



## Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 10:45 AM EDT

PDB ID : 9B36  
EMDB ID : EMD-44129  
Title : Open state of kainate receptor GluK2 in complex with agonist glutamate and positive allosteric modulator BPAM344 bound to two concanavalin A dimers. Composite map.  
Authors : Nadezhdin, K.D.; Gangwar, S.P.; Sobolevsky, A.I.  
Deposited on : 2024-03-18  
Resolution : 4.29 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

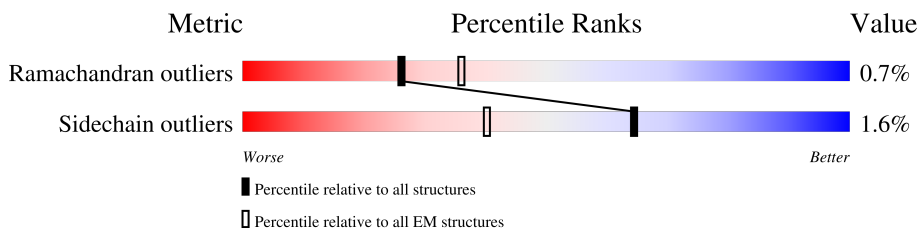
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.29 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	912	89% 8%
1	B	912	91% 8%
1	C	912	89% 8%
1	D	912	91% 8%
2	E	237	94% 5%
2	F	237	94% 5%
2	G	237	94% 5%
2	H	237	94% 5%
3	I	7	14% 14% 86%


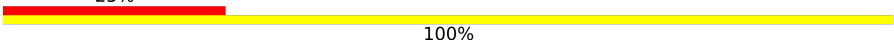
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Mol	Chain	Length	Quality of chain
3	W	7	14% 100%
4	J	2	50% 50%
4	L	2	50% 50%
4	N	2	50% 100%
4	O	2	50% 100%
4	Q	2	50% 50%
4	V	2	50% 100%
4	X	2	50% 50%
4	Z	2	50% 50%
4	b	2	50% 100%
4	c	2	100% 100%
4	e	2	50% 50%
4	j	2	50% 100%
5	K	8	62% 12% 88%
6	M	3	67% 33% 67%
6	S	3	67% 33% 67%
6	T	3	67% 67% 33%
6	a	3	67% 67% 33%
6	g	3	67% 33% 67%
7	P	4	25% 75%
7	d	4	50% 25% 75%
8	R	7	14% 100%
8	Y	7	14% 57% 43%
8	f	7	14% 14% 86%
9	U	4	25% 25% 75%

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Mol	Chain	Length	Quality of chain
9	h	4	 75% 50% 50%
9	i	4	 25% 100%

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 36342 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 Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	842	6684	4283	1117	1244	40	2	0
1	B	842	6680	4280	1117	1243	40	1	0
1	C	842	6684	4283	1117	1244	40	2	0
1	D	842	6680	4280	1117	1243	40	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	VAL	ILE	conflict	UNP P42260
A	571	CYS	TYR	conflict	UNP P42260
A	909	LEU	-	expression tag	UNP P42260
A	910	VAL	-	expression tag	UNP P42260
A	911	PRO	-	expression tag	UNP P42260
A	912	ARG	-	expression tag	UNP P42260
B	567	VAL	ILE	conflict	UNP P42260
B	571	CYS	TYR	conflict	UNP P42260
B	909	LEU	-	expression tag	UNP P42260
B	910	VAL	-	expression tag	UNP P42260
B	911	PRO	-	expression tag	UNP P42260
B	912	ARG	-	expression tag	UNP P42260
C	567	VAL	ILE	conflict	UNP P42260
C	571	CYS	TYR	conflict	UNP P42260
C	909	LEU	-	expression tag	UNP P42260
C	910	VAL	-	expression tag	UNP P42260
C	911	PRO	-	expression tag	UNP P42260
C	912	ARG	-	expression tag	UNP P42260
D	567	VAL	ILE	conflict	UNP P42260
D	571	CYS	TYR	conflict	UNP P42260
D	909	LEU	-	expression tag	UNP P42260
D	910	VAL	-	expression tag	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	911	PRO	-	expression tag	UNP P42260
D	912	ARG	-	expression tag	UNP P42260

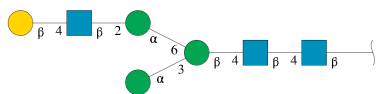
- Molecule 2 is a protein called Concanavalin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	237	Total	C	N	O	S	0	0
			1806	1140	302	362	2		
2	F	237	Total	C	N	O	S	0	0
			1809	1141	302	364	2		
2	G	237	Total	C	N	O	S	0	0
			1806	1140	302	362	2		
2	H	237	Total	C	N	O	S	0	0
			1809	1141	302	364	2		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	58	ASP	GLY	conflict	UNP C0HJY1
E	70	ALA	GLY	conflict	UNP C0HJY1
E	129	MET	VAL	conflict	UNP C0HJY1
E	192	GLU	ASP	conflict	UNP C0HJY1
F	58	ASP	GLY	conflict	UNP C0HJY1
F	70	ALA	GLY	conflict	UNP C0HJY1
F	129	MET	VAL	conflict	UNP C0HJY1
F	192	GLU	ASP	conflict	UNP C0HJY1
G	58	ASP	GLY	conflict	UNP C0HJY1
G	70	ALA	GLY	conflict	UNP C0HJY1
G	129	MET	VAL	conflict	UNP C0HJY1
G	192	GLU	ASP	conflict	UNP C0HJY1
H	58	ASP	GLY	conflict	UNP C0HJY1
H	70	ALA	GLY	conflict	UNP C0HJY1
H	129	MET	VAL	conflict	UNP C0HJY1
H	192	GLU	ASP	conflict	UNP C0HJY1

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	7	Total	C	N	O	0	0
			86	48	3	35		
3	W	7	Total	C	N	O	0	0
			86	48	3	35		

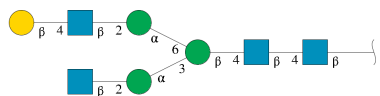
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		

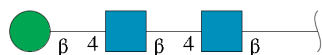
- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(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
			Total	C	N	O		
5	K	8	100	56	4	40	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	3	39	22	2	15	0	0
6	S	3	39	22	2	15	0	0
6	T	3	39	22	2	15	0	0
6	a	3	39	22	2	15	0	0
6	g	3	39	22	2	15	0	0

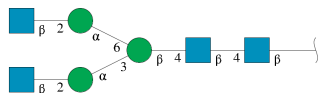
- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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



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



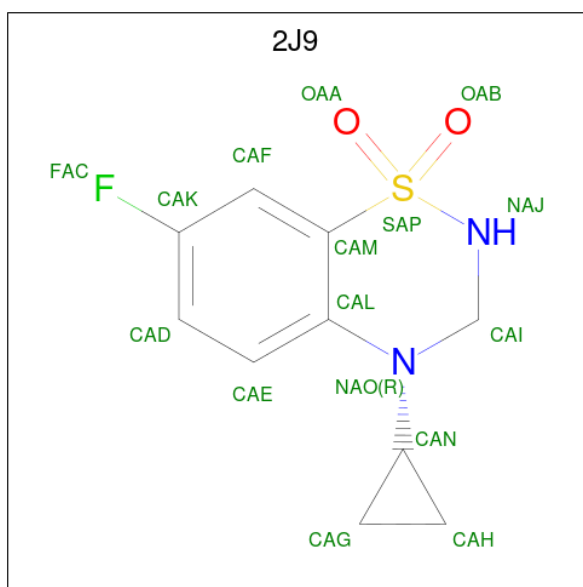
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	R	7	Total	C	N	O	0	0
			89	50	4	35		
8	Y	7	Total	C	N	O	0	0
			89	50	4	35		
8	f	7	Total	C	N	O	0	0
			89	50	4	35		

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



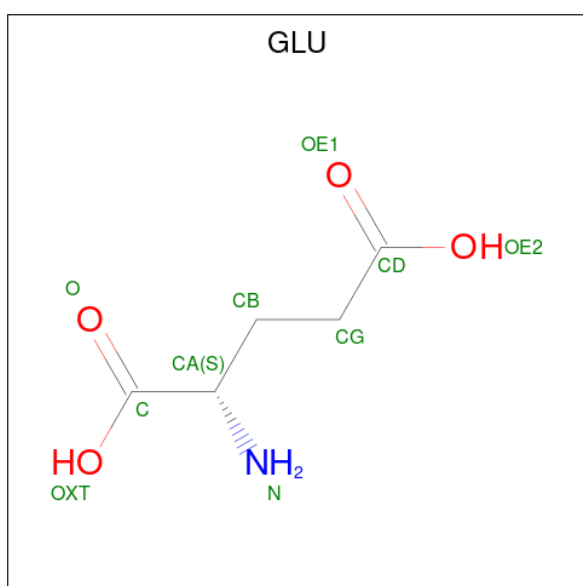
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	4	Total	C	N	O	0	0
			50	28	2	20		
9	h	4	Total	C	N	O	0	0
			50	28	2	20		
9	i	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 4-cyclopropyl-7-fluoro-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 2J9) (formula: C<sub>10</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



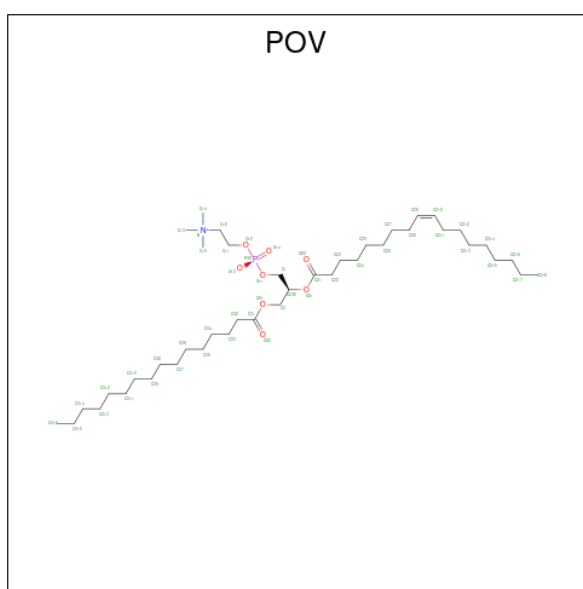
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	N	O		S
10	A	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
10	B	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
10	C	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	
10	D	1	Total	C	F	N	O	S	0
			16	10	1	2	2	1	

- Molecule 11 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	A	1	10	5	1	4	0
11	B	1	10	5	1	4	0
11	C	1	10	5	1	4	0
11	D	1	10	5	1	4	0

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



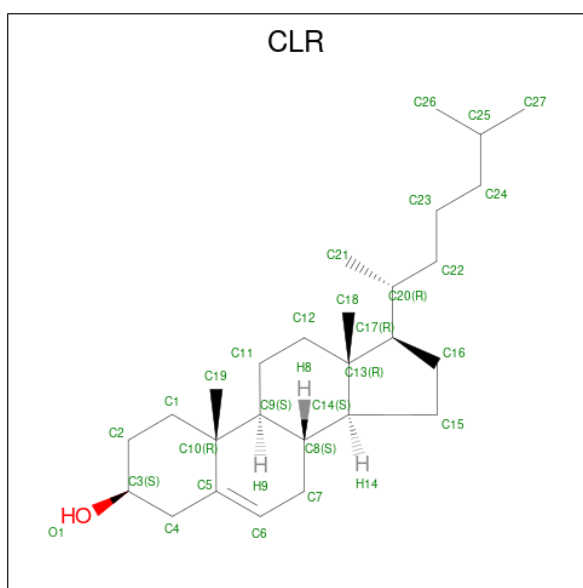
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	52	42	1	8	1	0
12	A	1	52	42	1	8	1	0
12	A	1	52	42	1	8	1	0
12	A	1	52	42	1	8	1	0
12	B	1	52	42	1	8	1	0
12	B	1	52	42	1	8	1	0
12	B	1	52	42	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 13 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			28	27	1	
13	A	1	Total	C	O	0
			28	27	1	
13	A	1	Total	C	O	0
			28	27	1	
13	A	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total	C	O	0
			28	27	1	
13	C	1	Total	C	O	0
			28	27	1	
13	C	1	Total	C	O	0
			28	27	1	
13	C	1	Total	C	O	0
			28	27	1	

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	1	Total	Zn	0
			1	1	
14	F	1	Total	Zn	0
			1	1	
14	G	1	Total	Zn	0
			1	1	
14	H	1	Total	Zn	0
			1	1	

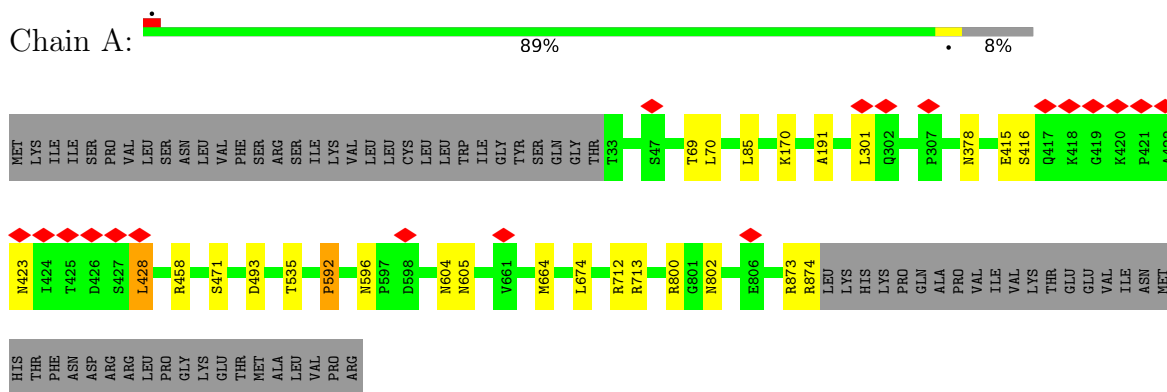
- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	E	1	Total	Ca	0
			1	1	
15	F	1	Total	Ca	0
			1	1	
15	G	1	Total	Ca	0
			1	1	
15	H	1	Total	Ca	0
			1	1	

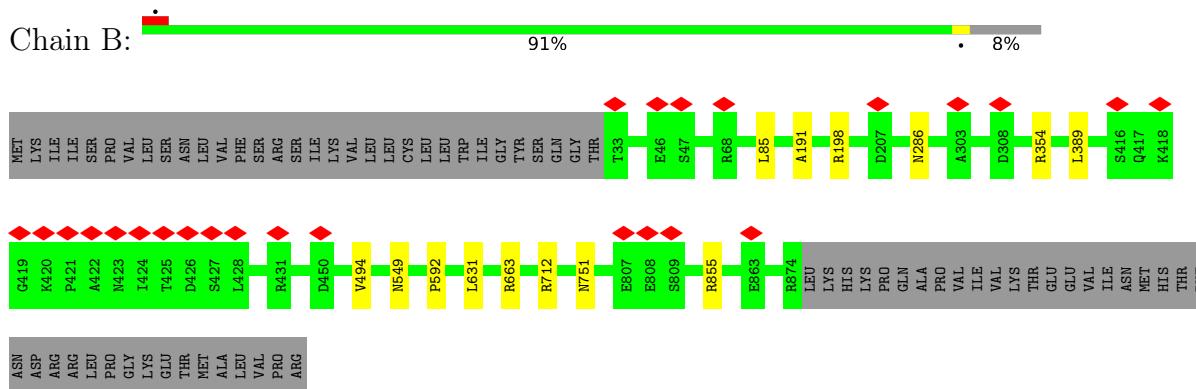
### 3 Residue-property plots [i](#)

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

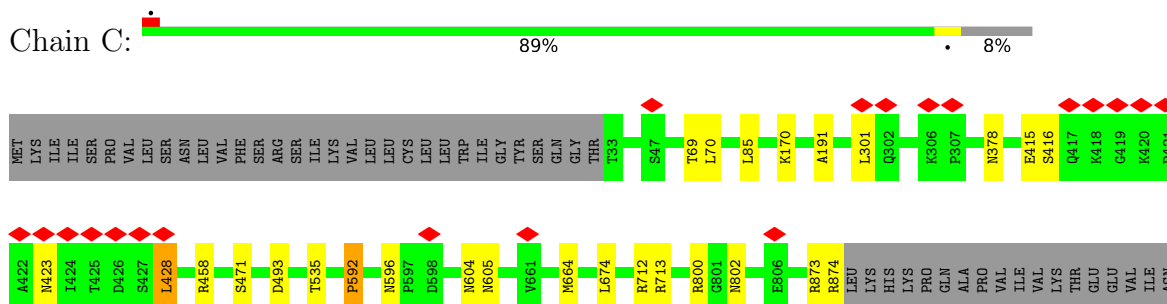
- Molecule 1: Glutamate receptor ionotropic, kainate 2



- Molecule 1: Glutamate receptor ionotropic, kainate 2



- Molecule 1: Glutamate receptor ionotropic, kainate 2



MET  
HIS  
THR  
PHE  
ASN  
ASP  
ARG  
ARG  
LEU  
PRO  
GLY  
LYS  
GLU  
THR  
MET  
ALA  
VAL  
PRO  
ARG

- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain D: 91% 8%

MET  
LYS  
ILE  
SER  
PRO  
VAL  
LEU  
SER  
ASN  
LEU  
VAL  
PHE  
SER  
ARG  
SER  
ILE  
LYS  
VAL  
LEU  
LEU  
CYS  
LEU  
LEU  
TRP  
ILE  
GLY  
TYR  
SER  
GLN  
GLY  
THR  
T33  
E46  
S47  
R68  
L85  
A191  
R198  
D207  
M286  
A303  
D308  
R354  
L389  
S416  
Q417  
K418

G419  
K420  
P421  
A422  
N423  
I424  
T425  
D426  
S427  
L428  
R431  
D450  
V494  
N549  
P592  
L631  
R663  
R712  
N751  
E807  
E808  
S809  
R855  
Q872  
R873  
R874  
LEU  
LYS  
HIS  
LYS  
PRO  
GLN  
ALA  
PRO  
VAL  
ILE  
VAL  
LYS  
THR  
GLU  
VAL  
ILE  
ASN  
MET  
HIS  
THR  
PHE

ASN  
ASP  
ARG  
ARG  
LEU  
PRO  
GLY  
LYS  
GLU  
THR  
MET  
ALA  
LEU  
VAL  
PRO  
ARG

- Molecule 2: Concanavalin A

Chain E: 94% 5%

A1  
V47  
G48  
K59  
L115  
N118  
Q132  
S161  
N162  
I181  
W182  
E183  
S184  
S185  
A186  
V187  
A207  
L230  
N237

- Molecule 2: Concanavalin A

Chain F: 94% 5%

A1  
V47  
G48  
K59  
G98  
L115  
K116  
S117  
N118  
S119  
E122  
Q132  
R158  
N162  
I181  
W182  
E183  
S184  
S185  
A186  
D203  
A207  
S223  
N237

- Molecule 2: Concanavalin A

Chain G: 94% 5%

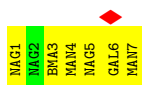
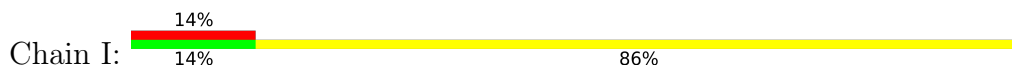
A1  
V47  
G48  
K59  
L115  
N118  
E122  
Q132  
S161  
N162  
I181  
W182  
E183  
S184  
S185  
A186  
V187  
A207  
L230  
N237

- Molecule 2: Concanavalin A

Chain H: 94% 5%

A1  
V47  
G48  
K59  
L115  
K116  
S117  
N118  
S119  
Q132  
S160  
S161  
N162  
I181  
W182  
E183  
S184  
S185  
A186  
A207  
N237

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



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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



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



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



- Molecule 7: beta-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 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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



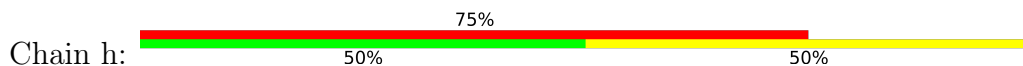
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	60.657	Depositor
Minimum map value	-32.589	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	1.320	Depositor
Recommended contour level	4.33	Depositor
Map size ( $\text{\AA}$ )	345.2672, 345.2672, 345.2672	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3487, 1.3487, 1.3487	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, ZN, CLR, MAN, CA, NAG, POV, GAL, 2J9

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	0.32	0/6840	0.62	6/9258 (0.1%)
1	B	0.32	0/6833	0.58	1/9248 (0.0%)
1	C	0.32	0/6840	0.62	7/9258 (0.1%)
1	D	0.32	0/6833	0.58	1/9248 (0.0%)
2	E	0.36	0/1848	0.76	2/2518 (0.1%)
2	F	0.36	0/1851	0.75	1/2522 (0.0%)
2	G	0.36	0/1848	0.76	2/2518 (0.1%)
2	H	0.36	0/1851	0.75	1/2522 (0.0%)
All	All	0.33	0/34744	0.63	21/47092 (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	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
2	E	0	8
2	F	0	8
2	G	0	8
2	H	0	8
All	All	0	42

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	48	GLY	N-CA-C	10.16	138.50	113.10
2	G	48	GLY	N-CA-C	10.14	138.44	113.10
1	A	428	LEU	CA-CB-CG	9.06	136.15	115.30
1	C	428	LEU	CA-CB-CG	9.04	136.09	115.30
2	H	48	GLY	N-CA-C	8.06	133.25	113.10
2	F	48	GLY	N-CA-C	8.05	133.23	113.10
1	A	301	LEU	CA-CB-CG	6.90	131.18	115.30
1	C	301	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	85	LEU	CA-CB-CG	5.95	128.97	115.30
1	C	85	LEU	CA-CB-CG	5.94	128.96	115.30
1	B	85	LEU	CA-CB-CG	5.78	128.58	115.30
1	D	85	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	493	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	493	ASP	CB-CG-OD1	5.60	123.34	118.30
2	E	230	LEU	CA-CB-CG	5.53	128.02	115.30
2	G	230	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	70	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	70	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	674	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	674	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	428	LEU	CB-CG-CD1	5.03	119.55	111.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ALA	Peptide
1	A	415	GLU	Peptide
1	A	592	PRO	Peptide
1	B	191	ALA	Peptide
1	B	751	ASN	Peptide
1	C	191	ALA	Peptide
1	C	415	GLU	Peptide
1	C	592	PRO	Peptide
1	D	191	ALA	Peptide
1	D	751	ASN	Peptide
2	E	115	LEU	Peptide
2	E	118	ASN	Peptide
2	E	181	ILE	Peptide
2	E	182	TRP	Peptide
2	E	185	SER	Peptide
2	E	186	ALA	Peptide
2	E	207	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	E	47	VAL	Peptide
2	F	115	LEU	Peptide
2	F	118	ASN	Peptide
2	F	181	ILE	Peptide
2	F	182	TRP	Peptide
2	F	185	SER	Peptide
2	F	186	ALA	Peptide
2	F	207	ALA	Peptide
2	F	47	VAL	Peptide
2	G	115	LEU	Peptide
2	G	118	ASN	Peptide
2	G	181	ILE	Peptide
2	G	182	TRP	Peptide
2	G	185	SER	Peptide
2	G	186	ALA	Peptide
2	G	207	ALA	Peptide
2	G	47	VAL	Peptide
2	H	115	LEU	Peptide
2	H	118	ASN	Peptide
2	H	181	ILE	Peptide
2	H	182	TRP	Peptide
2	H	185	SER	Peptide
2	H	186	ALA	Peptide
2	H	207	ALA	Peptide
2	H	47	VAL	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	842/912 (92%)	740 (88%)	98 (12%)	4 (0%)	29	68
1	B	841/912 (92%)	745 (89%)	93 (11%)	3 (0%)	34	72
1	C	842/912 (92%)	740 (88%)	98 (12%)	4 (0%)	29	68
1	D	841/912 (92%)	745 (89%)	93 (11%)	3 (0%)	34	72
2	E	235/237 (99%)	179 (76%)	52 (22%)	4 (2%)	9	43
2	F	235/237 (99%)	171 (73%)	59 (25%)	5 (2%)	7	39
2	G	235/237 (99%)	179 (76%)	52 (22%)	4 (2%)	9	43
2	H	235/237 (99%)	171 (73%)	59 (25%)	5 (2%)	7	39
All	All	4306/4596 (94%)	3670 (85%)	604 (14%)	32 (1%)	26	62

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	186	ALA
2	F	186	ALA
2	G	186	ALA
2	H	186	ALA
1	A	416	SER
1	B	631	LEU
1	C	416	SER
1	D	631	LEU
2	E	184	SER
2	F	119	SER
2	G	184	SER
2	H	119	SER
1	A	605	ASN
1	C	605	ASN
2	E	182	TRP
2	F	182	TRP
2	F	184	SER
2	G	182	TRP
2	H	182	TRP
2	H	184	SER
1	A	592	PRO
1	C	592	PRO
1	B	592	PRO
1	D	592	PRO
2	F	116	LYS
2	H	116	LYS
1	A	69	THR

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Mol	Chain	Res	Type
1	C	69	THR
1	B	494	VAL
1	D	494	VAL
2	E	187	VAL
2	G	187	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	735/798 (92%)	717 (98%)	18 (2%)	49 69
1	B	734/798 (92%)	726 (99%)	8 (1%)	73 85
1	C	735/798 (92%)	717 (98%)	18 (2%)	49 69
1	D	734/798 (92%)	726 (99%)	8 (1%)	73 85
2	E	202/203 (100%)	199 (98%)	3 (2%)	65 80
2	F	203/203 (100%)	200 (98%)	3 (2%)	65 80
2	G	202/203 (100%)	199 (98%)	3 (2%)	65 80
2	H	203/203 (100%)	200 (98%)	3 (2%)	65 80
All	All	3748/4004 (94%)	3684 (98%)	64 (2%)	64 78

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	378	ASN
1	A	423	ASN
1	A	428	LEU
1	A	458	ARG
1	A	471[A]	SER
1	A	471[B]	SER
1	A	535[A]	THR
1	A	535[B]	THR
1	A	596	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	604	ASN
1	A	664	MET
1	A	712	ARG
1	A	713	ARG
1	A	800	ARG
1	A	802	ASN
1	A	873	ARG
1	A	874	ARG
1	B	198	ARG
1	B	286	ASN
1	B	354	ARG
1	B	389	LEU
1	B	549	ASN
1	B	663	ARG
1	B	712	ARG
1	B	855	ARG
1	C	170	LYS
1	C	378	ASN
1	C	423	ASN
1	C	428	LEU
1	C	458	ARG
1	C	471[A]	SER
1	C	471[B]	SER
1	C	535[A]	THR
1	C	535[B]	THR
1	C	596	ASN
1	C	604	ASN
1	C	664	MET
1	C	712	ARG
1	C	713	ARG
1	C	800	ARG
1	C	802	ASN
1	C	873	ARG
1	C	874	ARG
1	D	198	ARG
1	D	286	ASN
1	D	354	ARG
1	D	389	LEU
1	D	549	ASN
1	D	663	ARG
1	D	712	ARG
1	D	855	ARG

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Mol	Chain	Res	Type
2	E	59	LYS
2	E	132	GLN
2	E	162	ASN
2	F	59	LYS
2	F	132	GLN
2	F	162	ASN
2	G	59	LYS
2	G	132	GLN
2	G	162	ASN
2	H	59	LYS
2	H	132	GLN
2	H	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	HIS
1	A	508	HIS
1	A	596	ASN
1	A	604	ASN
1	A	605	ASN
1	A	802	ASN
1	A	872	GLN
1	B	286	ASN
1	B	288	GLN
1	B	346	GLN
1	B	430	ASN
1	B	549	ASN
1	B	604	ASN
1	B	610	ASN
1	B	819	ASN
1	C	335	GLN
1	C	350	HIS
1	C	423	ASN
1	C	508	HIS
1	C	596	ASN
1	C	604	ASN
1	C	605	ASN
1	C	714	GLN
1	C	802	ASN
1	C	872	GLN
1	D	286	ASN

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Mol	Chain	Res	Type
1	D	288	GLN
1	D	346	GLN
1	D	430	ASN
1	D	549	ASN
1	D	604	ASN
1	D	610	ASN
1	D	819	ASN
2	E	162	ASN
2	F	162	ASN
2	G	162	ASN
2	H	162	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

102 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
3	NAG	I	1	1,3	14,14,15	1.28	1 (7%)	17,19,21	1.43	2 (11%)
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.49	0
3	BMA	I	3	3	11,11,12	1.82	3 (27%)	15,15,17	2.35	4 (26%)
3	MAN	I	4	3	11,11,12	2.85	3 (27%)	15,15,17	2.34	3 (20%)
3	NAG	I	5	3	14,14,15	1.27	2 (14%)	17,19,21	1.73	1 (5%)
3	GAL	I	6	3	11,11,12	0.56	0	15,15,17	1.39	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	I	7	3	11,11,12	1.40	2 (18%)	15,15,17	1.44	3 (20%)
4	NAG	J	1	4	14,14,15	1.20	1 (7%)	17,19,21	1.35	1 (5%)
4	NAG	J	2	4	14,14,15	0.35	0	17,19,21	0.54	0
5	NAG	K	1	1,5	14,14,15	0.44	0	17,19,21	0.72	0
5	NAG	K	2	5	14,14,15	0.25	0	17,19,21	0.88	1 (5%)
5	BMA	K	3	5	11,11,12	1.21	1 (9%)	15,15,17	1.62	4 (26%)
5	MAN	K	4	5	11,11,12	1.05	1 (9%)	15,15,17	0.92	1 (6%)
5	NAG	K	5	5	14,14,15	0.67	1 (7%)	17,19,21	0.89	1 (5%)
5	GAL	K	6	5	11,11,12	1.29	3 (27%)	15,15,17	1.43	4 (26%)
5	MAN	K	7	5	11,11,12	1.66	3 (27%)	15,15,17	2.11	4 (26%)
5	NAG	K	8	5	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
4	NAG	L	1	1,4	14,14,15	1.41	1 (7%)	17,19,21	1.51	1 (5%)
4	NAG	L	2	4	14,14,15	0.36	0	17,19,21	0.48	0
6	NAG	M	1	1,6	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
6	NAG	M	2	6	14,14,15	0.27	0	17,19,21	0.46	0
6	BMA	M	3	6	11,11,12	0.80	0	15,15,17	1.19	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.74	0
4	NAG	N	2	4	14,14,15	1.30	1 (7%)	17,19,21	2.24	3 (17%)
4	NAG	O	1	1,4	14,14,15	1.49	2 (14%)	17,19,21	1.51	1 (5%)
4	NAG	O	2	4	14,14,15	0.43	0	17,19,21	0.50	0
7	NAG	P	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	1.17	2 (11%)
7	NAG	P	2	7	14,14,15	0.84	1 (7%)	17,19,21	2.29	3 (17%)
7	BMA	P	3	7	11,11,12	1.12	1 (9%)	15,15,17	1.10	1 (6%)
7	BMA	P	4	7	11,11,12	0.83	0	15,15,17	0.85	0
4	NAG	Q	1	1,4	14,14,15	0.67	1 (7%)	17,19,21	1.49	1 (5%)
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.56	0
8	NAG	R	1	1,8	14,14,15	1.53	1 (7%)	17,19,21	1.63	5 (29%)
8	NAG	R	2	8	14,14,15	0.30	0	17,19,21	1.14	1 (5%)
8	BMA	R	3	8	11,11,12	1.72	2 (18%)	15,15,17	2.64	4 (26%)
8	MAN	R	4	8	11,11,12	0.95	0	15,15,17	1.62	3 (20%)
8	NAG	R	5	8	14,14,15	1.30	2 (14%)	17,19,21	2.43	4 (23%)
8	MAN	R	6	8	11,11,12	0.89	0	15,15,17	0.99	1 (6%)
8	NAG	R	7	8	14,14,15	1.57	2 (14%)	17,19,21	1.36	1 (5%)
6	NAG	S	1	1,6	14,14,15	0.46	0	17,19,21	0.68	0
6	NAG	S	2	6	14,14,15	0.29	0	17,19,21	0.92	1 (5%)
6	BMA	S	3	6	11,11,12	1.17	1 (9%)	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	T	1	1,6	14,14,15	0.26	0	17,19,21	0.56	0
6	NAG	T	2	6	14,14,15	0.29	0	17,19,21	0.53	0
6	BMA	T	3	6	11,11,12	1.24	2 (18%)	15,15,17	1.59	3 (20%)
9	NAG	U	1	1,9	14,14,15	0.52	0	17,19,21	0.90	0
9	NAG	U	2	9	14,14,15	1.58	2 (14%)	17,19,21	1.60	2 (11%)
9	BMA	U	3	9	11,11,12	1.15	1 (9%)	15,15,17	2.22	2 (13%)
9	MAN	U	4	9	11,11,12	1.69	2 (18%)	15,15,17	2.00	3 (20%)
4	NAG	V	1	1,4	14,14,15	1.59	2 (14%)	17,19,21	1.30	1 (5%)
4	NAG	V	2	4	14,14,15	0.50	0	17,19,21	0.65	1 (5%)
3	NAG	W	1	1,3	14,14,15	1.13	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	W	2	3	14,14,15	0.35	0	17,19,21	1.03	1 (5%)
3	BMA	W	3	3	11,11,12	2.13	4 (36%)	15,15,17	1.72	5 (33%)
3	MAN	W	4	3	11,11,12	1.62	3 (27%)	15,15,17	1.89	3 (20%)
3	NAG	W	5	3	14,14,15	0.16	0	17,19,21	1.47	1 (5%)
3	GAL	W	6	3	11,11,12	1.07	2 (18%)	15,15,17	1.77	2 (13%)
3	MAN	W	7	3	11,11,12	0.94	1 (9%)	15,15,17	1.67	3 (20%)
4	NAG	X	1	4	14,14,15	1.28	2 (14%)	17,19,21	1.33	1 (5%)
4	NAG	X	2	4	14,14,15	0.34	0	17,19,21	0.53	0
8	NAG	Y	1	1,8	14,14,15	0.49	0	17,19,21	0.66	0
8	NAG	Y	2	8	14,14,15	0.62	0	17,19,21	0.58	0
8	BMA	Y	3	8	11,11,12	2.05	3 (27%)	15,15,17	2.03	6 (40%)
8	MAN	Y	4	8	11,11,12	1.00	1 (9%)	15,15,17	1.20	2 (13%)
8	NAG	Y	5	8	14,14,15	0.38	0	17,19,21	0.54	0
8	MAN	Y	6	8	11,11,12	1.19	2 (18%)	15,15,17	1.58	2 (13%)
8	NAG	Y	7	8	14,14,15	0.52	0	17,19,21	0.48	0
4	NAG	Z	1	1,4	14,14,15	1.47	1 (7%)	17,19,21	1.41	1 (5%)
4	NAG	Z	2	4	14,14,15	0.38	0	17,19,21	0.49	0
6	NAG	a	1	1,6	14,14,15	0.27	0	17,19,21	0.61	0
6	NAG	a	2	6	14,14,15	0.27	0	17,19,21	0.52	0
6	BMA	a	3	6	11,11,12	0.97	1 (9%)	15,15,17	0.80	0
4	NAG	b	1	1,4	14,14,15	0.57	0	17,19,21	0.67	0
4	NAG	b	2	4	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	c	1	1,4	14,14,15	1.27	2 (14%)	17,19,21	1.63	2 (11%)
4	NAG	c	2	4	14,14,15	1.23	1 (7%)	17,19,21	1.23	1 (5%)
7	NAG	d	1	1,7	14,14,15	0.92	1 (7%)	17,19,21	1.22	2 (11%)
7	NAG	d	2	7	14,14,15	0.41	0	17,19,21	1.12	1 (5%)
7	BMA	d	3	7	11,11,12	0.87	0	15,15,17	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	d	4	7	11,11,12	0.84	0	15,15,17	0.79	0
4	NAG	e	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	1.11	2 (11%)
4	NAG	e	2	4	14,14,15	0.34	0	17,19,21	0.54	0
8	NAG	f	1	1,8	14,14,15	0.67	1 (7%)	17,19,21	1.31	3 (17%)
8	NAG	f	2	8	14,14,15	0.99	2 (14%)	17,19,21	0.59	0
8	BMA	f	3	8	11,11,12	1.49	3 (27%)	15,15,17	1.60	2 (13%)
8	MAN	f	4	8	11,11,12	0.86	0	15,15,17	1.26	1 (6%)
8	NAG	f	5	8	14,14,15	0.46	0	17,19,21	0.40	0
8	MAN	f	6	8	11,11,12	1.06	1 (9%)	15,15,17	1.58	3 (20%)
8	NAG	f	7	8	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
6	NAG	g	1	1,6	14,14,15	0.73	0	17,19,21	1.27	3 (17%)
6	NAG	g	2	6	14,14,15	1.65	1 (7%)	17,19,21	2.01	2 (11%)
6	BMA	g	3	6	11,11,12	0.76	0	15,15,17	0.85	0
9	NAG	h	1	1,9	14,14,15	0.25	0	17,19,21	0.55	0
9	NAG	h	2	9	14,14,15	0.36	0	17,19,21	0.48	0
9	BMA	h	3	9	11,11,12	1.62	4 (36%)	15,15,17	1.73	3 (20%)
9	MAN	h	4	9	11,11,12	1.46	3 (27%)	15,15,17	1.35	1 (6%)
9	NAG	i	1	1,9	14,14,15	0.49	0	17,19,21	1.12	2 (11%)
9	NAG	i	2	9	14,14,15	0.95	1 (7%)	17,19,21	2.29	4 (23%)
9	BMA	i	3	9	11,11,12	0.78	0	15,15,17	0.90	1 (6%)
9	MAN	i	4	9	11,11,12	1.46	2 (18%)	15,15,17	1.92	5 (33%)
4	NAG	j	1	1,4	14,14,15	1.55	2 (14%)	17,19,21	1.37	1 (5%)
4	NAG	j	2	4	14,14,15	0.50	0	17,19,21	0.69	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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	1/2/19/22	1/1/1/1
3	NAG	I	5	3	-	2/6/23/26	0/1/1/1
3	GAL	I	6	3	-	2/2/19/22	0/1/1/1
3	MAN	I	7	3	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	2/2/19/22	1/1/1/1
5	NAG	K	5	5	-	0/6/23/26	0/1/1/1
5	GAL	K	6	5	-	1/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1
5	NAG	K	8	5	-	1/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	5/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
7	NAG	P	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	5/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	BMA	P	4	7	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
8	NAG	R	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	0/2/19/22	0/1/1/1
8	MAN	R	4	8	-	2/2/19/22	0/1/1/1
8	NAG	R	5	8	-	5/6/23/26	0/1/1/1
8	MAN	R	6	8	-	0/2/19/22	0/1/1/1
8	NAG	R	7	8	-	3/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	3/6/23/26	0/1/1/1

