	122.90
6	r	1	NAG	O5-C1-C2	-2.32	107.63	111.29
7	X	2	NAG	C2-N2-C7	2.31	126.19	122.90
7	X	1	NAG	O7-C7-N2	2.29	126.17	121.95
6	m	1	NAG	O4-C4-C3	-2.29	105.05	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	l	3	BMA	C1-C2-C3	2.29	112.48	109.67
5	V	1	NAG	C3-C4-C5	2.28	114.31	110.24
7	X	3	BMA	C1-O5-C5	2.27	115.27	112.19
6	O	2	NAG	C1-O5-C5	2.27	115.27	112.19
5	M	2	NAG	C6-C5-C4	-2.27	107.70	113.00
6	m	1	NAG	C1-C2-N2	2.26	114.35	110.49
6	e	1	NAG	C1-O5-C5	-2.26	109.13	112.19
5	f	1	NAG	C3-C4-C5	2.25	114.25	110.24
6	Y	2	NAG	C2-N2-C7	2.25	126.11	122.90
6	b	1	NAG	C1-O5-C5	-2.25	109.15	112.19
6	l	2	NAG	O4-C4-C3	-2.24	105.17	110.35
6	Q	3	BMA	C1-C2-C3	2.24	112.42	109.67
7	s	2	NAG	C2-N2-C7	2.24	126.09	122.90
6	b	1	NAG	O5-C1-C2	-2.24	107.75	111.29
6	Z	1	NAG	C4-C3-C2	-2.23	107.74	111.02
6	P	2	NAG	C4-C3-C2	-2.23	107.75	111.02
6	j	3	BMA	C1-O5-C5	2.22	115.20	112.19
6	l	1	NAG	O5-C5-C6	-2.22	103.72	107.20
7	s	3	BMA	C1-O5-C5	2.21	115.18	112.19
6	P	2	NAG	O5-C1-C2	-2.21	107.81	111.29
5	M	2	NAG	O4-C4-C3	-2.21	105.25	110.35
6	O	3	BMA	C1-O5-C5	2.20	115.18	112.19
6	Q	1	NAG	O4-C4-C5	2.20	114.76	109.30
6	p	2	NAG	C3-C4-C5	2.19	114.14	110.24
6	Z	2	NAG	C1-O5-C5	2.19	115.15	112.19
6	Z	1	NAG	O4-C4-C5	2.18	114.72	109.30
6	U	1	NAG	O5-C1-C2	-2.17	107.86	111.29
5	f	1	NAG	C1-O5-C5	-2.17	109.25	112.19
6	P	2	NAG	O4-C4-C3	2.17	115.36	110.35
6	m	1	NAG	C3-C4-C5	2.16	114.09	110.24
6	O	1	NAG	C1-O5-C5	2.16	115.12	112.19
7	c	1	NAG	C4-C3-C2	2.16	114.18	111.02
5	V	1	NAG	C1-O5-C5	-2.15	109.28	112.19
6	T	1	NAG	O5-C5-C6	2.15	110.58	107.20
6	j	2	NAG	C2-N2-C7	2.15	125.96	122.90
6	U	1	NAG	O4-C4-C3	-2.14	105.40	110.35
6	m	1	NAG	C2-N2-C7	2.14	125.94	122.90
6	g	2	NAG	O5-C5-C4	-2.11	105.70	110.83
6	p	1	NAG	O4-C4-C5	-2.10	104.08	109.30
6	Z	2	NAG	C4-C3-C2	-2.09	107.95	111.02
6	N	2	NAG	C1-O5-C5	2.08	115.01	112.19
7	X	2	NAG	O3-C3-C2	-2.08	105.16	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	m	1	NAG	O5-C1-C2	-2.08	108.00	111.29
6	Z	2	NAG	O4-C4-C3	2.08	115.15	110.35
6	k	2	NAG	C1-O5-C5	2.06	114.98	112.19
6	k	1	NAG	C4-C3-C2	-2.05	108.01	111.02
6	U	2	NAG	C3-C4-C5	2.04	113.88	110.24
6	d	2	NAG	C1-O5-C5	2.04	114.96	112.19
7	S	2	NAG	C3-C4-C5	2.04	113.88	110.24
6	R	1	NAG	O4-C4-C5	-2.04	104.23	109.30
7	c	2	NAG	C3-C4-C5	2.03	113.86	110.24
7	h	2	NAG	O3-C3-C2	-2.02	105.28	109.47
6	k	2	NAG	O5-C1-C2	-2.01	108.11	111.29
6	k	2	NAG	C4-C3-C2	-2.01	108.07	111.02
7	s	2	NAG	O3-C3-C2	-2.01	105.31	109.47
6	o	2	NAG	O5-C5-C4	-2.01	105.94	110.83
6	j	3	BMA	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	k	1	NAG	C3-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7
7	h	1	NAG	C1-C2-N2-C7
7	h	2	NAG	C1-C2-N2-C7
7	s	1	NAG	C1-C2-N2-C7
7	h	3	BMA	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	X	3	BMA	O5-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
7	X	3	BMA	C4-C5-C6-O6
7	h	3	BMA	C4-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
6	l	2	NAG	C1-C2-N2-C7
6	N	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	s	3	BMA	O5-C5-C6-O6
7	s	3	BMA	C4-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C1-C2-N2-C7
6	Q	2	NAG	C1-C2-N2-C7
5	M	2	NAG	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
6	o	1	NAG	C1-C2-N2-C7
7	s	1	NAG	C4-C5-C6-O6
6	k	1	NAG	O5-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	C1-C2-N2-C7
6	a	2	NAG	C1-C2-N2-C7
7	S	3	BMA	O5-C5-C6-O6
6	k	1	NAG	C4-C5-C6-O6
6	m	1	NAG	C1-C2-N2-C7
7	c	3	BMA	O5-C5-C6-O6
7	n	3	BMA	O5-C5-C6-O6
6	T	3	BMA	C4-C5-C6-O6
6	m	1	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	k	1	NAG	C1-C2-N2-C7
6	b	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C1-C2-N2-C7
7	S	1	NAG	O5-C5-C6-O6
5	V	1	NAG	C3-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	q	1	NAG	C3-C2-N2-C7
6	O	2	NAG	C3-C2-N2-C7
6	o	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	n	2	NAG	C3-C2-N2-C7
6	l	1	NAG	O5-C5-C6-O6
6	R	1	NAG	C1-C2-N2-C7

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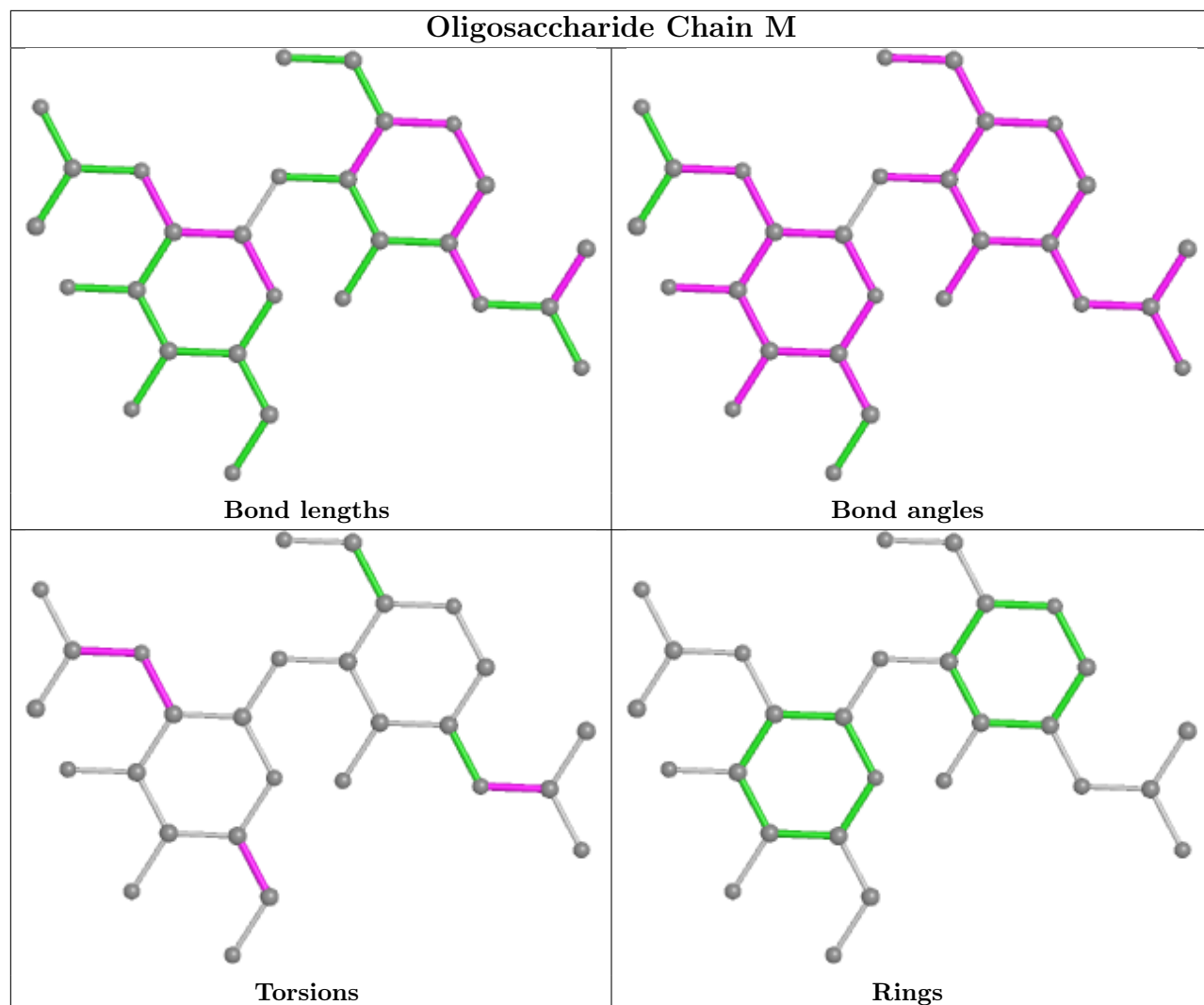
Mol	Chain	Res	Type	Atoms
6	T	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C1-C2-N2-C7
7	c	2	NAG	C1-C2-N2-C7
6	Q	1	NAG	C4-C5-C6-O6
7	S	2	NAG	C1-C2-N2-C7
6	U	1	NAG	C1-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
6	T	2	NAG	C3-C2-N2-C7
6	Y	2	NAG	C3-C2-N2-C7
6	Z	1	NAG	C3-C2-N2-C7
6	b	1	NAG	C3-C2-N2-C7
6	d	2	NAG	C3-C2-N2-C7
6	j	2	NAG	C3-C2-N2-C7
6	o	1	NAG	C3-C2-N2-C7
7	S	2	NAG	C3-C2-N2-C7
7	c	2	NAG	C3-C2-N2-C7
7	s	2	NAG	C3-C2-N2-C7
6	l	2	NAG	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
6	o	2	NAG	C1-C2-N2-C7

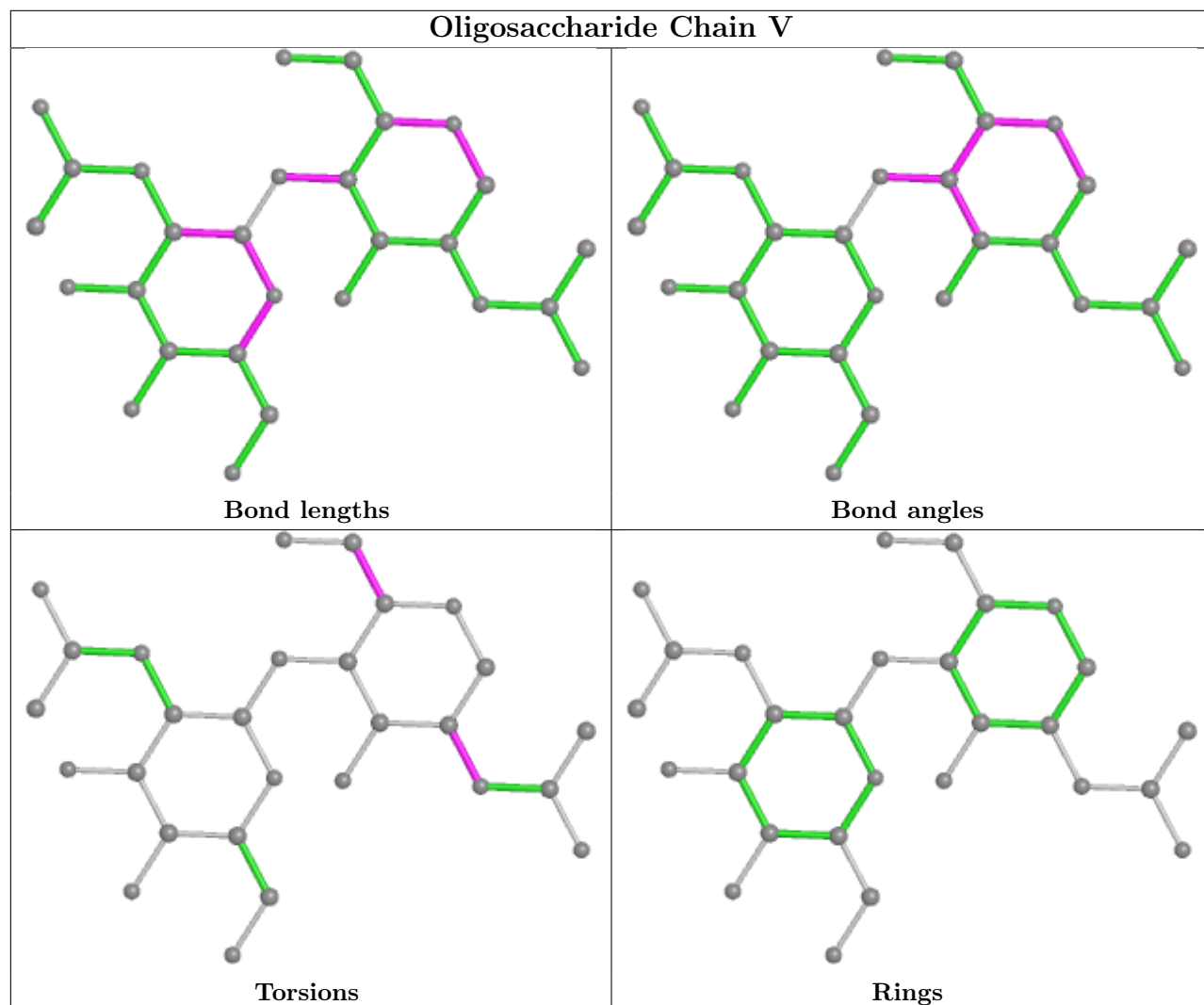
There are no ring outliers.

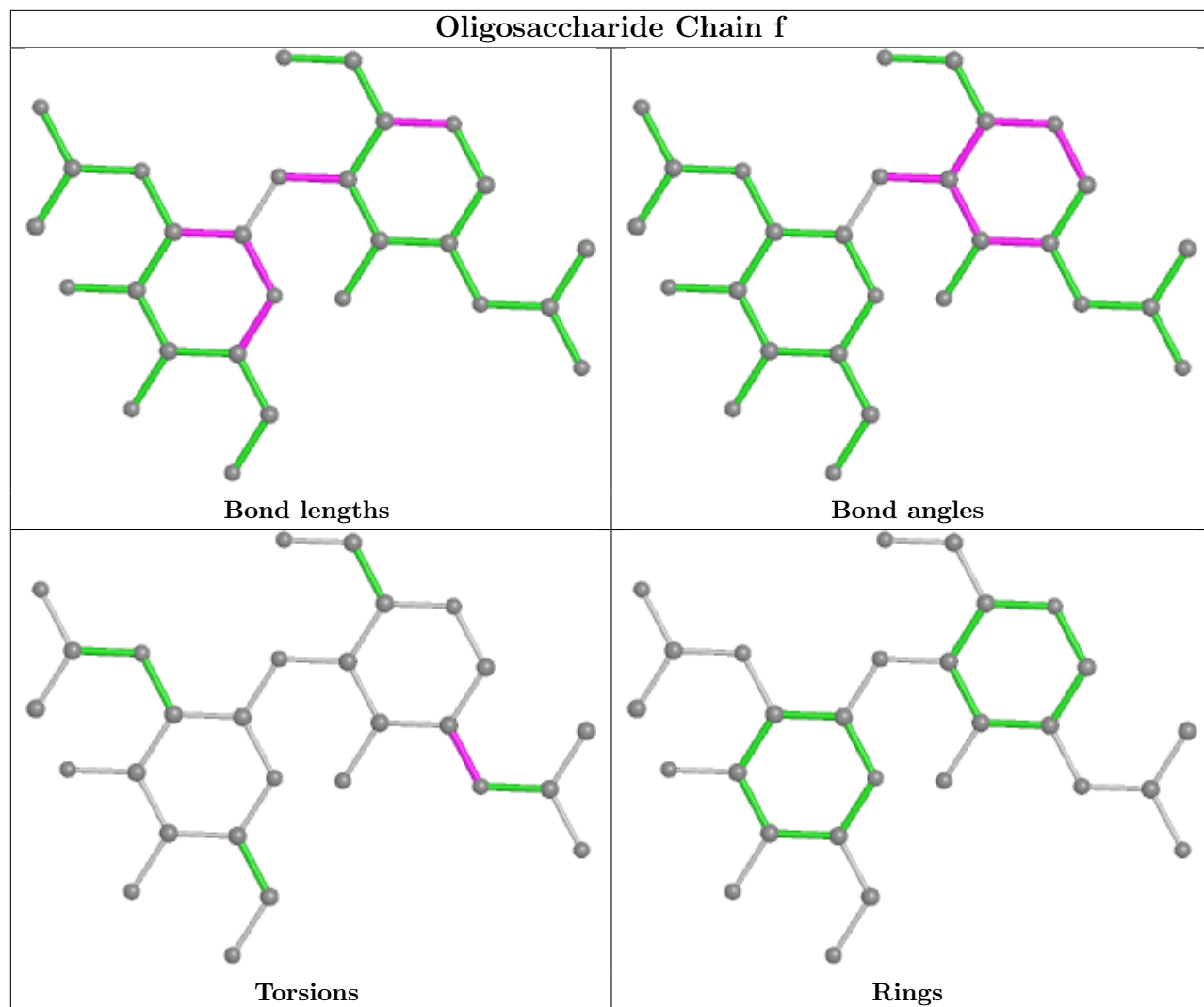
1 monomer is involved in 2 short contacts:

