



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:47 AM UTC

PDB ID : 8OZP / pdb_00008ozp
EMDB ID : EMD-17317
Title : In situ subtomogram average of Prototype Foamy Virus Env pentamer of trimers
Authors : Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on : 2023-05-09
Resolution : 11.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

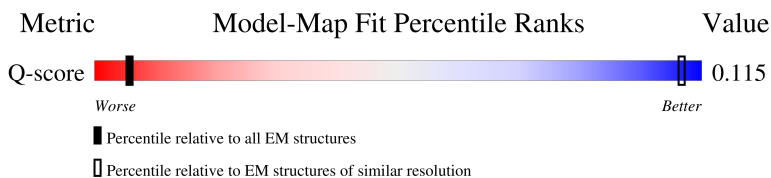
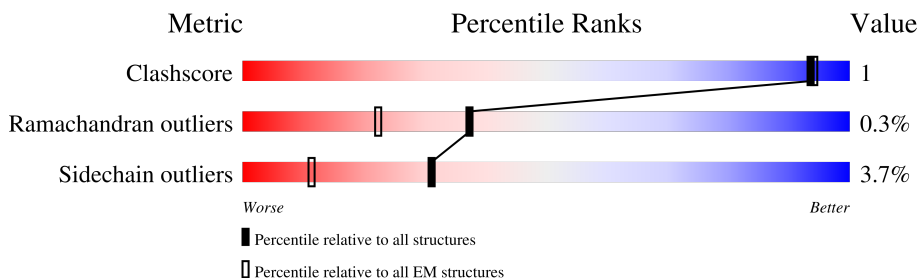
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 11.90 Å.

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



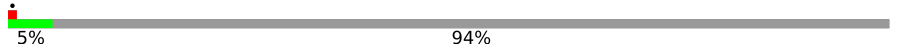
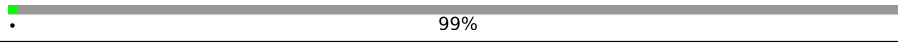
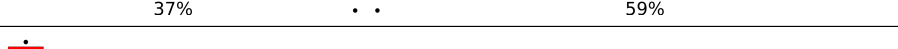
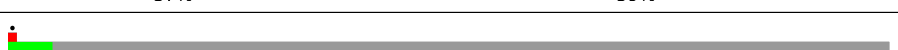
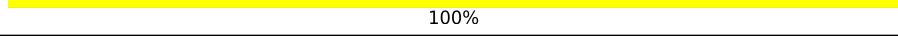
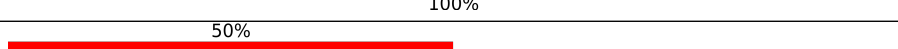
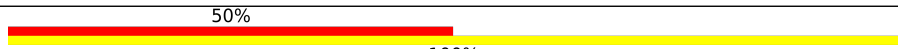
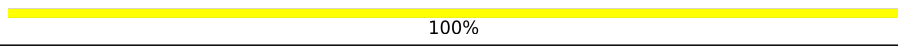
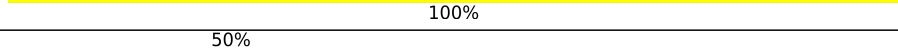
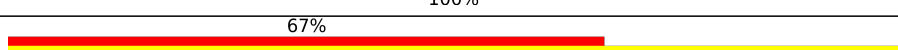
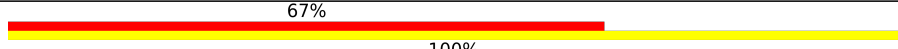
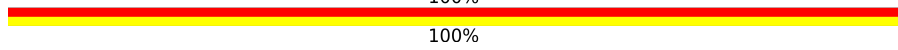
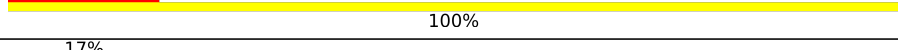
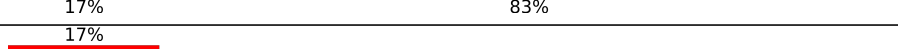
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	86 (11.40 - 12.40)

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	988	
1	B	988	
1	C	988	
1	D	988	

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Mol	Chain	Length	Quality of chain
1	E	988	 5% 94%
1	F	988	 99%
1	G	988	 37% 59%
1	H	988	 37% 59%
1	I	988	 5% 94%
1	L	988	 37% 59%
2	M	2	 50% 100%
2	N	2	 50% 100%
2	O	2	 100%
2	Y	2	 50% 100%
2	Z	2	 50% 100%
2	a	2	 50% 100%
2	b	2	 100%
2	c	2	 100%
2	d	2	 50% 100%
3	S	3	 67% 100%
3	T	3	 67% 100%
3	U	3	 100% 100%
4	V	6	 17% 100%
4	W	6	 17% 83%
4	X	6	 17% 100%
5	P	4	 75% 100%
5	Q	4	 25% 75%
5	R	4	 75% 100%
6	e	8	12% 88%

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Mol	Chain	Length	Quality of chain
6	f	8	50% 100%
6	g	8	38% 100%
7	h	6	67% 100%
7	i	6	83% 100%
7	j	6	67% 100%

2 Entry composition [i](#)

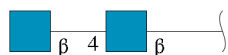
There are 10 unique types of molecules in this entry. The entry contains 22752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	B	411	Total	C	N	O	S	0	0
			3380	2164	561	636	19		
1	D	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	F	11	Total	C	N	O	S	0	0
			94	61	18	14	1		
1	H	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	L	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	E	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	I	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	C	411	Total	C	N	O	S	0	0
			3380	2164	561	636	19		
1	G	405	Total	C	N	O	S	0	0
			3328	2133	549	628	18		

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



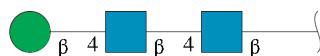
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		

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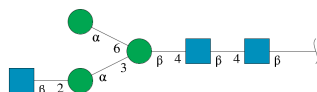
Mol	Chain	Residues	Atoms				AltConf	Trace
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	T	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	X	6	Total	C	N	O	0	0
			75	42	3	30		

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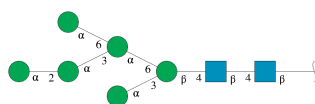
Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	6	Total	C	N	O	0	0
			75	42	3	30		
4	W	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 5 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.



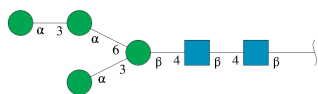
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



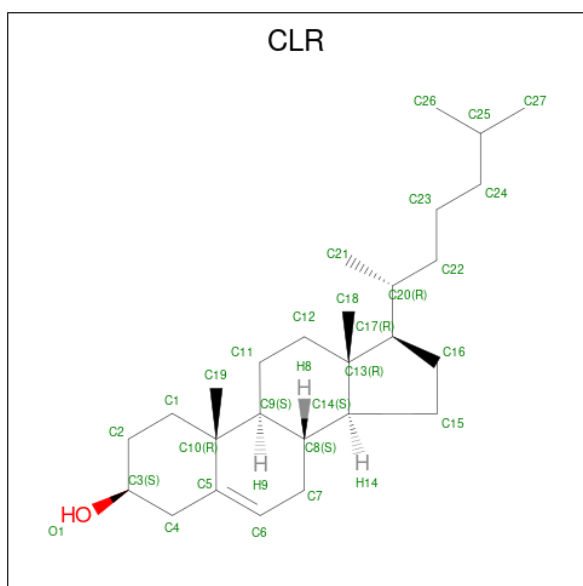
Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	g	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 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.



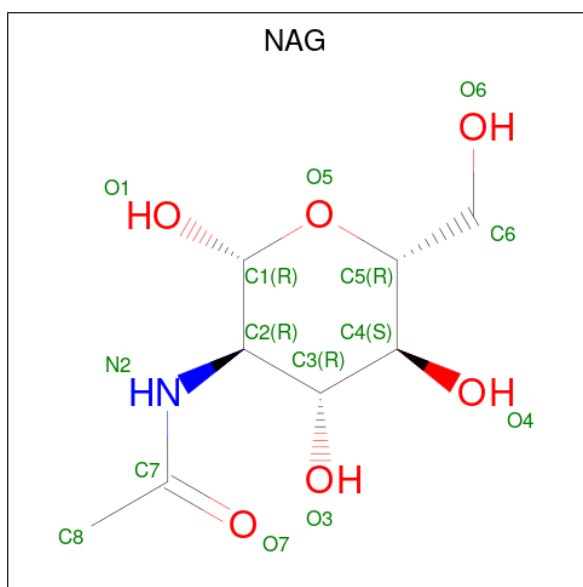
Mol	Chain	Residues	Atoms				AltConf	Trace
7	h	6	Total	C	N	O	0	0
			72	40	2	30		
7	i	6	Total	C	N	O	0	0
			72	40	2	30		
7	j	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



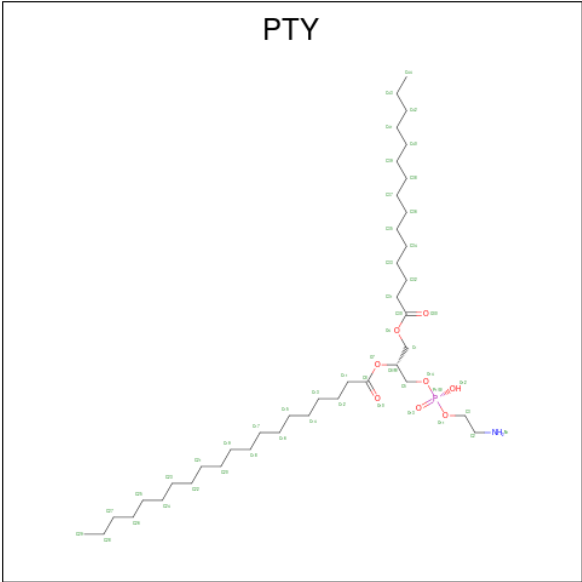
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	28	27
			28	27	1		
8	D	1	Total	C	O	28	27
			28	27	1		
8	L	1	Total	C	O	28	27
			28	27	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).

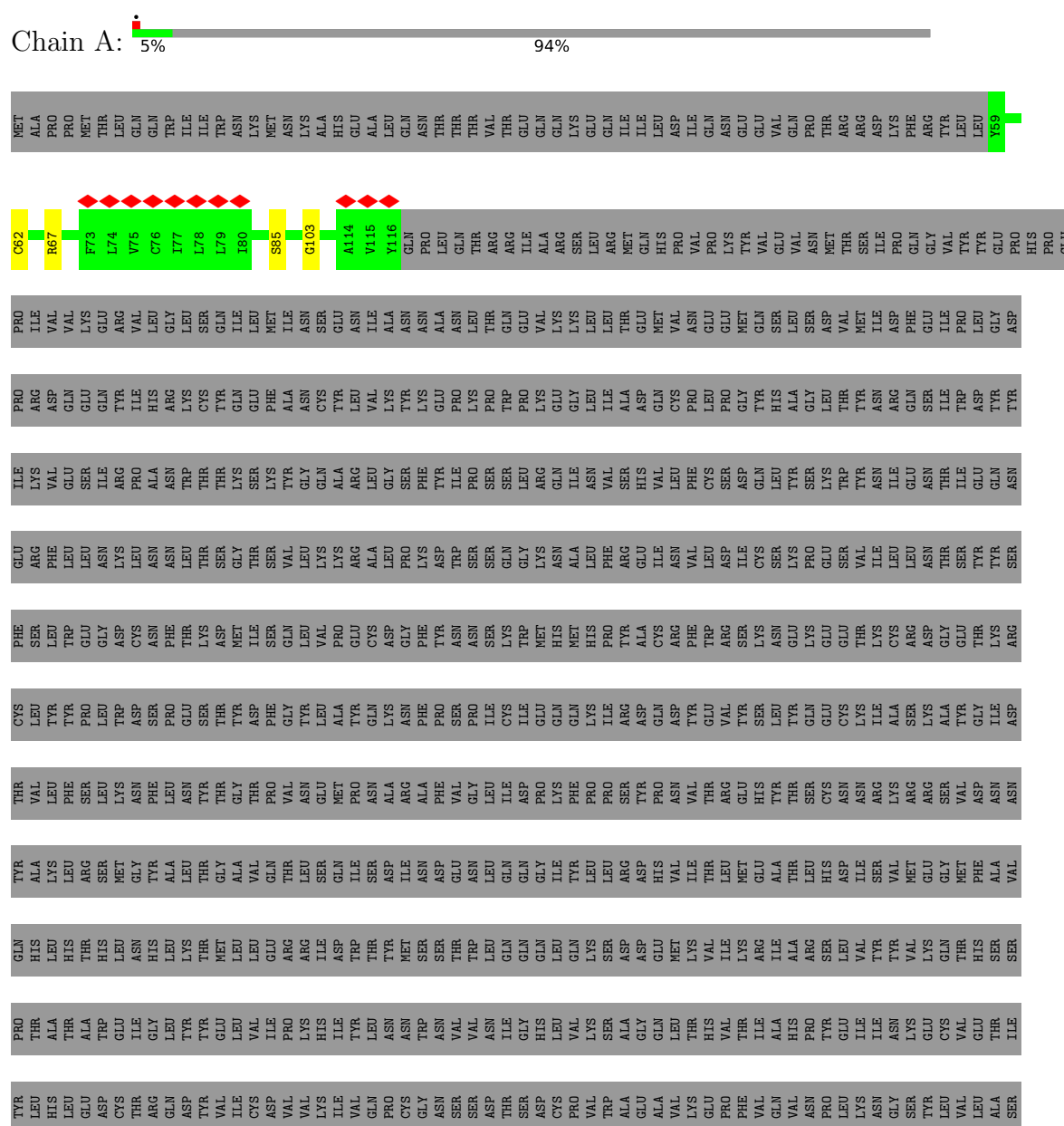


Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

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



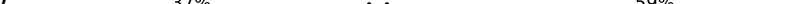
[illegible]

- Molecule 1: Envelope glycoprotein

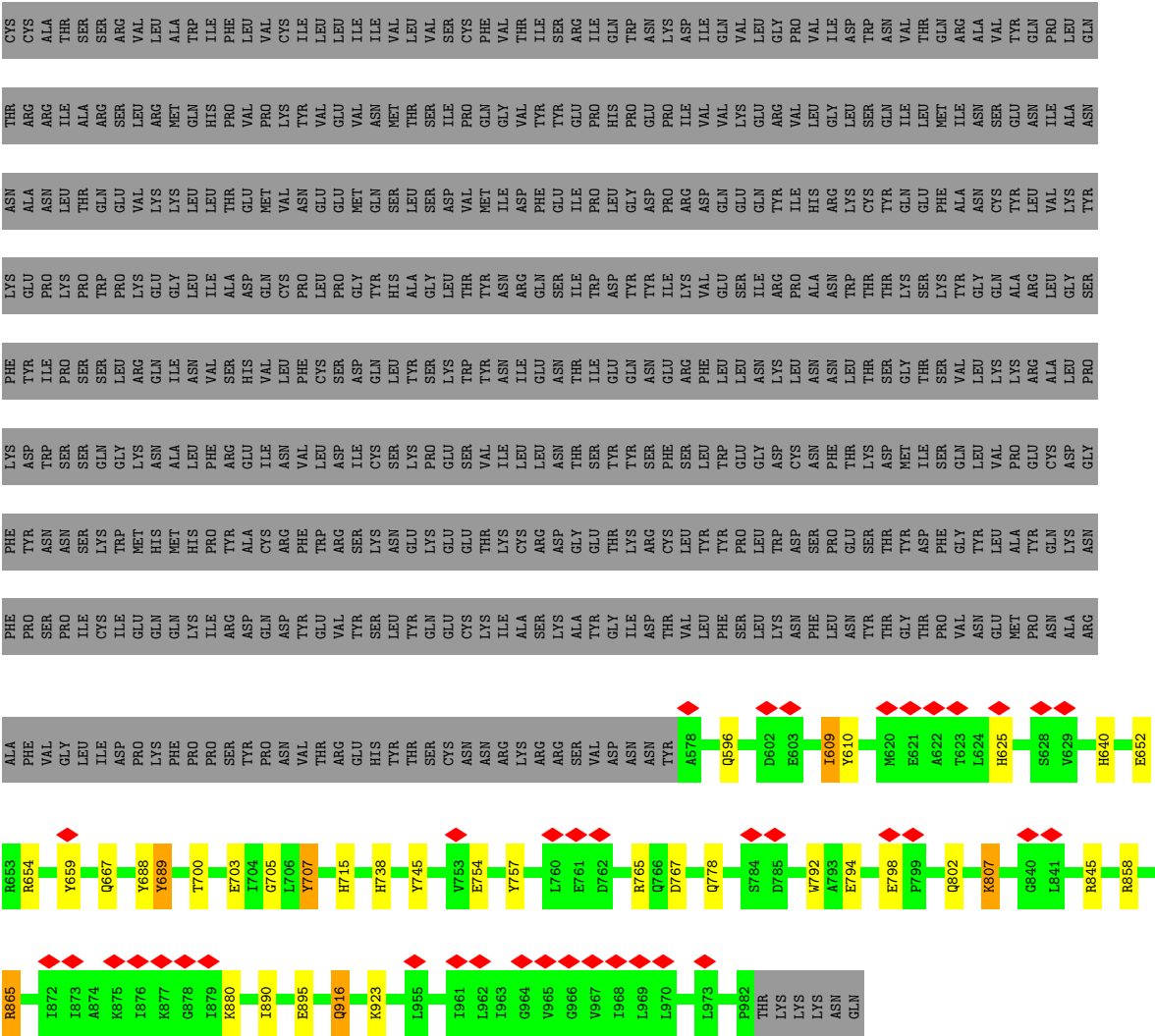
Chain B: 38% 58%

[illegible]

- Molecule 1: Envelope glycoprotein

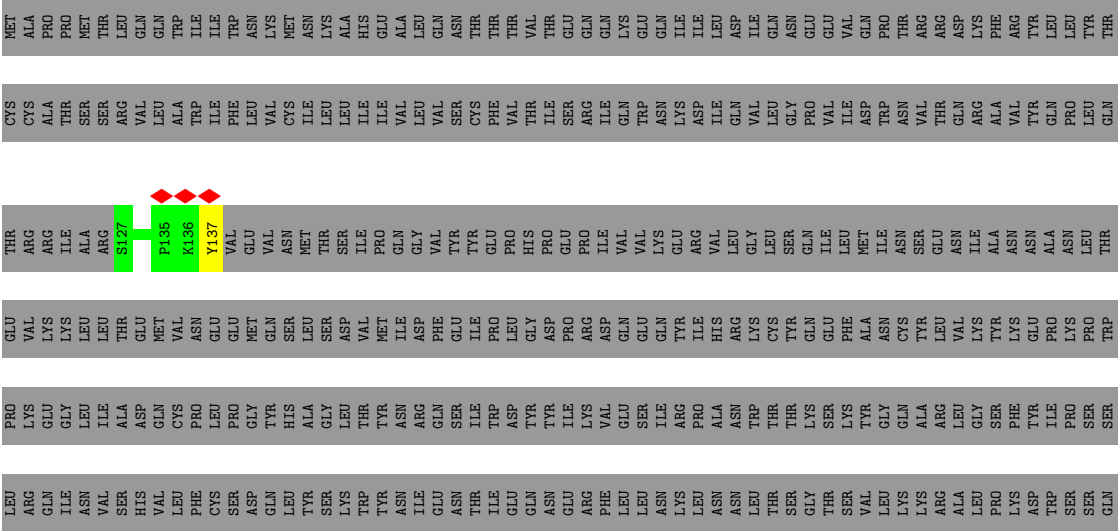
Chain D:  37% 59%

MET	ALA	PRO	PRO	MET	THR	THR	LEU	GLN	GLN	TRP	ILE	ILE	TRP	ASN	LYS	MET	ASN	LYS	ALA	HIS	GLU	GLU	LEU	GLN	ASN	THR	THR	THR	THR	GLU	GLN	GLN	LYS	GLN	GLN	ILE	ILE	GLN	ASP	LEU	LEU	ILE	ILE	GLN	ASN	GLN	PRO	THR	THR	ARG	ARG	ASP	LYS	PHE	ARG	TYR	LEU	LEU	TYR	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



● Molecule 1: Envelope glycoprotein

Chain F: 99%

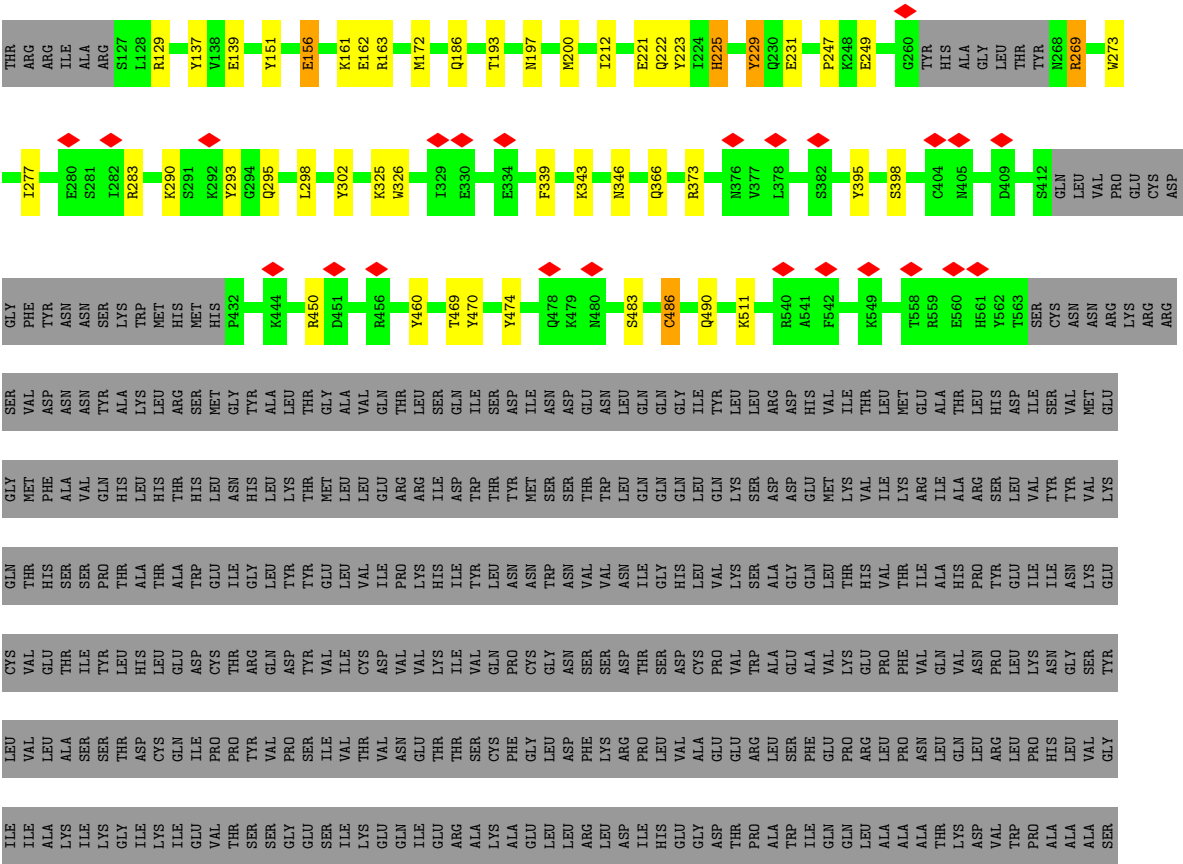




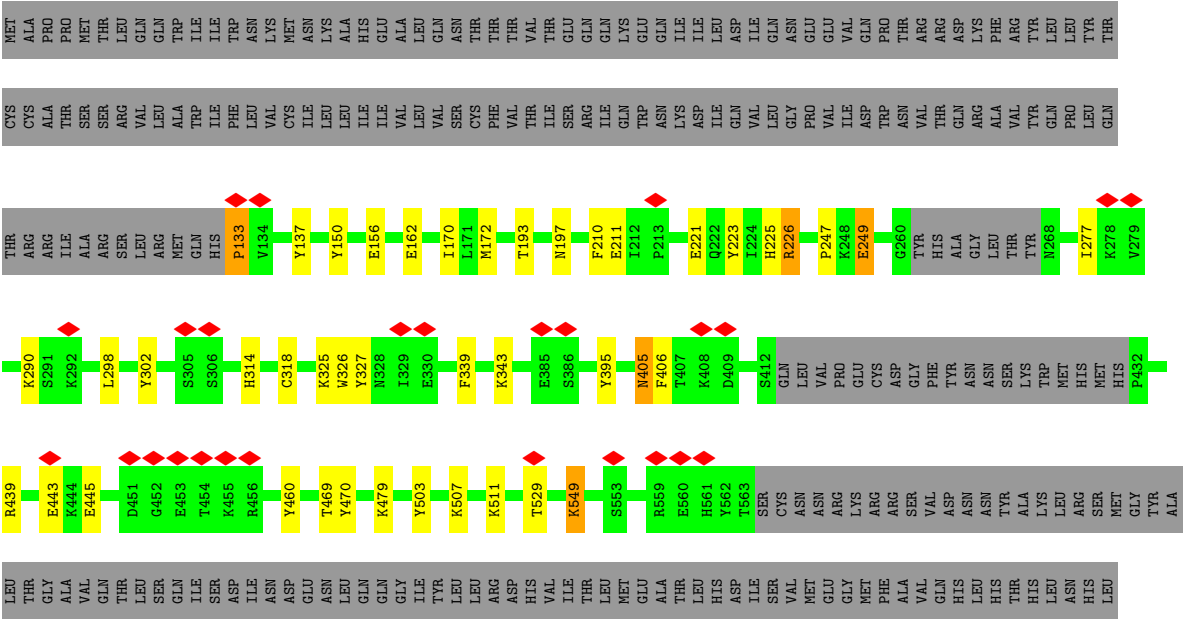
Chain E: 5% 94%





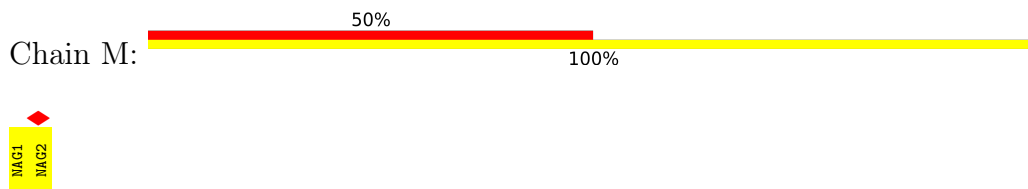


• Molecule 1: Envelope glycoprotein

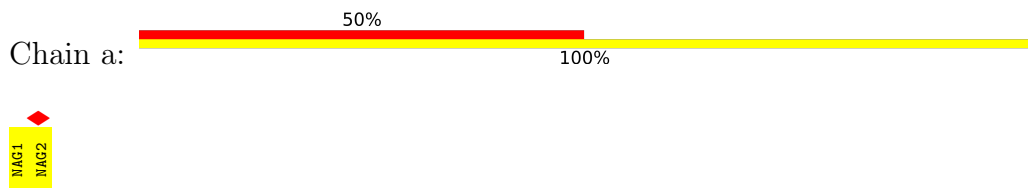


ILE	GLY	PRO	ASP	TYR	LYS
PHE	GLU	SER	TYR	GLU	THR
THR	SER	ILE	VAL	THR	MET
ALA	ILE	VAL	ILE	LEU	LEU
PHE	GLU	VAL	CYS	VAL	ARG
SER	GLN	ASN	ASP	PRO	ARG
LEU	ILE	GLU	VAL	LYS	ARG
LEU	GLU	THR	LYS	HIS	ILE
GLY	ARG	THR	ILE	ILE	ASP
TYR	ALA	SER	GLN	TYR	THR
LEU	ALA	CYS	VAL	LEU	THR
LYS	ALA	PHE	PRO	ASN	TYR
PRO	GLU	GLY	CYS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

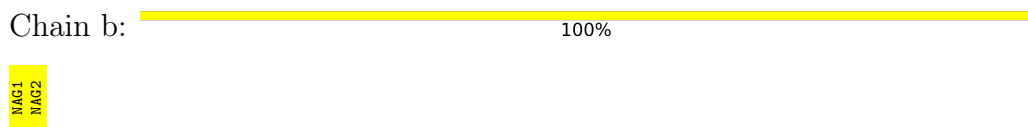
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



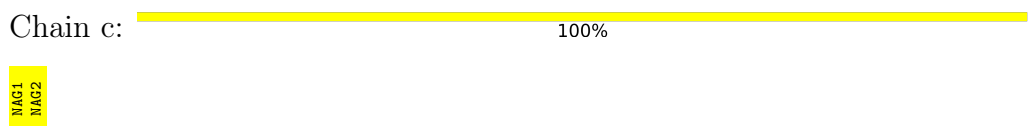
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



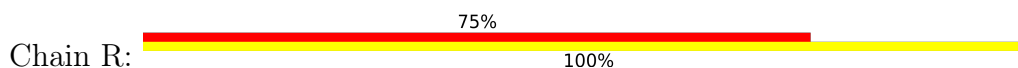
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

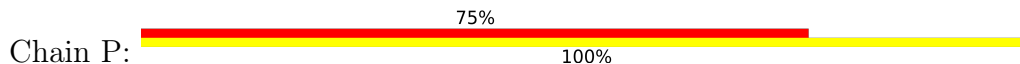


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





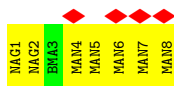
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



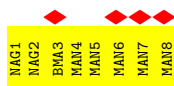
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

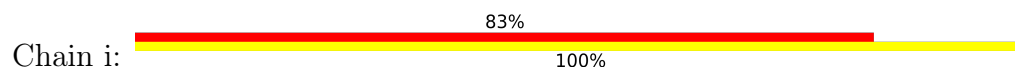




- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 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 7: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of subtomograms used	2220	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 ($e^-/\text{\AA}^2$)	107.42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.064	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.76, 2.76, 2.76	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/476	1.36	2/653 (0.3%)
1	B	0.79	0/3469	1.34	7/4705 (0.1%)
1	C	0.78	0/3469	1.32	9/4705 (0.2%)
1	D	0.78	0/3260	1.35	10/4441 (0.2%)
1	E	0.78	0/476	1.42	4/653 (0.6%)
1	F	0.90	0/97	1.57	0/130
1	G	0.78	0/3416	1.32	10/4634 (0.2%)
1	H	0.78	0/3260	1.34	8/4441 (0.2%)
1	I	0.83	0/476	1.43	3/653 (0.5%)
1	L	0.79	0/3260	1.37	10/4441 (0.2%)
All	All	0.79	0/21659	1.35	63/29456 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	10
1	C	0	11
1	D	0	11
1	E	0	1
1	G	0	9
1	H	0	10
1	I	0	1
1	L	0	5
All	All	0	58

