



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 02:04 PM EST

PDB ID : 6VI0  
EMDB ID : EMD-21208  
Title : Cryo-EM structure of VRC01.23 in complex with HIV-1 Env BG505 DS.SOSIP  
Authors : Gorman, J.; Kwong, P.D.  
Deposited on : 2020-01-10  
Resolution : 3.43 Å (reported)  
Based on initial model : 6NNF

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

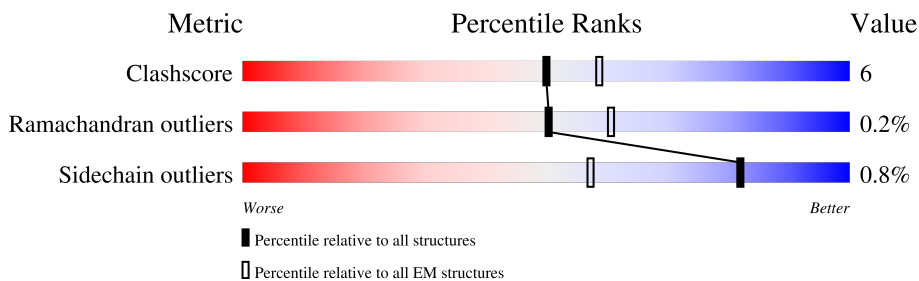
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.43 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.




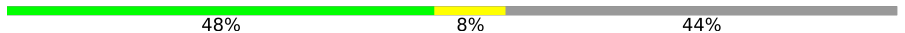
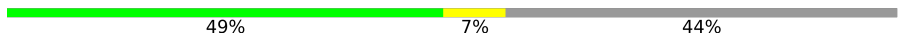


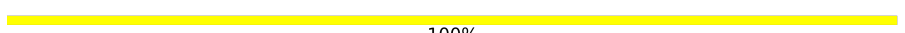
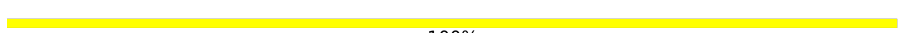




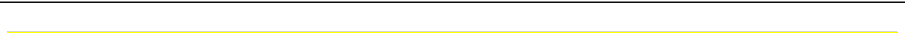



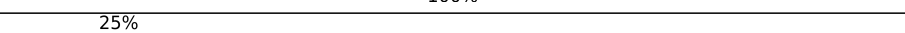
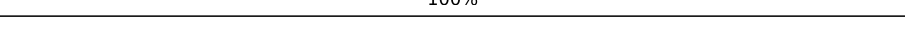
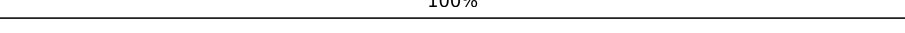
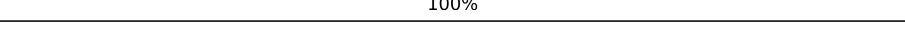
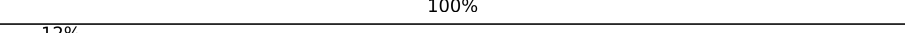





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	153	
1	B	153	
1	F	153	
2	C	481	
2	G	481	
2	I	481	
3	D	207	
3	J	207	




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Mol	Chain	Length	Quality of chain
3	L	207	 40% 7% 54%
4	E	229	 48% 8% 44%
4	H	229	 49% 7% 44%
4	K	229	 49% 7% 44%
5	M	2	 50% 50%
5	Q	2	 100%
5	T	2	 100%
5	U	2	 50% 50%
5	Y	2	 100%
5	b	2	 50% 50%
5	c	2	 50% 50%
5	g	2	 100%
5	j	2	 50% 50%
6	N	4	 25% 100%
6	V	4	 25% 100%
6	d	4	 25% 100%
7	O	6	 100%
7	W	6	 100%
7	e	6	 100%
8	P	8	 12% 62% 25% 12%
8	X	8	 12% 62% 25% 12%
8	f	8	 12% 75% 25%
9	R	6	 17% 33% 50% 17%
9	Z	6	 17% 33% 50% 17%
9	h	6	 17% 33% 67%

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Mol	Chain	Length	Quality of chain
10	S	3	 67% 33%
10	a	3	 67% 33%
10	i	3	 67% 33%

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 20823 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 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	131	1044	663	180	195	6	0	0
1	A	131	1044	663	180	195	6	0	0
1	F	131	1044	663	180	195	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
A	559	PRO	ILE	conflict	UNP Q2N0S6
A	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called BG505 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	450	3535	2215	626	664	30	0	0
2	C	450	3535	2215	626	664	30	0	0
2	I	450	3535	2215	626	664	30	0	0

There are 24 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	GLU	conflict	UNP Q2N0S6
G	510	ARG	LYS	conflict	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	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
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
I	201	CYS	ILE	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	433	CYS	ALA	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6
I	509	ARG	GLU	conflict	UNP Q2N0S6
I	510	ARG	LYS	conflict	UNP Q2N0S6
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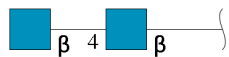
- Molecule 3 is a protein called VRC01.23 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	96	Total	C	N	O	S	0	0
			744	469	128	145	2		
3	D	96	Total	C	N	O	S	0	0
			744	469	128	145	2		
3	J	96	Total	C	N	O	S	0	0
			744	469	128	145	2		

- Molecule 4 is a protein called VRC01.23 Heavy chain.

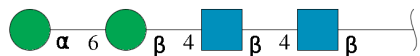
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	129	Total	C	N	O	S	0	0
			1039	656	187	188	8		
4	E	129	Total	C	N	O	S	0	0
			1039	656	187	188	8		
4	K	129	Total	C	N	O	S	0	0
			1039	656	187	188	8		

- 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	Q	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	Y	2	28	16	2	10	0	0
5	b	2	28	16	2	10	0	0
5	c	2	28	16	2	10	0	0
5	g	2	28	16	2	10	0	0
5	j	2	28	16	2	10	0	0

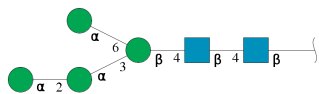
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	N	4	50	28	2	20	0	0
6	V	4	50	28	2	20	0	0
6	d	4	50	28	2	20	0	0

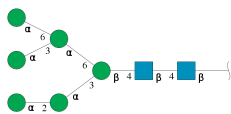
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

ose-(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.



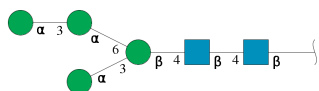
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
7	O	6	72	40	2	30	0	0
7	W	6	72	40	2	30	0	0
7	e	6	72	40	2	30	0	0

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



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
8	P	8	94	52	2	40	0	0
8	X	8	94	52	2	40	0	0
8	f	8	94	52	2	40	0	0

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



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

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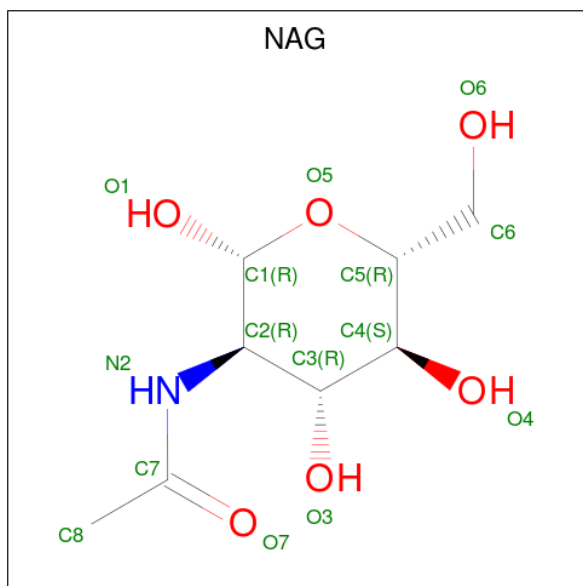
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	6	Total	C	N	O	0	0
			72	40	2	30		
9	h	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	N	O	0
			28	16	2	10	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	Total 28	C 16	N 2	O 10	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	G	1	Total 126	C 72	N 9	O 45	0
11	L	1	Total 14	C 8	N 1	O 5	0
11	A	1	Total 28	C 16	N 2	O 10	0
11	A	1	Total 28	C 16	N 2	O 10	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0
11	C	1	Total 126	C 72	N 9	O 45	0

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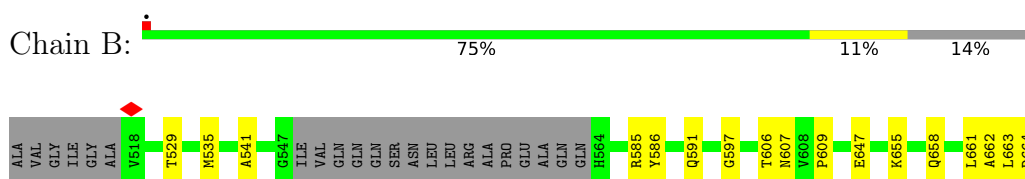
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
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11	D	1	Total 14	C 8	N 1	O 5	0
11	F	1	Total 28	C 16	N 2	O 10	0
11	F	1	Total 28	C 16	N 2	O 10	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	I	1	Total 126	C 72	N 9	O 45	0
11	J	1	Total 14	C 8	N 1	O 5	0

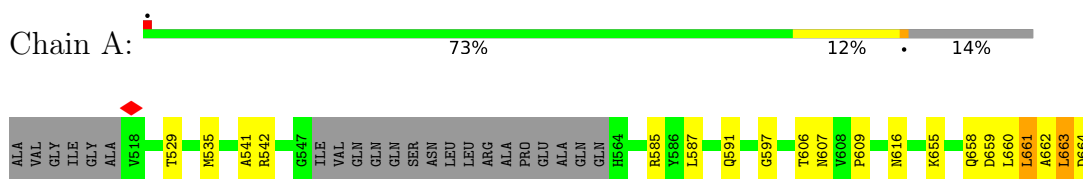
### 3 Residue-property plots [i](#)

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.

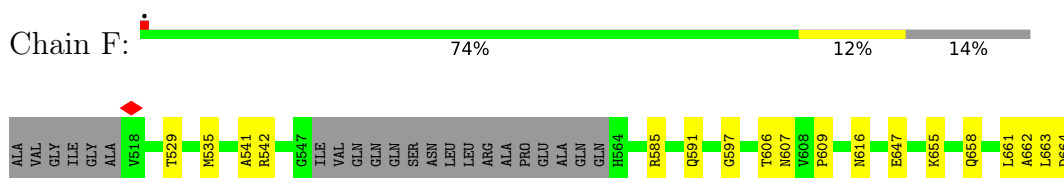
- Molecule 1: Envelope glycoprotein gp41



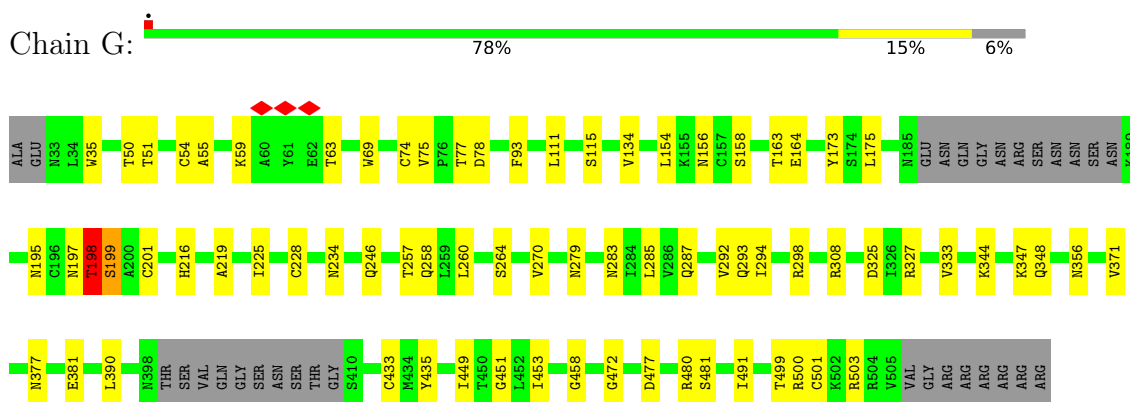
- Molecule 1: Envelope glycoprotein gp41



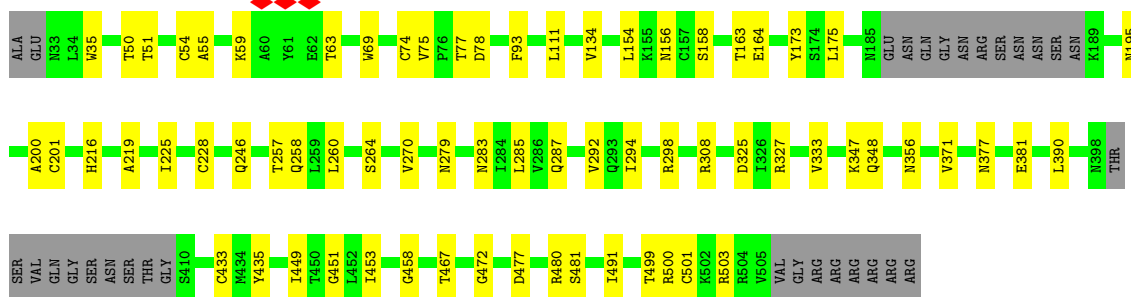
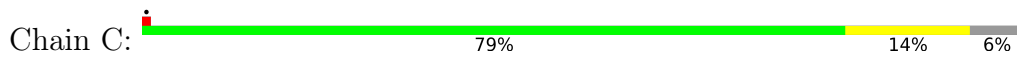
- Molecule 1: Envelope glycoprotein gp41



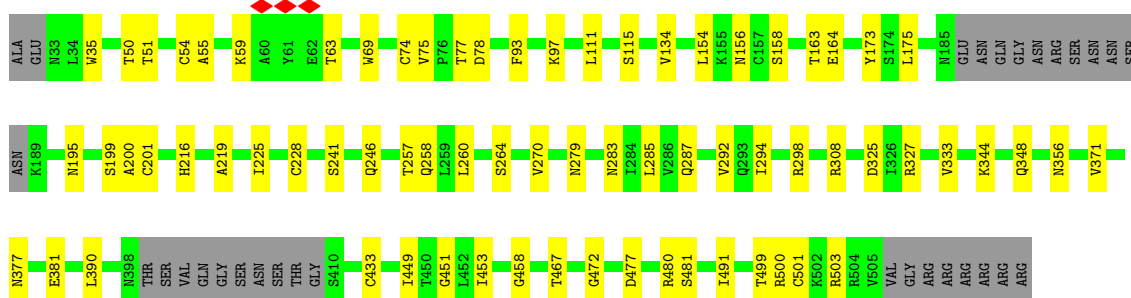
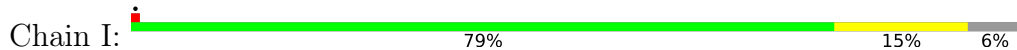
- Molecule 2: BG505 gp120



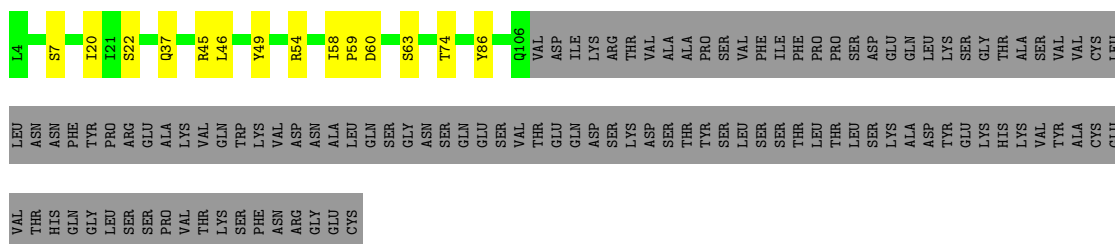
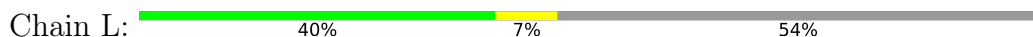
- Molecule 2: BG505 gp120



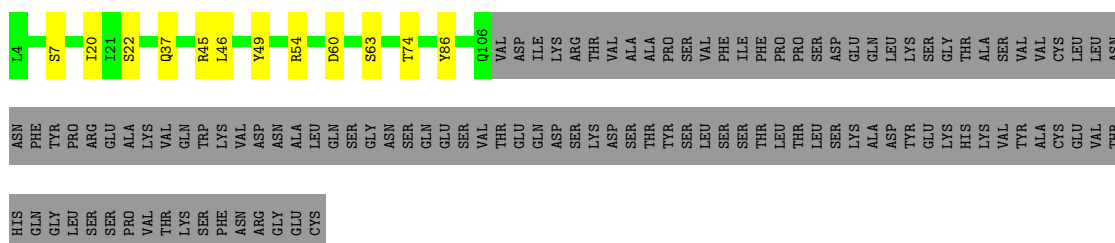
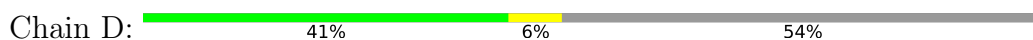
• Molecule 2: BG505 gp120



• Molecule 3: VRC01.23 Light chain



• Molecule 3: VRC01.23 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



- 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 g:  100%



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

Chain j:  50% 50%



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

Chain N:  25% 100%



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

Chain V:  25% 100%




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

Chain d:  25% 100%



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain O:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain P:  12% 62% 25% 12%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

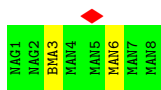
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  12% 62% 25% 12%

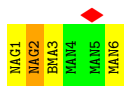
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

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

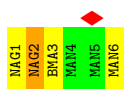
Chain f:  12% 75% 25%



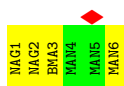
- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