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

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

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	MAN	O2-C2	7.42	1.59	1.43
6	g	2	NAG	O5-C1	5.79	1.53	1.43
8	R	1	NAG	O5-C1	-5.58	1.34	1.43
4	Z	1	NAG	O5-C1	5.29	1.52	1.43
8	Y	3	BMA	C1-C2	5.17	1.64	1.52
4	L	1	NAG	O5-C1	5.13	1.51	1.43
4	V	1	NAG	O5-C1	5.07	1.51	1.43
9	U	2	NAG	O5-C1	5.04	1.51	1.43
4	j	1	NAG	O5-C1	4.95	1.51	1.43
4	O	1	NAG	O5-C1	4.89	1.51	1.43
8	R	7	NAG	O5-C1	4.81	1.51	1.43
3	I	4	MAN	C2-C3	4.68	1.59	1.52
8	R	3	BMA	O5-C1	4.36	1.50	1.43
3	I	1	NAG	O5-C1	-4.28	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	2	NAG	C1-C2	4.27	1.58	1.52
4	X	1	NAG	O5-C1	4.17	1.50	1.43
4	c	2	NAG	O5-C1	4.15	1.50	1.43
3	I	5	NAG	O5-C1	3.96	1.50	1.43
3	W	1	NAG	O5-C1	-3.93	1.37	1.43
4	c	1	NAG	O5-C1	3.86	1.49	1.43
4	J	1	NAG	O5-C1	3.82	1.49	1.43
3	W	3	BMA	C4-C3	3.72	1.61	1.52
9	U	4	MAN	C1-C2	3.61	1.60	1.52
8	Y	3	BMA	C2-C3	3.58	1.57	1.52
3	W	3	BMA	O5-C1	-3.48	1.38	1.43
3	W	3	BMA	C4-C5	3.48	1.60	1.53
5	K	7	MAN	C1-C2	3.35	1.59	1.52
8	R	5	NAG	O5-C1	-3.29	1.38	1.43
8	f	3	BMA	C1-C2	3.22	1.59	1.52
5	K	7	MAN	O5-C5	3.16	1.49	1.43
3	W	4	MAN	C1-C2	3.16	1.59	1.52
8	R	7	NAG	C1-C2	3.07	1.56	1.52
9	i	4	MAN	C2-C3	3.06	1.57	1.52
7	d	1	NAG	O5-C1	3.03	1.48	1.43
9	U	4	MAN	C2-C3	3.01	1.56	1.52
3	I	3	BMA	O5-C1	2.98	1.48	1.43
9	i	2	NAG	C1-C2	2.91	1.56	1.52
3	I	3	BMA	O5-C5	2.86	1.49	1.43
8	R	5	NAG	C1-C2	2.85	1.56	1.52
9	h	3	BMA	C2-C3	2.84	1.56	1.52
8	Y	6	MAN	C1-C2	2.79	1.58	1.52
9	U	2	NAG	C1-C2	2.78	1.56	1.52
4	V	1	NAG	C1-C2	2.77	1.56	1.52
5	K	7	MAN	O5-C1	2.73	1.48	1.43
9	U	3	BMA	O5-C5	2.73	1.49	1.43
4	j	1	NAG	C1-C2	2.72	1.56	1.52
5	K	6	GAL	C2-C3	2.65	1.56	1.52
3	W	3	BMA	C2-C3	2.64	1.56	1.52
9	h	4	MAN	C2-C3	2.63	1.56	1.52
3	I	7	MAN	O5-C1	-2.63	1.39	1.43
8	f	6	MAN	C2-C3	2.62	1.56	1.52
5	K	3	BMA	O3-C3	2.61	1.49	1.43
3	I	4	MAN	C1-C2	2.60	1.58	1.52
4	N	1	NAG	O5-C1	2.59	1.47	1.43
9	h	4	MAN	O5-C5	2.58	1.48	1.43
8	Y	4	MAN	C1-C2	2.57	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5	NAG	C1-C2	2.57	1.56	1.52
4	c	1	NAG	C1-C2	2.57	1.56	1.52
4	e	1	NAG	C1-C2	2.53	1.56	1.52
3	I	3	BMA	C4-C5	2.53	1.58	1.53
8	f	2	NAG	O5-C1	2.51	1.47	1.43
8	f	2	NAG	C1-C2	2.50	1.56	1.52
7	P	1	NAG	O5-C1	2.46	1.47	1.43
3	W	4	MAN	O5-C1	2.44	1.47	1.43
6	S	3	BMA	C2-C3	2.44	1.56	1.52
3	W	6	GAL	C1-C2	2.41	1.57	1.52
9	h	3	BMA	O5-C5	2.40	1.48	1.43
3	W	4	MAN	C2-C3	2.38	1.56	1.52
3	W	7	MAN	C1-C2	2.38	1.57	1.52
7	P	3	BMA	C1-C2	2.36	1.57	1.52
4	Q	1	NAG	O5-C1	2.35	1.47	1.43
9	h	3	BMA	C1-C2	2.34	1.57	1.52
9	i	4	MAN	C1-C2	2.34	1.57	1.52
4	O	1	NAG	C1-C2	2.32	1.55	1.52
7	P	2	NAG	C1-C2	2.29	1.55	1.52
3	I	7	MAN	C4-C5	2.29	1.57	1.53
8	f	3	BMA	C2-C3	2.25	1.55	1.52
6	T	3	BMA	C1-C2	2.22	1.57	1.52
8	Y	6	MAN	O5-C5	2.19	1.47	1.43
8	R	3	BMA	O5-C5	2.17	1.47	1.43
5	K	5	NAG	O5-C1	-2.17	1.40	1.43
8	f	1	NAG	C1-C2	2.15	1.55	1.52
9	h	4	MAN	C1-C2	2.15	1.57	1.52
6	a	3	BMA	C1-C2	2.14	1.57	1.52
6	T	3	BMA	C4-C3	2.13	1.57	1.52
3	W	6	GAL	O5-C1	2.13	1.47	1.43
5	K	6	GAL	C4-C3	2.12	1.57	1.52
9	h	3	BMA	O5-C1	2.10	1.47	1.43
5	K	4	MAN	C1-C2	2.09	1.57	1.52
5	K	6	GAL	C1-C2	2.08	1.56	1.52
8	f	3	BMA	C6-C5	2.08	1.58	1.51
8	Y	3	BMA	C4-C3	2.03	1.57	1.52
4	X	1	NAG	C1-C2	2.01	1.55	1.52

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	2	NAG	C2-N2-C7	7.92	134.18	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C2-N2-C7	7.81	134.03	122.90
9	i	2	NAG	C2-N2-C7	7.77	133.96	122.90
8	R	5	NAG	C2-N2-C7	7.53	133.62	122.90
3	I	3	BMA	C1-O5-C5	7.32	122.11	112.19
9	U	3	BMA	C1-O5-C5	7.31	122.09	112.19
6	g	2	NAG	C1-O5-C5	7.06	121.75	112.19
8	R	3	BMA	C1-O5-C5	7.02	121.71	112.19
3	I	4	MAN	C1-O5-C5	6.82	121.43	112.19
3	I	5	NAG	C1-O5-C5	6.33	120.77	112.19
9	U	2	NAG	C1-O5-C5	5.83	120.10	112.19
4	L	1	NAG	C1-O5-C5	5.75	119.99	112.19
4	Q	1	NAG	C1-O5-C5	5.70	119.91	112.19
9	U	4	MAN	C1-O5-C5	5.57	119.74	112.19
4	Z	1	NAG	C1-O5-C5	5.56	119.73	112.19
9	i	4	MAN	C1-O5-C5	5.50	119.64	112.19
5	K	7	MAN	C1-O5-C5	5.49	119.63	112.19
3	W	4	MAN	C1-O5-C5	5.41	119.53	112.19
4	O	1	NAG	C1-O5-C5	5.39	119.49	112.19
4	c	1	NAG	C1-O5-C5	5.30	119.37	112.19
4	j	1	NAG	C1-O5-C5	5.29	119.36	112.19
3	W	5	NAG	C1-O5-C5	5.13	119.14	112.19
8	R	7	NAG	C1-O5-C5	5.12	119.13	112.19
8	Y	6	MAN	C1-O5-C5	5.10	119.10	112.19
4	J	1	NAG	C1-O5-C5	5.06	119.05	112.19
4	V	1	NAG	C1-O5-C5	5.00	118.97	112.19
9	h	3	BMA	C1-O5-C5	5.00	118.96	112.19
4	X	1	NAG	C1-O5-C5	4.99	118.95	112.19
3	W	6	GAL	C1-O5-C5	4.91	118.85	112.19
4	c	2	NAG	C1-O5-C5	4.91	118.84	112.19
3	W	7	MAN	C1-O5-C5	4.57	118.39	112.19
8	R	3	BMA	C3-C4-C5	-4.49	102.22	110.24
5	K	7	MAN	O2-C2-C3	-4.32	101.49	110.14
3	I	6	GAL	C1-O5-C5	4.27	117.98	112.19
3	I	1	NAG	C3-C4-C5	4.16	117.66	110.24
8	R	5	NAG	C1-C2-N2	3.87	117.10	110.49
8	R	3	BMA	O5-C1-C2	3.85	116.71	110.77
6	T	3	BMA	C1-O5-C5	3.83	117.38	112.19
3	I	4	MAN	O2-C2-C3	3.73	117.61	110.14
8	Y	3	BMA	C1-C2-C3	3.73	114.25	109.67
4	N	2	NAG	C1-C2-N2	3.70	116.80	110.49
3	W	1	NAG	C3-C4-C5	3.67	116.79	110.24
9	h	4	MAN	C1-O5-C5	3.65	117.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	4	MAN	C1-O5-C5	3.65	117.13	112.19
8	f	6	MAN	O2-C2-C1	-3.60	101.79	109.15
3	I	4	MAN	O2-C2-C1	3.57	116.45	109.15
8	R	1	NAG	C3-C4-C5	3.53	116.54	110.24
3	W	3	BMA	C2-C3-C4	3.51	116.97	110.89
3	W	4	MAN	O2-C2-C1	-3.50	102.00	109.15
7	P	2	NAG	C1-C2-N2	3.47	116.42	110.49
8	R	4	MAN	O2-C2-C1	3.43	116.17	109.15
8	f	3	BMA	O5-C5-C6	3.42	112.57	107.20
8	Y	3	BMA	C2-C3-C4	3.41	116.80	110.89
5	K	3	BMA	O3-C3-C2	3.32	116.35	109.99
5	K	3	BMA	C1-O5-C5	3.30	116.66	112.19
3	W	6	GAL	C1-C2-C3	3.23	113.64	109.67
8	f	1	NAG	O4-C4-C3	3.22	117.78	110.35
9	U	4	MAN	O2-C2-C3	-3.18	103.77	110.14
8	R	1	NAG	C2-N2-C7	3.17	127.42	122.90
8	Y	4	MAN	O2-C2-C3	-3.16	103.81	110.14
8	R	5	NAG	C4-C3-C2	3.14	115.62	111.02
7	d	1	NAG	C1-O5-C5	3.13	116.43	112.19
6	g	1	NAG	C2-N2-C7	3.13	127.35	122.90
7	d	2	NAG	C2-N2-C7	3.12	127.34	122.90
5	K	8	NAG	C2-N2-C7	3.10	127.32	122.90
8	f	7	NAG	C1-O5-C5	3.10	116.39	112.19
8	R	5	NAG	C3-C4-C5	3.10	115.77	110.24
6	g	2	NAG	C2-N2-C7	3.08	127.29	122.90
8	R	2	NAG	C1-O5-C5	3.08	116.36	112.19
3	W	2	NAG	O4-C4-C5	-3.04	101.75	109.30
5	K	2	NAG	C1-O5-C5	3.04	116.31	112.19
9	U	3	BMA	O5-C1-C2	3.02	115.43	110.77
7	P	1	NAG	C1-O5-C5	2.99	116.24	112.19
4	c	1	NAG	C2-N2-C7	2.98	127.15	122.90
8	f	1	NAG	C2-N2-C7	2.98	127.15	122.90
9	i	2	NAG	C1-C2-N2	2.96	115.54	110.49
8	f	3	BMA	C1-C2-C3	2.92	113.25	109.67
3	I	3	BMA	O5-C1-C2	2.91	115.26	110.77
4	e	1	NAG	C2-N2-C7	2.89	127.02	122.90
8	R	4	MAN	C1-O5-C5	2.89	116.11	112.19
5	K	6	GAL	O5-C1-C2	-2.89	106.31	110.77
6	S	3	BMA	C2-C3-C4	2.88	115.88	110.89
3	I	7	MAN	C1-O5-C5	2.86	116.07	112.19
8	R	6	MAN	O2-C2-C3	-2.85	104.43	110.14
8	Y	3	BMA	C1-O5-C5	-2.82	108.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	3	BMA	O5-C5-C6	2.81	111.61	107.20
3	I	7	MAN	O2-C2-C3	-2.79	104.55	110.14
3	W	3	BMA	O5-C1-C2	-2.76	106.52	110.77
4	e	1	NAG	C1-O5-C5	2.75	115.92	112.19
7	d	1	NAG	O4-C4-C5	2.71	116.02	109.30
8	Y	4	MAN	C1-O5-C5	2.70	115.84	112.19
3	I	3	BMA	C3-C4-C5	2.69	115.04	110.24
8	f	6	MAN	O3-C3-C2	2.69	115.15	109.99
3	I	1	NAG	C4-C3-C2	2.67	114.93	111.02
6	M	3	BMA	C1-O5-C5	2.66	115.79	112.19
8	R	3	BMA	O5-C5-C6	2.63	111.33	107.20
8	R	1	NAG	O4-C4-C3	-2.62	104.28	110.35
8	f	6	MAN	O5-C1-C2	-2.62	106.73	110.77
5	K	6	GAL	C1-C2-C3	2.61	112.87	109.67
8	Y	3	BMA	O2-C2-C1	2.56	114.40	109.15
9	i	4	MAN	C1-C2-C3	2.54	112.78	109.67
9	i	4	MAN	O5-C1-C2	2.54	114.69	110.77
3	W	3	BMA	C3-C4-C5	2.51	114.72	110.24
5	K	3	BMA	C1-C2-C3	-2.50	106.59	109.67
5	K	4	MAN	C1-O5-C5	2.50	115.58	112.19
9	i	3	BMA	C1-O5-C5	2.50	115.58	112.19
6	T	3	BMA	O5-C1-C2	2.49	114.61	110.77
7	P	1	NAG	O4-C4-C5	2.48	115.46	109.30
6	T	3	BMA	C2-C3-C4	2.47	115.17	110.89
5	K	3	BMA	O3-C3-C4	2.45	116.01	110.35
3	W	7	MAN	O2-C2-C3	-2.43	105.28	110.14
9	i	1	NAG	C1-C2-N2	2.38	114.55	110.49
4	V	2	NAG	C1-O5-C5	2.34	115.36	112.19
9	i	2	NAG	C1-O5-C5	2.33	115.35	112.19
8	R	1	NAG	C4-C3-C2	2.32	114.42	111.02
6	g	1	NAG	C1-O5-C5	2.32	115.34	112.19
5	K	7	MAN	C3-C4-C5	-2.32	106.10	110.24
3	W	4	MAN	O3-C3-C2	2.32	114.43	109.99
9	U	2	NAG	C4-C3-C2	2.31	114.40	111.02
3	W	3	BMA	C1-O5-C5	2.31	115.32	112.19
5	K	7	MAN	O2-C2-C1	2.30	113.86	109.15
9	h	3	BMA	C2-C3-C4	2.27	114.83	110.89
3	W	1	NAG	O4-C4-C3	-2.27	105.10	110.35
6	S	3	BMA	O2-C2-C3	-2.26	105.60	110.14
7	d	3	BMA	C1-C2-C3	-2.26	106.88	109.67
3	I	7	MAN	C2-C3-C4	2.26	114.81	110.89
8	Y	6	MAN	O2-C2-C3	-2.26	105.61	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	4	MAN	C2-C3-C4	2.23	114.76	110.89
9	i	1	NAG	O3-C3-C4	2.20	115.44	110.35
9	i	2	NAG	C8-C7-N2	2.18	119.79	116.10
7	P	2	NAG	C8-C7-N2	2.16	119.76	116.10
6	g	1	NAG	C1-C2-N2	2.16	114.17	110.49
3	I	3	BMA	O3-C3-C4	2.14	115.31	110.35
5	K	6	GAL	C2-C3-C4	2.14	114.60	110.89
9	h	3	BMA	O5-C1-C2	2.14	114.08	110.77
3	W	3	BMA	C6-C5-C4	2.14	118.01	113.00
6	M	1	NAG	C1-O5-C5	2.13	115.08	112.19
7	P	3	BMA	O2-C2-C3	-2.12	105.89	110.14
4	N	2	NAG	C8-C7-N2	2.12	119.69	116.10
9	i	4	MAN	C2-C3-C4	2.10	114.54	110.89
4	j	2	NAG	C1-O5-C5	2.10	115.04	112.19
9	i	4	MAN	O2-C2-C3	-2.09	105.94	110.14
5	K	5	NAG	O4-C4-C3	-2.08	105.53	110.35
3	W	7	MAN	C1-C2-C3	2.08	112.23	109.67
8	R	4	MAN	C3-C4-C5	-2.08	106.53	110.24
6	S	2	NAG	C3-C4-C5	2.04	113.88	110.24
8	R	1	NAG	O4-C4-C5	-2.04	104.22	109.30
8	Y	3	BMA	C3-C4-C5	2.04	113.88	110.24
8	f	1	NAG	C1-O5-C5	2.03	114.94	112.19
5	K	6	GAL	C1-O5-C5	-2.00	109.48	112.19

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	3	BMA	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
9	i	3	BMA	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
3	W	3	BMA	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
5	K	4	MAN	C4-C5-C6-O6
8	f	4	MAN	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
3	I	7	MAN	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
6	M	3	BMA	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
3	W	3	BMA	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
5	K	4	MAN	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
8	R	4	MAN	O5-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
8	f	4	MAN	O5-C5-C6-O6
9	i	3	BMA	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6
3	I	5	NAG	C4-C5-C6-O6
3	I	7	MAN	C4-C5-C6-O6
9	U	3	BMA	C4-C5-C6-O6
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	O	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	O	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	e	2	NAG	C8-C7-N2-C2
4	e	2	NAG	O7-C7-N2-C2
4	j	2	NAG	C8-C7-N2-C2
4	j	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	T	2	NAG	C8-C7-N2-C2
6	T	2	NAG	O7-C7-N2-C2
6	a	1	NAG	C8-C7-N2-C2
6	a	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
8	R	2	NAG	C8-C7-N2-C2
8	R	2	NAG	O7-C7-N2-C2
8	R	5	NAG	C8-C7-N2-C2
8	R	5	NAG	O7-C7-N2-C2
8	R	7	NAG	C8-C7-N2-C2
8	R	7	NAG	O7-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
8	Y	5	NAG	C8-C7-N2-C2
8	Y	5	NAG	O7-C7-N2-C2
8	Y	7	NAG	C8-C7-N2-C2
8	Y	7	NAG	O7-C7-N2-C2
8	f	2	NAG	C8-C7-N2-C2
8	f	2	NAG	O7-C7-N2-C2
8	f	7	NAG	C8-C7-N2-C2
8	f	7	NAG	O7-C7-N2-C2
9	U	1	NAG	C8-C7-N2-C2
9	U	1	NAG	O7-C7-N2-C2
9	h	1	NAG	C8-C7-N2-C2
9	h	1	NAG	O7-C7-N2-C2
9	i	1	NAG	C8-C7-N2-C2
9	i	1	NAG	O7-C7-N2-C2
9	i	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	i	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
8	f	6	MAN	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
8	Y	4	MAN	O5-C5-C6-O6
3	W	7	MAN	O5-C5-C6-O6
9	h	4	MAN	O5-C5-C6-O6
8	f	7	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
8	R	5	NAG	O5-C5-C6-O6
7	P	4	BMA	O5-C5-C6-O6
8	Y	6	MAN	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
4	j	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
8	f	6	MAN	O5-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
8	Y	6	MAN	O5-C5-C6-O6
7	P	4	BMA	C4-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
3	I	6	GAL	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
3	W	4	MAN	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
5	K	6	GAL	C4-C5-C6-O6

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

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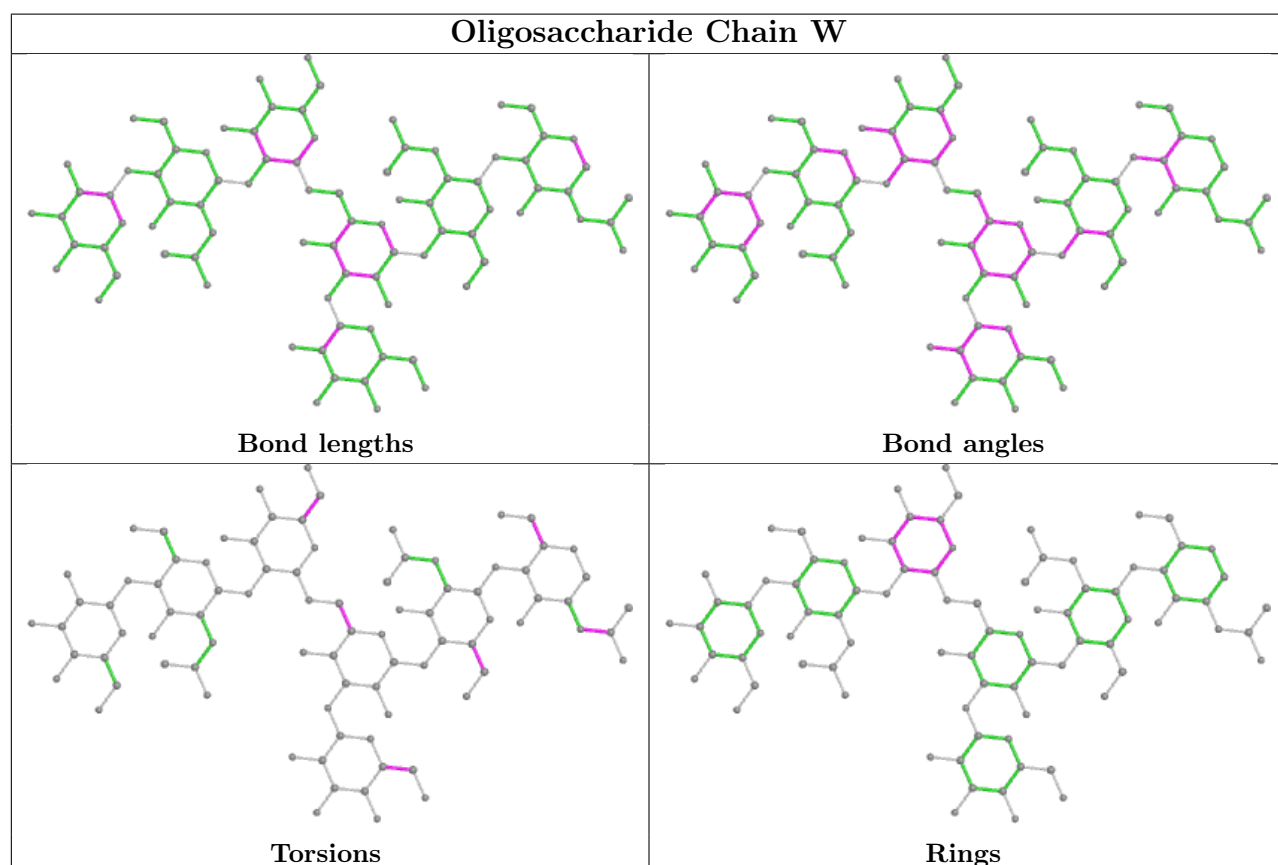
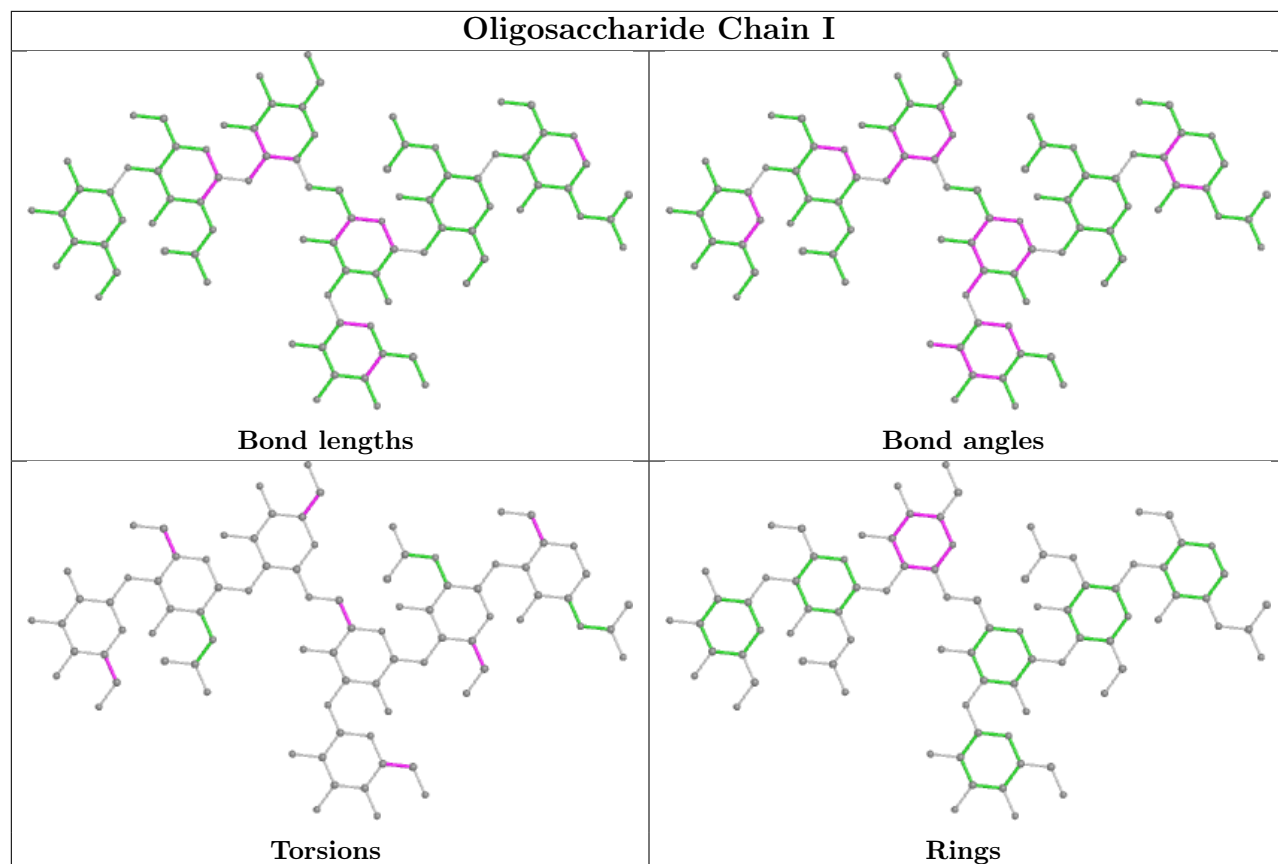
Mol	Chain	Res	Type	Atoms
4	c	1	NAG	C3-C2-N2-C7
5	K	8	NAG	C3-C2-N2-C7
7	P	2	NAG	C3-C2-N2-C7
7	d	2	NAG	C3-C2-N2-C7
8	R	1	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
9	i	2	NAG	C3-C2-N2-C7
9	U	2	NAG	O5-C5-C6-O6
9	U	2	NAG	C4-C5-C6-O6
6	g	2	NAG	C1-C2-N2-C7

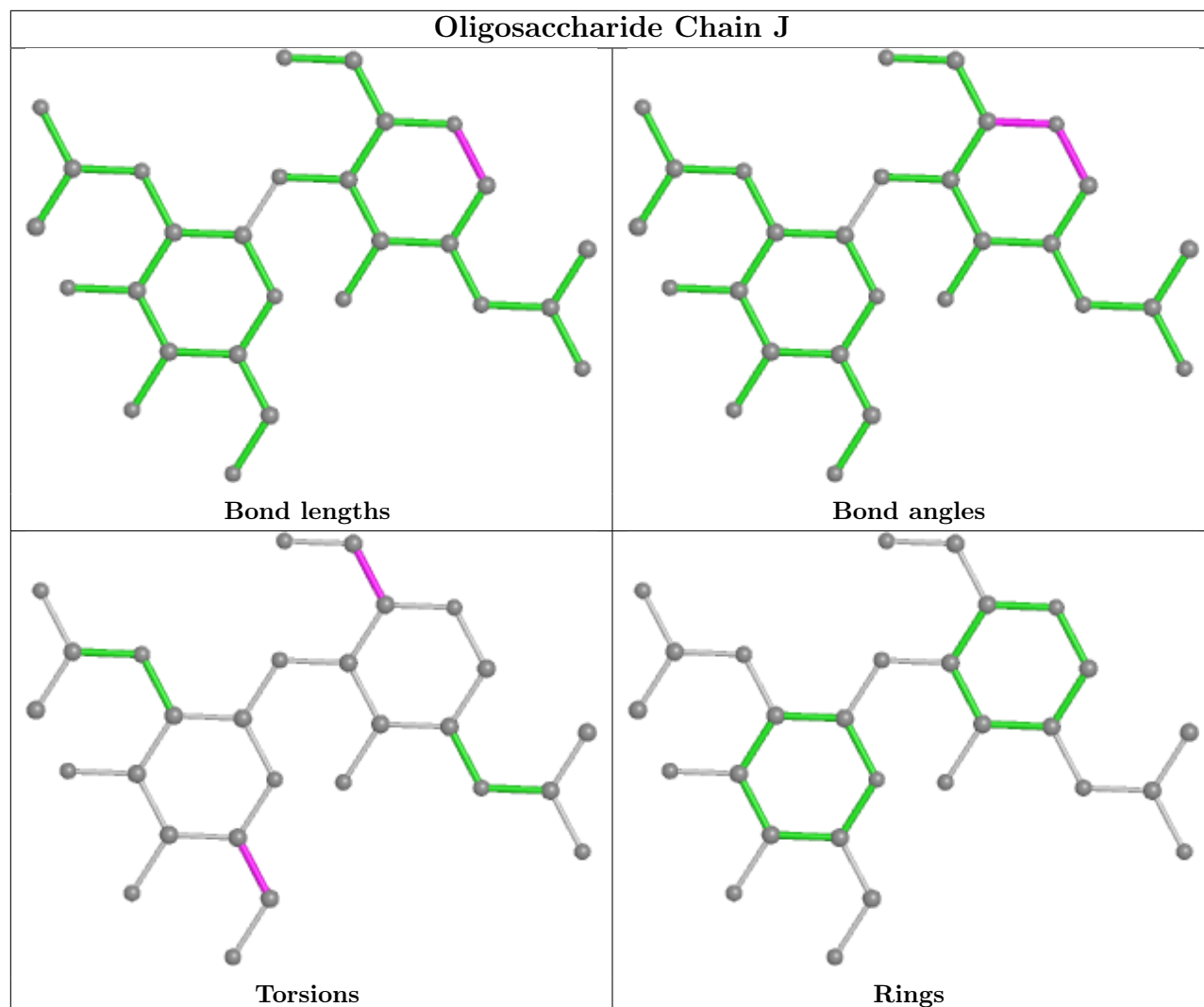
All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	4	MAN	C1-C2-C3-C4-C5-O5
8	Y	6	MAN	C1-C2-C3-C4-C5-O5
8	f	4	MAN	C1-C2-C3-C4-C5-O5
3	I	4	MAN	C1-C2-C3-C4-C5-O5
3	W	4	MAN	C1-C2-C3-C4-C5-O5

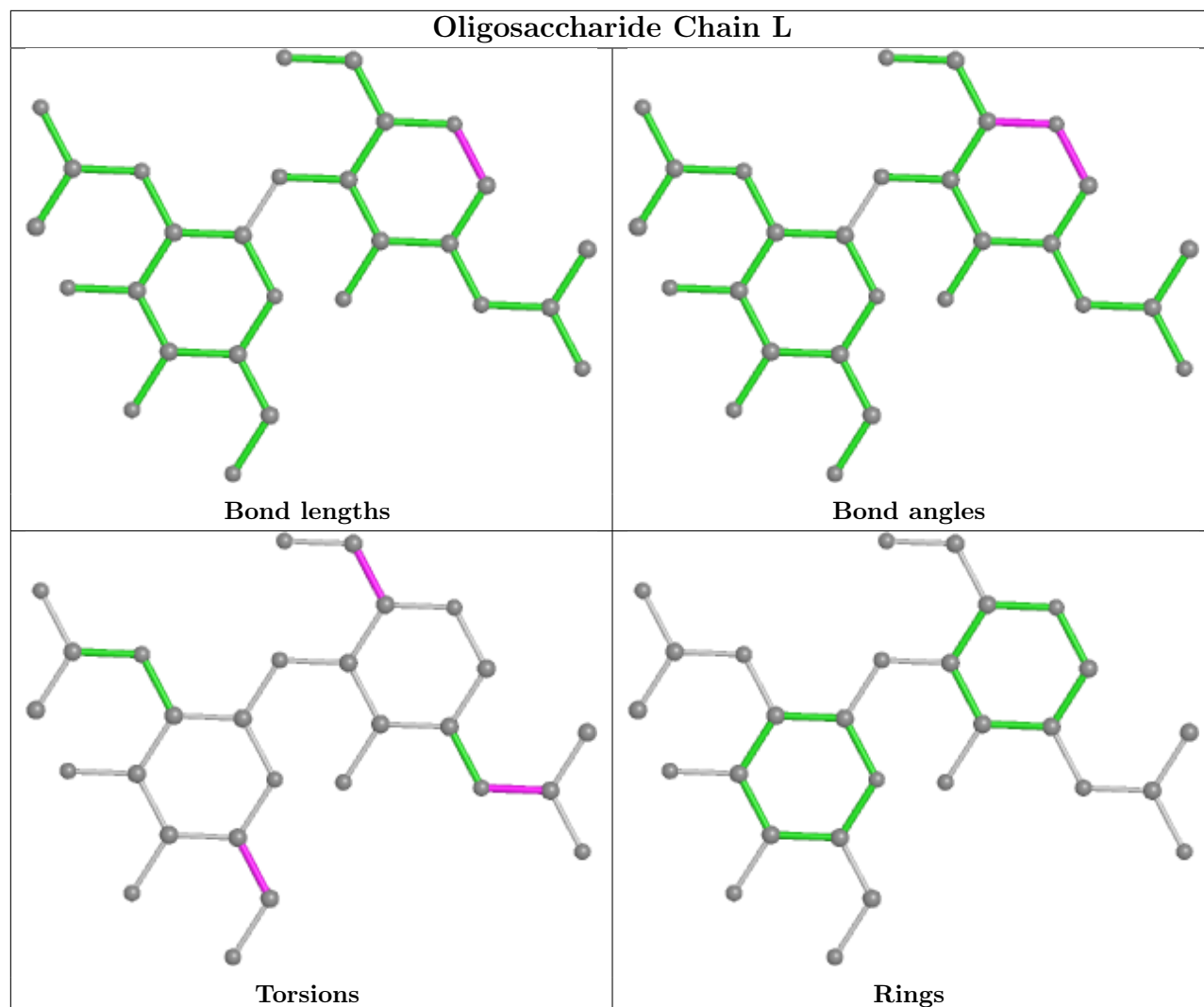
No monomer is involved in short contacts.