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	738	HIS	CB-CG-CD2	-7.92	120.91	131.20
1	C	339	PHE	CA-CB-CG	6.84	120.64	113.80
1	B	226	ARG	CD-NE-CZ	6.70	133.78	124.40
1	B	405	ASN	CA-CB-CG	6.69	119.29	112.60
1	D	625	HIS	CB-CG-CD2	-6.67	122.52	131.20
1	L	670	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	B	339	PHE	CA-CB-CG	6.51	120.31	113.80
1	G	226	ARG	CD-NE-CZ	6.42	133.38	124.40
1	D	802	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	L	916	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	G	133	PRO	CA-N-CD	-6.14	103.41	112.00
1	I	92	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	A	103	GLY	CA-C-N	5.98	125.95	120.21
1	A	103	GLY	C-N-CA	5.98	125.95	120.21
1	L	802	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	L	738	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	E	92	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	C	469	THR	CA-C-N	5.84	132.70	121.54
1	C	469	THR	C-N-CA	5.84	132.70	121.54
1	E	103	GLY	CA-C-N	5.79	125.77	120.21
1	E	103	GLY	C-N-CA	5.79	125.77	120.21
1	L	715	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	H	916	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	D	916	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	H	802	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	I	112	GLN	CB-CG-CD	-5.65	103.00	112.60
1	B	314	HIS	CB-CG-CD2	-5.63	123.89	131.20
1	H	667	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	G	339	PHE	CA-CB-CG	5.53	119.33	113.80
1	D	738	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	D	596	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	D	640	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	G	469	THR	CA-C-N	5.48	132.01	121.54
1	G	469	THR	C-N-CA	5.48	132.01	121.54
1	C	483	SER	N-CA-C	5.39	113.07	108.22
1	D	895	GLU	CA-C-N	5.38	127.75	120.44
1	D	895	GLU	C-N-CA	5.38	127.75	120.44
1	G	529	THR	CA-CB-CG2	5.37	119.63	110.50
1	L	752	CYS	CA-C-O	5.35	121.04	117.94
1	C	186	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	C	225	HIS	CA-CB-CG	-5.32	108.48	113.80
1	L	625	HIS	CB-CG-CD2	-5.30	124.30	131.20
1	C	295	GLN	OE1-CD-NE2	-5.30	117.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	694	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	G	406	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	139	GLU	CB-CG-CD	-5.21	103.75	112.60
1	G	318	CYS	CA-CB-SG	5.19	126.35	114.40
1	D	802	GLN	CB-CA-C	5.19	118.73	109.65
1	B	295	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	I	100	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	H	735	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	225	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	H	766	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	H	823	PRO	N-CA-CB	5.13	106.06	103.19
1	G	314	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	G	405	ASN	CA-CB-CG	5.09	117.69	112.60
1	E	100	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	L	952	PHE	CA-CB-CG	5.01	118.81	113.80
1	B	356	LYS	CA-C-N	5.01	127.25	120.38
1	B	356	LYS	C-N-CA	5.01	127.25	120.38
1	D	715	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	H	596	GLN	CB-CG-CD	-5.01	104.09	112.60
1	L	596	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	TYR	Sidechain
1	B	225	HIS	Sidechain
1	B	283	ARG	Sidechain
1	B	293	TYR	Sidechain
1	B	338	ARG	Sidechain
1	B	395	TYR	Sidechain
1	B	433	TYR	Sidechain
1	B	456	ARG	Sidechain
1	B	470	TYR	Sidechain
1	B	513	TYR	Sidechain
1	C	137	TYR	Sidechain
1	C	223	TYR	Sidechain
1	C	225	HIS	Sidechain
1	C	229	TYR	Sidechain
1	C	283	ARG	Sidechain
1	C	293	TYR	Sidechain
1	C	302	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	373	ARG	Sidechain
1	C	395	TYR	Sidechain
1	C	460	TYR	Sidechain
1	C	474	TYR	Sidechain
1	D	610	TYR	Sidechain
1	D	659	TYR	Sidechain
1	D	688	TYR	Sidechain
1	D	689	TYR	Sidechain
1	D	707	TYR	Sidechain
1	D	745	TYR	Sidechain
1	D	757	TYR	Sidechain
1	D	765	ARG	Sidechain
1	D	845	ARG	Sidechain
1	D	858	ARG	Sidechain
1	D	865	ARG	Sidechain
1	E	113	ARG	Sidechain
1	G	137	TYR	Sidechain
1	G	150	TYR	Sidechain
1	G	223	TYR	Sidechain
1	G	225	HIS	Sidechain
1	G	302	TYR	Sidechain
1	G	327	TYR	Sidechain
1	G	395	TYR	Sidechain
1	G	439	ARG	Sidechain
1	G	460	TYR	Sidechain
1	H	585	TYR	Sidechain
1	H	653	ARG	Sidechain
1	H	659	TYR	Sidechain
1	H	681	ARG	Sidechain
1	H	688	TYR	Sidechain
1	H	689	TYR	Sidechain
1	H	707	TYR	Sidechain
1	H	738	HIS	Sidechain
1	H	757	TYR	Sidechain
1	H	825	TYR	Sidechain
1	I	113	ARG	Sidechain
1	L	659	TYR	Sidechain
1	L	689	TYR	Sidechain
1	L	707	TYR	Sidechain
1	L	745	TYR	Sidechain
1	L	757	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	466	0	488	1	0
1	B	3380	0	3293	10	0
1	C	3380	0	3293	12	0
1	D	3190	0	3242	10	0
1	E	466	0	488	0	0
1	F	94	0	97	1	0
1	G	3328	0	3241	11	0
1	H	3190	0	3242	12	0
1	I	466	0	488	0	0
1	L	3190	0	3242	11	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
3	S	39	0	34	0	0
3	T	39	0	34	0	0
3	U	39	0	34	0	0
4	V	75	0	64	0	0
4	W	75	0	64	0	0
4	X	75	0	64	0	0
5	P	50	0	43	0	0
5	Q	50	0	43	0	0
5	R	50	0	43	0	0
6	e	94	0	79	0	0
6	f	94	0	79	0	0
6	g	94	0	79	0	0
7	h	72	0	61	0	0
7	i	72	0	61	1	0
7	j	72	0	61	0	0
8	A	28	0	46	1	0
8	D	28	0	46	3	0
8	L	28	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	42	0	39	0	0
9	C	42	0	39	0	0
9	G	42	0	39	0	0
10	D	50	0	79	0	0
10	H	50	0	79	0	0
10	L	50	0	79	0	0
All	All	22752	0	22674	61	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 1.

All (61) 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:B:326:TRP:CG	1:B:343:LYS:HE3	2.31	0.65
1:G:326:TRP:CG	1:G:343:LYS:HE3	2.33	0.65
8:D:1100:CLR:H192	1:L:960:PRO:HB3	1.79	0.64
1:L:660:MET:HE3	1:L:661:SER:H	1.67	0.59
1:L:660:MET:HE2	1:L:664:TRP:CE3	2.40	0.56
1:C:277:ILE:HG21	1:C:298:LEU:HD12	1.87	0.55
1:L:620:MET:HE1	1:L:659:TYR:CE1	2.44	0.52
1:D:865:ARG:HE	1:D:890:ILE:HD11	1.75	0.52
1:G:277:ILE:HG21	1:G:298:LEU:HD12	1.92	0.52
1:L:620:MET:HE1	1:L:659:TYR:CD1	2.45	0.51
1:B:277:ILE:HD11	1:B:302:TYR:HB2	1.93	0.50
1:D:700:THR:HG23	1:C:193:THR:HG23	1.93	0.50
1:L:792:TRP:CG	1:L:880:LYS:HE2	2.47	0.50
1:D:792:TRP:CG	1:D:880:LYS:HE2	2.47	0.49
1:H:700:THR:HG23	1:G:193:THR:HG23	1.95	0.49
8:D:1100:CLR:H192	1:L:960:PRO:CB	2.42	0.47
1:B:249:GLU:H	1:B:249:GLU:CD	2.22	0.47
1:H:807:LYS:HE3	1:H:807:LYS:HA	1.95	0.47
1:C:398:SER:HB3	1:C:486:CYS:SG	2.55	0.47
1:C:156:GLU:H	1:C:156:GLU:CD	2.22	0.47
1:G:549:LYS:HE3	1:G:549:LYS:HA	1.96	0.47
1:L:760:LEU:HD22	1:L:774:VAL:HG22	1.97	0.47
8:D:1100:CLR:H212	8:D:1100:CLR:H121	1.97	0.46
1:B:503:TYR:CE2	1:B:507:LYS:HE2	2.50	0.46
1:F:137:TYR:CE1	1:G:133:PRO:HD3	2.52	0.45
1:H:623:THR:HG21	1:H:659:TYR:CD1	2.52	0.44
1:G:156:GLU:CD	1:G:156:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:TYR:CE2	1:C:212:ILE:HD12	2.53	0.44
1:H:681:ARG:HA	1:H:681:ARG:NE	2.33	0.44
1:L:609:ILE:N	1:L:609:ILE:HD12	2.33	0.44
1:B:325:LYS:HA	1:B:325:LYS:HE3	2.00	0.43
1:D:609:ILE:HD12	1:D:609:ILE:N	2.33	0.43
1:H:864:LEU:HD12	7:i:1:NAG:H81	2.00	0.43
1:H:700:THR:HG21	1:G:197:ASN:OD1	2.18	0.43
1:H:793:ALA:C	1:H:880:LYS:HE3	2.43	0.43
1:C:326:TRP:CG	1:C:343:LYS:HE3	2.54	0.43
1:H:585:TYR:CE1	1:G:210:PHE:CE2	3.07	0.43
1:H:681:ARG:HA	1:H:681:ARG:CZ	2.49	0.43
1:D:700:THR:HG21	1:C:197:ASN:OD1	2.18	0.43
1:G:503:TYR:CE2	1:G:507:LYS:HE2	2.54	0.43
1:G:326:TRP:CB	1:G:343:LYS:HE3	2.48	0.42
1:B:139:GLU:CD	1:C:129:ARG:HE	2.27	0.42
1:D:807:LYS:HE3	1:D:807:LYS:HA	2.02	0.42
1:B:438:TRP:CE2	1:B:472:PHE:HB3	2.55	0.42
1:B:385:GLU:H	1:B:385:GLU:CD	2.27	0.42
1:C:161:LYS:HE3	1:C:163:ARG:C	2.45	0.42
1:A:85:SER:HA	8:A:1100:CLR:C2	2.49	0.42
1:L:757:TYR:CD1	1:L:779:PRO:HD3	2.55	0.42
1:D:792:TRP:CB	1:D:880:LYS:HE2	2.50	0.41
1:D:689:TYR:CE2	1:D:705:GLY:HA3	2.56	0.41
1:L:923:LYS:HE3	1:L:927:PRO:HA	2.03	0.41
1:H:911:THR:HB	1:H:912:PRO:HD3	2.02	0.41
1:G:249:GLU:H	1:G:249:GLU:CD	2.27	0.41
1:C:277:ILE:CG2	1:C:298:LEU:HD12	2.49	0.41
1:B:156:GLU:H	1:B:156:GLU:CD	2.29	0.41
1:D:689:TYR:CD1	1:D:689:TYR:C	2.99	0.41
1:C:269:ARG:HA	1:C:273:TRP:CZ3	2.56	0.41
1:B:244:LYS:HE3	1:B:244:LYS:HB3	1.95	0.41
1:C:229:TYR:CD2	1:C:229:TYR:C	2.99	0.40
1:H:689:TYR:C	1:H:689:TYR:CD1	2.99	0.40
1:H:770:ILE:N	1:H:770:ILE:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	56/988 (6%)	54 (96%)	2 (4%)	0	100	100
1	B	405/988 (41%)	382 (94%)	22 (5%)	1 (0%)	43	78
1	C	405/988 (41%)	379 (94%)	24 (6%)	2 (0%)	24	63
1	D	403/988 (41%)	387 (96%)	15 (4%)	1 (0%)	43	78
1	E	56/988 (6%)	54 (96%)	2 (4%)	0	100	100
1	F	9/988 (1%)	9 (100%)	0	0	100	100
1	G	399/988 (40%)	374 (94%)	23 (6%)	2 (0%)	24	63
1	H	403/988 (41%)	387 (96%)	15 (4%)	1 (0%)	43	78
1	I	56/988 (6%)	53 (95%)	3 (5%)	0	100	100
1	L	403/988 (41%)	386 (96%)	16 (4%)	1 (0%)	43	78
All	All	2595/9880 (26%)	2465 (95%)	122 (5%)	8 (0%)	37	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	470	TYR
1	G	470	TYR
1	B	470	TYR
1	L	767	ASP
1	H	767	ASP
1	C	247	PRO
1	D	767	ASP
1	G	247	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/899 (6%)	52 (96%)	2 (4%)	30	51
1	B	382/899 (42%)	367 (96%)	15 (4%)	28	49
1	C	382/899 (42%)	364 (95%)	18 (5%)	23	45
1	D	356/899 (40%)	344 (97%)	12 (3%)	32	54
1	E	54/899 (6%)	53 (98%)	1 (2%)	50	67
1	F	11/899 (1%)	11 (100%)	0	100	100
1	G	376/899 (42%)	361 (96%)	15 (4%)	28	49
1	H	356/899 (40%)	342 (96%)	14 (4%)	28	49
1	I	54/899 (6%)	53 (98%)	1 (2%)	50	67
1	L	356/899 (40%)	345 (97%)	11 (3%)	35	56
All	All	2381/8990 (26%)	2292 (96%)	89 (4%)	31	51

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	CYS
1	A	67	ARG
1	B	151	TYR
1	B	156	GLU
1	B	176	GLU
1	B	200	MET
1	B	222	GLN
1	B	226	ARG
1	B	235	CYS
1	B	242	GLU
1	B	249	GLU
1	B	290	LYS
1	B	318	CYS
1	B	325	LYS
1	B	366	GLN
1	B	405	ASN
1	B	410	MET
1	D	609	ILE
1	D	652	GLU
1	D	654	ARG
1	D	667	GLN
1	D	703	GLU

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Mol	Chain	Res	Type
1	D	754	GLU
1	D	778	GLN
1	D	794	GLU
1	D	798	GLU
1	D	807	LYS
1	D	916	GLN
1	D	923	LYS
1	H	596	GLN
1	H	609	ILE
1	H	652	GLU
1	H	667	GLN
1	H	670	GLN
1	H	692	GLN
1	H	703	GLU
1	H	714	LYS
1	H	754	GLU
1	H	807	LYS
1	H	876	ILE
1	H	880	LYS
1	H	892	GLU
1	H	916	GLN
1	L	579	LYS
1	L	609	ILE
1	L	652	GLU
1	L	654	ARG
1	L	667	GLN
1	L	670	GLN
1	L	754	GLU
1	L	802	GLN
1	L	885	SER
1	L	916	GLN
1	L	923	LYS
1	E	113	ARG
1	I	100	GLN
1	C	151	TYR
1	C	156	GLU
1	C	162	GLU
1	C	172	MET
1	C	200	MET
1	C	221	GLU
1	C	222	GLN
1	C	231	GLU

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Mol	Chain	Res	Type
1	C	249	GLU
1	C	269	ARG
1	C	290	LYS
1	C	325	LYS
1	C	346	ASN
1	C	366	GLN
1	C	450	ARG
1	C	486	CYS
1	C	490	GLN
1	C	511	LYS
1	G	162	GLU
1	G	170	ILE
1	G	172	MET
1	G	211	GLU
1	G	221	GLU
1	G	226	ARG
1	G	249	GLU
1	G	290	LYS
1	G	325	LYS
1	G	405	ASN
1	G	443	GLU
1	G	445	GLU
1	G	479	LYS
1	G	511	LYS
1	G	549	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	186	GLN
1	B	230	GLN
1	B	309	GLN
1	B	561	HIS
1	D	692	GLN
1	D	821	GLN
1	D	893	GLN
1	D	934	GLN
1	H	692	GLN
1	L	670	GLN
1	L	692	GLN
1	L	802	GLN

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Mol	Chain	Res	Type
1	L	804	ASN
1	L	893	GLN
1	L	934	GLN
1	C	201	GLN
1	C	230	GLN
1	C	309	GLN
1	C	489	GLN
1	C	495	GLN
1	G	295	GLN
1	G	309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

99 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	M	1	1,2	14,14,15	1.22	1 (7%)	17,19,21	1.27	2 (11%)
2	NAG	M	2	2	14,14,15	1.38	2 (14%)	17,19,21	0.74	0
2	NAG	N	1	1,2	14,14,15	1.25	2 (14%)	17,19,21	0.85	0
2	NAG	N	2	2	14,14,15	1.23	1 (7%)	17,19,21	0.69	0
2	NAG	O	1	1,2	14,14,15	1.10	2 (14%)	17,19,21	1.27	2 (11%)
2	NAG	O	2	2	14,14,15	1.11	1 (7%)	17,19,21	0.87	0
5	NAG	P	1	1,5	14,14,15	1.11	2 (14%)	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	P	2	5	14,14,15	1.42	4 (28%)	17,19,21	1.01	2 (11%)
5	BMA	P	3	5	11,11,12	1.11	1 (9%)	15,15,17	0.98	1 (6%)
5	MAN	P	4	5	11,11,12	1.33	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	Q	1	1,5	14,14,15	1.02	0	17,19,21	0.68	0
5	NAG	Q	2	5	14,14,15	1.17	1 (7%)	17,19,21	1.08	2 (11%)
5	BMA	Q	3	5	11,11,12	1.17	1 (9%)	15,15,17	0.95	1 (6%)
5	MAN	Q	4	5	11,11,12	1.36	2 (18%)	15,15,17	1.06	2 (13%)
5	NAG	R	1	1,5	14,14,15	1.16	3 (21%)	17,19,21	0.90	0
5	NAG	R	2	5	14,14,15	1.56	4 (28%)	17,19,21	0.78	0
5	BMA	R	3	5	11,11,12	1.19	1 (9%)	15,15,17	0.99	0
5	MAN	R	4	5	11,11,12	1.27	2 (18%)	15,15,17	0.85	1 (6%)
3	NAG	S	1	1,3	14,14,15	1.22	1 (7%)	17,19,21	1.58	2 (11%)
3	NAG	S	2	3	14,14,15	1.19	1 (7%)	17,19,21	0.69	0
3	BMA	S	3	3	11,11,12	1.15	2 (18%)	15,15,17	1.00	1 (6%)
3	NAG	T	1	1,3	14,14,15	1.10	0	17,19,21	1.54	3 (17%)
3	NAG	T	2	3	14,14,15	1.29	2 (14%)	17,19,21	0.90	0
3	BMA	T	3	3	11,11,12	1.31	2 (18%)	15,15,17	0.78	0
3	NAG	U	1	1,3	14,14,15	1.30	3 (21%)	17,19,21	0.90	1 (5%)
3	NAG	U	2	3	14,14,15	1.17	1 (7%)	17,19,21	1.17	2 (11%)
3	BMA	U	3	3	11,11,12	1.35	2 (18%)	15,15,17	0.71	0
4	NAG	V	1	1,4	14,14,15	1.27	3 (21%)	17,19,21	0.84	0
4	NAG	V	2	4	14,14,15	1.00	1 (7%)	17,19,21	0.99	1 (5%)
4	BMA	V	3	4	11,11,12	1.21	1 (9%)	15,15,17	0.74	0
4	MAN	V	4	4	11,11,12	1.51	3 (27%)	15,15,17	1.30	2 (13%)
4	NAG	V	5	4	14,14,15	0.88	0	17,19,21	1.24	2 (11%)
4	MAN	V	6	4	11,11,12	1.47	2 (18%)	15,15,17	1.18	1 (6%)
4	NAG	W	1	1,4	14,14,15	1.04	0	17,19,21	1.11	0
4	NAG	W	2	4	14,14,15	1.10	1 (7%)	17,19,21	1.01	1 (5%)
4	BMA	W	3	4	11,11,12	1.11	1 (9%)	15,15,17	0.88	0
4	MAN	W	4	4	11,11,12	1.47	3 (27%)	15,15,17	1.17	2 (13%)
4	NAG	W	5	4	14,14,15	0.84	1 (7%)	17,19,21	1.21	3 (17%)
4	MAN	W	6	4	11,11,12	1.40	2 (18%)	15,15,17	0.87	1 (6%)
4	NAG	X	1	1,4	14,14,15	1.31	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	X	2	4	14,14,15	1.06	1 (7%)	17,19,21	1.17	2 (11%)
4	BMA	X	3	4	11,11,12	1.17	1 (9%)	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	X	4	4	11,11,12	1.58	3 (27%)	15,15,17	1.25	2 (13%)
4	NAG	X	5	4	14,14,15	0.87	1 (7%)	17,19,21	1.17	2 (11%)
4	MAN	X	6	4	11,11,12	1.40	2 (18%)	15,15,17	1.03	1 (6%)
2	NAG	Y	1	1,2	14,14,15	1.07	2 (14%)	17,19,21	0.81	1 (5%)
2	NAG	Y	2	2	14,14,15	1.21	2 (14%)	17,19,21	1.20	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.17	2 (14%)	17,19,21	0.92	1 (5%)
2	NAG	Z	2	2	14,14,15	1.23	3 (21%)	17,19,21	0.83	0
2	NAG	a	1	1,2	14,14,15	1.44	3 (21%)	17,19,21	0.71	0
2	NAG	a	2	2	14,14,15	1.07	1 (7%)	17,19,21	0.99	2 (11%)
2	NAG	b	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	1.91	6 (35%)
2	NAG	b	2	2	14,14,15	1.33	3 (21%)	17,19,21	1.70	3 (17%)
2	NAG	c	1	1,2	14,14,15	1.26	3 (21%)	17,19,21	1.28	3 (17%)
2	NAG	c	2	2	14,14,15	1.29	1 (7%)	17,19,21	1.23	1 (5%)
2	NAG	d	1	1,2	14,14,15	0.99	1 (7%)	17,19,21	1.67	5 (29%)
2	NAG	d	2	2	14,14,15	1.23	2 (14%)	17,19,21	1.44	2 (11%)
6	NAG	e	1	1,6	14,14,15	1.27	2 (14%)	17,19,21	1.40	2 (11%)
6	NAG	e	2	6	14,14,15	1.03	1 (7%)	17,19,21	0.76	0
6	BMA	e	3	6	11,11,12	1.08	0	15,15,17	0.87	0
6	MAN	e	4	6	11,11,12	1.30	1 (9%)	15,15,17	0.85	0
6	MAN	e	5	6	11,11,12	1.20	1 (9%)	15,15,17	1.63	5 (33%)
6	MAN	e	6	6	11,11,12	1.18	1 (9%)	15,15,17	1.19	1 (6%)
6	MAN	e	7	6	11,11,12	1.34	2 (18%)	15,15,17	0.65	0
6	MAN	e	8	6	11,11,12	1.29	1 (9%)	15,15,17	0.70	0
6	NAG	f	1	1,6	14,14,15	1.29	2 (14%)	17,19,21	1.17	2 (11%)
6	NAG	f	2	6	14,14,15	1.10	1 (7%)	17,19,21	0.87	1 (5%)
6	BMA	f	3	6	11,11,12	1.19	1 (9%)	15,15,17	0.64	0
6	MAN	f	4	6	11,11,12	1.17	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	f	5	6	11,11,12	1.26	2 (18%)	15,15,17	1.28	2 (13%)
6	MAN	f	6	6	11,11,12	1.31	2 (18%)	15,15,17	0.91	1 (6%)
6	MAN	f	7	6	11,11,12	1.29	1 (9%)	15,15,17	0.76	0
6	MAN	f	8	6	11,11,12	1.21	1 (9%)	15,15,17	0.76	1 (6%)
6	NAG	g	1	1,6	14,14,15	1.13	1 (7%)	17,19,21	1.19	2 (11%)
6	NAG	g	2	6	14,14,15	1.27	3 (21%)	17,19,21	0.77	0
6	BMA	g	3	6	11,11,12	1.12	1 (9%)	15,15,17	0.97	0
6	MAN	g	4	6	11,11,12	1.26	1 (9%)	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	g	5	6	11,11,12	1.19	1 (9%)	15,15,17	1.32	3 (20%)
6	MAN	g	6	6	11,11,12	1.19	1 (9%)	15,15,17	0.91	1 (6%)
6	MAN	g	7	6	11,11,12	1.28	1 (9%)	15,15,17	0.85	1 (6%)
6	MAN	g	8	6	11,11,12	1.16	1 (9%)	15,15,17	0.75	1 (6%)
7	NAG	h	1	1,7	14,14,15	1.00	0	17,19,21	1.33	2 (11%)
7	NAG	h	2	7	14,14,15	0.97	1 (7%)	17,19,21	1.02	1 (5%)
7	BMA	h	3	7	11,11,12	1.22	2 (18%)	15,15,17	1.05	1 (6%)
7	MAN	h	4	7	11,11,12	1.23	1 (9%)	15,15,17	0.86	1 (6%)
7	MAN	h	5	7	11,11,12	1.37	1 (9%)	15,15,17	1.04	1 (6%)
7	MAN	h	6	7	11,11,12	1.33	1 (9%)	15,15,17	0.80	1 (6%)
7	NAG	i	1	1,7	14,14,15	1.04	0	17,19,21	0.83	0
7	NAG	i	2	7	14,14,15	1.24	2 (14%)	17,19,21	0.84	1 (5%)
7	BMA	i	3	7	11,11,12	1.40	2 (18%)	15,15,17	1.14	1 (6%)
7	MAN	i	4	7	11,11,12	1.28	2 (18%)	15,15,17	1.16	1 (6%)
7	MAN	i	5	7	11,11,12	1.41	2 (18%)	15,15,17	1.15	2 (13%)
7	MAN	i	6	7	11,11,12	1.36	2 (18%)	15,15,17	0.48	0
7	NAG	j	1	1,7	14,14,15	1.07	1 (7%)	17,19,21	1.16	2 (11%)
7	NAG	j	2	7	14,14,15	1.26	2 (14%)	17,19,21	0.91	0
7	BMA	j	3	7	11,11,12	1.36	1 (9%)	15,15,17	1.52	2 (13%)
7	MAN	j	4	7	11,11,12	1.20	1 (9%)	15,15,17	1.28	1 (6%)
7	MAN	j	5	7	11,11,12	1.39	2 (18%)	15,15,17	1.20	1 (6%)
7	MAN	j	6	7	11,11,12	1.33	2 (18%)	15,15,17	1.01	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
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1

