



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 05:04 AM UTC

PDB ID : 8OZJ / pdb_00008ozj
EMDB ID : EMD-17311
Title : In situ cryoEM structure of Prototype Foamy Virus Env dimer of trimers
Authors : Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on : 2023-05-09
Resolution : 3.70 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

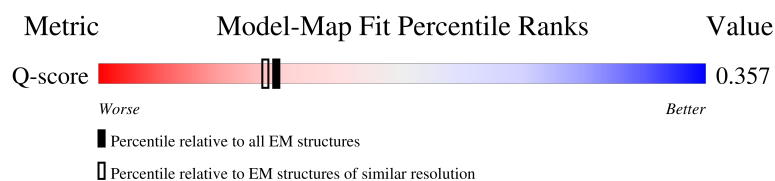
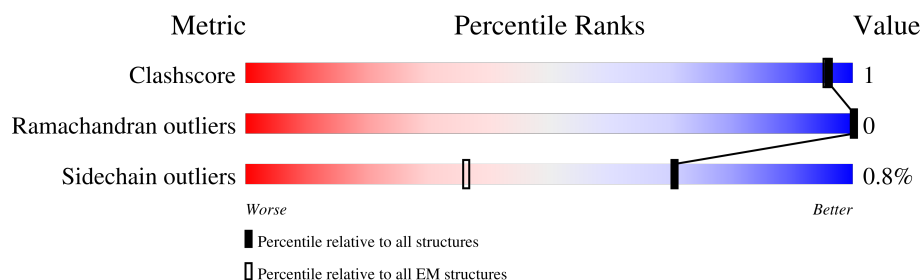
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

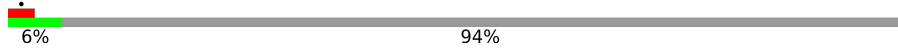
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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	 6% 94%
1	C	988	 11% 40% 58%
1	D	988	 40% 59%
1	E	988	 6% 94%

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Mol	Chain	Length	Quality of chain
1	F	988	
1	G	988	
1	H	988	
1	I	988	
1	J	988	
1	K	988	
1	L	988	
2	M	2	
2	N	2	
2	O	2	
2	Y	2	
2	Z	2	
2	a	2	
2	b	2	
2	c	2	
2	d	2	
3	e	8	
3	f	8	
3	g	8	
4	h	6	
4	i	6	
4	j	6	
5	S	3	
5	T	3	
5	U	3	

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Mol	Chain	Length	Quality of chain
6	V	6	50%33%67%
6	W	6	67%33%67%
6	X	6	67%50%50%
7	P	4	75%25%75%
7	Q	4	50%25%75%
7	R	4	75%25%75%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22794 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	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	J	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		
1	K	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.



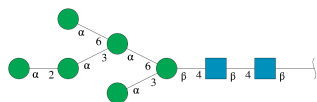
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

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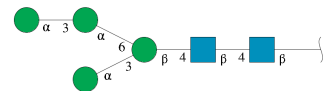
Mol	Chain	Residues	Atoms				AltConf	Trace
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16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

- Molecule 3 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.



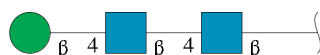
Mol	Chain	Residues	Atoms				AltConf	Trace
3	e	8	Total	C	N	O	0	0
			94	52	2	40		
3	f	8	Total	C	N	O	0	0
			94	52	2	40		
3	g	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 4 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.



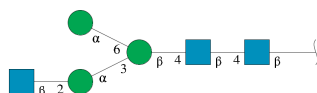
Mol	Chain	Residues	Atoms				AltConf	Trace
4	h	6	Total	C	N	O	0	0
			72	40	2	30		
4	i	6	Total	C	N	O	0	0
			72	40	2	30		
4	j	6	Total	C	N	O	0	0
			72	40	2	30		

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



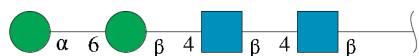
Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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.



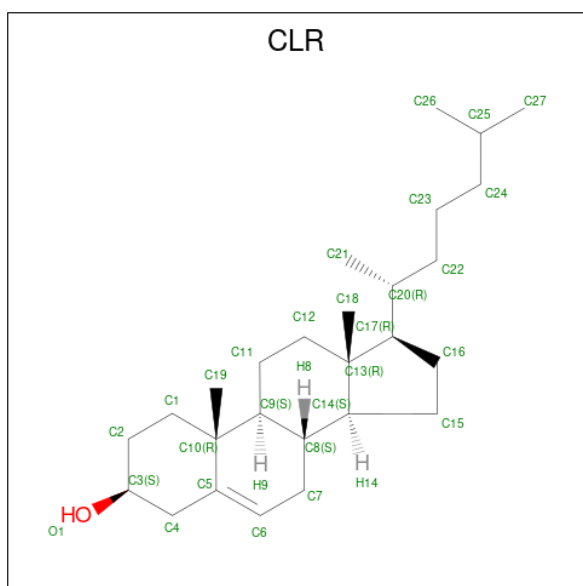
Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	6	Total	C	N	O	0	0
			75	42	3	30		
6	W	6	Total	C	N	O	0	0
			75	42	3	30		
6	X	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 7 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.



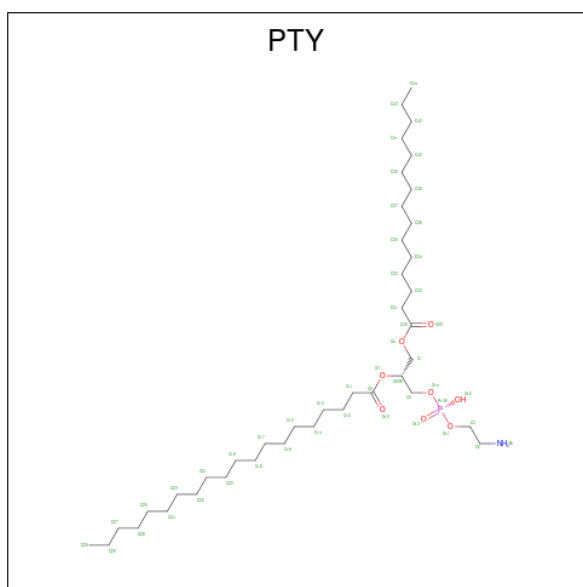
Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	4	Total	C	N	O	0	0
			50	28	2	20		
7	Q	4	Total	C	N	O	0	0
			50	28	2	20		
7	R	4	Total	C	N	O	0	0
			50	28	2	20		

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



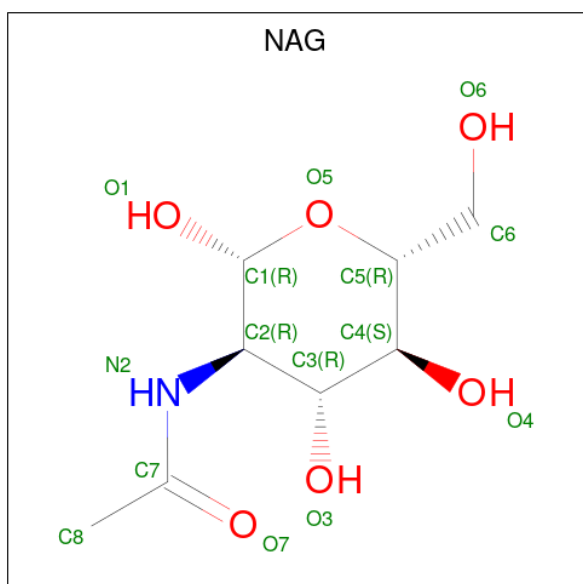
Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	O		0
			28	27	1		
8	H	1	Total	C	O		0
			28	27	1		
8	L	1	Total	C	O		0
			28	27	1		

- Molecule 9 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

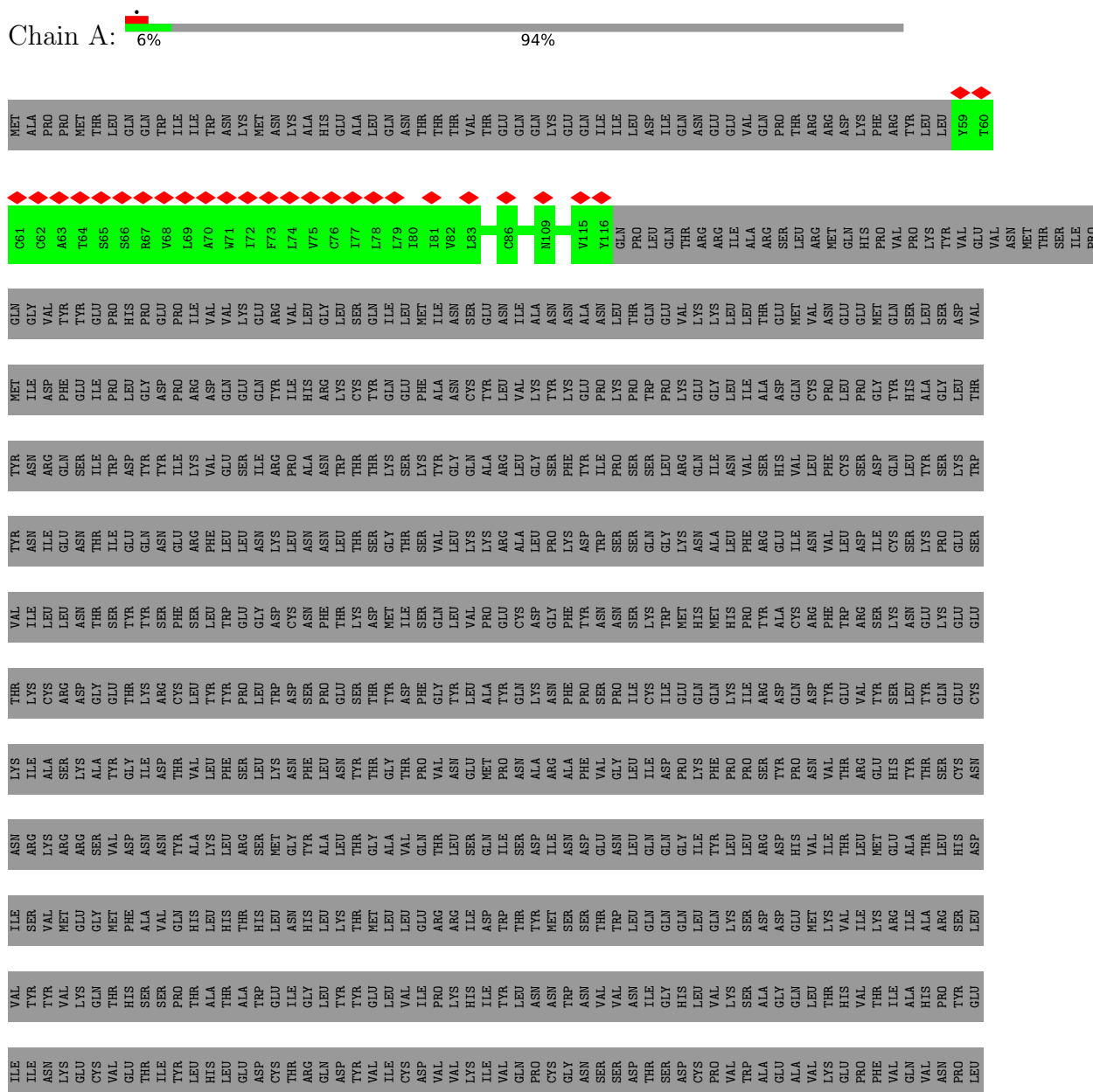


Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	K	1	Total	C	N	O	0
			14	8	1	5	
10	K	1	Total	C	N	O	0
			14	8	1	5	
10	K	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

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

• Molecule 1: Envelope glycoprotein



[illegible]

- Molecule 1: Envelope glycoprotein



L862	ALA	PHE	PRO	PHE	PHE	PHE	PHE	TYR	ASP	TYR	LYS	ASN	ASN	ARG	THR	LYS	ASN	THR	CYS	MET
K891	VAL	SER	ASN	THR	ASN	TRP	ASN	TYR	TRP	ASN	PRO	GLU	ASN	ARG	ARG	ILE	ASN	PRO	ALA	ALA
A899	GLY	PRO	PRO	ILE	SER	SER	SER	ASN	SER	SER	SER	PRO	THR	ALA	ILE	THR	LEU	THR	THR	PRO
T911	ILE	CYS	ILE	ILE	LYS	GLN	TRP	TRP	GLY	LEU	GLY	LEU	GLU	TRP	PRO	PRO	ARG	ARG	THR	LEU
P912	ASP	PRO	GLU	GLU	MET	LYS	MET	ASN	LYS	ASN	GLN	GLU	VAL	VAL	LYS	VAL	VAL	VAL	VAL	GLN
T922	PHE	GLN	GLN	MET	MET	ALA	ILE	ILE	GLY	GLN	GLY	LYS	LYS	ASN	THR	LEU	GLN	TRP	TRP	LEU
A926	PRO	ILE	PRO	HIS	HIS	PHE	ASN	ASN	LEU	VAL	ILE	LEU	LEU	GLN	HIS	PRO	THR	ILE	ILE	ILE
P927	PRO	ARG	ARG	TYR	TYR	ARG	ARG	SER	ARG	SER	ALA	ALA	THR	THR	THR	VAL	PRO	PHE	THR	TRP
A928	TYR	ASP	GLN	CYS	ALA	GLU	GLU	HIS	GLN	HIS	GLN	GLN	GLU	VAL	VAL	GLN	ASP	LEU	ASN	ASN
A929	ASN	ASP	ASN	ARG	ARG	ASN	PHE	TYR	VAL	PHE	VAL	CYS	ASN	VAL	LYS	VAL	THR	CYS	MET	VAL
A932	VAL	THR	GLU	TRP	TRP	LEU	TRP	GLU	LEU	CYS	GLY	GLU	GLU	GLU	VAL	GLU	VAL	LEU	LEU	ALA
L933	ARG	ARG	VAL	ARG	SER	ASP	ARG	SER	ASP	SER	PRO	PRO	PRO	PRO	PRO	GLU	GLU	LEU	LEU	ALA
Q934	GLU	GLU	TYR	TYR	TYR	ILE	TYR	ASP	ILE	ASP	GLY	GLY	MET	MET	VAL	VAL	GLN	ILE	ILE	HIS
Q935	HIS	THR	LEU	ASN	ASN	CYS	LYS	GLN	SER	GLN	HIS	THR	SER	SER	ASN	THR	LEU	VAL	VAL	ALA
F939	THR	SER	GLN	GLU	LYS	PRO	GLU	TYR	GLY	SER	ALA	GLY	SER	SER	ASN	THR	LEU	VAL	VAL	GLN
L940	CYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	THR	THR	THR	THR	THR	THR	VAL	PRO	CYS	THR	THR	ASN
S941	ASN	ASN	LYS	THR	THR	VAL	VAL	LYS	ASN	THR	ASN	ASN	ILE	ILE	GLY	VAL	THR	THR	THR	THR
G942	ARG	LYS	ILE	CYS	CYS	LEU	ILE	ILE	ASN	ASP	ASP	ASP	PHE	PHE	THR	THR	THR	THR	THR	VAL
T943	ARG	SER	ALA	ARG	ARG	LEU	LEU	ILE	GLU	GLU	GLN	PHE	PHE	THR	THR	THR	THR	THR	THR	VAL
A944	ARG	LYS	LYS	ASP	ASP	THR	ASN	ASN	SER	ASN	SER	GLU	GLU	THR	THR	THR	THR	THR	THR	GLN
Q945	ARG	ALA	ALA	GLY	GLY	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
G946	VAL	SER	TYR	GLU	GLU	SER	ILE	THR	GLY	GLU	GLY	LEU	LEU	GLY	HIS	PRO	CYS	THR	THR	GLN
L947	ASP	ASP	GLY	THR	THR	THR	LYS	THR	TYR	GLN	GLN	GLY	GLY	THR	PRO	GLU	TRP	TRP	TRP	LYS
F948	ASN	ASN	ILE	ARG	ARG	TYR	ASN	ASN	SER	ASN	THR	THR	THR	THR	PRO	GLU	ASN	ASN	LYS	ILE
A951	ASN	ASP	ASP	THR	CYS	PHE	SER	GLU	ILE	PRO	PRO	PRO	PRO	GLU	GLU	ASN	ASN	LYS	LYS	ILE
F952	THR	VAL	VAL	THR	LEU	LEU	THR	TYR	SER	ARG	VAL	LYS	ASP	VAL	VAL	VAL	GLY	ASP	ASP	ILE
S953	LEU	LEU	LEU	PHE	TYR	LEU	THR	TYR	THR	PHE	LEU	GLU	GLN	GLN	VAL	VAL	GLN	GLN	GLN	THR
L954	SER	SER	SER	SER	PRO	GLY	LEU	LEU	GLY	LEU	SER	SER	GLU	LYS	VAL	VAL	VAL	VAL	VAL	THR
L955	LEU	LEU	LEU	LEU	LEU	GLY	GLY	ASN	ILE	ASN	ILE	GLN	GLN	GLN	GLY	GLY	LEU	LEU	LEU	GLN
L958	LYS	LYS	TRP	TRP	TRP	ASP	ASP	ARG	ARG	ARG	ARG	THR	THR	THR	THR	THR	THR	THR	THR	ASN
I961	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
G964	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
V965	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
G966	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
V967	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
L968	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
I969	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
A976	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
I977	LYS	LYS	TRP	TRP	TRP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN

ASN
GLN

- Molecule 1: Envelope glycoprotein





[illegible]

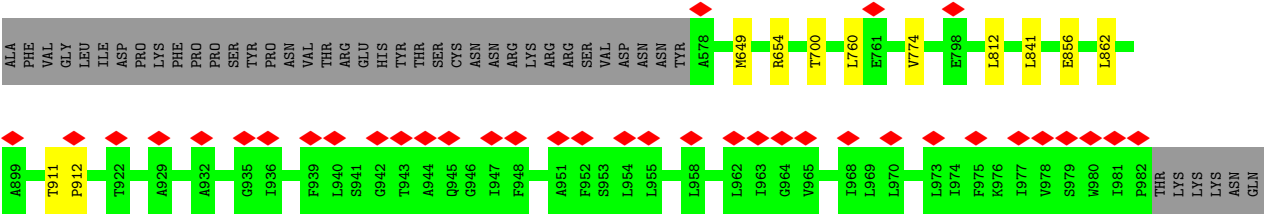
- Molecule 1: Envelope glycoprotein

[illegible]

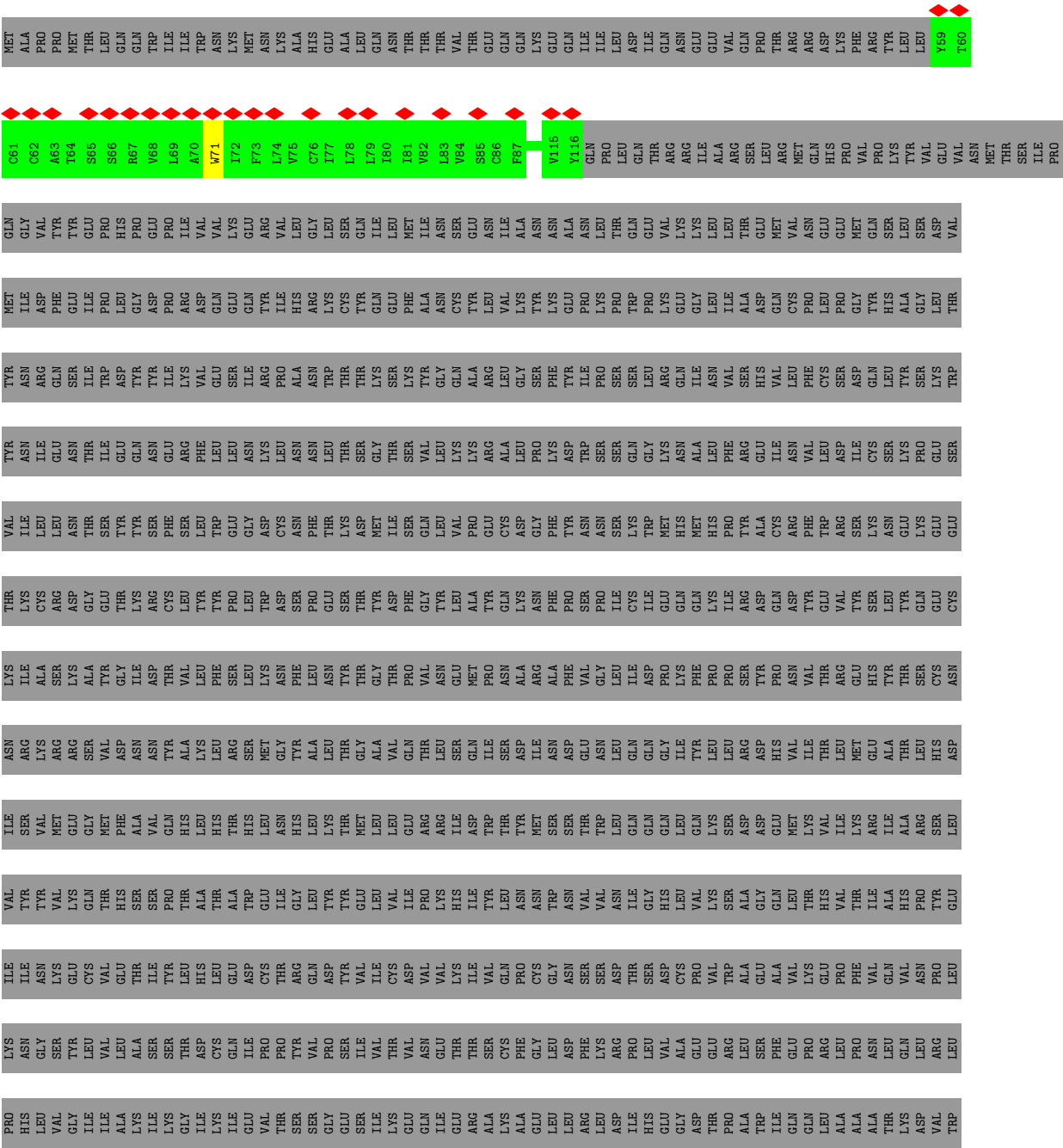
- Molecule 1: Envelope glycoprotein

40%





• Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

[illegible]

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



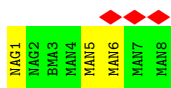
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



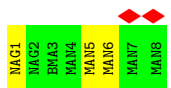
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



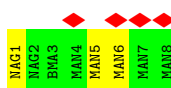
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



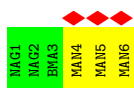
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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

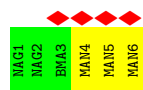


- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

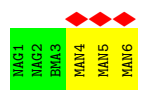


- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

ido-2-deoxy-beta-D-glucopyranose



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



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



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

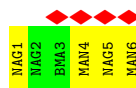


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

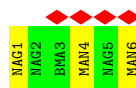




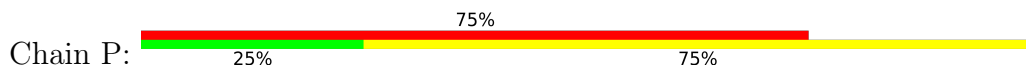
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 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



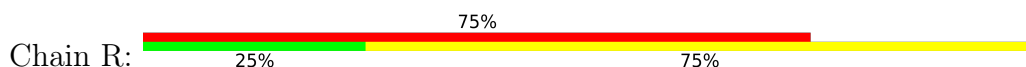
- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	324976	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.064	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0149	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.11	0/476	1.62	0/653
1	C	1.06	0/3469	1.38	3/4705 (0.1%)
1	D	1.07	0/3260	1.40	0/4441
1	E	1.10	0/476	1.62	0/653
1	F	1.03	0/97	1.15	0/130
1	G	1.05	0/3416	1.38	1/4634 (0.0%)
1	H	1.08	0/3260	1.40	0/4441
1	I	1.11	0/476	1.62	0/653
1	J	0.98	0/97	1.11	0/130
1	K	1.05	0/3416	1.37	1/4634 (0.0%)
1	L	1.08	0/3260	1.40	0/4441
All	All	1.07	0/21703	1.40	5/29515 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	PRO	N-CA-C	5.77	120.28	111.34
1	K	135	PRO	N-CA-C	5.70	120.17	111.34
1	C	135	PRO	N-CA-C	5.68	120.15	111.34
1	C	158	ILE	CA-C-N	5.26	129.55	122.93
1	C	158	ILE	C-N-CA	5.26	129.55	122.93

There are no chirality outliers.

There are no planarity outliers.

