



## Full wwPDB EM Validation Report ⓘ

Oct 18, 2023 – 03:46 PM JST

PDB ID : 8HFZ  
EMDB ID : EMD-34729  
Title : Cryo-EM structure of SARS-CoV-2 prototype spike protein in complex with white-tailed deer ACE2  
Authors : Han, P.; Meng, Y.M.; Qi, J.X.  
Deposited on : 2022-11-13  
Resolution : 2.71 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>.

---

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

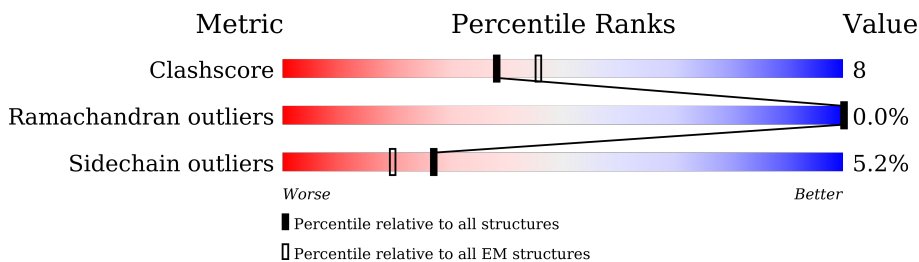
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.71 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.



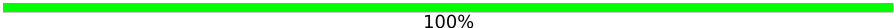


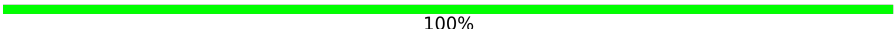
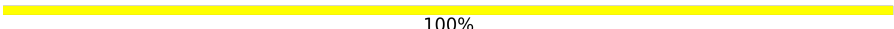

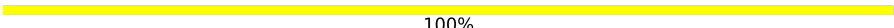

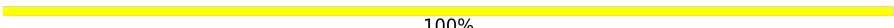

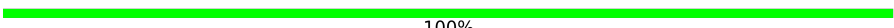






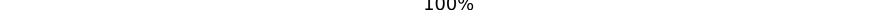
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1217	71% 14% 13% 7%
1	B	1217	71% 15% 13% 7%
1	C	1217	70% 16% 12% 7%
2	E	661	59% 28% 10% 5%
3	D	2	100%
3	F	2	50% 50%
3	G	2	100%
3	H	2	100%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 50% 50%
3	K	2	 50% 50%
3	L	2	 100%
3	M	2	 100%
3	N	2	 50% 50%
3	O	2	 100%
3	P	2	 50% 100%
3	Q	2	 100%
3	R	2	 50% 50%
3	S	2	 100%
3	T	2	 50% 50%
3	U	2	 50% 50%
3	V	2	 50% 50%
3	W	2	 50% 50%
3	X	2	 50% 50%
3	Y	2	 100%  100%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30704 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1061	8290	5290	1383	1580	37	0	0
1	B	1061	8292	5292	1383	1579	38	0	0
1	C	1065	8322	5312	1388	1584	38	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	595	4889	3124	804	931	30	0	0

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



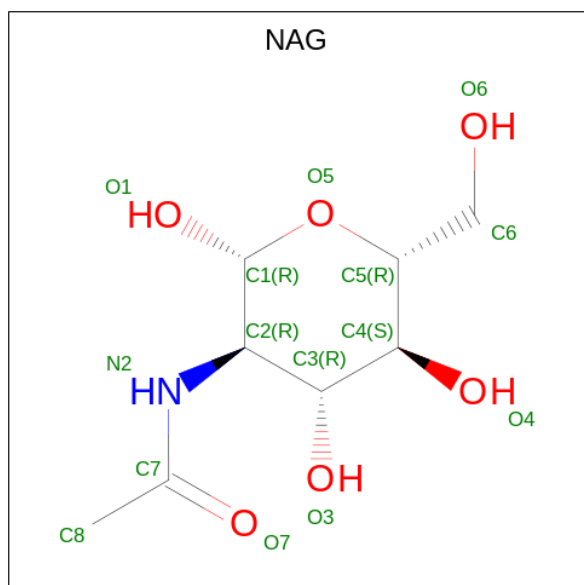
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

*Continued from previous page...*

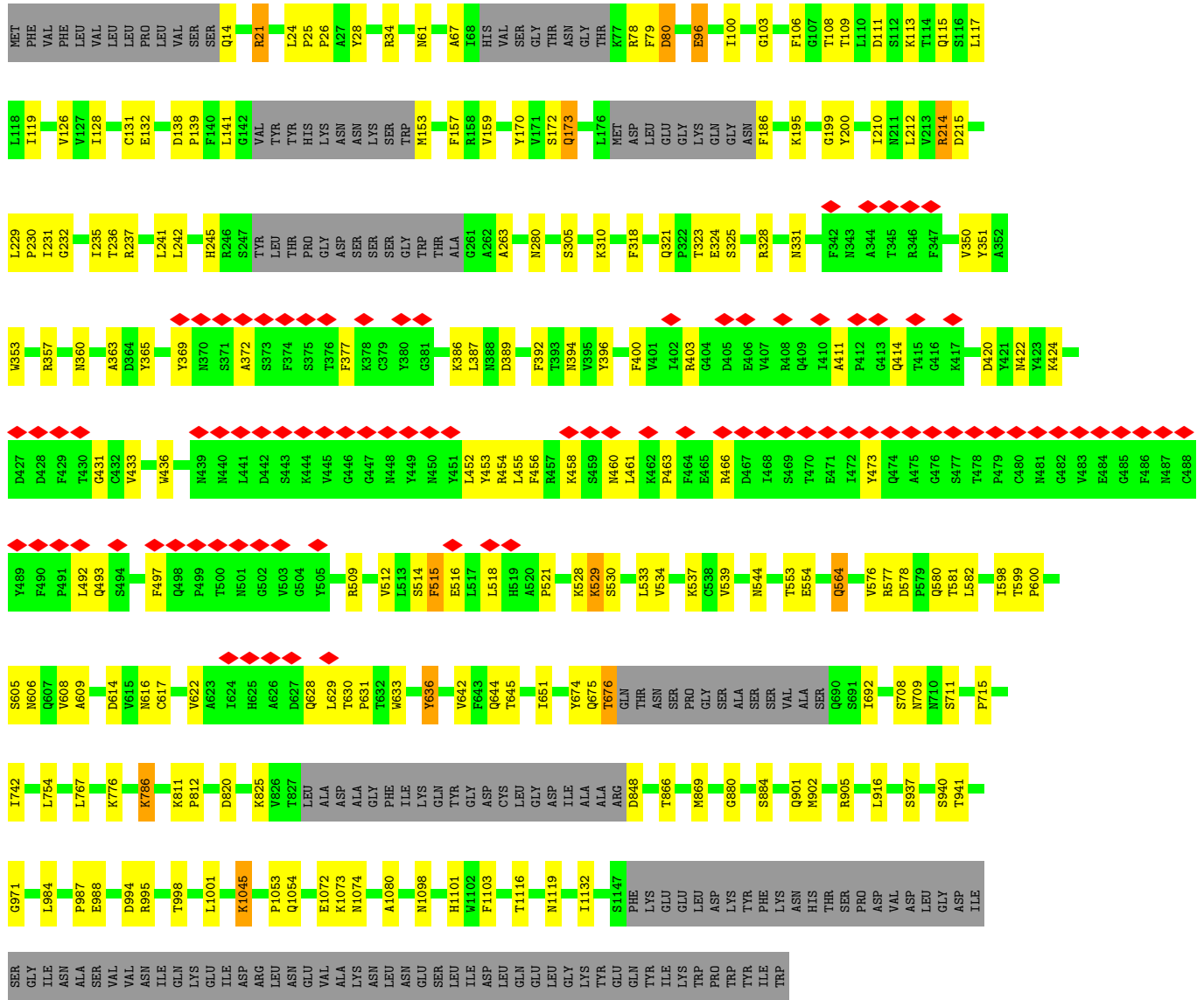
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

