



Full wwPDB EM Validation Report ⓘ

Aug 11, 2026 – 04:34 PM EDT

PDB ID : 9NPM / pdb_00009npm
EMDB ID : EMD-49628
Title : Composite map of three pairs of dimeric VRC36 Fabs bound to HIV-1 BG505.T332N DS-SOSIP.664 Env trimer
Authors : Cheng, J.; Cale, E.M.; Longo, N.; Sutton, M.S.; Lei, H.; Huang, R.; Morton, A.J.; Lang, Z.C.; Morano, N.C.; Roark, R.S.; Becker, J.E.; Tsybovsky, Y.; Li, N.; Zhang, B.; Du, H.; Rubin, S.; Shapiro, L.; Pierson, T.C.; Doria-Rose, N.A.; Zhou, T.; Kwong, P.D.
Deposited on : 2025-03-11
Resolution : 3.59 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:

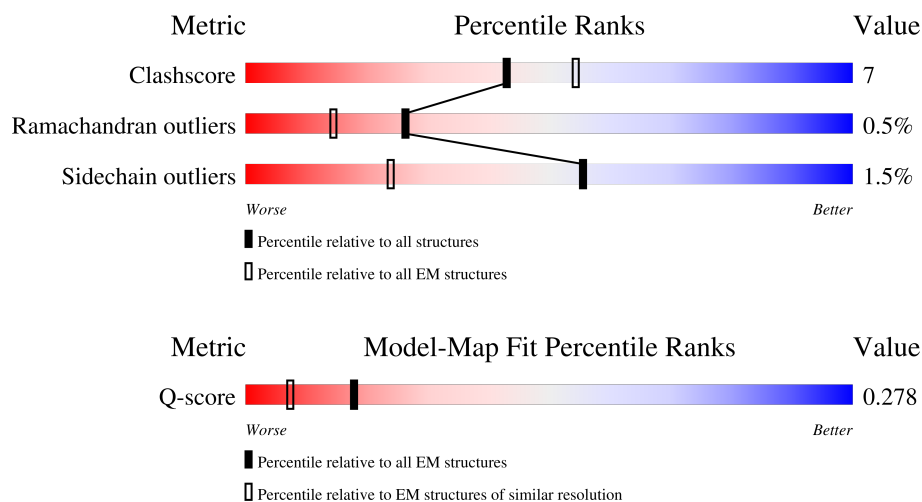
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.59 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	12565 (3.09 - 4.09)

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	473	 82% 13% . .
1	C	473	 80% 15% .
1	E	473	 58% 30% 7% . .

Continued on next page...

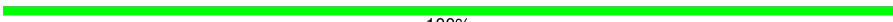
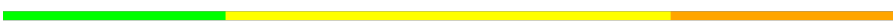
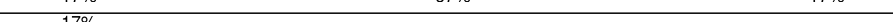
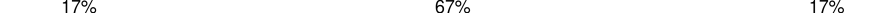
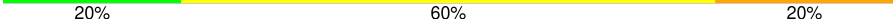
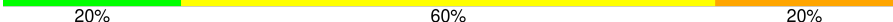
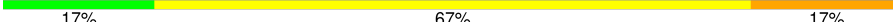
Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	153	
2	D	153	
2	F	153	
3	G	223	
3	I	223	
3	K	223	
3	M	223	
3	O	223	
3	Q	223	
4	H	214	
4	J	214	
4	L	214	
4	N	214	
4	P	214	
4	R	214	
5	S	2	
5	T	2	
5	V	2	
5	W	2	
5	d	2	
5	e	2	
5	g	2	
5	h	2	
5	o	2	
5	p	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	r	2	 100%
5	s	2	 100%
6	U	4	 25% 50% 25%
6	f	4	 50% 25% 25%
6	q	4	 25% 50% 25%
7	X	9	 22% 67% 11%
7	i	9	 11% 78% 11%
7	t	9	 22% 78%
8	Y	8	 12% 62% 25%
8	Z	8	 50% 50%
8	j	8	 25% 62% 12%
8	k	8	 25% 50% 25%
8	v	8	 38% 62%
9	a	6	 17% 67% 17%
9	b	6	 17% 50% 50%
9	l	6	 33% 50% 17%
9	m	6	 33% 50% 50%
9	w	6	 17% 67% 17%
9	x	6	 17% 50% 50%
10	c	5	 40% 40% 20%
10	n	5	 20% 60% 20%
10	z	5	 20% 60% 20%
11	u	6	 17% 67% 17%
12	y	2	 50% 50%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35931 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 HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	454	Total	C	N	O	S	0	0
			3573	2238	631	674	30		
1	E	454	Total	C	N	O	S	0	0
			3573	2238	631	674	30		
1	A	454	Total	C	N	O	S	0	0
			3573	2238	631	674	30		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP A0A6H1VH54
C	?	-	GLN	deletion	UNP A0A6H1VH54
C	?	-	GLY	deletion	UNP A0A6H1VH54
C	?	-	ASN	deletion	UNP A0A6H1VH54
C	?	-	ARG	deletion	UNP A0A6H1VH54
C	?	-	SER	deletion	UNP A0A6H1VH54
C	?	-	ASN	deletion	UNP A0A6H1VH54
C	?	-	ASN	deletion	UNP A0A6H1VH54
C	201	CYS	ILE	conflict	UNP A0A6H1VH54
C	375	SER	TYR	conflict	UNP A0A6H1VH54
C	433	CYS	ALA	conflict	UNP A0A6H1VH54
C	501	CYS	ALA	conflict	UNP A0A6H1VH54
C	509	ARG	-	expression tag	UNP A0A6H1VH54
C	510	ARG	-	expression tag	UNP A0A6H1VH54
C	511	ARG	-	expression tag	UNP A0A6H1VH54
C	512	ARG	-	expression tag	UNP A0A6H1VH54
C	513	ARG	-	expression tag	UNP A0A6H1VH54
E	?	-	ASN	deletion	UNP A0A6H1VH54
E	?	-	GLN	deletion	UNP A0A6H1VH54
E	?	-	GLY	deletion	UNP A0A6H1VH54
E	?	-	ASN	deletion	UNP A0A6H1VH54
E	?	-	ARG	deletion	UNP A0A6H1VH54
E	?	-	SER	deletion	UNP A0A6H1VH54
E	?	-	ASN	deletion	UNP A0A6H1VH54

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASN	deletion	UNP A0A6H1VH54
E	201	CYS	ILE	conflict	UNP A0A6H1VH54
E	375	SER	TYR	conflict	UNP A0A6H1VH54
E	433	CYS	ALA	conflict	UNP A0A6H1VH54
E	501	CYS	ALA	conflict	UNP A0A6H1VH54
E	509	ARG	-	expression tag	UNP A0A6H1VH54
E	510	ARG	-	expression tag	UNP A0A6H1VH54
E	511	ARG	-	expression tag	UNP A0A6H1VH54
E	512	ARG	-	expression tag	UNP A0A6H1VH54
E	513	ARG	-	expression tag	UNP A0A6H1VH54
A	?	-	ASN	deletion	UNP A0A6H1VH54
A	?	-	GLN	deletion	UNP A0A6H1VH54
A	?	-	GLY	deletion	UNP A0A6H1VH54
A	?	-	ASN	deletion	UNP A0A6H1VH54
A	?	-	ARG	deletion	UNP A0A6H1VH54
A	?	-	SER	deletion	UNP A0A6H1VH54
A	?	-	ASN	deletion	UNP A0A6H1VH54
A	?	-	ASN	deletion	UNP A0A6H1VH54
A	201	CYS	ILE	conflict	UNP A0A6H1VH54
A	375	SER	TYR	conflict	UNP A0A6H1VH54
A	433	CYS	ALA	conflict	UNP A0A6H1VH54
A	501	CYS	ALA	conflict	UNP A0A6H1VH54
A	509	ARG	-	expression tag	UNP A0A6H1VH54
A	510	ARG	-	expression tag	UNP A0A6H1VH54
A	511	ARG	-	expression tag	UNP A0A6H1VH54
A	512	ARG	-	expression tag	UNP A0A6H1VH54
A	513	ARG	-	expression tag	UNP A0A6H1VH54

- Molecule 2 is a protein called HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			1002	634	172	190	6		
2	F	126	Total	C	N	O	S	0	0
			1002	634	172	190	6		
2	B	126	Total	C	N	O	S	0	0
			1002	634	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	engineered mutation	UNP Q2N0S5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	605	CYS	THR	engineered mutation	UNP Q2N0S5
F	559	PRO	ILE	engineered mutation	UNP Q2N0S5
F	605	CYS	THR	engineered mutation	UNP Q2N0S5
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

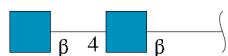
- Molecule 3 is a protein called VRC36 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		
3	M	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		
3	O	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		
3	Q	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		
3	G	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		
3	I	223	Total	C	N	O	S	0	0
			1696	1065	300	324	7		

- Molecule 4 is a protein called VRC36 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		
4	N	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		
4	P	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		
4	R	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		
4	H	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		
4	J	214	Total	C	N	O	S	0	0
			1640	1017	282	334	7		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	r	2	Total	C	N	O	0	0
			28	16	2	10		
5	s	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called 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.



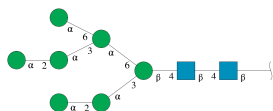
Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	4	Total	C	N	O	0	0
			50	28	2	20		
6	f	4	Total	C	N	O	0	0
			50	28	2	20		

Continued on next page...

Continued from previous page...

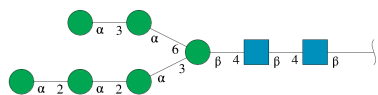
Mol	Chain	Residues	Atoms				AltConf	Trace
6	q	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 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-(1-2)-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	X	9	Total	C	N	O	0	0
			105	58	2	45		
7	i	9	Total	C	N	O	0	0
			105	58	2	45		
7	t	9	Total	C	N	O	0	0
			105	58	2	45		

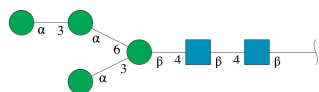
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	8	Total	C	N	O	0	0
			94	52	2	40		
8	Z	8	Total	C	N	O	0	0
			94	52	2	40		
8	j	8	Total	C	N	O	0	0
			94	52	2	40		
8	k	8	Total	C	N	O	0	0
			94	52	2	40		
8	v	8	Total	C	N	O	0	0
			94	52	2	40		

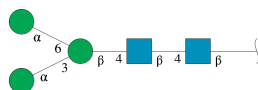
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran

ose-(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
9	a	6	Total	C	N	O	0	0
			72	40	2	30		
9	b	6	Total	C	N	O	0	0
			72	40	2	30		
9	l	6	Total	C	N	O	0	0
			72	40	2	30		
9	m	6	Total	C	N	O	0	0
			72	40	2	30		
9	w	6	Total	C	N	O	0	0
			72	40	2	30		
9	x	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called 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
10	c	5	Total	C	N	O	0	0
			61	34	2	25		
10	n	5	Total	C	N	O	0	0
			61	34	2	25		
10	z	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.



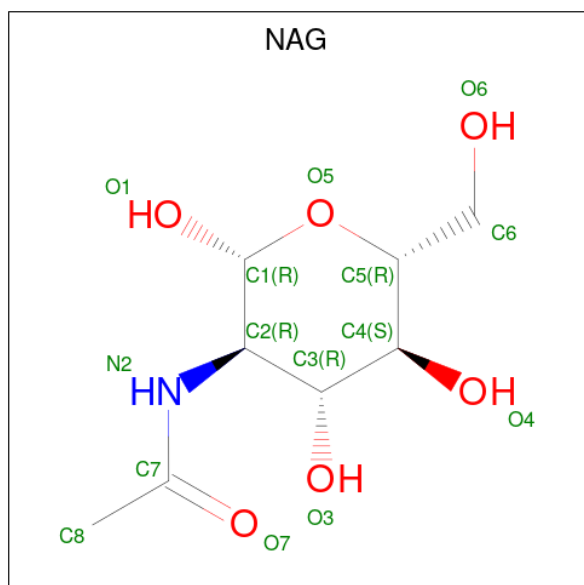
Mol	Chain	Residues	Atoms				AltConf	Trace
11	u	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
12	y	2	Total	C	O	0	0
			22	12	10		

- Molecule 13 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
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

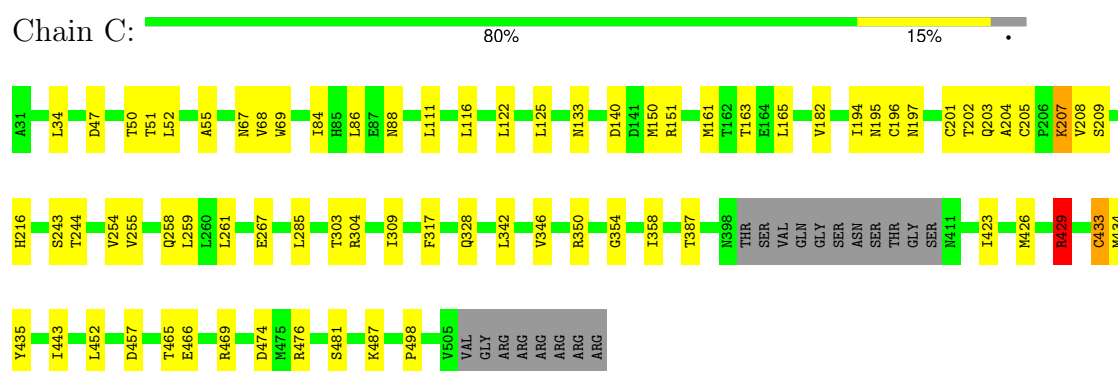
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0
13	A	1	Total 14	C 8	N 1	O 5	0

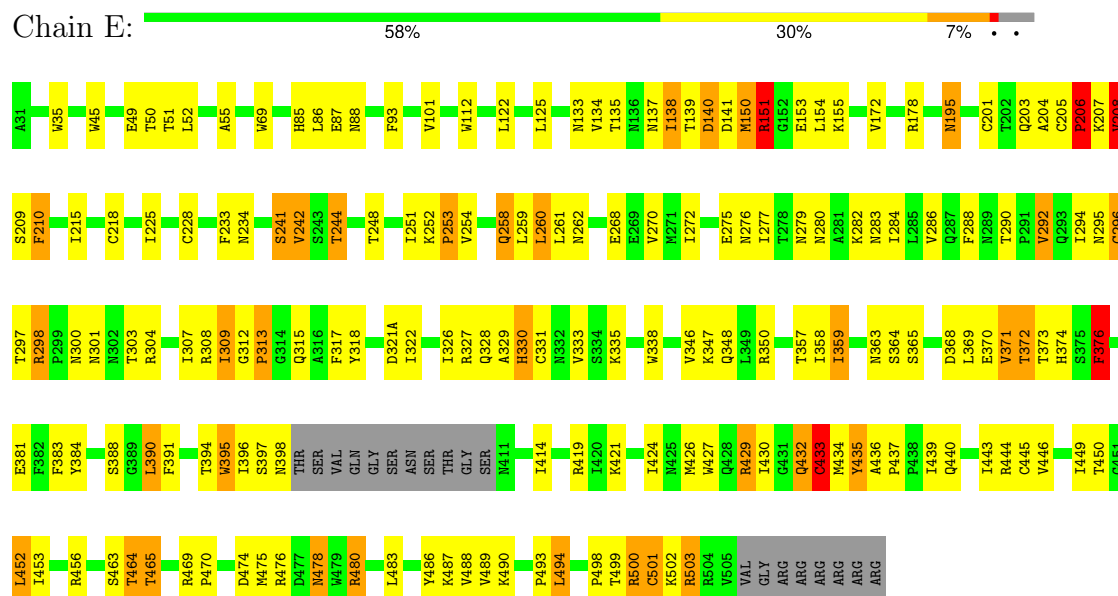
3 Residue-property plots

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: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp120

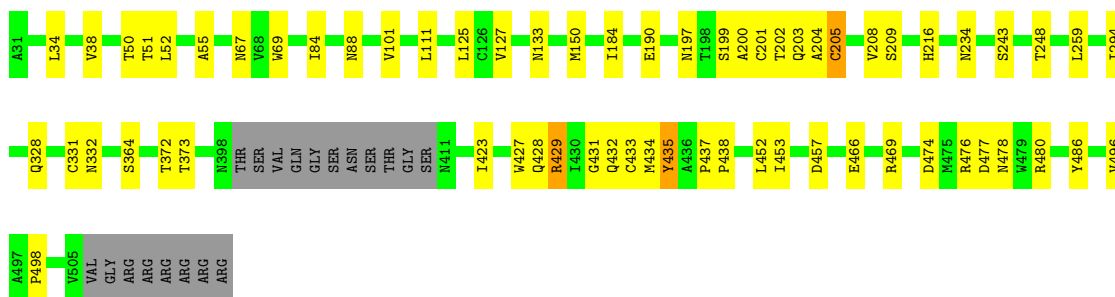


- Molecule 1: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp120

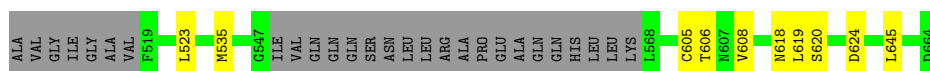


- Molecule 1: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp120

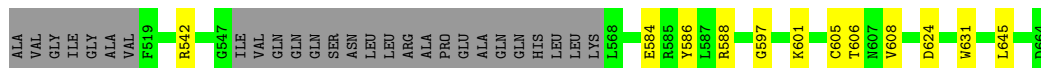




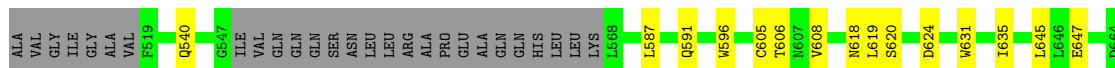
- Molecule 2: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp41



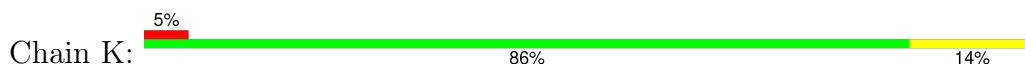
- Molecule 2: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp41



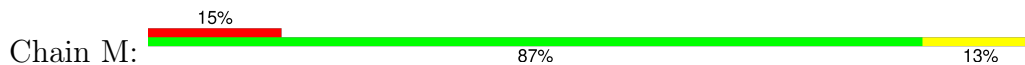
- Molecule 2: HIV-1 BG505.T332N DS-SOSIP.664 Env glycoprotein gp41

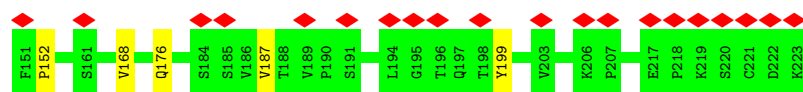


- Molecule 3: VRC36 Fab heavy chain

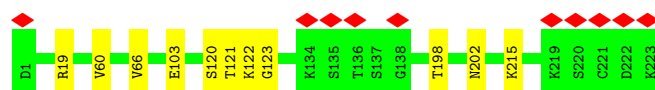


- Molecule 3: VRC36 Fab heavy chain

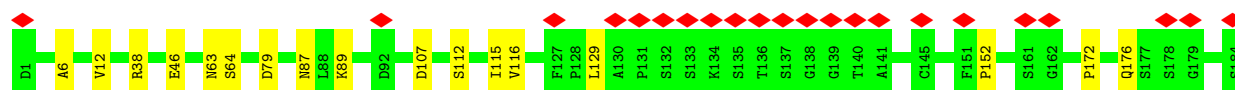
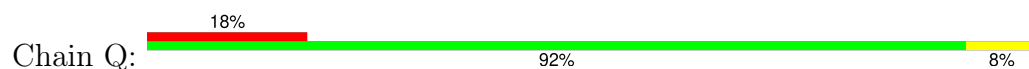




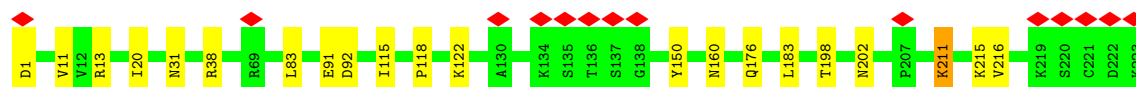
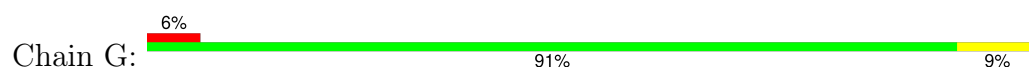
- Molecule 3: VRC36 Fab heavy chain



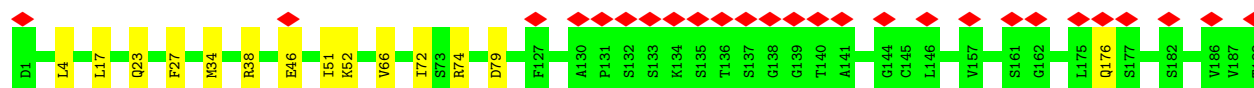
- Molecule 3: VRC36 Fab heavy chain



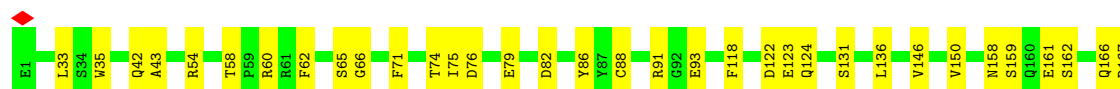
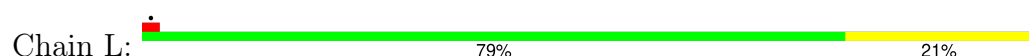
- Molecule 3: VRC36 Fab heavy chain

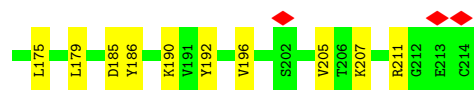


- Molecule 3: VRC36 Fab heavy chain

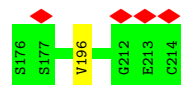
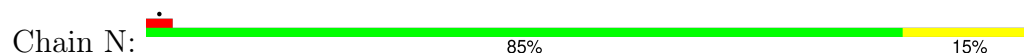


- Molecule 4: VRC36 Fab light chain

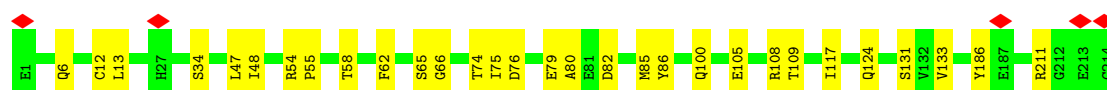
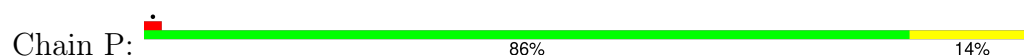




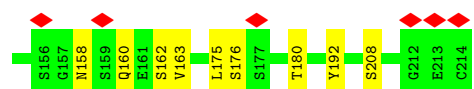
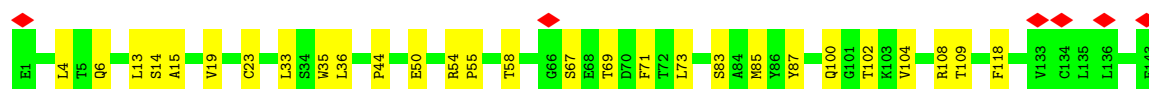
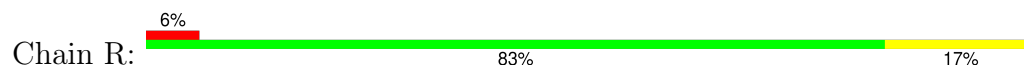
- Molecule 4: VRC36 Fab light chain



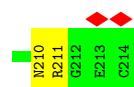
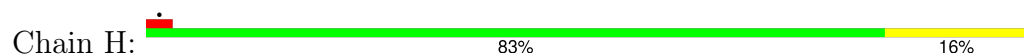
- Molecule 4: VRC36 Fab light chain



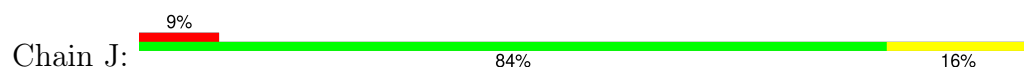
- Molecule 4: VRC36 Fab light chain

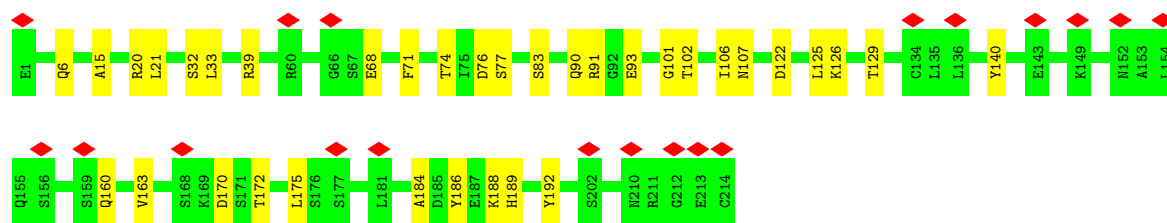


- Molecule 4: VRC36 Fab light chain



- Molecule 4: VRC36 Fab light chain





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

Chain S: 



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

Chain T: 

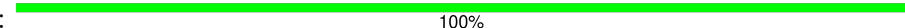


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain W: 

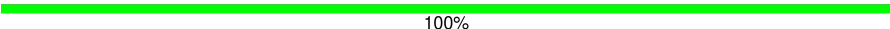


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 



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

Chain e: 



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

Chain g:  100%



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

Chain h:  100%



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

Chain o:  50% 50%



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

Chain p:  50% 50%



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

Chain r:  100%

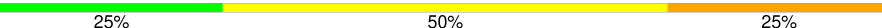


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  100%



- Molecule 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

Chain U: 

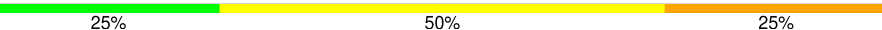


- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 



- Molecule 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

Chain q: 

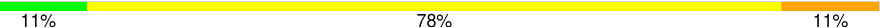


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

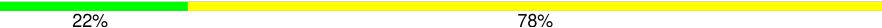


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 

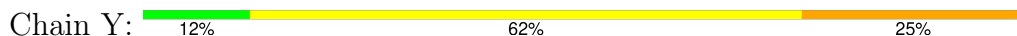


- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



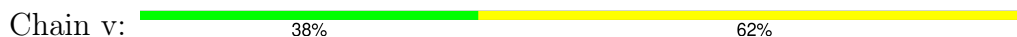
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



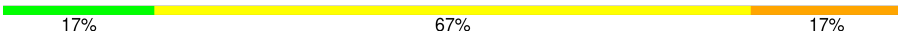
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



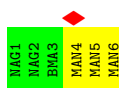
• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

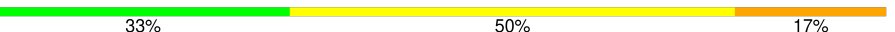


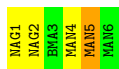
• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 



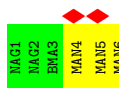
• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 

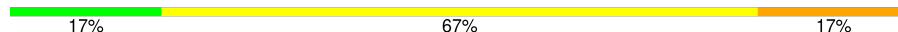


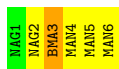
• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m: 

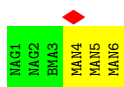


• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 



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



- Molecule 10: 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



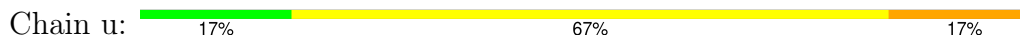
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	84.527	Depositor
Minimum map value	-10.531	Depositor
Average map value	0.050	Depositor
Map value standard deviation	1.459	Depositor
Recommended contour level	1.8	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/3648	0.54	2/4954 (0.0%)
1	C	0.29	0/3648	0.54	3/4954 (0.1%)
1	E	0.76	0/3648	1.14	9/4954 (0.2%)
2	B	0.18	0/1020	0.39	0/1383
2	D	0.18	0/1020	0.39	0/1383
2	F	0.20	0/1020	0.42	0/1383
3	G	0.23	0/1739	0.49	0/2366
3	I	0.20	0/1739	0.47	0/2366
3	K	0.21	0/1739	0.45	0/2366
3	M	0.24	0/1739	0.52	0/2366
3	O	0.21	0/1739	0.48	0/2366
3	Q	0.22	0/1739	0.48	0/2366
4	H	0.23	0/1674	0.54	1/2275 (0.0%)
4	J	0.21	0/1674	0.47	0/2275
4	L	0.24	0/1674	0.52	0/2275
4	N	0.22	0/1674	0.50	1/2275 (0.0%)
4	P	0.23	0/1674	0.50	0/2275
4	R	0.23	0/1674	0.49	1/2275 (0.0%)
All	All	0.33	0/34482	0.60	17/46857 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	11
All	All	0	12

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	433	CYS	CB-CA-C	-12.27	86.00	110.42
1	C	197	ASN	CB-CA-C	-10.65	93.11	110.79
1	A	197	ASN	CB-CA-C	-10.05	95.10	110.88
4	R	55	PRO	CA-N-CD	-6.81	102.46	112.00
1	E	268	GLU	CB-CA-C	-6.24	109.40	116.63
1	C	197	ASN	N-CA-C	-5.99	104.75	111.28
1	A	197	ASN	N-CA-C	-5.93	104.72	111.07
4	N	95	PRO	CA-N-CD	-5.89	103.25	111.50
1	E	390	LEU	N-CA-C	-5.86	106.29	113.50
1	E	296	CYS	CB-CA-C	-5.68	99.12	110.42
1	C	196	CYS	CB-CA-C	5.58	117.71	109.29
4	H	50	GLU	CA-CB-CG	5.55	125.21	114.10
1	E	253	PRO	N-CA-CB	-5.51	98.90	102.65
1	E	376	PHE	CA-CB-CG	5.49	119.29	113.80
1	E	141	ASP	N-CA-C	-5.18	108.22	114.75
1	E	437	PRO	N-CA-C	-5.17	105.04	110.58
1	E	464	THR	N-CA-C	-5.15	107.02	113.15

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	429	ARG	Sidechain
1	E	151	ARG	Sidechain
1	E	298	ARG	Sidechain
1	E	304	ARG	Sidechain
1	E	308	ARG	Sidechain
1	E	327	ARG	Sidechain
1	E	419	ARG	Sidechain
1	E	429	ARG	Sidechain
1	E	444	ARG	Sidechain
1	E	456	ARG	Sidechain
1	E	500	ARG	Sidechain
1	E	503	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3573	0	3496	45	0
1	C	3573	0	3496	44	0
1	E	3573	0	3497	129	0
2	B	1002	0	981	11	0
2	D	1002	0	981	7	0
2	F	1002	0	981	12	0
3	G	1696	0	1668	13	0
3	I	1696	0	1668	11	0
3	K	1696	0	1668	24	0
3	M	1696	0	1668	21	0
3	O	1696	0	1668	8	0
3	Q	1696	0	1668	12	0
4	H	1640	0	1589	23	0
4	J	1640	0	1589	23	0
4	L	1640	0	1589	32	0
4	N	1640	0	1589	18	0
4	P	1640	0	1589	19	0
4	R	1640	0	1589	23	0
5	S	28	0	25	0	0
5	T	28	0	25	1	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
5	o	28	0	25	0	0
5	p	28	0	25	0	0
5	r	28	0	25	0	0
5	s	28	0	25	0	0
6	U	50	0	43	2	0
6	f	50	0	43	2	0
6	q	50	0	43	1	0
7	X	105	0	88	1	0
7	i	105	0	88	2	0
7	t	105	0	88	0	0
8	Y	94	0	79	3	0
8	Z	94	0	79	0	0
8	j	94	0	79	1	0
8	k	94	0	79	2	0
8	v	94	0	79	0	0
9	a	72	0	61	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	b	72	0	61	0	0
9	l	72	0	61	1	0
9	m	72	0	61	0	0
9	w	72	0	61	1	0
9	x	72	0	61	0	0
10	c	61	0	52	1	0
10	n	61	0	52	2	0
10	z	61	0	52	2	0
11	u	72	0	61	3	0
12	y	22	0	19	1	0
13	A	70	0	65	2	0
13	C	70	0	65	2	0
13	E	70	0	65	2	0
All	All	35931	0	34859	469	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 7.