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

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

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

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	j	5	MAN	O5-C5	3.30	1.49	1.43
4	V	6	MAN	O5-C5	3.30	1.49	1.43
7	i	5	MAN	O5-C5	3.28	1.49	1.43
7	h	5	MAN	O5-C5	3.27	1.49	1.43
2	c	2	NAG	O5-C5	3.15	1.49	1.43
4	X	6	MAN	O5-C5	3.13	1.49	1.43
2	M	2	NAG	O5-C5	3.08	1.49	1.43
6	f	7	MAN	O5-C5	3.05	1.49	1.43
6	e	5	MAN	O5-C5	3.05	1.49	1.43
7	i	6	MAN	O5-C5	3.04	1.49	1.43
7	h	6	MAN	O5-C5	3.04	1.49	1.43
2	b	2	NAG	O5-C5	3.01	1.49	1.43
4	W	6	MAN	O5-C5	3.00	1.49	1.43
4	X	4	MAN	O5-C1	2.97	1.48	1.43
6	e	8	MAN	O5-C5	2.91	1.49	1.43
7	j	6	MAN	O5-C5	2.88	1.49	1.43
7	j	2	NAG	O4-C4	2.87	1.50	1.43
2	N	2	NAG	O5-C5	2.86	1.49	1.43
6	g	7	MAN	O5-C5	2.86	1.49	1.43
6	f	5	MAN	O5-C5	2.85	1.49	1.43
6	e	7	MAN	O5-C5	2.84	1.49	1.43
5	P	4	MAN	O5-C5	2.84	1.49	1.43
6	f	8	MAN	O5-C5	2.82	1.48	1.43
6	g	5	MAN	O5-C5	2.81	1.48	1.43
6	g	8	MAN	O5-C5	2.79	1.48	1.43
6	f	6	MAN	O5-C5	2.79	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	i	2	NAG	O5-C5	2.79	1.48	1.43
2	M	1	NAG	O5-C5	2.76	1.48	1.43
4	V	4	MAN	O5-C5	2.75	1.48	1.43
4	W	4	MAN	O5-C1	2.73	1.48	1.43
4	X	4	MAN	O5-C5	2.73	1.48	1.43
6	e	4	MAN	O5-C5	2.72	1.48	1.43
3	S	2	NAG	O5-C5	2.72	1.48	1.43
2	d	2	NAG	O5-C5	2.71	1.48	1.43
5	R	3	BMA	O5-C5	2.70	1.48	1.43
4	V	6	MAN	O5-C1	2.69	1.48	1.43
7	j	3	BMA	O5-C5	2.68	1.48	1.43
5	R	2	NAG	O5-C5	2.68	1.48	1.43
3	T	3	BMA	O5-C5	2.67	1.48	1.43
4	W	4	MAN	O5-C5	2.66	1.48	1.43
5	R	4	MAN	O5-C5	2.65	1.48	1.43
6	e	6	MAN	O5-C5	2.65	1.48	1.43
6	e	1	NAG	O5-C5	2.65	1.48	1.43
3	U	2	NAG	O5-C5	2.64	1.48	1.43
4	V	3	BMA	O5-C5	2.63	1.48	1.43
7	i	3	BMA	O5-C5	2.63	1.48	1.43
3	S	3	BMA	O5-C5	2.61	1.48	1.43
7	i	2	NAG	O4-C4	2.61	1.49	1.43
3	T	2	NAG	O5-C5	2.60	1.48	1.43
2	N	1	NAG	O5-C5	2.59	1.48	1.43
2	a	1	NAG	O5-C5	2.57	1.48	1.43
5	R	2	NAG	O5-C1	2.57	1.48	1.43
5	P	2	NAG	C1-C2	2.57	1.55	1.52
6	g	4	MAN	O5-C5	2.56	1.48	1.43
7	j	4	MAN	O5-C5	2.56	1.48	1.43
4	W	3	BMA	O5-C5	2.55	1.48	1.43
4	V	4	MAN	O5-C1	2.54	1.48	1.43
7	j	2	NAG	O5-C5	2.54	1.48	1.43
3	U	3	BMA	O5-C5	2.53	1.48	1.43
2	a	1	NAG	O4-C4	2.52	1.49	1.43
4	X	4	MAN	O2-C2	2.52	1.48	1.43
5	P	3	BMA	O5-C5	2.51	1.48	1.43
6	g	6	MAN	O5-C5	2.51	1.48	1.43
4	X	1	NAG	O5-C5	2.50	1.48	1.43
7	h	4	MAN	O5-C5	2.49	1.48	1.43
2	Z	2	NAG	O5-C5	2.48	1.48	1.43
5	R	2	NAG	C1-C2	2.48	1.55	1.52
6	f	1	NAG	O5-C5	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	NAG	O5-C5	2.47	1.48	1.43
4	X	2	NAG	O5-C5	2.46	1.48	1.43
5	R	2	NAG	O4-C4	2.46	1.49	1.43
5	Q	4	MAN	O5-C1	2.45	1.47	1.43
5	Q	4	MAN	O5-C5	2.45	1.48	1.43
3	U	3	BMA	O5-C1	2.45	1.47	1.43
5	P	2	NAG	O5-C5	2.44	1.48	1.43
6	f	4	MAN	O5-C5	2.44	1.48	1.43
4	X	3	BMA	O5-C5	2.43	1.48	1.43
2	Y	2	NAG	O5-C5	2.42	1.48	1.43
4	W	6	MAN	O5-C1	2.41	1.47	1.43
4	W	4	MAN	O2-C2	2.40	1.48	1.43
4	V	4	MAN	O2-C2	2.40	1.48	1.43
5	P	2	NAG	O4-C4	2.40	1.48	1.43
4	V	1	NAG	C1-C2	2.40	1.55	1.52
6	f	3	BMA	O5-C5	2.39	1.48	1.43
6	g	1	NAG	O5-C5	2.39	1.48	1.43
4	X	1	NAG	C1-C2	2.38	1.55	1.52
6	g	2	NAG	O5-C5	2.38	1.48	1.43
3	T	2	NAG	O4-C4	2.37	1.48	1.43
2	M	2	NAG	O5-C1	2.34	1.47	1.43
7	i	4	MAN	O5-C5	2.34	1.48	1.43
2	c	1	NAG	O4-C4	2.34	1.48	1.43
4	W	2	NAG	O5-C5	2.34	1.48	1.43
2	a	1	NAG	C1-C2	2.32	1.55	1.52
7	h	2	NAG	O5-C5	2.31	1.47	1.43
5	Q	2	NAG	O5-C1	2.30	1.47	1.43
5	P	4	MAN	O5-C1	2.30	1.47	1.43
5	Q	3	BMA	O5-C5	2.30	1.47	1.43
6	f	6	MAN	O5-C1	2.28	1.47	1.43
7	i	4	MAN	O3-C3	2.28	1.48	1.43
2	N	1	NAG	O4-C4	2.27	1.48	1.43
4	X	5	NAG	O5-C5	2.27	1.47	1.43
6	f	2	NAG	O5-C5	2.27	1.47	1.43
3	U	1	NAG	O5-C5	2.27	1.47	1.43
3	S	1	NAG	C1-C2	2.27	1.55	1.52
4	V	1	NAG	O5-C5	2.27	1.47	1.43
6	e	7	MAN	O5-C1	2.27	1.47	1.43
6	e	1	NAG	C1-C2	2.26	1.55	1.52
4	W	5	NAG	O5-C5	2.25	1.47	1.43
7	i	5	MAN	O5-C1	2.25	1.47	1.43
7	h	3	BMA	O5-C5	2.24	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	2	NAG	C1-C2	2.23	1.55	1.52
3	U	1	NAG	C1-C2	2.22	1.55	1.52
5	R	4	MAN	O5-C1	2.22	1.47	1.43
2	Z	1	NAG	C1-C2	2.22	1.55	1.52
6	g	3	BMA	O5-C5	2.21	1.47	1.43
4	X	6	MAN	O5-C1	2.21	1.47	1.43
6	g	2	NAG	C1-C2	2.20	1.55	1.52
2	b	1	NAG	O4-C4	2.20	1.48	1.43
6	f	1	NAG	C1-C2	2.20	1.55	1.52
2	Y	1	NAG	O5-C5	2.18	1.47	1.43
2	d	1	NAG	O4-C4	2.18	1.48	1.43
6	g	2	NAG	O5-C1	2.18	1.47	1.43
2	Y	1	NAG	O4-C4	2.18	1.48	1.43
7	j	6	MAN	O5-C1	2.18	1.47	1.43
2	a	2	NAG	O5-C5	2.18	1.47	1.43
2	Z	2	NAG	O5-C1	2.17	1.47	1.43
4	V	1	NAG	O5-C1	2.17	1.47	1.43
3	T	3	BMA	O5-C1	2.17	1.47	1.43
3	U	1	NAG	O4-C4	2.16	1.48	1.43
7	i	6	MAN	O5-C1	2.15	1.47	1.43
5	R	1	NAG	O5-C5	2.14	1.47	1.43
5	R	1	NAG	O4-C4	2.13	1.48	1.43
2	c	1	NAG	O5-C5	2.13	1.47	1.43
5	P	1	NAG	O4-C4	2.12	1.48	1.43
2	Z	1	NAG	O5-C5	2.12	1.47	1.43
2	d	2	NAG	C1-C2	2.11	1.55	1.52
2	b	2	NAG	O5-C1	2.10	1.47	1.43
7	j	1	NAG	O5-C5	2.09	1.47	1.43
4	V	2	NAG	O5-C5	2.09	1.47	1.43
7	j	5	MAN	O5-C1	2.09	1.47	1.43
2	O	1	NAG	O5-C5	2.08	1.47	1.43
6	f	5	MAN	O2-C2	2.07	1.47	1.43
5	P	2	NAG	O5-C1	2.06	1.47	1.43
7	i	3	BMA	O3-C3	2.06	1.48	1.43
2	Z	2	NAG	C1-C2	2.05	1.55	1.52
5	P	1	NAG	O5-C5	2.05	1.47	1.43
2	Y	2	NAG	C1-C2	2.04	1.55	1.52
2	c	1	NAG	C1-C2	2.03	1.55	1.52
2	O	1	NAG	C1-C2	2.02	1.55	1.52
3	S	3	BMA	O5-C1	2.01	1.47	1.43
5	R	1	NAG	C1-C2	2.01	1.55	1.52
7	h	3	BMA	O5-C1	2.01	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	2	NAG	C1-C2	2.00	1.55	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C2-N2-C7	4.95	129.53	122.90
3	S	1	NAG	C2-N2-C7	4.86	129.41	122.90
7	j	3	BMA	C1-O5-C5	4.58	118.32	112.19
7	j	4	MAN	C1-O5-C5	4.47	118.18	112.19
2	b	2	NAG	C2-N2-C7	4.39	128.78	122.90
6	e	6	MAN	C1-O5-C5	4.22	117.84	112.19
4	V	6	MAN	C1-O5-C5	3.83	117.32	112.19
7	i	4	MAN	C1-O5-C5	3.83	117.31	112.19
2	Y	2	NAG	C1-O5-C5	3.74	117.20	112.19
2	d	1	NAG	C1-O5-C5	3.65	117.08	112.19
2	d	1	NAG	O5-C5-C6	-3.64	100.58	107.66
7	h	1	NAG	C2-N2-C7	3.57	127.69	122.90
6	e	1	NAG	C1-O5-C5	3.57	116.97	112.19
2	b	1	NAG	C4-C3-C2	-3.56	105.81	111.02
2	d	2	NAG	C2-N2-C7	3.54	127.64	122.90
6	f	5	MAN	C1-O5-C5	3.42	116.77	112.19
2	c	2	NAG	C2-N2-C7	-3.42	118.32	122.90
2	b	1	NAG	O5-C5-C6	-3.41	101.02	107.66
2	b	1	NAG	C3-C4-C5	-3.39	104.09	110.23
2	b	2	NAG	C1-C2-N2	3.34	115.70	110.43
4	X	3	BMA	C1-O5-C5	3.31	116.62	112.19
2	b	1	NAG	C1-O5-C5	3.29	116.60	112.19
2	d	2	NAG	C1-C2-N2	3.27	115.59	110.43
4	X	6	MAN	C1-O5-C5	3.26	116.56	112.19
3	S	1	NAG	C1-C2-N2	3.25	115.56	110.43
4	W	4	MAN	C1-O5-C5	3.25	116.54	112.19
3	U	2	NAG	C2-N2-C7	-3.23	118.57	122.90
4	V	5	NAG	O4-C4-C3	-3.21	102.81	110.38
6	g	6	MAN	C1-O5-C5	3.20	116.47	112.19
6	e	1	NAG	C4-C3-C2	-3.18	106.36	111.02
6	f	1	NAG	C1-O5-C5	3.16	116.42	112.19
4	X	4	MAN	C1-O5-C5	3.14	116.40	112.19
5	Q	2	NAG	C1-O5-C5	3.13	116.38	112.19
6	e	5	MAN	O4-C4-C3	-3.09	103.09	110.38
6	g	1	NAG	C4-C3-C2	-3.06	106.53	111.02
5	P	4	MAN	C1-O5-C5	3.05	116.27	112.19
4	W	5	NAG	O4-C4-C3	-3.05	103.19	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	NAG	O4-C4-C3	-3.04	103.22	110.38
4	V	4	MAN	O2-C2-C1	2.99	116.08	109.22
7	i	3	BMA	C1-O5-C5	2.93	116.11	112.19
6	f	6	MAN	C1-O5-C5	2.92	116.09	112.19
2	c	1	NAG	C1-O5-C5	2.89	116.06	112.19
4	X	5	NAG	O4-C4-C3	-2.88	103.58	110.38
6	e	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	V	2	NAG	O4-C4-C3	-2.87	103.62	110.38
7	i	5	MAN	C1-O5-C5	2.86	116.01	112.19
7	j	6	MAN	C1-O5-C5	2.85	116.01	112.19
7	j	1	NAG	C1-O5-C5	2.84	115.99	112.19
4	W	6	MAN	C1-O5-C5	2.79	115.93	112.19
6	g	5	MAN	C1-O5-C5	2.75	115.87	112.19
5	Q	3	BMA	C1-O5-C5	2.69	115.79	112.19
4	X	1	NAG	C1-O5-C5	2.68	115.77	112.19
7	h	4	MAN	C1-O5-C5	2.66	115.75	112.19
4	V	4	MAN	C1-O5-C5	2.65	115.73	112.19
2	M	1	NAG	C1-O5-C5	2.64	115.72	112.19
7	h	2	NAG	C2-N2-C7	-2.62	119.39	122.90
5	Q	4	MAN	C1-O5-C5	2.60	115.67	112.19
6	g	1	NAG	C1-O5-C5	2.59	115.65	112.19
7	j	5	MAN	C1-O5-C5	2.58	115.64	112.19
2	c	1	NAG	C3-C4-C5	-2.56	105.59	110.23
6	f	1	NAG	C2-N2-C7	2.56	126.33	122.90
7	h	1	NAG	C1-O5-C5	2.55	115.61	112.19
7	h	3	BMA	C1-O5-C5	2.55	115.61	112.19
2	M	1	NAG	C4-C3-C2	-2.53	107.30	111.02
2	b	2	NAG	C1-O5-C5	2.53	115.57	112.19
4	W	2	NAG	O4-C4-C3	-2.52	104.44	110.38
2	c	1	NAG	C4-C3-C2	-2.50	107.36	111.02
2	O	1	NAG	C3-C4-C5	2.48	114.72	110.23
2	a	2	NAG	O5-C1-C2	-2.48	107.46	111.29
6	g	5	MAN	O4-C4-C3	-2.47	104.55	110.38
5	R	4	MAN	C1-O5-C5	2.46	115.49	112.19
5	P	2	NAG	C1-O5-C5	2.46	115.48	112.19
3	T	1	NAG	C1-C2-N2	2.46	114.30	110.43
4	V	5	NAG	C3-C4-C5	2.44	114.66	110.23
2	Y	1	NAG	C2-N2-C7	-2.44	119.63	122.90
7	h	5	MAN	C1-C2-C3	2.43	113.18	109.64
4	X	2	NAG	O4-C4-C3	-2.42	104.67	110.38
3	U	1	NAG	C2-N2-C7	2.42	126.14	122.90
2	d	1	NAG	C6-C5-C4	2.40	118.92	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	1	NAG	C6-C5-C4	2.39	118.90	113.02
6	e	5	MAN	O2-C2-C1	-2.39	103.76	109.22
7	h	6	MAN	C1-O5-C5	2.38	115.38	112.19
5	P	3	BMA	C1-O5-C5	2.38	115.38	112.19
2	d	1	NAG	C3-C4-C5	-2.38	105.92	110.23
6	g	7	MAN	C1-O5-C5	2.36	115.35	112.19
4	X	2	NAG	C2-N2-C7	-2.34	119.76	122.90
6	e	5	MAN	C1-C2-C3	2.33	113.04	109.64
6	f	5	MAN	O4-C4-C3	-2.32	104.91	110.38
5	P	1	NAG	C6-C5-C4	2.30	118.67	113.02
7	i	2	NAG	C2-N2-C7	-2.29	119.83	122.90
2	Z	1	NAG	C4-C3-C2	2.26	114.33	111.02
7	j	3	BMA	O3-C3-C2	2.24	114.62	110.05
5	Q	4	MAN	C1-C2-C3	2.23	112.90	109.64
3	S	3	BMA	C1-O5-C5	2.22	115.16	112.19
2	a	2	NAG	C1-O5-C5	2.20	115.14	112.19
3	T	1	NAG	C1-O5-C5	2.18	115.10	112.19
3	U	2	NAG	O4-C4-C3	-2.17	105.27	110.38
6	f	4	MAN	C1-O5-C5	2.16	115.08	112.19
6	f	8	MAN	C1-O5-C5	2.15	115.07	112.19
2	b	1	NAG	O4-C4-C5	2.14	114.60	109.32
2	d	1	NAG	C4-C3-C2	-2.13	107.89	111.02
7	j	1	NAG	O4-C4-C3	-2.12	105.38	110.38
6	e	5	MAN	C2-C3-C4	2.11	114.58	110.86
6	g	8	MAN	C1-O5-C5	2.11	115.02	112.19
6	g	5	MAN	O2-C2-C1	-2.11	104.39	109.22
4	W	5	NAG	C2-N2-C7	-2.10	120.09	122.90
4	X	4	MAN	O2-C2-C1	2.09	114.02	109.22
5	P	1	NAG	C2-N2-C7	2.09	125.70	122.90
6	f	2	NAG	C1-O5-C5	2.08	114.98	112.19
4	W	5	NAG	C3-C4-C5	2.07	113.99	110.23
7	i	5	MAN	C1-C2-C3	2.06	112.64	109.64
4	X	5	NAG	C3-C4-C5	2.05	113.96	110.23
5	Q	2	NAG	O5-C5-C4	-2.05	105.85	110.83
5	P	2	NAG	C3-C4-C5	-2.04	106.53	110.23
4	W	4	MAN	O2-C2-C1	2.03	113.87	109.22

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	b	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	d	2	NAG	C1-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7
3	T	1	NAG	C3-C2-N2-C7
2	Z	2	NAG	C4-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
4	W	5	NAG	O5-C5-C6-O6
6	f	6	MAN	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
4	X	5	NAG	O5-C5-C6-O6
5	R	1	NAG	C8-C7-N2-C2
4	X	4	MAN	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
4	W	4	MAN	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
4	V	4	MAN	O5-C5-C6-O6
7	h	4	MAN	O5-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
3	S	1	NAG	C3-C2-N2-C7
7	i	4	MAN	O5-C5-C6-O6
7	j	4	MAN	O5-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
4	V	5	NAG	O5-C5-C6-O6
4	V	6	MAN	O5-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
4	W	6	MAN	O5-C5-C6-O6
6	f	8	MAN	O5-C5-C6-O6

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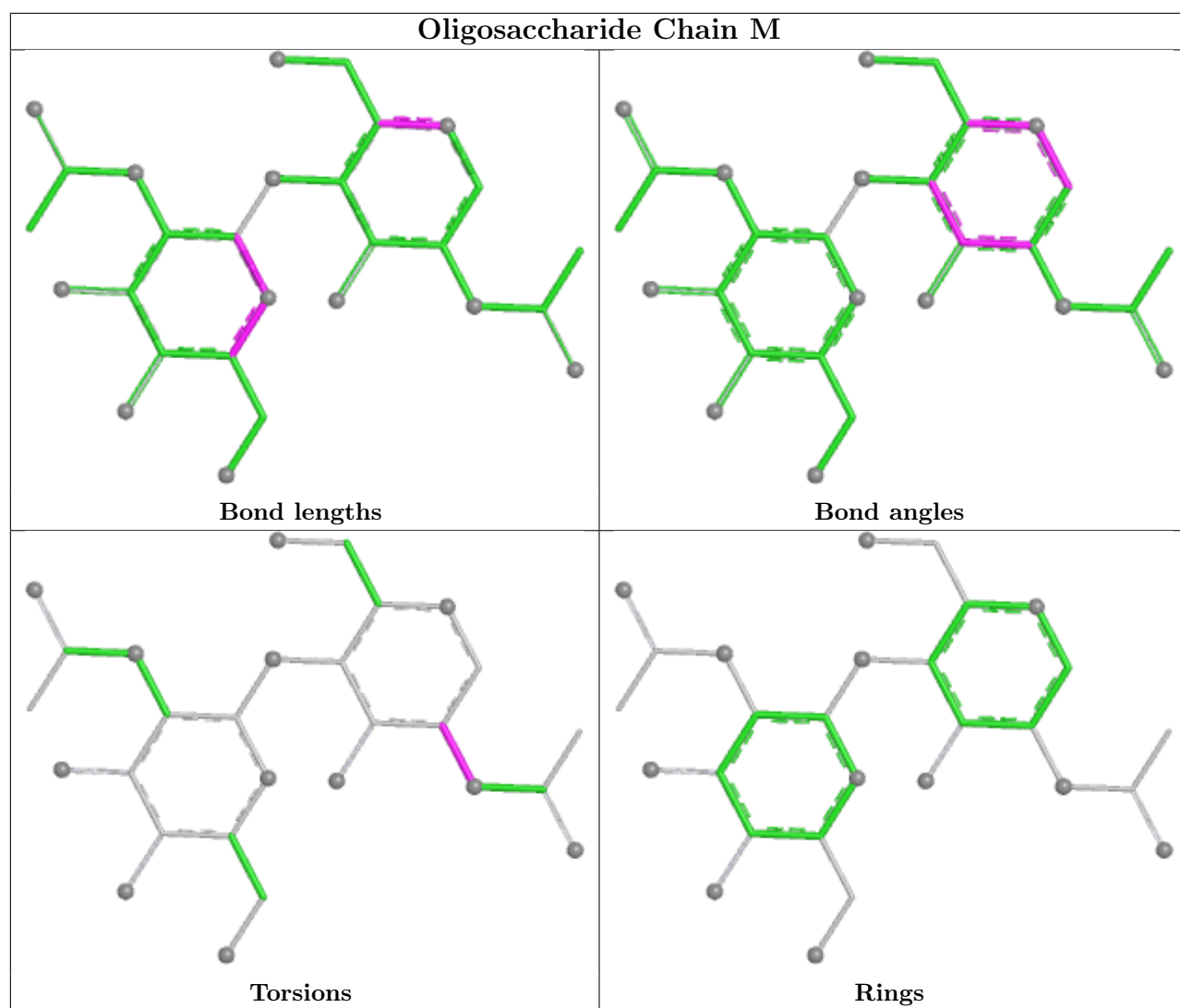
Mol	Chain	Res	Type	Atoms
2	M	1	NAG	C1-C2-N2-C7
2	O	1	NAG	C1-C2-N2-C7
3	S	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C8-C7-N2-C2
2	b	2	NAG	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
7	i	6	MAN	C4-C5-C6-O6
4	W	5	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C3-C2-N2-C7
6	e	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O7-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
6	f	6	MAN	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
6	g	8	MAN	O5-C5-C6-O6
3	T	1	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
2	d	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	c	2	NAG	C4-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	f	5	MAN	O5-C5-C6-O6
4	X	5	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
4	V	5	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6

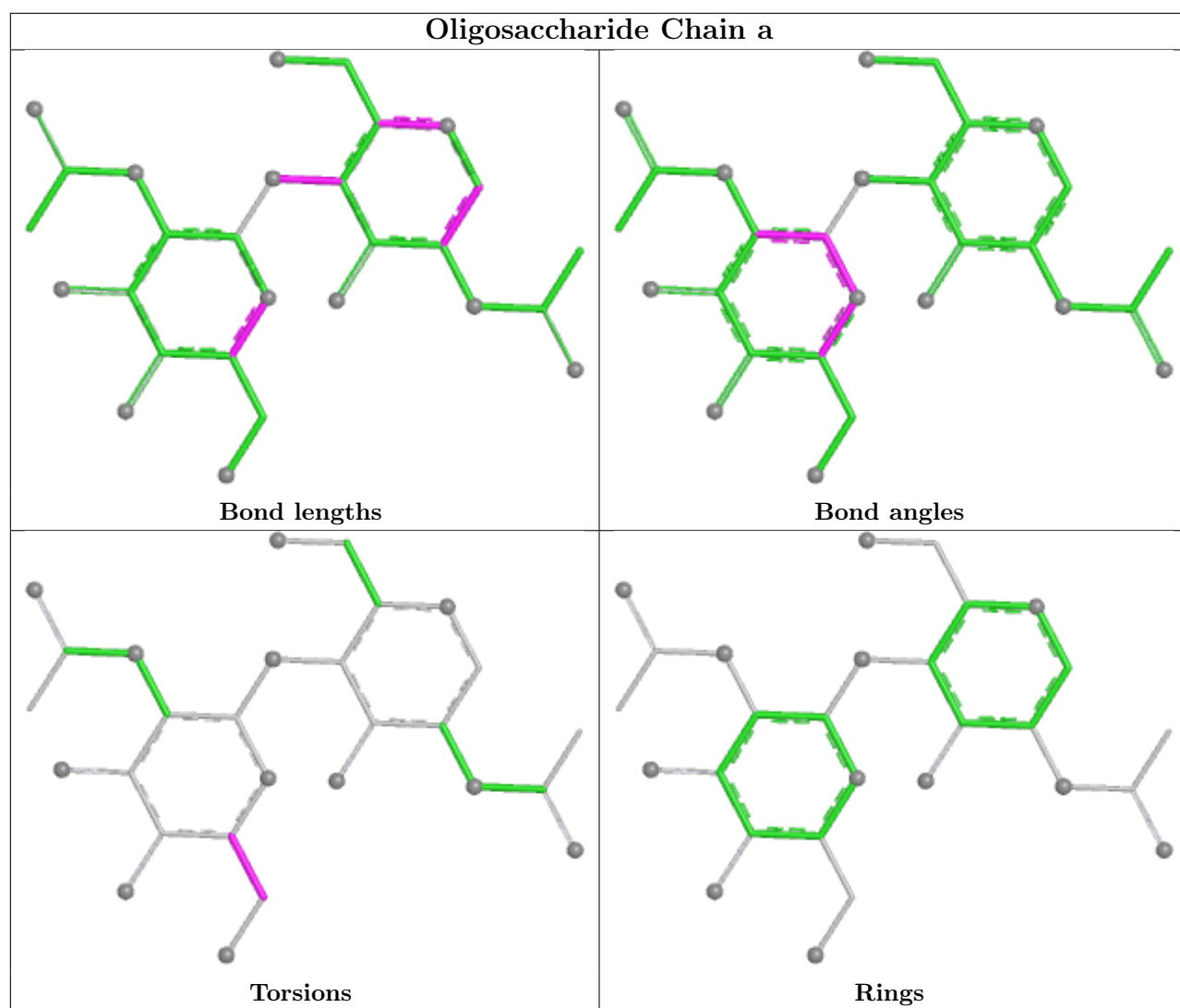
There are no ring outliers.

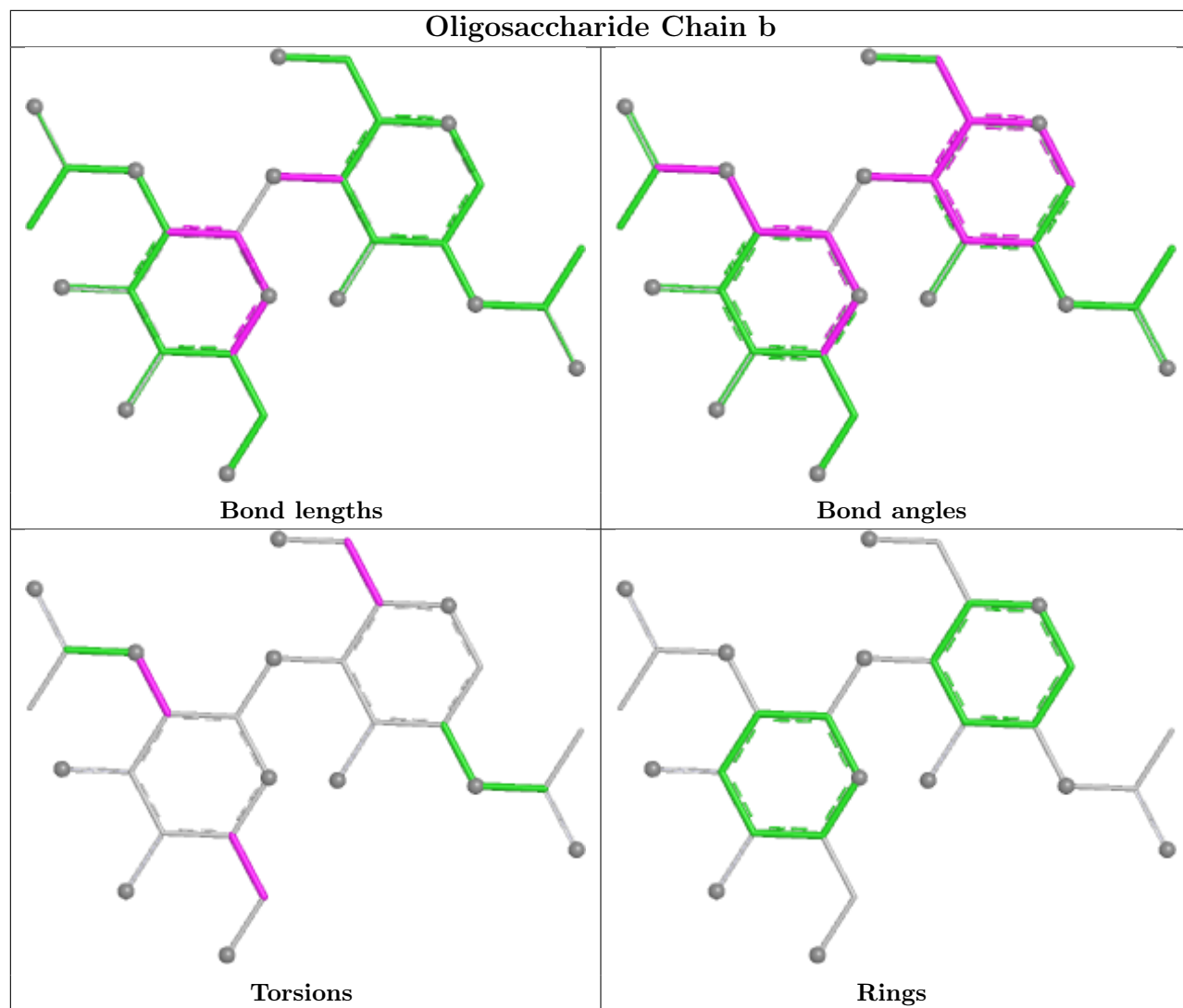
1 monomer is involved in 1 short contact:

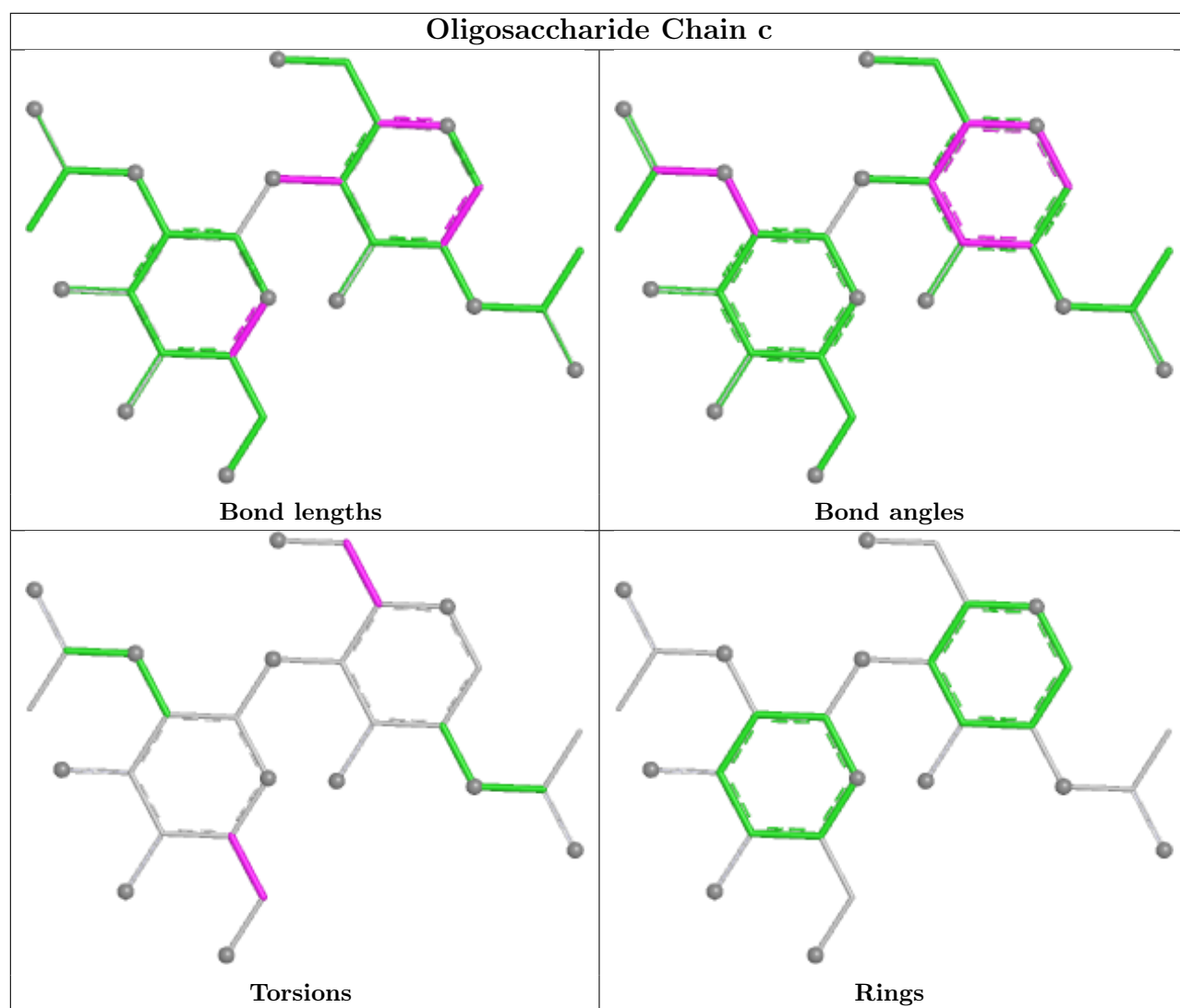
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	i	1	NAG	1	0

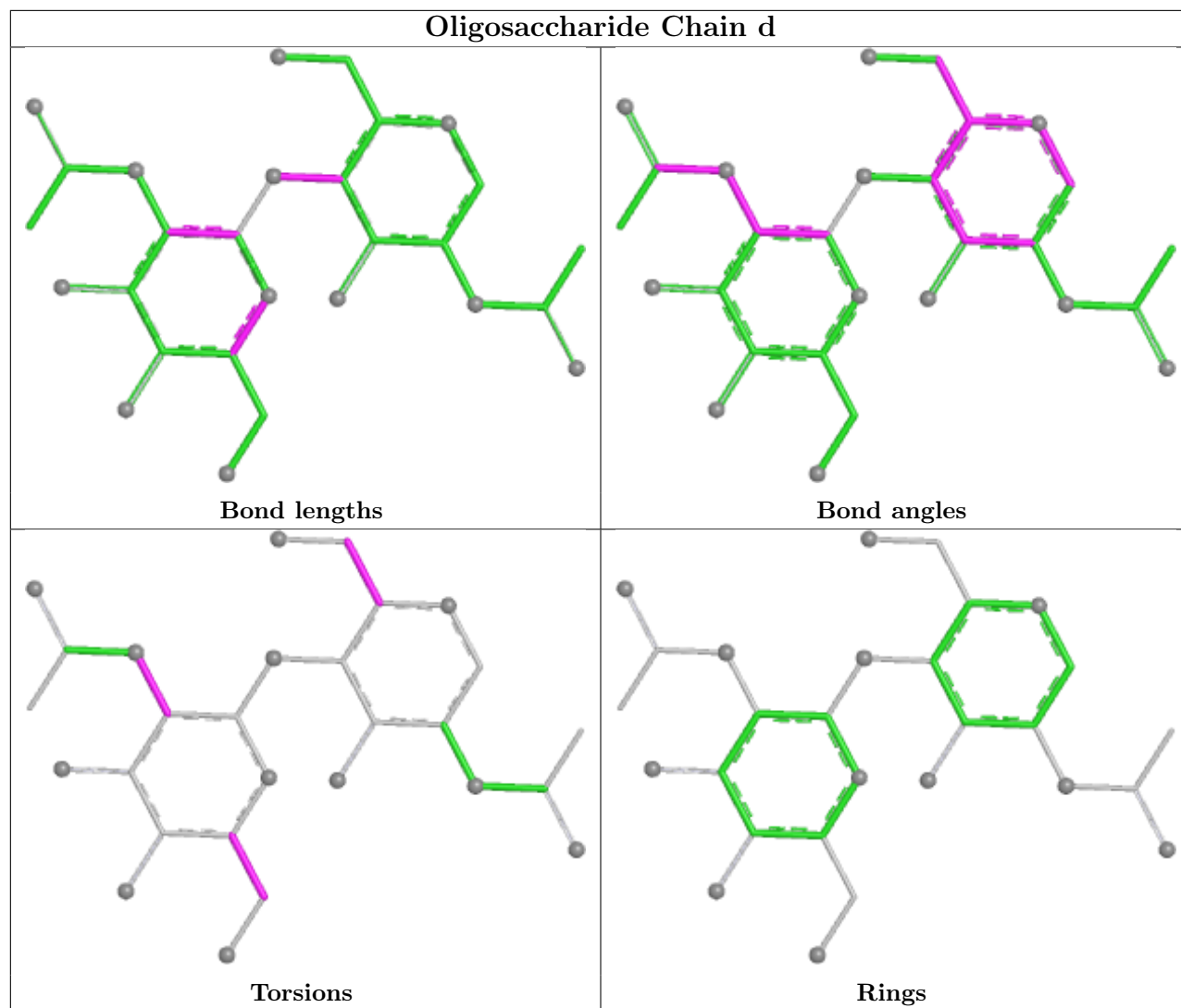
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