Chain i:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	55046	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 ( $e^-/\text{\AA}^2$ )	70.41	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.529	Depositor
Minimum map value	-1.487	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	334.854, 334.854, 334.854	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07325, 1.07325, 1.07325	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	0.33	0/1063	0.51	0/1441
1	B	0.32	0/1063	0.52	0/1441
1	F	0.32	0/1063	0.52	0/1441
2	C	0.42	0/3608	0.57	0/4898
2	G	0.42	0/3608	0.57	0/4898
2	I	0.41	0/3608	0.57	0/4898
3	D	0.36	0/764	0.55	0/1038
3	J	0.36	0/764	0.55	0/1038
3	L	0.36	0/764	0.54	0/1038
4	E	0.40	0/1070	0.56	0/1454
4	H	0.40	0/1070	0.56	0/1454
4	K	0.40	0/1070	0.56	0/1454
All	All	0.39	0/19515	0.56	0/26493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1044	0	1029	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1044	0	1029	19	0
1	F	1044	0	1029	17	0
2	C	3535	0	3464	50	0
2	G	3535	0	3464	57	0
2	I	3535	0	3464	53	0
3	D	744	0	701	7	0
3	J	744	0	701	7	0
3	L	744	0	701	9	0
4	E	1039	0	997	11	0
4	H	1039	0	997	10	0
4	K	1039	0	997	10	0
5	M	28	0	25	0	0
5	Q	28	0	25	0	0
5	T	28	0	25	1	0
5	U	28	0	25	0	0
5	Y	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	g	28	0	25	0	0
5	j	28	0	25	0	0
6	N	50	0	43	0	0
6	V	50	0	43	0	0
6	d	50	0	43	0	0
7	O	72	0	61	0	0
7	W	72	0	61	0	0
7	e	72	0	61	0	0
8	P	94	0	79	1	0
8	X	94	0	79	1	0
8	f	94	0	79	0	0
9	R	72	0	61	1	0
9	Z	72	0	61	1	0
9	h	72	0	61	0	0
10	S	39	0	34	0	0
10	a	39	0	34	0	0
10	i	39	0	34	0	0
11	A	28	0	26	0	0
11	B	28	0	26	0	0
11	C	126	0	117	0	0
11	D	14	0	13	0	0
11	F	28	0	26	0	0
11	G	126	0	117	0	0
11	I	126	0	117	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	14	0	13	0	0
11	L	14	0	13	0	0
All	All	20823	0	20100	243	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 6.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:LEU:HD23	1:A:660:LEU:O	1.74	0.88
1:F:661:LEU:O	1:F:664:ASP:HB2	1.82	0.80
1:F:661:LEU:O	1:F:661:LEU:HD12	1.82	0.78
1:B:661:LEU:HD12	1:B:661:LEU:O	1.87	0.75
1:B:661:LEU:O	1:B:664:ASP:HB2	1.87	0.74
1:A:661:LEU:O	1:A:664:ASP:HB2	1.92	0.69
1:F:661:LEU:HD12	1:F:661:LEU:C	2.15	0.66
2:I:156:ASN:HA	2:I:175:LEU:HD23	1.79	0.65
2:G:156:ASN:HA	2:G:175:LEU:HD23	1.79	0.64
2:C:156:ASN:HA	2:C:175:LEU:HD23	1.79	0.63
1:A:659:ASP:O	1:A:663:LEU:HD23	1.98	0.63
2:I:74:CYS:SG	2:I:75:VAL:N	2.73	0.62
1:A:660:LEU:O	1:A:660:LEU:CD2	2.48	0.62
2:I:134:VAL:HG11	2:I:154:LEU:HG	1.82	0.62
1:B:661:LEU:HD12	1:B:661:LEU:C	2.20	0.62
2:C:74:CYS:SG	2:C:75:VAL:N	2.73	0.61
1:A:660:LEU:HA	1:A:663:LEU:HD21	1.83	0.61
2:G:74:CYS:SG	2:G:75:VAL:N	2.73	0.61
2:G:134:VAL:HG11	2:G:154:LEU:HG	1.82	0.61
2:C:134:VAL:HG11	2:C:154:LEU:HG	1.82	0.61
1:A:658:GLN:HA	1:A:661:LEU:HD11	1.84	0.59
2:C:200:ALA:O	2:C:201:CYS:SG	2.60	0.59
2:G:195:ASN:ND2	2:G:201:CYS:SG	2.76	0.59
2:C:55:ALA:HB3	2:C:216:HIS:HB2	1.85	0.59
2:G:198:THR:O	2:G:199:SER:HB2	2.02	0.58
2:I:279:ASN:OD1	4:K:100(B):TRP:NE1	2.36	0.58
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.85	0.58
2:I:55:ALA:HB3	2:I:216:HIS:HB2	1.85	0.58
4:K:7:SER:OG	4:K:8:GLY:N	2.37	0.57
2:I:458:GLY:HA2	4:K:47:TRP:HZ3	1.70	0.57
2:G:458:GLY:HA2	4:H:47:TRP:HZ3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:GLY:HA2	4:E:47:TRP:HZ3	1.70	0.57
1:B:663:LEU:HD23	1:B:663:LEU:C	2.25	0.56
2:G:500:ARG:O	1:A:662:ALA:HA	2.05	0.56
2:C:195:ASN:ND2	2:C:201:CYS:SG	2.78	0.56
4:E:7:SER:OG	4:E:8:GLY:N	2.37	0.56
2:C:279:ASN:OD1	4:E:100(B):TRP:NE1	2.36	0.56
3:D:63:SER:OG	3:D:74:THR:OG1	2.24	0.56
2:I:195:ASN:ND2	2:I:201:CYS:SG	2.79	0.56
2:G:298:ARG:NH1	2:G:381:GLU:OE1	2.39	0.55
1:B:585:ARG:NH2	2:G:491:ILE:O	2.39	0.55
4:H:7:SER:OG	4:H:8:GLY:N	2.37	0.55
2:C:298:ARG:NH1	2:C:381:GLU:OE1	2.40	0.55
2:G:279:ASN:OD1	4:H:100(B):TRP:NE1	2.36	0.55
3:J:63:SER:OG	3:J:74:THR:OG1	2.24	0.55
1:F:585:ARG:NH2	2:I:491:ILE:O	2.39	0.54
1:B:658:GLN:NE2	2:I:501:CYS:SG	2.62	0.54
1:A:585:ARG:NH2	2:C:491:ILE:O	2.39	0.54
2:I:298:ARG:NH1	2:I:381:GLU:OE1	2.40	0.54
1:B:535:MET:SD	1:A:655:LYS:NZ	2.74	0.54
3:L:7:SER:HG	3:L:22:SER:HG	1.53	0.54
1:B:597:GLY:O	2:G:503:ARG:NH2	2.42	0.53
1:F:597:GLY:O	2:I:503:ARG:NH2	2.42	0.53
2:G:197:ASN:CG	2:G:197:ASN:O	2.47	0.53
3:L:37:GLN:NE2	3:L:86:TYR:OH	2.42	0.53
3:D:20:ILE:HG22	3:D:74:THR:HG22	1.92	0.52
3:D:37:GLN:NE2	3:D:86:TYR:OH	2.42	0.52
3:J:37:GLN:NE2	3:J:86:TYR:OH	2.43	0.52
1:A:597:GLY:O	2:C:503:ARG:NH2	2.42	0.52
1:B:655:LYS:NZ	1:F:535:MET:SD	2.73	0.52
2:C:325:ASP:OD2	2:C:327:ARG:NH2	2.43	0.52
2:C:264:SER:O	2:C:287:GLN:NE2	2.41	0.52
3:J:20:ILE:HG22	3:J:74:THR:HG22	1.92	0.52
2:I:325:ASP:OD2	2:I:327:ARG:NH2	2.43	0.51
2:G:78:ASP:OD1	2:G:78:ASP:N	2.43	0.51
2:G:325:ASP:OD2	2:G:327:ARG:NH2	2.43	0.51
2:G:54:CYS:SG	2:G:55:ALA:N	2.84	0.51
2:G:198:THR:O	2:G:198:THR:CG2	2.57	0.51
2:C:50:THR:OG1	2:C:51:THR:N	2.43	0.51
2:C:54:CYS:SG	2:C:55:ALA:N	2.84	0.51
2:C:164:GLU:OE1	2:C:308:ARG:NH1	2.44	0.51
3:L:20:ILE:HG22	3:L:74:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:198:THR:O	2:G:198:THR:HG23	2.10	0.51
4:H:87:THR:HG23	4:H:110:ILE:HA	1.93	0.51
2:I:50:THR:OG1	2:I:51:THR:N	2.43	0.51
4:K:87:THR:HG23	4:K:110:ILE:HA	1.93	0.51
2:I:54:CYS:SG	2:I:55:ALA:N	2.83	0.50
1:A:535:MET:SD	1:F:655:LYS:NZ	2.75	0.50
2:G:50:THR:OG1	2:G:51:THR:N	2.43	0.50
2:G:164:GLU:OE1	2:G:308:ARG:NH1	2.44	0.50
2:I:164:GLU:OE1	2:I:308:ARG:NH1	2.44	0.50
2:I:264:SER:O	2:I:287:GLN:NE2	2.41	0.50
2:G:283:ASN:ND2	2:G:477:ASP:OD2	2.45	0.49
2:C:283:ASN:ND2	2:C:477:ASP:OD2	2.45	0.49
4:E:87:THR:HG23	4:E:110:ILE:HA	1.93	0.49
2:C:294:ILE:HD12	2:C:449:ILE:HD11	1.95	0.49
2:I:477:ASP:OD1	2:I:480:ARG:NH1	2.45	0.49
1:B:658:GLN:O	1:B:662:ALA:HB2	2.13	0.49
4:H:35:ASN:OD1	4:H:47:TRP:NE1	2.42	0.49
1:B:662:ALA:HA	2:I:500:ARG:O	2.13	0.48
2:I:154:LEU:HD23	2:I:154:LEU:H	1.78	0.48
2:I:283:ASN:ND2	2:I:477:ASP:OD2	2.45	0.48
2:I:294:ILE:HD12	2:I:449:ILE:HD11	1.94	0.48
4:H:6:GLN:NE2	4:H:90:TYR:O	2.45	0.48
2:G:260:LEU:HD12	2:G:451:GLY:HA3	1.96	0.48
2:C:163:THR:OG1	2:C:164:GLU:N	2.47	0.48
2:C:154:LEU:HD23	2:C:154:LEU:H	1.78	0.48
2:I:260:LEU:HD12	2:I:451:GLY:HA3	1.96	0.48
1:B:663:LEU:HD23	1:B:663:LEU:O	2.14	0.47
2:C:260:LEU:HD12	2:C:451:GLY:HA3	1.96	0.47
1:F:658:GLN:O	1:F:662:ALA:HB2	2.14	0.47
2:G:154:LEU:HD23	2:G:154:LEU:H	1.78	0.47
2:G:264:SER:O	2:G:287:GLN:NE2	2.41	0.47
2:C:200:ALA:C	2:C:201:CYS:SG	2.92	0.47
2:I:163:THR:OG1	2:I:164:GLU:N	2.47	0.47
1:B:541:ALA:O	1:A:591:GLN:NE2	2.47	0.47
2:G:294:ILE:HD12	2:G:449:ILE:HD11	1.94	0.47
3:L:63:SER:OG	3:L:74:THR:OG1	2.24	0.47
2:C:500:ARG:O	1:F:662:ALA:HA	2.14	0.47
2:C:69:TRP:HA	2:C:111:LEU:HD13	1.97	0.47
4:H:32:CYS:HB3	4:H:98:CYS:HB3	1.77	0.47
2:G:163:THR:OG1	2:G:164:GLU:N	2.47	0.47
9:Z:2:NAG:O3	9:Z:2:NAG:C7	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.45	0.46
1:A:541:ALA:O	1:F:591:GLN:NE2	2.48	0.46
9:R:2:NAG:C7	9:R:2:NAG:O3	2.63	0.46
2:C:501:CYS:SG	1:F:658:GLN:NE2	2.63	0.46
2:G:356:ASN:OD1	2:G:356:ASN:N	2.49	0.46
4:K:6:GLN:NE2	4:K:90:TYR:O	2.45	0.46
2:C:477:ASP:OD1	2:C:480:ARG:NH1	2.45	0.46
2:I:199:SER:OG	2:I:200:ALA:N	2.49	0.46
2:G:69:TRP:HA	2:G:111:LEU:HD13	1.97	0.46
2:G:293:GLN:NE2	5:T:1:NAG:O7	2.48	0.46
2:I:69:TRP:HA	2:I:111:LEU:HD13	1.97	0.46
2:I:356:ASN:OD1	2:I:356:ASN:N	2.49	0.46
1:B:591:GLN:NE2	1:F:541:ALA:O	2.49	0.45
2:C:356:ASN:N	2:C:356:ASN:OD1	2.49	0.45
2:I:270:VAL:HG13	2:I:348:GLN:HG3	1.98	0.45
2:G:377:ASN:OD1	2:G:377:ASN:N	2.49	0.45
2:C:93:PHE:CE2	2:C:228:CYS:HB2	2.52	0.45
2:C:270:VAL:HG13	2:C:348:GLN:HG3	1.98	0.45
4:E:32:CYS:SG	4:E:94:ARG:NH2	2.90	0.45
2:G:158:SER:HA	2:G:173:TYR:HA	1.99	0.45
4:E:6:GLN:NE2	4:E:90:TYR:O	2.45	0.45
4:K:32:CYS:SG	4:K:94:ARG:NH2	2.90	0.45
2:G:501:CYS:SG	1:A:658:GLN:NE2	2.64	0.45
2:C:134:VAL:CG1	2:C:154:LEU:HG	2.47	0.45
3:D:7:SER:OG	3:D:22:SER:OG	2.32	0.45
2:I:219:ALA:HB2	2:I:225:ILE:HG13	1.99	0.45
2:G:115:SER:O	2:G:115:SER:OG	2.35	0.44
2:I:134:VAL:CG1	2:I:154:LEU:HG	2.47	0.44
2:C:158:SER:HA	2:C:173:TYR:HA	1.99	0.44
2:C:219:ALA:HB2	2:C:225:ILE:HG13	1.99	0.44
2:I:93:PHE:CE2	2:I:228:CYS:HB2	2.52	0.44
3:J:46:LEU:HD11	3:J:49:TYR:HB3	1.99	0.44
2:G:93:PHE:CE2	2:G:228:CYS:HB2	2.52	0.44
2:G:134:VAL:CG1	2:G:154:LEU:HG	2.47	0.44
4:H:32:CYS:SG	4:H:94:ARG:NH2	2.90	0.44
2:I:285:LEU:HD23	2:I:481:SER:HB2	1.99	0.44
2:C:285:LEU:HD23	2:C:481:SER:HB2	1.99	0.44
2:G:219:ALA:HB2	2:G:225:ILE:HG13	1.99	0.44
3:D:46:LEU:HD11	3:D:49:TYR:HB3	1.99	0.44
2:I:115:SER:O	2:I:115:SER:OG	2.35	0.44
2:G:270:VAL:HG13	2:G:348:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:LYS:O	2:G:63:THR:OG1	2.32	0.44
3:L:46:LEU:HD11	3:L:49:TYR:HB3	1.99	0.44
3:D:37:GLN:OE1	3:D:45:ARG:NH2	2.51	0.43
2:I:78:ASP:OD1	2:I:78:ASP:N	2.43	0.43
2:C:78:ASP:OD1	2:C:78:ASP:N	2.43	0.43
2:C:499:THR:OG1	2:C:500:ARG:N	2.51	0.43
2:I:77:THR:OG1	2:I:78:ASP:OD1	2.36	0.43
2:G:499:THR:OG1	2:G:500:ARG:N	2.51	0.43
2:I:158:SER:HA	2:I:173:TYR:HA	1.99	0.43
8:X:6:MAN:H62	8:X:8:MAN:H2	1.79	0.43
2:G:78:ASP:OD2	2:G:246:GLN:NE2	2.52	0.43
2:C:257:THR:HG23	2:C:472:GLY:HA3	2.00	0.43
3:J:37:GLN:OE1	3:J:45:ARG:NH2	2.51	0.43
2:G:257:THR:HG23	2:G:472:GLY:HA3	2.00	0.43
2:C:77:THR:OG1	2:C:78:ASP:OD1	2.36	0.43
2:I:78:ASP:OD2	2:I:246:GLN:NE2	2.52	0.43
2:C:59:LYS:HD2	2:C:59:LYS:HA	1.80	0.43
4:E:35:ASN:OD1	4:E:47:TRP:NE1	2.42	0.43
1:F:606:THR:HG22	1:F:607:ASN:H	1.84	0.43
2:G:77:THR:OG1	2:G:78:ASP:OD1	2.36	0.43
4:K:47:TRP:HZ2	4:K:50:TRP:HD1	1.67	0.43
4:H:47:TRP:HZ2	4:H:50:TRP:HD1	1.67	0.42
2:C:78:ASP:OD2	2:C:246:GLN:NE2	2.52	0.42
2:I:257:THR:HG23	2:I:472:GLY:HA3	2.00	0.42
1:B:606:THR:HG22	1:B:607:ASN:H	1.84	0.42
4:E:47:TRP:HZ2	4:E:50:TRP:HD1	1.67	0.42
2:I:377:ASN:OD1	2:I:377:ASN:N	2.49	0.42
2:G:285:LEU:HD23	2:G:481:SER:HB2	1.99	0.42
1:A:606:THR:HG22	1:A:607:ASN:H	1.84	0.42
4:K:32:CYS:HB3	4:K:98:CYS:HB3	1.77	0.42
1:A:660:LEU:HA	1:A:663:LEU:CD2	2.49	0.42
2:G:260:LEU:HD21	2:G:453:ILE:HD11	2.02	0.42
3:L:37:GLN:OE1	3:L:45:ARG:NH2	2.50	0.42
2:I:499:THR:OG1	2:I:500:ARG:N	2.51	0.42
1:B:647:GLU:OE2	1:F:542:ARG:NH1	2.52	0.42
1:B:658:GLN:HG2	2:I:501:CYS:SG	2.60	0.42
2:I:59:LYS:O	2:I:63:THR:OG1	2.33	0.42
2:G:501:CYS:SG	1:A:661:LEU:HD13	2.60	0.42
2:C:377:ASN:OD1	2:C:377:ASN:N	2.49	0.42
4:E:82(C):LEU:HD23	4:E:82(C):LEU:HA	1.90	0.42
3:J:58:ILE:HD13	3:J:58:ILE:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:292:VAL:HG22	2:G:449:ILE:HB	2.02	0.42
2:C:260:LEU:HD21	2:C:453:ILE:HD11	2.02	0.42
2:I:260:LEU:HD21	2:I:453:ILE:HD11	2.02	0.42
2:G:270:VAL:HG11	2:G:344:LYS:HB3	2.02	0.41
1:A:609:PRO:HA	2:C:35:TRP:HA	2.02	0.41
2:I:270:VAL:HG11	2:I:344:LYS:HB3	2.02	0.41
3:J:54:ARG:NH1	3:J:60:ASP:OD1	2.53	0.41
1:B:609:PRO:HA	2:G:35:TRP:HA	2.02	0.41
2:G:234:ASN:OD1	2:G:234:ASN:N	2.53	0.41
4:E:40:ALA:HB3	4:E:43:LYS:HB2	2.02	0.41
2:I:257:THR:HG22	2:I:258:GLN:HG3	2.02	0.41
2:I:292:VAL:HG22	2:I:449:ILE:HB	2.02	0.41
2:I:333:VAL:HG11	2:I:390:LEU:HD21	2.03	0.41
2:G:111:LEU:HD23	2:G:111:LEU:HA	1.93	0.41
3:L:58:ILE:HA	3:L:59:PRO:HD3	1.92	0.41
2:C:257:THR:HG22	2:C:258:GLN:HG3	2.02	0.41
3:D:54:ARG:NH1	3:D:60:ASP:OD1	2.53	0.41
1:F:609:PRO:HA	2:I:35:TRP:HA	2.02	0.41
8:P:6:MAN:H62	8:P:8:MAN:H2	1.79	0.41
2:C:257:THR:HG21	2:C:371:VAL:HA	2.02	0.41
3:L:58:ILE:HA	3:L:58:ILE:HD13	1.92	0.41
4:E:32:CYS:HB3	4:E:98:CYS:HB3	1.77	0.41
2:I:241:SER:O	2:I:241:SER:OG	2.36	0.41
1:B:586:TYR:HE2	1:A:587:LEU:HD22	1.85	0.41
2:G:257:THR:HG22	2:G:258:GLN:HG3	2.02	0.41
3:L:54:ARG:NH1	3:L:60:ASP:OD1	2.53	0.41
2:C:333:VAL:HG11	2:C:390:LEU:HD21	2.03	0.41
2:G:134:VAL:HG12	2:G:154:LEU:O	2.21	0.41
2:G:333:VAL:HG11	2:G:390:LEU:HD21	2.03	0.41
1:A:542:ARG:NH1	1:F:647:GLU:OE2	2.54	0.41
2:C:292:VAL:HG22	2:C:449:ILE:HB	2.02	0.41
4:K:40:ALA:HB3	4:K:43:LYS:HB2	2.02	0.41
2:G:501:CYS:SG	1:A:658:GLN:HG2	2.60	0.41
2:C:134:VAL:HG12	2:C:154:LEU:O	2.21	0.41
2:I:257:THR:HG21	2:I:371:VAL:HA	2.02	0.41
2:G:257:THR:HG21	2:G:371:VAL:HA	2.03	0.40
2:G:347:LYS:HB3	2:G:347:LYS:HE2	1.92	0.40
2:C:59:LYS:O	2:C:63:THR:OG1	2.32	0.40
2:I:134:VAL:HG12	2:I:154:LEU:O	2.21	0.40
2:C:467:THR:O	2:C:467:THR:OG1	2.37	0.40
2:I:59:LYS:HD2	2:I:59:LYS:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:40:ALA:HB3	4:H:43:LYS:HB2	2.02	0.40
2:C:347:LYS:HB3	2:C:347:LYS:HE2	1.92	0.40
2:I:97:LYS:HD3	2:I:97:LYS:HA	1.83	0.40
2:I:467:THR:O	2:I:467:THR:OG1	2.37	0.40
1:A:616:ASN:OD1	1:A:616:ASN:N	2.55	0.40
1:F:616:ASN:OD1	1:F:616:ASN:N	2.55	0.40
4:K:35:ASN:OD1	4:K:47:TRP:NE1	2.42	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	127/153 (83%)	123 (97%)	4 (3%)	0	100	100
1	B	127/153 (83%)	123 (97%)	4 (3%)	0	100	100
1	F	127/153 (83%)	123 (97%)	4 (3%)	0	100	100
2	C	444/481 (92%)	402 (90%)	41 (9%)	1 (0%)	47	80
2	G	444/481 (92%)	402 (90%)	39 (9%)	3 (1%)	22	60
2	I	444/481 (92%)	406 (91%)	38 (9%)	0	100	100
3	D	94/207 (45%)	87 (93%)	7 (7%)	0	100	100
3	J	94/207 (45%)	87 (93%)	7 (7%)	0	100	100
3	L	94/207 (45%)	87 (93%)	7 (7%)	0	100	100
4	E	127/229 (56%)	116 (91%)	11 (9%)	0	100	100
4	H	127/229 (56%)	116 (91%)	11 (9%)	0	100	100
4	K	127/229 (56%)	115 (91%)	12 (9%)	0	100	100
All	All	2376/3210 (74%)	2187 (92%)	185 (8%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	198	THR
2	G	435	TYR
2	G	199	SER
2	C	435	TYR

### 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	113/129 (88%)	110 (97%)	3 (3%)	44	73
1	B	113/129 (88%)	112 (99%)	1 (1%)	78	90
1	F	113/129 (88%)	111 (98%)	2 (2%)	59	81
2	C	402/429 (94%)	401 (100%)	1 (0%)	93	98
2	G	402/429 (94%)	400 (100%)	2 (0%)	88	95
2	I	402/429 (94%)	401 (100%)	1 (0%)	93	98
3	D	79/179 (44%)	79 (100%)	0	100	100
3	J	79/179 (44%)	79 (100%)	0	100	100
3	L	79/179 (44%)	79 (100%)	0	100	100
4	E	111/198 (56%)	109 (98%)	2 (2%)	59	81
4	H	111/198 (56%)	109 (98%)	2 (2%)	59	81
4	K	111/198 (56%)	109 (98%)	2 (2%)	59	81
All	All	2115/2805 (75%)	2099 (99%)	16 (1%)	82	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	529	THR
2	G	198	THR
2	G	433	CYS
4	H	71	ARG
4	H	83	THR
1	A	529	THR
1	A	661	LEU

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Mol	Chain	Res	Type
1	A	663	LEU
2	C	433	CYS
4	E	71	ARG
4	E	83	THR
1	F	529	THR
1	F	663	LEU
2	I	433	CYS
4	K	71	ARG
4	K	83	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	591	GLN
2	G	114	GLN
2	G	293	GLN
3	L	37	GLN
3	L	90	GLN
4	H	100(A)	ASN
1	A	591	GLN
2	C	99	ASN
2	C	114	GLN
2	C	293	GLN
3	D	37	GLN
3	D	90	GLN
4	E	100(A)	ASN
1	F	591	GLN
2	I	114	GLN
2	I	293	GLN
3	J	37	GLN
3	J	90	GLN
4	K	100(A)	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

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	5,2	14,14,15	0.20	0	17,19,21	0.64	1 (5%)
5	NAG	M	2	5	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	N	1	6,2	14,14,15	0.37	0	17,19,21	0.66	1 (5%)
6	NAG	N	2	6	14,14,15	0.47	0	17,19,21	0.62	1 (5%)
6	BMA	N	3	6	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
6	MAN	N	4	6	11,11,12	0.90	0	15,15,17	1.19	2 (13%)
7	NAG	O	1	7,2	14,14,15	0.65	0	17,19,21	1.97	3 (17%)
7	NAG	O	2	7	14,14,15	0.66	0	17,19,21	1.62	4 (23%)
7	BMA	O	3	7	11,11,12	0.56	0	15,15,17	1.42	3 (20%)
7	MAN	O	4	7	11,11,12	0.31	0	15,15,17	1.56	5 (33%)
7	MAN	O	5	7	11,11,12	0.29	0	15,15,17	0.78	1 (6%)
7	MAN	O	6	7	11,11,12	0.25	0	15,15,17	1.01	1 (6%)
8	NAG	P	1	8,2	14,14,15	0.46	0	17,19,21	0.81	0
8	NAG	P	2	8	14,14,15	0.46	0	17,19,21	0.95	0
8	BMA	P	3	8	11,11,12	0.40	0	15,15,17	1.50	4 (26%)
8	MAN	P	4	8	11,11,12	0.26	0	15,15,17	0.84	0
8	MAN	P	5	8	11,11,12	0.25	0	15,15,17	0.92	0
8	MAN	P	6	8	11,11,12	0.38	0	15,15,17	1.14	1 (6%)
8	MAN	P	7	8	11,11,12	0.23	0	15,15,17	0.71	0
8	MAN	P	8	8	11,11,12	0.25	0	15,15,17	0.83	0
5	NAG	Q	1	5,2	14,14,15	0.74	1 (7%)	17,19,21	2.25	4 (23%)
5	NAG	Q	2	5	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
9	NAG	R	1	9,2	14,14,15	1.15	1 (7%)	17,19,21	1.30	3 (17%)
9	NAG	R	2	9	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
9	BMA	R	3	9	11,11,12	0.46	0	15,15,17	1.37	3 (20%)
9	MAN	R	4	9	11,11,12	0.22	0	15,15,17	0.88	0
9	MAN	R	5	9	11,11,12	0.32	0	15,15,17	0.91	0
9	MAN	R	6	9	11,11,12	0.23	0	15,15,17	1.06	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	S	1	2,10	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
10	NAG	S	2	10	14,14,15	0.26	0	17,19,21	0.52	0
10	BMA	S	3	10	11,11,12	0.77	0	15,15,17	0.96	0
5	NAG	T	1	5,2	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	T	2	5	14,14,15	0.44	0	17,19,21	0.63	1 (5%)
5	NAG	U	1	5,2	14,14,15	0.19	0	17,19,21	0.64	1 (5%)
5	NAG	U	2	5	14,14,15	0.24	0	17,19,21	0.47	0
6	NAG	V	1	6,2	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
6	NAG	V	2	6	14,14,15	0.47	0	17,19,21	0.62	1 (5%)
6	BMA	V	3	6	11,11,12	0.73	0	15,15,17	0.95	1 (6%)
6	MAN	V	4	6	11,11,12	0.90	0	15,15,17	1.18	2 (13%)
7	NAG	W	1	7,2	14,14,15	0.66	0	17,19,21	1.98	3 (17%)
7	NAG	W	2	7	14,14,15	0.67	0	17,19,21	1.59	4 (23%)
7	BMA	W	3	7	11,11,12	0.59	0	15,15,17	1.40	3 (20%)
7	MAN	W	4	7	11,11,12	0.30	0	15,15,17	1.56	5 (33%)
7	MAN	W	5	7	11,11,12	0.30	0	15,15,17	0.78	1 (6%)
7	MAN	W	6	7	11,11,12	0.25	0	15,15,17	1.01	1 (6%)
8	NAG	X	1	8,2	14,14,15	0.44	0	17,19,21	0.80	0
8	NAG	X	2	8	14,14,15	0.49	0	17,19,21	0.95	0
8	BMA	X	3	8	11,11,12	0.38	0	15,15,17	1.52	4 (26%)
8	MAN	X	4	8	11,11,12	0.26	0	15,15,17	0.82	0
8	MAN	X	5	8	11,11,12	0.26	0	15,15,17	0.93	0
8	MAN	X	6	8	11,11,12	0.36	0	15,15,17	1.15	1 (6%)
8	MAN	X	7	8	11,11,12	0.24	0	15,15,17	0.72	0
8	MAN	X	8	8	11,11,12	0.27	0	15,15,17	0.82	0
5	NAG	Y	1	5,2	14,14,15	0.73	1 (7%)	17,19,21	2.25	4 (23%)
5	NAG	Y	2	5	14,14,15	0.45	0	17,19,21	0.94	1 (5%)
9	NAG	Z	1	9,2	14,14,15	1.15	2 (14%)	17,19,21	1.28	3 (17%)
9	NAG	Z	2	9	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
9	BMA	Z	3	9	11,11,12	0.46	0	15,15,17	1.38	3 (20%)
9	MAN	Z	4	9	11,11,12	0.25	0	15,15,17	0.88	0
9	MAN	Z	5	9	11,11,12	0.30	0	15,15,17	0.92	0
9	MAN	Z	6	9	11,11,12	0.23	0	15,15,17	1.07	2 (13%)
10	NAG	a	1	2,10	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
10	NAG	a	2	10	14,14,15	0.25	0	17,19,21	0.52	0
10	BMA	a	3	10	11,11,12	0.75	0	15,15,17	0.97	0
5	NAG	b	1	5,2	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	b	2	5	14,14,15	0.44	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	c	1	5,2	14,14,15	0.19	0	17,19,21	0.65	1 (5%)
5	NAG	c	2	5	14,14,15	0.24	0	17,19,21	0.47	0
6	NAG	d	1	6,2	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
6	NAG	d	2	6	14,14,15	0.46	0	17,19,21	0.61	1 (5%)
6	BMA	d	3	6	11,11,12	0.73	0	15,15,17	0.96	1 (6%)
6	MAN	d	4	6	11,11,12	0.90	0	15,15,17	1.19	2 (13%)
7	NAG	e	1	7,2	14,14,15	0.66	0	17,19,21	1.98	3 (17%)
7	NAG	e	2	7	14,14,15	0.68	0	17,19,21	1.58	4 (23%)
7	BMA	e	3	7	11,11,12	0.57	0	15,15,17	1.42	4 (26%)
7	MAN	e	4	7	11,11,12	0.30	0	15,15,17	1.56	5 (33%)
7	MAN	e	5	7	11,11,12	0.31	0	15,15,17	0.78	1 (6%)
7	MAN	e	6	7	11,11,12	0.25	0	15,15,17	1.02	1 (6%)
8	NAG	f	1	8,2	14,14,15	0.44	0	17,19,21	0.80	0
8	NAG	f	2	8	14,14,15	0.49	0	17,19,21	0.94	0
8	BMA	f	3	8	11,11,12	0.39	0	15,15,17	1.50	4 (26%)
8	MAN	f	4	8	11,11,12	0.25	0	15,15,17	0.82	0
8	MAN	f	5	8	11,11,12	0.25	0	15,15,17	0.92	0
8	MAN	f	6	8	11,11,12	0.36	0	15,15,17	1.15	1 (6%)
8	MAN	f	7	8	11,11,12	0.22	0	15,15,17	0.71	0
8	MAN	f	8	8	11,11,12	0.27	0	15,15,17	0.83	0
5	NAG	g	1	5,2	14,14,15	0.75	1 (7%)	17,19,21	2.26	4 (23%)
5	NAG	g	2	5	14,14,15	0.46	0	17,19,21	0.94	1 (5%)
9	NAG	h	1	9,2	14,14,15	1.16	2 (14%)	17,19,21	1.29	3 (17%)
9	NAG	h	2	9	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
9	BMA	h	3	9	11,11,12	0.47	0	15,15,17	1.37	3 (20%)
9	MAN	h	4	9	11,11,12	0.22	0	15,15,17	0.89	0
9	MAN	h	5	9	11,11,12	0.29	0	15,15,17	0.92	0
9	MAN	h	6	9	11,11,12	0.23	0	15,15,17	1.06	2 (13%)
10	NAG	i	1	2,10	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
10	NAG	i	2	10	14,14,15	0.25	0	17,19,21	0.52	0
10	BMA	i	3	10	11,11,12	0.76	0	15,15,17	0.96	0
5	NAG	j	1	5,2	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	j	2	5	14,14,15	0.44	0	17,19,21	0.61	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
5	NAG	M	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
6	NAG	N	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,2	-	3/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	2/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	0/1/1/1
7	MAN	O	6	7	-	1/2/19/22	0/1/1/1
8	NAG	P	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	2/6/23/26	0/1/1/1
8	BMA	P	3	8	-	0/2/19/22	0/1/1/1
8	MAN	P	4	8	-	0/2/19/22	0/1/1/1
8	MAN	P	5	8	-	1/2/19/22	0/1/1/1
8	MAN	P	6	8	-	2/2/19/22	0/1/1/1
8	MAN	P	7	8	-	0/2/19/22	0/1/1/1
8	MAN	P	8	8	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	5,2	-	5/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	3/6/23/26	0/1/1/1
9	NAG	R	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	6/6/23/26	0/1/1/1
9	BMA	R	3	9	-	2/2/19/22	0/1/1/1
9	MAN	R	4	9	-	0/2/19/22	0/1/1/1
9	MAN	R	5	9	-	0/2/19/22	0/1/1/1
9	MAN	R	6	9	-	2/2/19/22	0/1/1/1
10	NAG	S	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	1/6/23/26	0/1/1/1
10	BMA	S	3	10	-	2/2/19/22	0/1/1/1
5	NAG	T	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
6	NAG	V	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	g	1	NAG	C1-C2	2.17	1.55	1.52
9	h	1	NAG	C1-C2	-2.14	1.49	1.52
5	Q	1	NAG	C1-C2	2.12	1.55	1.52
9	Z	1	NAG	C1-C2	-2.12	1.49	1.52
9	R	1	NAG	C1-C2	-2.08	1.49	1.52
5	Y	1	NAG	C1-C2	2.07	1.55	1.52
9	h	1	NAG	C2-N2	-2.06	1.42	1.46
9	Z	1	NAG	C2-N2	-2.06	1.42	1.46

