



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:10 PM UTC

PDB ID : 8OZQ / pdb_00008ozq
EMDB ID : EMD-17318
Title : In situ subtomogram average of Prototype Foamy Virus Env hexamer of trimers
Authors : Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on : 2023-05-09
Resolution : 10.00 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:

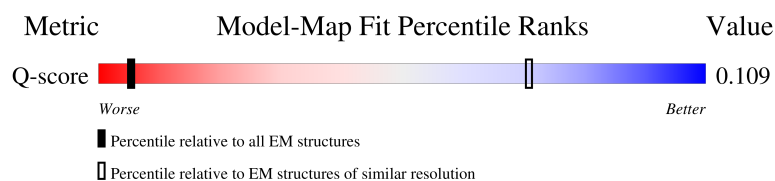
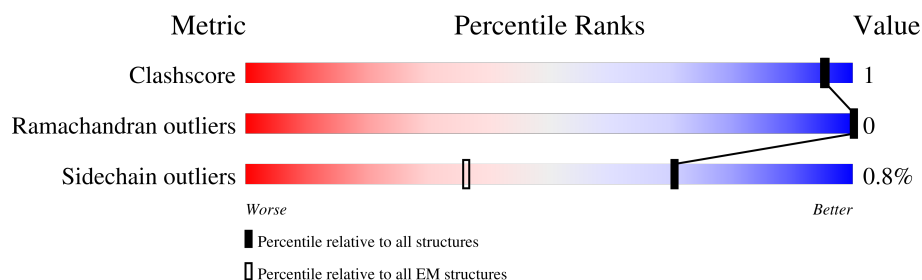
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 10.00 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.



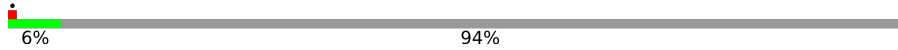
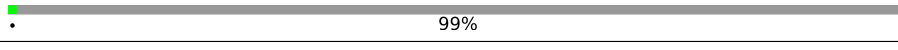
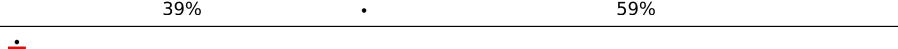
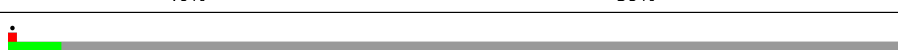
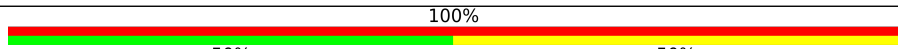
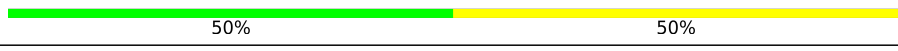
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	147 (9.50 - 10.50)

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	B	988	 40% 58%
1	C	988	 40% 58%
1	D	988	 40% 59%

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Mol	Chain	Length	Quality of chain
1	E	988	
1	F	988	
1	G	988	
1	H	988	
1	I	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	S	3	
3	T	3	
3	U	3	
4	V	6	
4	W	6	
4	X	6	
5	P	4	
5	Q	4	
5	R	4	
6	e	8	

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Mol	Chain	Length	Quality of chain
6	f	8	38% 62% 38%
6	g	8	25% 62% 38%
7	h	6	67% 50% 50%
7	i	6	67% 50% 50%
7	j	6	67% 50% 50%

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.



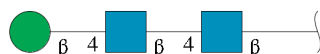
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		

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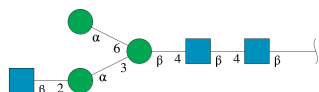
Mol	Chain	Residues	Atoms				AltConf	Trace
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	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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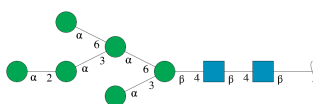
Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	6	Total	C	N	O	0	0
			75	42	3	30		
4	W	6	Total	C	N	O	0	0
			75	42	3	30		

- 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.



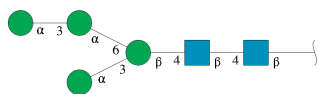
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



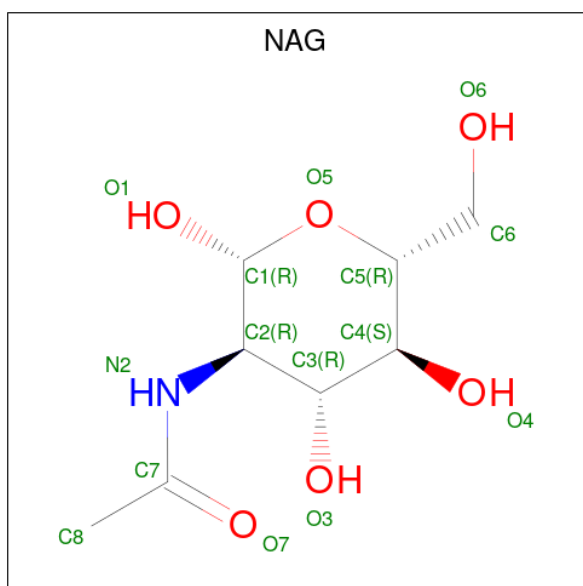
Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	g	8	Total	C	N	O	0	0
			94	52	2	40		

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



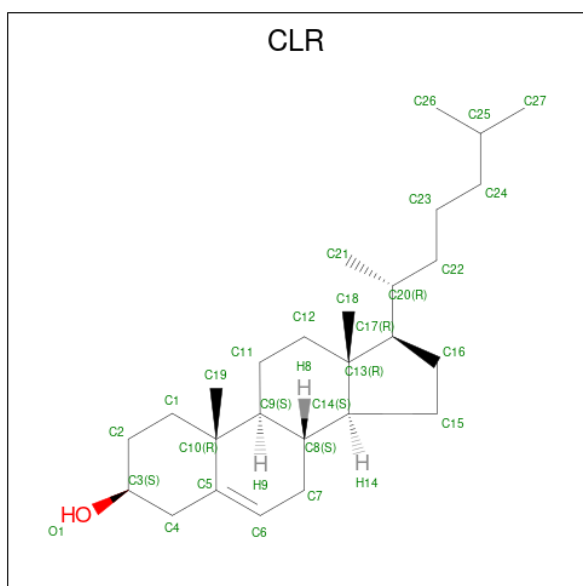
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

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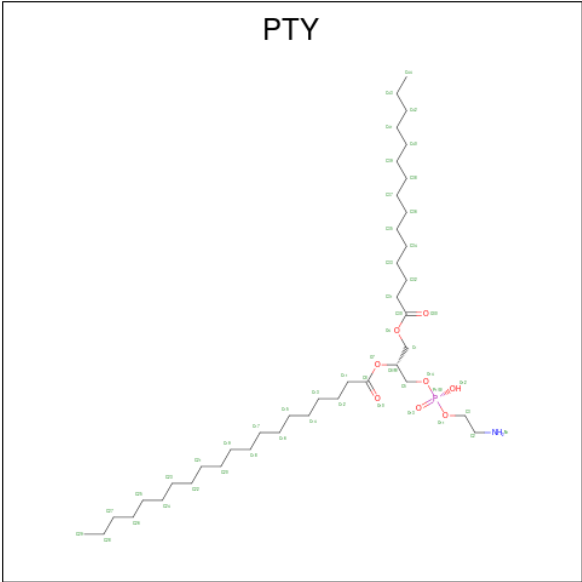
Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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

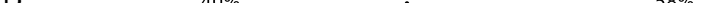
- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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	

LEU SER GLY THR ALA GLN GLY ILE PHE GLY GLY THR ALA PHE SER LEU LEU TYR LYS PRO ILE LEU LEU ILE GLY VAL GLY VAL ILE LEU LEU VAL ILE LEU LEU PHE LYS VAL SER TRP ILE PRO THR LYS LYS ASN GN

- Molecule 1: Envelope glycoprotein

Chain B: 

MET	ALA	PRO	PRO	MET	THR	LEU	GLN	GLN	TRP	TRP	ILE	ILE	TRP	LYS	ASN	ASN	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	ILE	GLN	ASN	GLU	GLU	GLU	VAL	VAL	PRO	THR	THR	ARG	ARG	ASP	LYS	PHE	ARG	TYR	LEU	LEU	LEU	TYR	THR
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CYS	CYS	ALA	THR	SER	SER	ARG	VAL	LEU	LEU	ALA	ALA	TRP	PHE	ILE	LEU	VAL	CYS	ILE	LEU	LEU	LEU	SER	CYS	PHE	VAL	VAL	THR	THR	ILE	SER	ARG	ARG	ILE	GLN	GLN	VAL	LEU	LEU	GLY	PRO	VAL	VAL	ILE	ILE	ASP	TRP	ASN	ASN	VAL	THR	THR	GLN	GLN	ARG	ALA	VAL	Tyr	VAL	Gln	PRO	PRO	LEU	TYR
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The diagram illustrates the interaction between a set of 120 amino acids (arranged in a grid) and various proteins. The amino acids are color-coded: green for those with specific interactions (indicated by red diamonds) and yellow for others. The proteins are listed on the left and right sides of the grid.

Proteins on the left: F406, T407, K408, D409, M410, L411, S412, GLN, LEU, VAL, PRO, GLU, CYS, ASP, GLY, PHE, TYR, ASN, SER, LYS, TRP, MET, HIS, MET, HIS, P432.

Proteins on the right: THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.

Interactions (Red Diamonds):

- F406 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- T407 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- K408 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- D409 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- M410 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- L411 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- S412 interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- GLN interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- LEU interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- VAL interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- PRO interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- GLU interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- CYS interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- ASP interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- GLY interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- PHE interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- TYR interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- ASN interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- SER interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L341, S349, G350, A358, A370, C404, M405.
- LYS interacts with THR, ARG, ARG, ILE, ALA, ARG, S127, V134, P135, K136, Y137, V138, Y151, E211, K241, E242, G260, TYR, HIS, ALA, GLY, LEU, THR, N268, D274, I277, N286, S291, K292, L298, Y302, S305, S306, E337, L34

E560
T563
SER
CYS
ASN
ASN
ARG
LYS
ARG
ARG
SER
VAL
ASP
ASN
ASN
TYR
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LYS
LEU
ARG
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GLU ALA THR THR HIS LEU ASP ILE SER VAL MET MET GLY GLU MET PHE ALA ALA VAL GLN GLN HIS LEU HIS HIS HIS HIS LEU LEU LEU THR THR MET LEU LEU GLU ARG ARG ARG ARG ASP ASP TRP THR TYR MET MET SER SER THR THR TRP TRP LEU LEU GLN GLN GLN GLN LEU LEU GLN GLN LYS LYS MET MET ASP ASP GLU GLU VAL VAL ILE ILE

ARG ILE ALA ARG SER LEU VAL TYR TYR VAL VAL LYS GLN THR HIS SER SER PRO THR ALA THR ALA TRP TRP GLU GLE ILE GLY TYR TYR TYR GLU LEU VAL VAL ILE PRO PRO LYS LYS HIS ILE TYR LEU LEU ASN ASN ASN VAL VAL ASN ILE GLY HIS LEU VAL VAL LYS SER SER ALA ALA GLY GLN LEU THR HIS VAL THR

ILE ALA HIS PRO GUU ILE ILE ASN GLU VAL CYS ASP THR ARG GNL ASP ASP THR VAL ILE CYS ASP VAL VAL LYS ILE ILE GNL PRG VAL VAL LYS ASP SER SER ASP THR ASP CYS PRG VAL TRP ALA GLU PHE

VAL	GLN	VAL	ASN	PRO	LEU	LYS	ASN	GLY	SER	THR	LEU	VAL	LEU	ALA	ALA	SER	SER	THR	ASP	CYS	GLN	PRO	PRO	PRO	TYR	VAL	VAL	PRO	PRO	ILE	ILE	VAL	THR	THR	THR	THR	THR	SER	SER	CYS	PHE	GLY	LEU	ASP	PHE	LYS	ARG	PRO	PRO	LEU	VAL	ALA	GLU	GLU	ARG	ARG	SER	PHE	GLU	PRO	PRO	LEU	LEU
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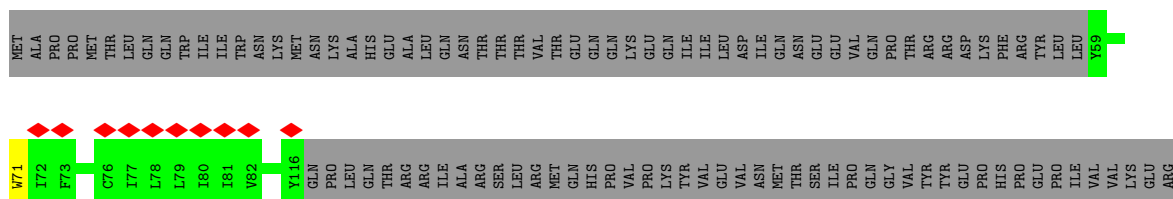
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FILE	PRO	THR	LYS	LYS	LYS	ASN	GLN
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- Molecule 1: Envelope glycoprotein

Chain D: 40% 59%

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

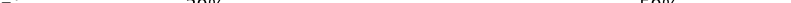
- Molecule 1: Envelope glycoprotein

Chain I: 6% 94%

[illegible]

[illegible]

- Molecule 1: Envelope glycoprotein

Chain G:  39% 59%

ALA	HIS	ASN	ILE	TYR	SER	ARG	CYS	THR	MET
ALA	LEU	GLY	ASN	TYR	VAL	ARG	A370	ARG	ALA
ALA	VAL	SER	LYS	VAL	MET	ARG	B405	ARG	PRO
SER	GLY	TYR	GLU	LYS	GLY	SER	F406	ALA	MET
LEU	ILE	VAL	VAL	THR	MET	VAL	F407	ARG	THR
GLN	ALA	LEU	THR	HIS	PHE	ASP	K408	SER	LEU
GLY	LYS	SER	ALA	SER	VAL	ASN	K409	LEU	GLN
GLY	LYS	SER	TYR	PRO	GLN	TYR	D409	ARG	VAL
ASN	GLY	THR	LEU	THR	HIS	ALA	S412	MET	ALA
PHE	ILE	ASP	HIS	ALA	LEU	LYS	GLN	HIS	TRP
LEU	LYS	CYS	LEU	THR	HIS	LEU	LEU	P133	PHE
GLY	ILE	GLN	GLU	ALA	THR	ARG	VAL	V134	ASN
SER	GLU	ILE	ASP	TRP	HIS	SER	PRO	P135	VAL
THR	VAL	PRO	CYS	GLY	MET	MET	GLU	K136	CYS
ALA	THR	PRO	THR	ILE	ASN	GLY	CYS	K137	ASN
GLN	SER	TYR	ARG	GLY	HIS	TYR	ASP	Y137	LYS
GLY	SER	VAL	THR	GLY	LEU	ALA	PHE	Y151	LEU
ILE	GLY	PRO	ASP	TYR	LEU	LEU	GLY	Y151	LEU
PHE	GLU	SER	VAL	THR	THR	THR	TYR	E187	GLU
GLY	SER	ILE	VAL	GLY	MET	GLY	ASN	E187	VAL
THR	ILE	VAL	ILE	LEU	LEU	ALA	ASN	T193	LEU
ALA	LYS	THR	CYS	VAL	LEU	VAL	SER	T193	GLN
PHE	GLY	VAL	VAL	ILE	GLU	GLU	LYS	N197	ASN
GLN	GLN	ASN	VAL	PRO	ARG	THR	TRP	N197	SER
LEU	ILE	GLU	VAL	LYS	ARG	LEU	MET	E211	THR
GLY	GLU	THR	LYS	HIS	ILE	ILE	HIS	E211	VAL
GLY	ARG	THR	ILE	ILE	ASP	GLN	MET	C260	VAL
TYR	ALA	SER	VAL	TYR	TRP	ILE	HIS	C260	THR
LEU	LYS	CYS	GLN	LEU	THR	ASP	F432	TYR	THR
LYS	ALA	PHE	PRO	ASN	THR	SER	F432	HIS	GLU
PRO	GLU	GLY	CYS	ASN	MET	ILE	E443	ALA	GLN
ILE	LEU	LEU	GLY	TRP	SER	ASN	E443	GLY	LYS
LEU	LEU	ASP	ASN	ASN	SER	ASP	D451	LEU	TRP
ILE	ARG	PHE	SER	VAL	THR	GLU	D451	THR	GLN
GLY	LEU	LYS	SER	VAL	TRP	ASN	G452	ASN	ASN
VAL	ASP	ARG	ASP	ASN	LEU	LEU	G452	LYS	TRP
GLY	ILE	PRO	THR	ILE	GLN	GLN	F453	ASP	ILE
VAL	HIS	LEU	SER	GLY	GLN	GLN	F454	ILE	LEU
ILE	GLY	VAL	ASP	HIS	GLN	GLY	K455	GLN	ASP
LEU	GLY	ALA	CYS	LEU	LEU	ILE	R456	ILE	GLN
LEU	ASP	GLU	PRO	VAL	GLN	TYR	R456	LEU	ASN
VAL	THR	GLU	VAL	VAL	LYS	LEU	S468	PRO	GLY
ILE	PRO	ARG	VAL	LYS	SER	LEU	S468	GLU	GLU
LEU	ALA	LEU	ALA	ALA	ASP	ARG	T529	ILE	VAL
ILE	TRP	SER	ALA	GLY	ASP	ASP	T529	ASP	GLN
PHE	ILE	PHE	ALA	GLN	GLU	HIS	R540	ASN	TRP
LYS	GLN	GLU	VAL	LEU	MET	VAL	R540	THR	THR
ILE	GLN	PRO	GLY	THR	LYS	ILE	V543	VAL	ARG
VAL	LEU	ARG	GLU	HIS	VAL	THR	V543	THR	ARG
SER	ALA	LEU	PRO	VAL	ILE	LEU	LEU	MET	ASP
TRP	ALA	PRO	PHE	THR	ARG	GLU	I546	LYS	GLN
ILE	ALA	ASN	VAL	ILE	ARG	GLU	I546	ALA	ARG
PRO	THR	GLN	VAL	ALA	ILE	ALA	D547	VAL	ALA
THR	LYS	GLN	VAL	HIS	ALA	THR	D547	TYR	THR
PRO	THR	LEU	VAL	HIS	ALA	THR	T558	GLN	ARG
LYS	ASP	LEU	ASN	PRO	ARG	LEU	R559	LEU	LEU
LYS	VAL	LEU	PRO	TYR	SER	HIS	E560	LEU	PRO
ASN	PRO	LEU	LYS	ILE	VAL	ILE	T563	GLN	THR
							SER		
							CYS		
							ASN		

GLN

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

- 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

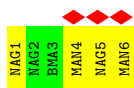


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

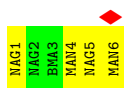




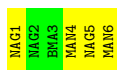
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



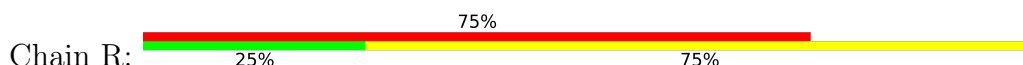
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



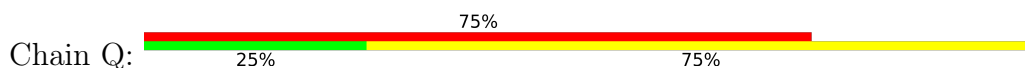
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



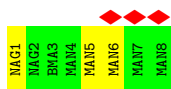
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



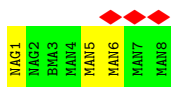
- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



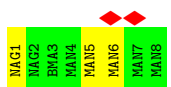
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



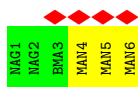
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



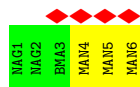
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



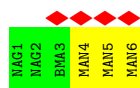
- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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, C6	Depositor
Number of subtomograms used	5697	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	0.198	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0702	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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.10	0/476	1.62	0/653
1	B	1.06	0/3469	1.37	1/4705 (0.0%)
1	C	1.06	0/3469	1.37	1/4705 (0.0%)
1	D	1.08	0/3260	1.40	0/4441
1	E	1.10	0/476	1.62	0/653
1	F	1.02	0/97	1.15	0/130
1	G	1.05	0/3416	1.38	1/4634 (0.0%)
1	H	1.07	0/3260	1.40	0/4441
1	I	1.10	0/476	1.62	0/653
1	L	1.08	0/3260	1.40	0/4441
All	All	1.07	0/21659	1.40	3/29456 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	PRO	N-CA-C	5.73	120.22	111.34
1	B	135	PRO	N-CA-C	5.70	120.17	111.34
1	G	135	PRO	N-CA-C	5.70	120.17	111.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	466	0	488	0	0
1	B	3380	0	3293	9	0
1	C	3380	0	3293	14	0
1	D	3190	0	3242	9	0
1	E	466	0	488	1	0
1	F	94	0	97	3	0
1	G	3328	0	3241	11	0
1	H	3190	0	3242	8	0
1	I	466	0	488	0	0
1	L	3190	0	3242	5	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	0	0
7	j	72	0	61	0	0
8	B	42	0	39	0	0
8	C	42	0	39	0	0
8	G	42	0	39	0	0
9	D	28	0	46	0	0
9	H	28	0	46	0	0
9	L	28	0	46	0	0
10	D	50	0	79	0	0
10	H	50	0	79	0	0
10	L	50	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22752	0	22674	43	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 (43) 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:D:700:THR:HG21	1:C:197:ASN:OD1	1.96	0.64
1:B:134:VAL:HG21	1:C:138:VAL:HG23	1.80	0.64
1:H:700:THR:HG21	1:G:197:ASN:OD1	1.98	0.62
1:B:138:VAL:HG23	1:C:134:VAL:HG21	1.80	0.62
1:D:700:THR:HG23	1:C:193:THR:HG23	1.83	0.60
1:F:137:TYR:HE1	1:G:133:PRO:HG3	1.67	0.59
1:G:136:LYS:HG2	1:G:137:TYR:H	1.71	0.56
1:C:136:LYS:HG2	1:C:137:TYR:H	1.71	0.56
1:H:700:THR:HG23	1:G:193:THR:HG23	1.88	0.55
1:G:277:ILE:HG21	1:G:298:LEU:HD12	1.89	0.55
1:B:136:LYS:HG2	1:B:137:TYR:H	1.71	0.54
1:B:277:ILE:HG21	1:B:298:LEU:HD12	1.89	0.53
1:C:277:ILE:HG21	1:C:298:LEU:HD12	1.88	0.53
1:F:137:TYR:CE1	1:G:133:PRO:HG3	2.48	0.49
1:D:652:GLU:OE2	1:L:654:ARG:NH1	2.47	0.48
1:B:358:ALA:HA	1:B:370:ALA:HB3	1.97	0.46
1:G:358:ALA:HA	1:G:370:ALA:HB3	1.97	0.46
1:C:358:ALA:HA	1:C:370:ALA:HB3	1.97	0.45
1:L:760:LEU:HD22	1:L:774:VAL:HG22	1.99	0.45
1:B:134:VAL:HG21	1:C:138:VAL:CG2	2.47	0.44
1:C:277:ILE:HD11	1:C:302:TYR:HB2	2.00	0.44
1:D:760:LEU:HD22	1:D:774:VAL:HG22	1.99	0.44
1:G:277:ILE:HD11	1:G:302:TYR:HB2	2.00	0.44
1:B:277:ILE:HD11	1:B:302:TYR:HB2	2.00	0.43
1:F:131:GLN:HB3	1:G:137:TYR:CD1	2.53	0.43
1:H:760:LEU:HD22	1:H:774:VAL:HG22	1.99	0.43
1:D:654:ARG:NH1	1:H:652:GLU:OE2	2.52	0.43
1:C:337:GLU:O	1:C:341:LEU:HG	2.20	0.42
1:G:136:LYS:HG2	1:G:137:TYR:N	2.34	0.42
1:D:911:THR:HB	1:D:912:PRO:HD3	2.02	0.42
1:D:774:VAL:HG21	1:C:160:VAL:HG22	2.02	0.42
1:G:337:GLU:O	1:G:341:LEU:HG	2.20	0.42
1:H:975:PHE:CE2	1:E:71:TRP:CH2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:911:THR:HB	1:H:912:PRO:HD3	2.02	0.41
1:L:911:THR:HB	1:L:912:PRO:HD3	2.02	0.41
1:H:649:MET:HA	1:H:649:MET:HE2	2.02	0.41
1:B:337:GLU:O	1:B:341:LEU:HG	2.20	0.41
1:D:649:MET:HA	1:D:649:MET:HE2	2.02	0.41
1:L:649:MET:HA	1:L:649:MET:HE2	2.02	0.41
1:B:138:VAL:CG2	1:C:134:VAL:HG21	2.47	0.41
1:D:700:THR:HG21	1:C:197:ASN:CG	2.46	0.40
1:H:654:ARG:NH1	1:L:652:GLU:OE2	2.53	0.40
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	B	405/988 (41%)	379 (94%)	26 (6%)	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
1	L	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
All	All	2595/9880 (26%)	2435 (94%)	160 (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	B	382/899 (42%)	379 (99%)	3 (1%)	73	80
1	C	382/899 (42%)	379 (99%)	3 (1%)	73	80
1	D	356/899 (40%)	353 (99%)	3 (1%)	73	80
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	80
1	H	356/899 (40%)	353 (99%)	3 (1%)	73	80
1	I	54/899 (6%)	54 (100%)	0	100	100
1	L	356/899 (40%)	353 (99%)	3 (1%)	73	80
All	All	2381/8990 (26%)	2363 (99%)	18 (1%)	70	80

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

Mol	Chain	Res	Type
1	B	151	TYR
1	B	211	GLU
1	B	405	ASN
1	D	812	LEU
1	D	841	LEU
1	D	862	LEU
1	H	812	LEU
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

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Mol	Chain	Res	Type
1	C	405	ASN
1	G	151	TYR
1	G	211	GLU
1	G	405	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	GLN
1	B	321	GLN
1	B	335	GLN
1	B	478	GLN
1	B	538	ASN
1	D	606	GLN
1	D	625	HIS
1	D	644	ASN
1	D	893	GLN
1	F	131	GLN
1	H	644	ASN
1	H	893	GLN
1	L	640	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