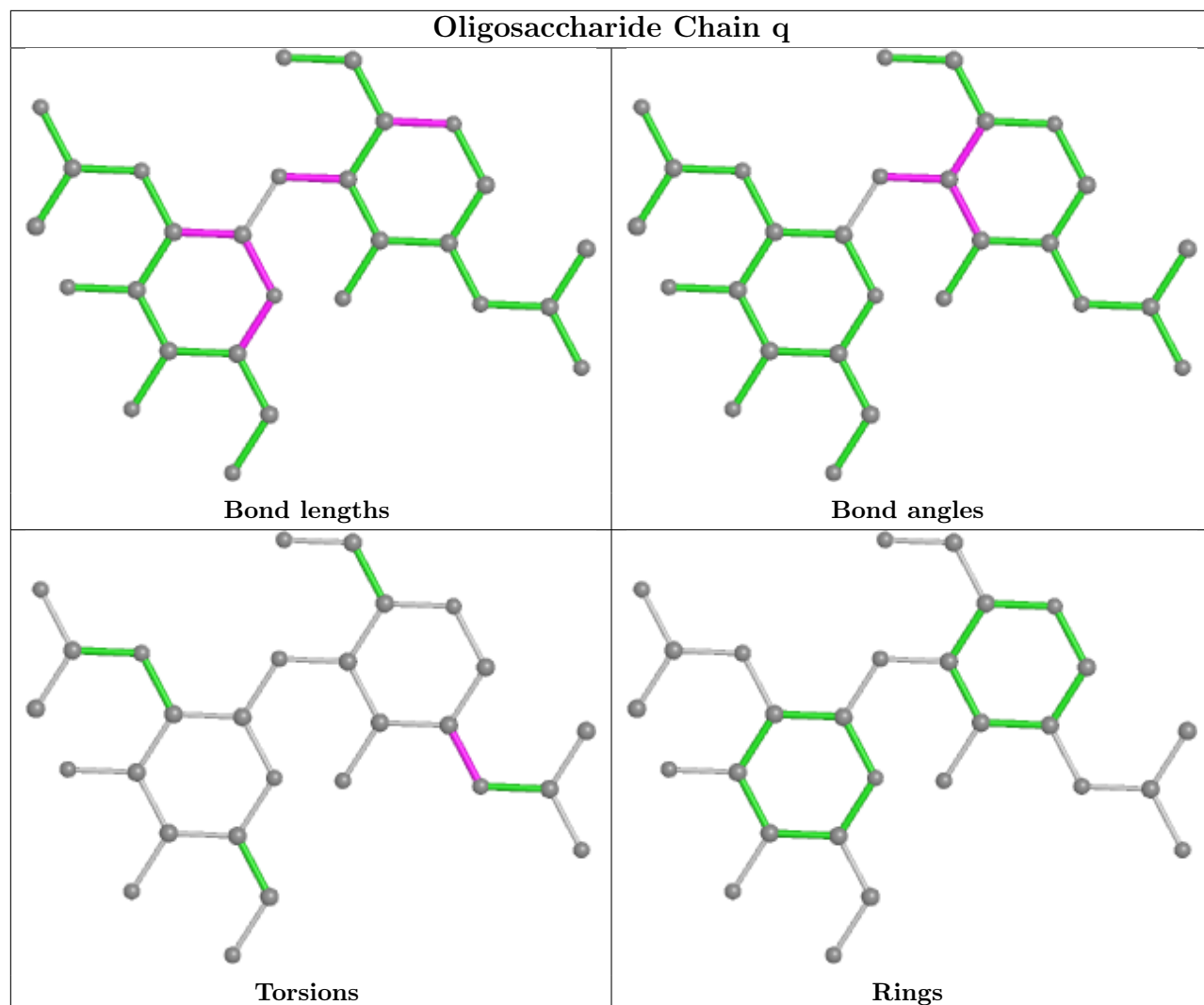
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	1	NAG	2	0

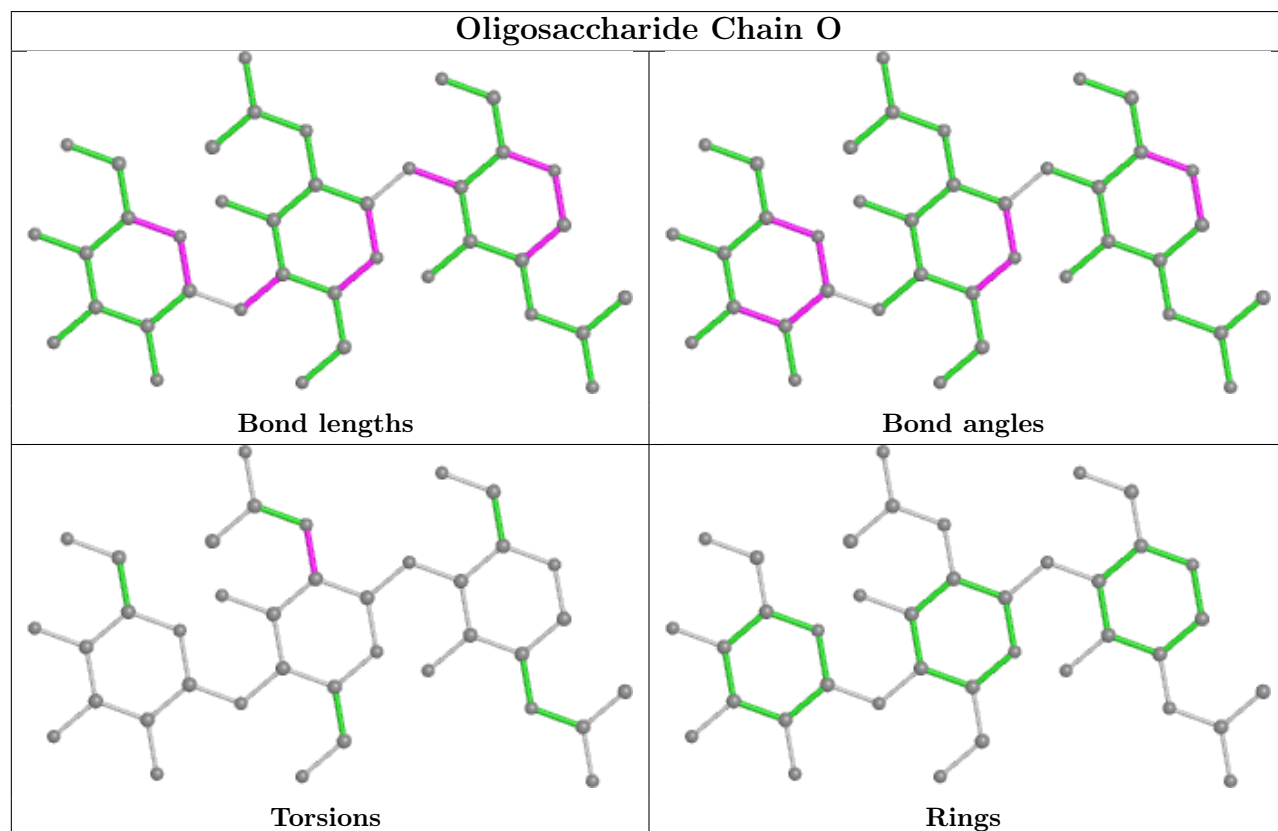
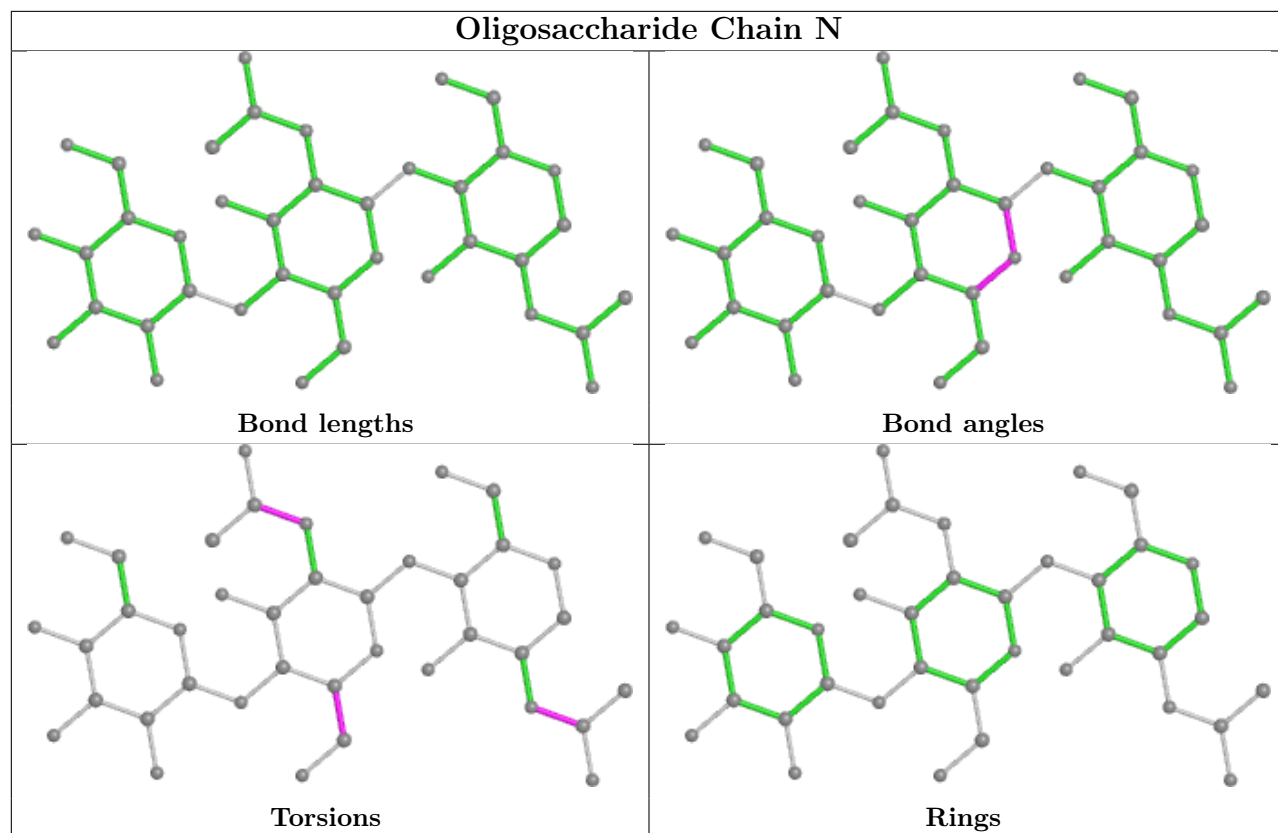
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

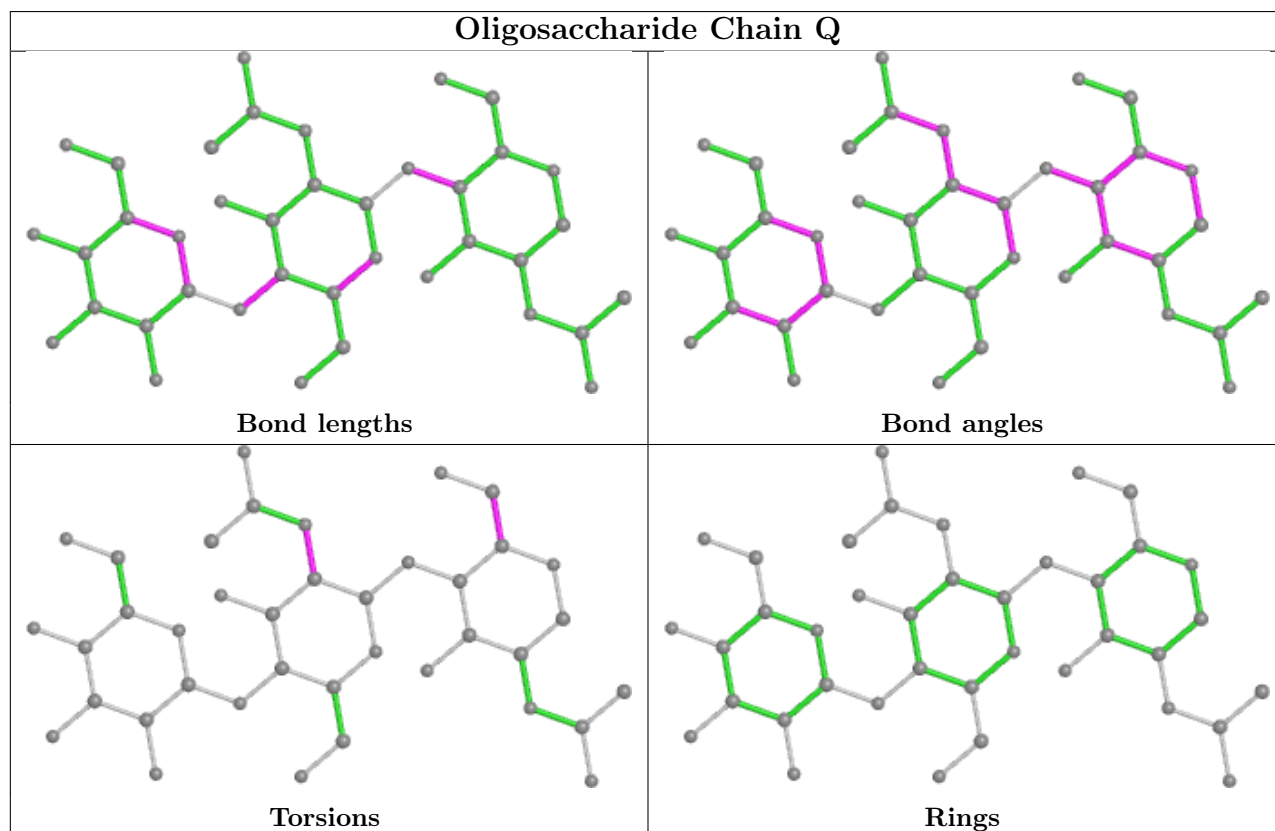
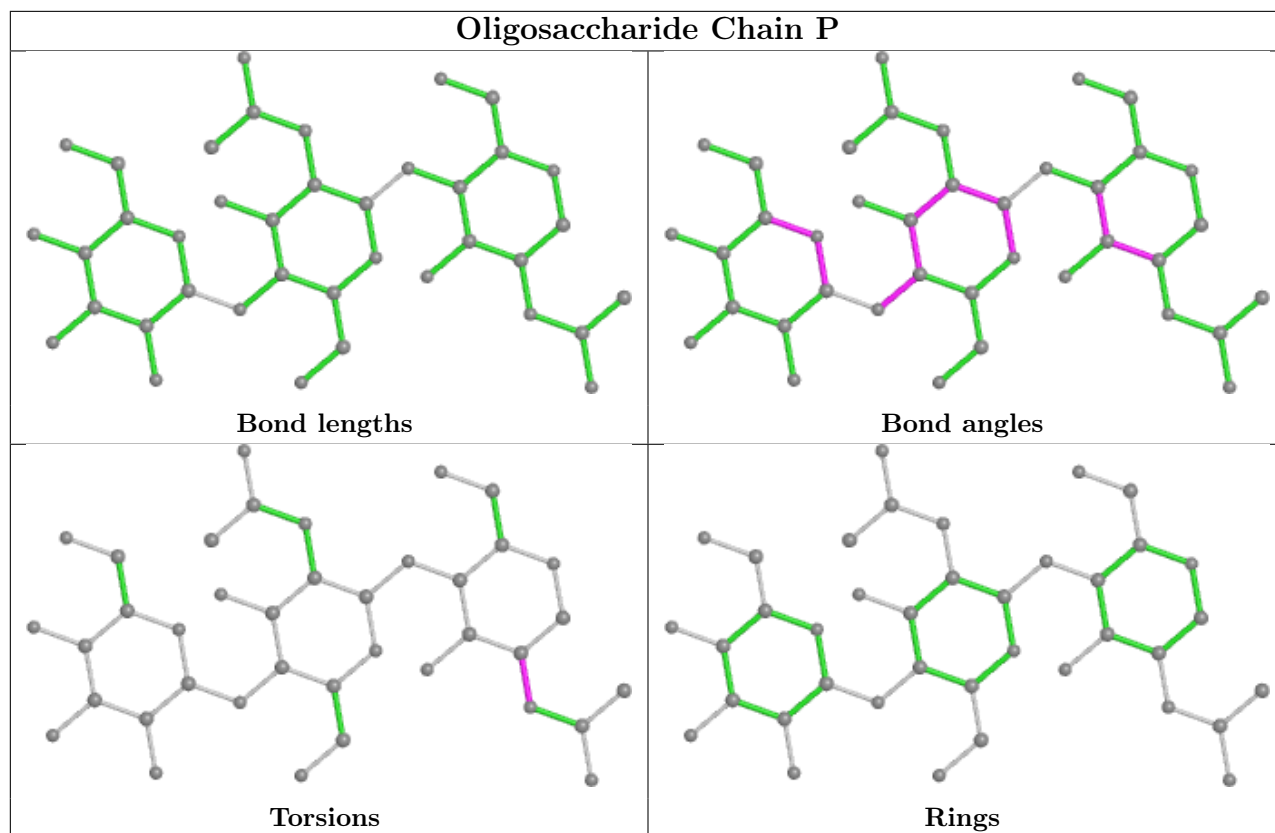


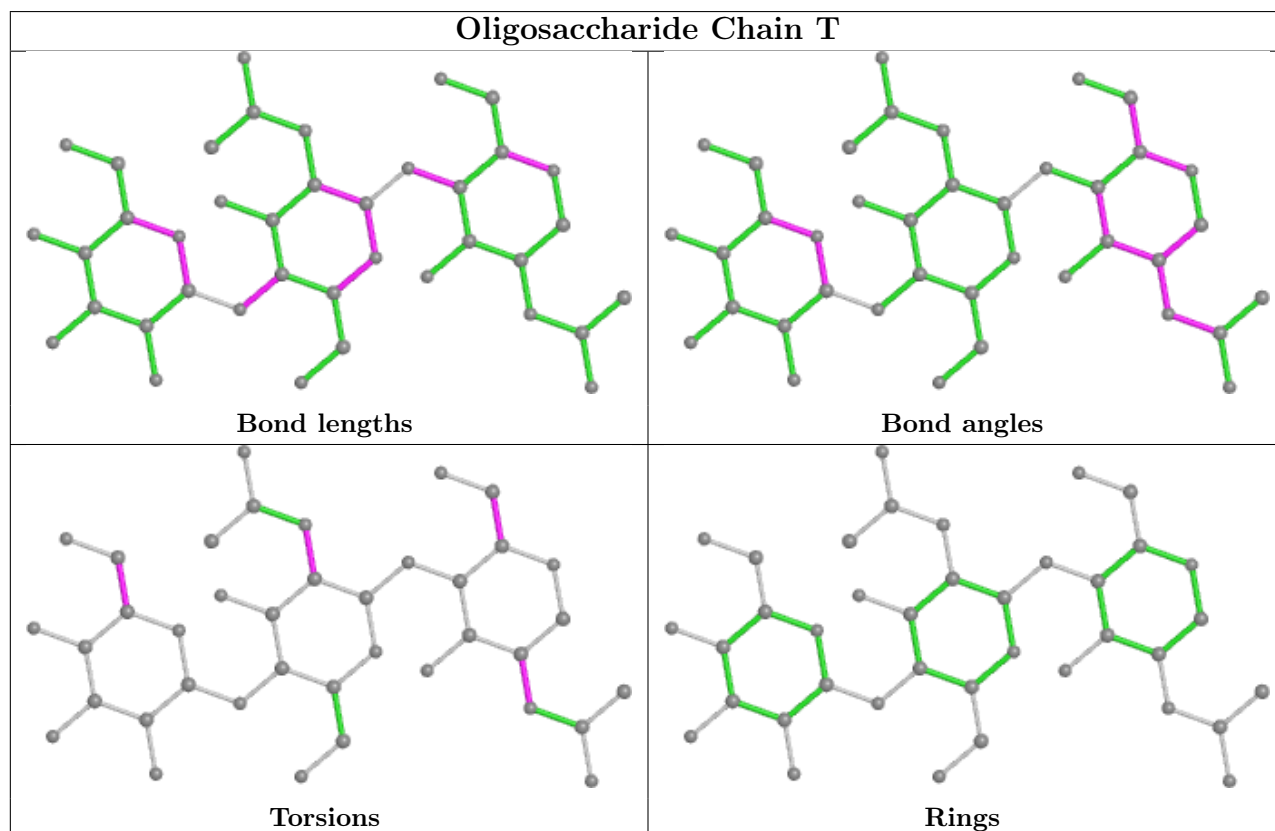
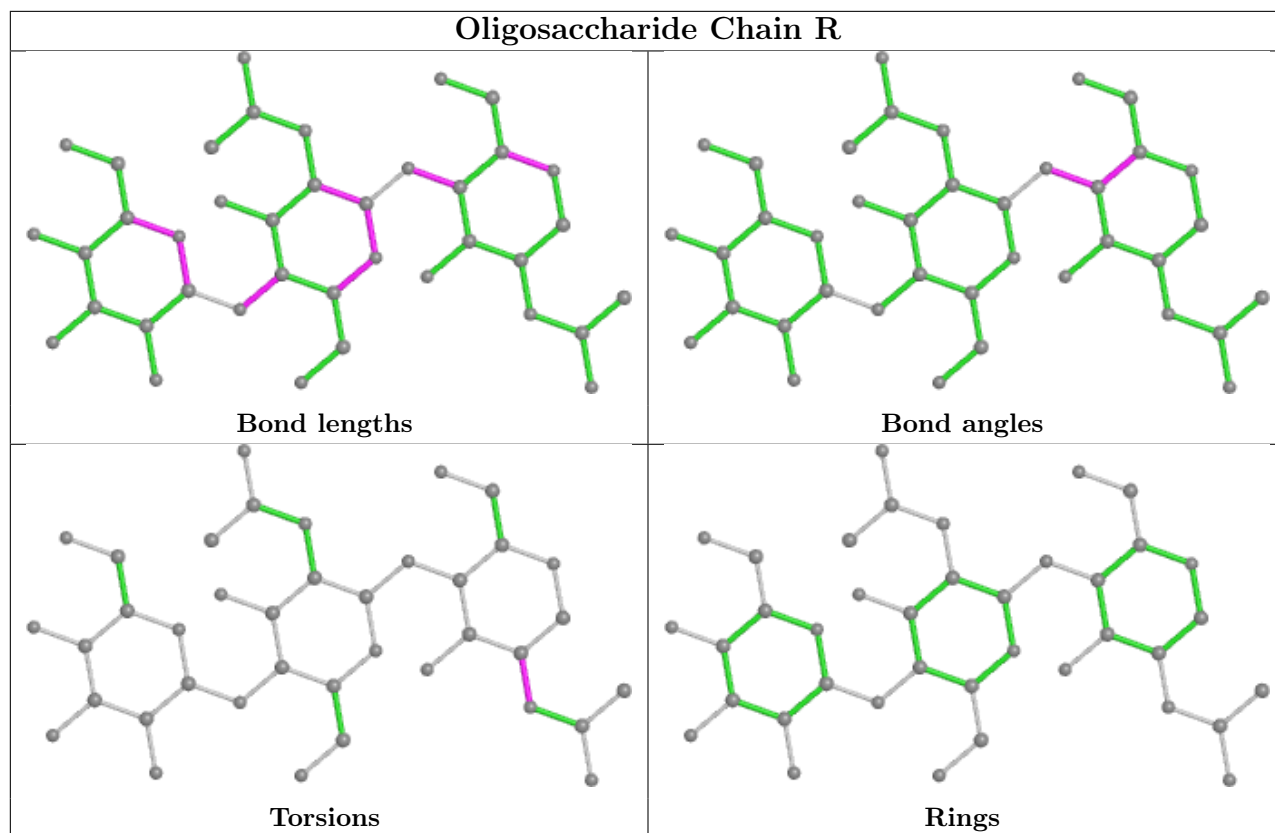