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	1	NAG	C2-N2-C7	7.83	134.06	122.90
5	Q	1	NAG	C2-N2-C7	7.81	134.02	122.90
5	Y	1	NAG	C2-N2-C7	7.80	134.00	122.90
7	O	1	NAG	C2-N2-C7	4.90	129.88	122.90
7	e	1	NAG	C2-N2-C7	4.89	129.87	122.90
7	W	1	NAG	C2-N2-C7	4.87	129.84	122.90
7	O	2	NAG	C2-N2-C7	-4.84	116.01	122.90
7	e	2	NAG	C2-N2-C7	-4.69	116.22	122.90
7	W	2	NAG	C2-N2-C7	-4.68	116.24	122.90
5	g	1	NAG	C1-C2-N2	3.54	116.53	110.49
5	Y	1	NAG	C1-C2-N2	3.52	116.50	110.49
5	Q	1	NAG	C1-C2-N2	3.50	116.47	110.49
8	P	3	BMA	O3-C3-C2	-3.22	103.83	109.99
8	X	3	BMA	O3-C3-C2	-3.21	103.85	109.99
8	f	3	BMA	O3-C3-C2	-3.18	103.90	109.99
7	e	1	NAG	C1-C2-N2	3.03	115.66	110.49
5	Q	2	NAG	C2-N2-C7	3.02	127.20	122.90
7	W	1	NAG	C1-C2-N2	3.01	115.64	110.49
7	O	1	NAG	C1-C2-N2	3.01	115.63	110.49
5	g	2	NAG	C2-N2-C7	2.95	127.11	122.90
5	Y	2	NAG	C2-N2-C7	2.95	127.10	122.90
7	e	4	MAN	C3-C4-C5	-2.88	105.10	110.24
7	W	4	MAN	C3-C4-C5	-2.88	105.11	110.24
7	O	4	MAN	C3-C4-C5	-2.87	105.12	110.24
6	d	4	MAN	C1-O5-C5	2.84	116.03	112.19
6	V	4	MAN	C1-O5-C5	2.78	115.96	112.19
6	N	4	MAN	C1-O5-C5	2.78	115.96	112.19
9	Z	3	BMA	C6-C5-C4	-2.73	106.60	113.00
9	R	3	BMA	C6-C5-C4	-2.73	106.62	113.00
9	h	3	BMA	C6-C5-C4	-2.72	106.64	113.00
7	e	2	NAG	C1-C2-N2	2.59	114.91	110.49
7	e	4	MAN	O5-C5-C6	2.56	111.22	107.20
9	Z	3	BMA	C2-C3-C4	-2.56	106.46	110.89
7	O	3	BMA	O5-C5-C6	-2.56	103.19	107.20
7	O	2	NAG	C1-C2-N2	2.55	114.84	110.49
7	W	2	NAG	C1-C2-N2	2.55	114.84	110.49
9	R	3	BMA	C2-C3-C4	-2.54	106.49	110.89
7	O	4	MAN	O5-C5-C6	2.54	111.19	107.20
6	N	3	BMA	C1-O5-C5	2.54	115.63	112.19
8	f	6	MAN	C3-C4-C5	-2.53	105.72	110.24
7	O	4	MAN	O5-C1-C2	-2.53	106.86	110.77
8	X	6	MAN	C3-C4-C5	-2.53	105.73	110.24
9	h	3	BMA	C2-C3-C4	-2.53	106.52	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	4	MAN	O5-C1-C2	-2.53	106.87	110.77
7	W	4	MAN	O5-C5-C6	2.52	111.15	107.20
7	W	4	MAN	O5-C1-C2	-2.51	106.89	110.77
7	O	3	BMA	C6-C5-C4	-2.50	107.14	113.00
7	W	3	BMA	C6-C5-C4	-2.49	107.17	113.00
6	V	3	BMA	C1-O5-C5	2.49	115.56	112.19
9	R	2	NAG	C1-C2-N2	-2.49	106.24	110.49
8	P	6	MAN	C3-C4-C5	-2.49	105.80	110.24
7	e	3	BMA	C6-C5-C4	-2.49	107.18	113.00
7	e	3	BMA	O5-C5-C6	-2.48	103.31	107.20
6	d	3	BMA	C1-O5-C5	2.48	115.55	112.19
9	h	2	NAG	C1-C2-N2	-2.47	106.28	110.49
7	W	3	BMA	O5-C5-C6	-2.47	103.34	107.20
7	e	1	NAG	O5-C1-C2	-2.46	107.41	111.29
7	W	1	NAG	O5-C1-C2	-2.46	107.41	111.29
7	O	1	NAG	O5-C1-C2	-2.45	107.43	111.29
8	f	3	BMA	O3-C3-C4	-2.43	104.72	110.35
9	Z	2	NAG	C1-C2-N2	-2.42	106.35	110.49
8	X	3	BMA	O3-C3-C4	-2.42	104.75	110.35
8	P	3	BMA	O3-C3-C4	-2.39	104.81	110.35
7	W	3	BMA	O6-C6-C5	-2.38	103.11	111.29
7	e	3	BMA	O6-C6-C5	-2.38	103.13	111.29
8	f	3	BMA	C6-C5-C4	-2.37	107.46	113.00
7	O	3	BMA	O6-C6-C5	-2.36	103.18	111.29
8	X	3	BMA	C6-C5-C4	-2.36	107.47	113.00
8	P	3	BMA	C6-C5-C4	-2.36	107.48	113.00
6	d	1	NAG	C1-O5-C5	2.34	115.37	112.19
6	V	1	NAG	C1-O5-C5	2.34	115.36	112.19
9	R	6	MAN	O5-C5-C6	2.32	110.83	107.20
5	M	1	NAG	C1-O5-C5	2.30	115.31	112.19
9	Z	6	MAN	O5-C5-C6	2.30	110.81	107.20
5	c	1	NAG	C1-O5-C5	2.30	115.31	112.19
6	N	1	NAG	C1-O5-C5	2.29	115.30	112.19
5	U	1	NAG	C1-O5-C5	2.29	115.29	112.19
8	X	3	BMA	C2-C3-C4	-2.28	106.94	110.89
8	f	3	BMA	C2-C3-C4	-2.27	106.96	110.89
9	h	6	MAN	O5-C5-C6	2.26	110.75	107.20
8	P	3	BMA	C2-C3-C4	-2.25	107.01	110.89
10	S	1	NAG	C1-O5-C5	2.24	115.23	112.19
7	e	6	MAN	O5-C5-C6	2.23	110.71	107.20
10	a	1	NAG	C1-O5-C5	2.23	115.21	112.19
7	W	4	MAN	O3-C3-C2	2.21	114.23	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	6	MAN	O5-C5-C6	2.21	110.67	107.20
7	W	6	MAN	O5-C5-C6	2.21	110.67	107.20
7	O	2	NAG	C4-C3-C2	-2.21	107.78	111.02
9	Z	6	MAN	O5-C1-C2	-2.20	107.37	110.77
7	W	2	NAG	C4-C3-C2	-2.20	107.80	111.02
9	R	1	NAG	O4-C4-C3	-2.19	105.28	110.35
7	O	2	NAG	O4-C4-C3	-2.19	105.28	110.35
9	h	1	NAG	O4-C4-C3	-2.19	105.28	110.35
10	i	1	NAG	C1-O5-C5	2.19	115.16	112.19
7	W	2	NAG	O4-C4-C3	-2.19	105.30	110.35
9	Z	1	NAG	O4-C4-C3	-2.18	105.30	110.35
7	e	4	MAN	O3-C3-C2	2.18	114.17	109.99
7	O	4	MAN	O3-C3-C2	2.18	114.17	109.99
9	h	3	BMA	O3-C3-C4	-2.17	105.33	110.35
5	g	1	NAG	C8-C7-N2	2.17	119.77	116.10
5	Q	1	NAG	C8-C7-N2	2.17	119.77	116.10
9	Z	3	BMA	O3-C3-C4	-2.16	105.35	110.35
9	R	3	BMA	O3-C3-C4	-2.16	105.36	110.35
9	h	6	MAN	O5-C1-C2	-2.15	107.45	110.77
9	h	1	NAG	C2-N2-C7	-2.15	119.84	122.90
5	Y	1	NAG	C8-C7-N2	2.15	119.73	116.10
7	e	2	NAG	O4-C4-C3	-2.14	105.39	110.35
9	R	6	MAN	O5-C1-C2	-2.14	107.47	110.77
9	Z	1	NAG	C2-N2-C7	-2.14	119.86	122.90
9	R	1	NAG	C2-N2-C7	-2.13	119.86	122.90
6	N	2	NAG	C1-O5-C5	2.13	115.08	112.19
5	T	2	NAG	C1-O5-C5	2.11	115.05	112.19
5	Y	1	NAG	C1-O5-C5	2.10	115.04	112.19
7	e	4	MAN	O2-C2-C1	-2.09	104.88	109.15
6	V	2	NAG	C1-O5-C5	2.09	115.02	112.19
7	e	2	NAG	C4-C3-C2	-2.08	107.97	111.02
5	g	1	NAG	C1-O5-C5	2.08	115.00	112.19
7	W	4	MAN	O2-C2-C1	-2.07	104.91	109.15
5	Q	1	NAG	C1-O5-C5	2.07	115.00	112.19
6	d	2	NAG	C1-O5-C5	2.07	115.00	112.19
5	b	2	NAG	C1-O5-C5	2.07	114.99	112.19
7	e	5	MAN	C2-C3-C4	-2.06	107.32	110.89
7	O	4	MAN	O2-C2-C1	-2.06	104.94	109.15
9	h	1	NAG	C3-C4-C5	-2.06	106.57	110.24
5	j	2	NAG	C1-O5-C5	2.05	114.97	112.19
7	O	5	MAN	C2-C3-C4	-2.05	107.34	110.89
9	R	1	NAG	C3-C4-C5	-2.05	106.58	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	4	MAN	O2-C2-C3	-2.05	106.03	110.14
6	N	4	MAN	O2-C2-C3	-2.05	106.04	110.14
7	W	5	MAN	C2-C3-C4	-2.05	107.36	110.89
6	d	4	MAN	O2-C2-C3	-2.04	106.06	110.14
7	e	3	BMA	C2-C3-C4	-2.03	107.39	110.89
9	Z	1	NAG	C3-C4-C5	-2.01	106.66	110.24

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
9	R	2	NAG	C8-C7-N2-C2
9	R	2	NAG	O7-C7-N2-C2
9	Z	2	NAG	C8-C7-N2-C2
9	Z	2	NAG	O7-C7-N2-C2
9	h	2	NAG	C8-C7-N2-C2
9	h	2	NAG	O7-C7-N2-C2
9	R	1	NAG	C8-C7-N2-C2
9	R	1	NAG	O7-C7-N2-C2
9	Z	1	NAG	C8-C7-N2-C2
9	Z	1	NAG	O7-C7-N2-C2
9	h	1	NAG	C8-C7-N2-C2
9	h	1	NAG	O7-C7-N2-C2
10	S	1	NAG	O5-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
10	i	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	j	1	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	a	1	NAG	C4-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
8	P	6	MAN	O5-C5-C6-O6
8	X	6	MAN	O5-C5-C6-O6
8	f	6	MAN	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	d	2	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
5	j	1	NAG	C4-C5-C6-O6
8	P	8	MAN	C4-C5-C6-O6
8	X	8	MAN	C4-C5-C6-O6
8	f	8	MAN	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
8	P	6	MAN	C4-C5-C6-O6
8	X	6	MAN	C4-C5-C6-O6
8	f	6	MAN	C4-C5-C6-O6
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
7	W	2	NAG	C8-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
5	Q	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	e	4	MAN	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
8	X	2	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	P	1	NAG	C8-C7-N2-C2
8	X	1	NAG	C8-C7-N2-C2
8	f	1	NAG	C8-C7-N2-C2
5	T	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
9	R	2	NAG	C1-C2-N2-C7
9	Z	2	NAG	C1-C2-N2-C7
9	h	2	NAG	C1-C2-N2-C7
8	P	8	MAN	O5-C5-C6-O6
8	f	8	MAN	O5-C5-C6-O6
7	O	2	NAG	O7-C7-N2-C2
7	W	2	NAG	O7-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
8	f	1	NAG	O7-C7-N2-C2
8	X	8	MAN	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
9	h	3	BMA	O5-C5-C6-O6
9	R	3	BMA	O5-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
9	R	6	MAN	C4-C5-C6-O6
9	Z	6	MAN	C4-C5-C6-O6
9	h	6	MAN	C4-C5-C6-O6
10	S	3	BMA	C4-C5-C6-O6
10	i	3	BMA	C4-C5-C6-O6
10	a	3	BMA	C4-C5-C6-O6
7	O	6	MAN	O5-C5-C6-O6
7	W	6	MAN	O5-C5-C6-O6
7	e	6	MAN	O5-C5-C6-O6
8	f	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	P	5	MAN	O5-C5-C6-O6
8	X	5	MAN	O5-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	Z	3	BMA	C4-C5-C6-O6
9	R	3	BMA	C4-C5-C6-O6
9	h	3	BMA	C4-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	Z	6	MAN	O5-C5-C6-O6
9	R	6	MAN	O5-C5-C6-O6
9	h	6	MAN	O5-C5-C6-O6
10	S	3	BMA	O5-C5-C6-O6
10	i	3	BMA	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	d	1	NAG	C4-C5-C6-O6
8	P	2	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
8	X	2	NAG	C4-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
7	O	1	NAG	C3-C2-N2-C7
7	W	1	NAG	C3-C2-N2-C7
7	e	1	NAG	C3-C2-N2-C7
9	R	2	NAG	C3-C2-N2-C7
9	Z	2	NAG	C3-C2-N2-C7
9	h	2	NAG	C3-C2-N2-C7
10	S	2	NAG	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	i	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	Y	1	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	g	1	NAG	C3-C2-N2-C7
5	g	2	NAG	C3-C2-N2-C7
7	O	4	MAN	C4-C5-C6-O6

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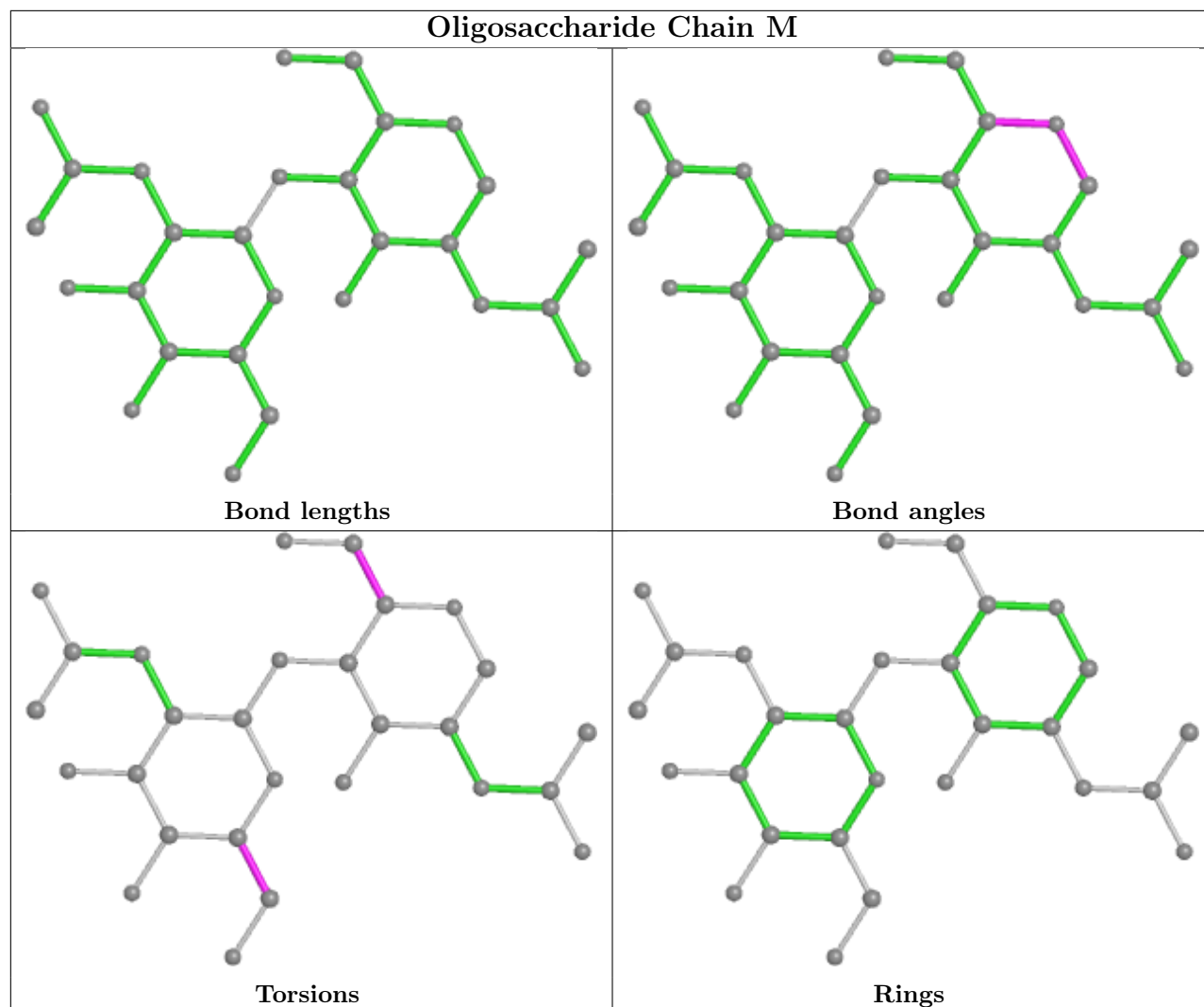
Mol	Chain	Res	Type	Atoms
7	W	4	MAN	C4-C5-C6-O6

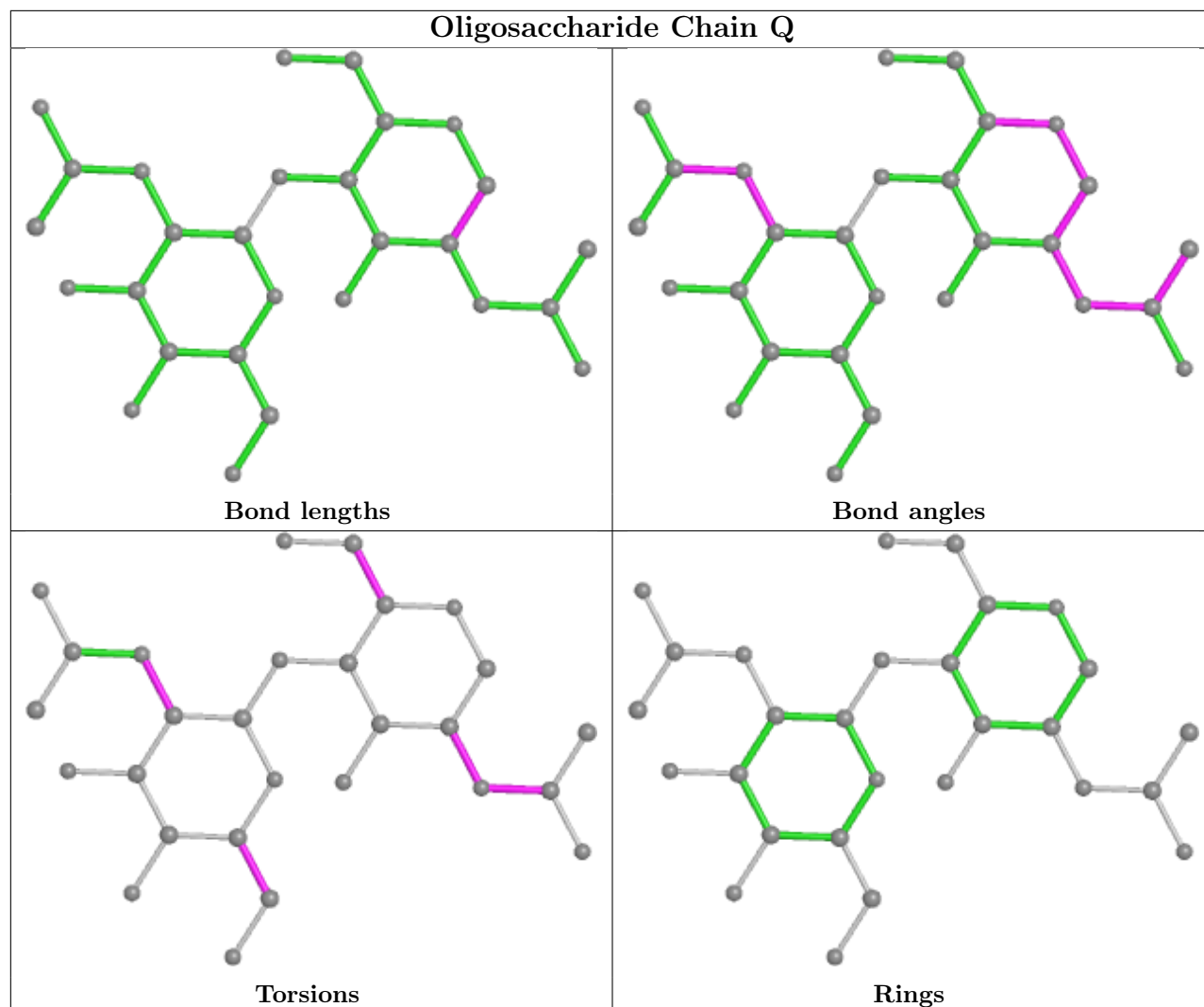
There are no ring outliers.