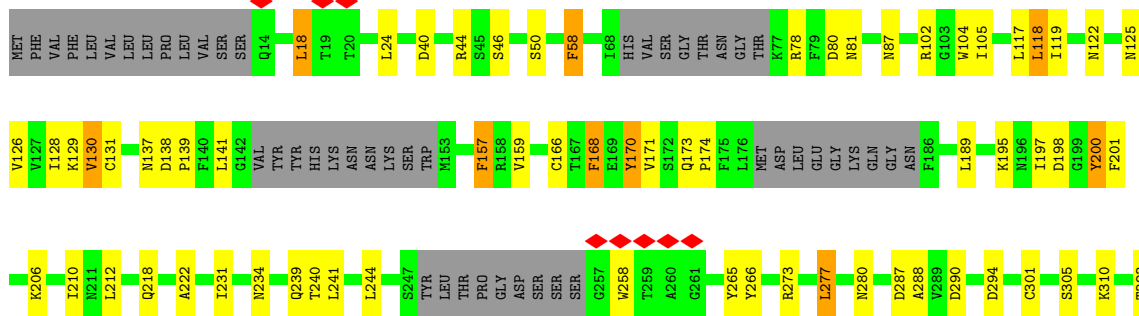
Mol	Chain	Residues	Atoms		AltConf
5	E	1	Total 1	Zn 1	0