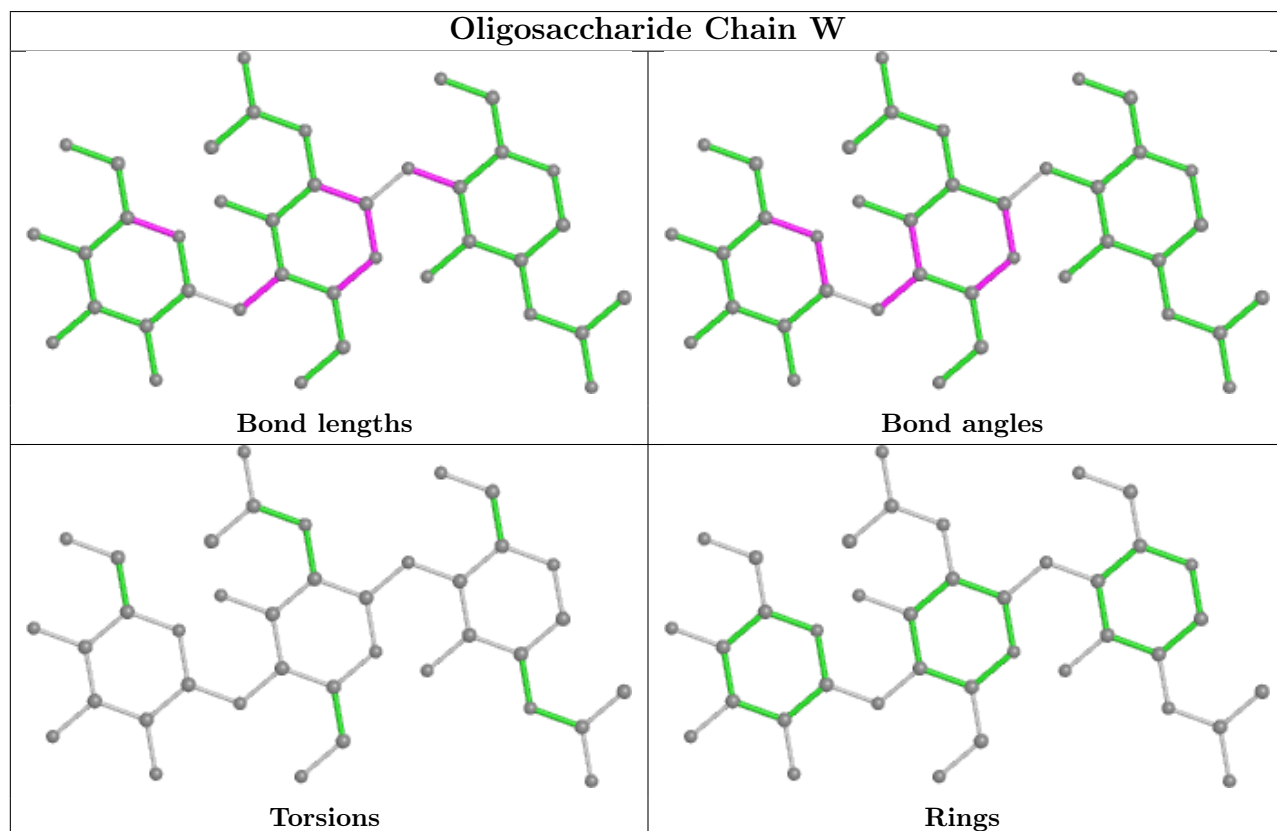
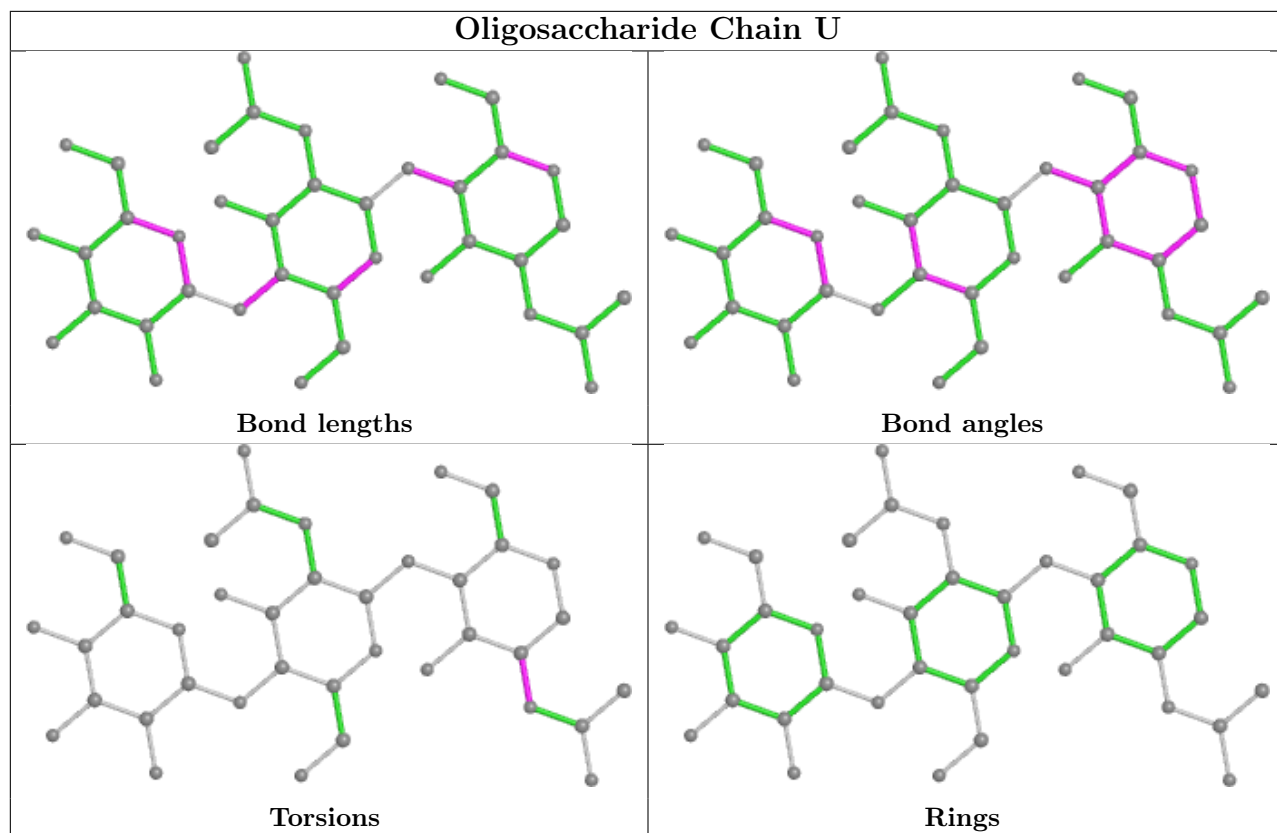


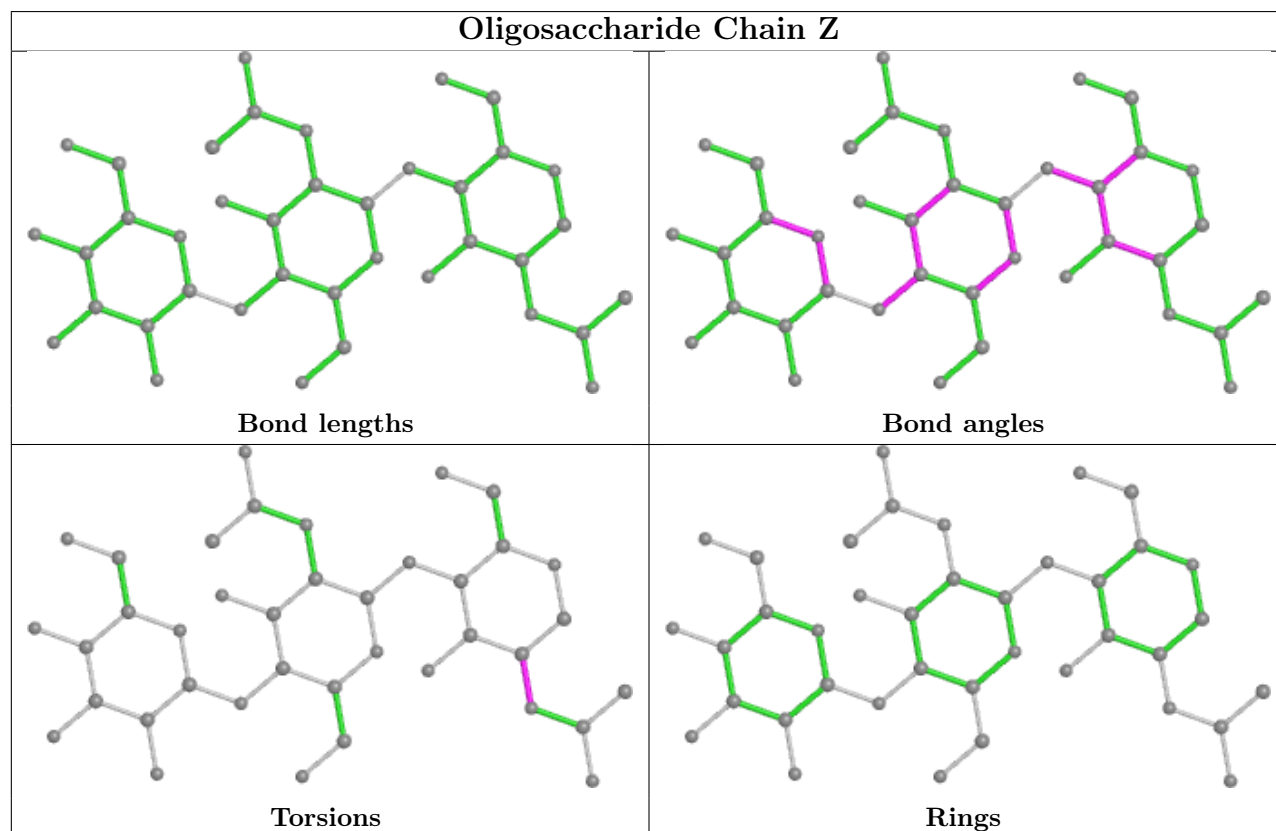
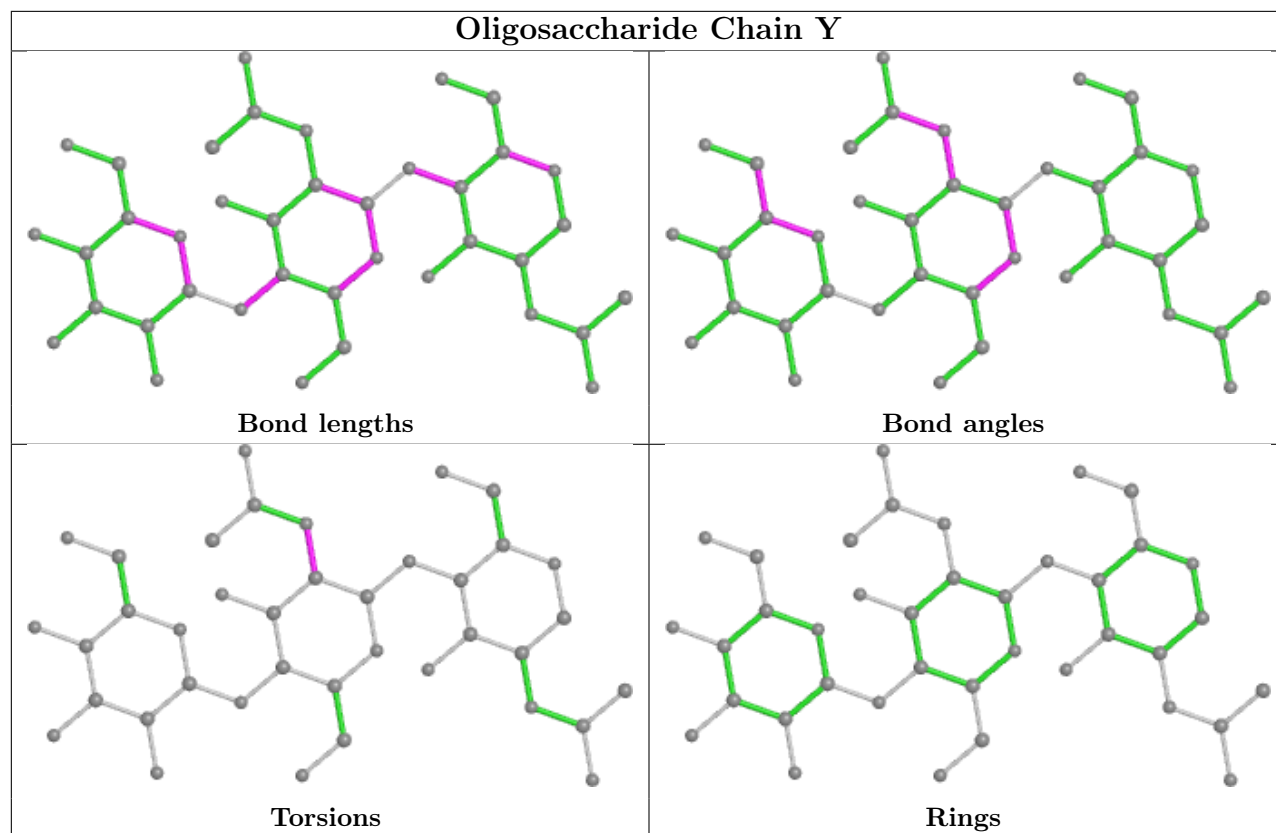


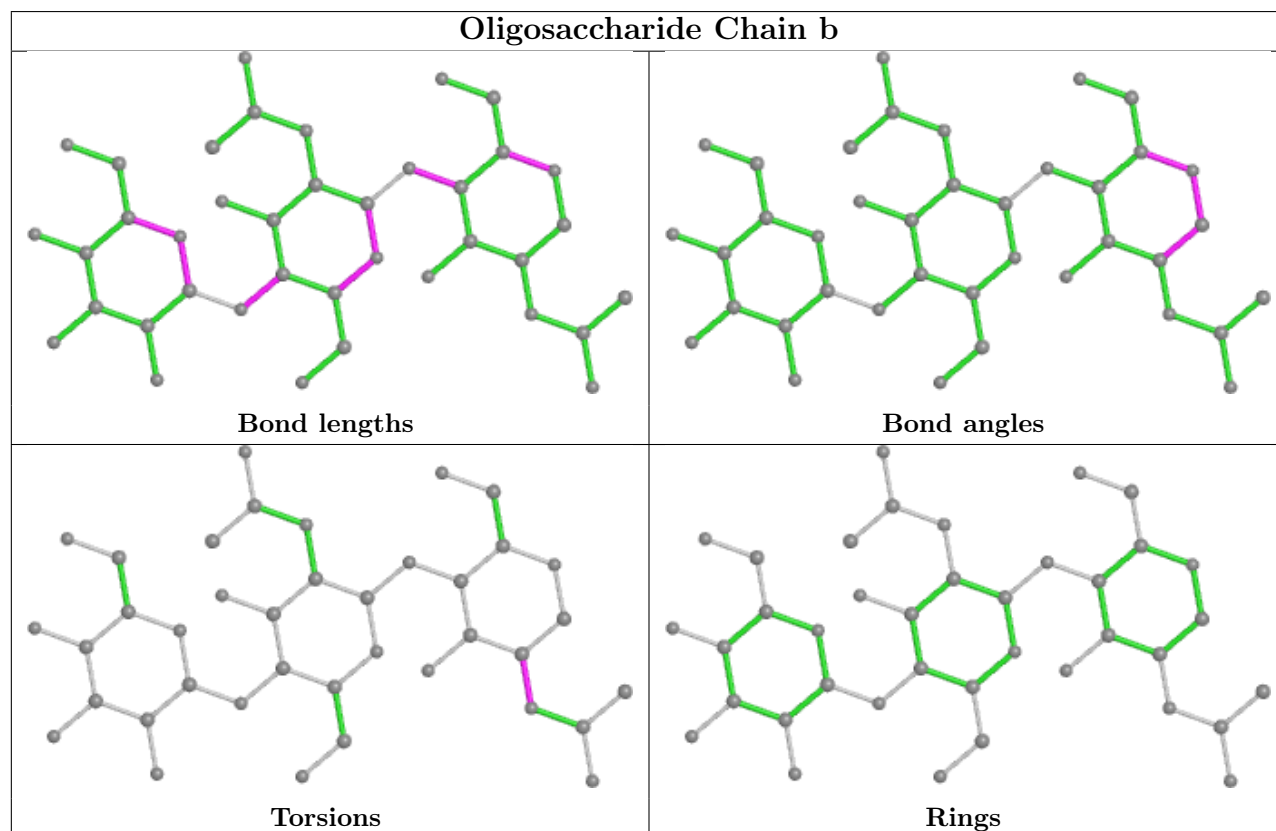
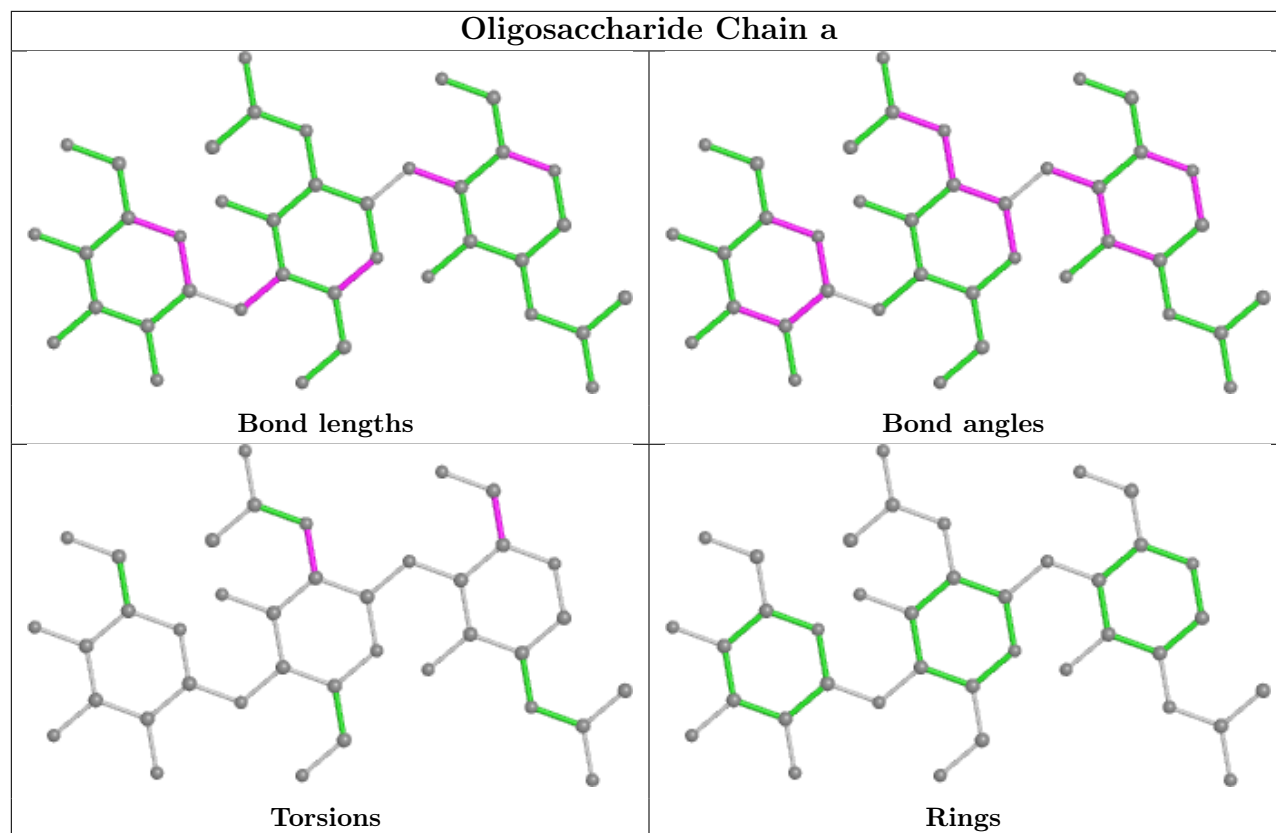