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	0	0
1	C	3380	0	3293	8	0
1	D	3190	0	3242	6	0
1	E	466	0	488	1	0
1	F	94	0	97	2	0
1	G	3328	0	3241	10	0
1	H	3190	0	3242	7	0
1	I	466	0	488	0	0
1	J	94	0	97	3	0
1	K	3328	0	3241	12	0
1	L	3190	0	3242	7	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	e	94	0	79	0	0
3	f	94	0	79	0	0
3	g	94	0	79	0	0
4	h	72	0	61	0	0
4	i	72	0	61	0	0
4	j	72	0	61	0	0
5	S	39	0	34	0	0
5	T	39	0	34	0	0
5	U	39	0	34	0	0
6	V	75	0	64	0	0
6	W	75	0	64	0	0
6	X	75	0	64	0	0
7	P	50	0	43	0	0
7	Q	50	0	43	0	0
7	R	50	0	43	0	0
8	D	28	0	46	0	0
8	H	28	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	28	0	46	0	0
9	D	50	0	79	0	0
9	H	50	0	79	0	0
9	L	50	0	79	0	0
10	C	42	0	39	0	0
10	G	42	0	39	0	0
10	K	42	0	39	0	0
All	All	22794	0	22719	41	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 (41) 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:J:137:TYR:HE1	1:K:133:PRO:HG3	1.32	0.94
1:J:137:TYR:CE1	1:K:133:PRO:HG3	2.20	0.75
1:F:137:TYR:HE1	1:G:133:PRO:HG3	1.52	0.74
1:D:700:THR:HG23	1:C:193:THR:HG23	1.71	0.73
1:L:700:THR:HG23	1:K:193:THR:HG23	1.78	0.65
1:H:700:THR:HG23	1:G:193:THR:HG23	1.80	0.63
1:L:700:THR:HG21	1:K:197:ASN:OD1	2.00	0.62
1:F:137:TYR:CE1	1:G:133:PRO:HG3	2.36	0.61
1:G:136:LYS:HG2	1:G:137:TYR:H	1.71	0.56
1:D:700:THR:HG21	1:C:197:ASN:OD1	2.05	0.56
1:C:136:LYS:HG2	1:C:137:TYR:H	1.71	0.56
1:G:277:ILE:HG21	1:G:298:LEU:HD12	1.89	0.55
1:K:136:LYS:HG2	1:K:137:TYR:H	1.71	0.55
1:C:277:ILE:HG21	1:C:298:LEU:HD12	1.89	0.54
1:K:277:ILE:HG21	1:K:298:LEU:HD12	1.89	0.54
1:H:700:THR:HG21	1:G:197:ASN:OD1	2.09	0.53
1:J:130:MET:HG3	1:K:142:MET:HE1	1.96	0.47
1:D:652:GLU:OE2	1:L:654:ARG:NH1	2.48	0.47
1:C:358:ALA:HA	1:C:370:ALA:HB3	1.97	0.47
1:L:856:GLU:OE2	1:K:151:TYR:OH	2.20	0.46
1:G:358:ALA:HA	1:G:370:ALA:HB3	1.97	0.45
1:H:760:LEU:HD22	1:H:774:VAL:HG22	1.99	0.45
1:L:760:LEU:HD22	1:L:774:VAL:HG22	1.99	0.45
1:K:358:ALA:HA	1:K:370:ALA:HB3	1.97	0.45
1:D:760:LEU:HD22	1:D:774:VAL:HG22	1.99	0.45
1:G:277:ILE:HD11	1:G:302:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:LYS:HG2	1:K:137:TYR:N	2.34	0.42
1:D:654:ARG:NH1	1:H:652:GLU:OE2	2.52	0.42
1:G:337:GLU:O	1:G:341:LEU:HG	2.20	0.42
1:K:277:ILE:HD11	1:K:302:TYR:HB2	2.00	0.42
1:L:911:THR:HB	1:L:912:PRO:HD3	2.02	0.42
1:C:337:GLU:O	1:C:341:LEU:HG	2.20	0.42
1:C:277:ILE:HD11	1:C:302:TYR:HB2	2.00	0.42
1:L:649:MET:HA	1:L:649:MET:HE2	2.02	0.42
1:H:911:THR:HB	1:H:912:PRO:HD3	2.02	0.41
1:G:136:LYS:HG2	1:G:137:TYR:N	2.34	0.41
1:K:337:GLU:O	1:K:341:LEU:HG	2.20	0.41
1:D:911:THR:HB	1:D:912:PRO:HD3	2.02	0.41
1:H:649:MET:HA	1:H:649:MET:HE2	2.03	0.41
1:H:975:PHE:CE2	1:E:71:TRP:CH2	3.09	0.41
1:C:136:LYS:HG2	1:C:137:TYR:N	2.35	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%)	55 (98%)	1 (2%)	0	100	100
1	C	405/988 (41%)	379 (94%)	26 (6%)	0	100	100
1	D	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
1	E	56/988 (6%)	55 (98%)	1 (2%)	0	100	100
1	F	9/988 (1%)	7 (78%)	2 (22%)	0	100	100
1	G	399/988 (40%)	374 (94%)	25 (6%)	0	100	100
1	H	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
1	I	56/988 (6%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	9/988 (1%)	7 (78%)	2 (22%)	0	100	100
1	K	399/988 (40%)	374 (94%)	25 (6%)	0	100	100
1	L	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
All	All	2598/10868 (24%)	2437 (94%)	161 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/899 (6%)	54 (100%)	0	100	100
1	C	382/899 (42%)	379 (99%)	3 (1%)	73	76
1	D	356/899 (40%)	353 (99%)	3 (1%)	73	76
1	E	54/899 (6%)	54 (100%)	0	100	100
1	F	11/899 (1%)	11 (100%)	0	100	100
1	G	376/899 (42%)	373 (99%)	3 (1%)	73	76
1	H	356/899 (40%)	353 (99%)	3 (1%)	73	76
1	I	54/899 (6%)	54 (100%)	0	100	100
1	J	11/899 (1%)	11 (100%)	0	100	100
1	K	376/899 (42%)	373 (99%)	3 (1%)	73	76
1	L	356/899 (40%)	353 (99%)	3 (1%)	73	76
All	All	2386/9889 (24%)	2368 (99%)	18 (1%)	70	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	812	LEU
1	D	841	LEU
1	D	862	LEU
1	H	812	LEU

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Mol	Chain	Res	Type
1	H	841	LEU
1	H	862	LEU
1	L	812	LEU
1	L	841	LEU
1	L	862	LEU
1	C	151	TYR
1	C	211	GLU
1	C	405	ASN
1	G	151	TYR
1	G	211	GLU
1	G	405	ASN
1	K	151	TYR
1	K	211	GLU
1	K	405	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	606	GLN
1	D	644	ASN
1	D	743	HIS
1	D	893	GLN
1	H	625	HIS
1	H	644	ASN
1	H	645	HIS
1	H	743	HIS
1	H	893	GLN
1	L	625	HIS
1	L	644	ASN
1	L	743	HIS
1	L	893	GLN
1	C	270	GLN
1	C	321	GLN
1	C	335	GLN
1	C	478	GLN
1	C	538	ASN
1	G	270	GLN
1	G	321	GLN
1	G	335	GLN
1	G	478	GLN
1	G	538	ASN
1	K	270	GLN

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Mol	Chain	Res	Type
1	K	321	GLN
1	K	335	GLN
1	K	478	GLN
1	K	538	ASN

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	0.32	0	17,19,21	1.37	2 (11%)
2	NAG	M	2	2	14,14,15	0.35	0	17,19,21	0.76	0
2	NAG	N	1	1,2	14,14,15	0.33	0	17,19,21	1.37	2 (11%)
2	NAG	N	2	2	14,14,15	0.34	0	17,19,21	0.76	0
2	NAG	O	1	1,2	14,14,15	0.33	0	17,19,21	1.38	2 (11%)
2	NAG	O	2	2	14,14,15	0.34	0	17,19,21	0.76	0
7	NAG	P	1	1,7	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
7	NAG	P	2	7	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
7	BMA	P	3	7	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
7	MAN	P	4	7	11,11,12	0.43	0	15,15,17	0.76	0
7	NAG	Q	1	1,7	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
7	NAG	Q	2	7	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
7	BMA	Q	3	7	11,11,12	0.40	0	15,15,17	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	Q	4	7	11,11,12	0.43	0	15,15,17	0.76	0
7	NAG	R	1	1,7	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
7	NAG	R	2	7	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
7	BMA	R	3	7	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
7	MAN	R	4	7	11,11,12	0.43	0	15,15,17	0.76	0
5	NAG	S	1	5,1	14,14,15	0.43	0	17,19,21	1.44	2 (11%)
5	NAG	S	2	5	14,14,15	0.44	0	17,19,21	1.59	3 (17%)
5	BMA	S	3	5	11,11,12	0.33	0	15,15,17	0.54	0
5	NAG	T	1	5,1	14,14,15	0.44	0	17,19,21	1.44	2 (11%)
5	NAG	T	2	5	14,14,15	0.42	0	17,19,21	1.59	3 (17%)
5	BMA	T	3	5	11,11,12	0.33	0	15,15,17	0.54	0
5	NAG	U	1	5,1	14,14,15	0.44	0	17,19,21	1.44	2 (11%)
5	NAG	U	2	5	14,14,15	0.42	0	17,19,21	1.59	3 (17%)
5	BMA	U	3	5	11,11,12	0.33	0	15,15,17	0.55	0
6	NAG	V	1	1,6	14,14,15	0.51	0	17,19,21	1.12	1 (5%)
6	NAG	V	2	6	14,14,15	0.31	0	17,19,21	0.80	0
6	BMA	V	3	6	11,11,12	0.36	0	15,15,17	0.70	0
6	MAN	V	4	6	11,11,12	0.64	0	15,15,17	1.26	2 (13%)
6	NAG	V	5	6	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
6	MAN	V	6	6	11,11,12	0.35	0	15,15,17	0.79	1 (6%)
6	NAG	W	1	1,6	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
6	NAG	W	2	6	14,14,15	0.30	0	17,19,21	0.80	0
6	BMA	W	3	6	11,11,12	0.35	0	15,15,17	0.70	0
6	MAN	W	4	6	11,11,12	0.64	0	15,15,17	1.25	2 (13%)
6	NAG	W	5	6	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
6	MAN	W	6	6	11,11,12	0.36	0	15,15,17	0.79	1 (6%)
6	NAG	X	1	1,6	14,14,15	0.49	0	17,19,21	1.11	1 (5%)
6	NAG	X	2	6	14,14,15	0.33	0	17,19,21	0.80	0
6	BMA	X	3	6	11,11,12	0.36	0	15,15,17	0.70	0
6	MAN	X	4	6	11,11,12	0.64	0	15,15,17	1.25	2 (13%)
6	NAG	X	5	6	14,14,15	0.26	0	17,19,21	0.85	0
6	MAN	X	6	6	11,11,12	0.35	0	15,15,17	0.79	1 (6%)
2	NAG	Y	1	1,2	14,14,15	0.40	0	17,19,21	0.74	0
2	NAG	Y	2	2	14,14,15	0.31	0	17,19,21	0.99	2 (11%)
2	NAG	Z	1	1,2	14,14,15	0.40	0	17,19,21	0.74	0
2	NAG	Z	2	2	14,14,15	0.32	0	17,19,21	0.99	2 (11%)
2	NAG	a	1	1,2	14,14,15	0.40	0	17,19,21	0.74	0
2	NAG	a	2	2	14,14,15	0.30	0	17,19,21	0.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	b	1	1,2	14,14,15	0.38	0	17,19,21	0.75	0
2	NAG	b	2	2	14,14,15	0.31	0	17,19,21	1.18	2 (11%)
2	NAG	c	1	1,2	14,14,15	0.38	0	17,19,21	0.75	0
2	NAG	c	2	2	14,14,15	0.32	0	17,19,21	1.18	2 (11%)
2	NAG	d	1	1,2	14,14,15	0.37	0	17,19,21	0.75	0
2	NAG	d	2	2	14,14,15	0.31	0	17,19,21	1.17	2 (11%)
3	NAG	e	1	3,1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
3	NAG	e	2	3	14,14,15	0.44	0	17,19,21	0.85	0
3	BMA	e	3	3	11,11,12	0.36	0	15,15,17	0.56	0
3	MAN	e	4	3	11,11,12	0.35	0	15,15,17	0.72	0
3	MAN	e	5	3	11,11,12	0.35	0	15,15,17	0.86	1 (6%)
3	MAN	e	6	3	11,11,12	0.34	0	15,15,17	0.80	1 (6%)
3	MAN	e	7	3	11,11,12	0.39	0	15,15,17	0.62	0
3	MAN	e	8	3	11,11,12	0.34	0	15,15,17	0.64	0
3	NAG	f	1	3,1	14,14,15	0.39	0	17,19,21	1.17	1 (5%)
3	NAG	f	2	3	14,14,15	0.44	0	17,19,21	0.85	0
3	BMA	f	3	3	11,11,12	0.38	0	15,15,17	0.55	0
3	MAN	f	4	3	11,11,12	0.36	0	15,15,17	0.72	0
3	MAN	f	5	3	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
3	MAN	f	6	3	11,11,12	0.33	0	15,15,17	0.80	1 (6%)
3	MAN	f	7	3	11,11,12	0.39	0	15,15,17	0.62	0
3	MAN	f	8	3	11,11,12	0.33	0	15,15,17	0.63	0
3	NAG	g	1	3,1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
3	NAG	g	2	3	14,14,15	0.44	0	17,19,21	0.85	0
3	BMA	g	3	3	11,11,12	0.37	0	15,15,17	0.57	0
3	MAN	g	4	3	11,11,12	0.35	0	15,15,17	0.71	0
3	MAN	g	5	3	11,11,12	0.34	0	15,15,17	0.88	1 (6%)
3	MAN	g	6	3	11,11,12	0.35	0	15,15,17	0.80	1 (6%)
3	MAN	g	7	3	11,11,12	0.40	0	15,15,17	0.61	0
3	MAN	g	8	3	11,11,12	0.33	0	15,15,17	0.64	0
4	NAG	h	1	1,4	14,14,15	0.52	0	17,19,21	1.09	0
4	NAG	h	2	4	14,14,15	0.48	0	17,19,21	0.81	0
4	BMA	h	3	4	11,11,12	0.39	0	15,15,17	0.58	0
4	MAN	h	4	4	11,11,12	0.37	0	15,15,17	0.83	1 (6%)
4	MAN	h	5	4	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
4	MAN	h	6	4	11,11,12	0.36	0	15,15,17	0.70	1 (6%)
4	NAG	i	1	1,4	14,14,15	0.52	0	17,19,21	1.09	0
4	NAG	i	2	4	14,14,15	0.46	0	17,19,21	0.81	0
4	BMA	i	3	4	11,11,12	0.39	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	i	4	4	11,11,12	0.37	0	15,15,17	0.83	1 (6%)
4	MAN	i	5	4	11,11,12	0.33	0	15,15,17	0.80	1 (6%)
4	MAN	i	6	4	11,11,12	0.36	0	15,15,17	0.71	1 (6%)
4	NAG	j	1	1,4	14,14,15	0.52	0	17,19,21	1.09	0
4	NAG	j	2	4	14,14,15	0.48	0	17,19,21	0.82	0
4	BMA	j	3	4	11,11,12	0.39	0	15,15,17	0.58	0
4	MAN	j	4	4	11,11,12	0.38	0	15,15,17	0.84	1 (6%)
4	MAN	j	5	4	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
4	MAN	j	6	4	11,11,12	0.35	0	15,15,17	0.71	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
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	1/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	NAG	R	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1

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

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

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	2	NAG	C2-N2-C7	4.10	128.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	2	NAG	C2-N2-C7	4.07	128.36	122.90
5	S	2	NAG	C2-N2-C7	4.07	128.35	122.90
6	W	4	MAN	O2-C2-C1	3.58	117.41	109.22
6	V	4	MAN	O2-C2-C1	3.57	117.40	109.22
6	X	4	MAN	O2-C2-C1	3.56	117.36	109.22
5	T	1	NAG	C2-N2-C7	3.47	127.56	122.90
5	U	1	NAG	C2-N2-C7	3.47	127.56	122.90
5	S	1	NAG	C2-N2-C7	3.46	127.54	122.90
6	V	1	NAG	C1-O5-C5	3.44	116.79	112.19
6	X	1	NAG	C1-O5-C5	3.42	116.77	112.19
6	W	1	NAG	C1-O5-C5	3.39	116.73	112.19
2	O	1	NAG	C1-O5-C5	3.39	116.73	112.19
2	N	1	NAG	C1-O5-C5	3.37	116.70	112.19
2	M	1	NAG	C1-O5-C5	3.36	116.69	112.19
7	R	1	NAG	C1-C2-N2	-3.10	105.55	110.43
7	Q	1	NAG	C1-C2-N2	-3.08	105.58	110.43
7	P	1	NAG	C1-C2-N2	-3.07	105.60	110.43
3	f	1	NAG	C1-O5-C5	3.05	116.27	112.19
3	e	1	NAG	C1-O5-C5	3.01	116.22	112.19
3	g	1	NAG	C1-O5-C5	2.98	116.18	112.19
2	d	2	NAG	C2-N2-C7	2.94	126.84	122.90
2	b	2	NAG	C2-N2-C7	2.93	126.82	122.90
2	c	2	NAG	C2-N2-C7	2.93	126.82	122.90
5	U	1	NAG	C8-C7-N2	2.85	120.85	116.12
5	S	1	NAG	C8-C7-N2	2.84	120.83	116.12
5	T	1	NAG	C8-C7-N2	2.83	120.82	116.12
6	V	4	MAN	C1-O5-C5	2.83	115.98	112.19
6	W	4	MAN	C1-O5-C5	2.82	115.97	112.19
6	X	4	MAN	C1-O5-C5	2.80	115.94	112.19
3	g	5	MAN	C1-O5-C5	2.69	115.80	112.19
5	S	2	NAG	C4-C3-C2	2.67	114.93	111.02
3	f	5	MAN	C1-O5-C5	2.66	115.76	112.19
2	O	1	NAG	O5-C1-C2	-2.65	107.19	111.29
5	U	2	NAG	C4-C3-C2	2.65	114.90	111.02
5	T	2	NAG	C4-C3-C2	2.65	114.90	111.02
2	N	1	NAG	O5-C1-C2	-2.65	107.20	111.29
2	M	1	NAG	O5-C1-C2	-2.64	107.21	111.29
5	T	2	NAG	C1-C2-N2	-2.63	106.29	110.43
3	e	5	MAN	C1-O5-C5	2.61	115.69	112.19
4	j	4	MAN	C1-O5-C5	2.57	115.63	112.19
5	S	2	NAG	C1-C2-N2	-2.57	106.39	110.43
5	U	2	NAG	C1-C2-N2	-2.56	106.40	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	h	4	MAN	C1-O5-C5	2.55	115.60	112.19
4	i	4	MAN	C1-O5-C5	2.53	115.58	112.19
7	R	2	NAG	C1-O5-C5	2.53	115.58	112.19
3	e	6	MAN	C1-O5-C5	2.52	115.56	112.19
3	f	6	MAN	C1-O5-C5	2.52	115.56	112.19
3	g	6	MAN	C1-O5-C5	2.50	115.54	112.19
7	P	2	NAG	C1-O5-C5	2.50	115.53	112.19
7	Q	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	b	2	NAG	C8-C7-N2	2.47	120.21	116.12
2	c	2	NAG	C8-C7-N2	2.45	120.18	116.12
2	d	2	NAG	C8-C7-N2	2.44	120.16	116.12
4	i	5	MAN	C1-O5-C5	2.42	115.43	112.19
4	h	5	MAN	C1-O5-C5	2.38	115.37	112.19
6	V	6	MAN	C1-O5-C5	2.37	115.36	112.19
4	j	5	MAN	C1-O5-C5	2.36	115.35	112.19
6	X	6	MAN	C1-O5-C5	2.35	115.34	112.19
6	W	6	MAN	C1-O5-C5	2.35	115.34	112.19
4	j	6	MAN	C1-O5-C5	2.31	115.29	112.19
4	i	6	MAN	C1-O5-C5	2.31	115.28	112.19
4	h	6	MAN	C1-O5-C5	2.26	115.21	112.19
7	Q	3	BMA	C1-O5-C5	2.21	115.15	112.19
7	R	3	BMA	C1-O5-C5	2.17	115.09	112.19
7	P	3	BMA	C1-O5-C5	2.16	115.08	112.19
2	Z	2	NAG	O5-C1-C2	-2.13	108.00	111.29
2	Y	2	NAG	O5-C1-C2	-2.12	108.01	111.29
2	a	2	NAG	O5-C1-C2	-2.12	108.02	111.29
2	Z	2	NAG	C1-O5-C5	2.03	114.90	112.19
6	W	5	NAG	O5-C1-C2	-2.02	108.17	111.29
2	Y	2	NAG	C1-O5-C5	2.02	114.89	112.19
2	a	2	NAG	C1-O5-C5	2.01	114.88	112.19
6	V	5	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
2	b	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	b	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	b	2	NAG	C8-C7-N2-C2
2	b	2	NAG	O7-C7-N2-C2
2	c	2	NAG	C8-C7-N2-C2
2	c	2	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
3	g	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
4	h	4	MAN	O5-C5-C6-O6
4	i	4	MAN	O5-C5-C6-O6
4	j	4	MAN	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
6	V	4	MAN	O5-C5-C6-O6
6	W	4	MAN	O5-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	W	1	NAG	C4-C5-C6-O6

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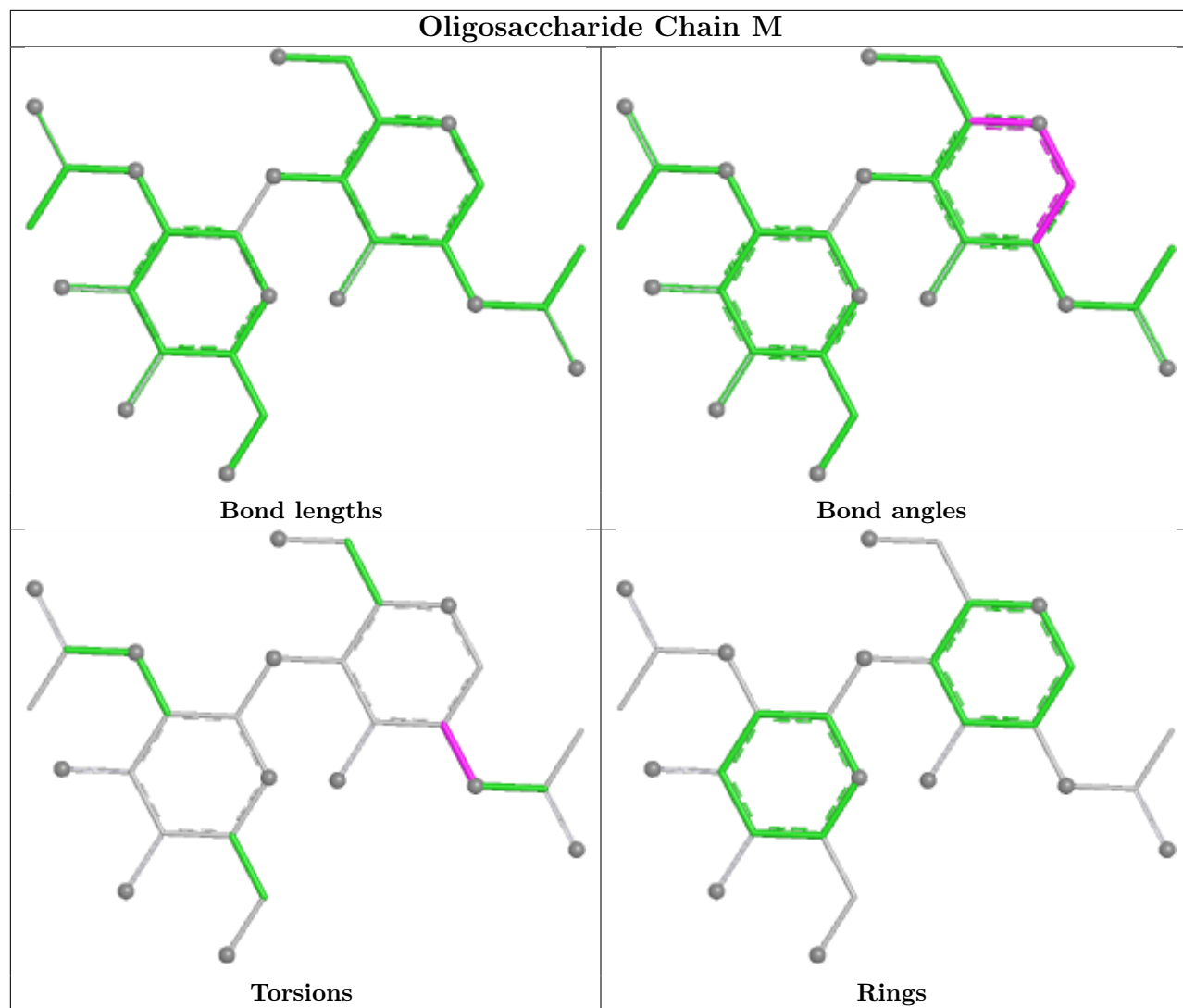
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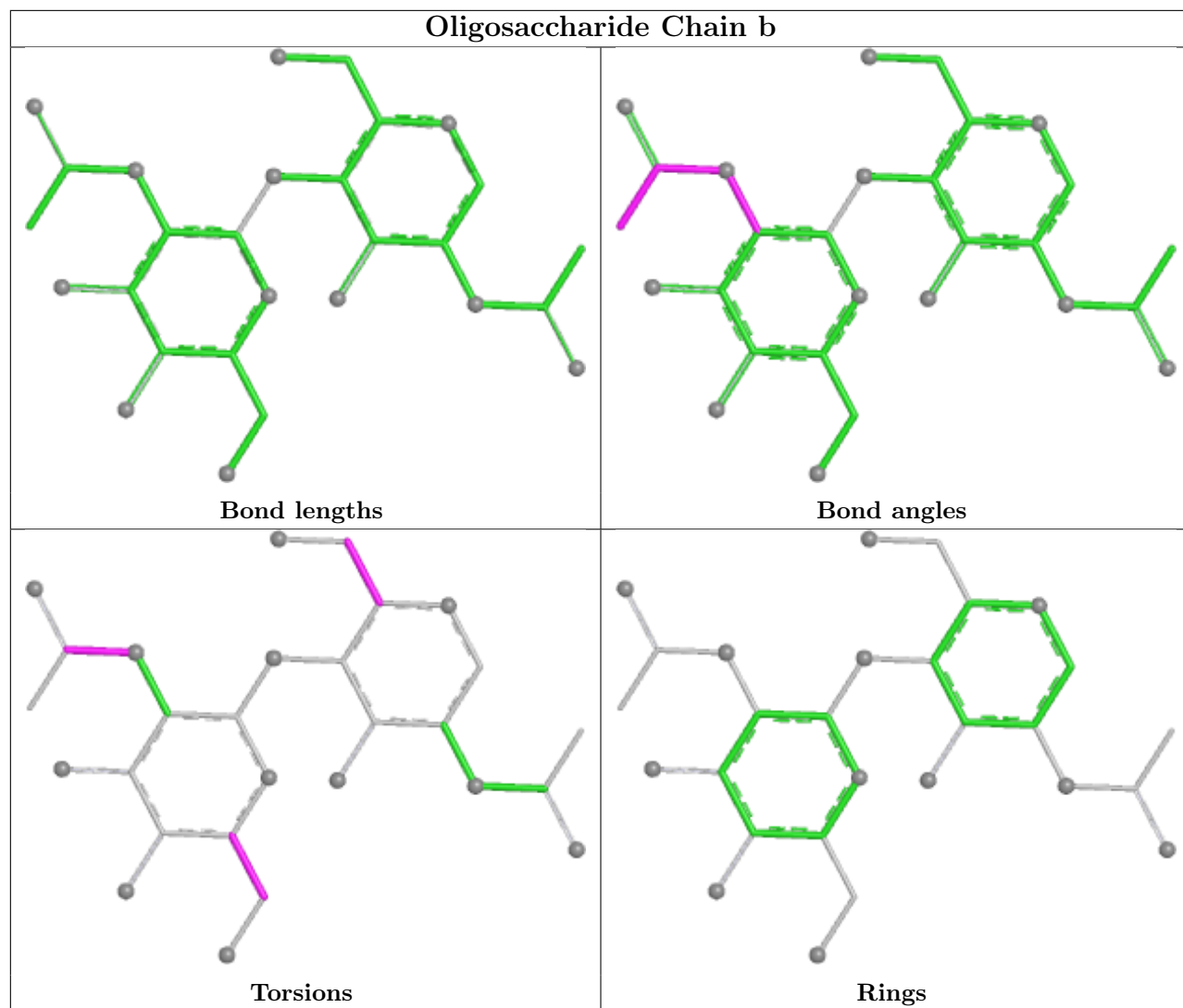
Mol	Chain	Res	Type	Atoms
3	e	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	M	1	NAG	C3-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
6	W	5	NAG	O5-C5-C6-O6
6	V	5	NAG	O5-C5-C6-O6
6	X	5	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6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

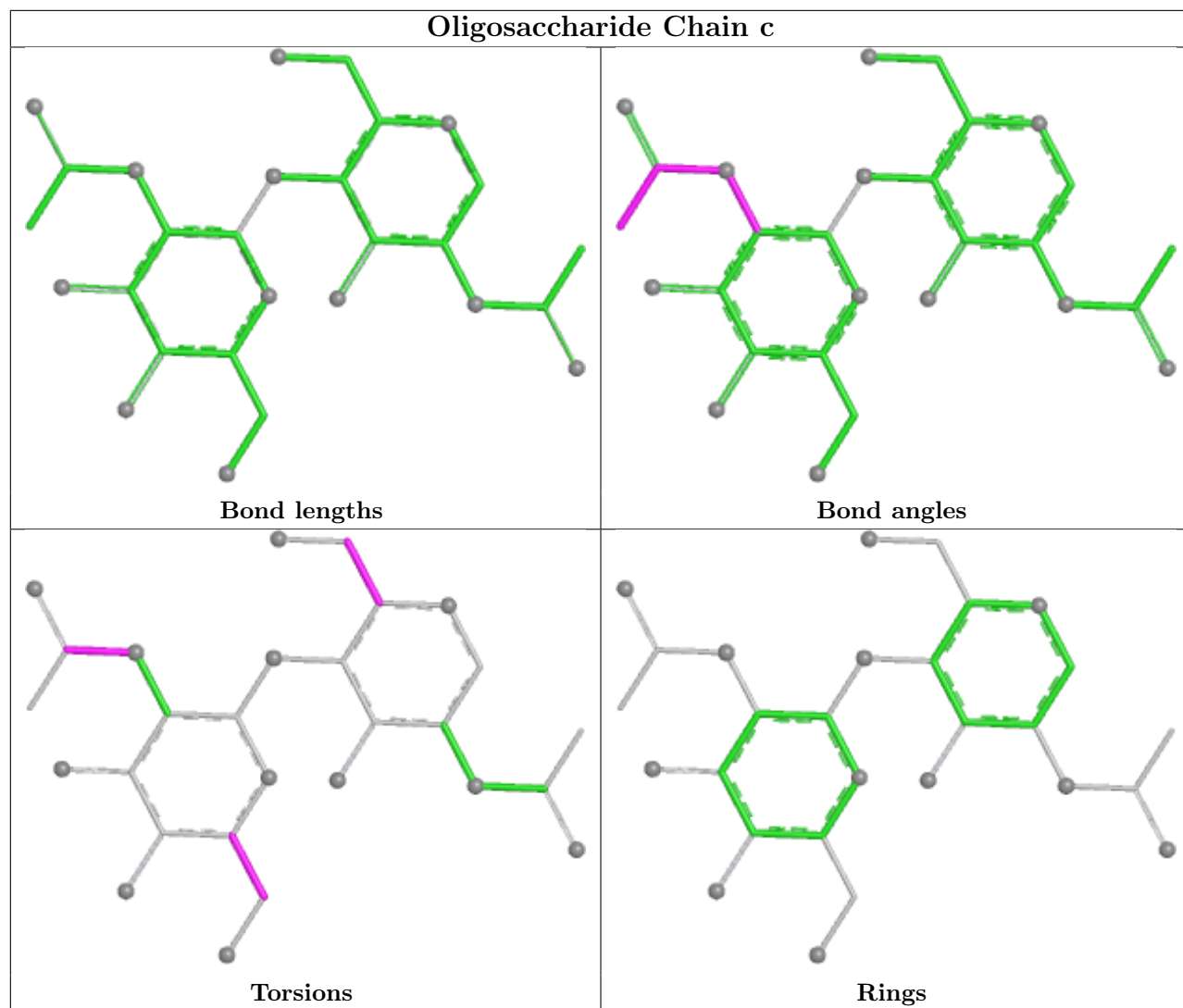
There are no ring outliers.