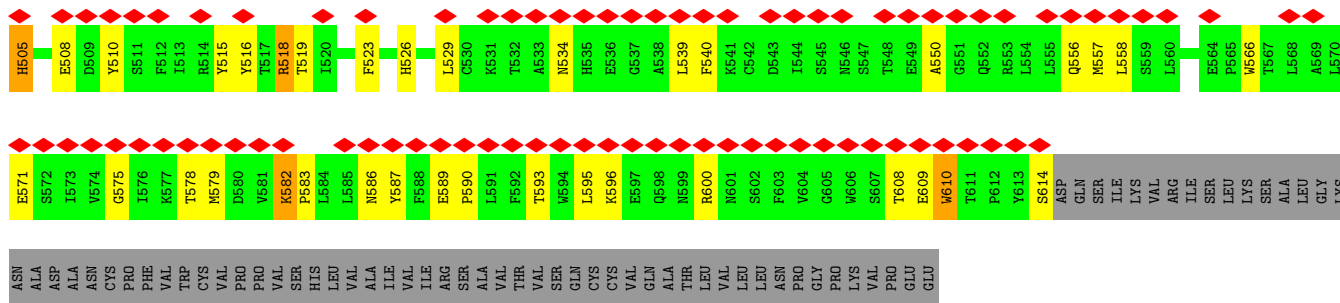




• Molecule 1: Spike glycoprotein







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



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



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



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



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



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

Chain J:  50% 50%

MAG1  
MAG2

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

Chain K:  50% 50%

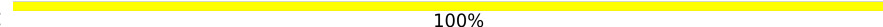
MAG1  
MAG2

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

Chain L:  100%


MAG1  
MAG2

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

Chain M:  100%

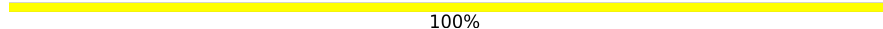
MAG1  
MAG2

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

Chain N:  50% 50%

MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

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

Chain P:  50% 100%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  50% 50%



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

Chain V:  50% 50%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:  100% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123232	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	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	1.278	Depositor
Minimum map value	-0.388	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	380.80002, 380.80002, 380.80002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: ZN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/8483	0.53	0/11556
1	B	0.37	0/8484	0.54	1/11553 (0.0%)
1	C	0.35	0/8516	0.54	2/11598 (0.0%)
2	E	0.31	1/5024 (0.0%)	0.58	2/6812 (0.0%)
All	All	0.35	1/30507 (0.0%)	0.54	5/41519 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	469	PRO	CG-CD	-5.30	1.33	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	469	PRO	CA-N-CD	-13.12	93.14	111.50
2	E	469	PRO	N-CD-CG	-8.32	90.72	103.20
1	B	614	ASP	CB-CG-OD1	6.79	124.42	118.30
1	C	614	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	629	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8290	0	8083	114	0
1	B	8292	0	8089	118	0
1	C	8322	0	8118	125	0
2	E	4889	0	4657	122	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	2	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
3	Q	28	0	25	3	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	2	0
3	U	28	0	25	2	0
3	V	28	0	25	1	0
3	W	28	0	25	3	0
3	X	28	0	25	1	0
3	Y	28	0	25	0	0
4	A	56	0	52	0	0
4	B	126	0	117	2	0
4	C	98	0	91	6	0
4	E	42	0	39	5	0
5	E	1	0	0	0	0
All	All	30704	0	29771	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:THR:HG1	1:C:690:GLN:N	1.70	0.89
2:E:207:TYR:HB3	2:E:219:ARG:HD3	1.56	0.85
2:E:436:ILE:HG22	2:E:438:PHE:H	1.46	0.78
1:C:457:ARG:NH1	1:C:459:SER:OG	2.17	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ASN:HD21	1:B:454:ARG:H	1.35	0.74
2:E:342:VAL:HG21	2:E:359:LYS:HG2	1.71	0.72
2:E:27:LYS:HE3	2:E:98:LEU:HD11	1.71	0.72
1:C:676:THR:HG23	1:C:690:GLN:HG2	1.71	0.72
2:E:269:ASP:HB3	2:E:272:GLY:H	1.55	0.72
1:B:24:LEU:HD12	1:B:78:ARG:HE	1.54	0.71
1:A:426:PRO:HA	1:A:463:PRO:HB3	1.72	0.71
2:E:110:SER:HB3	2:E:113:LYS:HG3	1.70	0.70
1:C:1103:PHE:HZ	3:W:1:NAG:H61	1.56	0.70
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.09	0.70
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.72	0.70
1:A:634:ARG:NH1	1:A:636:TYR:O	2.25	0.69
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.73	0.69
3:T:1:NAG:H61	3:T:2:NAG:HN2	1.57	0.69
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.23	0.68
1:C:417:LYS:HE2	1:C:455:LEU:HD23	1.75	0.68
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.74	0.68
1:C:189:LEU:HB2	1:C:210:ILE:HD11	1.74	0.68
1:B:321:GLN:H	1:B:628:GLN:HE22	1.41	0.68
2:E:372:ALA:HA	2:E:375:GLU:HB2	1.75	0.68
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.27	0.68
2:E:90:GLN:OE1	2:E:90:GLN:N	2.21	0.68
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.27	0.67
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.41	0.67
1:B:987:PRO:HD3	1:C:413:GLY:HA3	1.77	0.66
1:A:501:ASN:HB3	1:A:505:TYR:HB3	1.76	0.66
1:A:578:ASP:OD2	1:A:581:THR:N	2.28	0.66
1:C:117:LEU:HA	1:C:130:VAL:HA	1.78	0.65
1:A:452:LEU:HD21	1:A:492:LEU:HD12	1.78	0.65
1:B:1098:ASN:OD1	3:Q:1:NAG:N2	2.29	0.65
2:E:482:ARG:HD3	2:E:488:VAL:HG13	1.78	0.65
1:B:21:ARG:HE	1:B:21:ARG:H	1.44	0.65
1:C:356:LYS:NZ	1:C:357:ARG:O	2.30	0.65
1:A:155:SER:HB3	1:A:158:ARG:HB2	1.78	0.65
1:A:318:PHE:HA	1:A:629:LEU:HD22	1.78	0.64
2:E:505:HIS:HB3	2:E:510:TYR:HB3	1.79	0.64
1:C:1051:SER:HG	1:C:1064:HIS:HD1	1.46	0.64
2:E:335:GLU:HG3	2:E:337:GLY:H	1.62	0.64
1:B:323:THR:HB	1:B:539:VAL:HG12	1.79	0.64
1:B:436:TRP:HB3	1:B:509:ARG:HB2	1.79	0.63
1:C:605:SER:OG	1:C:606:ASN:N	2.30	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:703:NAG:H3	4:E:703:NAG:H83	1.79	0.63
1:A:454:ARG:NH1	1:A:467:ASP:OD2	2.33	0.62
1:C:206:LYS:NZ	1:C:222:ALA:O	2.31	0.62
2:E:494:ASP:H	2:E:497:TYR:HD2	1.47	0.62
1:A:336:CYS:N	1:A:361:CYS:SG	2.72	0.62
1:C:615:VAL:HG13	1:C:619:GLU:HG2	1.81	0.62
1:B:521:PRO:HG3	1:B:564:GLN:HG3	1.80	0.62
1:B:394:ASN:ND2	1:C:200:TYR:OH	2.32	0.62
1:C:745:ASP:OD1	1:C:745:ASP:N	2.22	0.62
1:A:236:THR:HG22	3:D:1:NAG:HN2	1.63	0.62
1:A:386:LYS:HD2	1:A:390:LEU:HD22	1.80	0.62
2:E:24:GLU:O	2:E:28:THR:OG1	2.16	0.61
1:A:498:GLN:OE1	1:A:501:ASN:ND2	2.26	0.61
1:B:577:ARG:HD3	1:B:582:LEU:HD12	1.82	0.61
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.81	0.61
2:E:407:ILE:HG23	2:E:526:HIS:HA	1.83	0.61
2:E:244:VAL:HG22	2:E:440:LEU:HD21	1.82	0.61
2:E:282:THR:O	2:E:437:ASN:ND2	2.34	0.61
1:C:409:GLN:HE22	1:C:417:LYS:H	1.48	0.60
2:E:95:LYS:HA	2:E:98:LEU:HD12	1.82	0.60
1:C:635:VAL:HG23	1:C:636:TYR:HD2	1.65	0.60
2:E:571:GLU:HA	2:E:575:GLY:HA2	1.83	0.60
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.84	0.60
1:C:418:ILE:HG22	1:C:422:ASN:HD22	1.65	0.60
1:B:96:GLU:OE1	1:B:100:ILE:N	2.33	0.59
1:A:122:ASN:OD1	1:A:125:ASN:N	2.36	0.59
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.85	0.59
1:C:1134:ASN:OD1	3:X:1:NAG:N2	2.35	0.59
1:A:1142:GLN:HE22	1:A:1145:LEU:HD13	1.68	0.59
3:H:2:NAG:H3	3:H:2:NAG:H83	1.85	0.59