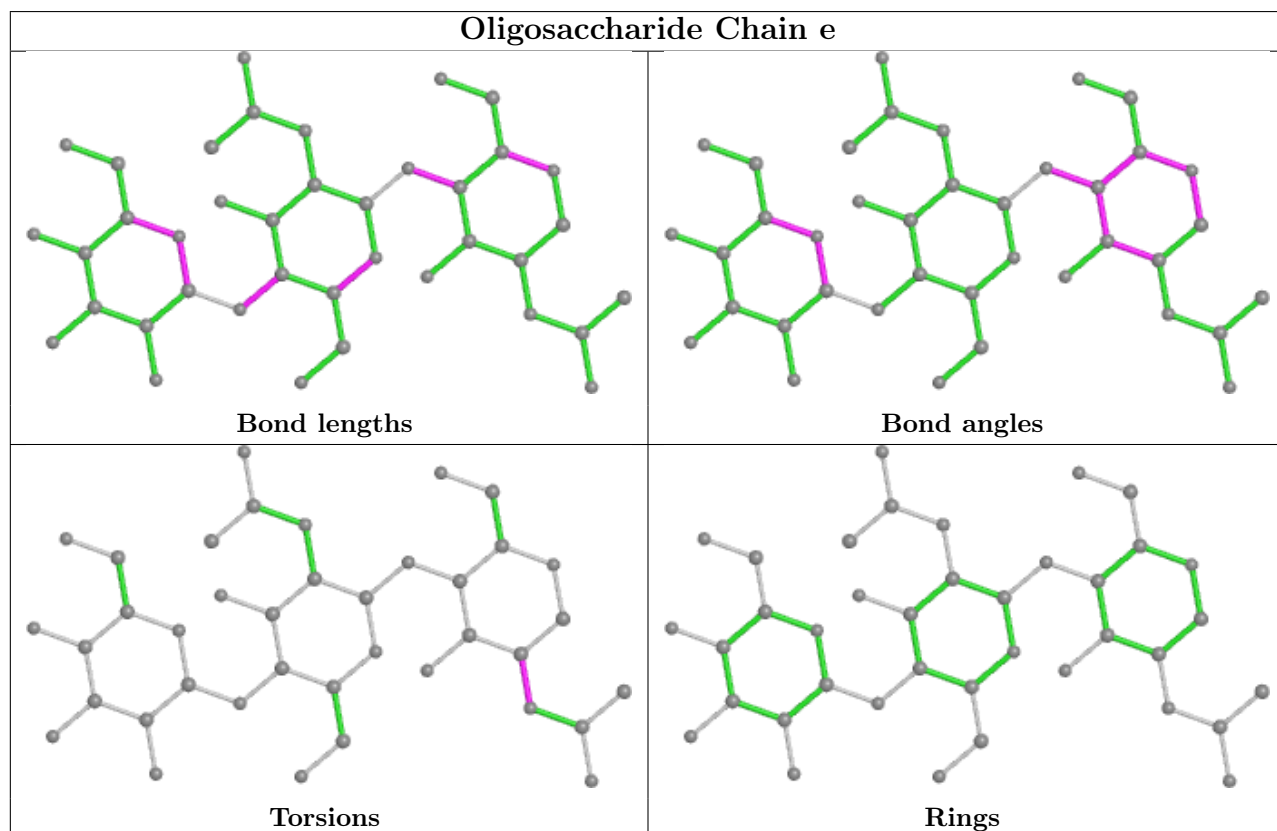
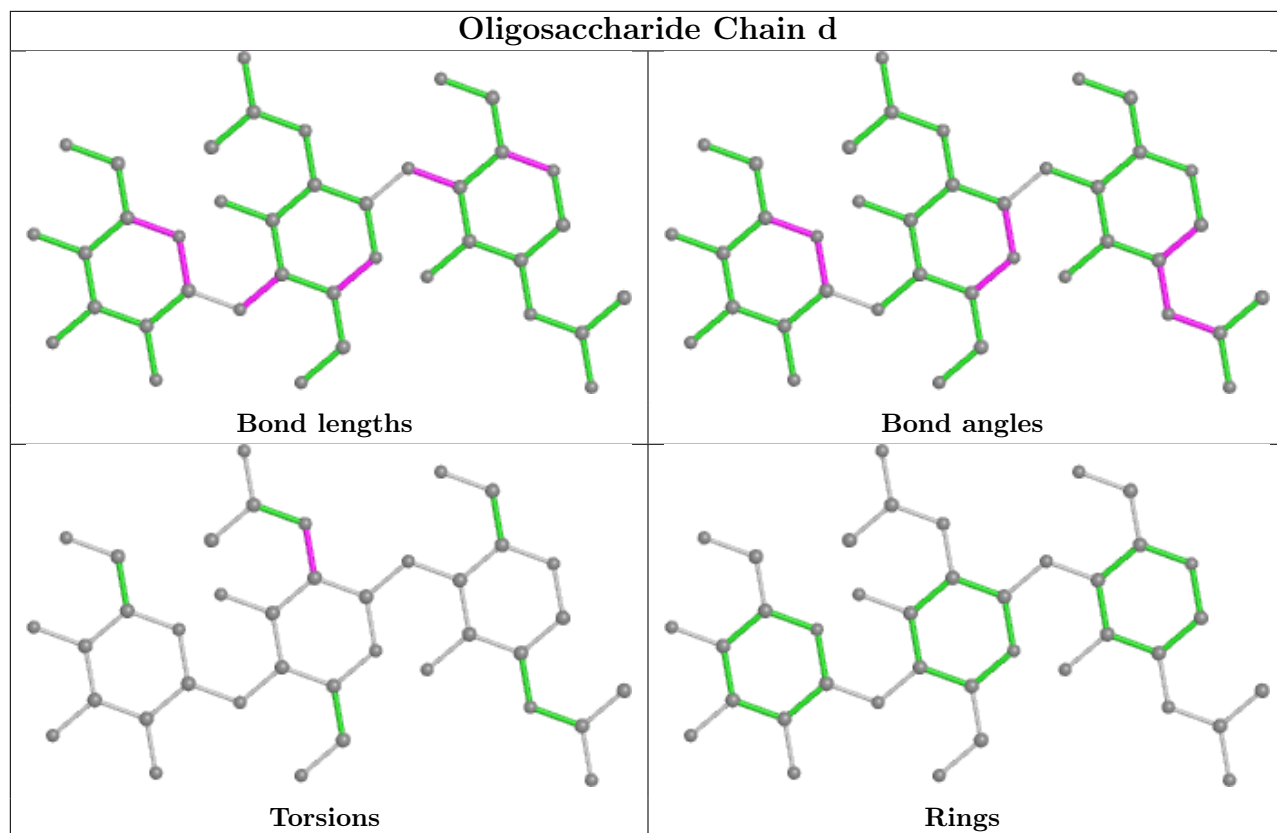


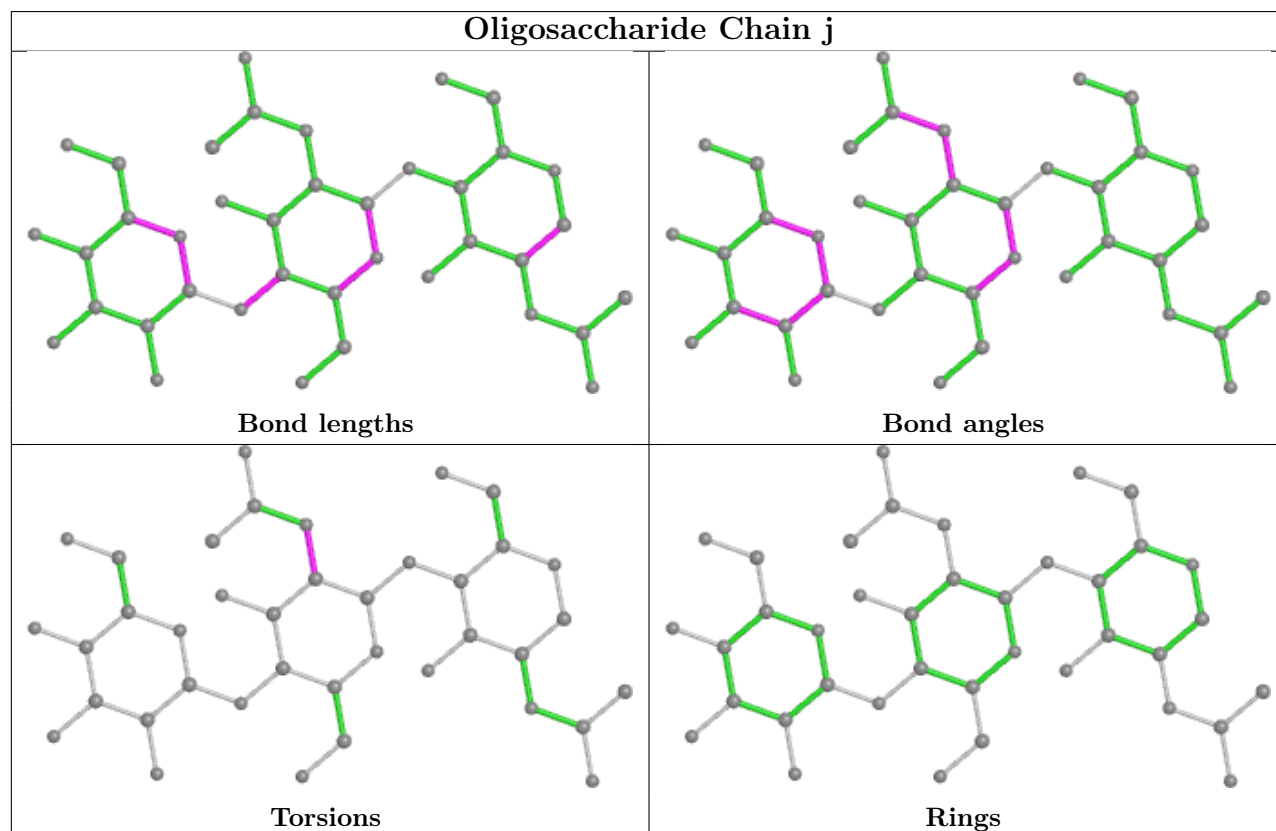
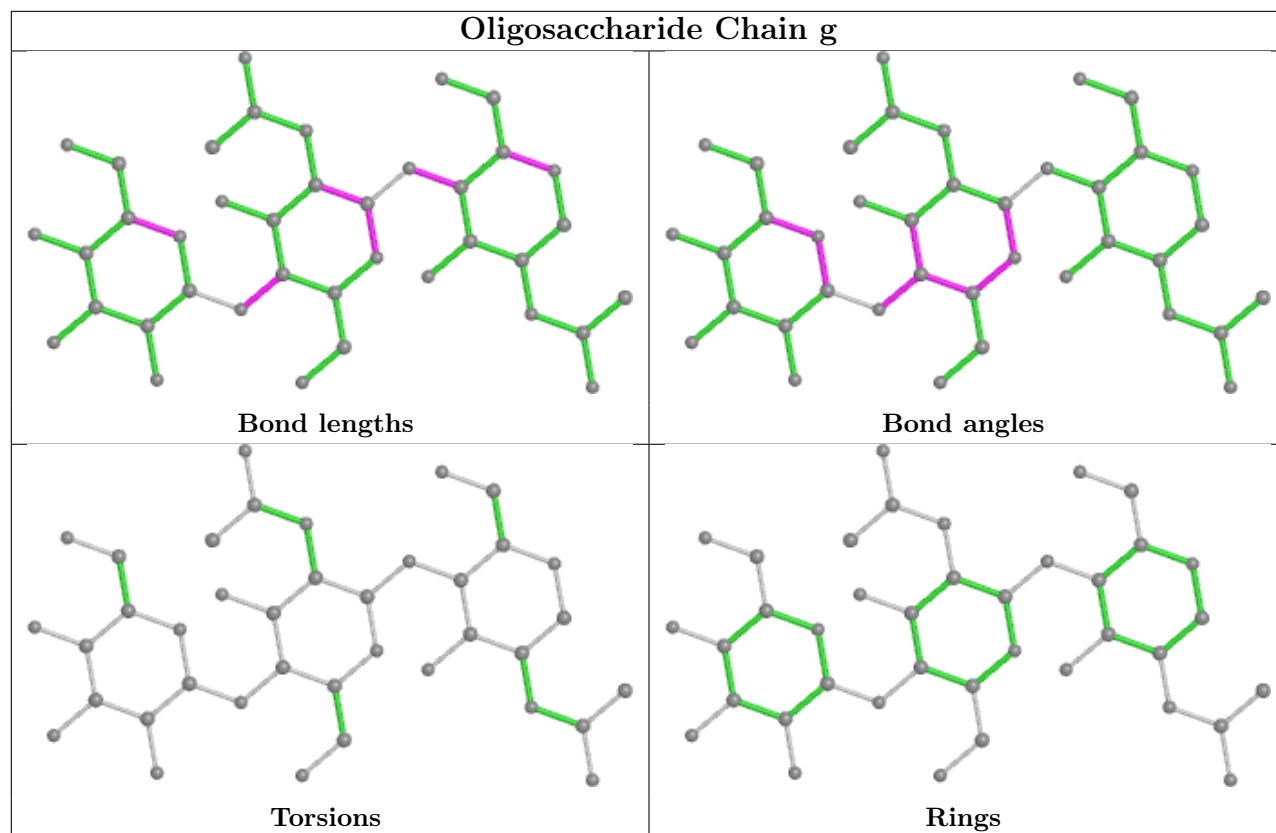


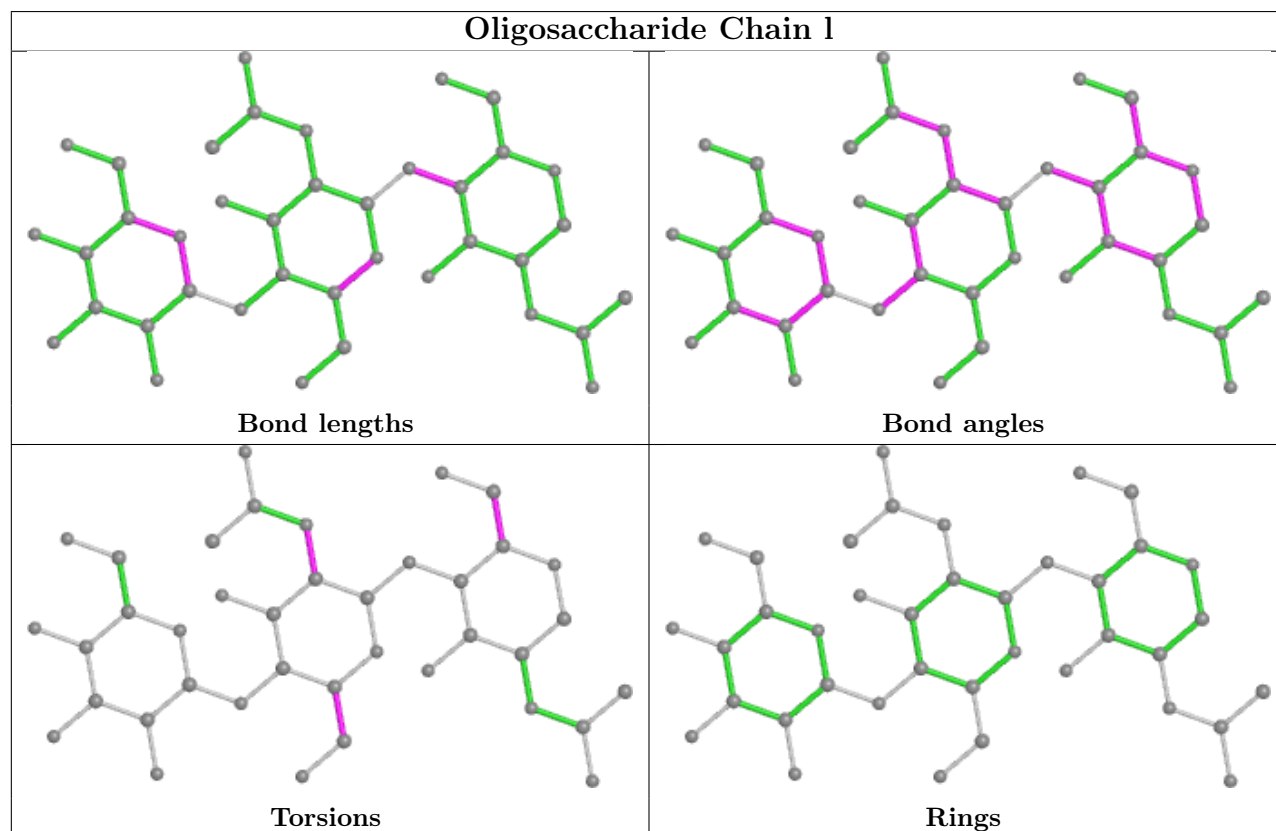
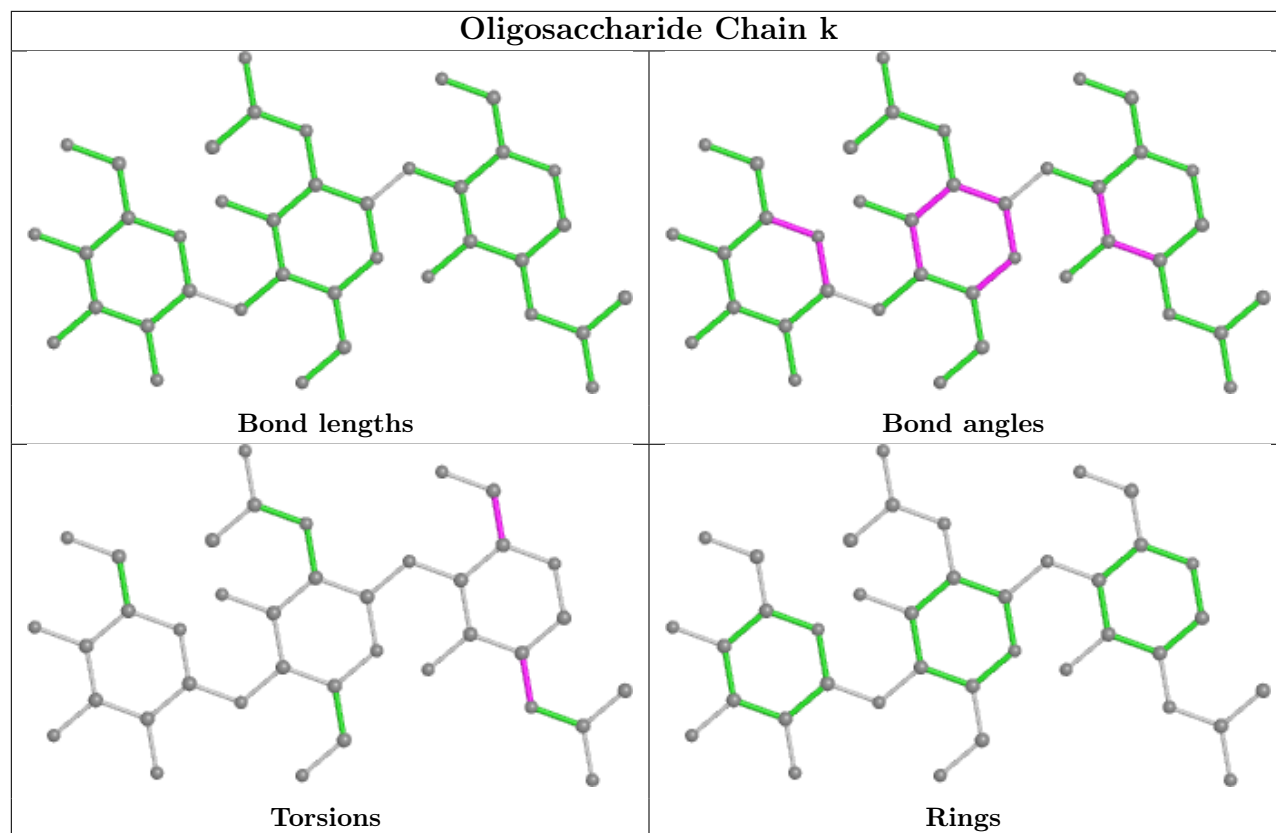