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	0.33	0	17,19,21	1.38	2 (11%)
2	NAG	M	2	2	14,14,15	0.34	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	0.35	0	17,19,21	0.77	0
2	NAG	O	1	1,2	14,14,15	0.33	0	17,19,21	1.37	2 (11%)
2	NAG	O	2	2	14,14,15	0.36	0	17,19,21	0.76	0
5	NAG	P	1	1,5	14,14,15	0.35	0	17,19,21	1.03	1 (5%)
5	NAG	P	2	5	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
5	BMA	P	3	5	11,11,12	0.41	0	15,15,17	0.76	1 (6%)
5	MAN	P	4	5	11,11,12	0.43	0	15,15,17	0.76	0
5	NAG	Q	1	1,5	14,14,15	0.35	0	17,19,21	1.03	1 (5%)
5	NAG	Q	2	5	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
5	BMA	Q	3	5	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
5	MAN	Q	4	5	11,11,12	0.44	0	15,15,17	0.75	0
5	NAG	R	1	1,5	14,14,15	0.34	0	17,19,21	1.03	1 (5%)
5	NAG	R	2	5	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
5	BMA	R	3	5	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
5	MAN	R	4	5	11,11,12	0.43	0	15,15,17	0.76	0
3	NAG	S	1	1,3	14,14,15	0.41	0	17,19,21	1.44	2 (11%)
3	NAG	S	2	3	14,14,15	0.42	0	17,19,21	1.58	3 (17%)
3	BMA	S	3	3	11,11,12	0.33	0	15,15,17	0.53	0
3	NAG	T	1	1,3	14,14,15	0.43	0	17,19,21	1.44	2 (11%)
3	NAG	T	2	3	14,14,15	0.42	0	17,19,21	1.59	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	T	3	3	11,11,12	0.34	0	15,15,17	0.54	0
3	NAG	U	1	1,3	14,14,15	0.42	0	17,19,21	1.44	2 (11%)
3	NAG	U	2	3	14,14,15	0.42	0	17,19,21	1.59	3 (17%)
3	BMA	U	3	3	11,11,12	0.34	0	15,15,17	0.54	0
4	NAG	V	1	1,4	14,14,15	0.51	0	17,19,21	1.12	1 (5%)
4	NAG	V	2	4	14,14,15	0.31	0	17,19,21	0.78	0
4	BMA	V	3	4	11,11,12	0.35	0	15,15,17	0.71	0
4	MAN	V	4	4	11,11,12	0.64	0	15,15,17	1.26	2 (13%)
4	NAG	V	5	4	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
4	MAN	V	6	4	11,11,12	0.36	0	15,15,17	0.80	1 (6%)
4	NAG	W	1	1,4	14,14,15	0.50	0	17,19,21	1.11	1 (5%)
4	NAG	W	2	4	14,14,15	0.30	0	17,19,21	0.80	0
4	BMA	W	3	4	11,11,12	0.35	0	15,15,17	0.70	0
4	MAN	W	4	4	11,11,12	0.65	0	15,15,17	1.26	2 (13%)
4	NAG	W	5	4	14,14,15	0.28	0	17,19,21	0.85	1 (5%)
4	MAN	W	6	4	11,11,12	0.35	0	15,15,17	0.79	1 (6%)
4	NAG	X	1	1,4	14,14,15	0.50	0	17,19,21	1.12	2 (11%)
4	NAG	X	2	4	14,14,15	0.28	0	17,19,21	0.78	0
4	BMA	X	3	4	11,11,12	0.35	0	15,15,17	0.71	0
4	MAN	X	4	4	11,11,12	0.63	0	15,15,17	1.26	2 (13%)
4	NAG	X	5	4	14,14,15	0.25	0	17,19,21	0.85	1 (5%)
4	MAN	X	6	4	11,11,12	0.34	0	15,15,17	0.80	1 (6%)
2	NAG	Y	1	1,2	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	Y	2	2	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
2	NAG	Z	1	1,2	14,14,15	0.42	0	17,19,21	0.74	0
2	NAG	Z	2	2	14,14,15	0.33	0	17,19,21	0.99	2 (11%)
2	NAG	a	1	1,2	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	a	2	2	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
2	NAG	b	1	1,2	14,14,15	0.38	0	17,19,21	0.76	0
2	NAG	b	2	2	14,14,15	0.32	0	17,19,21	1.17	2 (11%)
2	NAG	c	1	1,2	14,14,15	0.37	0	17,19,21	0.77	0
2	NAG	c	2	2	14,14,15	0.31	0	17,19,21	1.18	2 (11%)
2	NAG	d	1	1,2	14,14,15	0.37	0	17,19,21	0.76	0
2	NAG	d	2	2	14,14,15	0.31	0	17,19,21	1.17	2 (11%)
6	NAG	e	1	6,1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
6	NAG	e	2	6	14,14,15	0.43	0	17,19,21	0.86	0
6	BMA	e	3	6	11,11,12	0.37	0	15,15,17	0.56	0
6	MAN	e	4	6	11,11,12	0.35	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	e	5	6	11,11,12	0.33	0	15,15,17	0.87	1 (6%)
6	MAN	e	6	6	11,11,12	0.34	0	15,15,17	0.80	1 (6%)
6	MAN	e	7	6	11,11,12	0.40	0	15,15,17	0.63	0
6	MAN	e	8	6	11,11,12	0.33	0	15,15,17	0.64	0
6	NAG	f	1	6,1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
6	NAG	f	2	6	14,14,15	0.44	0	17,19,21	0.85	0
6	BMA	f	3	6	11,11,12	0.37	0	15,15,17	0.56	0
6	MAN	f	4	6	11,11,12	0.36	0	15,15,17	0.72	0
6	MAN	f	5	6	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
6	MAN	f	6	6	11,11,12	0.35	0	15,15,17	0.79	1 (6%)
6	MAN	f	7	6	11,11,12	0.40	0	15,15,17	0.61	0
6	MAN	f	8	6	11,11,12	0.34	0	15,15,17	0.64	0
6	NAG	g	1	6,1	14,14,15	0.37	0	17,19,21	1.18	1 (5%)
6	NAG	g	2	6	14,14,15	0.44	0	17,19,21	0.84	0
6	BMA	g	3	6	11,11,12	0.36	0	15,15,17	0.56	0
6	MAN	g	4	6	11,11,12	0.35	0	15,15,17	0.72	0
6	MAN	g	5	6	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
6	MAN	g	6	6	11,11,12	0.35	0	15,15,17	0.80	1 (6%)
6	MAN	g	7	6	11,11,12	0.39	0	15,15,17	0.62	0
6	MAN	g	8	6	11,11,12	0.32	0	15,15,17	0.64	0
7	NAG	h	1	1,7	14,14,15	0.54	0	17,19,21	1.08	0
7	NAG	h	2	7	14,14,15	0.47	0	17,19,21	0.81	0
7	BMA	h	3	7	11,11,12	0.40	0	15,15,17	0.58	0
7	MAN	h	4	7	11,11,12	0.37	0	15,15,17	0.83	1 (6%)
7	MAN	h	5	7	11,11,12	0.33	0	15,15,17	0.78	1 (6%)
7	MAN	h	6	7	11,11,12	0.36	0	15,15,17	0.70	1 (6%)
7	NAG	i	1	1,7	14,14,15	0.52	0	17,19,21	1.09	0
7	NAG	i	2	7	14,14,15	0.48	0	17,19,21	0.81	0
7	BMA	i	3	7	11,11,12	0.39	0	15,15,17	0.58	0
7	MAN	i	4	7	11,11,12	0.38	0	15,15,17	0.83	1 (6%)
7	MAN	i	5	7	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
7	MAN	i	6	7	11,11,12	0.36	0	15,15,17	0.69	1 (6%)
7	NAG	j	1	1,7	14,14,15	0.52	0	17,19,21	1.09	0
7	NAG	j	2	7	14,14,15	0.48	0	17,19,21	0.82	0
7	BMA	j	3	7	11,11,12	0.40	0	15,15,17	0.58	0
7	MAN	j	4	7	11,11,12	0.38	0	15,15,17	0.84	1 (6%)
7	MAN	j	5	7	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
7	MAN	j	6	7	11,11,12	0.36	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
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	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	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	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	-	1/6/23/26	0/1/1/1
4	MAN	V	6	4	-	0/2/19/22	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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/2/19/22	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
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	-	0/2/19/22	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

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	NAG	C2-N2-C7	4.09	128.38	122.90
3	T	2	NAG	C2-N2-C7	4.07	128.35	122.90
3	S	2	NAG	C2-N2-C7	4.03	128.30	122.90
4	V	4	MAN	O2-C2-C1	3.59	117.43	109.22
4	W	4	MAN	O2-C2-C1	3.58	117.41	109.22
4	X	4	MAN	O2-C2-C1	3.57	117.39	109.22
3	S	1	NAG	C2-N2-C7	3.47	127.55	122.90
3	U	1	NAG	C2-N2-C7	3.46	127.53	122.90
3	T	1	NAG	C2-N2-C7	3.45	127.53	122.90
4	V	1	NAG	C1-O5-C5	3.44	116.80	112.19
4	X	1	NAG	C1-O5-C5	3.43	116.79	112.19
4	W	1	NAG	C1-O5-C5	3.39	116.73	112.19
2	M	1	NAG	C1-O5-C5	3.38	116.72	112.19
2	O	1	NAG	C1-O5-C5	3.36	116.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	NAG	C1-O5-C5	3.34	116.66	112.19
5	Q	1	NAG	C1-C2-N2	-3.05	105.62	110.43
5	P	1	NAG	C1-C2-N2	-3.05	105.63	110.43
6	f	1	NAG	C1-O5-C5	3.04	116.26	112.19
5	R	1	NAG	C1-C2-N2	-3.03	105.67	110.43
6	g	1	NAG	C1-O5-C5	3.01	116.22	112.19
6	e	1	NAG	C1-O5-C5	2.99	116.19	112.19
2	b	2	NAG	C2-N2-C7	2.93	126.83	122.90
2	d	2	NAG	C2-N2-C7	2.92	126.81	122.90
2	c	2	NAG	C2-N2-C7	2.91	126.79	122.90
3	T	1	NAG	C8-C7-N2	2.87	120.87	116.12
3	S	1	NAG	C8-C7-N2	2.85	120.84	116.12
4	X	4	MAN	C1-O5-C5	2.85	116.00	112.19
4	V	4	MAN	C1-O5-C5	2.85	116.00	112.19
4	W	4	MAN	C1-O5-C5	2.83	115.98	112.19
3	U	1	NAG	C8-C7-N2	2.83	120.81	116.12
2	M	1	NAG	O5-C1-C2	-2.68	107.14	111.29
6	g	5	MAN	C1-O5-C5	2.67	115.76	112.19
3	S	2	NAG	C4-C3-C2	2.67	114.93	111.02
6	f	5	MAN	C1-O5-C5	2.66	115.75	112.19
3	U	2	NAG	C4-C3-C2	2.65	114.90	111.02
6	e	5	MAN	C1-O5-C5	2.65	115.73	112.19
3	T	2	NAG	C4-C3-C2	2.63	114.87	111.02
2	O	1	NAG	O5-C1-C2	-2.62	107.23	111.29
2	N	1	NAG	O5-C1-C2	-2.62	107.24	111.29
3	S	2	NAG	C1-C2-N2	-2.61	106.33	110.43
3	T	2	NAG	C1-C2-N2	-2.59	106.35	110.43
7	j	4	MAN	C1-O5-C5	2.58	115.64	112.19
3	U	2	NAG	C1-C2-N2	-2.56	106.40	110.43
6	e	6	MAN	C1-O5-C5	2.53	115.58	112.19
7	i	4	MAN	C1-O5-C5	2.53	115.58	112.19
7	h	4	MAN	C1-O5-C5	2.52	115.57	112.19
5	P	2	NAG	C1-O5-C5	2.52	115.56	112.19
5	Q	2	NAG	C1-O5-C5	2.51	115.55	112.19
6	g	6	MAN	C1-O5-C5	2.49	115.52	112.19
6	f	6	MAN	C1-O5-C5	2.49	115.52	112.19
5	R	2	NAG	C1-O5-C5	2.48	115.50	112.19
2	c	2	NAG	C8-C7-N2	2.45	120.17	116.12
2	b	2	NAG	C8-C7-N2	2.43	120.15	116.12
2	d	2	NAG	C8-C7-N2	2.43	120.15	116.12
4	V	6	MAN	C1-O5-C5	2.39	115.39	112.19
7	i	5	MAN	C1-O5-C5	2.39	115.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	6	MAN	C1-O5-C5	2.38	115.38	112.19
4	W	6	MAN	C1-O5-C5	2.37	115.36	112.19
7	h	5	MAN	C1-O5-C5	2.36	115.35	112.19
7	j	5	MAN	C1-O5-C5	2.35	115.34	112.19
7	j	6	MAN	C1-O5-C5	2.31	115.28	112.19
7	h	6	MAN	C1-O5-C5	2.27	115.22	112.19
7	i	6	MAN	C1-O5-C5	2.26	115.22	112.19
5	Q	3	BMA	C1-O5-C5	2.16	115.09	112.19
5	R	3	BMA	C1-O5-C5	2.16	115.08	112.19
5	P	3	BMA	C1-O5-C5	2.16	115.08	112.19
2	Y	2	NAG	O5-C1-C2	-2.15	107.96	111.29
2	Z	2	NAG	O5-C1-C2	-2.15	107.96	111.29
2	a	2	NAG	O5-C1-C2	-2.14	107.98	111.29
2	a	2	NAG	C1-O5-C5	2.07	114.96	112.19
4	X	5	NAG	O5-C1-C2	-2.05	108.12	111.29
2	Y	2	NAG	C1-O5-C5	2.04	114.92	112.19
4	W	5	NAG	O5-C1-C2	-2.04	108.14	111.29
4	V	5	NAG	O5-C1-C2	-2.02	108.17	111.29
2	Z	2	NAG	C1-O5-C5	2.01	114.89	112.19
4	X	1	NAG	C1-C2-N2	2.01	113.59	110.43

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C3-C2-N2-C7
3	S	2	NAG	C3-C2-N2-C7
3	T	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
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
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2

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

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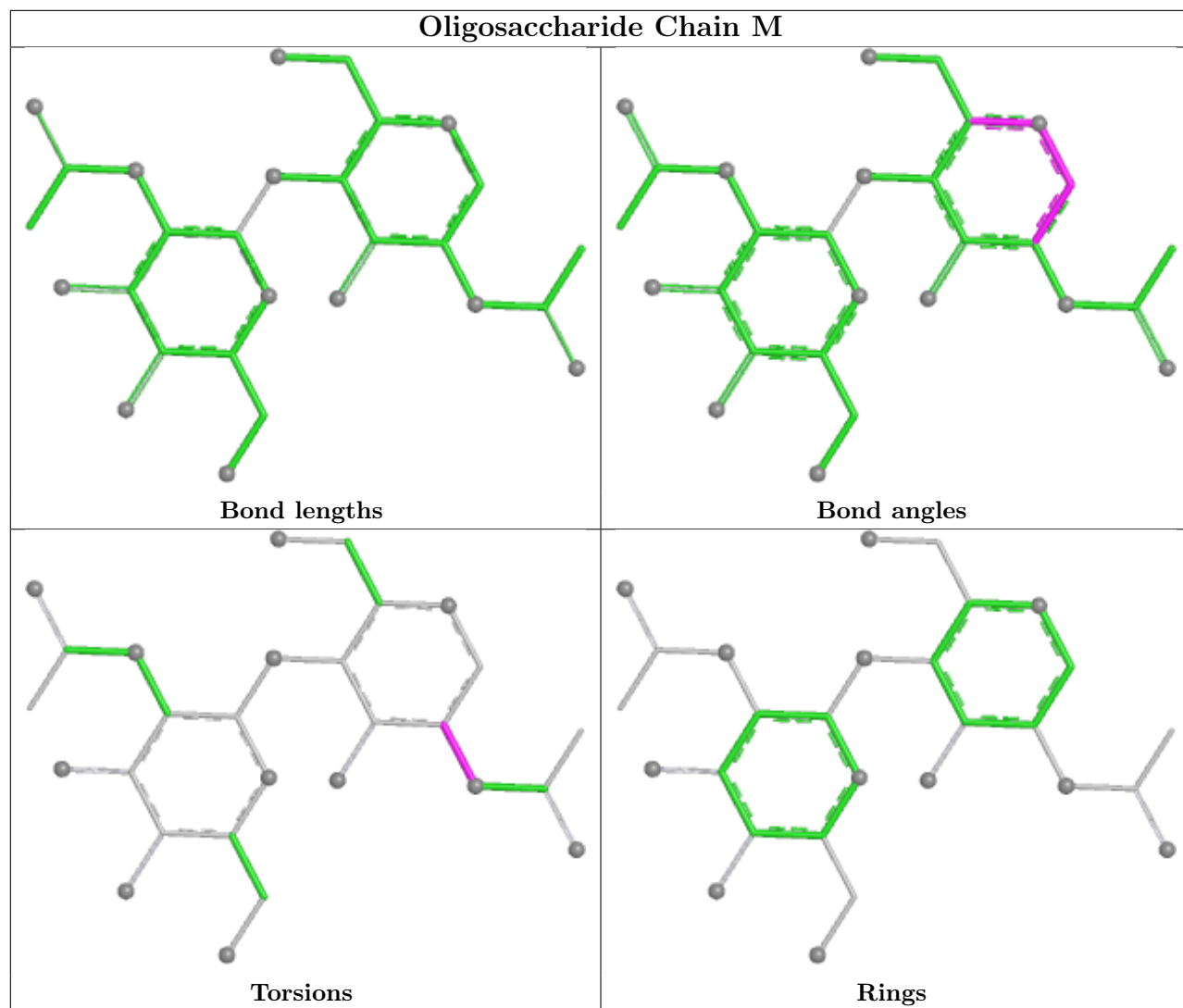
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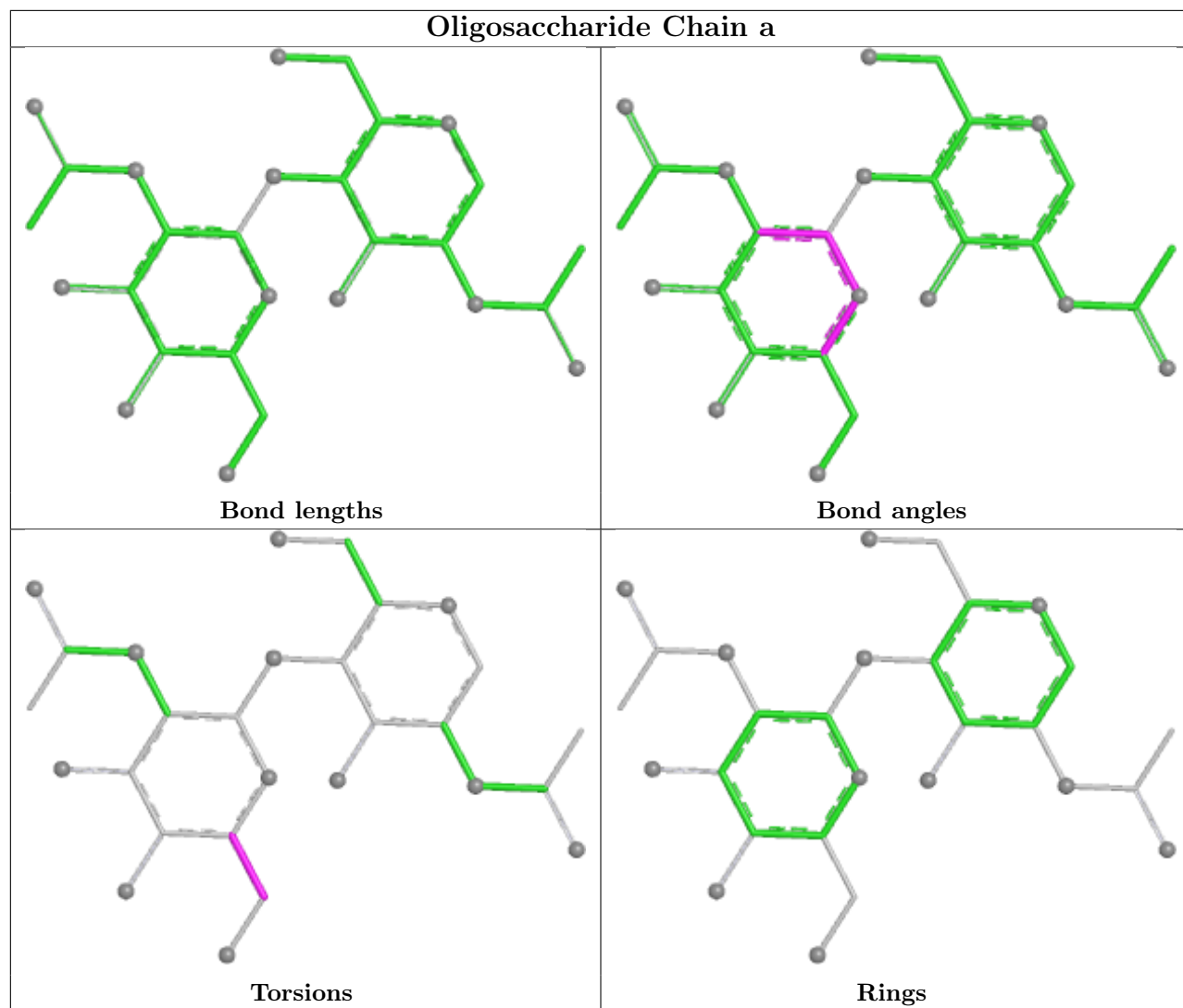
Mol	Chain	Res	Type	Atoms
4	V	5	NAG	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C1-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7
2	O	1	NAG	C1-C2-N2-C7
4	X	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6

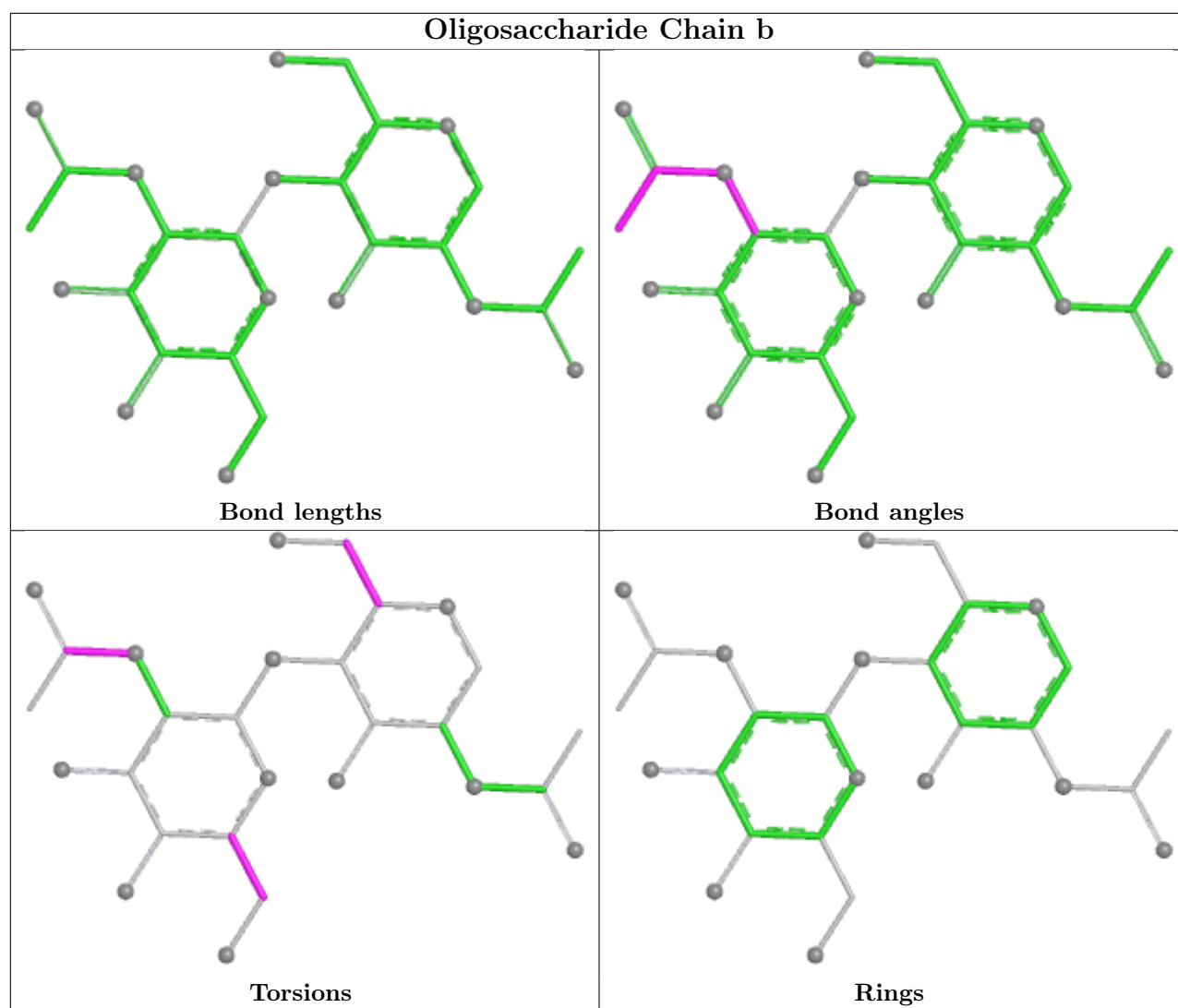
There are no ring outliers.

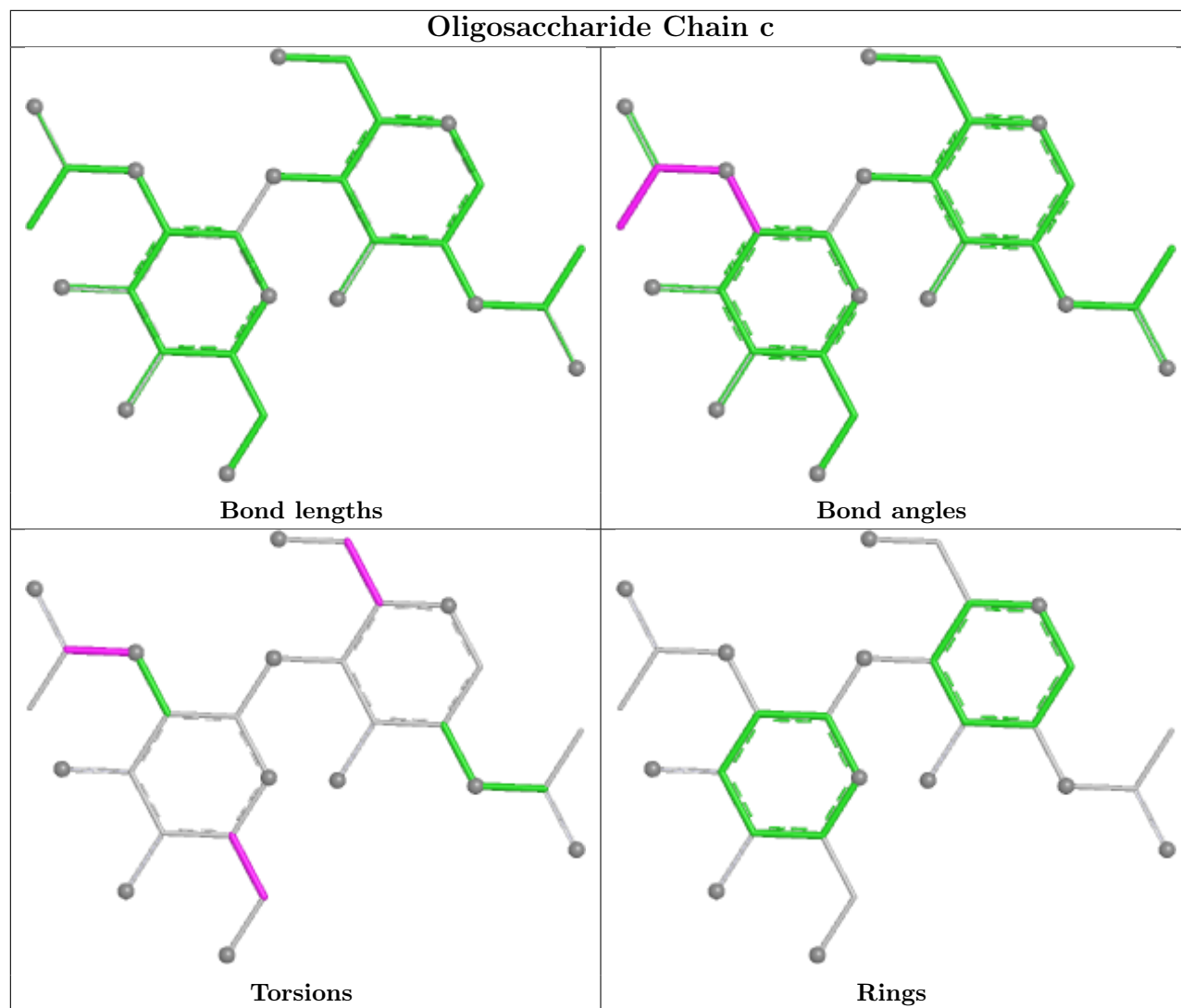
No monomer is involved in short contacts.