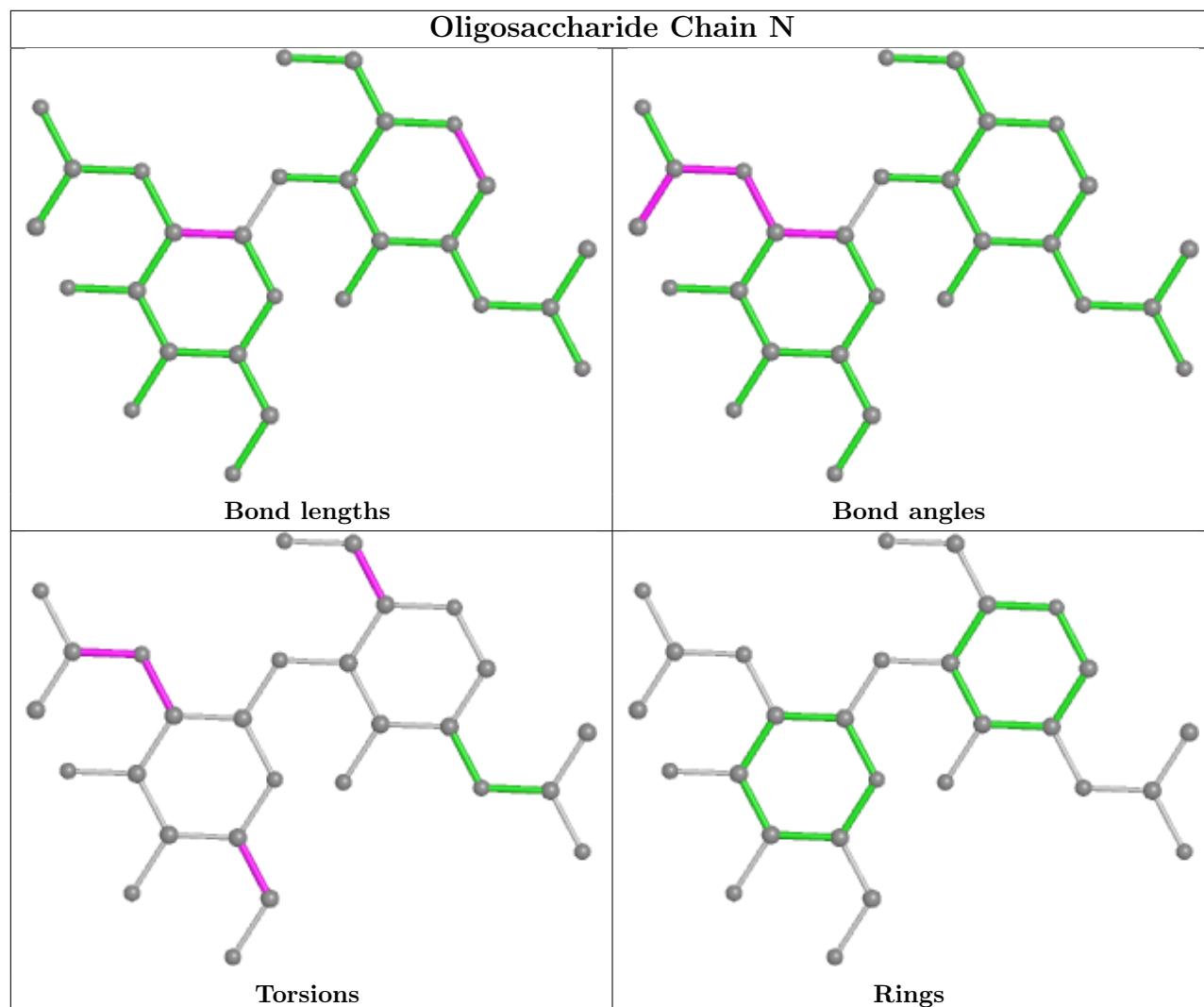
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