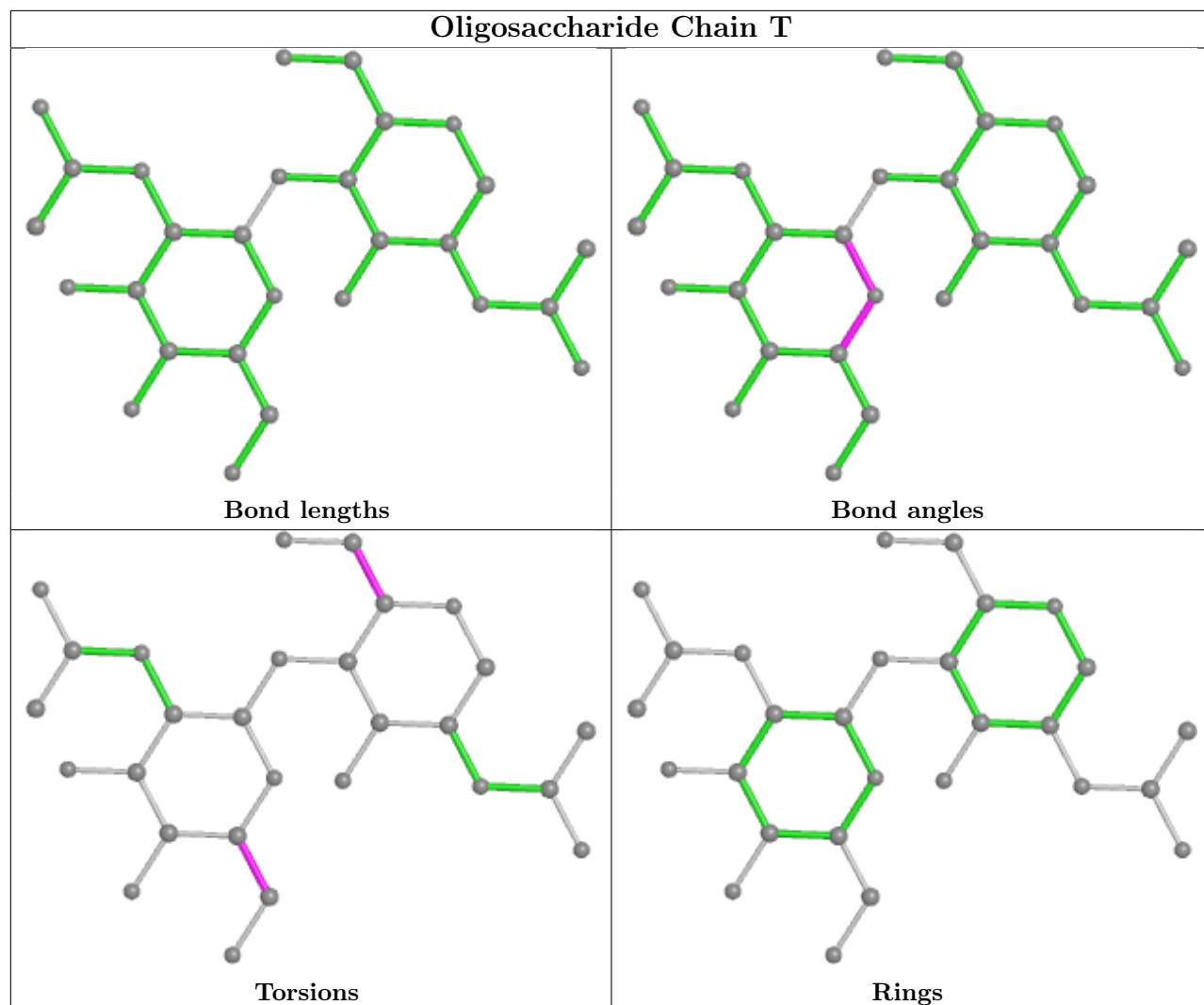
7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	8	MAN	1	0
5	T	1	NAG	1	0
8	P	8	MAN	1	0
8	P	6	MAN	1	0
8	X	6	MAN	1	0
9	Z	2	NAG	1	0
9	R	2	NAG	1	0

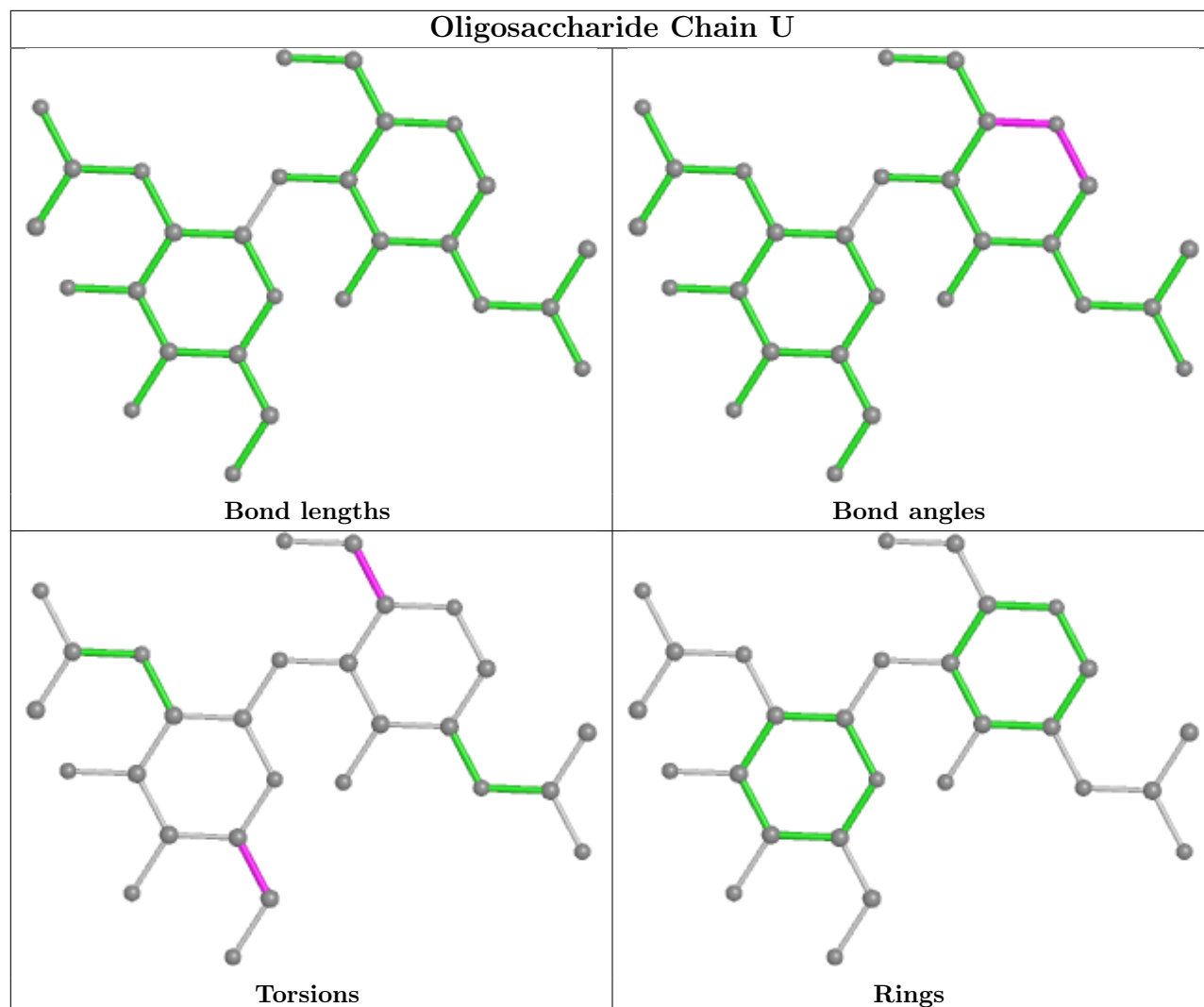
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