1:C:703:ASN:OD1	1:C:704:SER:N	2.36	0.58
1:B:674:TYR:HD1	1:B:692:ILE:HG12	1.68	0.58
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.36	0.58
1:B:389:ASP:OD1	1:B:389:ASP:N	2.36	0.58
3:W:1:NAG:H83	3:W:1:NAG:H3	1.85	0.58
1:C:1092:GLU:N	1:C:1092:GLU:OE1	2.36	0.58
2:E:27:LYS:HD2	2:E:94:LEU:HD23	1.86	0.58
1:C:139:PRO:HB3	1:C:159:VAL:HG12	1.84	0.57
2:E:188:ASN:HD21	2:E:464:PHE:HB3	1.69	0.57
2:E:358:ILE:HD11	2:E:379:ILE:HG21	1.86	0.57
1:A:86:PHE:N	1:A:236:THR:O	2.25	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:471:GLU:OE1	2:E:471:GLU:N	2.35	0.57
2:E:81:ALA:O	2:E:102:GLN:NE2	2.31	0.57
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.87	0.57
1:B:424:LYS:HG2	1:B:463:PRO:HG3	1.86	0.57
1:A:353:TRP:O	1:A:466:ARG:NH2	2.36	0.57
2:E:383:MET:CE	2:E:383:MET:H	2.18	0.57
3:H:1:NAG:H83	3:H:1:NAG:H3	1.87	0.57
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.87	0.57
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.87	0.57
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.87	0.57
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.22	0.57
1:C:1127:ASP:OD1	1:C:1127:ASP:N	2.36	0.57
1:A:529:LYS:HE3	1:A:529:LYS:HA	1.87	0.56
1:A:461:LEU:HD21	1:A:467:ASP:HB2	1.87	0.56
1:A:154:GLU:HA	1:A:245:HIS:HA	1.86	0.56
1:C:118:LEU:N	1:C:129:LYS:O	2.25	0.56
1:B:866:THR:H	1:B:869:MET:HE2	1.70	0.56
1:C:141:LEU:HD23	1:C:157:PHE:HA	1.86	0.56
1:A:477:SER:HG	2:E:20:SER:N	2.02	0.56
1:B:403:ARG:HD3	1:B:497:PHE:HE1	1.71	0.56
1:A:294:ASP:OD1	1:A:294:ASP:N	2.38	0.56
2:E:87:GLU:O	2:E:88:GLU:HG3	2.06	0.56
1:B:372:ALA:HB3	1:B:436:TRP:HH2	1.71	0.55
2:E:515:TYR:HA	2:E:518:ARG:HG2	1.87	0.55
1:C:81:ASN:O	1:C:239:GLN:NE2	2.40	0.55
2:E:388:GLN:HB3	2:E:392:LEU:HB2	1.86	0.55
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.70	0.55
1:A:132:GLU:HB2	1:A:164:ASN:HB2	1.89	0.55
1:B:80:ASP:N	1:B:80:ASP:OD1	2.39	0.55
1:C:125:ASN:HD21	4:C:1303:NAG:H62	1.70	0.55
1:B:138:ASP:OD1	1:B:138:ASP:N	2.39	0.55
1:A:361:CYS:SG	1:A:362:VAL:N	2.80	0.55
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.88	0.55
1:A:354:ASN:OD1	1:A:354:ASN:N	2.40	0.54
1:C:168:PHE:CE2	1:C:170:TYR:HB2	2.42	0.54
2:E:87:GLU:O	2:E:89:ILE:HG12	2.08	0.54
2:E:582:LYS:H	2:E:582:LYS:HD3	1.72	0.54
1:A:16:VAL:O	1:A:18:LEU:HD12	2.07	0.54
1:C:277:LEU:HD12	1:C:277:LEU:H	1.71	0.54
1:A:491:PRO:HG2	1:A:492:LEU:HD22	1.90	0.54
1:B:323:THR:HG22	1:B:324:GLU:HG2	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:VAL:HA	1:B:636:TYR:HE2	1.73	0.54
1:C:195:LYS:HG2	1:C:197:ILE:HG13	1.90	0.54
1:C:448:ASN:HD22	1:C:450:ASN:HD22	1.55	0.54
1:C:1103:PHE:CZ	3:W:1:NAG:H61	2.41	0.54
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.91	0.54
1:C:802:PHE:N	3:U:1:NAG:O7	2.41	0.54
2:E:260:GLY:HA2	2:E:610:TRP:CH2	2.43	0.54
1:A:716:THR:HG21	1:A:1073:LYS:HE2	1.90	0.53
2:E:145:GLU:N	2:E:145:GLU:OE1	2.40	0.53
1:C:138:ASP:N	1:C:138:ASP:OD1	2.40	0.53
2:E:200:GLY:HA2	2:E:203:TRP:CE3	2.44	0.53
1:B:516:GLU:HG2	1:B:518:LEU:HG	1.90	0.53
1:B:984:LEU:HD11	1:B:988:GLU:OE1	2.08	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.89	0.53
2:E:384:ALA:HB1	2:E:558:LEU:HB3	1.91	0.53
1:B:529:LYS:HG2	1:B:530:SER:N	2.24	0.53
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.90	0.53
1:A:406:GLU:N	1:A:406:GLU:OE1	2.41	0.53
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.90	0.53
2:E:142:LEU:HD21	2:E:164:ALA:HA	1.89	0.53
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.91	0.52
1:B:742:ILE:HD11	1:B:1001:LEU:HD13	1.89	0.52
1:B:1073:LYS:HG2	1:B:1074:ASN:H	1.74	0.52
1:B:811:LYS:NZ	1:B:812:PRO:O	2.28	0.52
1:B:599:THR:HB	1:B:608:VAL:HG12	1.90	0.52
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.92	0.52
1:B:848:ASP:OD1	1:B:848:ASP:N	2.42	0.52
1:C:402:ILE:HG23	1:C:406:GLU:HG2	1.91	0.52
2:E:389:PRO:HD2	2:E:392:LEU:HD12	1.92	0.52
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.28	0.51
1:C:378:LYS:HZ3	1:C:379:CYS:C	2.13	0.51
2:E:593:THR:HA	2:E:596:LYS:HE2	1.92	0.51
1:B:386:LYS:NZ	1:C:981:LEU:O	2.43	0.51
2:E:87:GLU:OE1	2:E:87:GLU:N	2.40	0.51
1:A:526:GLY:O	1:A:528:LYS:NZ	2.37	0.51
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.75	0.51
1:C:802:PHE:H	3:U:1:NAG:H81	1.75	0.51
2:E:396:ALA:HB1	2:E:566:TRP:HB3	1.93	0.51
1:B:880:GLY:O	1:B:884:SER:OG	2.24	0.51
1:C:80:ASP:O	1:C:265:TYR:OH	2.17	0.51
2:E:92:LEU:HD12	2:E:95:LYS:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:1:NAG:H61	3:T:2:NAG:N2	2.26	0.51
1:A:383:SER:OG	1:A:385:THR:O	2.28	0.51
2:E:326:GLY:O	2:E:330:ASN:ND2	2.44	0.51
1:B:786:LYS:H	1:B:786:LYS:HD3	1.76	0.50
2:E:303:ASP:OD1	2:E:303:ASP:N	2.44	0.50
1:C:128:ILE:O	1:C:129:LYS:HD2	2.11	0.50
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.74	0.50
1:A:21:ARG:NH2	1:A:81:ASN:OD1	2.44	0.50
1:A:345:THR:O	1:A:509:ARG:NH2	2.40	0.50
2:E:608:THR:HG22	2:E:609:GLU:HG2	1.94	0.50
2:E:271:TRP:HD1	2:E:273:ARG:HH11	1.59	0.50
1:A:408:ARG:HH21	1:A:414:GLN:HE22	1.59	0.50
1:B:245:HIS:H	1:B:245:HIS:CD2	2.30	0.50
1:C:173:GLN:OE1	1:C:174:PRO:HD2	2.12	0.50
1:C:786:LYS:HG2	1:C:787:GLN:HG2	1.93	0.50
2:E:226:VAL:HG13	2:E:454:TYR:CE1	2.47	0.50
1:B:1103:PHE:HZ	3:Q:1:NAG:H61	1.77	0.50
1:B:108:THR:HG22	1:B:236:THR:HG23	1.94	0.50
4:C:1307:NAG:H5	4:C:1307:NAG:HN2	1.75	0.50
1:B:436:TRP:N	1:B:509:ARG:O	2.37	0.50
1:B:994:ASP:O	1:B:998:THR:OG1	2.24	0.50
1:C:104:TRP:N	1:C:119:ILE:O	2.39	0.50
1:C:474:GLN:NE2	1:C:476:GLY:O	2.44	0.50
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.35	0.50
2:E:190:MET:SD	2:E:191:ALA:N	2.85	0.50
1:A:102:ARG:HE	1:A:121:ASN:HD22	1.58	0.49
1:A:336:CYS:HB2	1:A:338:PHE:CE2	2.47	0.49
1:A:287:ASP:OD1	1:A:288:ALA:N	2.45	0.49
2:E:315:PHE:HZ	2:E:373:HIS:HA	1.78	0.49
2:E:378:HIS:HD2	2:E:378:HIS:O	1.95	0.49
1:A:470:THR:HG21	1:A:492:LEU:HD11	1.94	0.49
1:B:186:PHE:HB3	1:B:212:LEU:HD11	1.94	0.49
1:C:752:LEU:HD11	1:C:993:ILE:HD11	1.95	0.49
1:A:350:VAL:HG13	1:A:402:ILE:HD11	1.95	0.49
1:B:629:LEU:H	1:B:629:LEU:HD23	1.77	0.49
1:B:21:ARG:H	1:B:21:ARG:NE	2.08	0.49
1:B:605:SER:OG	1:B:606:ASN:N	2.46	0.49
1:C:24:LEU:HD22	1:C:78:ARG:HD2	1.93	0.49
2:E:156:ARG:HB3	2:E:252:TYR:HE2	1.78	0.49
2:E:369:PHE:HZ	2:E:417:TYR:HH	1.61	0.49
2:E:540:PHE:HE1	2:E:590:PRO:HG2	1.77	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:SER:OG	1:A:811:LYS:NZ	2.41	0.49