All (469) 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:E:357:THR:HA	1:E:464:THR:HB	1.47	0.95
1:E:93:PHE:HE2	1:E:228:CYS:HB2	1.37	0.90
2:B:608:VAL:HG11	2:B:645:LEU:HD21	1.52	0.89
1:E:138:ILE:HG23	1:E:326:ILE:HD11	1.59	0.84
1:E:150:MET:HB3	1:E:153:GLU:HB3	1.62	0.81
1:E:346:VAL:HG13	1:E:359:ILE:HD11	1.63	0.78
1:E:93:PHE:CE2	1:E:228:CYS:HB2	2.19	0.78
1:E:292:VAL:HG23	1:E:449:ILE:HB	1.65	0.77
2:D:608:VAL:HG11	2:D:645:LEU:HD21	1.67	0.76
4:H:54:ARG:NH2	4:H:62:PHE:O	2.20	0.74
1:E:433:CYS:SG	1:E:434:MET:N	2.57	0.74
4:L:42:GLN:OE1	4:L:43:ALA:N	2.19	0.74
1:E:396:ILE:HG12	1:E:397:SER:H	1.53	0.73
4:L:166:GLN:OE1	4:L:167:ASP:N	2.20	0.73
1:E:498:PRO:HD2	2:F:631:TRP:HZ2	1.54	0.72
1:C:255:VAL:HG11	1:C:426:MET:HE1	1.70	0.71
1:C:195:ASN:ND2	1:C:201:CYS:SG	2.63	0.71
4:J:122:ASP:OD1	4:J:126:LYS:NZ	2.22	0.71
4:L:186:TYR:O	4:L:211:ARG:NH2	2.23	0.71
3:M:23:GLN:OE1	3:M:24:ALA:N	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:34:SER:OG	4:P:48:ILE:O	2.07	0.69
2:B:618:ASN:OD1	2:B:620:SER:OG	2.09	0.69
4:H:190:LYS:NZ	4:H:210:ASN:OD1	2.24	0.68
4:J:6:GLN:NE2	4:J:102:THR:OG1	2.27	0.68
3:K:28:ASN:ND2	3:K:31:ASN:OD1	2.26	0.68
4:L:82:ASP:O	4:L:86:TYR:OH	2.12	0.68
4:N:42:GLN:N	4:N:42:GLN:OE1	2.27	0.68
1:A:477:ASP:OD1	1:A:478:ASN:N	2.27	0.67
4:L:60:ARG:O	4:L:60:ARG:NH1	2.28	0.66
3:K:215:LYS:NZ	3:K:216:VAL:O	2.28	0.66
3:M:39:GLN:NE2	3:M:43:ARG:O	2.29	0.65
1:E:150:MET:O	1:E:151:ARG:C	2.39	0.65
4:H:17:GLU:OE1	4:H:18:THR:N	2.29	0.65
4:H:82:ASP:O	4:H:86:TYR:OH	2.14	0.65
4:P:186:TYR:O	4:P:211:ARG:NH2	2.30	0.65
3:K:82:TYR:OH	7:X:4:MAN:O2	2.14	0.64
1:E:391:PHE:CE2	1:E:470:PRO:HB3	2.33	0.64
4:R:108:ARG:NH1	4:R:109:THR:O	2.30	0.64
4:J:20:ARG:NE	4:J:74:THR:OG1	2.31	0.64
1:C:433:CYS:SG	1:C:434:MET:N	2.68	0.64
1:E:463:SER:HB3	1:E:465:THR:HG23	1.80	0.64
3:G:13:ARG:NH2	3:G:118:PRO:O	2.30	0.64
3:G:176:GLN:N	3:G:176:GLN:OE1	2.31	0.63
1:E:424:ILE:HD12	1:E:426:MET:HG2	1.80	0.63
4:N:6:GLN:OE1	4:N:102:THR:OG1	2.17	0.63
4:L:124:GLN:NE2	4:L:131:SER:OG	2.32	0.63
1:E:86:LEU:HD11	1:E:244:THR:HG22	1.81	0.63
1:E:259:LEU:HB2	1:E:374:HIS:CD2	2.34	0.63
1:E:394:THR:O	1:E:395:TRP:C	2.41	0.63
1:E:270:VAL:HG12	1:E:288:PHE:HA	1.81	0.62
4:P:82:ASP:O	4:P:86:TYR:OH	2.15	0.62
1:E:138:ILE:HA	1:E:326:ILE:HD11	1.81	0.62
2:F:608:VAL:HG21	2:F:645:LEU:HD21	1.82	0.62
1:E:335:LYS:HD3	1:E:414:ILE:HD11	1.80	0.62
2:F:542:ARG:NH2	2:B:647:GLU:OE2	2.32	0.62
3:O:19:ARG:NH2	7:i:7:MAN:O6	2.33	0.62
3:I:79:ASP:OD2	10:z:4:MAN:O3	2.16	0.62
1:E:55:ALA:HB2	1:E:218:CYS:SG	2.40	0.62
4:P:79:GLU:OE2	4:P:80:ALA:N	2.33	0.61
4:R:192:TYR:O	4:R:208:SER:OG	2.14	0.61
3:K:20:ILE:HD11	3:K:83:LEU:HD23	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:197:GLN:N	3:K:197:GLN:OE1	2.33	0.61
1:E:397:SER:O	1:E:398:ASN:C	2.44	0.61
1:E:138:ILE:HG23	1:E:326:ILE:CD1	2.29	0.61
4:P:105:GLU:OE2	4:P:105:GLU:N	2.34	0.61
4:L:33:LEU:HD13	4:L:71:PHE:CE2	2.36	0.61
1:E:251:ILE:O	1:E:252:LYS:C	2.43	0.61
4:N:6:GLN:NE2	4:N:101:GLY:O	2.34	0.60
1:E:172:VAL:HG21	1:E:307:ILE:HG12	1.84	0.60
1:E:205:CYS:HB2	1:E:208:VAL:HG13	1.83	0.60
1:E:122:LEU:HD21	1:E:125:LEU:HD13	1.82	0.60
4:R:4:LEU:HD11	4:R:23:CYS:SG	2.42	0.60
3:I:176:GLN:NE2	4:J:160:GLN:OE1	2.34	0.60
3:K:176:GLN:N	3:K:176:GLN:OE1	2.34	0.60
3:M:125:SER:OG	3:M:148:LYS:O	2.17	0.59
1:E:434:MET:O	1:E:436:ALA:N	2.36	0.59
3:M:31:ASN:ND2	8:Y:4:MAN:O5	2.34	0.59
1:E:155:LYS:HE2	1:E:178:ARG:HH22	1.67	0.59
4:J:125:LEU:HD21	4:J:186:TYR:HD2	1.66	0.59
3:G:150:TYR:OH	3:G:183:LEU:HD23	2.03	0.59
2:D:618:ASN:OD1	2:D:620:SER:OG	2.14	0.58
3:K:13:ARG:NH1	3:K:117:SER:O	2.36	0.58
4:R:163:VAL:HG22	4:R:175:LEU:HD13	1.85	0.58
3:I:38:ARG:O	3:I:46:GLU:N	2.35	0.58
1:E:69:TRP:NE1	1:E:253:PRO:HG3	2.19	0.58
1:C:358:ILE:HD11	1:C:465:THR:HG22	1.86	0.58
1:E:260:LEU:HD12	1:E:478:ASN:HD22	1.69	0.58
1:E:330:HIS:CD2	7:i:1:NAG:HN2	2.20	0.58
3:K:196:THR:OG1	3:K:197:GLN:OE1	2.19	0.58
3:O:198:THR:OG1	3:O:215:LYS:NZ	2.35	0.58
1:E:276:ASN:ND2	1:E:279:ASN:HB2	2.19	0.58
4:P:12:CYS:O	4:P:13:LEU:HD23	2.04	0.57
3:M:11:VAL:HG21	3:M:152:PRO:HG3	1.86	0.57
4:J:15:ALA:HA	4:J:106:ILE:HD11	1.85	0.57
3:M:38:ARG:O	3:M:46:GLU:N	2.36	0.57
1:E:427:TRP:HZ3	1:E:475:MET:HG2	1.69	0.57
1:E:282:LYS:O	1:E:283:ASN:C	2.48	0.57
4:L:190:LYS:NZ	4:L:190:LYS:O	2.36	0.57
1:C:457:ASP:OD2	1:C:469:ARG:NH2	2.38	0.57
1:E:49:GLU:N	1:E:49:GLU:OE2	2.37	0.57
1:E:275:GLU:HB3	1:E:282:LYS:HD2	1.85	0.57
4:L:93:GLU:N	4:L:93:GLU:OE1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:46:GLU:N	3:K:46:GLU:OE2	2.37	0.56
1:E:261:LEU:O	1:E:262:ASN:C	2.48	0.56
1:E:365:SER:HA	1:E:469:ARG:HD3	1.86	0.56
3:Q:129:LEU:HD11	4:R:118:PHE:CG	2.40	0.56
3:G:160:ASN:ND2	3:G:198:THR:O	2.38	0.56
1:C:84:ILE:O	1:C:243:SER:OG	2.23	0.56
1:E:295:ASN:O	1:E:296:CYS:SG	2.64	0.56
13:E:604:NAG:H83	13:E:604:NAG:H3	1.86	0.56
4:P:54:ARG:HB3	4:P:58:THR:HG21	1.87	0.56
3:Q:38:ARG:O	3:Q:46:GLU:N	2.39	0.56
3:Q:79:ASP:OD2	10:n:4:MAN:O3	2.17	0.56
2:D:624:ASP:OD1	2:D:624:ASP:N	2.39	0.56
3:K:129:LEU:HD21	4:L:118:PHE:CG	2.41	0.56
1:E:338:TRP:CE2	1:E:390:LEU:HG	2.41	0.56
1:A:201:CYS:SG	1:A:434:MET:N	2.79	0.56
1:A:372:THR:HG23	1:A:373:THR:HG23	1.88	0.56
4:N:13:LEU:HD12	4:N:19:VAL:HG12	1.88	0.55
1:E:376:PHE:HD1	1:E:383:PHE:HB2	1.71	0.55
4:L:54:ARG:NH1	4:L:58:THR:O	2.39	0.55
4:L:76:ASP:OD1	4:L:76:ASP:N	2.40	0.55
1:E:101:VAL:HG11	1:E:480:ARG:HD3	1.88	0.55
1:E:260:LEU:HD21	1:E:453:ILE:HG23	1.88	0.55
4:P:55:PRO:O	4:P:58:THR:HG22	2.07	0.55
4:J:68:GLU:N	4:J:68:GLU:OE1	2.38	0.55
4:J:107:ASN:OD1	4:J:140:TYR:OH	2.18	0.55
1:C:116:LEU:HD13	1:C:434:MET:HE2	1.89	0.55
1:E:328:GLN:HG3	1:E:329:ALA:H	1.70	0.55
3:Q:87:ASN:OD1	3:Q:89:LYS:NZ	2.19	0.55
1:E:205:CYS:O	1:E:206:PRO:C	2.49	0.55
1:E:469:ARG:HG3	1:E:470:PRO:HD2	1.89	0.55
3:M:64:SER:OG	3:M:65:ARG:NH1	2.40	0.55
4:P:124:GLN:NE2	4:P:131:SER:OG	2.40	0.55
4:R:100:GLN:OE1	4:R:100:GLN:N	2.39	0.55
3:K:8:GLY:O	3:K:112:SER:OG	2.22	0.55
4:R:6:GLN:NE2	4:R:102:THR:OG1	2.40	0.55
4:L:136:LEU:HD22	4:L:175:LEU:HD22	1.88	0.55
3:K:18:VAL:O	3:K:85:THR:OG1	2.19	0.55
1:E:258:GLN:NE2	1:E:470:PRO:HB2	2.22	0.55
2:F:601:LYS:NZ	2:B:591:GLN:OE1	2.32	0.55
4:R:13:LEU:HD12	4:R:19:VAL:HG12	1.89	0.55
11:u:2:NAG:O3	11:u:3:BMA:O5	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:VAL:O	1:E:348:GLN:HG3	2.07	0.54
4:J:163:VAL:HG22	4:J:175:LEU:HD22	1.89	0.54
4:R:35:TRP:CE3	4:R:73:LEU:HD22	2.43	0.54
4:H:76:ASP:OD1	4:H:76:ASP:N	2.40	0.54
4:N:105:GLU:OE2	4:N:173:TYR:OH	2.21	0.54
4:R:54:ARG:NH2	4:R:58:THR:O	2.40	0.54
1:C:258:GLN:NE2	1:C:387:THR:HG21	2.23	0.54
1:E:133:ASN:HB2	13:E:605:NAG:N2	2.23	0.54
4:P:62:PHE:CD1	4:P:75:ILE:HG23	2.43	0.53
2:B:624:ASP:OD1	2:B:624:ASP:N	2.41	0.53
1:E:204:ALA:O	1:E:205:CYS:C	2.51	0.53
1:A:208:VAL:HG23	1:A:209:SER:H	1.73	0.53
1:E:45:TRP:HB2	1:E:489:VAL:CG2	2.38	0.53
1:C:207:LYS:HE3	1:C:207:LYS:H	1.73	0.53
1:E:391:PHE:CD2	1:E:470:PRO:HB3	2.43	0.53
1:E:474:ASP:O	1:E:475:MET:C	2.51	0.53
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.89	0.53
3:O:103:GLU:N	3:O:103:GLU:OE1	2.41	0.53
4:R:158:ASN:ND2	4:R:180:THR:O	2.41	0.53
1:E:259:LEU:HD13	1:E:449:ILE:HD13	1.89	0.53
4:H:42:GLN:OE1	4:H:42:GLN:N	2.42	0.53
4:J:189:HIS:O	4:J:192:TYR:OH	2.21	0.53
2:D:535:MET:HA	2:D:535:MET:HE3	1.89	0.53
1:E:434:MET:O	1:E:435:TYR:C	2.52	0.53
4:P:108:ARG:NH2	4:P:109:THR:OG1	2.42	0.53
4:R:33:LEU:HD13	4:R:71:PHE:CD2	2.44	0.53
3:Q:6:ALA:O	3:Q:112:SER:OG	2.25	0.52
3:Q:172:PRO:O	4:R:162:SER:OG	2.26	0.52
4:H:154:LEU:HD12	4:H:155:GLN:N	2.24	0.52
1:C:201:CYS:SG	1:C:423:ILE:HD12	2.49	0.52
4:N:21:LEU:HD12	4:N:73:LEU:HD11	1.90	0.52
1:C:317:PHE:HE1	1:C:435:TYR:HE1	1.58	0.52
1:E:138:ILE:CG2	1:E:326:ILE:HD11	2.37	0.52
1:A:101:VAL:HG21	1:A:480:ARG:HH21	1.75	0.52
1:A:457:ASP:OD2	1:A:469:ARG:NH2	2.43	0.52
4:L:150:VAL:HG13	4:L:192:TYR:CD1	2.45	0.52
3:O:120:SER:OG	3:O:121:THR:N	2.40	0.52
1:E:35:TRP:CE2	1:E:502:LYS:HB2	2.44	0.52
3:O:103:GLU:OE2	8:k:5:MAN:O4	2.20	0.52
1:E:225:ILE:HD13	1:E:488:VAL:HG12	1.91	0.52
3:Q:115:ILE:HG21	3:Q:152:PRO:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:176:GLN:NE2	4:N:160:GLN:OE1	2.44	0.52
1:E:309:ILE:HG23	1:E:315:GLN:HB2	1.92	0.52
1:A:453:ILE:HG21	1:A:477:ASP:OD2	2.10	0.52
4:H:168:SER:OG	4:H:169:LYS:NZ	2.42	0.52
4:J:39:ARG:NH1	4:J:83:SER:O	2.43	0.52
3:M:91:GLU:N	3:M:91:GLU:OE1	2.43	0.51
1:E:376:PHE:CD1	1:E:383:PHE:HB2	2.45	0.51
3:G:31:ASN:OD1	3:G:31:ASN:N	2.42	0.51
6:U:1:NAG:O6	6:U:2:NAG:N2	2.43	0.51
3:M:143:LEU:HD22	3:M:199:TYR:HD2	1.75	0.51
4:L:35:TRP:NE1	4:L:88:CYS:SG	2.81	0.51
4:L:146:VAL:HG21	4:L:175:LEU:HD21	1.93	0.51
1:C:202:THR:O	1:C:203:GLN:C	2.52	0.51
2:D:605:CYS:SG	2:D:606:THR:N	2.83	0.51
1:E:277:ILE:HD12	1:E:284:ILE:HD12	1.91	0.51
4:P:76:ASP:OD1	4:P:76:ASP:N	2.43	0.51
3:M:36:TRP:HE1	3:M:81:MET:HE1	1.76	0.51
3:Q:107:ASP:OD1	3:Q:107:ASP:N	2.43	0.51
4:J:33:LEU:HD13	4:J:71:PHE:CD2	2.46	0.51
1:E:317:PHE:O	1:E:318:TYR:C	2.54	0.51
1:E:335:LYS:HA	1:E:414:ILE:HG13	1.92	0.51
1:E:312:GLY:O	1:E:313:PRO:C	2.54	0.50
8:Y:2:NAG:H3	8:Y:2:NAG:H83	1.92	0.50
1:C:133:ASN:H	13:C:605:NAG:H82	1.77	0.50
1:E:369:LEU:O	1:E:370:GLU:C	2.55	0.50
4:J:33:LEU:HD22	4:J:71:PHE:CE2	2.47	0.50
1:E:45:TRP:HB2	1:E:489:VAL:HG22	1.93	0.50
4:R:14:SER:OG	4:R:15:ALA:N	2.43	0.50
4:H:85:MET:SD	4:H:86:TYR:N	2.85	0.50
4:H:136:LEU:HD13	4:H:175:LEU:CD2	2.42	0.50
8:j:2:NAG:H83	8:j:2:NAG:H3	1.93	0.50
2:B:540:GLN:N	2:B:540:GLN:OE1	2.45	0.50
11:u:2:NAG:H83	11:u:2:NAG:H3	1.94	0.50
1:C:259:LEU:HD22	1:C:452:LEU:HD22	1.94	0.50
1:E:295:ASN:O	1:E:331:CYS:HB3	2.12	0.50
1:E:329:ALA:O	1:E:330:HIS:ND1	2.44	0.50
9:w:2:NAG:O3	9:w:3:BMA:O2	2.26	0.50
1:A:50:THR:OG1	1:A:51:THR:N	2.45	0.49
4:J:21:LEU:HD22	4:J:102:THR:HG21	1.94	0.49
4:L:136:LEU:HD21	4:L:196:VAL:CG2	2.42	0.49
4:H:105:GLU:N	4:H:105:GLU:OE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:65:SER:OG	4:L:66:GLY:N	2.46	0.49
4:H:50:GLU:O	4:H:52:SER:N	2.44	0.49
4:J:76:ASP:OD1	4:J:77:SER:N	2.45	0.49
4:L:205:VAL:HG12	4:L:207:LYS:NZ	2.27	0.49
1:E:262:ASN:HB2	6:f:1:NAG:HN2	1.78	0.49
1:E:384:TYR:HE2	1:E:421:LYS:HD3	1.78	0.49
3:G:215:LYS:NZ	3:G:216:VAL:O	2.46	0.49
4:J:15:ALA:CA	4:J:106:ILE:HD11	2.42	0.49
1:E:215:ILE:O	1:E:251:ILE:HG12	2.13	0.49
1:A:259:LEU:HD22	1:A:452:LEU:HD22	1.95	0.49
6:q:1:NAG:O6	6:q:2:NAG:N2	2.45	0.49
1:E:122:LEU:HB3	1:E:201:CYS:O	2.12	0.49
1:A:423:ILE:HG23	1:A:433:CYS:SG	2.53	0.49
1:A:466:GLU:OE1	1:A:466:GLU:N	2.45	0.49
1:C:161:MET:HE2	1:C:309:ILE:HD12	1.95	0.48
3:M:79:ASP:OD2	10:c:4:MAN:O3	2.12	0.48
3:Q:63:ASN:OD1	3:Q:64:SER:N	2.46	0.48
3:Q:176:GLN:NE2	4:R:160:GLN:OE1	2.45	0.48
1:E:288:PHE:CZ	1:E:452:LEU:HD11	2.47	0.48
1:E:498:PRO:HD2	2:F:631:TRP:CZ2	2.43	0.48
4:N:73:LEU:HD12	4:N:73:LEU:O	2.13	0.48
4:N:82:ASP:O	4:N:86:TYR:OH	2.29	0.48
1:E:371:VAL:O	1:E:372:THR:HB	2.14	0.48
4:H:135:LEU:C	4:H:136:LEU:HD12	2.37	0.48
1:E:209:SER:OG	1:E:210:PHE:N	2.46	0.48
2:F:624:ASP:OD1	2:F:624:ASP:N	2.45	0.48
4:J:6:GLN:OE1	4:J:101:GLY:N	2.44	0.48
1:C:429:ARG:HG2	1:C:429:ARG:HH11	1.77	0.48
1:E:347:LYS:O	1:E:350:ARG:HB3	2.14	0.48
2:F:605:CYS:SG	2:F:606:THR:N	2.87	0.48
1:A:427:TRP:C	1:A:429:ARG:H	2.22	0.48
1:C:204:ALA:O	1:C:205:CYS:C	2.56	0.48
4:P:65:SER:OG	4:P:66:GLY:N	2.45	0.48
4:R:83:SER:OG	4:R:104:VAL:O	2.30	0.48
1:C:51:THR:C	1:C:52:LEU:HD12	2.39	0.48
1:E:381:GLU:HG2	1:E:439:ILE:HD13	1.95	0.48
3:O:66:VAL:HG22	3:O:66:VAL:O	2.14	0.48
1:A:133:ASN:H	13:A:605:NAG:H82	1.79	0.48
4:H:70:ASP:OD1	4:H:71:PHE:N	2.47	0.48
1:E:55:ALA:CB	1:E:218:CYS:SG	3.01	0.47
1:E:258:GLN:CD	1:E:470:PRO:HB2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:584:GLU:OE1	2:F:588:ARG:NH2	2.47	0.47
1:A:204:ALA:O	1:A:205:CYS:C	2.56	0.47
1:A:474:ASP:OD2	1:A:476:ARG:NE	2.45	0.47
1:E:493:PRO:O	1:E:494:LEU:HB2	2.14	0.47
1:A:34:LEU:HD21	2:B:619:LEU:HD21	1.96	0.47
1:A:433:CYS:SG	1:A:434:MET:N	2.88	0.47
3:G:202:ASN:OD1	3:G:211:LYS:NZ	2.28	0.47
3:I:209:ASN:O	3:I:209:ASN:ND2	2.47	0.47
1:E:358:ILE:N	1:E:464:THR:O	2.46	0.47
4:P:74:THR:C	4:P:75:ILE:HD13	2.39	0.47
3:M:106:ASP:OD1	4:N:91:ARG:NH2	2.48	0.47
1:C:474:ASP:OD2	1:C:476:ARG:NE	2.45	0.47
3:K:75:ASP:OD1	3:K:75:ASP:N	2.48	0.47
3:K:210:THR:HG22	3:K:212:VAL:HG23	1.97	0.47
1:E:137:ASN:O	1:E:139:THR:N	2.45	0.47
3:M:34:MET:C	3:M:34:MET:HE2	2.40	0.47
1:E:50:THR:OG1	1:E:51:THR:N	2.48	0.47
1:C:267:GLU:N	1:C:267:GLU:OE1	2.48	0.47
1:E:150:MET:SD	1:E:153:GLU:HG2	2.55	0.47
4:P:47:LEU:HD11	4:P:62:PHE:HD2	1.80	0.47
1:E:429:ARG:HD2	1:E:432:GLN:HG3	1.96	0.47
1:C:47:ASP:OD2	1:C:487:LYS:NZ	2.49	0.46
1:E:475:MET:O	1:E:476:ARG:C	2.58	0.46
1:E:503:ARG:NH2	2:F:597:GLY:O	2.49	0.46
3:Q:115:ILE:HG21	3:Q:152:PRO:CB	2.45	0.46
1:A:199:SER:HB3	1:A:431:GLY:O	2.16	0.46
3:G:1:ASP:OD1	3:G:1:ASP:N	2.47	0.46
4:R:175:LEU:HD12	4:R:176:SER:H	1.81	0.46
1:A:69:TRP:HA	1:A:111:LEU:HD21	1.98	0.46
1:A:429:ARG:HG3	1:A:432:GLN:NE2	2.30	0.46
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.97	0.46
1:C:122:LEU:HD21	1:C:125:LEU:HD13	1.98	0.46
1:C:285:LEU:HD21	1:C:481:SER:HB2	1.96	0.46
4:L:74:THR:C	4:L:75:ILE:HD13	2.41	0.46
1:E:85:HIS:ND1	1:E:87:GLU:OE2	2.49	0.46
4:L:136:LEU:HD21	4:L:196:VAL:HG21	1.97	0.46
3:K:194:LEU:HD13	3:K:218:PRO:HG2	1.97	0.46
4:L:158:ASN:N	4:L:158:ASN:OD1	2.49	0.46
3:M:107:ASP:OD1	3:M:107:ASP:N	2.43	0.46
1:E:259:LEU:HB2	1:E:374:HIS:NE2	2.31	0.46
4:H:186:TYR:O	4:H:211:ARG:NH2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:2:NAG:O3	8:Y:3:BMA:O5	2.34	0.46
4:H:32:SER:O	4:H:32:SER:OG	2.28	0.46
3:G:20:ILE:HD11	3:G:83:LEU:HD23	1.98	0.46
1:C:50:THR:OG1	1:C:51:THR:N	2.47	0.46
4:J:184:ALA:O	4:J:188:LYS:NZ	2.44	0.46
3:K:150:TYR:OH	3:K:183:LEU:N	2.45	0.45
1:E:303:THR:HG22	1:E:321(A):ASP:O	2.16	0.45
1:E:364:SER:OG	10:n:1:NAG:H82	2.16	0.45
13:A:604:NAG:H3	13:A:604:NAG:H83	1.98	0.45
2:B:605:CYS:SG	2:B:606:THR:N	2.88	0.45
5:T:1:NAG:O3	5:T:2:NAG:O5	2.29	0.45
1:E:363:ASN:HB2	1:E:388:SER:HB2	1.97	0.45
4:P:79:GLU:N	4:P:82:ASP:OD2	2.47	0.45
1:C:423:ILE:HG23	1:C:433:CYS:SG	2.56	0.45
1:A:67:ASN:OD1	1:A:69:TRP:N	2.48	0.45
3:I:23:GLN:NE2	3:I:79:ASP:O	2.50	0.45
9:a:2:NAG:HO3	9:a:3:BMA:HO2	1.57	0.45
1:C:34:LEU:HD21	2:D:619:LEU:HD21	1.99	0.45
1:E:261:LEU:HA	1:E:261:LEU:HD23	1.69	0.45
4:R:175:LEU:HD12	4:R:176:SER:N	2.32	0.45
4:J:170:ASP:OD1	4:J:172:THR:HG22	2.16	0.45
4:N:49:SER:O	4:N:53:ALA:HB3	2.17	0.45
1:E:288:PHE:HB2	1:E:450:THR:O	2.17	0.45
1:E:433:CYS:O	1:E:434:MET:C	2.60	0.45
1:A:84:ILE:O	1:A:243:SER:OG	2.35	0.45
4:J:125:LEU:HD21	4:J:186:TYR:CD2	2.48	0.45
8:k:4:MAN:O3	8:k:5:MAN:O5	2.28	0.45
1:E:300:ASN:O	1:E:301:ASN:C	2.60	0.45
1:A:150:MET:HE3	1:A:328:GLN:HB3	1.98	0.45
3:M:34:MET:HE2	3:M:35:SER:N	2.32	0.44
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.52	0.44
4:H:48:ILE:HD12	4:H:73:LEU:CD1	2.47	0.44
4:J:32:SER:O	4:J:91:ARG:N	2.50	0.44
4:R:163:VAL:CG2	4:R:175:LEU:HD13	2.46	0.44
4:H:67:SER:OG	4:H:68:GLU:N	2.50	0.44
13:C:604:NAG:H3	13:C:604:NAG:H83	1.98	0.44
1:E:93:PHE:HB2	1:E:233:PHE:CZ	2.53	0.44
4:P:117:ILE:HD12	4:P:133:VAL:O	2.18	0.44
1:E:452:LEU:HD12	1:E:452:LEU:H	1.82	0.44
1:E:501:CYS:O	2:F:605:CYS:SG	2.71	0.44
4:P:85:MET:SD	4:P:86:TYR:N	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:91:GLU:N	3:G:91:GLU:OE1	2.50	0.44
1:C:342:LEU:O	1:C:346:VAL:HG23	2.17	0.44
1:E:294:ILE:HD12	1:E:449:ILE:HD11	1.99	0.44
3:G:150:TYR:OH	3:G:183:LEU:N	2.49	0.44
1:C:254:VAL:HG21	6:U:1:NAG:H82	1.99	0.44
1:A:51:THR:C	1:A:52:LEU:HD23	2.42	0.44
2:B:631:TRP:O	2:B:635:ILE:HD12	2.17	0.44
4:H:185:ASP:OD1	4:H:185:ASP:N	2.51	0.44
1:E:329:ALA:O	1:E:330:HIS:CB	2.65	0.44
3:I:34:MET:SD	3:I:51:ILE:HD13	2.58	0.44
3:K:101:LEU:HD21	4:L:91:ARG:HD3	1.99	0.44
4:L:122:ASP:OD1	4:L:123:GLU:N	2.50	0.44
4:N:47:LEU:HD23	4:N:48:ILE:HG12	1.99	0.44
1:A:294:ILE:HD12	1:A:332:ASN:O	2.17	0.44
3:I:51:ILE:CG1	3:I:72:ILE:HD12	2.48	0.44
1:E:241:SER:O	1:E:242:VAL:C	2.61	0.44
1:E:487:LYS:HE3	1:E:487:LYS:HB2	1.38	0.44
3:Q:12:VAL:O	3:Q:116:VAL:HG23	2.18	0.44
4:L:161:GLU:OE2	4:L:162:SER:N	2.52	0.43
1:E:52:LEU:HG	1:E:218:CYS:O	2.18	0.43
1:E:338:TRP:HZ2	1:E:391:PHE:CE1	2.36	0.43
9:I:1:NAG:H61	9:I:5:MAN:O2	2.17	0.43
1:C:140:ASP:O	1:C:151:ARG:NH1	2.50	0.43
1:C:243:SER:OG	1:C:244:THR:N	2.51	0.43
3:K:87:ASN:ND2	3:K:87:ASN:O	2.52	0.43
1:A:101:VAL:HG11	1:A:480:ARG:HE	1.83	0.43
1:A:294:ILE:HD11	1:A:331:CYS:HB3	2.01	0.43
3:K:147:VAL:HG13	3:K:150:TYR:HE2	1.83	0.43
1:A:202:THR:O	1:A:203:GLN:C	2.61	0.43
3:G:38:ARG:NH1	3:G:92:ASP:OD1	2.47	0.43
4:L:205:VAL:HG12	4:L:207:LYS:HZ2	1.83	0.43
1:E:203:GLN:HE22	1:E:318:TYR:HD2	1.66	0.43
1:E:329:ALA:O	1:E:330:HIS:HB3	2.18	0.43
3:M:168:VAL:HG22	3:M:187:VAL:HG12	2.00	0.43
1:E:201:CYS:HB3	1:E:433:CYS:HB3	1.25	0.43
1:E:248:THR:HG22	1:E:486:TYR:CD1	2.54	0.43
1:E:272:ILE:HD13	1:E:348:GLN:HB2	2.00	0.43
1:E:433:CYS:HB2	1:E:435:TYR:H	1.83	0.43
1:A:38:VAL:HG12	1:A:496:VAL:HG12	2.01	0.43
4:L:79:GLU:N	4:L:82:ASP:OD1	2.46	0.43
1:E:298:ARG:HD2	1:E:443:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ASP:OD1	1:E:368:ASP:N	2.52	0.43
4:H:65:SER:OG	4:H:66:GLY:N	2.51	0.43
4:R:33:LEU:HD22	4:R:71:PHE:CD2	2.54	0.43
1:A:125:LEU:O	1:A:127:VAL:N	2.47	0.43
1:C:67:ASN:OD1	1:C:69:TRP:N	2.52	0.43
1:C:303:THR:OG1	1:C:304:ARG:N	2.51	0.43
1:C:161:MET:CE	1:C:309:ILE:HD12	2.48	0.43
4:R:67:SER:O	4:R:69:THR:N	2.50	0.43
3:M:143:LEU:HD22	3:M:199:TYR:CD2	2.54	0.42
1:E:390:LEU:HD12	1:E:390:LEU:HA	1.87	0.42
1:C:34:LEU:HD22	1:C:498:PRO:HB2	2.00	0.42
4:L:185:ASP:OD1	4:L:185:ASP:N	2.50	0.42
4:P:6:GLN:O	4:P:100:GLN:NE2	2.51	0.42
3:I:66:VAL:HG12	3:I:66:VAL:O	2.19	0.42
1:C:182:VAL:HG11	1:C:194:ILE:HD13	2.02	0.42
4:N:75:ILE:HD13	4:N:78:LEU:HD13	2.01	0.42
1:A:427:TRP:HB2	1:A:429:ARG:HG2	2.01	0.42
2:F:586:TYR:HD2	2:B:587:LEU:HD21	1.84	0.42
4:H:56:THR:OG1	4:J:93:GLU:OE1	2.37	0.42
4:N:129:THR:OG1	4:N:130:ALA:N	2.52	0.42
1:E:259:LEU:O	1:E:260:LEU:C	2.61	0.42
1:E:396:ILE:HG12	1:E:397:SER:N	2.29	0.42
1:A:435:TYR:HD1	1:A:435:TYR:C	2.28	0.42
3:I:52:LYS:O	3:I:74:ARG:NH1	2.52	0.42
3:K:194:LEU:HD12	3:K:195:GLY:N	2.33	0.42
1:E:262:ASN:HB2	6:f:1:NAG:N2	2.35	0.42
1:E:172:VAL:HG11	1:E:307:ILE:CG2	2.49	0.42
1:E:427:TRP:HA	1:E:427:TRP:CE3	2.54	0.42
4:H:48:ILE:HD12	4:H:73:LEU:HD11	2.02	0.42
3:K:147:VAL:HG13	3:K:150:TYR:CE2	2.54	0.42
1:A:364:SER:OG	10:z:1:NAG:H82	2.20	0.42
4:H:85:MET:HE2	4:H:103:LYS:HD2	2.02	0.42
1:C:68:VAL:O	1:C:111:LEU:HD21	2.20	0.42
1:A:423:ILE:CG2	1:A:433:CYS:SG	3.07	0.42
11:u:3:BMA:O6	12:y:1:MAN:O5	2.35	0.42
1:C:255:VAL:HG11	1:C:426:MET:CE	2.44	0.41
4:N:143:GLU:OE1	4:N:143:GLU:N	2.52	0.41
4:R:85:MET:HE2	4:R:87:TYR:HE1	1.84	0.41
1:A:427:TRP:C	1:A:429:ARG:N	2.78	0.41
1:C:350:ARG:O	1:C:354:GLY:N	2.50	0.41
1:E:137:ASN:HB3	1:E:139:THR:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:6:ALA:O	3:M:112:SER:OG	2.36	0.41
1:E:503:ARG:HD2	2:F:606:THR:HA	2.02	0.41
3:K:106:ASP:OD2	4:L:91:ARG:NH2	2.48	0.41
1:E:317:PHE:O	1:E:317:PHE:CG	2.72	0.41
4:L:150:VAL:HG13	4:L:192:TYR:CE1	2.56	0.41
3:M:95:ILE:HD12	3:M:112:SER:C	2.45	0.41
1:E:347:LYS:HB2	1:E:347:LYS:HE3	1.86	0.41
1:A:435:TYR:C	1:A:435:TYR:CD1	2.98	0.41
3:O:122:LYS:NZ	3:O:123:GLY:O	2.53	0.41
3:I:4:LEU:HD21	3:I:27:PHE:HE2	1.85	0.41
4:L:62:PHE:HD2	4:L:75:ILE:HD12	1.86	0.41
1:A:429:ARG:HG3	1:A:432:GLN:HE22	1.86	0.41
4:N:38:GLN:HB3	4:N:85:MET:HB3	2.03	0.41
1:E:150:MET:HE2	1:E:150:MET:HA	2.03	0.41
1:E:205:CYS:O	1:E:208:VAL:HG22	2.21	0.41
4:R:36:LEU:HD12	4:R:44:PRO:HB2	2.03	0.41
1:A:34:LEU:HD22	1:A:498:PRO:HB2	2.02	0.41
3:G:11:VAL:HG12	3:G:115:ILE:HD11	2.01	0.41
1:C:150:MET:HE3	1:C:328:GLN:HB3	2.01	0.41
1:C:255:VAL:O	1:C:261:LEU:HD12	2.21	0.41
1:E:112:TRP:CG	1:E:427:TRP:HE1	2.39	0.41
1:A:184:ILE:HG22	1:A:190:GLU:O	2.20	0.41
1:C:86:LEU:HD22	2:D:523:LEU:O	2.21	0.40
3:K:146:LEU:HD12	3:K:146:LEU:O	2.21	0.40
3:M:63:ASN:OD1	3:M:65:ARG:N	2.48	0.40
1:E:134:VAL:HB	1:E:154:LEU:O	2.20	0.40
1:C:466:GLU:N	1:C:466:GLU:OE1	2.54	0.40
1:A:437:PRO:HA	1:A:438:PRO:HD3	1.93	0.40
4:J:90:GLN:OE1	4:J:90:GLN:N	2.50	0.40
1:C:163:THR:HG23	1:C:165:LEU:H	1.86	0.40
4:N:67:SER:O	4:N:69:THR:N	2.55	0.40
1:A:453:ILE:HD13	1:A:477:ASP:OD2	2.20	0.40
4:L:159:SER:HA	4:L:179:LEU:HD13	2.03	0.40
3:O:60:VAL:O	3:O:60:VAL:HG23	2.21	0.40
1:A:199:SER:OG	1:A:200:ALA:N	2.54	0.40
3:K:150:TYR:OH	3:K:183:LEU:HD23	2.22	0.40
4:N:136:LEU:HD21	4:N:196:VAL:HG21	2.03	0.40
1:A:38:VAL:HG11	2:B:596:TRP:CE3	2.57	0.40
3:I:17:LEU:O	3:I:17:LEU:HD12	2.22	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	450/473 (95%)	401 (89%)	49 (11%)	0	100	100
1	C	450/473 (95%)	404 (90%)	45 (10%)	1 (0%)	43	72
1	E	450/473 (95%)	359 (80%)	71 (16%)	20 (4%)	2	18
2	B	122/153 (80%)	112 (92%)	10 (8%)	0	100	100
2	D	122/153 (80%)	113 (93%)	9 (7%)	0	100	100
2	F	122/153 (80%)	113 (93%)	9 (7%)	0	100	100
3	G	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
3	I	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
3	K	221/223 (99%)	205 (93%)	16 (7%)	0	100	100
3	M	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
3	O	221/223 (99%)	209 (95%)	12 (5%)	0	100	100
3	Q	221/223 (99%)	217 (98%)	4 (2%)	0	100	100
4	H	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	J	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
4	N	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	24	57
4	P	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
4	R	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	24	57
All	All	4314/4500 (96%)	3982 (92%)	309 (7%)	23 (0%)	26	57

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	140	ASP
1	E	241	SER
1	E	330	HIS
1	E	372	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	494	LEU
1	C	209	SER
1	E	151	ARG
1	E	195	ASN
1	E	435	TYR
4	N	50	GLU
1	E	208	VAL
1	E	210	PHE
1	E	258	GLN
1	E	313	PRO
1	E	395	TRP
1	E	433	CYS
1	E	445	CYS
4	R	50	GLU
1	E	280	ASN
1	E	135	THR
1	E	138	ILE
1	E	206	PRO
1	E	446	VAL

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	406/422 (96%)	400 (98%)	6 (2%)	57	70
1	C	406/422 (96%)	400 (98%)	6 (2%)	57	70
1	E	406/422 (96%)	370 (91%)	36 (9%)	9	33
2	B	108/129 (84%)	108 (100%)	0	100	100
2	D	108/129 (84%)	108 (100%)	0	100	100
2	F	108/129 (84%)	108 (100%)	0	100	100
3	G	190/190 (100%)	188 (99%)	2 (1%)	65	74
3	I	190/190 (100%)	190 (100%)	0	100	100
3	K	190/190 (100%)	189 (100%)	1 (0%)	81	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	190/190 (100%)	190 (100%)	0	100	100
3	O	190/190 (100%)	189 (100%)	1 (0%)	81	80
3	Q	190/190 (100%)	190 (100%)	0	100	100
4	H	187/187 (100%)	185 (99%)	2 (1%)	65	74
4	J	187/187 (100%)	186 (100%)	1 (0%)	81	80
4	L	187/187 (100%)	187 (100%)	0	100	100
4	N	187/187 (100%)	186 (100%)	1 (0%)	81	80
4	P	187/187 (100%)	187 (100%)	0	100	100
4	R	187/187 (100%)	187 (100%)	0	100	100
All	All	3804/3915 (97%)	3748 (98%)	56 (2%)	55	70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	C	207	LYS
1	C	208	VAL
1	C	429	ARG
1	C	433	CYS
1	C	443	ILE
3	K	115	ILE
4	N	175	LEU
1	E	88	ASN
1	E	140	ASP
1	E	150	MET
1	E	195	ASN
1	E	206	PRO
1	E	207	LYS
1	E	208	VAL
1	E	234	ASN
1	E	242	VAL
1	E	244	THR
1	E	254	VAL
1	E	260	LEU
1	E	286	VAL
1	E	290	THR
1	E	292	VAL
1	E	297	THR
1	E	309	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	322	ILE
1	E	333	VAL
1	E	359	ILE
1	E	371	VAL
1	E	373	THR
1	E	376	PHE
1	E	430	ILE
1	E	432	GLN
1	E	433	CYS
1	E	440	GLN
1	E	452	LEU
1	E	465	THR
1	E	478	ASN
1	E	480	ARG
1	E	483	LEU
1	E	490	LYS
1	E	499	THR
1	E	500	ARG
1	E	501	CYS
3	O	202	ASN
1	A	88	ASN
1	A	205	CYS
1	A	234	ASN
1	A	428	GLN
1	A	429	ARG
1	A	435	TYR
3	G	122	LYS
3	G	211	LYS
4	H	47	LEU
4	H	50	GLU
4	J	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN
1	C	293	GLN
3	M	176	GLN
3	M	202	ASN
4	N	152	ASN
1	E	82	GLN
1	E	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	103	GLN
1	E	428	GLN
2	F	651	ASN
2	F	653	GLN
4	P	124	GLN
3	Q	23	GLN
4	R	6	GLN
1	A	82	GLN
1	A	99	ASN
1	A	103	GLN
1	A	300	ASN
1	A	352	HIS
4	H	137	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 ⓘ