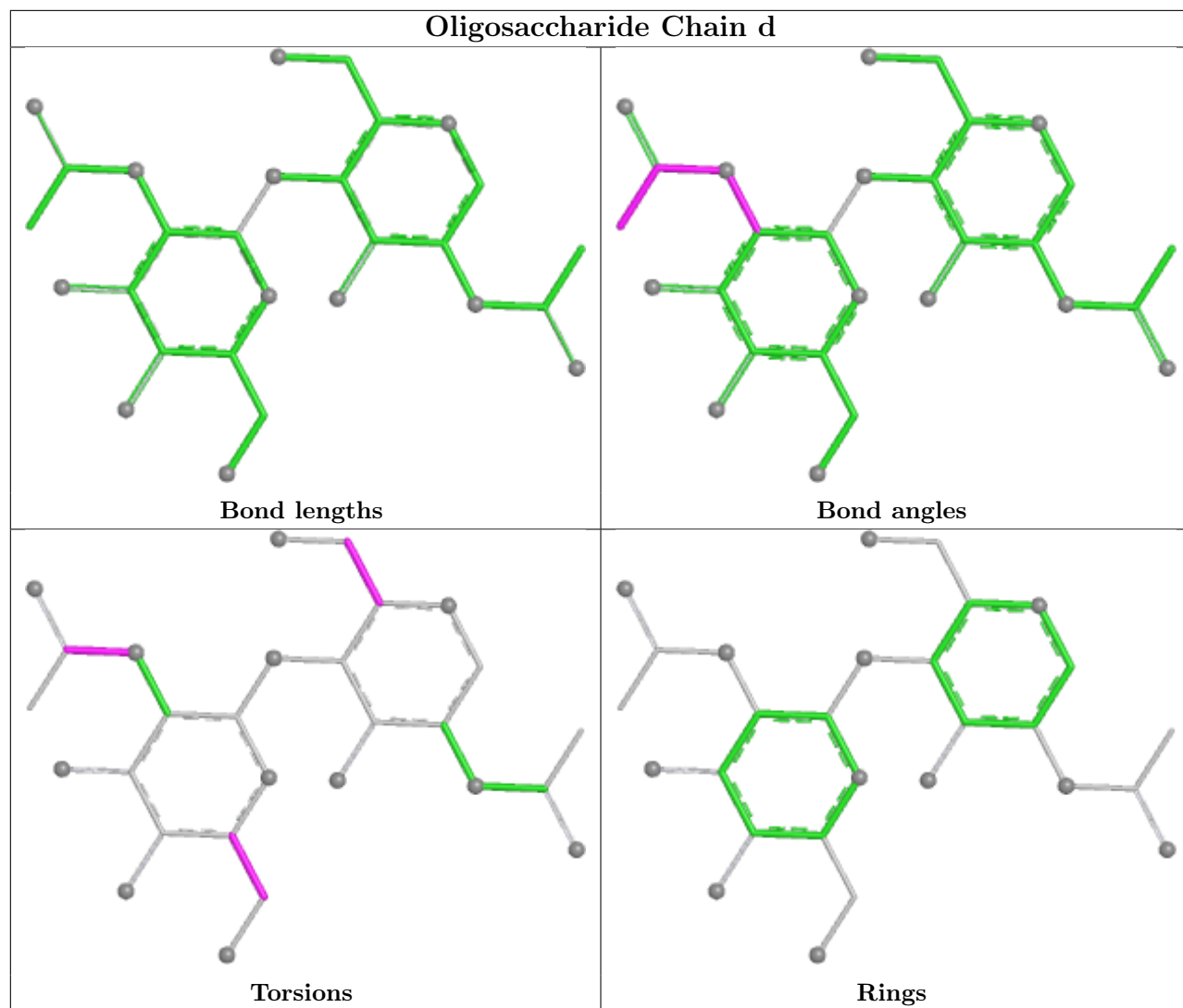
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

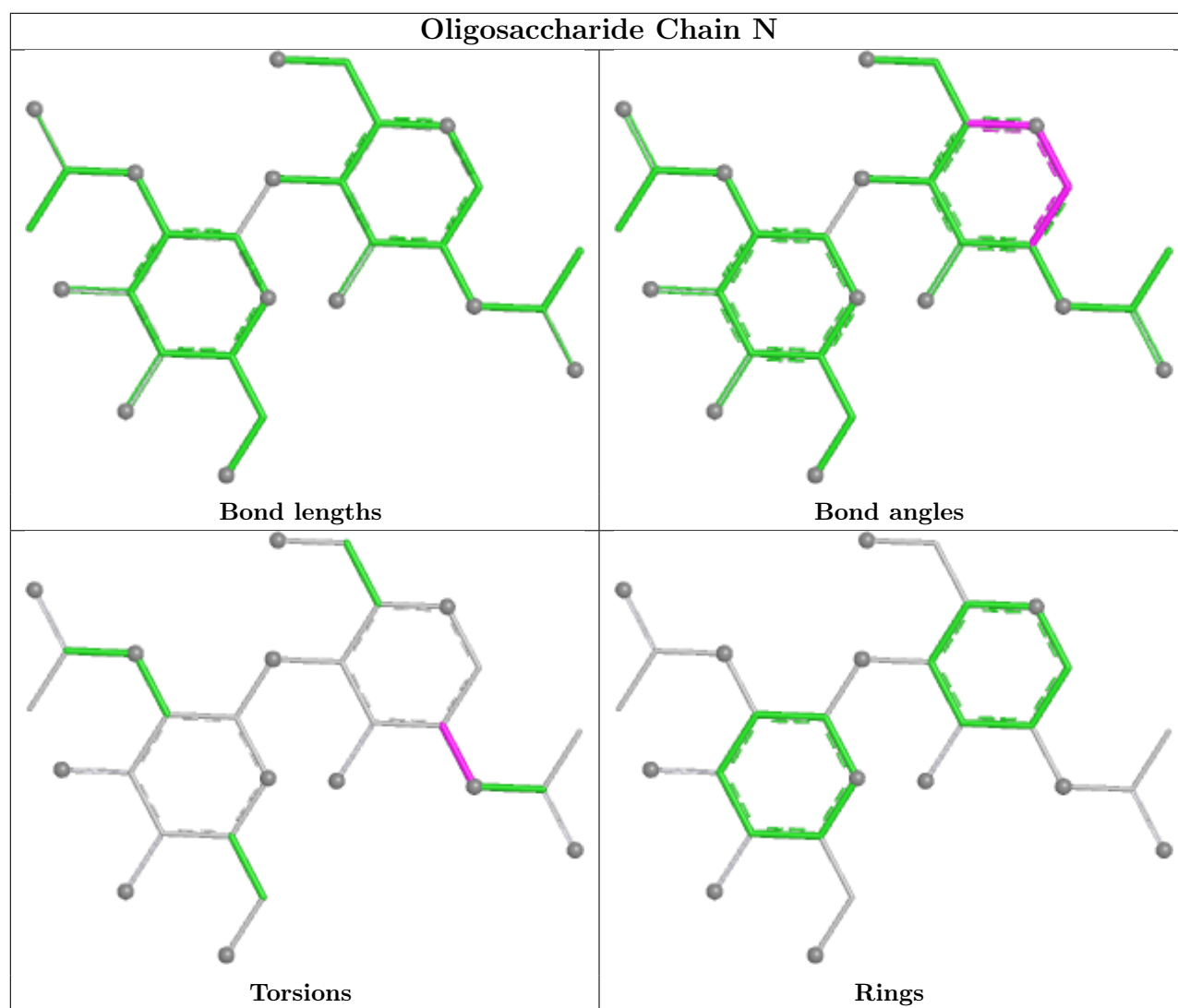


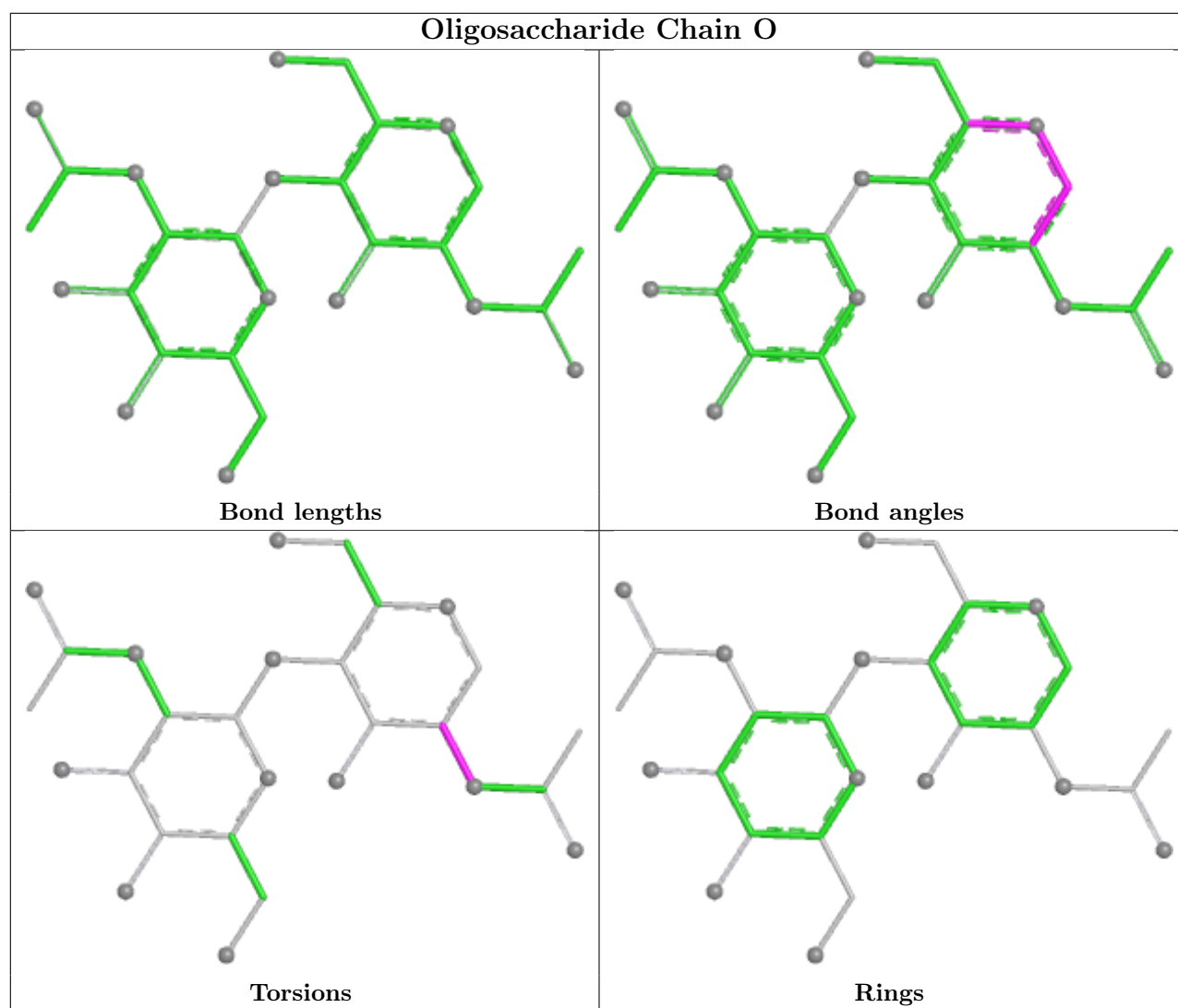


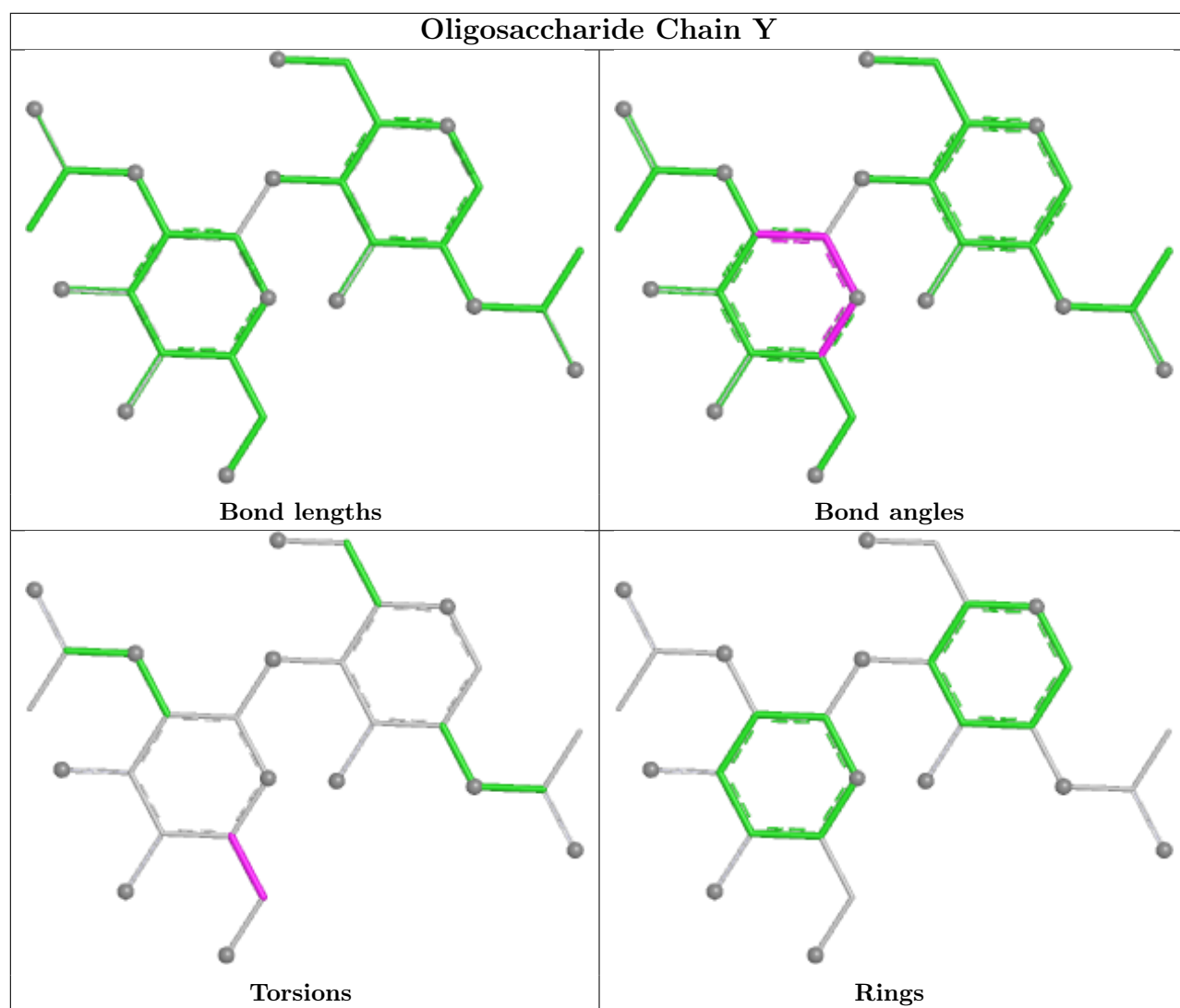


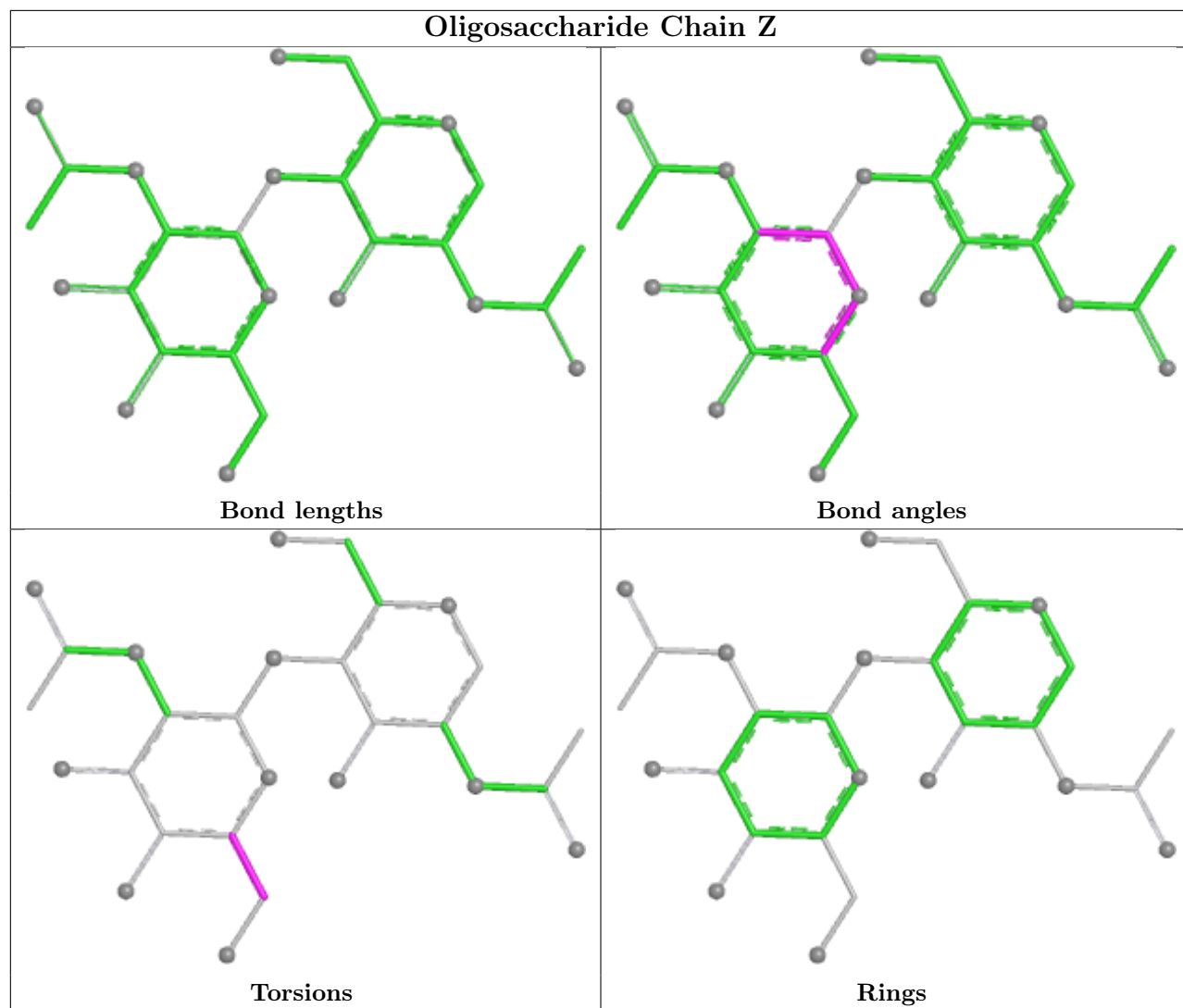


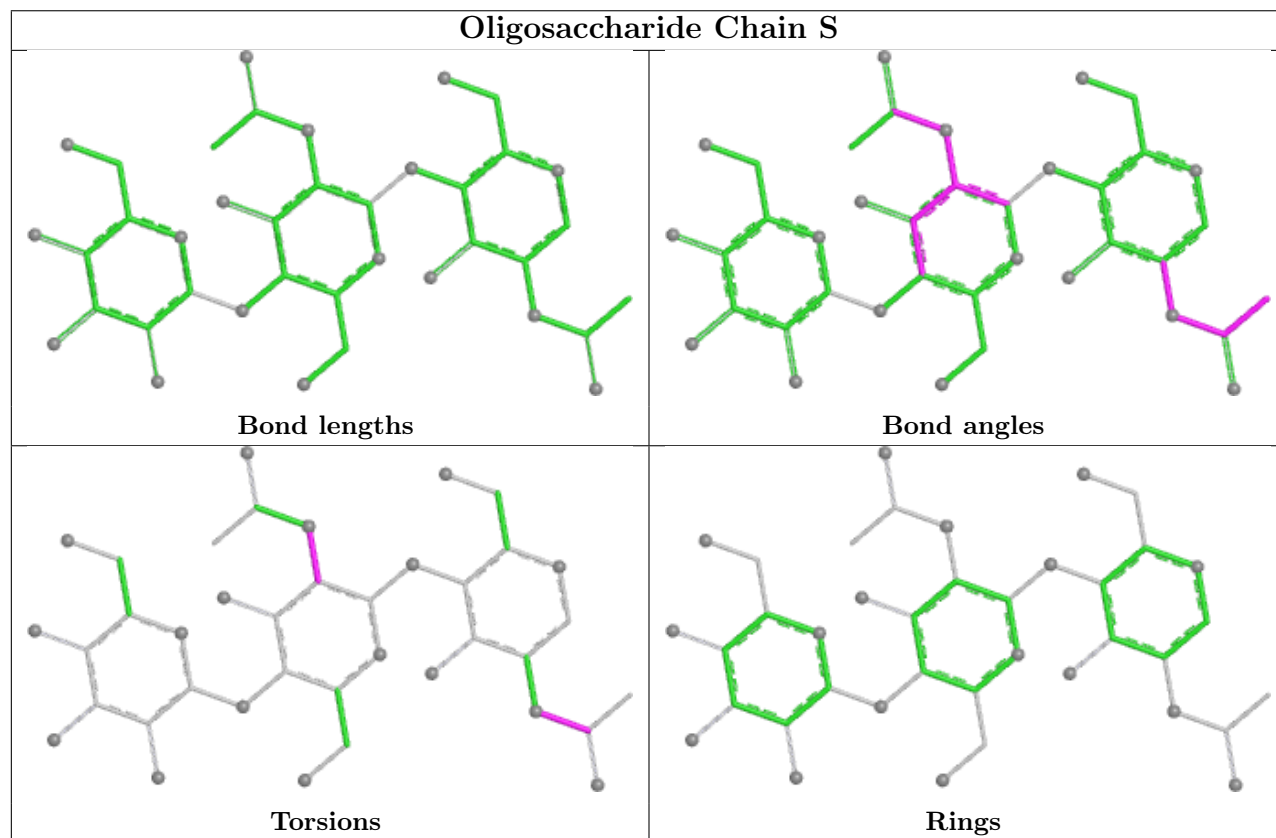
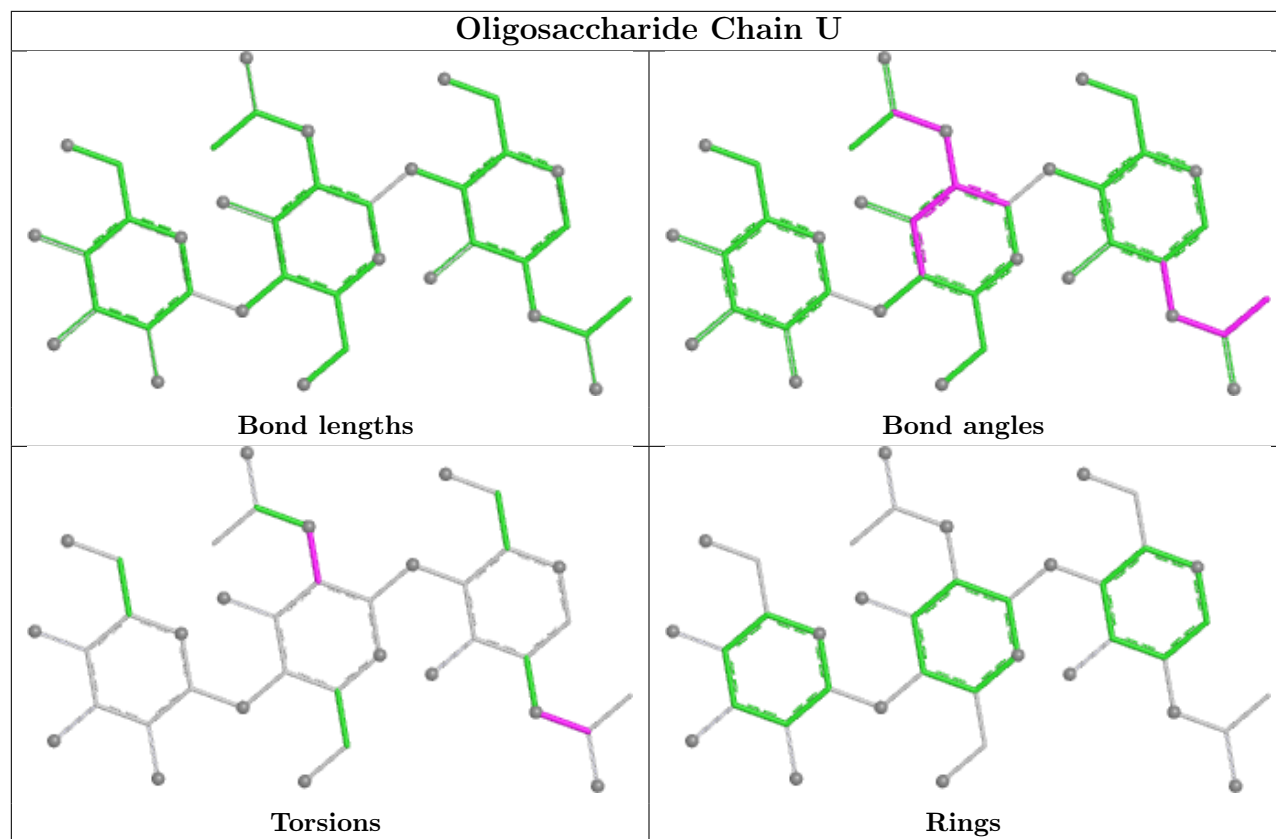