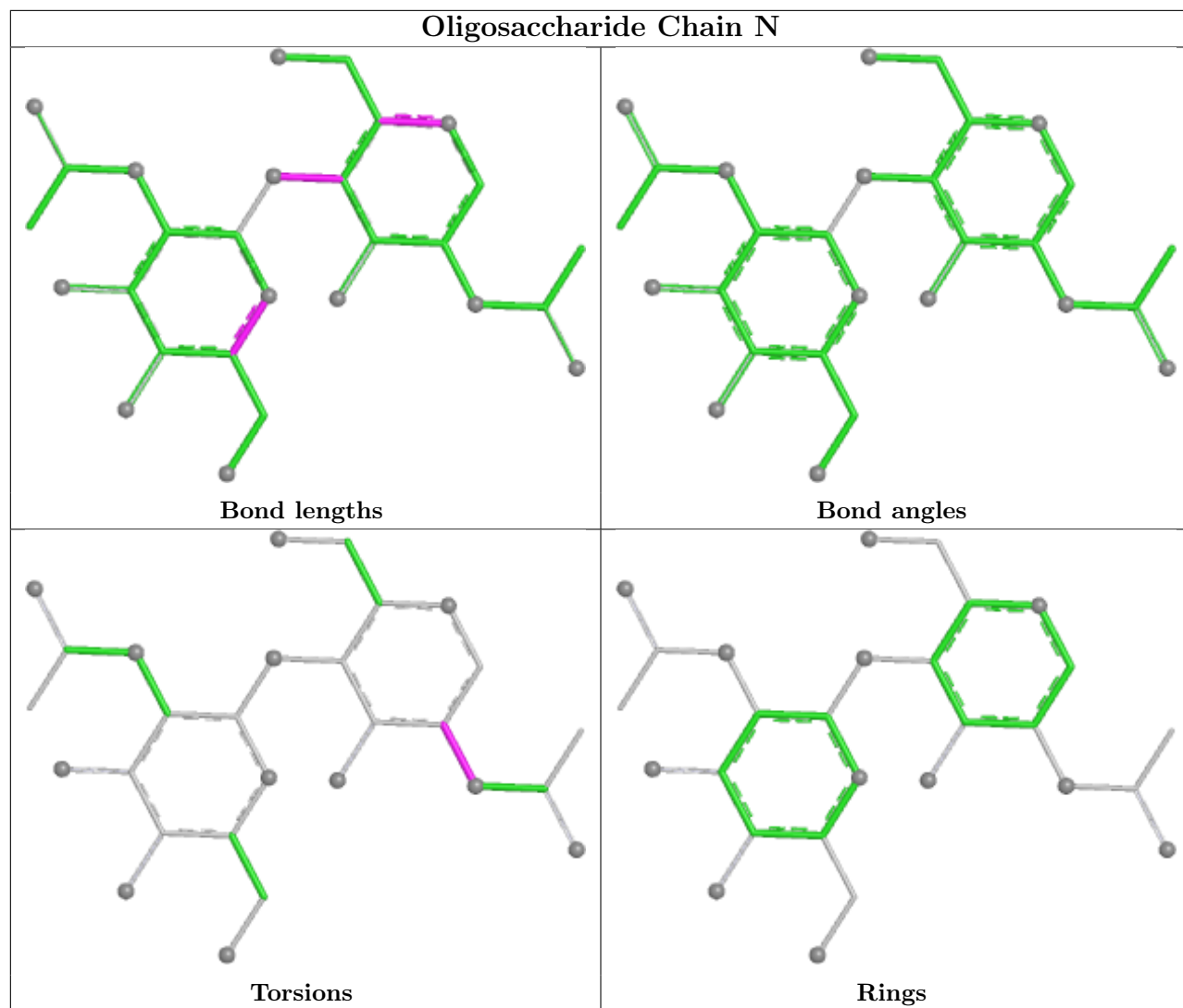


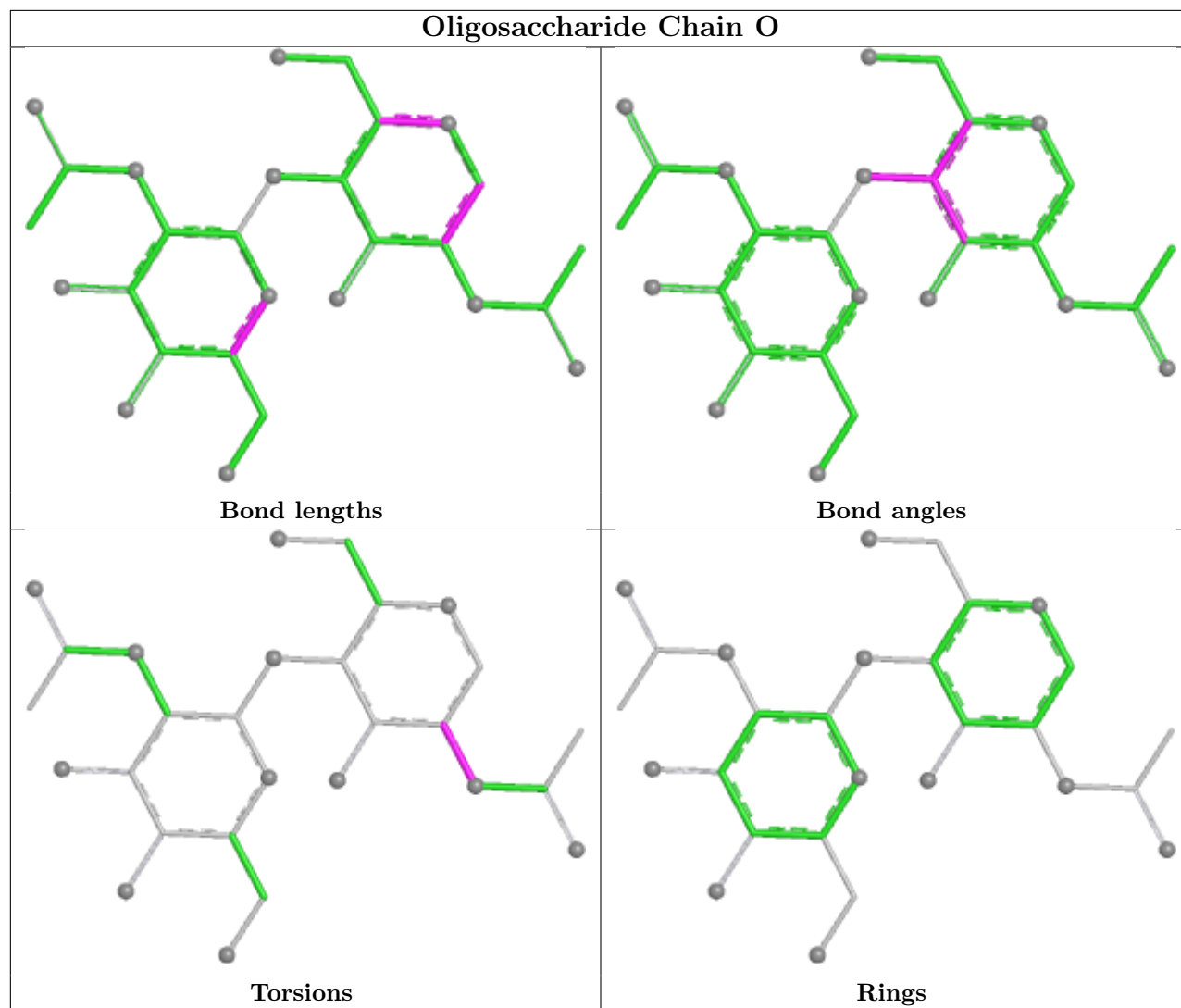


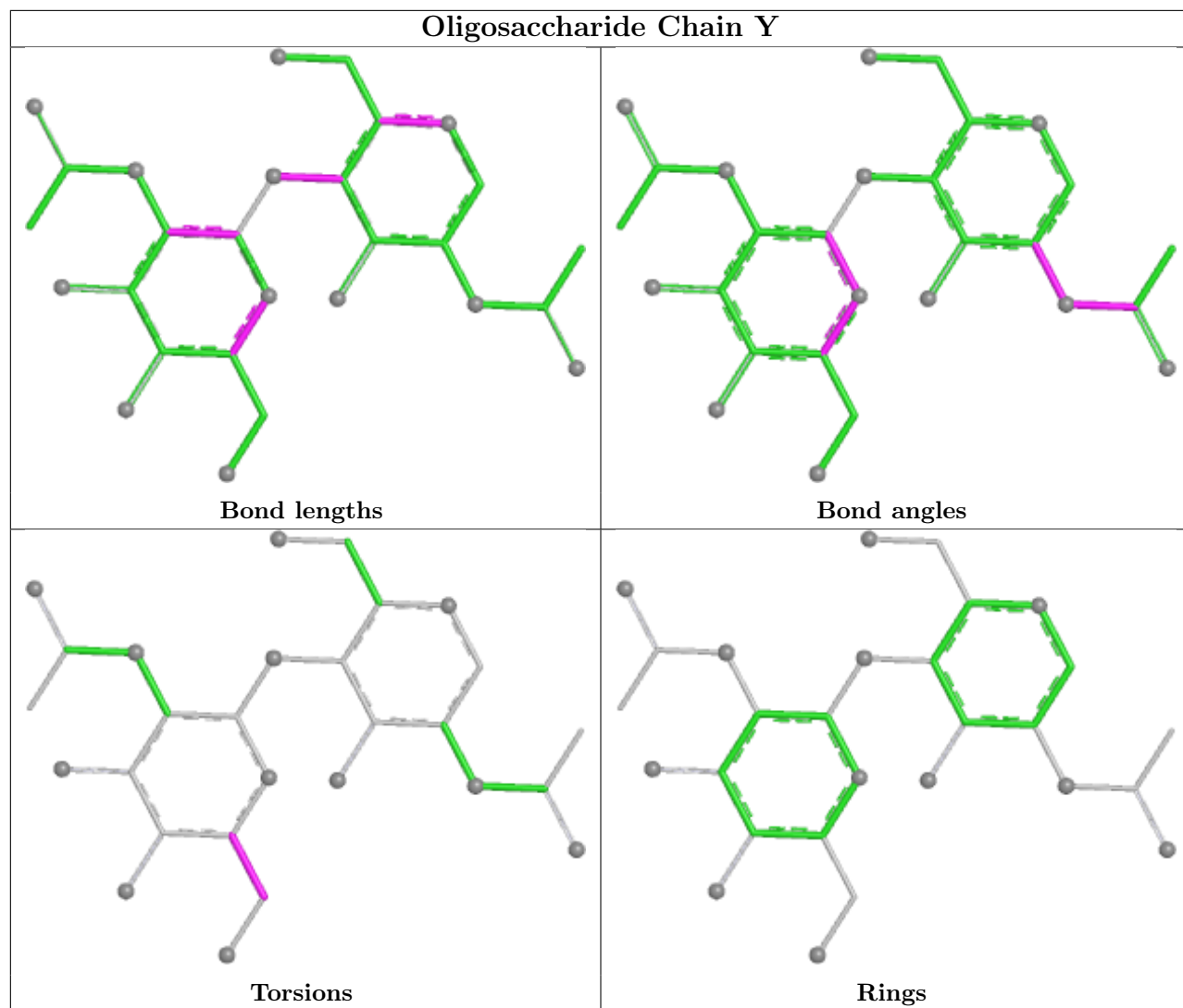


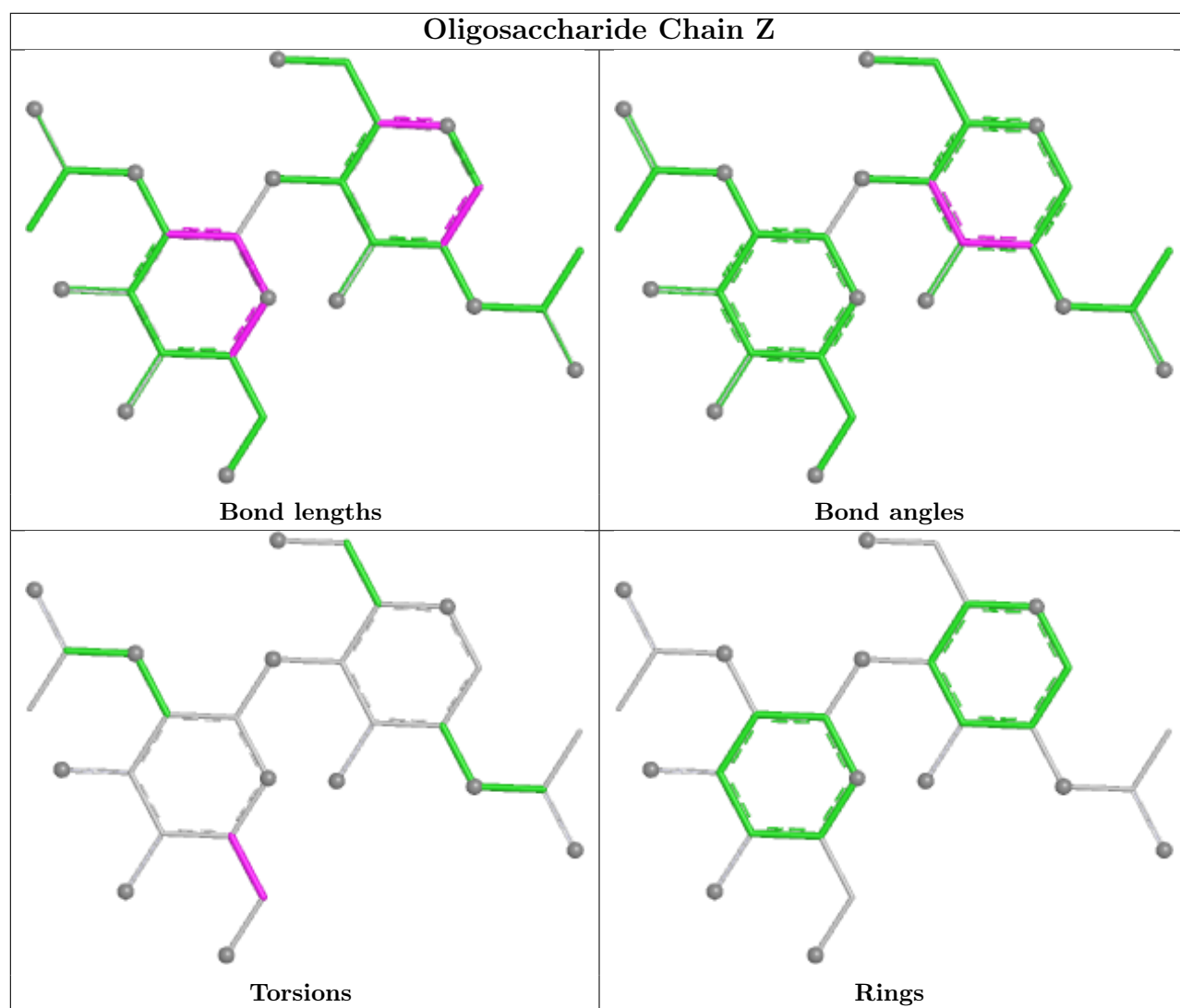


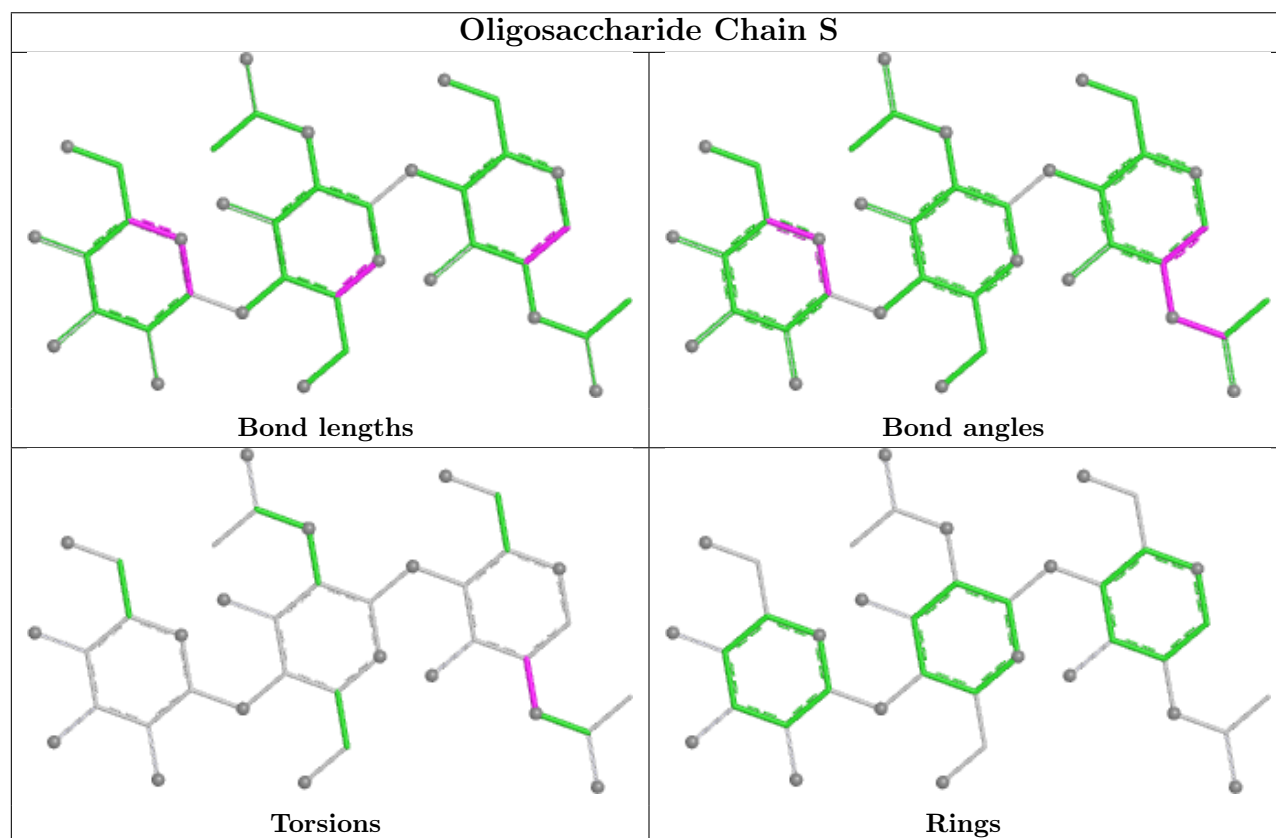
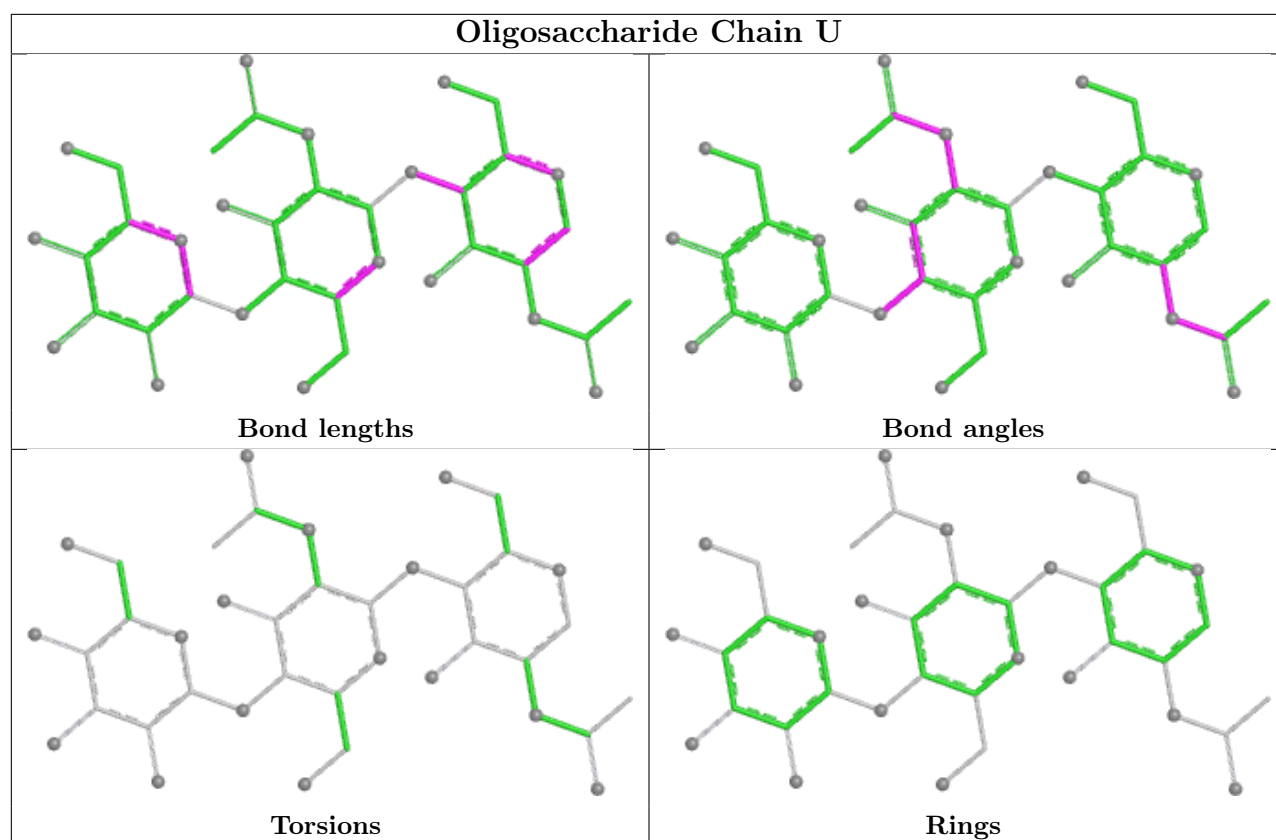