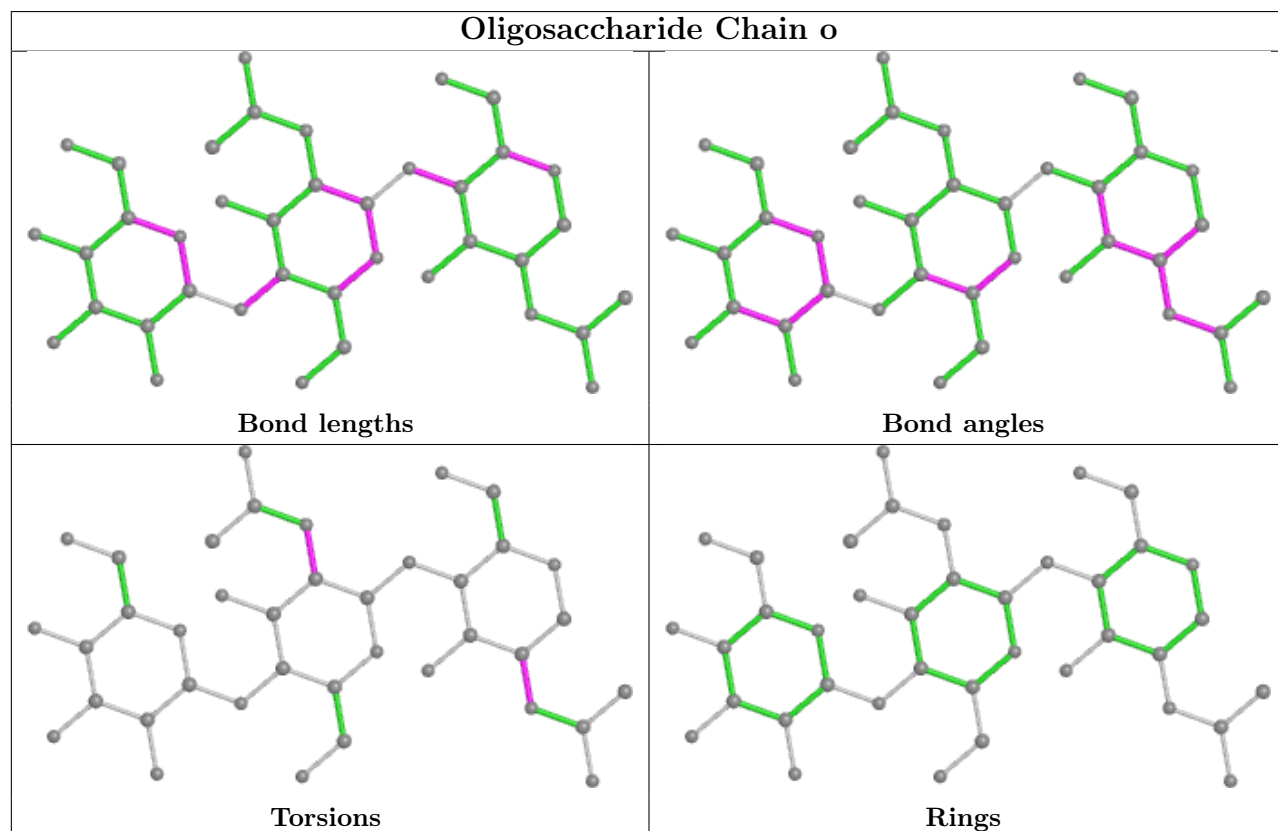
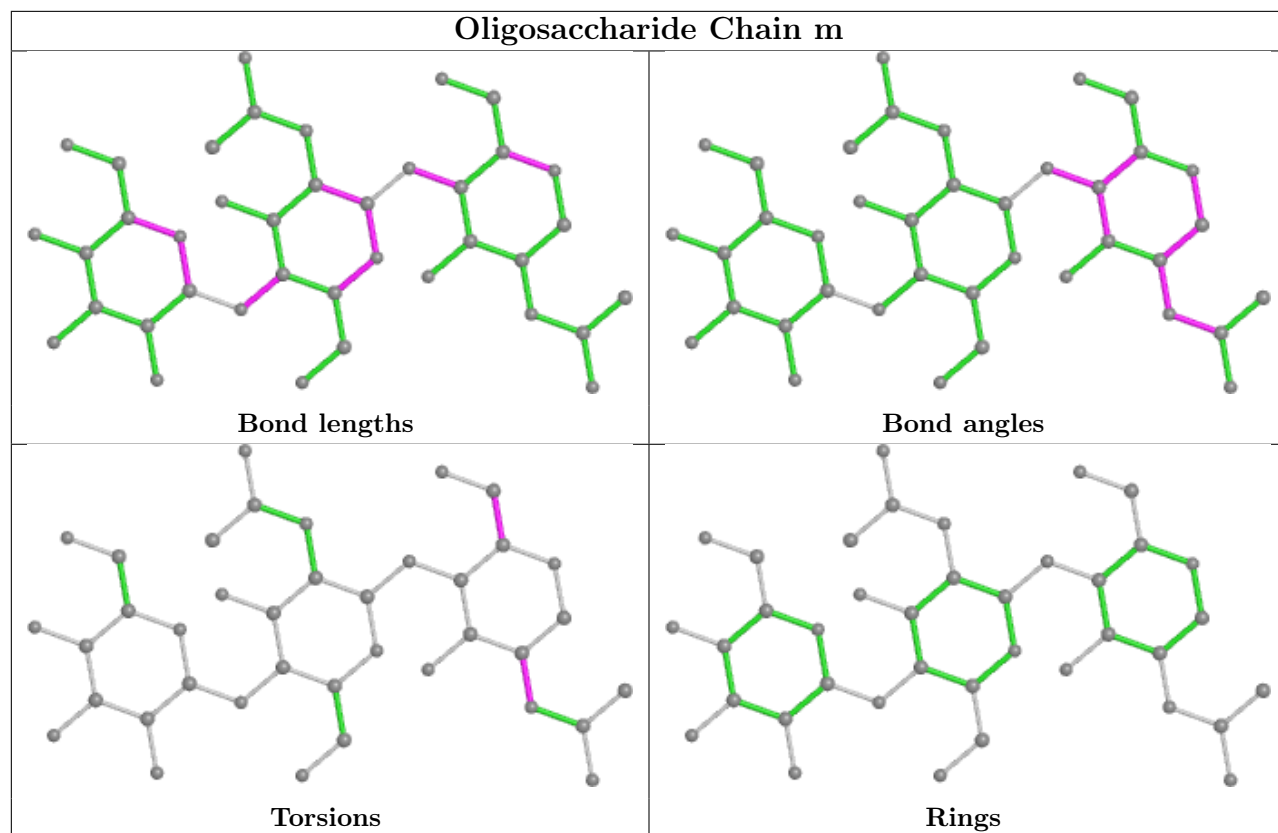


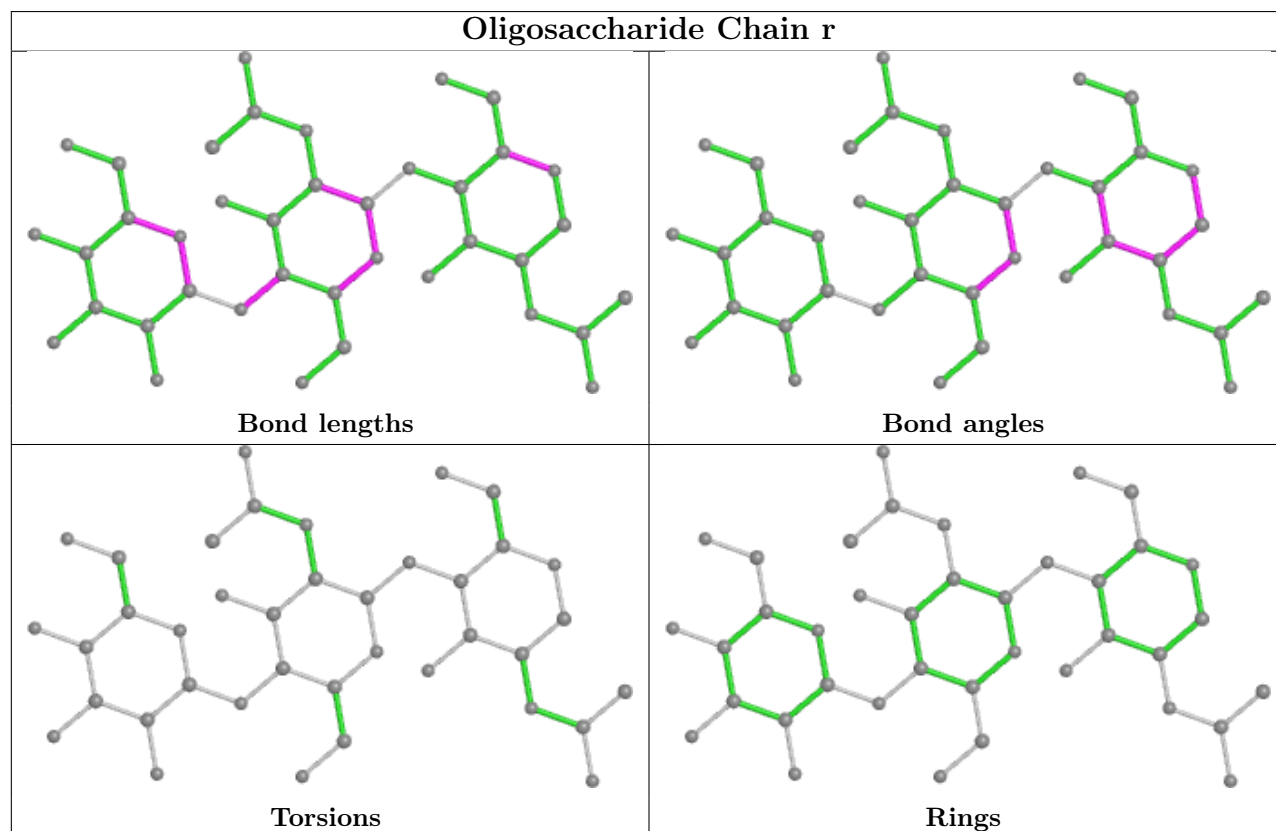
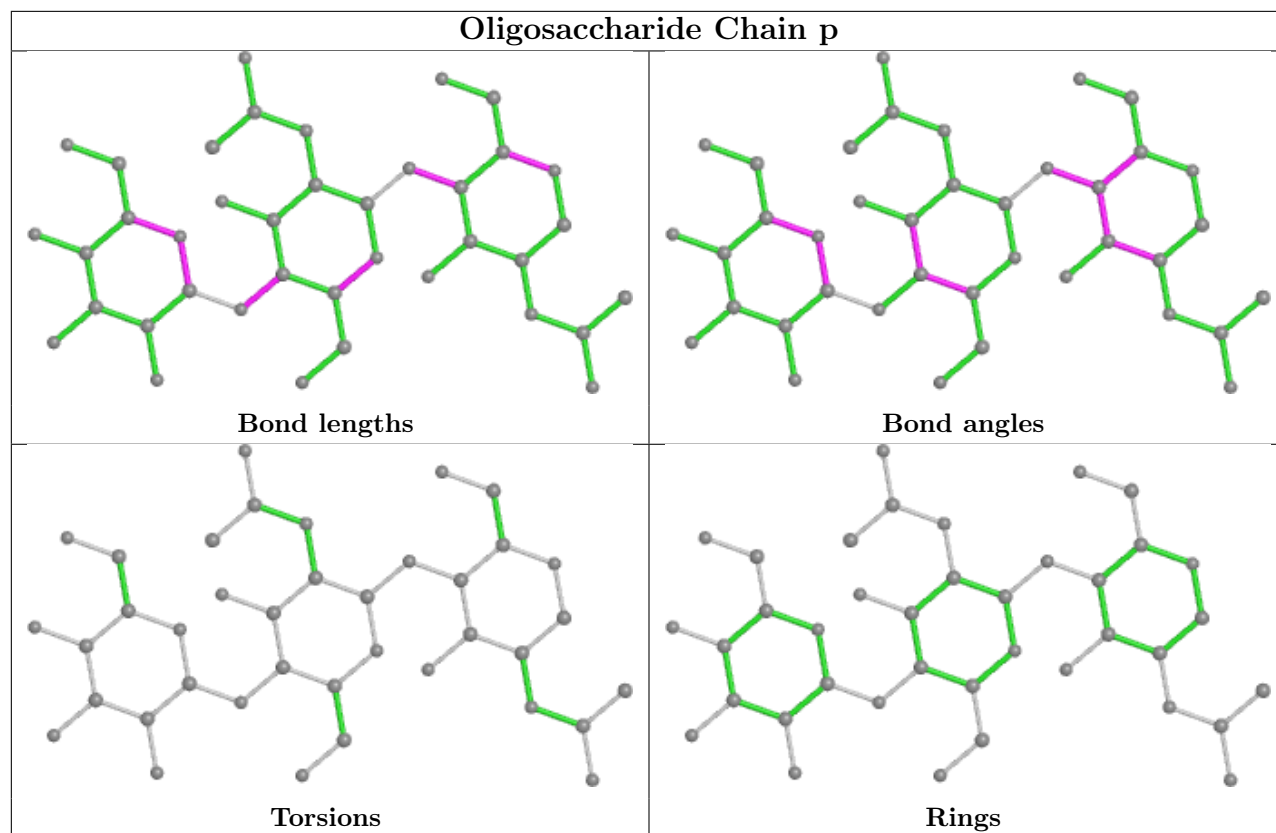


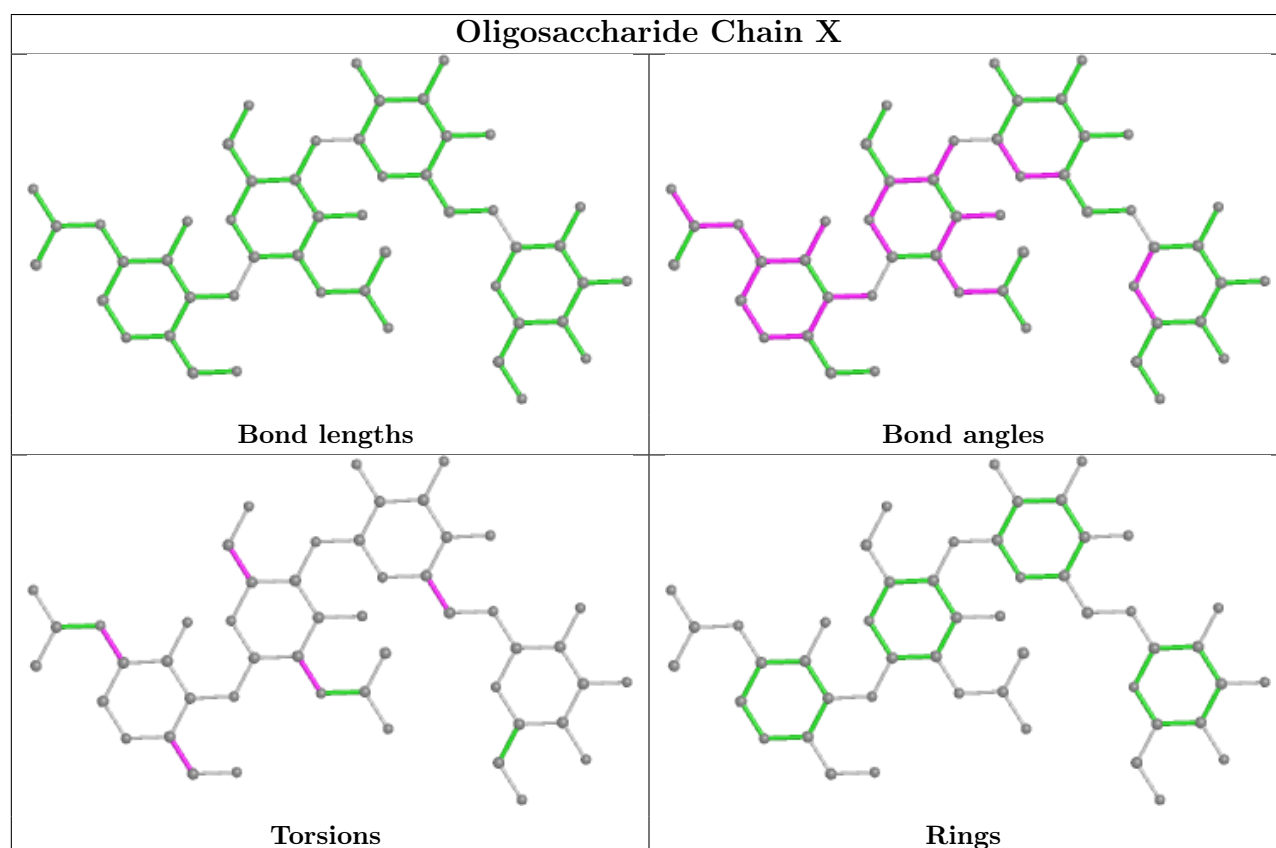
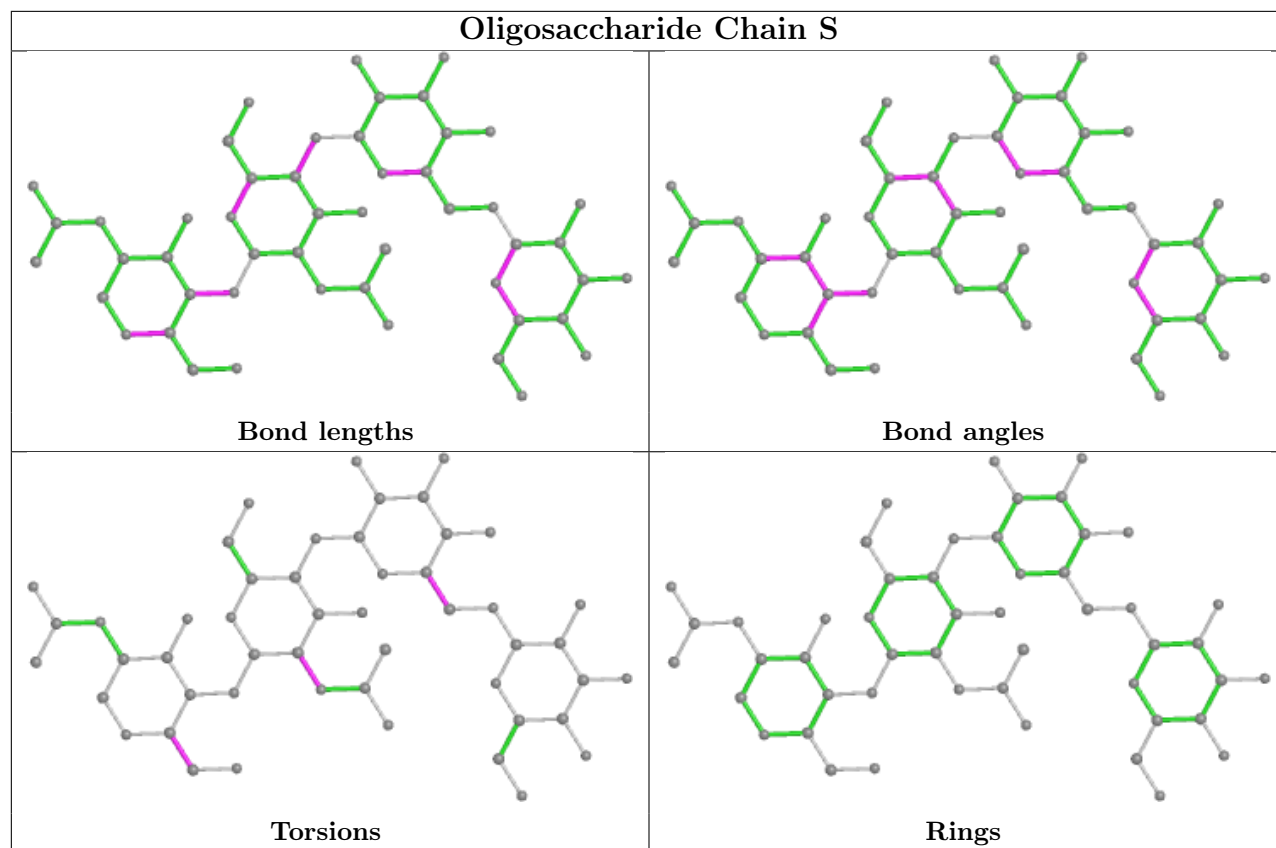