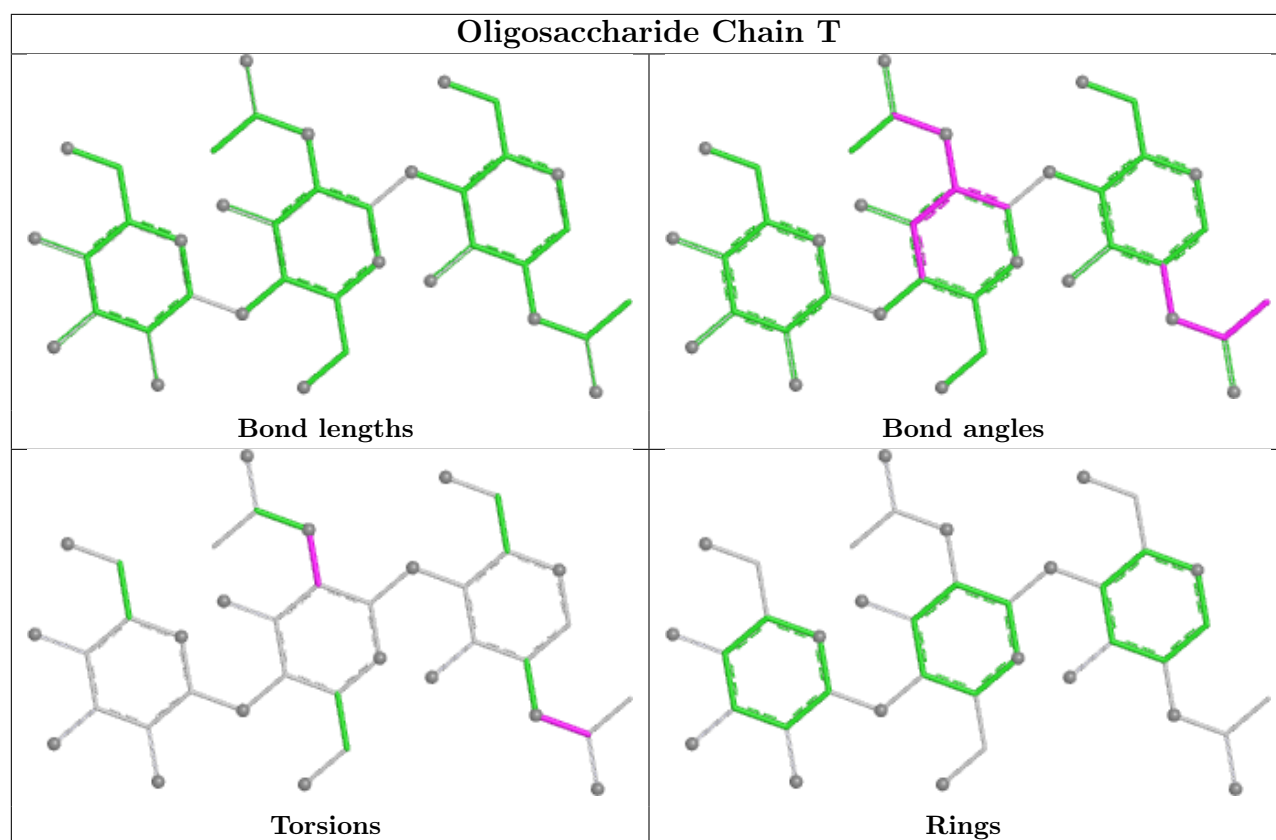


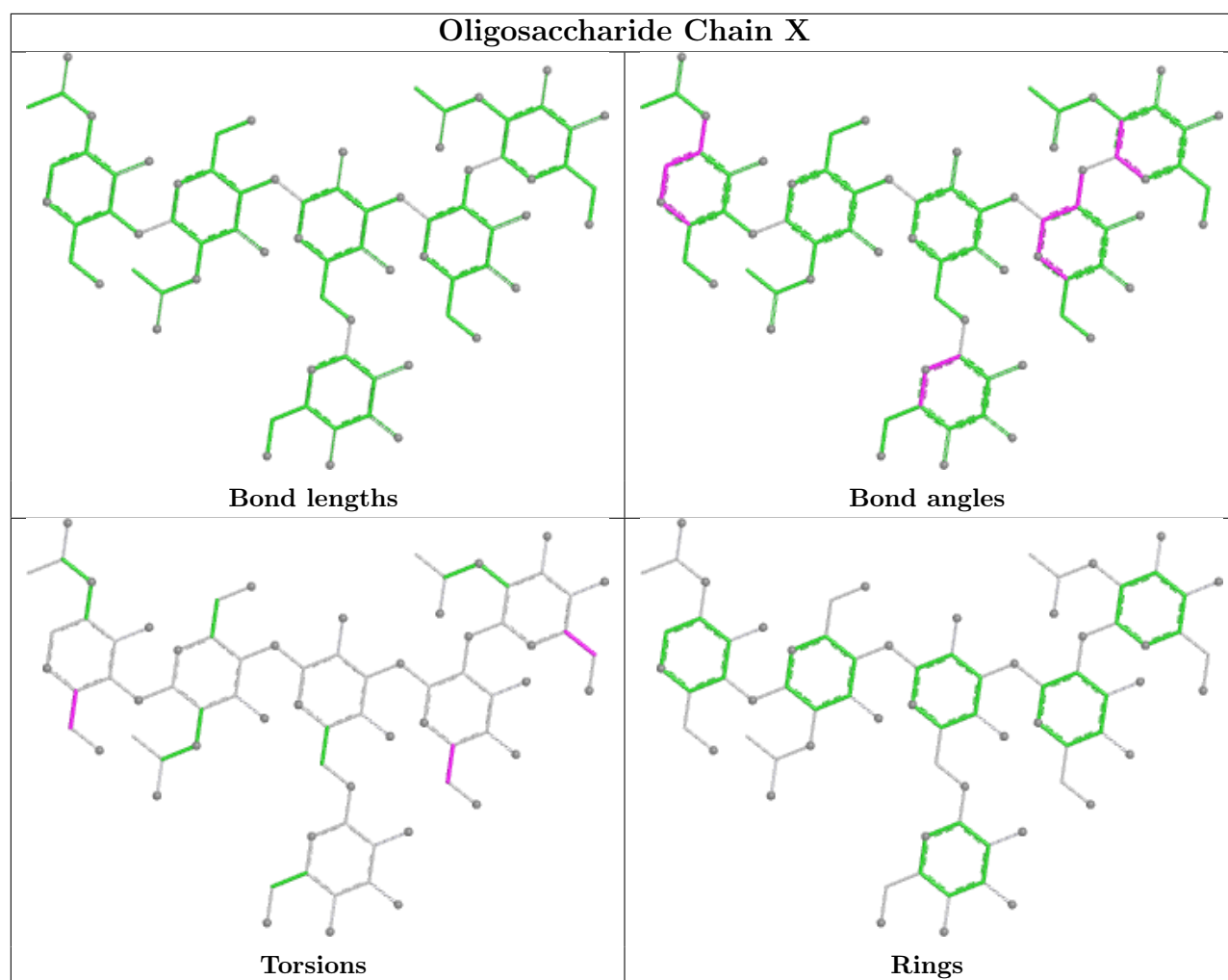


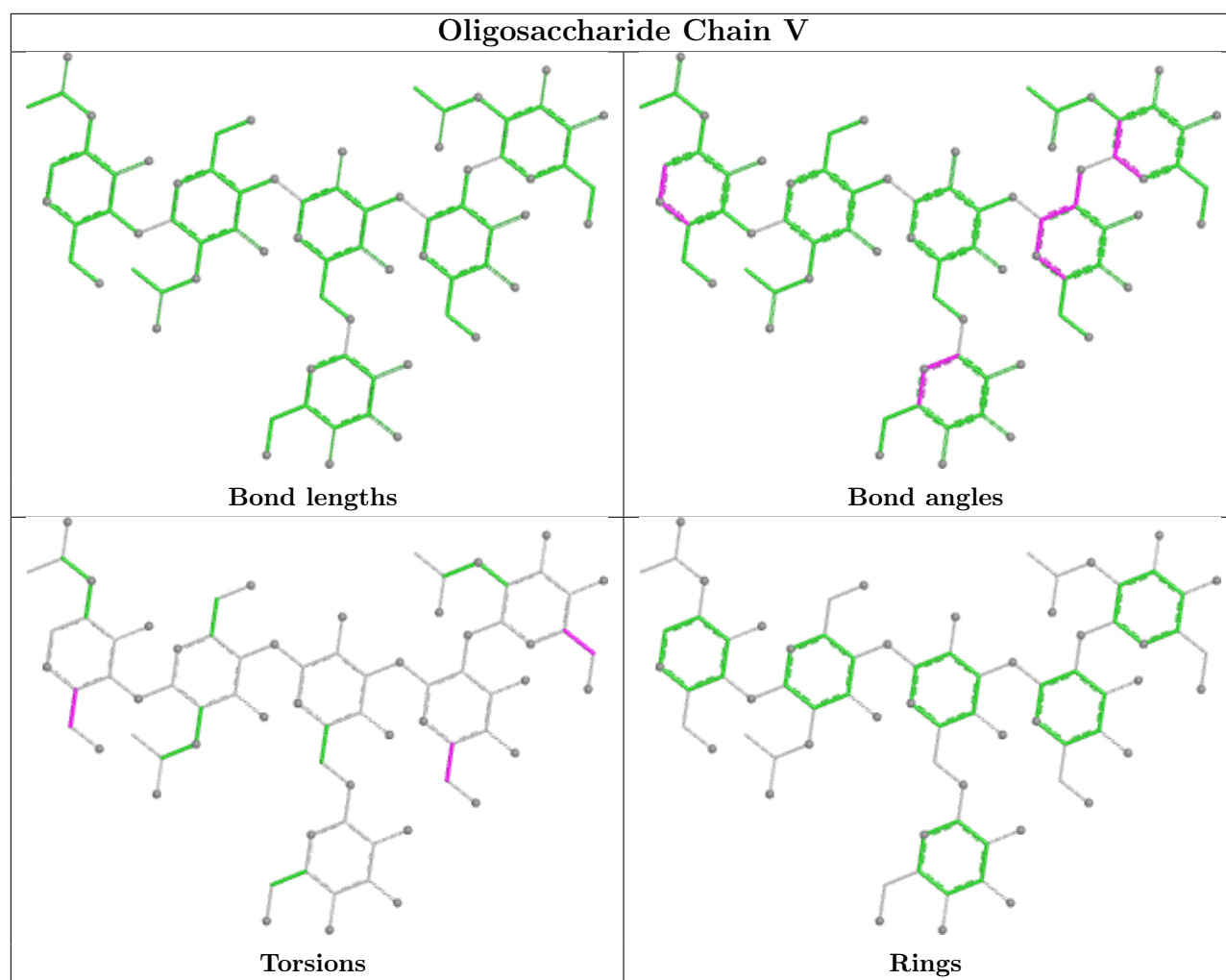


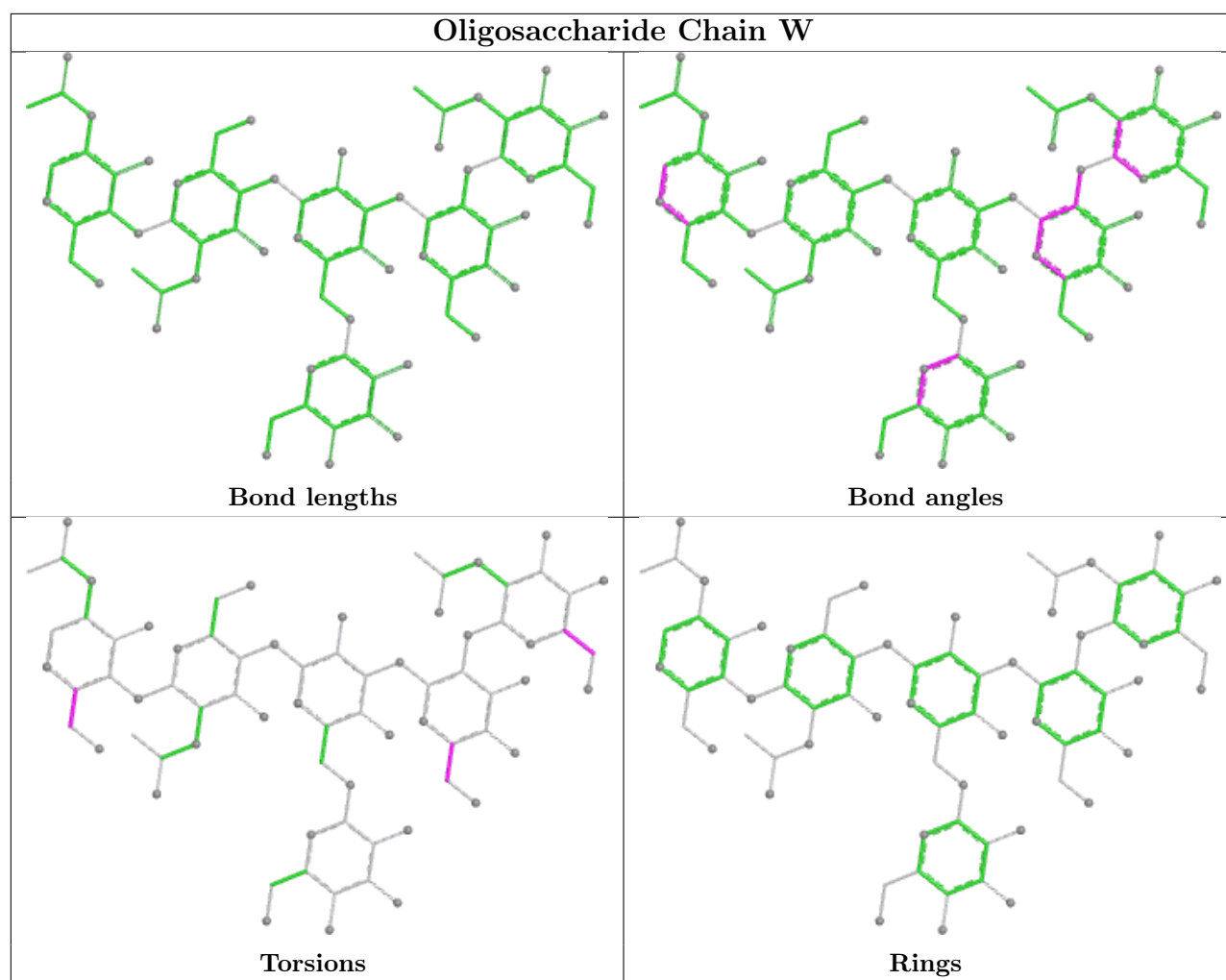


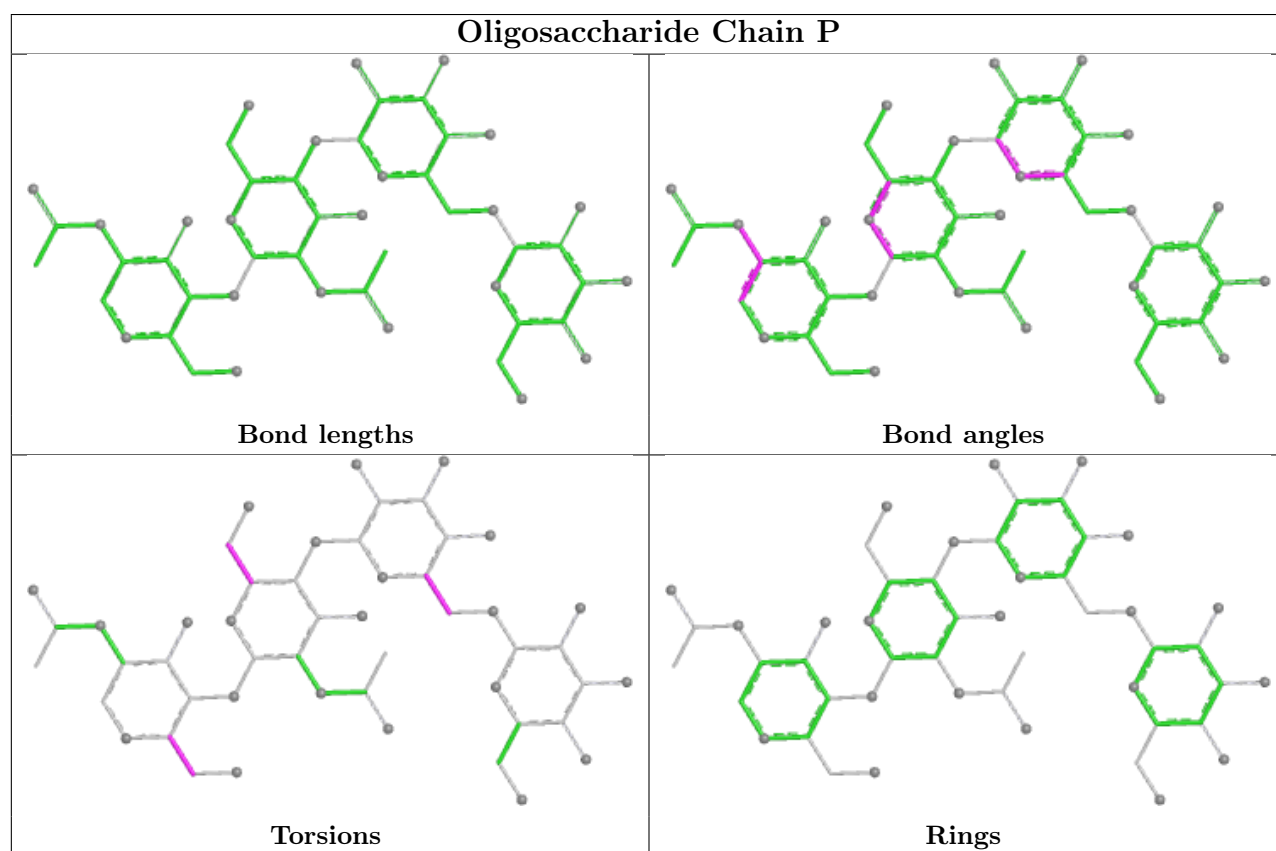
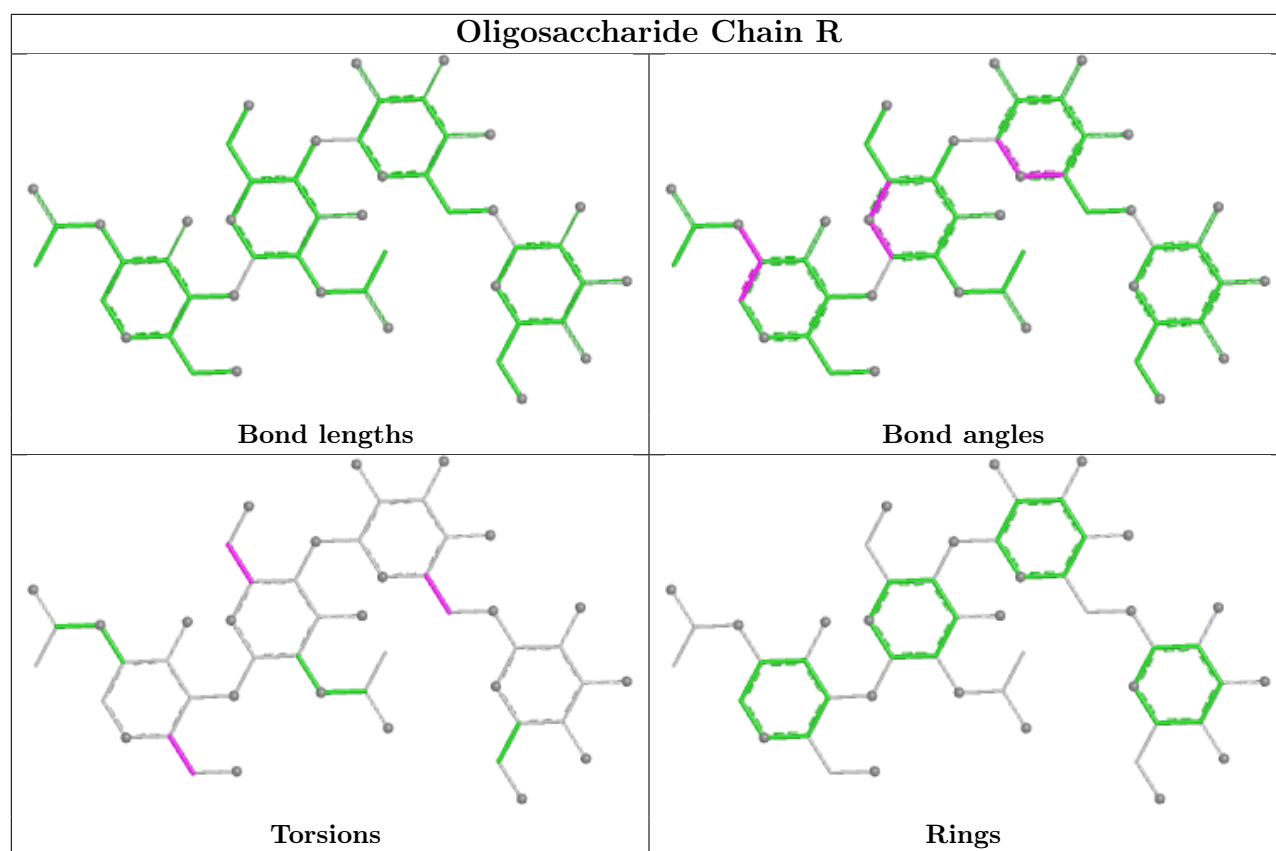