162 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	S	1	5,1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	S	2	5	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
5	NAG	T	1	5,1	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	T	2	5	14,14,15	0.29	0	17,19,21	0.79	1 (5%)
6	NAG	U	1	6,1	14,14,15	0.63	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	U	2	6	14,14,15	0.20	0	17,19,21	0.41	0
6	BMA	U	3	6	11,11,12	0.53	0	15,15,17	0.71	0
6	MAN	U	4	6	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
5	NAG	V	1	5,1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	W	1	5,1	14,14,15	0.19	0	17,19,21	0.50	0
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	X	1	7,1	14,14,15	0.18	0	17,19,21	0.86	1 (5%)
7	NAG	X	2	7	14,14,15	0.29	0	17,19,21	0.52	0
7	BMA	X	3	7	11,11,12	0.71	0	15,15,17	0.78	0
7	MAN	X	4	7	11,11,12	0.81	0	15,15,17	0.87	1 (6%)
7	MAN	X	5	7	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
7	MAN	X	6	7	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
7	MAN	X	7	7	11,11,12	0.96	1 (9%)	15,15,17	1.25	3 (20%)
7	MAN	X	8	7	11,11,12	0.66	0	15,15,17	0.89	2 (13%)
7	MAN	X	9	7	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
8	NAG	Y	1	8,1	14,14,15	0.23	0	17,19,21	0.52	0
8	NAG	Y	2	8	14,14,15	0.36	0	17,19,21	1.46	2 (11%)
8	BMA	Y	3	8	11,11,12	0.53	0	15,15,17	0.74	0
8	MAN	Y	4	8	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
8	MAN	Y	5	8	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
8	MAN	Y	6	8	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
8	MAN	Y	7	8	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
8	MAN	Y	8	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
8	NAG	Z	1	8,1	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	Z	2	8	14,14,15	0.22	0	17,19,21	0.42	0
8	BMA	Z	3	8	11,11,12	0.63	0	15,15,17	0.80	0
8	MAN	Z	4	8	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
8	MAN	Z	5	8	11,11,12	0.93	0	15,15,17	0.81	0
8	MAN	Z	6	8	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
8	MAN	Z	7	8	11,11,12	0.58	0	15,15,17	0.98	2 (13%)
8	MAN	Z	8	8	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
9	NAG	a	1	9,1	14,14,15	0.19	0	17,19,21	0.53	0
9	NAG	a	2	9	14,14,15	0.26	0	17,19,21	0.45	0
9	BMA	a	3	9	11,11,12	0.58	0	15,15,17	0.90	1 (6%)
9	MAN	a	4	9	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
9	MAN	a	5	9	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
9	MAN	a	6	9	11,11,12	0.68	0	15,15,17	1.13	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	b	1	9,1	14,14,15	0.18	0	17,19,21	0.40	0
9	NAG	b	2	9	14,14,15	0.22	0	17,19,21	0.46	0
9	BMA	b	3	9	11,11,12	0.54	0	15,15,17	0.80	0
9	MAN	b	4	9	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
9	MAN	b	5	9	11,11,12	0.58	0	15,15,17	0.97	2 (13%)
9	MAN	b	6	9	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
10	NAG	c	1	10,1	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	c	2	10	14,14,15	0.23	0	17,19,21	0.85	1 (5%)
10	BMA	c	3	10	11,11,12	0.54	0	15,15,17	0.73	0
10	MAN	c	4	10	11,11,12	0.62	0	15,15,17	0.98	2 (13%)
10	MAN	c	5	10	11,11,12	0.68	0	15,15,17	0.92	2 (13%)
5	NAG	d	1	5,1	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
5	NAG	d	2	5	14,14,15	0.38	0	17,19,21	0.30	0
5	NAG	e	1	5,1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	e	2	5	14,14,15	0.40	0	17,19,21	0.34	0
6	NAG	f	1	6,1	14,14,15	0.44	0	17,19,21	1.02	2 (11%)
6	NAG	f	2	6	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
6	BMA	f	3	6	11,11,12	0.25	0	15,15,17	0.47	0
6	MAN	f	4	6	11,11,12	0.26	0	15,15,17	0.48	0
5	NAG	g	1	5,1	14,14,15	0.39	0	17,19,21	0.53	0
5	NAG	g	2	5	14,14,15	0.38	0	17,19,21	0.35	0
5	NAG	h	1	5,1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	h	2	5	14,14,15	0.39	0	17,19,21	0.51	0
7	NAG	i	1	7,1	14,14,15	0.40	0	17,19,21	0.66	0
7	NAG	i	2	7	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
7	BMA	i	3	7	11,11,12	0.28	0	15,15,17	0.65	0
7	MAN	i	4	7	11,11,12	0.92	0	15,15,17	1.01	1 (6%)
7	MAN	i	5	7	11,11,12	0.61	0	15,15,17	1.13	2 (13%)
7	MAN	i	6	7	11,11,12	0.63	0	15,15,17	0.90	2 (13%)
7	MAN	i	7	7	11,11,12	0.75	1 (9%)	15,15,17	1.10	2 (13%)
7	MAN	i	8	7	11,11,12	0.63	0	15,15,17	0.93	2 (13%)
7	MAN	i	9	7	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
8	NAG	j	1	8,1	14,14,15	0.39	0	17,19,21	0.66	0
8	NAG	j	2	8	14,14,15	0.35	0	17,19,21	1.57	1 (5%)
8	BMA	j	3	8	11,11,12	0.52	0	15,15,17	0.75	0
8	MAN	j	4	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
8	MAN	j	5	8	11,11,12	0.67	0	15,15,17	0.99	1 (6%)
8	MAN	j	6	8	11,11,12	0.61	0	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	j	7	8	11,11,12	0.59	0	15,15,17	0.94	2 (13%)
8	MAN	j	8	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
8	NAG	k	1	8,1	14,14,15	0.41	0	17,19,21	0.95	2 (11%)
8	NAG	k	2	8	14,14,15	0.21	0	17,19,21	0.43	0
8	BMA	k	3	8	11,11,12	0.57	0	15,15,17	0.72	0
8	MAN	k	4	8	11,11,12	0.57	0	15,15,17	0.92	1 (6%)
8	MAN	k	5	8	11,11,12	0.97	0	15,15,17	0.91	1 (6%)
8	MAN	k	6	8	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
8	MAN	k	7	8	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
8	MAN	k	8	8	11,11,12	0.59	0	15,15,17	0.95	2 (13%)
9	NAG	l	1	9,1	14,14,15	0.41	0	17,19,21	0.55	0
9	NAG	l	2	9	14,14,15	0.41	0	17,19,21	0.71	1 (5%)
9	BMA	l	3	9	11,11,12	0.27	0	15,15,17	0.60	0
9	MAN	l	4	9	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
9	MAN	l	5	9	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
9	MAN	l	6	9	11,11,12	0.27	0	15,15,17	0.46	0
9	NAG	m	1	9,1	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	m	2	9	14,14,15	0.23	0	17,19,21	0.47	0
9	BMA	m	3	9	11,11,12	0.56	0	15,15,17	0.79	0
9	MAN	m	4	9	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
9	MAN	m	5	9	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
9	MAN	m	6	9	11,11,12	0.62	0	15,15,17	0.95	2 (13%)
10	NAG	n	1	10,1	14,14,15	0.19	0	17,19,21	0.44	0
10	NAG	n	2	10	14,14,15	0.34	0	17,19,21	0.89	1 (5%)
10	BMA	n	3	10	11,11,12	0.51	0	15,15,17	0.75	0
10	MAN	n	4	10	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
10	MAN	n	5	10	11,11,12	0.69	0	15,15,17	0.90	1 (6%)
5	NAG	o	1	5,1	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	o	2	5	14,14,15	0.32	0	17,19,21	0.79	1 (5%)
5	NAG	p	1	5,1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	p	2	5	14,14,15	0.27	0	17,19,21	0.79	1 (5%)
6	NAG	q	1	6,1	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
6	NAG	q	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	q	3	6	11,11,12	0.54	0	15,15,17	0.72	0
6	MAN	q	4	6	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
5	NAG	r	1	5,1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	r	2	5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	s	1	5,1	14,14,15	0.21	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	s	2	5	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	t	1	7,1	14,14,15	0.18	0	17,19,21	0.85	1 (5%)
7	NAG	t	2	7	14,14,15	0.27	0	17,19,21	0.51	0
7	BMA	t	3	7	11,11,12	0.69	0	15,15,17	0.83	0
7	MAN	t	4	7	11,11,12	0.74	0	15,15,17	0.87	1 (6%)
7	MAN	t	5	7	11,11,12	0.64	0	15,15,17	0.98	2 (13%)
7	MAN	t	6	7	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
7	MAN	t	7	7	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
7	MAN	t	8	7	11,11,12	0.63	0	15,15,17	0.89	2 (13%)
7	MAN	t	9	7	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
11	NAG	u	1	11,1	14,14,15	0.24	0	17,19,21	0.53	0
11	NAG	u	2	11	14,14,15	0.35	0	17,19,21	1.46	2 (11%)
11	BMA	u	3	11	11,11,12	0.61	0	15,15,17	0.74	0
11	MAN	u	4	11	11,11,12	0.56	0	15,15,17	1.02	2 (13%)
11	MAN	u	5	11	11,11,12	0.63	0	15,15,17	1.01	1 (6%)
11	MAN	u	6	11	11,11,12	0.56	0	15,15,17	0.96	2 (13%)
8	NAG	v	1	8,1	14,14,15	0.24	0	17,19,21	0.46	0
8	NAG	v	2	8	14,14,15	0.22	0	17,19,21	0.43	0
8	BMA	v	3	8	11,11,12	0.63	0	15,15,17	0.76	0
8	MAN	v	4	8	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
8	MAN	v	5	8	11,11,12	0.96	0	15,15,17	0.80	1 (6%)
8	MAN	v	6	8	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
8	MAN	v	7	8	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
8	MAN	v	8	8	11,11,12	0.58	0	15,15,17	0.97	2 (13%)
9	NAG	w	1	9,1	14,14,15	0.19	0	17,19,21	0.52	0
9	NAG	w	2	9	14,14,15	0.26	0	17,19,21	0.46	0
9	BMA	w	3	9	11,11,12	0.62	0	15,15,17	0.86	1 (6%)
9	MAN	w	4	9	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
9	MAN	w	5	9	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
9	MAN	w	6	9	11,11,12	0.67	0	15,15,17	1.13	2 (13%)
9	NAG	x	1	9,1	14,14,15	0.20	0	17,19,21	0.40	0
9	NAG	x	2	9	14,14,15	0.23	0	17,19,21	0.47	0
9	BMA	x	3	9	11,11,12	0.54	0	15,15,17	0.80	0
9	MAN	x	4	9	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
9	MAN	x	5	9	11,11,12	0.59	0	15,15,17	0.97	2 (13%)
9	MAN	x	6	9	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
12	MAN	y	1	12	11,11,12	0.72	0	15,15,17	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	y	2	12	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
10	NAG	z	1	10,1	14,14,15	0.21	0	17,19,21	0.42	0
10	NAG	z	2	10	14,14,15	0.20	0	17,19,21	0.84	1 (5%)
10	BMA	z	3	10	11,11,12	0.57	0	15,15,17	0.77	0
10	MAN	z	4	10	11,11,12	0.64	0	15,15,17	0.98	2 (13%)
10	MAN	z	5	10	11,11,12	0.74	0	15,15,17	0.90	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	S	2	5	-	4/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	4/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	2/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
7	MAN	X	4	7	-	2/2/19/22	0/1/1/1
7	MAN	X	5	7	-	1/2/19/22	0/1/1/1
7	MAN	X	6	7	-	0/2/19/22	0/1/1/1
7	MAN	X	7	7	-	2/2/19/22	0/1/1/1
7	MAN	X	8	7	-	0/2/19/22	0/1/1/1
7	MAN	X	9	7	-	0/2/19/22	1/1/1/1
8	NAG	Y	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	4/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	n	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	n	2	10	-	4/6/23/26	0/1/1/1
10	BMA	n	3	10	-	2/2/19/22	0/1/1/1
10	MAN	n	4	10	-	0/2/19/22	0/1/1/1
10	MAN	n	5	10	-	1/2/19/22	0/1/1/1
5	NAG	o	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	o	2	5	-	4/6/23/26	0/1/1/1
5	NAG	p	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	4/6/23/26	0/1/1/1
6	NAG	q	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	q	4	6	-	0/2/19/22	0/1/1/1
5	NAG	r	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	r	2	5	-	2/6/23/26	0/1/1/1
5	NAG	s	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
7	NAG	t	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	t	2	7	-	2/6/23/26	0/1/1/1
7	BMA	t	3	7	-	0/2/19/22	0/1/1/1
7	MAN	t	4	7	-	2/2/19/22	0/1/1/1
7	MAN	t	5	7	-	1/2/19/22	0/1/1/1
7	MAN	t	6	7	-	0/2/19/22	0/1/1/1
7	MAN	t	7	7	-	2/2/19/22	0/1/1/1
7	MAN	t	8	7	-	0/2/19/22	0/1/1/1
7	MAN	t	9	7	-	0/2/19/22	1/1/1/1
11	NAG	u	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	u	2	11	-	4/6/23/26	0/1/1/1
11	BMA	u	3	11	-	1/2/19/22	0/1/1/1
11	MAN	u	4	11	-	2/2/19/22	0/1/1/1
11	MAN	u	5	11	-	1/2/19/22	0/1/1/1
11	MAN	u	6	11	-	0/2/19/22	0/1/1/1
8	NAG	v	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	v	2	8	-	2/6/23/26	0/1/1/1
8	BMA	v	3	8	-	2/2/19/22	0/1/1/1
8	MAN	v	4	8	-	0/2/19/22	0/1/1/1
8	MAN	v	5	8	-	1/2/19/22	0/1/1/1
8	MAN	v	6	8	-	1/2/19/22	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	v	7	8	-	0/2/19/22	0/1/1/1
8	MAN	v	8	8	-	0/2/19/22	0/1/1/1
9	NAG	w	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	w	2	9	-	0/6/23/26	0/1/1/1
9	BMA	w	3	9	-	2/2/19/22	0/1/1/1
9	MAN	w	4	9	-	0/2/19/22	0/1/1/1
9	MAN	w	5	9	-	0/2/19/22	0/1/1/1
9	MAN	w	6	9	-	0/2/19/22	1/1/1/1
9	NAG	x	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	x	2	9	-	4/6/23/26	0/1/1/1
9	BMA	x	3	9	-	0/2/19/22	0/1/1/1
9	MAN	x	4	9	-	0/2/19/22	0/1/1/1
9	MAN	x	5	9	-	0/2/19/22	0/1/1/1
9	MAN	x	6	9	-	1/2/19/22	0/1/1/1
12	MAN	y	1	12	-	1/2/19/22	1/1/1/1
12	MAN	y	2	12	-	0/2/19/22	0/1/1/1
10	NAG	z	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	z	2	10	-	4/6/23/26	0/1/1/1
10	BMA	z	3	10	-	2/2/19/22	0/1/1/1
10	MAN	z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	z	5	10	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	7	MAN	C1-C2	2.64	1.58	1.52
7	i	7	MAN	C1-C2	2.22	1.57	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	2	NAG	C2-N2-C7	5.47	130.22	122.90
8	Y	2	NAG	C2-N2-C7	4.71	129.22	122.90
11	u	2	NAG	C2-N2-C7	4.71	129.22	122.90
12	y	1	MAN	C1-O5-C5	3.49	116.86	112.19
9	w	6	MAN	C1-O5-C5	3.42	116.77	112.19
9	a	6	MAN	C1-O5-C5	3.39	116.73	112.19
8	j	6	MAN	C1-O5-C5	3.13	116.38	112.19
7	X	9	MAN	C1-O5-C5	3.10	116.34	112.19
7	t	9	MAN	C1-O5-C5	3.06	116.29	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	1	NAG	O5-C1-C2	-3.04	106.58	111.29
6	U	1	NAG	C1-O5-C5	2.95	116.14	112.19
8	k	6	MAN	C1-O5-C5	2.94	116.13	112.19
8	v	6	MAN	C1-O5-C5	2.90	116.07	112.19
10	n	2	NAG	C2-N2-C7	2.88	126.76	122.90
7	i	9	MAN	C1-O5-C5	2.85	116.00	112.19
11	u	4	MAN	C1-O5-C5	2.85	116.00	112.19
11	u	5	MAN	C1-O5-C5	2.84	116.00	112.19
8	Z	6	MAN	C1-O5-C5	2.81	115.95	112.19
8	Y	6	MAN	C1-O5-C5	2.77	115.89	112.19
8	j	5	MAN	C1-O5-C5	2.77	115.89	112.19
8	Y	4	MAN	C1-O5-C5	2.76	115.89	112.19
7	i	5	MAN	C1-O5-C5	2.75	115.87	112.19
10	z	2	NAG	C2-N2-C7	2.74	126.57	122.90
9	b	4	MAN	C1-O5-C5	2.73	115.84	112.19
7	X	1	NAG	C2-N2-C7	2.73	126.56	122.90
10	c	2	NAG	C2-N2-C7	2.73	126.56	122.90
9	l	4	MAN	C1-O5-C5	2.71	115.81	112.19
7	t	1	NAG	C2-N2-C7	2.70	126.52	122.90
7	X	7	MAN	C1-O5-C5	2.70	115.81	112.19
6	f	1	NAG	O5-C1-C2	2.70	115.47	111.29
5	p	2	NAG	C2-N2-C7	2.68	126.49	122.90
9	x	4	MAN	C1-O5-C5	2.67	115.76	112.19
9	m	4	MAN	C1-O5-C5	2.67	115.76	112.19
5	o	2	NAG	C2-N2-C7	2.67	126.47	122.90
5	T	2	NAG	C2-N2-C7	2.67	126.47	122.90
5	S	2	NAG	C2-N2-C7	2.66	126.47	122.90
9	w	4	MAN	C1-O5-C5	2.65	115.74	112.19
7	X	5	MAN	O2-C2-C3	-2.65	104.67	110.15
9	a	4	MAN	C1-O5-C5	2.65	115.73	112.19
7	i	7	MAN	C1-O5-C5	2.64	115.72	112.19
7	i	5	MAN	O2-C2-C3	-2.63	104.70	110.15
6	q	1	NAG	C1-O5-C5	2.60	115.67	112.19
9	l	2	NAG	O5-C1-C2	-2.58	107.29	111.29
8	k	4	MAN	C1-O5-C5	2.56	115.62	112.19
8	j	4	MAN	C1-O5-C5	2.52	115.56	112.19
8	k	7	MAN	C1-O5-C5	2.51	115.55	112.19
9	a	3	BMA	C1-O5-C5	2.51	115.55	112.19
7	X	5	MAN	C1-O5-C5	2.50	115.54	112.19
8	Y	5	MAN	C1-O5-C5	2.50	115.54	112.19
8	Z	4	MAN	C1-O5-C5	2.49	115.52	112.19
7	i	4	MAN	C1-O5-C5	2.47	115.50	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	v	7	MAN	C1-O5-C5	2.47	115.50	112.19
7	t	5	MAN	O2-C2-C3	-2.46	105.06	110.15
8	Z	7	MAN	C1-O5-C5	2.45	115.48	112.19
7	t	7	MAN	C1-O5-C5	2.45	115.47	112.19
8	v	8	MAN	C1-O5-C5	2.45	115.47	112.19
6	f	1	NAG	C1-O5-C5	2.44	115.46	112.19
6	U	4	MAN	C1-O5-C5	2.43	115.45	112.19
6	q	4	MAN	C1-O5-C5	2.43	115.45	112.19
8	v	4	MAN	C1-O5-C5	2.43	115.44	112.19
8	k	5	MAN	C1-O5-C5	2.43	115.44	112.19
10	n	4	MAN	C1-O5-C5	2.42	115.43	112.19
8	Y	8	MAN	C1-O5-C5	2.42	115.43	112.19
8	j	8	MAN	C1-O5-C5	2.41	115.41	112.19
5	d	1	NAG	C2-N2-C7	2.40	126.12	122.90
7	X	7	MAN	O2-C2-C3	-2.40	105.18	110.15
9	x	5	MAN	C1-O5-C5	2.40	115.40	112.19
9	b	5	MAN	C1-O5-C5	2.39	115.39	112.19
7	X	7	MAN	C1-C2-C3	2.39	113.12	109.64
11	u	6	MAN	C1-O5-C5	2.37	115.37	112.19
9	m	5	MAN	C1-O5-C5	2.37	115.36	112.19
8	k	8	MAN	C1-O5-C5	2.36	115.35	112.19
8	Z	8	MAN	C1-O5-C5	2.36	115.34	112.19
10	z	5	MAN	O2-C2-C3	-2.33	105.32	110.15
10	c	4	MAN	C1-O5-C5	2.33	115.31	112.19
9	w	3	BMA	C1-O5-C5	2.32	115.29	112.19
11	u	2	NAG	C1-C2-N2	2.31	114.08	110.43
10	z	4	MAN	C1-O5-C5	2.31	115.28	112.19
12	y	2	MAN	C1-O5-C5	2.31	115.28	112.19
8	Y	2	NAG	C1-C2-N2	2.30	114.06	110.43
7	t	6	MAN	C1-O5-C5	2.29	115.26	112.19
7	i	2	NAG	C2-N2-C7	2.29	125.97	122.90
9	m	6	MAN	C1-O5-C5	2.28	115.24	112.19
10	n	5	MAN	O2-C2-C3	-2.27	105.45	110.15
10	c	5	MAN	O2-C2-C3	-2.26	105.47	110.15
9	w	5	MAN	C1-O5-C5	2.26	115.22	112.19
7	i	7	MAN	O2-C2-C3	-2.26	105.47	110.15
9	b	6	MAN	C1-O5-C5	2.26	115.21	112.19
9	l	5	MAN	C1-O5-C5	2.25	115.19	112.19
9	x	6	MAN	C1-O5-C5	2.24	115.19	112.19
7	t	7	MAN	O2-C2-C3	-2.24	105.50	110.15
9	a	5	MAN	C1-O5-C5	2.23	115.17	112.19
8	Y	7	MAN	C1-O5-C5	2.23	115.17	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	v	7	MAN	O2-C2-C3	-2.20	105.59	110.15
7	t	5	MAN	C1-O5-C5	2.20	115.13	112.19
10	z	4	MAN	O2-C2-C3	-2.19	105.61	110.15
9	l	4	MAN	O2-C2-C3	-2.19	105.62	110.15
9	a	4	MAN	O2-C2-C3	-2.19	105.62	110.15
8	k	7	MAN	O2-C2-C3	-2.18	105.64	110.15
9	w	4	MAN	O2-C2-C3	-2.18	105.64	110.15
8	j	7	MAN	C1-O5-C5	2.18	115.11	112.19
8	Y	4	MAN	O2-C2-C3	-2.18	105.64	110.15
7	i	8	MAN	C1-O5-C5	2.17	115.10	112.19
12	y	1	MAN	O2-C2-C3	-2.16	105.67	110.15
9	l	5	MAN	O2-C2-C3	-2.16	105.68	110.15
9	w	5	MAN	O2-C2-C3	-2.16	105.68	110.15
10	c	4	MAN	O2-C2-C3	-2.16	105.68	110.15
8	j	6	MAN	O2-C2-C3	-2.16	105.68	110.15
9	a	5	MAN	O2-C2-C3	-2.16	105.69	110.15
8	Y	8	MAN	O2-C2-C3	-2.15	105.69	110.15
6	U	4	MAN	O2-C2-C3	-2.15	105.69	110.15
9	b	6	MAN	O2-C2-C3	-2.15	105.69	110.15
8	j	8	MAN	O2-C2-C3	-2.15	105.69	110.15
9	b	5	MAN	O2-C2-C3	-2.15	105.70	110.15
6	q	4	MAN	O2-C2-C3	-2.15	105.70	110.15
7	t	6	MAN	O2-C2-C3	-2.15	105.70	110.15
9	x	6	MAN	O2-C2-C3	-2.15	105.70	110.15
12	y	2	MAN	O2-C2-C3	-2.15	105.70	110.15
8	j	7	MAN	O2-C2-C3	-2.14	105.71	110.15
8	v	4	MAN	O2-C2-C3	-2.14	105.71	110.15
9	w	6	MAN	O2-C2-C3	-2.14	105.71	110.15
8	k	8	MAN	O2-C2-C3	-2.14	105.71	110.15
7	X	6	MAN	O2-C2-C3	-2.14	105.72	110.15
7	t	4	MAN	O2-C2-C3	-2.14	105.72	110.15
7	X	6	MAN	C1-O5-C5	2.14	115.06	112.19
9	m	5	MAN	O2-C2-C3	-2.14	105.72	110.15
9	m	6	MAN	O2-C2-C3	-2.14	105.72	110.15
9	x	5	MAN	O2-C2-C3	-2.14	105.72	110.15
7	i	6	MAN	O2-C2-C3	-2.13	105.73	110.15
11	u	4	MAN	O2-C2-C3	-2.13	105.73	110.15
8	k	6	MAN	O2-C2-C3	-2.13	105.74	110.15
9	x	4	MAN	O2-C2-C3	-2.13	105.74	110.15
8	v	8	MAN	O2-C2-C3	-2.13	105.75	110.15
8	Z	8	MAN	O2-C2-C3	-2.13	105.75	110.15
9	m	4	MAN	O2-C2-C3	-2.13	105.75	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	n	4	MAN	O2-C2-C3	-2.13	105.75	110.15
9	a	6	MAN	O2-C2-C3	-2.12	105.75	110.15
9	b	4	MAN	O2-C2-C3	-2.12	105.76	110.15
8	Y	7	MAN	O2-C2-C3	-2.12	105.76	110.15
8	Z	7	MAN	O2-C2-C3	-2.12	105.76	110.15
8	Y	6	MAN	O2-C2-C3	-2.11	105.78	110.15
7	t	9	MAN	O2-C2-C3	-2.11	105.78	110.15
7	X	9	MAN	O2-C2-C3	-2.11	105.79	110.15
8	Z	4	MAN	O2-C2-C3	-2.10	105.80	110.15
7	i	9	MAN	O2-C2-C3	-2.10	105.80	110.15
11	u	6	MAN	O2-C2-C3	-2.10	105.80	110.15
8	j	4	MAN	O2-C2-C3	-2.10	105.80	110.15
7	X	8	MAN	O2-C2-C3	-2.10	105.81	110.15
8	k	1	NAG	C2-N2-C7	-2.09	120.10	122.90
8	Z	6	MAN	O2-C2-C3	-2.08	105.83	110.15
8	v	6	MAN	O2-C2-C3	-2.08	105.84	110.15
7	i	6	MAN	C1-O5-C5	2.07	114.97	112.19
7	t	8	MAN	C1-O5-C5	2.06	114.95	112.19
7	X	4	MAN	O2-C2-C3	-2.06	105.88	110.15
7	t	8	MAN	O2-C2-C3	-2.06	105.89	110.15
8	v	5	MAN	C1-O5-C5	2.03	114.91	112.19
6	f	2	NAG	O5-C1-C2	-2.02	108.16	111.29
7	i	8	MAN	O2-C2-C3	-2.02	105.96	110.15
7	X	8	MAN	C1-O5-C5	2.00	114.87	112.19
10	c	5	MAN	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	j	2	NAG	C8-C7-N2-C2
8	j	2	NAG	O7-C7-N2-C2
8	Y	3	BMA	C4-C5-C6-O6
8	Y	5	MAN	C4-C5-C6-O6
8	j	3	BMA	C4-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6
5	r	2	NAG	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
7	t	7	MAN	O5-C5-C6-O6
8	Y	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	b	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
7	i	4	MAN	O5-C5-C6-O6
8	j	3	BMA	O5-C5-C6-O6
8	k	2	NAG	O5-C5-C6-O6
9	m	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	o	1	NAG	O5-C5-C6-O6
9	x	2	NAG	O5-C5-C6-O6
10	z	1	NAG	O5-C5-C6-O6
7	X	4	MAN	C4-C5-C6-O6
7	i	7	MAN	O5-C5-C6-O6
8	j	5	MAN	O5-C5-C6-O6
9	w	1	NAG	O5-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6
8	k	2	NAG	C4-C5-C6-O6
8	v	3	BMA	C4-C5-C6-O6
9	m	2	NAG	C4-C5-C6-O6
9	x	1	NAG	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
10	z	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
9	a	1	NAG	O5-C5-C6-O6
9	x	2	NAG	C4-C5-C6-O6
10	n	1	NAG	O5-C5-C6-O6
5	r	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
9	m	2	NAG	O5-C5-C6-O6
8	Z	3	BMA	C4-C5-C6-O6
5	r	1	NAG	O5-C5-C6-O6
7	t	4	MAN	O5-C5-C6-O6
9	a	3	BMA	O5-C5-C6-O6
9	l	3	BMA	O5-C5-C6-O6
10	c	2	NAG	O5-C5-C6-O6
10	n	3	BMA	C4-C5-C6-O6
8	k	3	BMA	C4-C5-C6-O6
9	m	1	NAG	C4-C5-C6-O6
10	z	3	BMA	C4-C5-C6-O6
9	w	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	T	2	NAG	C4-C5-C6-O6
9	a	1	NAG	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
9	w	1	NAG	C4-C5-C6-O6
10	c	3	BMA	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
7	i	7	MAN	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	o	1	NAG	C4-C5-C6-O6
5	o	2	NAG	C4-C5-C6-O6
7	i	4	MAN	C4-C5-C6-O6
7	t	7	MAN	C4-C5-C6-O6
10	z	1	NAG	C4-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
10	n	3	BMA	O5-C5-C6-O6
9	l	3	BMA	C4-C5-C6-O6
7	X	7	MAN	O5-C5-C6-O6
10	c	3	BMA	O5-C5-C6-O6
10	z	3	BMA	O5-C5-C6-O6
5	p	2	NAG	C4-C5-C6-O6
10	c	1	NAG	C4-C5-C6-O6
10	z	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
9	x	1	NAG	C4-C5-C6-O6
10	n	1	NAG	C4-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
9	a	3	BMA	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
9	w	3	BMA	C4-C5-C6-O6
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
5	e	2	NAG	C8-C7-N2-C2
5	e	2	NAG	O7-C7-N2-C2
5	o	2	NAG	C8-C7-N2-C2
5	o	2	NAG	O7-C7-N2-C2
5	p	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	p	2	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	i	1	NAG	C8-C7-N2-C2
7	i	1	NAG	O7-C7-N2-C2
7	t	1	NAG	C8-C7-N2-C2
7	t	1	NAG	O7-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
10	c	2	NAG	C8-C7-N2-C2
10	c	2	NAG	O7-C7-N2-C2
10	n	2	NAG	C8-C7-N2-C2
10	n	2	NAG	O7-C7-N2-C2
10	z	2	NAG	C8-C7-N2-C2
10	z	2	NAG	O7-C7-N2-C2
11	u	2	NAG	C8-C7-N2-C2
11	u	2	NAG	O7-C7-N2-C2
11	u	5	MAN	O5-C5-C6-O6
6	q	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	r	1	NAG	C4-C5-C6-O6
7	t	4	MAN	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
8	v	3	BMA	O5-C5-C6-O6
10	c	2	NAG	C4-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
8	Z	3	BMA	O5-C5-C6-O6
7	X	7	MAN	C4-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
8	k	3	BMA	O5-C5-C6-O6
11	u	3	BMA	O5-C5-C6-O6
8	j	5	MAN	C4-C5-C6-O6
10	n	2	NAG	O5-C5-C6-O6
8	v	2	NAG	O5-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
8	k	5	MAN	O5-C5-C6-O6
12	y	1	MAN	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
7	t	5	MAN	O5-C5-C6-O6
7	X	5	MAN	O5-C5-C6-O6
8	Z	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	z	5	MAN	O5-C5-C6-O6
10	c	5	MAN	O5-C5-C6-O6
8	j	7	MAN	O5-C5-C6-O6
8	k	6	MAN	O5-C5-C6-O6
8	j	2	NAG	C3-C2-N2-C7
7	i	5	MAN	O5-C5-C6-O6
8	v	5	MAN	O5-C5-C6-O6
8	Y	7	MAN	O5-C5-C6-O6
8	v	6	MAN	O5-C5-C6-O6
9	b	6	MAN	O5-C5-C6-O6
9	m	6	MAN	O5-C5-C6-O6
9	x	6	MAN	O5-C5-C6-O6
8	Z	6	MAN	O5-C5-C6-O6
10	n	5	MAN	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C1-C2-N2-C7
5	o	1	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	t	2	NAG	C1-C2-N2-C7
8	Y	1	NAG	C1-C2-N2-C7
9	b	2	NAG	C1-C2-N2-C7
9	m	2	NAG	C1-C2-N2-C7
9	x	2	NAG	C1-C2-N2-C7
11	u	1	NAG	C1-C2-N2-C7
5	S	1	NAG	C3-C2-N2-C7
5	d	1	NAG	C3-C2-N2-C7
5	o	1	NAG	C3-C2-N2-C7
6	f	1	NAG	C3-C2-N2-C7
7	i	2	NAG	C3-C2-N2-C7
8	Y	1	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
9	b	2	NAG	C3-C2-N2-C7
9	m	2	NAG	C3-C2-N2-C7
9	x	2	NAG	C3-C2-N2-C7
11	u	2	NAG	C3-C2-N2-C7
5	s	1	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
10	n	2	NAG	C4-C5-C6-O6
11	u	4	MAN	O5-C5-C6-O6
5	r	1	NAG	C1-C2-N2-C7
8	Y	2	NAG	C1-C2-N2-C7
9	a	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	u	2	NAG	C1-C2-N2-C7
8	v	2	NAG	C4-C5-C6-O6
11	u	4	MAN	C4-C5-C6-O6
5	h	1	NAG	C3-C2-N2-C7
5	h	2	NAG	C3-C2-N2-C7
6	f	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	t	2	NAG	C3-C2-N2-C7
8	Y	2	NAG	C3-C2-N2-C7
11	u	1	NAG	C3-C2-N2-C7

All (10) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	v	6	MAN	C1-C2-C3-C4-C5-O5
9	l	6	MAN	C1-C2-C3-C4-C5-O5
12	y	1	MAN	C1-C2-C3-C4-C5-O5
7	i	9	MAN	C1-C2-C3-C4-C5-O5
8	Z	6	MAN	C1-C2-C3-C4-C5-O5
9	w	6	MAN	C1-C2-C3-C4-C5-O5
9	a	6	MAN	C1-C2-C3-C4-C5-O5
7	X	9	MAN	C1-C2-C3-C4-C5-O5
7	t	9	MAN	C1-C2-C3-C4-C5-O5
8	k	6	MAN	C1-C2-C3-C4-C5-O5

30 monomers are involved in 26 short contacts:

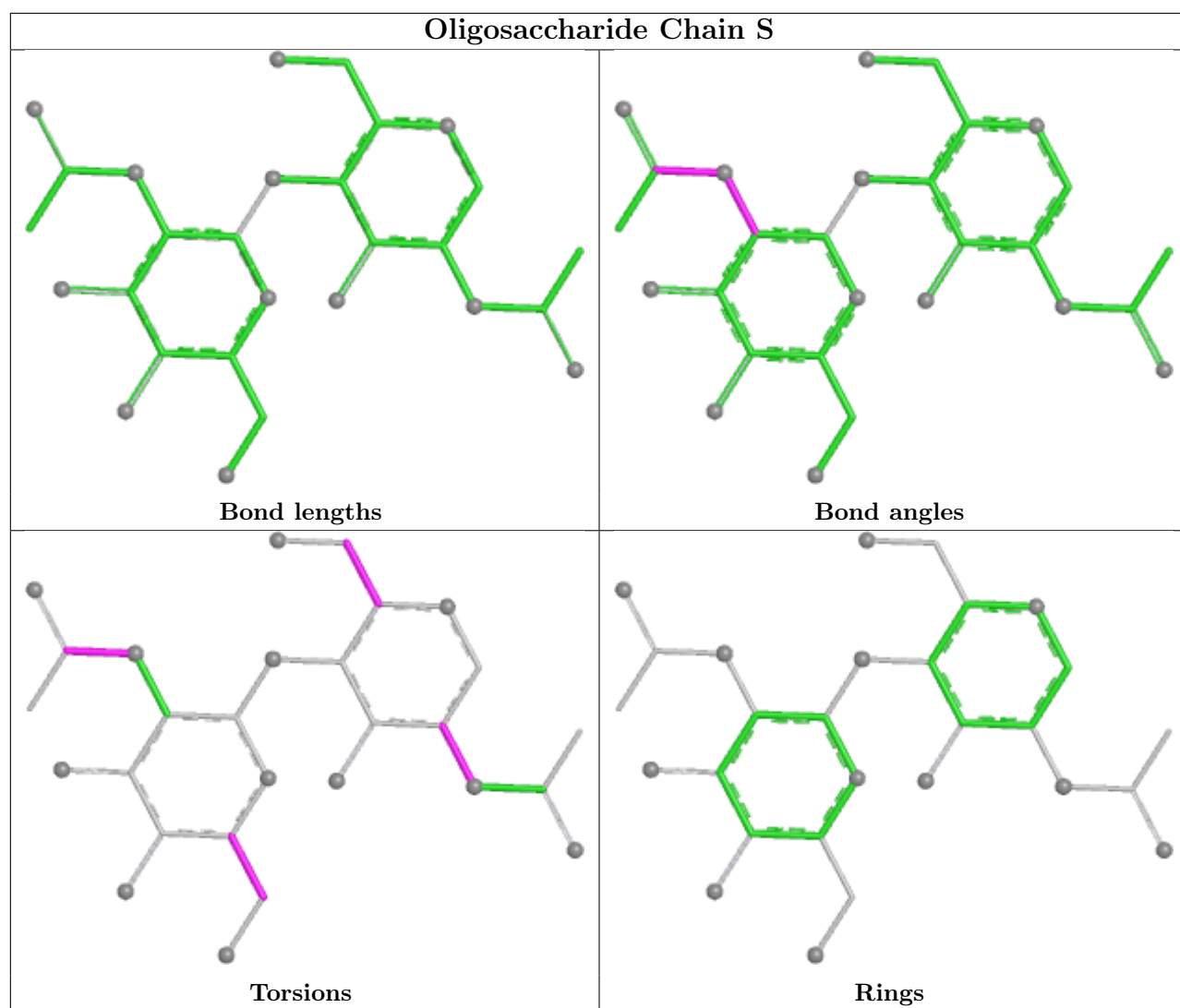
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	n	1	NAG	1	0
9	l	1	NAG	1	0
5	T	2	NAG	1	0
8	Y	4	MAN	1	0
7	i	1	NAG	1	0
10	z	4	MAN	1	0
12	y	1	MAN	1	0
6	U	1	NAG	2	0
6	f	1	NAG	2	0
7	i	7	MAN	1	0
6	U	2	NAG	1	0
6	q	2	NAG	1	0
7	X	4	MAN	1	0
6	q	1	NAG	1	0

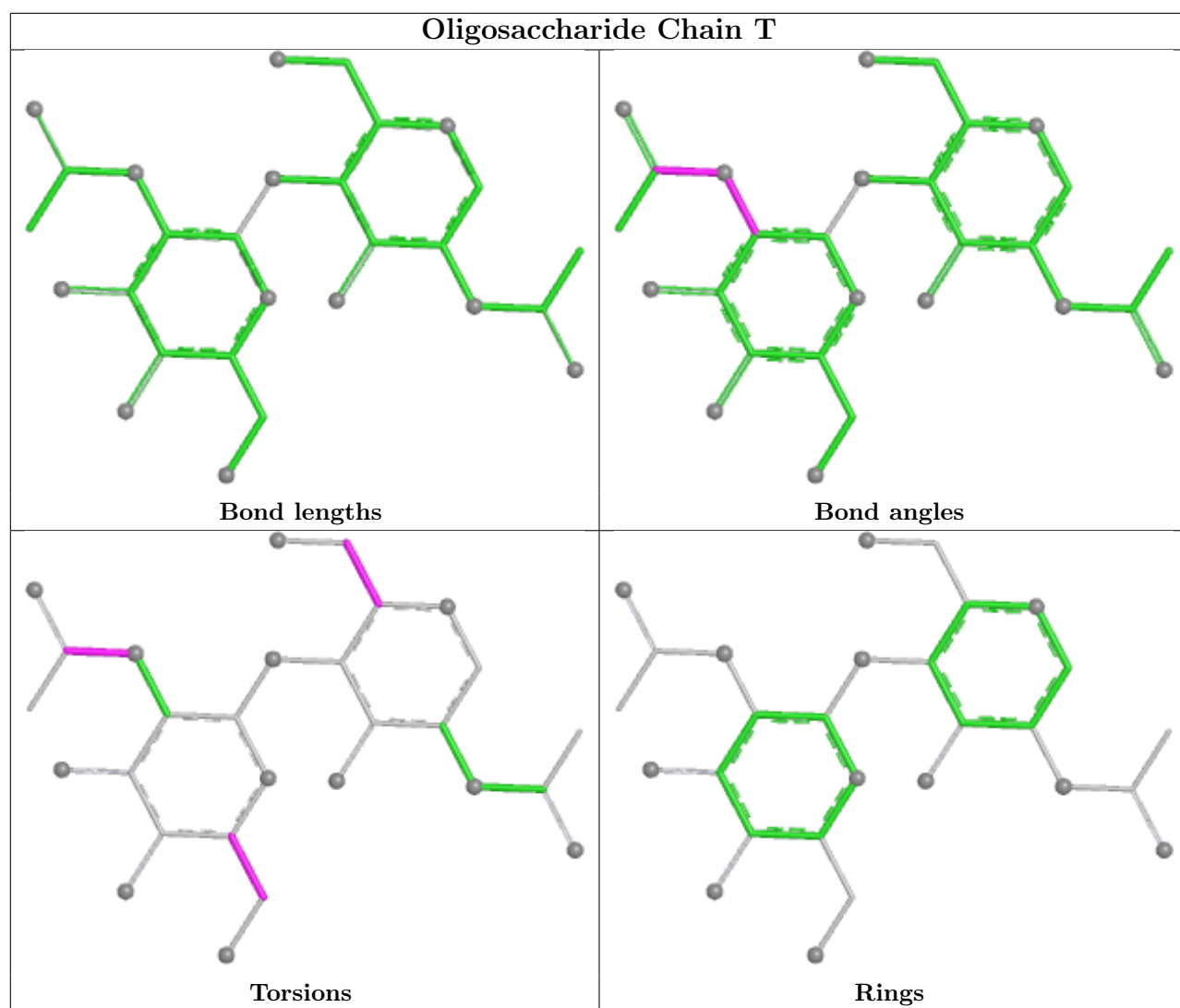
Continued on next page...