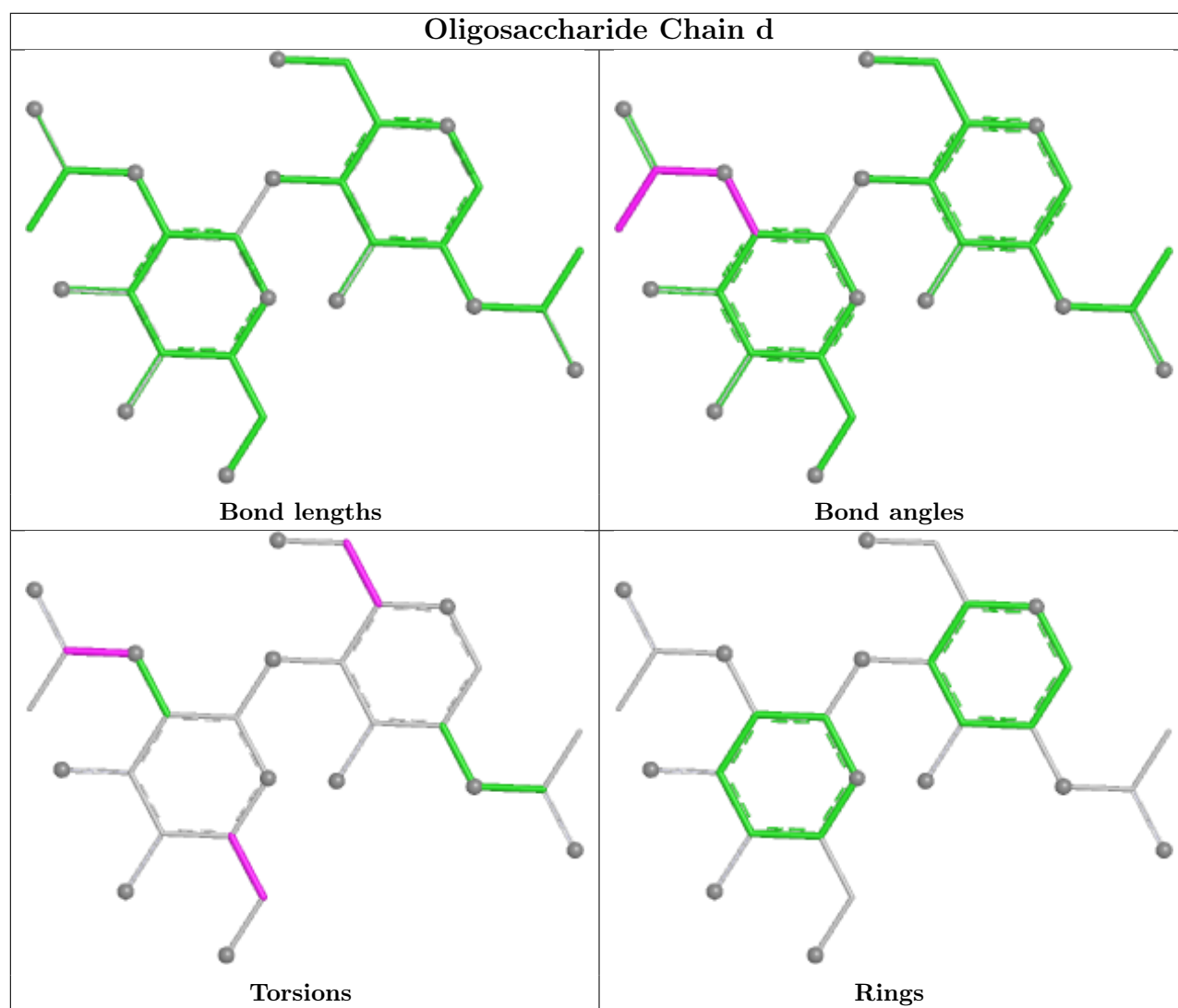
No monomer is involved in short contacts.

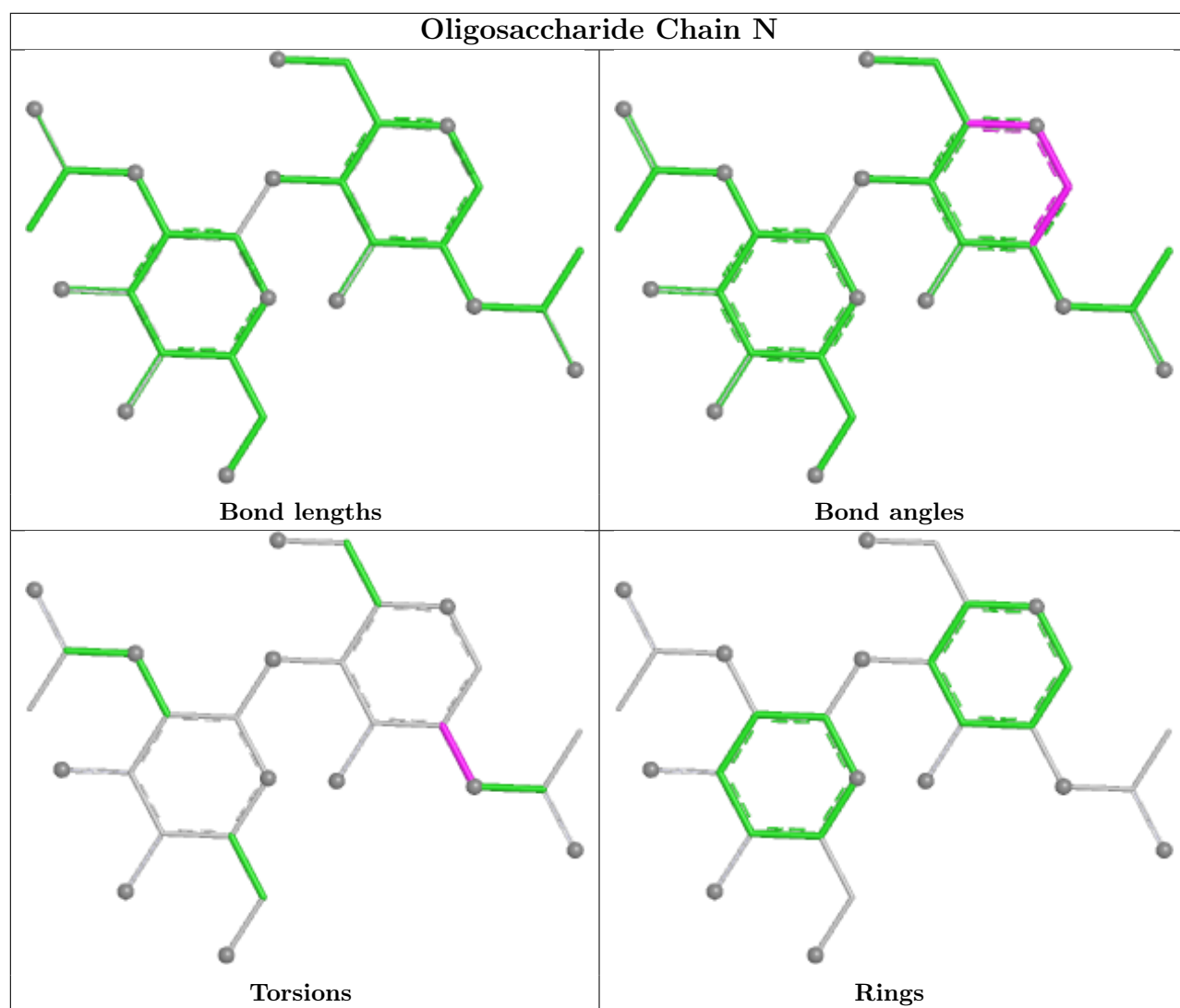
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