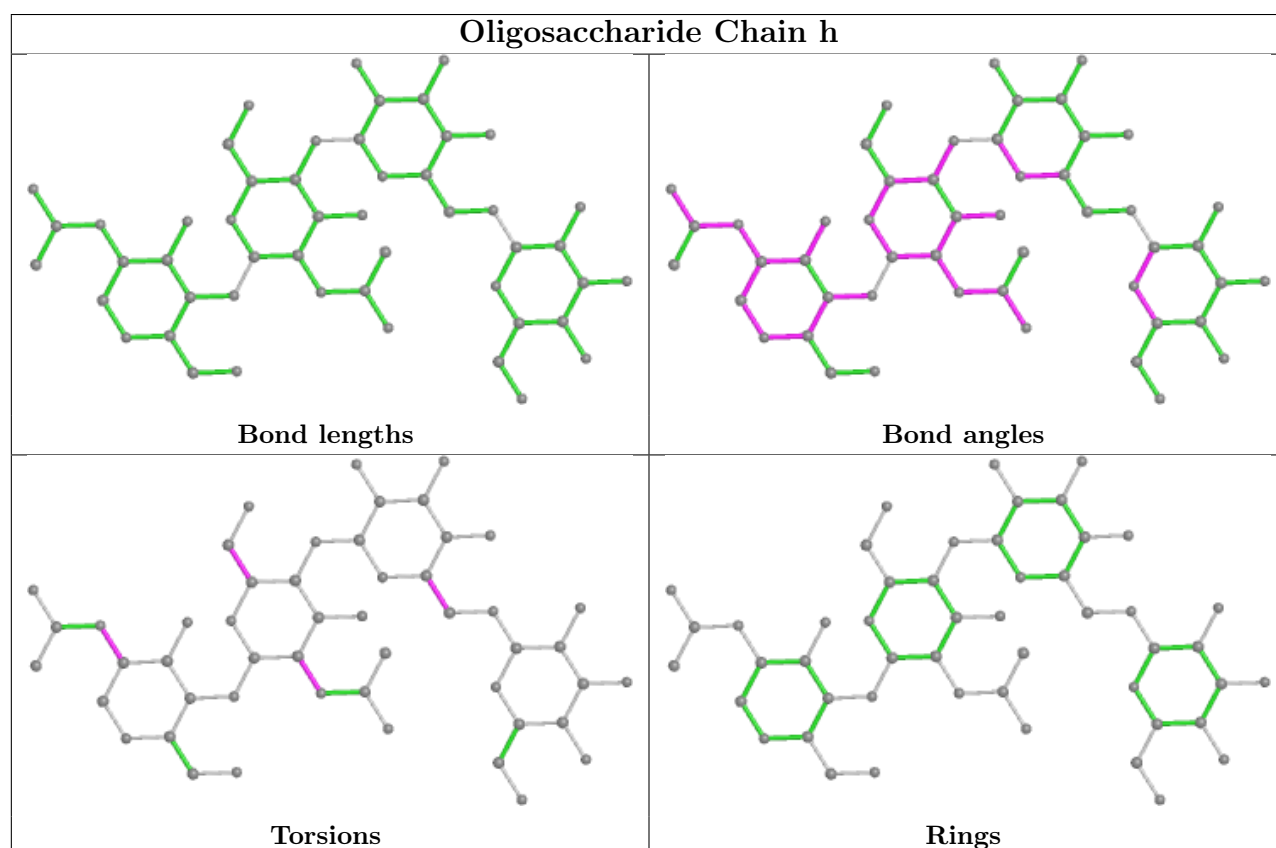
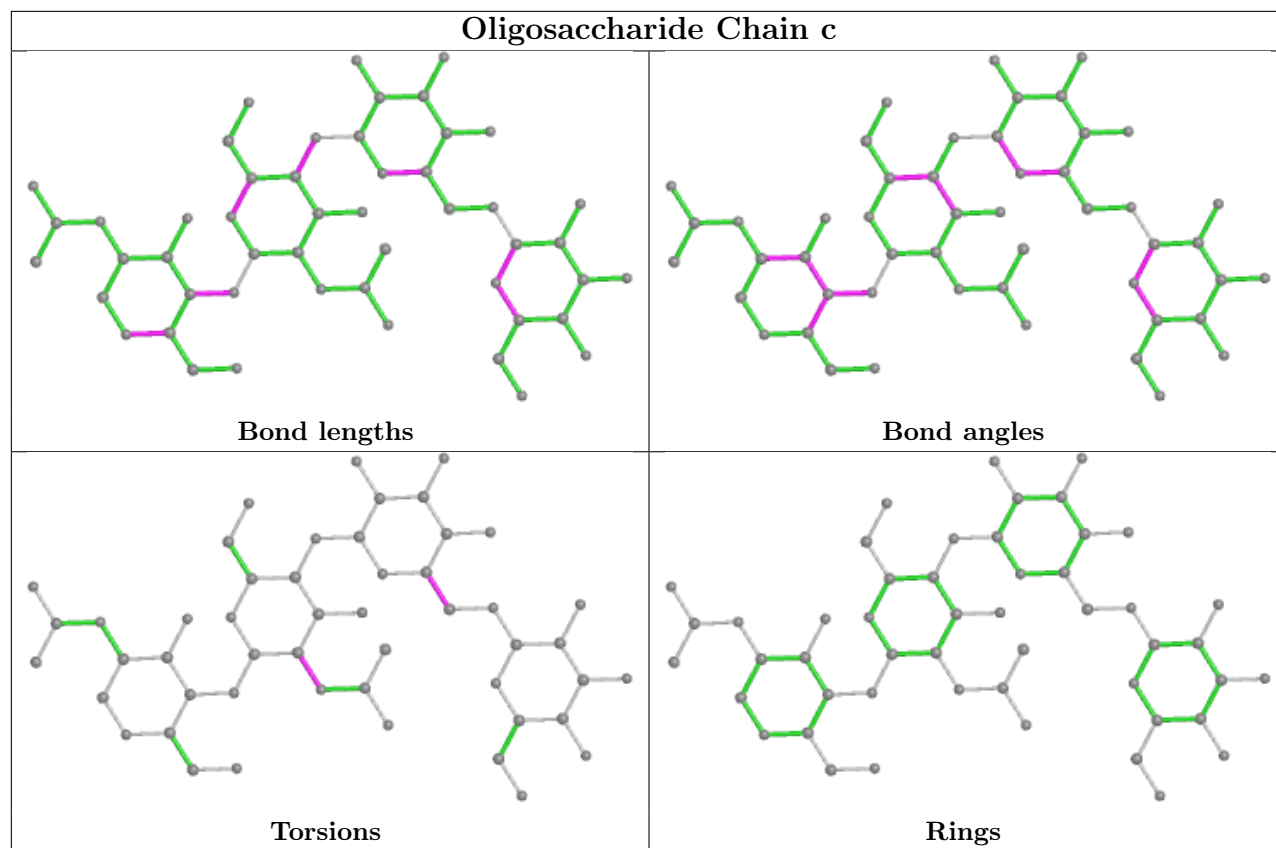


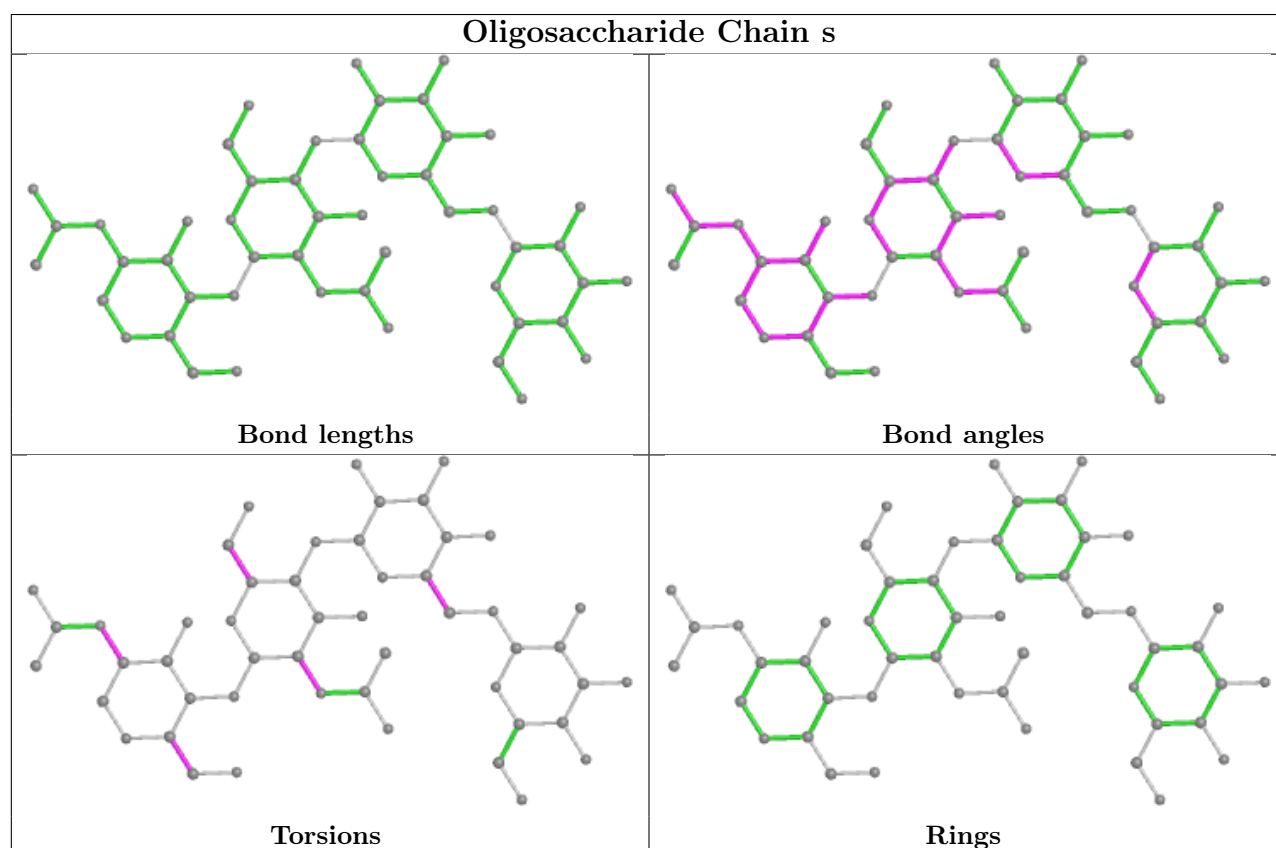
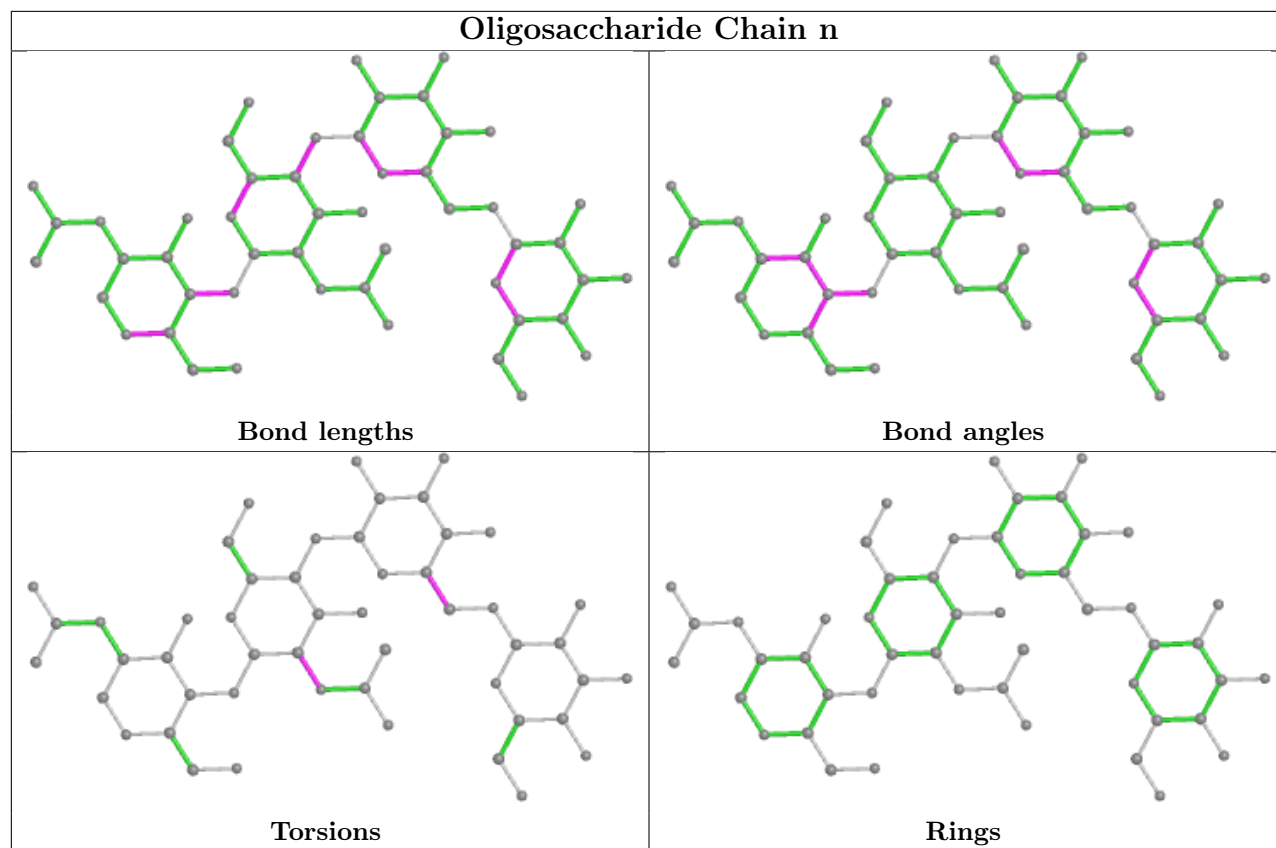












5.6 Ligand geometry

10 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
8	NAG	A	604	1	14,14,15	0.45	0	17,19,21	1.37	4 (23%)
8	NAG	A	602	1	14,14,15	1.21	2 (14%)	17,19,21	1.11	1 (5%)
8	NAG	A	603	1	14,14,15	1.20	2 (14%)	17,19,21	1.10	1 (5%)
8	NAG	I	603	1	14,14,15	1.21	2 (14%)	17,19,21	1.16	1 (5%)
8	NAG	E	601	1	14,14,15	1.06	1 (7%)	17,19,21	0.94	1 (5%)
8	NAG	E	602	1	14,14,15	1.23	3 (21%)	17,19,21	1.16	2 (11%)
8	NAG	I	601	1	14,14,15	1.21	3 (21%)	17,19,21	0.88	1 (5%)
8	NAG	A	601	1	14,14,15	1.21	2 (14%)	17,19,21	0.97	2 (11%)
8	NAG	E	603	1	14,14,15	1.17	1 (7%)	17,19,21	1.01	1 (5%)
8	NAG	I	602	1	14,14,15	1.26	3 (21%)	17,19,21	1.31	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	604	1	-	4/6/23/26	0/1/1/1
8	NAG	A	602	1	-	1/6/23/26	0/1/1/1
8	NAG	A	603	1	-	0/6/23/26	0/1/1/1
8	NAG	I	603	1	-	1/6/23/26	0/1/1/1
8	NAG	E	601	1	-	0/6/23/26	0/1/1/1
8	NAG	E	602	1	-	1/6/23/26	0/1/1/1
8	NAG	I	601	1	-	0/6/23/26	0/1/1/1
8	NAG	A	601	1	-	0/6/23/26	0/1/1/1
8	NAG	E	603	1	-	0/6/23/26	0/1/1/1
8	NAG	I	602	1	-	1/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	603	NAG	O5-C5	2.99	1.49	1.43
8	A	603	NAG	O5-C5	2.75	1.49	1.43
8	E	603	NAG	O5-C5	2.71	1.48	1.43
8	I	602	NAG	O5-C5	2.58	1.48	1.43
8	E	602	NAG	O5-C5	2.49	1.48	1.43
8	A	602	NAG	O5-C5	2.47	1.48	1.43
8	I	601	NAG	O5-C5	2.43	1.48	1.43
8	A	601	NAG	O5-C5	2.43	1.48	1.43
8	I	602	NAG	C1-C2	2.37	1.55	1.52
8	A	602	NAG	C1-C2	2.29	1.55	1.52
8	E	602	NAG	C1-C2	2.22	1.55	1.52
8	A	603	NAG	O5-C1	2.21	1.47	1.43
8	E	601	NAG	O5-C5	2.20	1.47	1.43
8	I	602	NAG	O5-C1	2.14	1.47	1.43
8	A	601	NAG	C1-C2	2.09	1.55	1.52
8	E	602	NAG	O5-C1	2.08	1.47	1.43
8	I	601	NAG	O5-C1	2.07	1.47	1.43
8	I	603	NAG	O5-C1	2.06	1.47	1.43
8	I	601	NAG	C1-C2	2.01	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	602	NAG	C1-O5-C5	4.15	117.82	112.19
8	A	602	NAG	C1-O5-C5	3.58	117.05	112.19
8	E	602	NAG	C1-O5-C5	3.49	116.92	112.19
8	A	603	NAG	C1-O5-C5	2.97	116.21	112.19
8	I	603	NAG	C1-O5-C5	2.89	116.11	112.19
8	A	604	NAG	O5-C1-C2	2.75	115.64	111.29
8	E	601	NAG	O5-C1-C2	-2.48	107.37	111.29
8	A	604	NAG	C1-O5-C5	-2.44	108.88	112.19
8	A	601	NAG	C1-O5-C5	2.34	115.36	112.19
8	A	604	NAG	C4-C3-C2	-2.30	107.65	111.02
8	E	602	NAG	C2-N2-C7	2.27	126.14	122.90
8	A	601	NAG	O5-C1-C2	-2.26	107.72	111.29
8	E	603	NAG	C1-O5-C5	2.17	115.13	112.19
8	A	604	NAG	O4-C4-C5	2.17	114.69	109.30
8	I	601	NAG	O5-C1-C2	-2.06	108.04	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	604	NAG	C8-C7-N2-C2
8	A	604	NAG	O7-C7-N2-C2
8	A	604	NAG	O5-C5-C6-O6
8	A	604	NAG	C4-C5-C6-O6
8	A	602	NAG	C3-C2-N2-C7
8	I	602	NAG	C3-C2-N2-C7
8	I	603	NAG	O5-C5-C6-O6
8	E	602	NAG	C3-C2-N2-C7

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.