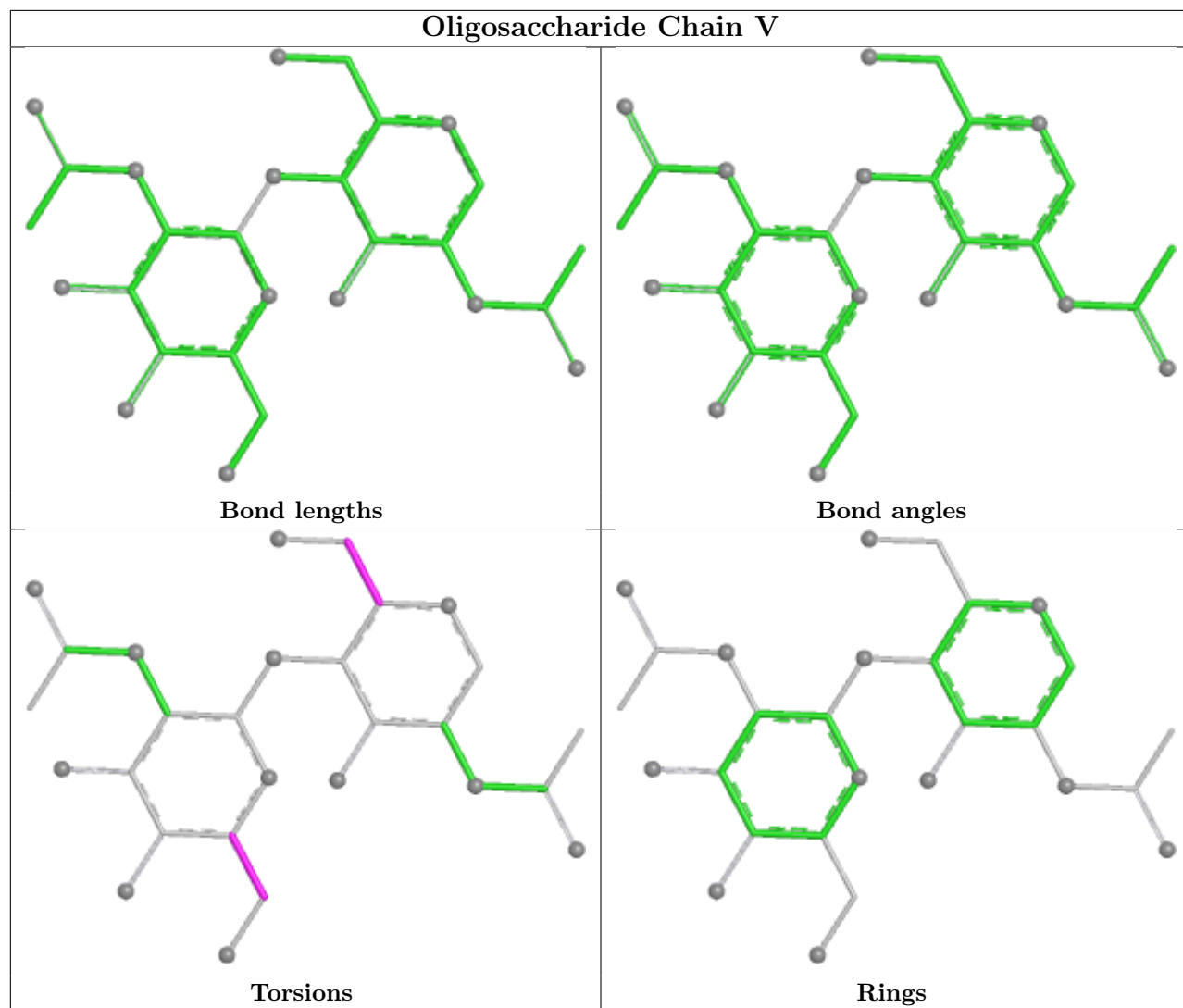
Continued from previous page...

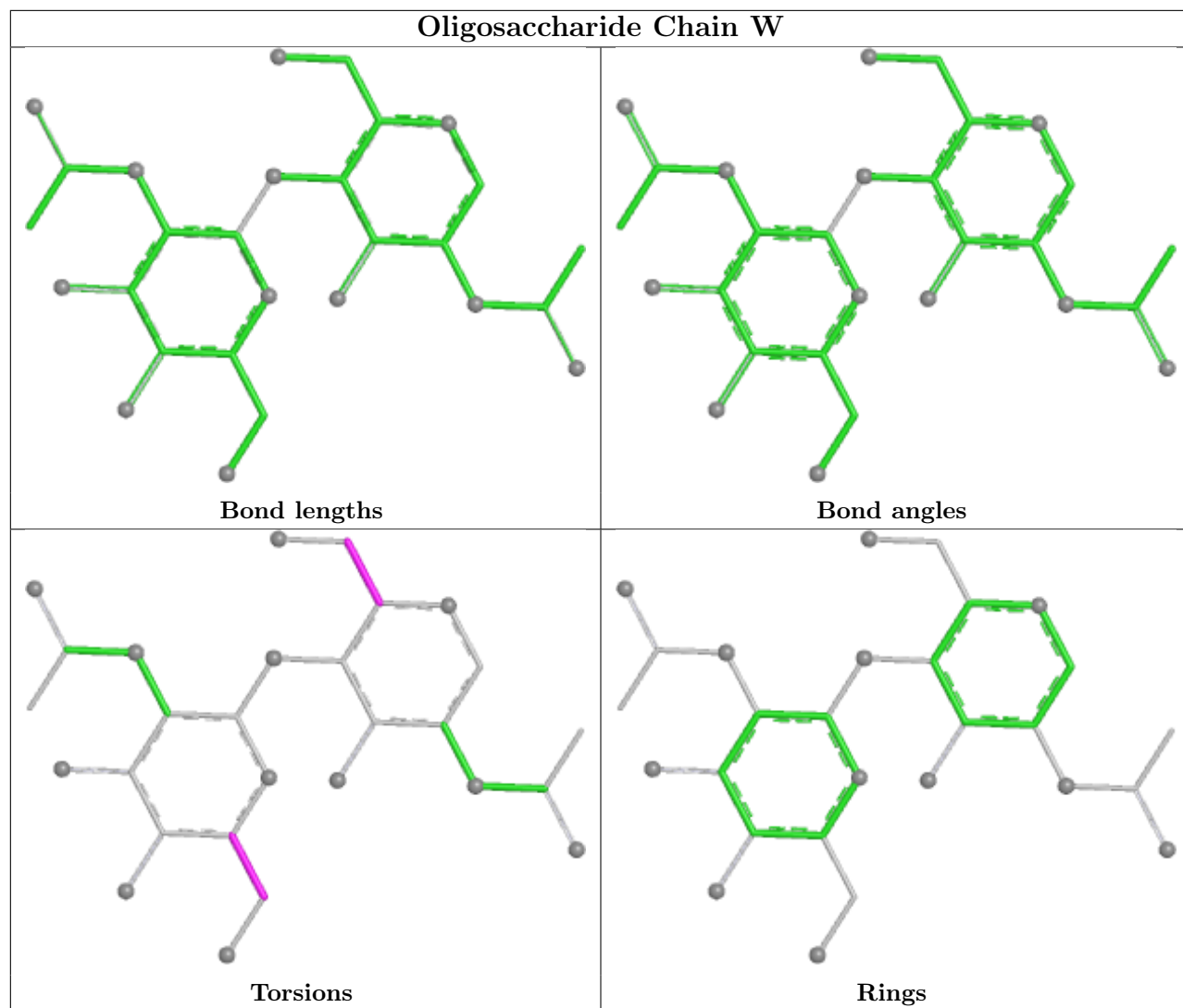
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	2	NAG	1	0
11	u	2	NAG	2	0
9	w	2	NAG	1	0
8	k	4	MAN	1	0
8	Y	3	BMA	1	0
10	z	1	NAG	1	0
8	Y	2	NAG	2	0
10	c	4	MAN	1	0
9	w	3	BMA	1	0
9	a	3	BMA	1	0
8	j	2	NAG	1	0
11	u	3	BMA	2	0
9	l	5	MAN	1	0
5	T	1	NAG	1	0
8	k	5	MAN	2	0
10	n	4	MAN	1	0

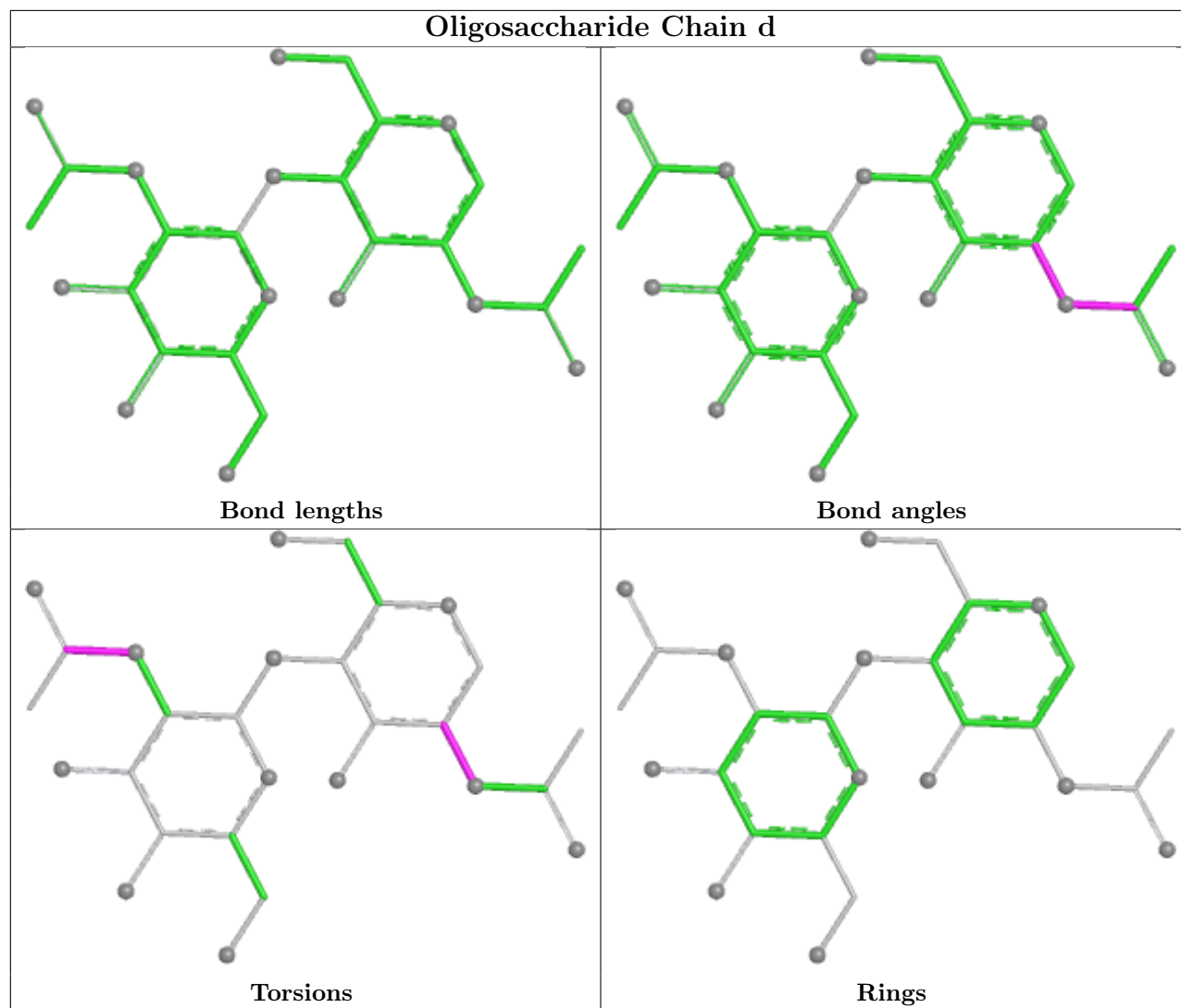
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

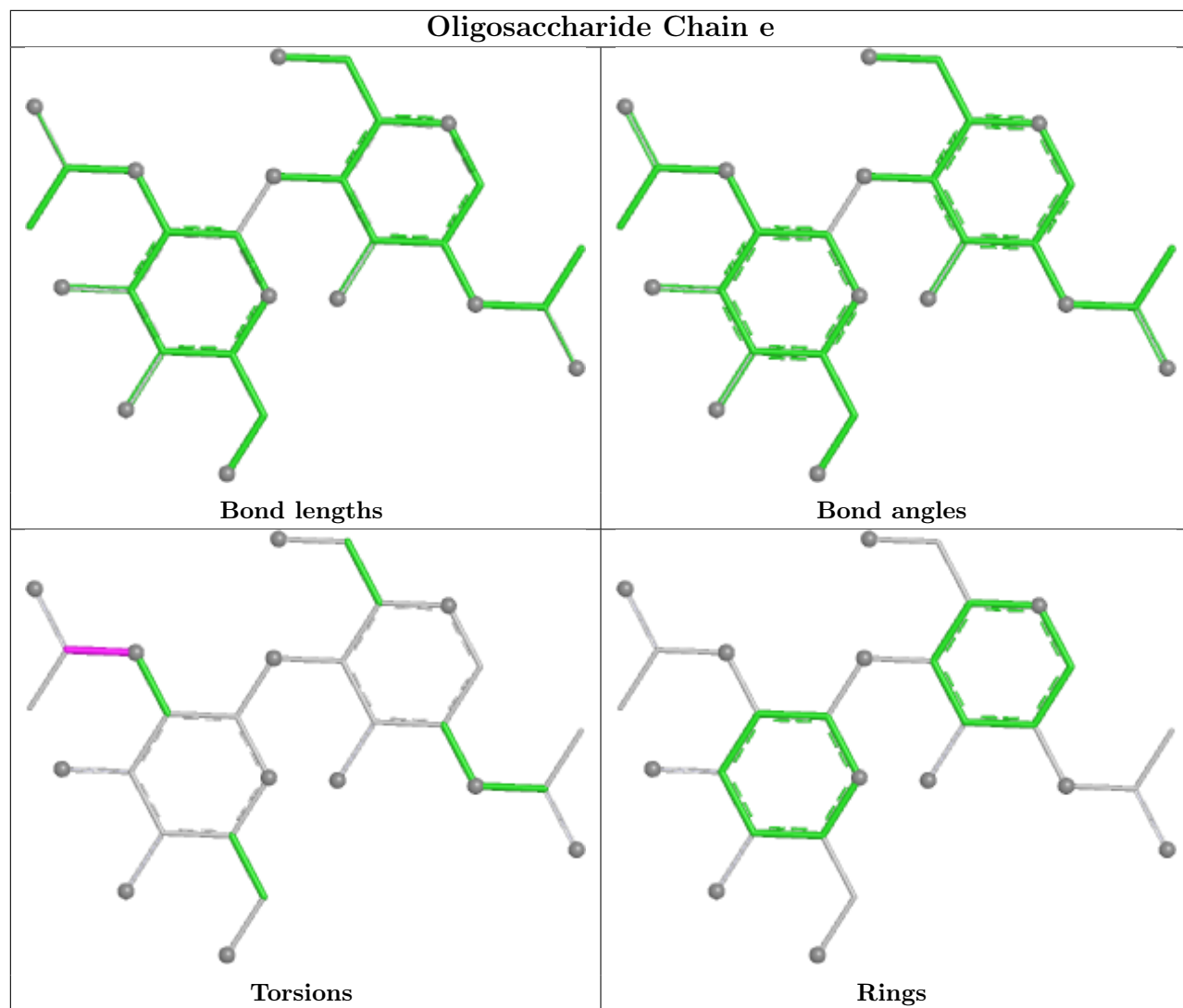


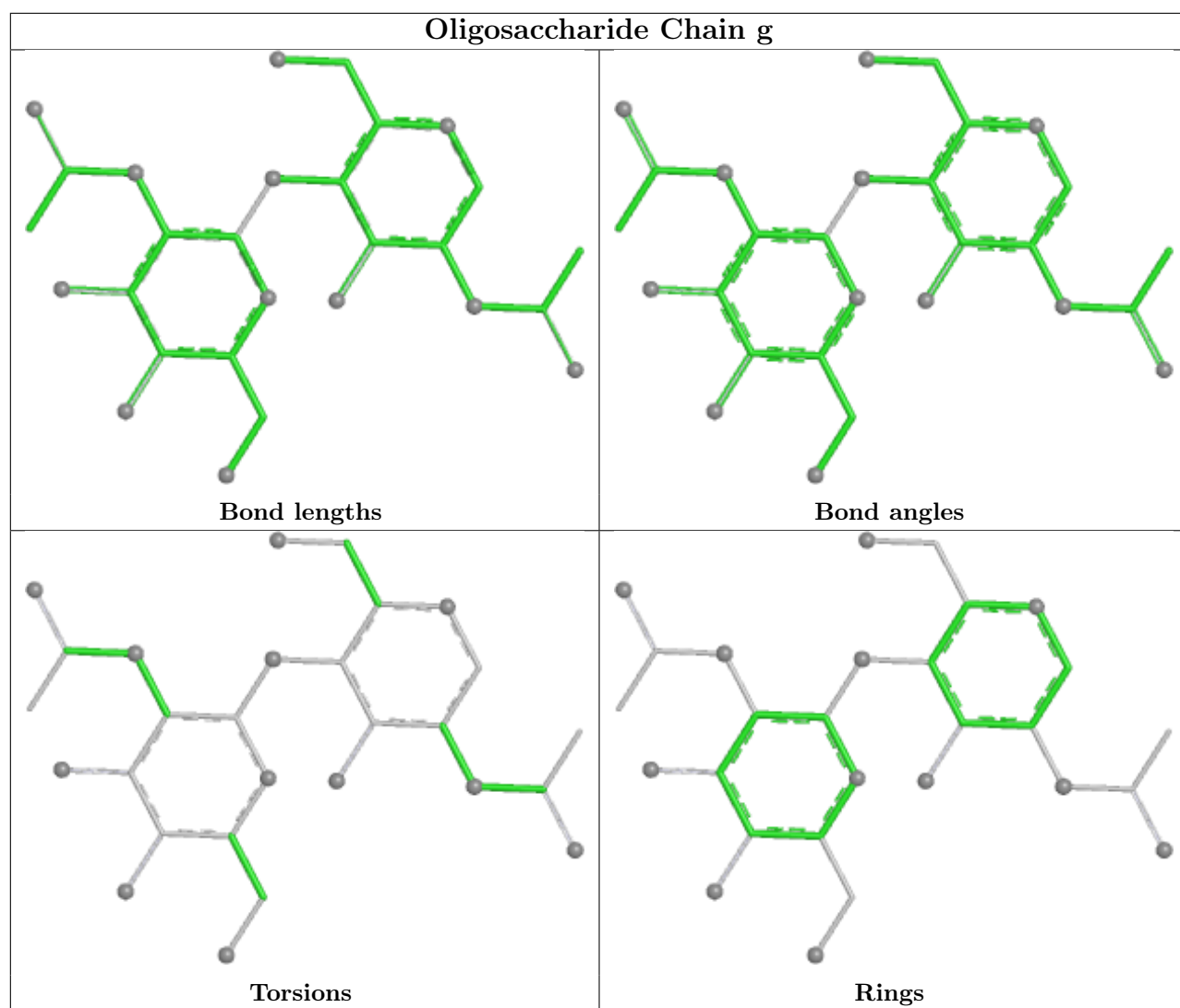


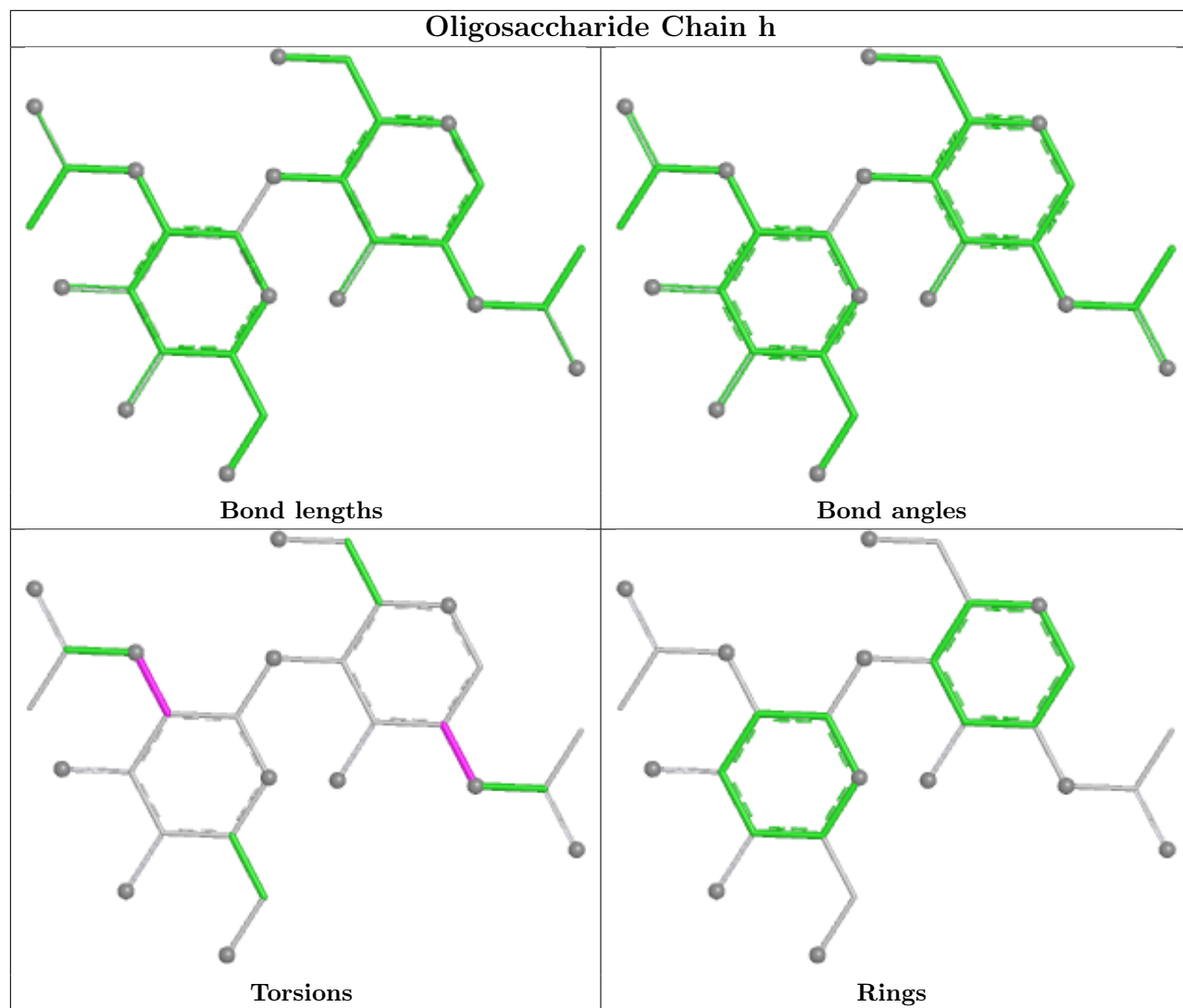


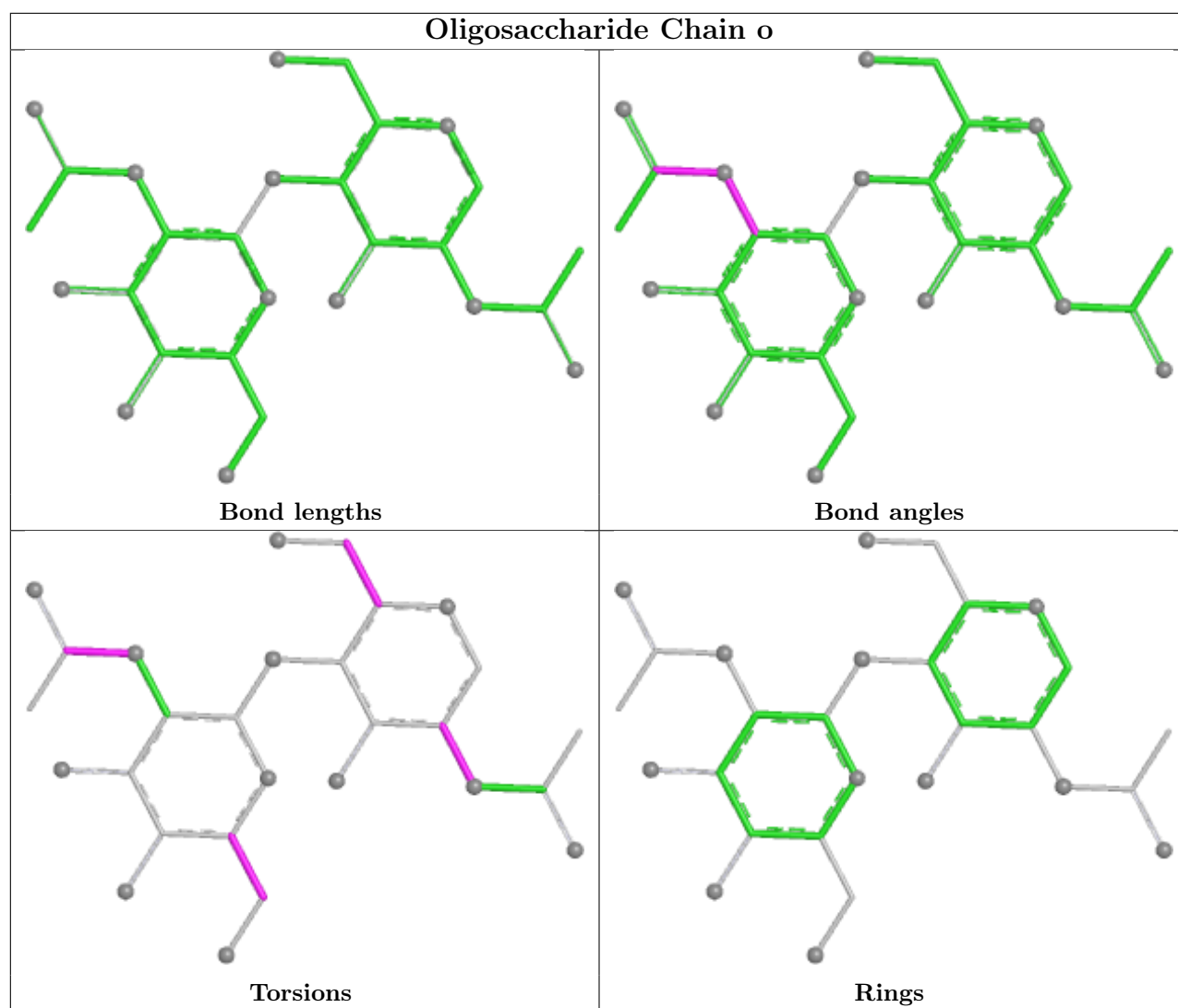


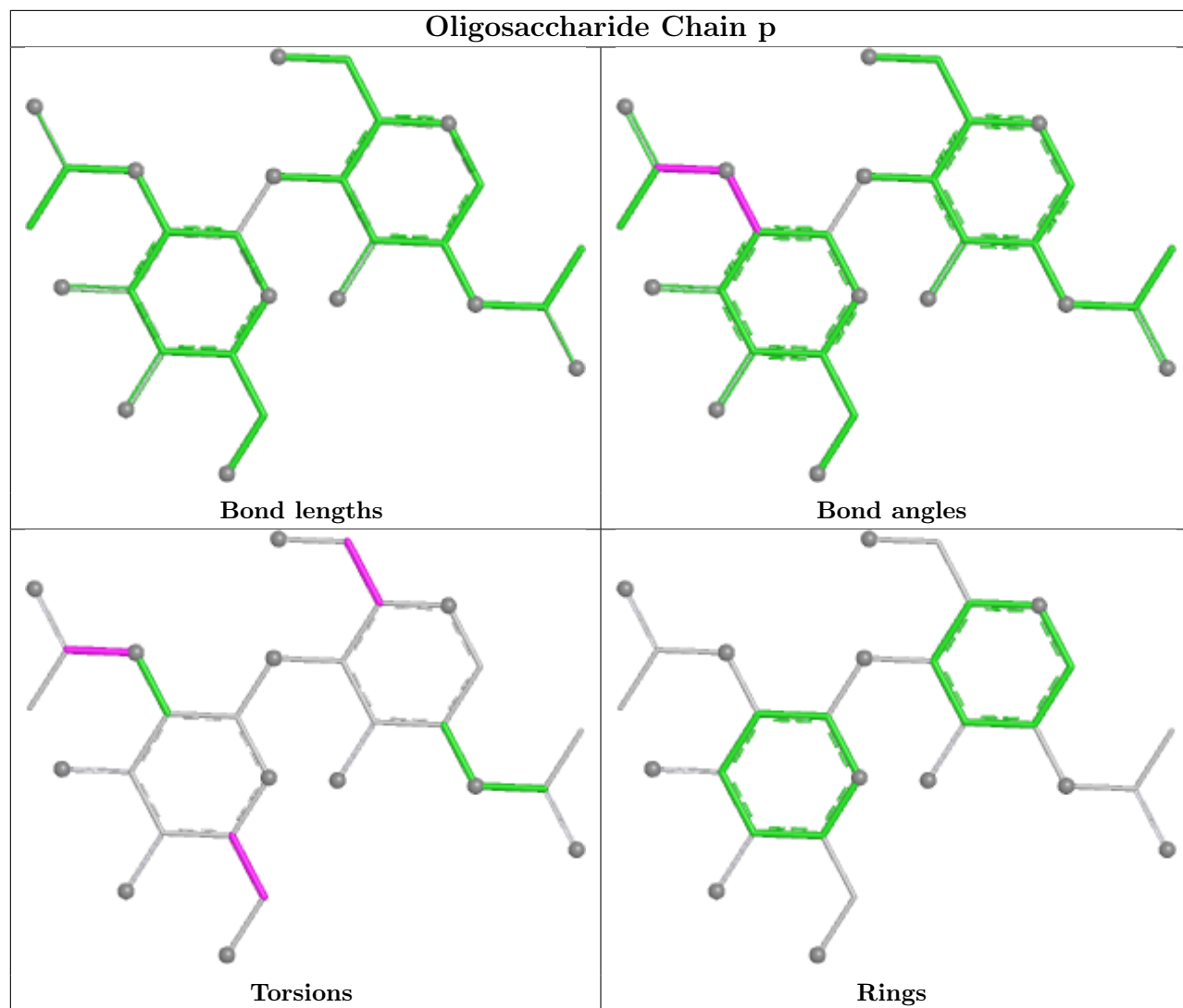


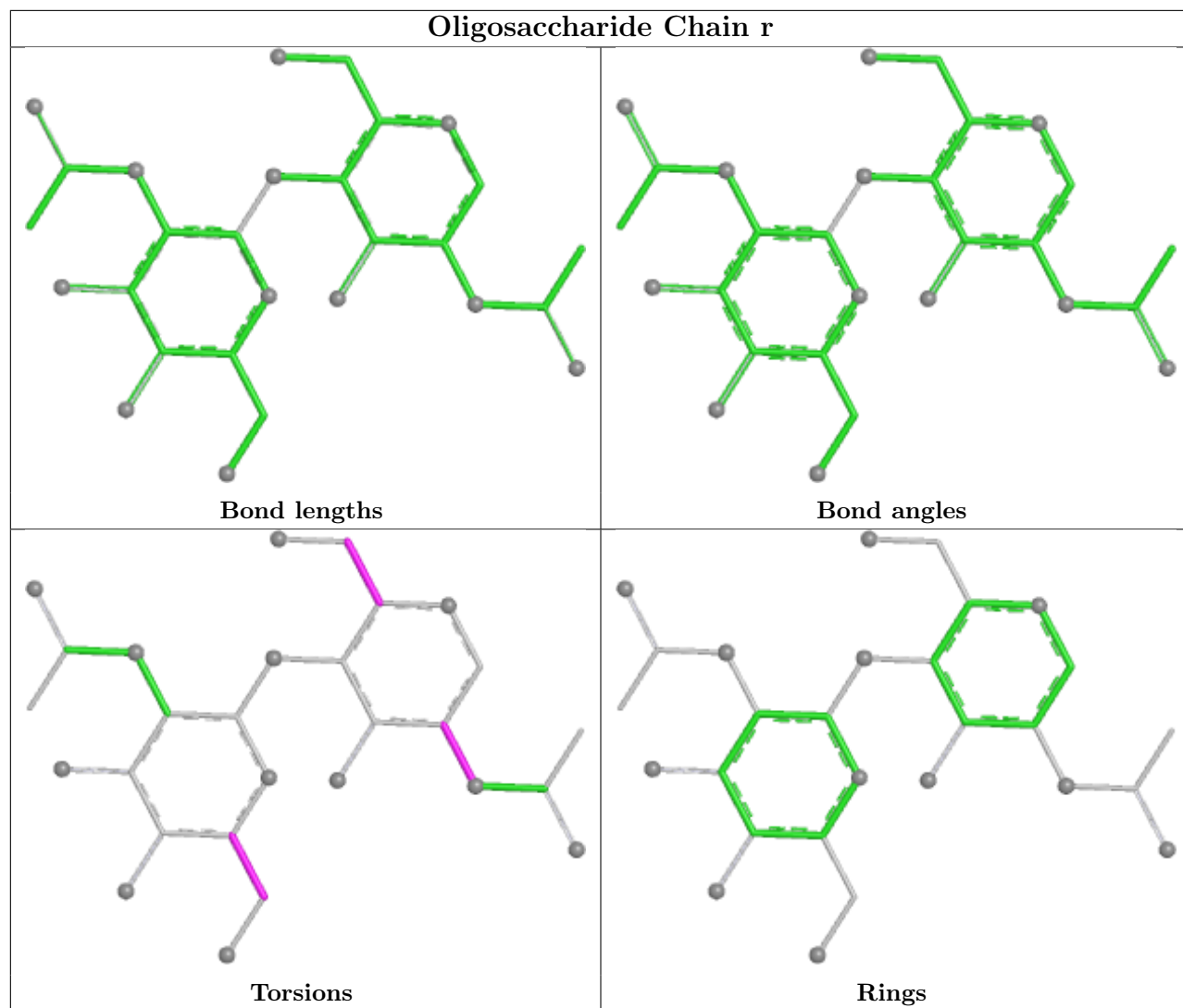


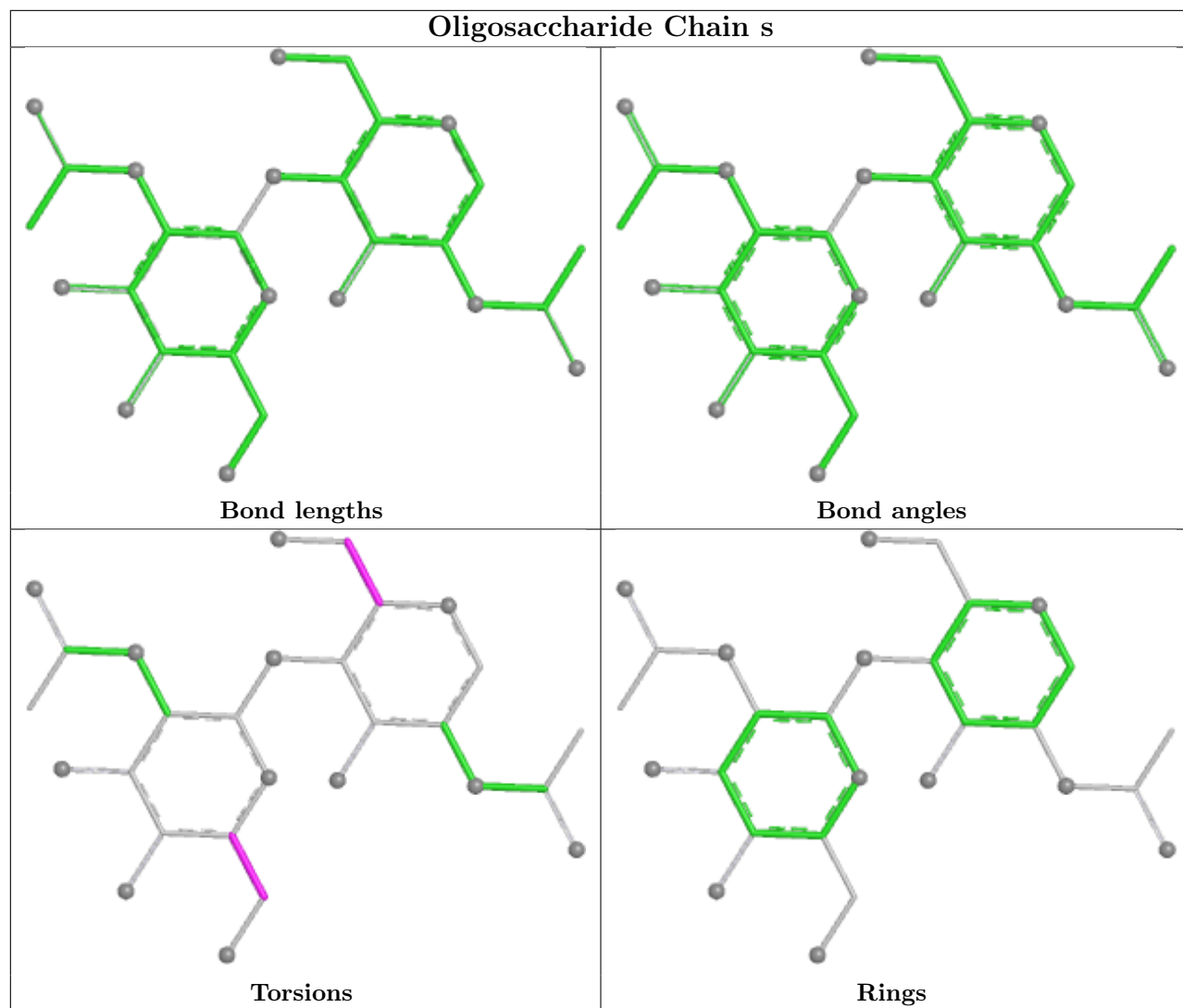


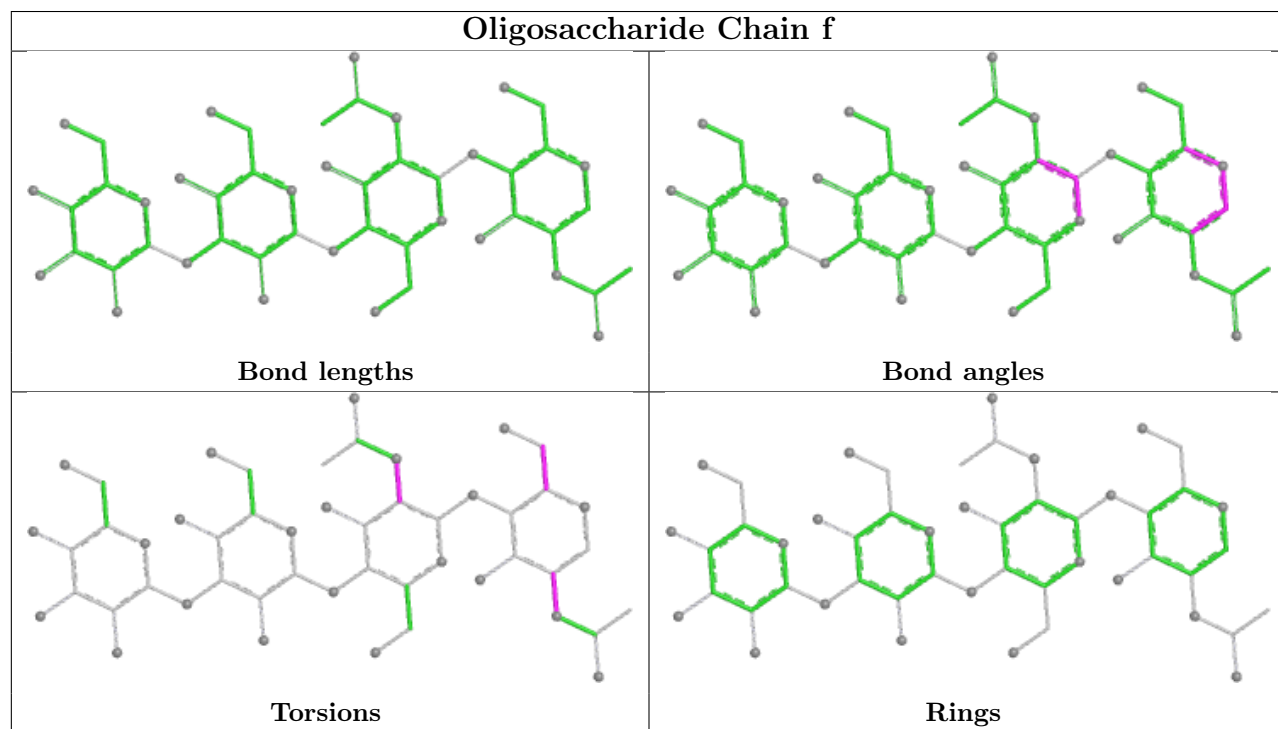
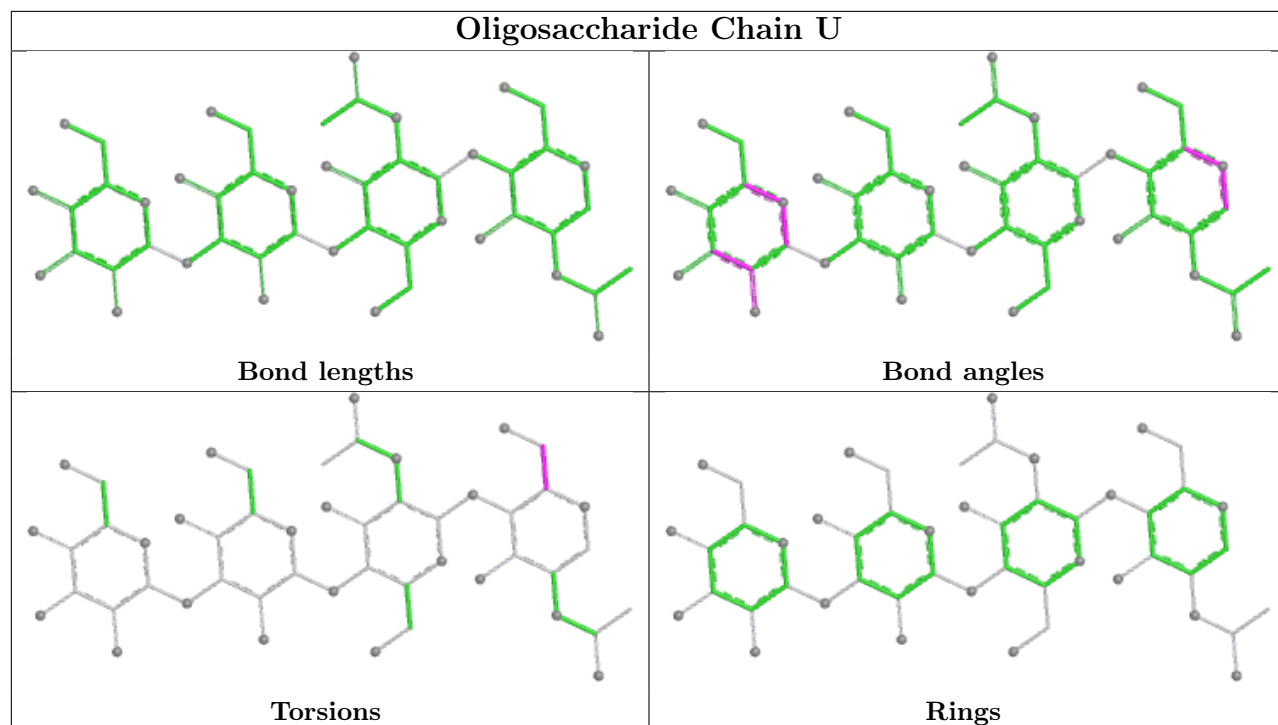