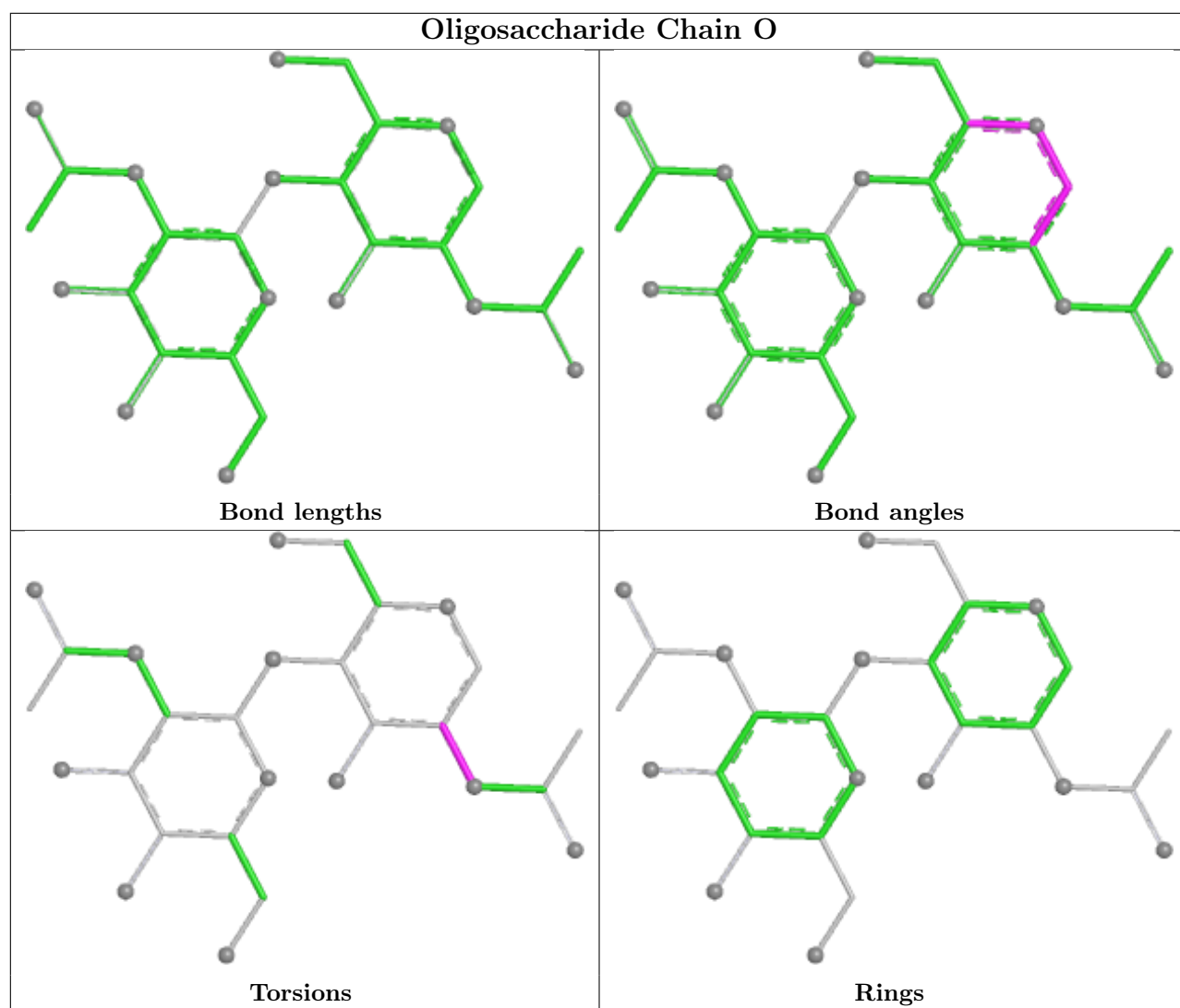


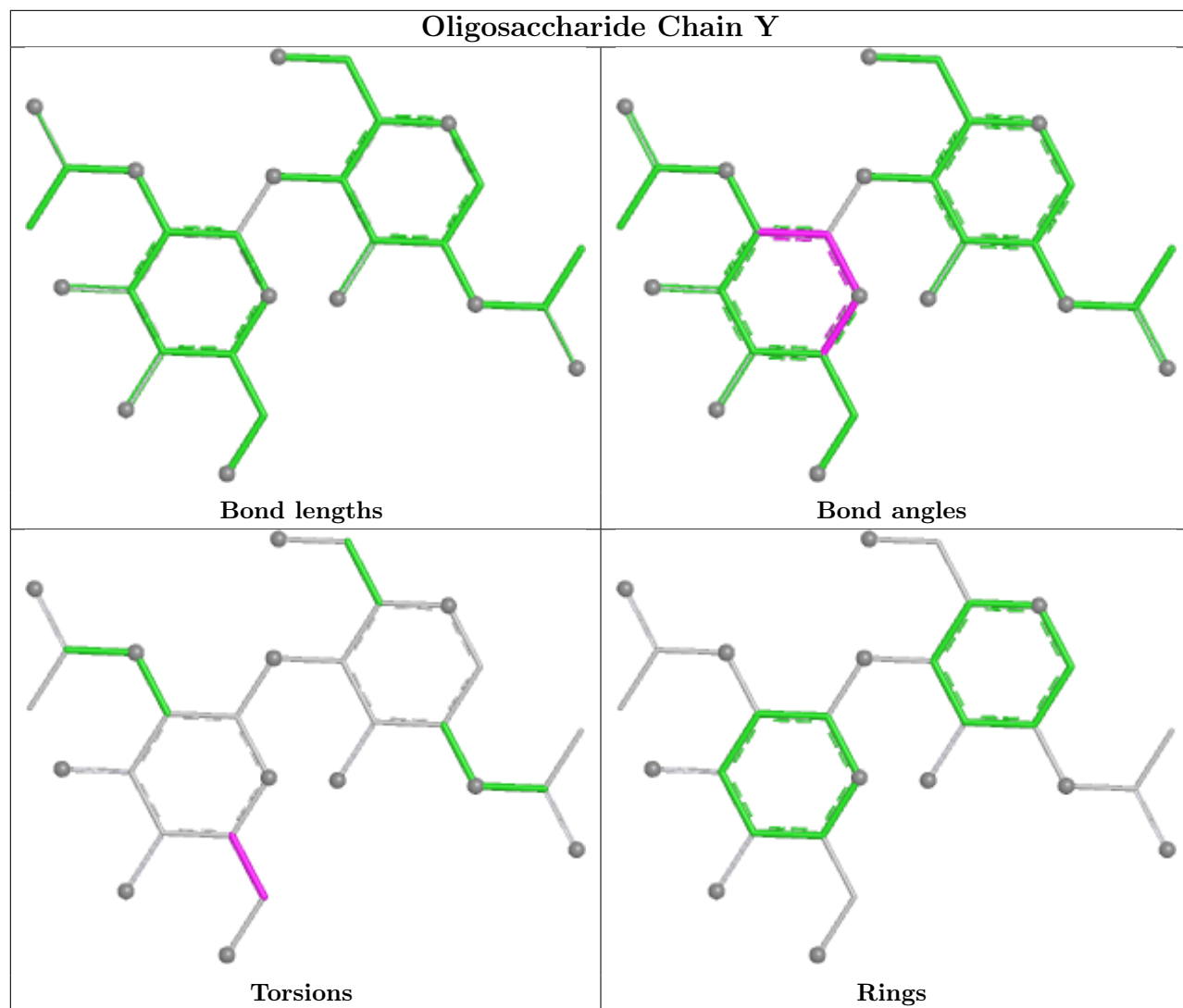


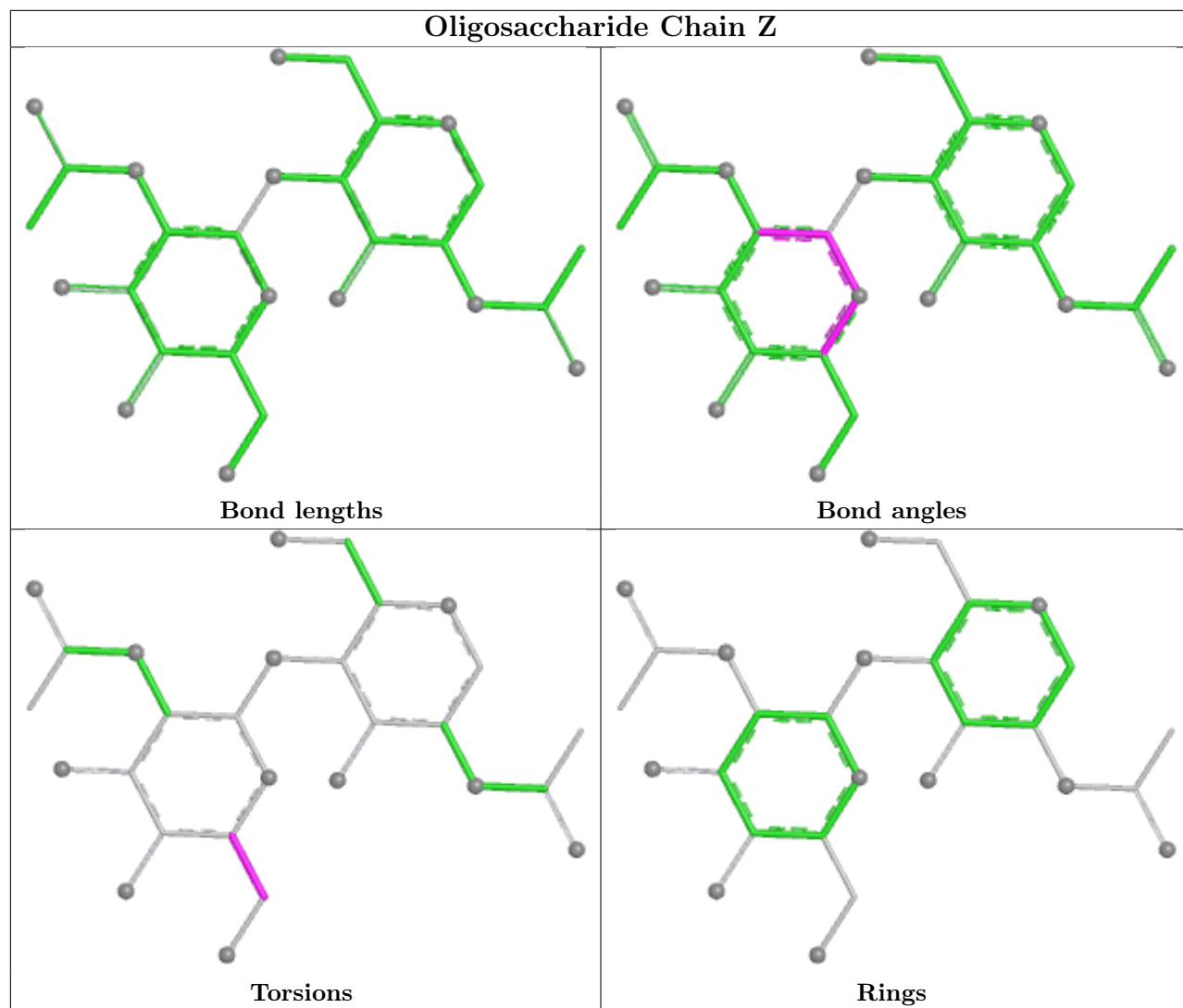


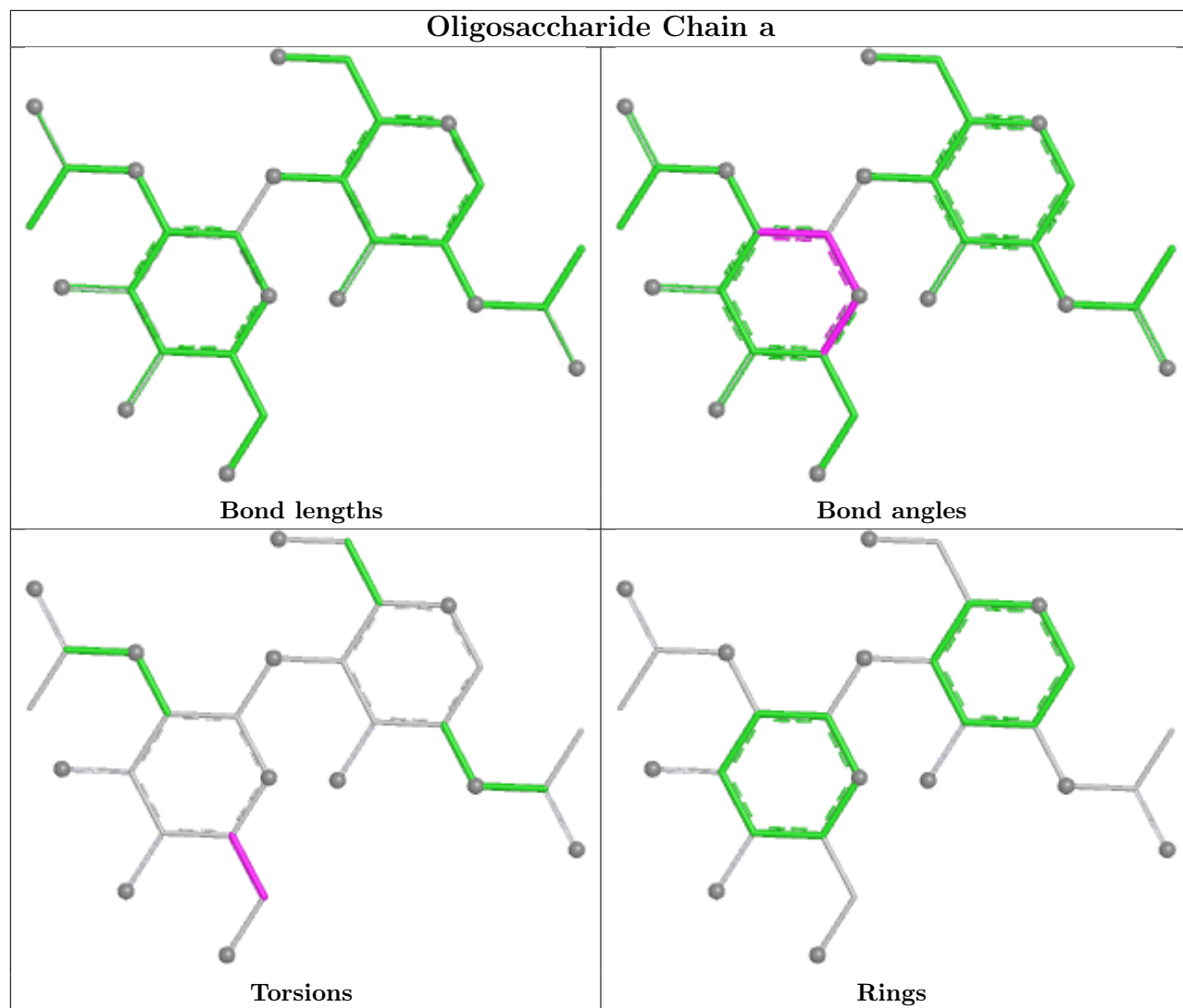


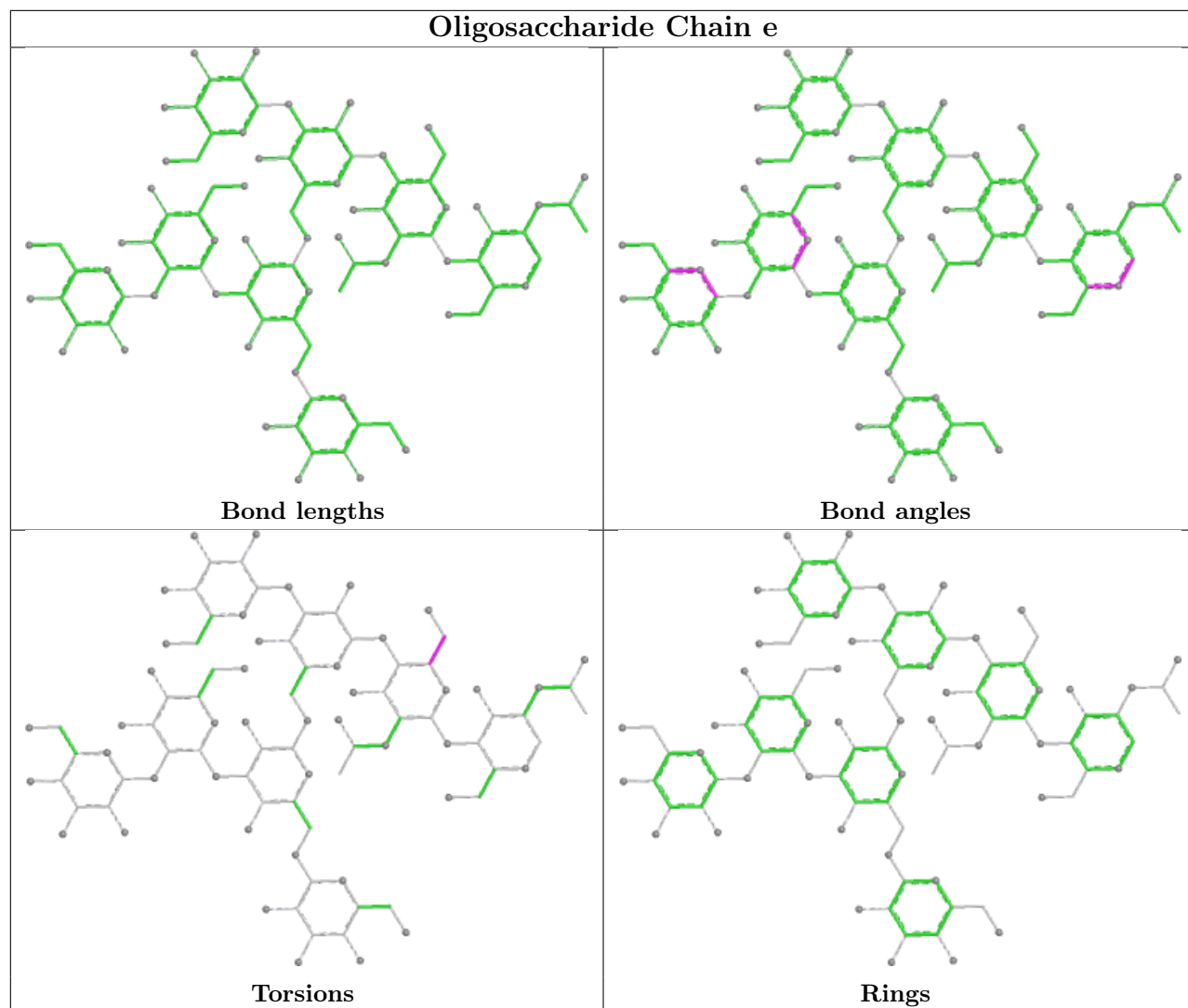


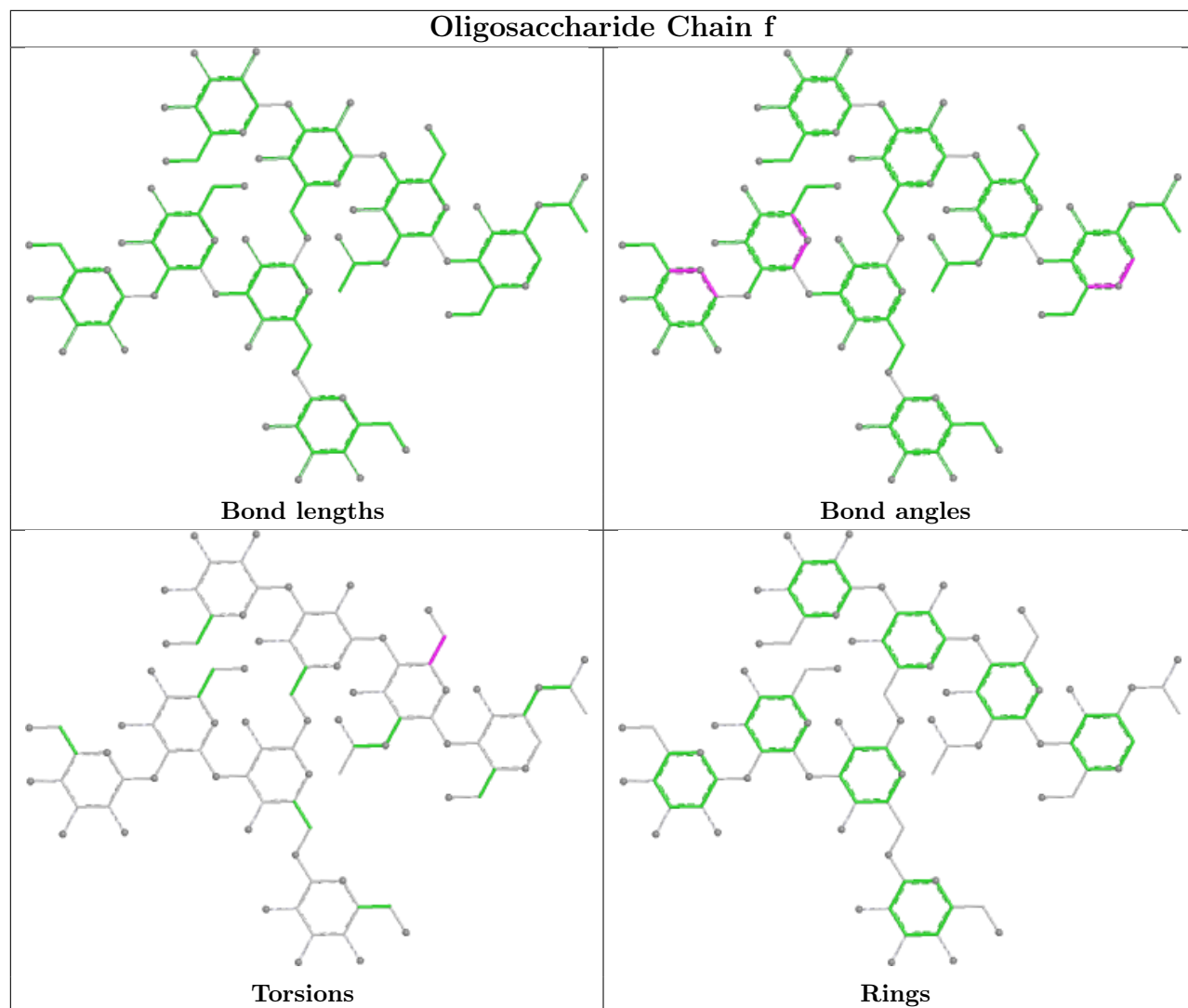


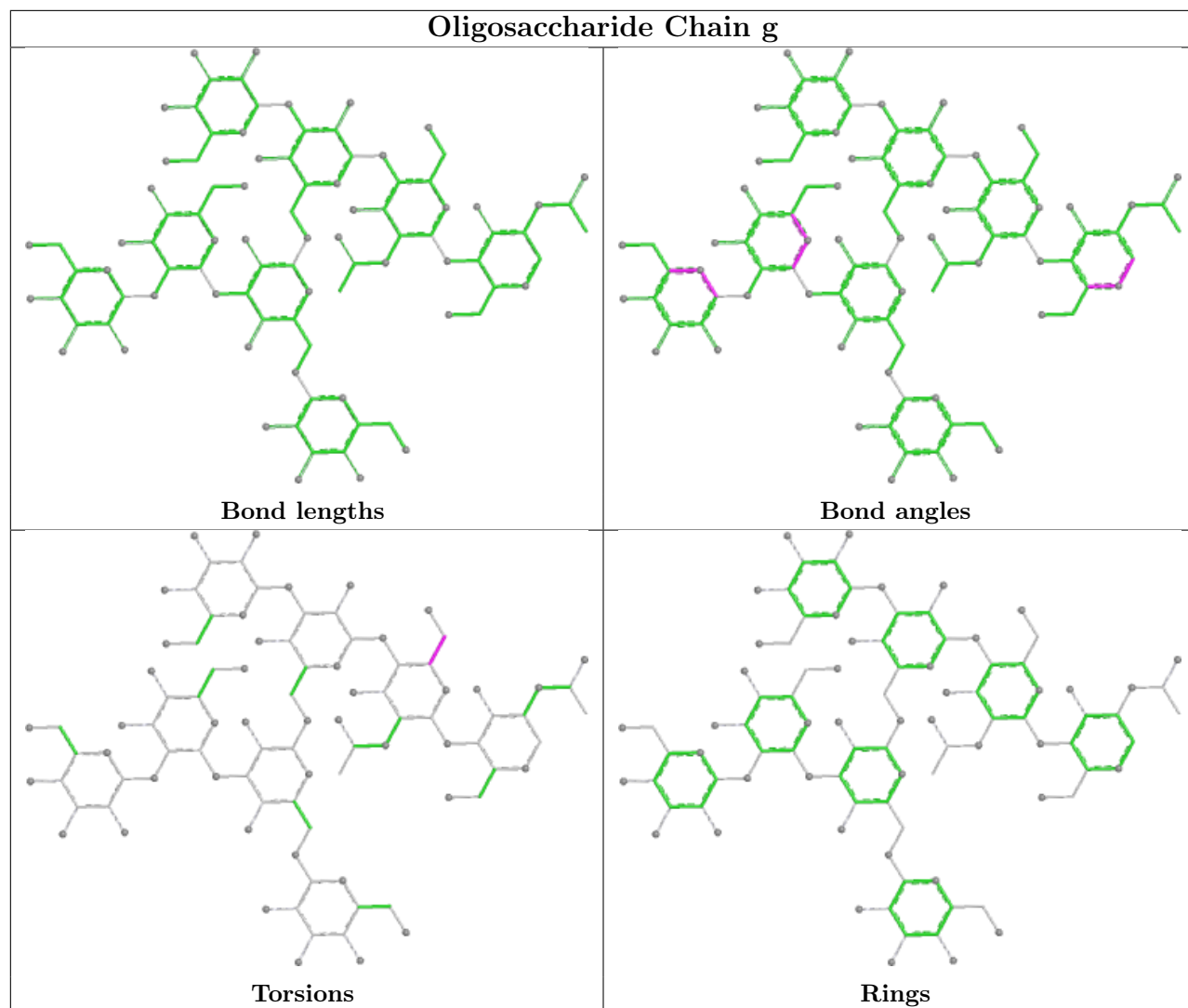


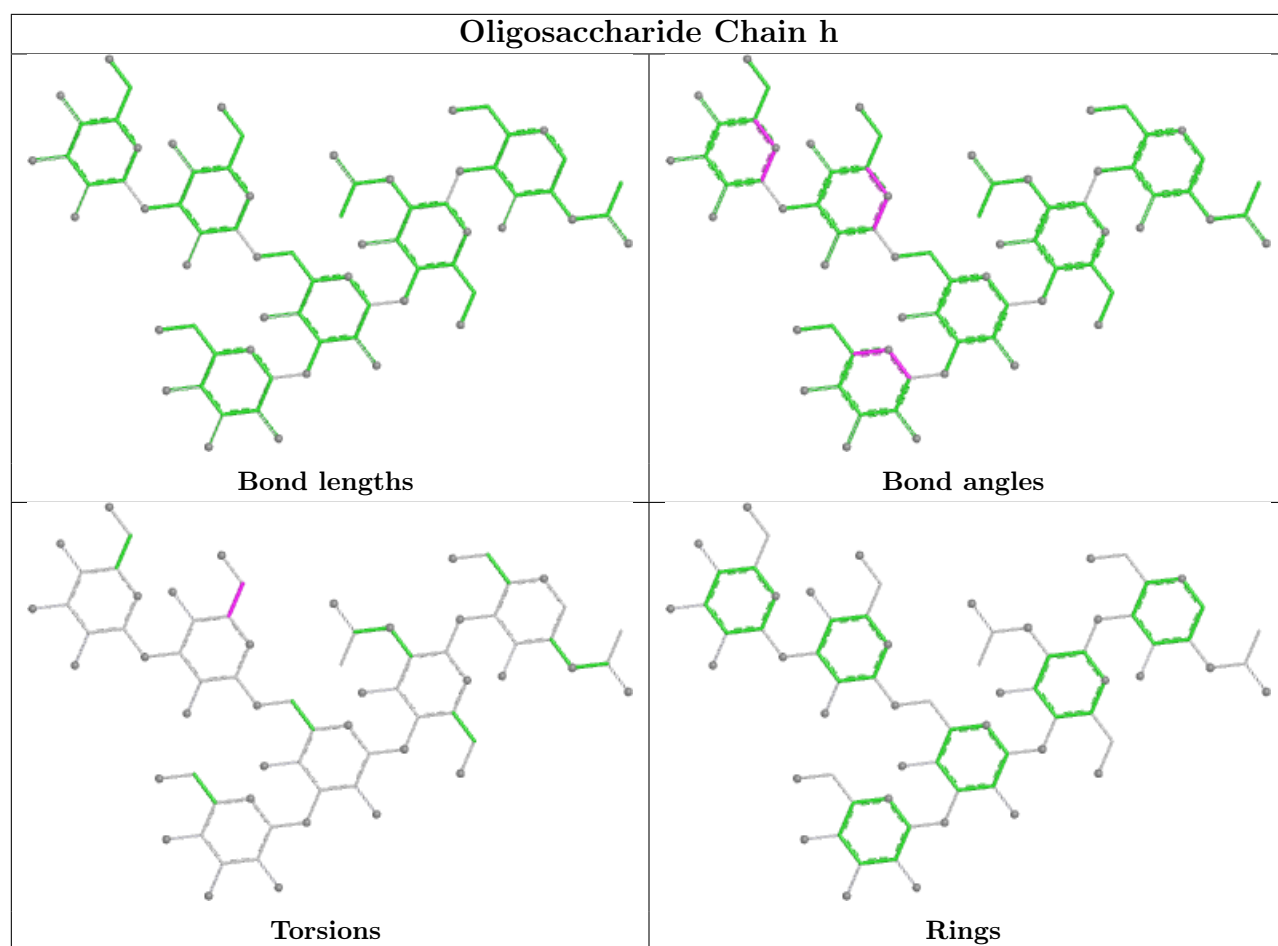


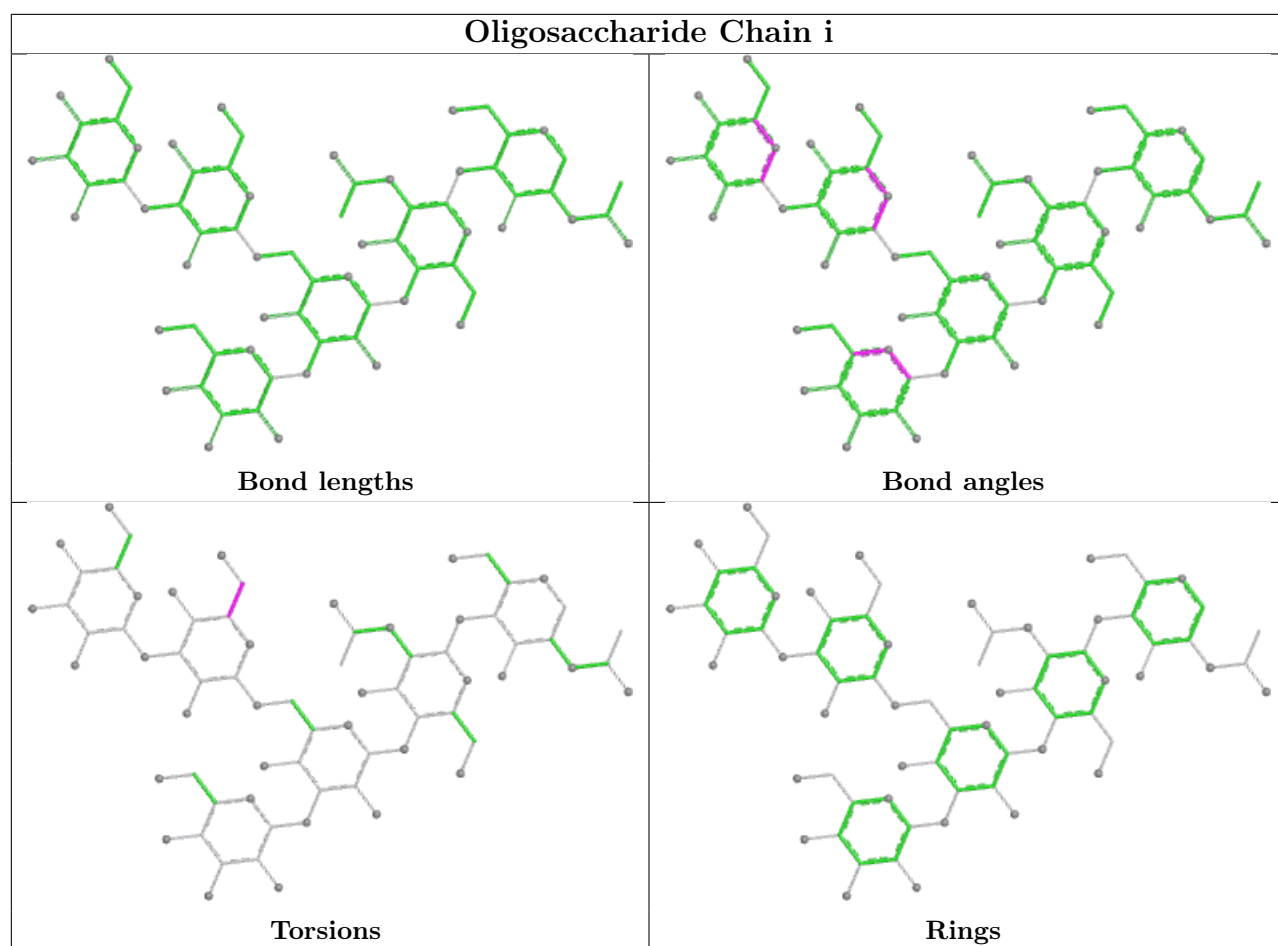


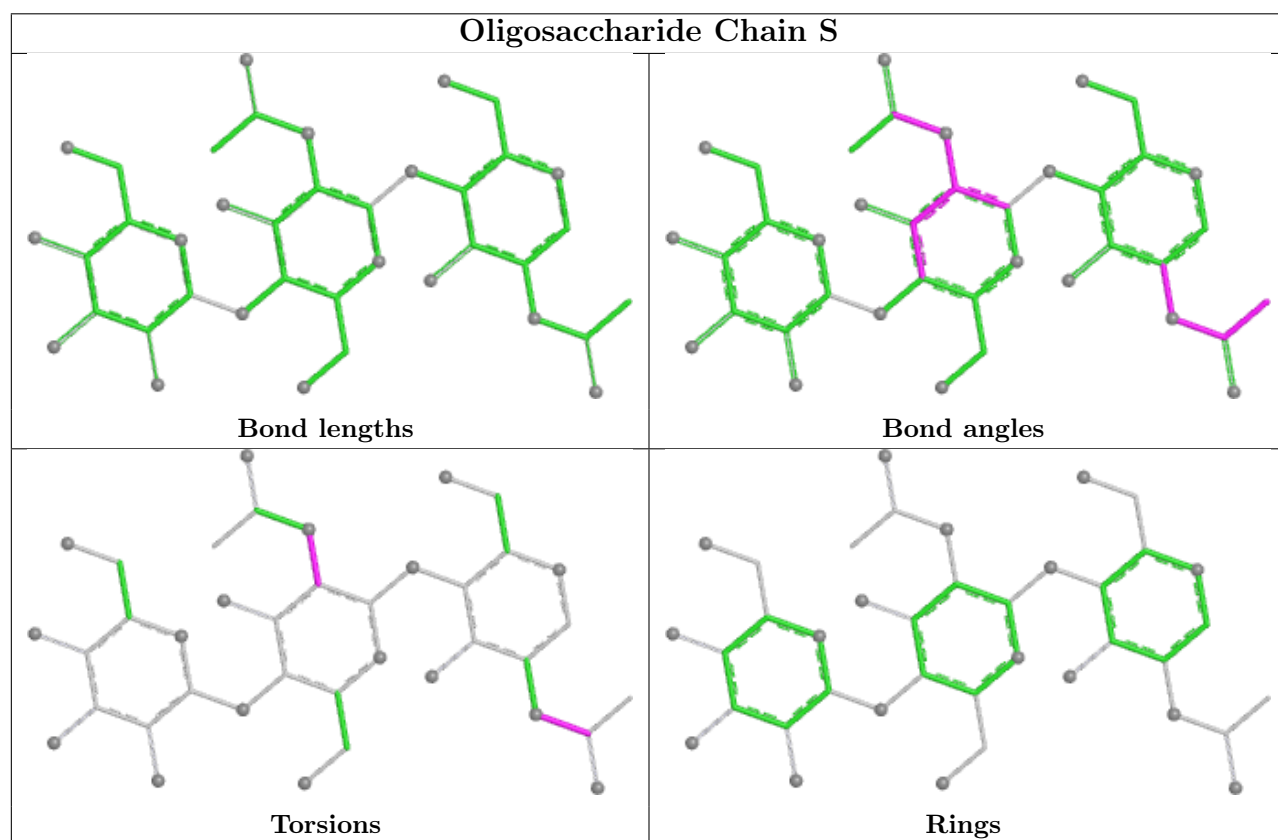
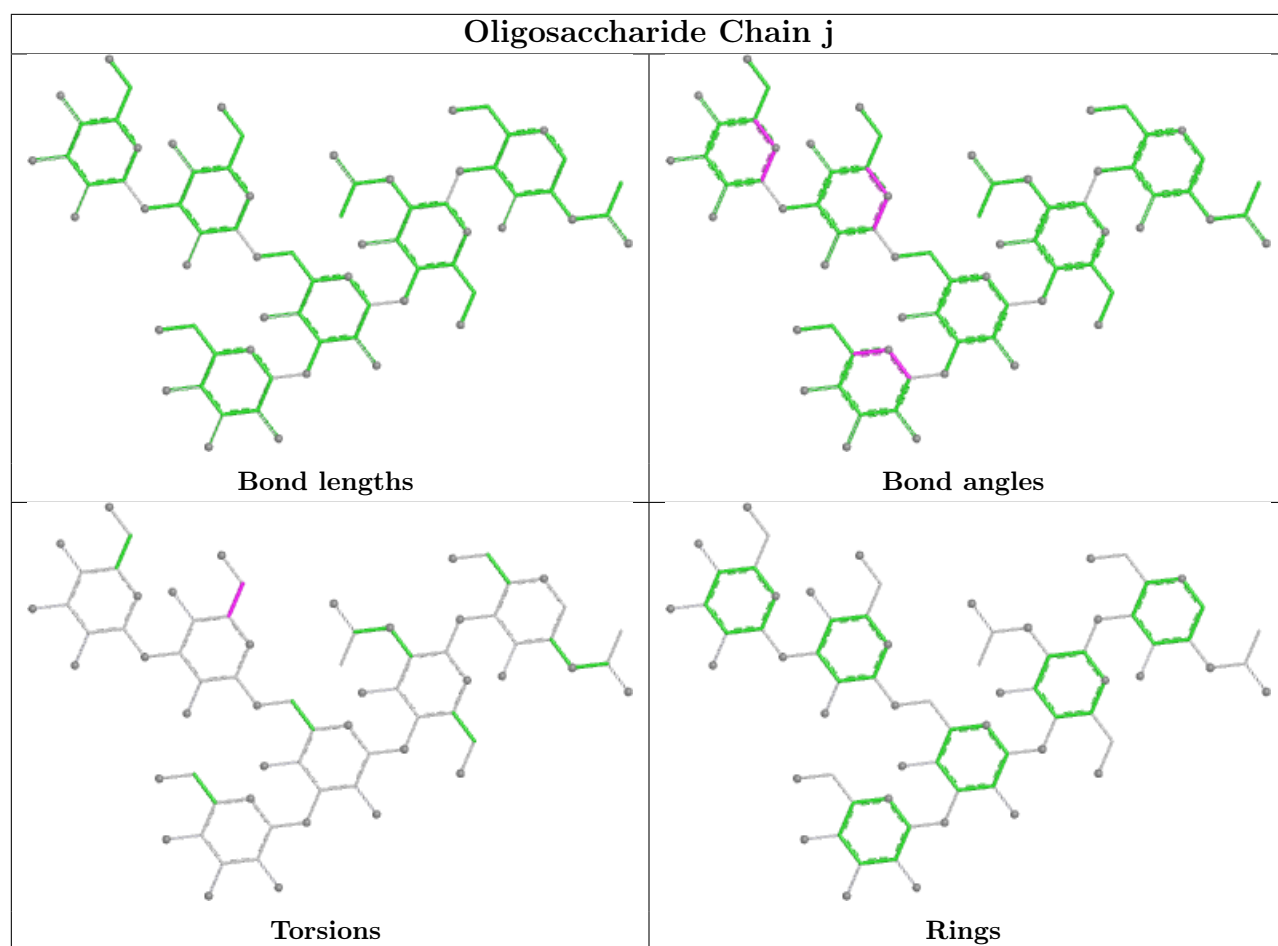


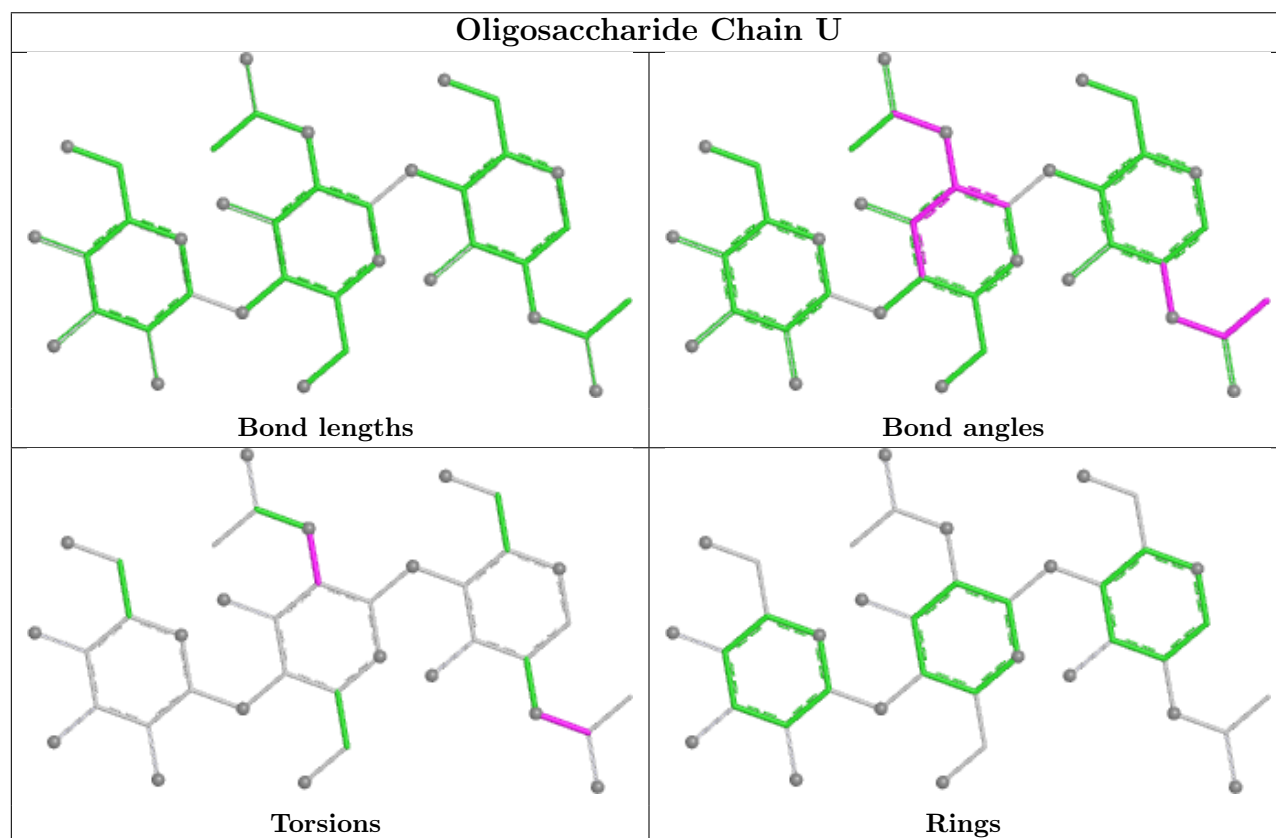
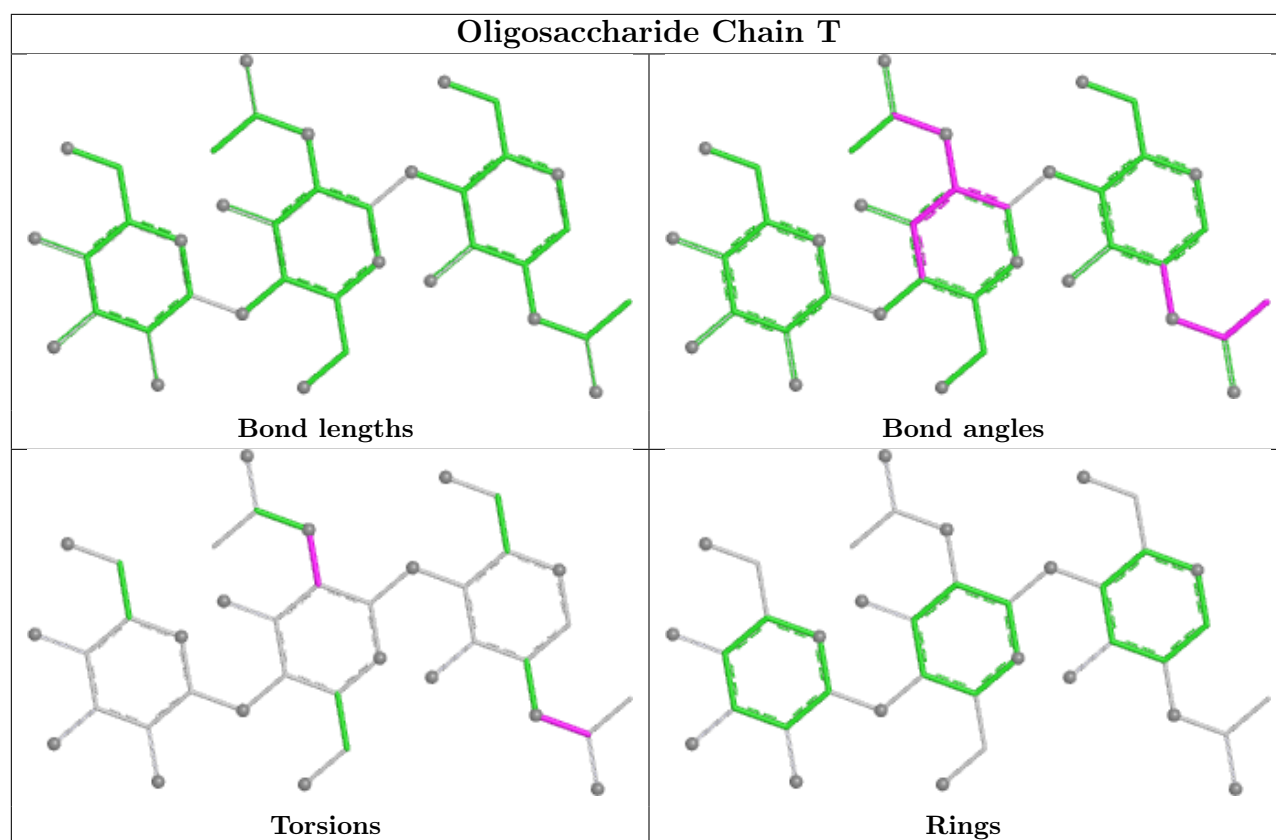