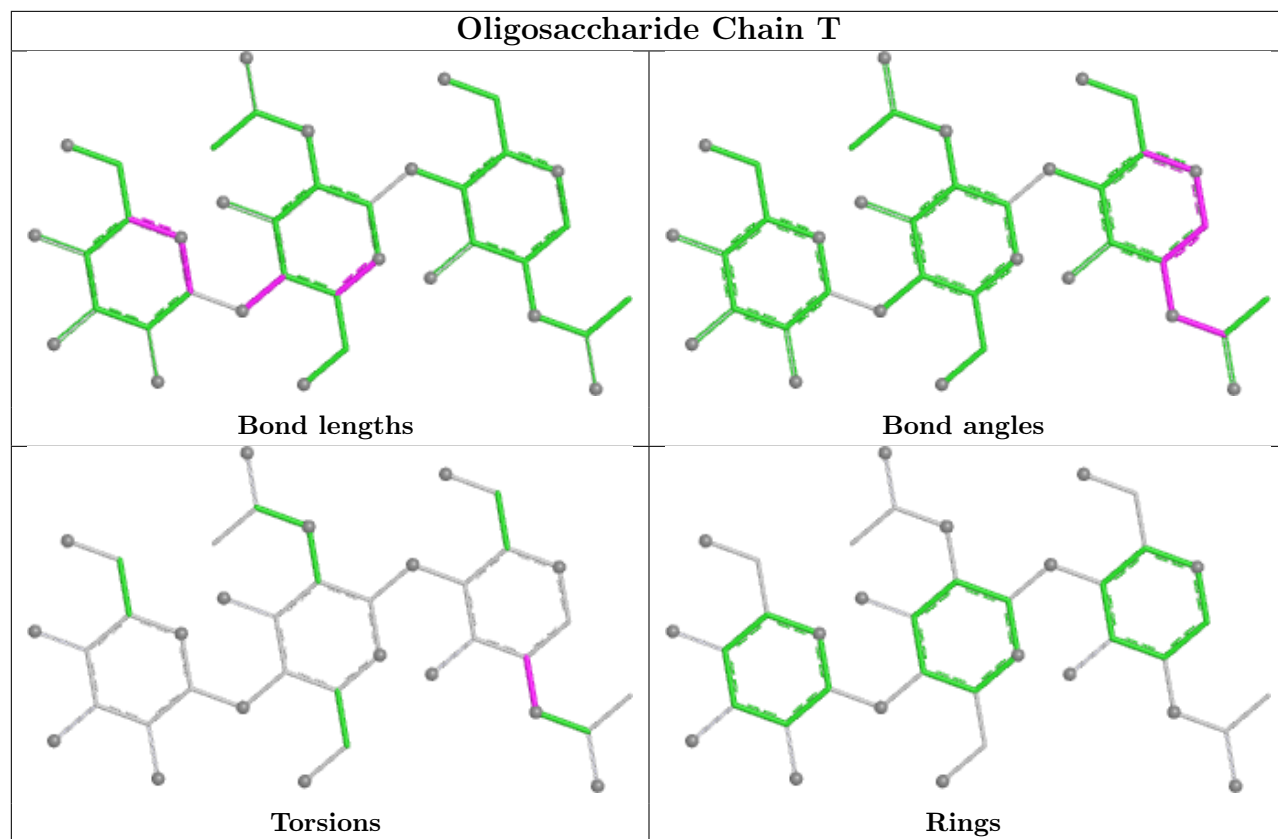


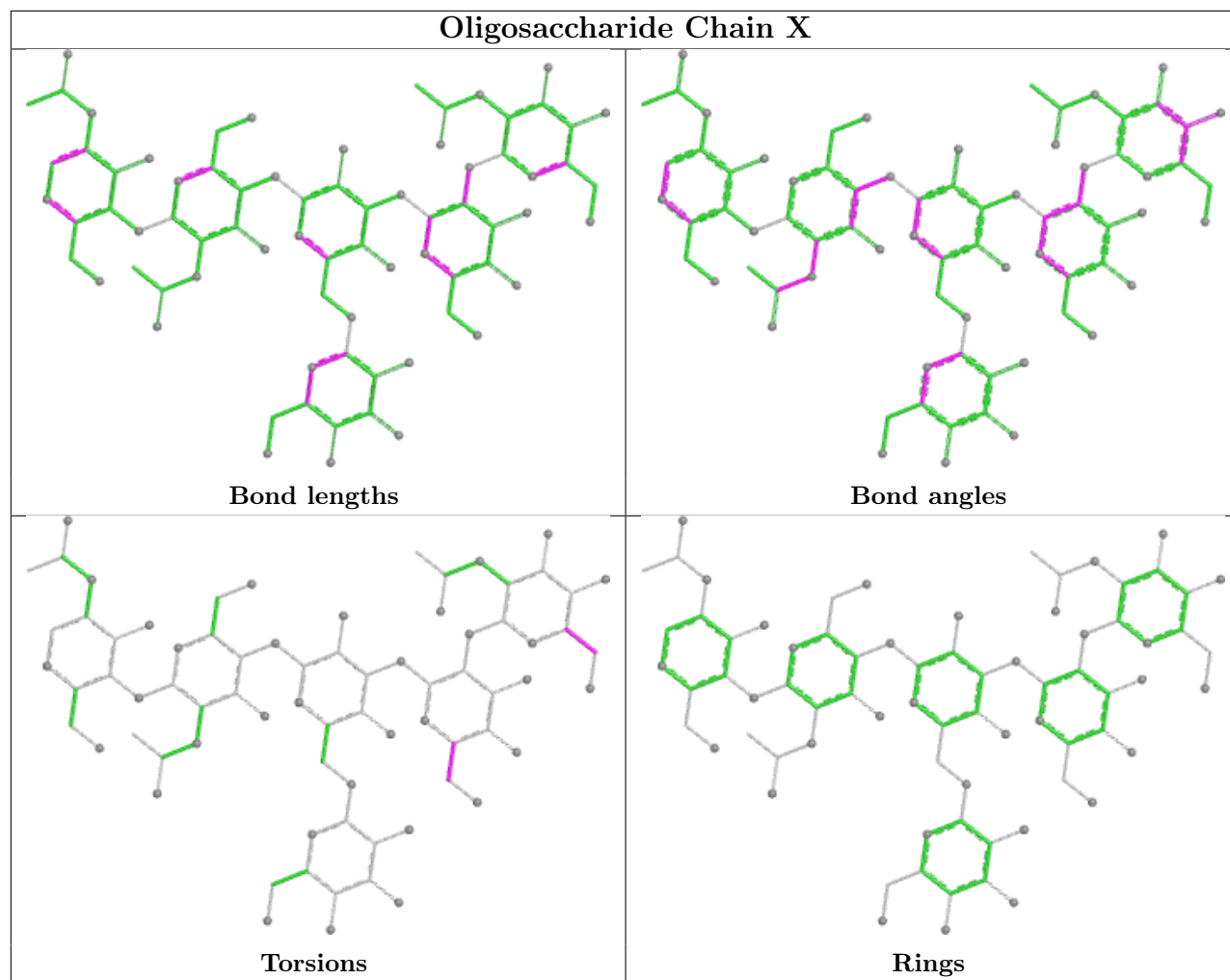


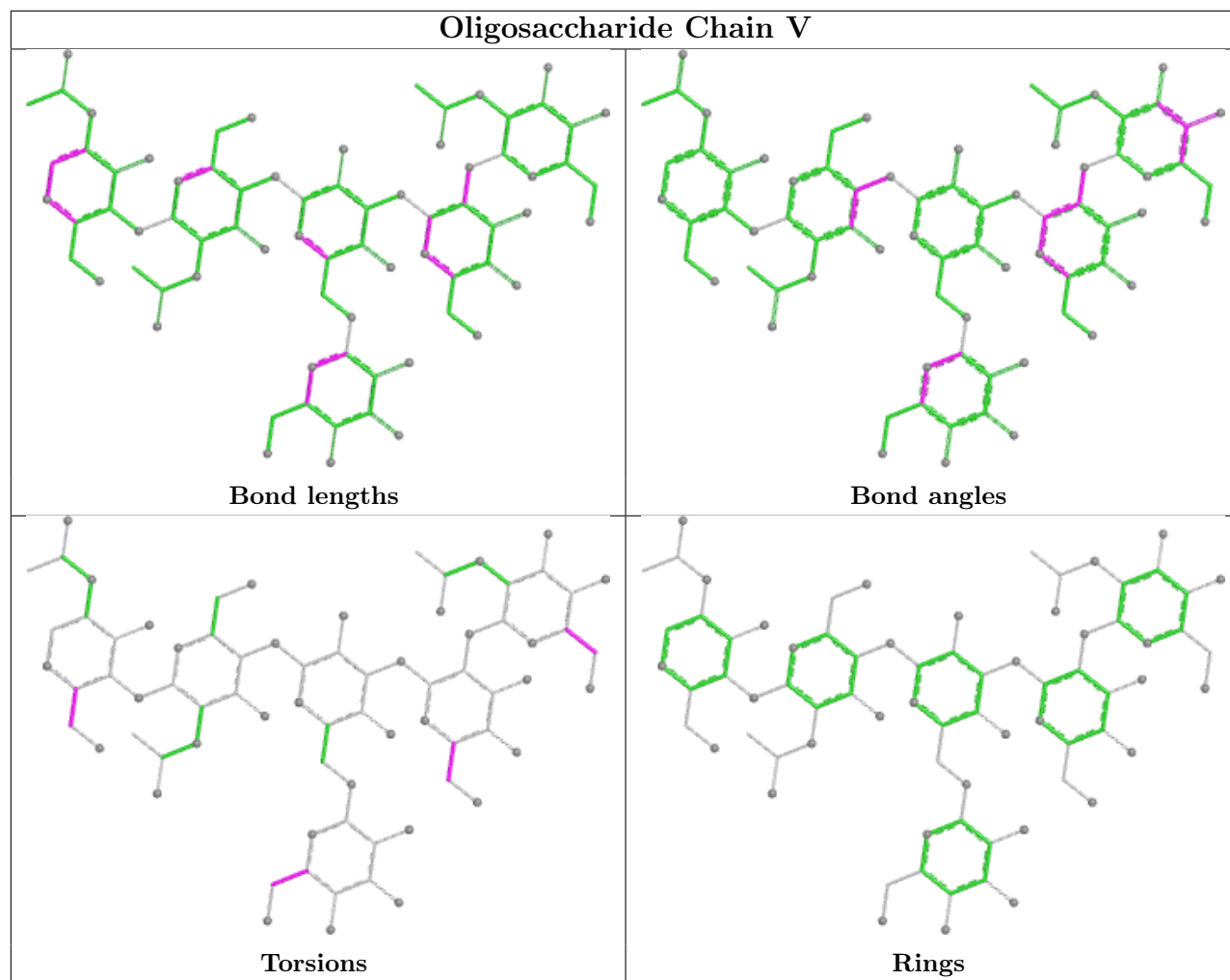


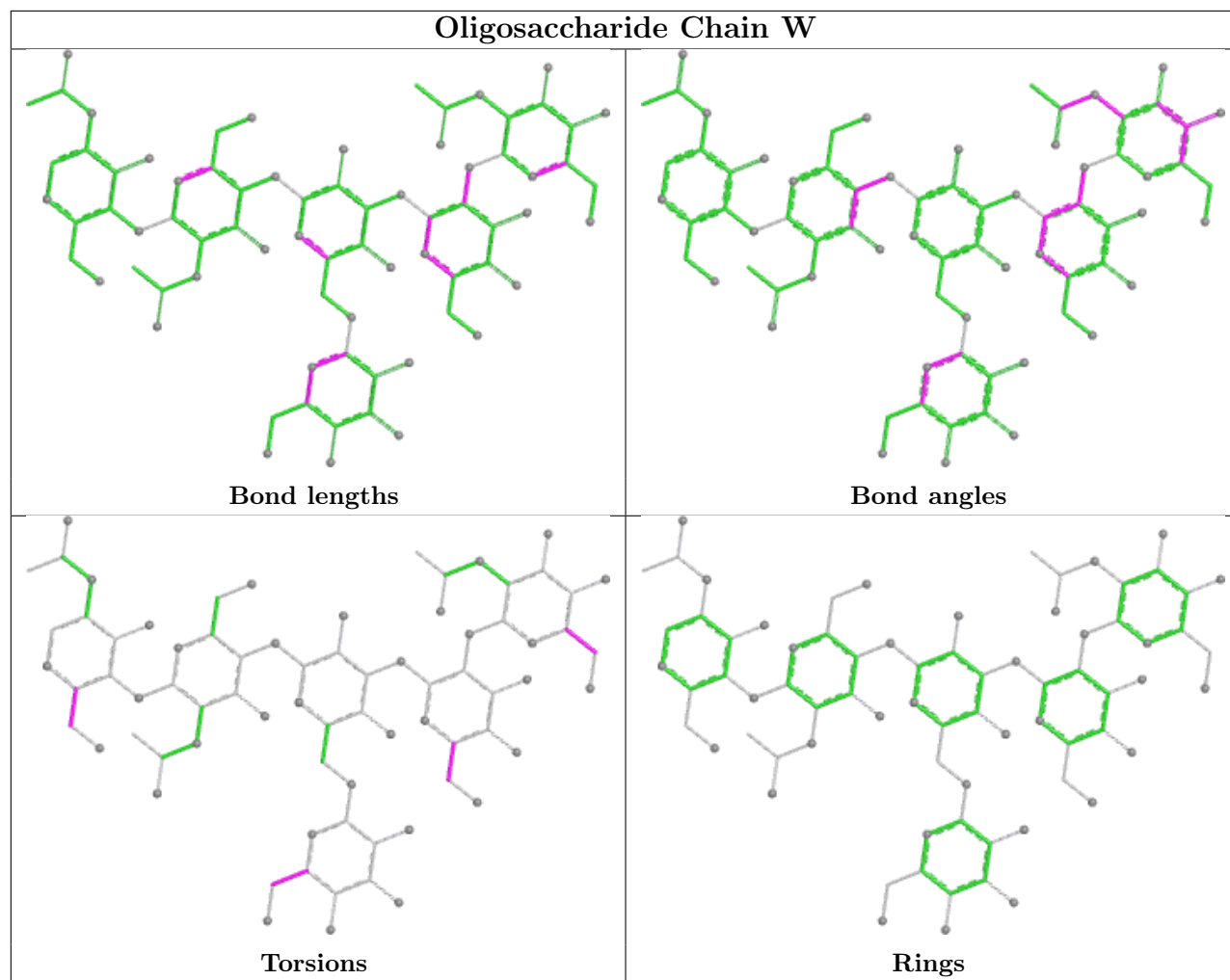


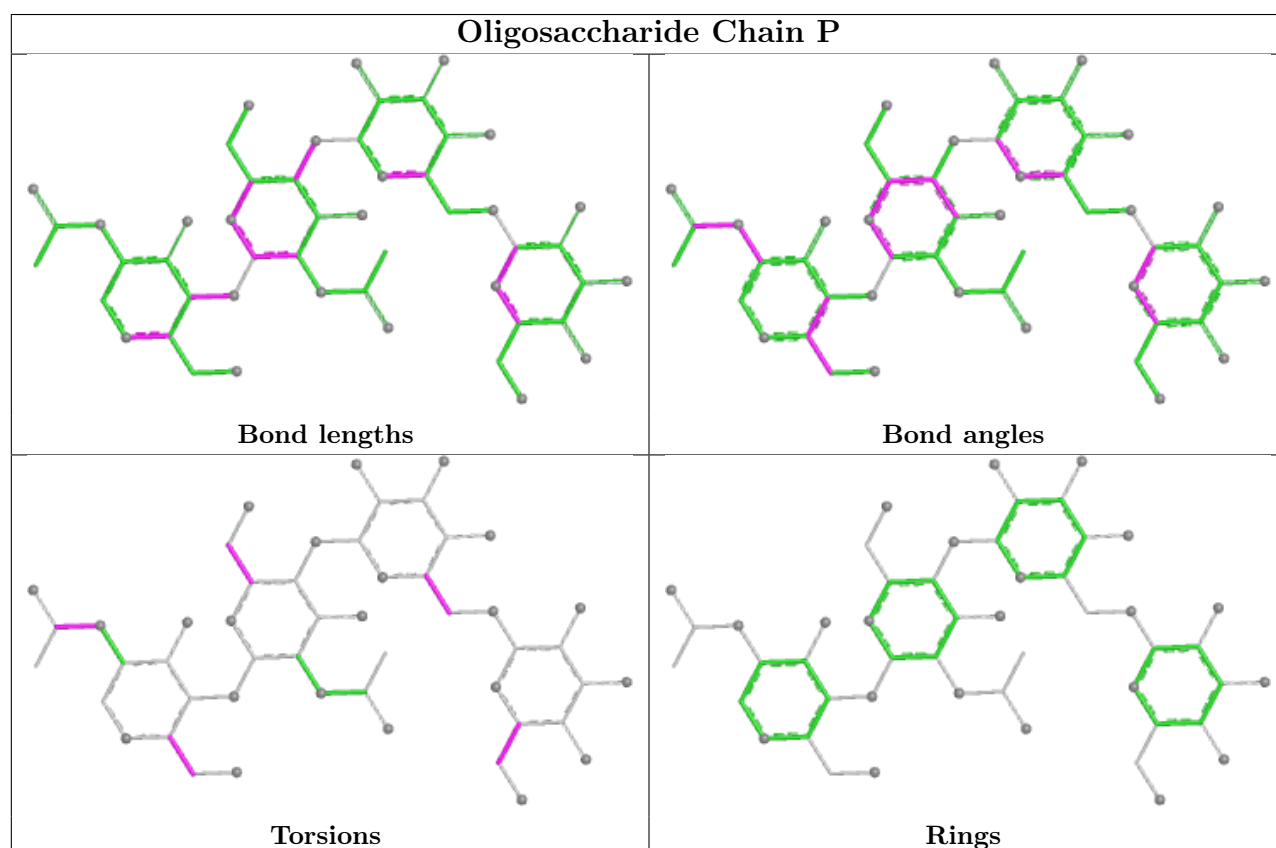
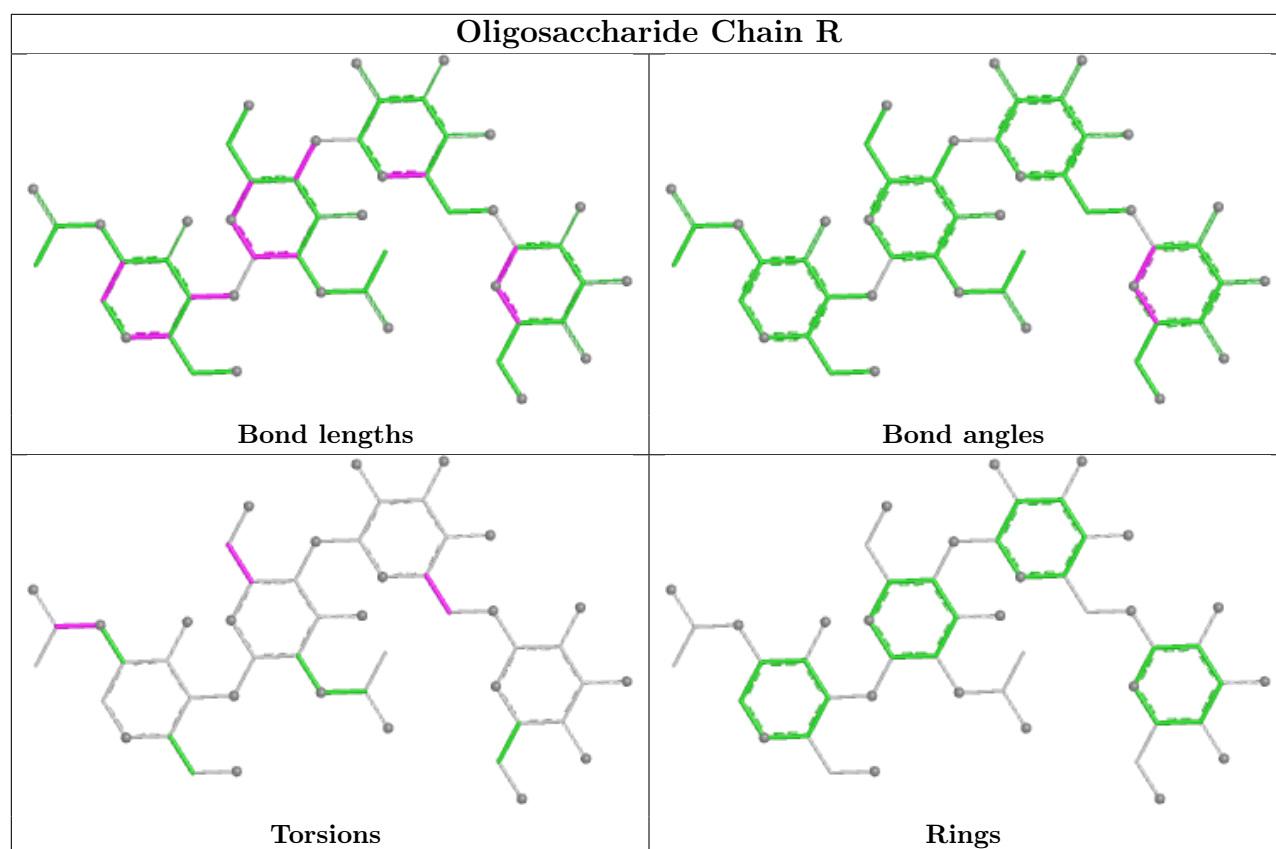