2:E:480:MET:SD	2:E:480:MET:N	2.67	0.49
1:A:66:HIS:O	1:A:80:ASP:HB2	2.13	0.49
1:B:111:ASP:OD1	1:B:113:LYS:HG2	2.13	0.49
1:B:331:ASN:HB3	1:B:580:GLN:HG2	1.95	0.48
1:C:128:ILE:O	1:C:128:ILE:HD12	2.12	0.48
2:E:263:PRO:HA	2:E:487:VAL:HG13	1.95	0.48
2:E:315:PHE:CZ	2:E:377:GLY:HA3	2.48	0.48
1:C:18:LEU:HA	1:C:137:ASN:HD21	1.79	0.48
2:E:475:GLU:CD	2:E:475:GLU:H	2.17	0.48
1:A:188:ASN:OD1	1:A:188:ASN:N	2.46	0.48
1:B:578:ASP:HB3	1:B:581:THR:O	2.13	0.48
1:B:622:VAL:HA	1:B:636:TYR:CE2	2.47	0.48
1:B:141:LEU:HD22	1:B:157:PHE:HA	1.95	0.48
1:B:357:ARG:CZ	1:B:357:ARG:HA	2.43	0.48
1:B:357:ARG:HA	1:B:357:ARG:NH1	2.29	0.48
1:C:406:GLU:HG3	1:C:418:ILE:HG12	1.96	0.48
1:B:411:ALA:HB3	1:B:414:GLN:HB3	1.95	0.48
1:C:821:LEU:HD22	1:C:935:GLN:HG3	1.96	0.48
2:E:157:ASP:OD1	2:E:157:ASP:N	2.47	0.48
1:B:754:LEU:HD23	1:B:754:LEU:H	1.78	0.48
1:A:195:LYS:HG2	1:A:197:ILE:HD13	1.95	0.48
1:A:786:LYS:CD	1:A:786:LYS:H	2.26	0.48
2:E:460:ARG:HA	2:E:463:VAL:HG12	1.96	0.48
1:A:936:ASP:N	1:A:936:ASP:OD1	2.47	0.48
1:C:719:THR:N	1:C:1068:VAL:O	2.42	0.48
1:A:346:ARG:HA	1:A:346:ARG:NH1	2.29	0.47
1:C:1074:ASN:OD1	3:V:1:NAG:N2	2.47	0.47
2:E:161:ARG:HA	2:E:266:LEU:HD21	1.96	0.47
2:E:192:ARG:NH2	2:E:465:LYS:O	2.47	0.47
1:B:103:GLY:H	1:B:241:LEU:HB2	1.80	0.47
1:C:125:ASN:HD22	1:C:171:VAL:HG22	1.78	0.47
1:C:210:ILE:HG22	1:C:212:LEU:H	1.80	0.47
2:E:383:MET:H	2:E:383:MET:HE3	1.79	0.47
1:A:359:SER:HA	1:A:524:VAL:HG12	1.95	0.47
1:C:122:ASN:OD1	4:C:1303:NAG:N2	2.47	0.47
1:C:294:ASP:OD1	1:C:294:ASP:N	2.48	0.47
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.61	0.47
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.97	0.47
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.14	0.47
1:B:436:TRP:HA	1:B:436:TRP:CE3	2.50	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ARG:NH1	1:C:409:GLN:HG2	2.29	0.47
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.96	0.47
1:B:452:LEU:HD13	1:B:492:LEU:HB3	1.96	0.47
1:B:629:LEU:HG	1:B:631:PRO:HG3	1.95	0.47
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.47
1:C:675:GLN:O	1:C:690:GLN:N	2.47	0.47
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.97	0.47
2:E:36:GLU:HB3	2:E:73:PHE:HE2	1.79	0.47
1:B:200:TYR:CZ	1:B:230:PRO:HB3	2.49	0.47
1:B:458:LYS:HA	1:B:473:TYR:CD1	2.49	0.47
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.96	0.46
1:C:417:LYS:O	1:C:417:LYS:NZ	2.46	0.46
2:E:144:LEU:HD22	2:E:144:LEU:H	1.79	0.46
1:A:444:LYS:C	1:A:499:PRO:HD3	2.36	0.46
1:C:986:PRO:N	1:C:987:PRO:HD2	2.30	0.46
2:E:293:VAL:O	2:E:418:LEU:HD22	2.15	0.46
1:A:985:ASP:OD2	1:A:987:PRO:HD2	2.14	0.46
1:B:172:SER:OG	1:B:173:GLN:N	2.48	0.46
1:C:661:GLU:O	1:C:695:TYR:OH	2.21	0.46
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.97	0.46
2:E:40:LEU:HD13	2:E:70:TRP:HA	1.96	0.46
1:A:599:THR:HB	1:A:608:VAL:HG12	1.98	0.46
1:B:420:ASP:O	1:B:461:LEU:N	2.44	0.46
1:A:138:ASP:N	1:A:138:ASP:OD1	2.47	0.46
2:E:27:LYS:HE2	4:E:703:NAG:O3	2.16	0.46
1:B:353:TRP:HB2	1:B:466:ARG:HH21	1.80	0.46
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.96	0.46
2:E:94:LEU:HB2	4:E:703:NAG:H4	1.97	0.46
1:B:363:ALA:HB1	1:B:365:TYR:CE2	2.51	0.46
1:B:1101:HIS:ND1	3:Q:1:NAG:H5	2.31	0.46
1:C:218:GLN:OE1	1:C:218:GLN:HA	2.16	0.46
2:E:176:LEU:HB3	2:E:498:CYS:SG	2.56	0.46
1:A:401:VAL:O	1:A:402:ILE:HD13	2.15	0.46
1:A:457:ARG:NE	1:A:459:SER:O	2.48	0.46
1:A:569:ILE:HD12	1:A:569:ILE:H	1.81	0.46
1:B:453:TYR:HE1	1:B:493:GLN:HB2	1.80	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.97	0.45
1:B:529:LYS:HG2	1:B:530:SER:H	1.81	0.45
1:C:125:ASN:ND2	1:C:171:VAL:HG22	2.31	0.45
2:E:321:PRO:O	2:E:380:GLN:HG2	2.16	0.45
2:E:452:PHE:CE2	2:E:456:LEU:HD22	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.99	0.45
1:A:30:ASN:HA	1:A:61:ASN:HA	1.98	0.45
1:A:102:ARG:NE	1:A:121:ASN:HD22	2.14	0.45
1:C:614:ASP:O	1:C:614:ASP:OD2	2.34	0.45
1:C:456:PHE:HB3	1:C:473:TYR:CD2	2.52	0.45
1:C:854:LYS:HB2	1:C:854:LYS:HE3	1.81	0.45
1:B:420:ASP:HB3	1:B:460:ASN:HB3	1.99	0.45
1:A:450:ASN:N	1:A:450:ASN:OD1	2.50	0.45
1:B:108:THR:O	1:B:237:ARG:NH1	2.50	0.45
1:C:444:LYS:HG3	1:C:447:GLY:H	1.82	0.45
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.52	0.45
2:E:36:GLU:HB3	2:E:73:PHE:CE2	2.51	0.45
1:A:336:CYS:HB2	1:A:338:PHE:CZ	2.51	0.45
1:B:21:ARG:HB3	1:B:79:PHE:CE1	2.51	0.45
1:C:280:ASN:ND2	4:C:1305:NAG:H82	2.32	0.45
2:E:47:ALA:HB1	2:E:50:ASN:HB2	1.98	0.45
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.99	0.44
1:A:329:PHE:O	1:A:580:GLN:NE2	2.50	0.44
1:B:1080:ALA:O	1:B:1132:ILE:HG13	2.17	0.44
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.99	0.44
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.16	0.44
2:E:222:LEU:HB3	2:E:223:MET:HE1	1.99	0.44
2:E:49:TRP:HE1	4:E:701:NAG:C8	2.30	0.44
2:E:225:ASP:OD1	2:E:225:ASP:N	2.51	0.44
2:E:586:ASN:HA	2:E:589:GLU:HG2	1.98	0.44
1:A:457:ARG:HH21	1:A:460:ASN:HA	1.81	0.44
1:B:528:LYS:HB2	1:B:528:LYS:HE3	1.53	0.44
1:B:786:LYS:H	1:B:786:LYS:CD	2.30	0.44
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.99	0.44
1:A:821:LEU:HD13	1:A:935:GLN:HE21	1.82	0.44
2:E:140:GLU:OE1	2:E:160:ARG:HB2	2.17	0.44
2:E:508:GLU:N	2:E:508:GLU:OE1	2.50	0.44
2:E:589:GLU:HB2	2:E:590:PRO:HD3	2.00	0.44
1:B:1119:ASN:OD1	1:B:1119:ASN:N	2.47	0.44
1:A:403:ARG:HE	1:A:505:TYR:HA	1.82	0.44
1:A:429:PHE:HE1	1:A:514:SER:HA	1.83	0.44
1:B:351:TYR:HA	1:B:454:ARG:NH2	2.33	0.44
1:C:708:SER:OG	1:C:709:ASN:N	2.50	0.44
2:E:53:THR:OG1	4:E:701:NAG:H2	2.18	0.44
2:E:316:VAL:HA	2:E:320:LEU:H	1.83	0.44
2:E:458:LYS:HG2	2:E:461:TRP:CZ3	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:O	1:A:421:TYR:HB2	2.18	0.44
1:B:96:GLU:OE2	1:B:100:ILE:HB	2.18	0.44
1:C:457:ARG:NH1	1:C:460:ASN:O	2.50	0.44
2:E:349:TRP:HE3	2:E:351:LEU:HD21	1.83	0.44
1:A:14:GLN:HE21	1:A:18:LEU:HD11	1.82	0.43
1:A:370:ASN:OD1	1:A:371:SER:N	2.51	0.43
1:B:215:ASP:OD1	1:B:215:ASP:N	2.44	0.43
2:E:458:LYS:HA	2:E:461:TRP:CE3	2.53	0.43
1:A:240:THR:OG1	1:A:241:LEU:N	2.50	0.43
1:B:61:ASN:HD21	4:B:1308:NAG:H83	1.82	0.43
1:B:675:GLN:HB3	1:B:676:THR:H	1.51	0.43
1:B:708:SER:HB3	1:B:711:SER:HB3	2.00	0.43
1:A:349:SER:OG	1:A:350:VAL:N	2.51	0.43
2:E:165:TRP:CZ2	2:E:493:HIS:HE1	2.37	0.43
2:E:318:ILE:HG22	2:E:550:ALA:HB3	2.01	0.43
1:A:346:ARG:CZ	1:A:347:PHE:H	2.31	0.43
1:B:229:LEU:HD12	1:B:231:ILE:HD11	2.00	0.43