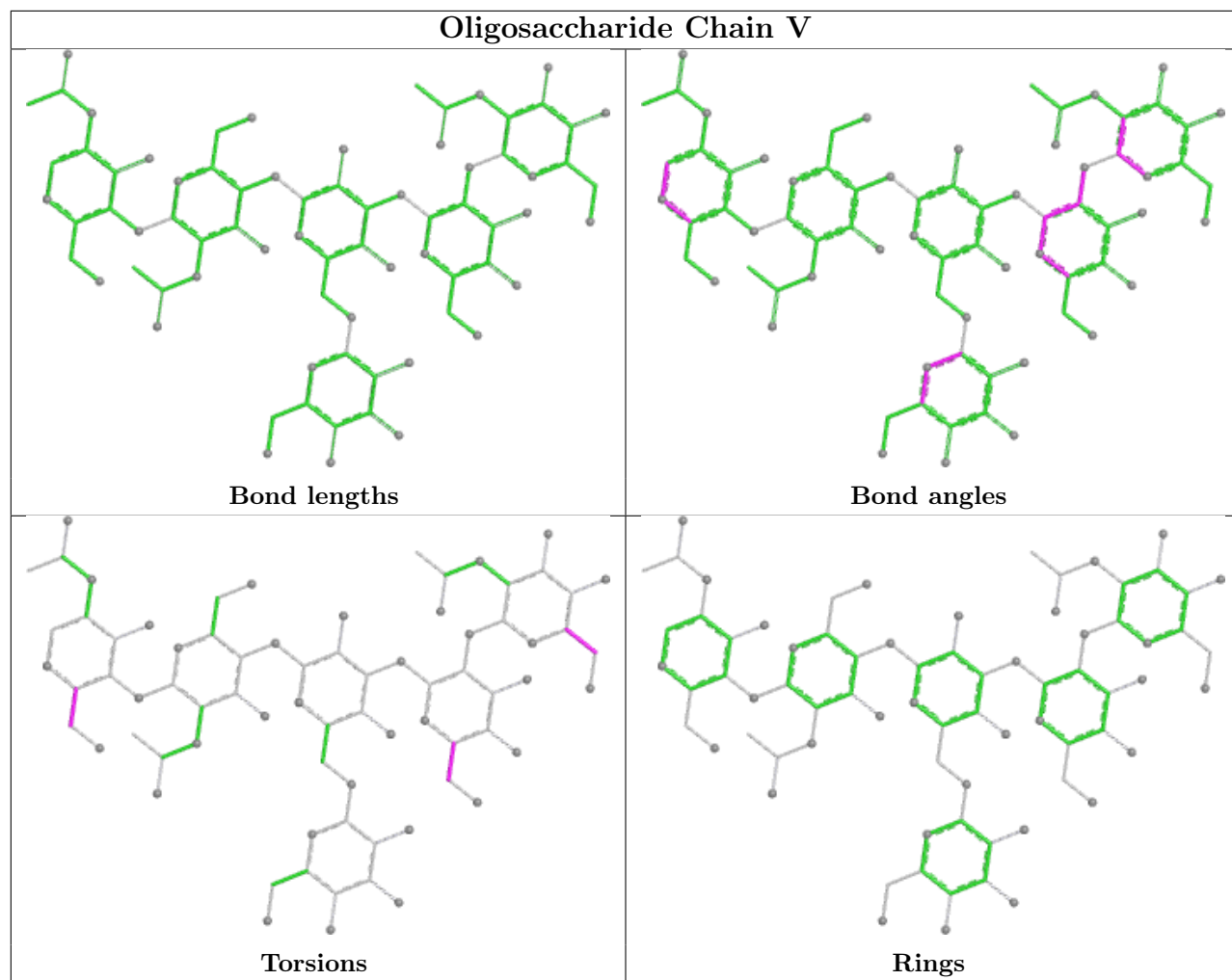


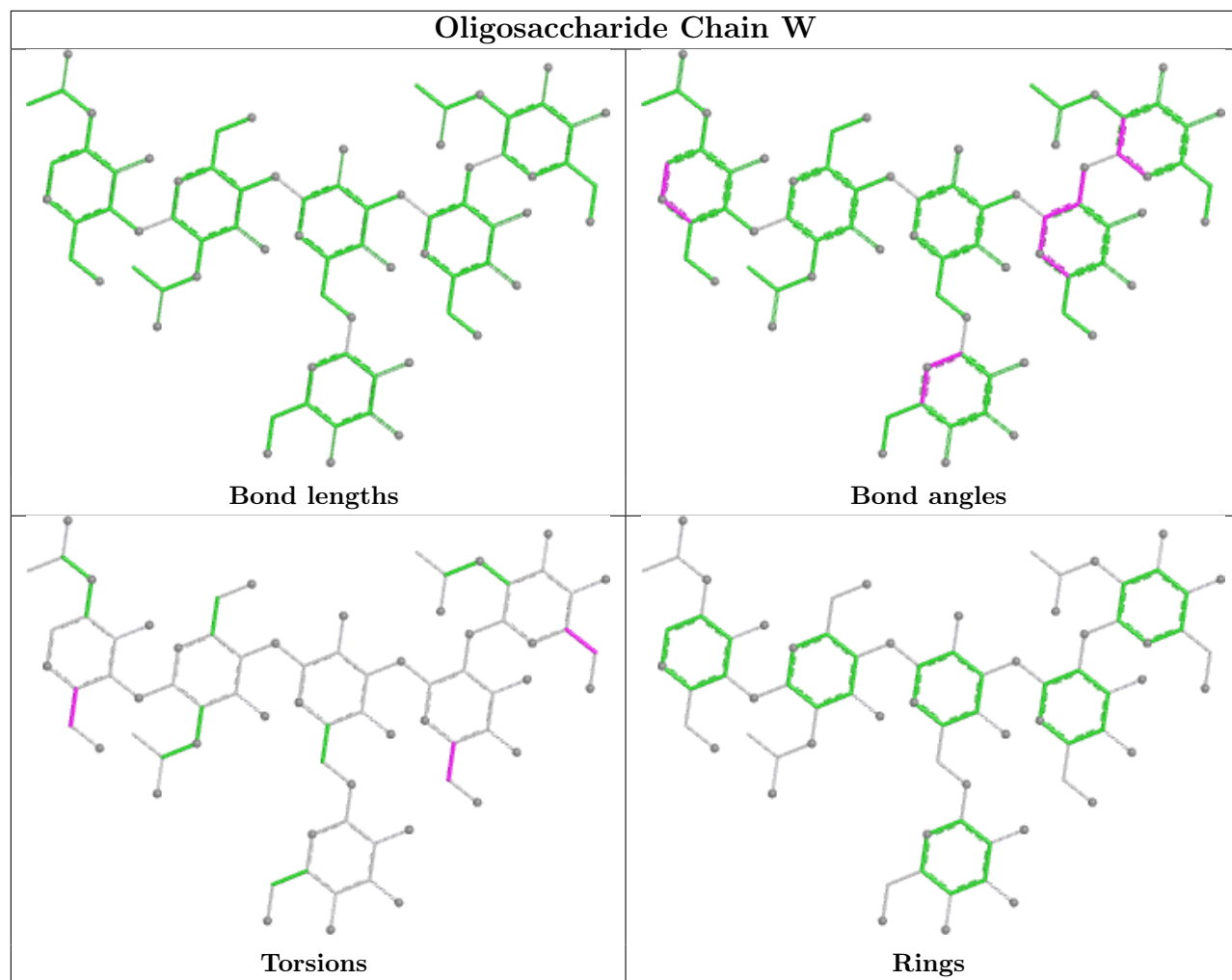


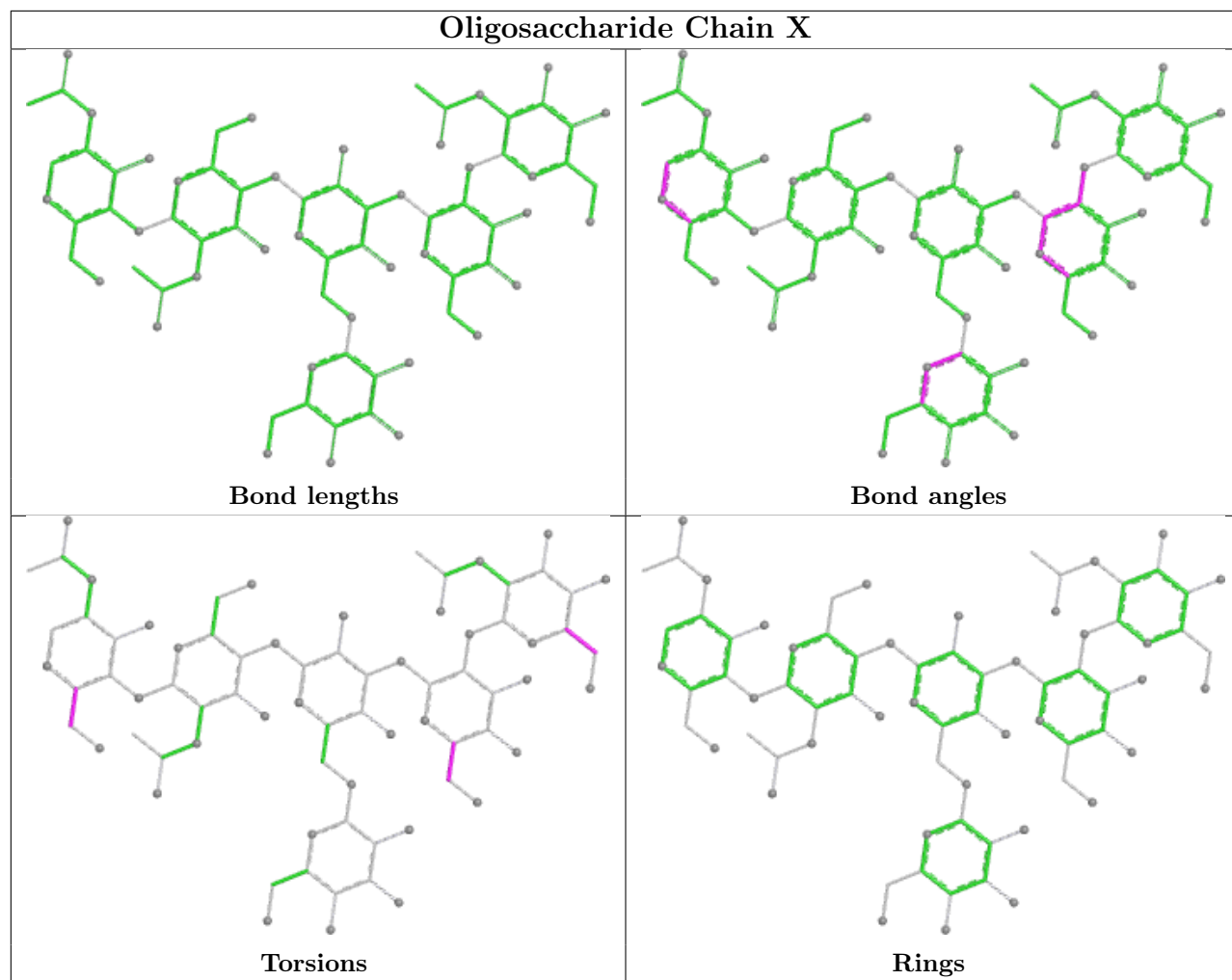


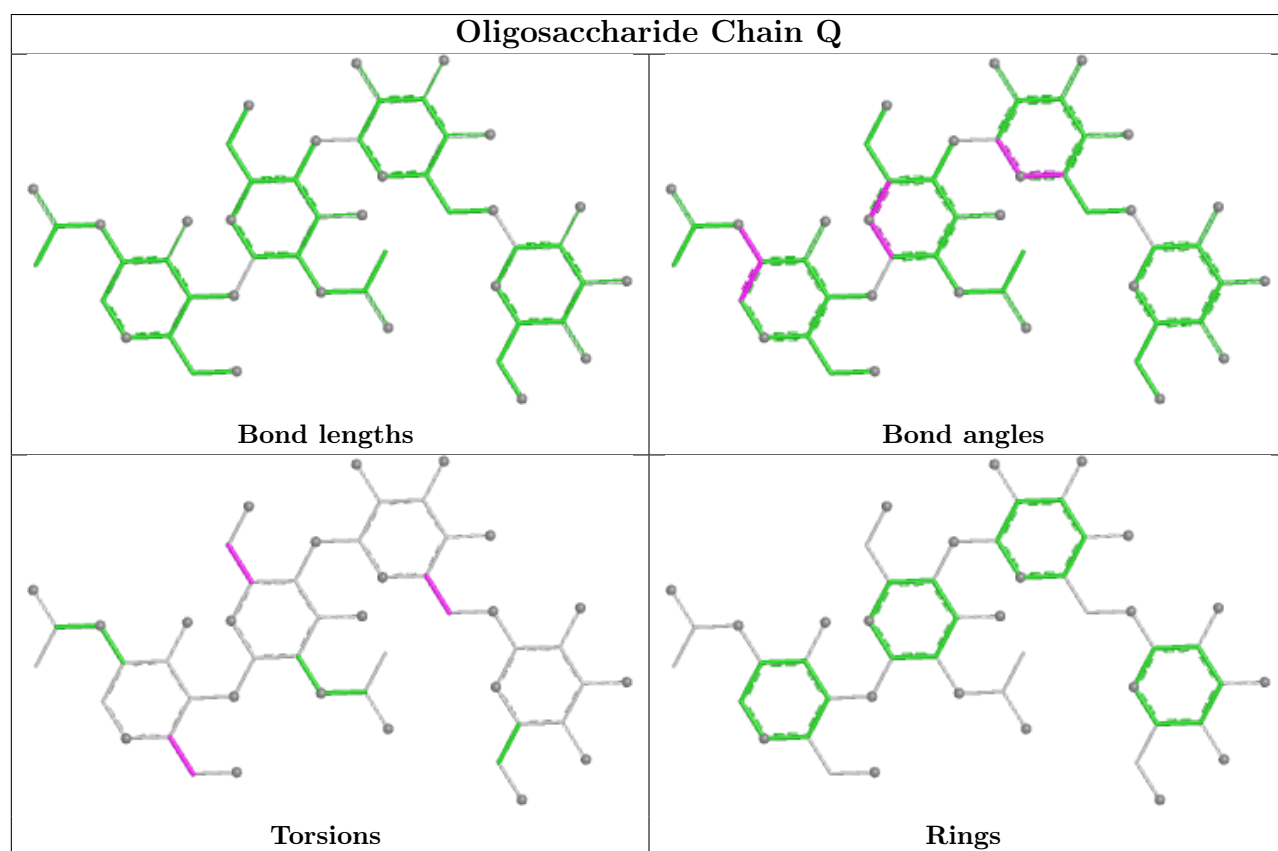
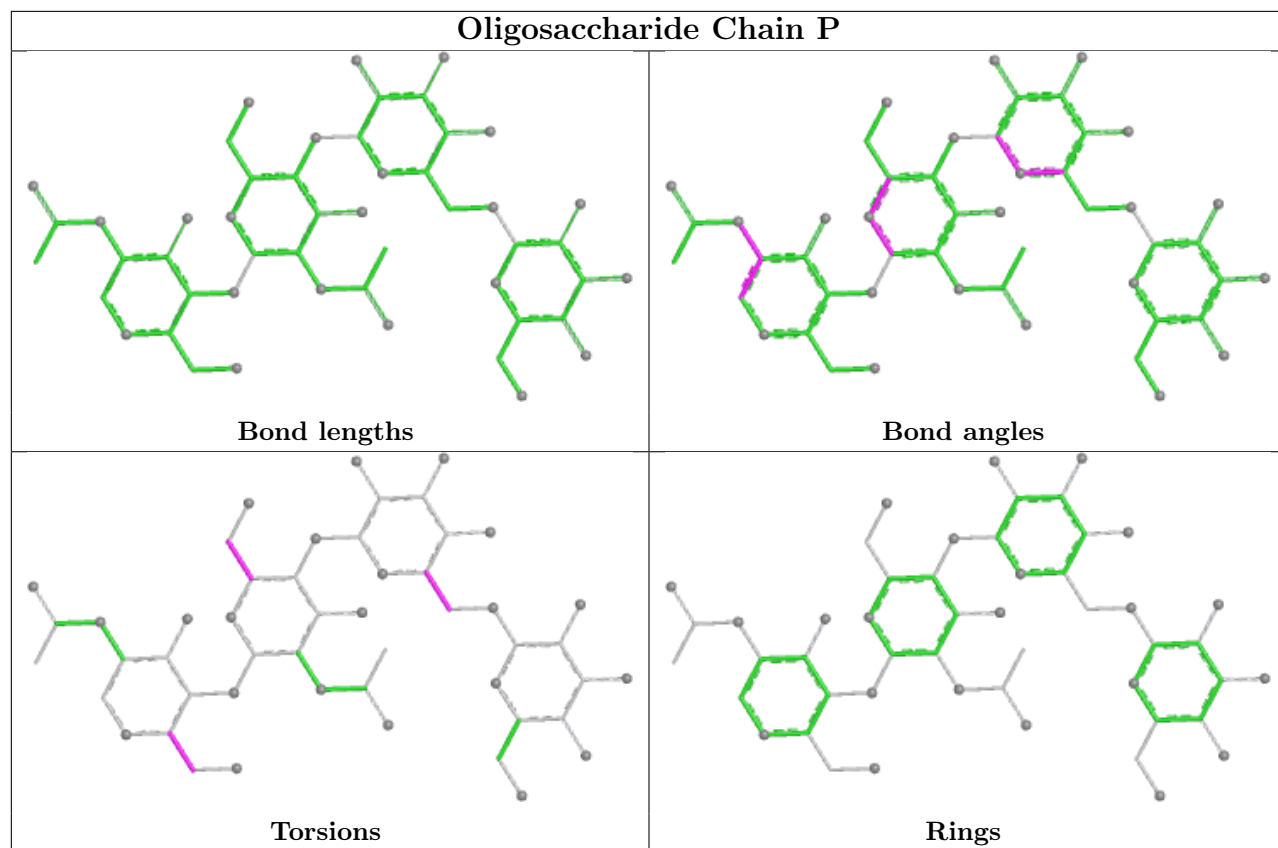


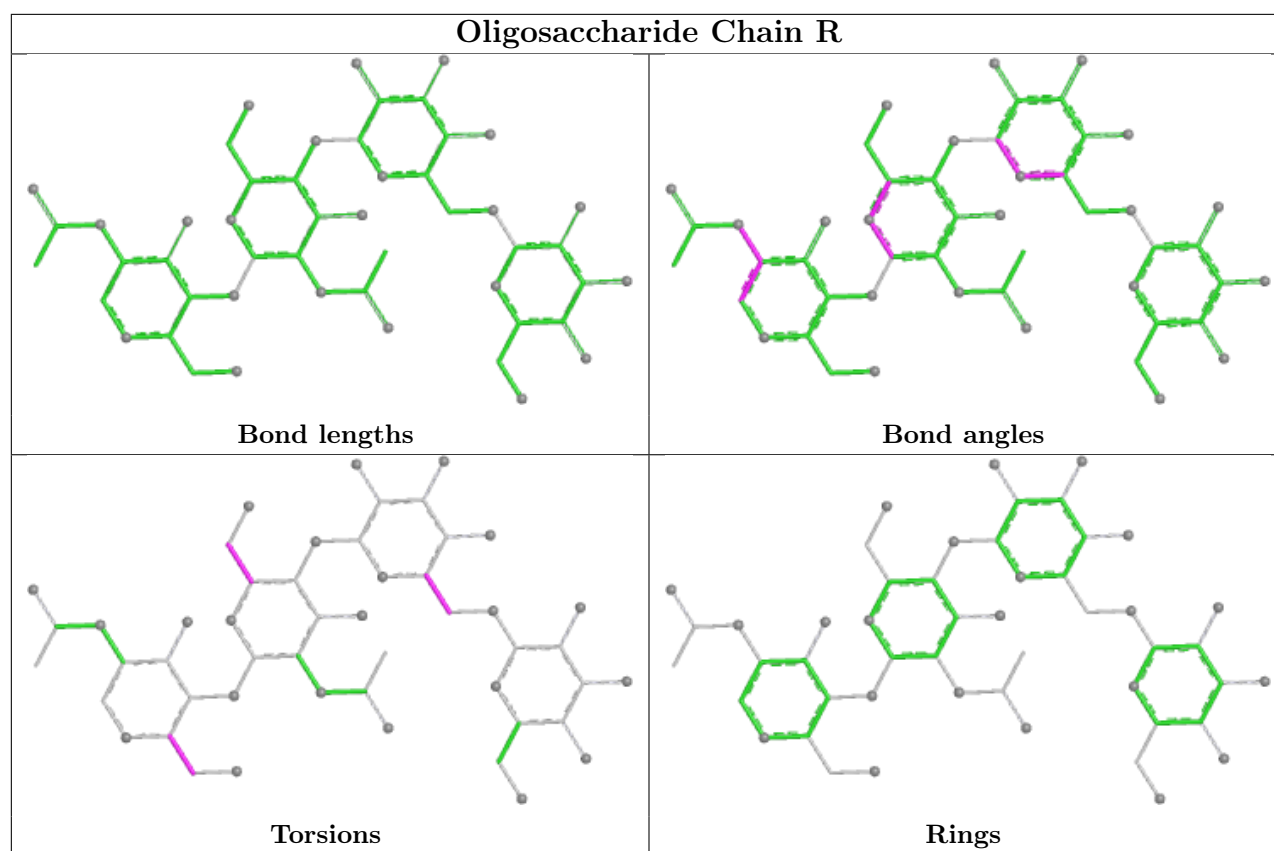












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
9	PTY	H	1101	-	49,49,49	0.27	0	52,54,54	0.31	0
8	CLR	H	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	NAG	C	1003	1	14,14,15	0.33	0	17,19,21	1.30	3 (17%)
10	NAG	K	1001	1	14,14,15	0.31	0	17,19,21	0.56	0
9	PTY	D	1101	-	49,49,49	0.27	0	52,54,54	0.30	0
10	NAG	C	1001	1	14,14,15	0.32	0	17,19,21	0.56	0
8	CLR	D	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	NAG	C	1002	1	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
9	PTY	L	1101	-	49,49,49	0.27	0	52,54,54	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	G	1001	1	14,14,15	0.32	0	17,19,21	0.56	0
8	CLR	L	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	NAG	G	1003	1	14,14,15	0.32	0	17,19,21	1.29	3 (17%)
10	NAG	G	1002	1	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
10	NAG	K	1002	1	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
10	NAG	K	1003	1	14,14,15	0.33	0	17,19,21	1.30	3 (17%)

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
9	PTY	H	1101	-	-	16/53/53/53	-
8	CLR	H	1100	-	-	6/10/68/68	0/4/4/4
10	NAG	C	1003	1	-	2/6/23/26	0/1/1/1
10	NAG	K	1001	1	-	1/6/23/26	0/1/1/1
9	PTY	D	1101	-	-	16/53/53/53	-
10	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
8	CLR	D	1100	-	-	6/10/68/68	0/4/4/4
10	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
9	PTY	L	1101	-	-	16/53/53/53	-
10	NAG	G	1001	1	-	1/6/23/26	0/1/1/1
8	CLR	L	1100	-	-	6/10/68/68	0/4/4/4
10	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
10	NAG	G	1002	1	-	2/6/23/26	0/1/1/1
10	NAG	K	1002	1	-	2/6/23/26	0/1/1/1
10	NAG	K	1003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1003	NAG	C2-N2-C7	2.86	126.73	122.90
10	C	1003	NAG	C2-N2-C7	2.84	126.70	122.90
10	G	1003	NAG	C2-N2-C7	2.81	126.67	122.90
10	G	1003	NAG	C8-C7-N2	2.61	120.45	116.12
10	C	1003	NAG	C8-C7-N2	2.61	120.45	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1003	NAG	C8-C7-N2	2.61	120.45	116.12
10	K	1003	NAG	C1-O5-C5	2.55	115.60	112.19
10	C	1003	NAG	C1-O5-C5	2.54	115.59	112.19
10	G	1003	NAG	C1-O5-C5	2.53	115.58	112.19
10	K	1002	NAG	C2-N2-C7	2.38	126.08	122.90
10	C	1002	NAG	C2-N2-C7	2.33	126.03	122.90
10	G	1002	NAG	C2-N2-C7	2.31	126.00	122.90

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1003	NAG	C8-C7-N2-C2
10	C	1003	NAG	O7-C7-N2-C2
10	G	1003	NAG	C8-C7-N2-C2
10	G	1003	NAG	O7-C7-N2-C2
10	K	1003	NAG	C8-C7-N2-C2
10	K	1003	NAG	O7-C7-N2-C2
8	D	1100	CLR	C20-C22-C23-C24
8	H	1100	CLR	C20-C22-C23-C24
8	L	1100	CLR	C20-C22-C23-C24
9	D	1101	PTY	C11-C8-O7-C6
9	H	1101	PTY	C11-C8-O7-C6
9	L	1101	PTY	C11-C8-O7-C6
9	D	1101	PTY	O10-C8-O7-C6
9	H	1101	PTY	O10-C8-O7-C6
9	L	1101	PTY	O10-C8-O7-C6
9	D	1101	PTY	C18-C19-C20-C21
9	H	1101	PTY	C18-C19-C20-C21
9	L	1101	PTY	C18-C19-C20-C21
9	D	1101	PTY	C25-C26-C27-C28
9	H	1101	PTY	C25-C26-C27-C28
9	L	1101	PTY	C25-C26-C27-C28
9	D	1101	PTY	C15-C16-C17-C18
9	H	1101	PTY	C15-C16-C17-C18
9	L	1101	PTY	C15-C16-C17-C18
9	H	1101	PTY	C40-C41-C42-C43
9	L	1101	PTY	C40-C41-C42-C43
9	D	1101	PTY	C40-C41-C42-C43
10	C	1001	NAG	O5-C5-C6-O6
10	G	1001	NAG	O5-C5-C6-O6
10	K	1001	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	D	1101	PTY	C12-C13-C14-C15
9	H	1101	PTY	C12-C13-C14-C15
9	L	1101	PTY	C12-C13-C14-C15
9	D	1101	PTY	C35-C36-C37-C38
9	H	1101	PTY	C35-C36-C37-C38
9	L	1101	PTY	C35-C36-C37-C38
9	D	1101	PTY	O4-C1-C6-O7
9	H	1101	PTY	O4-C1-C6-O7
9	L	1101	PTY	O4-C1-C6-O7
8	D	1100	CLR	C21-C20-C22-C23
8	H	1100	CLR	C21-C20-C22-C23
8	L	1100	CLR	C21-C20-C22-C23
8	D	1100	CLR	C13-C17-C20-C22
8	H	1100	CLR	C13-C17-C20-C22
8	L	1100	CLR	C13-C17-C20-C22
8	D	1100	CLR	C16-C17-C20-C22
8	H	1100	CLR	C16-C17-C20-C22
8	L	1100	CLR	C16-C17-C20-C22
9	D	1101	PTY	C6-C5-O14-P1
9	H	1101	PTY	C6-C5-O14-P1
9	L	1101	PTY	C6-C5-O14-P1
8	D	1100	CLR	C13-C17-C20-C21
8	H	1100	CLR	C13-C17-C20-C21
8	L	1100	CLR	C13-C17-C20-C21
9	D	1101	PTY	O14-C5-C6-O7
9	H	1101	PTY	O14-C5-C6-O7
9	L	1101	PTY	O14-C5-C6-O7
9	L	1101	PTY	C33-C34-C35-C36
9	H	1101	PTY	C33-C34-C35-C36
9	D	1101	PTY	C33-C34-C35-C36
9	H	1101	PTY	C26-C27-C28-C29
9	L	1101	PTY	C26-C27-C28-C29
9	D	1101	PTY	C26-C27-C28-C29
10	C	1002	NAG	C1-C2-N2-C7
10	G	1002	NAG	C1-C2-N2-C7
10	K	1002	NAG	C1-C2-N2-C7
10	C	1002	NAG	C3-C2-N2-C7
10	G	1002	NAG	C3-C2-N2-C7
10	K	1002	NAG	C3-C2-N2-C7
9	H	1101	PTY	C20-C21-C22-C23
9	L	1101	PTY	C20-C21-C22-C23
9	D	1101	PTY	C20-C21-C22-C23