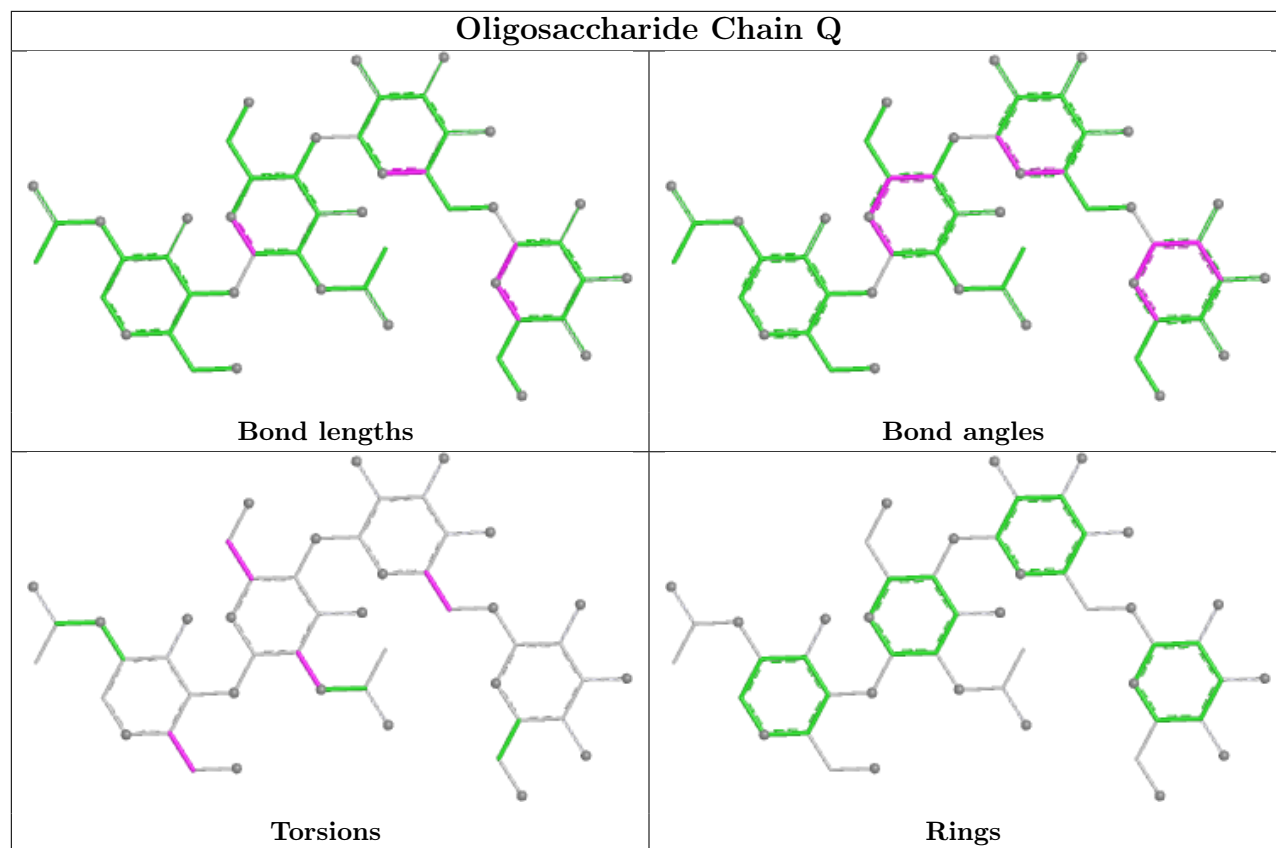


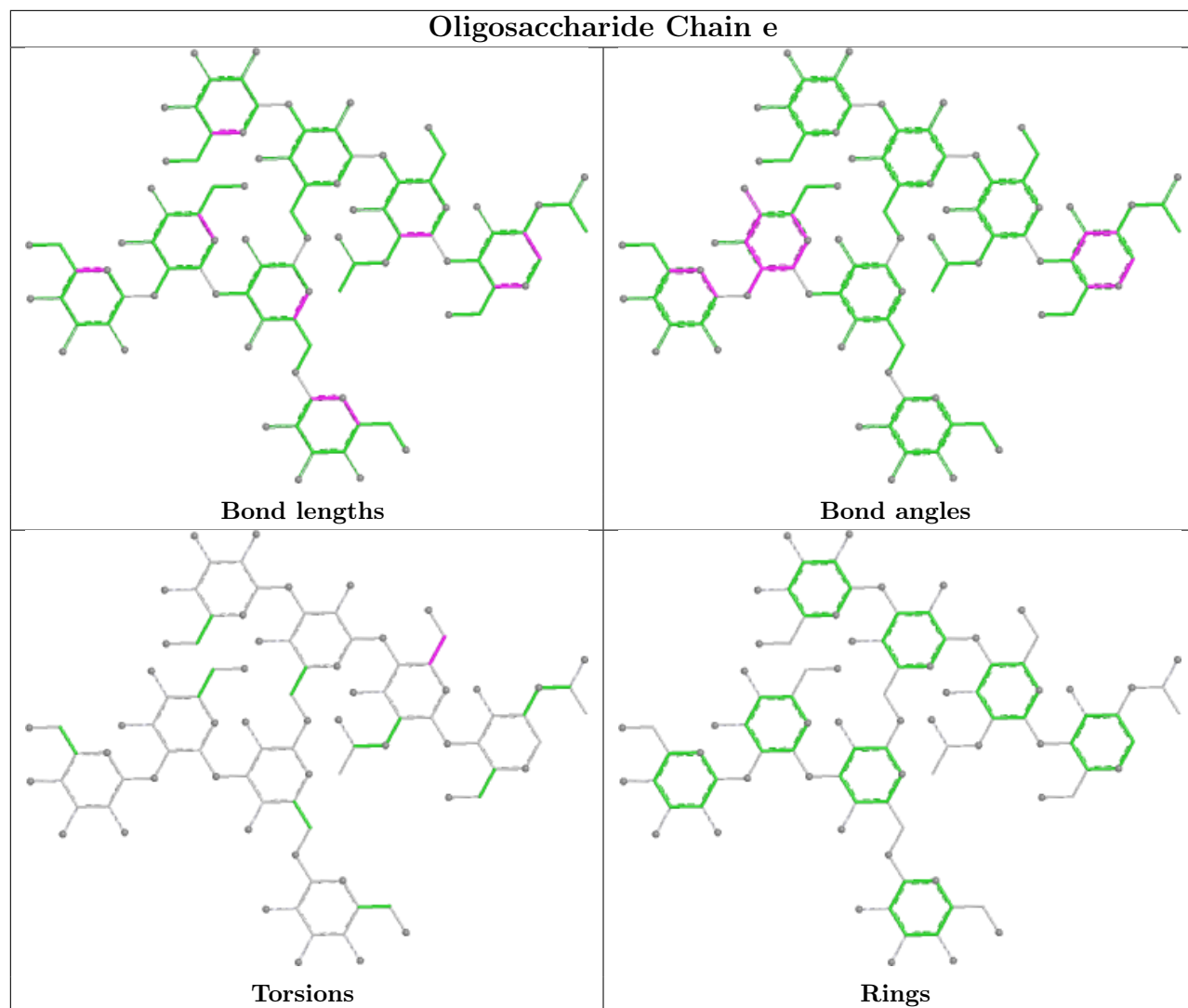


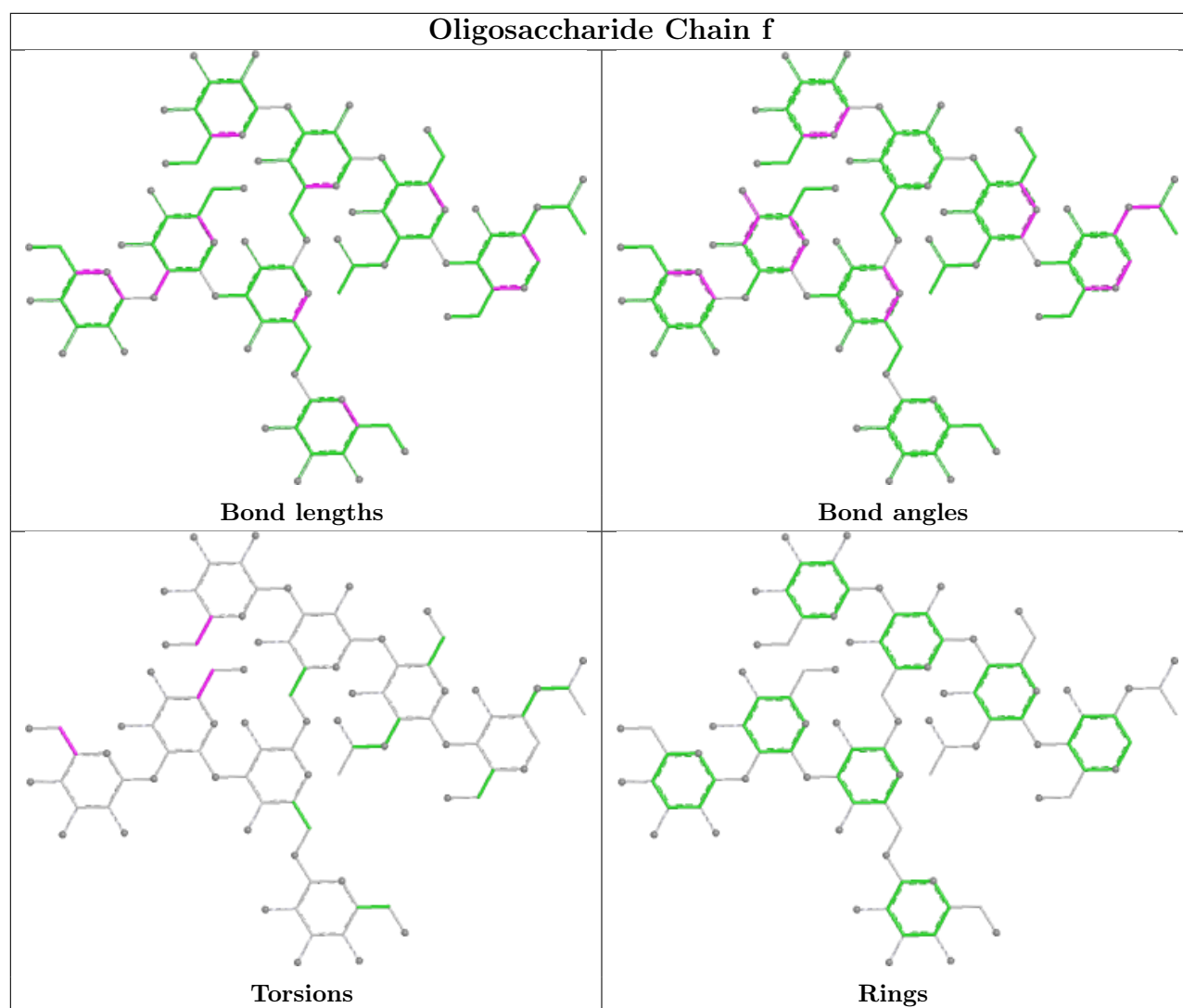


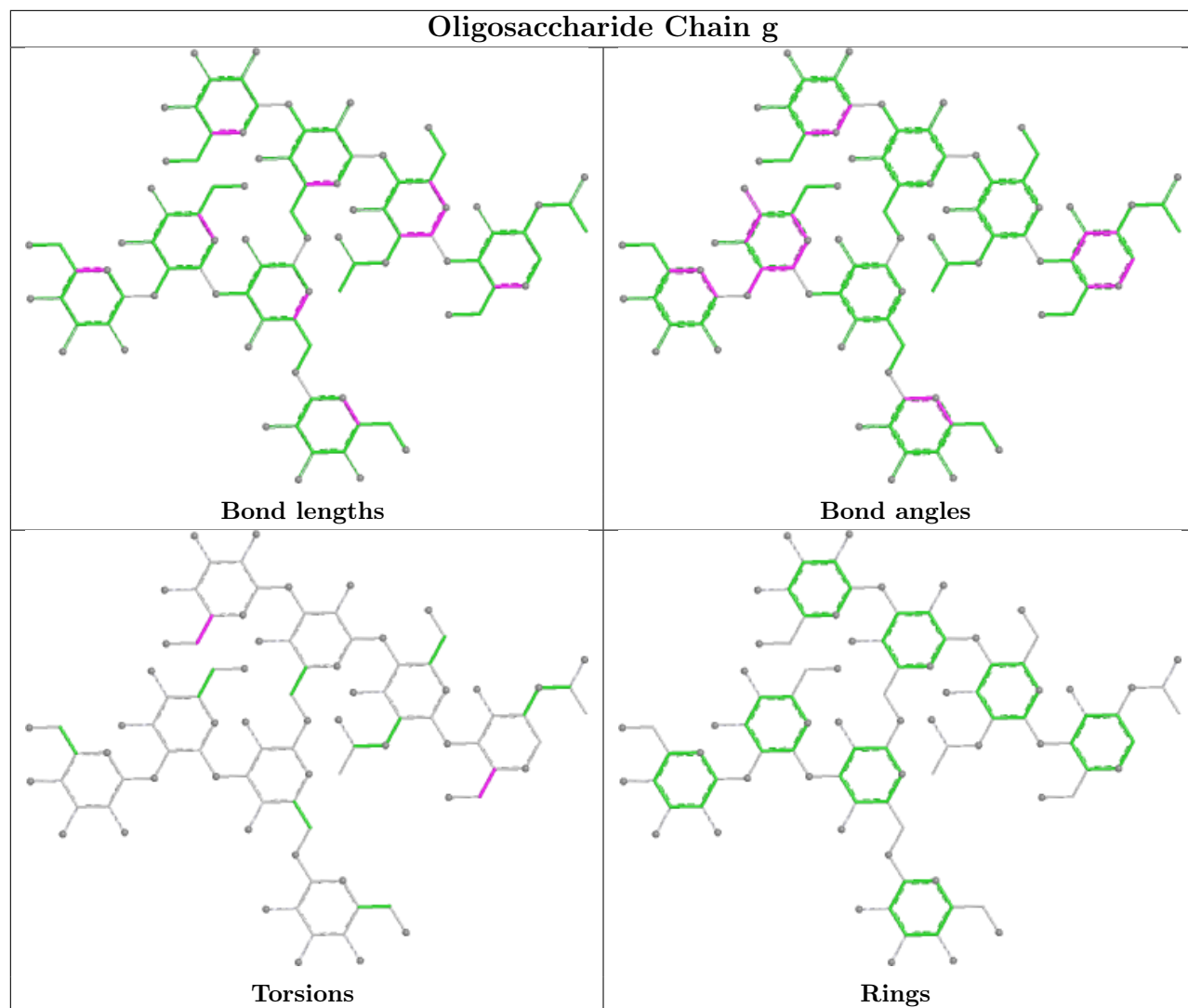


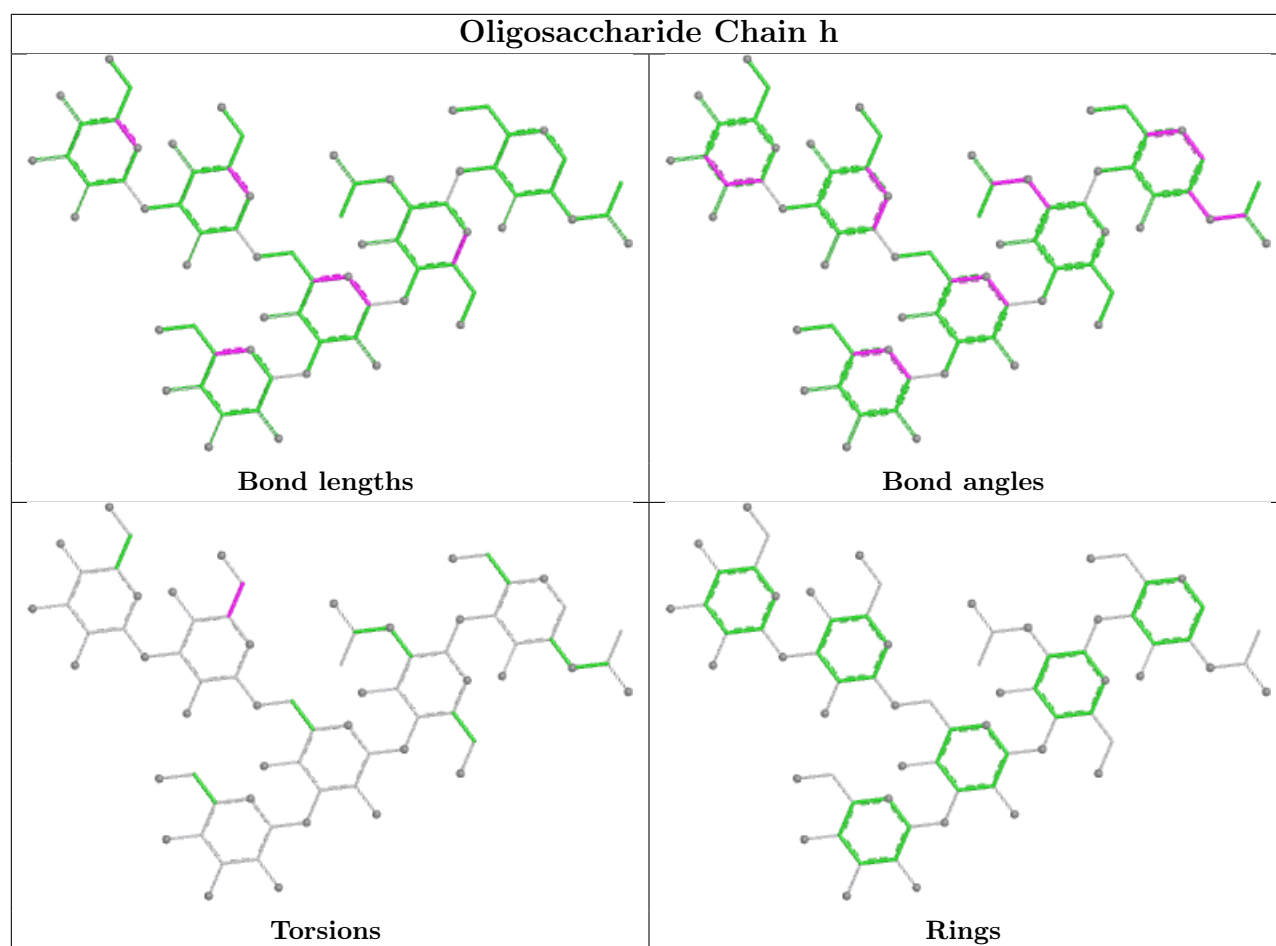


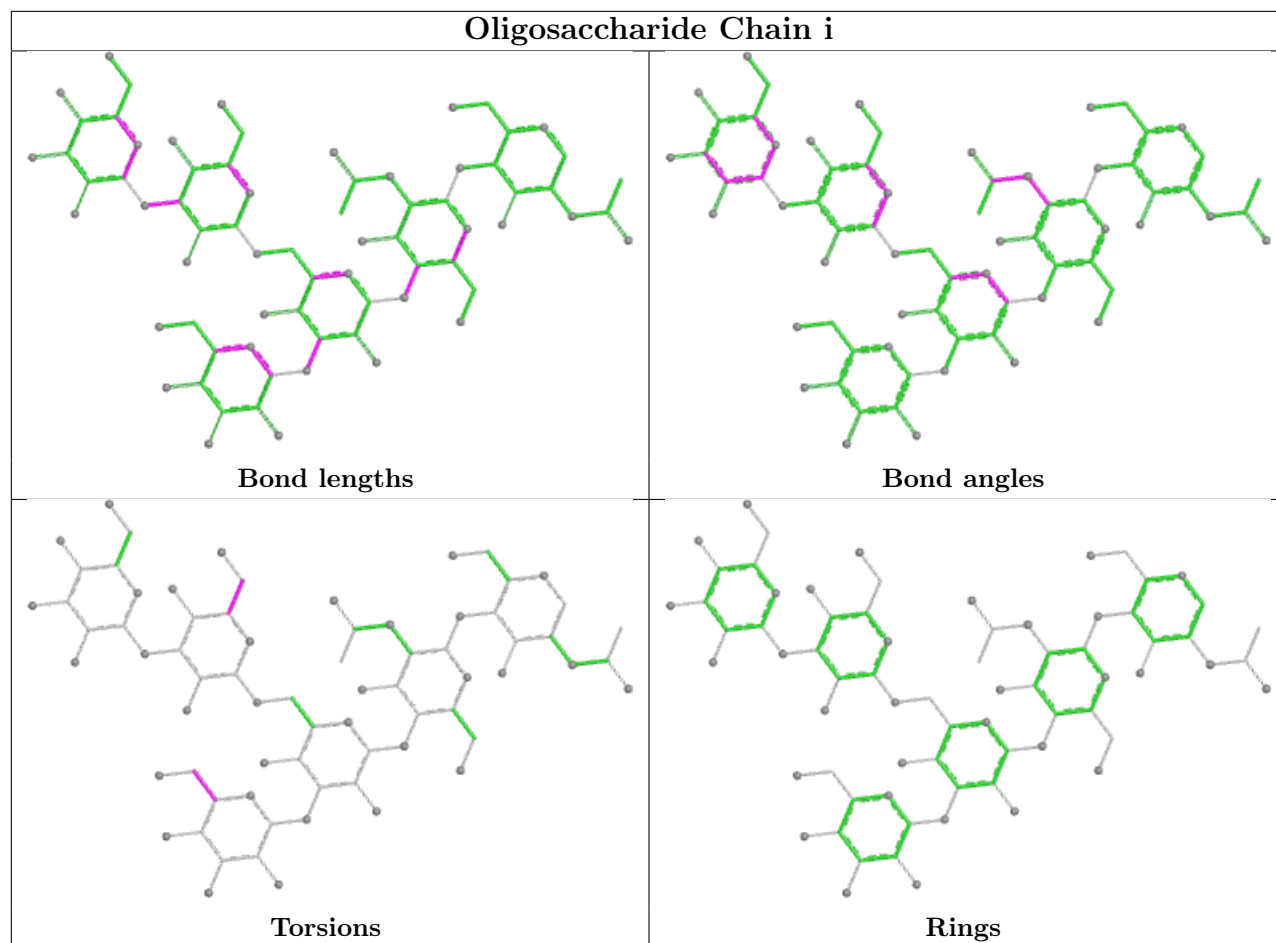


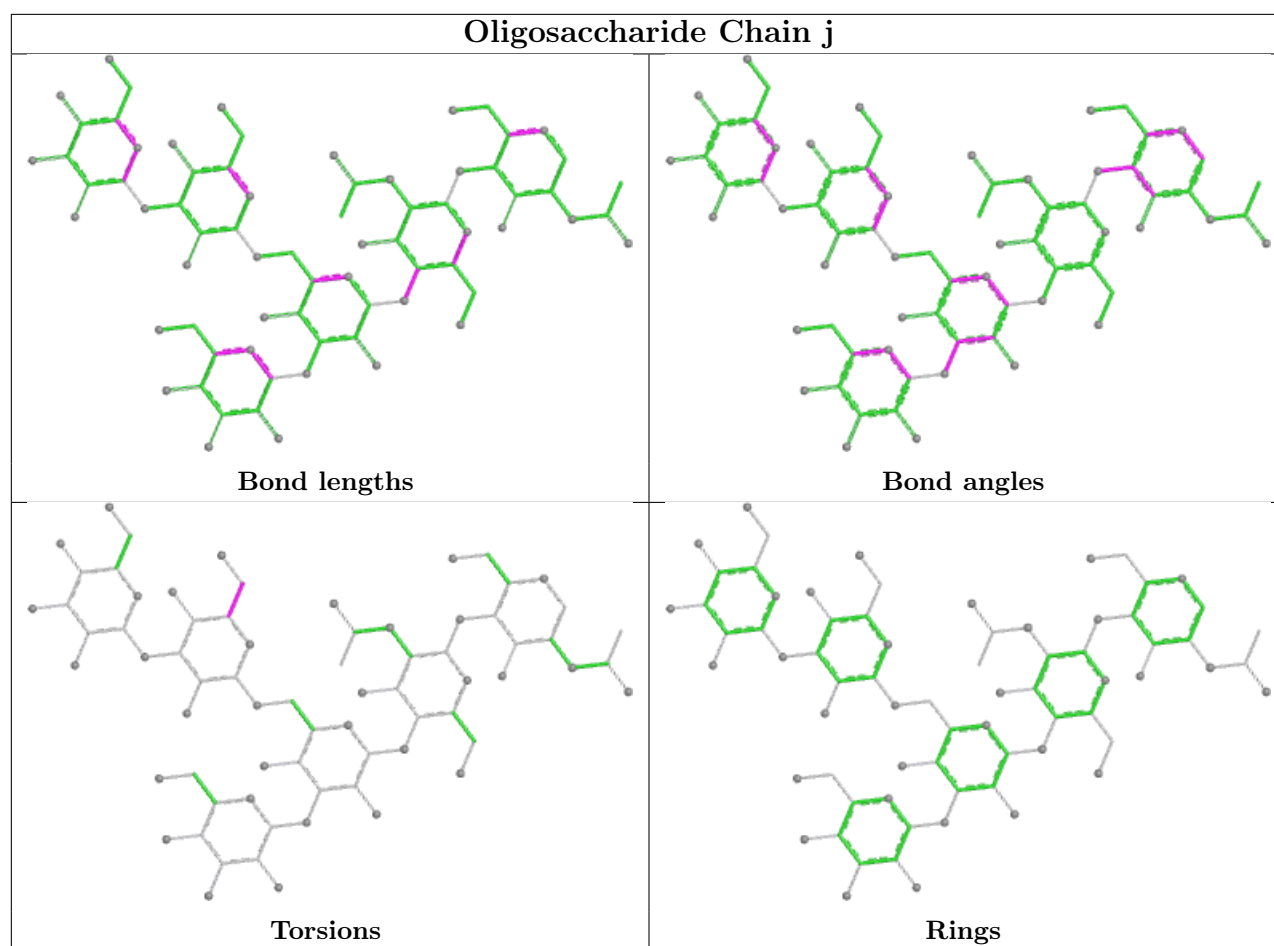












5.6 Ligand geometry [i](#)

15 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	CLR	A	1100	-	31,31,31	0.97	0	48,48,48	1.07	5 (10%)
9	NAG	G	1003	1	14,14,15	1.08	1 (7%)	17,19,21	1.03	1 (5%)
10	PTY	L	1101	-	49,49,49	0.82	0	52,54,54	0.63	0
8	CLR	L	1100	-	31,31,31	1.03	2 (6%)	48,48,48	0.99	5 (10%)
9	NAG	B	1002	1	14,14,15	1.25	2 (14%)	17,19,21	0.71	0
8	CLR	D	1100	-	31,31,31	1.07	3 (9%)	48,48,48	0.99	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	1001	1	14,14,15	1.43	3 (21%)	17,19,21	1.05	1 (5%)
9	NAG	B	1003	1	14,14,15	1.24	2 (14%)	17,19,21	1.19	1 (5%)
9	NAG	C	1001	1	14,14,15	1.31	2 (14%)	17,19,21	0.84	0
9	NAG	C	1002	1	14,14,15	1.19	2 (14%)	17,19,21	0.99	2 (11%)
9	NAG	G	1001	1	14,14,15	1.51	3 (21%)	17,19,21	0.97	1 (5%)
10	PTY	H	1101	-	49,49,49	0.70	0	52,54,54	0.45	0
9	NAG	C	1003	1	14,14,15	1.19	2 (14%)	17,19,21	0.90	1 (5%)
9	NAG	G	1002	1	14,14,15	1.23	2 (14%)	17,19,21	0.85	0
10	PTY	D	1101	-	49,49,49	0.77	0	52,54,54	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	A	1100	-	-	2/10/68/68	0/4/4/4
9	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
10	PTY	L	1101	-	-	8/53/53/53	-
8	CLR	L	1100	-	-	1/10/68/68	0/4/4/4
9	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
8	CLR	D	1100	-	-	0/10/68/68	0/4/4/4
9	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1003	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	C	1002	1	-	1/6/23/26	0/1/1/1
9	NAG	G	1001	1	-	1/6/23/26	0/1/1/1
10	PTY	H	1101	-	-	8/53/53/53	-
9	NAG	C	1003	1	-	1/6/23/26	0/1/1/1
9	NAG	G	1002	1	-	0/6/23/26	0/1/1/1
10	PTY	D	1101	-	-	13/53/53/53	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	1001	NAG	C1-C2	2.92	1.56	1.52
9	B	1001	NAG	O5-C5	2.92	1.49	1.43
9	C	1001	NAG	C1-C2	2.83	1.56	1.52
9	G	1001	NAG	O5-C5	2.83	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	NAG	C1-C2	2.69	1.56	1.52
8	D	1100	CLR	C11-C9	2.68	1.58	1.53
9	B	1003	NAG	O5-C5	2.66	1.48	1.43
9	G	1002	NAG	O5-C5	2.58	1.48	1.43
9	C	1003	NAG	C1-C2	2.58	1.55	1.52
9	B	1001	NAG	O5-C1	2.52	1.47	1.43
9	C	1003	NAG	O5-C5	2.50	1.48	1.43
9	B	1002	NAG	C1-C2	2.47	1.55	1.52
9	C	1002	NAG	O5-C5	2.47	1.48	1.43
9	C	1001	NAG	O5-C5	2.44	1.48	1.43
8	L	1100	CLR	C18-C13	2.39	1.58	1.54
9	B	1003	NAG	C1-C2	2.33	1.55	1.52
9	G	1001	NAG	O5-C1	2.30	1.47	1.43
9	B	1002	NAG	O5-C5	2.30	1.47	1.43
9	G	1002	NAG	C1-C2	2.28	1.55	1.52
9	G	1003	NAG	O5-C5	2.27	1.47	1.43
9	C	1002	NAG	C1-C2	2.23	1.55	1.52
8	L	1100	CLR	C11-C9	2.21	1.57	1.53
8	D	1100	CLR	C18-C13	2.04	1.57	1.54
8	D	1100	CLR	C10-C5	2.02	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1001	NAG	C1-O5-C5	3.37	116.70	112.19
9	B	1003	NAG	C1-C2-N2	3.30	115.64	110.43
9	G	1003	NAG	C1-C2-N2	3.01	115.18	110.43
9	G	1001	NAG	C1-O5-C5	2.87	116.03	112.19
8	A	1100	CLR	C19-C10-C1	2.60	113.38	109.43
8	A	1100	CLR	C1-C2-C3	2.56	113.87	110.48
8	A	1100	CLR	C7-C8-C9	2.49	112.60	109.72
8	A	1100	CLR	C15-C14-C13	2.49	106.77	103.84
8	D	1100	CLR	C19-C10-C9	-2.31	109.06	111.66
8	L	1100	CLR	C9-C10-C5	-2.26	106.34	109.65
8	L	1100	CLR	C21-C20-C22	2.26	113.84	110.34
8	L	1100	CLR	C11-C9-C8	2.20	114.85	111.78
8	D	1100	CLR	C11-C9-C8	2.19	114.84	111.78
8	D	1100	CLR	C15-C14-C13	2.17	106.39	103.84
8	L	1100	CLR	C1-C10-C5	2.14	112.43	108.74
8	A	1100	CLR	C1-C10-C5	-2.12	105.09	108.74
8	L	1100	CLR	C11-C9-C10	2.12	115.70	113.08
9	C	1002	NAG	O5-C1-C2	-2.11	108.03	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1002	NAG	C1-C2-N2	2.11	113.75	110.43
9	C	1003	NAG	C1-C2-N2	2.10	113.74	110.43

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1003	NAG	C1-C2-N2-C7
9	C	1002	NAG	C1-C2-N2-C7
9	C	1003	NAG	C1-C2-N2-C7
9	G	1003	NAG	C1-C2-N2-C7
10	D	1101	PTY	C2-C3-O11-P1
10	D	1101	PTY	C6-C5-O14-P1
10	H	1101	PTY	C6-C5-O14-P1
10	L	1101	PTY	N1-C2-C3-O11
10	L	1101	PTY	C6-C5-O14-P1
10	D	1101	PTY	C11-C8-O7-C6
9	B	1001	NAG	O5-C5-C6-O6
9	G	1001	NAG	O5-C5-C6-O6
10	D	1101	PTY	C11-C12-C13-C14
9	C	1001	NAG	O5-C5-C6-O6
8	L	1100	CLR	C20-C22-C23-C24
10	H	1101	PTY	C40-C41-C42-C43
10	L	1101	PTY	C34-C35-C36-C37
10	H	1101	PTY	C16-C17-C18-C19
10	L	1101	PTY	C31-C32-C33-C34
10	D	1101	PTY	O30-C30-O4-C1
10	H	1101	PTY	O14-C5-C6-C1
10	H	1101	PTY	O14-C5-C6-O7
10	D	1101	PTY	C30-C31-C32-C33
10	D	1101	PTY	C3-O11-P1-O12
10	D	1101	PTY	C3-O11-P1-O13
10	D	1101	PTY	C3-O11-P1-O14
8	A	1100	CLR	C17-C20-C22-C23
10	D	1101	PTY	O4-C1-C6-O7
10	L	1101	PTY	O4-C1-C6-O7
10	L	1101	PTY	C35-C36-C37-C38
8	A	1100	CLR	C21-C20-C22-C23
10	H	1101	PTY	C23-C24-C25-C26
9	G	1003	NAG	C3-C2-N2-C7
10	D	1101	PTY	C35-C36-C37-C38
10	D	1101	PTY	C41-C42-C43-C44

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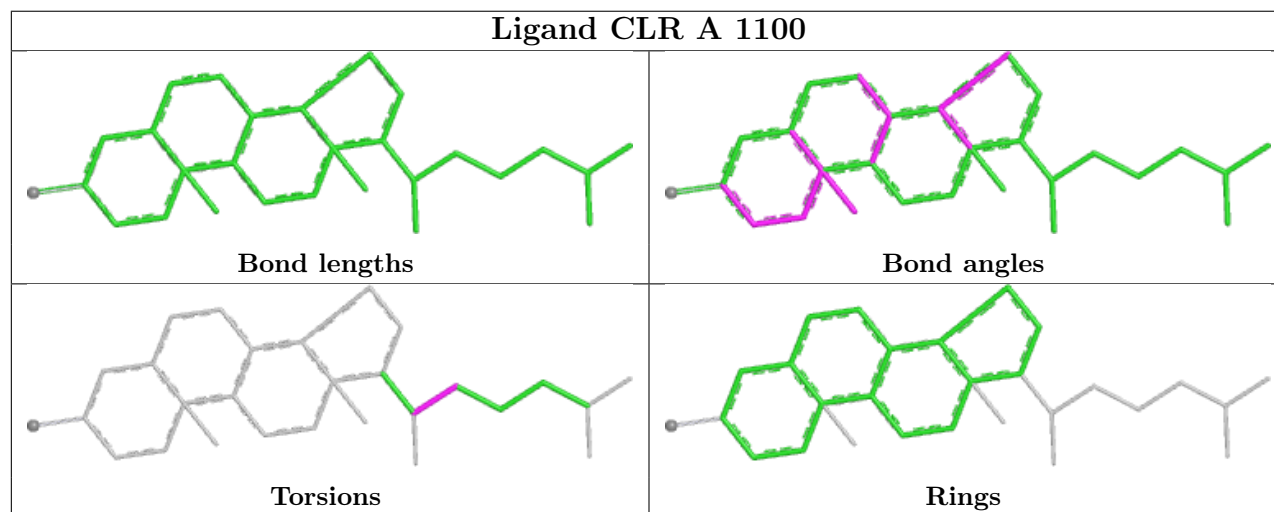
Mol	Chain	Res	Type	Atoms
10	L	1101	PTY	C41-C42-C43-C44
10	H	1101	PTY	C36-C37-C38-C39
10	D	1101	PTY	O4-C1-C6-C5
10	L	1101	PTY	O4-C1-C6-C5
10	H	1101	PTY	C19-C20-C21-C22

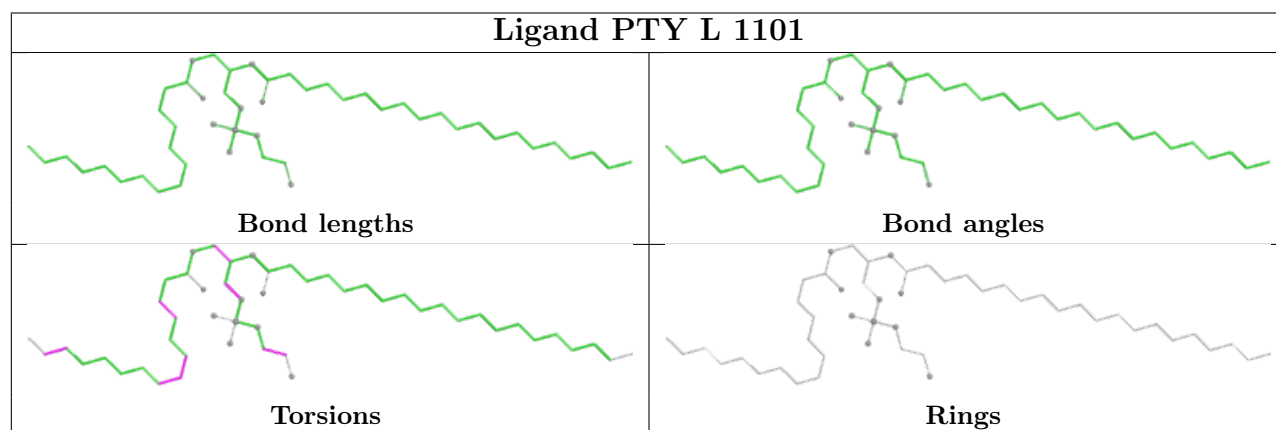
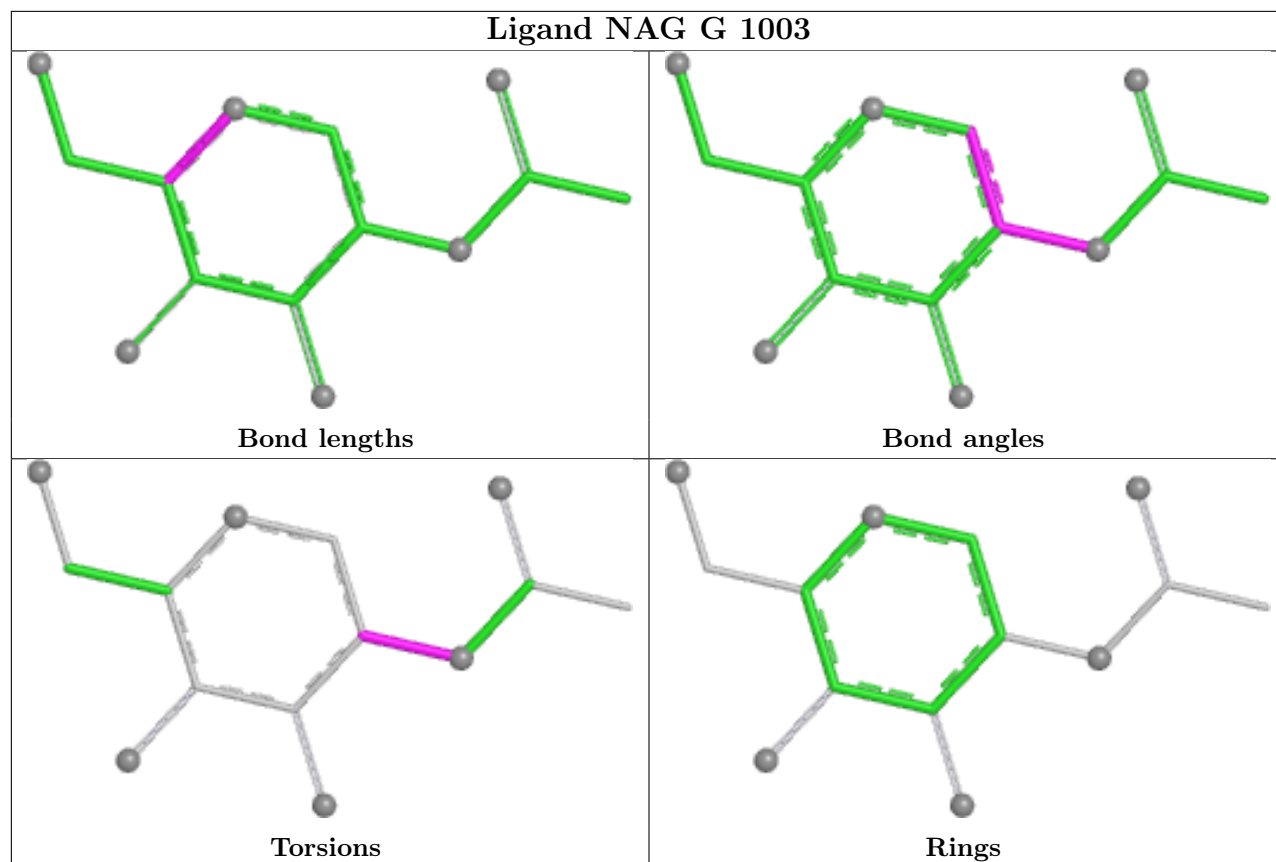
There are no ring outliers.

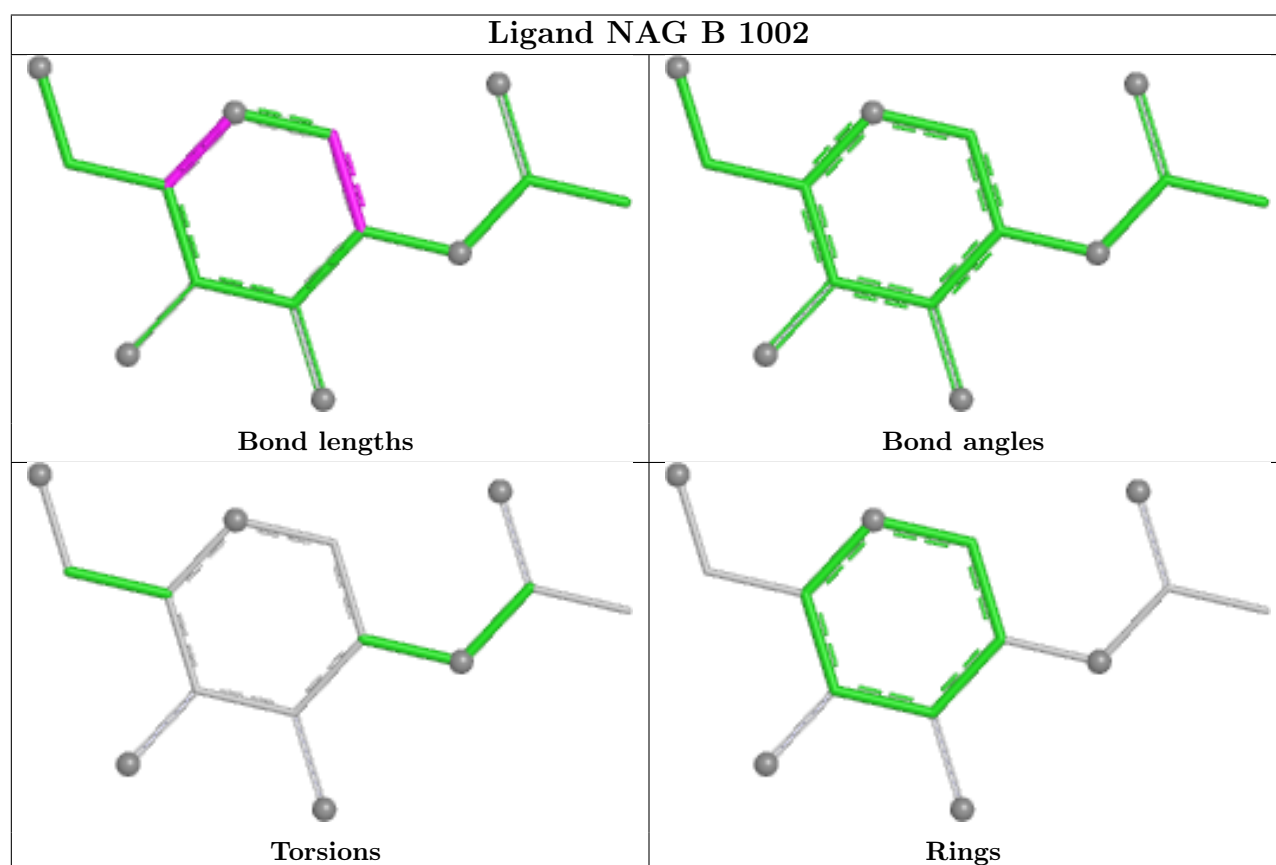
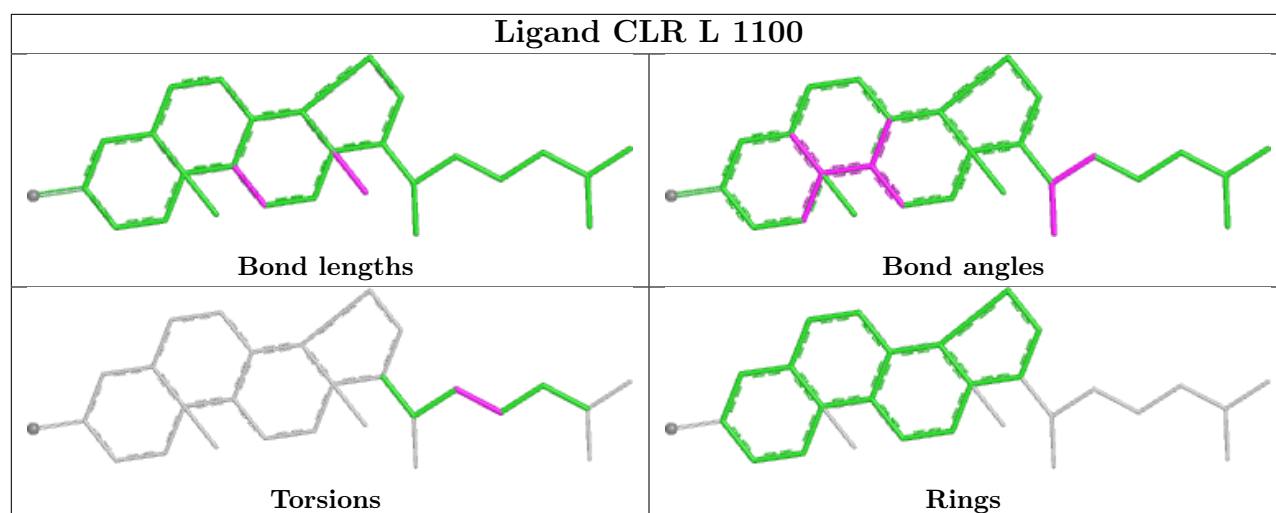
2 monomers are involved in 4 short contacts:

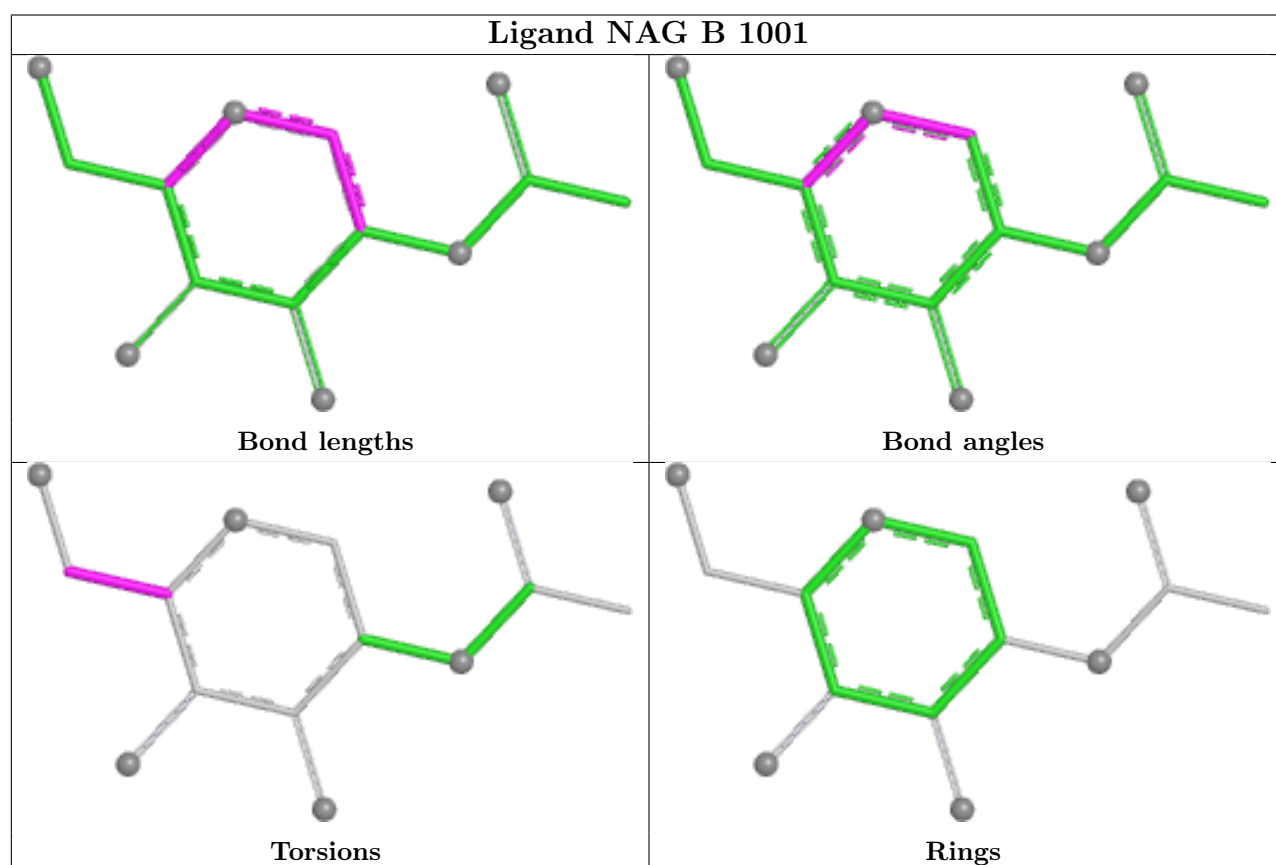
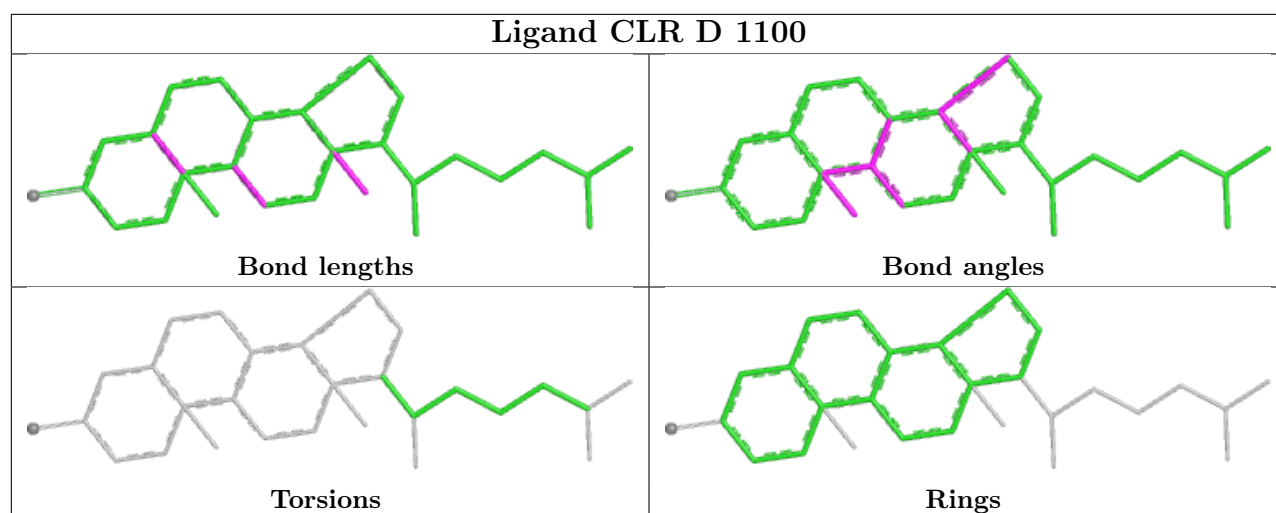
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1100	CLR	1	0
8	D	1100	CLR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