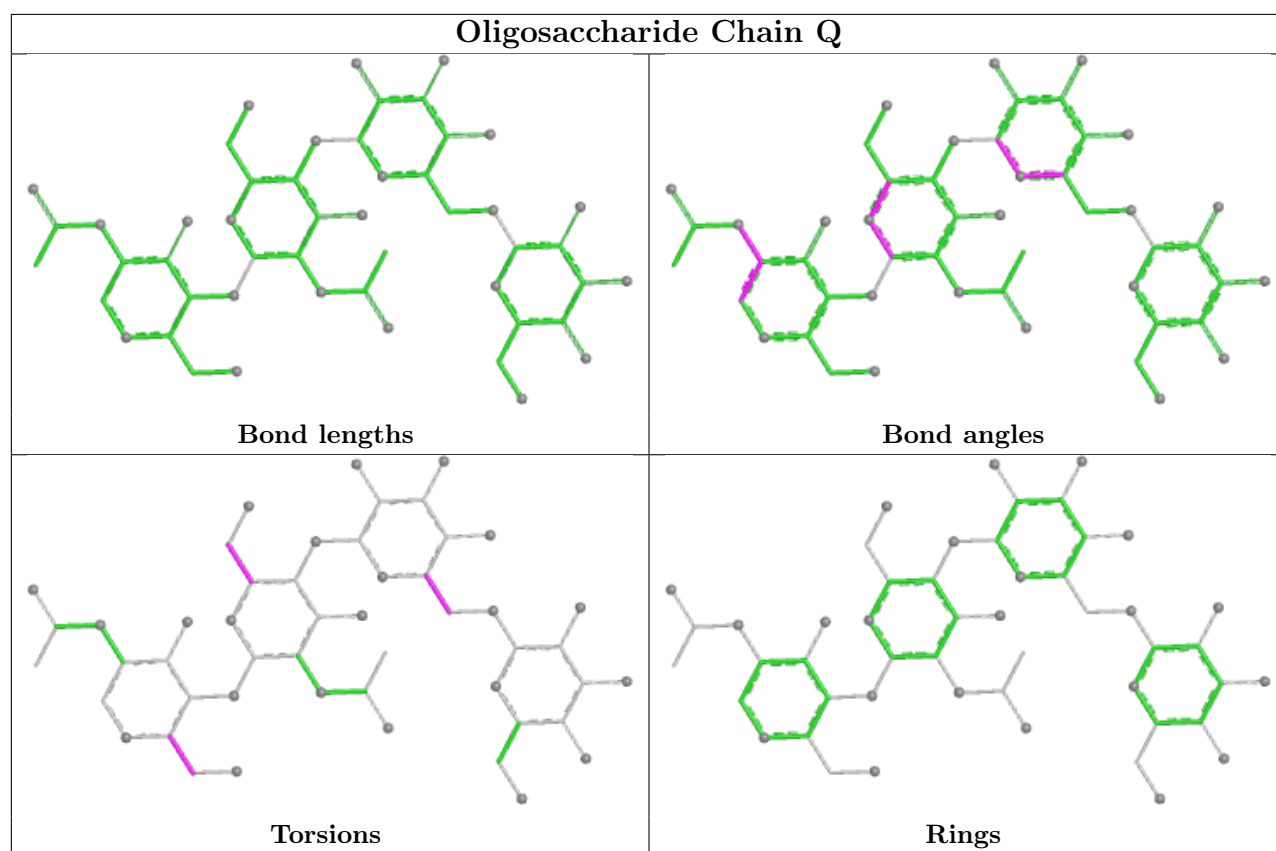


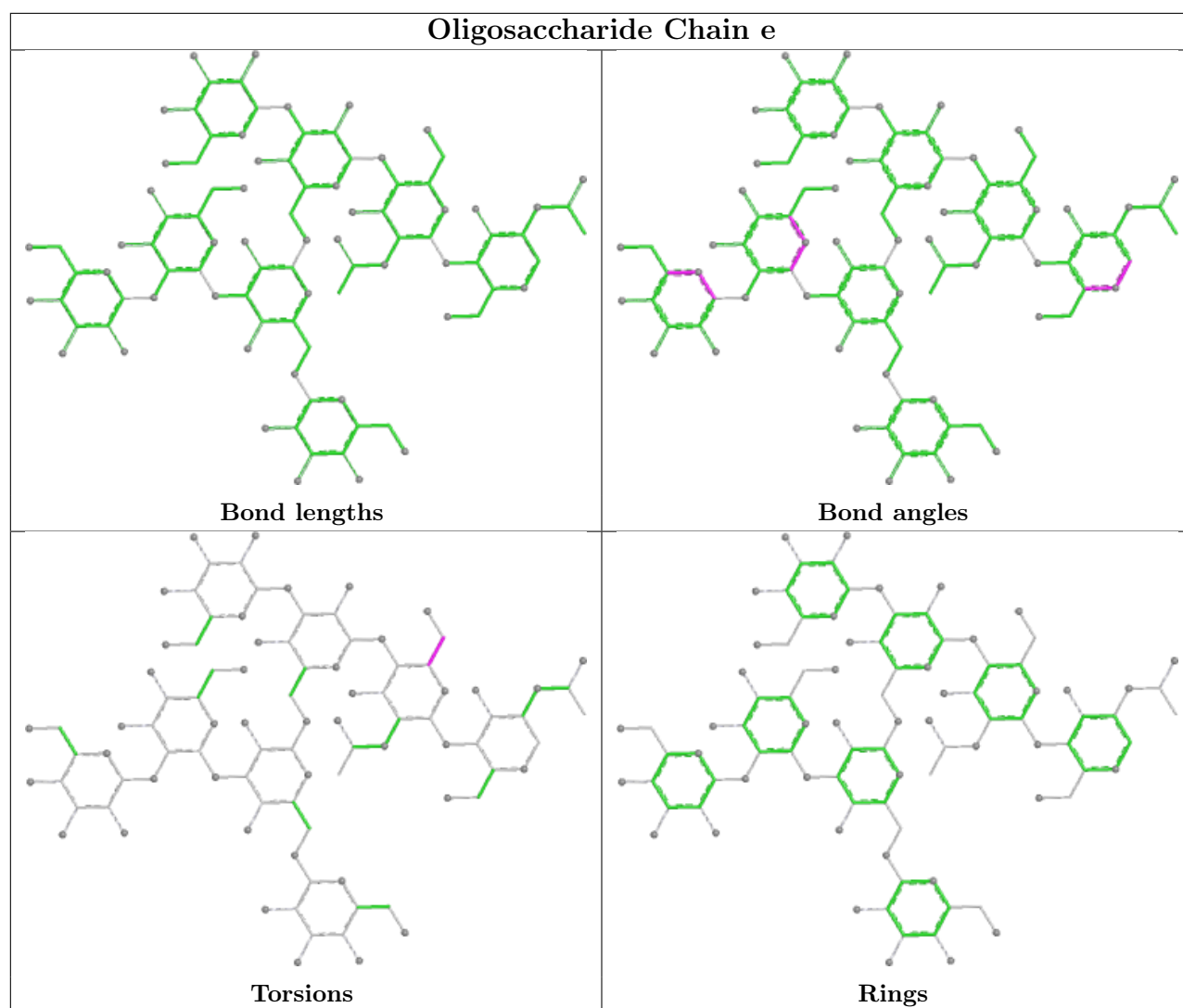


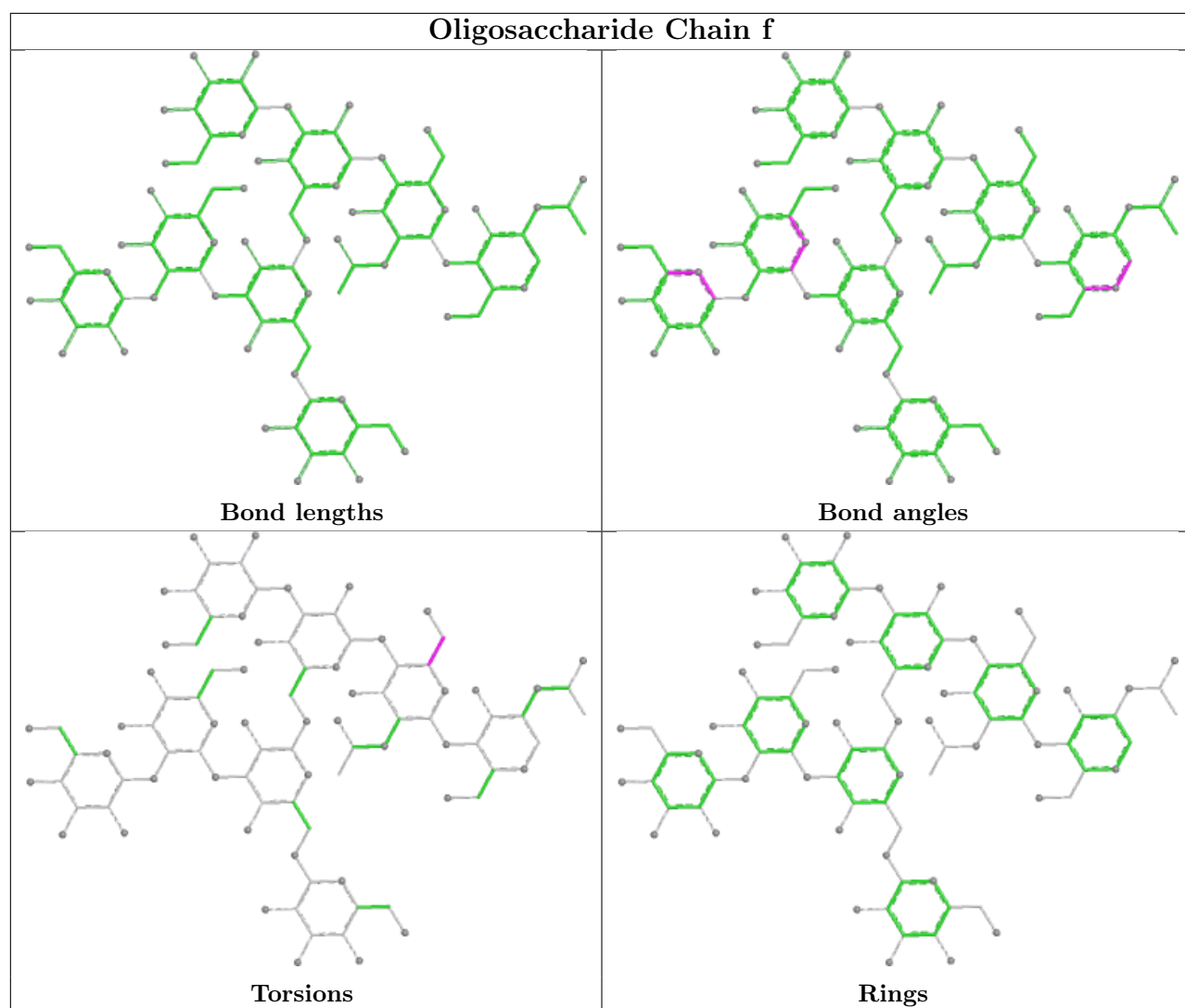


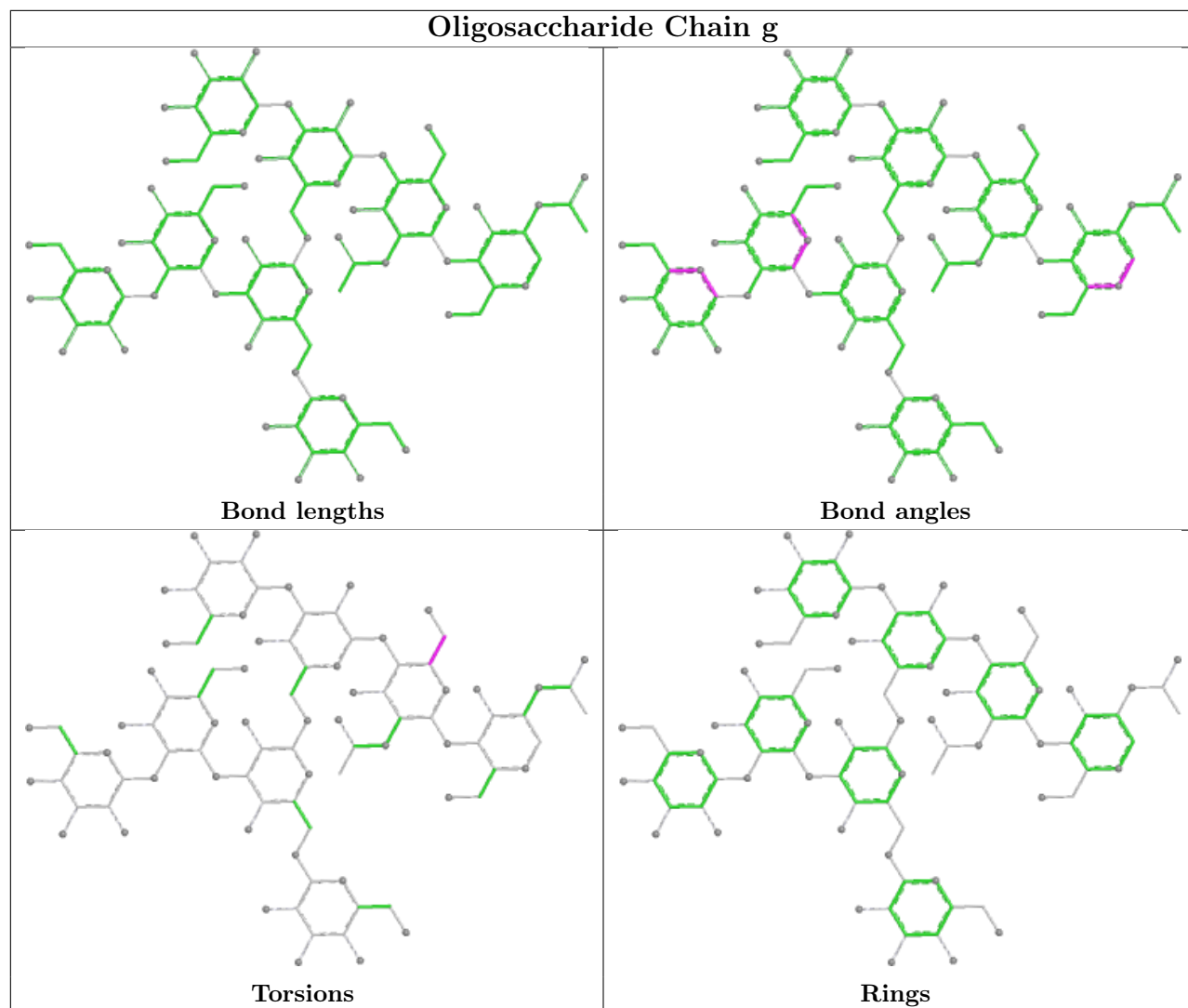


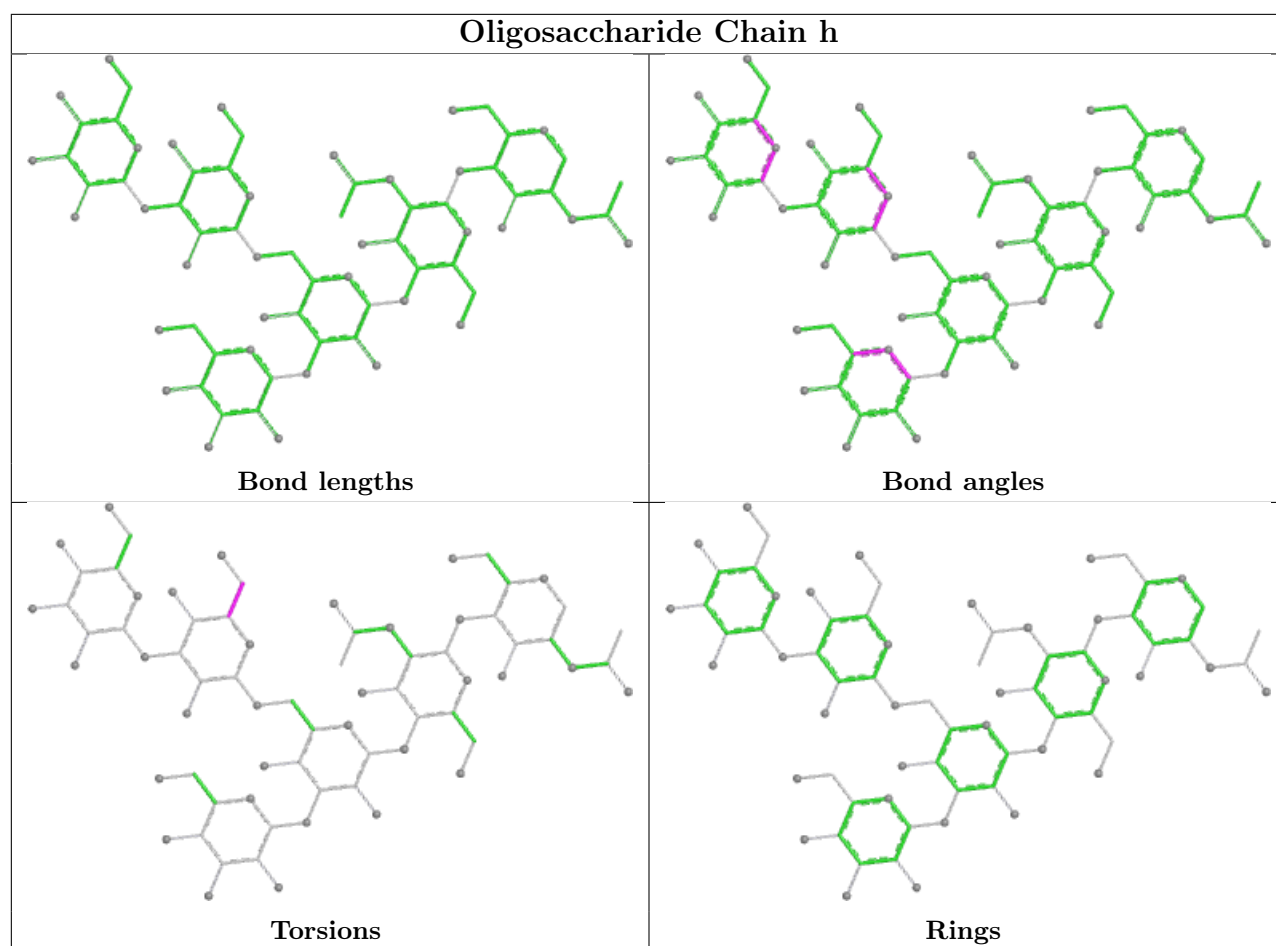


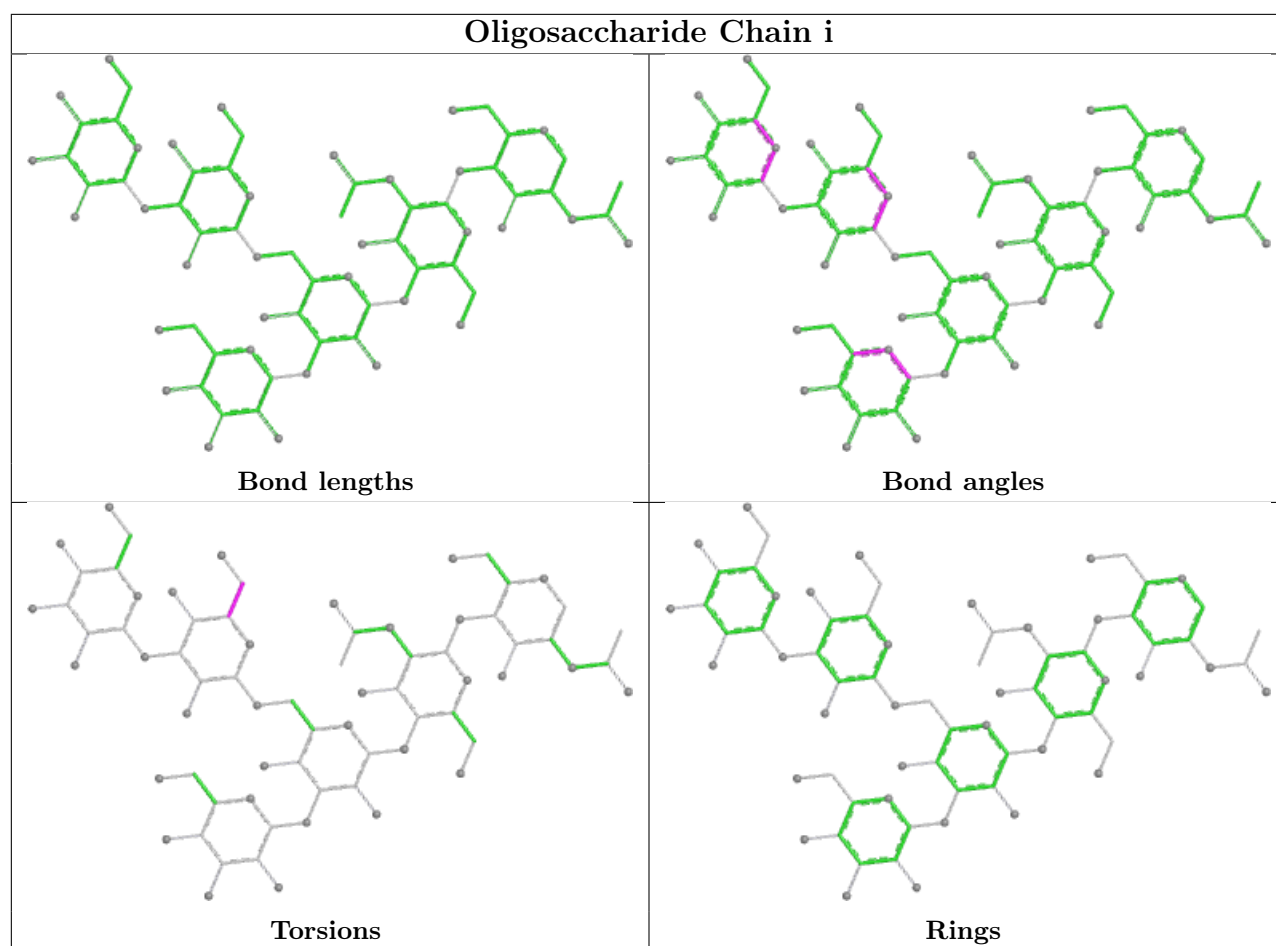


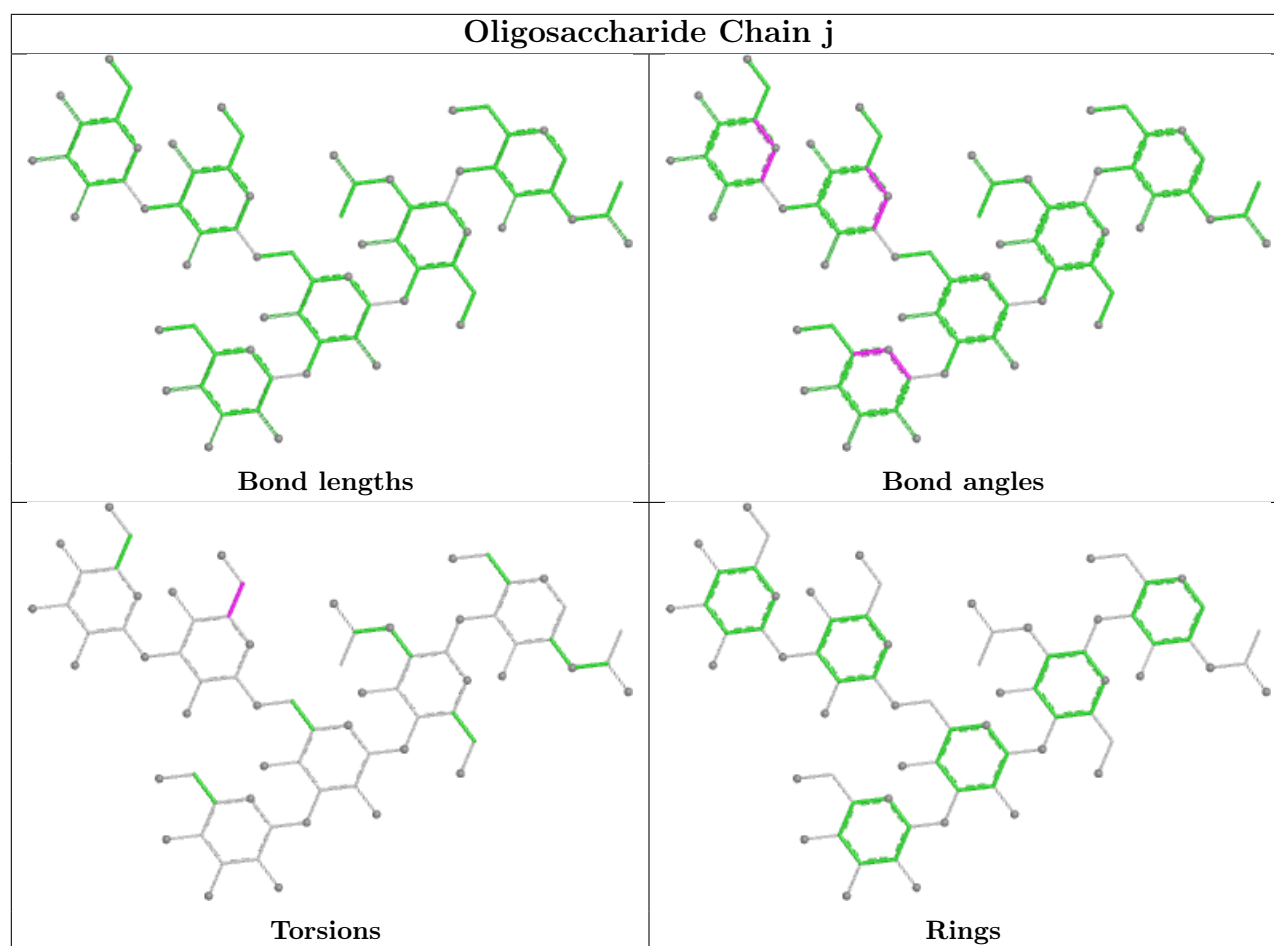












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	PTY	H	1101	-	49,49,49	0.27	0	52,54,54	0.31	0
8	NAG	G	1002	1	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
10	PTY	D	1101	-	49,49,49	0.27	0	52,54,54	0.31	0
8	NAG	B	1002	1	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
8	NAG	C	1001	1	14,14,15	0.33	0	17,19,21	0.57	0
8	NAG	G	1003	1	14,14,15	0.33	0	17,19,21	1.29	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	1001	1	14,14,15	0.33	0	17,19,21	0.56	0
8	NAG	C	1003	1	14,14,15	0.34	0	17,19,21	1.29	3 (17%)
9	CLR	L	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
8	NAG	G	1001	1	14,14,15	0.31	0	17,19,21	0.56	0
8	NAG	C	1002	1	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
9	CLR	H	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	PTY	L	1101	-	49,49,49	0.27	0	52,54,54	0.30	0
9	CLR	D	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
8	NAG	B	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
10	PTY	H	1101	-	-	16/53/53/53	-
8	NAG	G	1002	1	-	2/6/23/26	0/1/1/1
10	PTY	D	1101	-	-	16/53/53/53	-
8	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1003	1	-	2/6/23/26	0/1/1/1
9	CLR	L	1100	-	-	6/10/68/68	0/4/4/4
8	NAG	G	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
9	CLR	H	1100	-	-	6/10/68/68	0/4/4/4
10	PTY	L	1101	-	-	16/53/53/53	-
9	CLR	D	1100	-	-	6/10/68/68	0/4/4/4
8	NAG	B	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(°)
8	B	1003	NAG	C2-N2-C7	2.84	126.70	122.90
8	C	1003	NAG	C2-N2-C7	2.81	126.66	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1003	NAG	C2-N2-C7	2.80	126.65	122.90
8	B	1003	NAG	C8-C7-N2	2.63	120.47	116.12
8	C	1003	NAG	C8-C7-N2	2.62	120.46	116.12
8	G	1003	NAG	C8-C7-N2	2.60	120.42	116.12
8	B	1003	NAG	C1-O5-C5	2.53	115.57	112.19
8	G	1003	NAG	C1-O5-C5	2.53	115.57	112.19
8	C	1003	NAG	C1-O5-C5	2.49	115.53	112.19
8	C	1002	NAG	C2-N2-C7	2.37	126.07	122.90
8	B	1002	NAG	C2-N2-C7	2.32	126.00	122.90
8	G	1002	NAG	C2-N2-C7	2.30	125.98	122.90

There are no chirality outliers.