1:B:455:LEU:HG	1:B:456:PHE:HD1	1.84	0.43
1:C:117:LEU:H	1:C:117:LEU:HD23	1.84	0.43
2:E:294:THR:HG22	2:E:296:LYS:HB2	1.99	0.43
2:E:377:GLY:HA2	2:E:380:GLN:OE1	2.18	0.43
1:C:455:LEU:HB3	1:C:493:GLN:HE22	1.84	0.43
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.51	0.43
1:A:231:ILE:HG22	1:A:233:ILE:HG13	2.00	0.43
1:A:351:TYR:OH	1:A:454:ARG:HG2	2.18	0.43
1:A:717:ASN:HB2	1:A:1071:GLN:HB2	2.01	0.43
1:C:627:ASP:OD1	1:C:627:ASP:N	2.51	0.43
1:C:1114:ILE:H	1:C:1114:ILE:HG12	1.66	0.43
4:C:1307:NAG:H5	4:C:1307:NAG:N2	2.33	0.43
1:A:245:HIS:O	1:A:258:TRP:HB2	2.18	0.43
1:A:498:GLN:CD	1:A:498:GLN:H	2.22	0.43
1:B:119:ILE:HG12	1:B:128:ILE:HG12	2.01	0.43
1:B:360:ASN:OD1	1:B:360:ASN:O	2.37	0.43
1:C:346:ARG:NH1	1:C:346:ARG:HA	2.34	0.43
1:C:409:GLN:NE2	1:C:417:LYS:H	2.14	0.43
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.84	0.43
1:C:599:THR:HB	1:C:608:VAL:HG12	2.01	0.43
2:E:179:LEU:HD23	2:E:179:LEU:HA	1.82	0.42
2:E:457:GLU:OE1	2:E:461:TRP:NE1	2.52	0.42
1:A:388:ASN:OD1	1:A:528:LYS:NZ	2.47	0.42
1:B:115:GLN:HA	1:B:132:GLU:HG3	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HD13	1:C:198:ASP:OD2	2.19	0.42
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.85	0.42
2:E:446:ILE:HD13	2:E:523:PHE:HZ	1.84	0.42
2:E:518:ARG:HG3	2:E:519:THR:N	2.33	0.42
1:A:399:SER:HB3	1:A:511:VAL:HG22	2.00	0.42
2:E:418:LEU:HA	2:E:421:LEU:HD12	2.01	0.42
2:E:529:LEU:HD23	2:E:529:LEU:HA	1.88	0.42
1:B:940:SER:OG	1:B:941:THR:N	2.53	0.42
2:E:582:LYS:HD3	2:E:583:PRO:HD3	2.01	0.42
1:A:107:GLY:H	1:A:235:ILE:HG23	1.85	0.42
1:A:321:GLN:HE21	1:A:629:LEU:HB2	1.84	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.84	0.42
1:B:387:LEU:H	1:B:387:LEU:HD12	1.84	0.42
1:B:1045:LYS:HE2	1:B:1045:LYS:HB2	1.81	0.42
1:C:401:VAL:O	1:C:402:ILE:HD13	2.20	0.42
2:E:230:PHE:HZ	2:E:451:PRO:HG3	1.85	0.42
2:E:408:MET:CE	2:E:408:MET:H	2.33	0.42
1:C:117:LEU:HD13	1:C:231:ILE:HG21	2.01	0.42
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.86	0.42
1:C:884:SER:O	1:C:884:SER:OG	2.33	0.42
1:A:825:LYS:HA	1:A:825:LYS:HD2	1.89	0.42
1:C:280:ASN:HD22	4:C:1305:NAG:H82	1.85	0.42
1:C:426:PRO:HD3	1:C:463:PRO:HB3	2.01	0.42
1:C:428:ASP:OD1	1:C:428:ASP:N	2.45	0.42
2:E:370:LEU:O	2:E:373:HIS:ND1	2.43	0.42
2:E:407:ILE:HG21	2:E:529:LEU:HD12	2.01	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.52	0.42
1:A:411:ALA:H	1:A:425:LEU:HD22	1.85	0.42
1:A:880:GLY:O	1:A:884:SER:OG	2.28	0.42
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.87	0.42
1:B:776:LYS:HB3	1:B:776:LYS:HE3	1.82	0.42
1:C:81:ASN:HB3	1:C:239:GLN:HE21	1.85	0.42
2:E:108:VAL:HG11	2:E:190:MET:HG2	2.02	0.42
1:A:883:THR:O	1:A:895:GLN:HA	2.20	0.42
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	2.02	0.42
1:B:139:PRO:HB3	1:B:159:VAL:HB	2.00	0.42
1:B:616:ASN:OD1	1:B:617:CYS:N	2.53	0.42
1:C:58:PHE:HD1	1:C:58:PHE:HA	1.77	0.42
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.53	0.42
2:E:225:ASP:O	2:E:229:THR:HG23	2.19	0.42
2:E:539:LEU:HD12	2:E:587:TYR:HD1	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG23	1:A:77:LYS:HA	2.02	0.41
1:B:453:TYR:CE1	1:B:493:GLN:HB2	2.54	0.41
1:C:119:ILE:HG13	1:C:128:ILE:HG22	2.01	0.41
1:C:287:ASP:OD1	1:C:288:ALA:N	2.50	0.41
2:E:578:THR:OG1	2:E:579:MET:N	2.53	0.41
1:A:336:CYS:HB3	1:A:358:ILE:HG12	2.02	0.41
1:A:1142:GLN:NE2	1:A:1145:LEU:HD13	2.35	0.41
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.38	0.41
2:E:589:GLU:O	2:E:593:THR:HG23	2.20	0.41
1:B:433:VAL:HG22	1:B:512:VAL:HG13	2.02	0.41
1:C:529:LYS:HE2	1:C:529:LYS:HB2	1.89	0.41
2:E:152:MET:HB3	2:E:156:ARG:HH12	1.86	0.41
2:E:188:ASN:ND2	2:E:464:PHE:HB3	2.33	0.41
2:E:450:LEU:HD23	2:E:450:LEU:HA	1.90	0.41
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.90	0.41
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.53	0.41
1:C:544:ASN:OD1	1:C:544:ASN:N	2.53	0.41
1:C:417:LYS:CE	1:C:455:LEU:HD23	2.47	0.41
2:E:275:TRP:HB2	2:E:444:LEU:HB3	2.02	0.41
2:E:323:MET:SD	2:E:327:PHE:HB3	2.60	0.41
2:E:467:GLU:H	2:E:467:GLU:CD	2.21	0.41
1:A:195:LYS:HE3	1:A:195:LYS:HB3	1.84	0.41
1:A:1004:LEU:HD23	1:A:1004:LEU:HA	1.90	0.41
1:C:401:VAL:C	1:C:402:ILE:HD13	2.41	0.41
2:E:198:ASP:OD1	2:E:198:ASP:N	2.54	0.41
1:B:644:GLN:NE2	1:B:645:THR:O	2.53	0.41
1:C:985:ASP:HB3	1:C:987:PRO:HD2	2.02	0.41
1:B:25:PRO:HA	1:B:26:PRO:HD3	1.99	0.41
1:B:280:ASN:HD22	4:B:1303:NAG:H82	1.86	0.41
2:E:160:ARG:HH22	2:E:270:MET:HA	1.86	0.41
1:A:312:ILE:HD12	1:A:598:ILE:HG13	2.01	0.41
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.79	0.41
1:B:14:GLN:N	1:B:14:GLN:OE1	2.54	0.41
1:B:186:PHE:N	1:B:210:ILE:O	2.53	0.41
1:B:431:GLY:HA2	1:B:515:PHE:HD2	1.86	0.41
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.79	0.41
1:C:341:VAL:H	1:C:341:VAL:HG22	1.60	0.41
1:C:352:ALA:HA	1:C:466:ARG:HE	1.86	0.41
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.02	0.41
2:E:99:LYS:HE2	2:E:99:LYS:HB3	1.90	0.41
2:E:247:LYS:HE2	2:E:284:PRO:HA	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:HIS:HE1	2:E:349:TRP:CZ2	2.39	0.41
1:A:409:GLN:HB3	1:A:416:GLY:HA3	2.01	0.41
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.95	0.41
2:E:340:ARG:HH12	2:E:342:VAL:HG23	1.86	0.41
1:B:106:PHE:HB3	1:B:235:ILE:HD13	2.03	0.40
1:B:214:ARG:HA	1:B:214:ARG:HD3	1.85	0.40
1:B:328:ARG:NH1	1:B:533:LEU:HB2	2.35	0.40
1:B:630:THR:N	1:B:631:PRO:HD3	2.36	0.40
2:E:161:ARG:HH21	2:E:266:LEU:HD13	1.86	0.40
1:A:387:LEU:HD12	1:A:390:LEU:HD21	2.03	0.40
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.03	0.40
2:E:161:ARG:HH22	2:E:256:ILE:HD11	1.85	0.40
2:E:183:TYR:O	2:E:187:GLU:HB2	2.20	0.40
1:A:943:SER:O	1:A:943:SER:OG	2.39	0.40
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.40	0.40
1:C:335:LEU:HD23	1:C:336:CYS:N	2.36	0.40
1:C:621:PRO:HB3	1:C:628:GLN:NE2	2.36	0.40
2:E:398:GLU:H	2:E:398:GLU:HG2	1.63	0.40
3:O:1:NAG:O3	3:O:2:NAG:O5	2.34	0.40
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.03	0.40
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.96	0.40
1:C:410:ILE:H	1:C:410:ILE:HD12	1.85	0.40
2:E:55:ILE:O	2:E:55:ILE:HD12	2.22	0.40
2:E:62:LYS:HE2	2:E:62:LYS:HB3	1.91	0.40
2:E:378:HIS:O	2:E:378:HIS:CD2	2.74	0.40
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.87	0.40
3:N:1:NAG:H61	3:N:2:NAG:HN2	1.87	0.40