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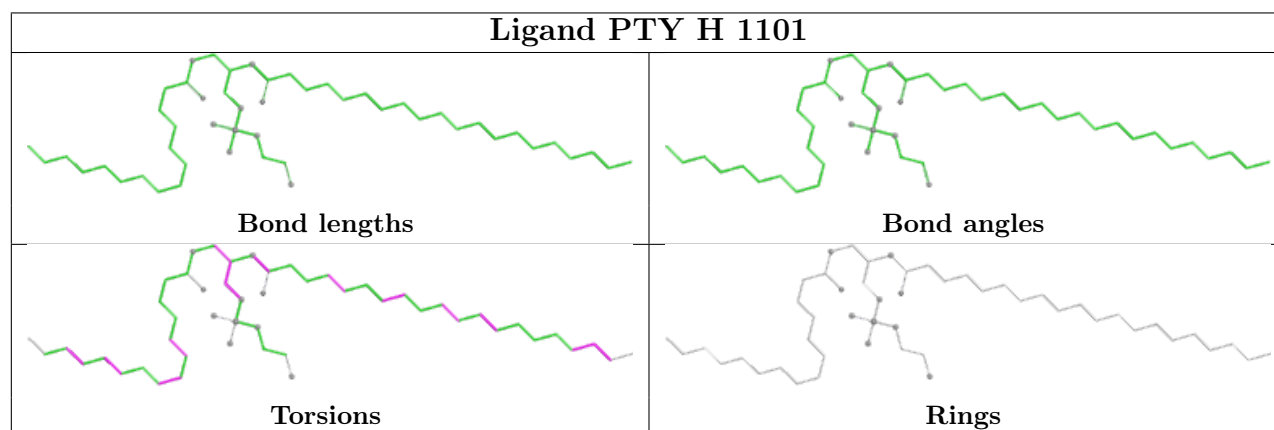
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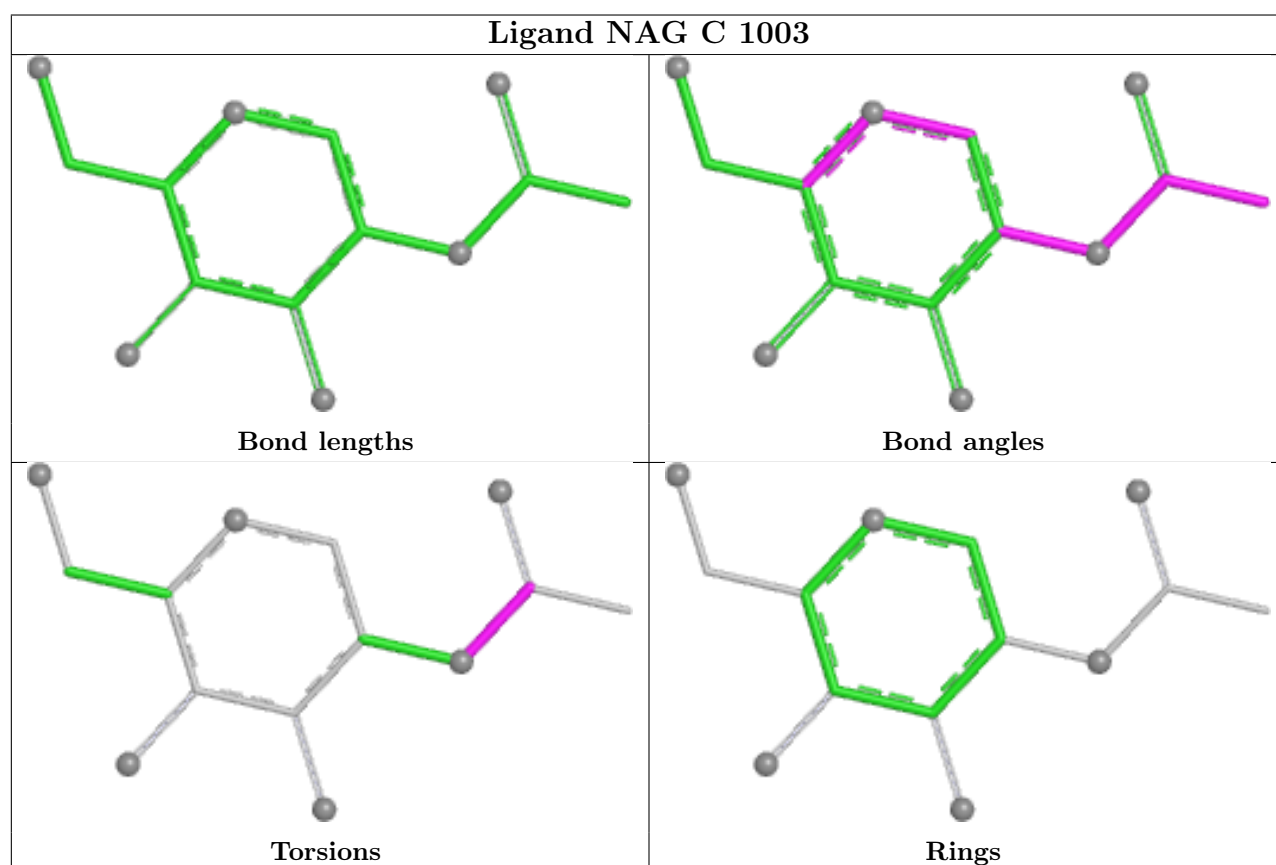
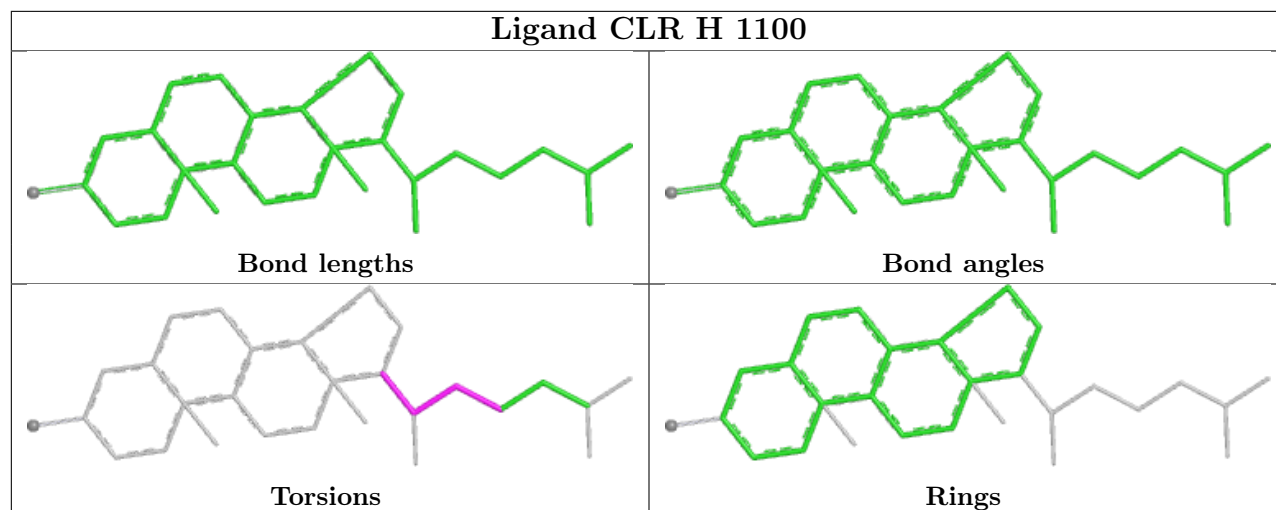
Mol	Chain	Res	Type	Atoms
8	D	1100	CLR	C16-C17-C20-C21
8	H	1100	CLR	C16-C17-C20-C21
8	L	1100	CLR	C16-C17-C20-C21
9	D	1101	PTY	O4-C1-C6-C5
9	H	1101	PTY	O4-C1-C6-C5
9	L	1101	PTY	O4-C1-C6-C5
9	H	1101	PTY	C38-C39-C40-C41
9	D	1101	PTY	C38-C39-C40-C41
9	L	1101	PTY	C38-C39-C40-C41

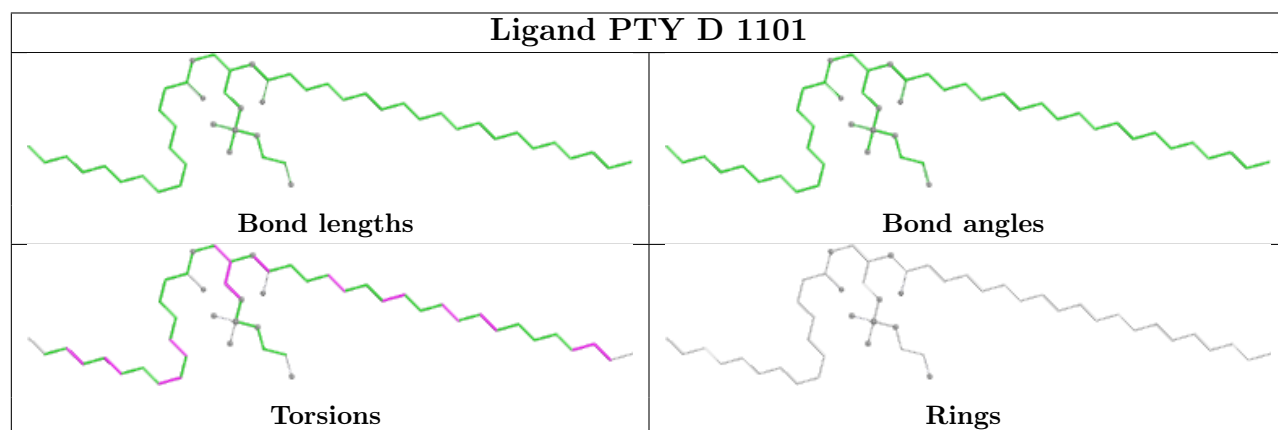
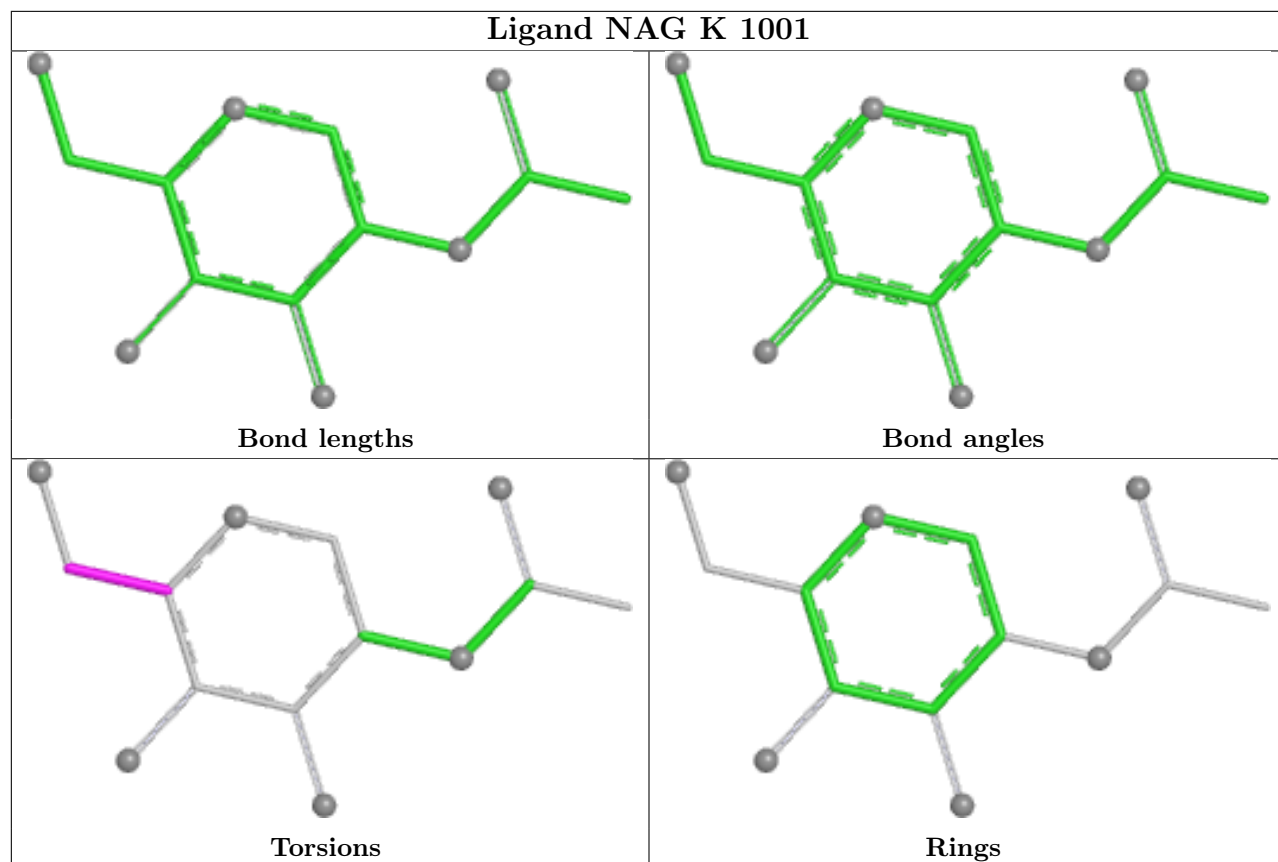
There are no ring outliers.

No monomer is involved in short contacts.

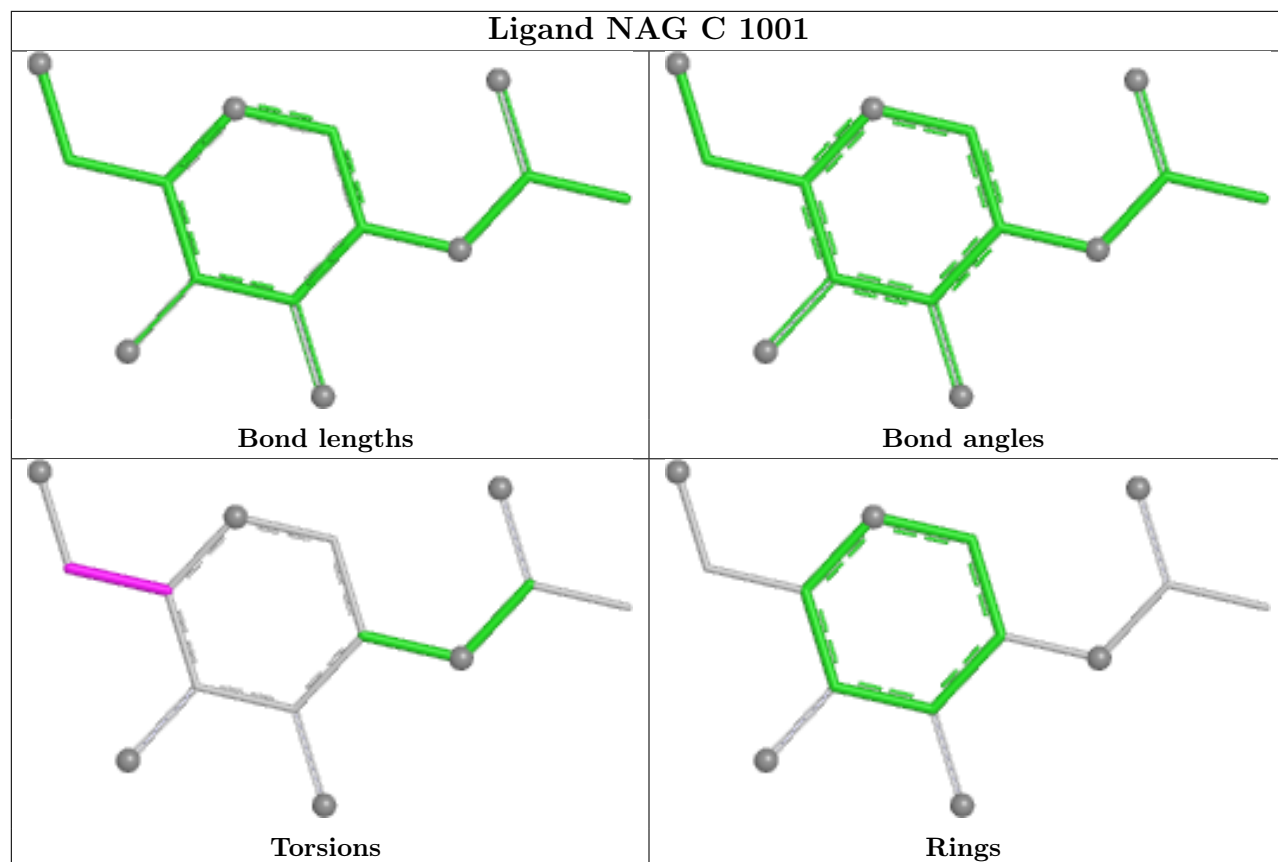
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



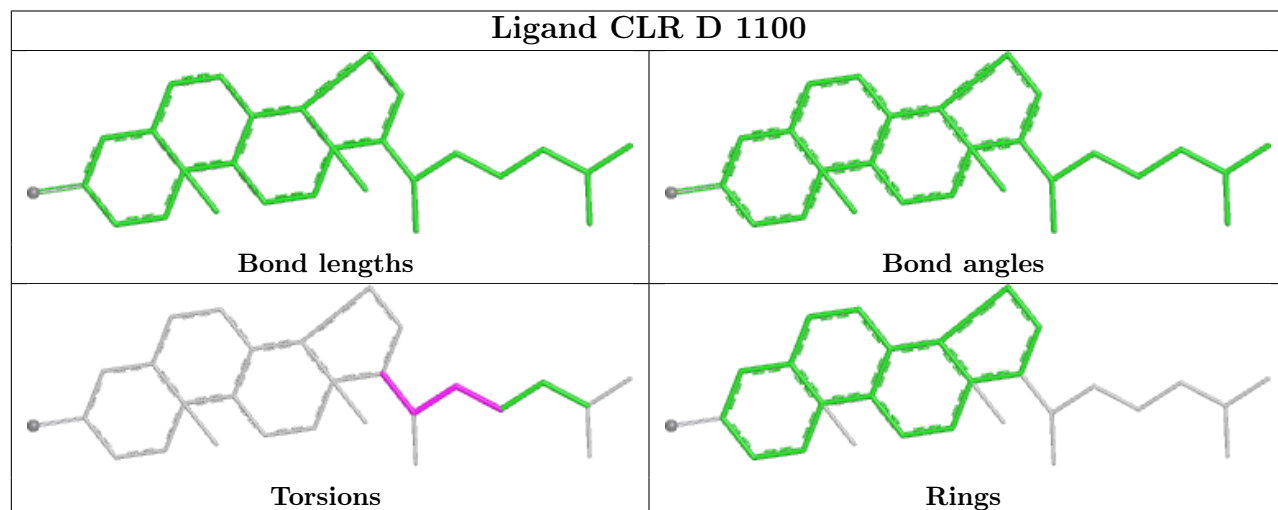


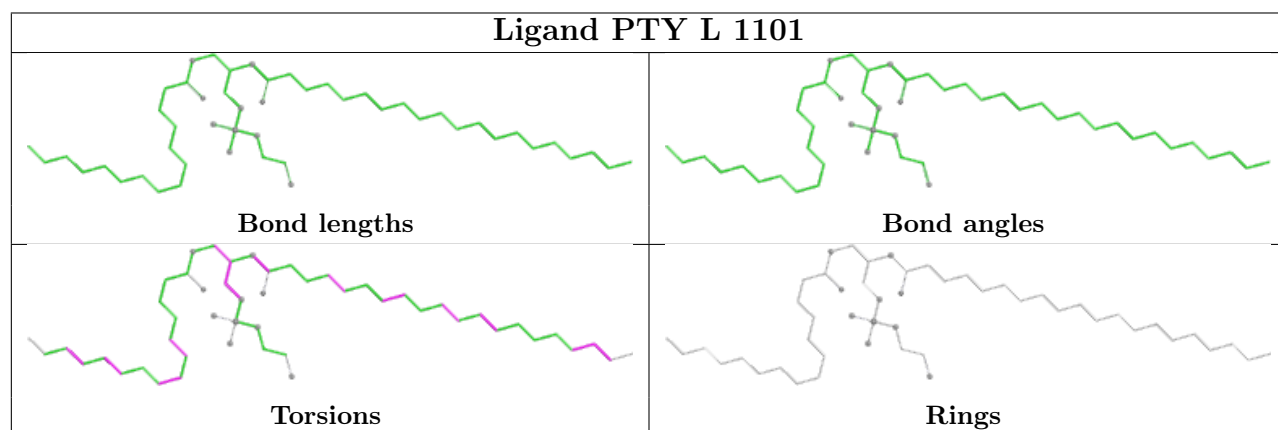
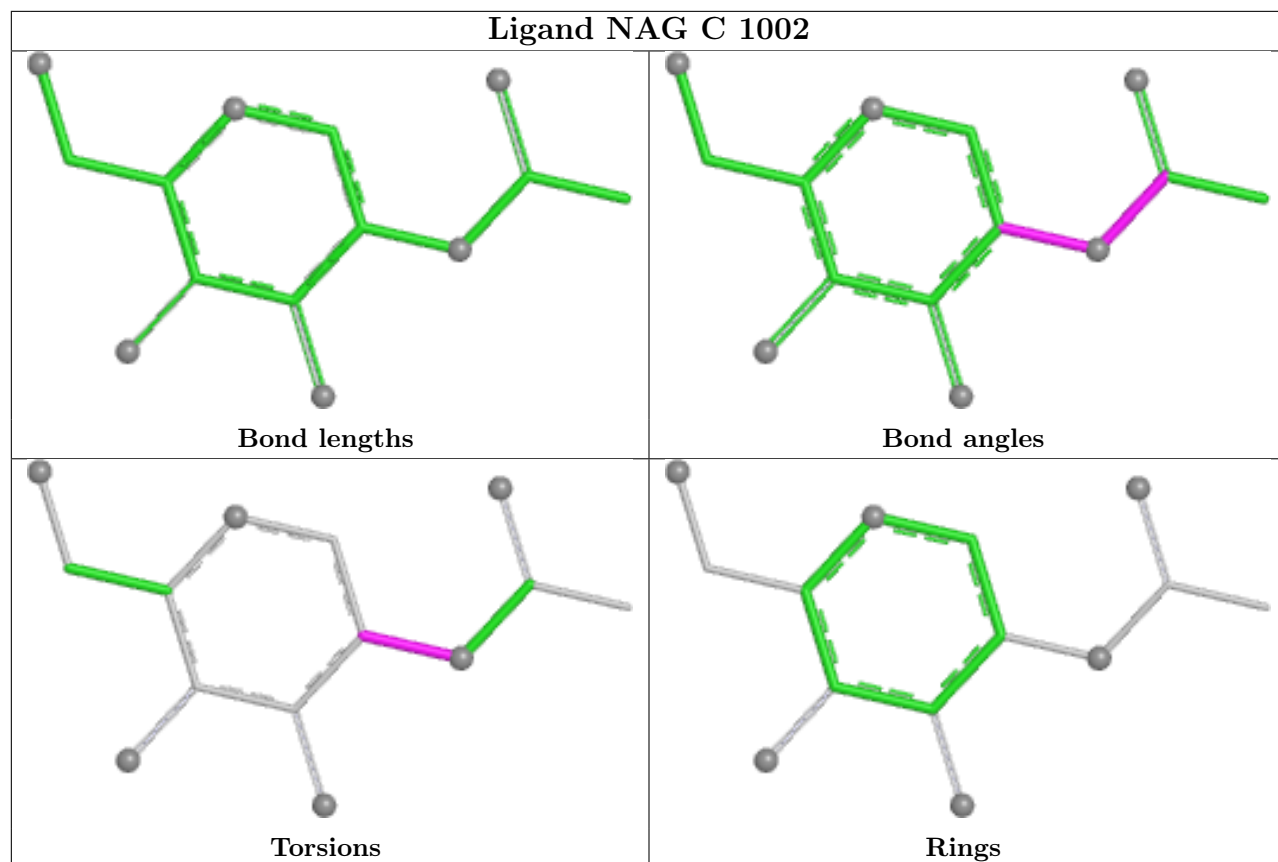


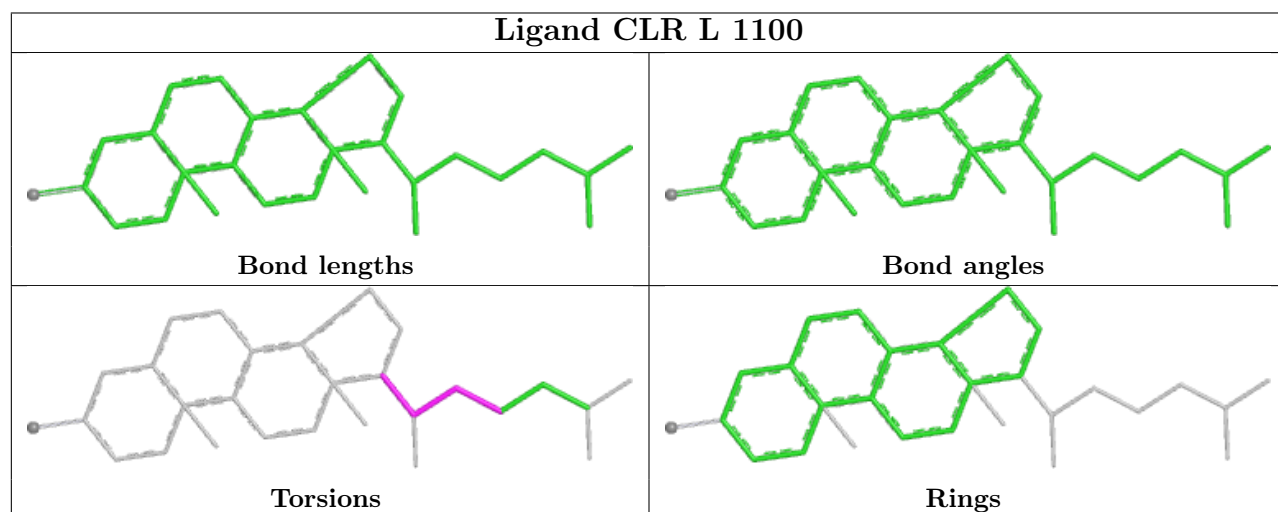
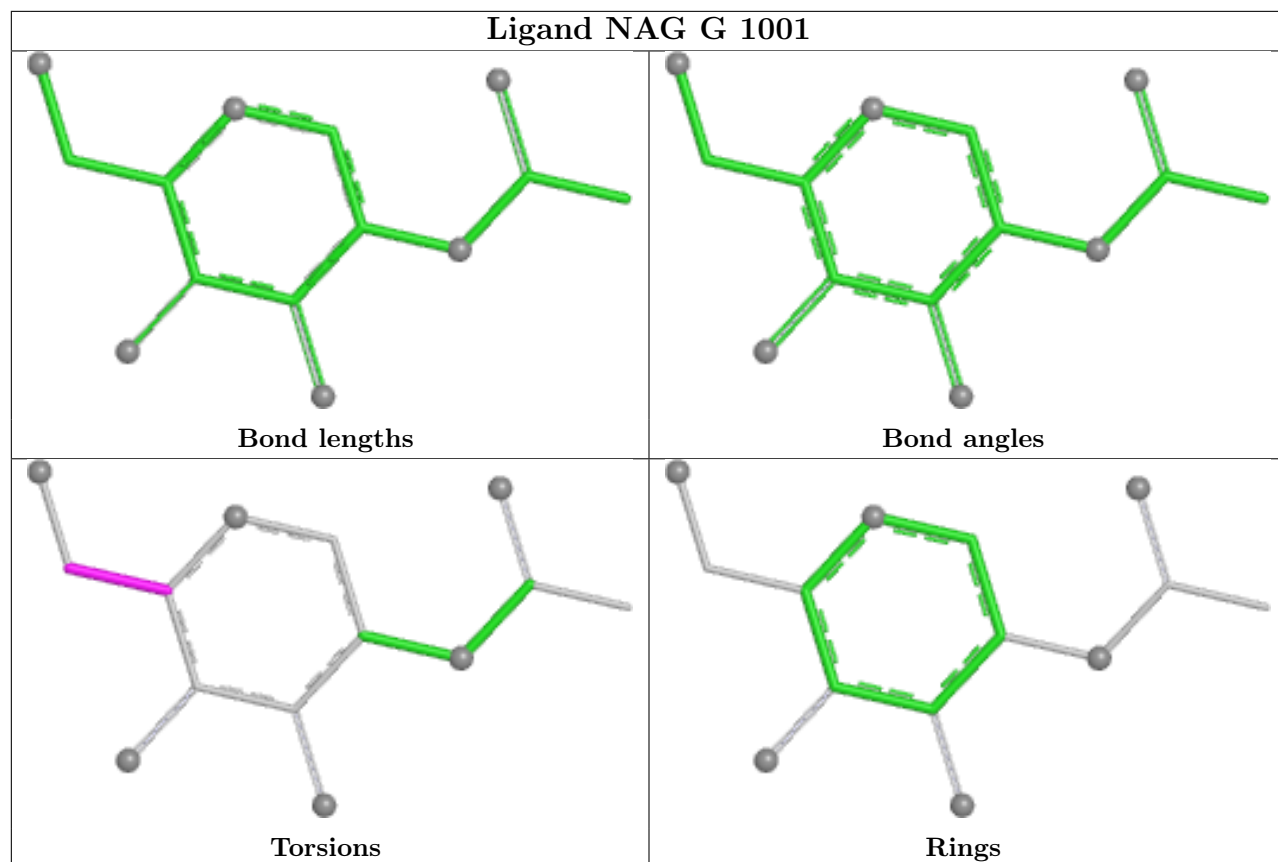
Ligand NAG C 1001