All (81) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
8	B	1001	NAG	O5-C5-C6-O6
8	C	1001	NAG	O5-C5-C6-O6
8	G	1001	NAG	O5-C5-C6-O6
10	D	1101	PTY	C12-C13-C14-C15
10	H	1101	PTY	C12-C13-C14-C15
10	L	1101	PTY	C12-C13-C14-C15
10	D	1101	PTY	C35-C36-C37-C38
10	H	1101	PTY	C35-C36-C37-C38
10	L	1101	PTY	C35-C36-C37-C38
10	D	1101	PTY	O4-C1-C6-O7
10	H	1101	PTY	O4-C1-C6-O7
10	L	1101	PTY	O4-C1-C6-O7
9	D	1100	CLR	C21-C20-C22-C23
9	H	1100	CLR	C21-C20-C22-C23
9	L	1100	CLR	C21-C20-C22-C23
9	D	1100	CLR	C13-C17-C20-C22
9	H	1100	CLR	C13-C17-C20-C22
9	L	1100	CLR	C13-C17-C20-C22
9	D	1100	CLR	C16-C17-C20-C22
9	H	1100	CLR	C16-C17-C20-C22
9	L	1100	CLR	C16-C17-C20-C22
10	D	1101	PTY	C6-C5-O14-P1
10	H	1101	PTY	C6-C5-O14-P1
10	L	1101	PTY	C6-C5-O14-P1
9	D	1100	CLR	C13-C17-C20-C21
9	H	1100	CLR	C13-C17-C20-C21
9	L	1100	CLR	C13-C17-C20-C21
10	D	1101	PTY	O14-C5-C6-O7
10	H	1101	PTY	O14-C5-C6-O7
10	L	1101	PTY	O14-C5-C6-O7
10	D	1101	PTY	C33-C34-C35-C36
10	H	1101	PTY	C33-C34-C35-C36
10	L	1101	PTY	C33-C34-C35-C36
10	D	1101	PTY	C26-C27-C28-C29
10	H	1101	PTY	C26-C27-C28-C29
10	L	1101	PTY	C26-C27-C28-C29
8	B	1002	NAG	C1-C2-N2-C7
8	C	1002	NAG	C1-C2-N2-C7
8	G	1002	NAG	C1-C2-N2-C7
8	B	1002	NAG	C3-C2-N2-C7
8	C	1002	NAG	C3-C2-N2-C7
8	G	1002	NAG	C3-C2-N2-C7

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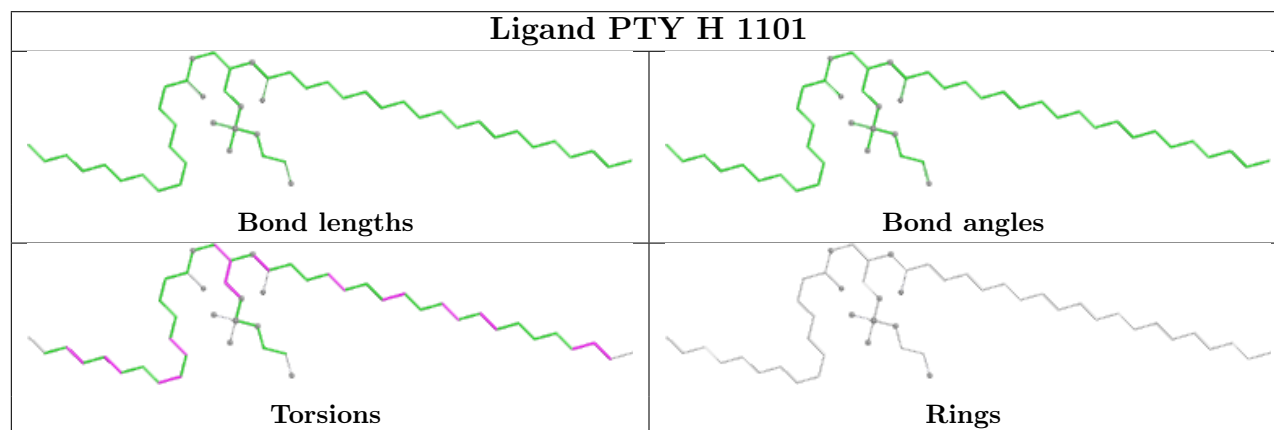
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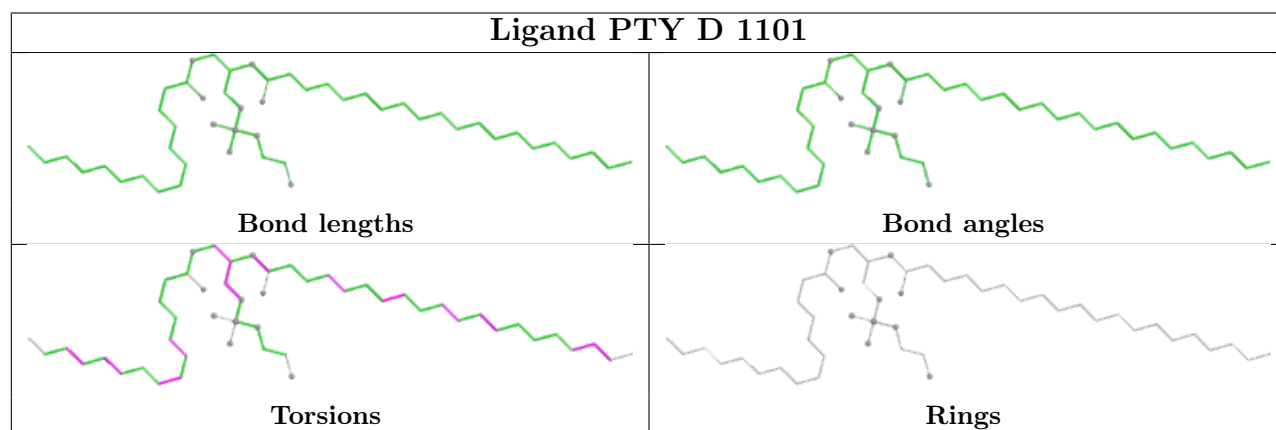
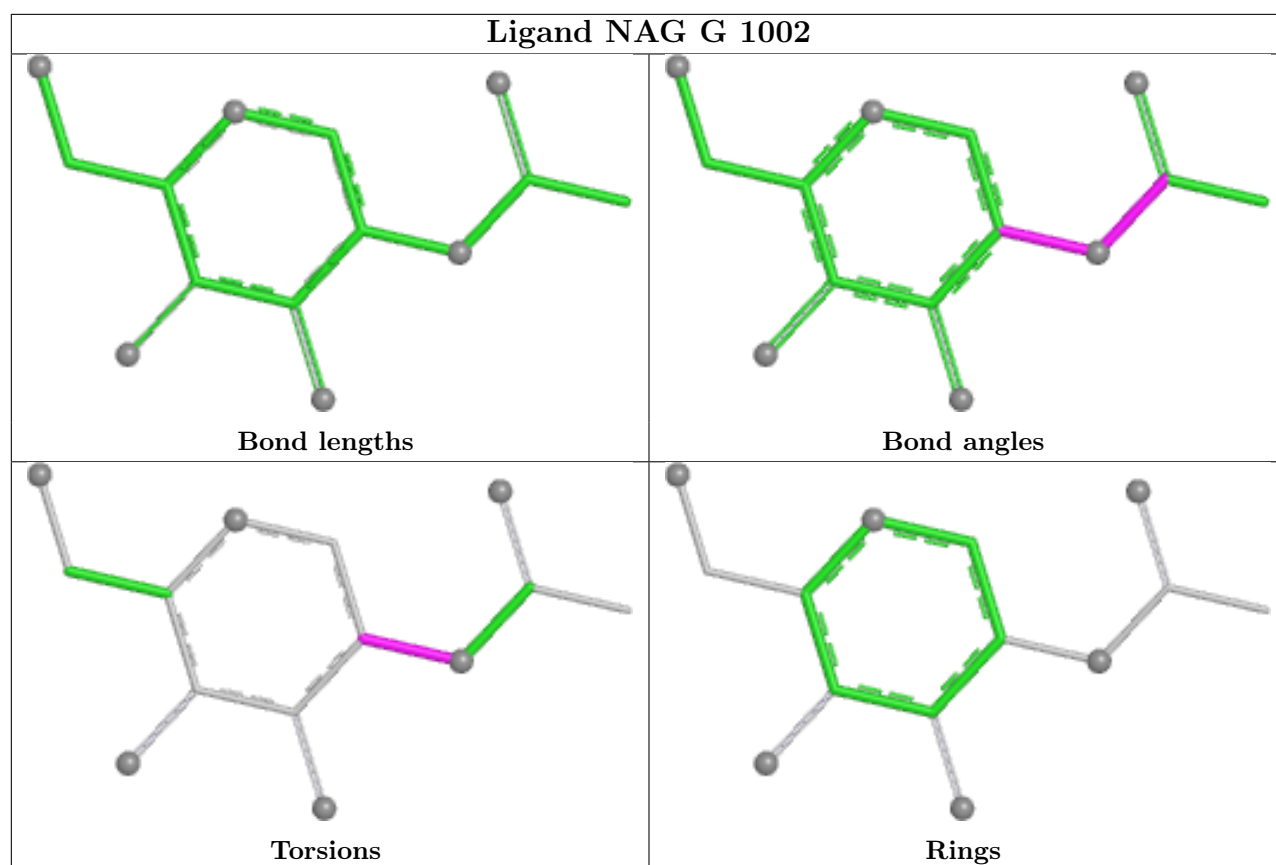
Mol	Chain	Res	Type	Atoms
10	L	1101	PTY	C20-C21-C22-C23
10	H	1101	PTY	C20-C21-C22-C23
10	D	1101	PTY	C20-C21-C22-C23
9	D	1100	CLR	C16-C17-C20-C21
9	L	1100	CLR	C16-C17-C20-C21
9	H	1100	CLR	C16-C17-C20-C21
10	D	1101	PTY	O4-C1-C6-C5
10	H	1101	PTY	O4-C1-C6-C5
10	L	1101	PTY	O4-C1-C6-C5
10	D	1101	PTY	C38-C39-C40-C41
10	H	1101	PTY	C38-C39-C40-C41
10	L	1101	PTY	C38-C39-C40-C41

There are no ring outliers.

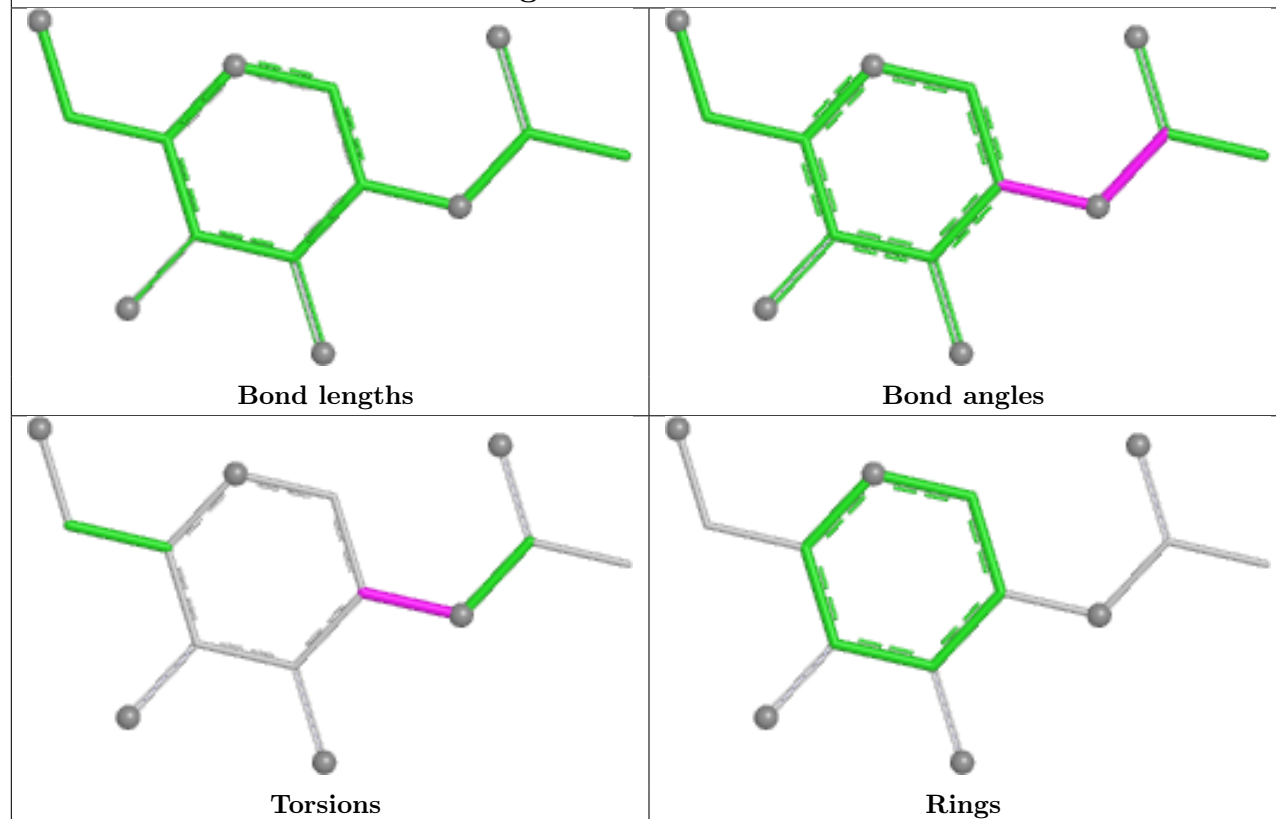
No monomer is involved in short contacts.

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.

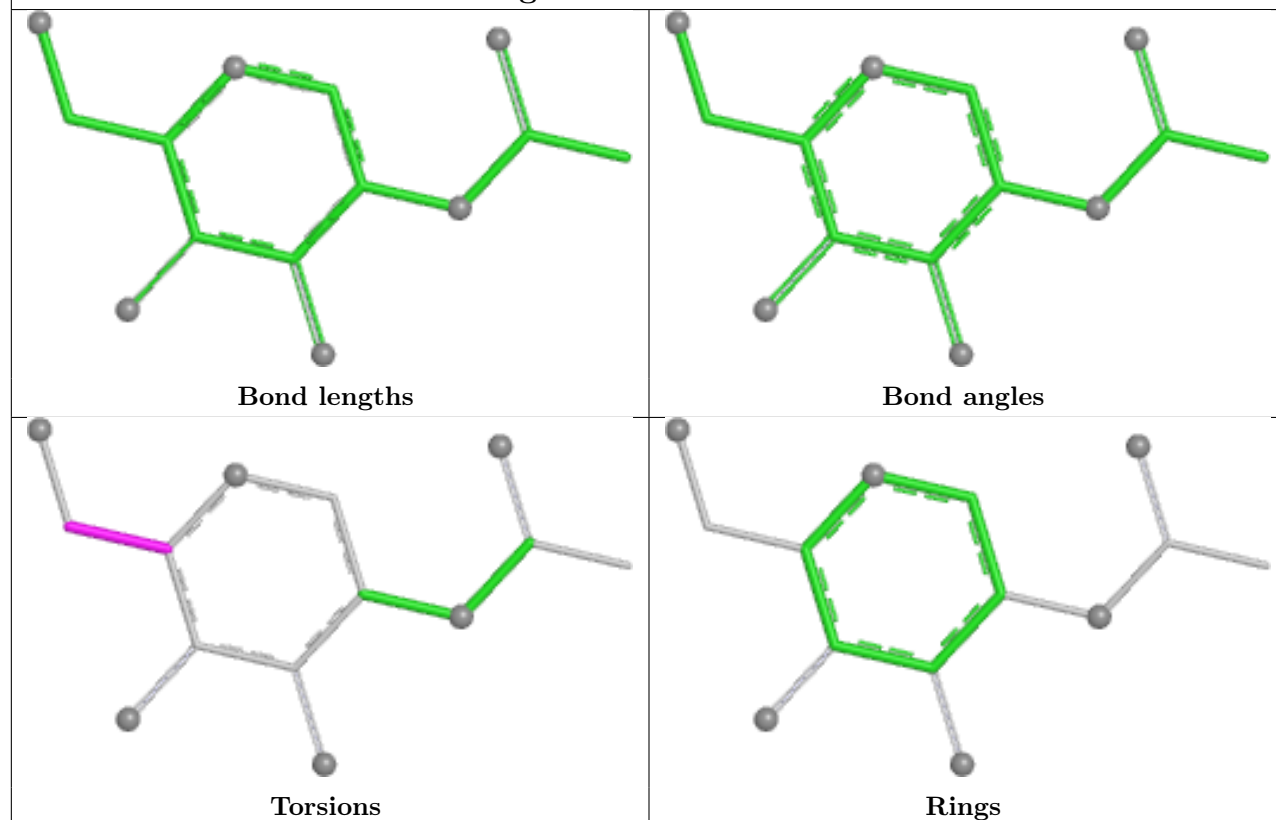


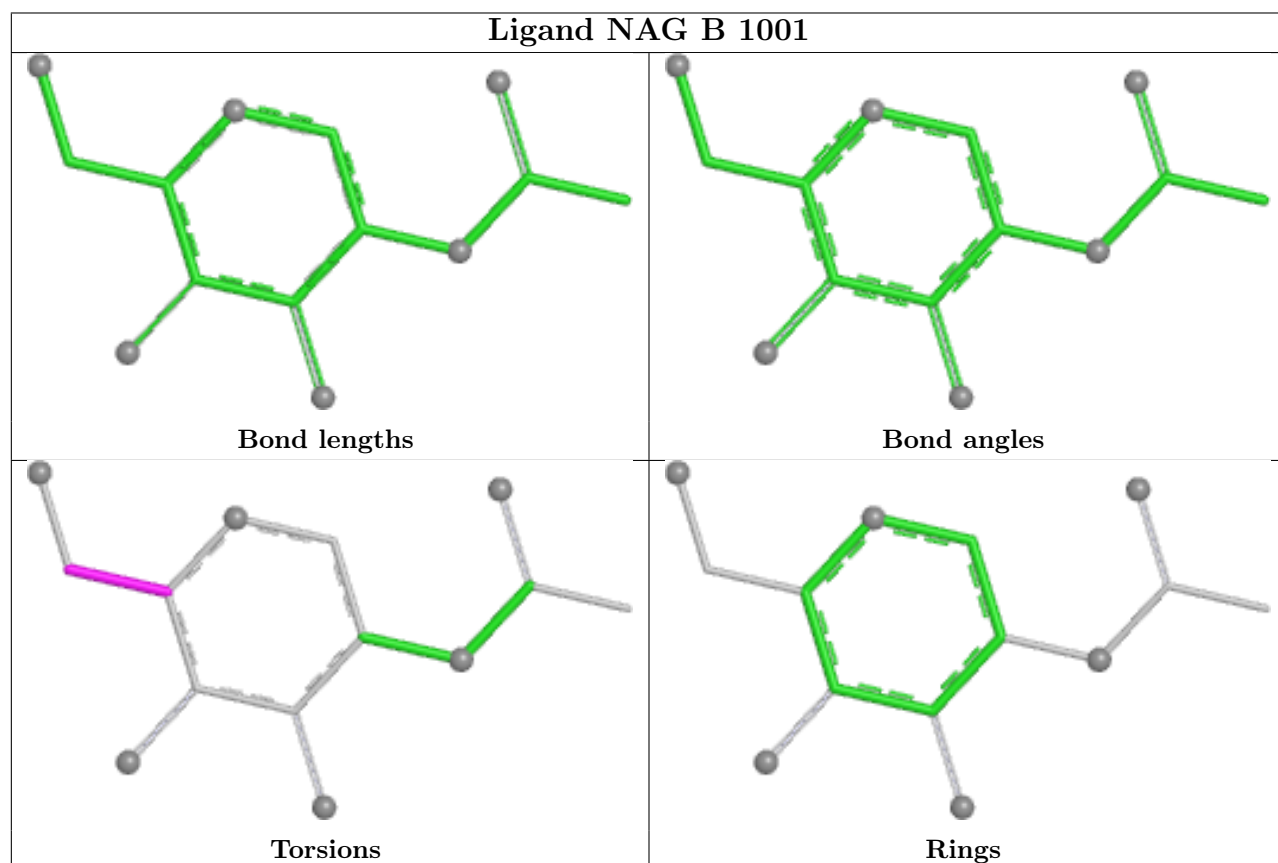
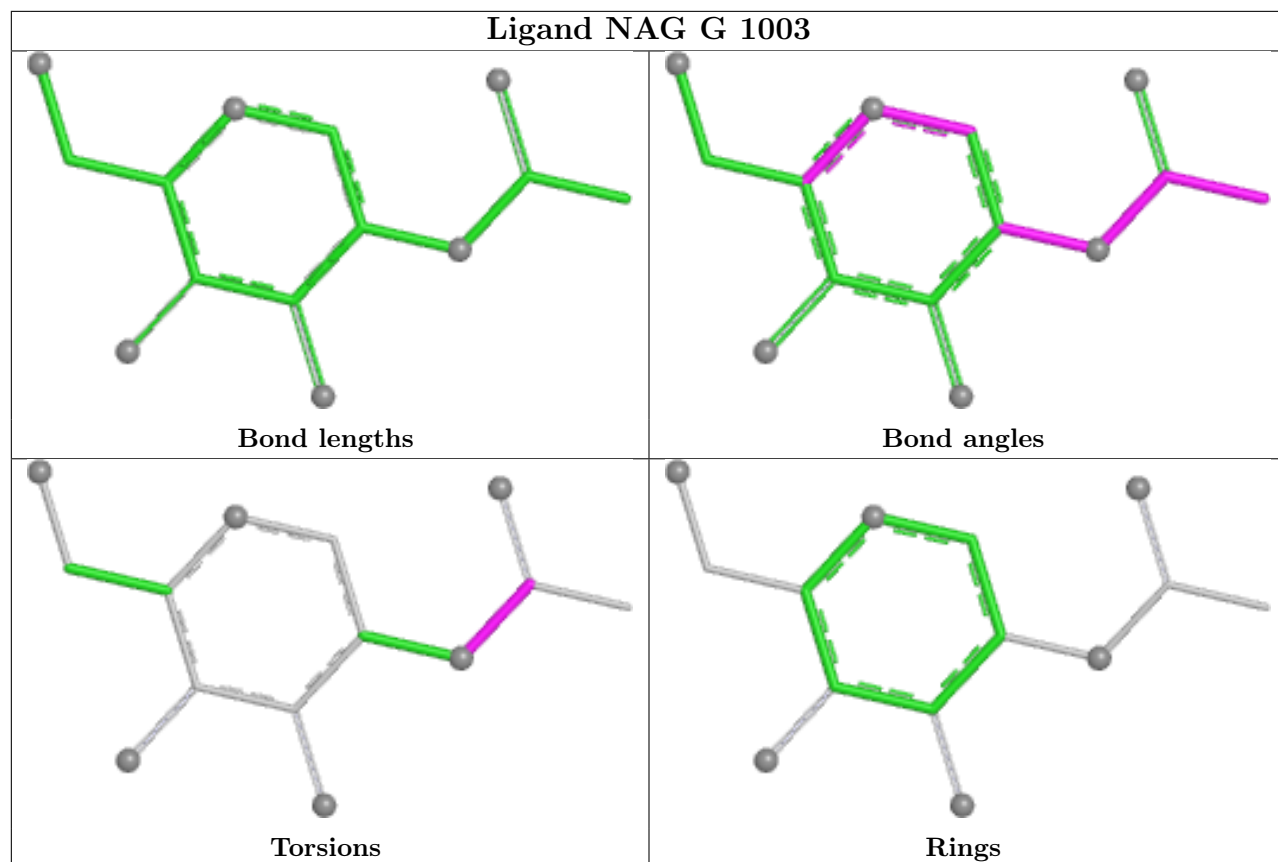


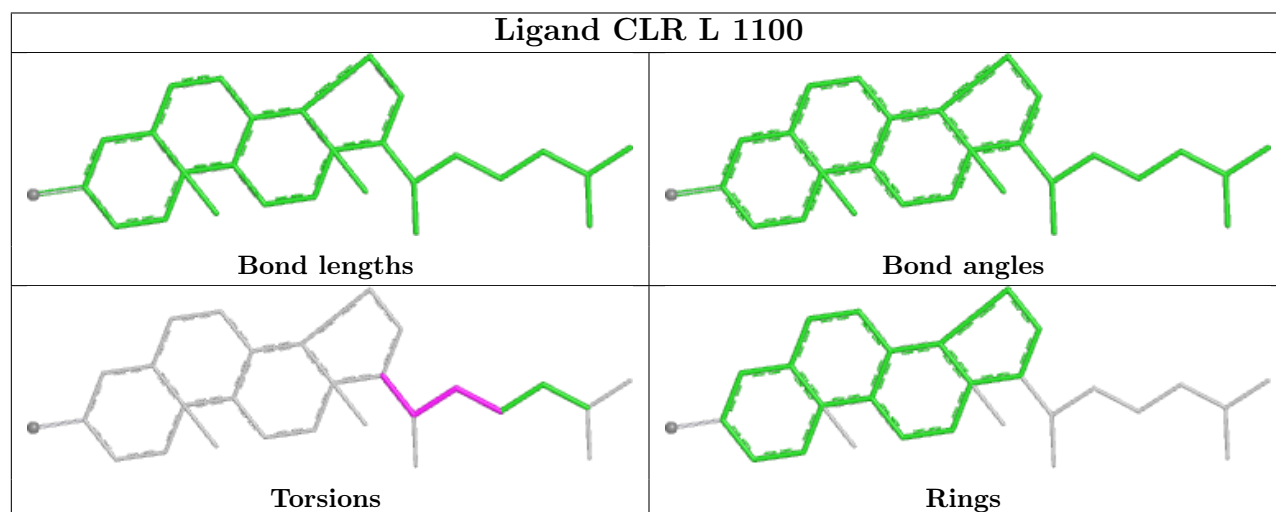
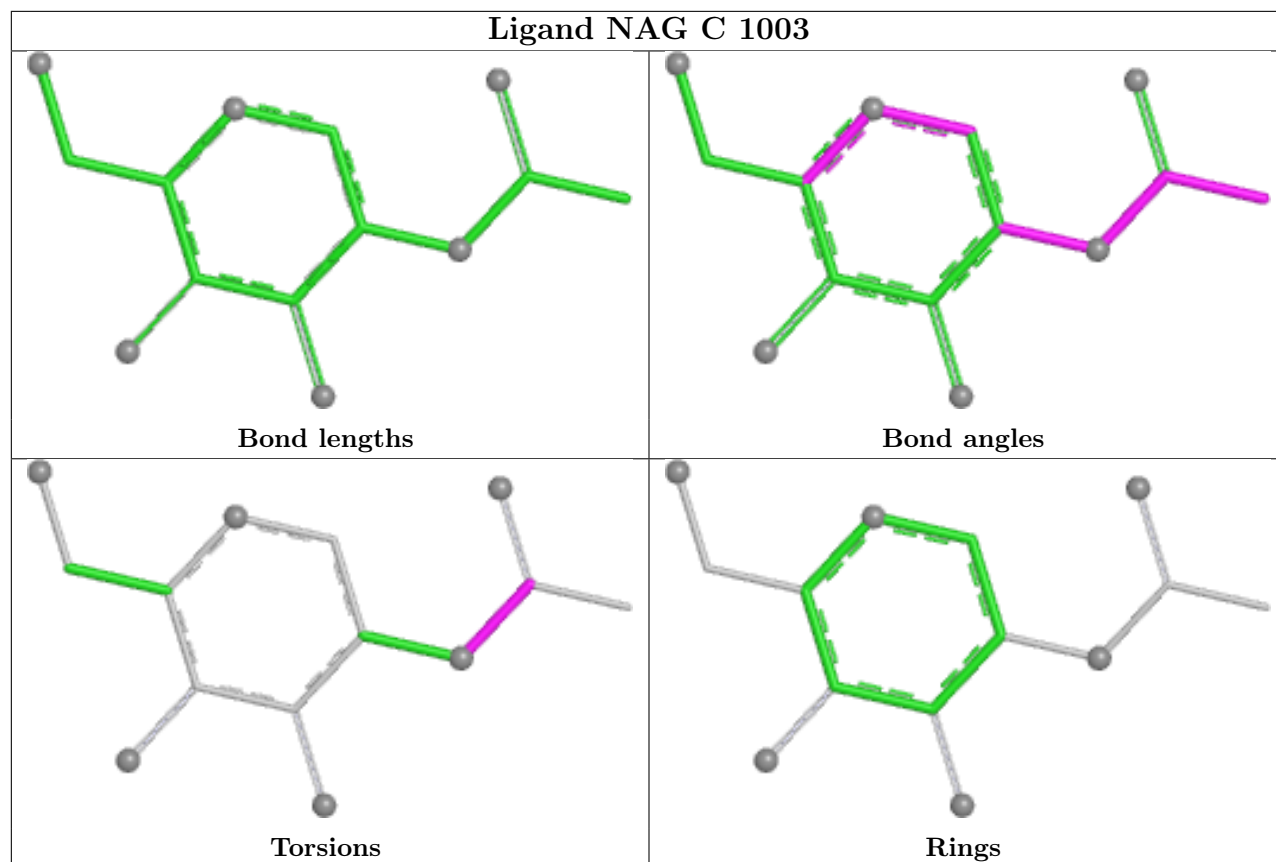
Ligand NAG B 1002