There are no symmetry-related clashes.

## 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	1047/1217 (86%)	999 (95%)	48 (5%)	0	100	100
1	B	1047/1217 (86%)	994 (95%)	53 (5%)	0	100	100
1	C	1051/1217 (86%)	993 (94%)	58 (6%)	0	100	100
2	E	593/661 (90%)	556 (94%)	36 (6%)	1 (0%)	47	72
All	All	3738/4312 (87%)	3542 (95%)	195 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	469	PRO

### 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	930/1065 (87%)	889 (96%)	41 (4%)	28	54
1	B	931/1065 (87%)	893 (96%)	38 (4%)	30	57
1	C	933/1065 (88%)	882 (94%)	51 (6%)	21	44
2	E	527/585 (90%)	484 (92%)	43 (8%)	11	25
All	All	3321/3780 (88%)	3148 (95%)	173 (5%)	27	47

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	24	LEU
1	A	50	SER
1	A	78	ARG
1	A	88	ASP
1	A	165	ASN
1	A	198	ASP
1	A	240	THR
1	A	246	ARG
1	A	277	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	305	SER
1	A	346	ARG
1	A	347	PHE
1	A	349	SER
1	A	369	TYR
1	A	373	SER
1	A	377	PHE
1	A	383	SER
1	A	385	THR
1	A	386	LYS
1	A	400	PHE
1	A	405	ASP
1	A	408	ARG
1	A	421	TYR
1	A	441	LEU
1	A	451	TYR
1	A	456	PHE
1	A	494	SER
1	A	505	TYR
1	A	528	LYS
1	A	586	ASP
1	A	634	ARG
1	A	636	TYR
1	A	731	MET
1	A	750	SER
1	A	786	LYS
1	A	813	SER
1	A	878	LEU
1	A	937	SER
1	A	985	ASP
1	A	1097	SER
1	B	21	ARG
1	B	34	ARG
1	B	80	ASP
1	B	96	GLU
1	B	126	VAL
1	B	131	CYS
1	B	153	MET
1	B	173	GLN
1	B	195	LYS
1	B	214	ARG
1	B	242	LEU

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	305	SER
1	B	318	PHE
1	B	325	SER
1	B	350	VAL
1	B	369	TYR
1	B	377	PHE
1	B	392	PHE
1	B	400	PHE
1	B	515	PHE
1	B	529	LYS
1	B	544	ASN
1	B	553	THR
1	B	554	GLU
1	B	564	GLN
1	B	576	VAL
1	B	633	TRP
1	B	636	TYR
1	B	676	THR
1	B	709	ASN
1	B	786	LYS
1	B	820	ASP
1	B	825	LYS
1	B	902	MET
1	B	916	LEU
1	B	937	SER
1	B	1045	LYS
1	B	1116	THR
1	C	18	LEU
1	C	46	SER
1	C	50	SER
1	C	58	PHE
1	C	87	ASN
1	C	102	ARG
1	C	118	LEU
1	C	130	VAL
1	C	157	PHE
1	C	168	PHE
1	C	170	TYR
1	C	200	TYR
1	C	201	PHE
1	C	234	ASN
1	C	240	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	244	LEU
1	C	258	TRP
1	C	266	TYR
1	C	277	LEU
1	C	301	CYS
1	C	305	SER
1	C	369	TYR
1	C	374	PHE
1	C	377	PHE
1	C	388	ASN
1	C	390	LEU
1	C	392	PHE
1	C	408	ARG
1	C	462	LYS
1	C	490	PHE
1	C	495	TYR
1	C	508	TYR
1	C	515	PHE
1	C	518	LEU
1	C	540	ASN
1	C	544	ASN
1	C	559	PHE
1	C	745	ASP
1	C	759	PHE
1	C	786	LYS
1	C	787	GLN
1	C	791	THR
1	C	800	PHE
1	C	803	SER
1	C	813	SER
1	C	820	ASP
1	C	875	SER
1	C	916	LEU
1	C	965	GLN
1	C	974	SER
1	C	1043	CYS
2	E	24	GLU
2	E	52	ASN
2	E	54	ASN
2	E	63	MET
2	E	83	THR
2	E	112	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	115	LYS
2	E	124	MET
2	E	152	MET
2	E	158	TYR
2	E	160	ARG
2	E	190	MET
2	E	223	MET
2	E	224	LYS
2	E	230	PHE
2	E	271	TRP
2	E	287	HIS
2	E	297	MET
2	E	306	ARG
2	E	323	MET
2	E	332	MET
2	E	357	ARG
2	E	360	MET
2	E	381	TYR
2	E	383	MET
2	E	385	TYR
2	E	408	MET
2	E	410	LEU
2	E	455	MET
2	E	462	MET
2	E	472	GLN
2	E	480	MET
2	E	505	HIS
2	E	516	TYR
2	E	518	ARG
2	E	534	ASN
2	E	556	GLN
2	E	557	MET
2	E	582	LYS
2	E	595	LEU
2	E	600	ARG
2	E	610	TRP
2	E	614	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	14	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	121	ASN
1	A	188	ASN
1	A	314	GLN
1	A	343	ASN
1	A	414	GLN
1	A	437	ASN
1	A	613	GLN
1	A	675	GLN
1	A	762	GLN
1	A	804	GLN
1	A	935	GLN
1	A	953	ASN
1	A	957	GLN
1	A	1142	GLN
1	B	14	GLN
1	B	173	GLN
1	B	218	GLN
1	B	245	HIS
1	B	317	ASN
1	B	354	ASN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	448	ASN
1	B	493	GLN
1	B	519	HIS
1	B	544	ASN
1	B	628	GLN
1	B	658	ASN
1	B	901	GLN
1	B	955	ASN
1	B	1002	GLN
1	C	87	ASN
1	C	137	ASN
1	C	239	GLN
1	C	422	ASN
1	C	450	ASN
1	C	519	HIS
1	C	580	GLN
1	C	658	ASN
1	C	675	GLN
1	C	901	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	C	965	GLN
1	C	1002	GLN
2	E	43	GLN
2	E	59	ASN
2	E	61	GLN
2	E	64	ASN
2	E	330	ASN
2	E	345	HIS
2	E	493	HIS
2	E	524	GLN