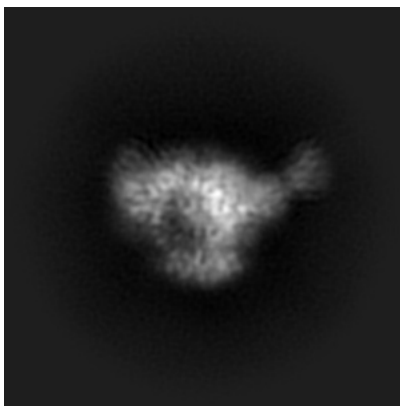
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23424. These allow visual inspection of the internal detail of the map and identification of artifacts.

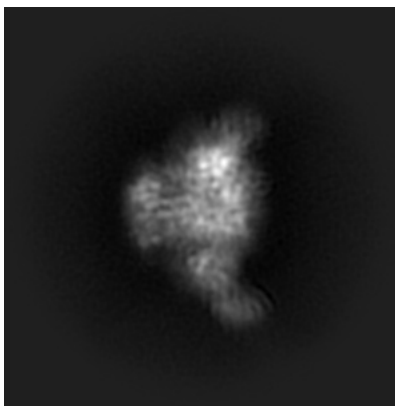
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

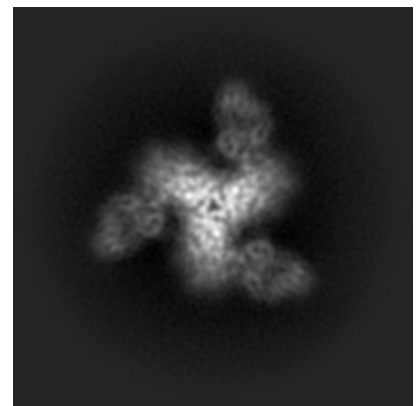
6.1.1 Primary map



X

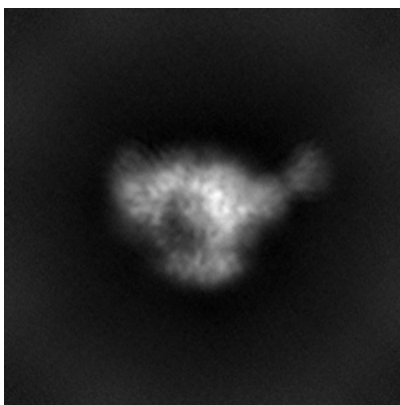


Y

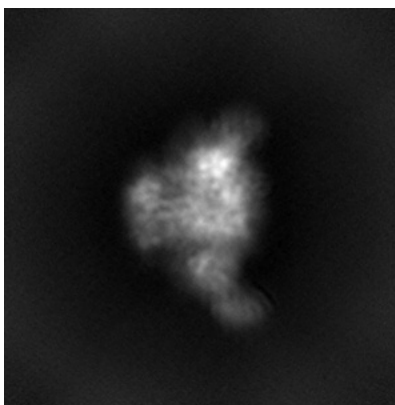


Z

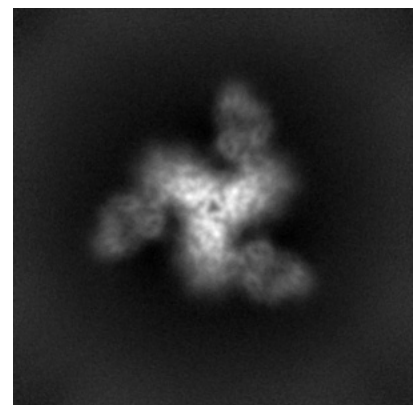
6.1.2 Raw map



X



Y

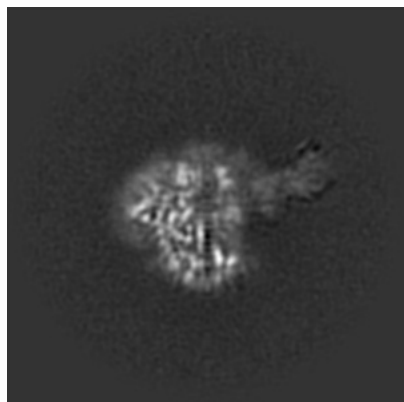


Z

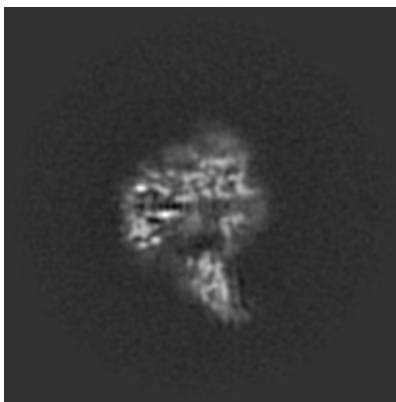
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

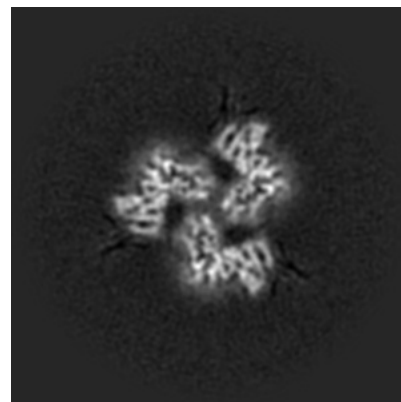
6.2.1 Primary map



X Index: 160

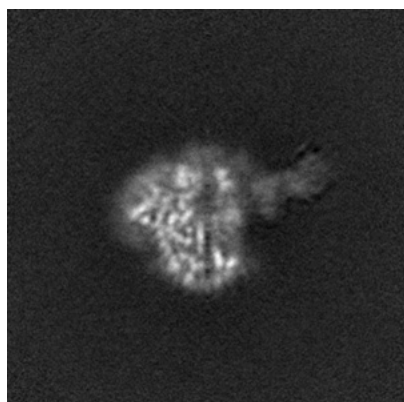


Y Index: 160

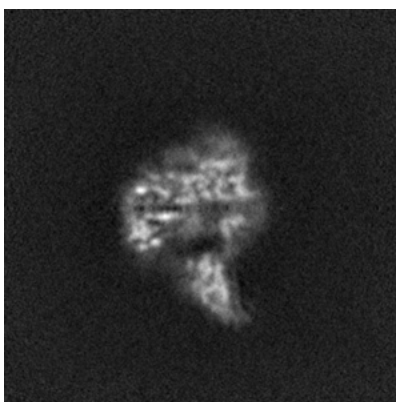


Z Index: 160

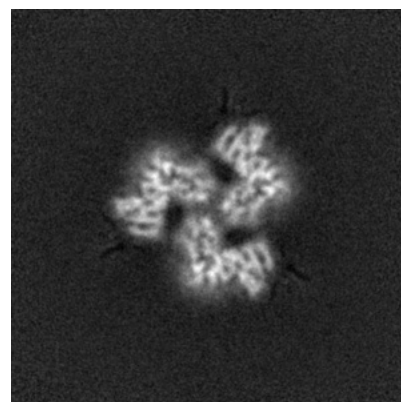
6.2.2 Raw map



X Index: 160



Y Index: 160

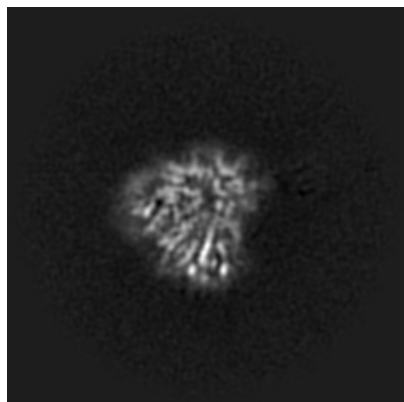


Z Index: 160

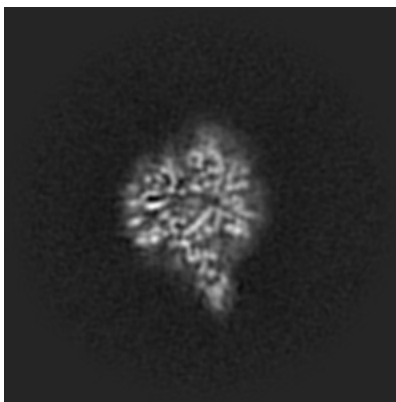
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

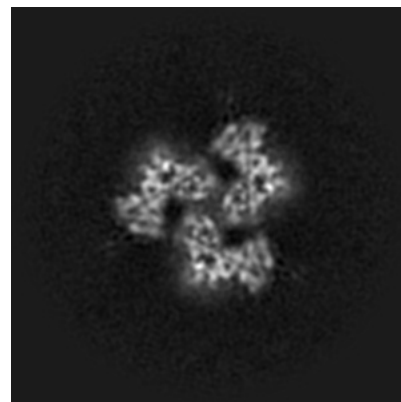
6.3.1 Primary map



X Index: 153

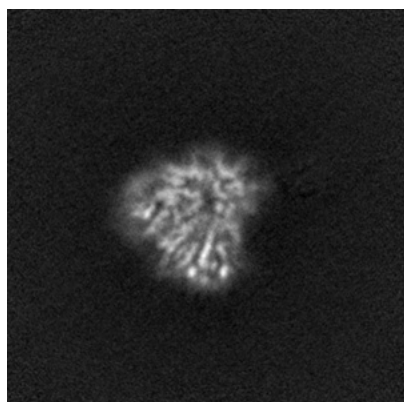


Y Index: 169

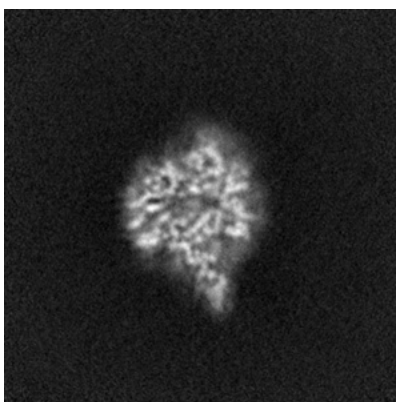


Z Index: 158

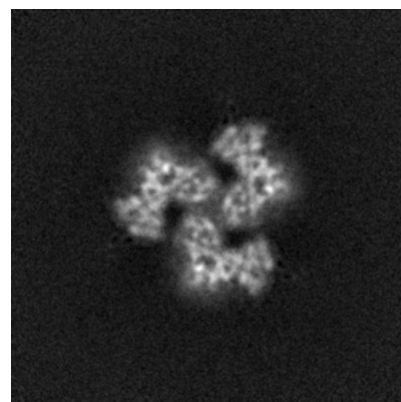
6.3.2 Raw map



X Index: 153



Y Index: 170

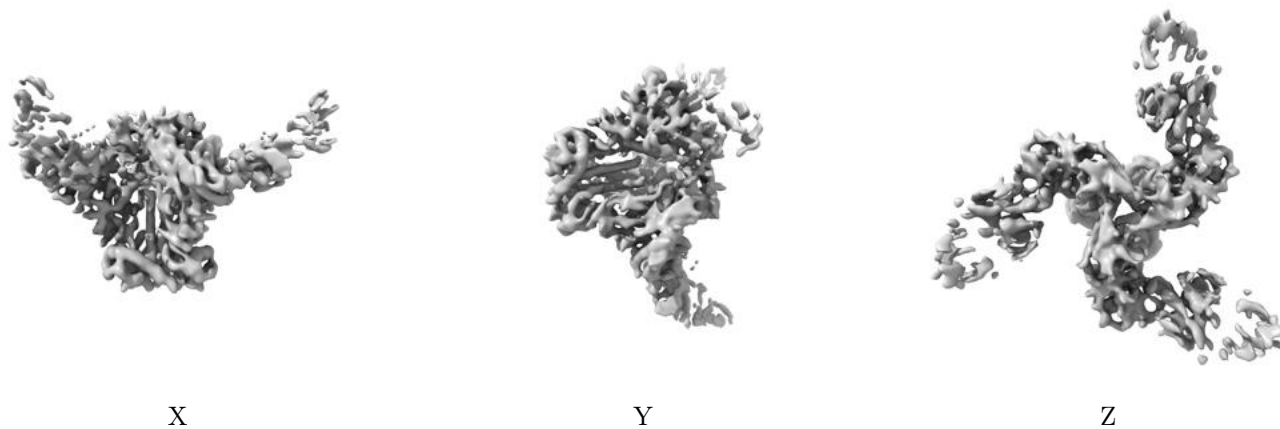


Z Index: 158

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

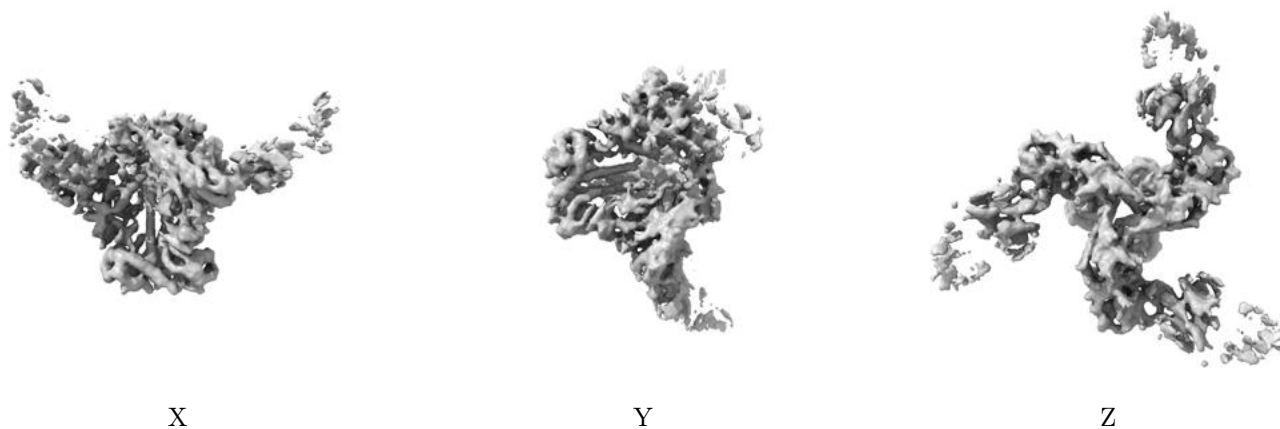
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

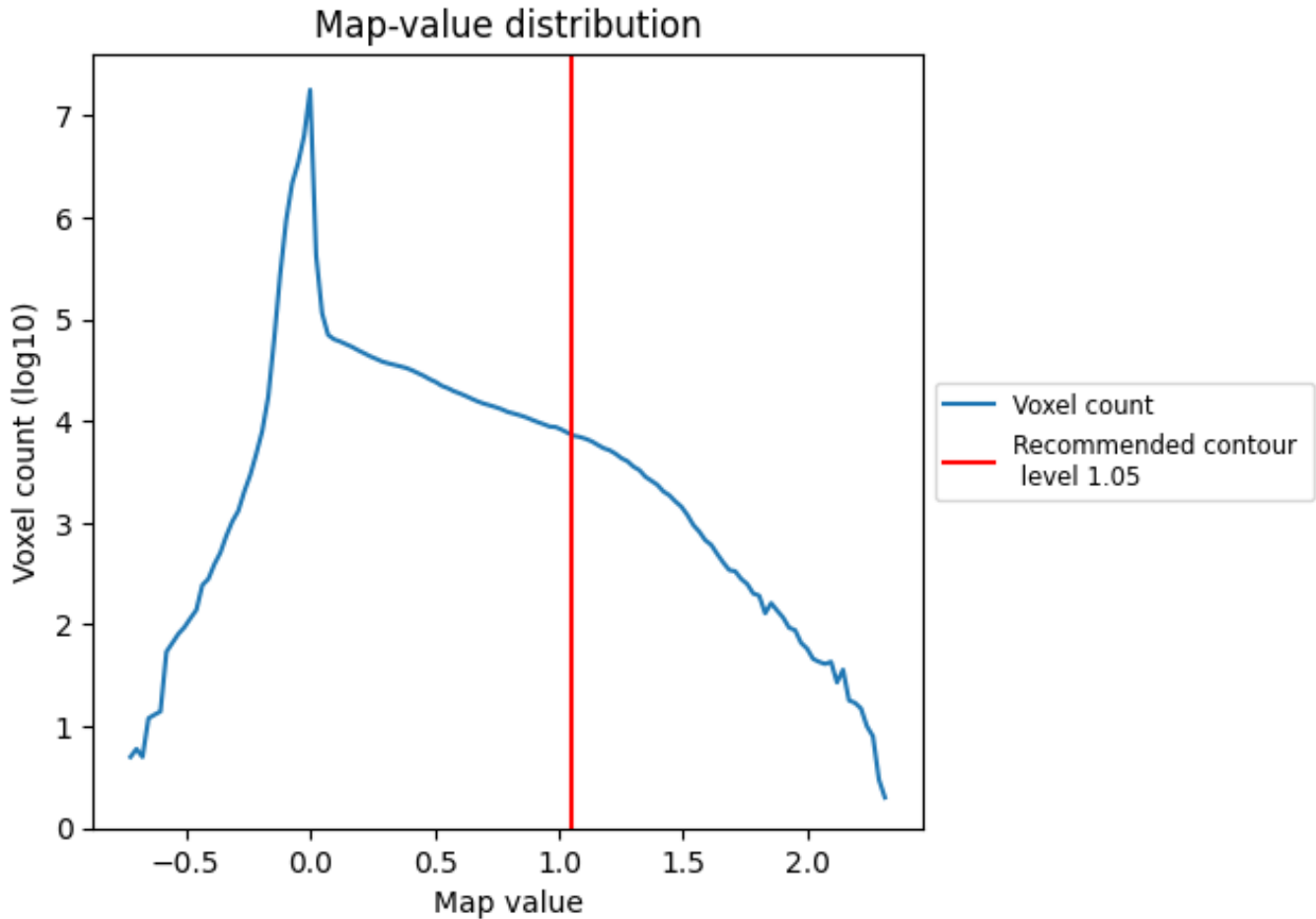
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