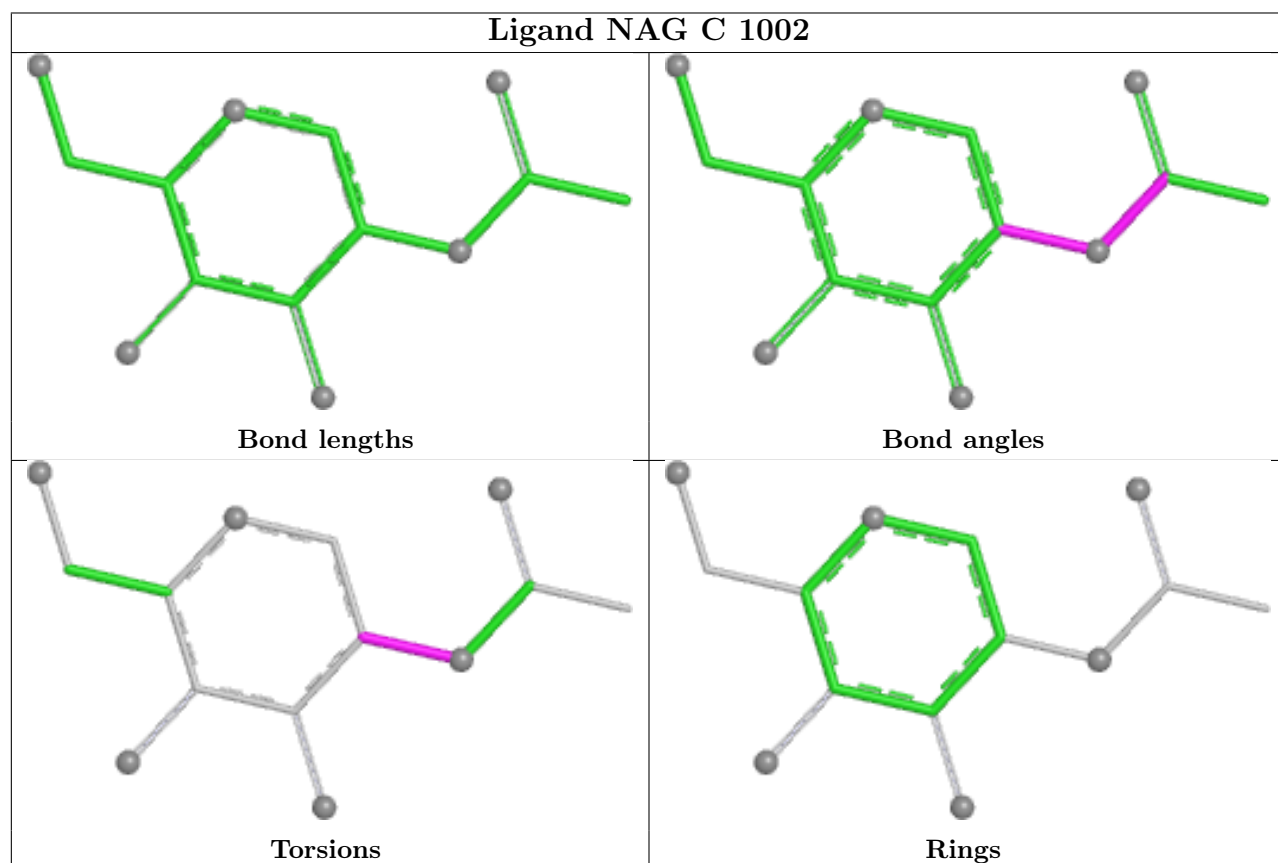
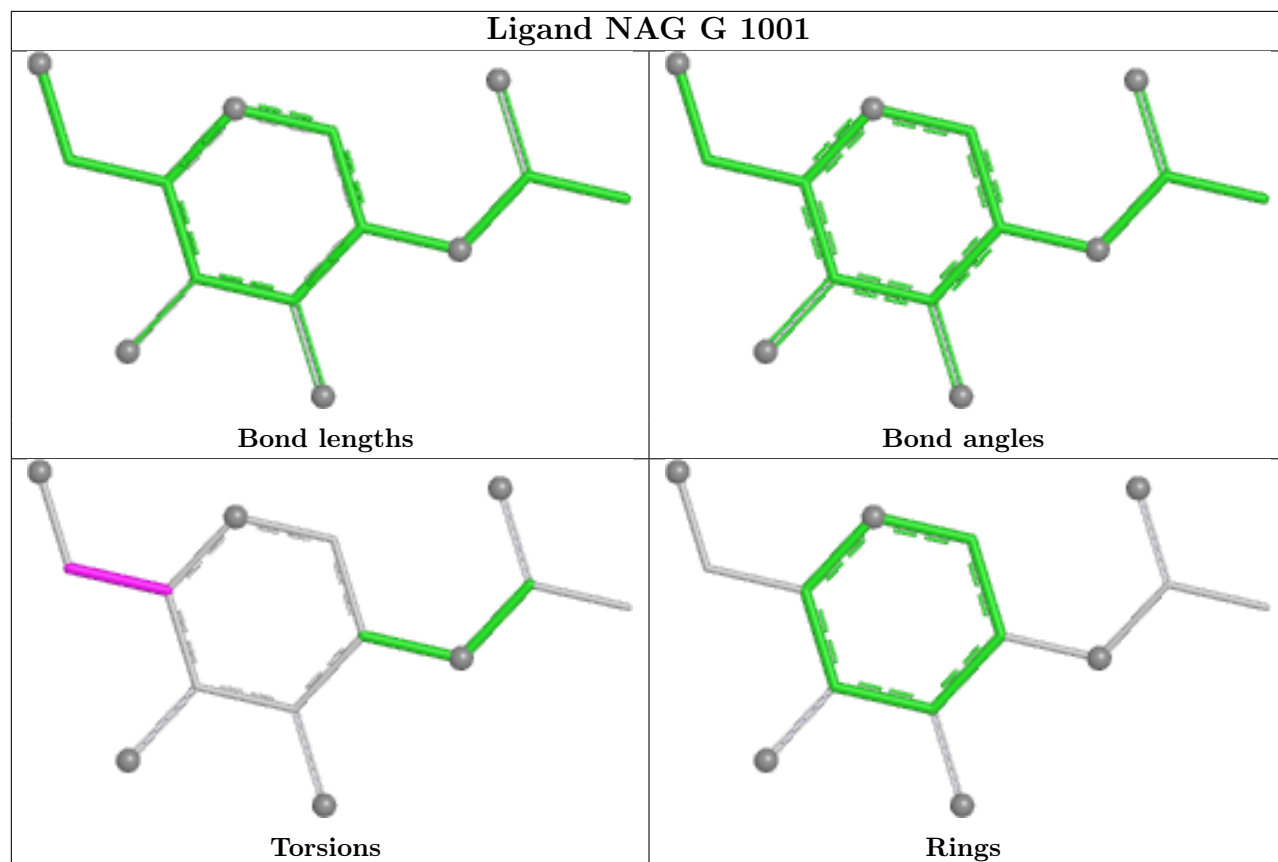


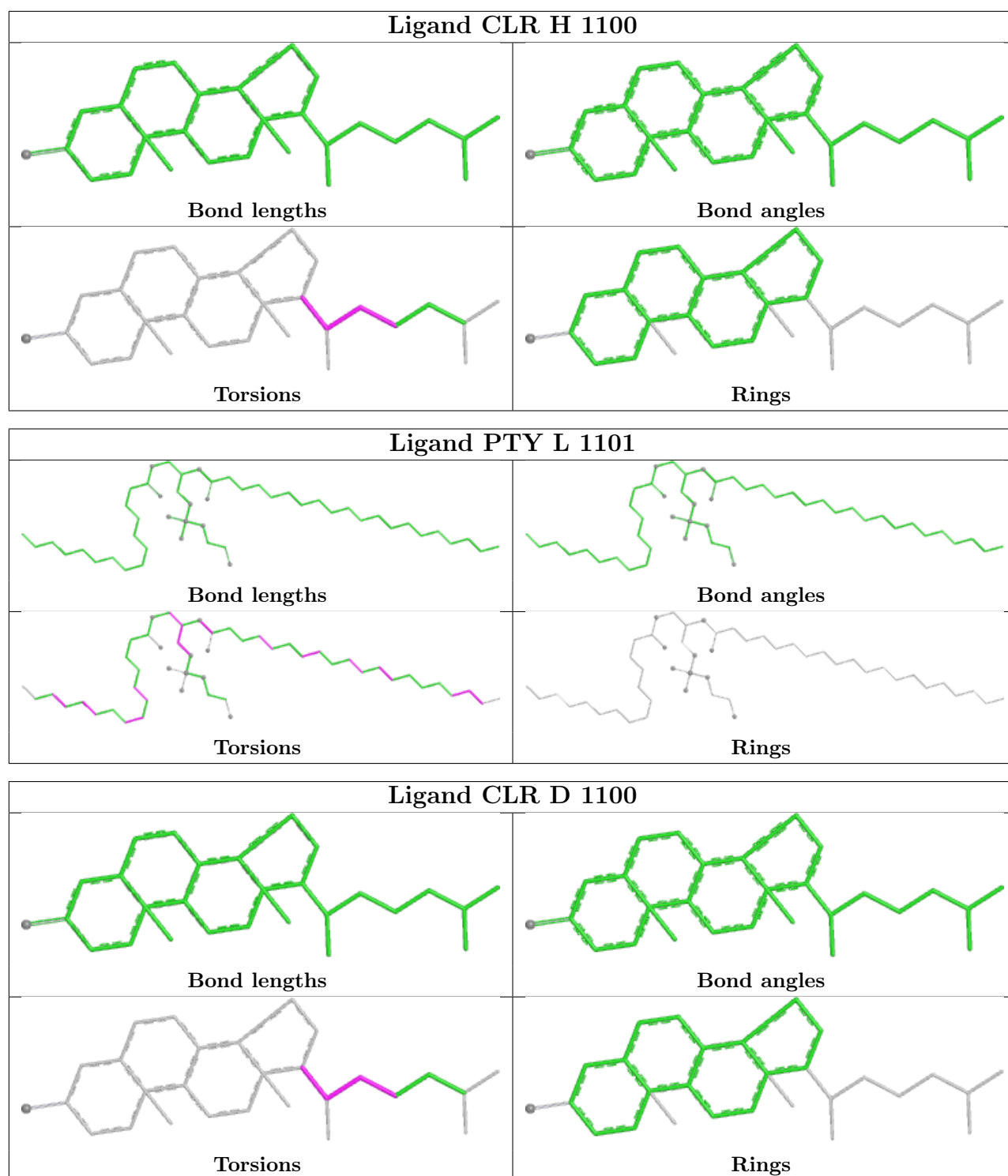
Ligand NAG C 1001

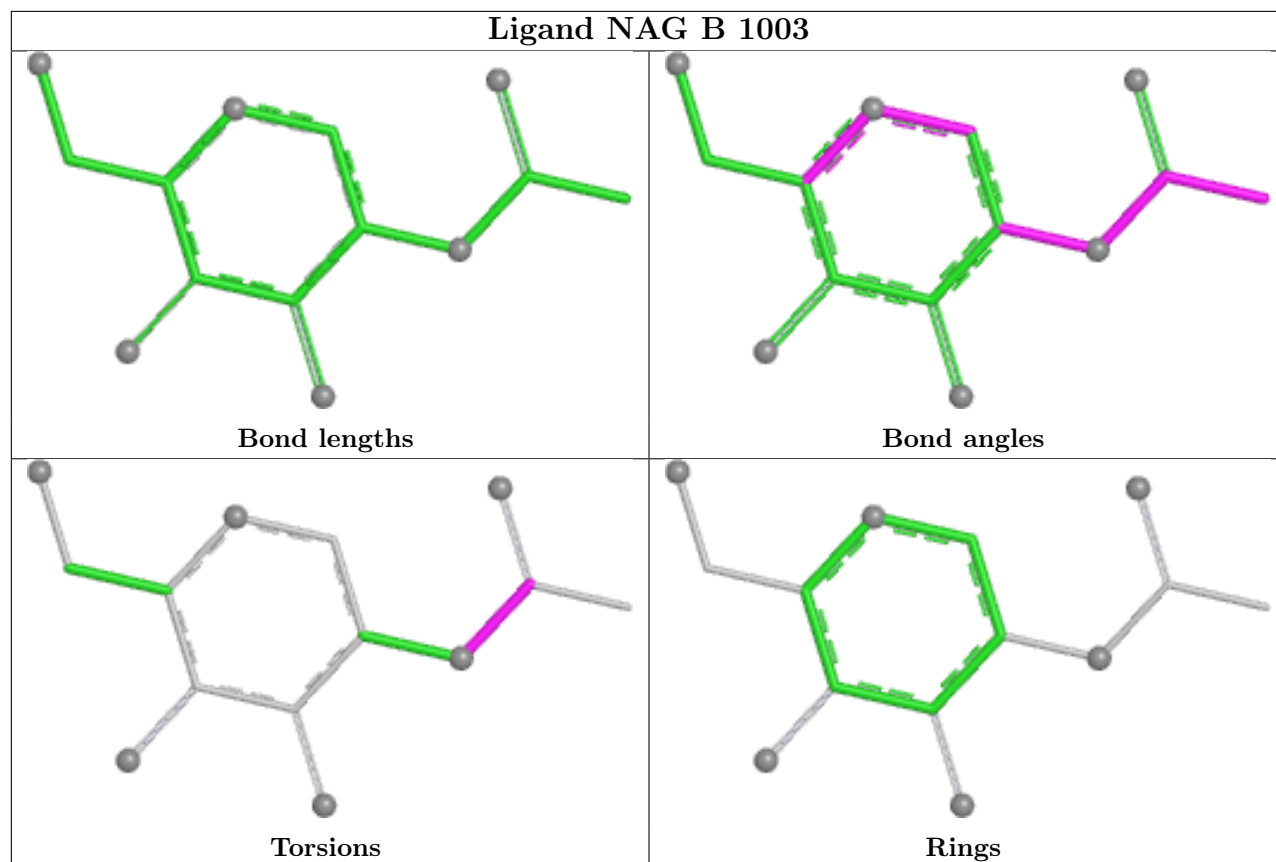












5.7 Other polymers [i](#)

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-17318. These allow visual inspection of the internal detail of the map and identification of artifacts.

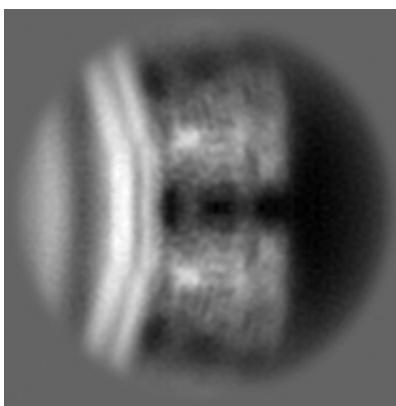
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

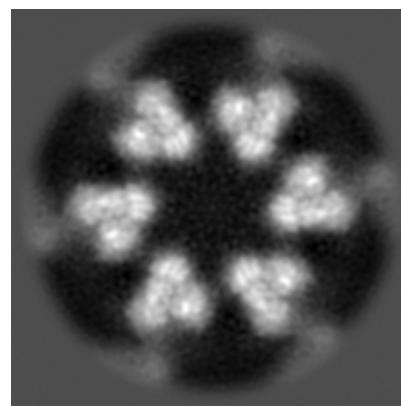
6.1.1 Primary map



X

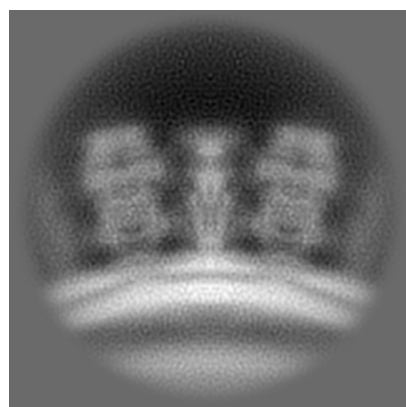


Y

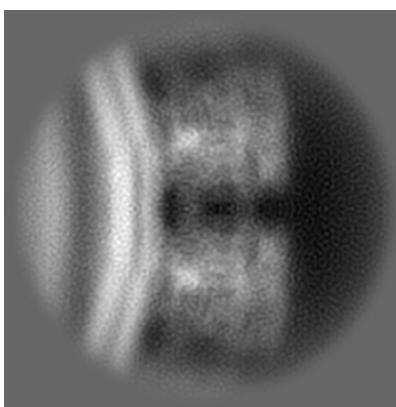


Z

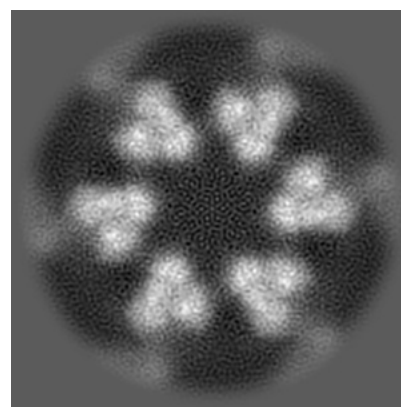
6.1.2 Raw map



X



Y



Z

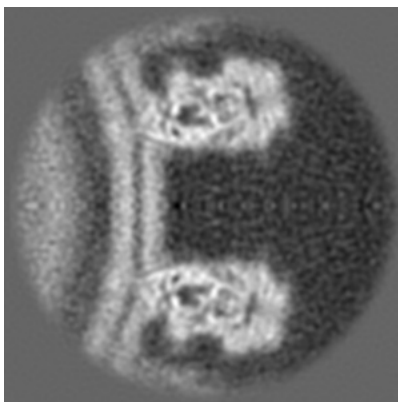
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

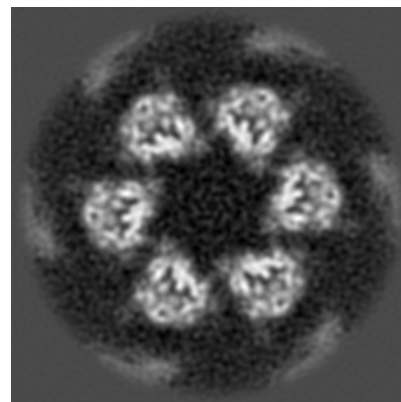
6.2.1 Primary map



X Index: 80

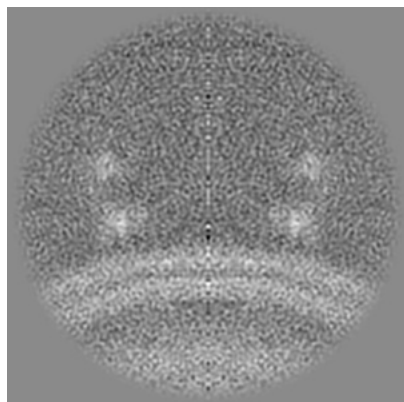


Y Index: 80

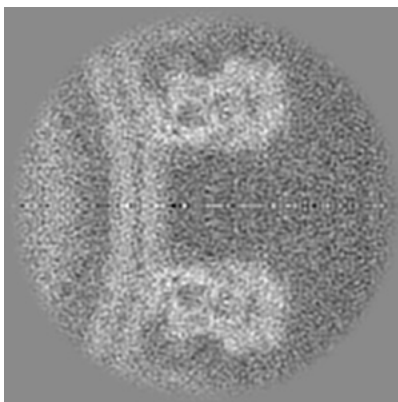


Z Index: 80

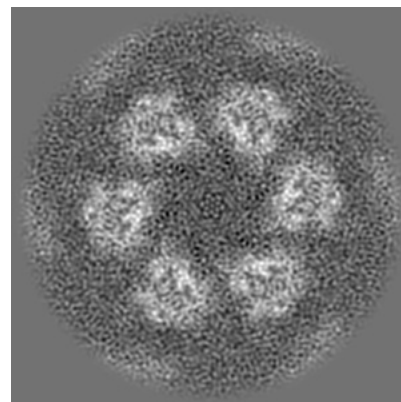
6.2.2 Raw map



X Index: 80



Y Index: 80

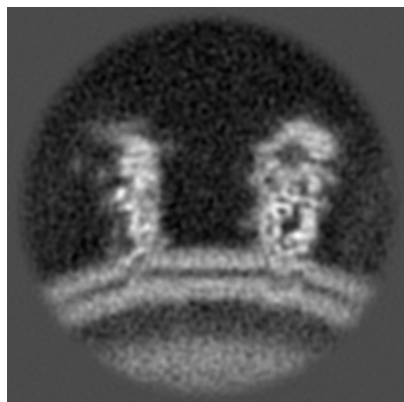


Z Index: 80

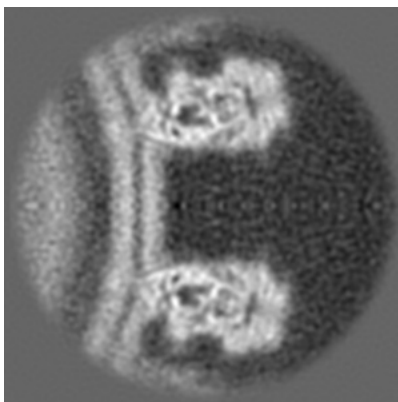
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

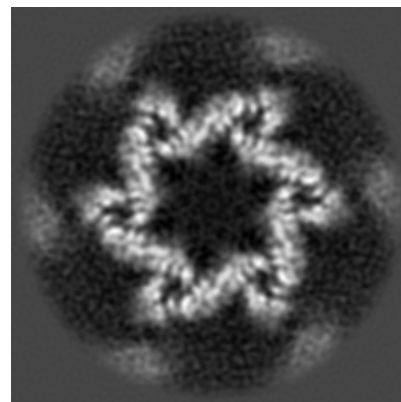
6.3.1 Primary map



X Index: 92

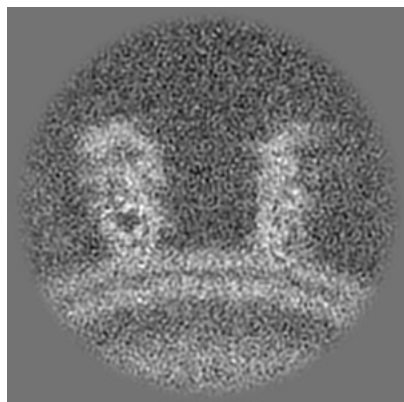


Y Index: 80

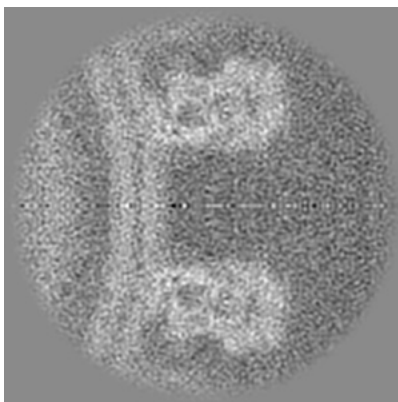


Z Index: 75

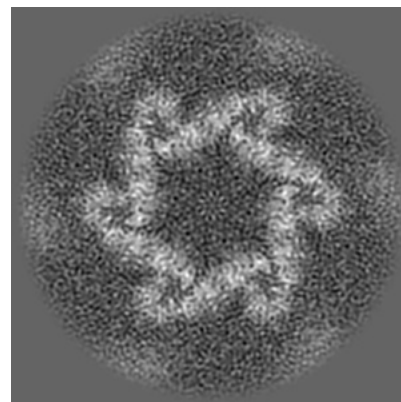
6.3.2 Raw map



X Index: 67



Y Index: 80

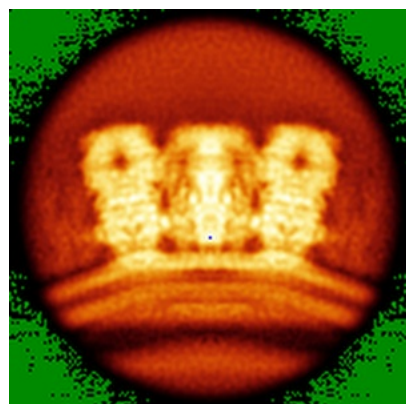


Z Index: 76

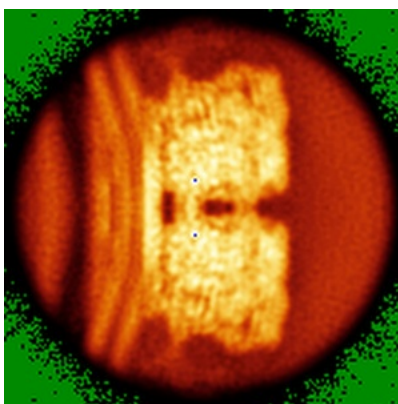
The images above show the largest variance slices of the map in three orthogonal directions.

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

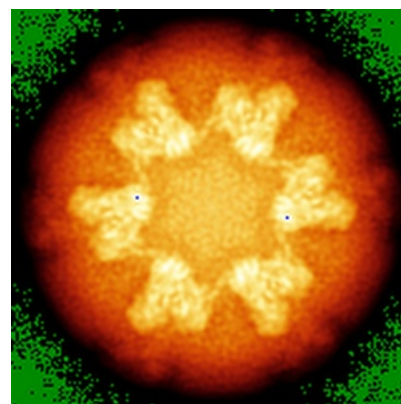
6.4.1 Primary map



X

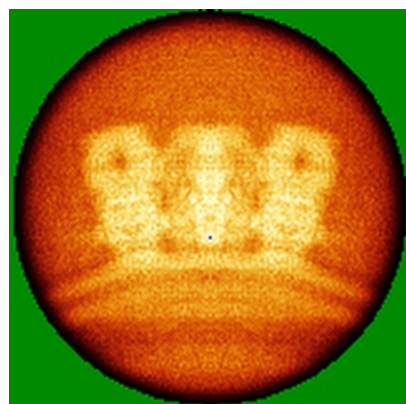


Y

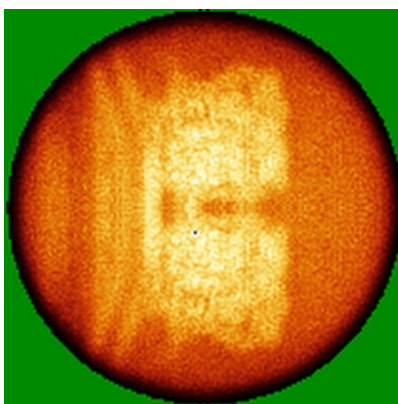


Z

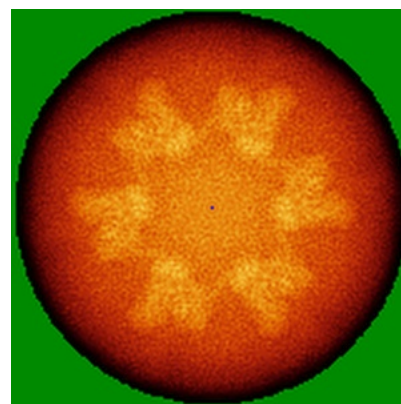
6.4.2 Raw map



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](#)

This section was not generated.