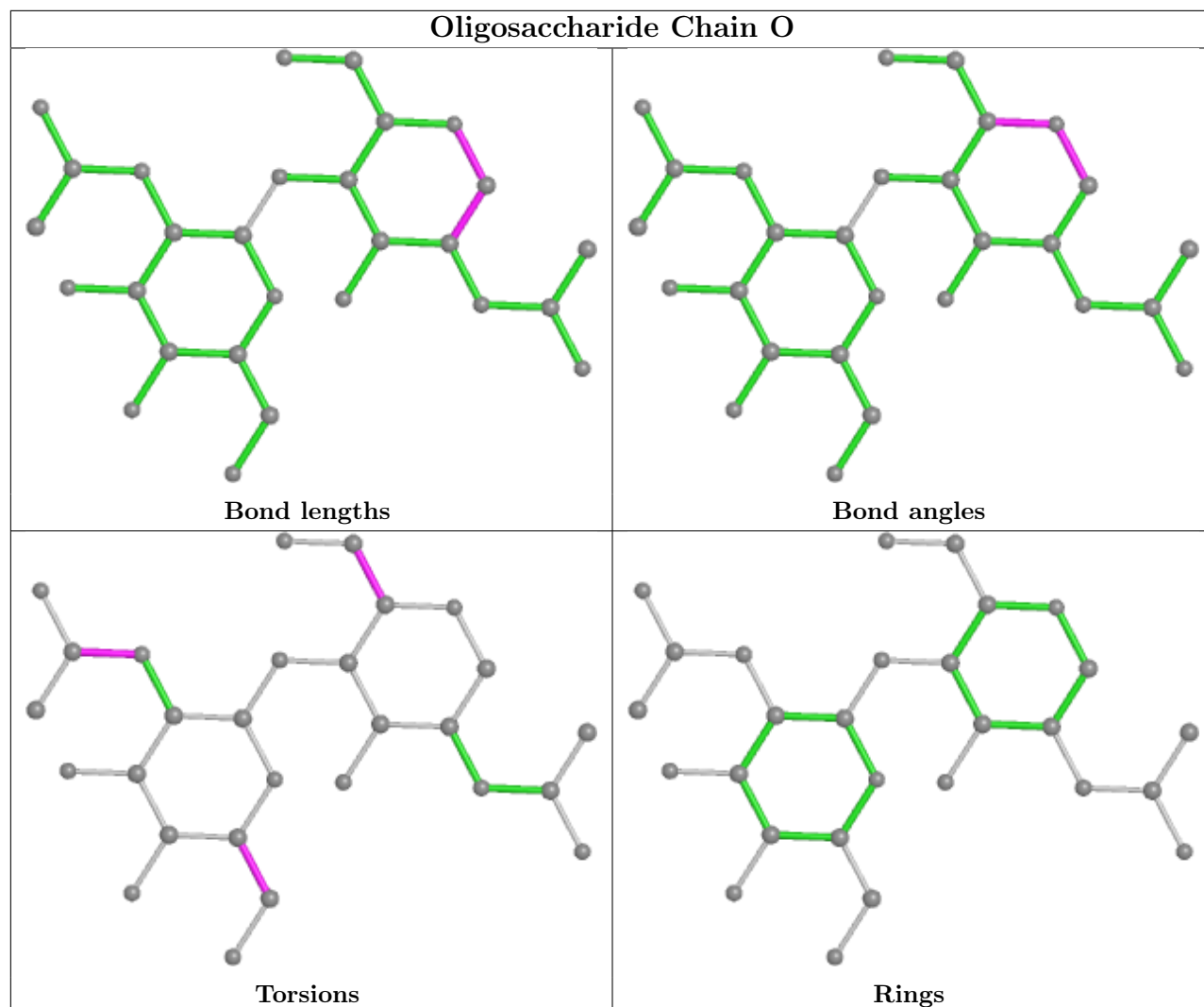


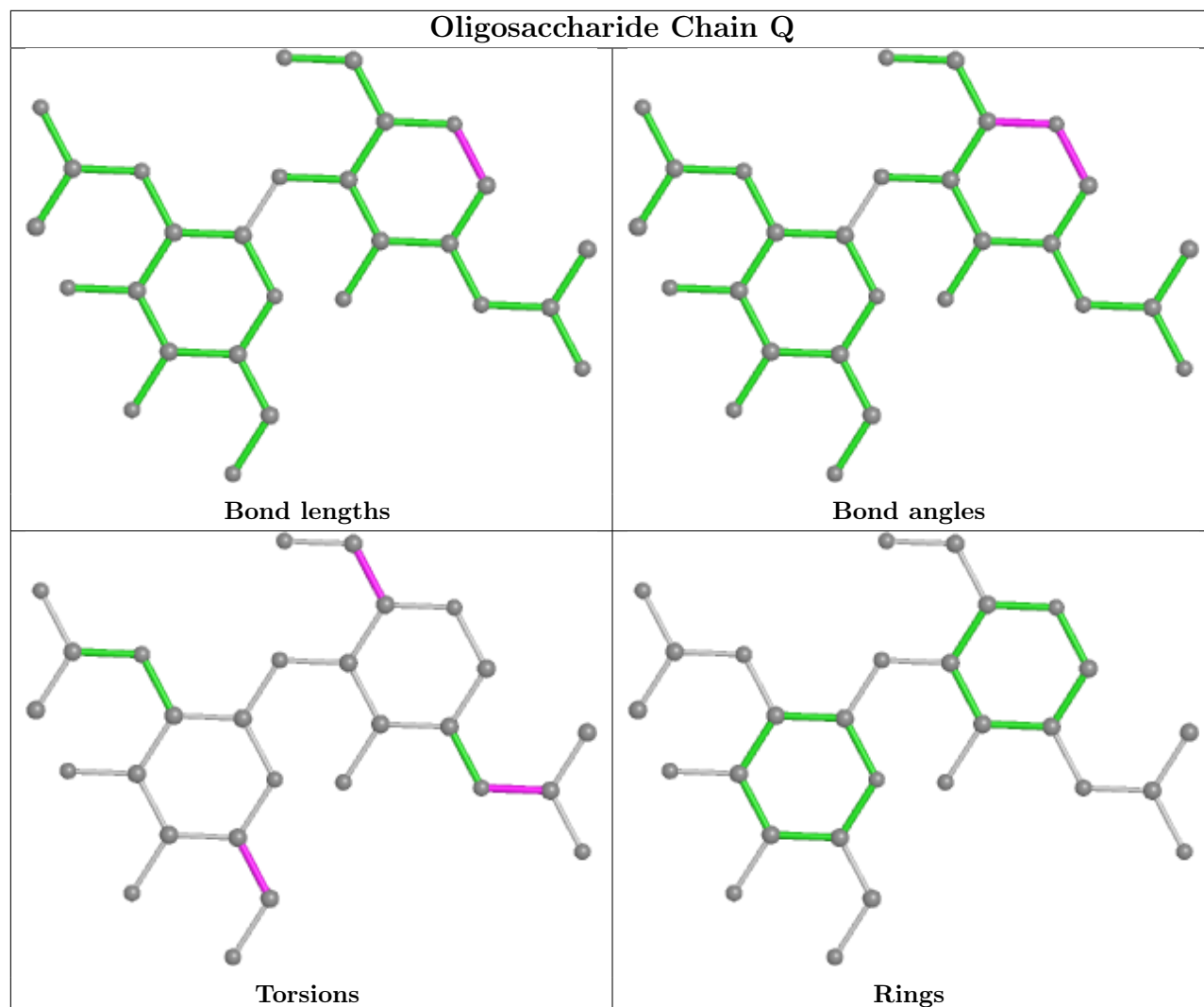


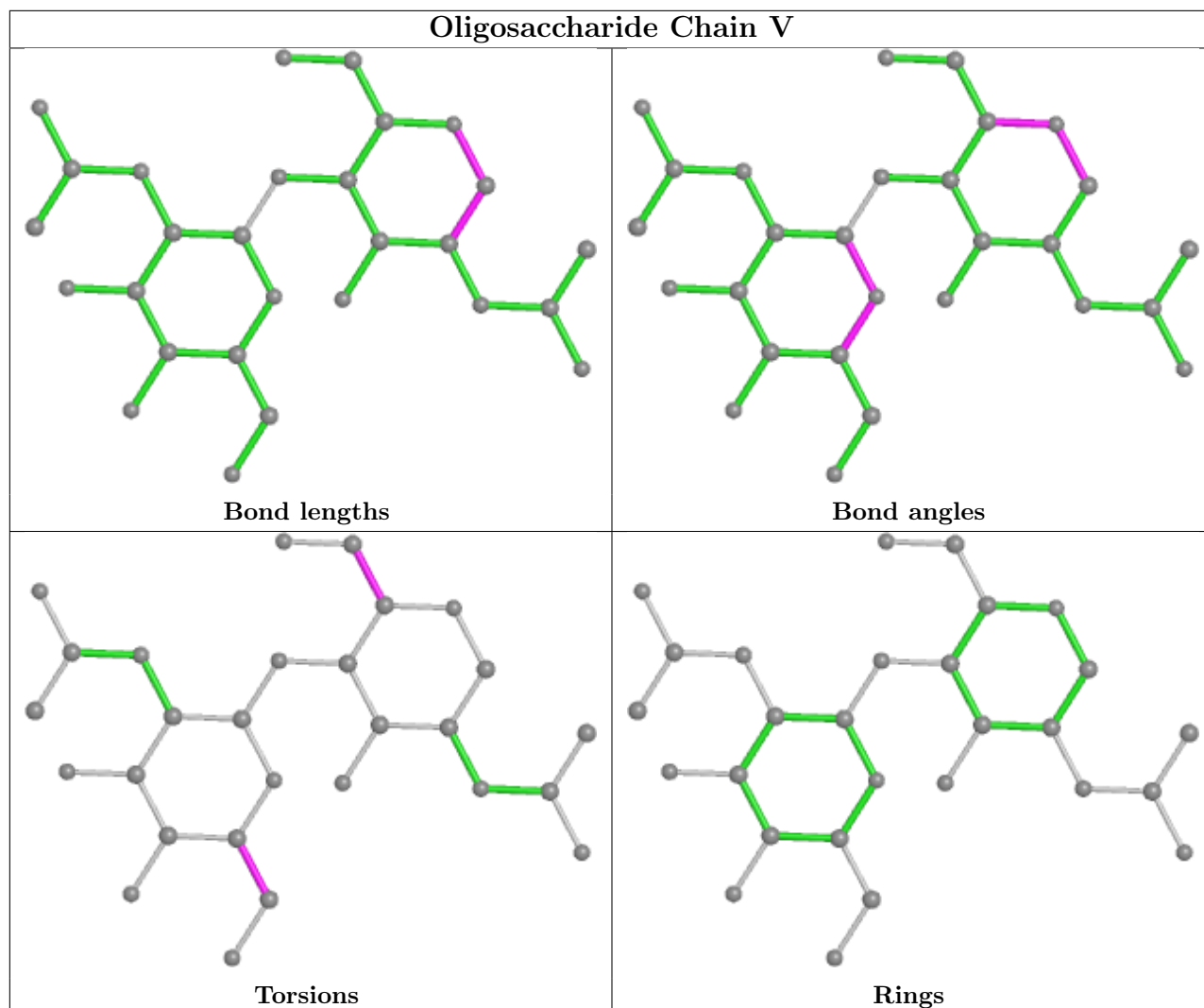


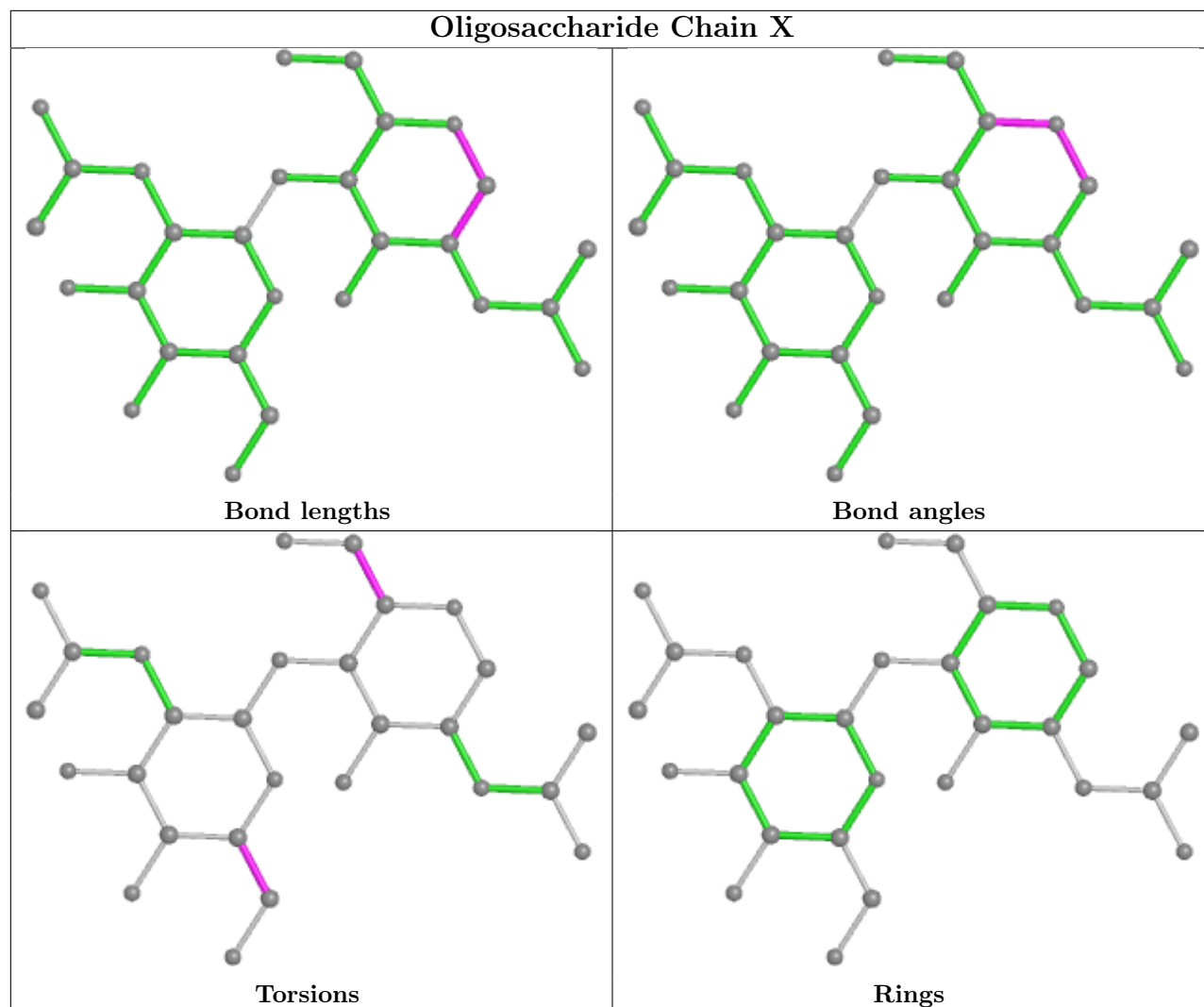


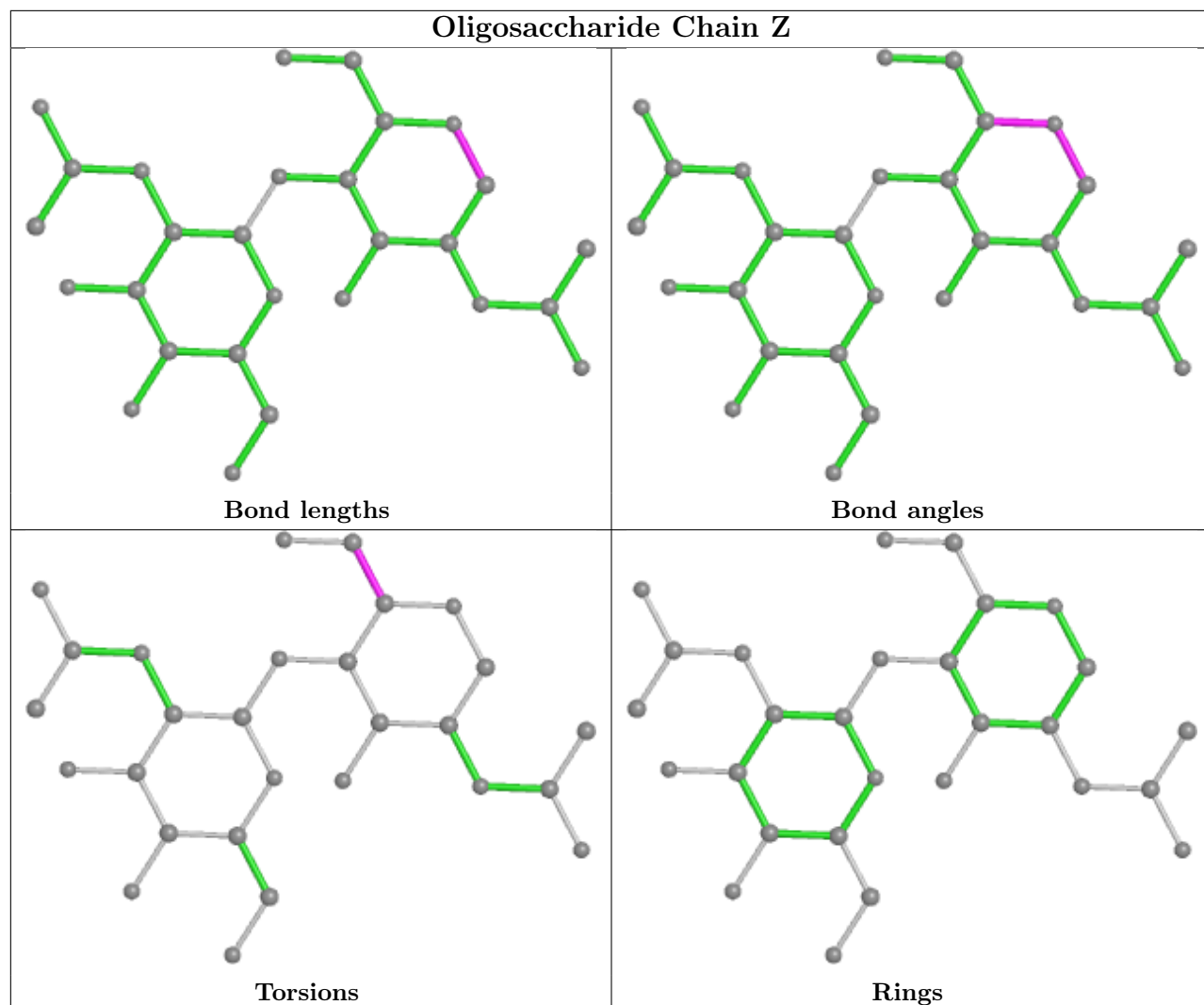


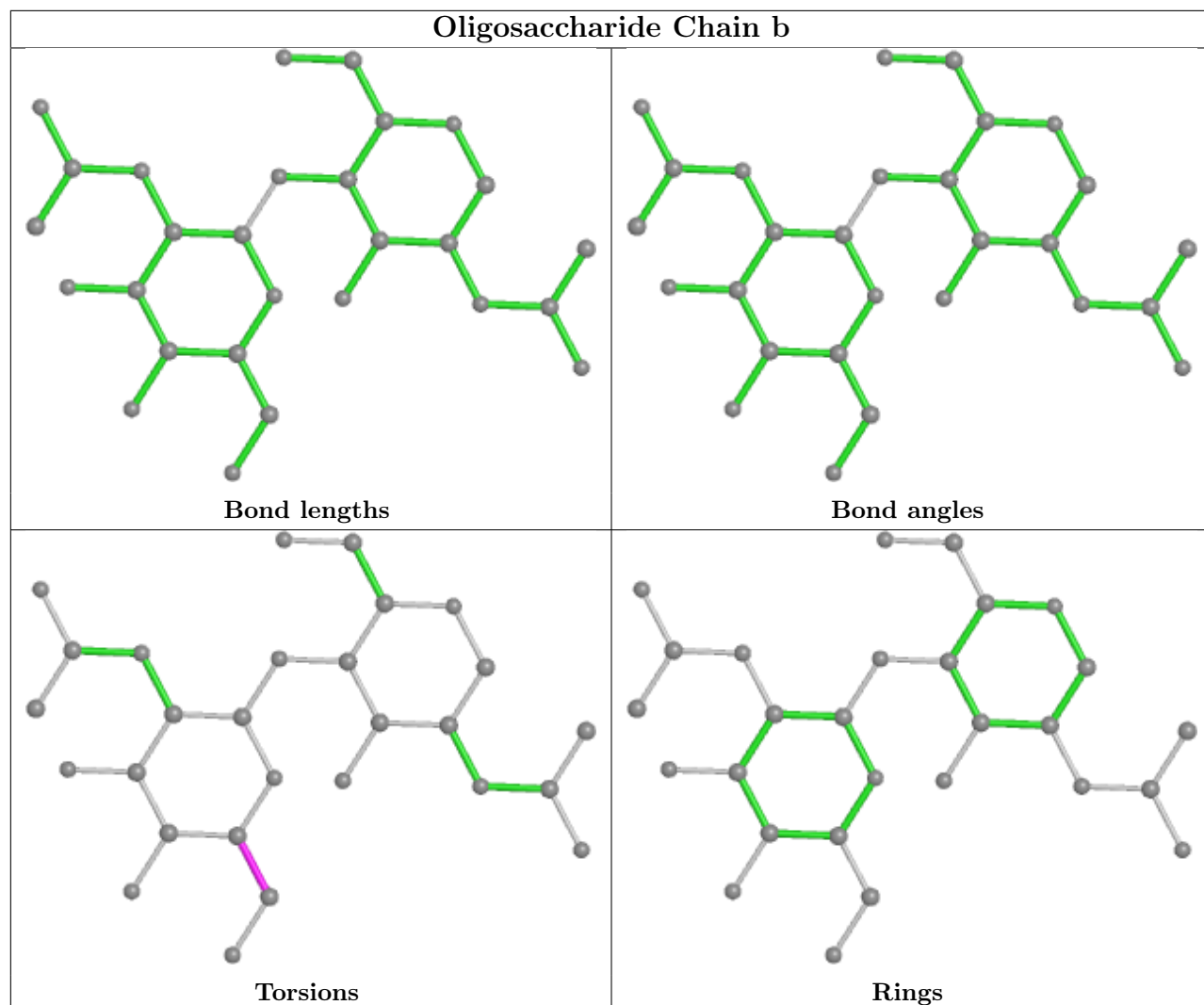




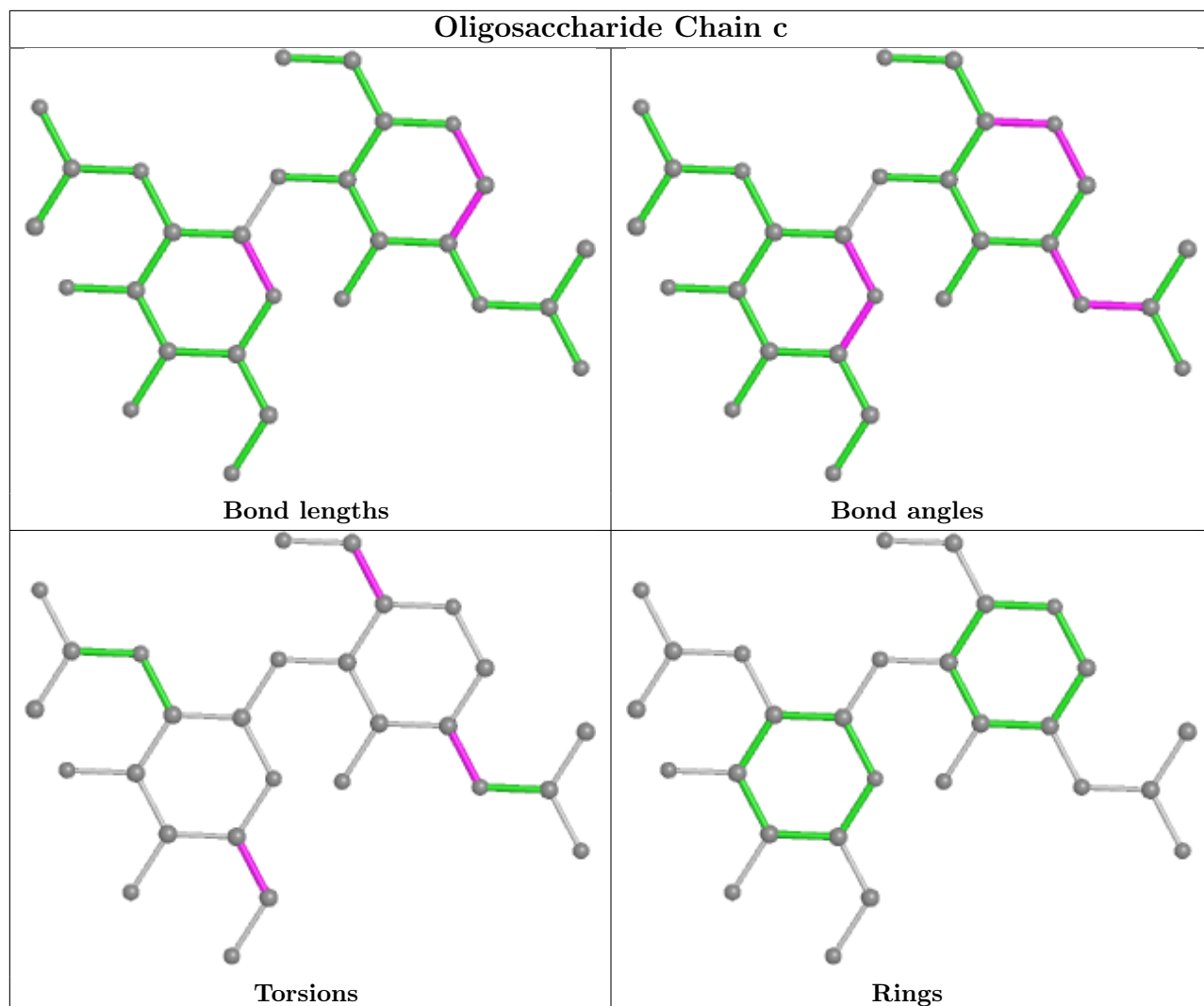


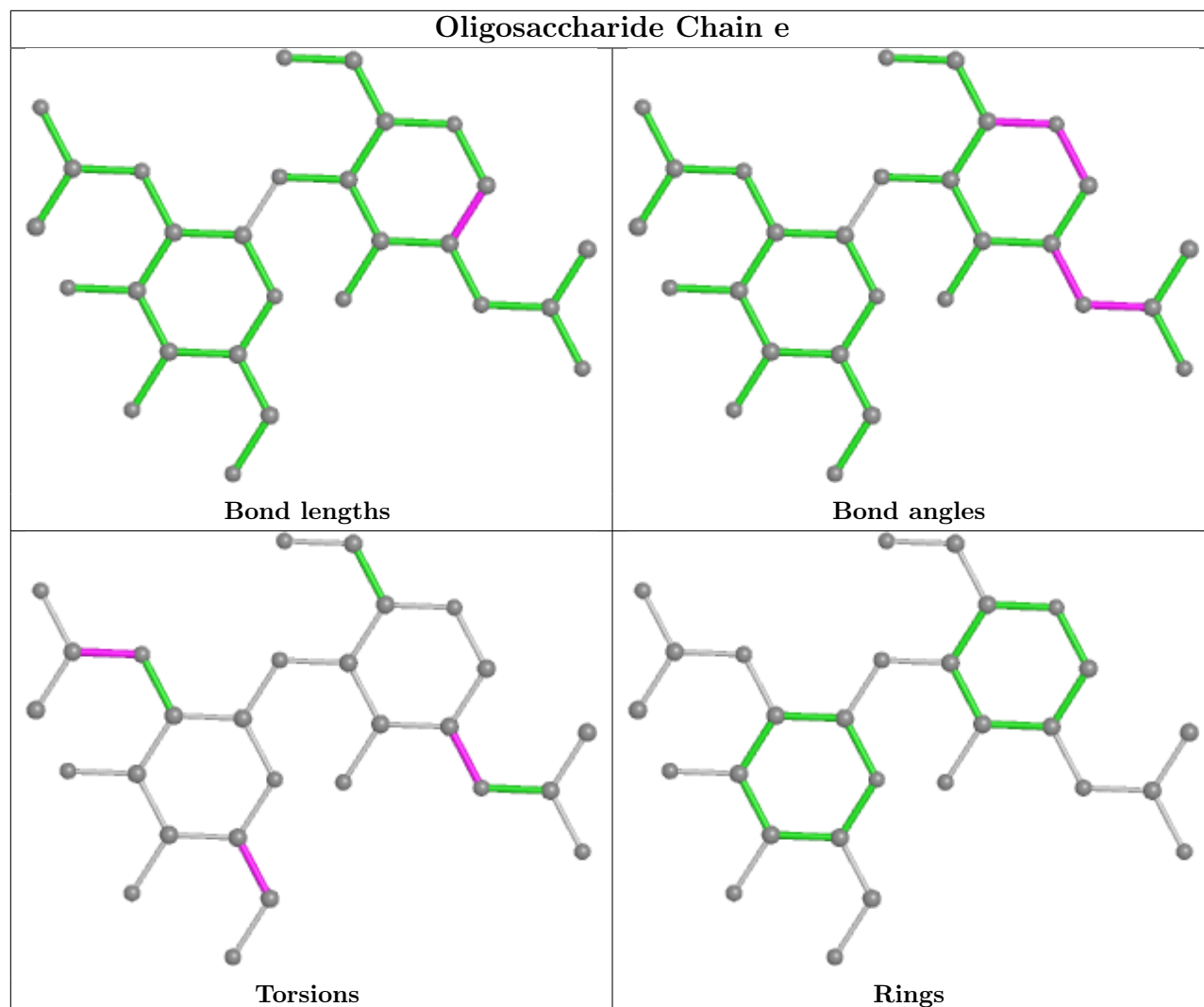


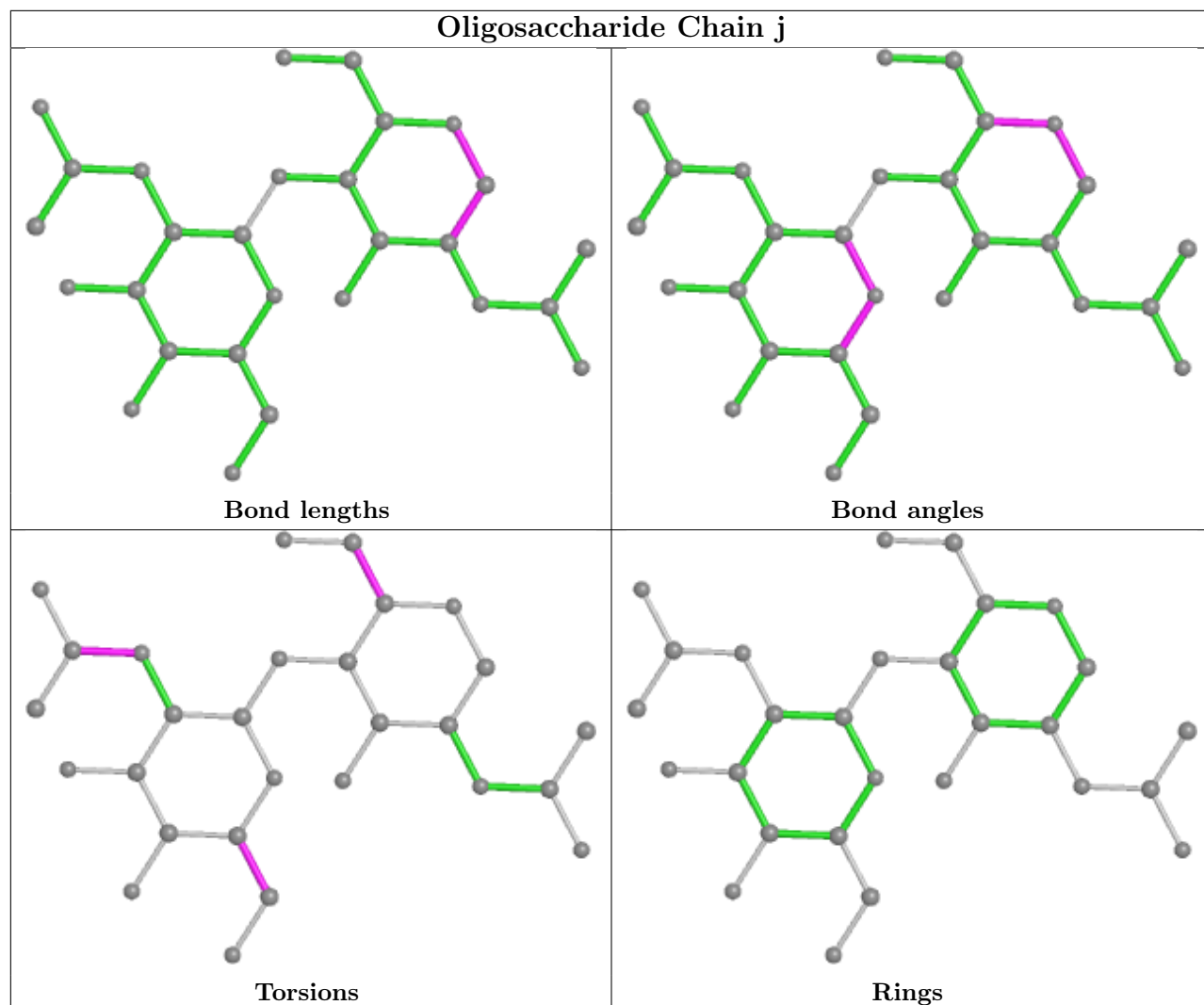


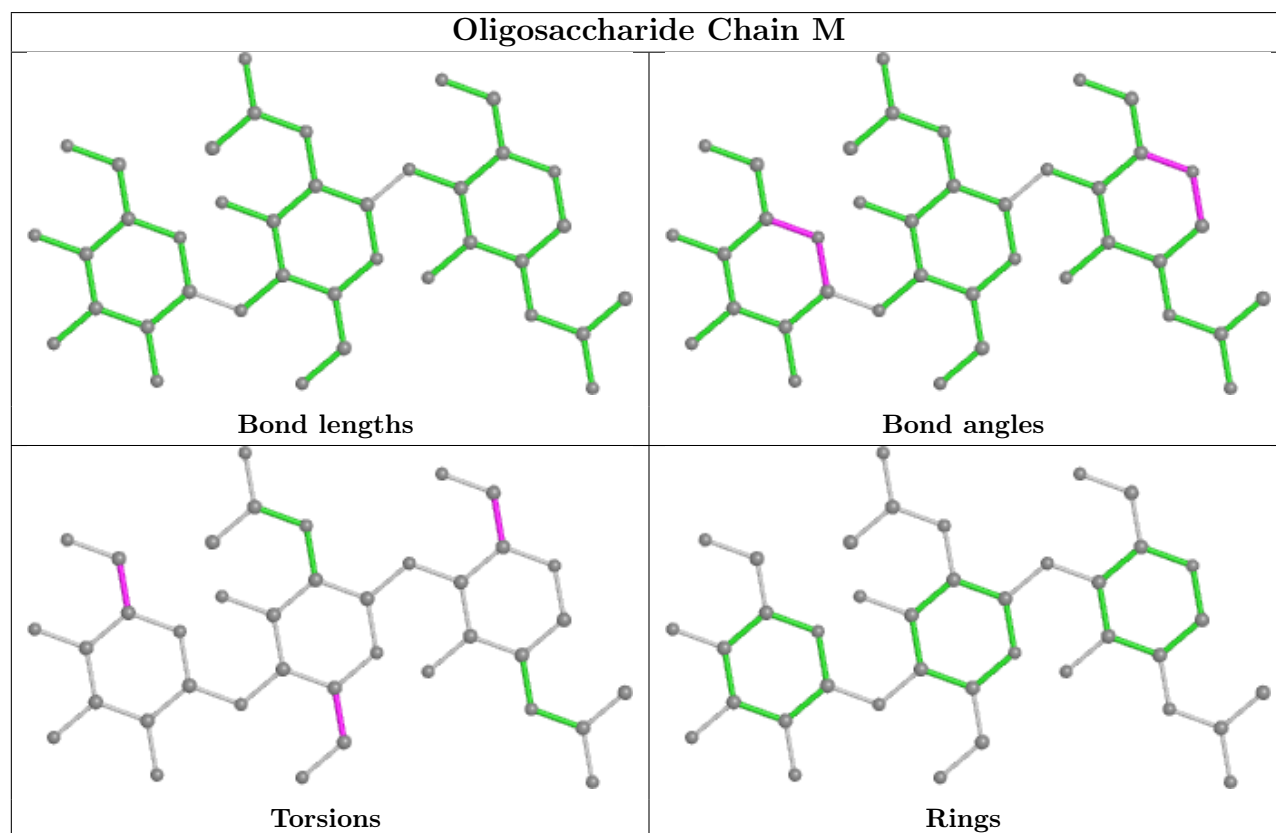
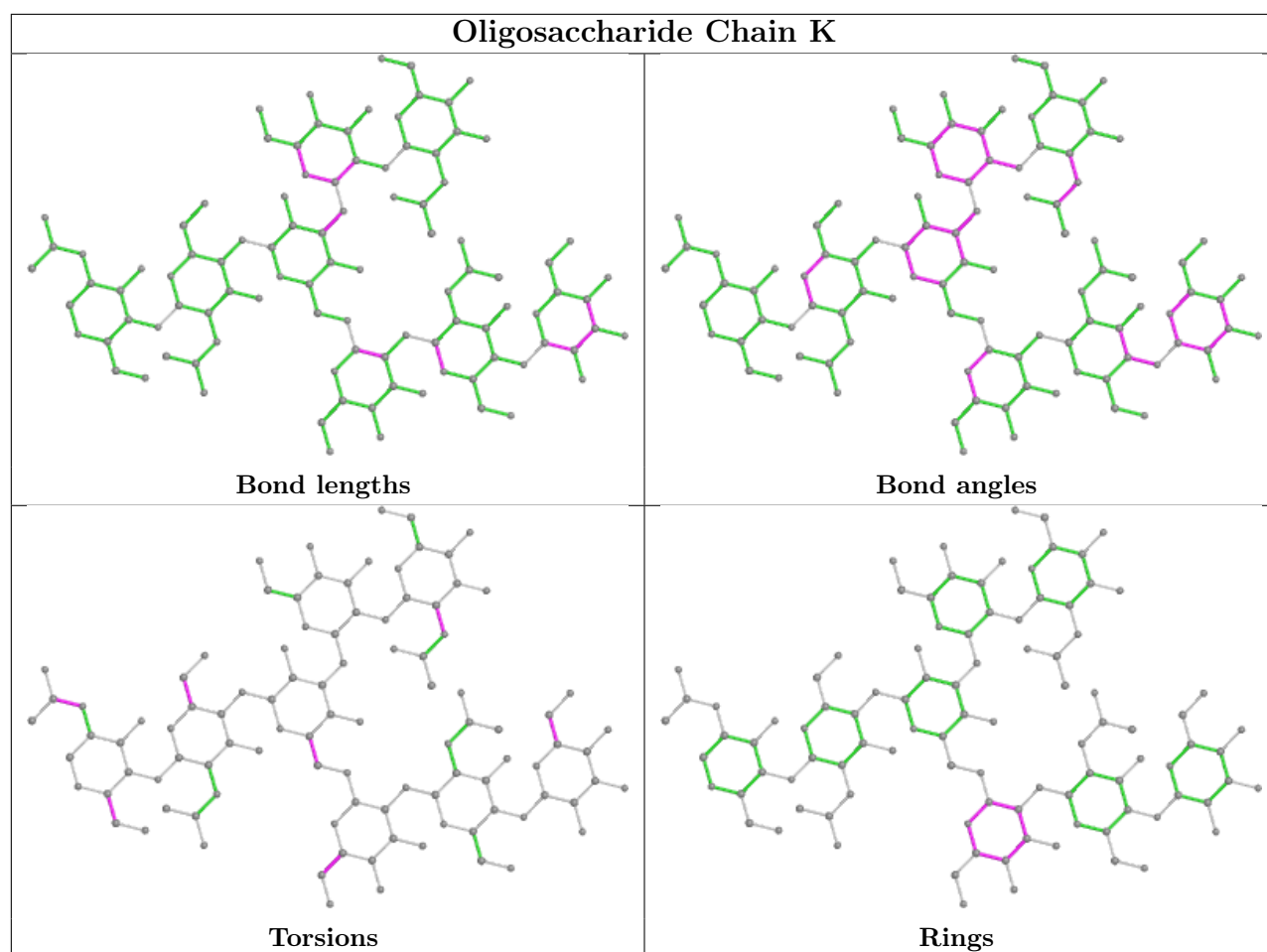


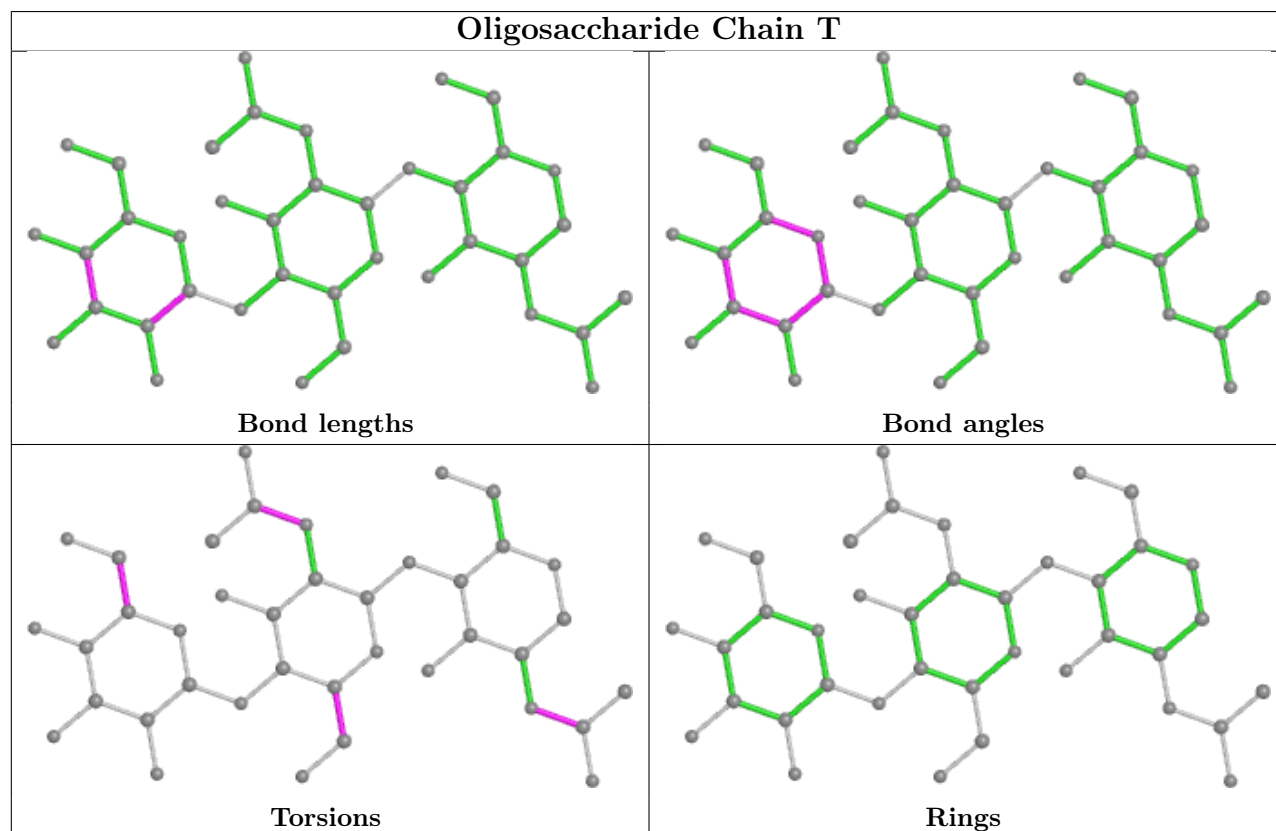
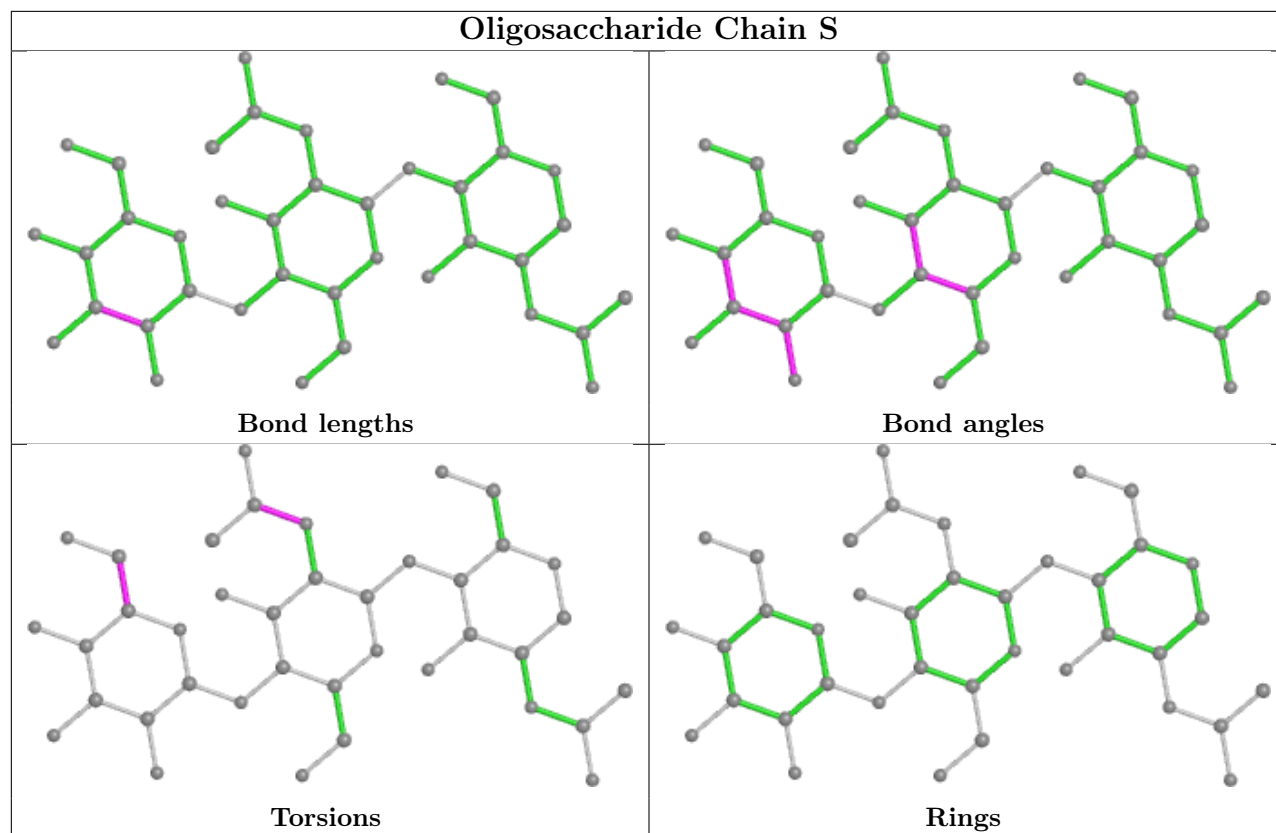


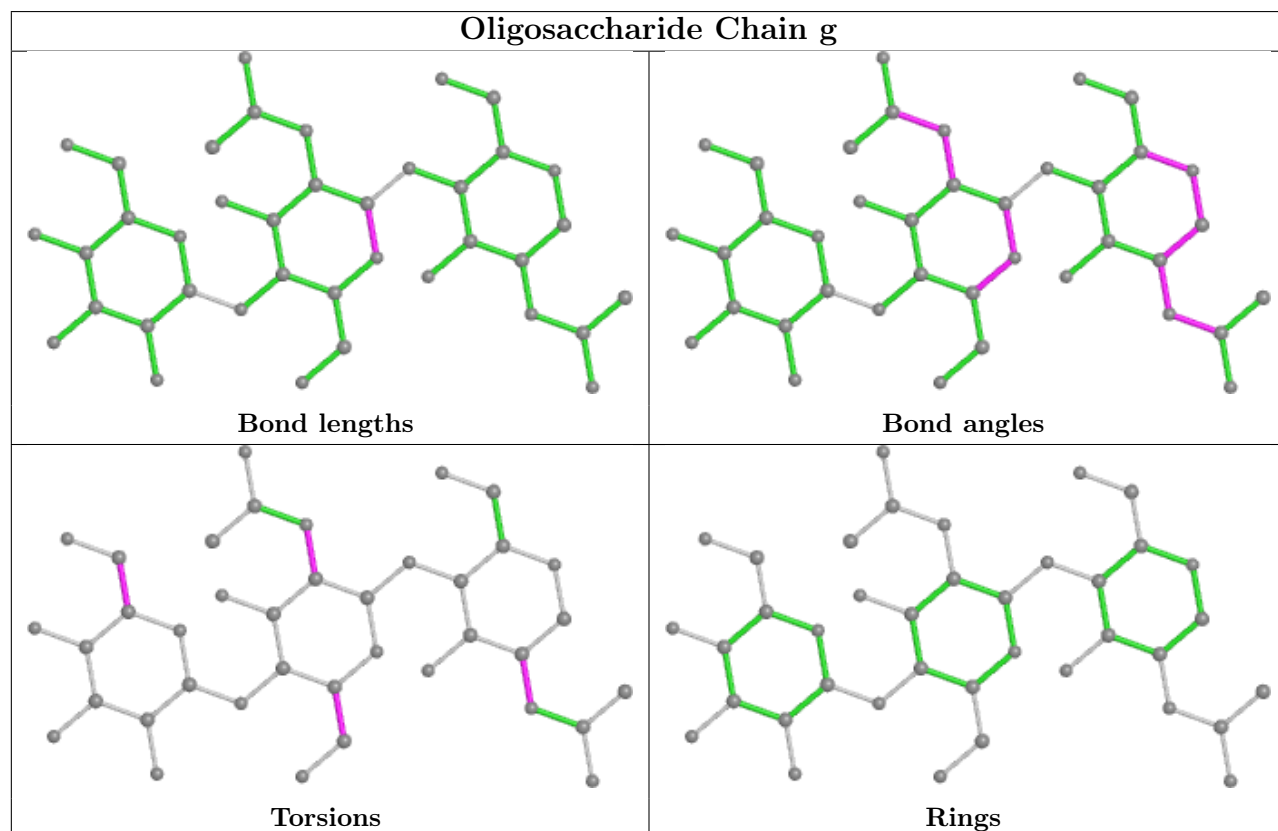
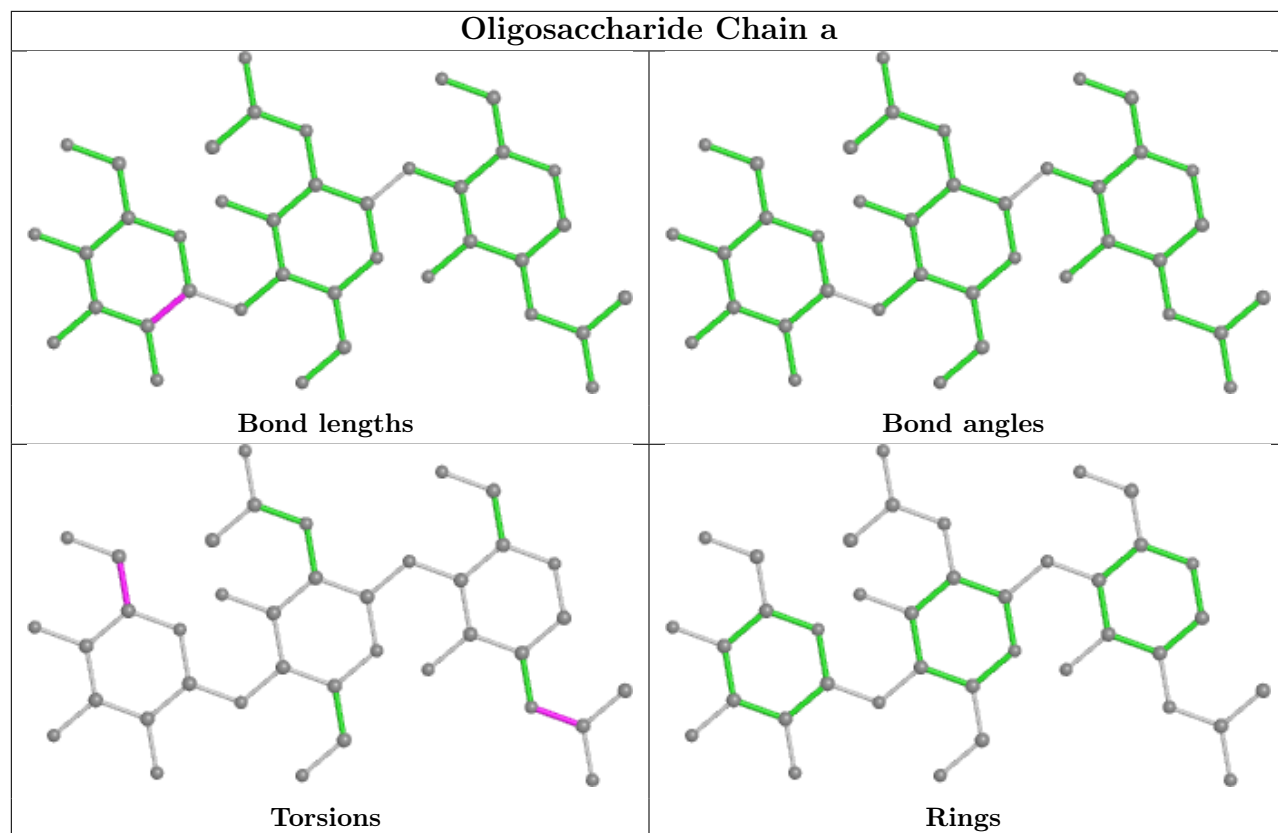


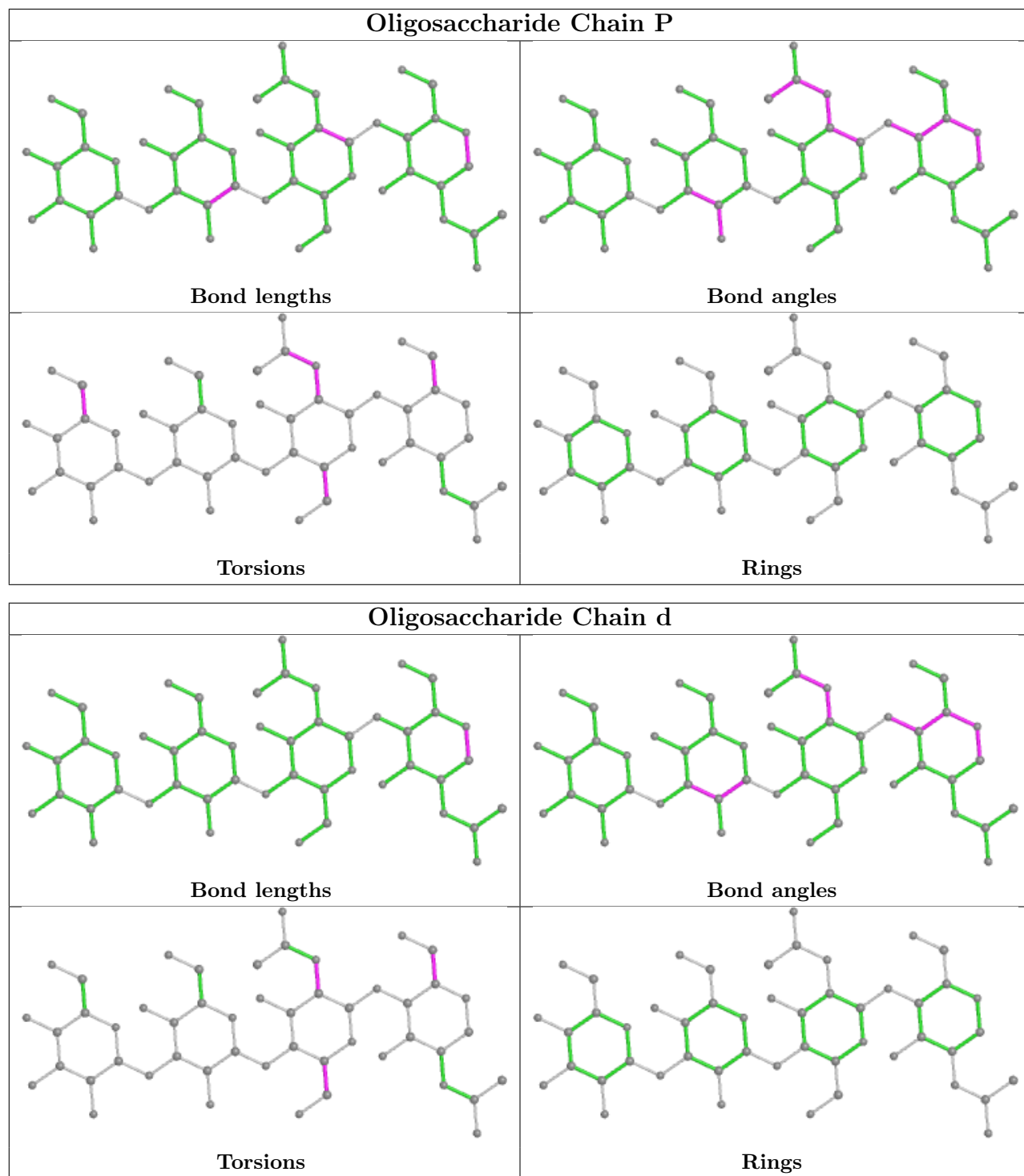


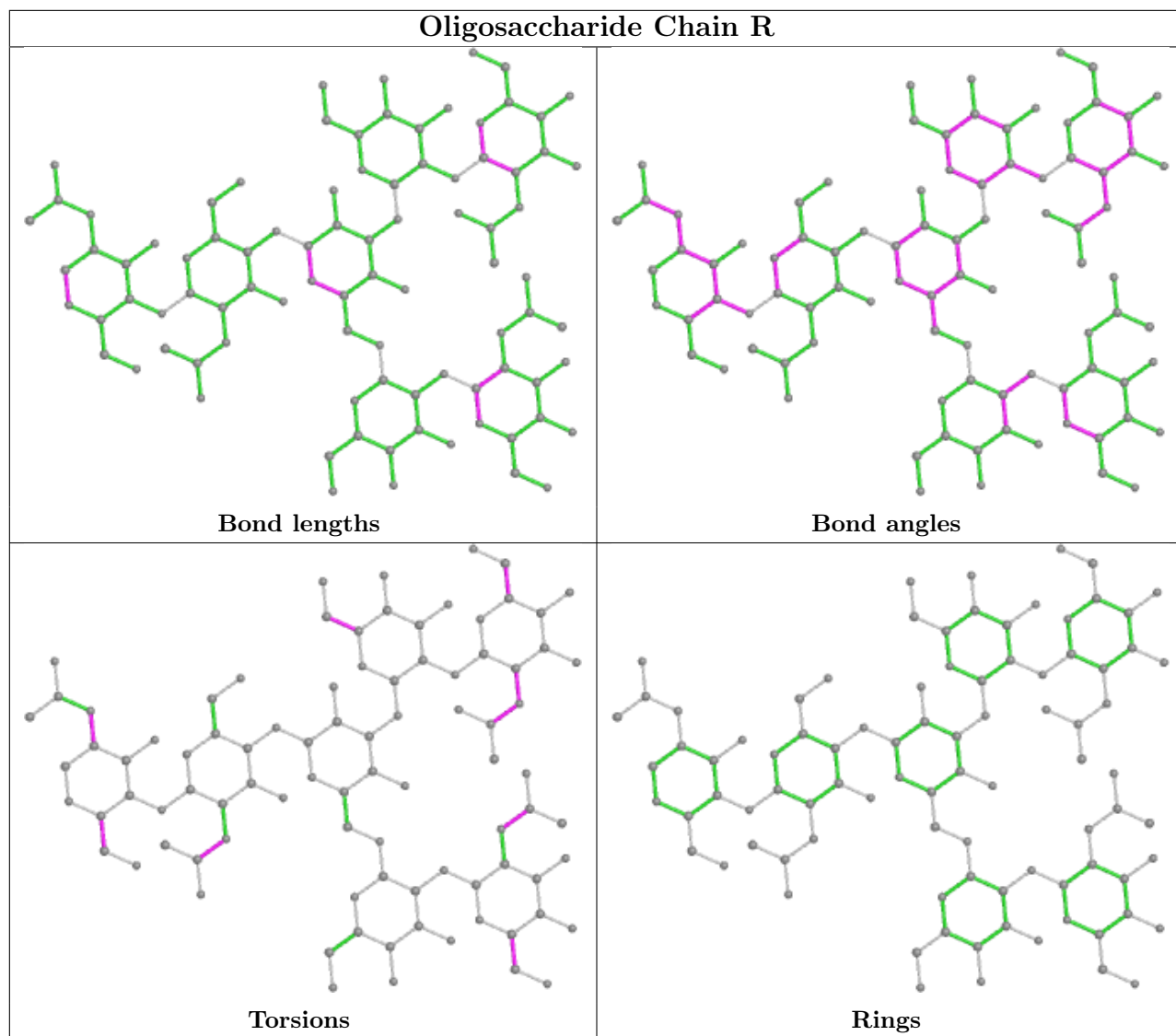




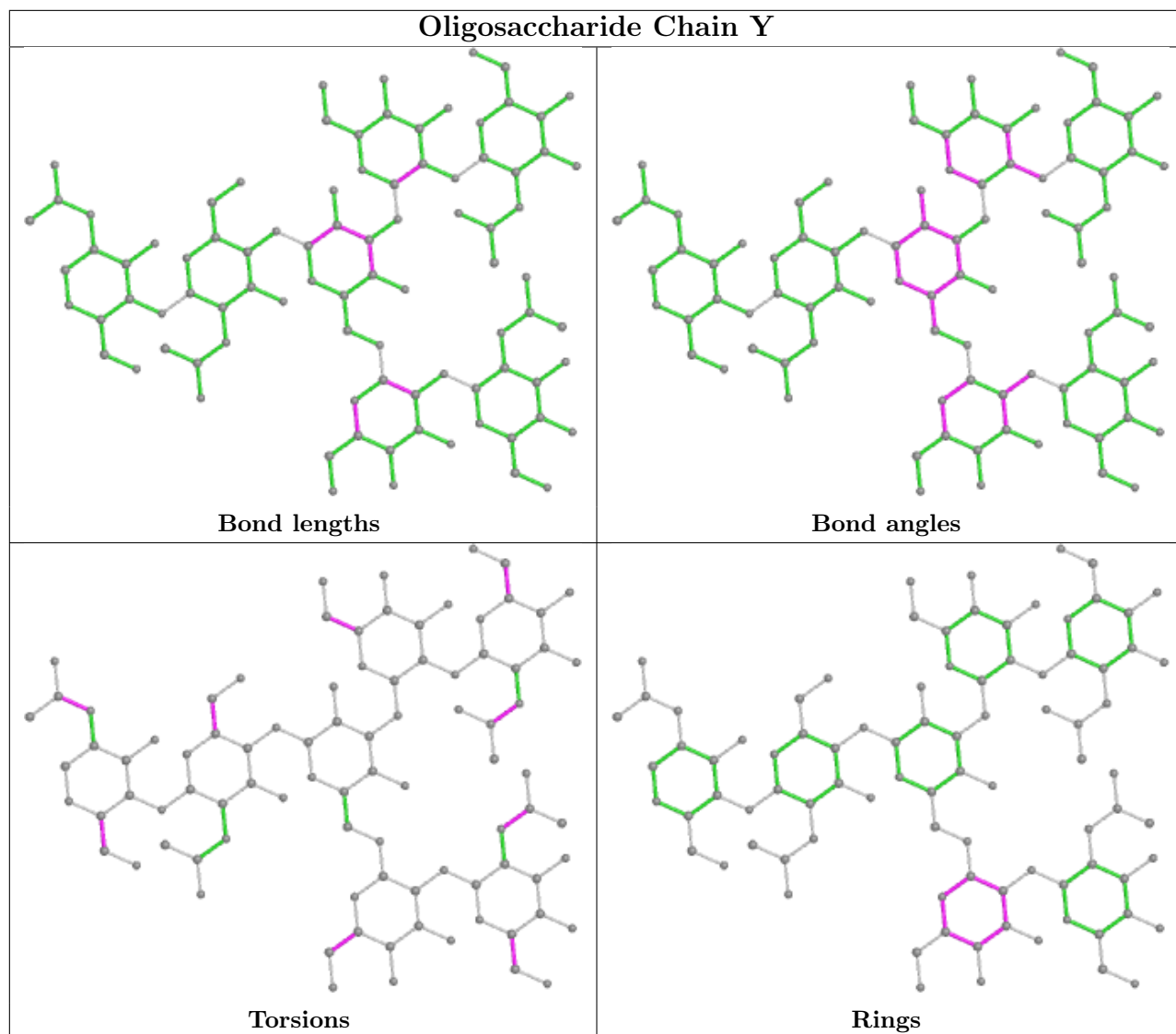


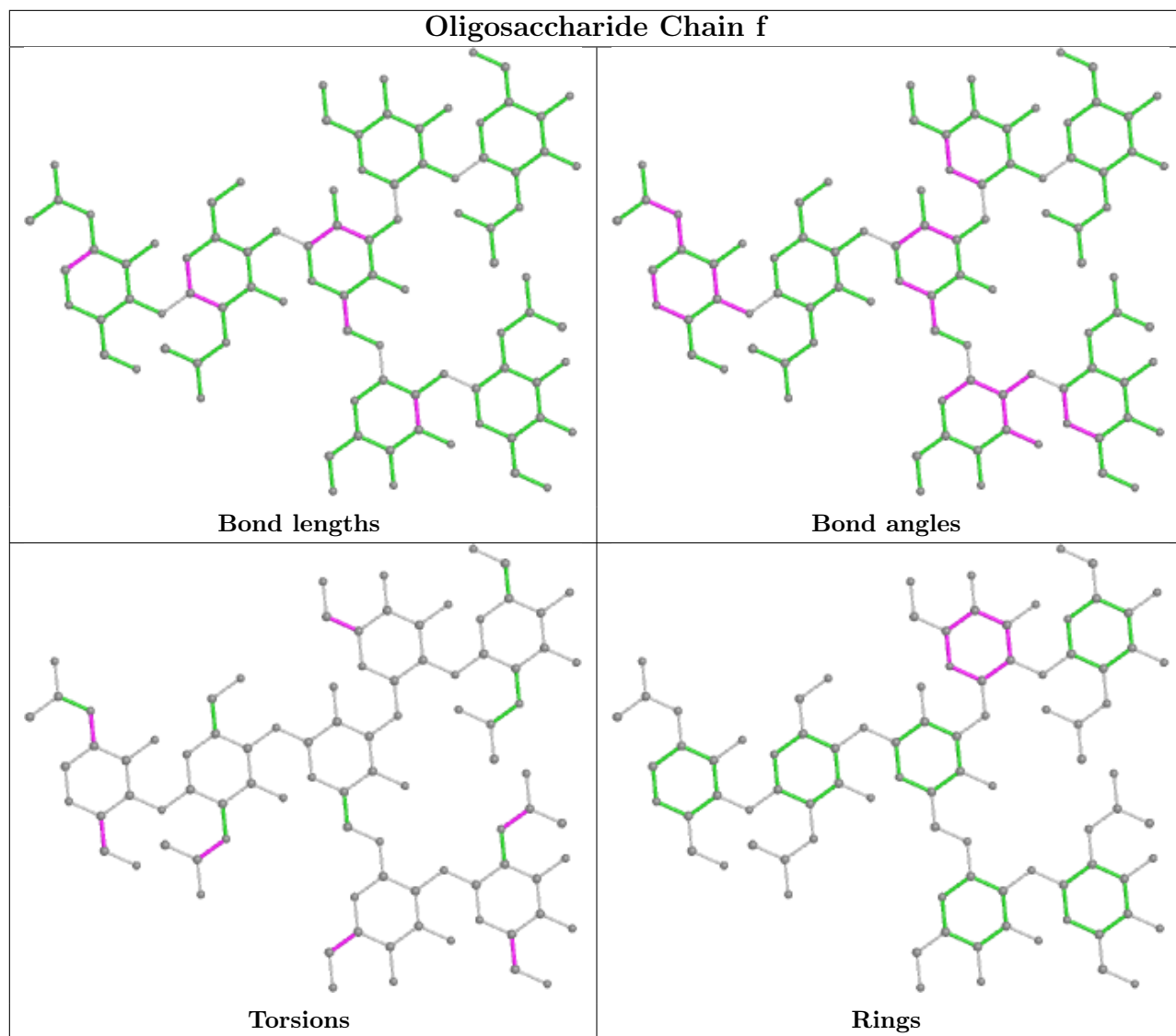


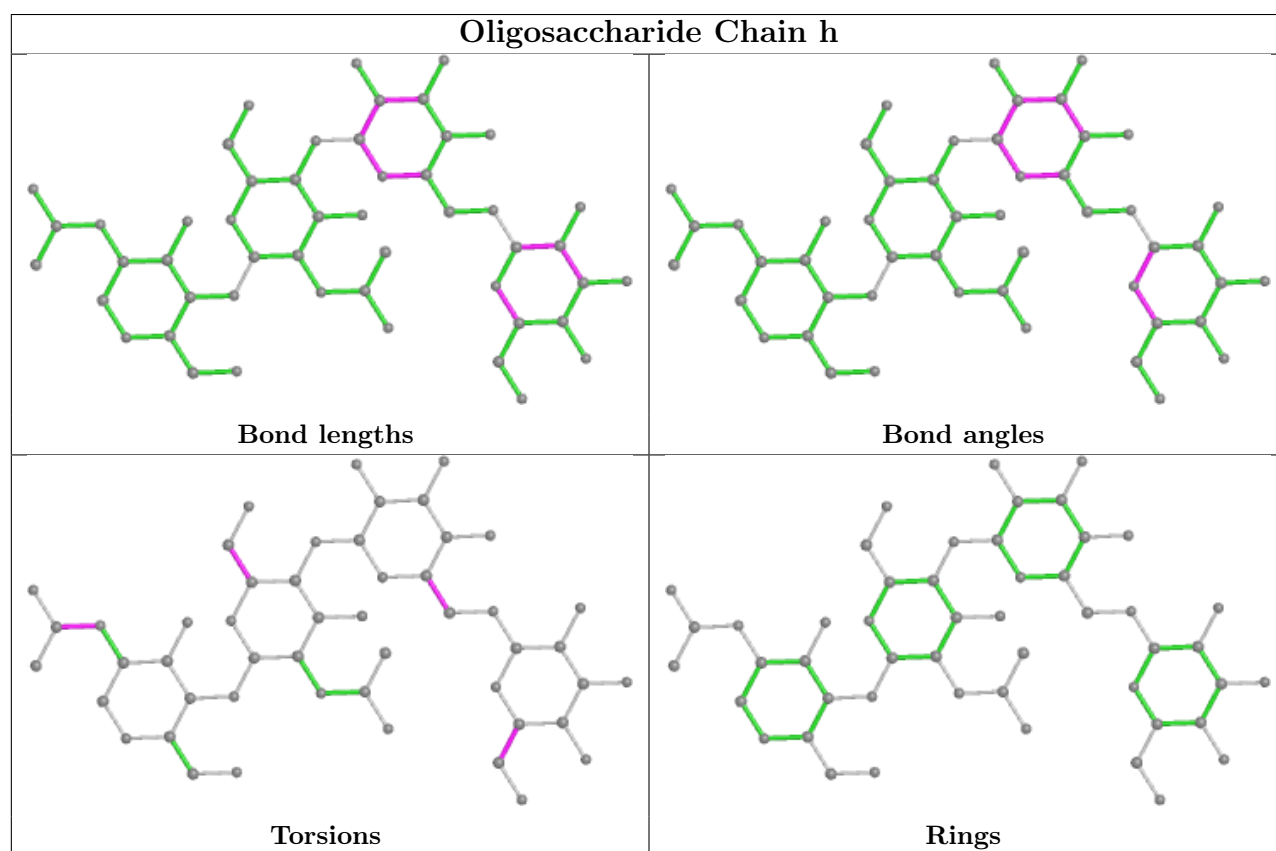
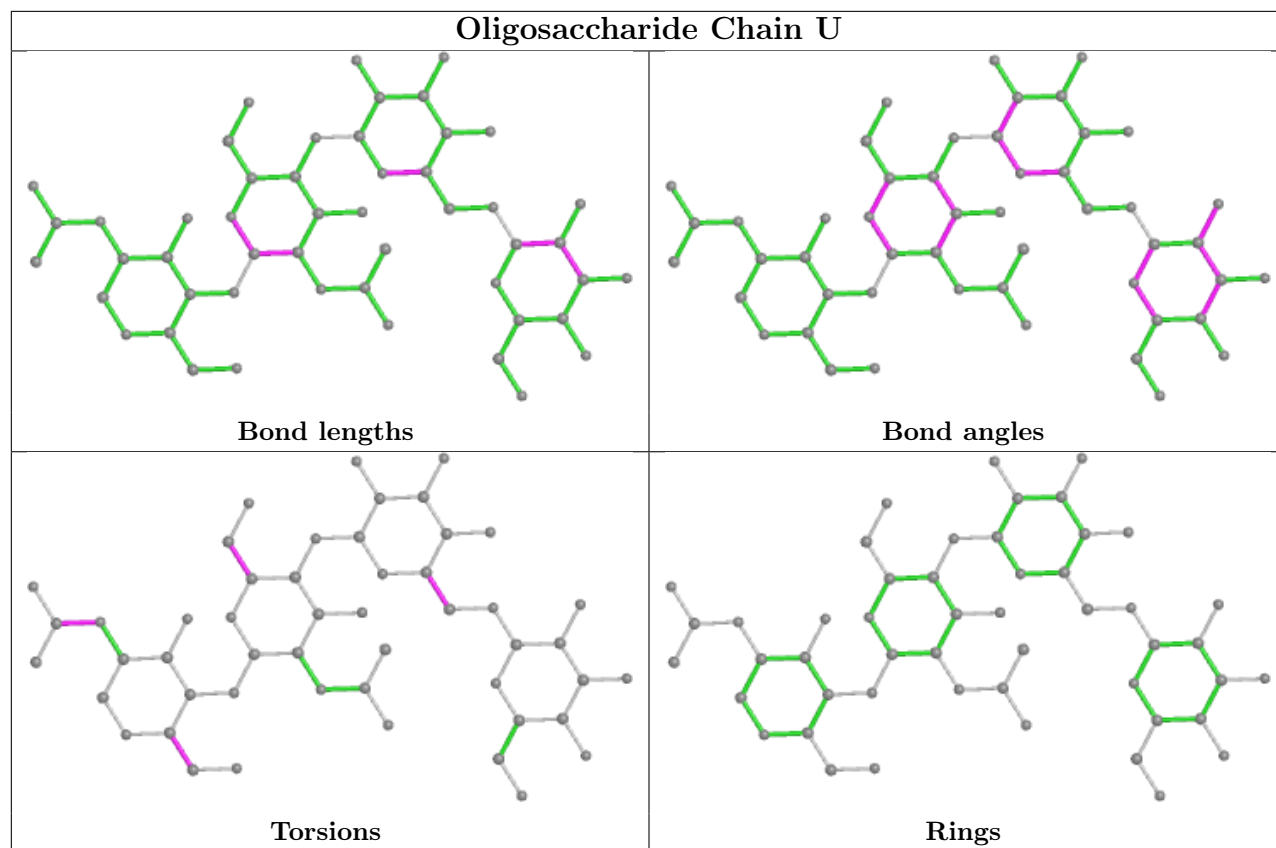