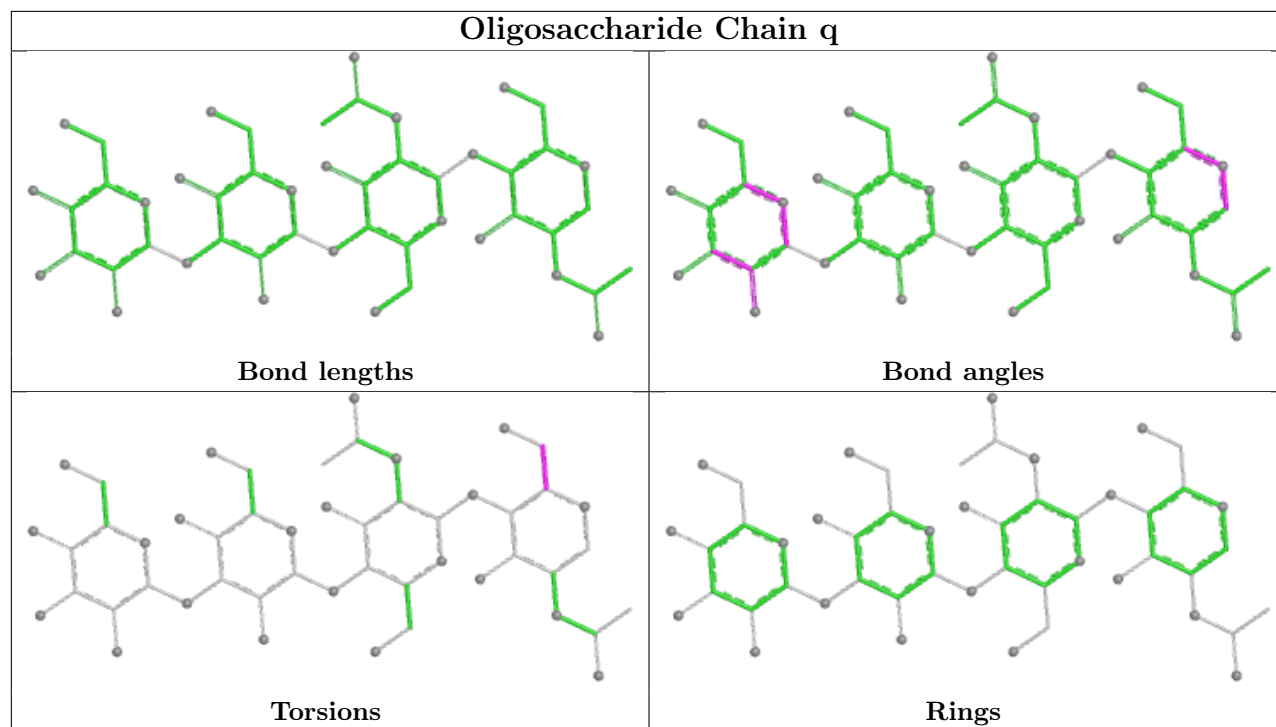


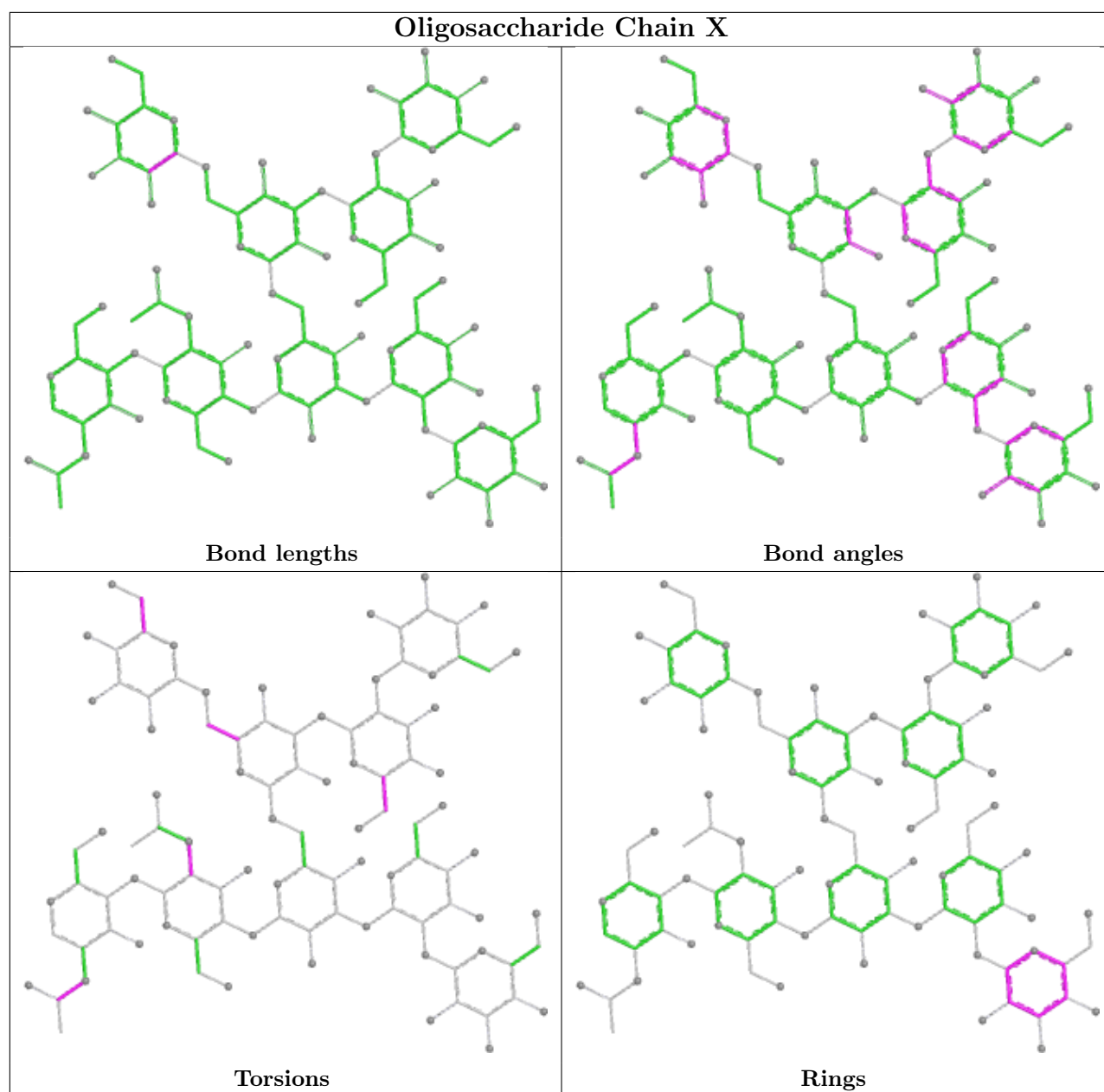


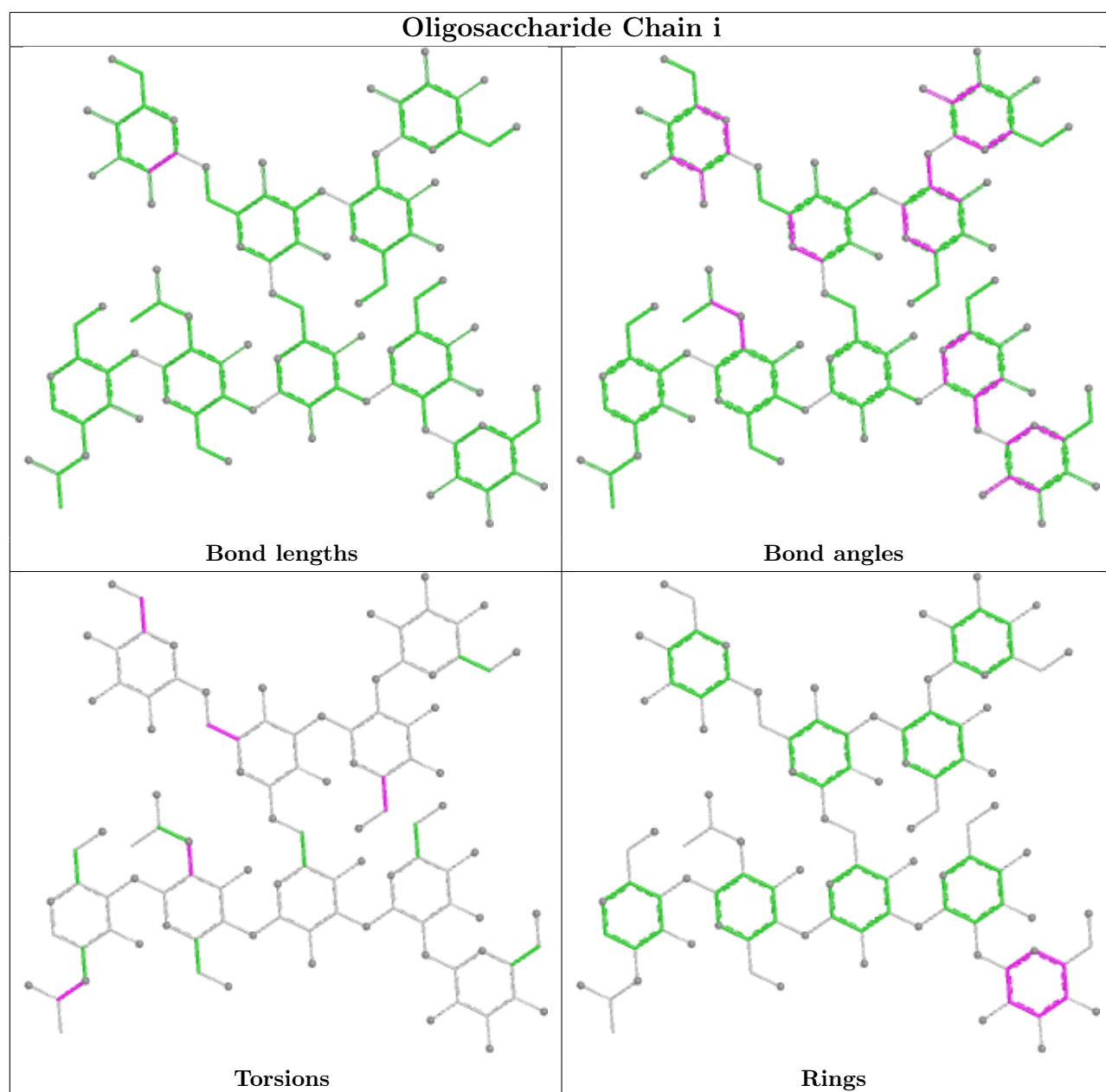


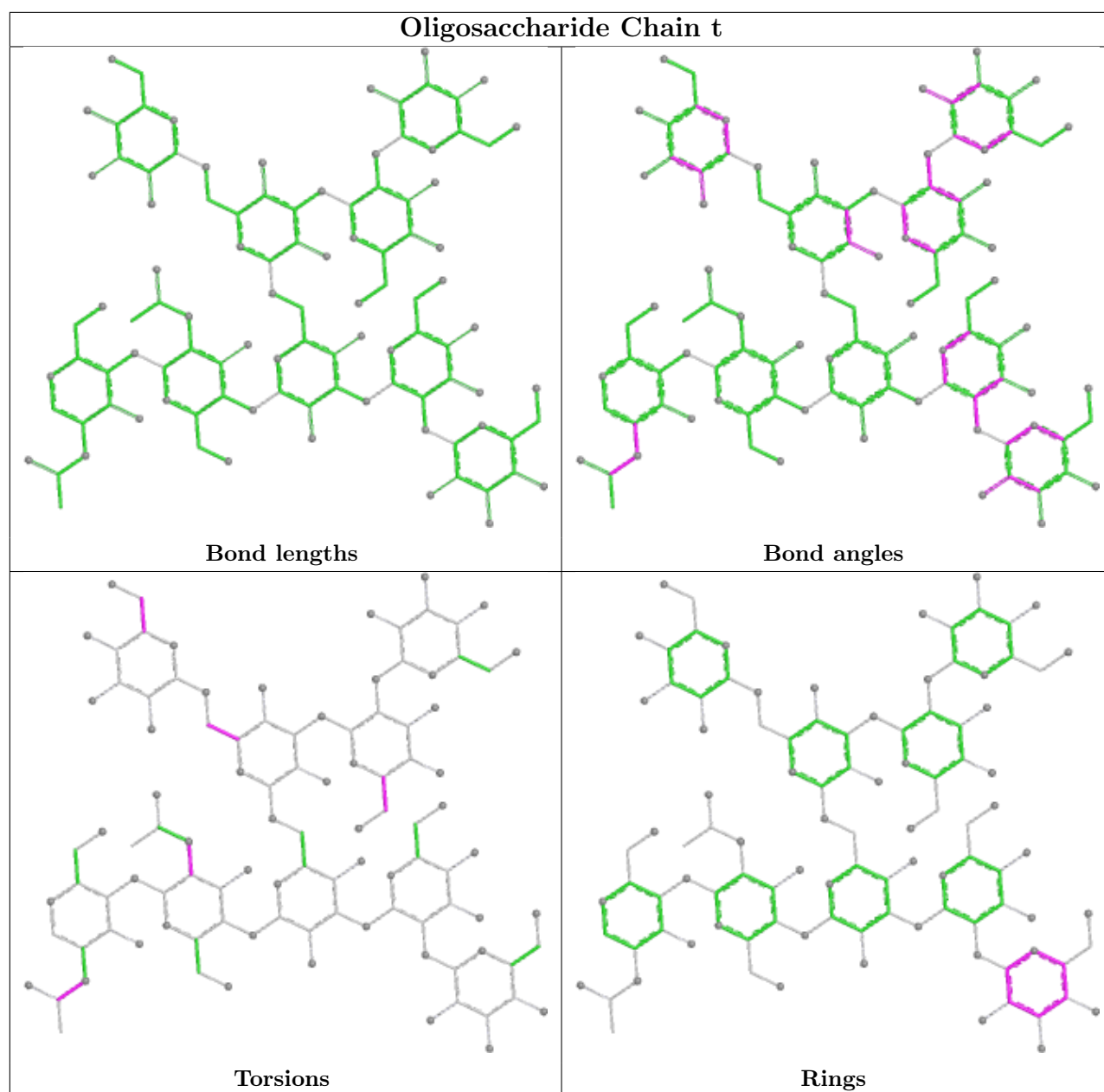


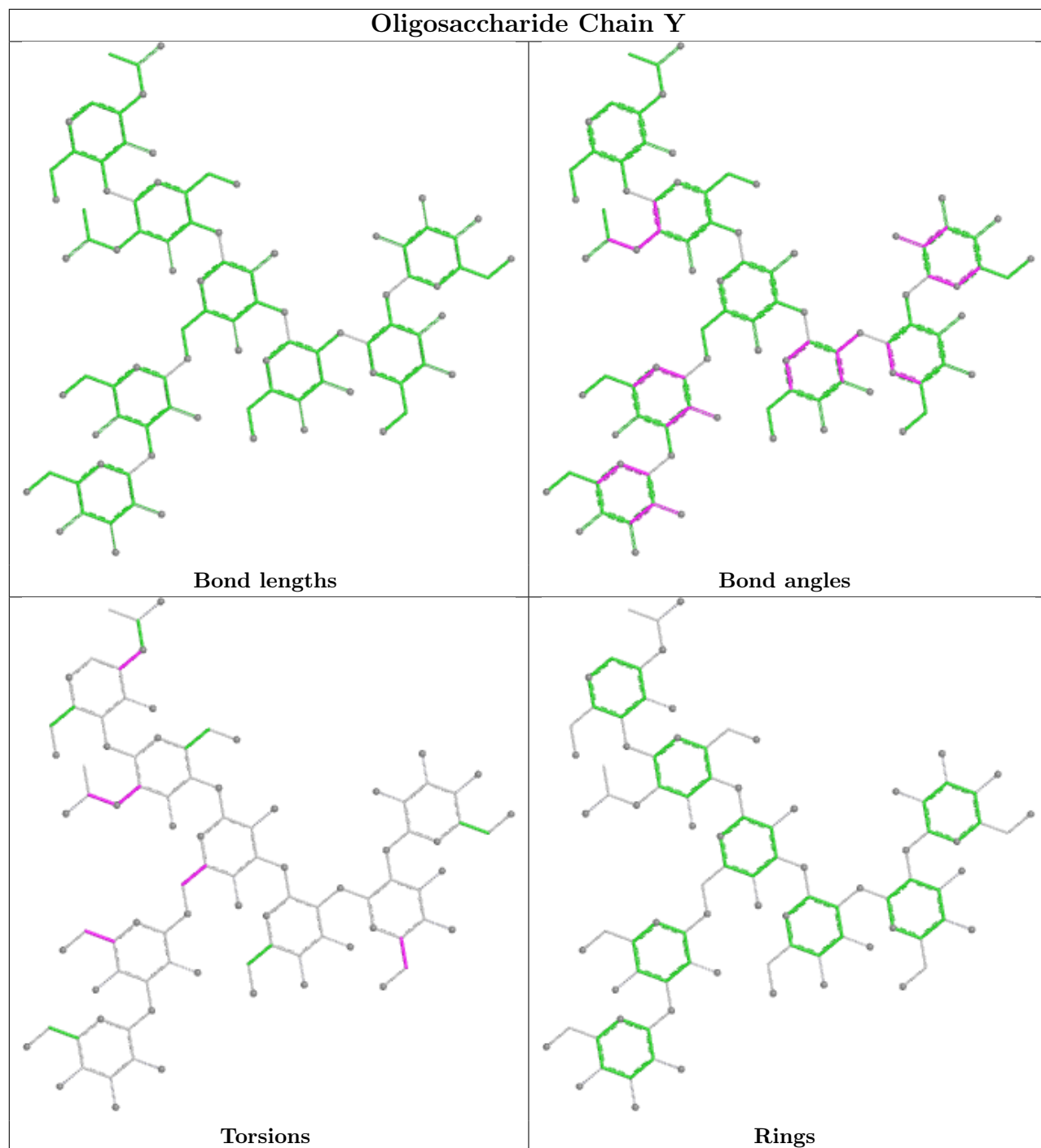


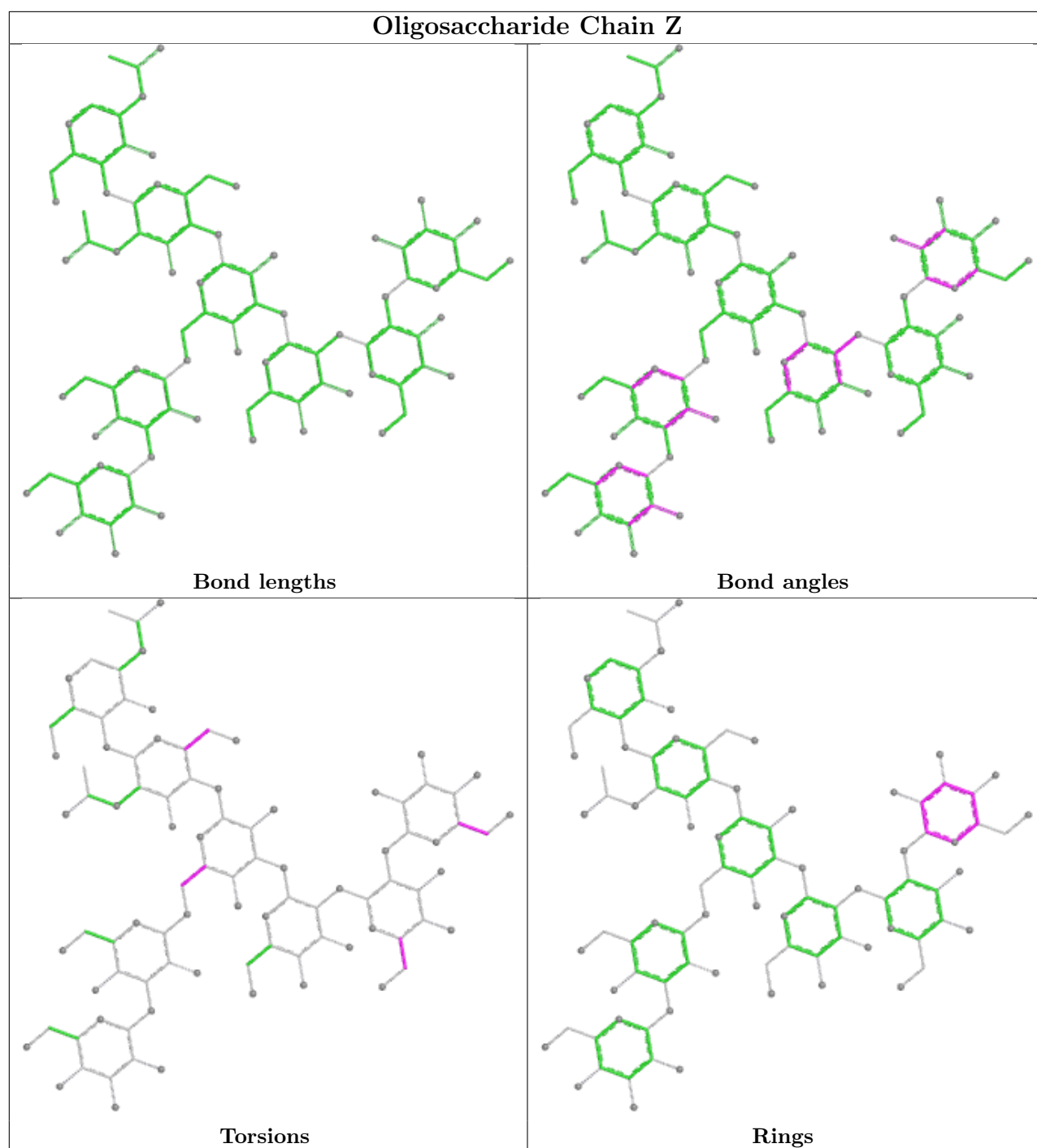


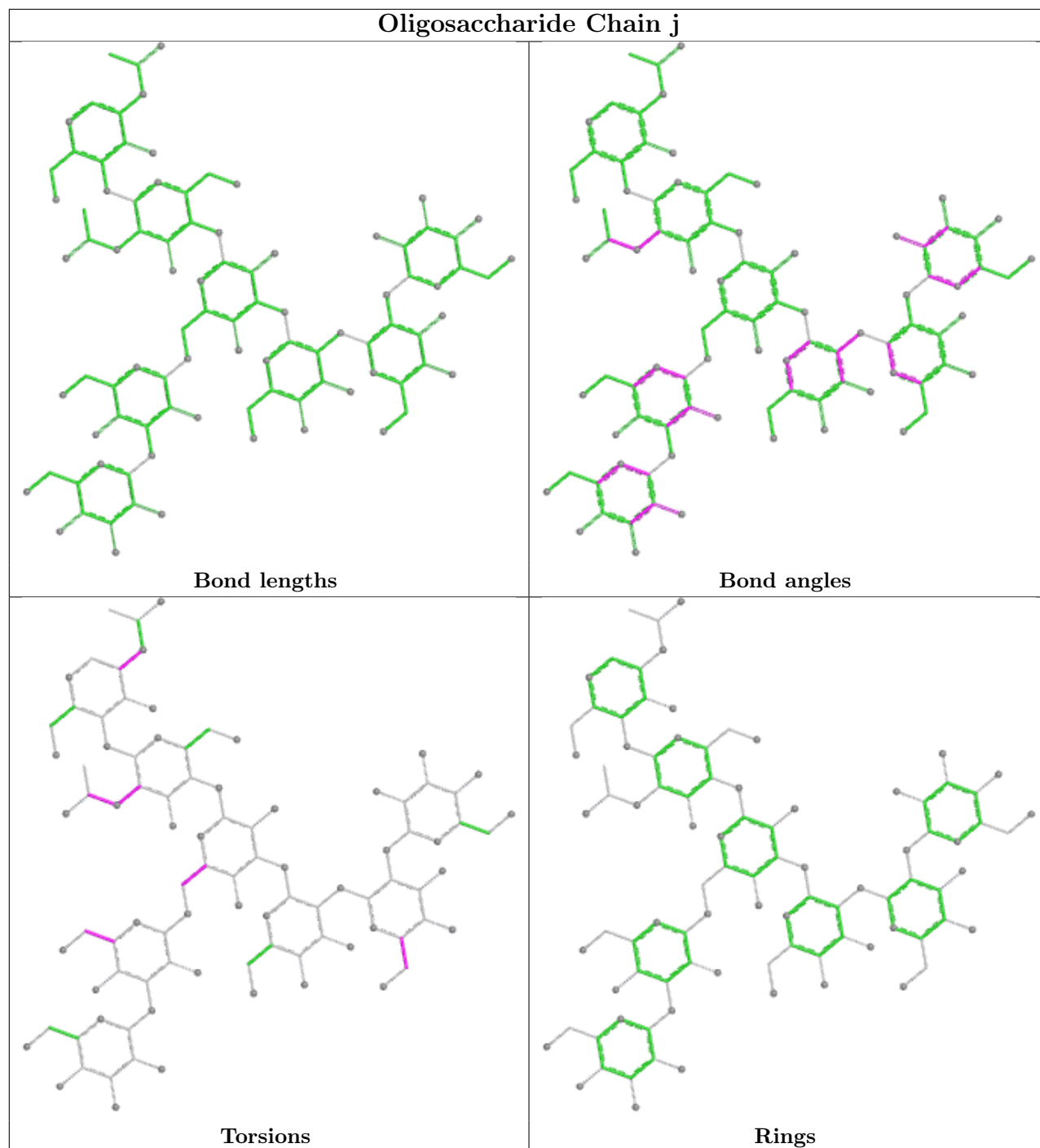


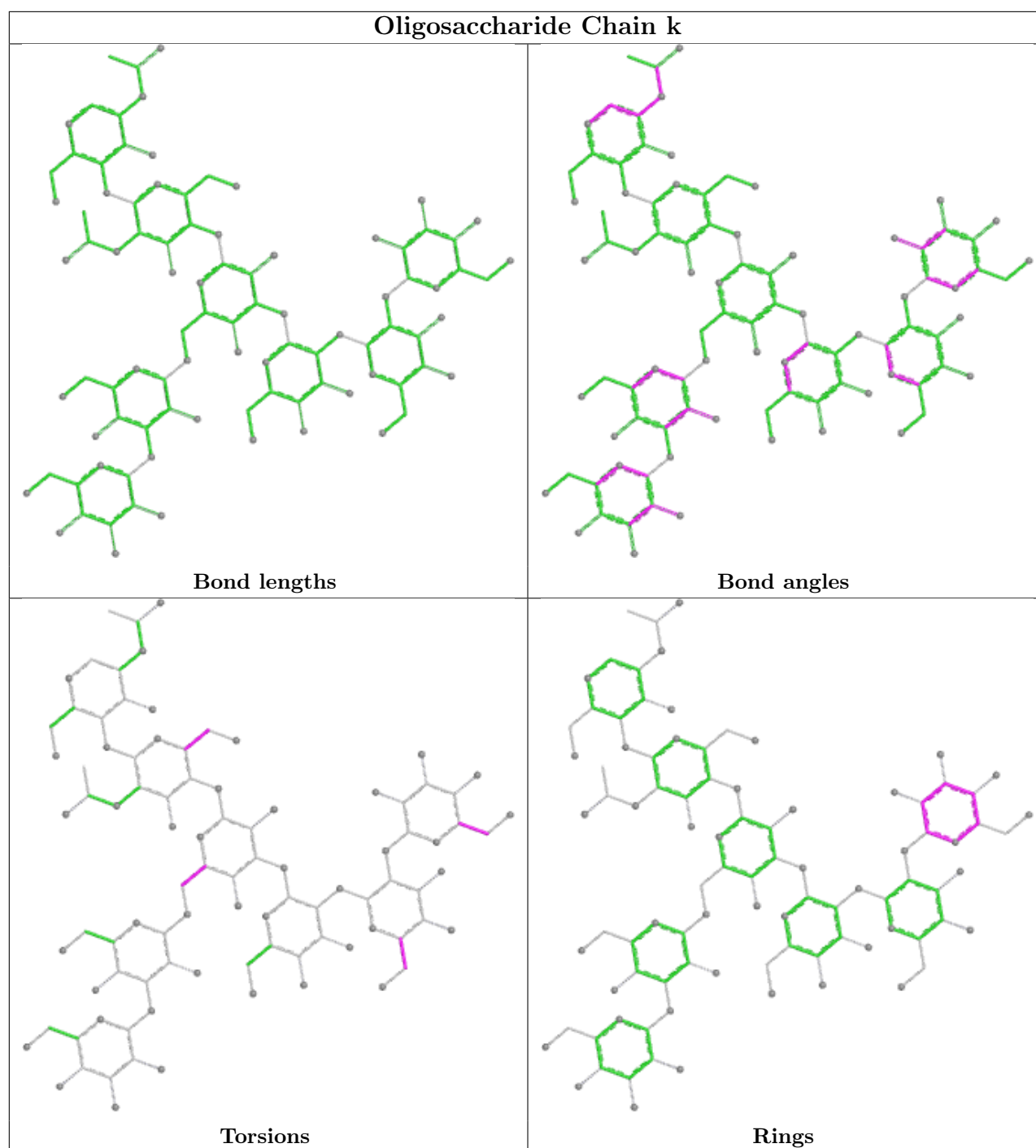


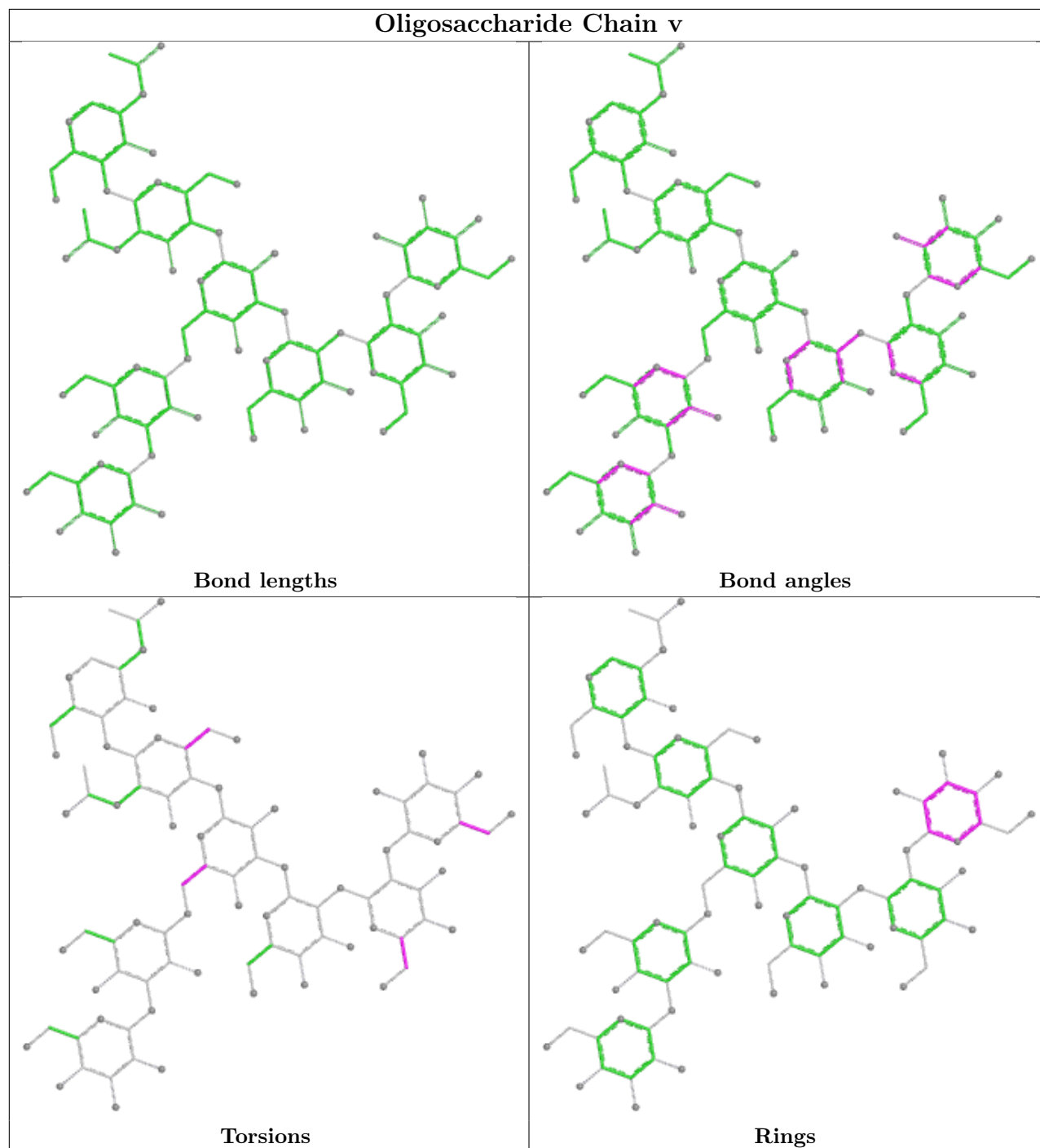


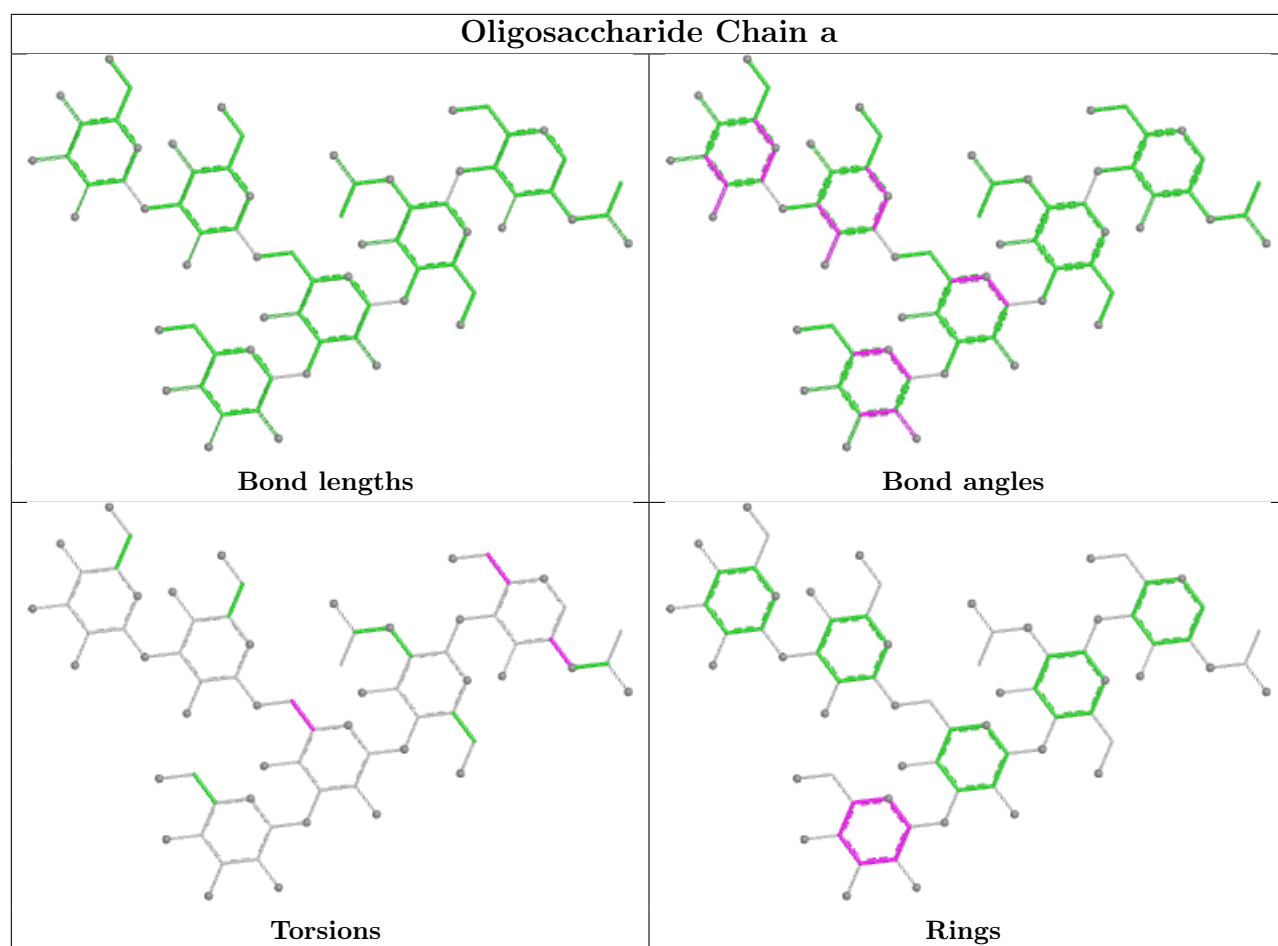


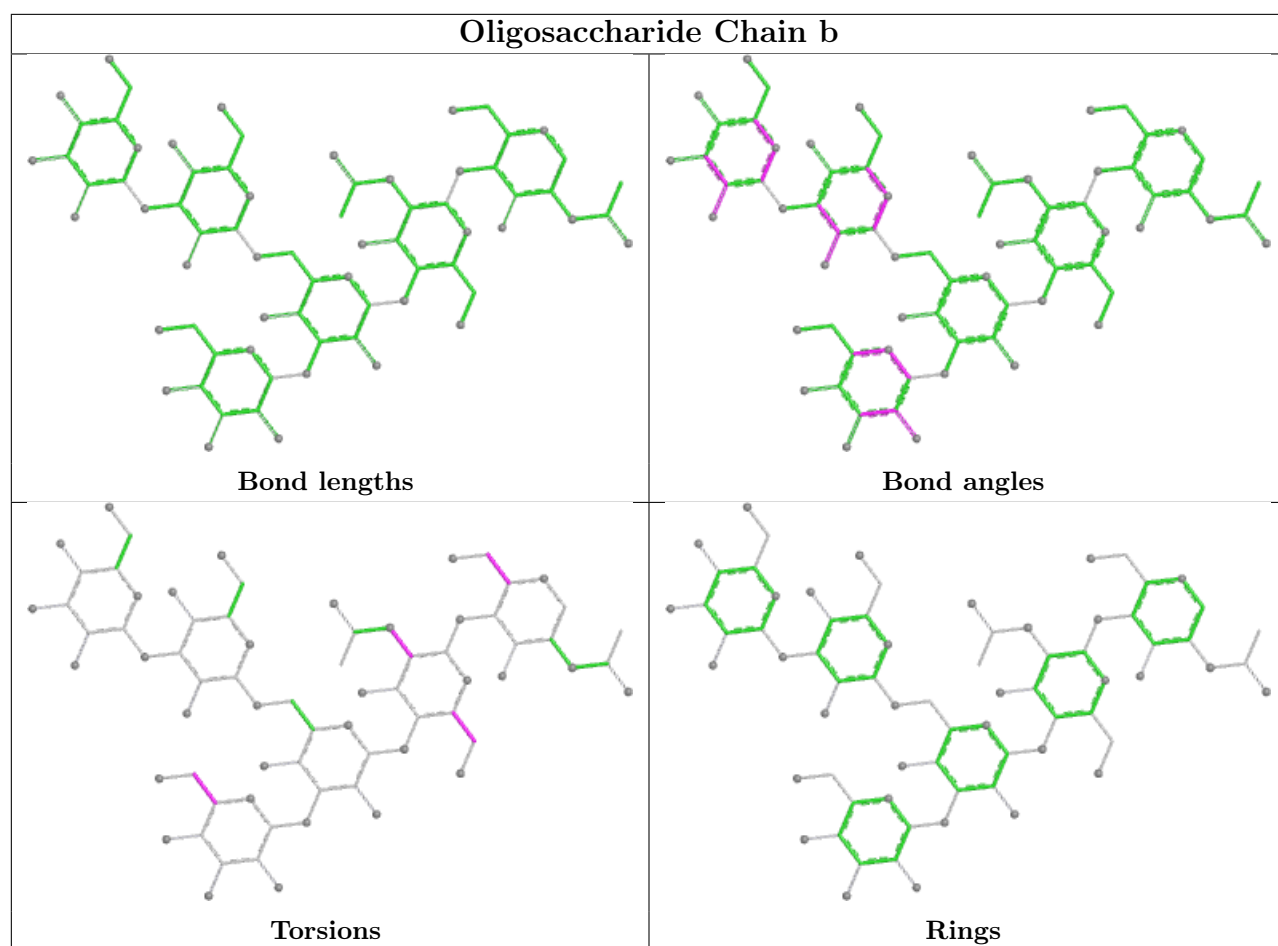


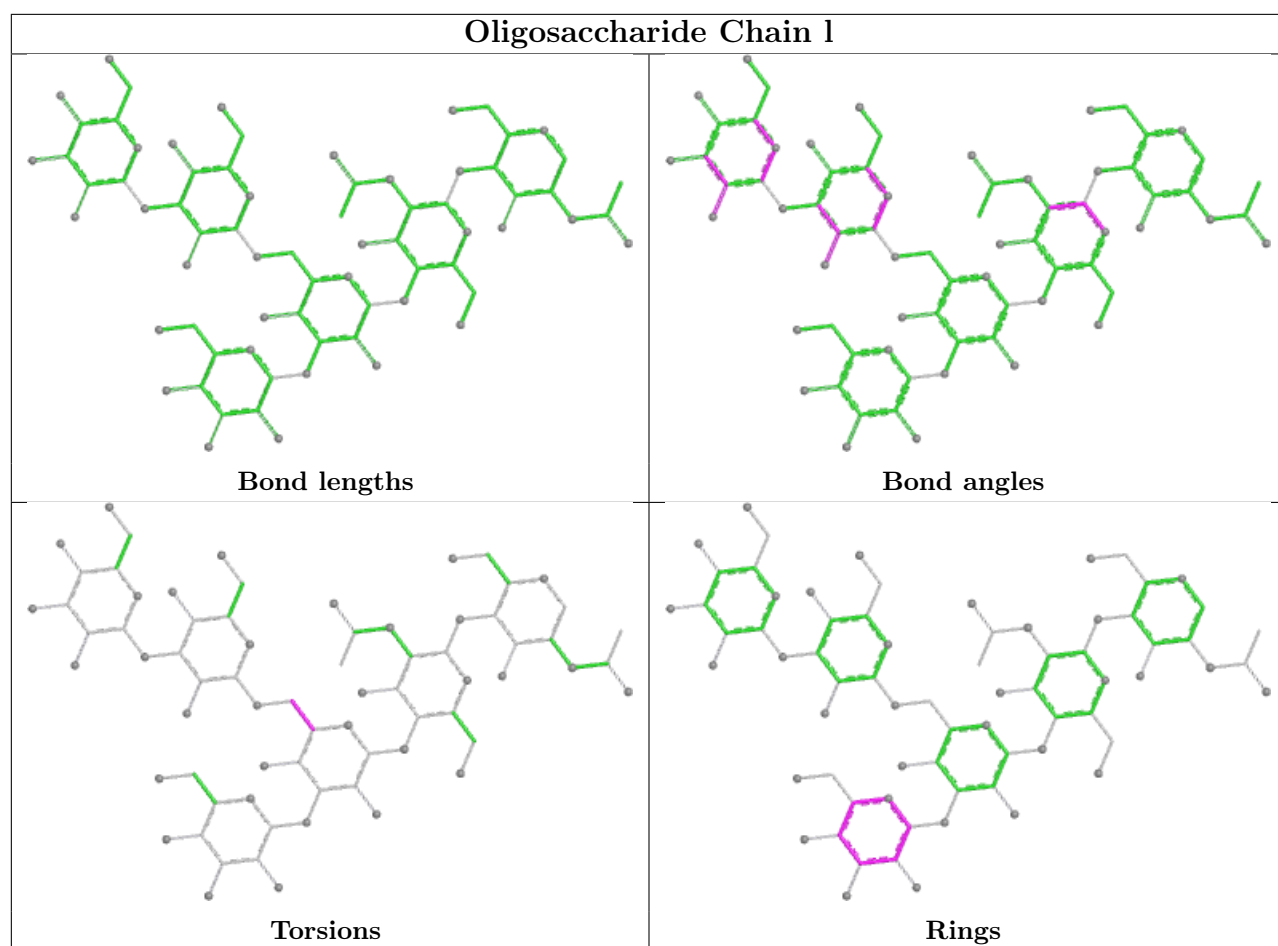


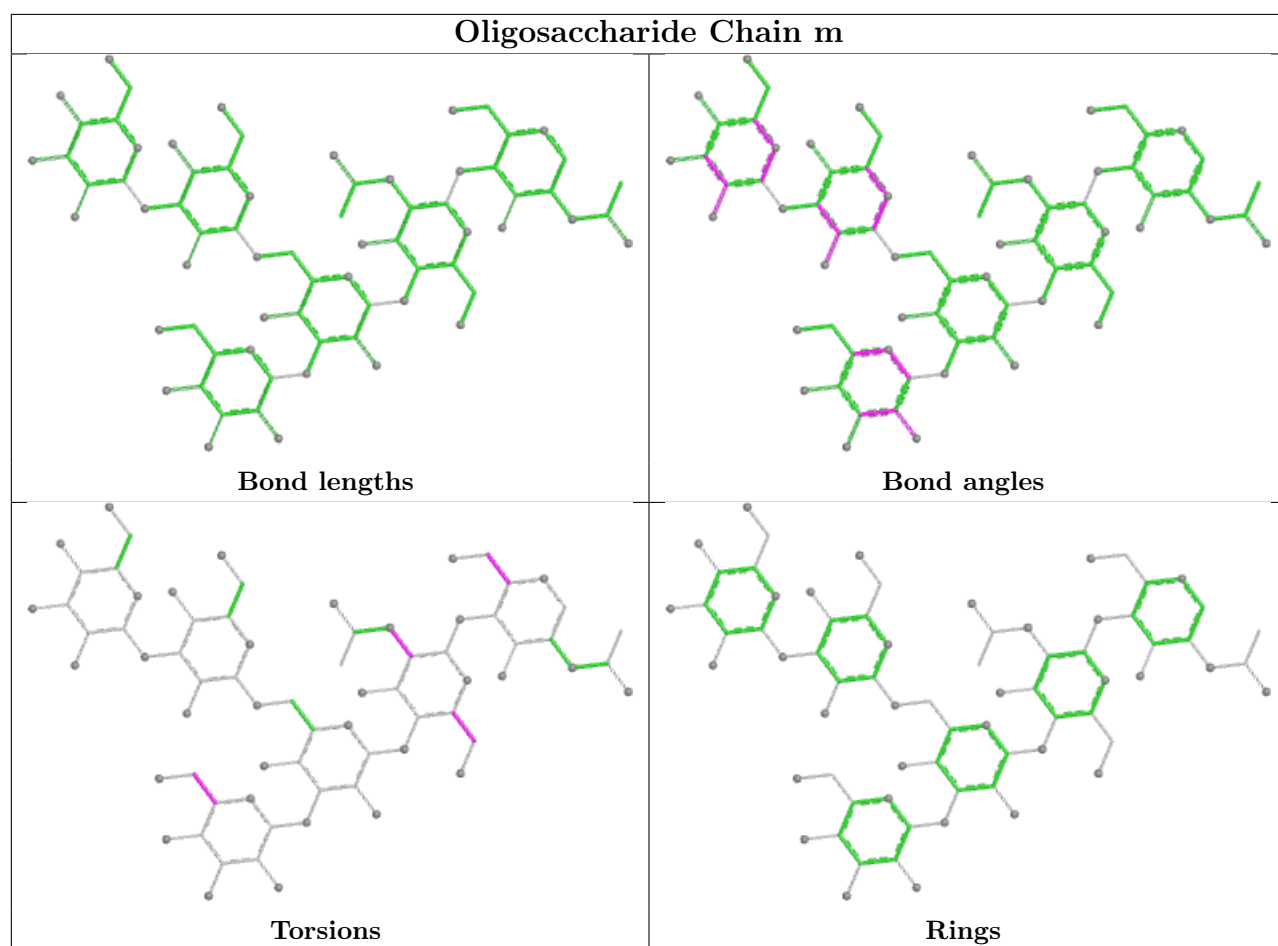


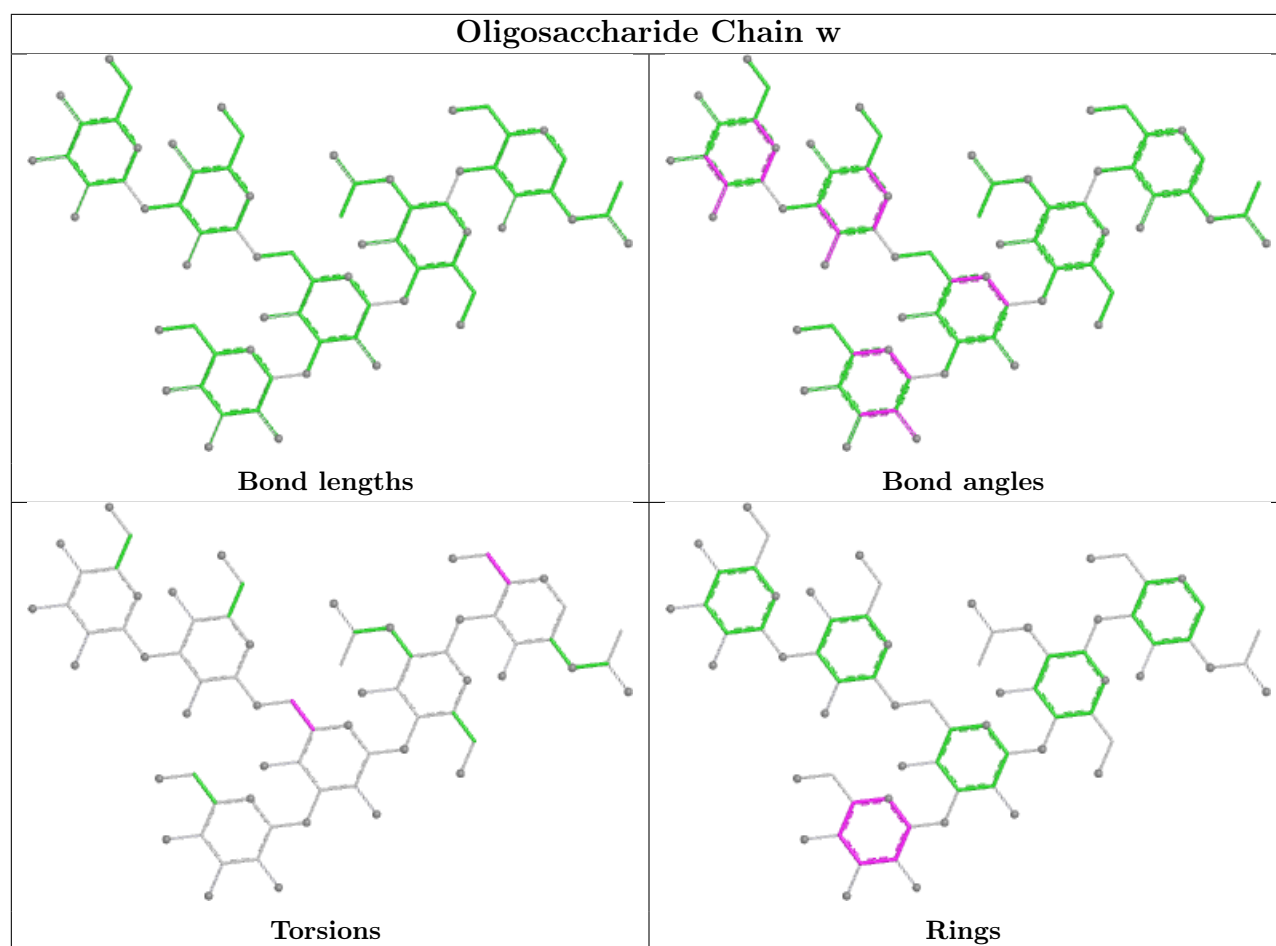


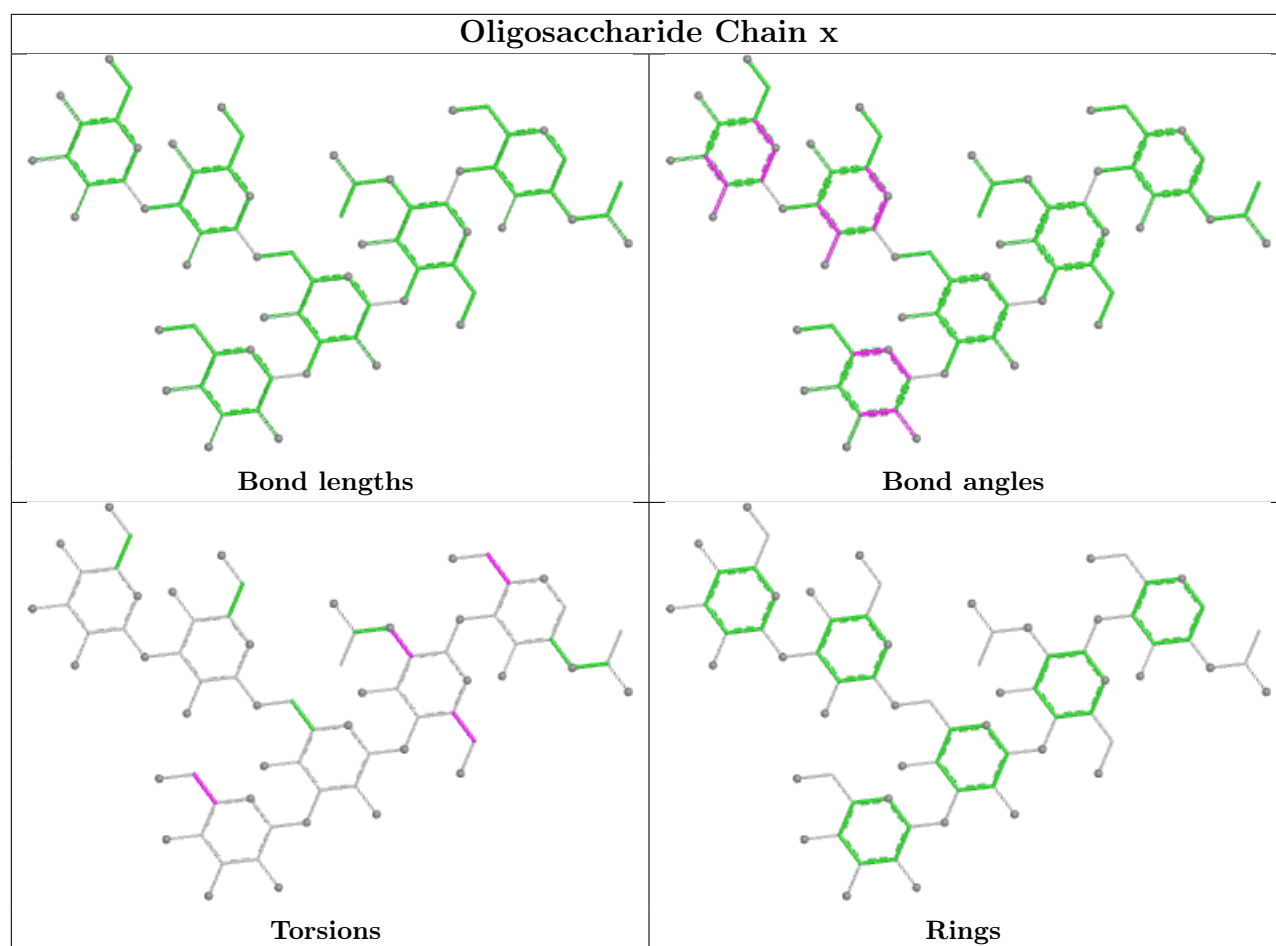


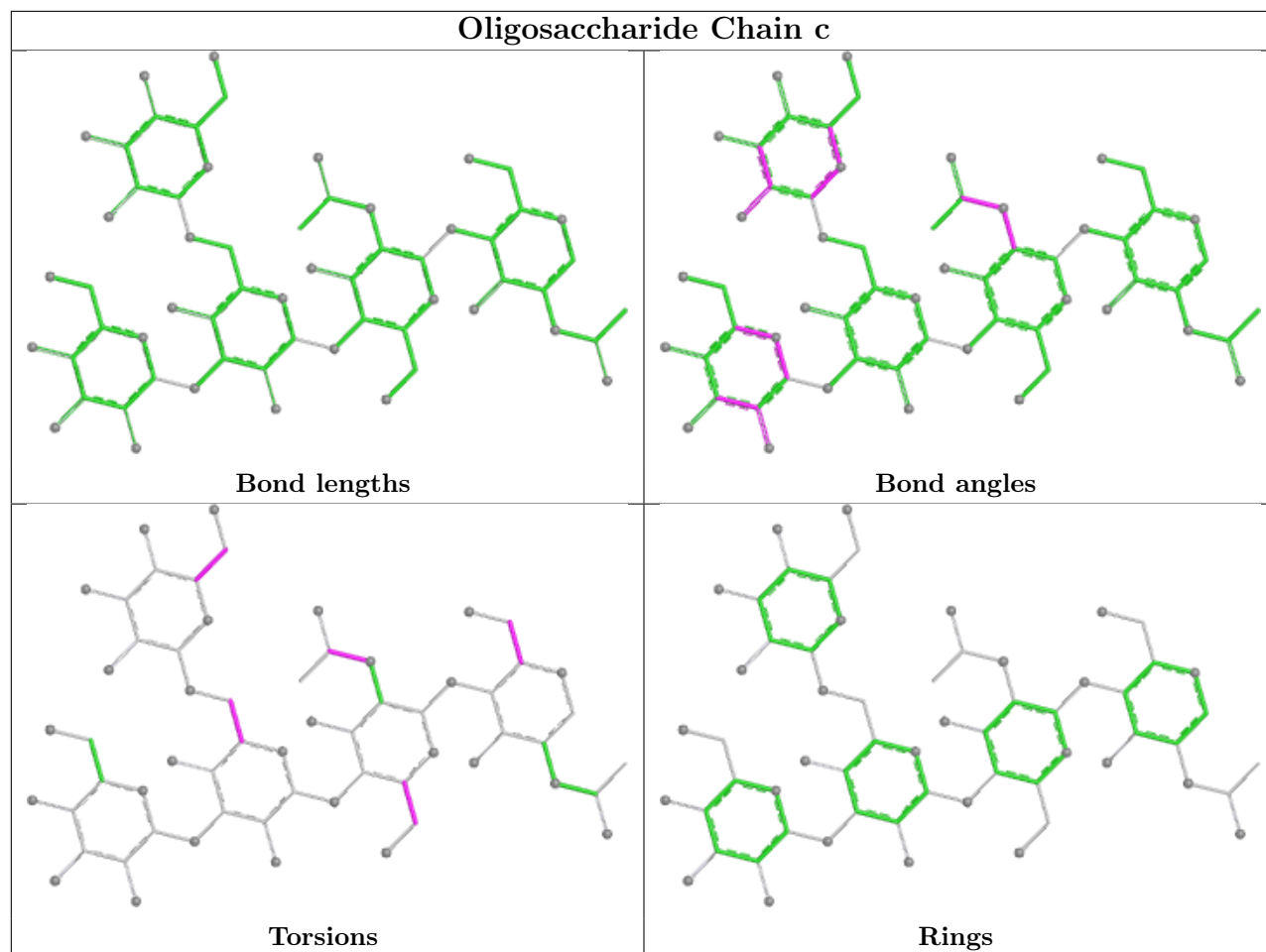


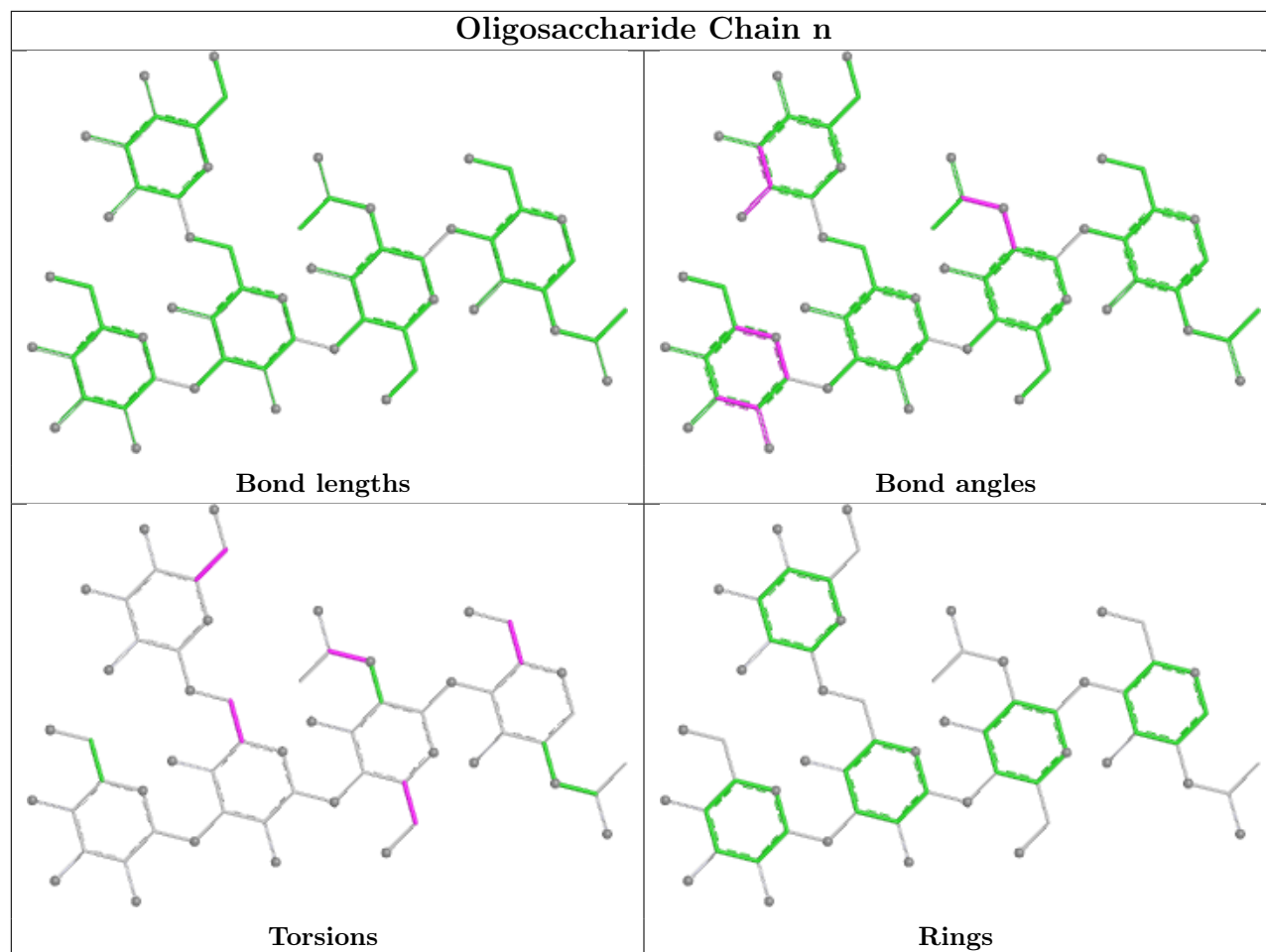


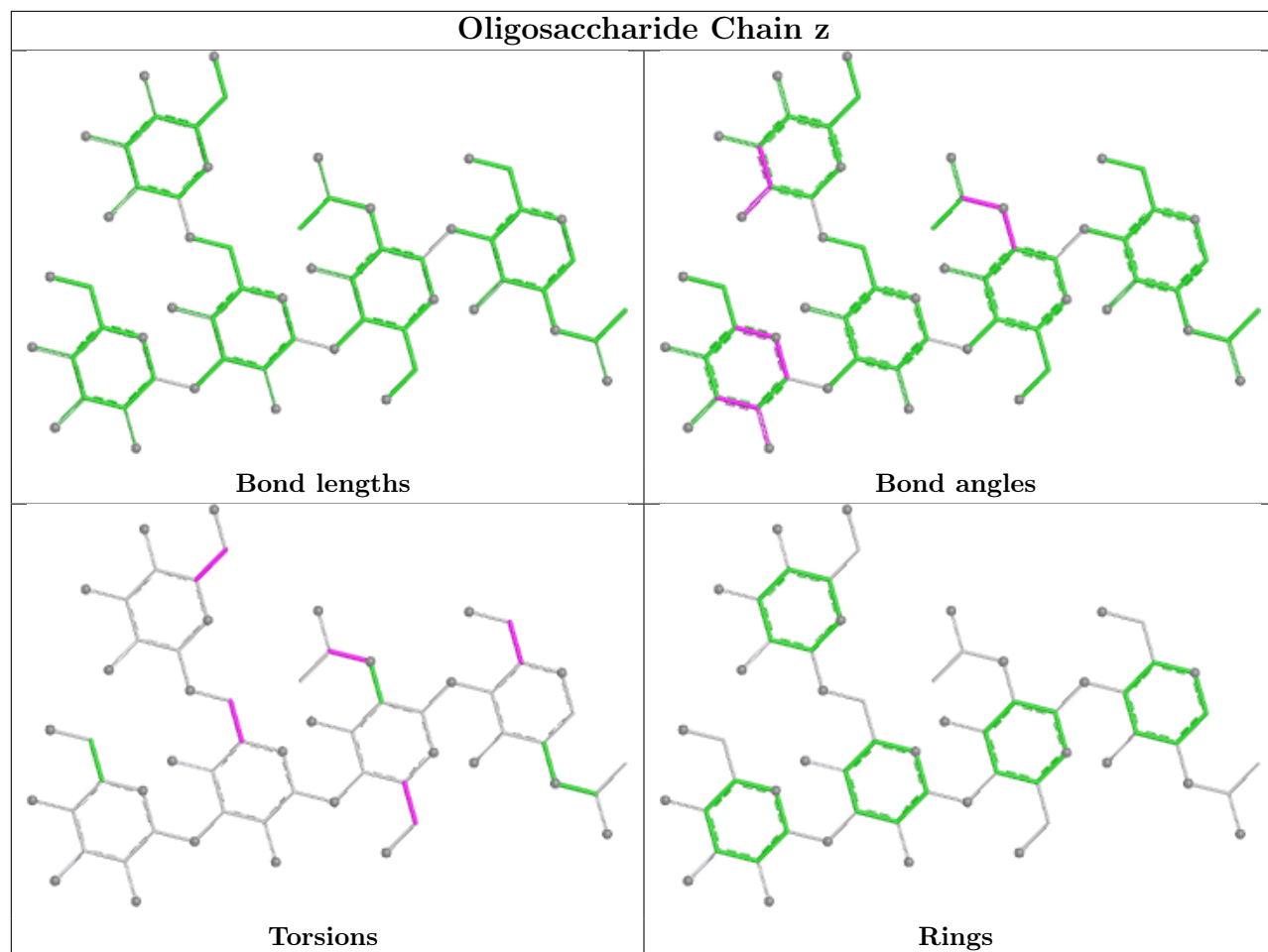


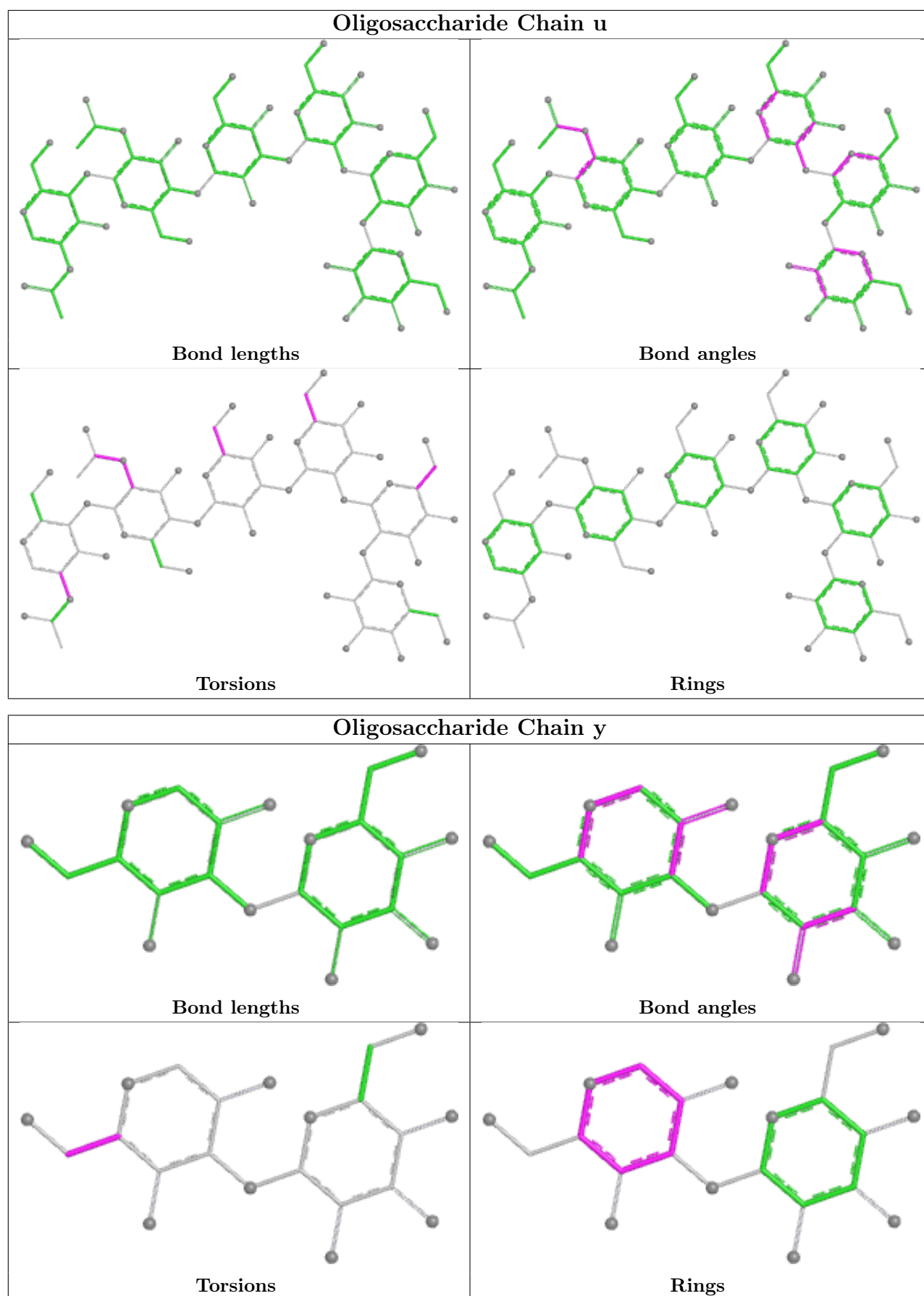












5.6 Ligand geometry

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
13	NAG	C	603	1	14,14,15	0.25	0	17,19,21	0.42	0
13	NAG	A	602	1	14,14,15	0.22	0	17,19,21	0.84	1 (5%)
13	NAG	C	605	1	14,14,15	0.79	1 (7%)	17,19,21	0.86	1 (5%)
13	NAG	C	604	1	14,14,15	0.36	0	17,19,21	1.41	2 (11%)
13	NAG	E	605	1	14,14,15	0.82	1 (7%)	17,19,21	0.85	1 (5%)
13	NAG	A	601	1	14,14,15	0.26	0	17,19,21	0.43	0
13	NAG	E	603	1	14,14,15	0.39	0	17,19,21	0.50	0
13	NAG	A	603	1	14,14,15	0.22	0	17,19,21	0.43	0
13	NAG	E	602	1	14,14,15	0.40	0	17,19,21	0.48	0
13	NAG	E	601	1	14,14,15	0.39	0	17,19,21	0.54	0
13	NAG	E	604	1	14,14,15	0.39	0	17,19,21	1.65	1 (5%)
13	NAG	C	601	1	14,14,15	0.28	0	17,19,21	0.44	0
13	NAG	A	605	1	14,14,15	0.78	1 (7%)	17,19,21	0.87	1 (5%)
13	NAG	A	604	1	14,14,15	0.32	0	17,19,21	1.41	2 (11%)
13	NAG	C	602	1	14,14,15	0.21	0	17,19,21	0.84	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	C	603	1	-	3/6/23/26	0/1/1/1
13	NAG	A	602	1	-	4/6/23/26	0/1/1/1
13	NAG	C	605	1	-	2/6/23/26	0/1/1/1
13	NAG	C	604	1	-	6/6/23/26	0/1/1/1
13	NAG	E	605	1	-	2/6/23/26	0/1/1/1
13	NAG	A	601	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	E	603	1	-	1/6/23/26	0/1/1/1