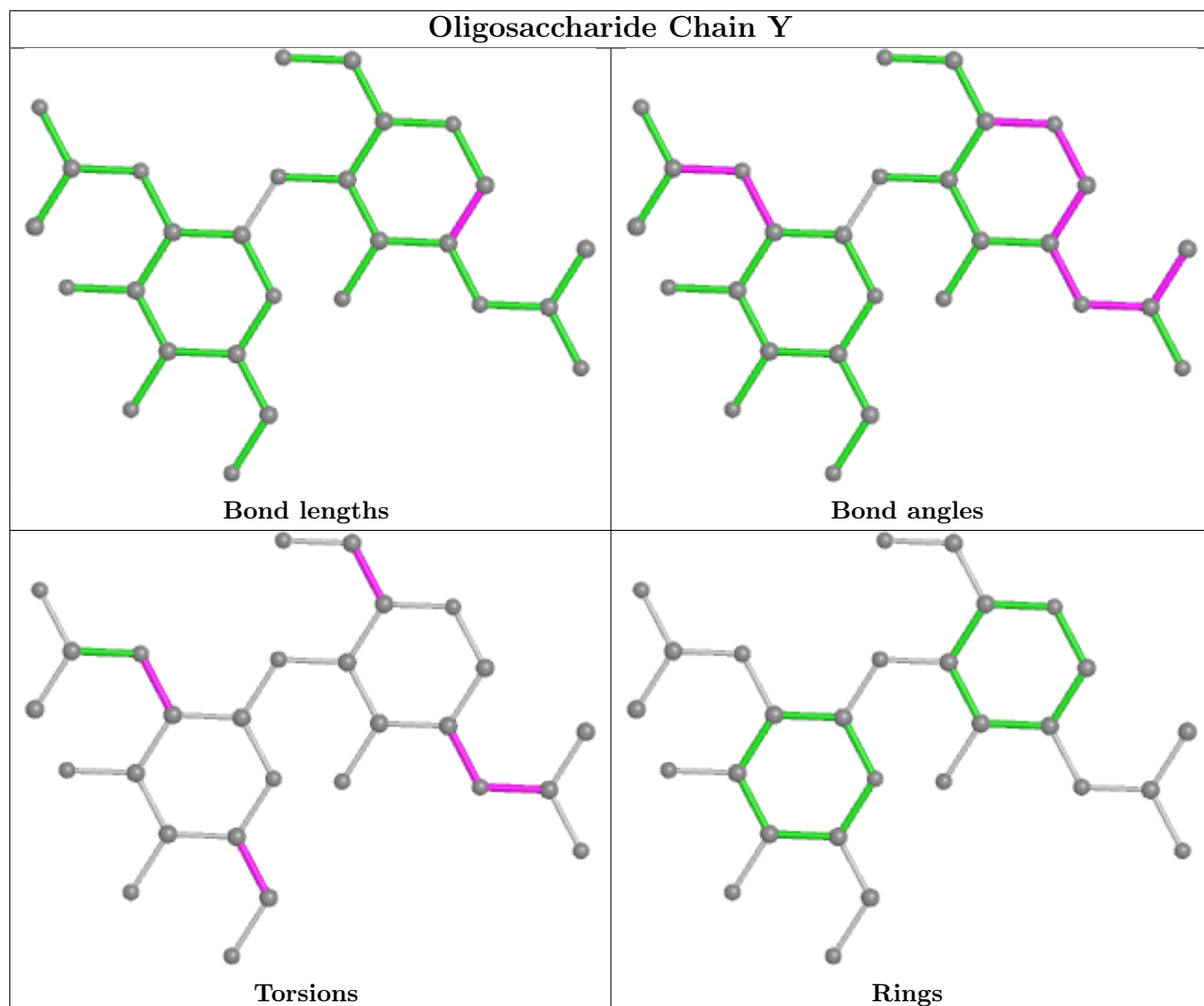


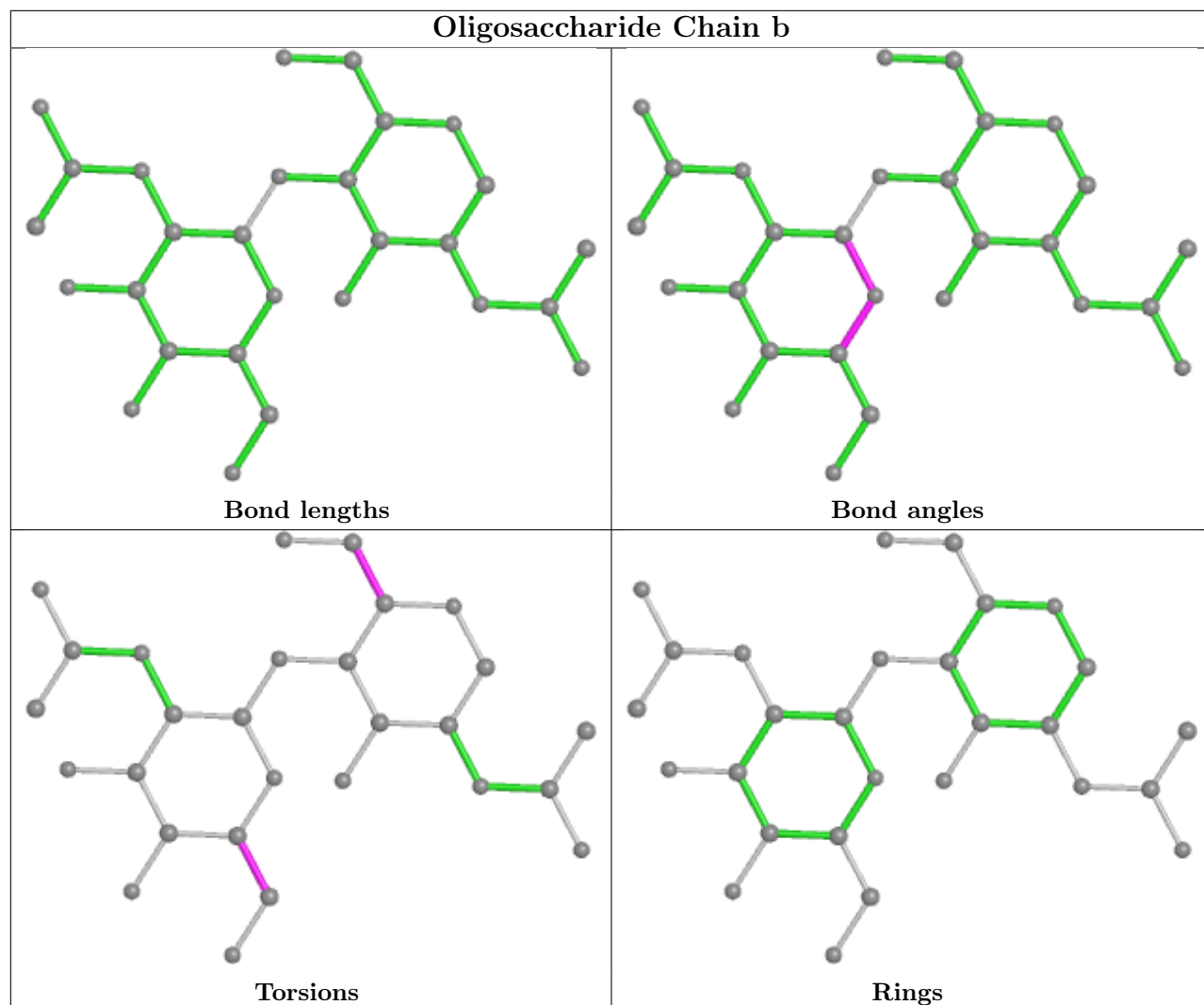


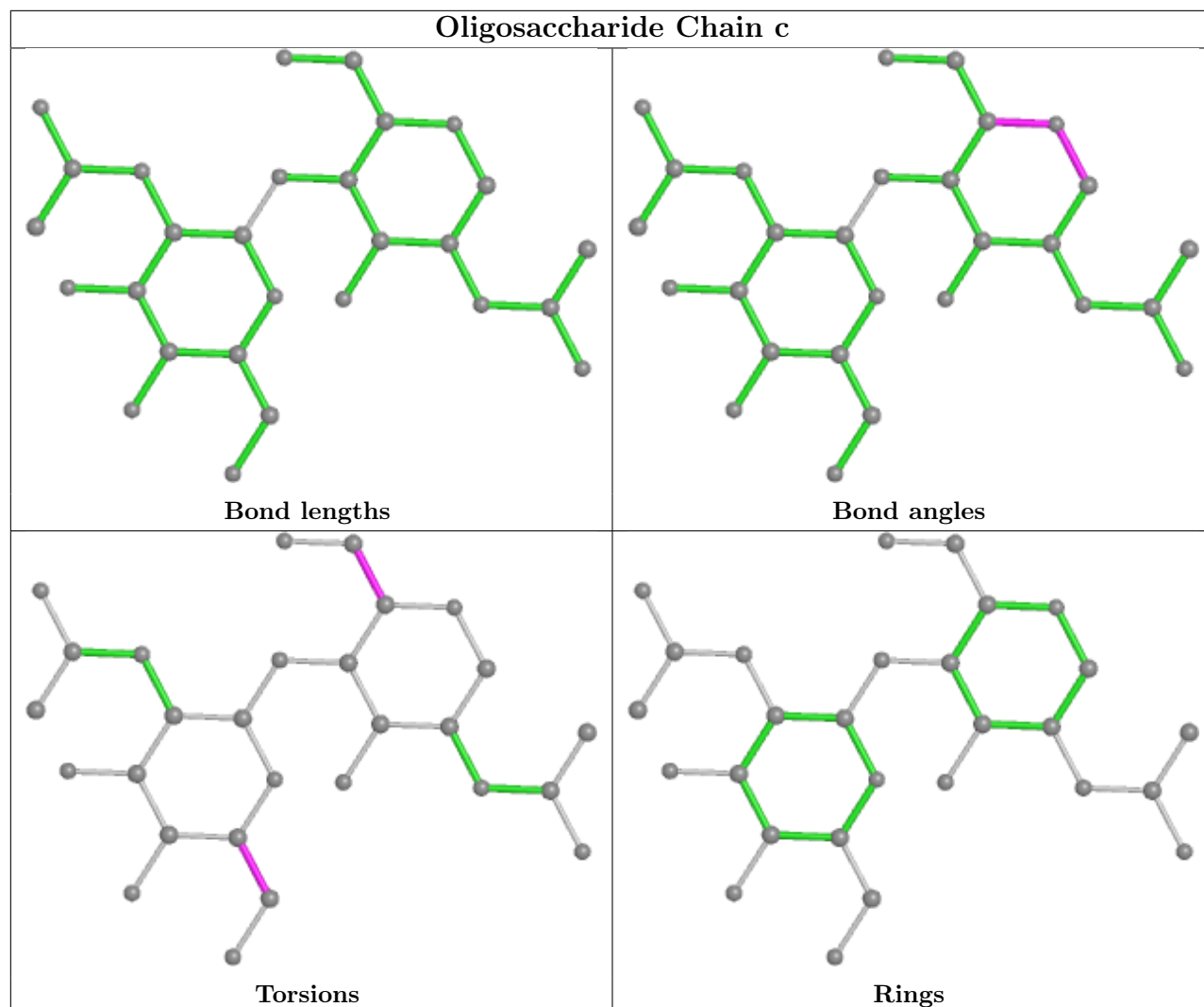


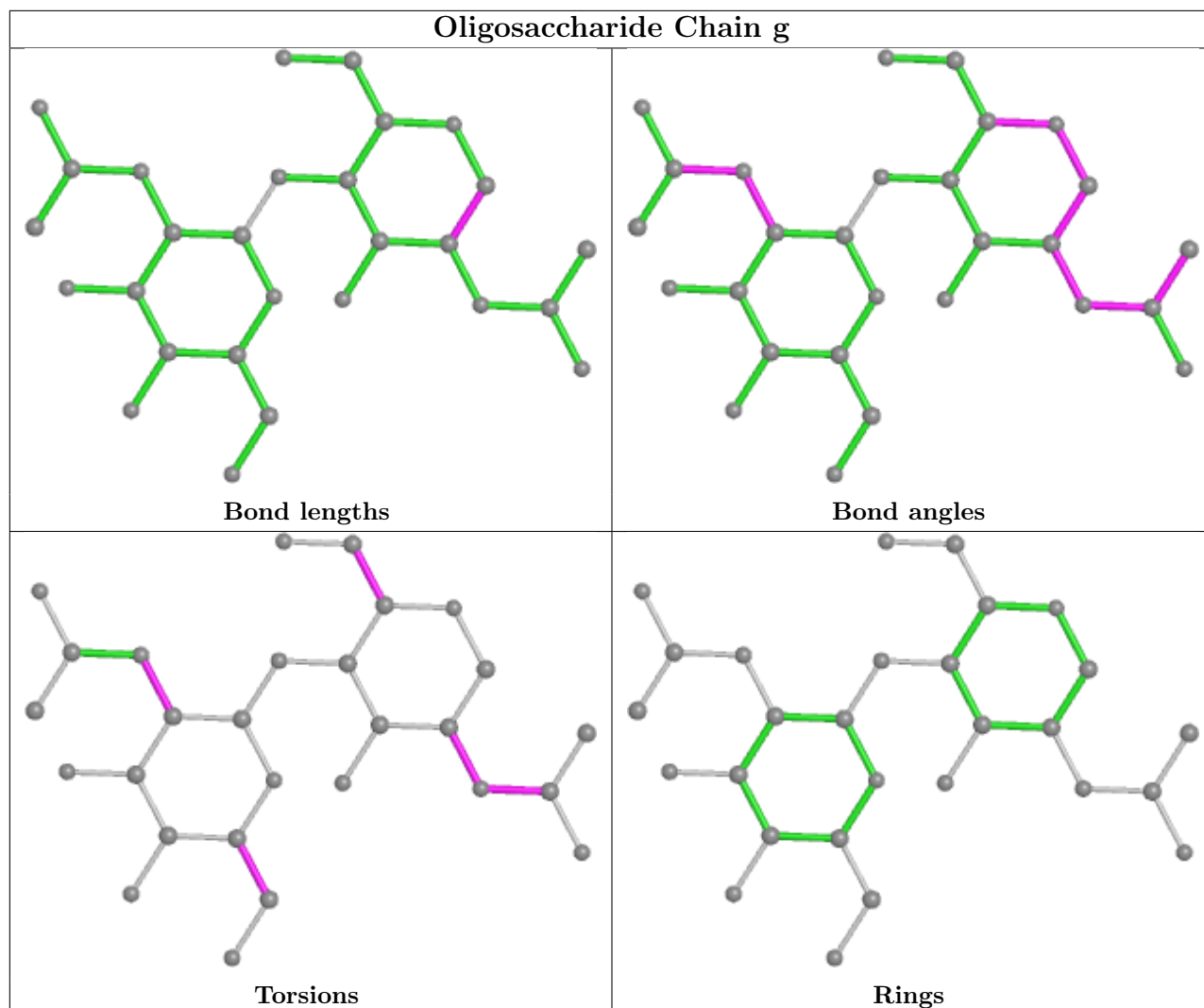


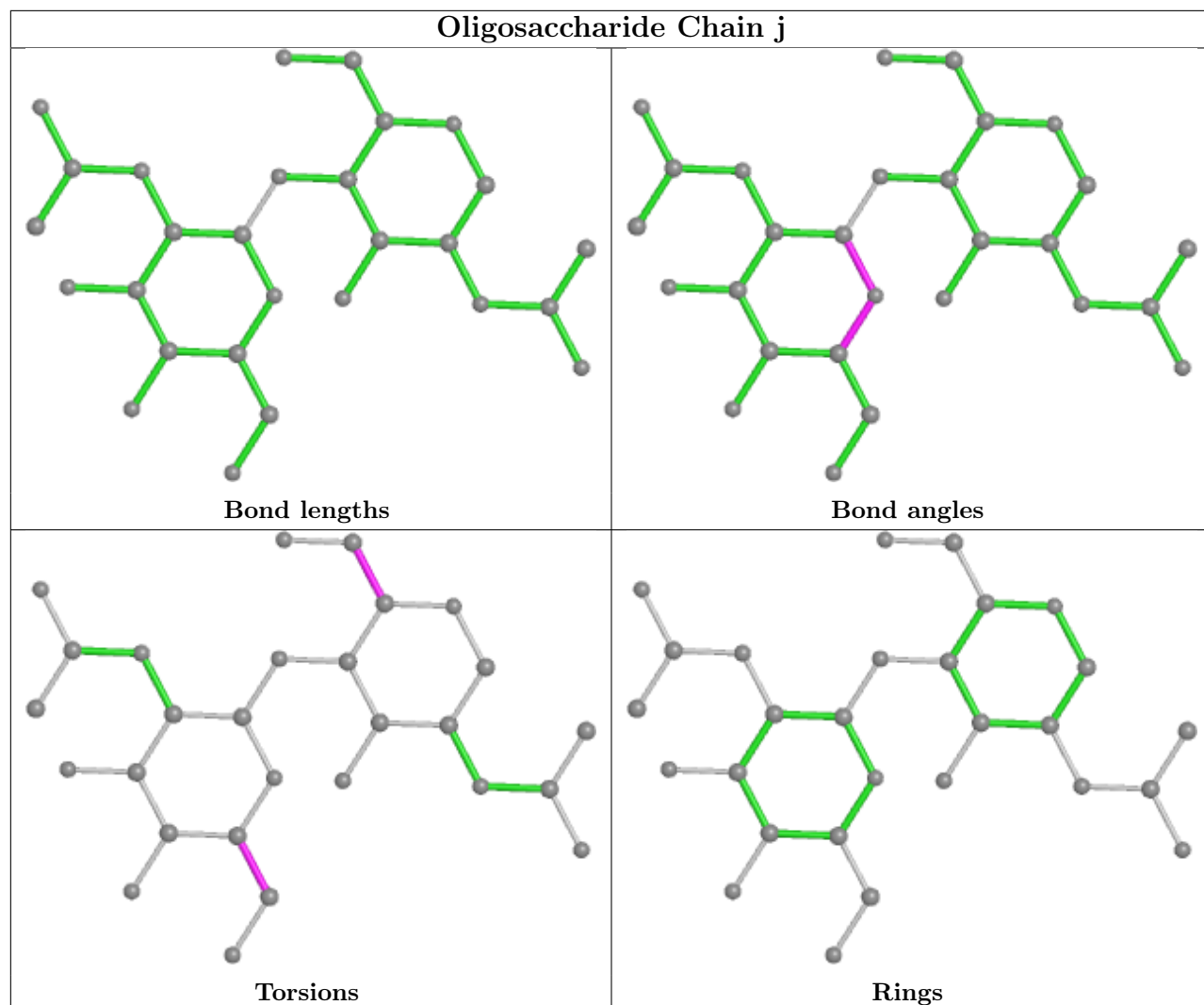


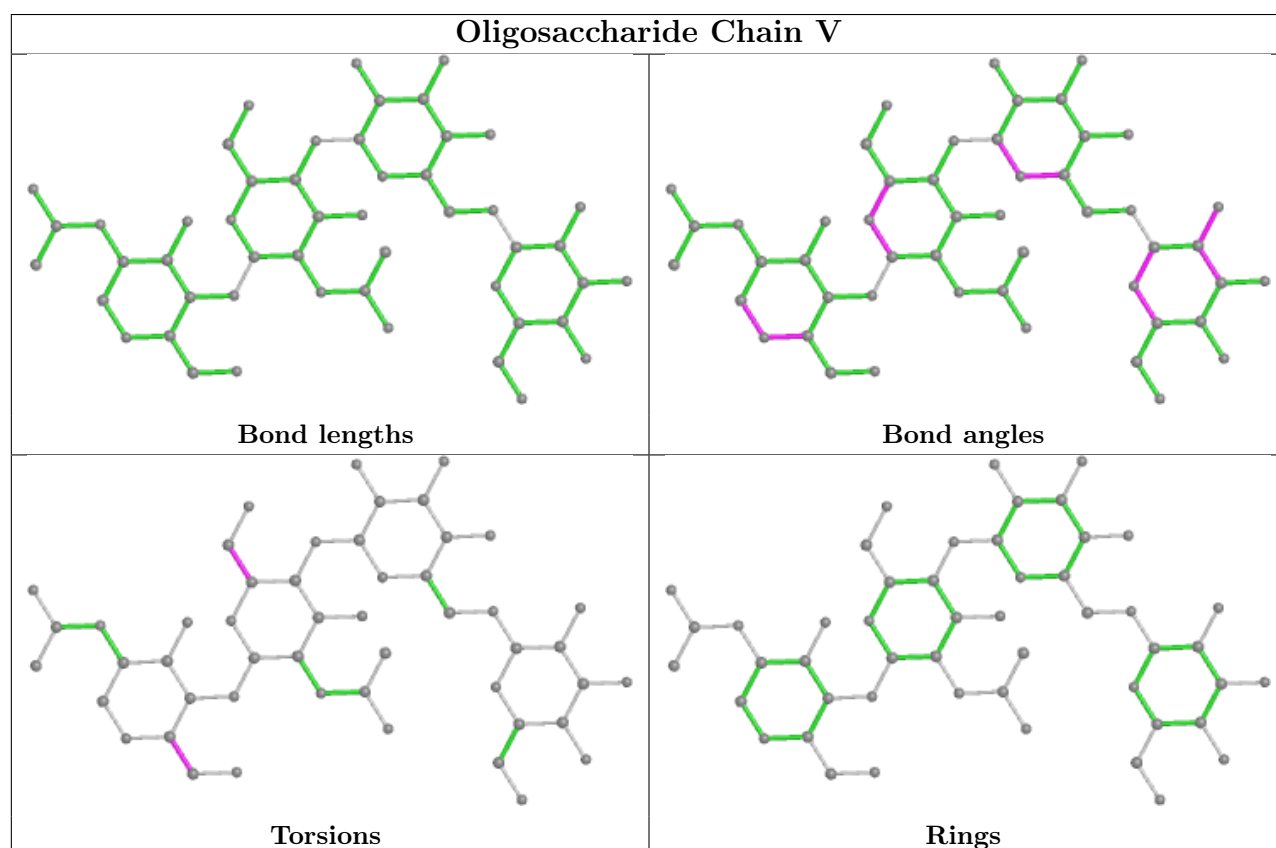
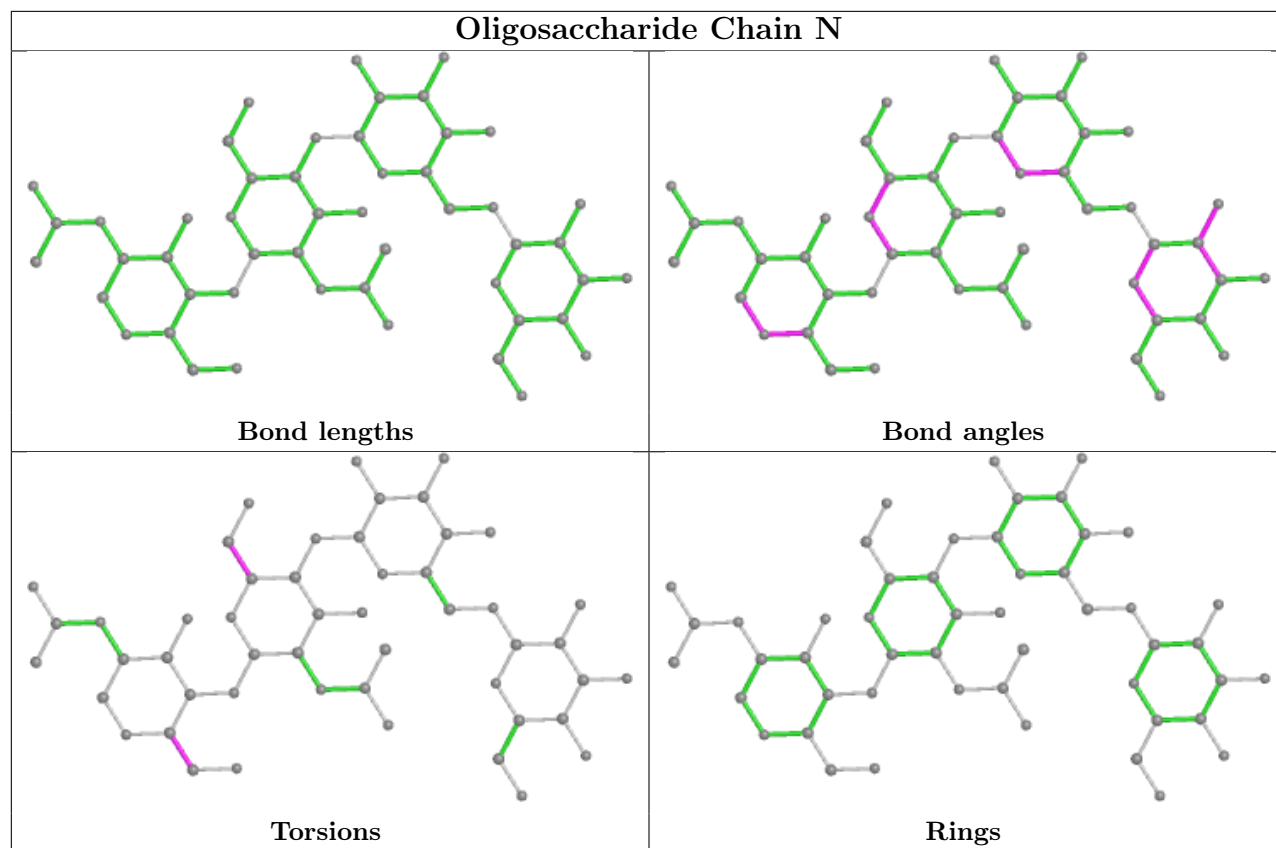