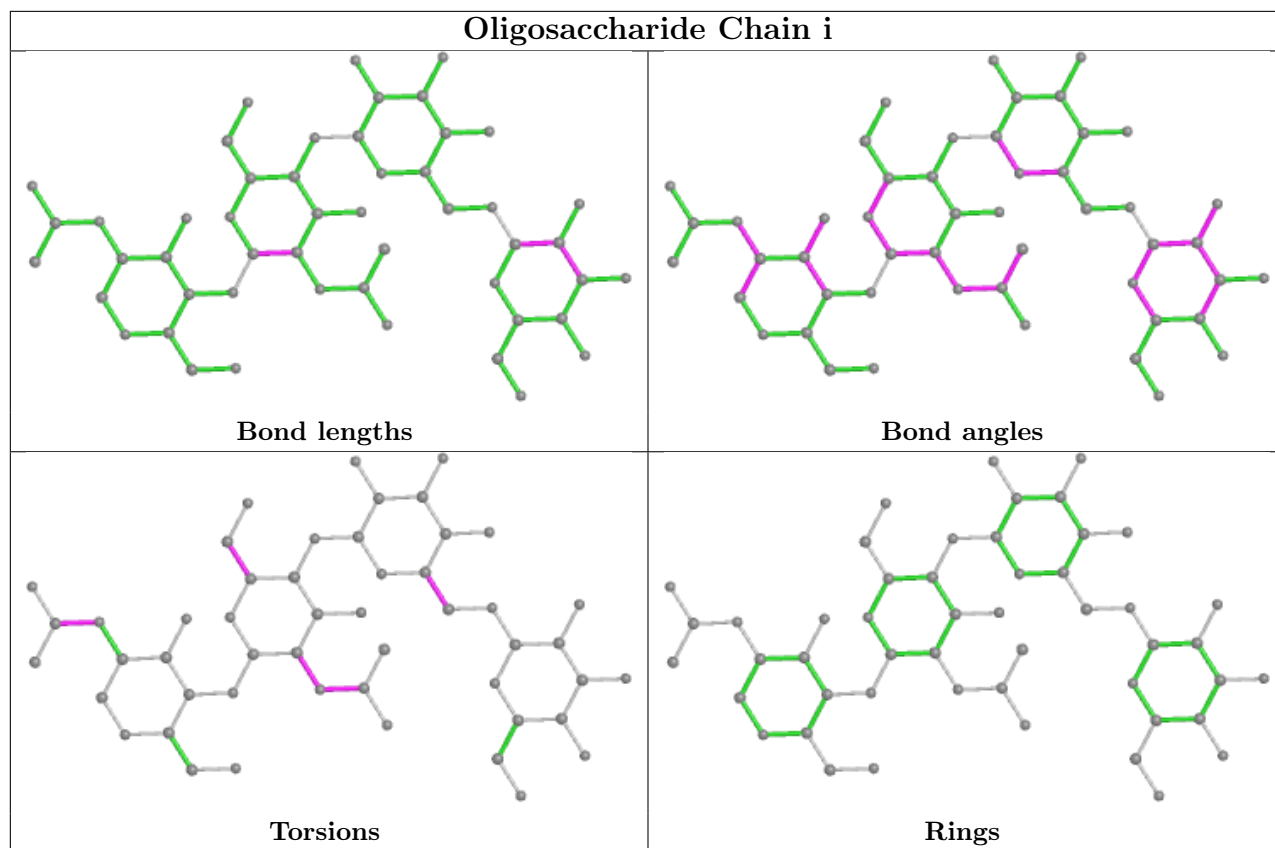












## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	2J9	D	1002	-	17,18,18	7.28	8 (47%)	23,28,28	5.81	6 (26%)
13	CLR	B	1006	-	31,31,31	0.15	0	48,48,48	0.34	0
13	CLR	C	1007	-	31,31,31	0.18	0	48,48,48	0.32	0
12	POV	D	1001	-	51,51,51	1.07	3 (5%)	57,59,59	0.92	4 (7%)
10	2J9	C	1002	-	17,18,18	7.23	8 (47%)	23,28,28	5.38	7 (30%)
10	2J9	B	1002	-	17,18,18	7.28	8 (47%)	23,28,28	5.65	7 (30%)
12	POV	C	1005	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
13	CLR	A	1009	-	31,31,31	0.16	0	48,48,48	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	POV	D	1005	-	51,51,51	1.08	3 (5%)	57,59,59	0.93	3 (5%)
13	CLR	A	1008	-	31,31,31	0.19	0	48,48,48	0.38	0
12	POV	B	1004	-	51,51,51	1.07	3 (5%)	57,59,59	0.92	3 (5%)
13	CLR	A	1006	-	31,31,31	0.15	0	48,48,48	0.34	0
11	GLU	B	1003	-	8,9,9	1.09	1 (12%)	10,11,11	1.24	2 (20%)
12	POV	B	1001	-	51,51,51	1.07	3 (5%)	57,59,59	0.93	4 (7%)
12	POV	C	1001	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
12	POV	D	1004	-	51,51,51	1.07	3 (5%)	57,59,59	0.94	3 (5%)
12	POV	A	1003	-	51,51,51	1.06	3 (5%)	57,59,59	0.91	3 (5%)
11	GLU	D	1003	-	8,9,9	1.08	1 (12%)	10,11,11	1.24	2 (20%)
12	POV	C	1004	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	3 (5%)
13	CLR	A	1007	-	31,31,31	0.18	0	48,48,48	0.32	0
13	CLR	C	1009	-	31,31,31	0.18	0	48,48,48	0.32	0
12	POV	C	1006	-	51,51,51	1.08	2 (3%)	57,59,59	0.95	3 (5%)
12	POV	B	1005	-	51,51,51	1.08	3 (5%)	57,59,59	0.94	3 (5%)
13	CLR	C	1008	-	31,31,31	0.19	0	48,48,48	0.37	0
10	2J9	A	1001	-	17,18,18	7.24	8 (47%)	23,28,28	5.60	6 (26%)
11	GLU	C	1003	-	8,9,9	1.13	1 (12%)	10,11,11	1.19	2 (20%)
12	POV	A	1005	-	51,51,51	1.08	2 (3%)	57,59,59	0.96	3 (5%)
12	POV	A	1004	-	51,51,51	1.07	3 (5%)	57,59,59	0.86	3 (5%)
11	GLU	A	1002	-	8,9,9	1.12	1 (12%)	10,11,11	1.20	2 (20%)
12	POV	A	1010	-	51,51,51	1.08	3 (5%)	57,59,59	0.91	3 (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
10	2J9	D	1002	-	-	1/4/22/22	0/3/3/3
13	CLR	B	1006	-	-	7/10/68/68	0/4/4/4
13	CLR	C	1007	-	-	7/10/68/68	0/4/4/4
12	POV	D	1001	-	-	29/55/55/55	-
10	2J9	C	1002	-	-	1/4/22/22	0/3/3/3
10	2J9	B	1002	-	-	2/4/22/22	0/3/3/3
12	POV	C	1005	-	-	22/55/55/55	-
13	CLR	A	1009	-	-	6/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	POV	D	1005	-	-	30/55/55/55	-
13	CLR	A	1008	-	-	2/10/68/68	0/4/4/4
12	POV	B	1004	-	-	31/55/55/55	-
13	CLR	A	1006	-	-	7/10/68/68	0/4/4/4
11	GLU	B	1003	-	-	3/9/9/9	-
12	POV	B	1001	-	-	28/55/55/55	-
12	POV	C	1001	-	-	26/55/55/55	-
12	POV	D	1004	-	-	29/55/55/55	-
12	POV	A	1003	-	-	32/55/55/55	-
11	GLU	D	1003	-	-	3/9/9/9	-
12	POV	C	1004	-	-	34/55/55/55	-
13	CLR	A	1007	-	-	7/10/68/68	0/4/4/4
13	CLR	C	1009	-	-	6/10/68/68	0/4/4/4
12	POV	C	1006	-	-	31/55/55/55	-
12	POV	B	1005	-	-	26/55/55/55	-
13	CLR	C	1008	-	-	2/10/68/68	0/4/4/4
10	2J9	A	1001	-	-	1/4/22/22	0/3/3/3
11	GLU	C	1003	-	-	1/9/9/9	-
12	POV	A	1005	-	-	30/55/55/55	-
12	POV	A	1004	-	-	28/55/55/55	-
11	GLU	A	1002	-	-	1/9/9/9	-
12	POV	A	1010	-	-	28/55/55/55	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1002	2J9	OAA-SAP	19.96	1.66	1.43
10	D	1002	2J9	OAA-SAP	19.86	1.66	1.43
10	A	1001	2J9	OAA-SAP	19.71	1.65	1.43
10	C	1002	2J9	OAA-SAP	19.68	1.65	1.43
10	C	1002	2J9	OAB-SAP	19.50	1.65	1.43
10	D	1002	2J9	OAB-SAP	19.49	1.65	1.43
10	A	1001	2J9	OAB-SAP	19.48	1.65	1.43
10	B	1002	2J9	OAB-SAP	19.42	1.65	1.43
10	B	1002	2J9	CAL-NAO	6.13	1.55	1.40
10	D	1002	2J9	CAL-NAO	6.07	1.55	1.40
10	C	1002	2J9	CAL-NAO	5.98	1.55	1.40
10	A	1001	2J9	CAL-NAO	5.94	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1002	2J9	CAL-CAM	-4.57	1.35	1.40
10	A	1001	2J9	CAH-CAN	-4.57	1.39	1.48
10	C	1002	2J9	CAH-CAN	-4.53	1.39	1.48
10	B	1002	2J9	CAG-CAN	-4.46	1.39	1.48
10	D	1002	2J9	CAG-CAN	-4.45	1.39	1.48
10	D	1002	2J9	CAH-CAN	-4.44	1.39	1.48
10	A	1001	2J9	CAL-CAM	-4.43	1.35	1.40
10	B	1002	2J9	CAH-CAN	-4.43	1.39	1.48
10	A	1001	2J9	CAG-CAN	-4.41	1.39	1.48
10	C	1002	2J9	CAG-CAN	-4.40	1.39	1.48
10	B	1002	2J9	CAL-CAM	-4.38	1.35	1.40
10	C	1002	2J9	CAL-CAM	-4.32	1.35	1.40
10	D	1002	2J9	CAM-SAP	-3.86	1.72	1.75
10	B	1002	2J9	CAM-SAP	-3.70	1.72	1.75
12	A	1005	POV	O21-C21	3.20	1.43	1.34
12	C	1006	POV	O21-C21	3.19	1.43	1.34
10	A	1001	2J9	CAM-SAP	-3.13	1.73	1.75
10	C	1002	2J9	CAM-SAP	-3.01	1.73	1.75
12	B	1005	POV	O21-C21	2.88	1.42	1.34
12	D	1004	POV	O21-C21	2.84	1.42	1.34
12	C	1004	POV	O21-C21	2.83	1.42	1.34
12	A	1003	POV	O21-C21	2.82	1.42	1.34
12	B	1004	POV	O21-C21	2.82	1.42	1.34
12	A	1010	POV	O31-C31	2.82	1.41	1.33
12	A	1010	POV	O21-C21	2.80	1.42	1.34
12	D	1005	POV	O21-C21	2.80	1.42	1.34
12	C	1005	POV	O21-C21	2.80	1.42	1.34
12	C	1001	POV	O21-C21	2.80	1.42	1.34
12	D	1001	POV	O21-C21	2.79	1.42	1.34
12	C	1001	POV	O31-C31	2.78	1.41	1.33
12	B	1001	POV	O21-C21	2.76	1.42	1.34
12	D	1001	POV	O31-C31	2.74	1.41	1.33
12	A	1005	POV	O31-C31	2.74	1.41	1.33
12	A	1004	POV	O31-C31	2.74	1.41	1.33
12	B	1004	POV	O31-C31	2.73	1.41	1.33
12	D	1004	POV	O31-C31	2.73	1.41	1.33
12	C	1006	POV	O31-C31	2.71	1.41	1.33
12	C	1005	POV	O31-C31	2.71	1.41	1.33
12	D	1005	POV	O31-C31	2.70	1.41	1.33
12	A	1004	POV	O21-C21	2.70	1.41	1.34
12	B	1001	POV	O31-C31	2.69	1.41	1.33
12	C	1004	POV	O31-C31	2.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1005	POV	O31-C31	2.69	1.41	1.33
12	A	1003	POV	O31-C31	2.67	1.41	1.33
10	C	1002	2J9	CAH-CAG	-2.59	1.39	1.48
10	A	1001	2J9	CAH-CAG	-2.58	1.39	1.48
10	B	1002	2J9	CAH-CAG	-2.57	1.39	1.48
10	D	1002	2J9	CAH-CAG	-2.56	1.39	1.48
12	B	1001	POV	O21-C2	-2.45	1.40	1.46
12	D	1001	POV	O21-C2	-2.44	1.40	1.46
12	A	1003	POV	O21-C2	-2.43	1.40	1.46
12	A	1004	POV	O21-C2	-2.42	1.40	1.46
12	C	1004	POV	O21-C2	-2.40	1.40	1.46
12	B	1005	POV	O21-C2	-2.40	1.40	1.46
12	D	1005	POV	O21-C2	-2.39	1.40	1.46
12	C	1001	POV	O21-C2	-2.39	1.40	1.46
12	C	1005	POV	O21-C2	-2.38	1.40	1.46
12	B	1004	POV	O21-C2	-2.37	1.40	1.46
12	D	1004	POV	O21-C2	-2.36	1.40	1.46
12	A	1010	POV	O21-C2	-2.36	1.40	1.46
11	C	1003	GLU	OXT-C	-2.31	1.23	1.30
11	A	1002	GLU	OXT-C	-2.28	1.23	1.30
11	B	1003	GLU	OXT-C	-2.21	1.23	1.30
11	D	1003	GLU	OXT-C	-2.21	1.23	1.30

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1002	2J9	CAI-NAO-CAL	23.84	120.92	110.25
10	B	1002	2J9	CAI-NAO-CAL	23.03	120.56	110.25
10	A	1001	2J9	CAI-NAO-CAL	22.19	120.18	110.25
10	C	1002	2J9	CAI-NAO-CAL	20.81	119.57	110.25
10	C	1002	2J9	CAM-SAP-NAJ	11.26	111.28	102.37
10	A	1001	2J9	CAM-SAP-NAJ	11.18	111.22	102.37
10	D	1002	2J9	CAM-SAP-NAJ	9.97	110.26	102.37
10	B	1002	2J9	CAM-SAP-NAJ	9.75	110.09	102.37
10	B	1002	2J9	OAB-SAP-OAA	-8.19	110.10	118.46
10	C	1002	2J9	OAB-SAP-OAA	-8.09	110.21	118.46
10	D	1002	2J9	OAB-SAP-OAA	-8.04	110.25	118.46
10	A	1001	2J9	OAB-SAP-OAA	-7.98	110.32	118.46
12	B	1005	POV	O21-C21-C22	4.33	120.82	111.50
12	D	1005	POV	O21-C21-C22	4.21	120.57	111.50
12	A	1005	POV	O21-C21-C22	4.19	120.54	111.50
12	C	1006	POV	O21-C21-C22	4.14	120.43	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1002	2J9	CAK-CAF-CAM	4.10	119.65	116.86
12	D	1004	POV	O21-C21-C22	4.07	120.28	111.50
10	A	1001	2J9	CAK-CAF-CAM	3.99	119.58	116.86
12	B	1004	POV	O21-C21-C22	3.97	120.06	111.50
12	A	1003	POV	O21-C21-C22	3.86	119.82	111.50
12	C	1005	POV	O21-C21-C22	3.84	119.78	111.50
12	C	1004	POV	O21-C21-C22	3.82	119.73	111.50
12	A	1010	POV	O21-C21-C22	3.71	119.50	111.50
12	A	1004	POV	O21-C21-C22	3.70	119.48	111.50
12	C	1001	POV	O21-C21-C22	3.67	119.41	111.50
12	B	1001	POV	O21-C21-C22	3.57	119.19	111.50
10	D	1002	2J9	CAK-CAF-CAM	3.53	119.27	116.86
12	D	1001	POV	O21-C21-C22	3.53	119.12	111.50
10	B	1002	2J9	OAB-SAP-NAJ	3.34	111.04	107.92
10	D	1002	2J9	OAB-SAP-NAJ	3.16	110.87	107.92
10	B	1002	2J9	CAK-CAF-CAM	3.09	118.97	116.86
11	B	1003	GLU	OXT-C-O	-2.73	117.89	124.09
11	D	1003	GLU	OXT-C-O	-2.72	117.90	124.09
12	B	1001	POV	O31-C31-C32	2.58	120.00	111.91
12	C	1006	POV	O31-C31-C32	2.55	119.90	111.91
12	D	1001	POV	O31-C31-C32	2.54	119.89	111.91
12	A	1010	POV	C14-N-C12	2.52	120.24	109.92
12	A	1005	POV	O31-C31-C32	2.52	119.81	111.91
12	A	1003	POV	O31-C31-C32	2.51	119.79	111.91
10	D	1002	2J9	CAD-CAK-CAF	-2.51	120.04	123.29
12	C	1001	POV	O31-C31-C32	2.50	119.76	111.91
12	C	1001	POV	C14-N-C12	2.49	120.11	109.92
12	A	1010	POV	O31-C31-C32	2.48	119.70	111.91
12	D	1004	POV	O31-C31-C32	2.48	119.68	111.91
12	B	1005	POV	O31-C31-C32	2.46	119.64	111.91
12	D	1005	POV	O31-C31-C32	2.46	119.64	111.91
10	C	1002	2J9	CAD-CAK-CAF	-2.46	120.10	123.29
10	A	1001	2J9	CAD-CAK-CAF	-2.46	120.10	123.29
12	C	1004	POV	O31-C31-C32	2.46	119.61	111.91
10	B	1002	2J9	CAD-CAK-CAF	-2.44	120.12	123.29
12	B	1004	POV	O31-C31-C32	2.43	119.54	111.91
12	C	1005	POV	O31-C31-C32	2.41	119.46	111.91
12	B	1004	POV	C14-N-C12	2.38	119.65	109.92
12	A	1004	POV	O31-C31-C32	2.37	119.36	111.91
12	D	1004	POV	C14-N-C12	2.34	119.51	109.92
12	B	1001	POV	C14-N-C12	2.25	119.13	109.92
12	D	1001	POV	C14-N-C12	2.25	119.12	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1002	2J9	OAB-SAP-NAJ	2.21	109.98	107.92
11	B	1003	GLU	OXT-C-CA	2.20	120.89	113.38
11	D	1003	GLU	OXT-C-CA	2.20	120.87	113.38
11	A	1002	GLU	OXT-C-O	-2.17	119.17	124.09
10	A	1001	2J9	OAB-SAP-NAJ	2.14	109.92	107.92
12	D	1001	POV	C2-O21-C21	-2.13	112.54	117.79
11	C	1003	GLU	OXT-C-O	-2.13	119.26	124.09
10	B	1002	2J9	FAC-CAK-CAF	2.13	121.29	118.25
12	B	1001	POV	C2-O21-C21	-2.12	112.57	117.79
10	C	1002	2J9	CAM-CAL-NAO	-2.10	119.83	121.57
12	C	1005	POV	C14-N-C12	2.09	118.45	109.92
12	A	1004	POV	C14-N-C12	2.08	118.44	109.92
12	A	1003	POV	C14-N-C12	2.08	118.42	109.92
12	C	1006	POV	C14-N-C12	2.08	118.41	109.92
12	C	1004	POV	C14-N-C12	2.07	118.38	109.92
12	A	1005	POV	C14-N-C12	2.07	118.37	109.92
12	B	1005	POV	C14-N-C12	2.06	118.33	109.92
11	A	1002	GLU	OXT-C-CA	2.03	120.30	113.38
12	D	1005	POV	C14-N-C12	2.03	118.20	109.92
11	C	1003	GLU	OXT-C-CA	2.02	120.27	113.38

There are no chirality outliers.

All (461) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1002	2J9	CAG-CAN-NAO-CAI
10	B	1002	2J9	CAH-CAN-NAO-CAL
10	C	1002	2J9	CAG-CAN-NAO-CAL
12	A	1003	POV	C1-O11-P-O13
12	A	1003	POV	C1-O11-P-O14
12	A	1003	POV	C11-O12-P-O11
12	A	1003	POV	C11-O12-P-O13
12	A	1003	POV	C11-O12-P-O14
12	A	1003	POV	O12-C11-C12-N
12	A	1004	POV	C1-O11-P-O13
12	A	1004	POV	C1-O11-P-O14
12	A	1004	POV	O12-C11-C12-N
12	A	1005	POV	C1-O11-P-O14
12	A	1005	POV	C22-C21-O21-C2
12	A	1010	POV	C1-O11-P-O12
12	A	1010	POV	C1-O11-P-O13
12	A	1010	POV	O22-C21-O21-C2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
12	B	1001	POV	C1-O11-P-O14
12	B	1001	POV	O12-C11-C12-N
12	B	1001	POV	O22-C21-O21-C2
12	B	1004	POV	C1-O11-P-O13
12	B	1004	POV	C1-O11-P-O14
12	B	1004	POV	C11-O12-P-O14
12	B	1004	POV	O21-C2-C3-O31
12	B	1005	POV	C1-O11-P-O12
12	B	1005	POV	C11-O12-P-O14
12	B	1005	POV	O22-C21-O21-C2
12	C	1001	POV	C12-C11-O12-P
12	C	1001	POV	O22-C21-O21-C2
12	C	1004	POV	C1-O11-P-O13
12	C	1004	POV	C1-O11-P-O14
12	C	1004	POV	C11-O12-P-O11
12	C	1004	POV	C11-O12-P-O13
12	C	1004	POV	C11-O12-P-O14
12	C	1004	POV	O12-C11-C12-N
12	C	1005	POV	O12-C11-C12-N
12	C	1005	POV	C22-C21-O21-C2
12	C	1006	POV	C1-O11-P-O14
12	C	1006	POV	C22-C21-O21-C2
12	D	1001	POV	C1-O11-P-O12
12	D	1001	POV	C1-O11-P-O14
12	D	1001	POV	O12-C11-C12-N
12	D	1001	POV	O22-C21-O21-C2
12	D	1004	POV	C1-O11-P-O13
12	D	1004	POV	C1-O11-P-O14
12	D	1004	POV	O21-C2-C3-O31
12	D	1005	POV	O22-C21-O21-C2
13	A	1006	CLR	C13-C17-C20-C21
13	A	1006	CLR	C16-C17-C20-C21
12	A	1005	POV	O32-C31-O31-C3
12	C	1006	POV	O32-C31-O31-C3
13	A	1006	CLR	C13-C17-C20-C22
12	A	1005	POV	O22-C21-O21-C2
12	C	1005	POV	O22-C21-O21-C2
12	C	1006	POV	O22-C21-O21-C2
12	A	1005	POV	C32-C31-O31-C3
12	C	1006	POV	C32-C31-O31-C3
12	A	1010	POV	C22-C21-O21-C2
12	B	1001	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
12	B	1005	POV	C22-C21-O21-C2
12	C	1001	POV	C22-C21-O21-C2
12	D	1001	POV	C22-C21-O21-C2
12	D	1005	POV	C22-C21-O21-C2
13	B	1006	CLR	C16-C17-C20-C21
13	B	1006	CLR	C13-C17-C20-C21
13	A	1006	CLR	C16-C17-C20-C22
13	A	1009	CLR	C13-C17-C20-C22
13	B	1006	CLR	C13-C17-C20-C22
13	C	1009	CLR	C13-C17-C20-C22
13	B	1006	CLR	C16-C17-C20-C22
13	A	1007	CLR	C17-C20-C22-C23
13	A	1009	CLR	C17-C20-C22-C23
13	C	1007	CLR	C17-C20-C22-C23
13	C	1009	CLR	C17-C20-C22-C23
12	C	1004	POV	C22-C21-O21-C2
13	A	1008	CLR	C17-C20-C22-C23
13	C	1008	CLR	C17-C20-C22-C23
13	A	1007	CLR	C21-C20-C22-C23
13	A	1009	CLR	C21-C20-C22-C23
13	C	1007	CLR	C21-C20-C22-C23
13	C	1009	CLR	C21-C20-C22-C23
10	A	1001	2J9	CAG-CAN-NAO-CAL
12	A	1003	POV	C22-C21-O21-C2
12	C	1004	POV	O22-C21-O21-C2
13	C	1008	CLR	C21-C20-C22-C23
12	A	1003	POV	C32-C31-O31-C3
12	C	1004	POV	C32-C31-O31-C3
13	A	1009	CLR	C16-C17-C20-C21
13	C	1009	CLR	C16-C17-C20-C21
13	A	1008	CLR	C21-C20-C22-C23
12	D	1001	POV	C21-C22-C23-C24
12	A	1003	POV	O32-C31-O31-C3
13	A	1009	CLR	C13-C17-C20-C21
13	C	1009	CLR	C13-C17-C20-C21
13	A	1009	CLR	C16-C17-C20-C22
12	A	1010	POV	C31-C32-C33-C34
12	B	1001	POV	C21-C22-C23-C24
12	C	1006	POV	C21-C22-C23-C24
12	C	1004	POV	O32-C31-O31-C3
12	A	1005	POV	C21-C22-C23-C24
13	C	1009	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
12	B	1001	POV	C31-C32-C33-C34
12	C	1001	POV	C31-C32-C33-C34
12	D	1001	POV	C31-C32-C33-C34
13	A	1007	CLR	C20-C22-C23-C24
12	A	1004	POV	C22-C23-C24-C25
12	C	1005	POV	C21-C22-C23-C24
12	A	1003	POV	O22-C21-O21-C2
13	C	1007	CLR	C20-C22-C23-C24
12	D	1005	POV	C210-C211-C212-C213
12	A	1003	POV	C1-O11-P-O12
12	A	1004	POV	C1-O11-P-O12
12	A	1005	POV	C11-O12-P-O11
12	B	1001	POV	C11-O12-P-O11
12	B	1004	POV	C1-O11-P-O12
12	B	1004	POV	C11-O12-P-O11
12	B	1005	POV	C11-O12-P-O11
12	C	1001	POV	C1-O11-P-O12
12	C	1004	POV	C1-O11-P-O12
12	C	1005	POV	C1-O11-P-O12
12	C	1006	POV	C11-O12-P-O11
12	D	1001	POV	C11-O12-P-O11
12	D	1004	POV	C1-O11-P-O12
12	D	1004	POV	C11-O12-P-O11
12	D	1005	POV	C1-O11-P-O12
12	C	1001	POV	C22-C23-C24-C25
12	A	1003	POV	C310-C311-C312-C313
12	A	1004	POV	C37-C38-C39-C310
12	C	1004	POV	C36-C37-C38-C39
12	C	1006	POV	C33-C34-C35-C36
12	A	1005	POV	C33-C34-C35-C36
12	C	1001	POV	C25-C26-C27-C28
13	B	1006	CLR	C20-C22-C23-C24
12	A	1010	POV	C213-C214-C215-C216
12	C	1005	POV	C39-C310-C311-C312
12	D	1004	POV	C39-C310-C311-C312
12	D	1005	POV	C212-C213-C214-C215
12	A	1010	POV	C22-C23-C24-C25
12	B	1005	POV	C213-C214-C215-C216
12	D	1005	POV	C24-C25-C26-C27
12	D	1005	POV	C21-C22-C23-C24
12	C	1001	POV	C213-C214-C215-C216
12	A	1004	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
12	C	1005	POV	C33-C34-C35-C36
12	C	1005	POV	C212-C213-C214-C215
12	A	1010	POV	C25-C26-C27-C28
12	A	1003	POV	C311-C310-C39-C38
12	B	1004	POV	C311-C310-C39-C38
12	B	1004	POV	C311-C312-C313-C314
12	B	1005	POV	C22-C23-C24-C25
12	B	1005	POV	C24-C25-C26-C27
12	C	1005	POV	C36-C37-C38-C39
12	A	1003	POV	C213-C214-C215-C216
12	A	1003	POV	C22-C23-C24-C25
12	A	1004	POV	C36-C37-C38-C39
12	B	1001	POV	C212-C213-C214-C215
12	B	1004	POV	C312-C313-C314-C315
12	C	1006	POV	C214-C215-C216-C217
12	D	1001	POV	C212-C213-C214-C215
13	A	1006	CLR	C23-C24-C25-C27
13	B	1006	CLR	C23-C24-C25-C26
13	B	1006	CLR	C23-C24-C25-C27
12	A	1004	POV	C25-C26-C27-C28
12	C	1006	POV	C36-C37-C38-C39
12	D	1001	POV	C34-C35-C36-C37
12	D	1004	POV	C311-C310-C39-C38
12	D	1005	POV	C311-C310-C39-C38
12	B	1005	POV	C311-C310-C39-C38
12	A	1004	POV	C32-C31-O31-C3
12	B	1001	POV	C39-C310-C311-C312
13	A	1006	CLR	C23-C24-C25-C26
12	A	1003	POV	C24-C25-C26-C27
12	A	1004	POV	C311-C310-C39-C38
12	A	1004	POV	C33-C34-C35-C36
12	D	1004	POV	C24-C25-C26-C27
12	A	1010	POV	C36-C37-C38-C39
12	A	1004	POV	C22-C21-O21-C2
12	A	1005	POV	C214-C215-C216-C217
12	C	1004	POV	C312-C313-C314-C315
12	C	1004	POV	C213-C214-C215-C216
12	A	1004	POV	C210-C211-C212-C213
12	D	1004	POV	C311-C312-C313-C314
12	D	1004	POV	C213-C214-C215-C216
12	D	1001	POV	C33-C34-C35-C36
12	A	1005	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
12	C	1001	POV	C35-C36-C37-C38
12	D	1001	POV	C312-C313-C314-C315
12	A	1003	POV	C36-C37-C38-C39
12	A	1004	POV	O22-C21-O21-C2
12	C	1006	POV	C2-C1-O11-P
12	B	1001	POV	C34-C35-C36-C37
13	A	1006	CLR	C20-C22-C23-C24
10	D	1002	2J9	CAH-CAN-NAO-CAL
12	B	1004	POV	C39-C310-C311-C312
12	D	1001	POV	C25-C26-C27-C28
12	D	1004	POV	C312-C313-C314-C315
12	A	1010	POV	C34-C35-C36-C37
12	A	1004	POV	O32-C31-O31-C3
12	B	1005	POV	C32-C31-O31-C3
12	D	1005	POV	C32-C31-O31-C3
12	B	1004	POV	C213-C214-C215-C216
12	D	1005	POV	C33-C34-C35-C36
12	C	1006	POV	C34-C35-C36-C37
12	A	1010	POV	C311-C312-C313-C314
12	C	1006	POV	C211-C212-C213-C214
12	B	1004	POV	C37-C38-C39-C310
12	A	1005	POV	C211-C212-C213-C214
12	C	1001	POV	C311-C312-C313-C314
12	C	1005	POV	C23-C24-C25-C26
12	A	1005	POV	C213-C214-C215-C216
12	A	1005	POV	C34-C35-C36-C37
12	D	1004	POV	C37-C38-C39-C310
12	D	1005	POV	C312-C313-C314-C315
12	A	1010	POV	C210-C211-C212-C213
12	C	1006	POV	C210-C211-C212-C213
12	A	1005	POV	C31-C32-C33-C34
12	B	1005	POV	C21-C22-C23-C24
12	C	1006	POV	C213-C214-C215-C216
12	B	1001	POV	C25-C26-C27-C28
12	C	1004	POV	C311-C310-C39-C38
12	B	1001	POV	C22-C23-C24-C25
12	C	1005	POV	C22-C23-C24-C25
12	C	1005	POV	C37-C38-C39-C310
12	A	1005	POV	C1-O11-P-O12
12	A	1003	POV	C21-C22-C23-C24
12	A	1005	POV	C2-C1-O11-P
12	C	1006	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
12	B	1004	POV	O11-C1-C2-C3
12	C	1001	POV	C36-C37-C38-C39
12	D	1004	POV	C23-C24-C25-C26
12	D	1004	POV	C26-C27-C28-C29
12	B	1005	POV	C212-C213-C214-C215
12	A	1003	POV	C32-C33-C34-C35
12	A	1004	POV	C23-C24-C25-C26
12	C	1006	POV	C35-C36-C37-C38
12	A	1004	POV	C1-C2-C3-O31
12	A	1010	POV	C310-C311-C312-C313
12	C	1006	POV	C31-C32-C33-C34
12	D	1005	POV	O32-C31-O31-C3
12	B	1005	POV	O32-C31-O31-C3
12	B	1001	POV	C313-C314-C315-C316
12	C	1004	POV	C22-C23-C24-C25
12	D	1005	POV	C213-C214-C215-C216
12	A	1005	POV	C35-C36-C37-C38
12	A	1005	POV	C210-C211-C212-C213
12	B	1005	POV	C312-C313-C314-C315
12	B	1004	POV	C22-C21-O21-C2
12	B	1005	POV	C37-C38-C39-C310
12	A	1010	POV	C35-C36-C37-C38
12	B	1004	POV	C310-C311-C312-C313
12	A	1003	POV	C27-C28-C29-C210
12	C	1004	POV	C24-C25-C26-C27
12	C	1005	POV	C32-C31-O31-C3
12	D	1005	POV	O11-C1-C2-O21
12	B	1004	POV	C36-C37-C38-C39
12	B	1001	POV	O21-C2-C3-O31
12	C	1001	POV	O21-C2-C3-O31
12	B	1004	POV	C23-C24-C25-C26
12	C	1001	POV	C34-C35-C36-C37
12	C	1004	POV	C311-C312-C313-C314
12	D	1005	POV	C37-C38-C39-C310
12	D	1005	POV	C23-C24-C25-C26
12	B	1001	POV	C33-C34-C35-C36
13	C	1007	CLR	C16-C17-C20-C22
12	A	1005	POV	C311-C310-C39-C38
12	A	1003	POV	O11-C1-C2-C3
12	B	1005	POV	O11-C1-C2-C3
12	C	1001	POV	O11-C1-C2-C3
12	D	1004	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	D	1005	POV	O11-C1-C2-C3
12	B	1005	POV	C214-C215-C216-C217
12	B	1004	POV	C24-C25-C26-C27
12	B	1001	POV	C32-C31-O31-C3
12	D	1005	POV	C22-C23-C24-C25
12	B	1004	POV	C2-C1-O11-P
12	D	1004	POV	C2-C1-O11-P
13	A	1007	CLR	C16-C17-C20-C22
12	A	1010	POV	C37-C38-C39-C310
12	C	1001	POV	C210-C211-C212-C213
12	B	1001	POV	C311-C310-C39-C38
12	A	1010	POV	C1-C2-C3-O31
12	B	1004	POV	C1-C2-C3-O31
12	D	1005	POV	C1-C2-C3-O31
12	C	1005	POV	O32-C31-O31-C3
12	B	1005	POV	C33-C34-C35-C36
12	C	1004	POV	C32-C33-C34-C35
12	A	1005	POV	C39-C310-C311-C312
12	C	1004	POV	C313-C314-C315-C316
12	C	1006	POV	C39-C310-C311-C312
12	A	1003	POV	C39-C310-C311-C312
12	A	1003	POV	O11-C1-C2-O21
12	B	1005	POV	O11-C1-C2-O21
12	D	1004	POV	O11-C1-C2-O21
12	A	1004	POV	O21-C2-C3-O31
12	C	1005	POV	O21-C2-C3-O31
12	D	1001	POV	O21-C2-C3-O31
12	C	1004	POV	C27-C28-C29-C210
13	A	1007	CLR	C13-C17-C20-C22
13	C	1007	CLR	C13-C17-C20-C22
12	B	1004	POV	O22-C21-O21-C2
13	C	1007	CLR	C16-C17-C20-C21
12	B	1004	POV	C22-C23-C24-C25
12	D	1004	POV	C22-C23-C24-C25
12	C	1001	POV	C27-C28-C29-C210
12	C	1001	POV	C32-C31-O31-C3
12	D	1004	POV	C22-C21-O21-C2
12	A	1003	POV	C211-C212-C213-C214
12	C	1005	POV	C35-C36-C37-C38
12	C	1004	POV	O11-C1-C2-C3
12	A	1010	POV	C27-C28-C29-C210
12	C	1001	POV	C310-C311-C312-C313