13	NAG	A	603	1	-	3/6/23/26	0/1/1/1
13	NAG	E	602	1	-	3/6/23/26	0/1/1/1
13	NAG	E	601	1	-	0/6/23/26	0/1/1/1
13	NAG	E	604	1	-	4/6/23/26	0/1/1/1
13	NAG	C	601	1	-	0/6/23/26	0/1/1/1
13	NAG	A	605	1	-	2/6/23/26	0/1/1/1
13	NAG	A	604	1	-	6/6/23/26	0/1/1/1
13	NAG	C	602	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	605	NAG	C1-C2	2.51	1.55	1.52
13	C	605	NAG	C1-C2	2.42	1.55	1.52
13	A	605	NAG	C1-C2	2.36	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	604	NAG	C2-N2-C7	6.39	131.46	122.90
13	C	604	NAG	C2-N2-C7	4.80	129.33	122.90
13	A	604	NAG	C2-N2-C7	4.76	129.28	122.90
13	A	605	NAG	C1-O5-C5	3.22	116.50	112.19
13	C	605	NAG	C1-O5-C5	3.16	116.42	112.19
13	E	605	NAG	C1-O5-C5	3.10	116.33	112.19
13	A	602	NAG	C2-N2-C7	2.76	126.59	122.90
13	C	602	NAG	C2-N2-C7	2.75	126.58	122.90
13	A	604	NAG	C1-C2-N2	2.41	114.23	110.43
13	C	604	NAG	C1-C2-N2	2.39	114.20	110.43

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	E	605	NAG	O5-C5-C6-O6
13	A	605	NAG	O5-C5-C6-O6
13	C	602	NAG	C4-C5-C6-O6
13	A	602	NAG	C4-C5-C6-O6
13	C	603	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	C	605	NAG	O5-C5-C6-O6
13	A	603	NAG	O5-C5-C6-O6
13	C	605	NAG	C4-C5-C6-O6
13	A	605	NAG	C4-C5-C6-O6
13	E	605	NAG	C4-C5-C6-O6
13	A	602	NAG	O5-C5-C6-O6
13	C	602	NAG	O5-C5-C6-O6
13	A	604	NAG	O5-C5-C6-O6
13	C	604	NAG	O5-C5-C6-O6
13	C	604	NAG	C4-C5-C6-O6
13	A	603	NAG	C4-C5-C6-O6
13	C	603	NAG	C4-C5-C6-O6
13	C	602	NAG	C8-C7-N2-C2
13	C	602	NAG	O7-C7-N2-C2
13	C	604	NAG	C8-C7-N2-C2
13	C	604	NAG	O7-C7-N2-C2
13	E	602	NAG	C8-C7-N2-C2
13	E	602	NAG	O7-C7-N2-C2
13	E	604	NAG	C8-C7-N2-C2
13	E	604	NAG	O7-C7-N2-C2
13	A	602	NAG	C8-C7-N2-C2
13	A	602	NAG	O7-C7-N2-C2
13	A	604	NAG	C8-C7-N2-C2
13	A	604	NAG	O7-C7-N2-C2
13	A	604	NAG	C4-C5-C6-O6
13	E	602	NAG	O5-C5-C6-O6
13	E	603	NAG	O5-C5-C6-O6
13	E	604	NAG	O5-C5-C6-O6
13	C	604	NAG	C1-C2-N2-C7
13	A	604	NAG	C1-C2-N2-C7
13	E	604	NAG	C3-C2-N2-C7
13	C	603	NAG	C1-C2-N2-C7
13	A	603	NAG	C1-C2-N2-C7
13	C	604	NAG	C3-C2-N2-C7
13	A	604	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