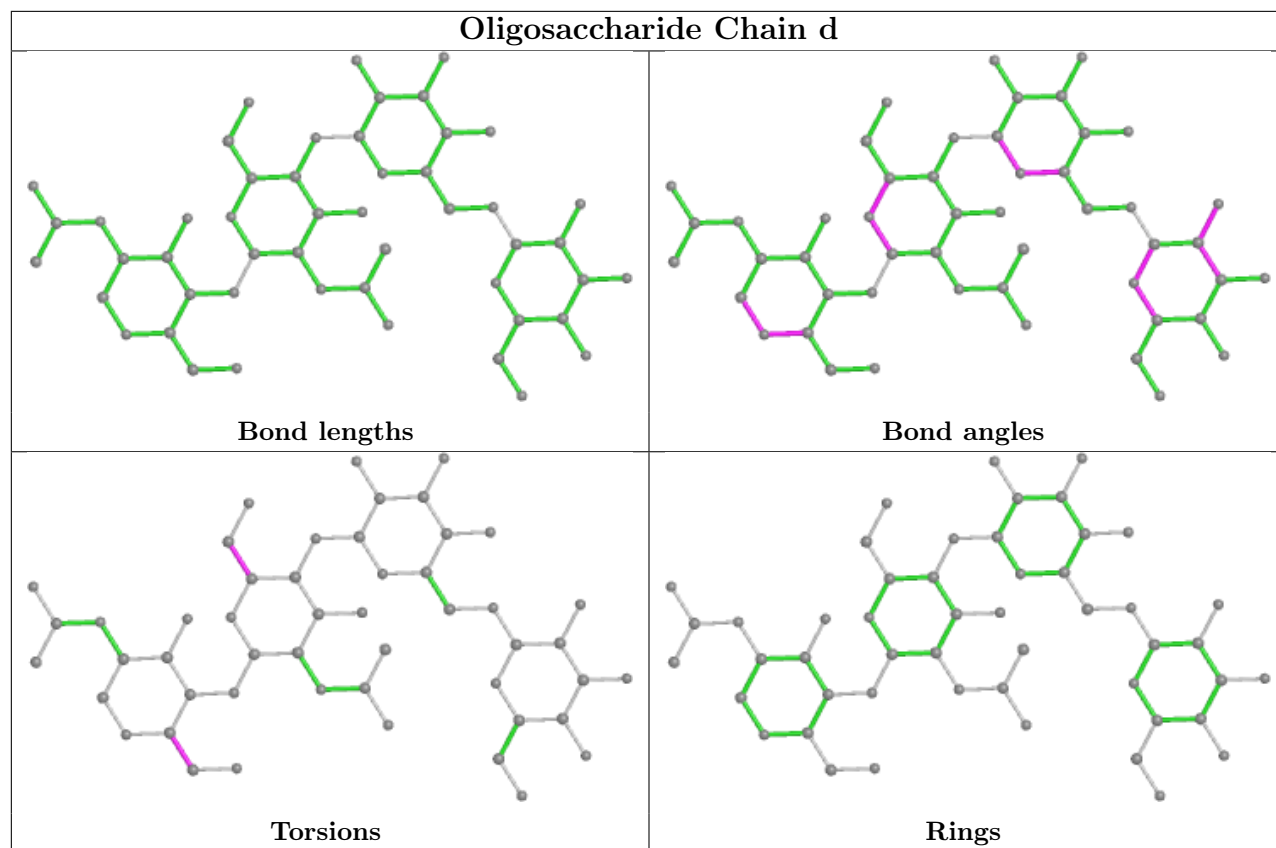




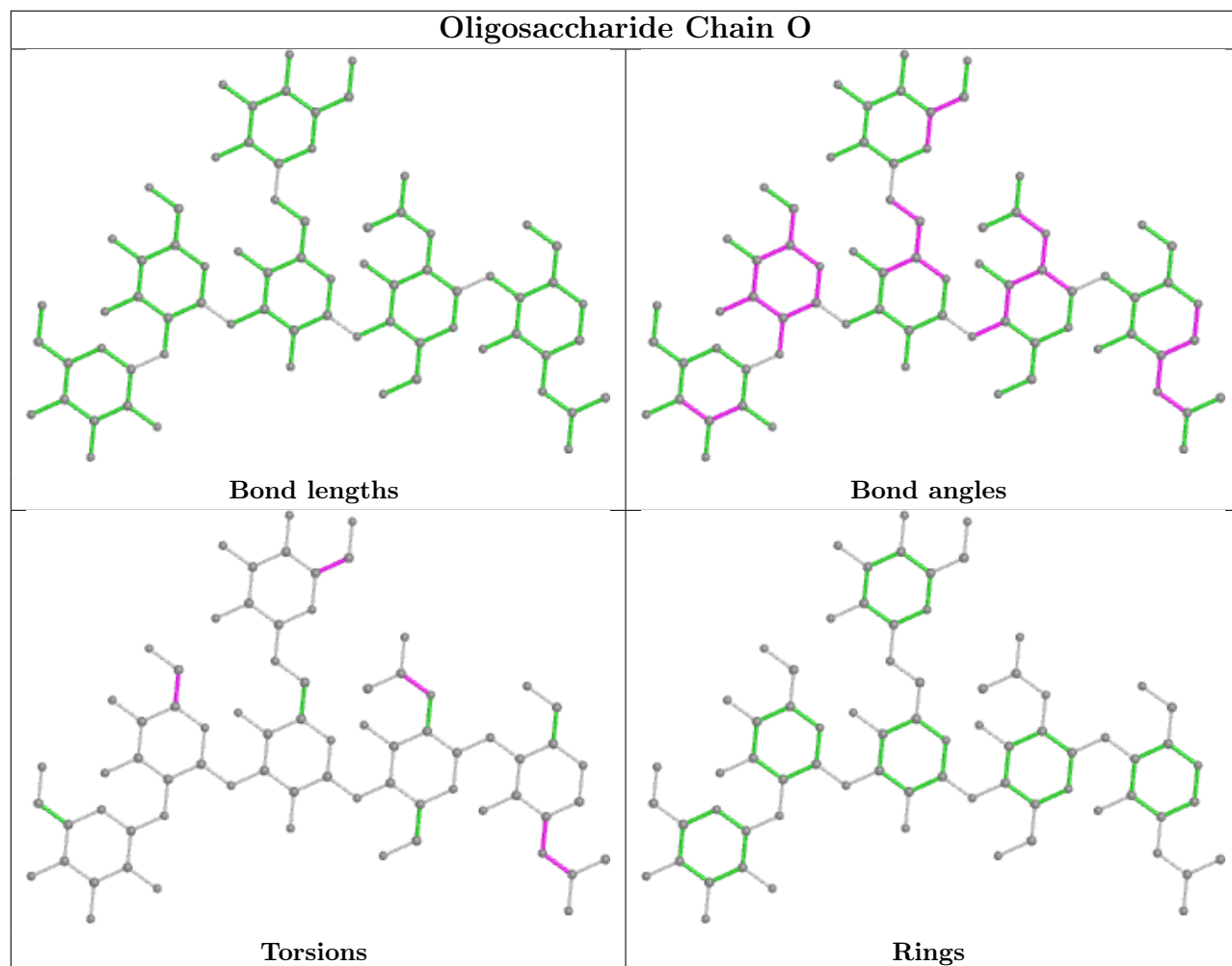


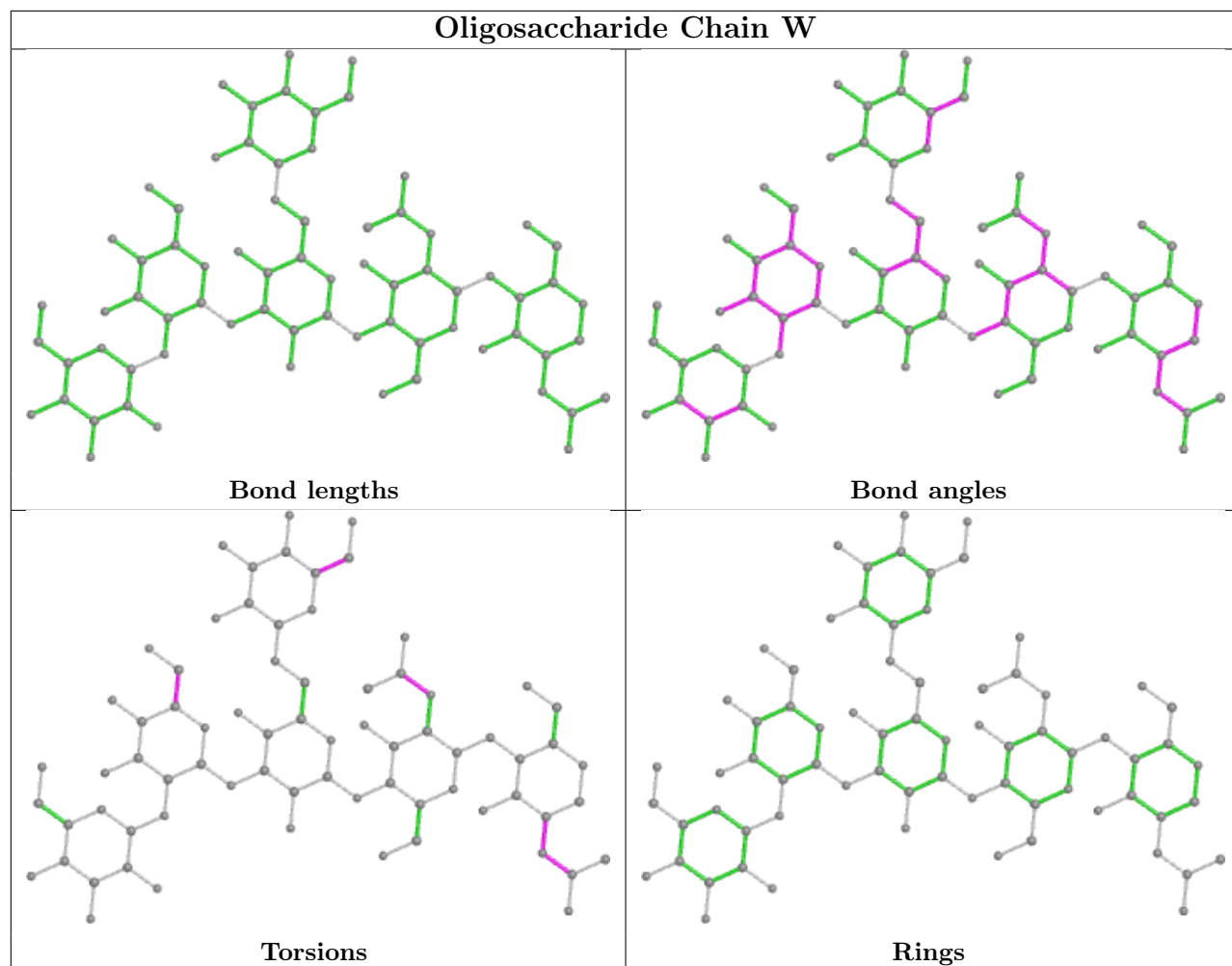


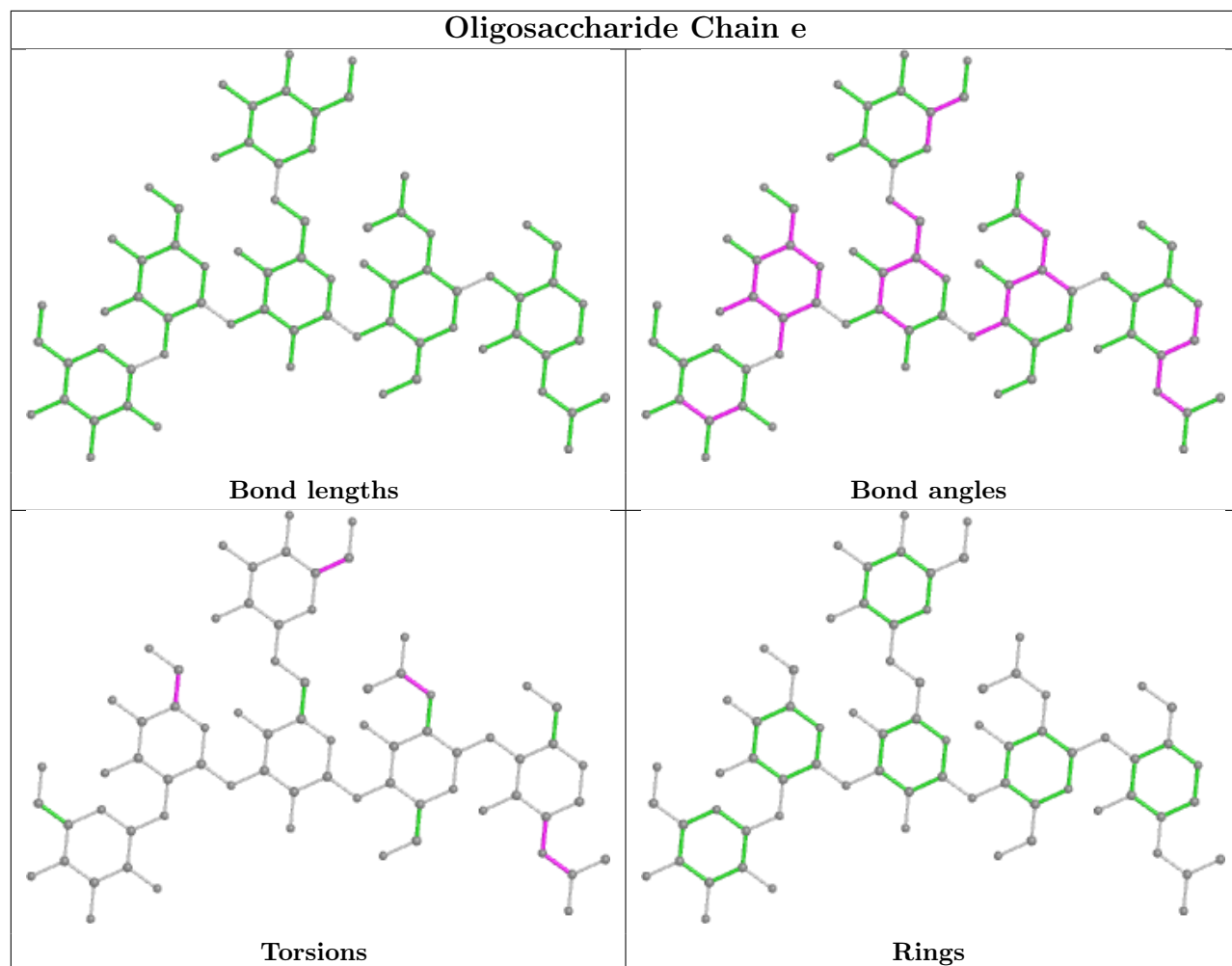


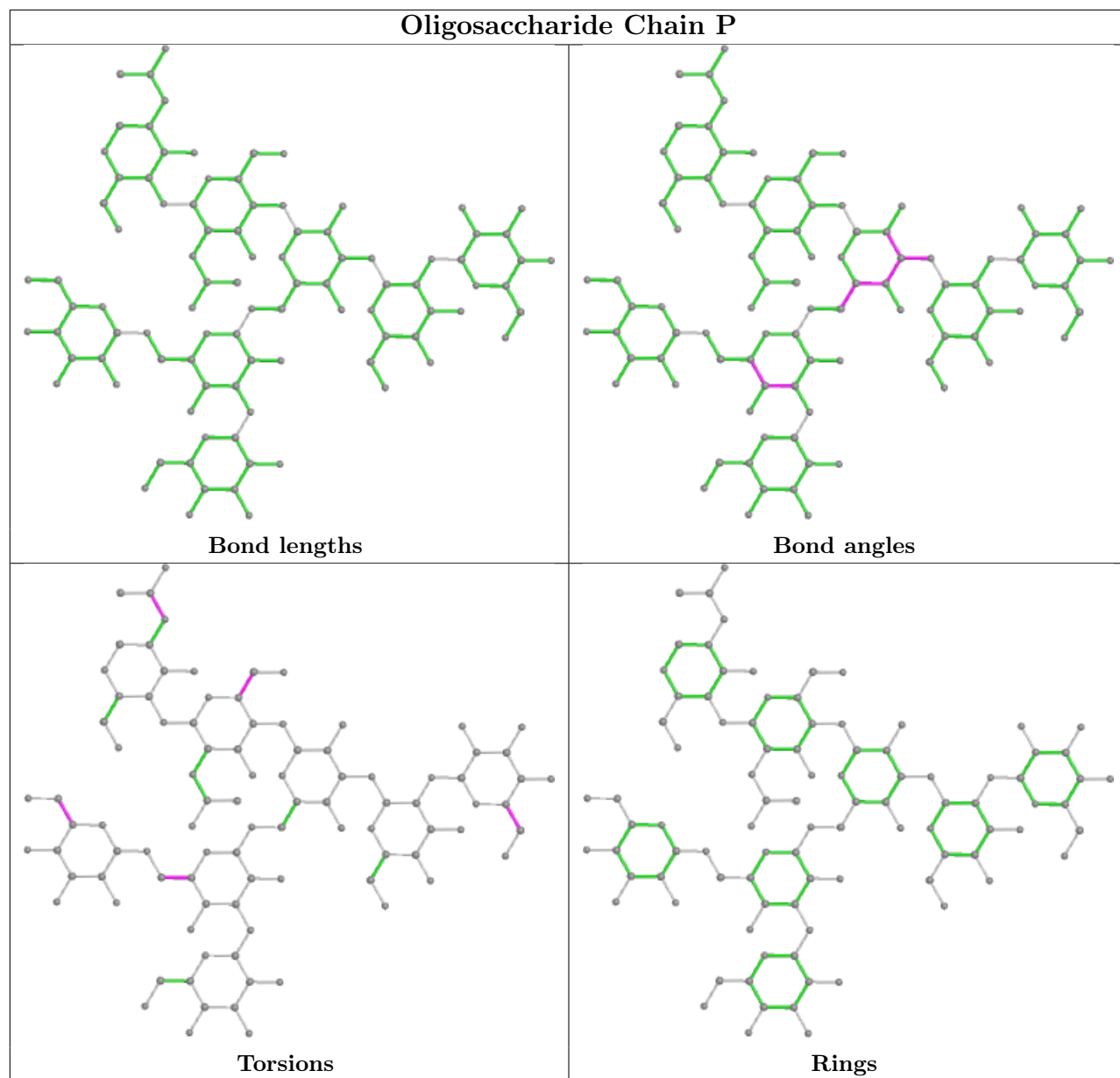


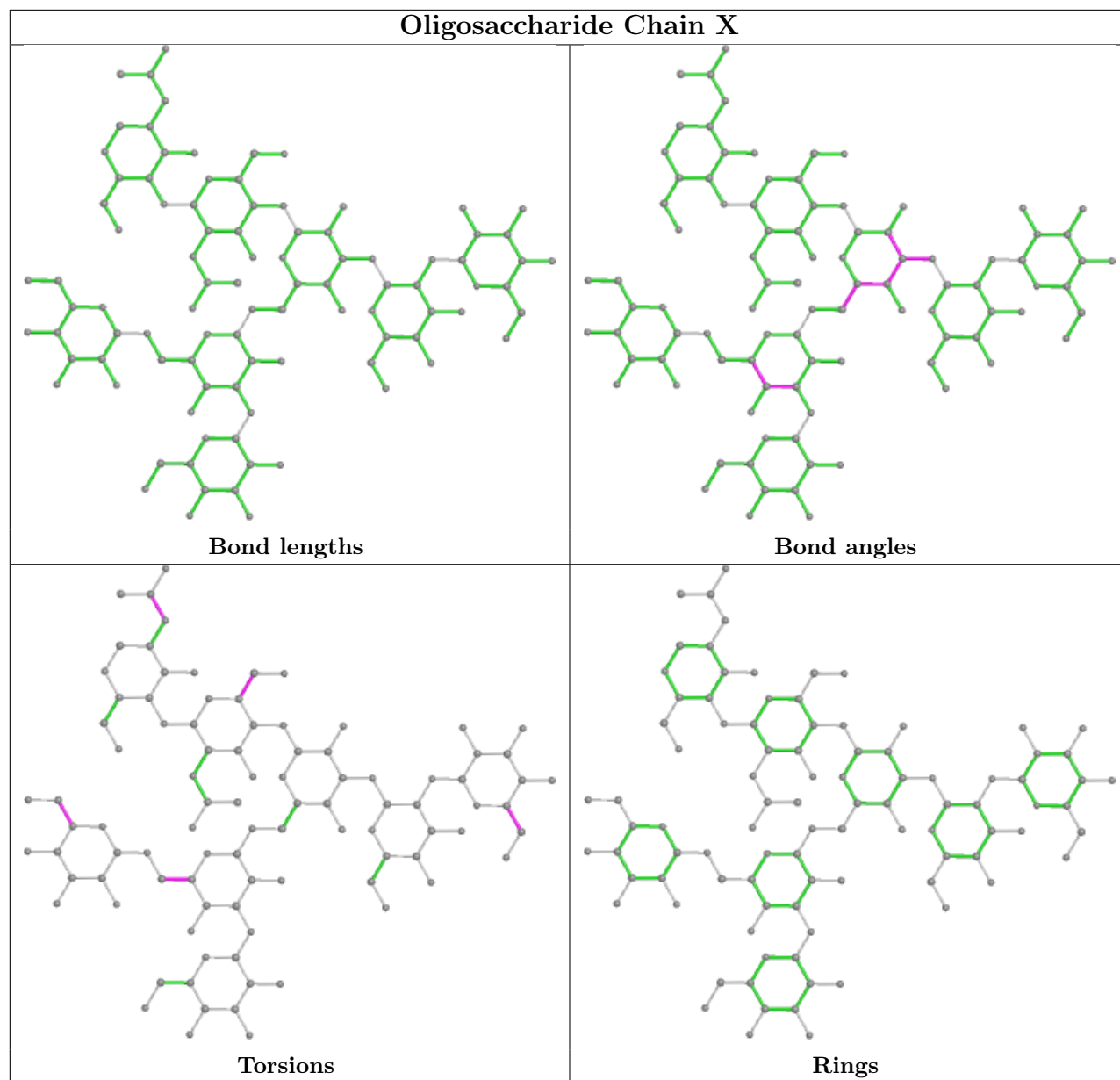


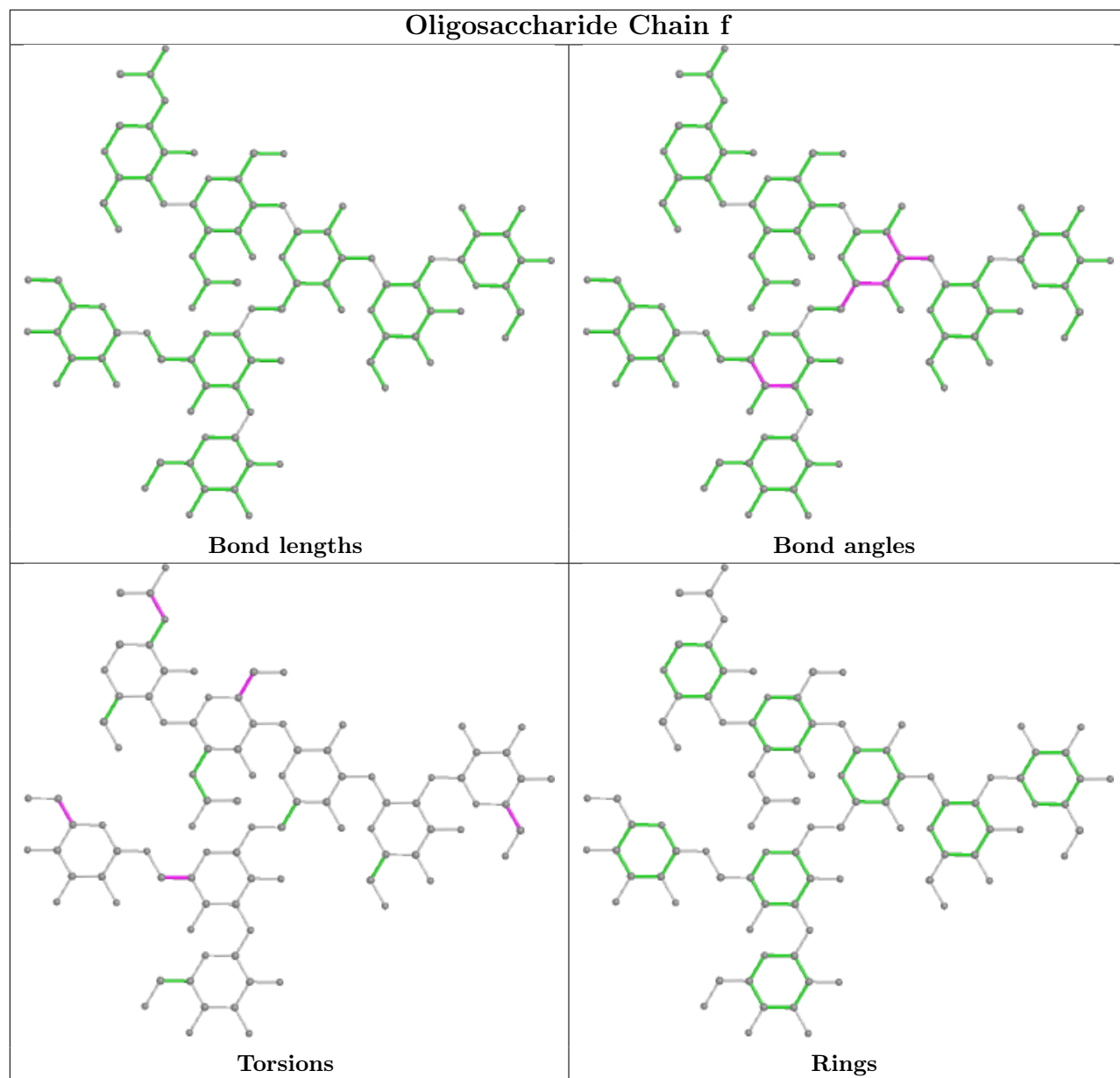


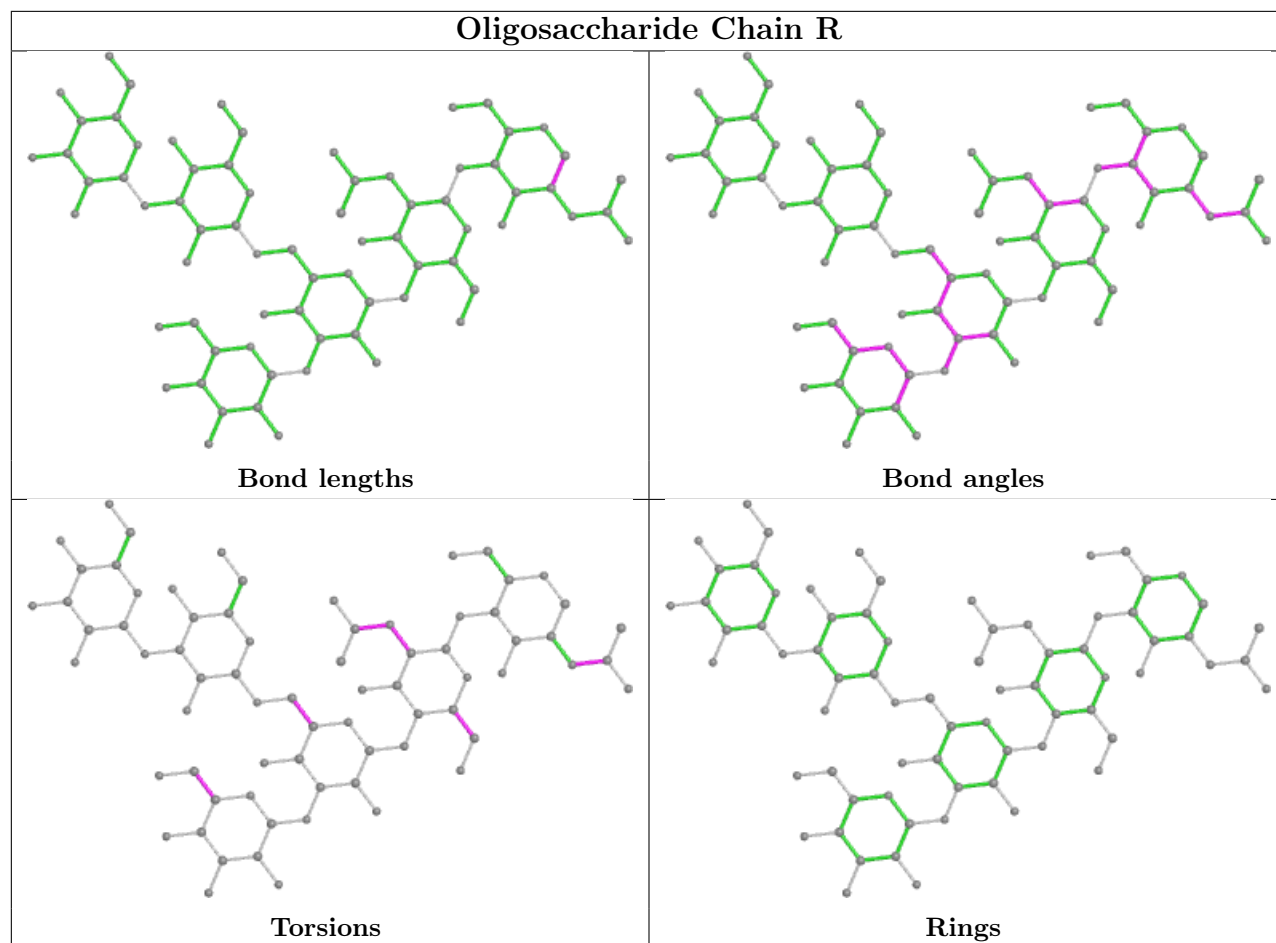


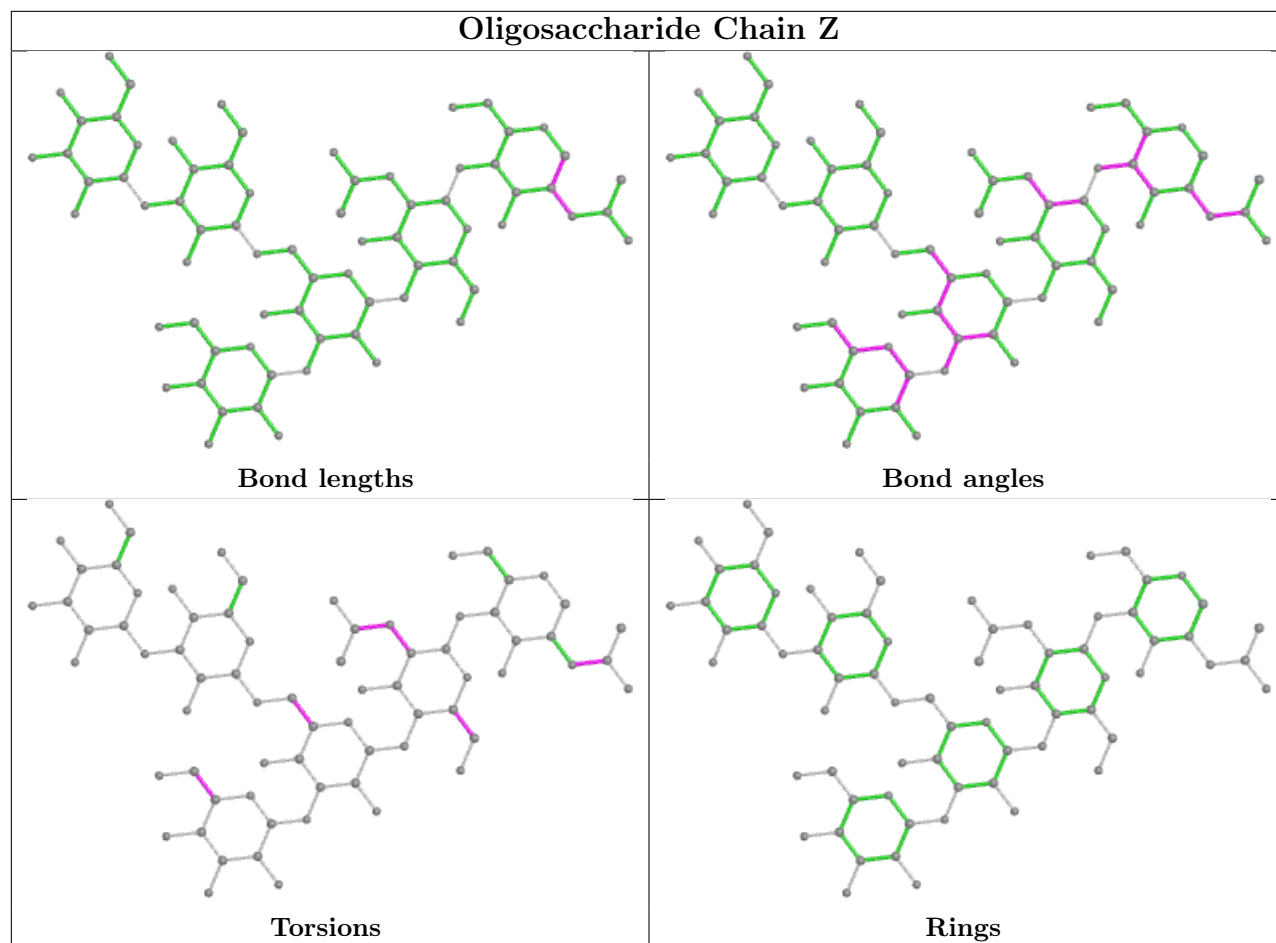




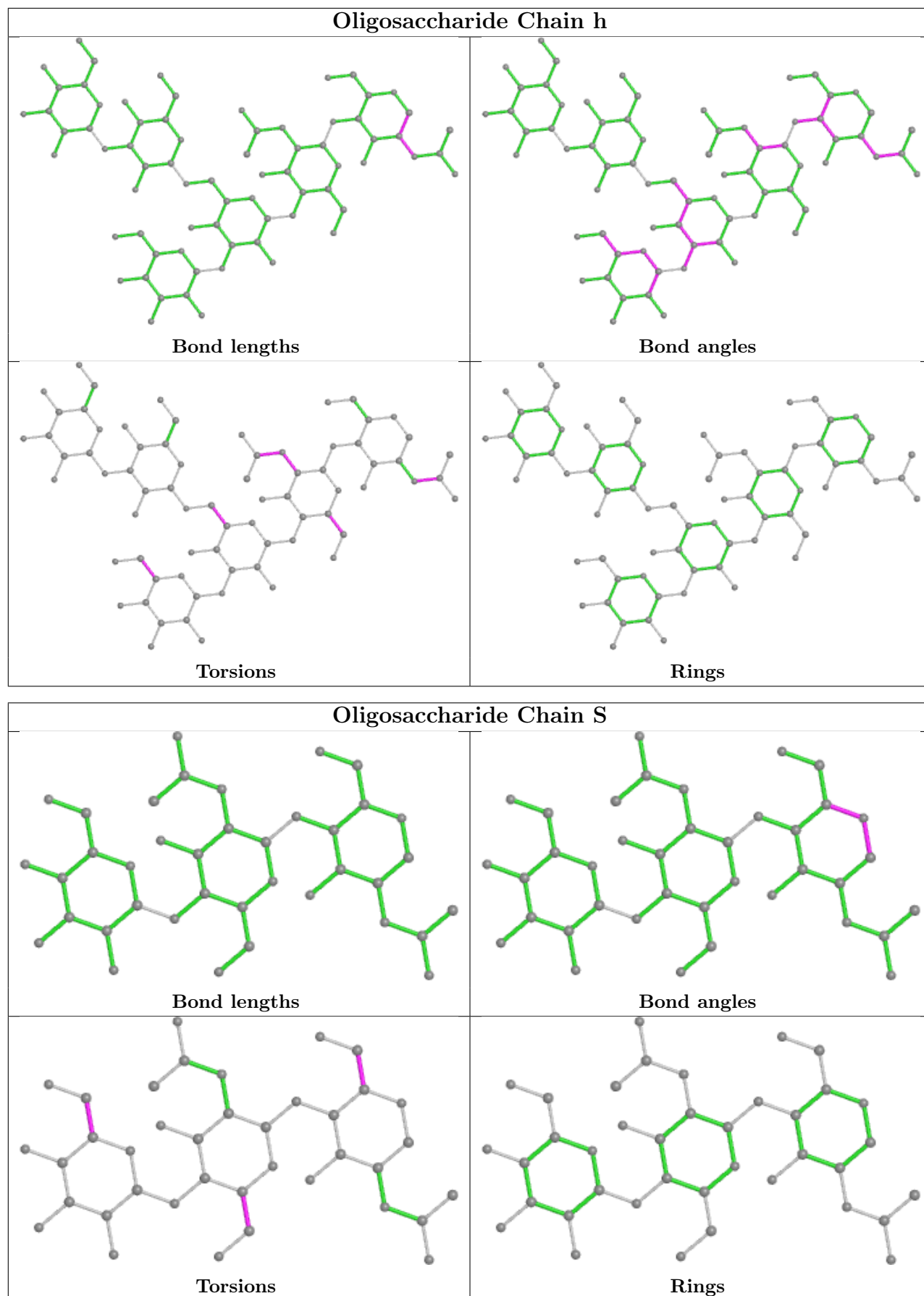


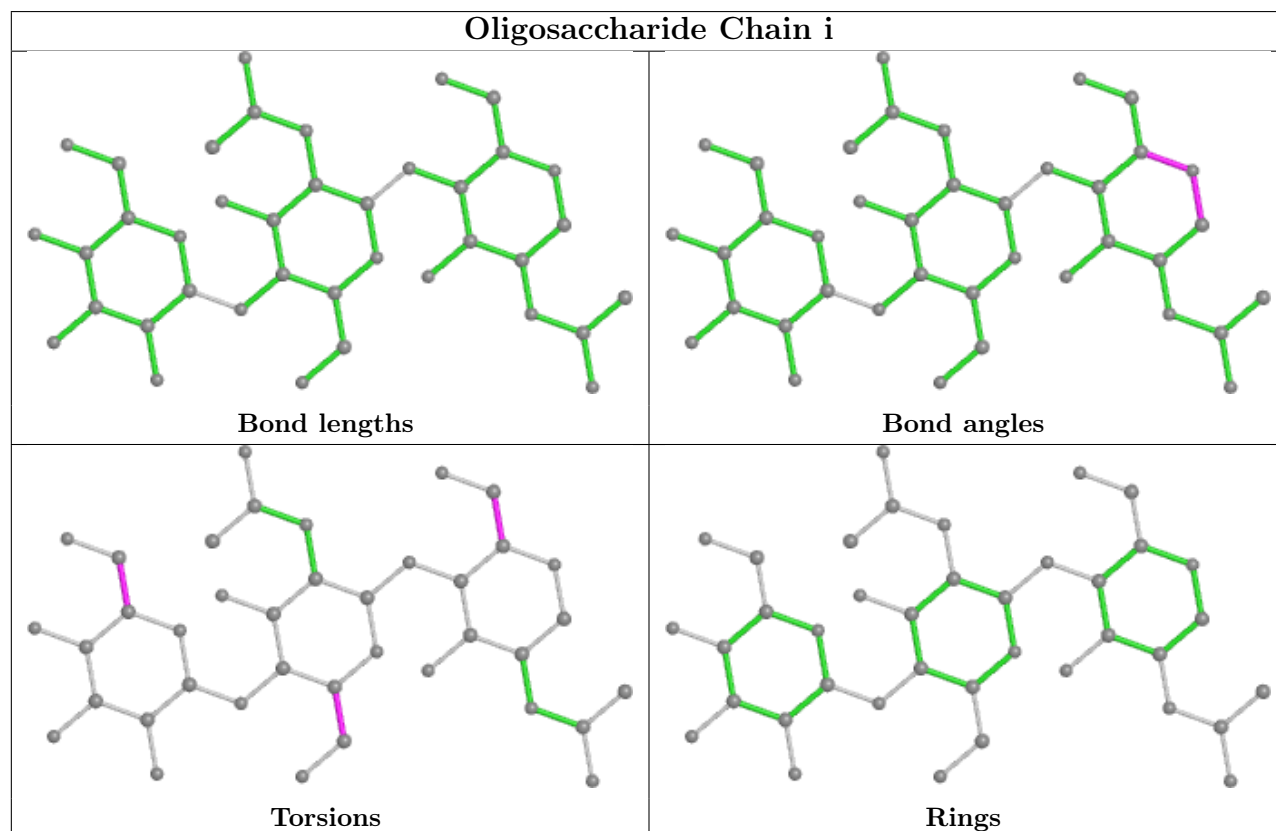
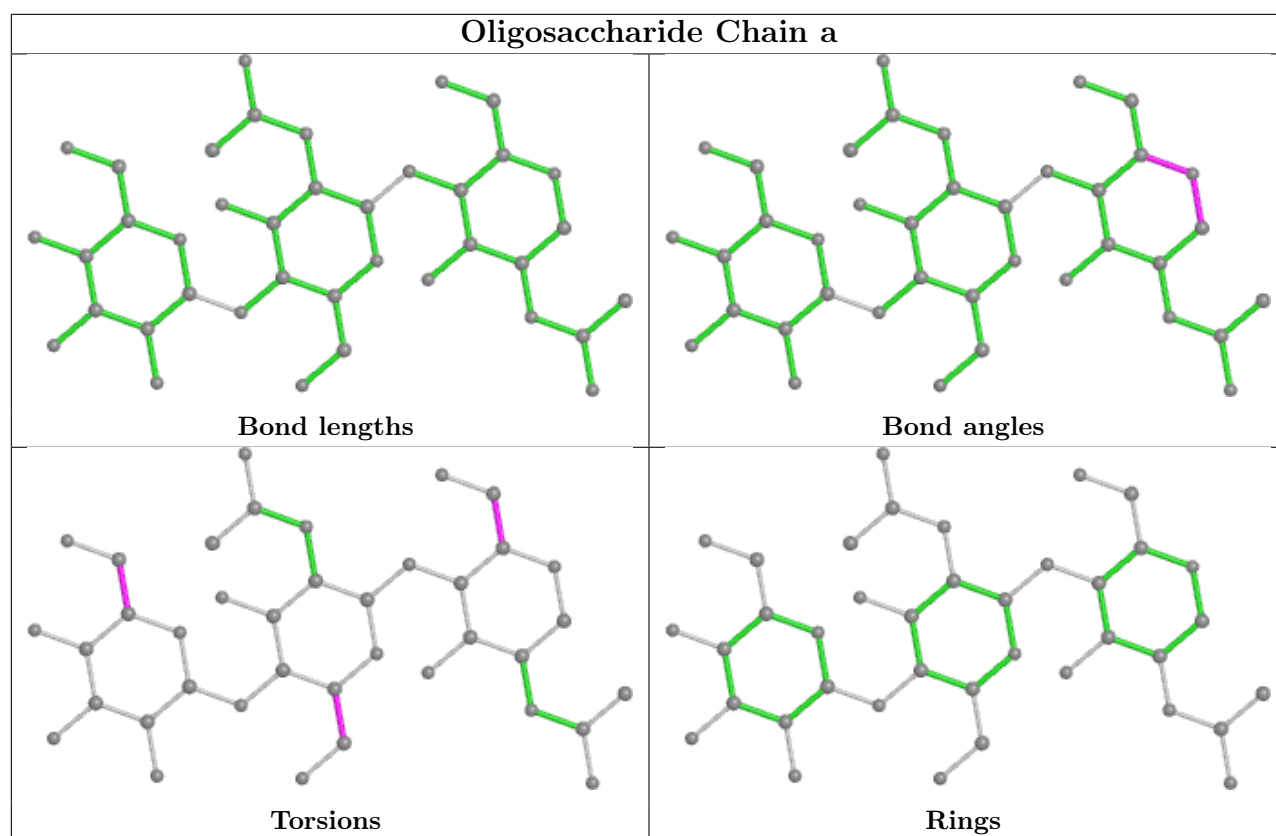