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
12	A	1004	POV	C35-C36-C37-C38
11	B	1003	GLU	OXT-C-CA-CB
11	D	1003	GLU	OXT-C-CA-CB
12	A	1003	POV	C37-C38-C39-C310
12	B	1004	POV	C26-C27-C28-C29
12	B	1005	POV	C2-C1-O11-P
12	C	1004	POV	C2-C1-O11-P
12	C	1005	POV	C1-C2-C3-O31
12	D	1004	POV	C1-C2-C3-O31
12	C	1001	POV	O11-C1-C2-O21
12	C	1004	POV	O11-C1-C2-O21
12	D	1001	POV	C32-C31-O31-C3
13	C	1007	CLR	C13-C17-C20-C21
12	C	1004	POV	C37-C38-C39-C310
12	C	1006	POV	C310-C311-C312-C313
12	D	1004	POV	O22-C21-O21-C2
12	B	1001	POV	O32-C31-O31-C3
12	A	1010	POV	O21-C2-C3-O31
12	B	1005	POV	O21-C2-C3-O31
12	D	1005	POV	O21-C2-C3-O31
13	A	1007	CLR	C16-C17-C20-C21
13	A	1007	CLR	C13-C17-C20-C21
12	A	1005	POV	C310-C311-C312-C313
12	C	1001	POV	O32-C31-O31-C3
12	D	1004	POV	C215-C216-C217-C218
12	D	1004	POV	C36-C37-C38-C39
12	B	1005	POV	C35-C36-C37-C38
12	C	1004	POV	C211-C212-C213-C214
12	B	1001	POV	C1-O11-P-O12
12	C	1006	POV	C1-O11-P-O12
12	A	1003	POV	C2-C1-O11-P
12	D	1001	POV	C2-C1-O11-P
12	D	1005	POV	C2-C1-O11-P
12	D	1001	POV	O32-C31-O31-C3
12	A	1005	POV	C1-O11-P-O13
12	A	1005	POV	C11-O12-P-O13
12	A	1010	POV	C1-O11-P-O14
12	A	1010	POV	C11-O12-P-O13
12	B	1001	POV	C11-O12-P-O13
12	C	1001	POV	C1-O11-P-O14
12	C	1001	POV	C11-O12-P-O13
12	C	1005	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
12	C	1006	POV	C1-O11-P-O13
12	C	1006	POV	C11-O12-P-O13
12	D	1001	POV	C11-O12-P-O13
12	D	1004	POV	C11-O12-P-O14
12	A	1004	POV	C34-C35-C36-C37
12	A	1004	POV	O11-C1-C2-C3
12	D	1005	POV	C313-C314-C315-C316
12	A	1004	POV	C213-C214-C215-C216
12	D	1005	POV	C211-C212-C213-C214
12	A	1003	POV	C12-C11-O12-P
12	A	1010	POV	C12-C11-O12-P
12	C	1004	POV	C12-C11-O12-P
12	D	1004	POV	C310-C311-C312-C313
12	C	1005	POV	C26-C27-C28-C29
12	C	1006	POV	C26-C27-C28-C29
12	C	1004	POV	C39-C310-C311-C312
12	A	1010	POV	O11-C1-C2-O21
12	A	1005	POV	C311-C312-C313-C314
12	B	1004	POV	C215-C216-C217-C218
12	A	1005	POV	O12-C11-C12-N
12	B	1001	POV	C1-C2-C3-O31
12	B	1004	POV	O12-C11-C12-N
12	C	1001	POV	C1-C2-C3-O31
12	C	1006	POV	O12-C11-C12-N
12	D	1001	POV	C1-C2-C3-O31
12	D	1004	POV	O12-C11-C12-N
11	B	1003	GLU	O-C-CA-CB
11	D	1003	GLU	O-C-CA-CB
12	C	1005	POV	C311-C312-C313-C314
12	A	1005	POV	C26-C27-C28-C29
12	B	1001	POV	C2-C1-O11-P
12	A	1010	POV	C33-C34-C35-C36
12	D	1001	POV	C311-C312-C313-C314
12	B	1005	POV	C31-C32-C33-C34
12	A	1003	POV	O21-C21-C22-C23
12	C	1004	POV	C31-C32-C33-C34
12	C	1005	POV	C25-C26-C27-C28
12	A	1005	POV	C1-C2-O21-C21
12	C	1006	POV	C1-C2-O21-C21
12	B	1004	POV	C34-C35-C36-C37
12	D	1005	POV	C35-C36-C37-C38
12	A	1004	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
12	B	1004	POV	O11-C1-C2-O21
12	B	1001	POV	C36-C37-C38-C39
12	C	1005	POV	C214-C215-C216-C217
12	C	1006	POV	C311-C312-C313-C314
12	D	1005	POV	C11-O12-P-O11
12	A	1004	POV	C31-C32-C33-C34
12	D	1001	POV	C22-C23-C24-C25
12	B	1001	POV	C311-C312-C313-C314
12	D	1005	POV	C26-C27-C28-C29
12	A	1010	POV	O11-C1-C2-C3
12	C	1004	POV	C33-C34-C35-C36
12	D	1001	POV	C39-C310-C311-C312
12	C	1004	POV	O21-C21-C22-C23
12	D	1005	POV	C31-C32-C33-C34
12	A	1004	POV	C310-C311-C312-C313
12	C	1001	POV	C37-C38-C39-C310
12	D	1001	POV	C313-C314-C315-C316
12	B	1005	POV	C39-C310-C311-C312
12	C	1004	POV	C21-C22-C23-C24
12	A	1004	POV	C29-C210-C211-C212
12	C	1004	POV	C26-C27-C28-C29
12	A	1003	POV	C212-C213-C214-C215
12	C	1004	POV	C310-C311-C312-C313
12	B	1001	POV	C35-C36-C37-C38
12	D	1005	POV	C39-C310-C311-C312
12	B	1005	POV	C313-C314-C315-C316
12	B	1005	POV	C1-C2-C3-O31
12	A	1010	POV	C313-C314-C315-C316
12	D	1001	POV	C32-C33-C34-C35
12	A	1005	POV	C27-C28-C29-C210
12	B	1004	POV	O31-C31-C32-C33
12	A	1003	POV	C26-C27-C28-C29
12	A	1003	POV	C25-C26-C27-C28
12	D	1001	POV	C37-C38-C39-C310
12	B	1001	POV	C27-C28-C29-C210
12	C	1006	POV	C27-C28-C29-C210
12	D	1004	POV	C27-C28-C29-C210
12	B	1001	POV	C24-C25-C26-C27
11	B	1003	GLU	OXT-C-CA-N
11	D	1003	GLU	OXT-C-CA-N
12	A	1010	POV	C11-C12-N-C14
12	D	1005	POV	C215-C216-C217-C218

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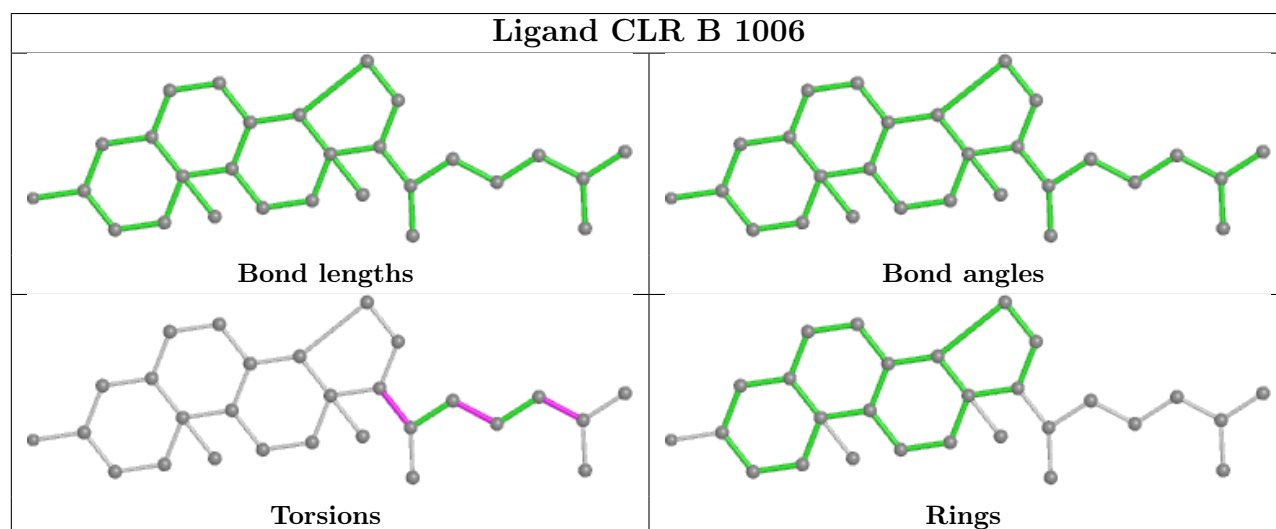
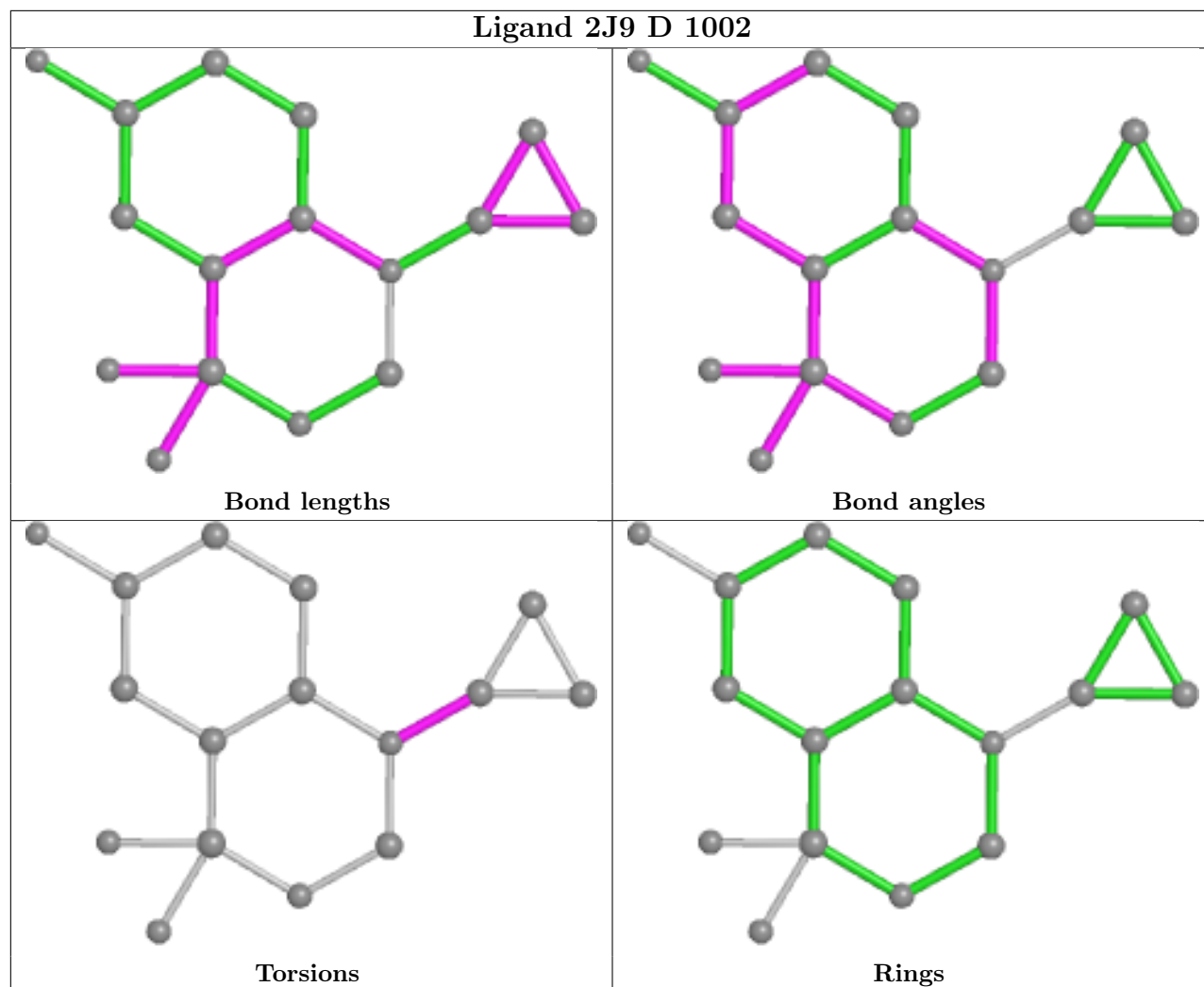
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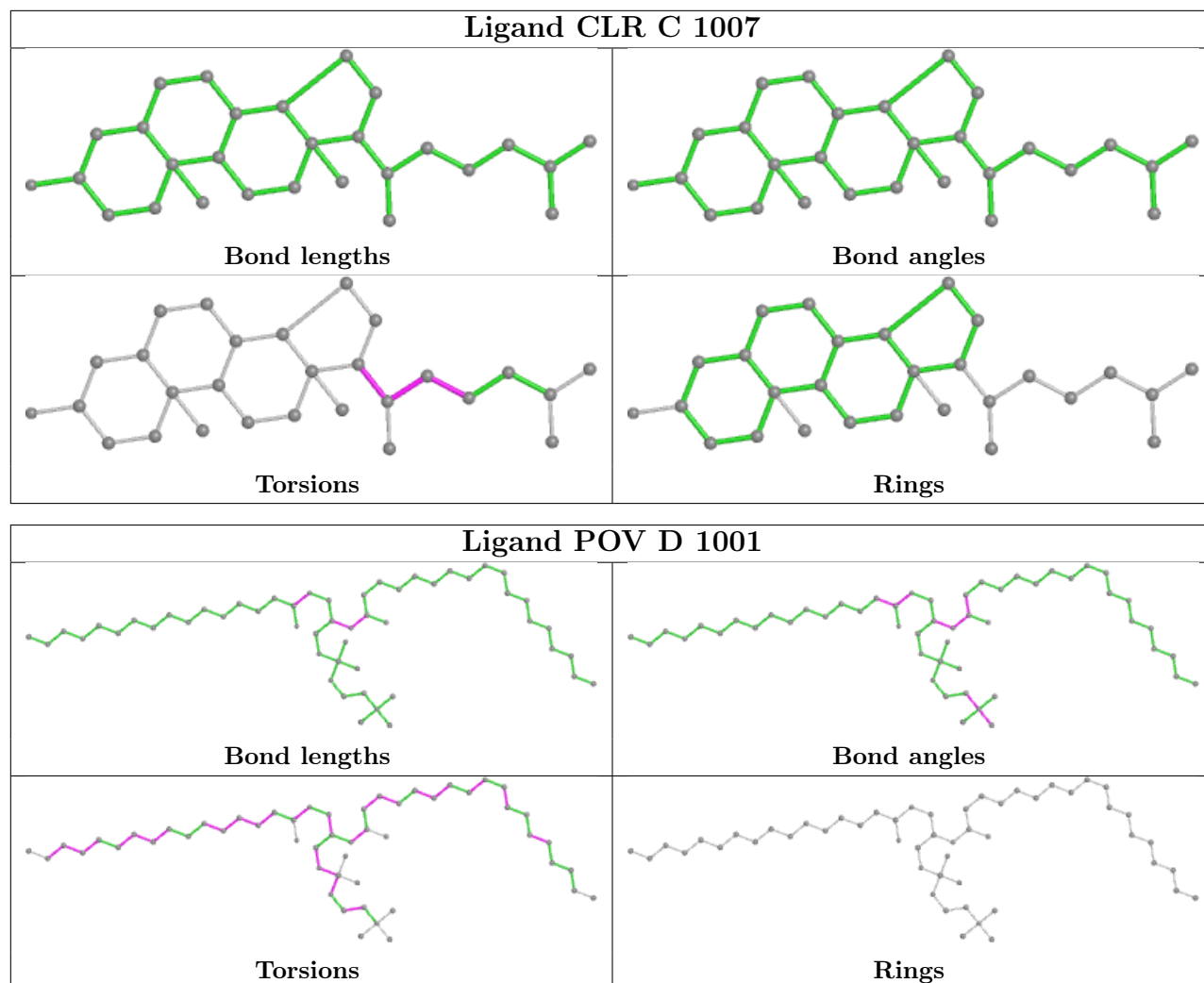
Mol	Chain	Res	Type	Atoms
12	B	1001	POV	C29-C210-C211-C212
12	D	1001	POV	C27-C28-C29-C210
12	D	1004	POV	C29-C210-C211-C212
12	C	1001	POV	C26-C27-C28-C29
12	D	1001	POV	C29-C210-C211-C212
12	A	1005	POV	O21-C21-C22-C23
12	B	1004	POV	O32-C31-C32-C33
12	C	1006	POV	O21-C21-C22-C23
12	A	1010	POV	C26-C27-C28-C29
12	A	1004	POV	C211-C212-C213-C214
12	C	1006	POV	C29-C210-C211-C212
12	A	1010	POV	C11-C12-N-C15
12	D	1005	POV	C11-O12-P-O14
12	D	1001	POV	C311-C310-C39-C38
12	B	1004	POV	C29-C210-C211-C212
12	B	1004	POV	C27-C28-C29-C210
12	C	1006	POV	C24-C25-C26-C27
12	D	1001	POV	C24-C25-C26-C27
12	A	1005	POV	C29-C210-C211-C212
11	A	1002	GLU	OE1-CD-CG-CB
11	C	1003	GLU	OE1-CD-CG-CB
12	C	1001	POV	C214-C215-C216-C217
12	A	1003	POV	C23-C24-C25-C26
12	D	1004	POV	O31-C31-C32-C33

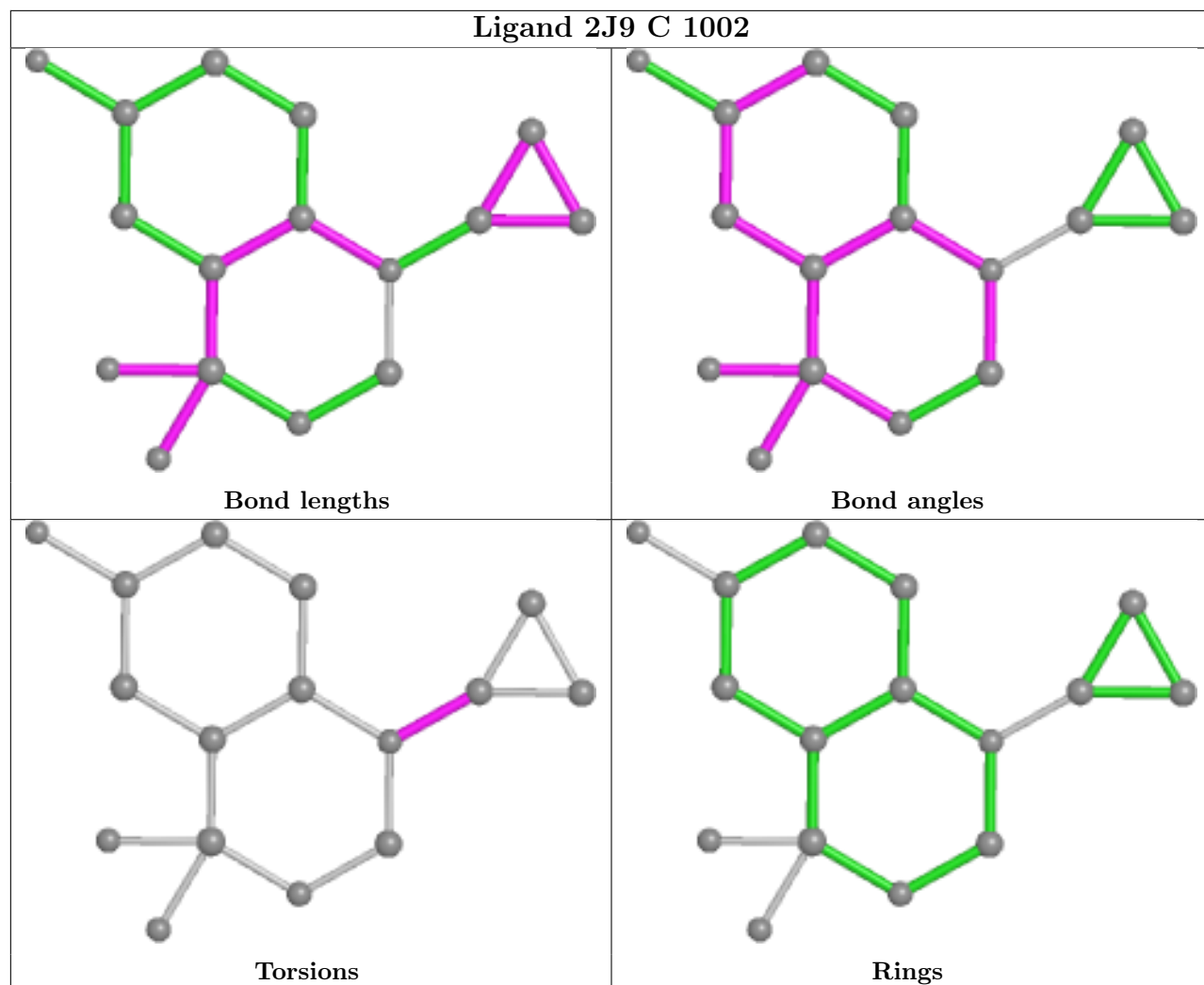
There are no ring outliers.

No monomer is involved in short contacts.

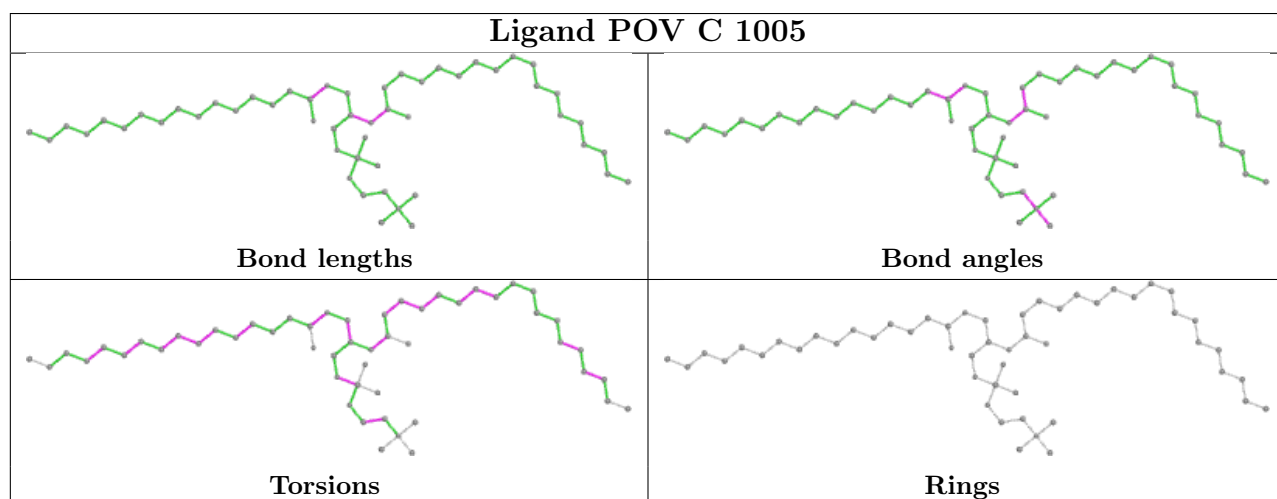
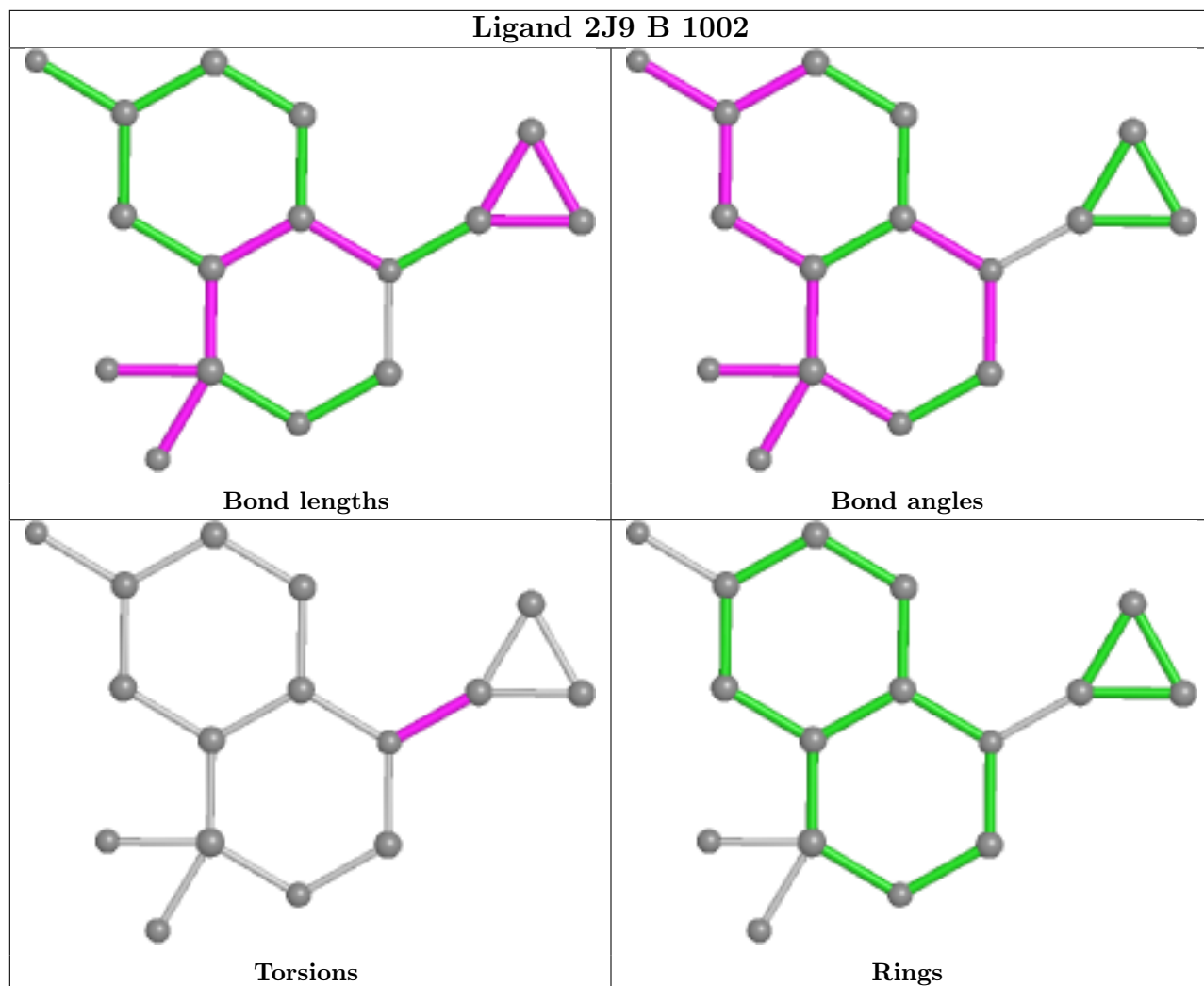
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

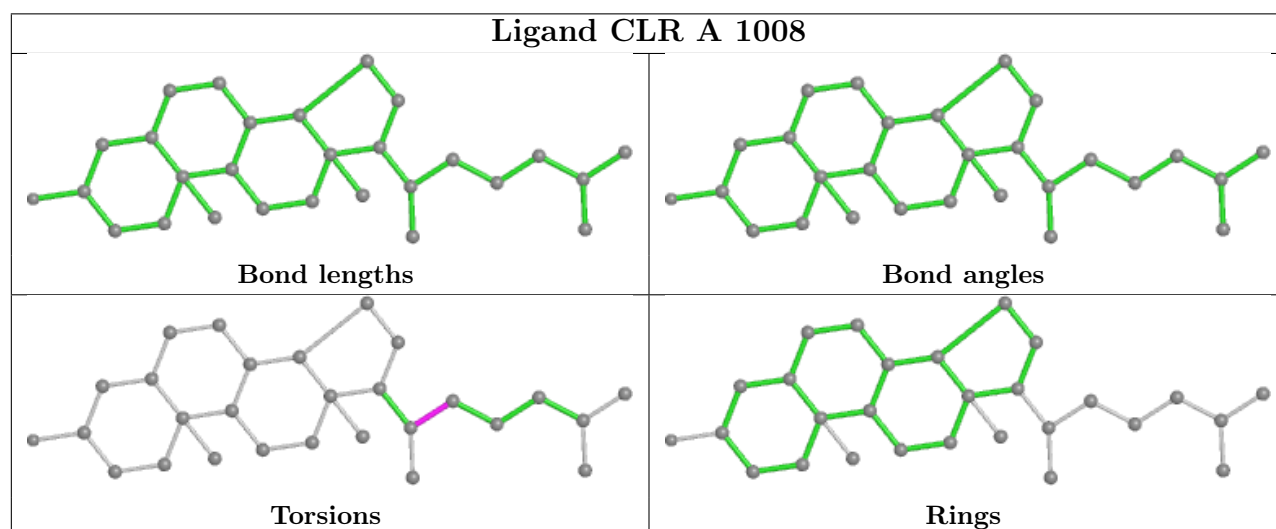
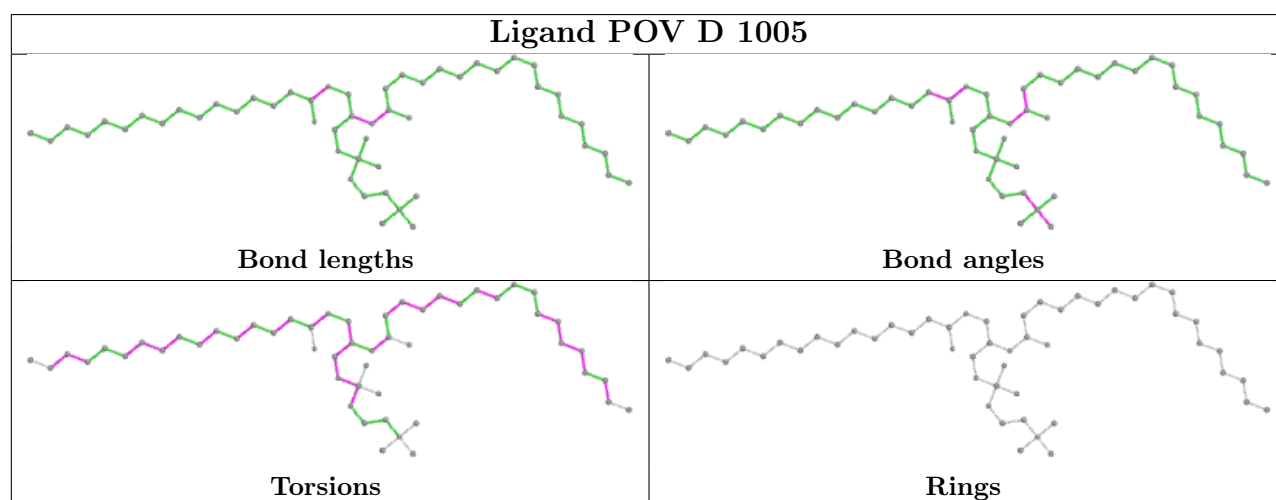
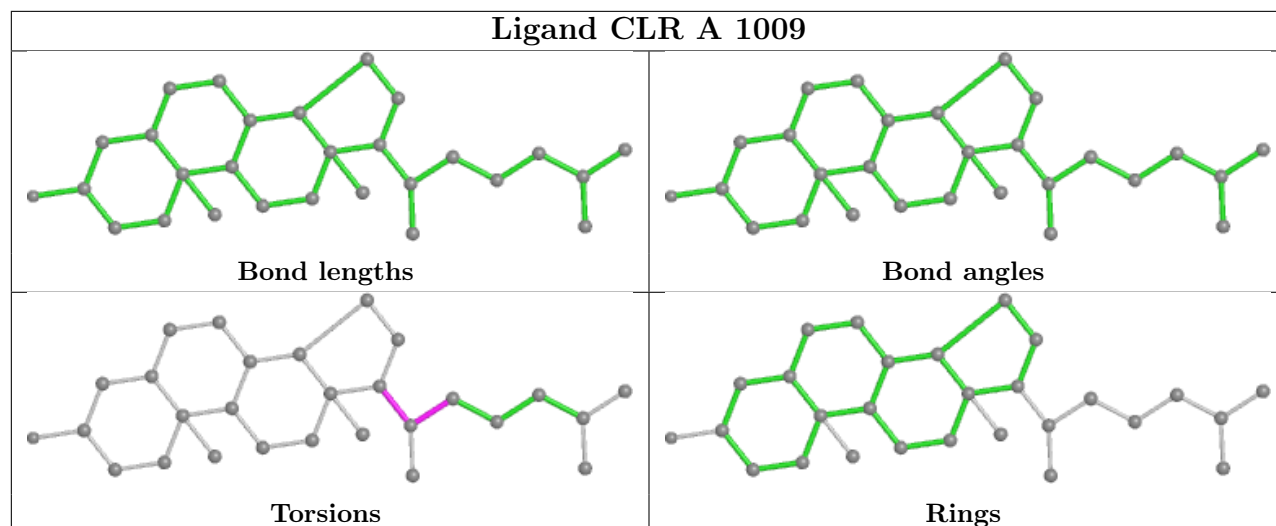