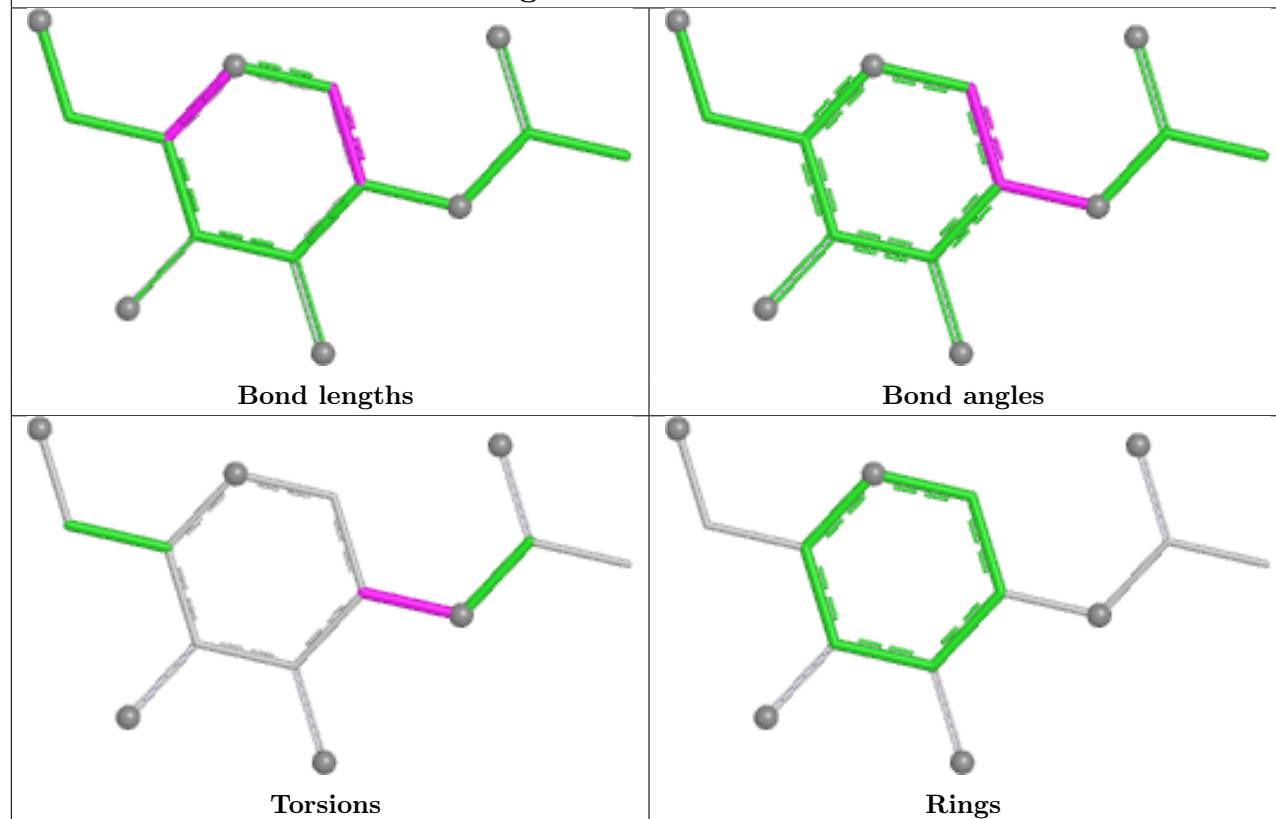




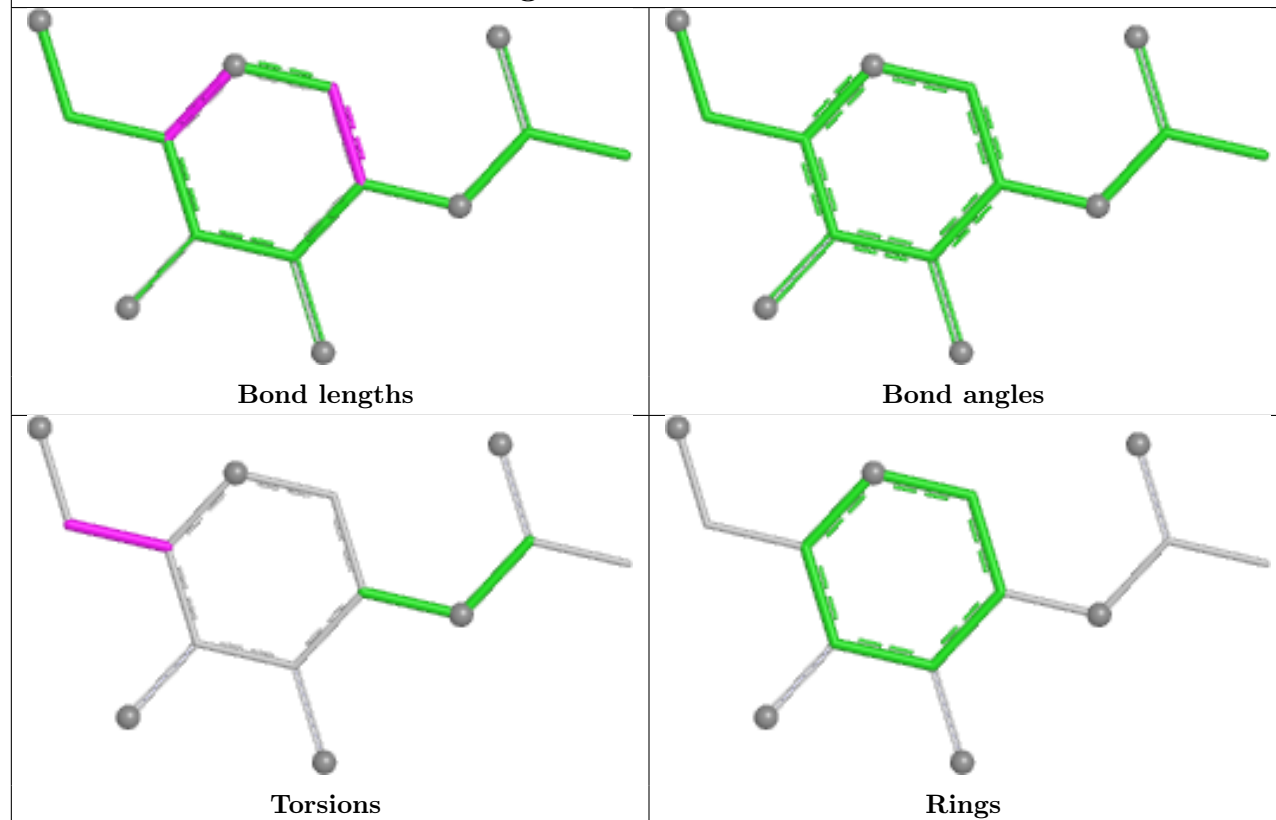


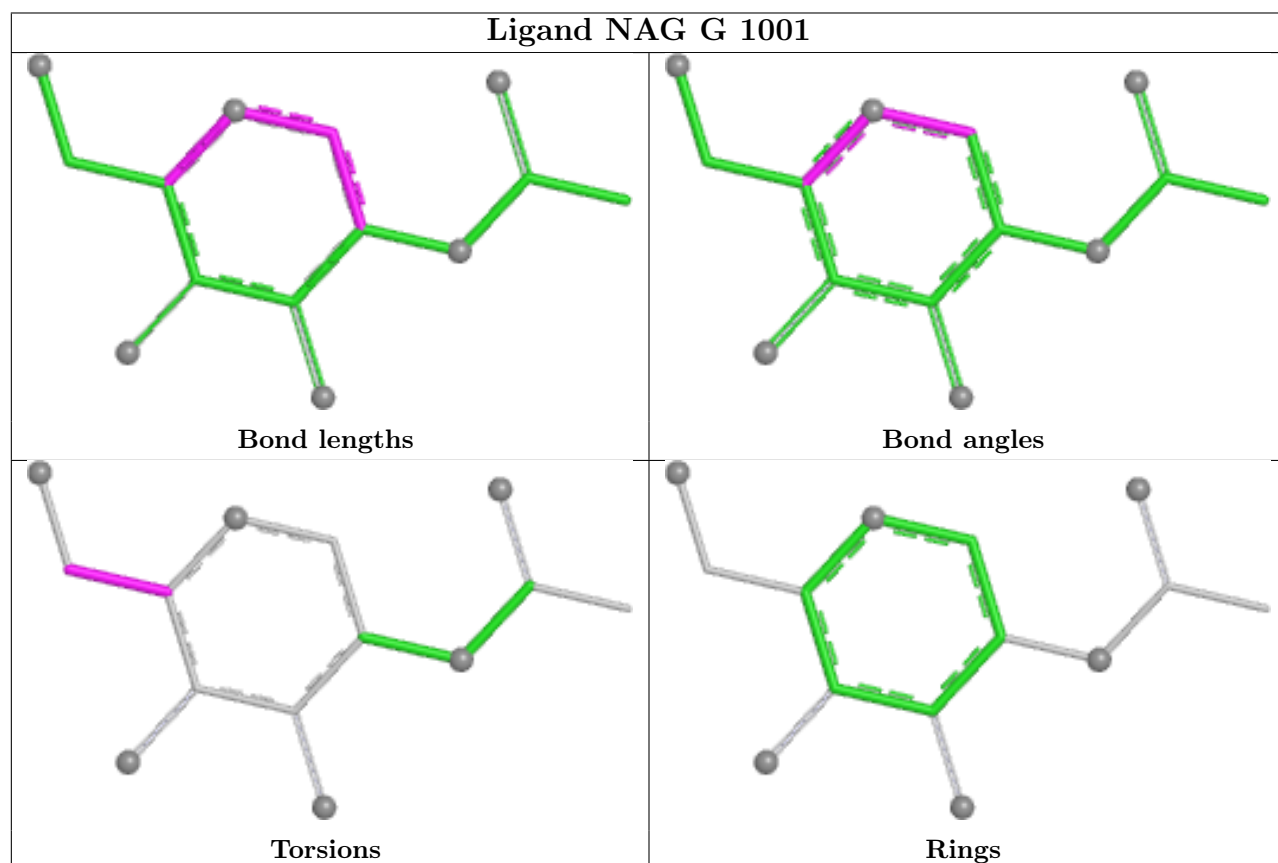
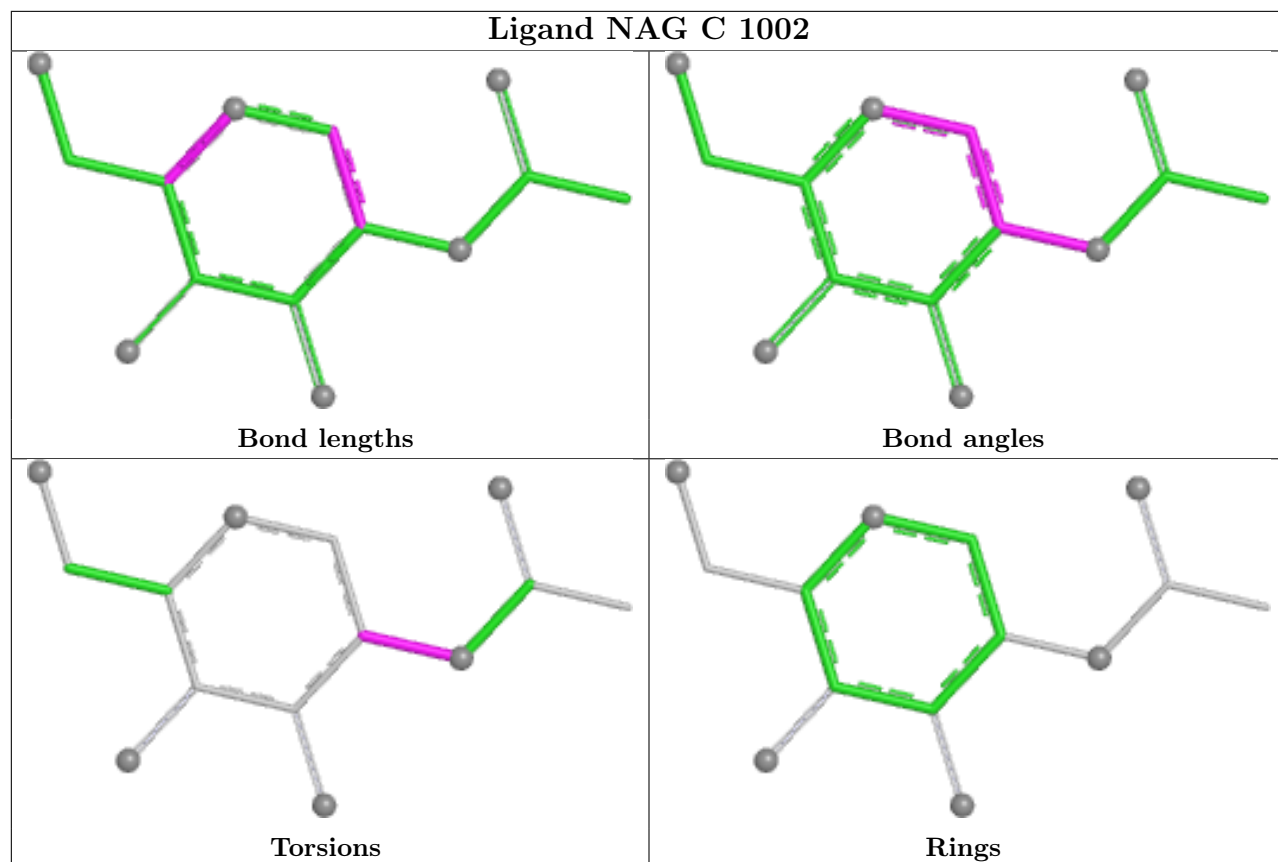


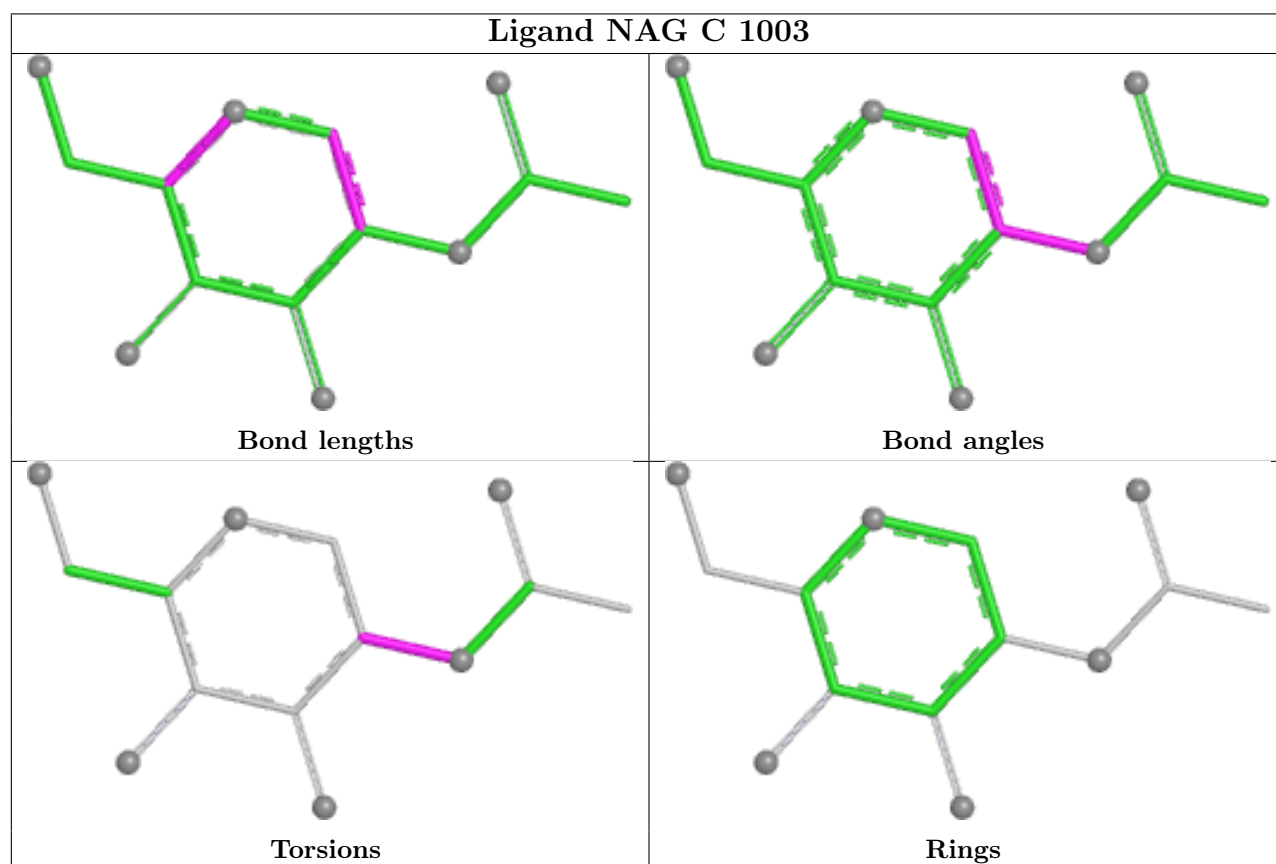
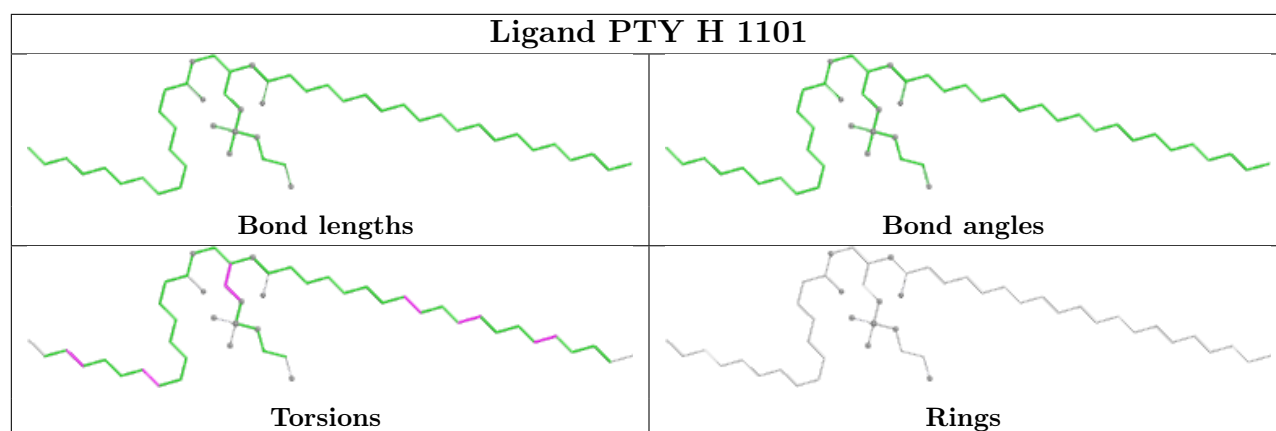
Ligand NAG B 1003

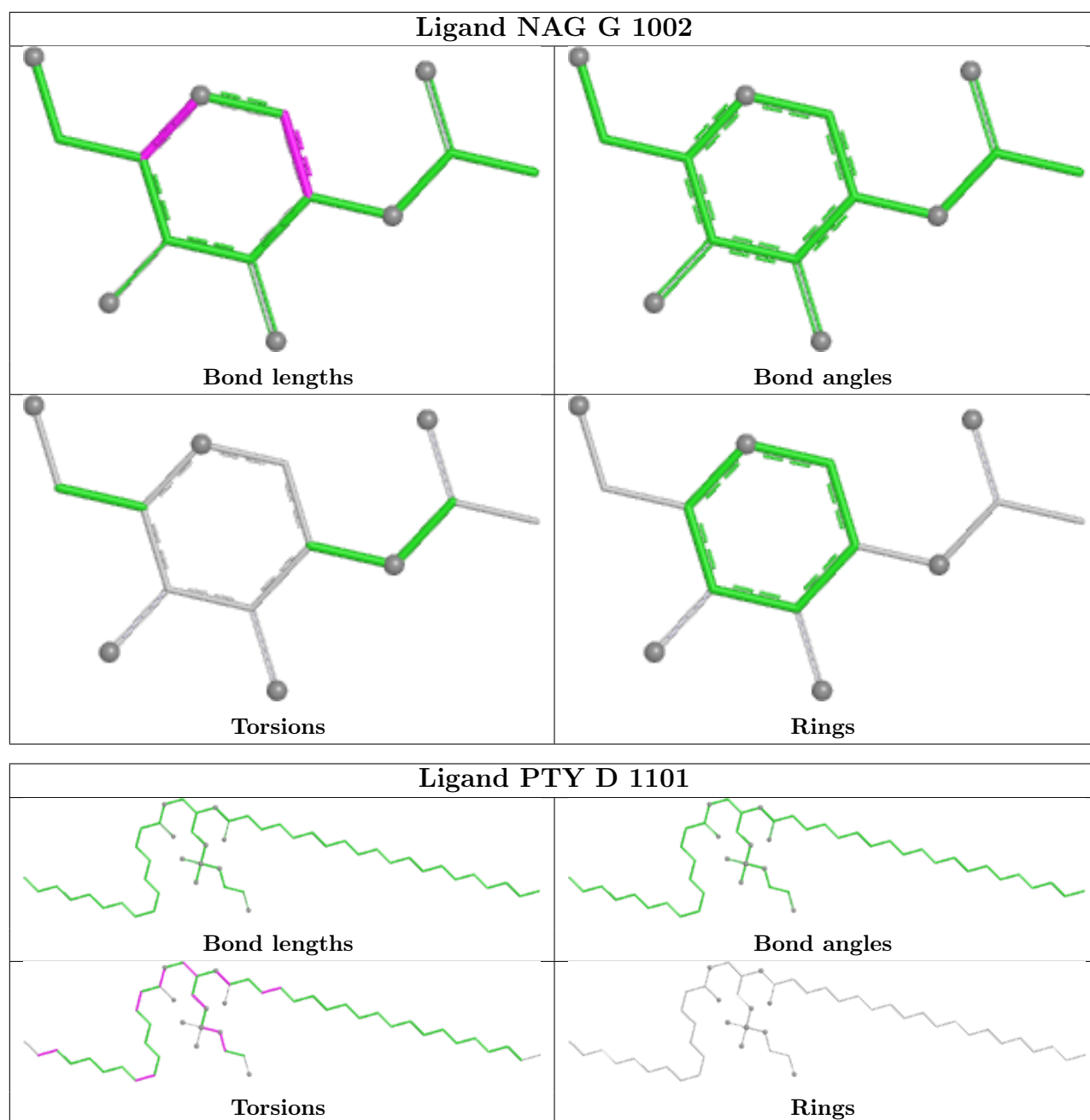


Ligand NAG C 1001









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.

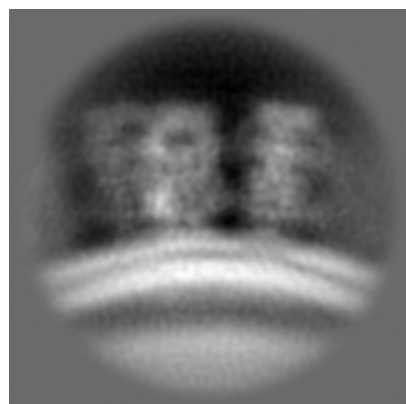
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17317. These allow visual inspection of the internal detail of the map and identification of artifacts.

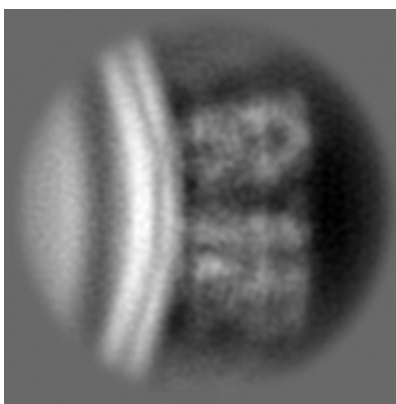
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

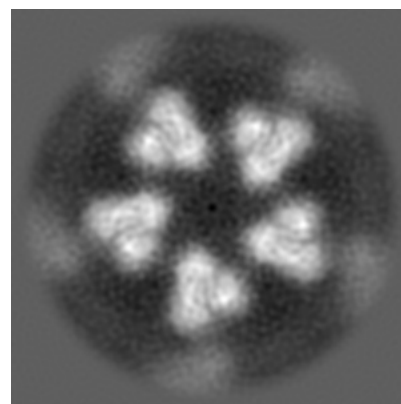
6.1.1 Primary map



X

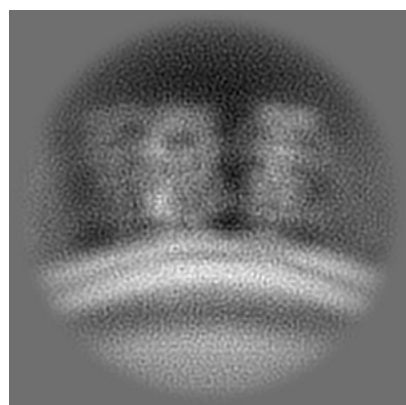


Y

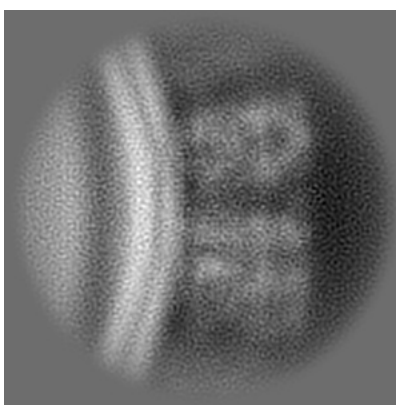


Z

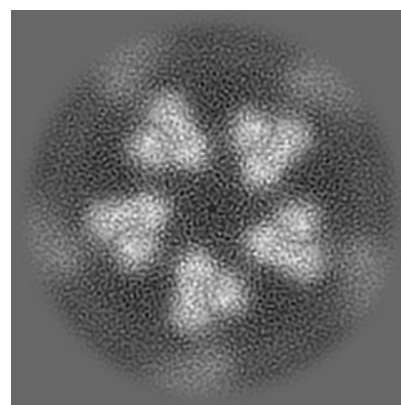
6.1.2 Raw map



X



Y

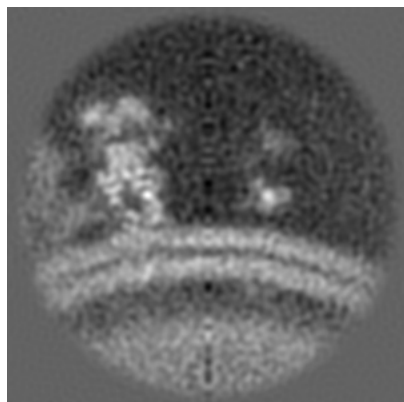


Z

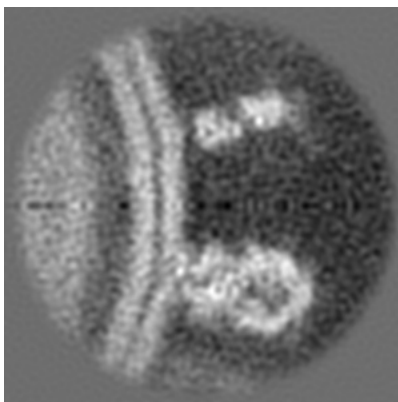
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

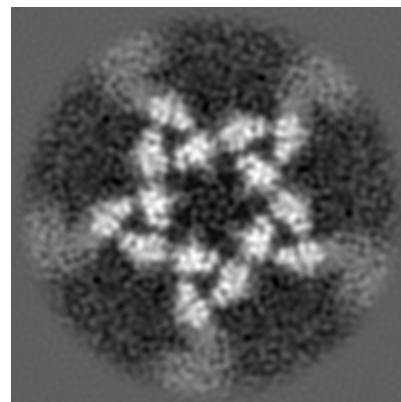
6.2.1 Primary map



X Index: 80

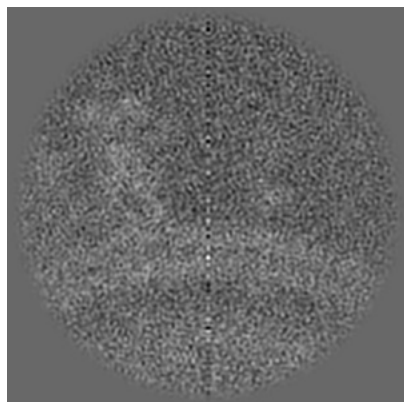


Y Index: 80

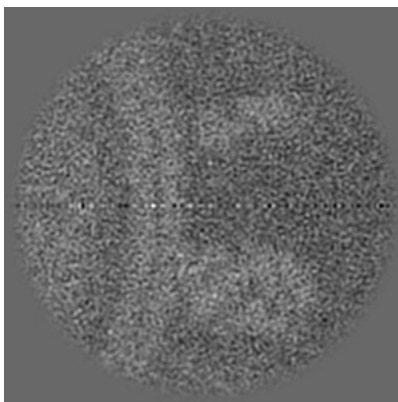


Z Index: 80

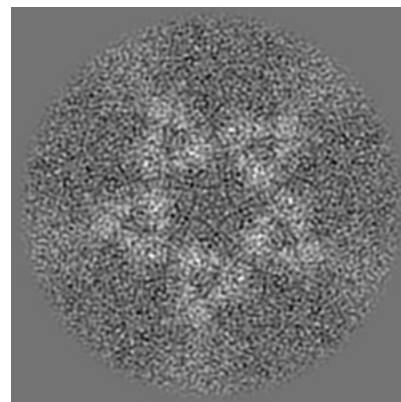
6.2.2 Raw map



X Index: 80



Y Index: 80

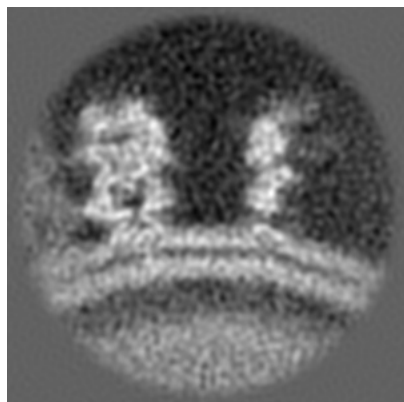


Z Index: 80

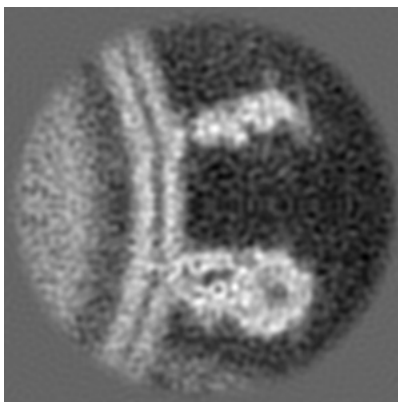
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

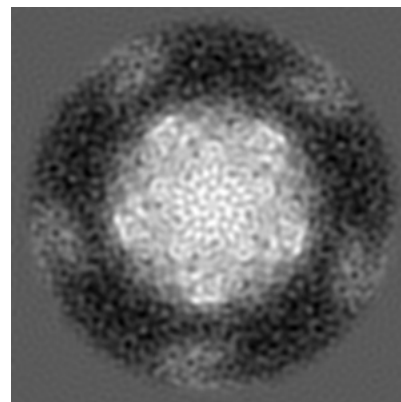
6.3.1 Primary map



X Index: 74

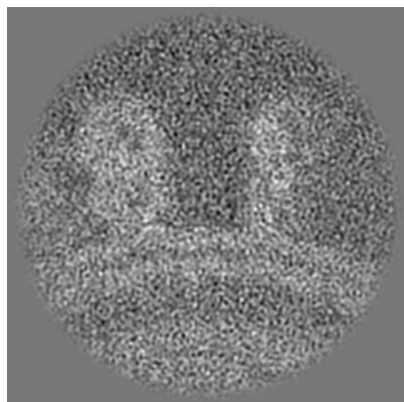


Y Index: 78

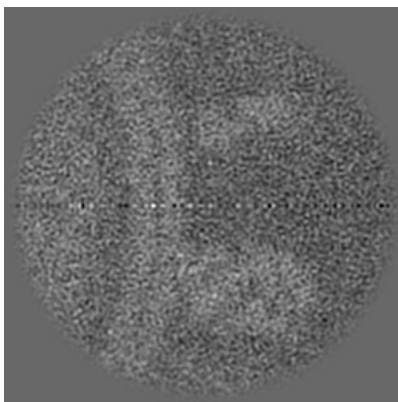


Z Index: 66

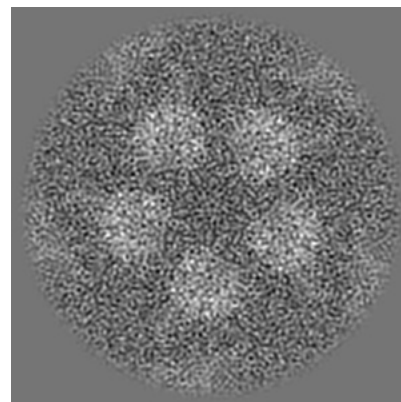
6.3.2 Raw map



X Index: 72



Y Index: 80

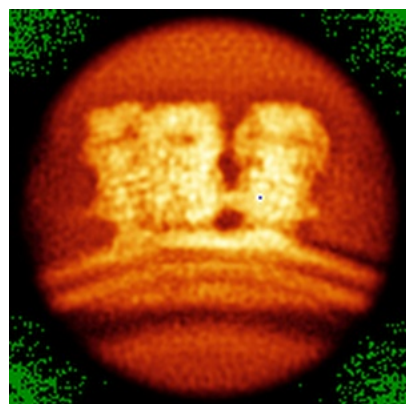


Z Index: 91

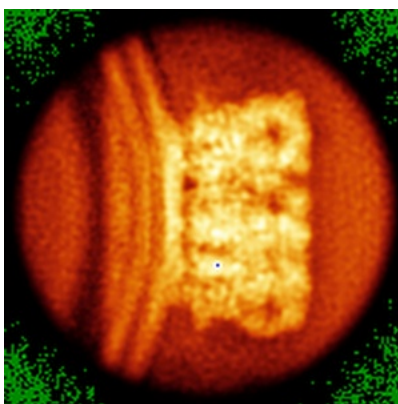
The images above show the largest variance slices of the map in three orthogonal directions.