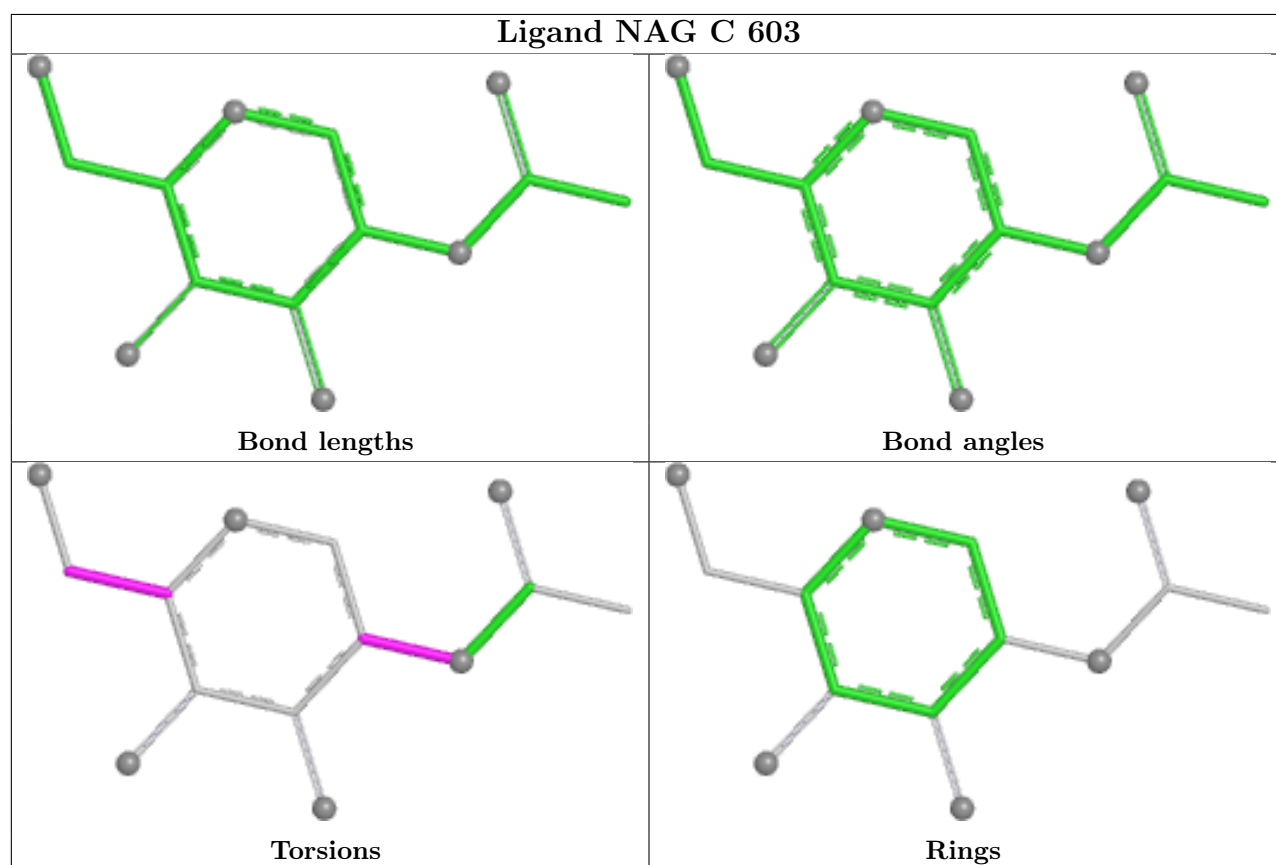
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	605	NAG	1	0
13	C	604	NAG	1	0

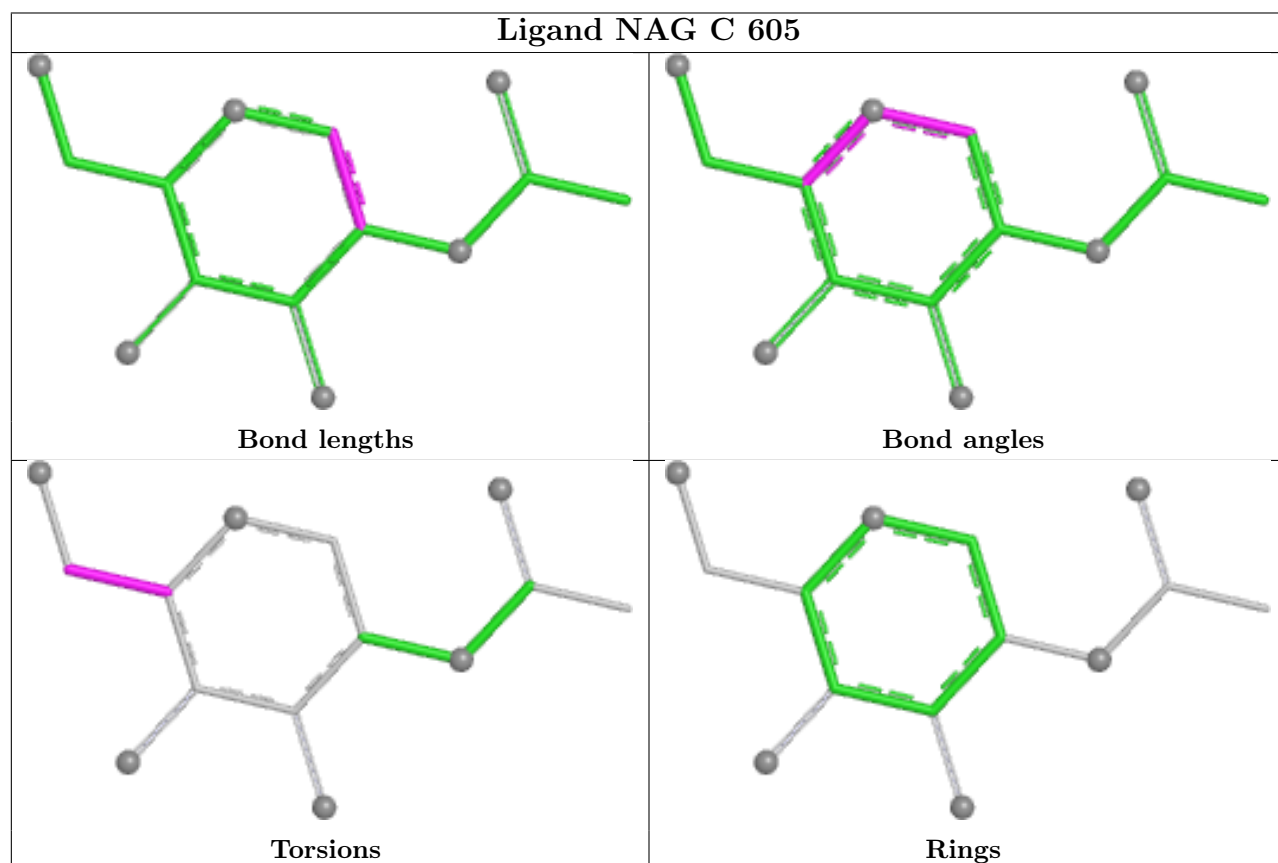
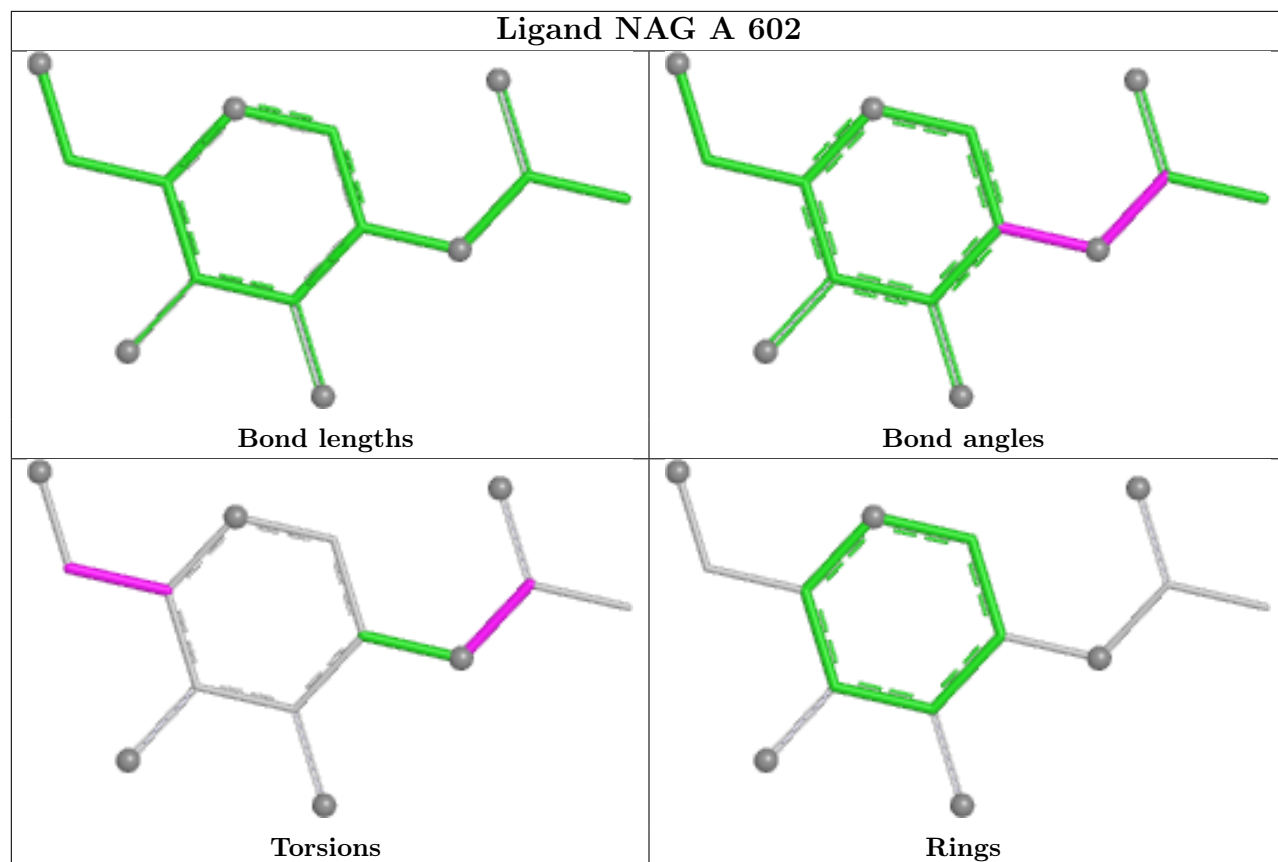
Continued on next page...

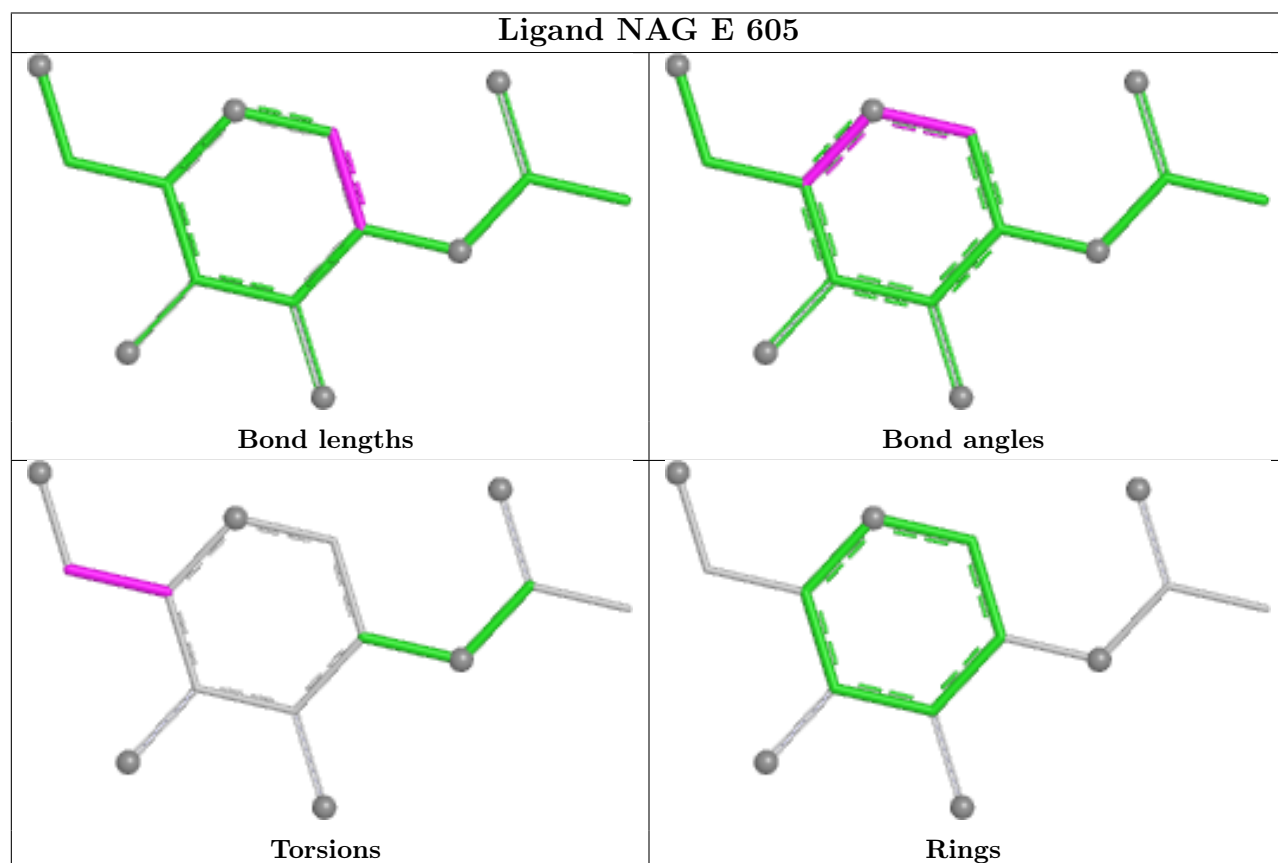
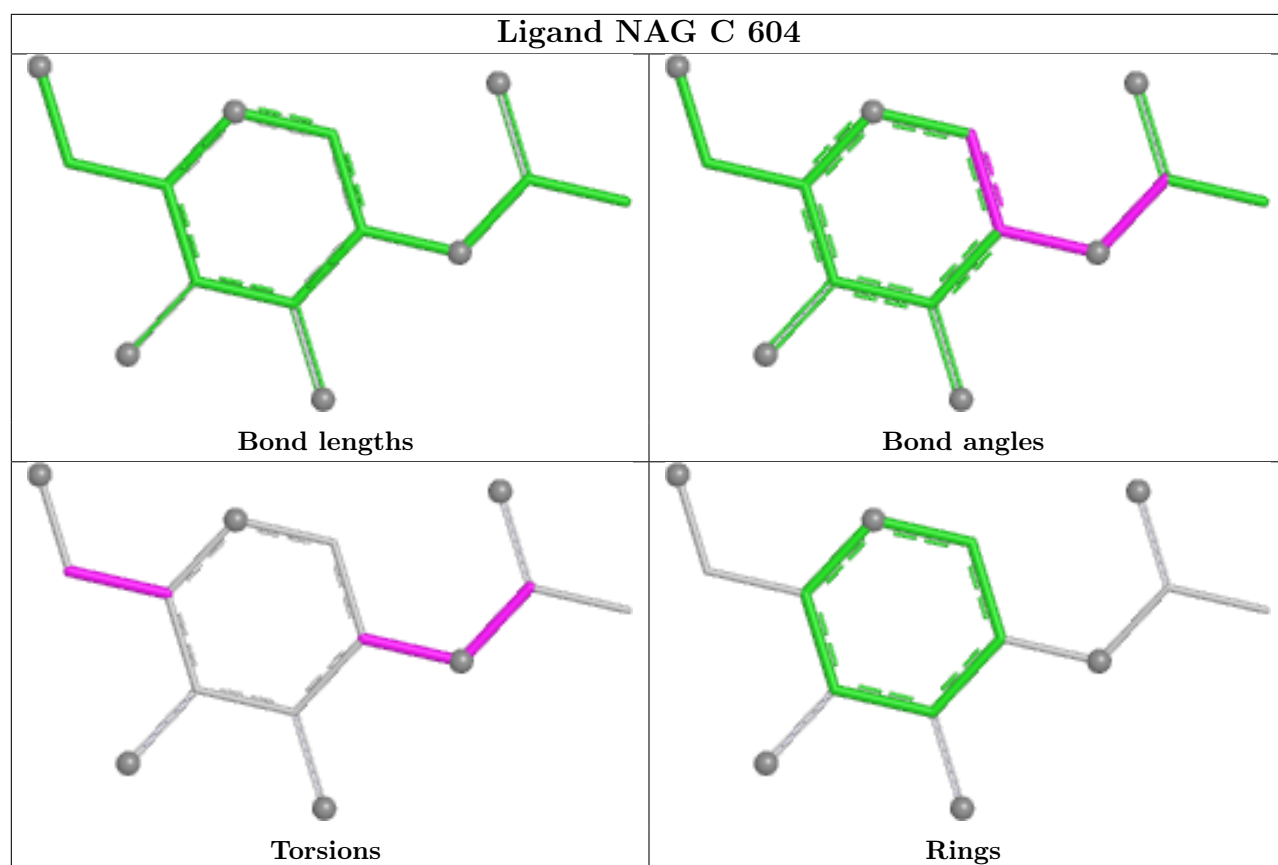
Continued from previous page...

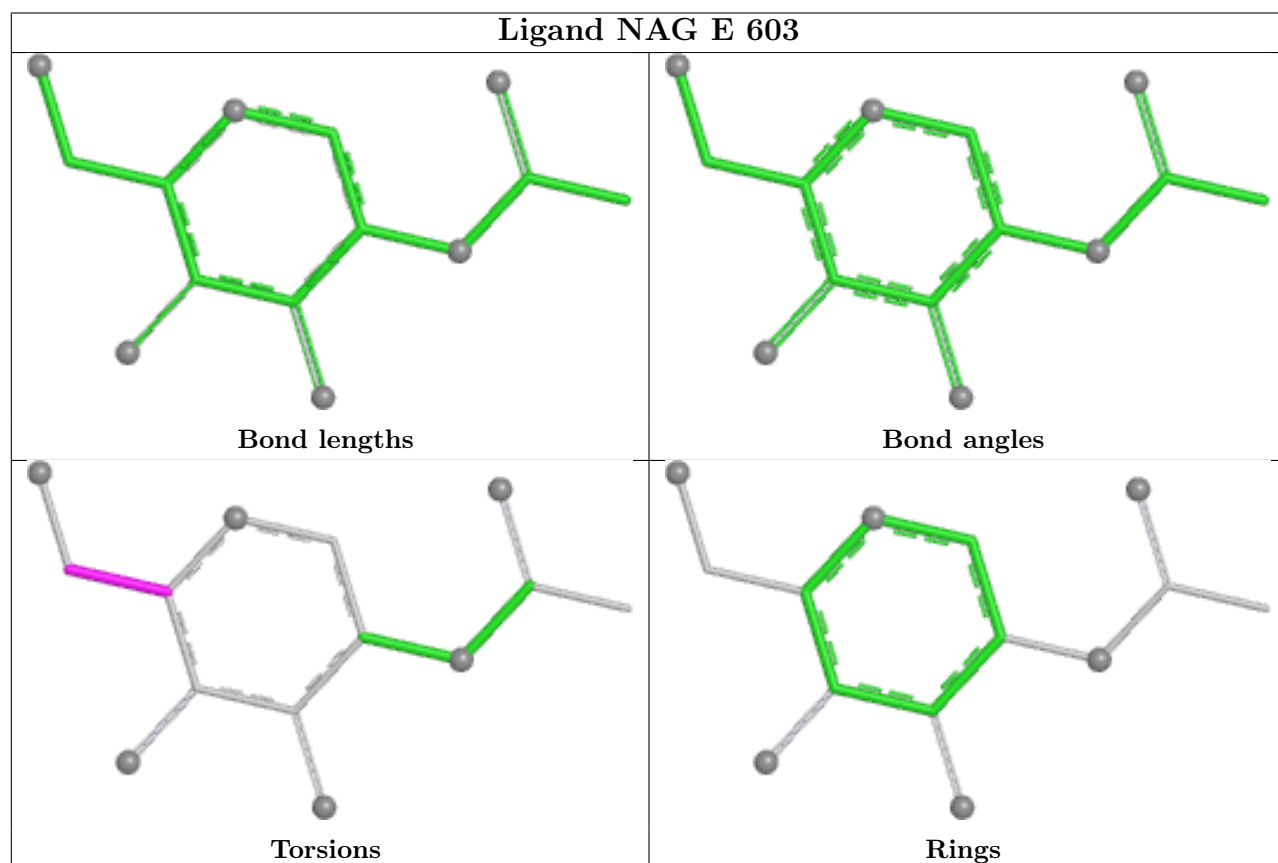
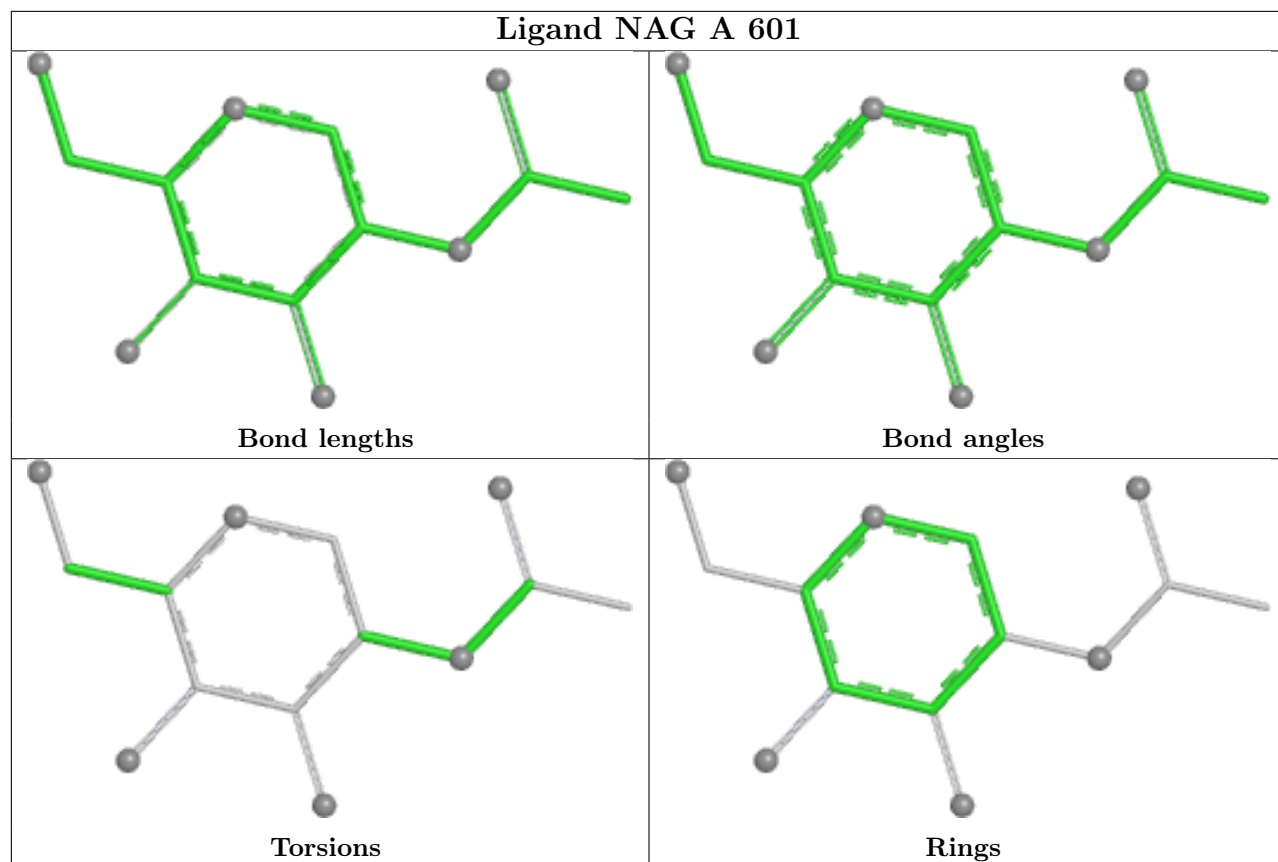
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	605	NAG	1	0
13	E	604	NAG	1	0
13	A	605	NAG	1	0
13	A	604	NAG	1	0

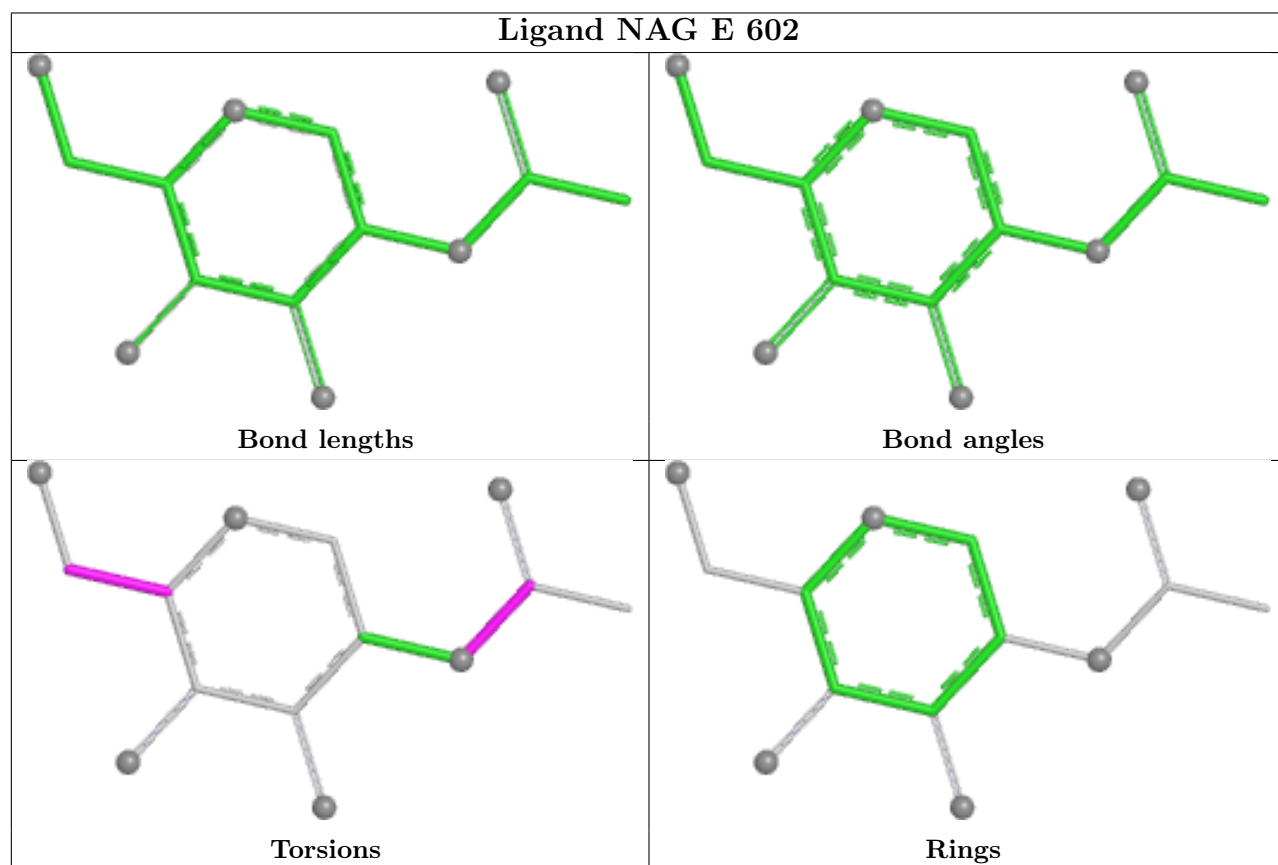
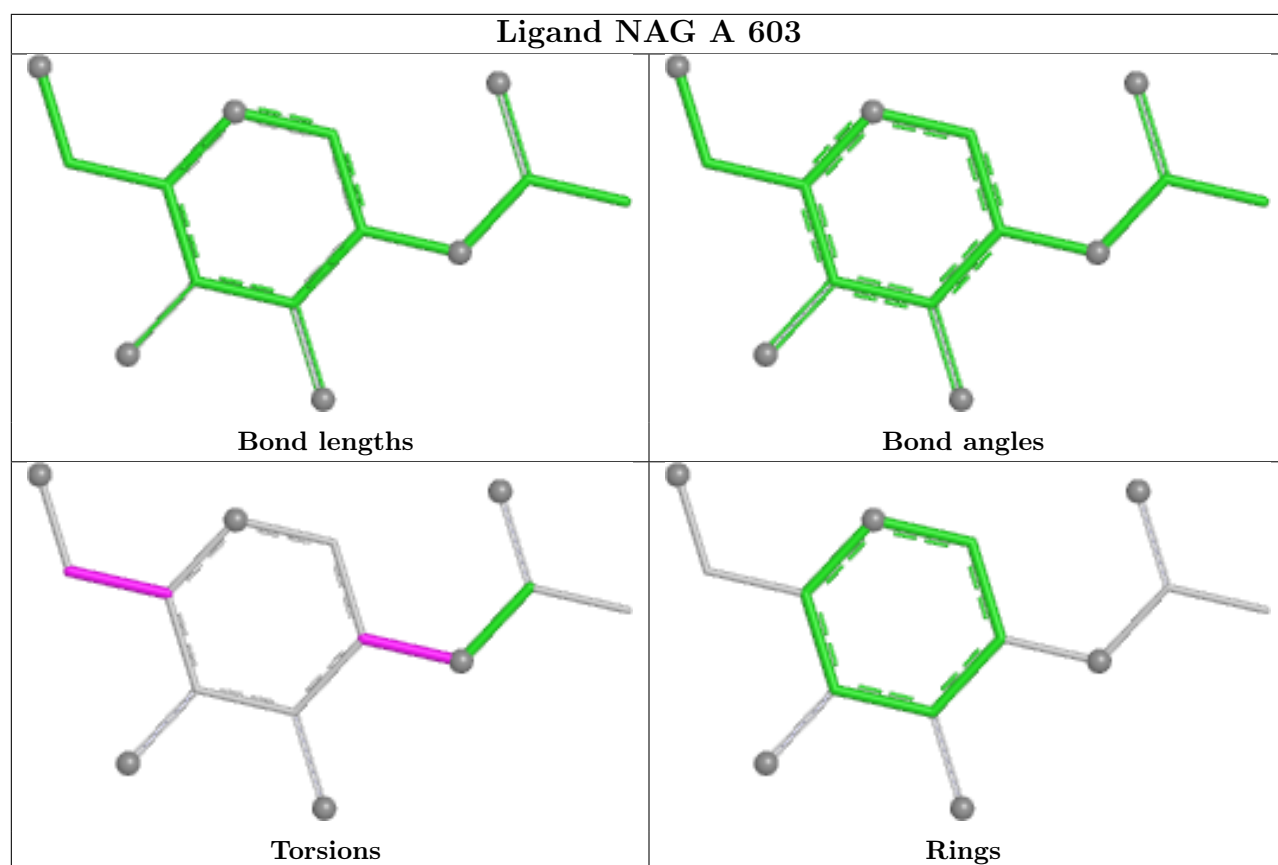
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

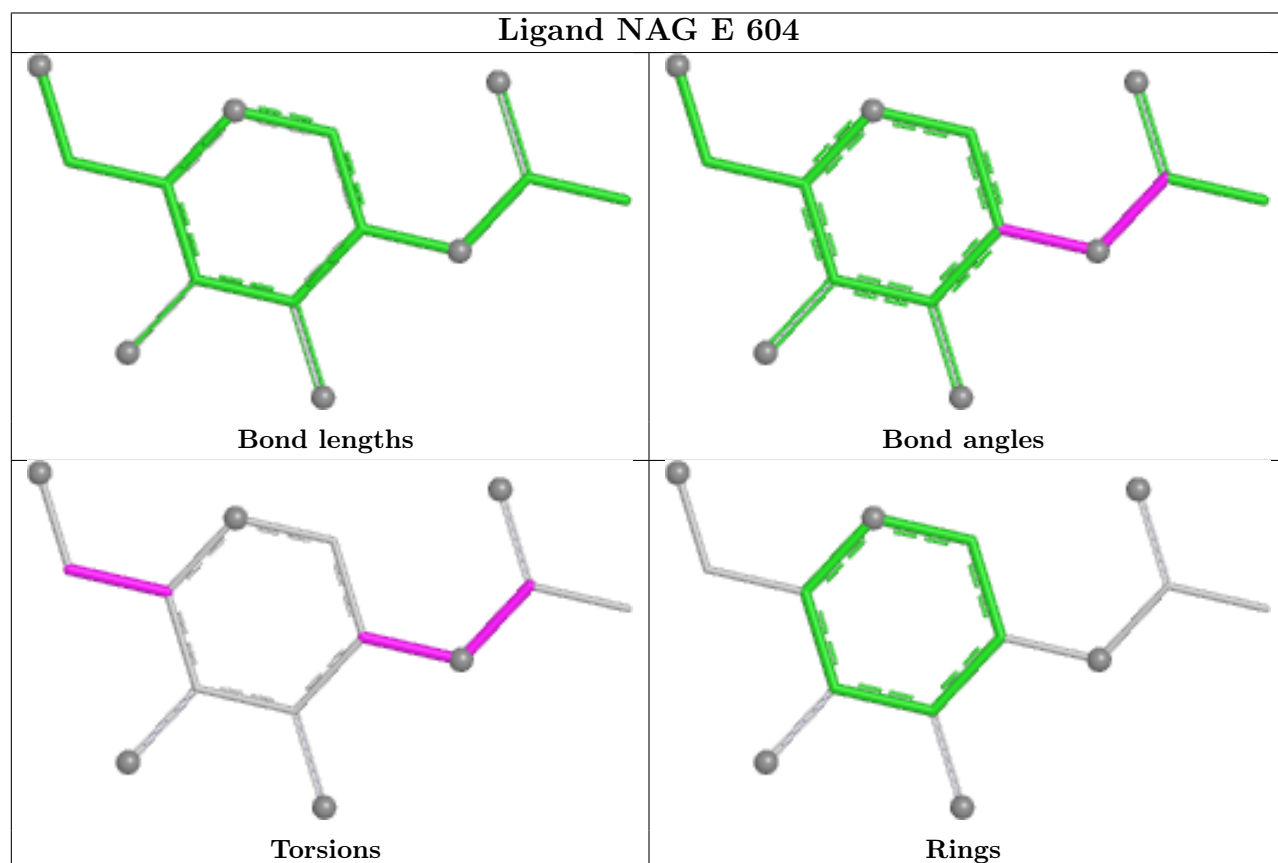
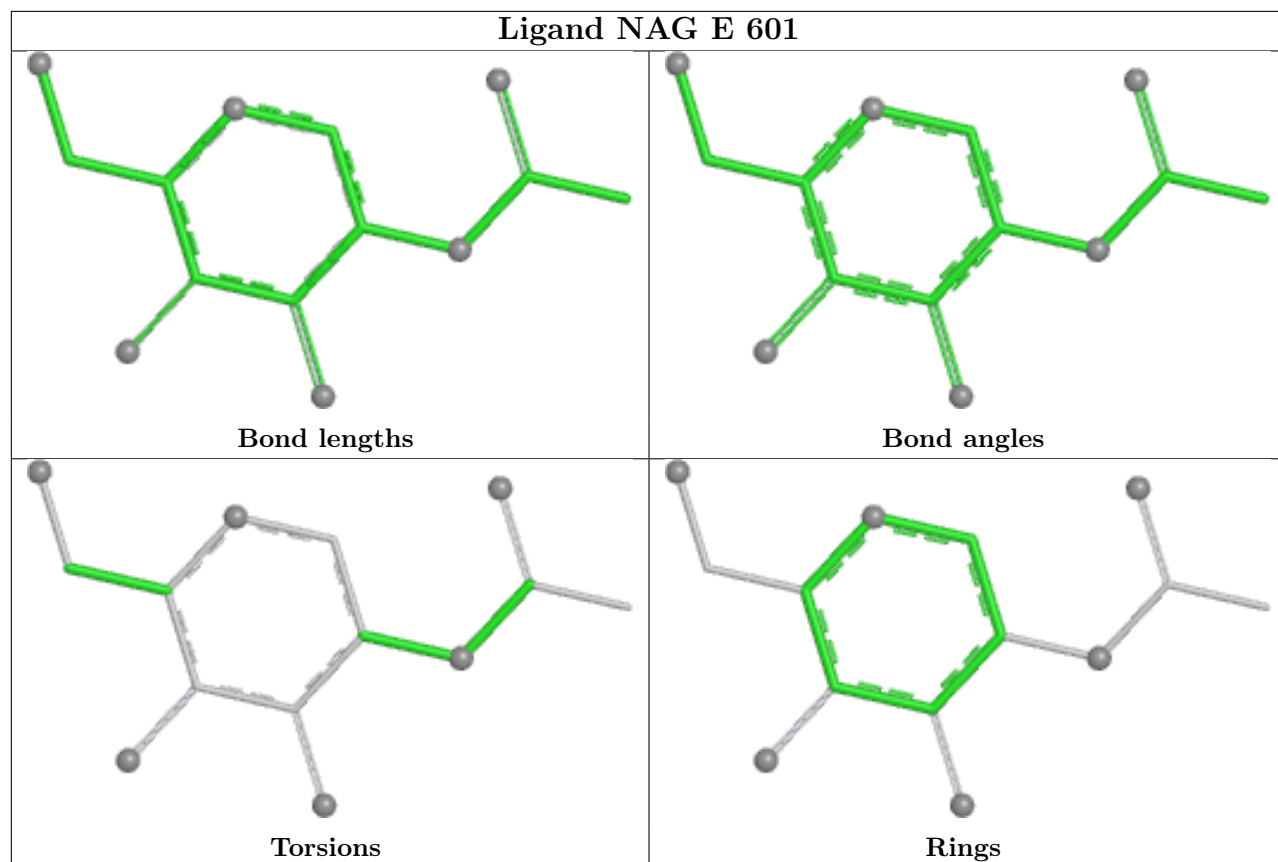