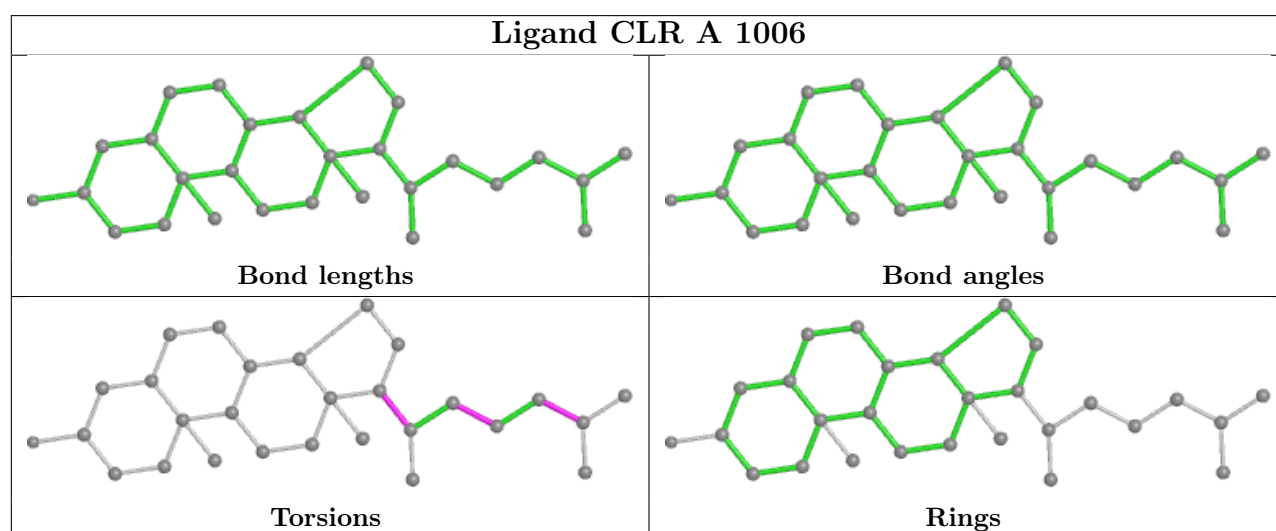
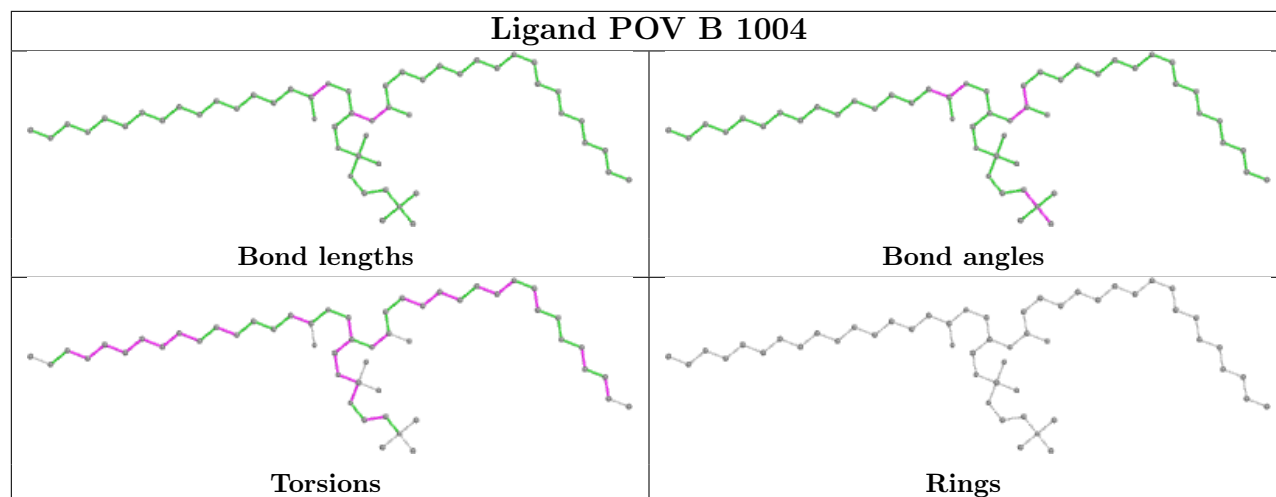


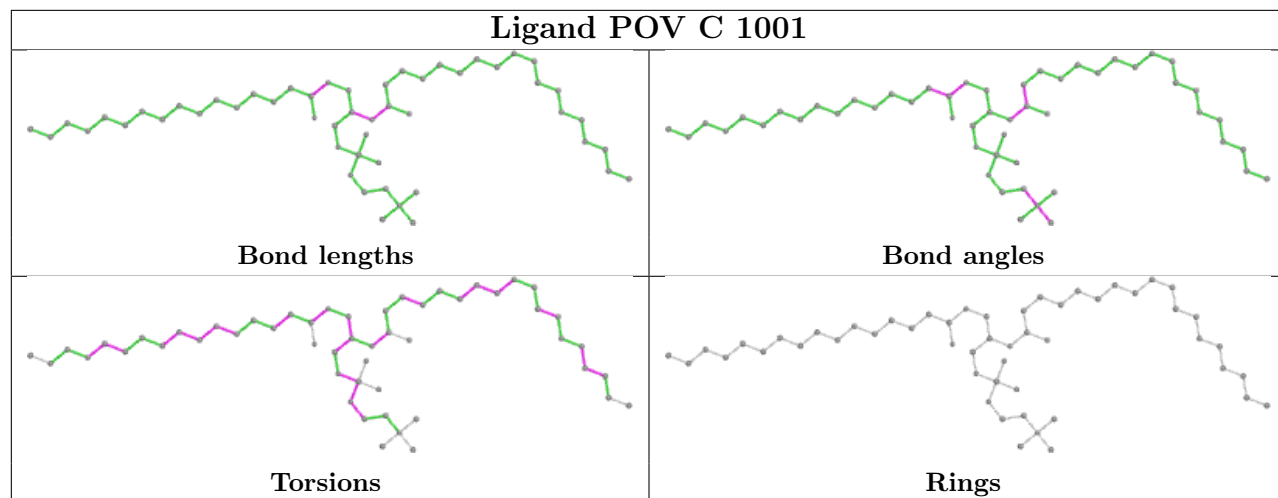
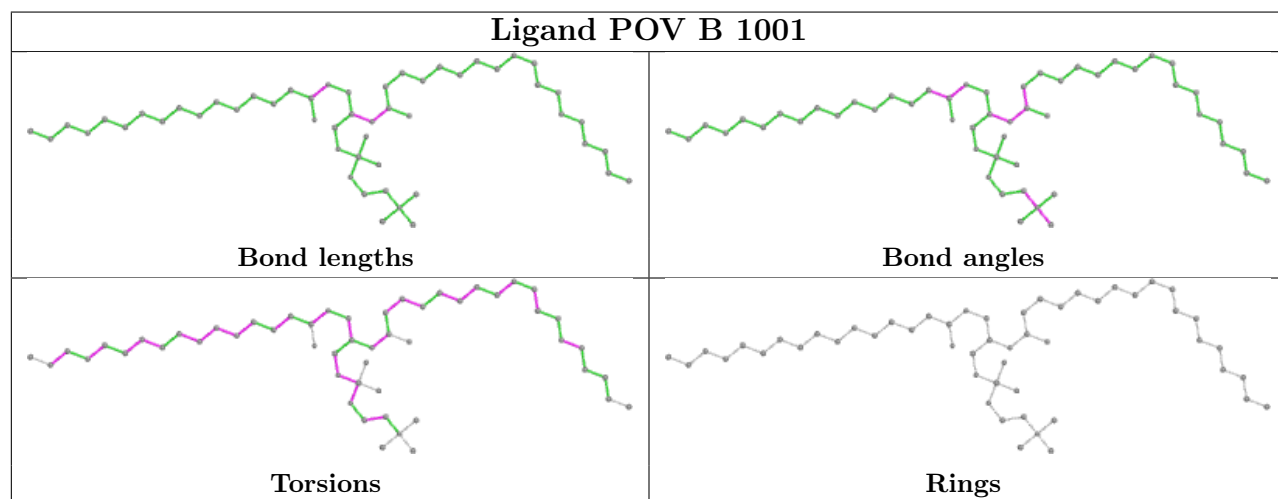
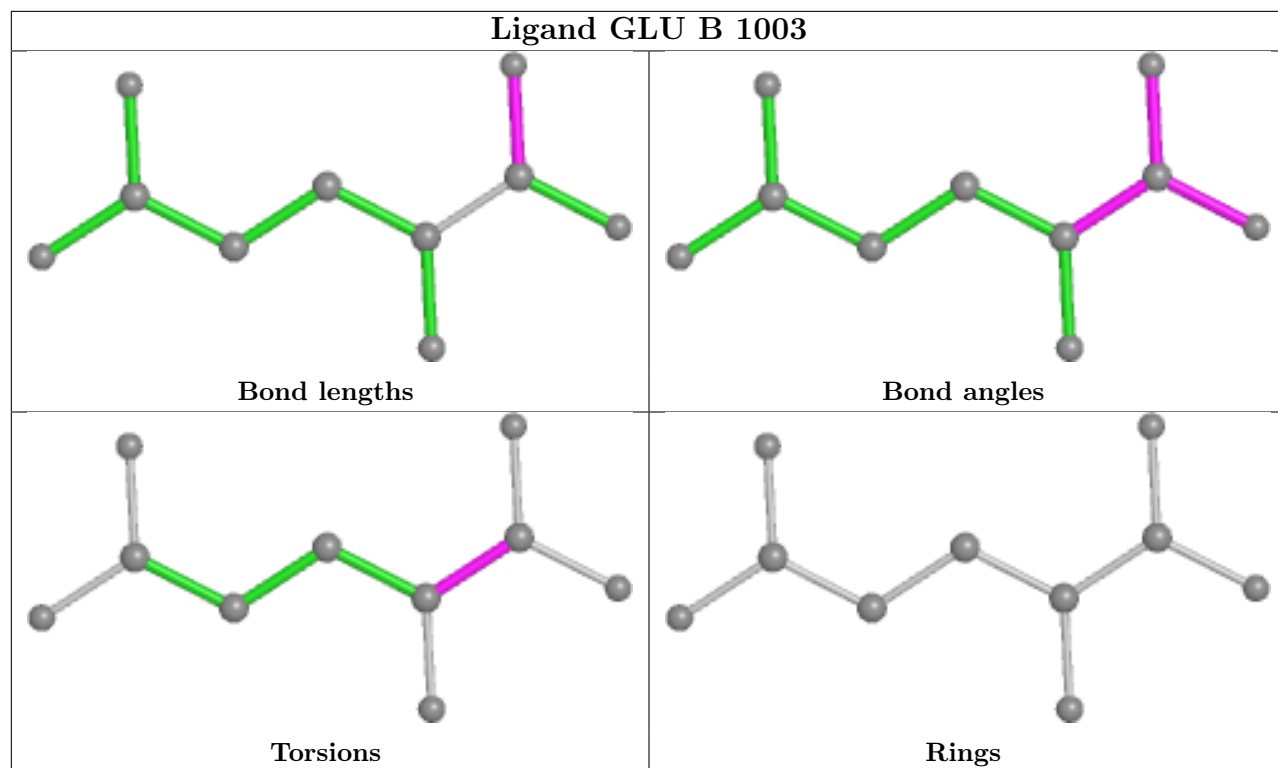


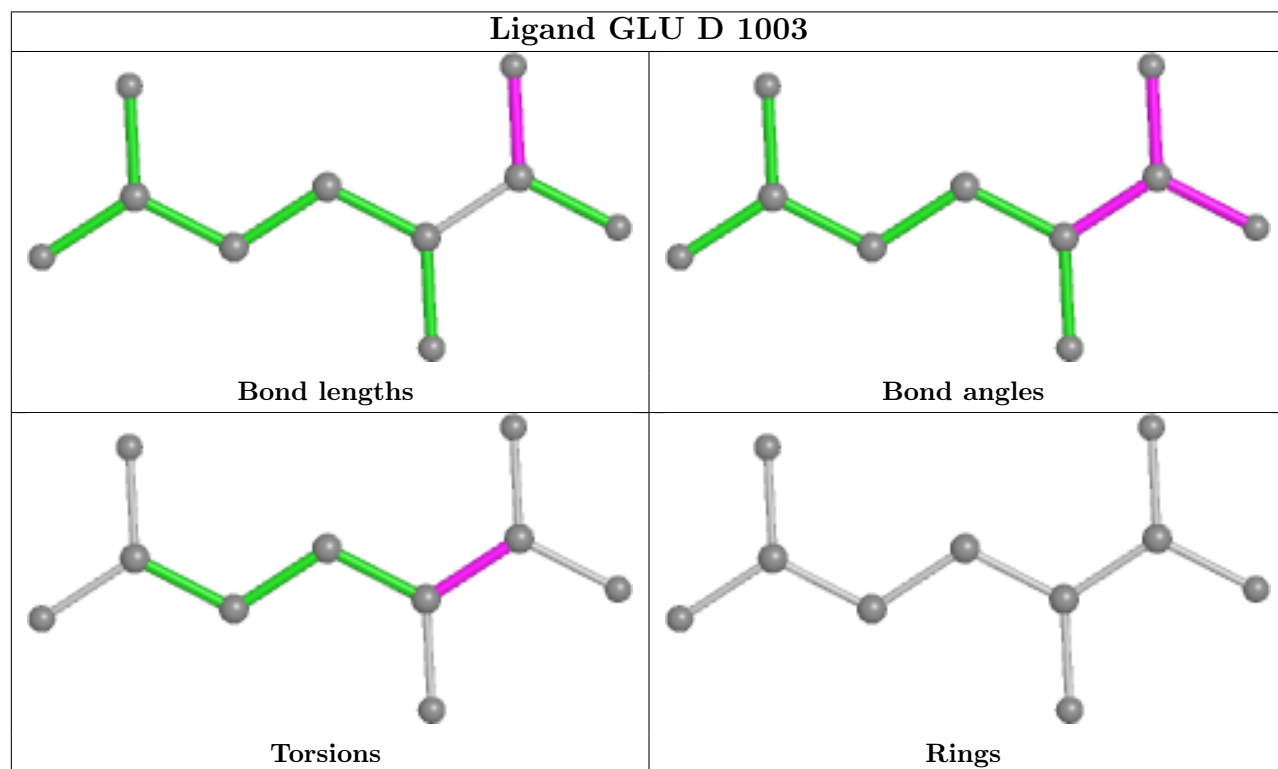
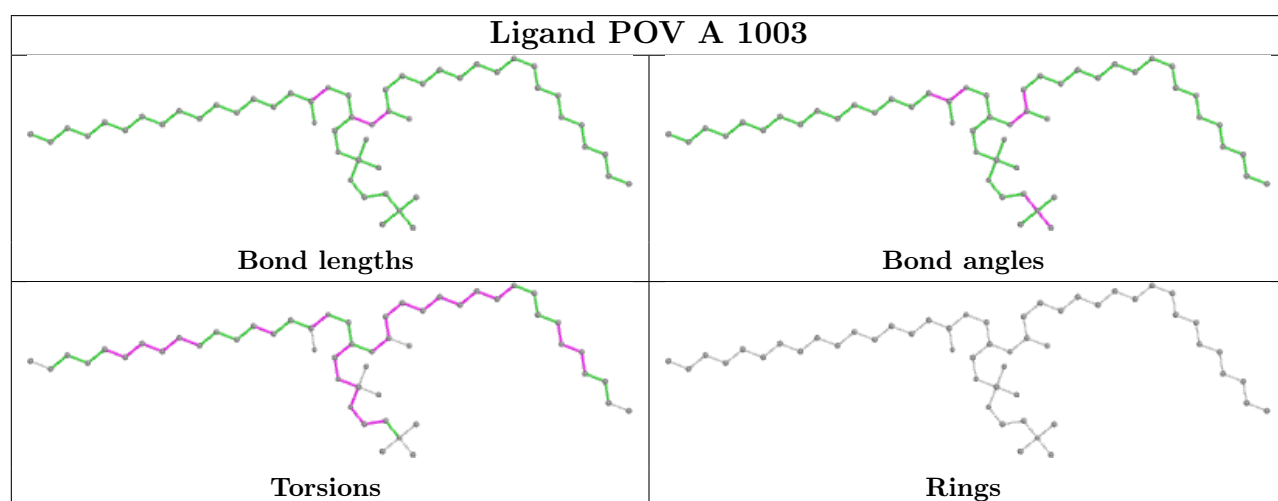
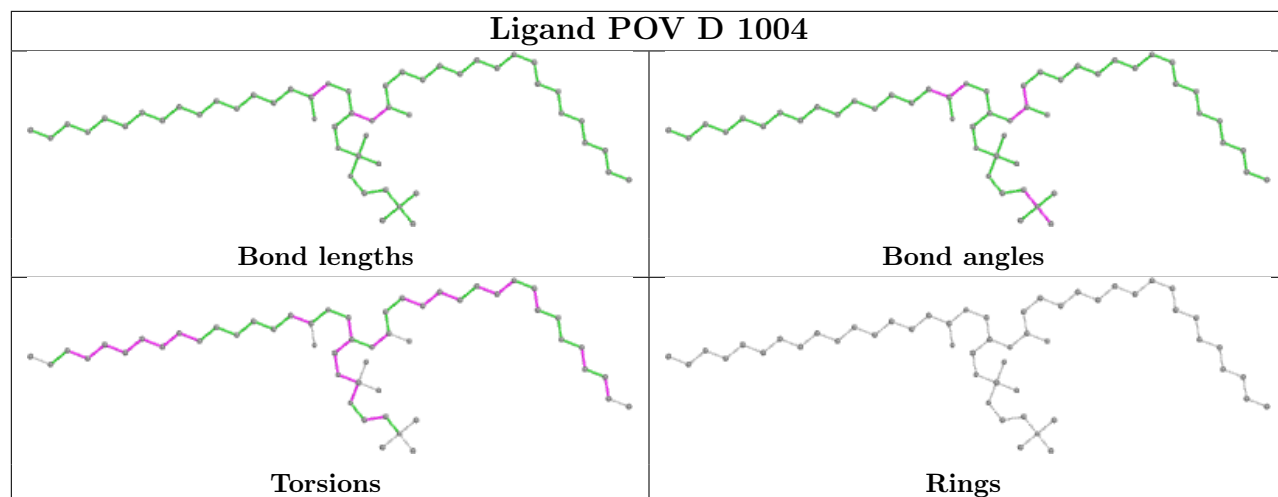


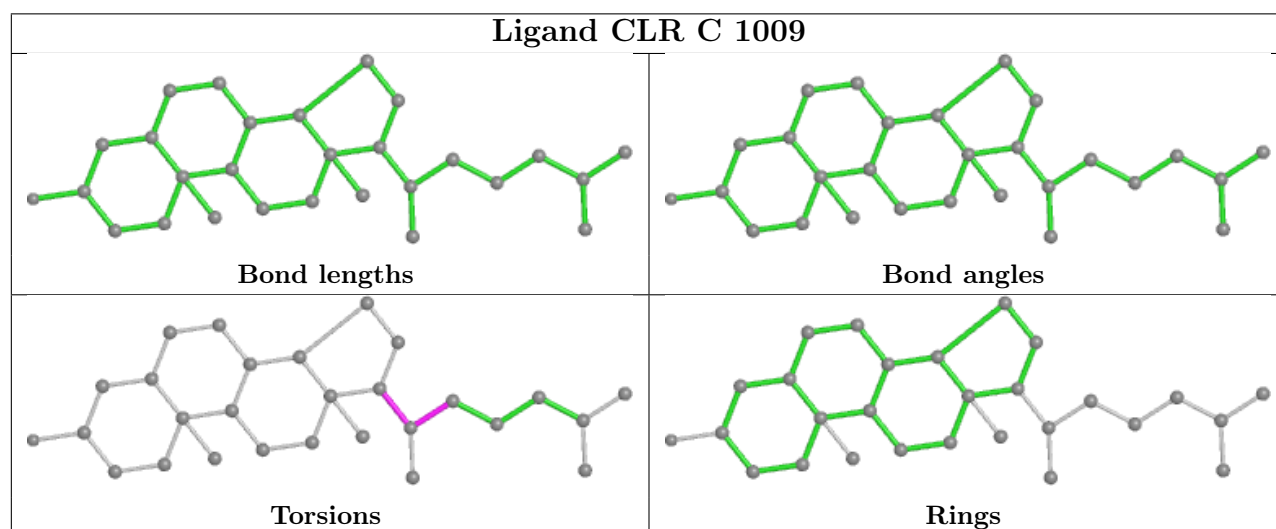
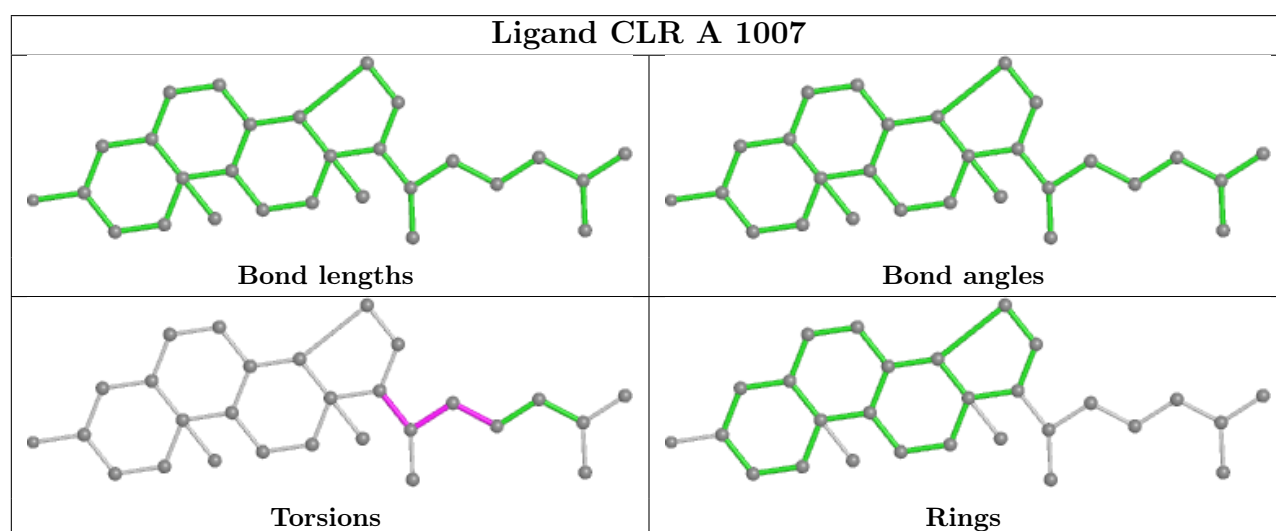
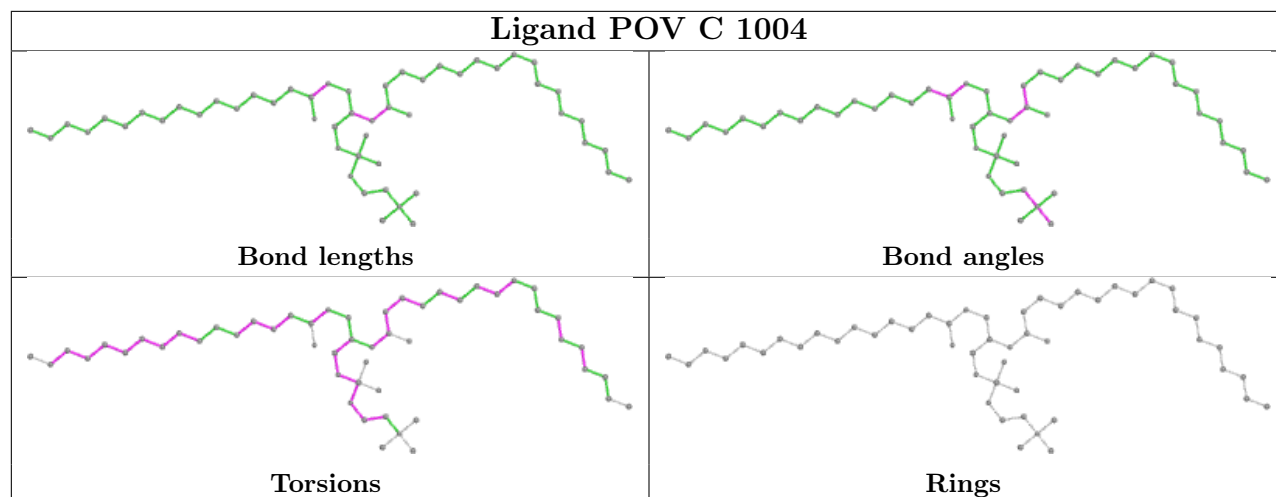


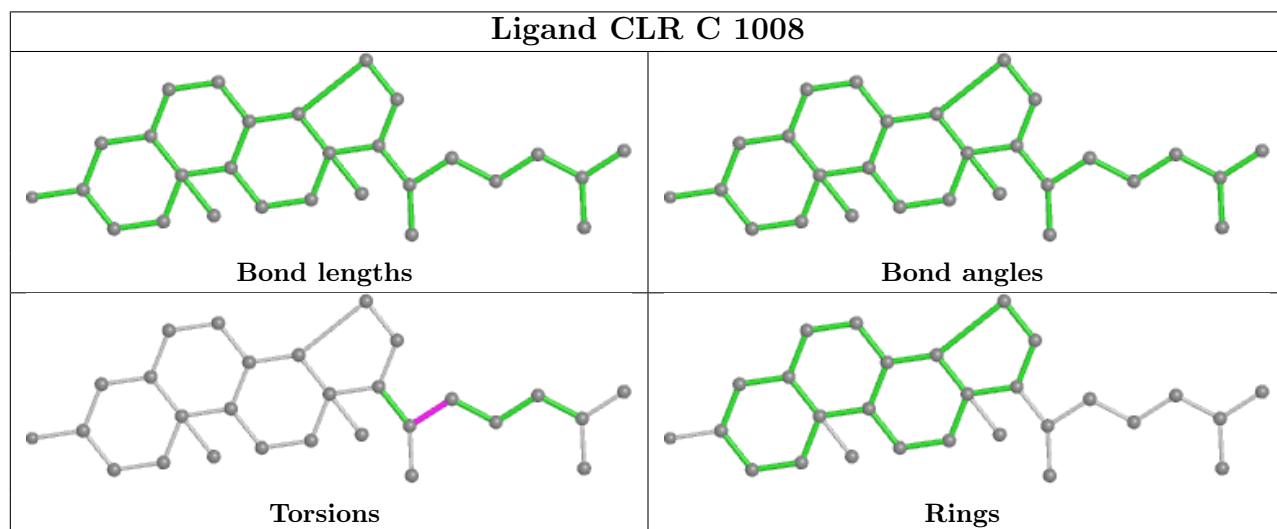
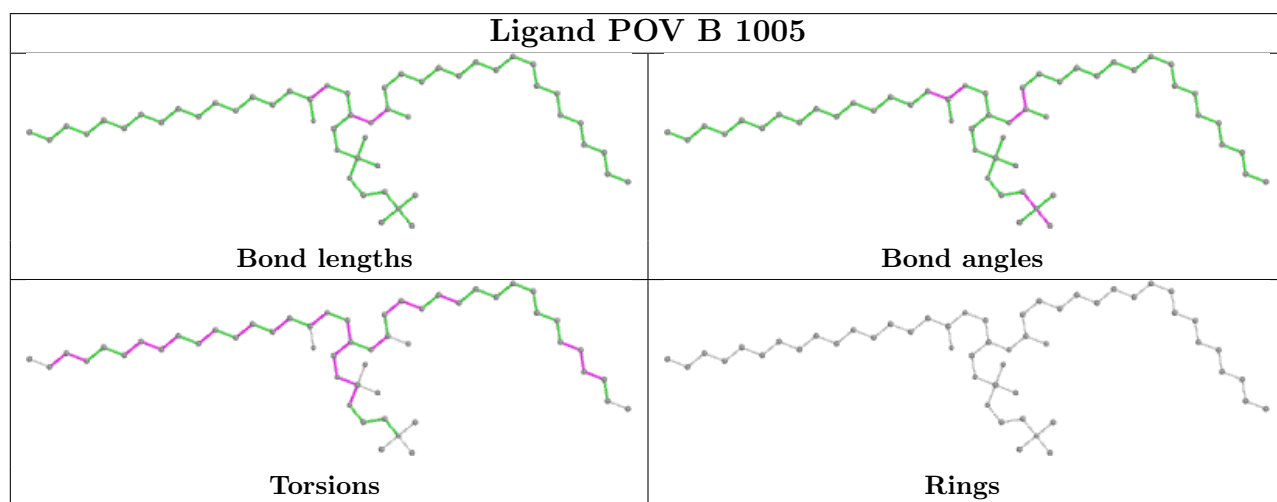
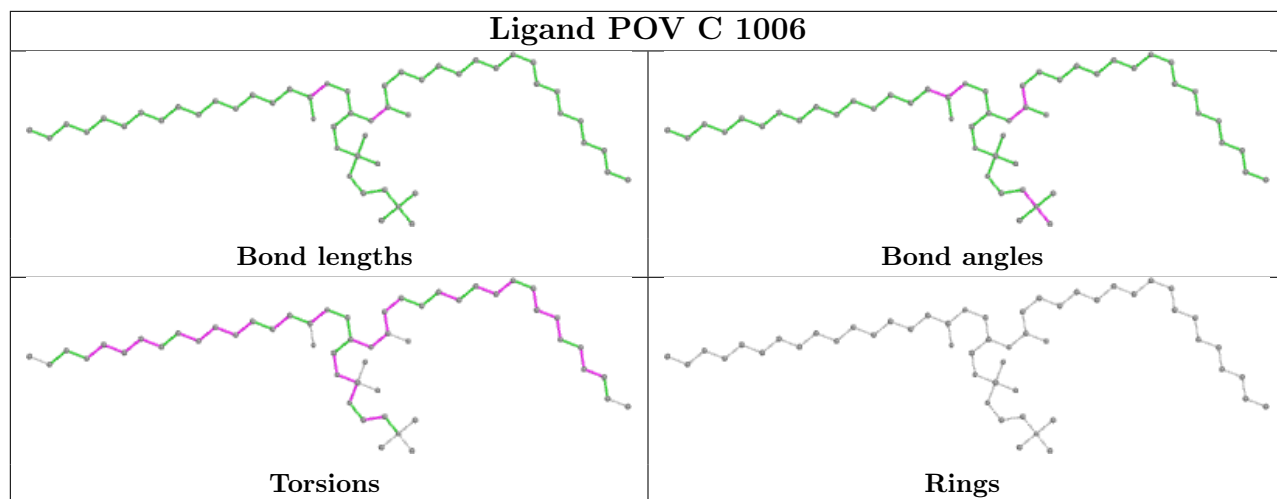


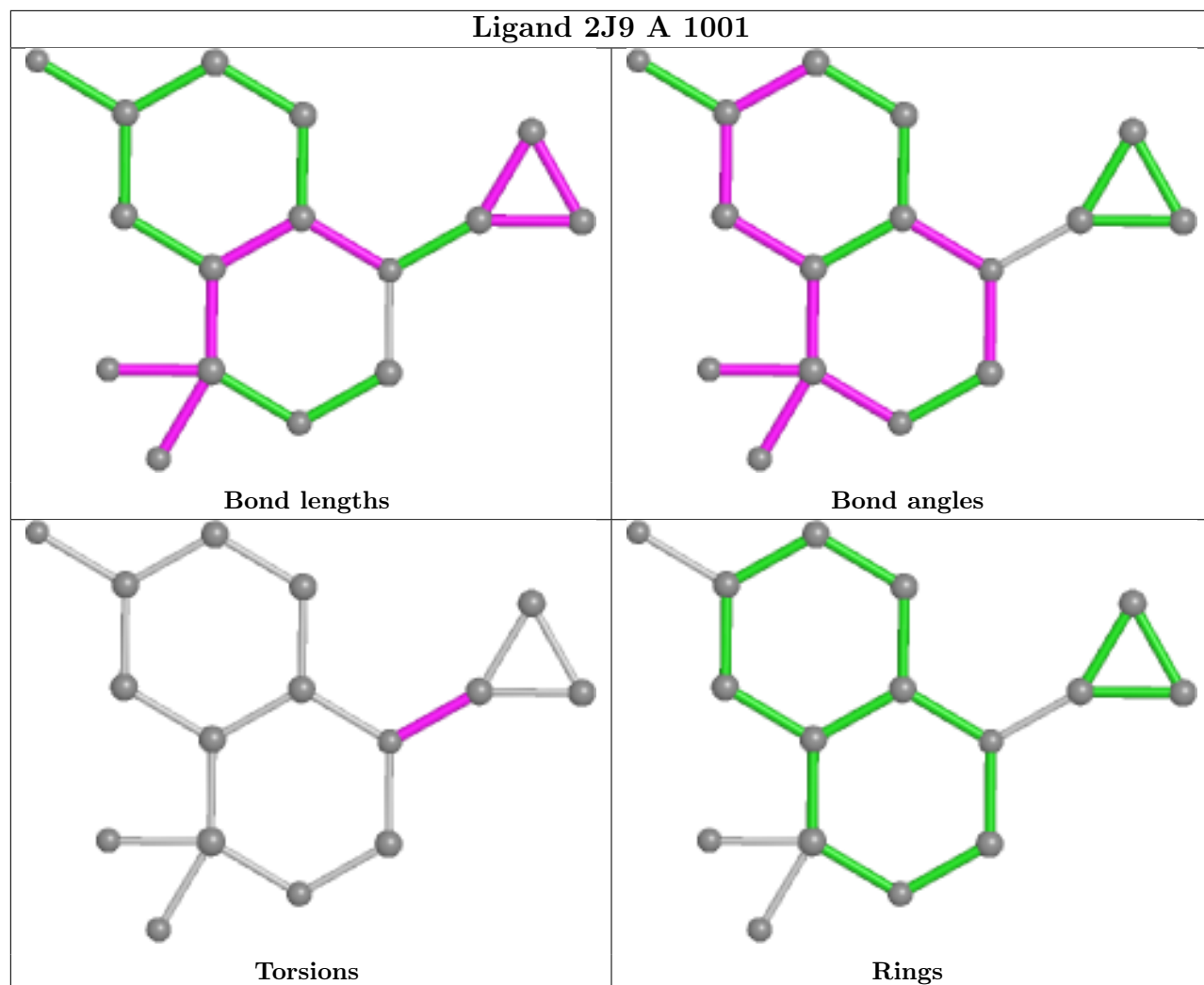




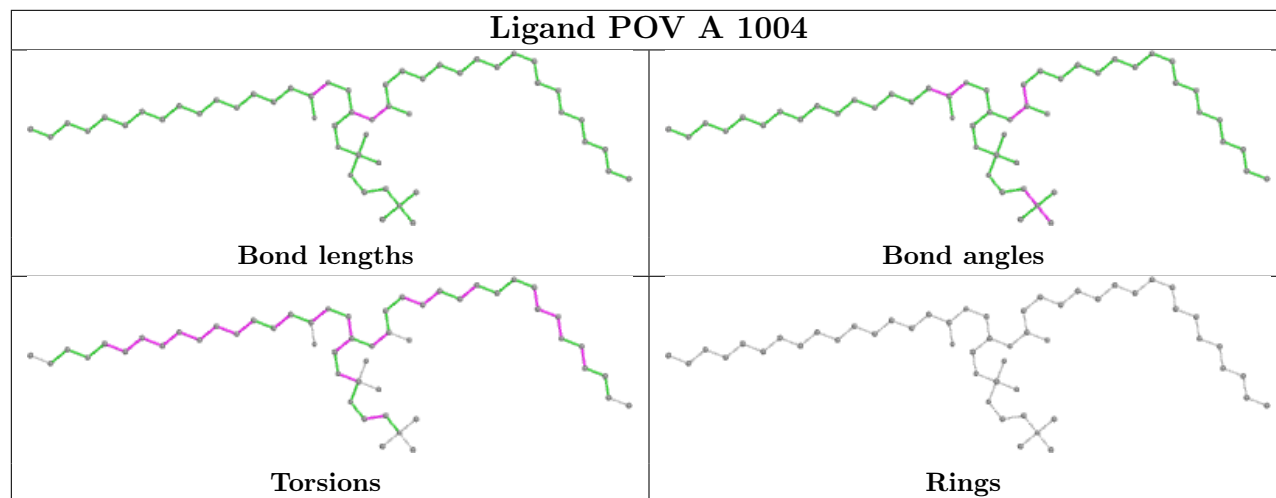
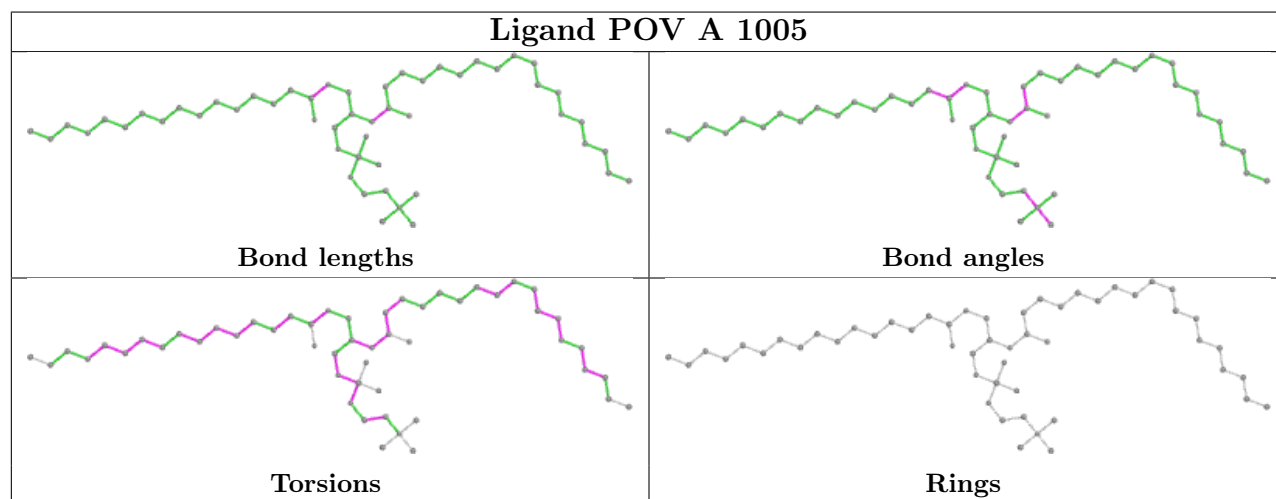
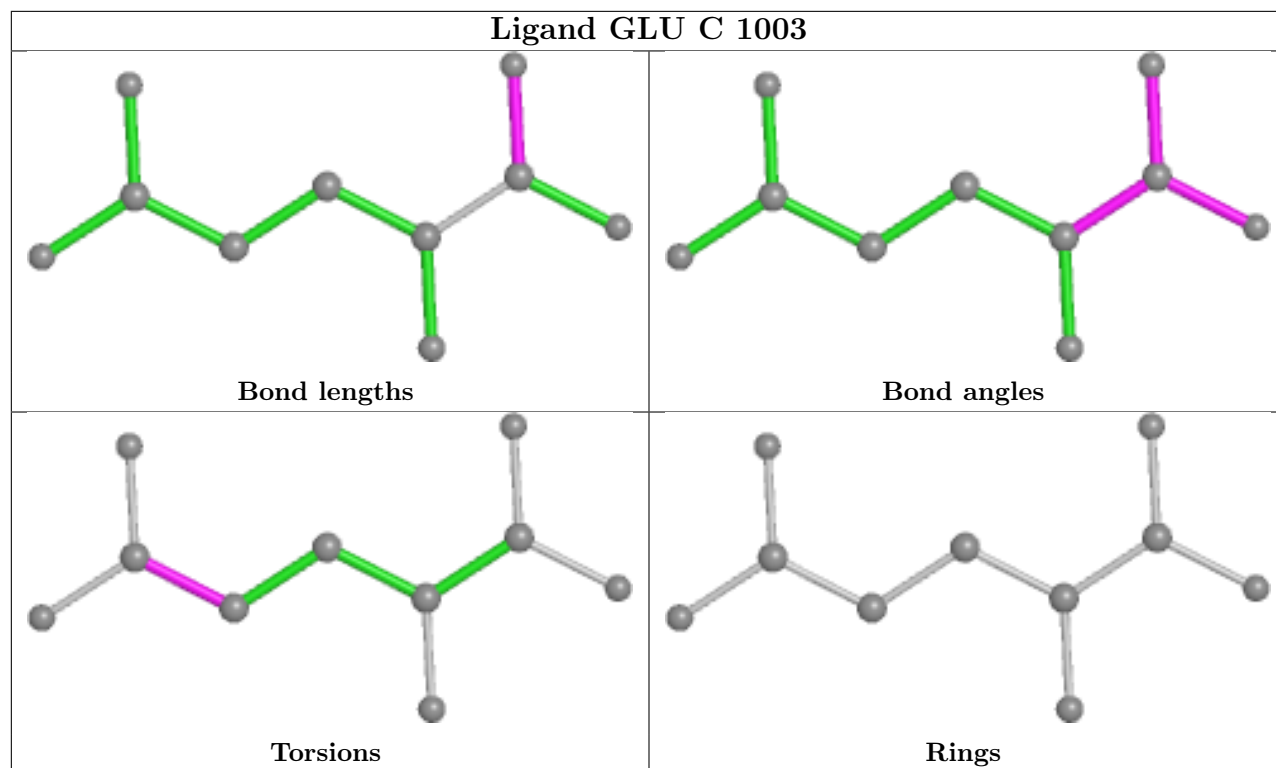