## 5.6 Ligand geometry

36 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
11	NAG	I	1234	2	14,14,15	0.28	0	17,19,21	0.52	0
11	NAG	I	1088	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
11	NAG	G	1301	2	14,14,15	0.24	0	17,19,21	0.59	0
11	NAG	I	1332	2	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
11	NAG	G	1088	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
11	NAG	I	1392	2	14,14,15	0.22	0	17,19,21	0.53	0
11	NAG	C	1301	2	14,14,15	0.23	0	17,19,21	0.58	0
11	NAG	C	1332	2	14,14,15	0.69	1 (7%)	17,19,21	0.98	1 (5%)
11	NAG	C	1355	2	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	G	1234	2	14,14,15	0.27	0	17,19,21	0.51	0
11	NAG	C	1339	2	14,14,15	0.34	0	17,19,21	0.53	0
11	NAG	D	1072	3	14,14,15	0.37	0	17,19,21	0.52	0
11	NAG	C	1156	2	14,14,15	0.57	0	17,19,21	1.35	3 (17%)
11	NAG	I	1156	2	14,14,15	0.59	0	17,19,21	1.34	3 (17%)
11	NAG	G	1339	2	14,14,15	0.35	0	17,19,21	0.55	0
11	NAG	I	1339	2	14,14,15	0.35	0	17,19,21	0.55	0
11	NAG	B	1637	1	14,14,15	0.29	0	17,19,21	0.48	0
11	NAG	G	1156	2	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
11	NAG	J	1072	3	14,14,15	0.35	0	17,19,21	0.52	0
11	NAG	L	1072	3	14,14,15	0.34	0	17,19,21	0.52	0
11	NAG	C	1234	2	14,14,15	0.26	0	17,19,21	0.51	0
11	NAG	F	1637	1	14,14,15	0.30	0	17,19,21	0.48	0
11	NAG	C	1088	2	14,14,15	0.58	0	17,19,21	0.99	1 (5%)
11	NAG	C	1133	2	14,14,15	0.29	0	17,19,21	0.48	0
11	NAG	B	1611	1	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
11	NAG	I	1301	2	14,14,15	0.24	0	17,19,21	0.59	0
11	NAG	I	1133	2	14,14,15	0.29	0	17,19,21	0.49	0
11	NAG	I	1355	2	14,14,15	0.29	0	17,19,21	0.46	0
11	NAG	A	1611	1	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
11	NAG	C	1392	2	14,14,15	0.21	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	A	1637	1	14,14,15	0.29	0	17,19,21	0.48	0
11	NAG	G	1133	2	14,14,15	0.29	0	17,19,21	0.48	0
11	NAG	G	1392	2	14,14,15	0.21	0	17,19,21	0.54	0
11	NAG	G	1355	2	14,14,15	0.32	0	17,19,21	0.46	0
11	NAG	F	1611	1	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
11	NAG	G	1332	2	14,14,15	0.69	0	17,19,21	0.98	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
11	NAG	I	1234	2	-	1/6/23/26	0/1/1/1
11	NAG	I	1088	2	-	2/6/23/26	0/1/1/1
11	NAG	G	1301	2	-	0/6/23/26	0/1/1/1
11	NAG	I	1332	2	-	3/6/23/26	0/1/1/1
11	NAG	G	1088	2	-	2/6/23/26	0/1/1/1
11	NAG	I	1392	2	-	2/6/23/26	0/1/1/1
11	NAG	C	1301	2	-	0/6/23/26	0/1/1/1
11	NAG	C	1332	2	-	3/6/23/26	0/1/1/1
11	NAG	C	1355	2	-	2/6/23/26	0/1/1/1
11	NAG	G	1234	2	-	1/6/23/26	0/1/1/1
11	NAG	C	1339	2	-	2/6/23/26	0/1/1/1
11	NAG	D	1072	3	-	2/6/23/26	0/1/1/1
11	NAG	C	1156	2	-	0/6/23/26	0/1/1/1
11	NAG	I	1156	2	-	0/6/23/26	0/1/1/1
11	NAG	G	1339	2	-	2/6/23/26	0/1/1/1
11	NAG	I	1339	2	-	2/6/23/26	0/1/1/1
11	NAG	B	1637	1	-	1/6/23/26	0/1/1/1
11	NAG	G	1156	2	-	0/6/23/26	0/1/1/1
11	NAG	J	1072	3	-	2/6/23/26	0/1/1/1
11	NAG	L	1072	3	-	2/6/23/26	0/1/1/1
11	NAG	C	1234	2	-	1/6/23/26	0/1/1/1
11	NAG	F	1637	1	-	1/6/23/26	0/1/1/1
11	NAG	C	1088	2	-	2/6/23/26	0/1/1/1
11	NAG	C	1133	2	-	2/6/23/26	0/1/1/1
11	NAG	B	1611	1	-	1/6/23/26	0/1/1/1
11	NAG	I	1301	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	I	1133	2	-	2/6/23/26	0/1/1/1
11	NAG	I	1355	2	-	2/6/23/26	0/1/1/1
11	NAG	A	1611	1	-	1/6/23/26	0/1/1/1
11	NAG	C	1392	2	-	2/6/23/26	0/1/1/1
11	NAG	A	1637	1	-	1/6/23/26	0/1/1/1
11	NAG	G	1133	2	-	2/6/23/26	0/1/1/1
11	NAG	G	1392	2	-	2/6/23/26	0/1/1/1
11	NAG	G	1355	2	-	2/6/23/26	0/1/1/1
11	NAG	F	1611	1	-	1/6/23/26	0/1/1/1
11	NAG	G	1332	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1332	NAG	C1-C2	2.01	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1332	NAG	C2-N2-C7	3.05	127.24	122.90
11	I	1332	NAG	C2-N2-C7	3.02	127.21	122.90
11	G	1332	NAG	C2-N2-C7	3.02	127.21	122.90
11	I	1088	NAG	C2-N2-C7	2.94	127.09	122.90
11	G	1088	NAG	C2-N2-C7	2.94	127.09	122.90
11	C	1088	NAG	C2-N2-C7	2.92	127.06	122.90
11	G	1156	NAG	C2-N2-C7	-2.88	118.80	122.90
11	C	1156	NAG	C2-N2-C7	-2.86	118.83	122.90
11	I	1156	NAG	C2-N2-C7	-2.83	118.87	122.90
11	C	1156	NAG	C1-O5-C5	2.42	115.47	112.19
11	G	1156	NAG	C1-O5-C5	2.39	115.44	112.19
11	I	1156	NAG	C1-O5-C5	2.38	115.41	112.19
11	G	1156	NAG	O5-C1-C2	-2.16	107.88	111.29
11	C	1156	NAG	O5-C1-C2	-2.14	107.91	111.29
11	A	1611	NAG	C1-O5-C5	2.13	115.08	112.19
11	F	1611	NAG	C1-O5-C5	2.12	115.06	112.19
11	I	1156	NAG	O5-C1-C2	-2.10	107.98	111.29
11	G	1088	NAG	C1-O5-C5	2.09	115.02	112.19
11	B	1611	NAG	C1-O5-C5	2.08	115.01	112.19
11	I	1088	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	1332	NAG	O5-C5-C6-O6
11	I	1332	NAG	O5-C5-C6-O6
11	G	1133	NAG	O5-C5-C6-O6
11	L	1072	NAG	O5-C5-C6-O6
11	C	1133	NAG	O5-C5-C6-O6
11	C	1332	NAG	O5-C5-C6-O6
11	D	1072	NAG	O5-C5-C6-O6
11	I	1133	NAG	O5-C5-C6-O6
11	J	1072	NAG	O5-C5-C6-O6
11	G	1332	NAG	C4-C5-C6-O6
11	C	1332	NAG	C4-C5-C6-O6
11	I	1332	NAG	C4-C5-C6-O6
11	G	1133	NAG	C4-C5-C6-O6
11	C	1133	NAG	C4-C5-C6-O6
11	I	1133	NAG	C4-C5-C6-O6
11	G	1355	NAG	O5-C5-C6-O6
11	C	1355	NAG	O5-C5-C6-O6
11	I	1355	NAG	O5-C5-C6-O6
11	G	1339	NAG	O5-C5-C6-O6
11	G	1392	NAG	O5-C5-C6-O6
11	C	1339	NAG	O5-C5-C6-O6
11	C	1392	NAG	O5-C5-C6-O6
11	I	1339	NAG	O5-C5-C6-O6
11	I	1392	NAG	O5-C5-C6-O6
11	C	1392	NAG	C4-C5-C6-O6
11	G	1392	NAG	C4-C5-C6-O6
11	I	1392	NAG	C4-C5-C6-O6
11	G	1088	NAG	O5-C5-C6-O6
11	I	1088	NAG	O5-C5-C6-O6
11	J	1072	NAG	C4-C5-C6-O6
11	C	1088	NAG	O5-C5-C6-O6
11	L	1072	NAG	C4-C5-C6-O6
11	D	1072	NAG	C4-C5-C6-O6
11	C	1234	NAG	O5-C5-C6-O6
11	G	1234	NAG	O5-C5-C6-O6
11	I	1234	NAG	O5-C5-C6-O6
11	G	1339	NAG	C4-C5-C6-O6
11	C	1339	NAG	C4-C5-C6-O6
11	I	1339	NAG	C4-C5-C6-O6
11	A	1611	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	F	1611	NAG	O5-C5-C6-O6
11	B	1611	NAG	O5-C5-C6-O6
11	G	1088	NAG	C3-C2-N2-C7
11	G	1332	NAG	C3-C2-N2-C7
11	C	1088	NAG	C3-C2-N2-C7
11	C	1332	NAG	C3-C2-N2-C7
11	I	1088	NAG	C3-C2-N2-C7
11	I	1332	NAG	C3-C2-N2-C7
11	G	1355	NAG	C4-C5-C6-O6
11	I	1355	NAG	C4-C5-C6-O6
11	C	1355	NAG	C4-C5-C6-O6
11	F	1637	NAG	O5-C5-C6-O6
11	B	1637	NAG	O5-C5-C6-O6
11	A	1637	NAG	O5-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.

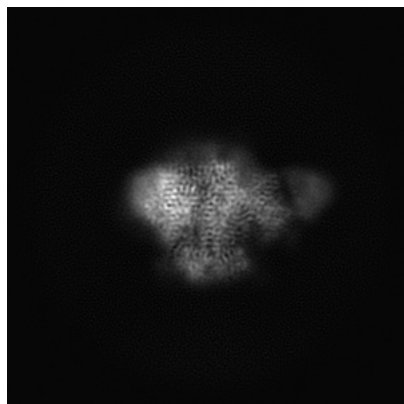
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21208. These allow visual inspection of the internal detail of the map and identification of artifacts.

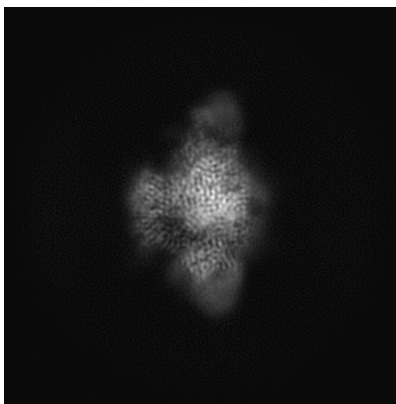
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

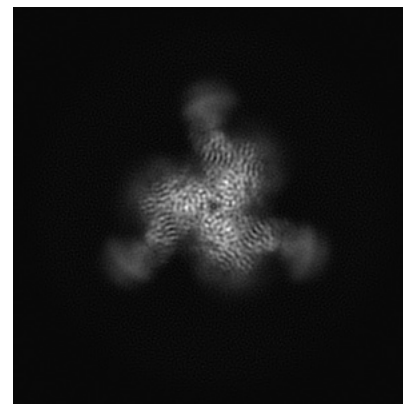
#### 6.1.1 Primary map



X

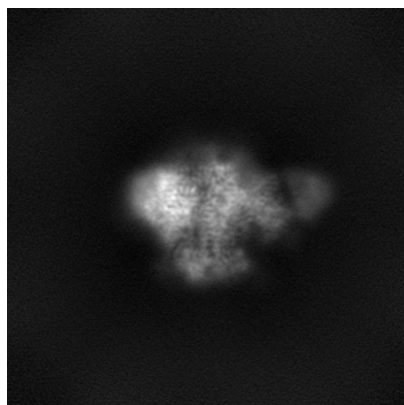


Y

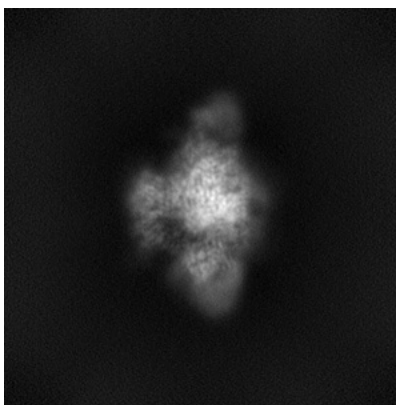


Z

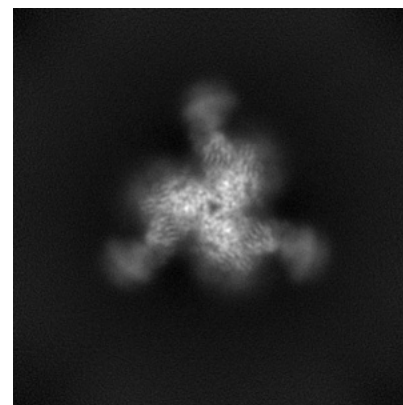
#### 6.1.2 Raw map



X



Y



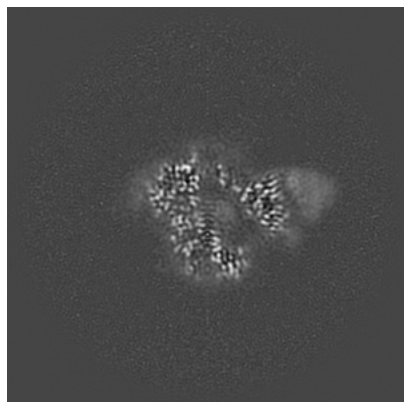
Z

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

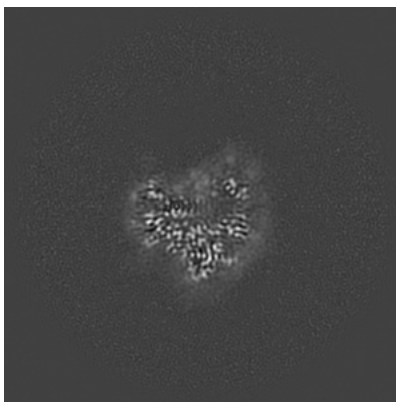


## 6.2 Central slices [i](#)

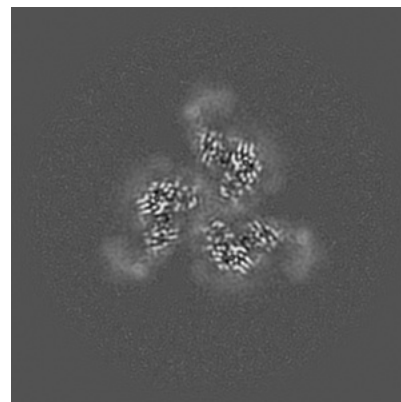
### 6.2.1 Primary map



X Index: 156

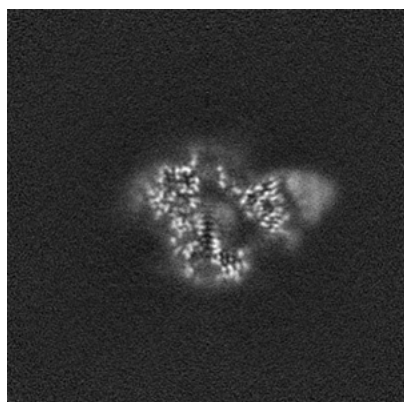


Y Index: 156

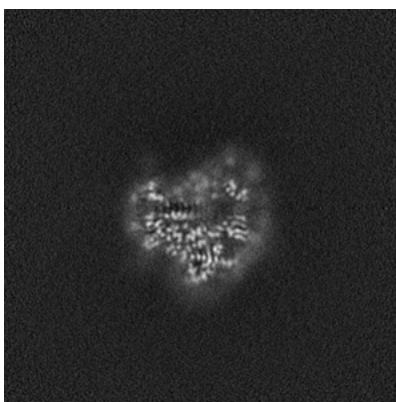


Z Index: 156

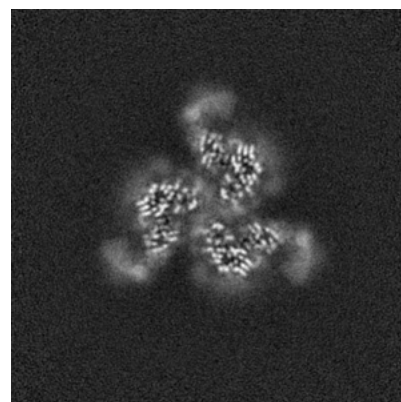
### 6.2.2 Raw map



X Index: 156



Y Index: 156

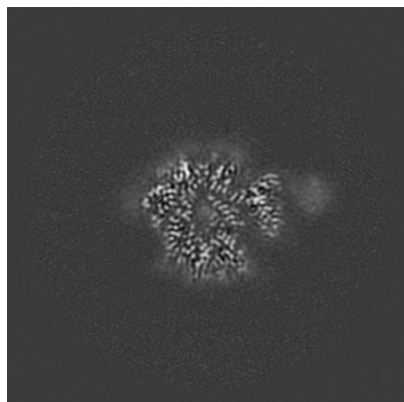


Z Index: 156

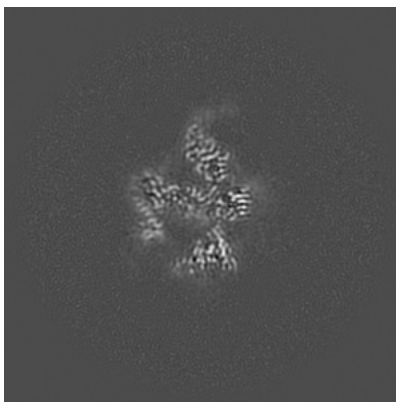
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

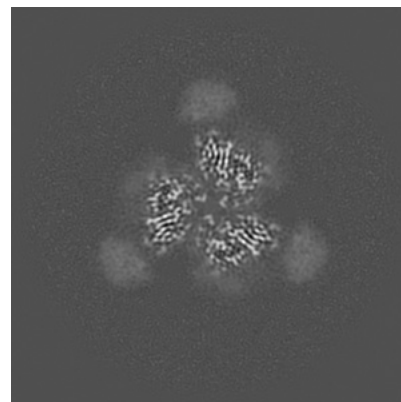
### 6.3.1 Primary map



X Index: 164

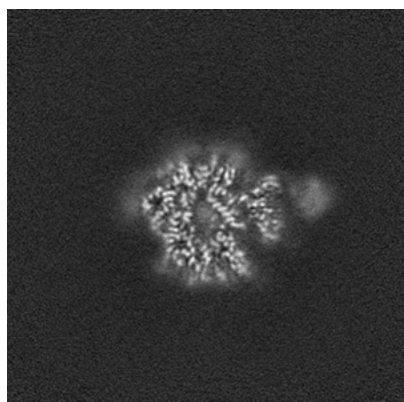


Y Index: 140

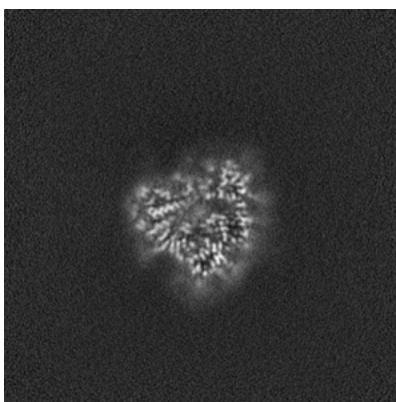


Z Index: 163

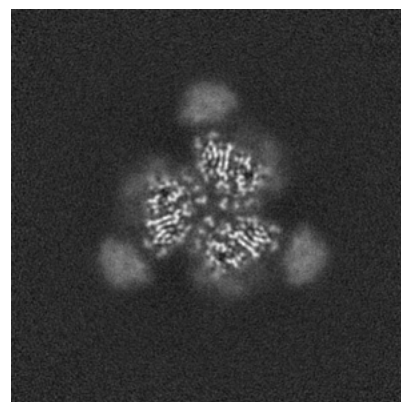
### 6.3.2 Raw map



X Index: 165



Y Index: 163

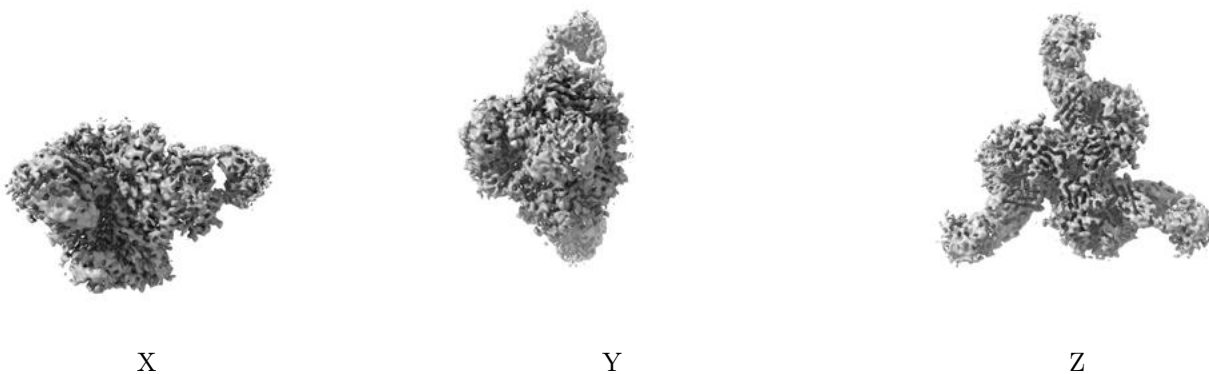


Z Index: 163

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

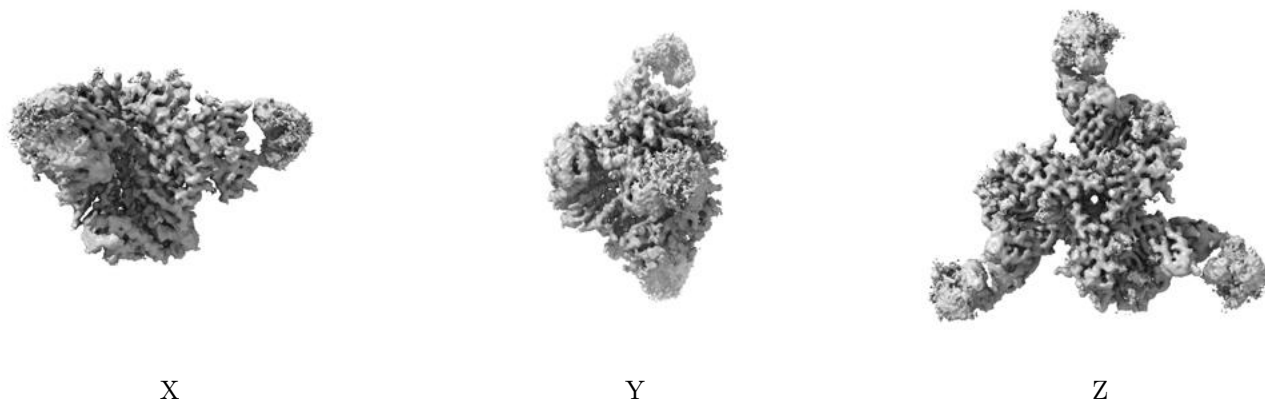
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

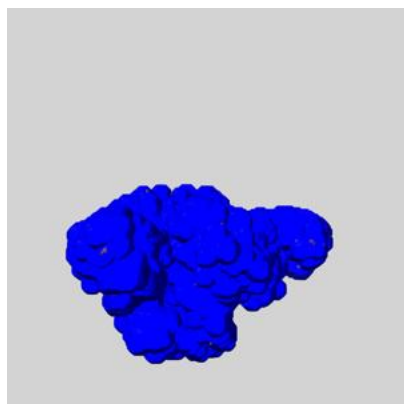
## 6.5 Mask visualisation [i](#)

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

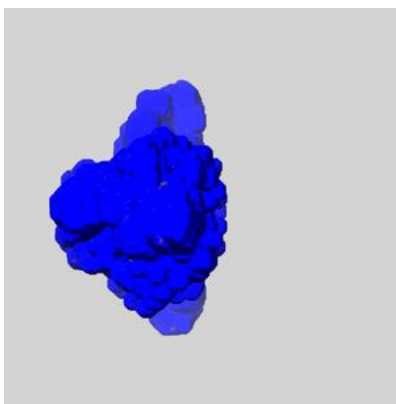
A mask typically either:

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

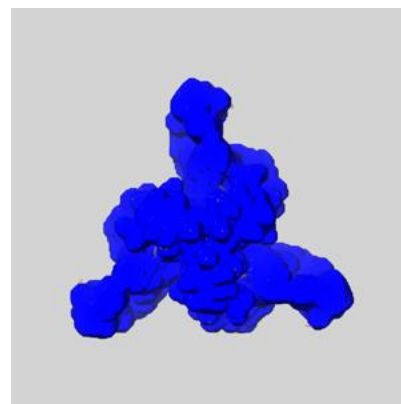
### 6.5.1 emd\_21208\_msk\_1.map [i](#)