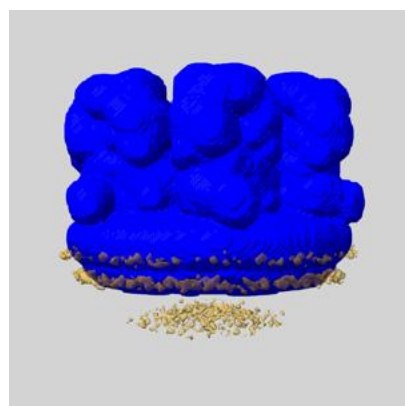
6.6 Mask visualisation [i](#)

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

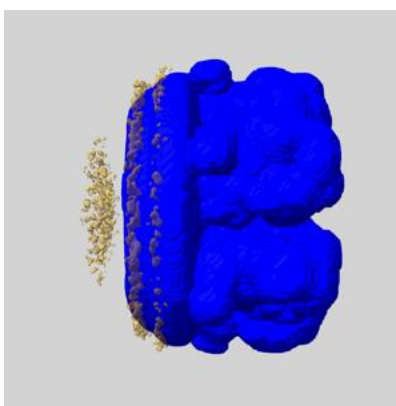
A mask typically either:

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

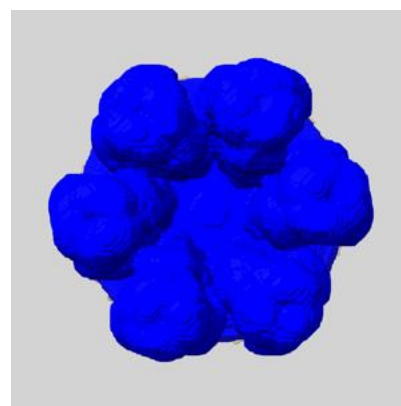
6.6.1 emd_17318_msk_1.map [i](#)



X



Y

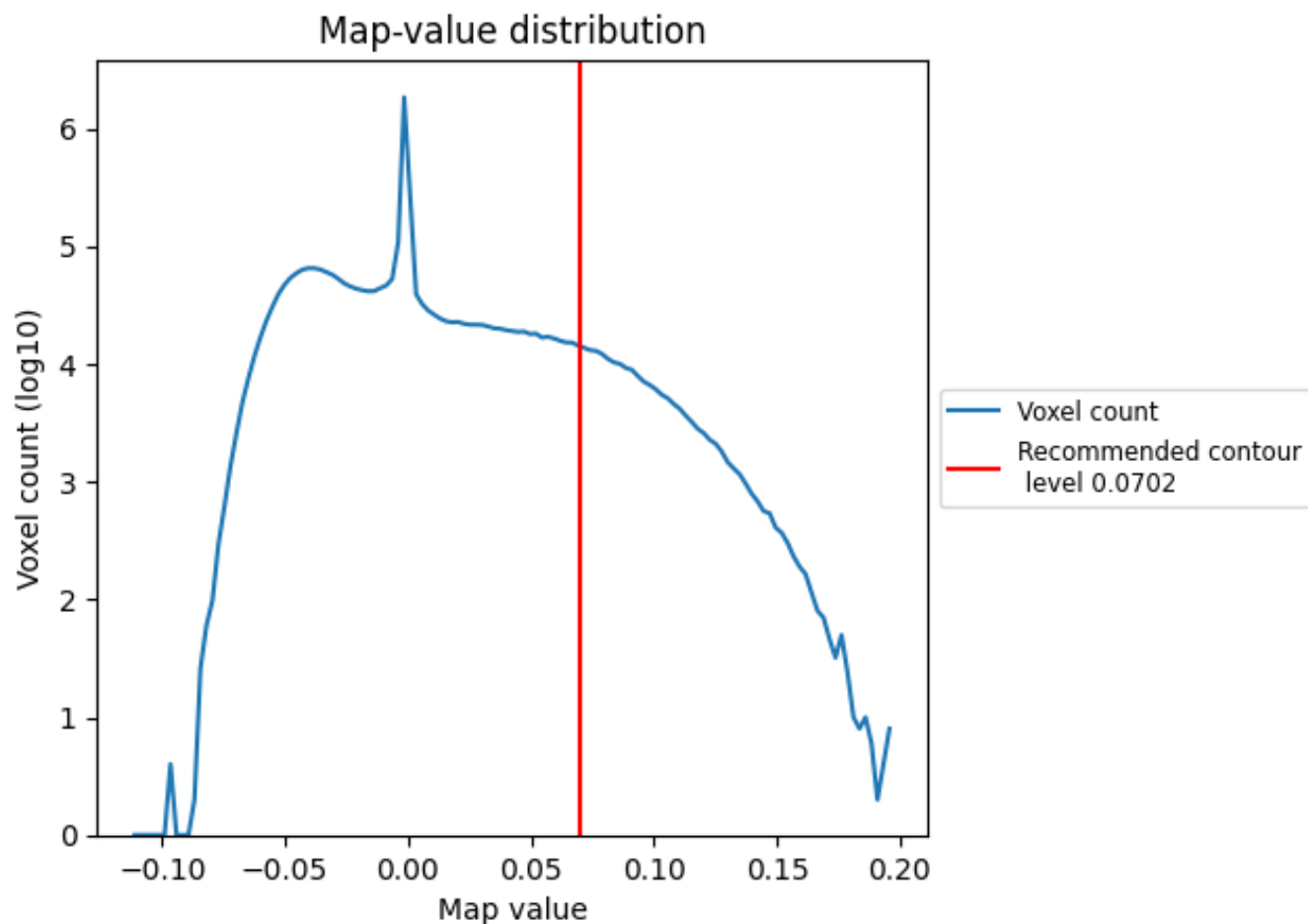


Z

7 Map analysis [i](#)

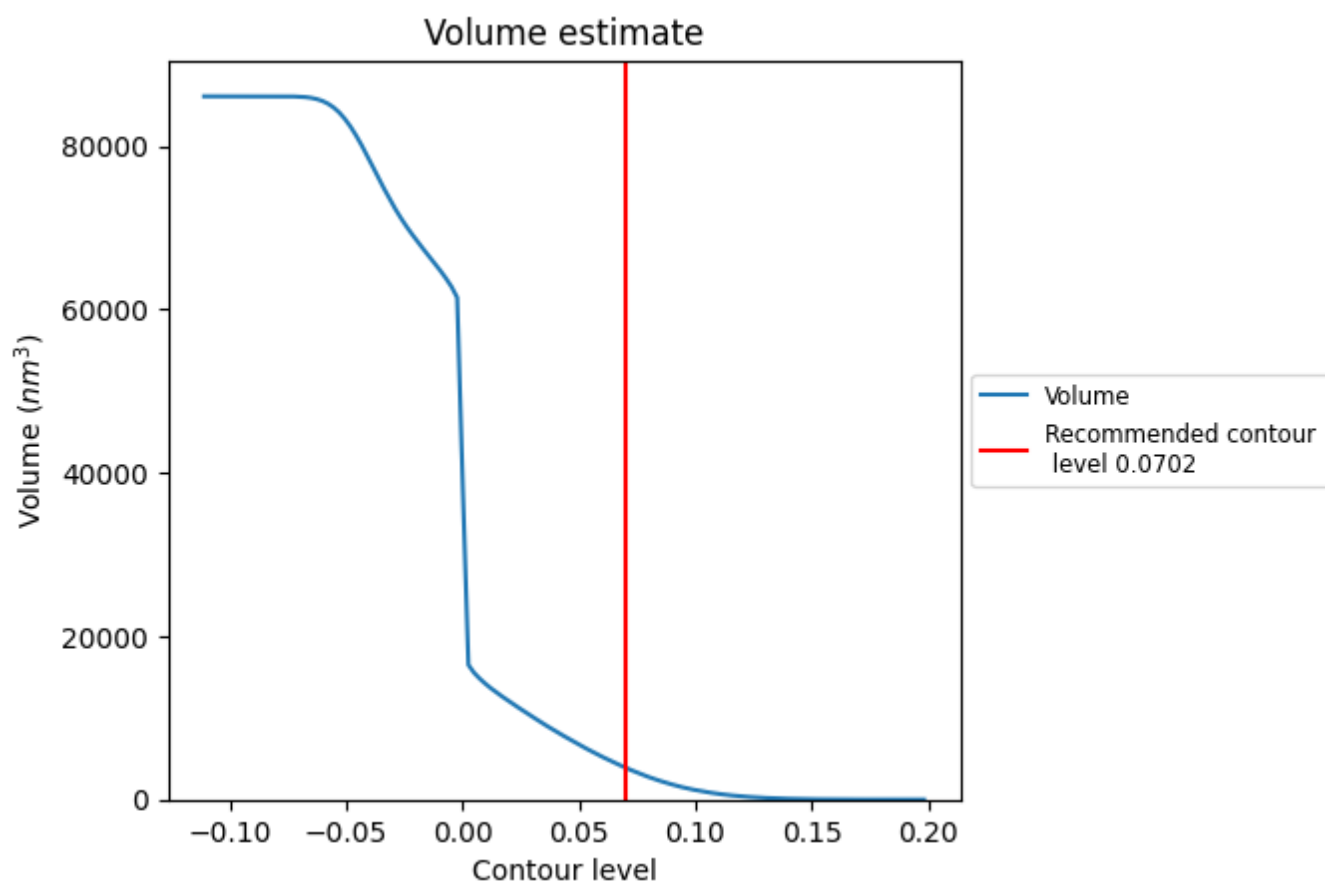
This section contains the results of statistical analysis of the map.

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.

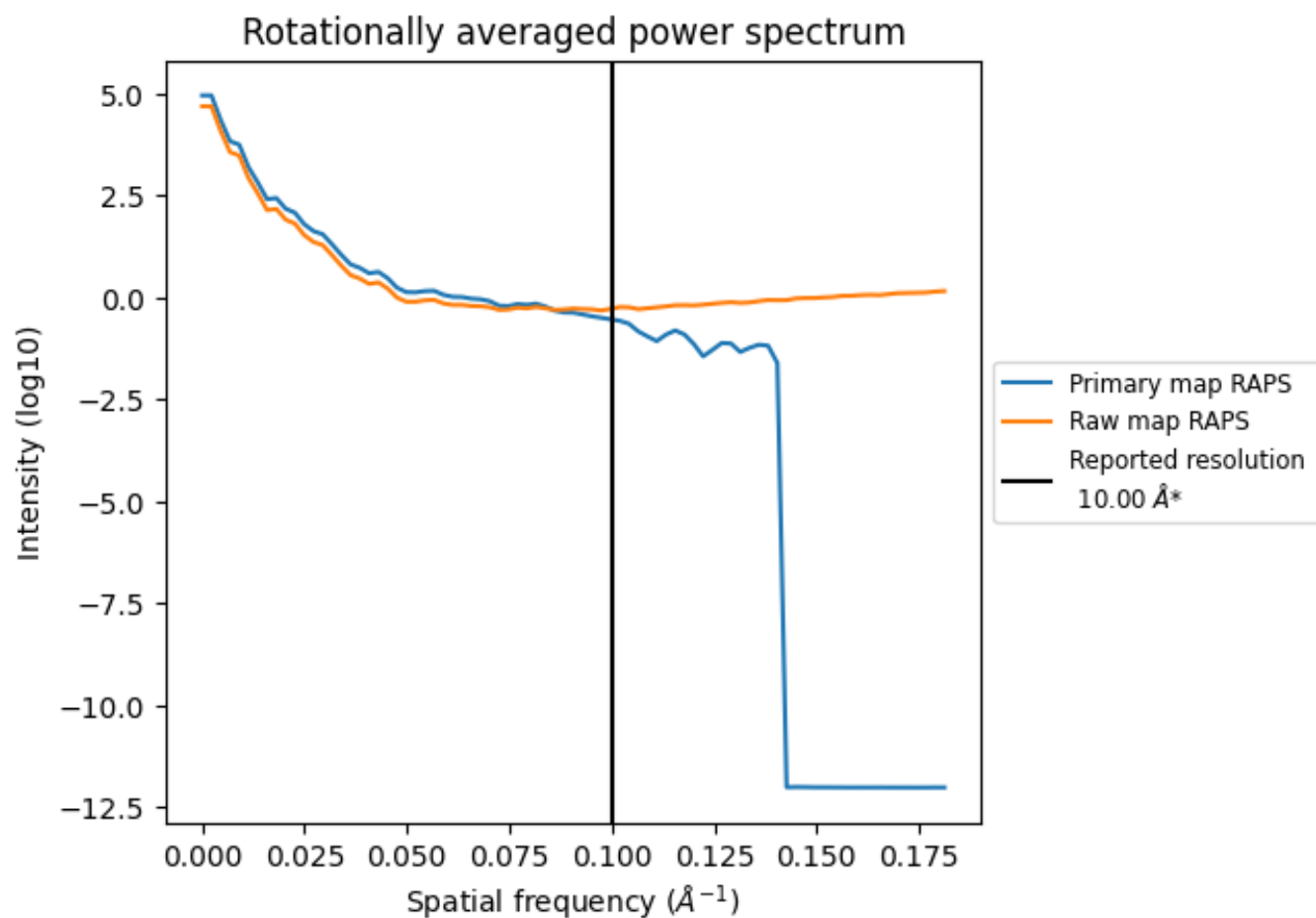
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3872 nm³; this corresponds to an approximate mass of 3497 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 ⓘ

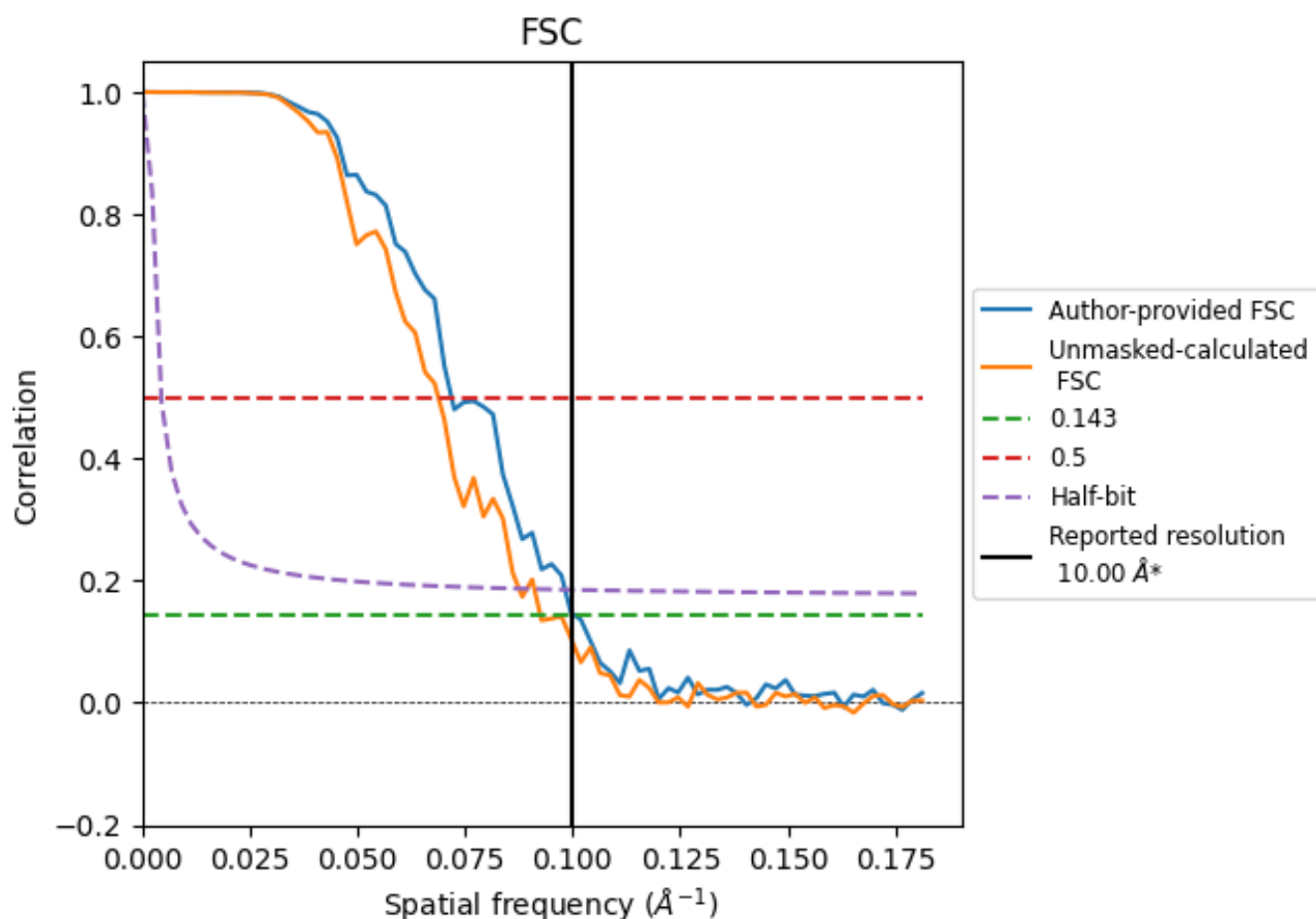


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

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 0.100 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.95	13.93	10.17
Unmasked-calculated*	10.80	14.53	11.43

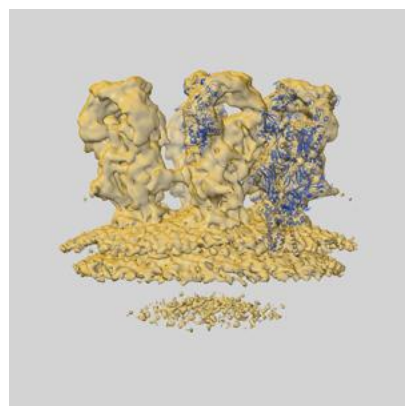
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

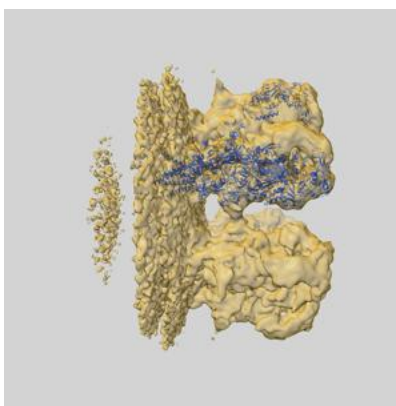
This section contains information regarding the fit between EMDB map EMD-17318 and PDB model 8OZQ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

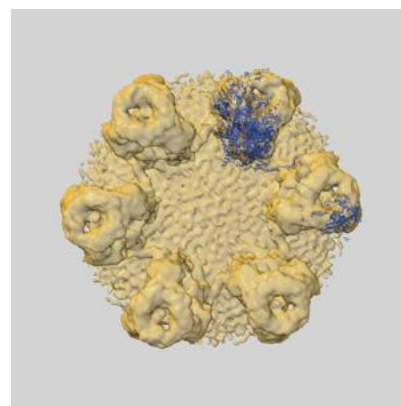
9.1.1 Map-model overlay ⓘ



X



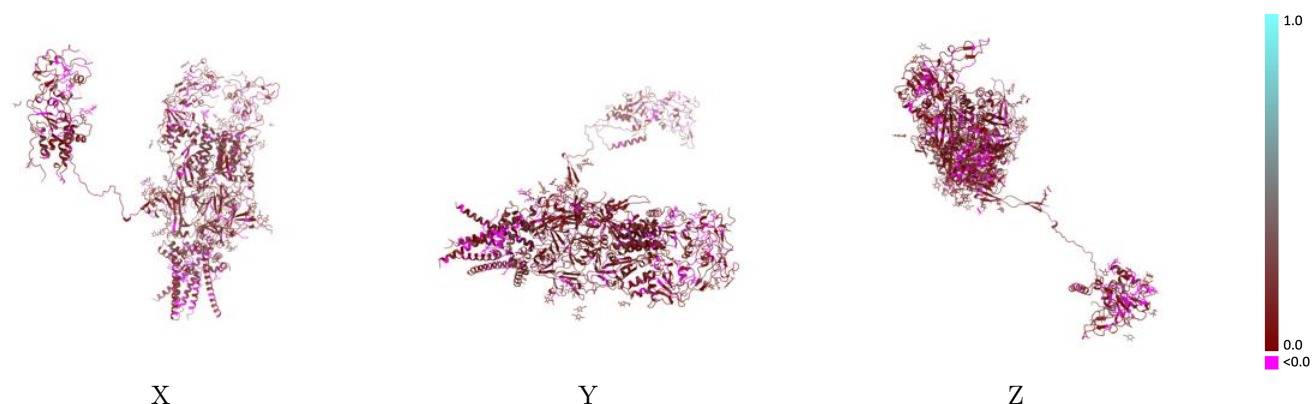
Y



Z

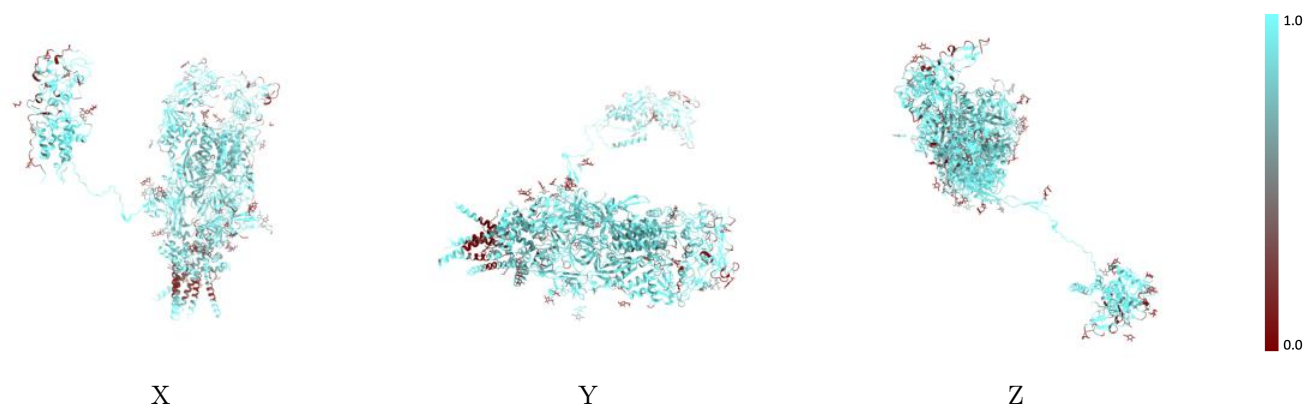
The images above show the 3D surface view of the map at the recommended contour level 0.0702 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



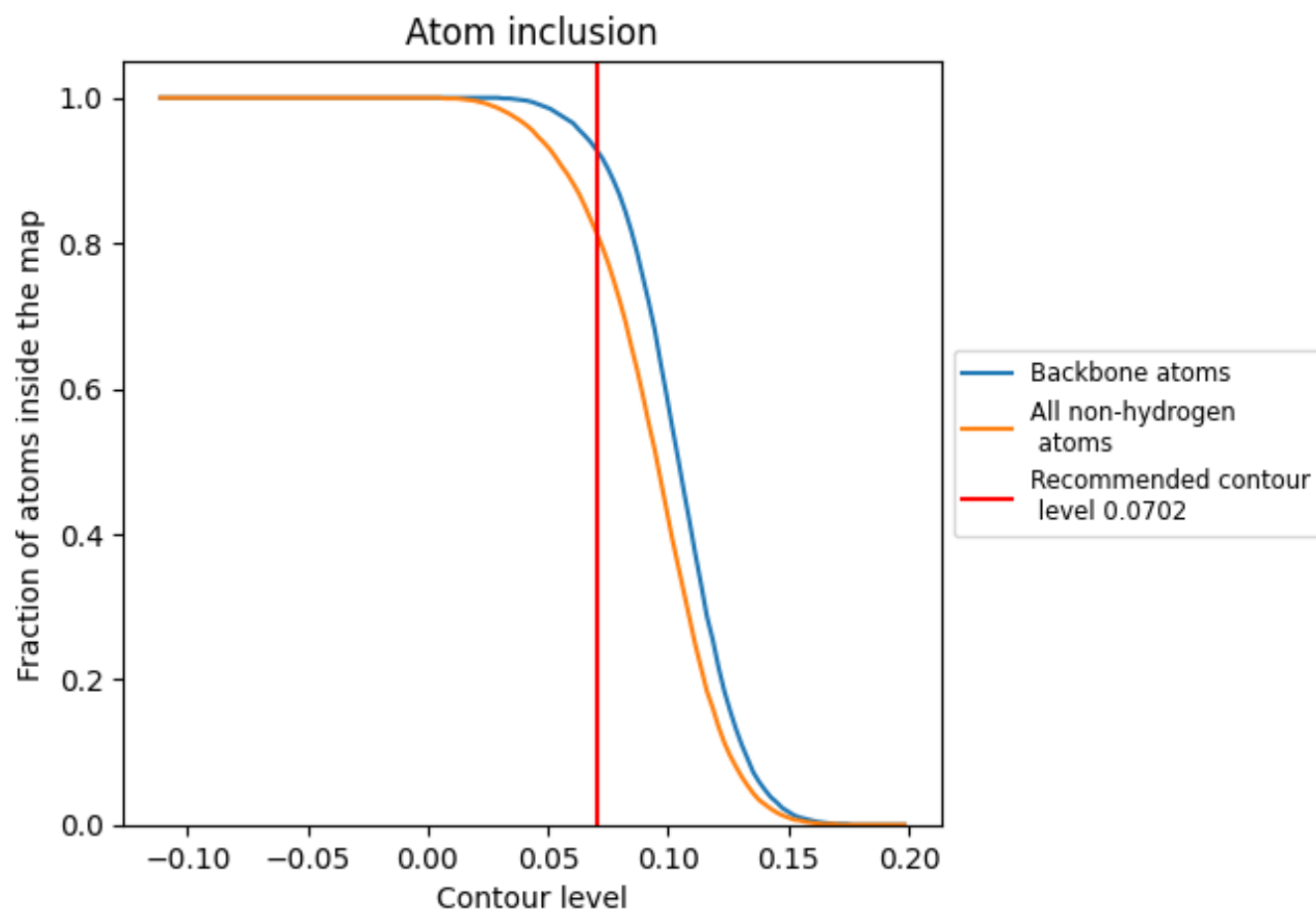
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0702).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% 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 (0.0702) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.1090
A	 0.7080	 0.0820
B	 0.8330	 0.1050
C	 0.8390	 0.1000
D	 0.8520	 0.1230
E	 0.7580	 0.1370
F	 0.7470	 0.1090
G	 0.8500	 0.0930
H	 0.8260	 0.1100
I	 0.7340	 0.1200
L	 0.8460	 0.1220
M	 0.2500	 0.0710
N	 0.5710	 0.0720
O	 0.8210	 0.2900
P	 0.4400	 0.1060
Q	 0.2600	 0.1390
R	 0.3600	 0.1600
S	 0.3080	 0.0800
T	 0.1540	 -0.0260
U	 0.1540	 -0.0450
V	 0.7470	 0.0530
W	 0.7870	 0.0400
X	 0.5470	 -0.0220
Y	 0.4290	 0.2140
Z	 0.0710	 0.1620
a	 0.4640	 0.2650
b	 0.5710	 0.0720
c	 0.5360	 0.1090
d	 0.7500	 0.1390
e	 0.6380	 0.1470
f	 0.5850	 0.1050
g	 0.7230	 0.1300
h	 0.3470	 0.1330
i	 0.2500	 0.0940
j	 0.2920	 0.2000