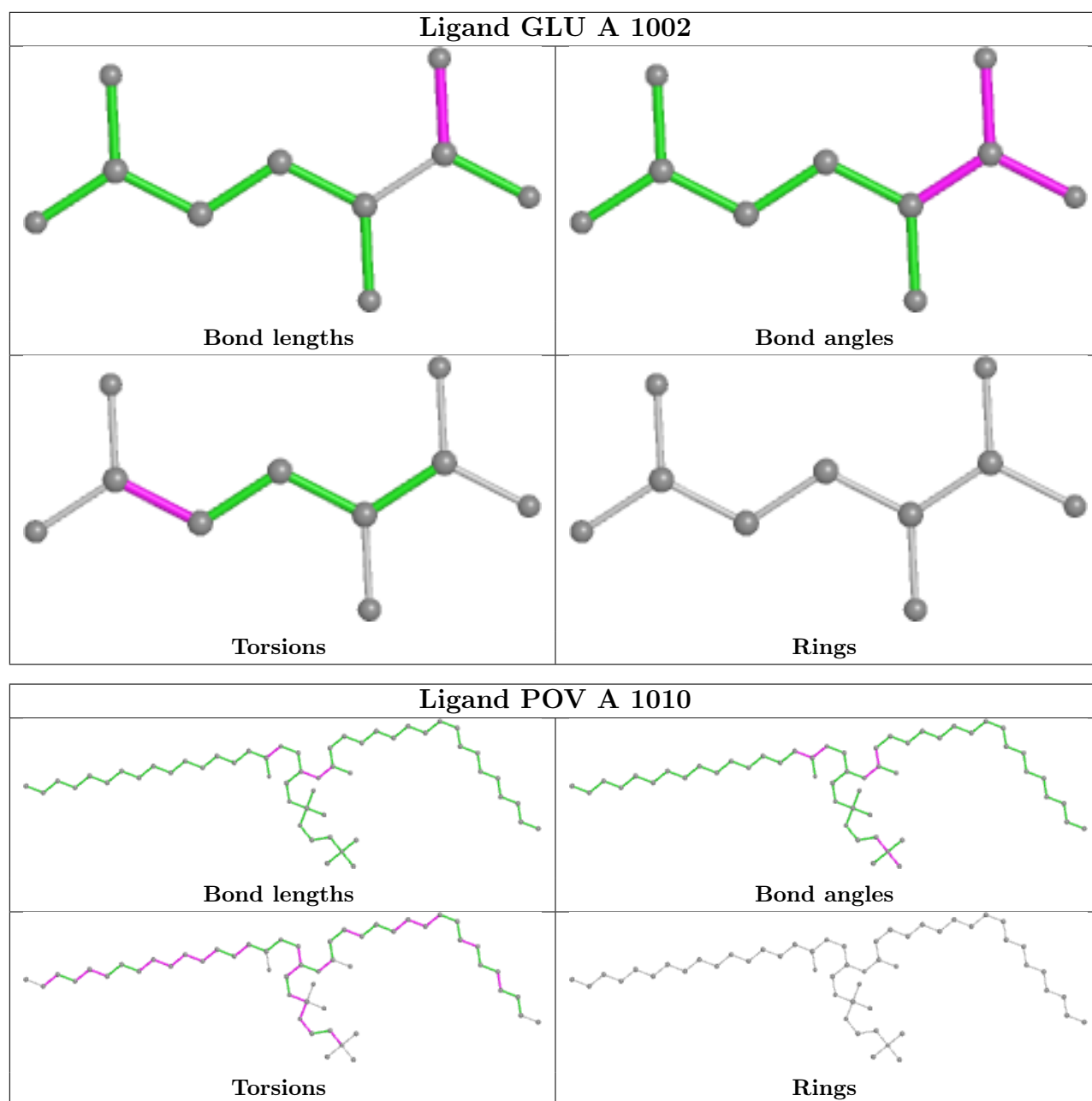












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

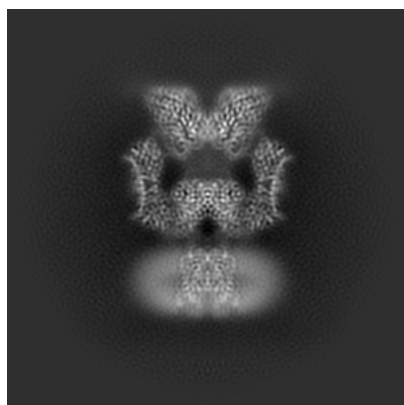
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44129. These allow visual inspection of the internal detail of the map and identification of artifacts.

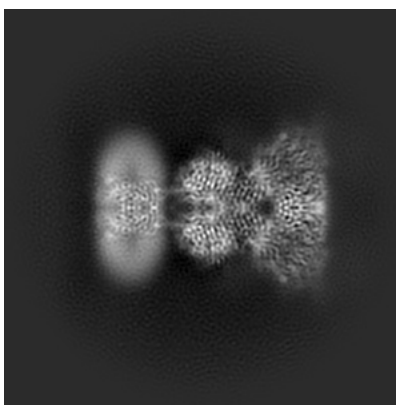
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

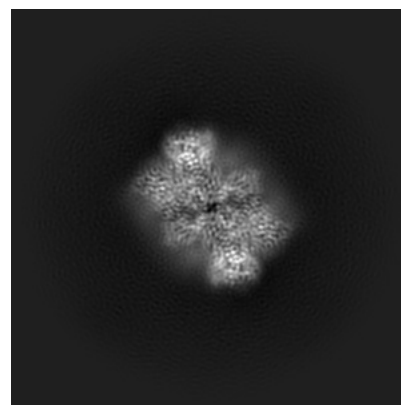
#### 6.1.1 Primary map



X



Y

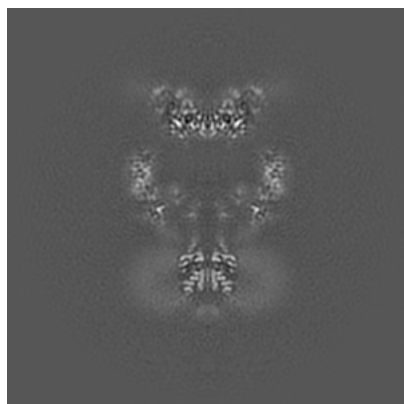


Z

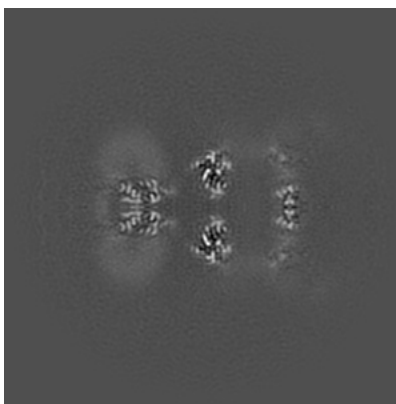
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

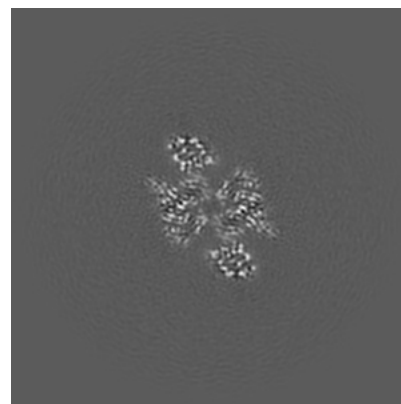
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

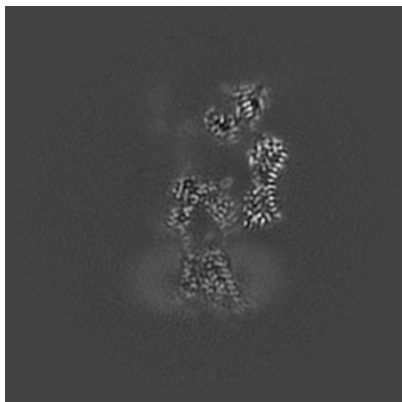


Z Index: 128

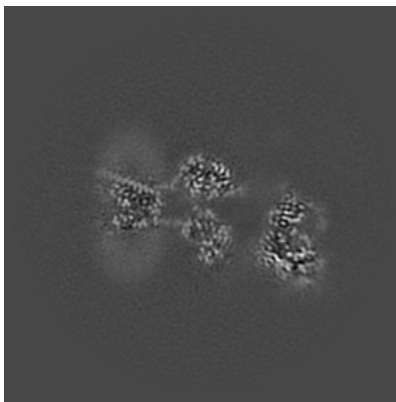
The images above show central slices of the map in three orthogonal directions.

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

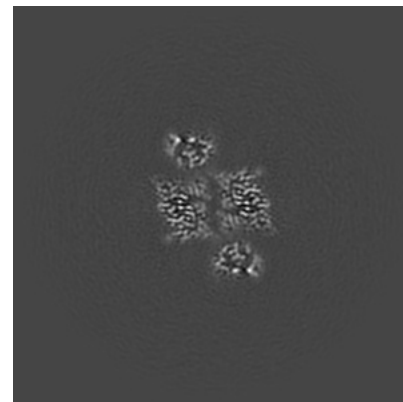
### 6.3.1 Primary map



X Index: 115



Y Index: 140



Z Index: 133

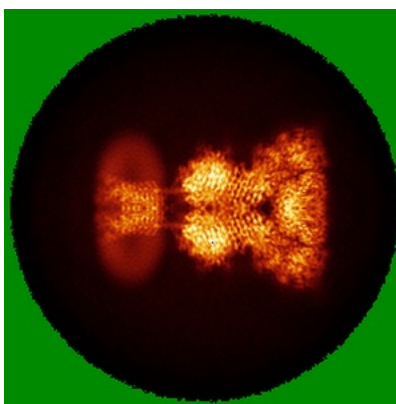
The images above show the largest variance slices of the map in three orthogonal directions.

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

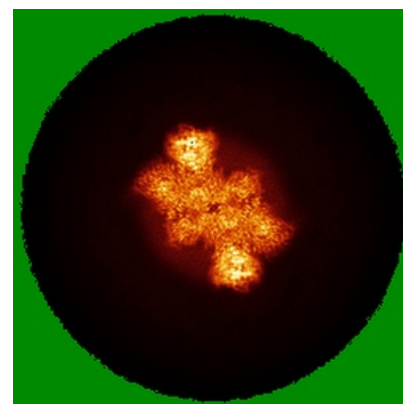
### 6.4.1 Primary map



X



Y

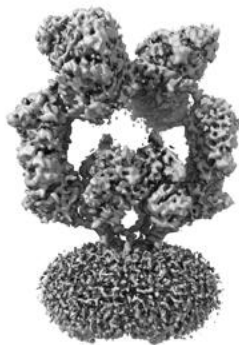


Z

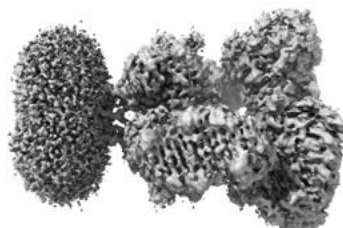
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

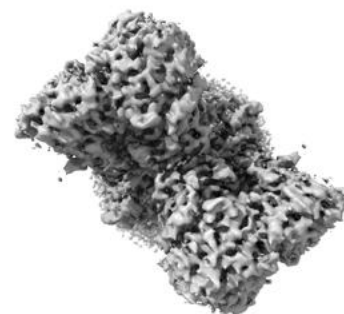
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

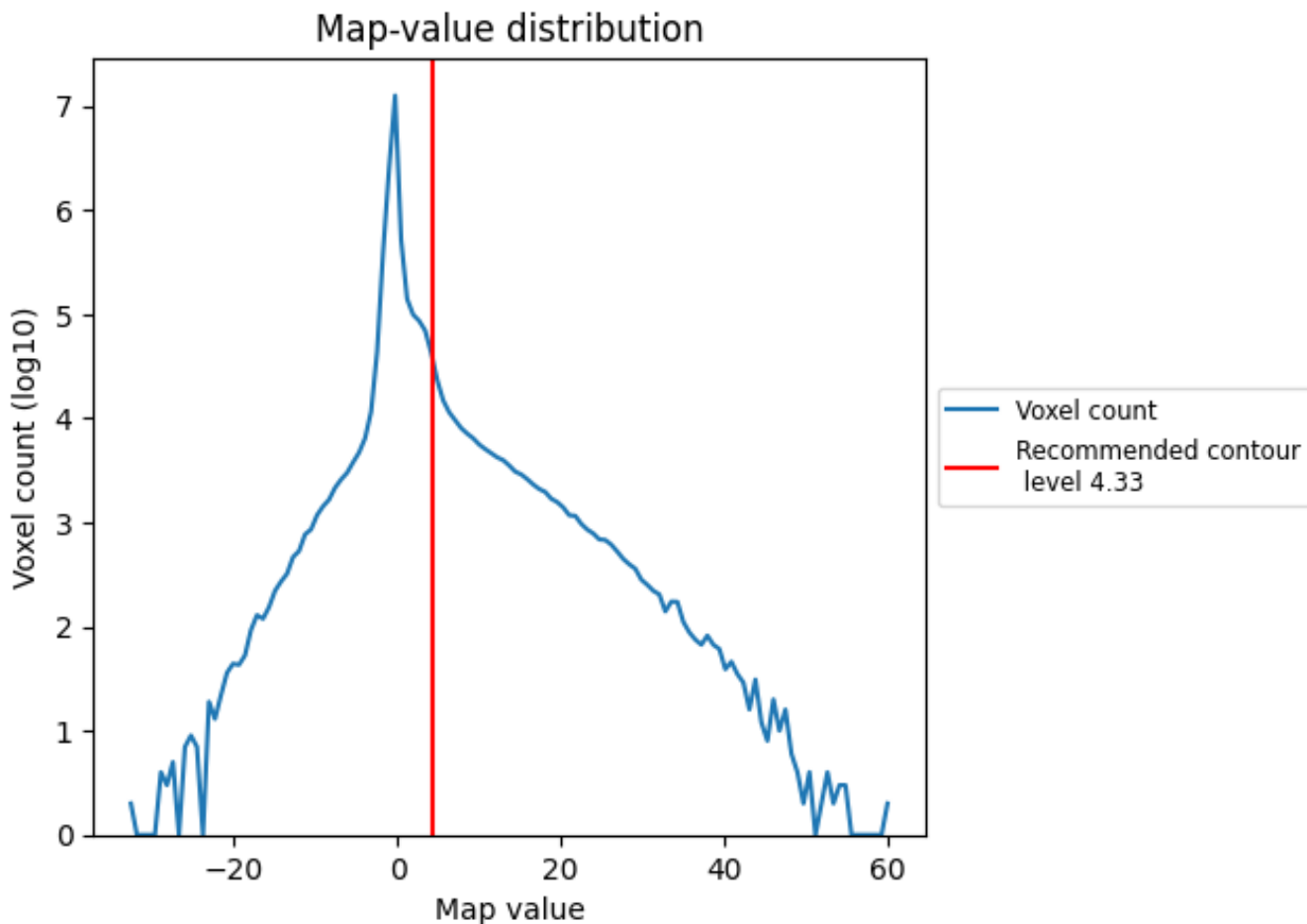
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

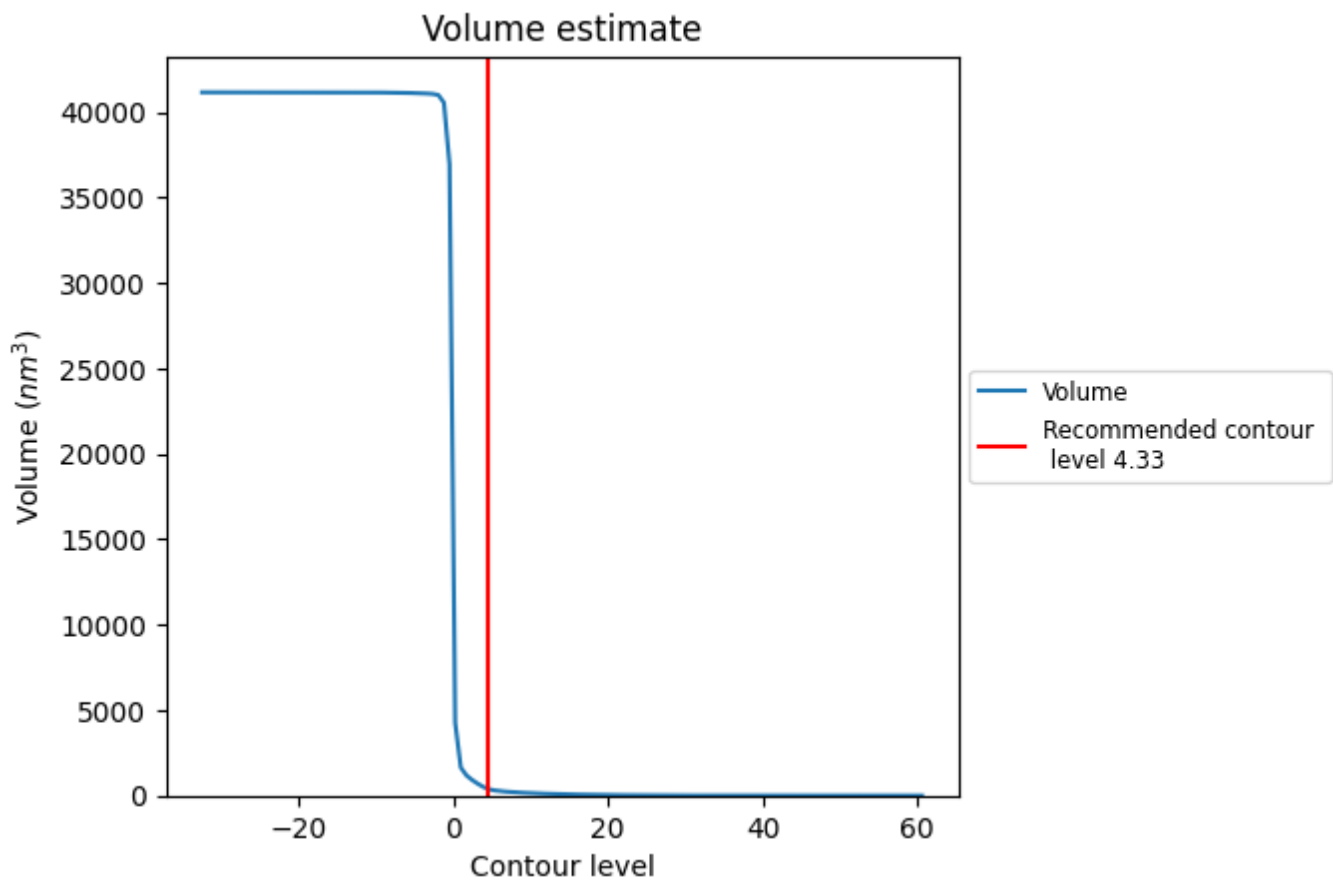
This section contains the results of statistical analysis of the map.

### 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.

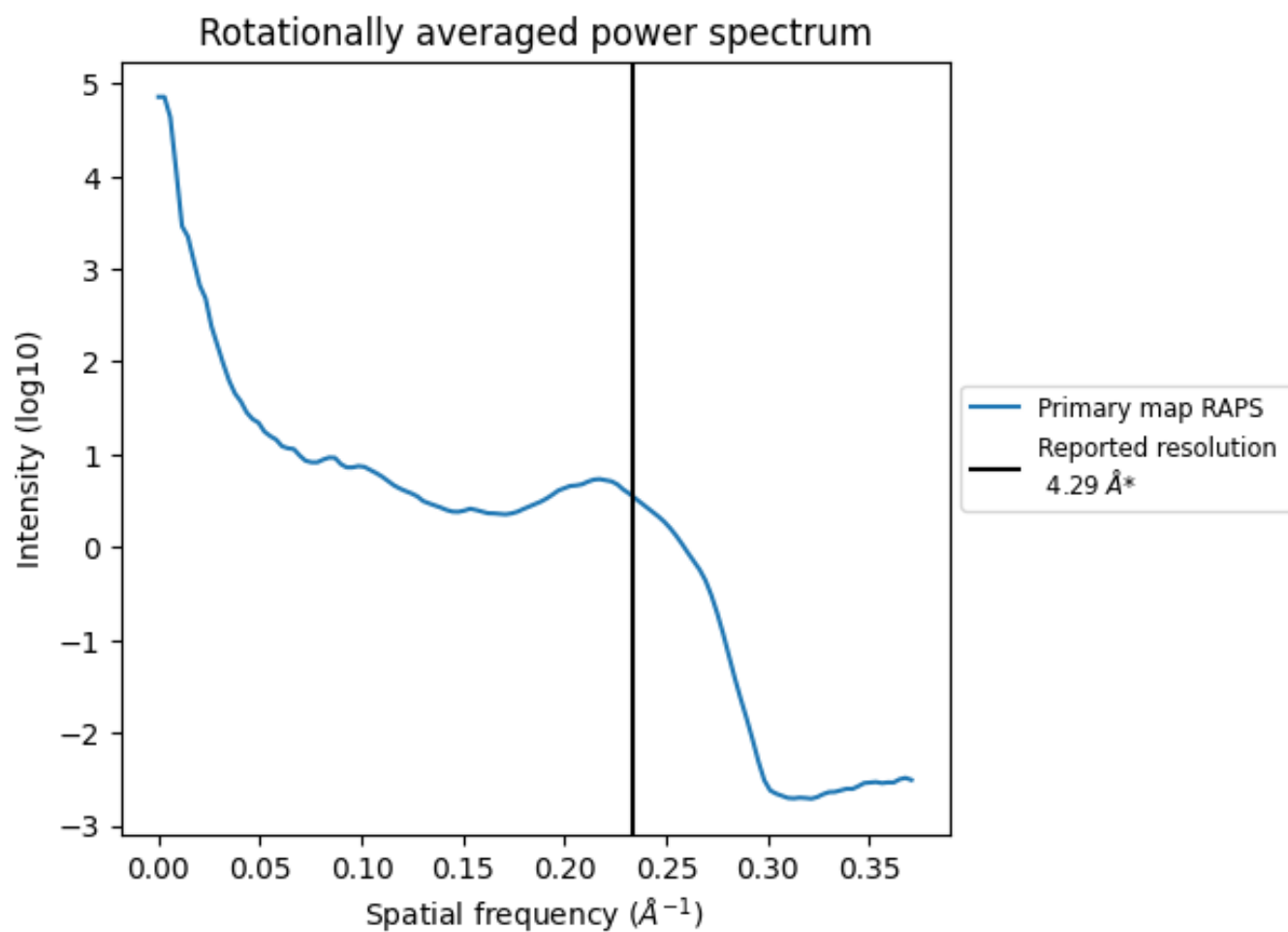
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 417  $\text{nm}^3$ ; this corresponds to an approximate mass of 377 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>



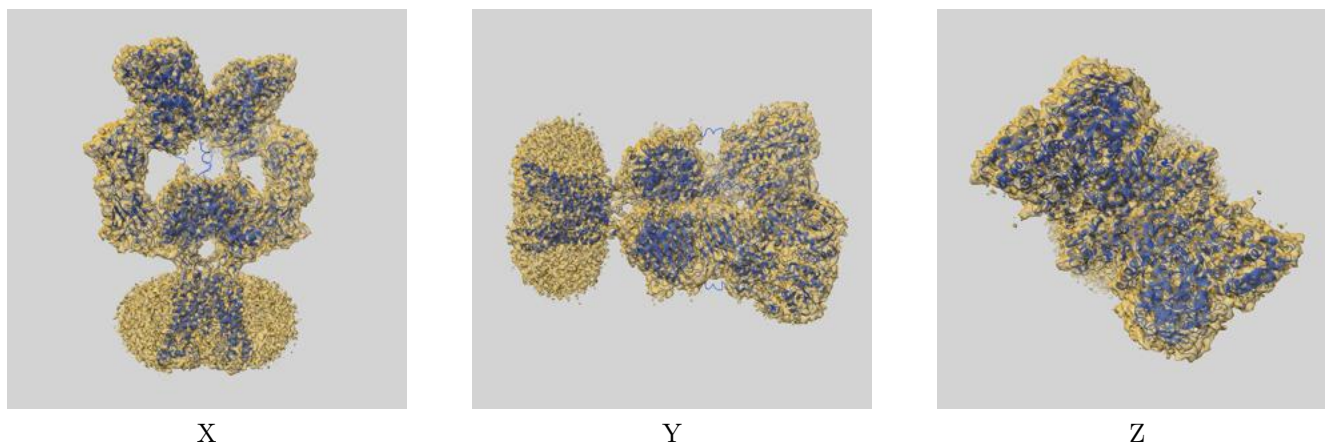
## 8 Fourier-Shell correlation

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

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

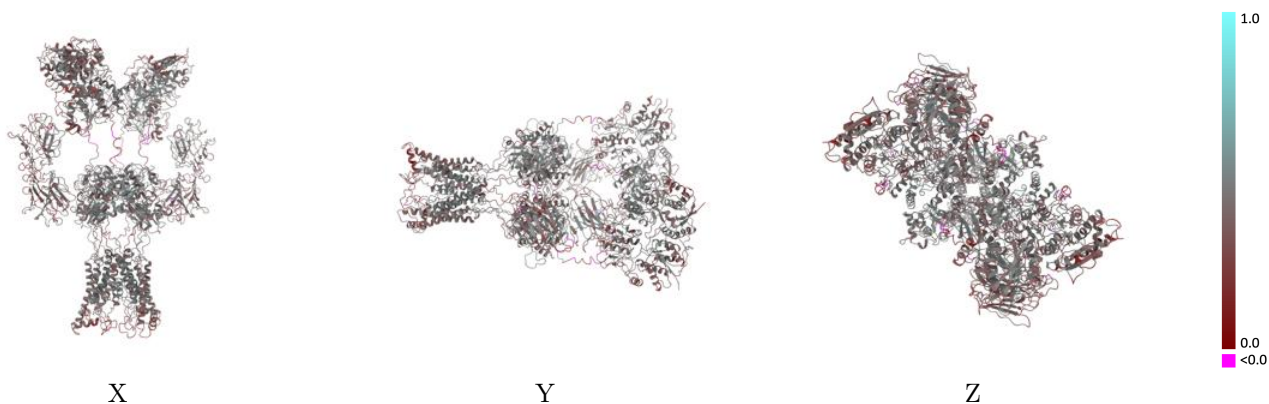
This section contains information regarding the fit between EMDB map EMD-44129 and PDB model 9B36. Per-residue inclusion information can be found in section 3 on page 14.

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



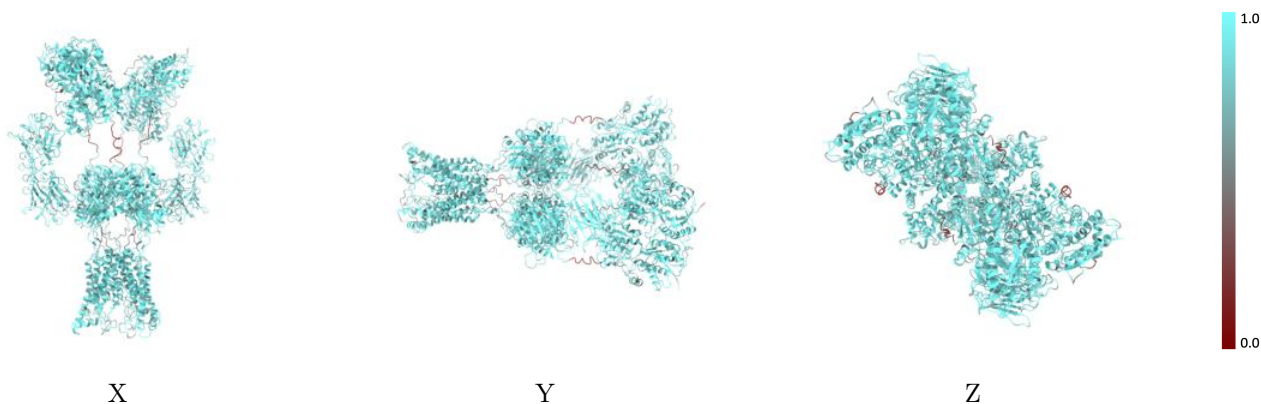
The images above show the 3D surface view of the map at the recommended contour level 4.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



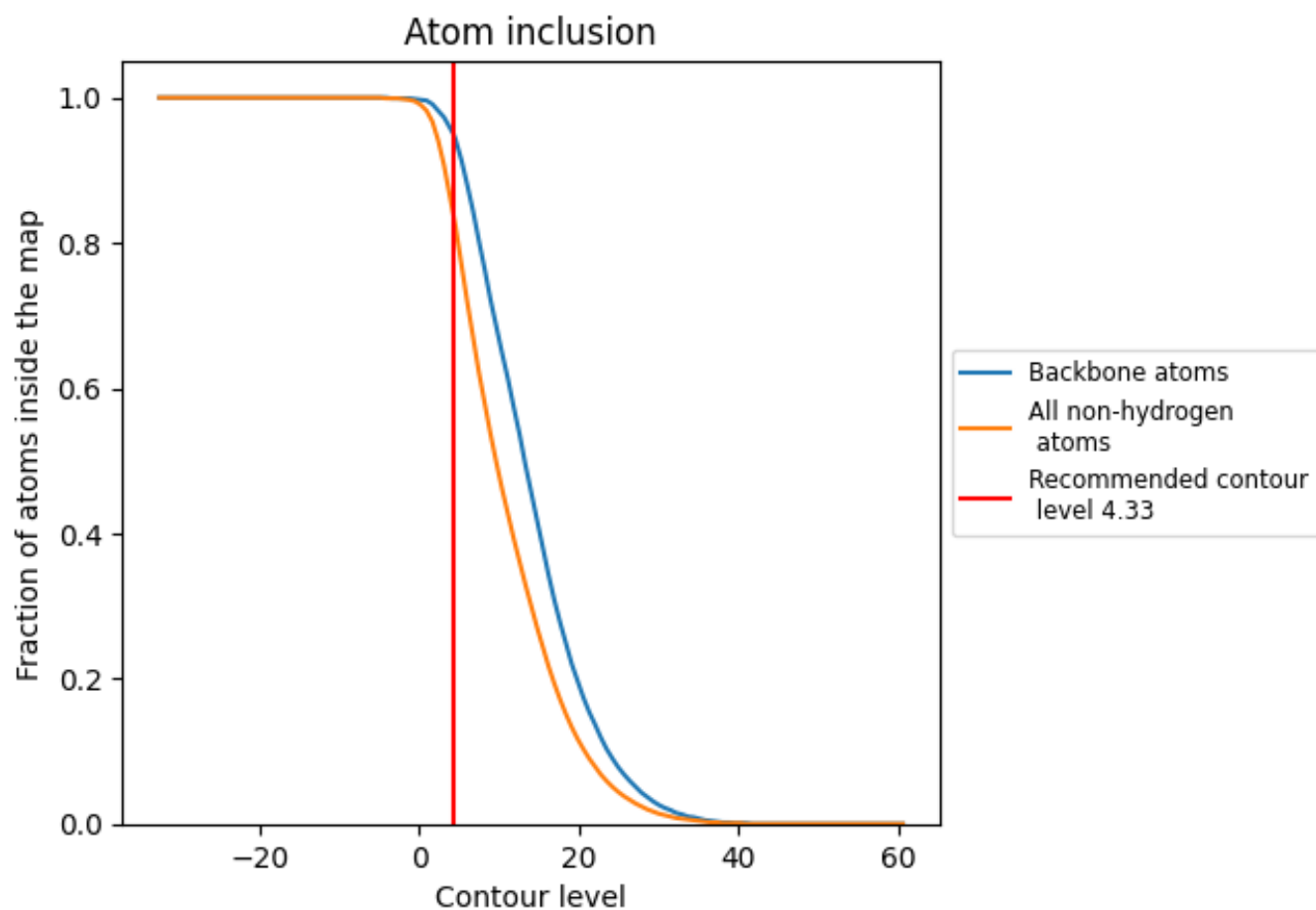
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.33).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (4.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.4020
A	 0.8440	 0.4100
B	 0.8580	 0.4280
C	 0.8440	 0.4090
D	 0.8570	 0.4270
E	 0.9000	 0.3970
F	 0.8100	 0.3350
G	 0.8640	 0.3630
H	 0.8330	 0.3570
I	 0.5930	 0.2600
J	 0.4640	 0.4500
K	 0.4300	 0.2370
L	 0.3930	 0.1120
M	 0.3850	 0.3340
N	 0.3930	 0.2700
O	 0.1070	 0.1580
P	 0.6000	 0.3480
Q	 0.2860	 0.3030
R	 0.7530	 0.2890
S	 0.3590	 0.2370
T	 0.4870	 0.2930
U	 0.4000	 0.2720
V	 0.3570	 0.1380
W	 0.6860	 0.3210
X	 0.4640	 0.4320
Y	 0.5510	 0.2730
Z	 0.3930	 0.1240
a	 0.3850	 0.3260
b	 0.3210	 0.2420
c	 0.1070	 0.2100
d	 0.4800	 0.3520
e	 0.2860	 0.3210
f	 0.7190	 0.3170
g	 0.3330	 0.2680
h	 0.3400	 0.2350



*Continued on next page...*

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Chain	Atom inclusion	Q-score
i	 0.4400	 0.2790
j	 0.3930	 0.1440