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

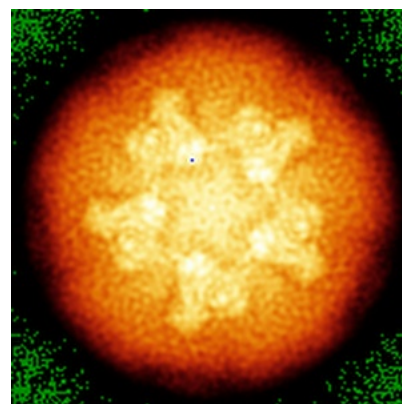
6.4.1 Primary map



X

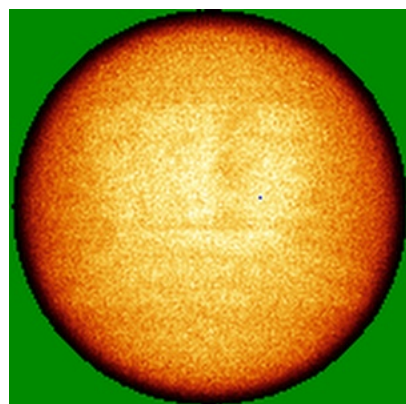


Y

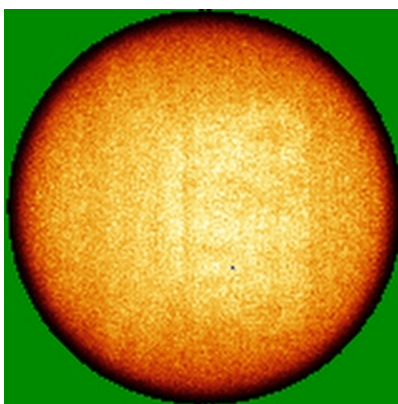


Z

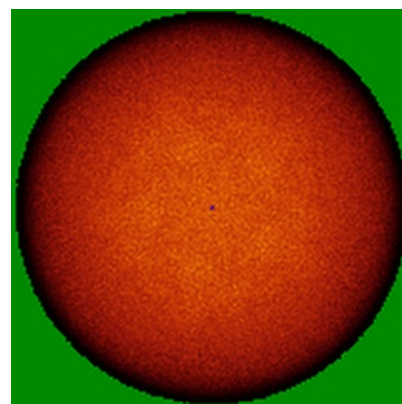
6.4.2 Raw map



X



Y

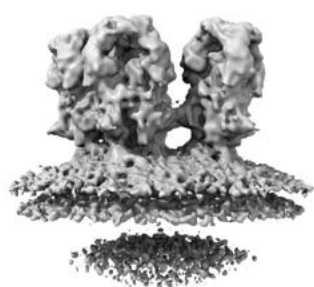


Z

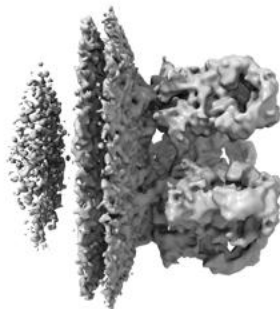
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

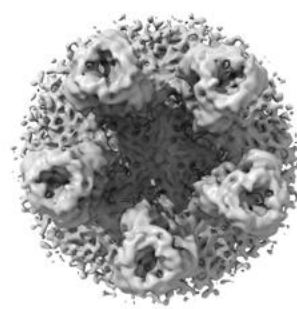
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.064. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

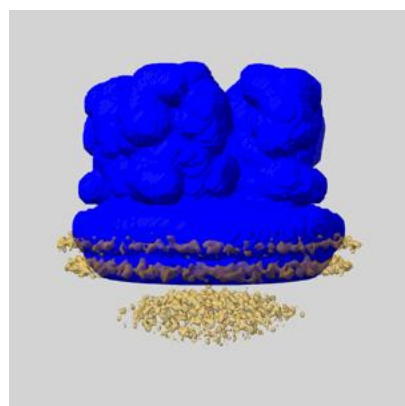
6.6 Mask visualisation [i](#)

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

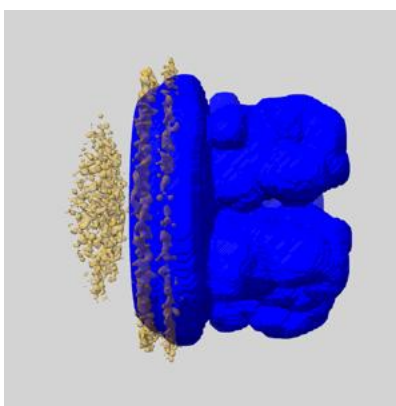
A mask typically either:

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

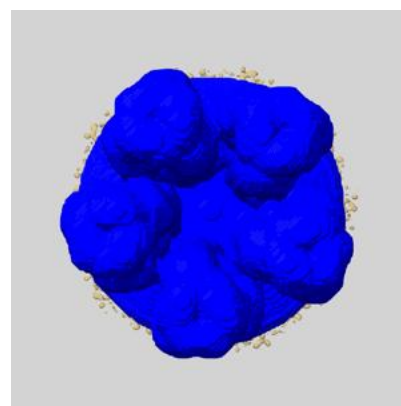
6.6.1 emd_17317_msk_1.map [i](#)



X



Y

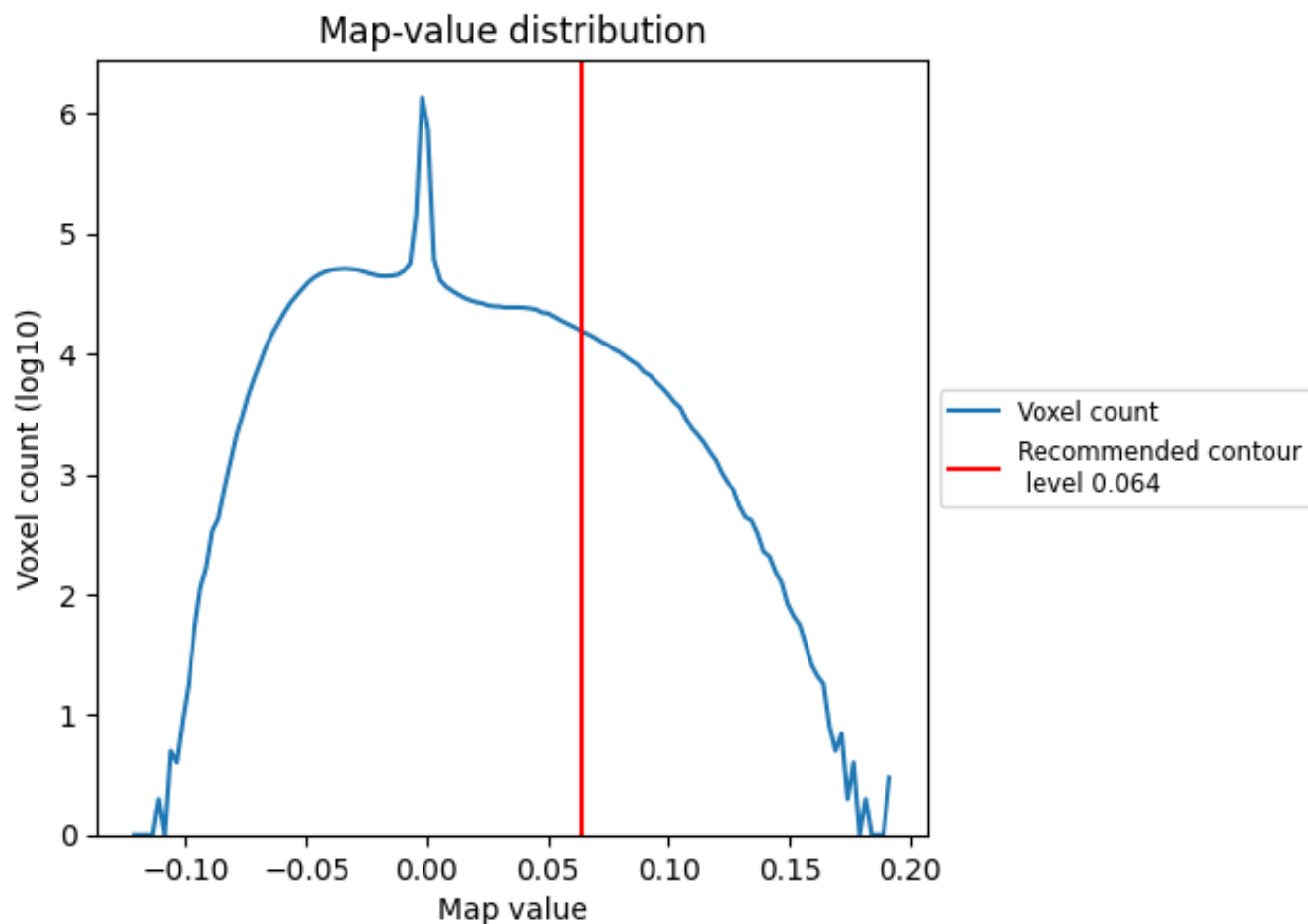


Z

7 Map analysis [i](#)

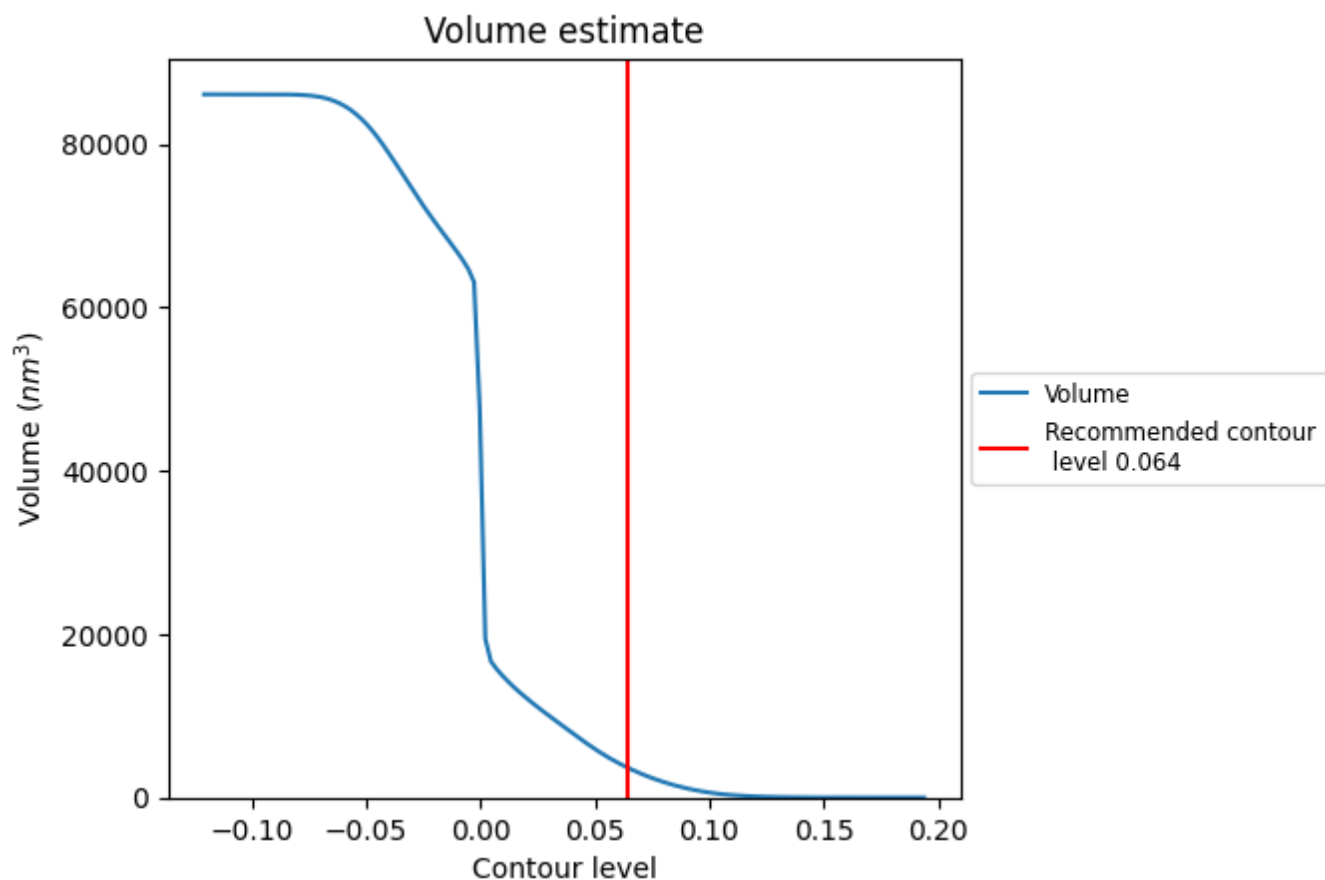
This section contains the results of statistical analysis of the map.

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.

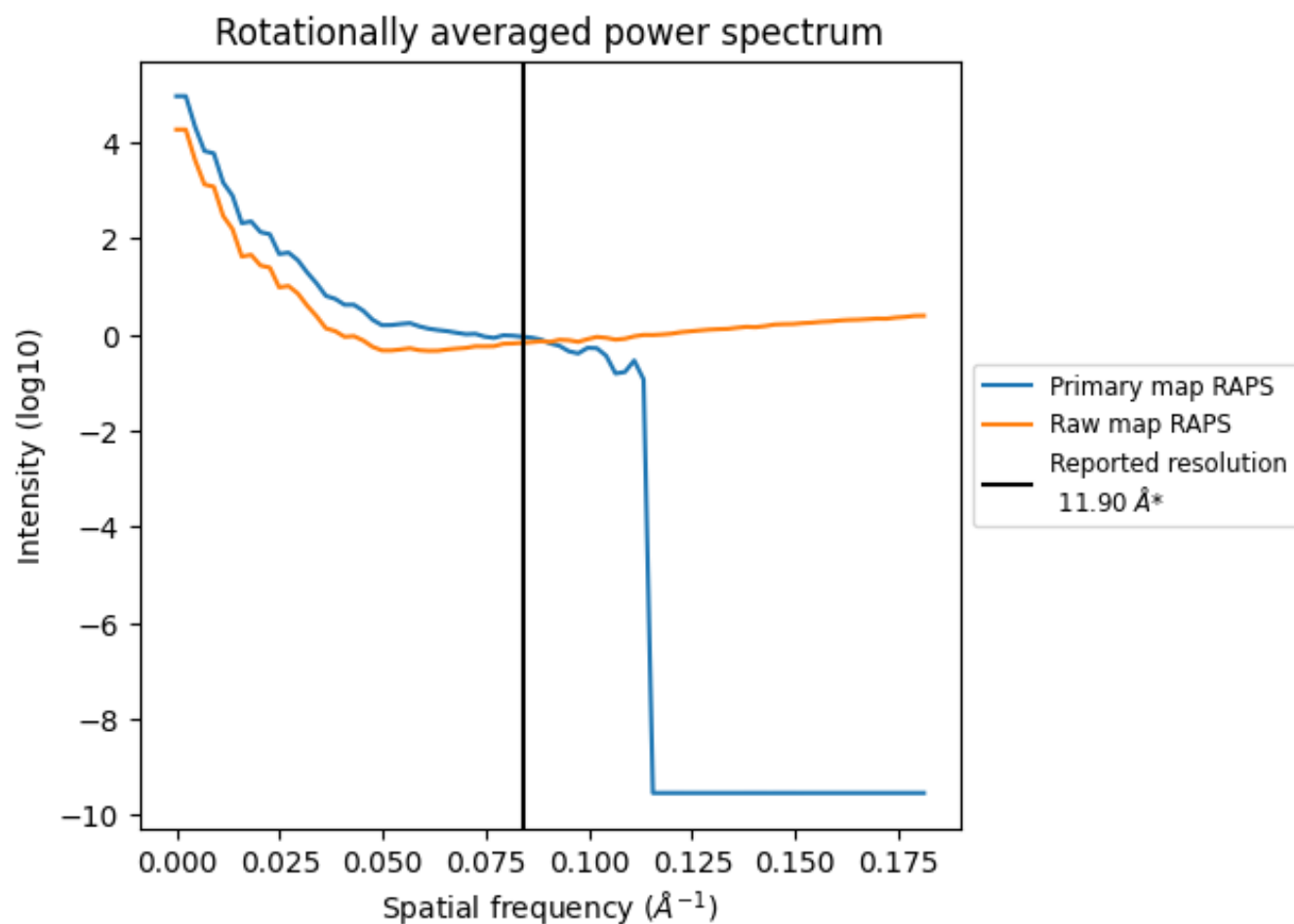
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3695 nm³; this corresponds to an approximate mass of 3337 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](#)

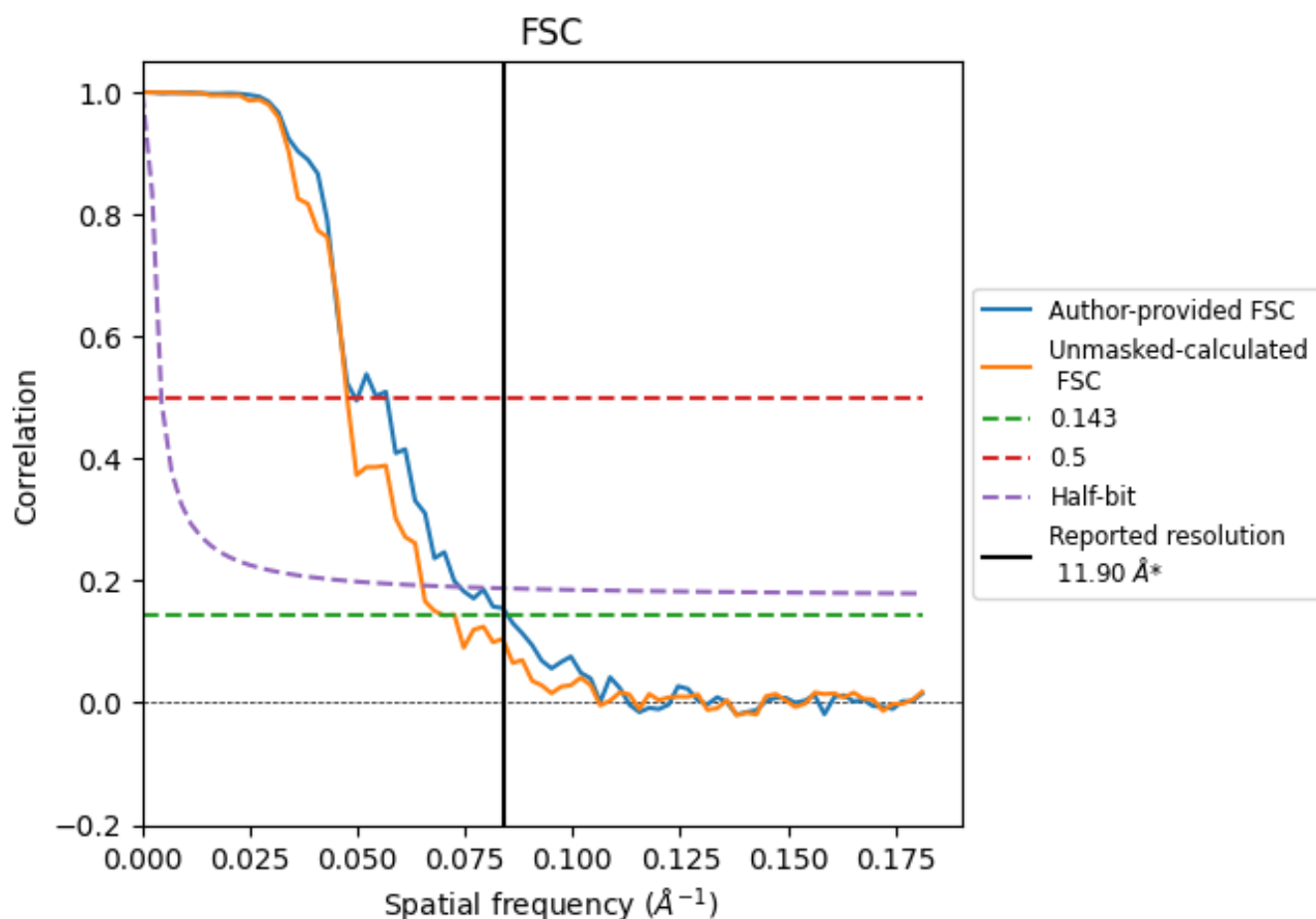


*Reported resolution corresponds to spatial frequency of 0.084 $\text{\AA}^{-1}$

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 0.084 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.90	-	-
Author-provided FSC curve	11.78	20.24	13.53
Unmasked-calculated*	14.25	21.01	15.36

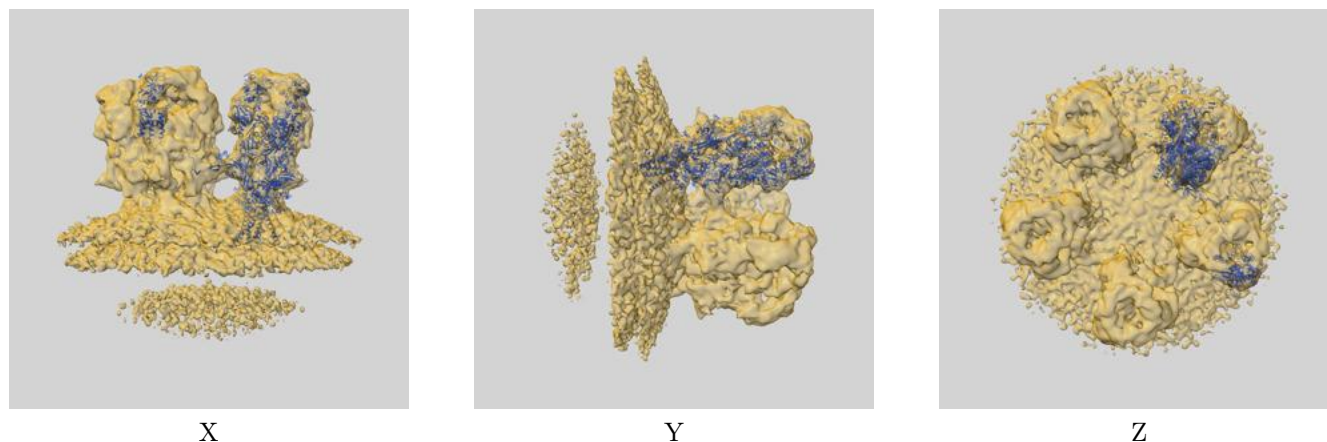
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.25 differs from the reported value 11.9 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17317 and PDB model 8OZP. Per-residue inclusion information can be found in section 3 on page 11.

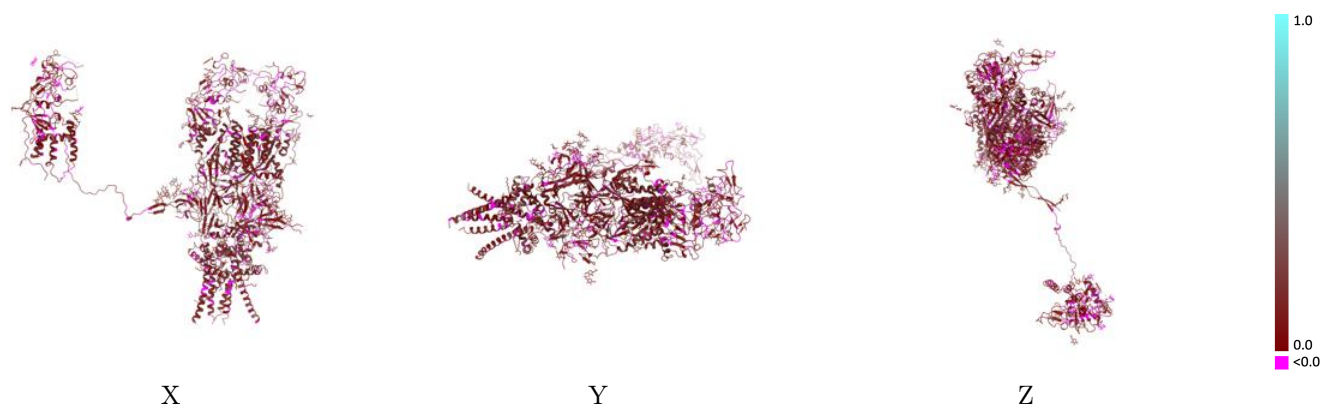
9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ



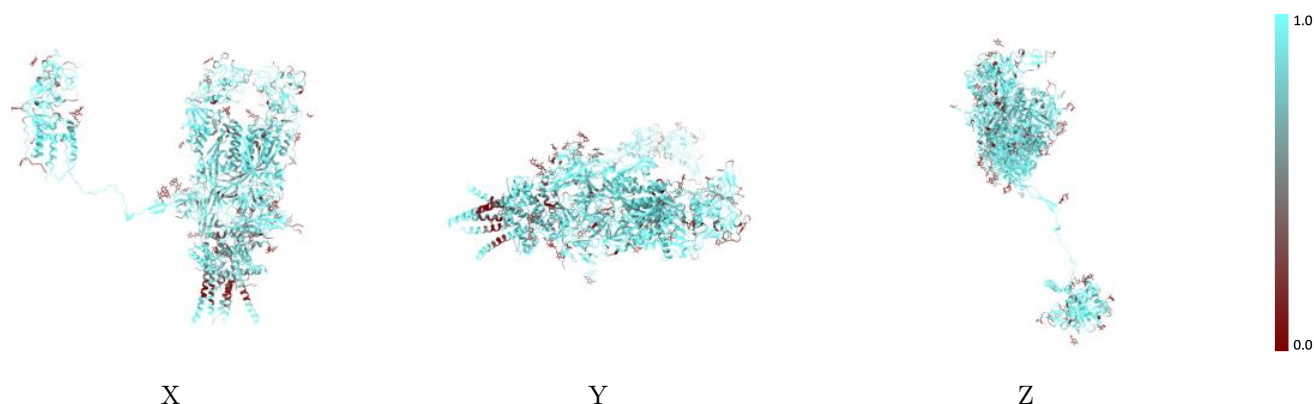
The images above show the 3D surface view of the map at the recommended contour level 0.064 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



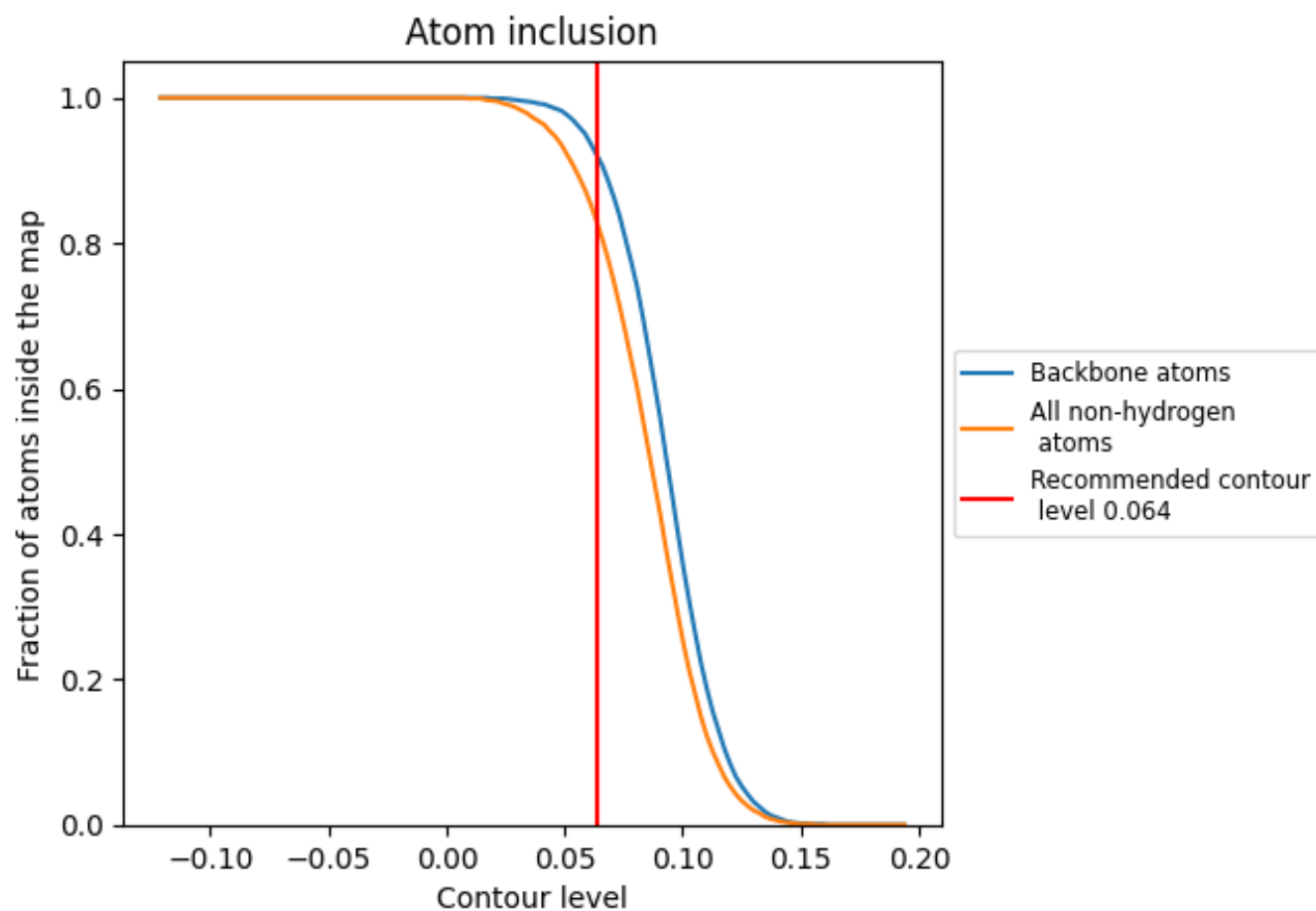
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.064).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.1150
A	 0.7270	 0.1210
B	 0.8600	 0.1000
C	 0.8680	 0.1160
D	 0.8400	 0.1270
E	 0.7800	 0.1330
F	 0.6590	 0.1300
G	 0.8530	 0.1030
H	 0.8470	 0.1210
I	 0.7320	 0.1070
L	 0.8660	 0.1250
M	 0.2140	 0.0540
N	 0.4290	 0.0990
O	 0.7860	 0.1960
P	 0.2600	 0.2070
Q	 0.4200	 0.2220
R	 0.2400	 0.1400
S	 0.2050	 0.1320
T	 0.1790	 0.1570
U	 0.1030	 0.0430
V	 0.6670	 0.0710
W	 0.6530	 0.1100
X	 0.6270	 0.0640
Y	 0.3570	 0.1410
Z	 0.3570	 0.2380
a	 0.2500	 0.2150
b	 0.7140	 0.1340
c	 0.7500	 0.0890
d	 0.6430	 0.0720
e	 0.5750	 0.0600
f	 0.5110	 0.0270
g	 0.6700	 0.0920
h	 0.3890	 0.1060
i	 0.2220	 0.1020
j	 0.3330	 0.1170