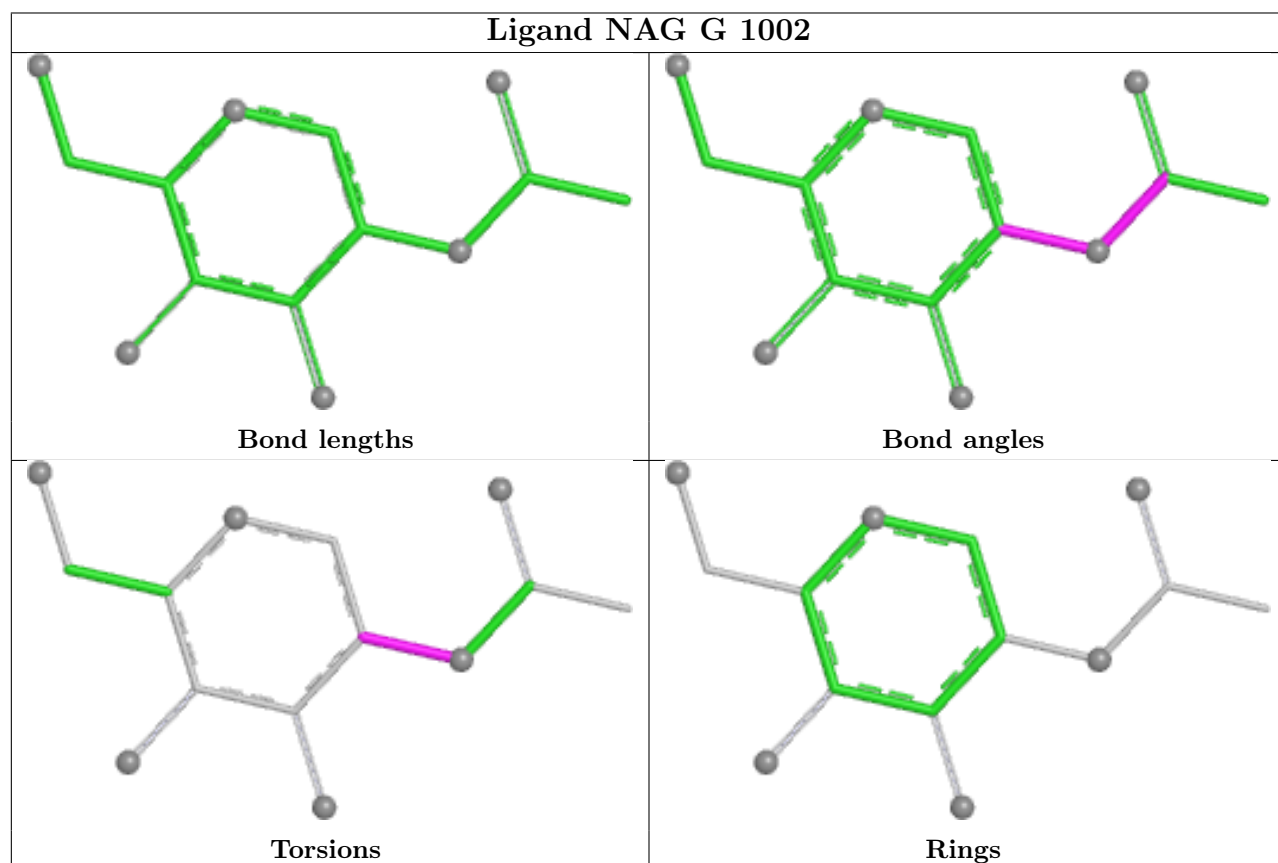
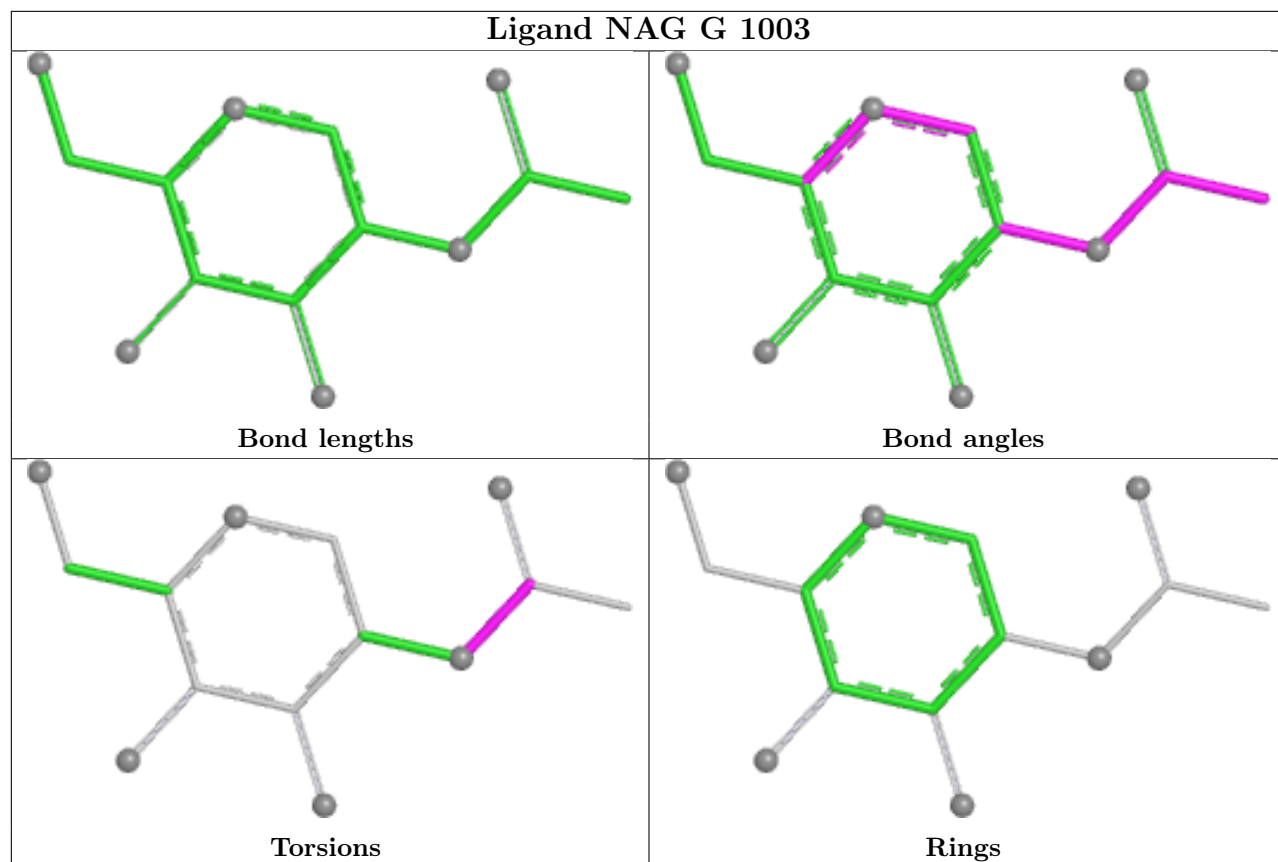


Ligand CLR D 1100

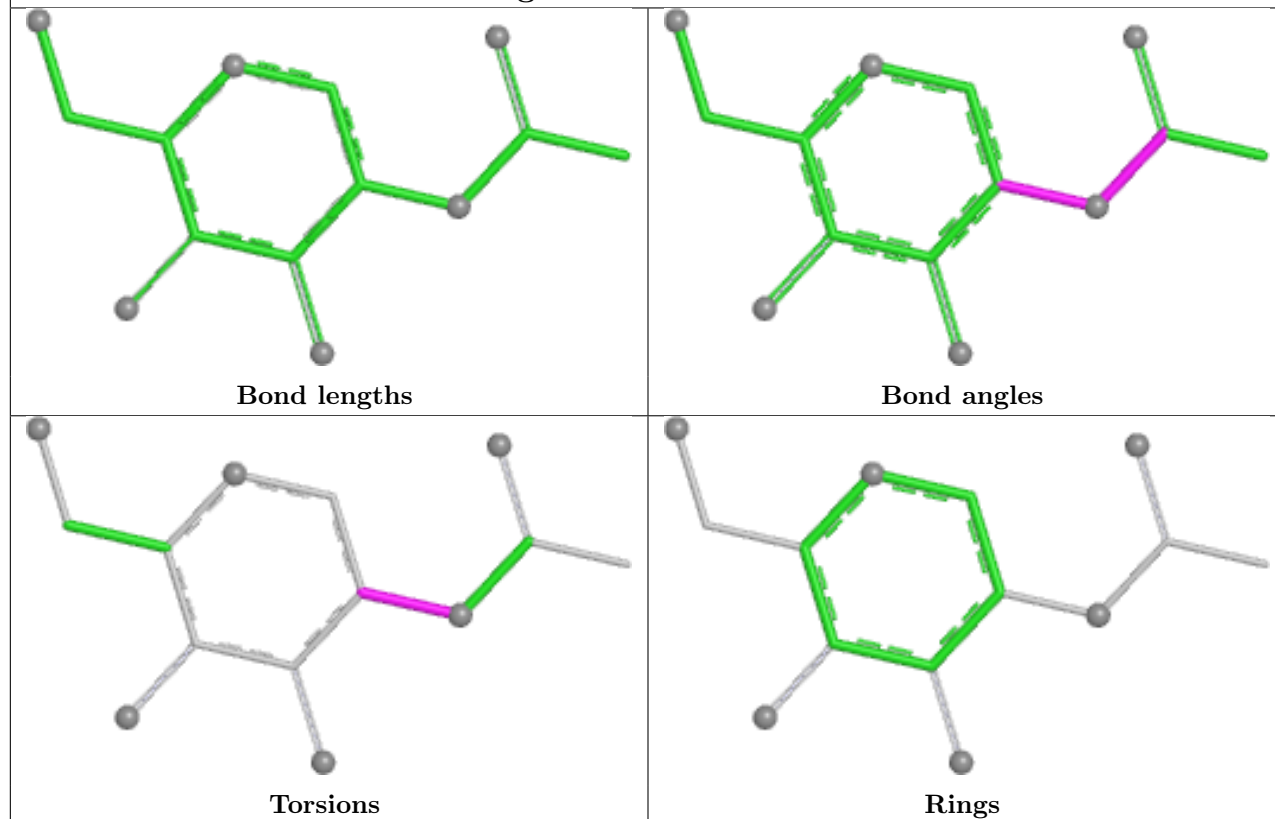




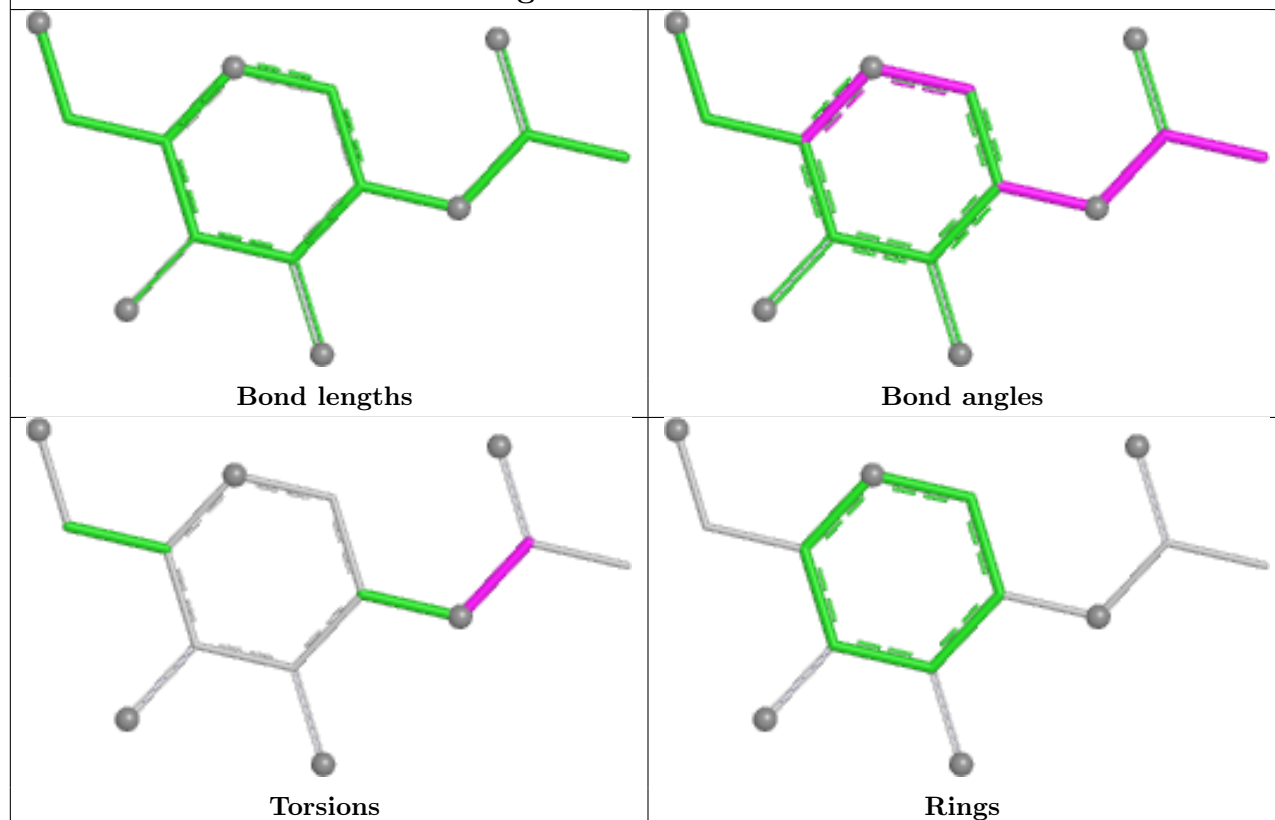




Ligand NAG K 1002



Ligand NAG K 1003



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.

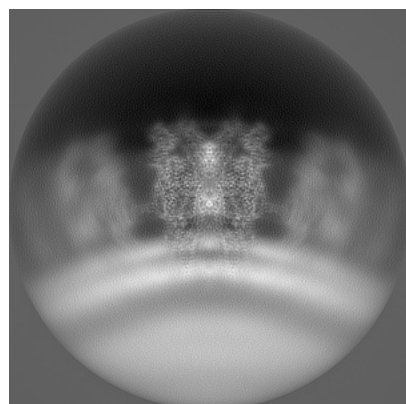
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17311. These allow visual inspection of the internal detail of the map and identification of artifacts.

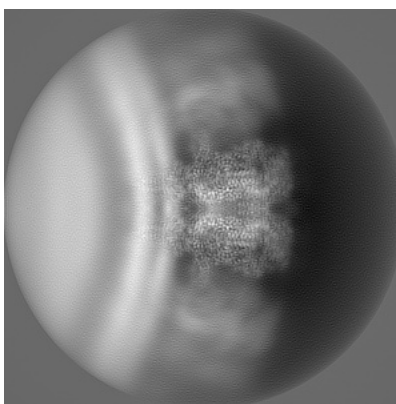
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

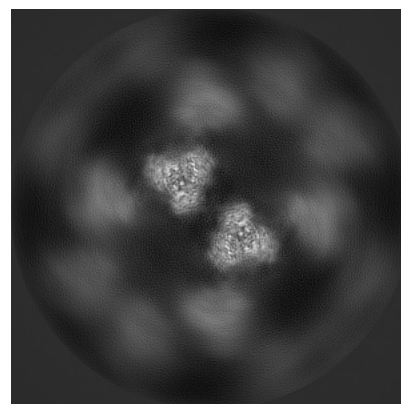
6.1.1 Primary map



X

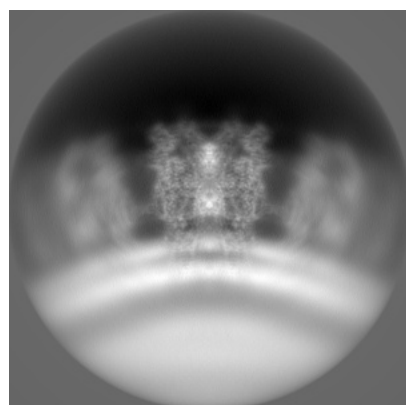


Y

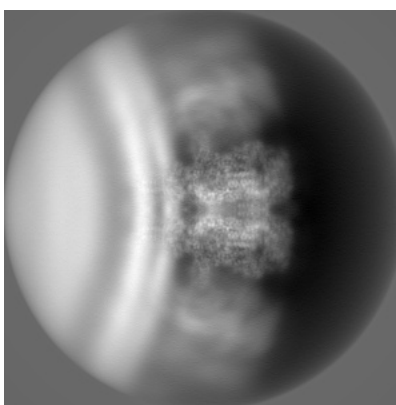


Z

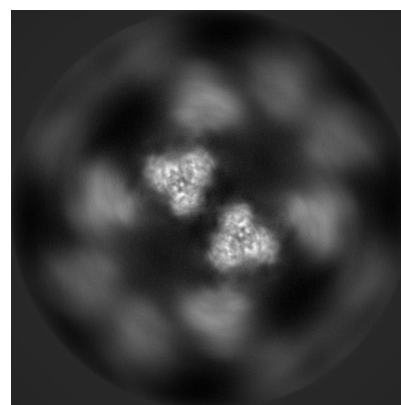
6.1.2 Raw map



X



Y

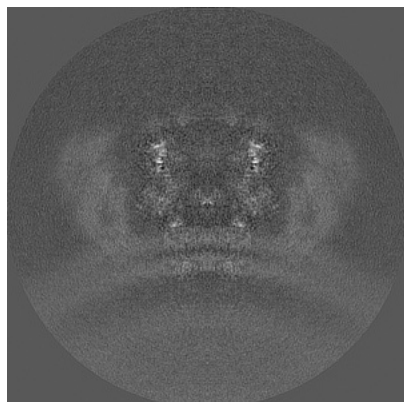


Z

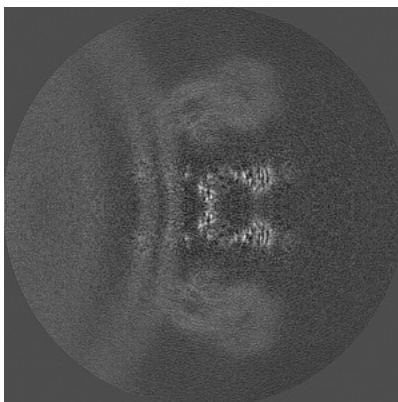
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

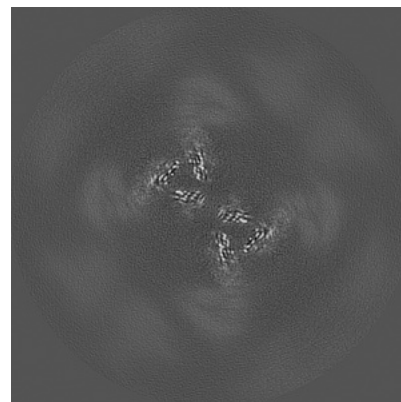
6.2.1 Primary map



X Index: 240

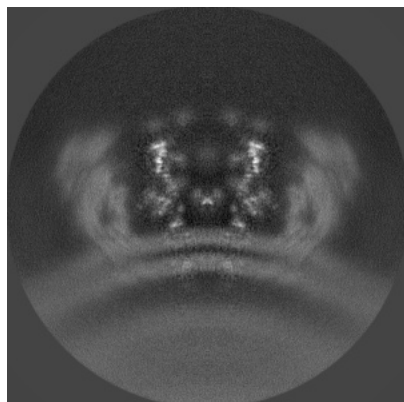


Y Index: 240

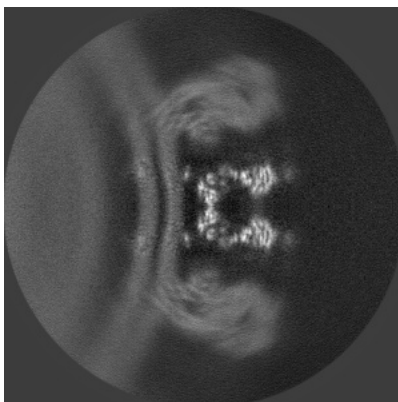


Z Index: 240

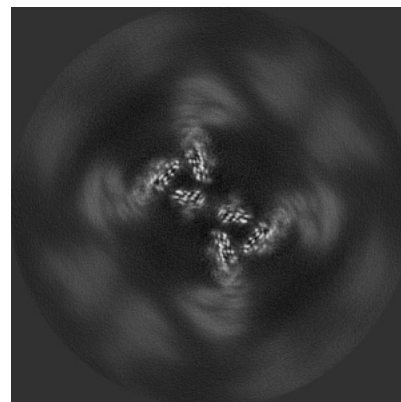
6.2.2 Raw map



X Index: 240



Y Index: 240

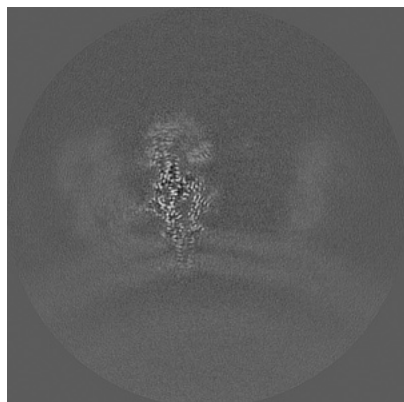


Z Index: 240

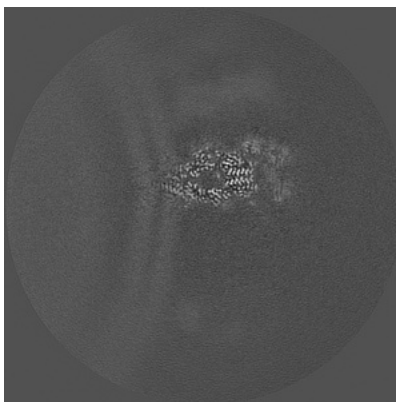
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

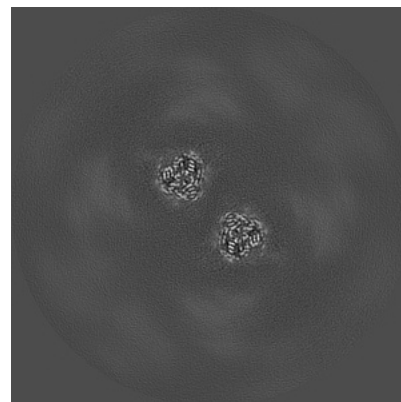
6.3.1 Primary map



X Index: 260

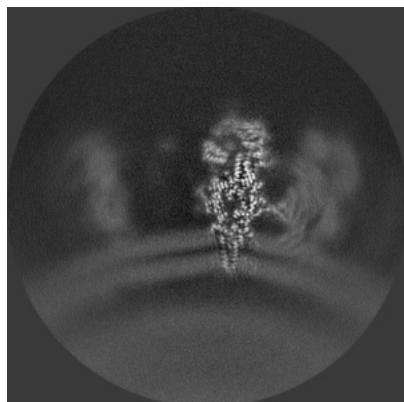


Y Index: 200

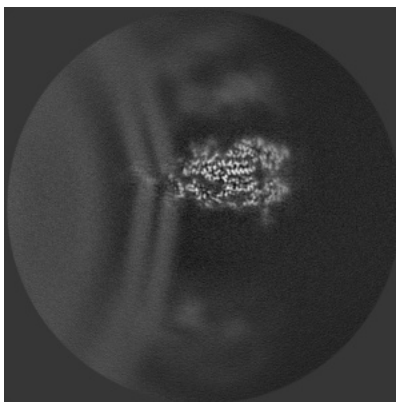


Z Index: 268

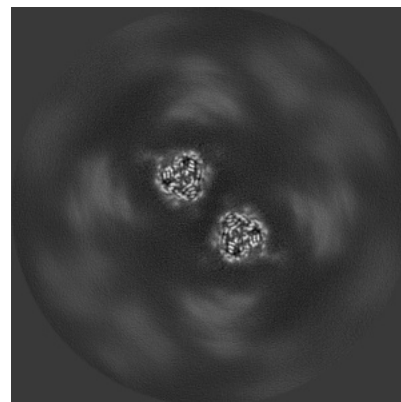
6.3.2 Raw map



X Index: 219



Y Index: 192

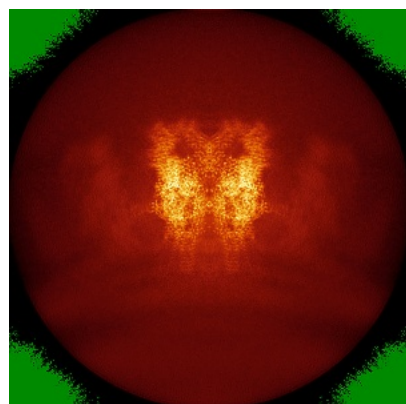


Z Index: 268

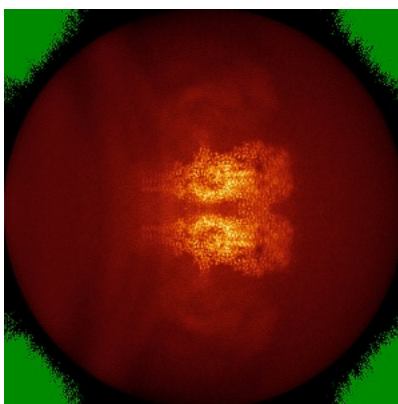
The images above show the largest variance slices of the map in three orthogonal directions.