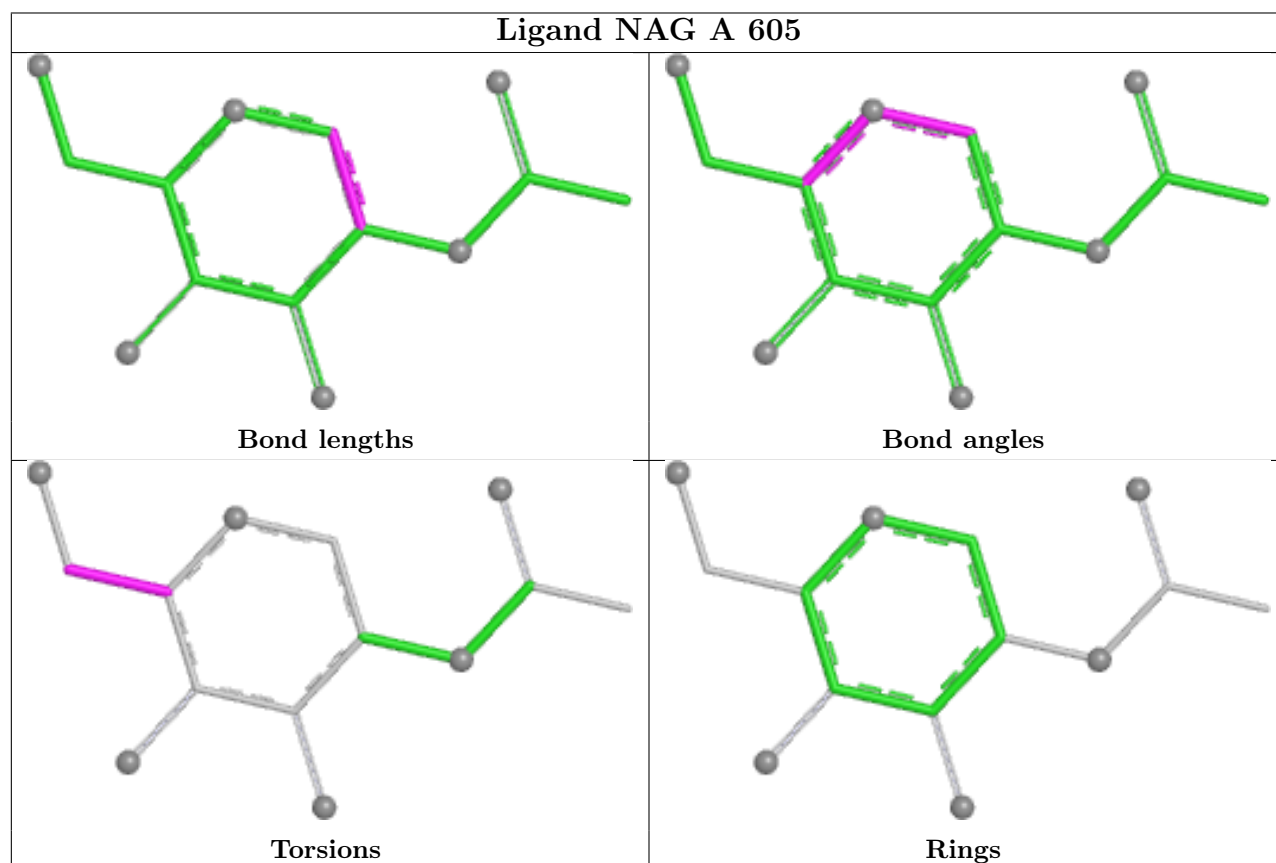
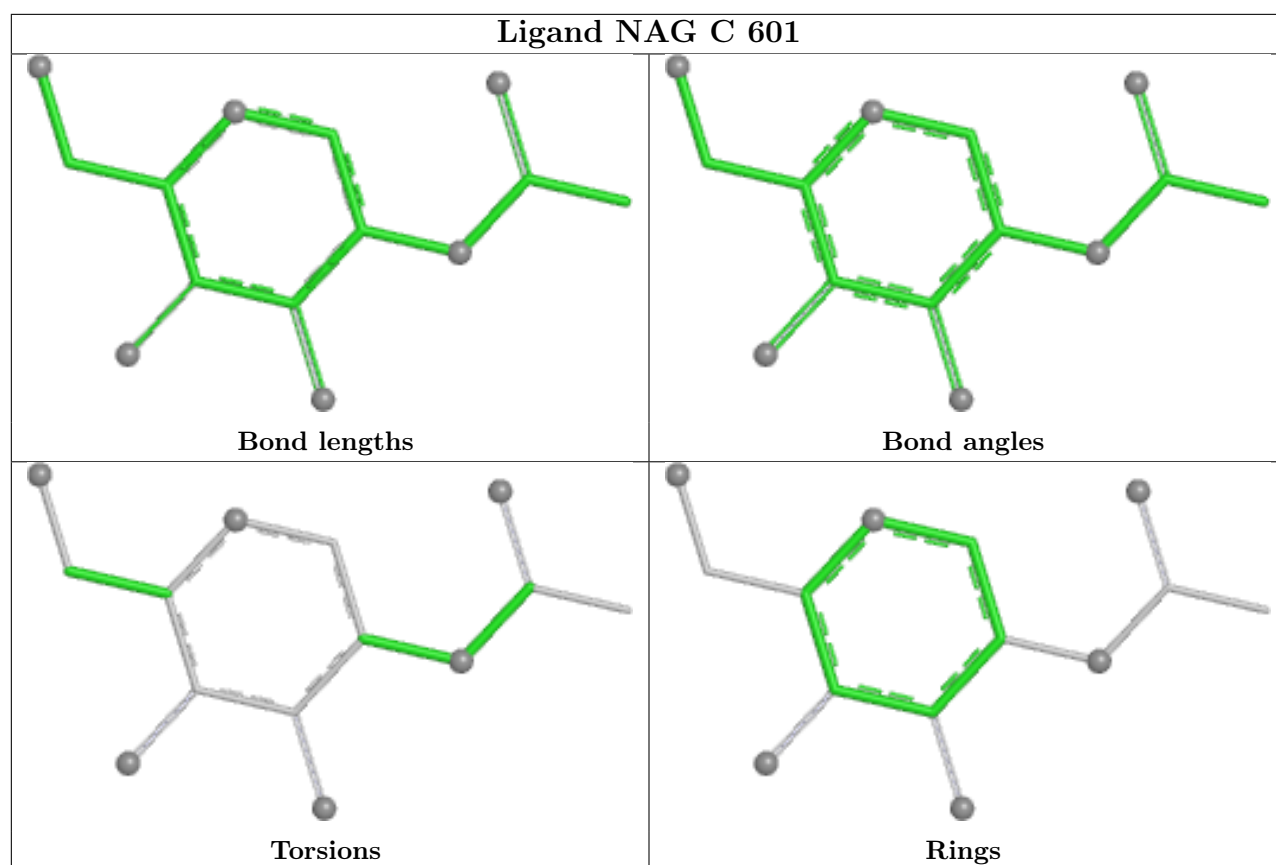


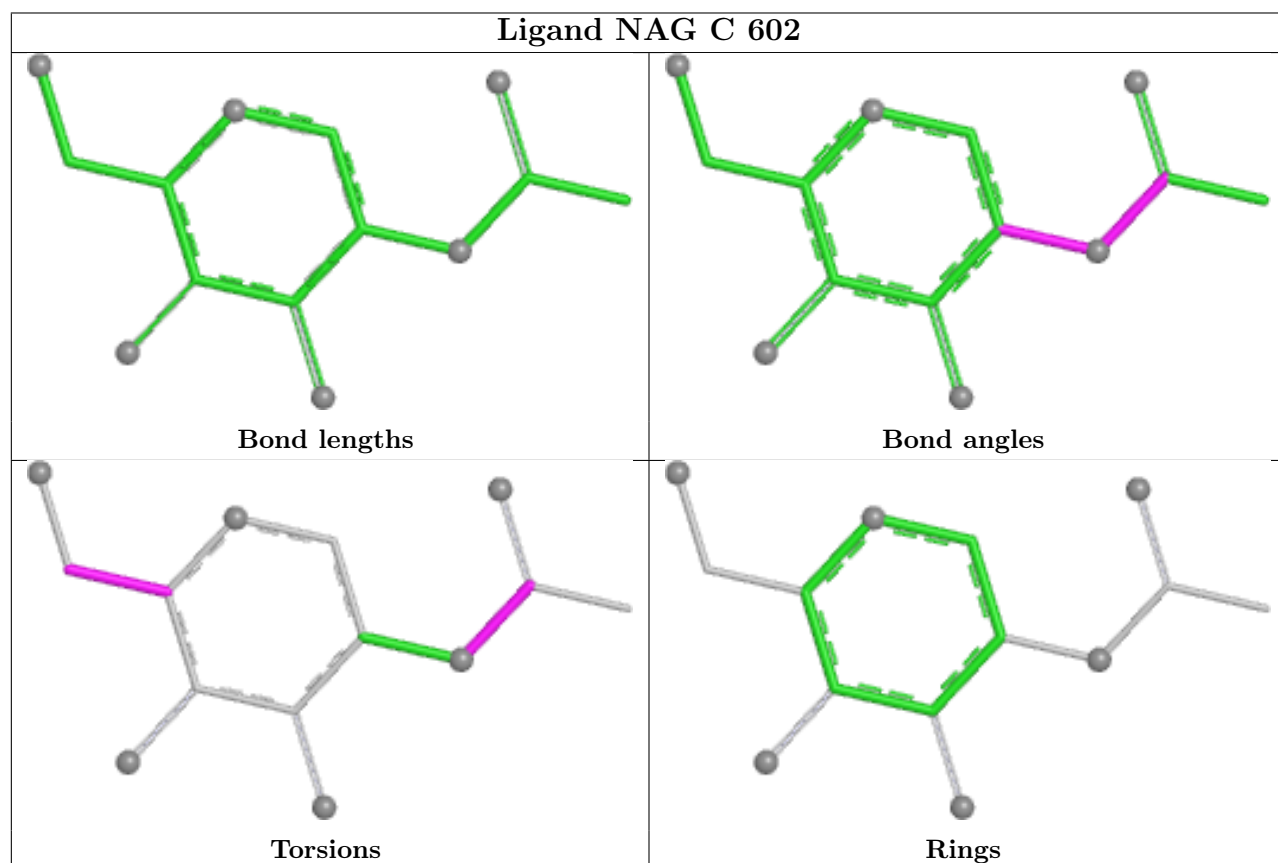
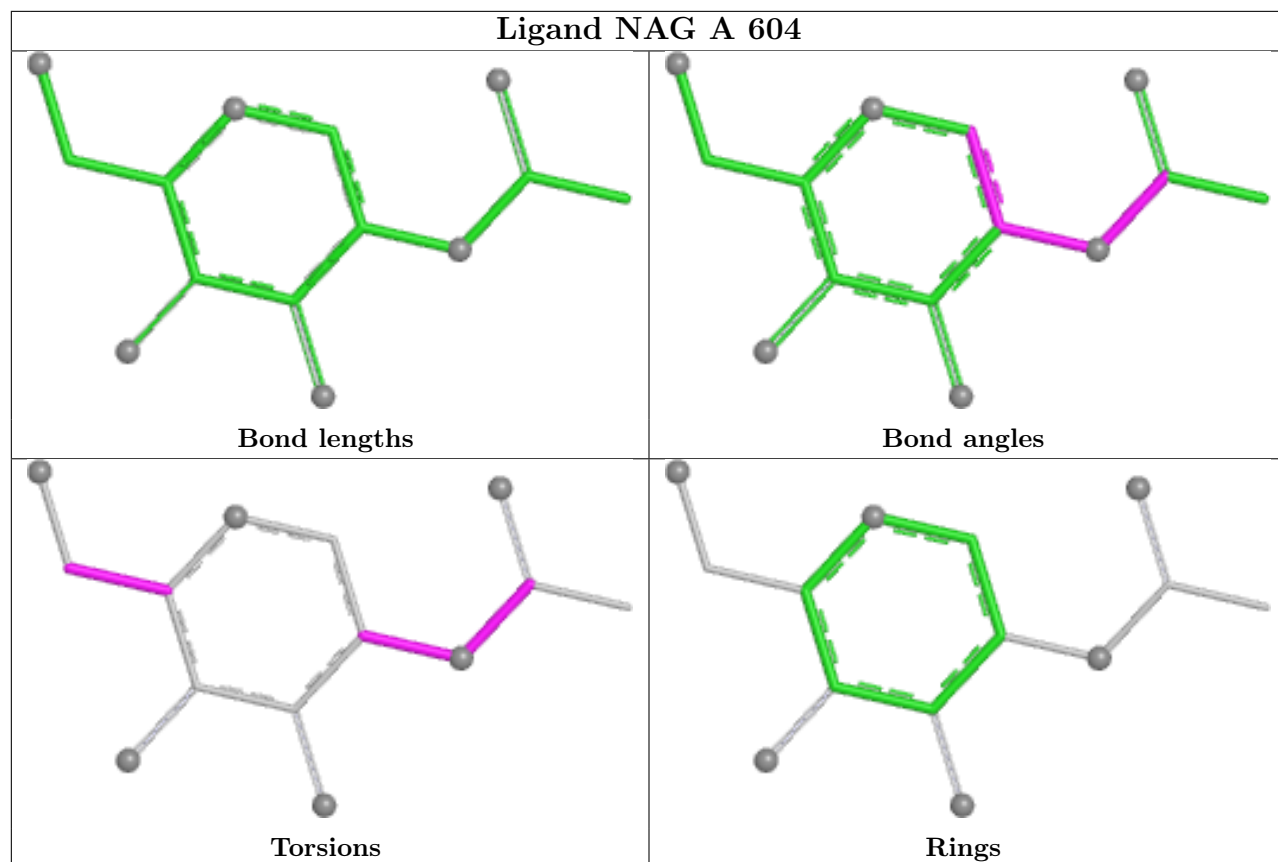












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

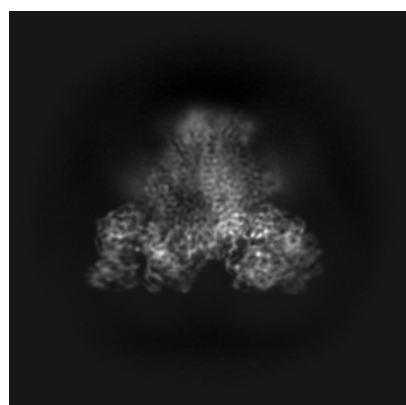
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49628. These allow visual inspection of the internal detail of the map and identification of artifacts.

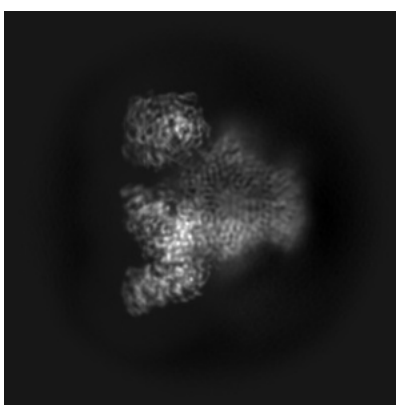
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

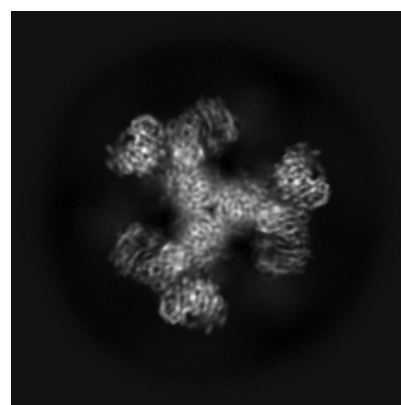
6.1.1 Primary map



X



Y

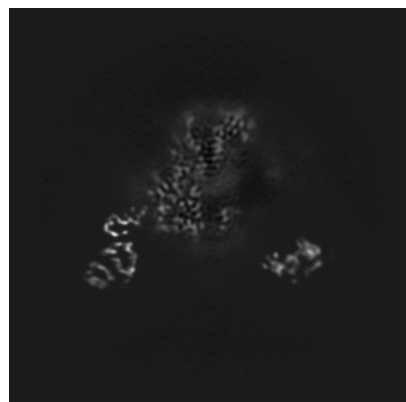


Z

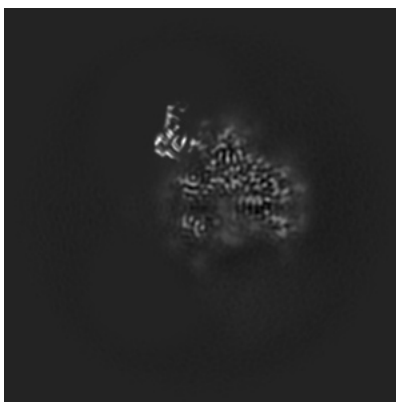
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

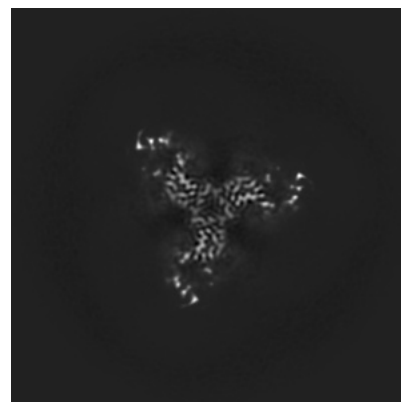
6.2.1 Primary map



X Index: 180



Y Index: 180

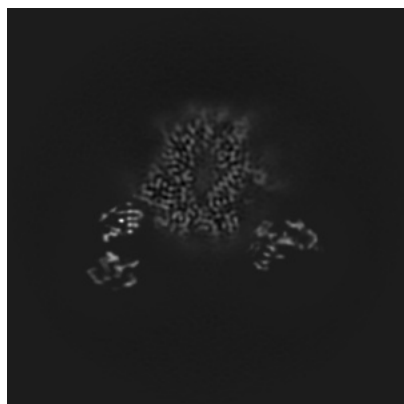


Z Index: 180

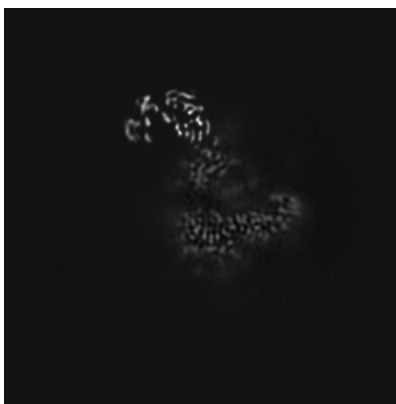
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

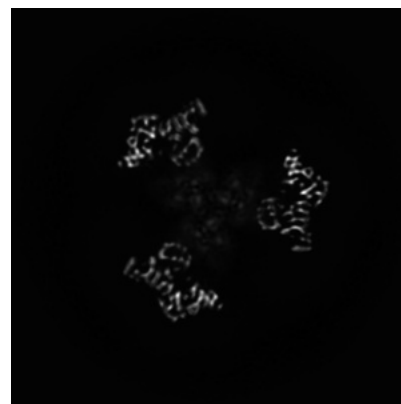
6.3.1 Primary map



X Index: 168



Y Index: 204

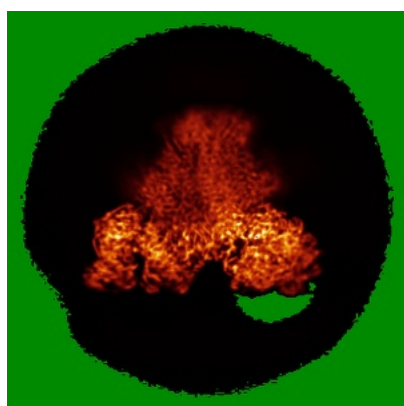


Z Index: 156

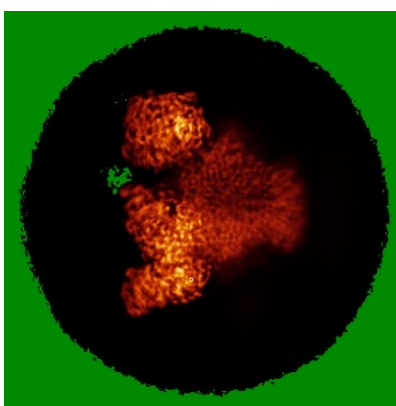
The images above show the largest variance slices of the map in three orthogonal directions.

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

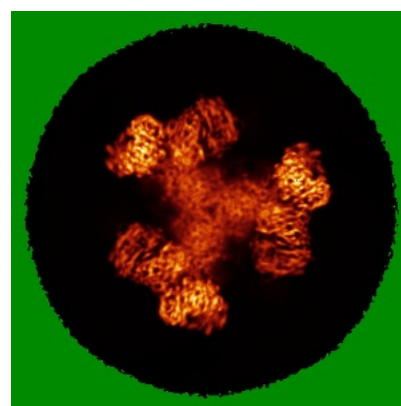
6.4.1 Primary map



X



Y



Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

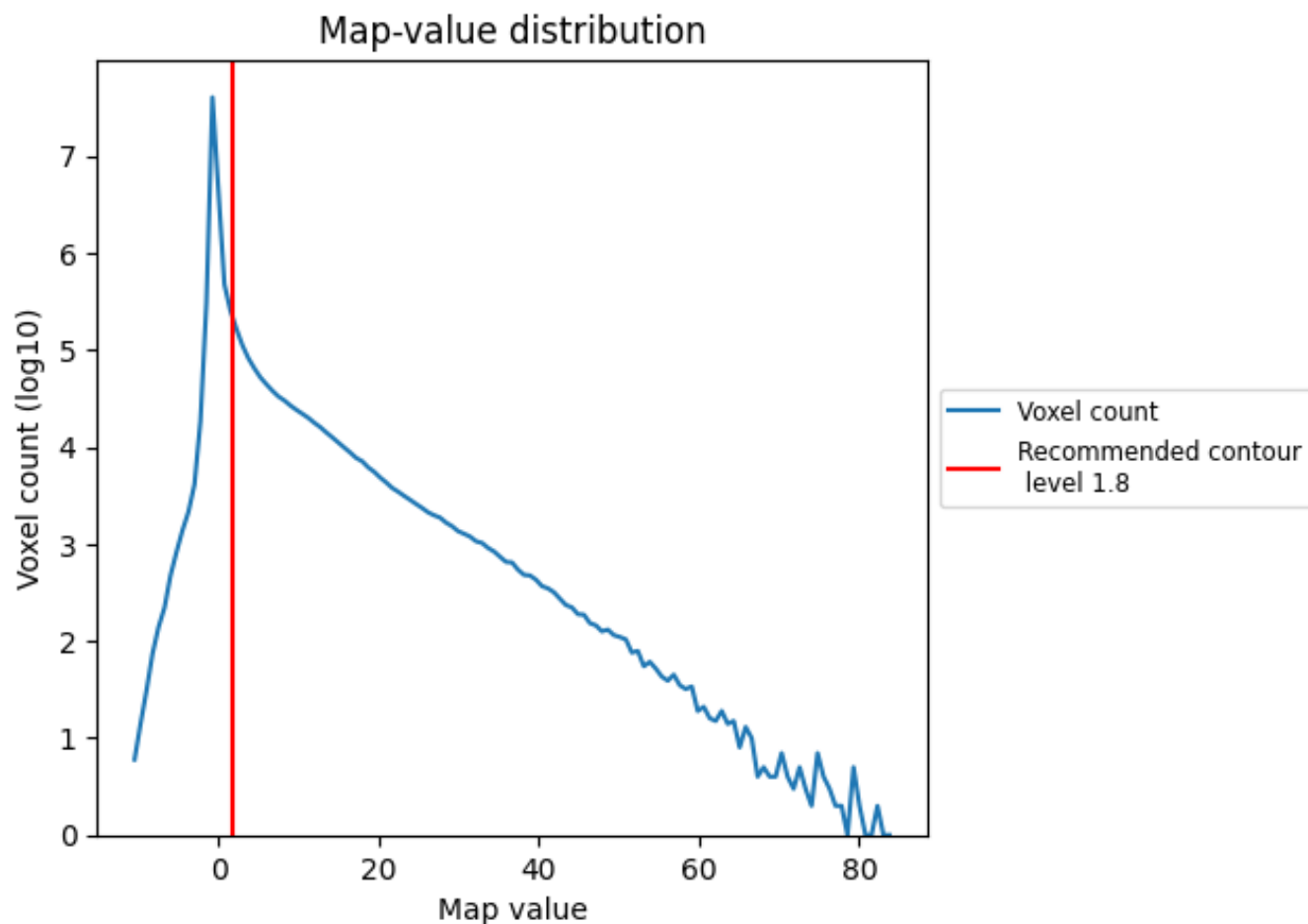
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

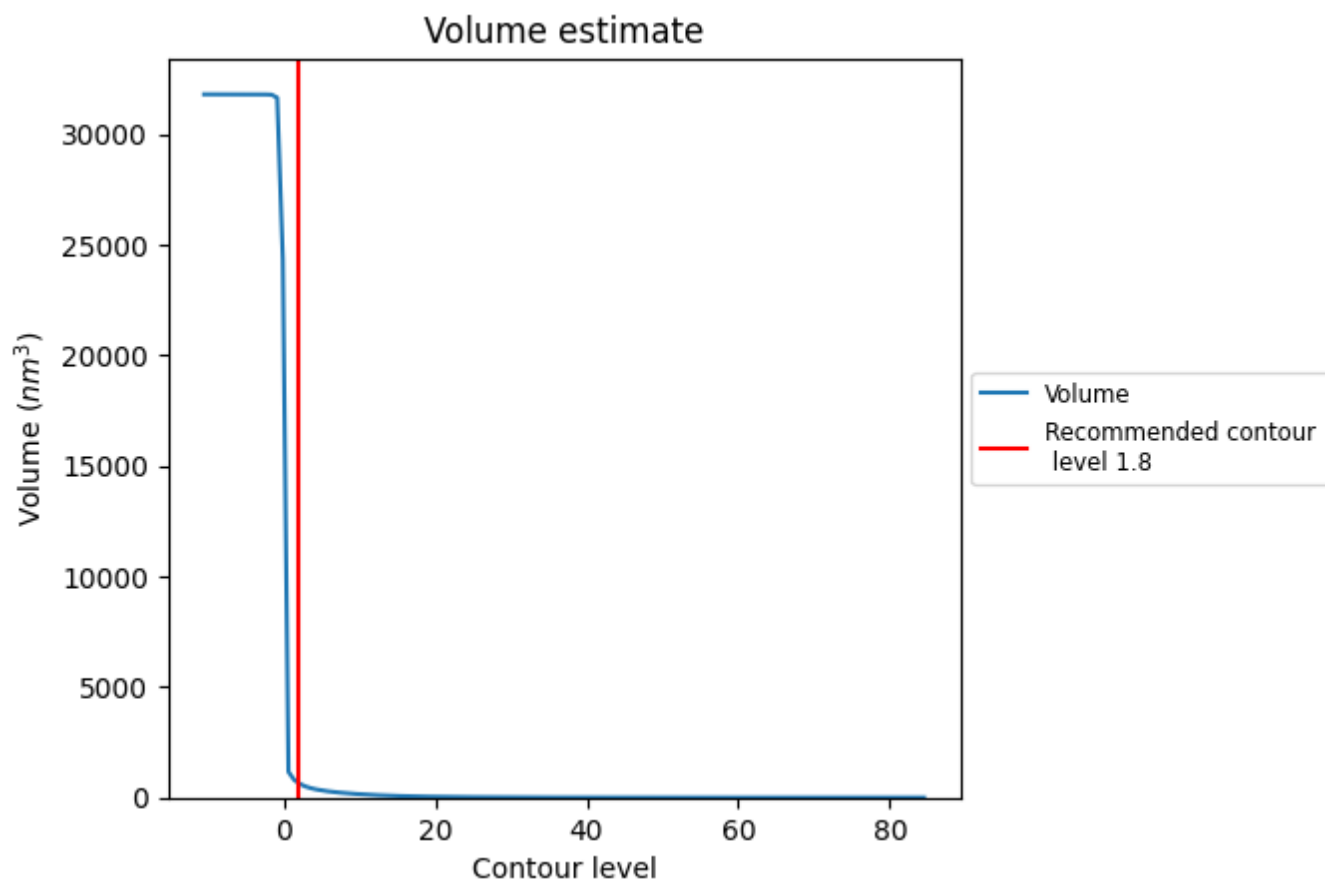
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

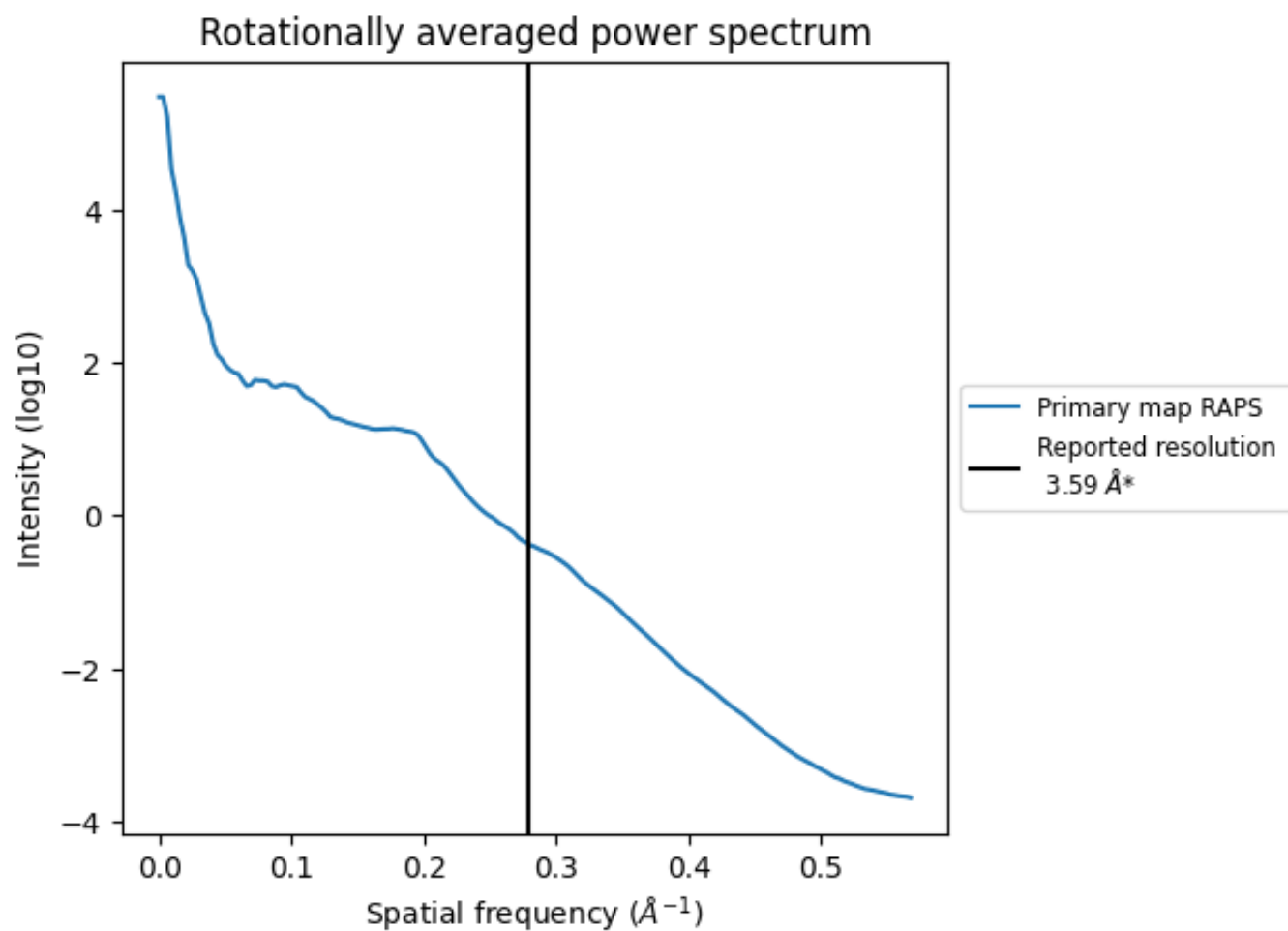
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 694 nm^3 ; this corresponds to an approximate mass of 627 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 0.279 Å⁻¹

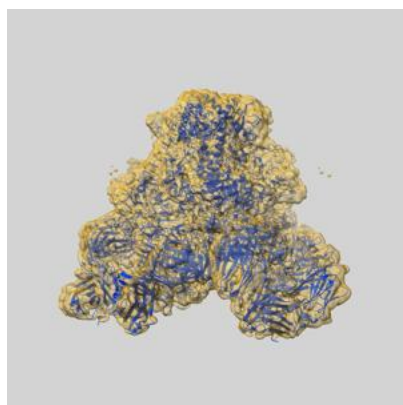
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

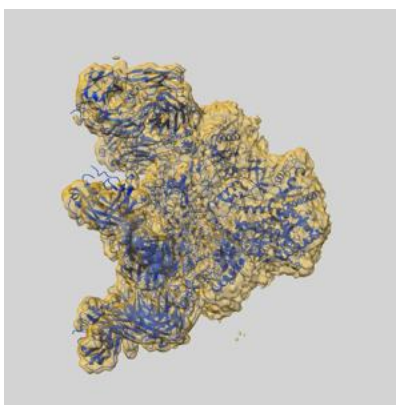
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49628 and PDB model 9NPM. Per-residue inclusion information can be found in section [3](#) on page [13](#).

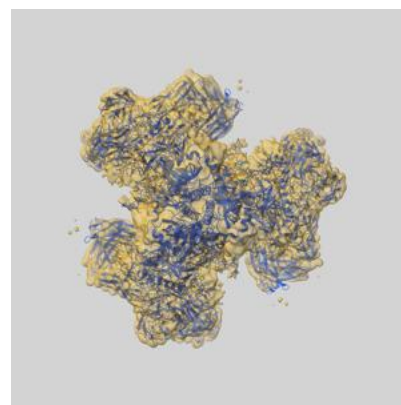
9.1 Map-model overlay [i](#)



X



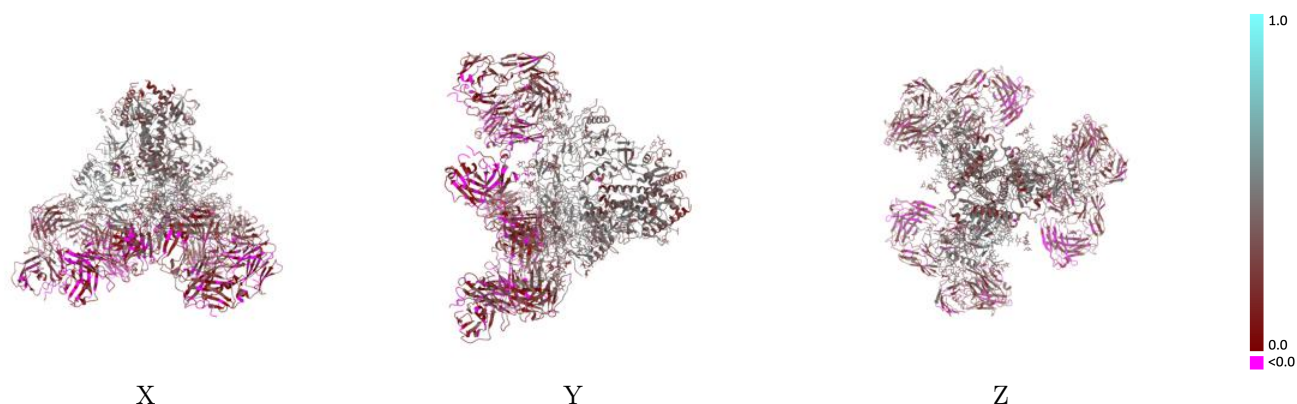
Y



Z

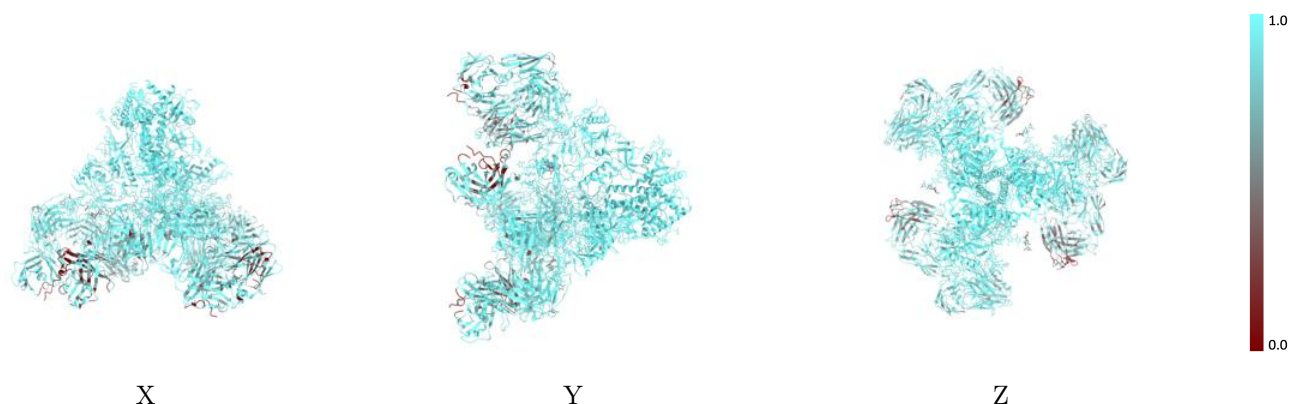
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



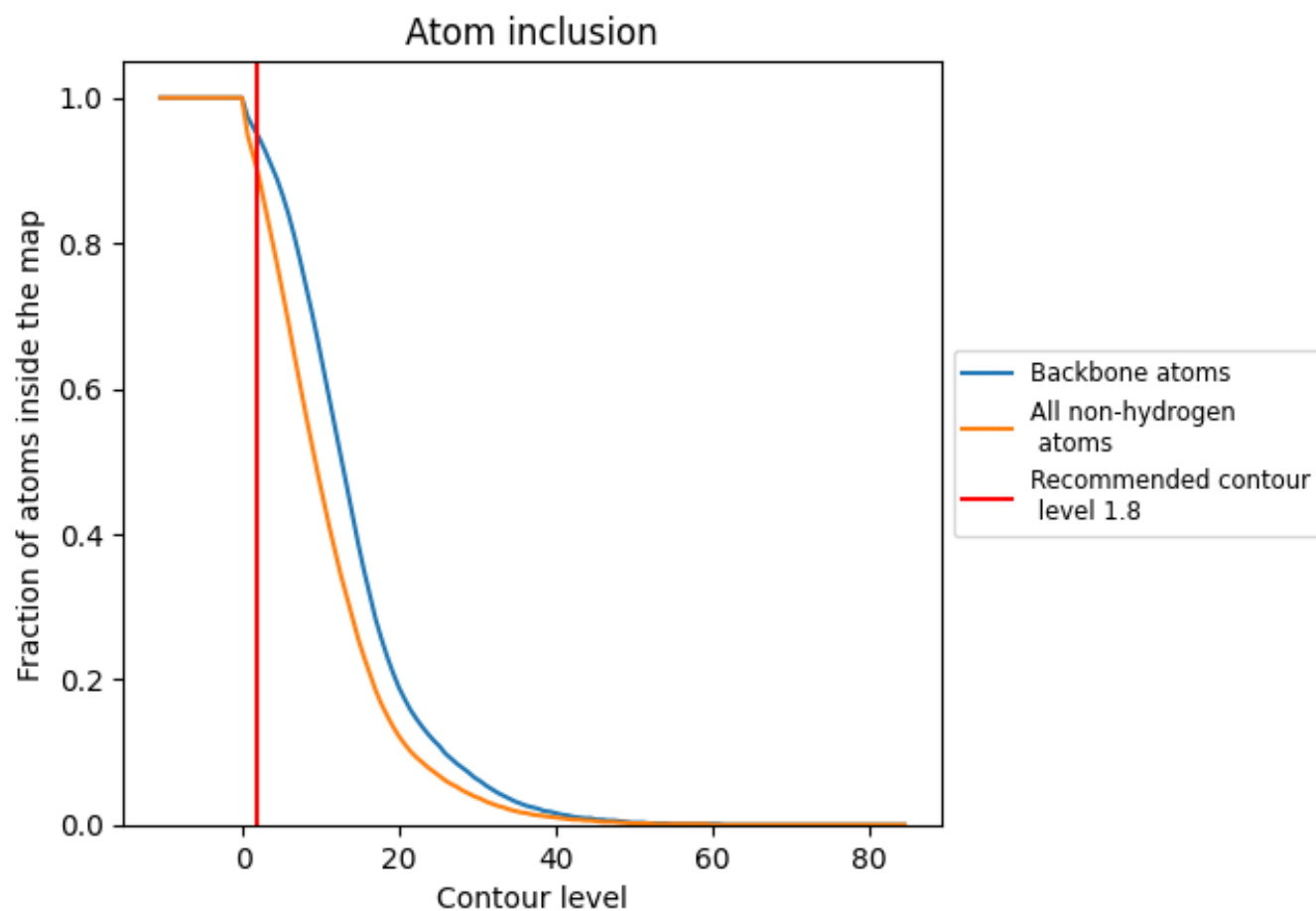
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.2780
A	 0.9920	 0.4050
B	 0.9890	 0.3400
C	 0.9930	 0.4070
D	 0.9890	 0.3500
E	 0.9930	 0.4340
F	 0.9910	 0.3440
G	 0.8470	 0.2400
H	 0.8410	 0.1970
I	 0.7210	 0.1060
J	 0.8070	 0.1570
K	 0.8850	 0.2480
L	 0.8620	 0.2150
M	 0.7860	 0.1580
N	 0.8750	 0.1640
O	 0.8930	 0.2420
P	 0.8860	 0.2030
Q	 0.7580	 0.1550
R	 0.8410	 0.1710
S	 0.9640	 0.3420
T	 0.9640	 0.3830
U	 1.0000	 0.4230
V	 1.0000	 0.3260
W	 0.9640	 0.2530
X	 0.9620	 0.3330
Y	 1.0000	 0.3840
Z	 0.9360	 0.3100
a	 0.9580	 0.2550
b	 0.7640	 0.3200
c	 0.9510	 0.2450
d	 1.0000	 0.3500
e	 0.9640	 0.4080
f	 1.0000	 0.4720
g	 1.0000	 0.3900
h	 1.0000	 0.3970



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9330	 0.3550
j	 1.0000	 0.4100
k	 0.9250	 0.3300
l	 0.9580	 0.2830
m	 0.7220	 0.3090
n	 0.9340	 0.2630
o	 0.9290	 0.3340
p	 0.9640	 0.3700
q	 1.0000	 0.4180
r	 1.0000	 0.3270
s	 0.9640	 0.2950
t	 0.9330	 0.3370
u	 1.0000	 0.3790
v	 0.9040	 0.3190
w	 0.9580	 0.2510
x	 0.7640	 0.3110
y	 1.0000	 0.3570
z	 0.9510	 0.2820