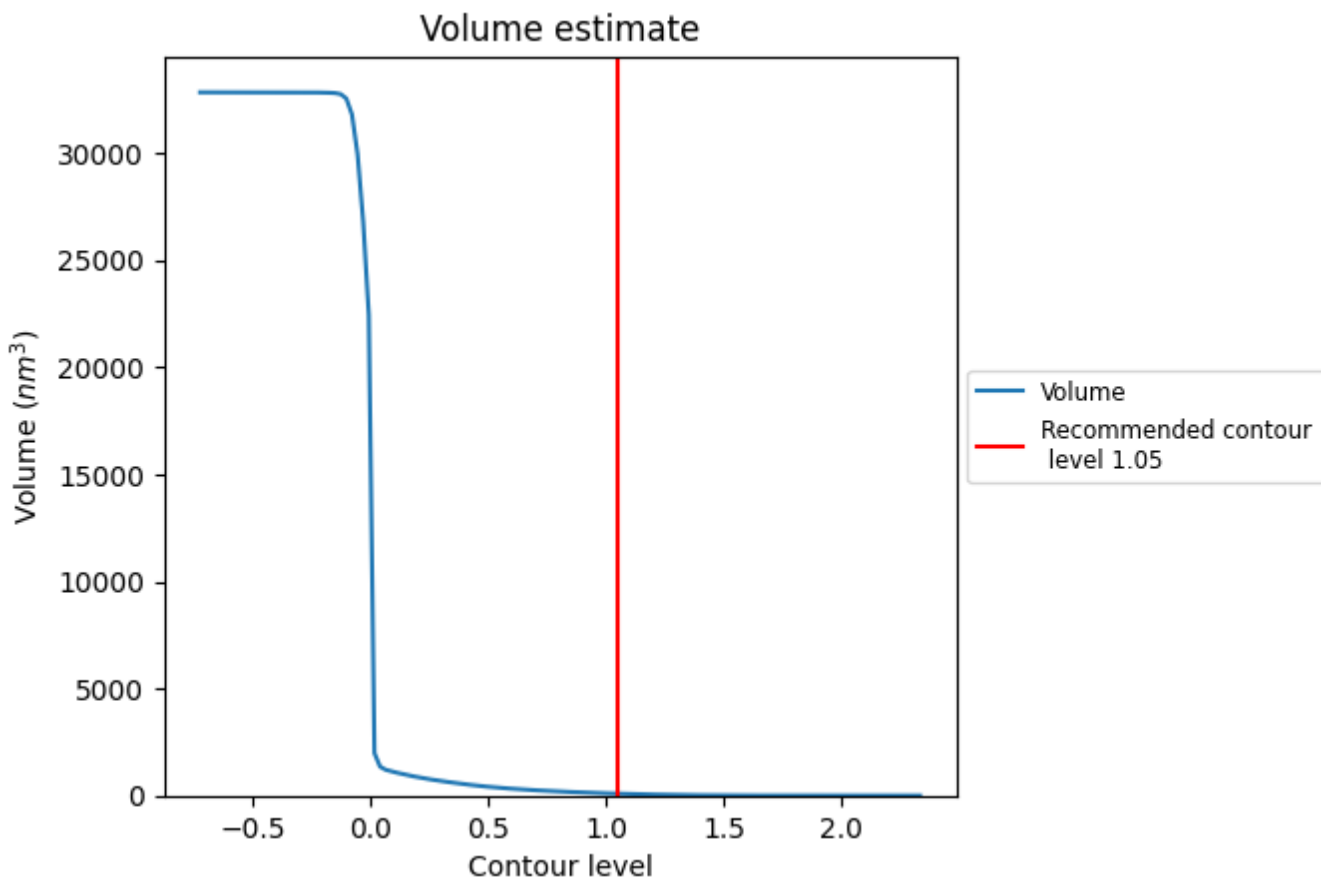
This section contains the results of statistical analysis of the map.

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.

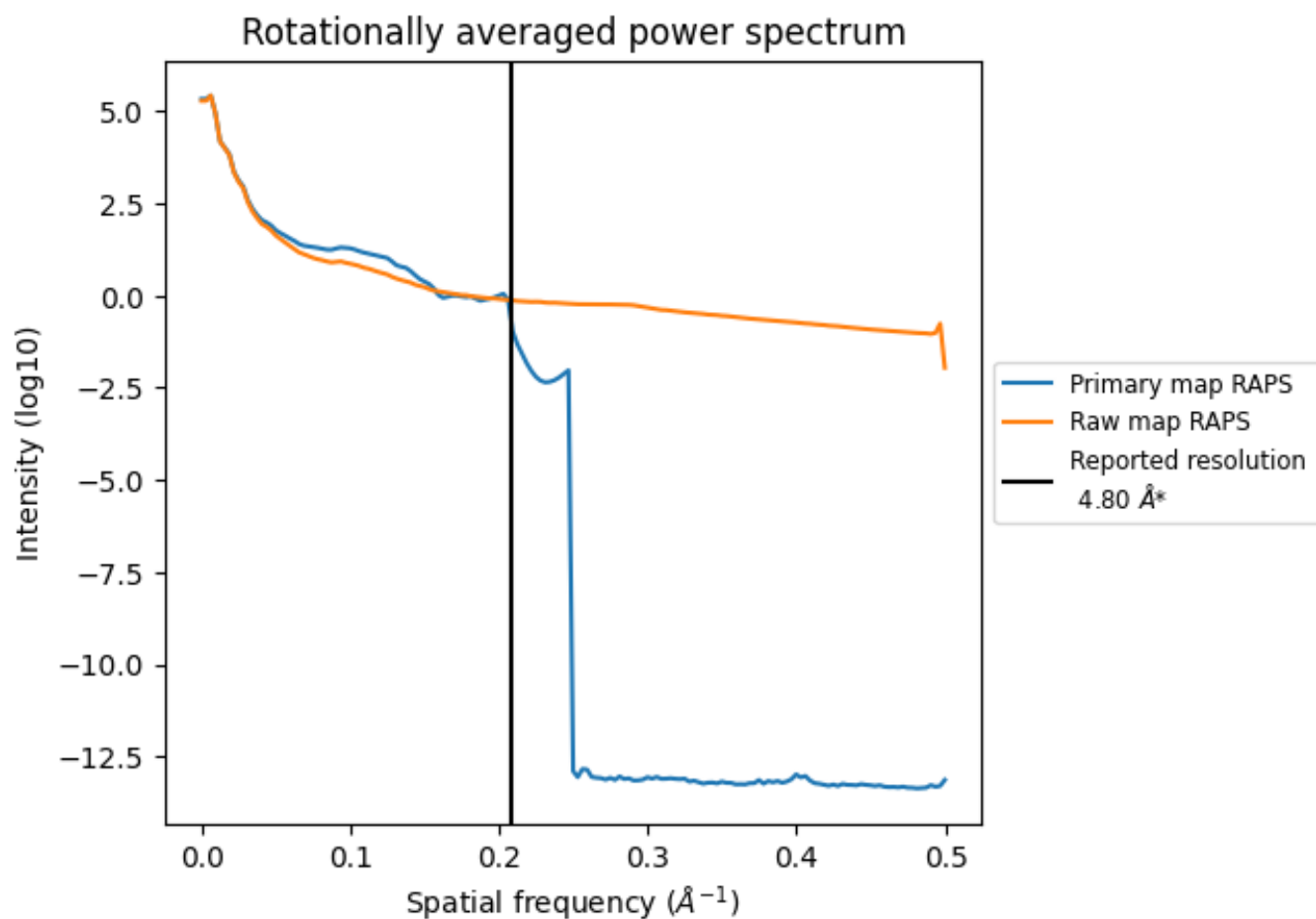
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

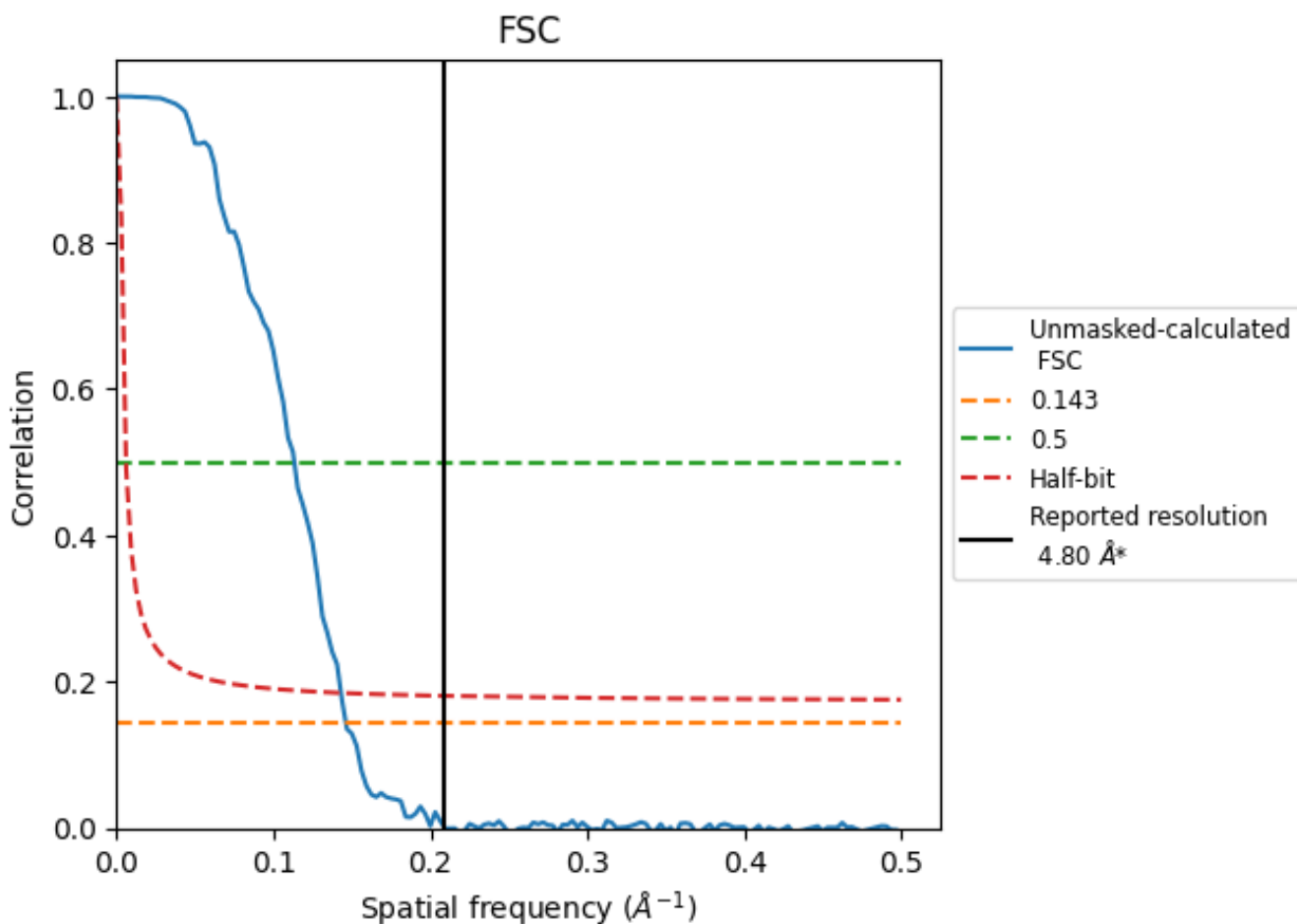


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

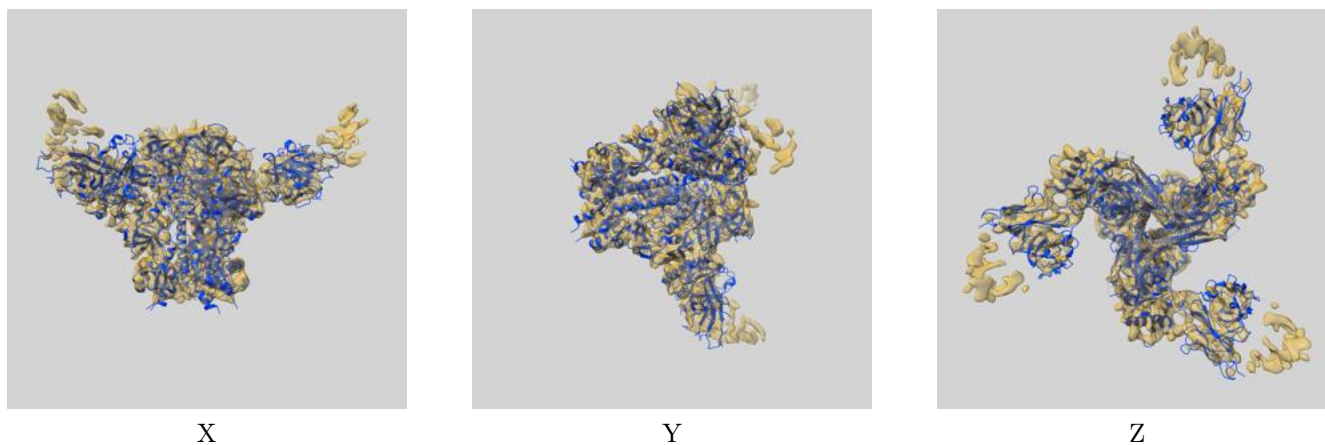
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.84	8.83	6.99

*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 6.84 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23424 and PDB model 7LLK. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



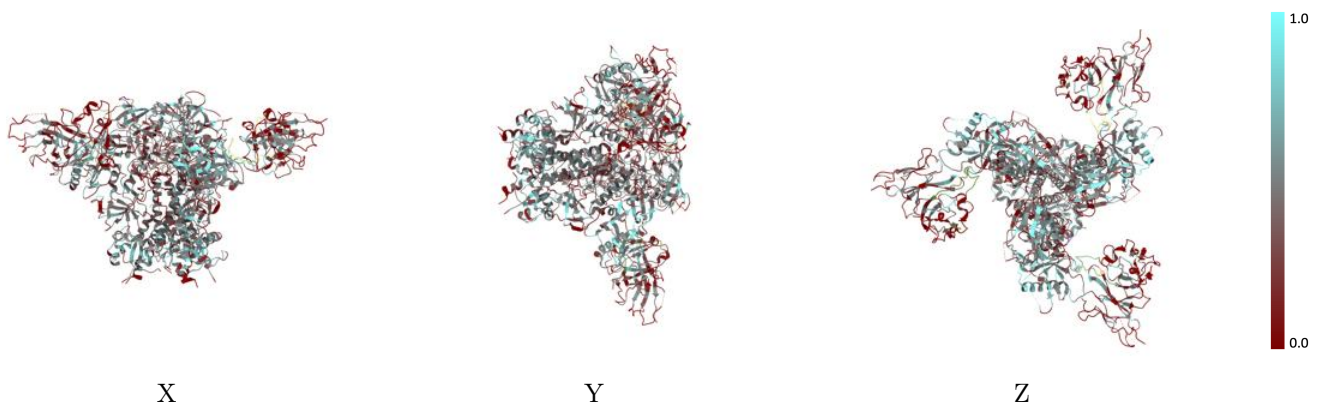
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



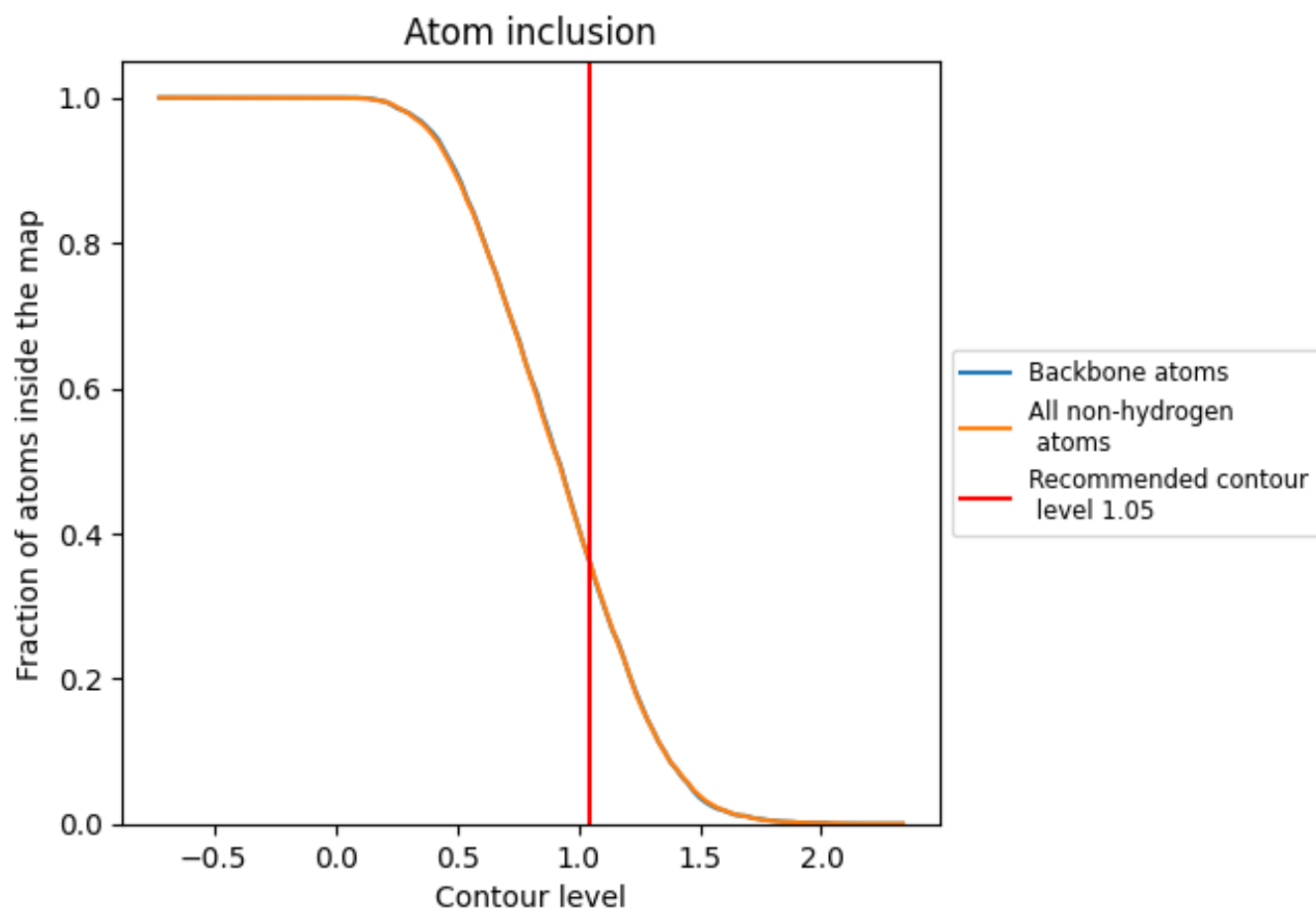
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 36% of all backbone atoms, 36% 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 (1.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3578	 0.2360
A	 0.4325	 0.2420
B	 0.4489	 0.2210
C	 0.2394	 0.2050
D	 0.2713	 0.2190
E	 0.4337	 0.2400
F	 0.4550	 0.2240
G	 0.2483	 0.2080
H	 0.2805	 0.2200
I	 0.4377	 0.2410
J	 0.4540	 0.2220
K	 0.2424	 0.2100
L	 0.2713	 0.2160
M	 0.0000	 0.4330
N	 0.0000	 0.3660
O	 0.1282	 0.2990
P	 0.0000	 0.3110
Q	 0.1026	 0.3500
R	 0.0769	 0.4020
S	 0.1200	 0.2850
T	 0.0000	 0.3250
U	 0.0769	 0.2540
V	 0.0000	 0.3740
W	 0.1282	 0.2930
X	 0.0400	 0.3870
Y	 0.1282	 0.3020
Z	 0.0000	 0.3280
a	 0.1026	 0.3510
b	 0.0769	 0.3940
c	 0.1400	 0.2920
d	 0.0000	 0.3220
e	 0.0769	 0.2650
f	 0.0000	 0.3690
g	 0.1282	 0.3050
h	 0.0600	 0.3880



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Chain	Atom inclusion	Q-score
j	 0.1026	 0.3030
k	 0.0000	 0.3030
l	 0.1282	 0.3660
m	 0.0769	 0.3640
n	 0.1400	 0.2940
o	 0.0000	 0.3270
p	 0.0769	 0.2450
q	 0.0000	 0.3630
r	 0.1538	 0.3260
s	 0.0600	 0.3750