X



Y

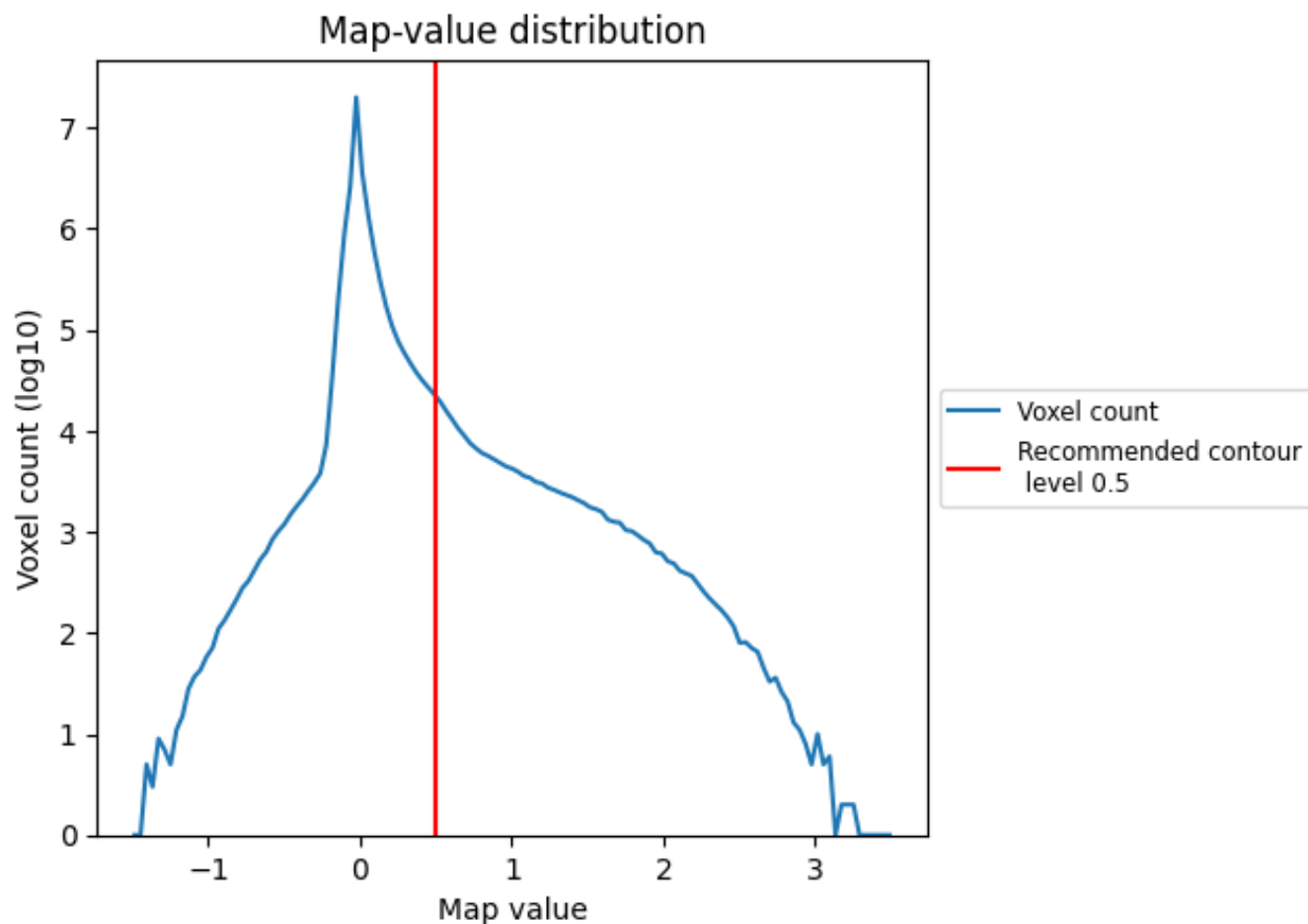


Z

## 7 Map analysis [i](#)

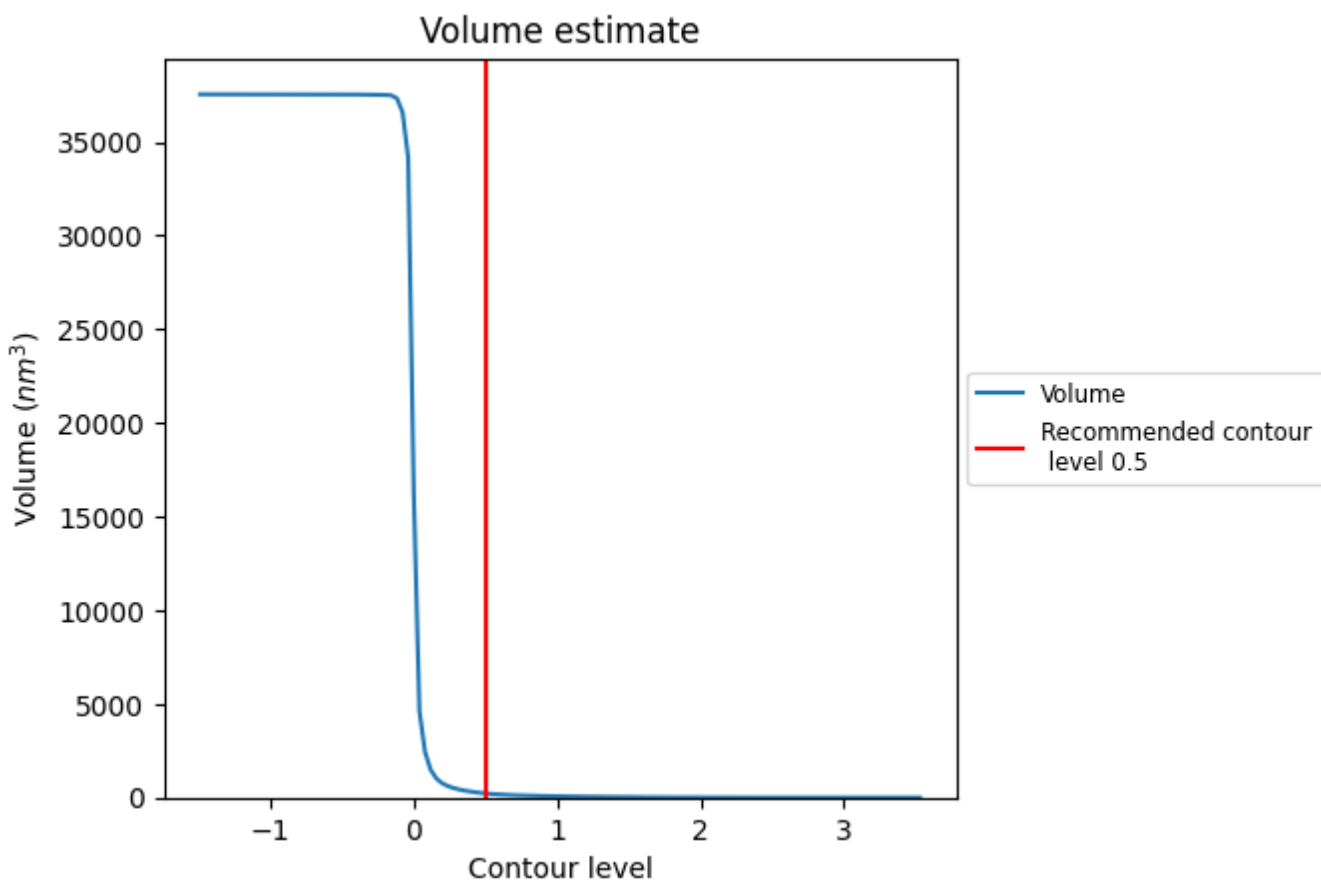
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

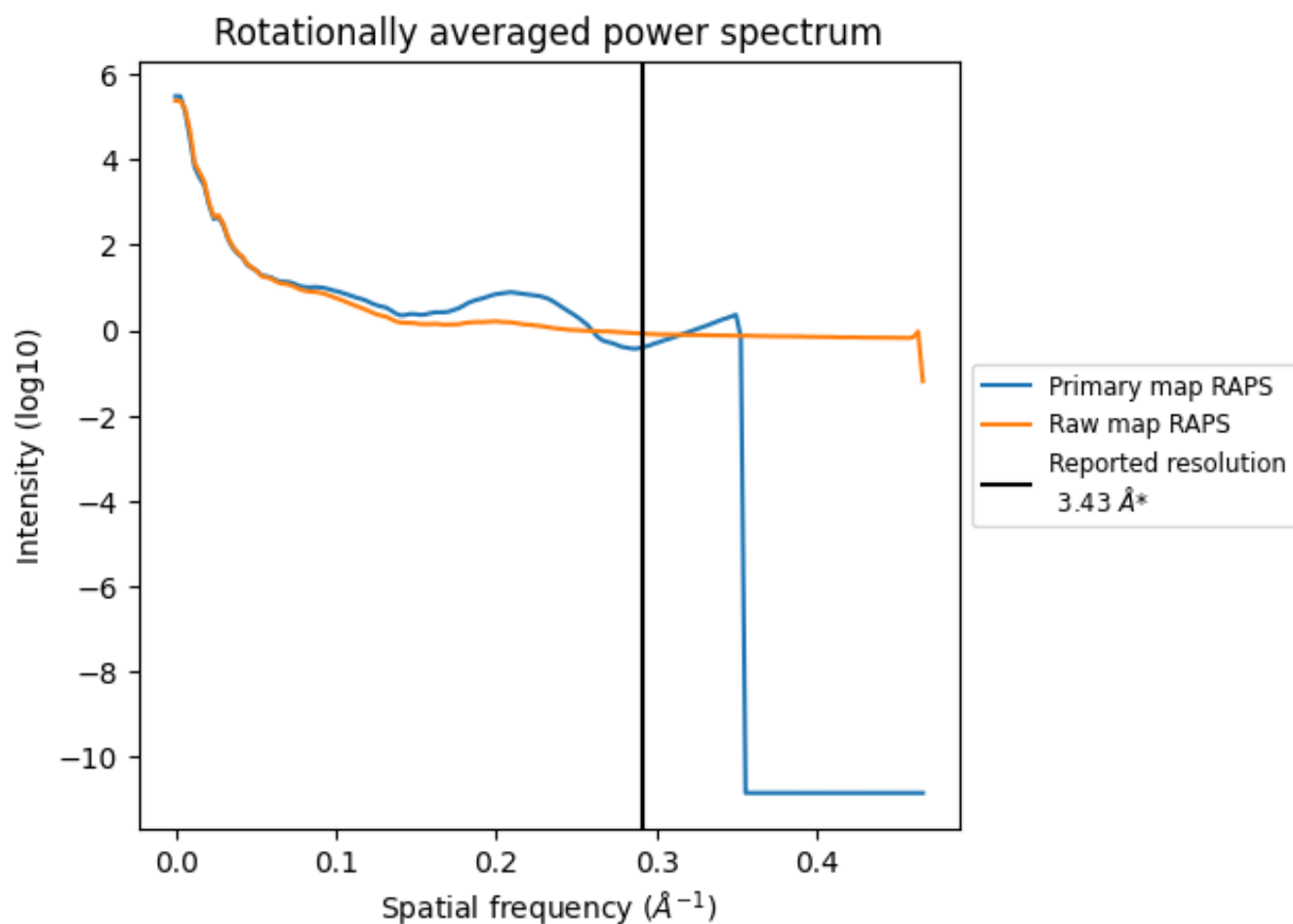
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224  $\text{nm}^3$ ; this corresponds to an approximate mass of 202 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](#)

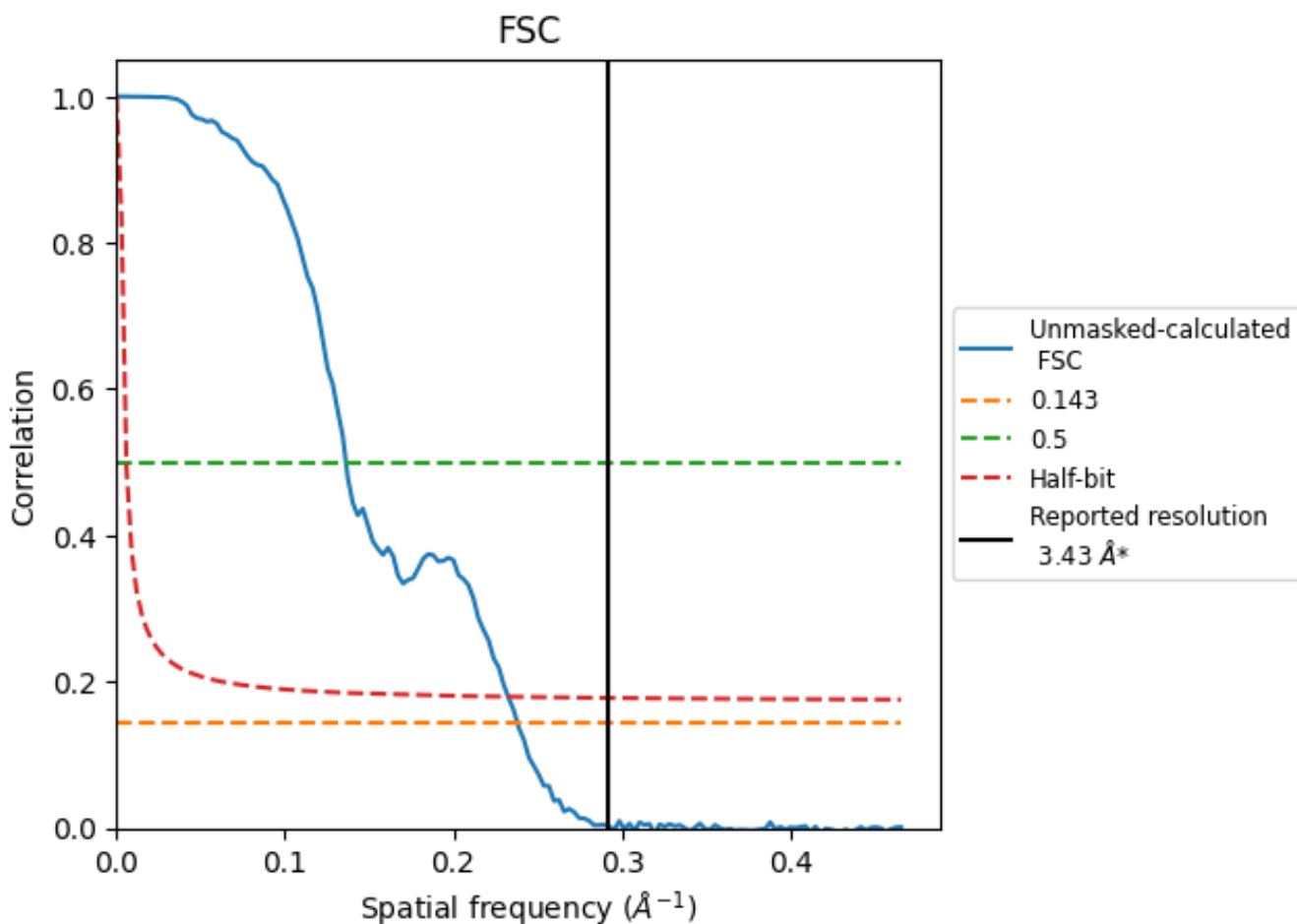


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 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 0.292 Å<sup>-1</sup>



## 8.2 Resolution estimates

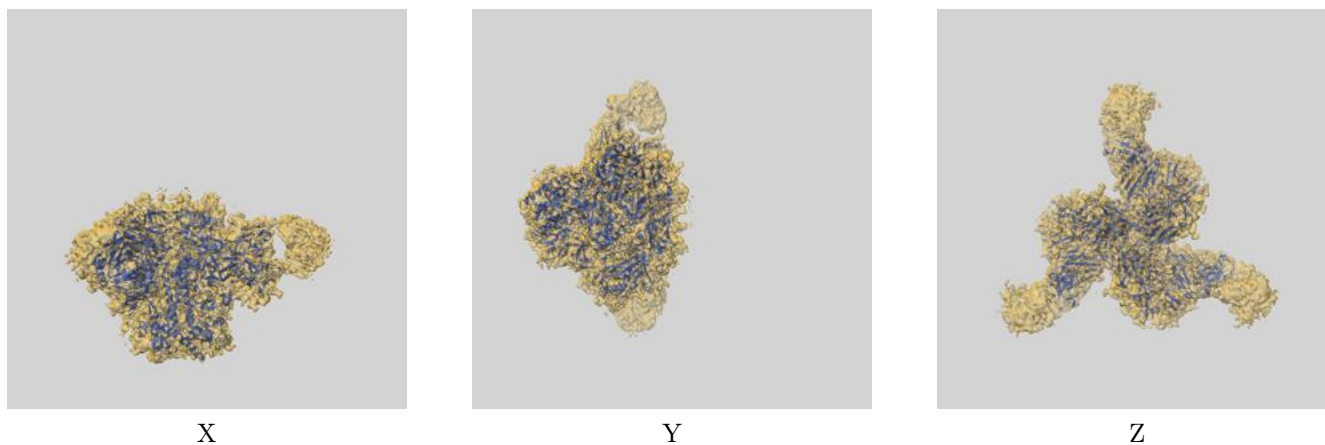
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.34	4.30

\*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 4.20 differs from the reported value 3.43 by more than 10 %

## 9 Map-model fit [i](#)

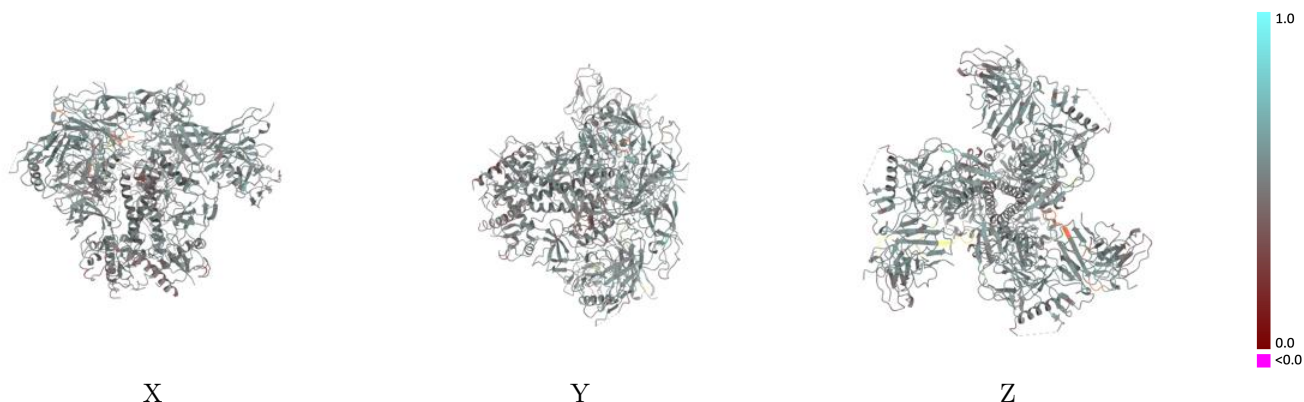
This section contains information regarding the fit between EMDB map EMD-21208 and PDB model 6VI0. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



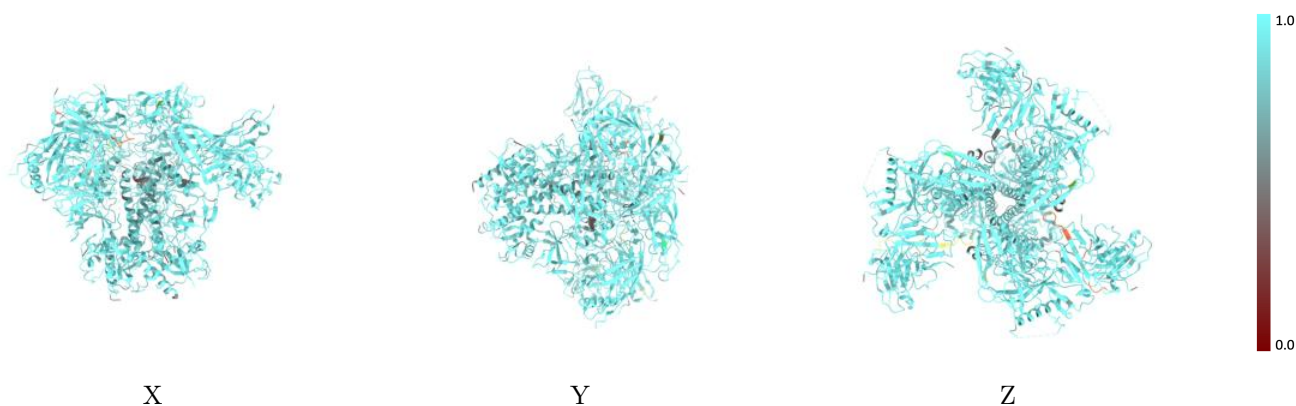
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



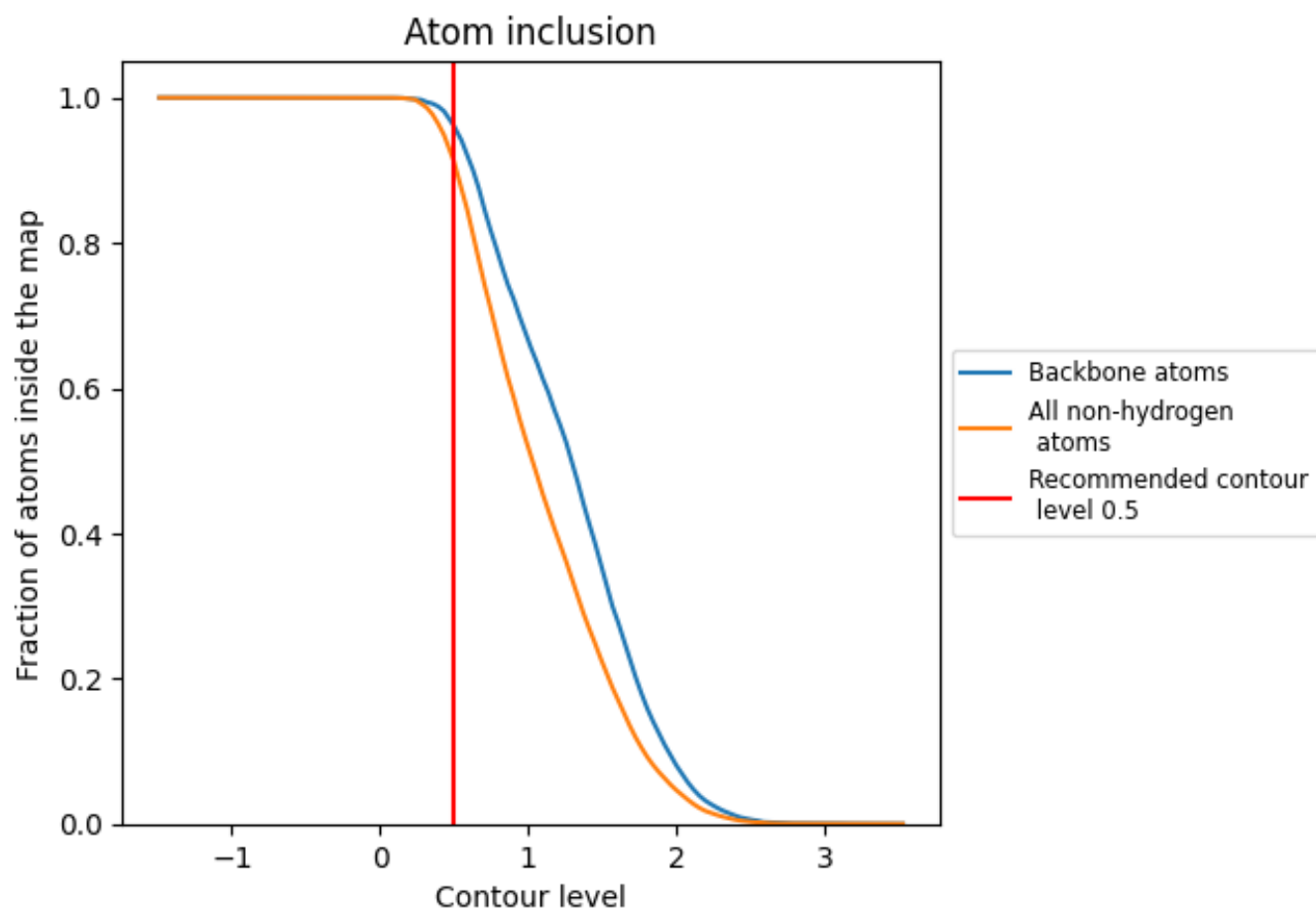
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9124	 0.5020
A	 0.8850	 0.4700
B	 0.8840	 0.4740
C	 0.9244	 0.5100
D	 0.9362	 0.4880
E	 0.9354	 0.5310
F	 0.8888	 0.4700
G	 0.9250	 0.5120
H	 0.9374	 0.5330
I	 0.9250	 0.5100
J	 0.9403	 0.4880
K	 0.9414	 0.5310
L	 0.9430	 0.4880
M	 0.6071	 0.4380
N	 0.5400	 0.4530
O	 0.8333	 0.4910
P	 0.7660	 0.4030
Q	 0.7857	 0.4890
R	 0.8611	 0.4780
S	 0.9487	 0.5350
T	 0.6071	 0.4170
U	 0.6071	 0.4610
V	 0.5000	 0.4470
W	 0.8333	 0.4980
X	 0.7766	 0.4030
Y	 0.7857	 0.4770
Z	 0.8333	 0.4720
a	 0.9487	 0.5190
b	 0.6786	 0.4170
c	 0.6071	 0.4520
d	 0.4800	 0.4590
e	 0.8194	 0.4900
f	 0.7660	 0.4000
g	 0.7857	 0.4830
h	 0.8472	 0.4760



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Chain	Atom inclusion	Q-score
i	 0.9487	 0.5200
j	 0.6429	 0.4260