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

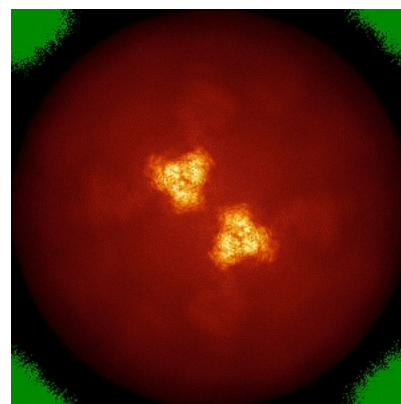
6.4.1 Primary map



X

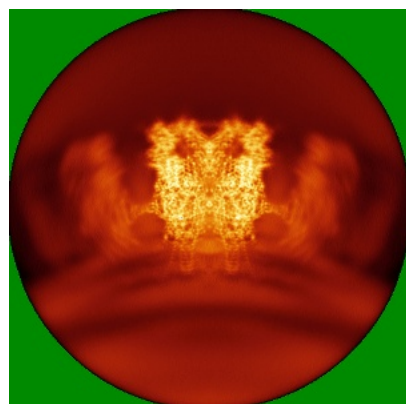


Y

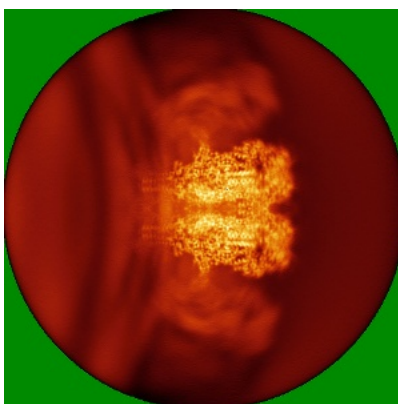


Z

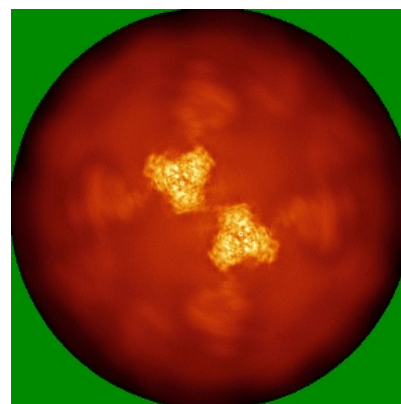
6.4.2 Raw map



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](#)

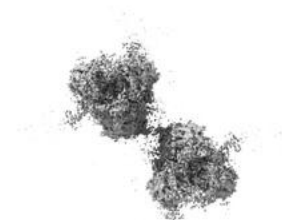
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

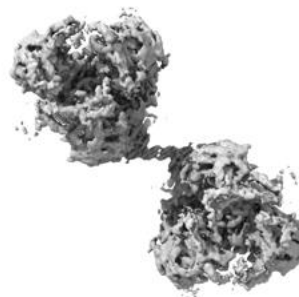
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

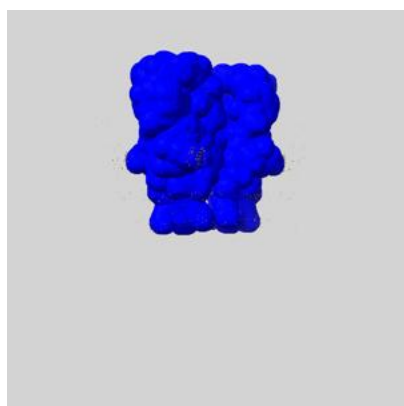
6.6 Mask visualisation [i](#)

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

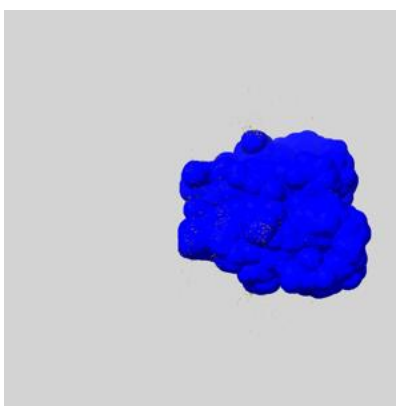
A mask typically either:

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

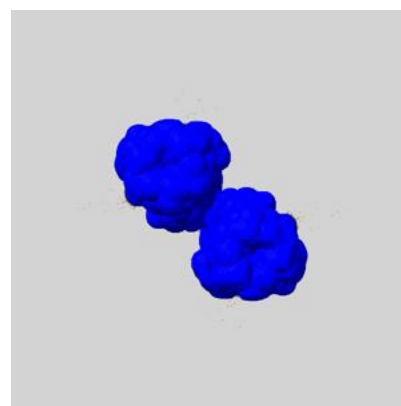
6.6.1 emd_17311_msk_1.map [i](#)



X



Y

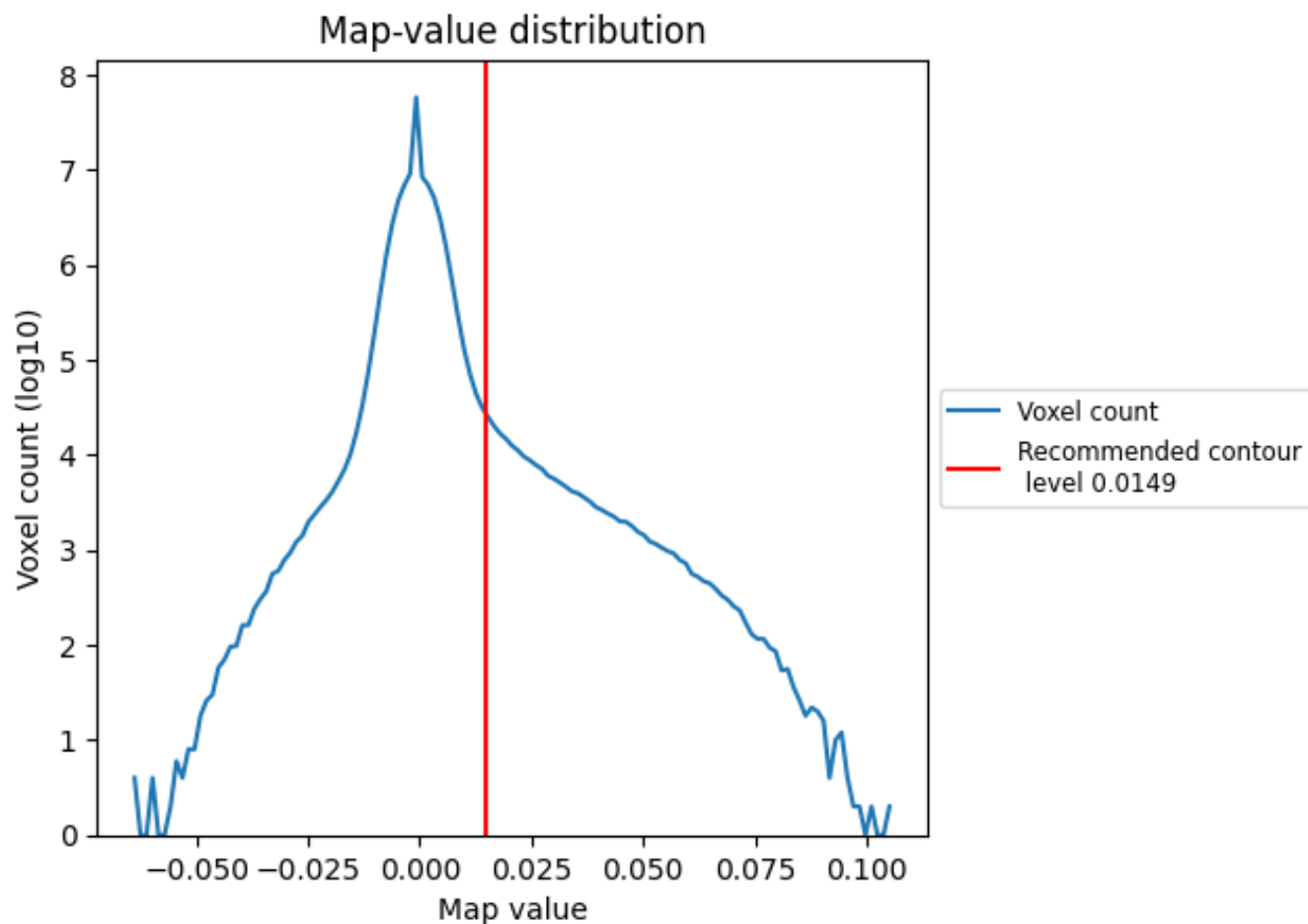


Z

7 Map analysis [i](#)

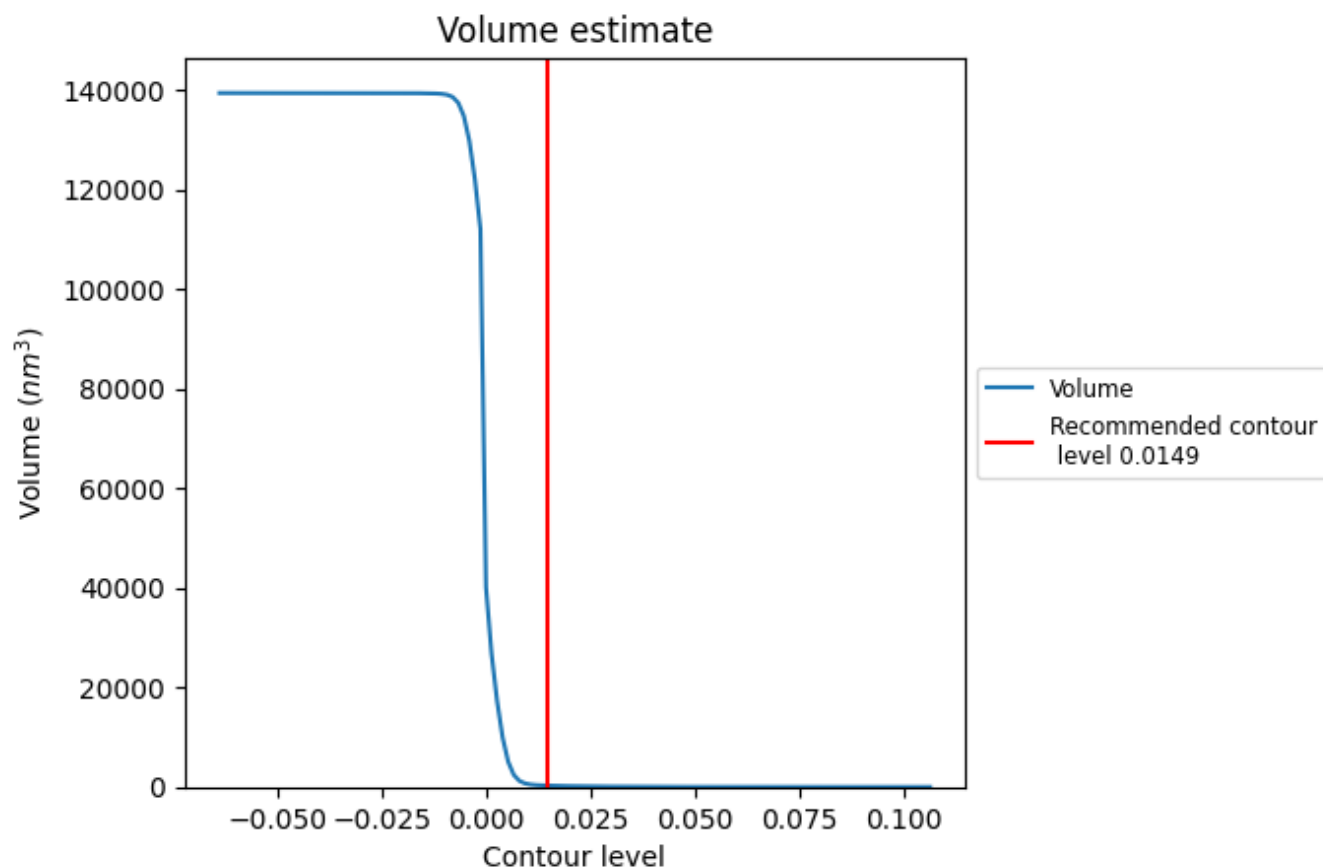
This section contains the results of statistical analysis of the map.

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.

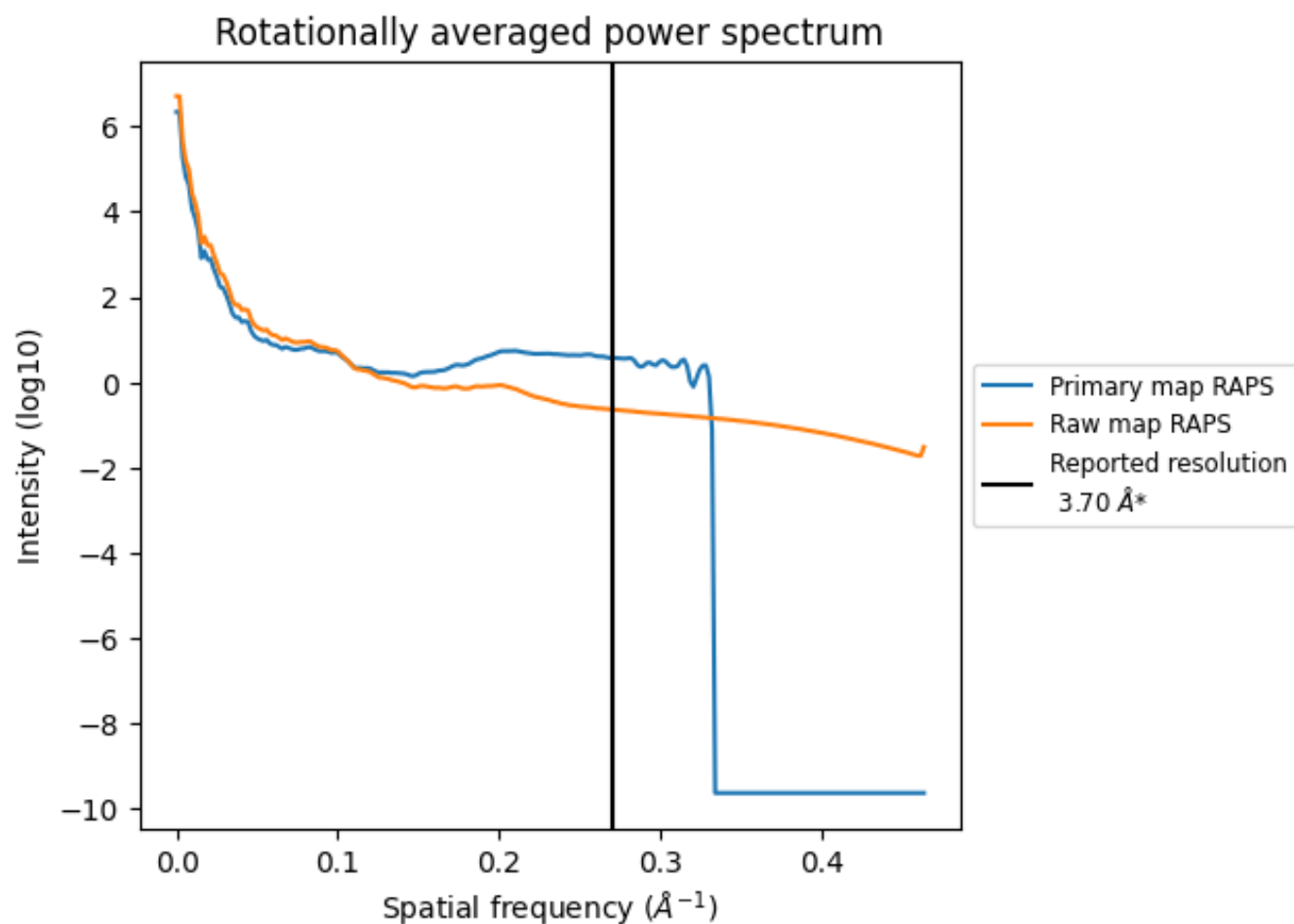
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm^3 ; this corresponds to an approximate mass of 240 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

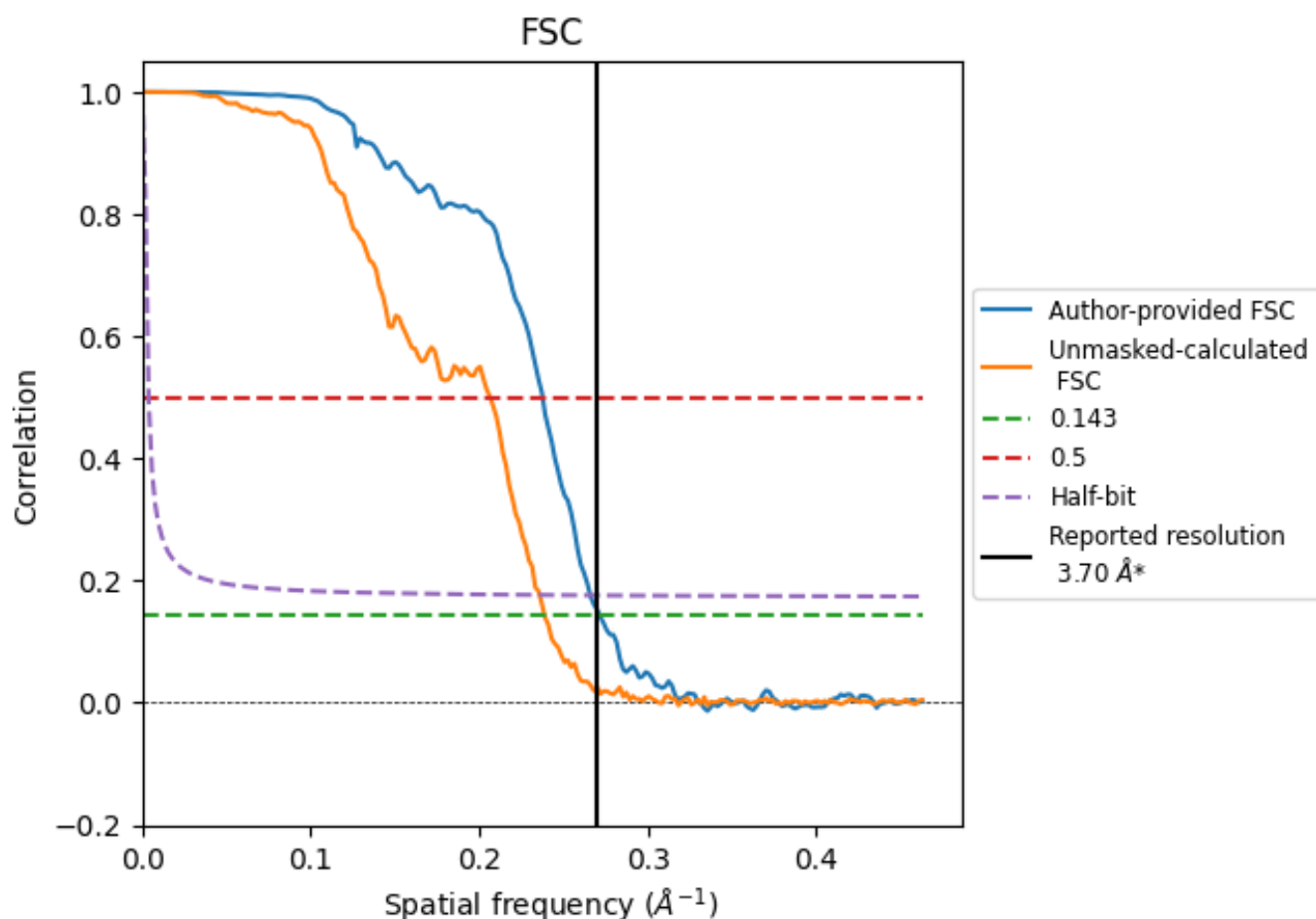


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.21	3.76
Unmasked-calculated*	4.19	4.84	4.24

*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 4.19 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

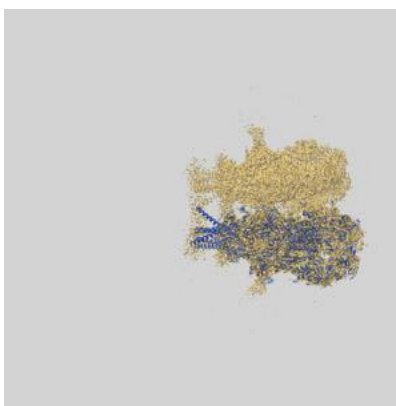
This section contains information regarding the fit between EMDB map EMD-17311 and PDB model 8OZJ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

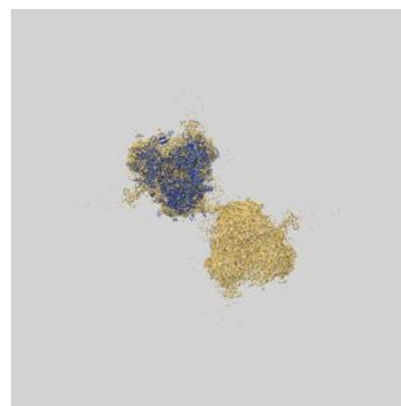
9.1.1 Map-model overlay [i](#)



X

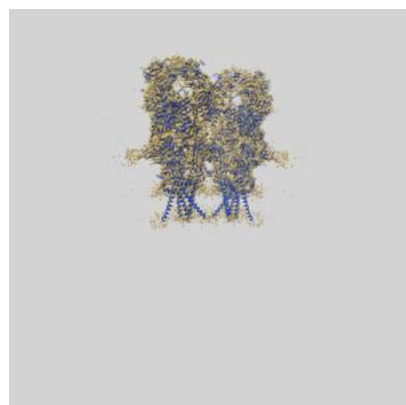


Y

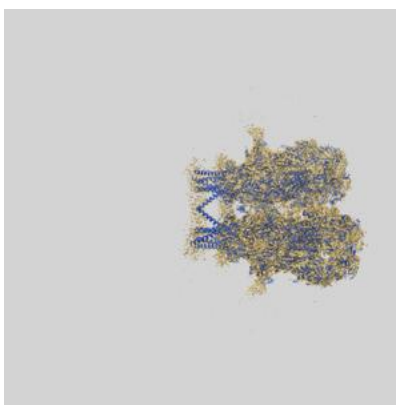


Z

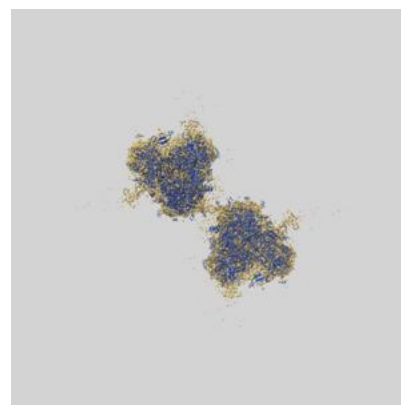
9.1.2 Map-model assembly overlay [i](#)



X



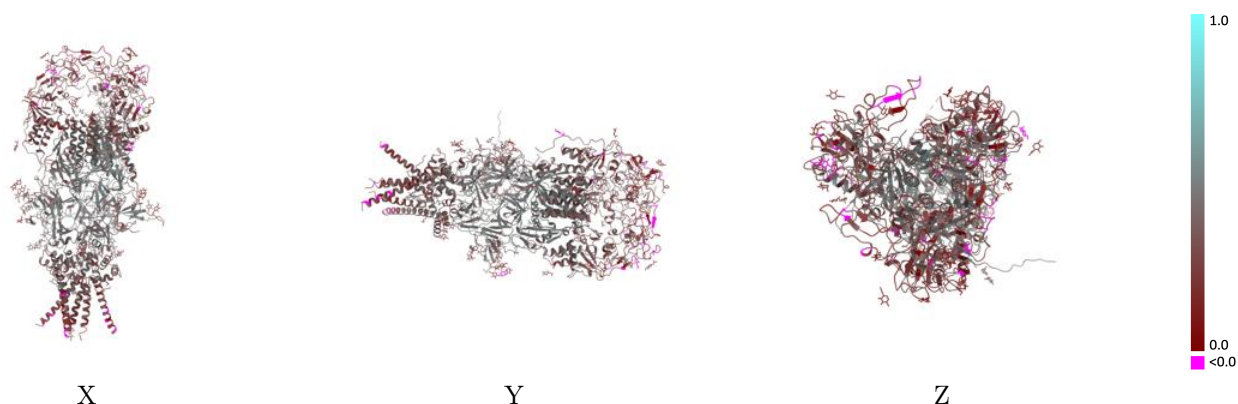
Y



Z

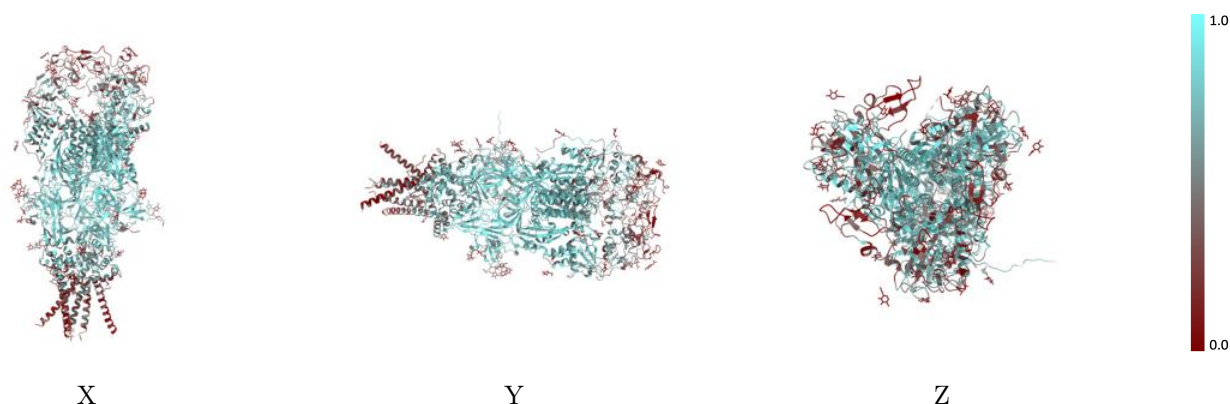
The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



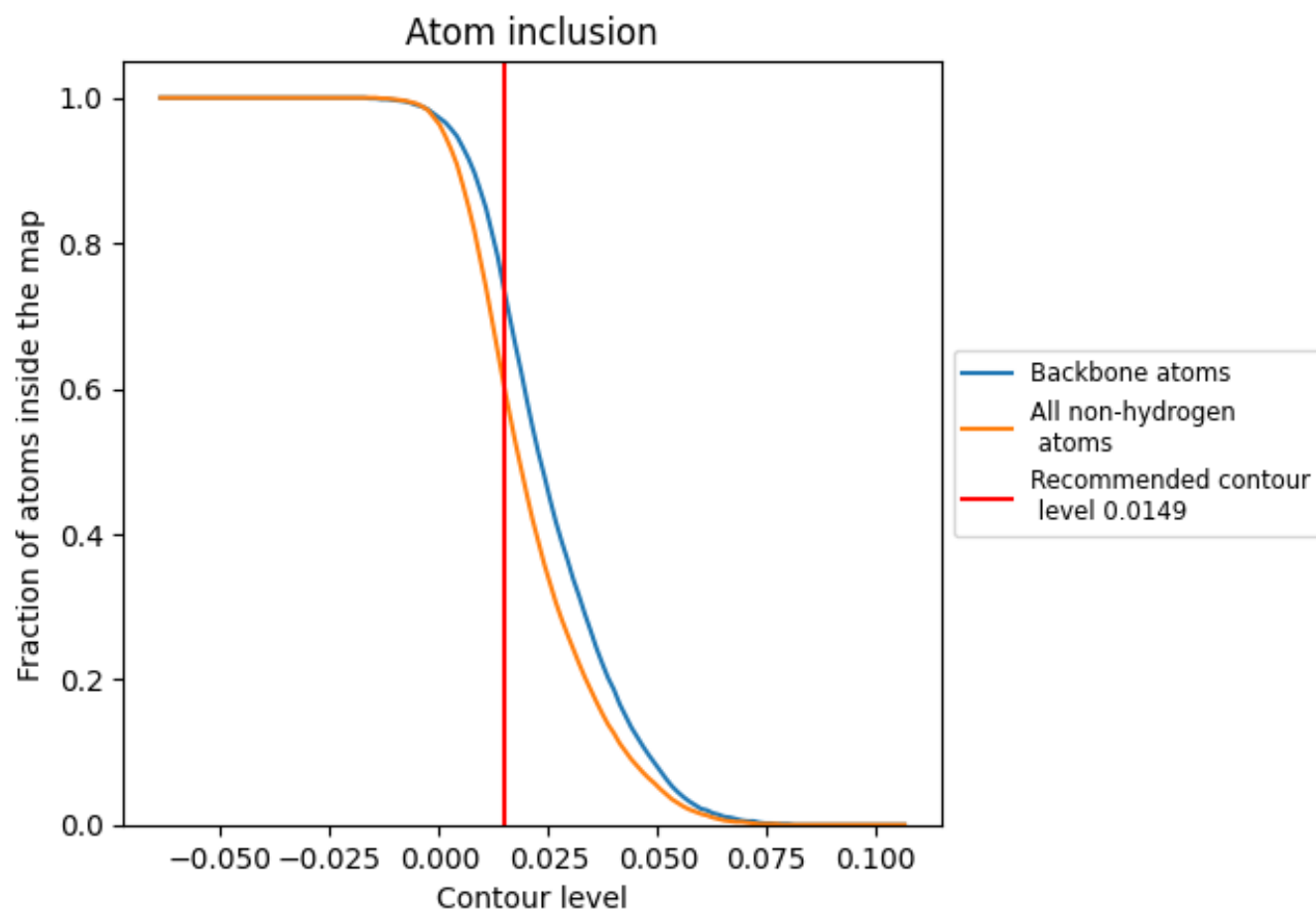
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0149).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6020	 0.3570
A	 0.4510	 0.3160
C	 0.5730	 0.3220
D	 0.7010	 0.4200
E	 0.4940	 0.3410
F	 0.5710	 0.4310
G	 0.5010	 0.2870
H	 0.7080	 0.4200
I	 0.4510	 0.3350
J	 0.6150	 0.3830
K	 0.5620	 0.3150
L	 0.7210	 0.4250
M	 0.3570	 0.3160
N	 0.3570	 0.2350
O	 0.2500	 0.2180
P	 0.2000	 0.1850
Q	 0.2800	 0.1750
R	 0.2400	 0.1200
S	 0.3080	 0.3330
T	 0.2560	 0.2370
U	 0.2820	 0.2730
V	 0.4400	 0.2430
W	 0.2930	 0.1970
X	 0.4000	 0.2390
Y	 0.3210	 0.3070
Z	 0.4640	 0.2670
a	 0.2860	 0.3340
b	 0.2860	 0.3610
c	 0.4290	 0.2180
d	 0.3930	 0.1810
e	 0.4470	 0.3380
f	 0.5000	 0.3720
g	 0.5110	 0.3720
h	 0.3470	 0.3520
i	 0.2920	 0.2920
j	 0.4170	 0.2840