### 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](#)

42 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	D	1	1,3	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.20	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	G	2	3	14,14,15	0.36	0	17,19,21	0.40	0
3	NAG	H	1	1,3	14,14,15	0.41	0	17,19,21	1.36	2 (11%)
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	1.22	2 (11%)

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	0.22	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.32	0	17,19,21	0.58	0
3	NAG	J	1	1,3	14,14,15	0.25	0	17,19,21	0.59	0
3	NAG	J	2	3	14,14,15	0.61	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.68	0	17,19,21	0.51	0
3	NAG	L	1	1,3	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.55	0
3	NAG	M	1	1,3	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
3	NAG	M	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.67	0
3	NAG	N	1	1,3	14,14,15	0.43	0	17,19,21	0.88	1 (5%)
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.55	0
3	NAG	O	1	1,3	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	O	2	3	14,14,15	0.52	0	17,19,21	0.42	0
3	NAG	P	1	1,3	14,14,15	0.37	0	17,19,21	0.78	0
3	NAG	P	2	3	14,14,15	0.40	0	17,19,21	0.53	0
3	NAG	Q	1	1,3	14,14,15	0.50	0	17,19,21	0.51	0
3	NAG	Q	2	3	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
3	NAG	R	1	1,3	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
3	NAG	R	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	S	1	1,3	14,14,15	0.22	0	17,19,21	0.57	0
3	NAG	S	2	3	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	T	1	1,3	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
3	NAG	T	2	3	14,14,15	0.54	0	17,19,21	0.48	0
3	NAG	U	1	1,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	U	2	3	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	V	1	1,3	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	V	2	3	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	W	1	1,3	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
3	NAG	W	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	X	1	1,3	14,14,15	0.26	0	17,19,21	0.64	1 (5%)
3	NAG	X	2	3	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	Y	1	2,3	14,14,15	0.39	0	17,19,21	0.50	0
3	NAG	Y	2	3	14,14,15	0.55	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	4/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Y	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	NAG	O5-C1	2.82	1.48	1.43
3	K	1	NAG	O5-C1	-2.29	1.40	1.43
3	J	2	NAG	O5-C1	-2.06	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C2-N2-C7	4.43	129.21	122.90
3	W	1	NAG	C2-N2-C7	4.21	128.89	122.90
3	H	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	J	2	NAG	C1-O5-C5	2.91	116.13	112.19
3	N	1	NAG	C1-O5-C5	2.86	116.07	112.19
3	Q	2	NAG	C1-O5-C5	2.59	115.70	112.19
3	F	2	NAG	C1-O5-C5	2.42	115.47	112.19
3	M	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	H	2	NAG	C1-C2-N2	2.25	114.34	110.49
3	D	2	NAG	C1-O5-C5	2.24	115.22	112.19
3	R	1	NAG	C1-O5-C5	2.18	115.14	112.19
3	H	1	NAG	C1-O5-C5	2.18	115.14	112.19
3	T	1	NAG	C1-O5-C5	2.11	115.06	112.19
3	X	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	W	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

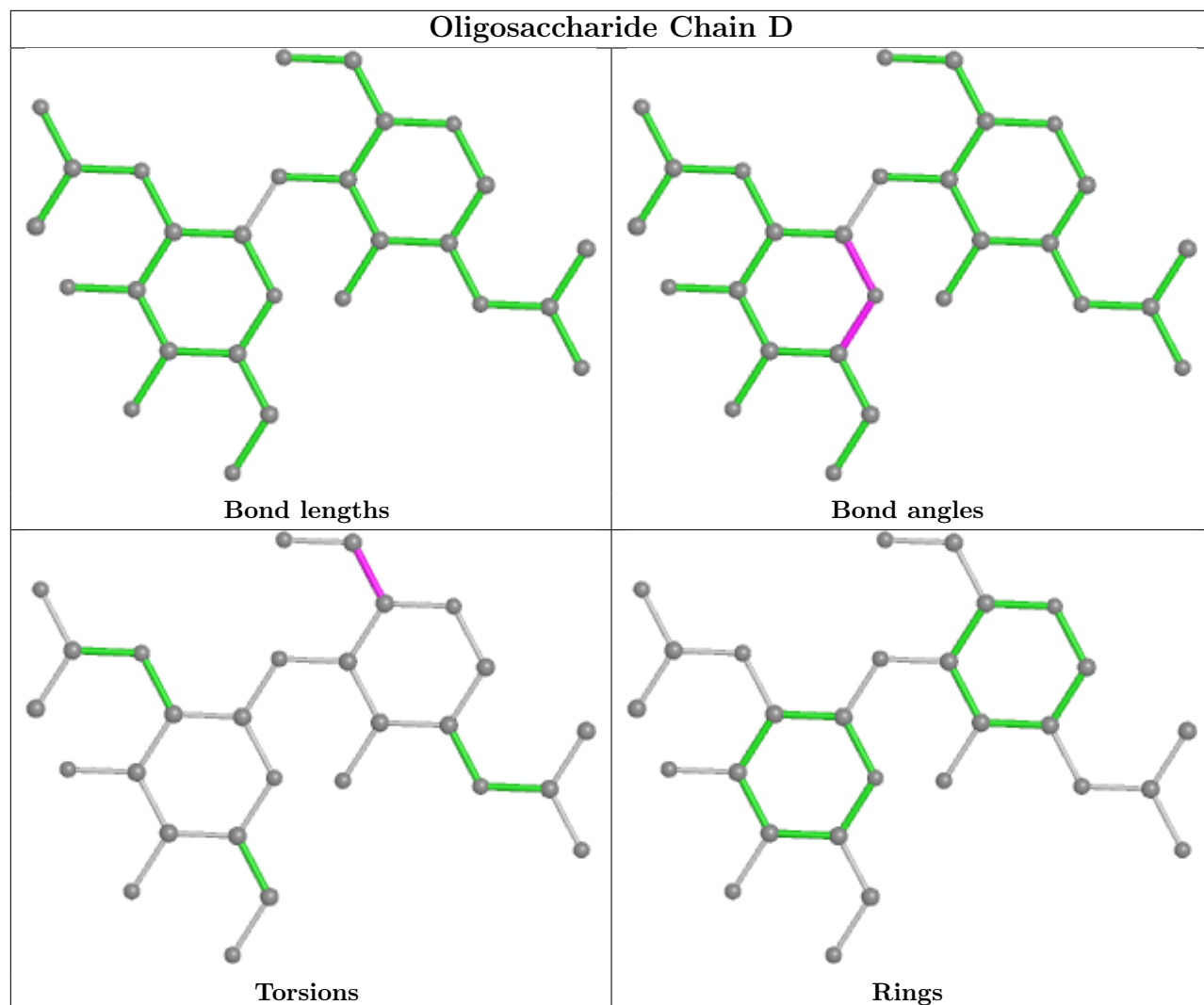
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C1-C2-N2-C7

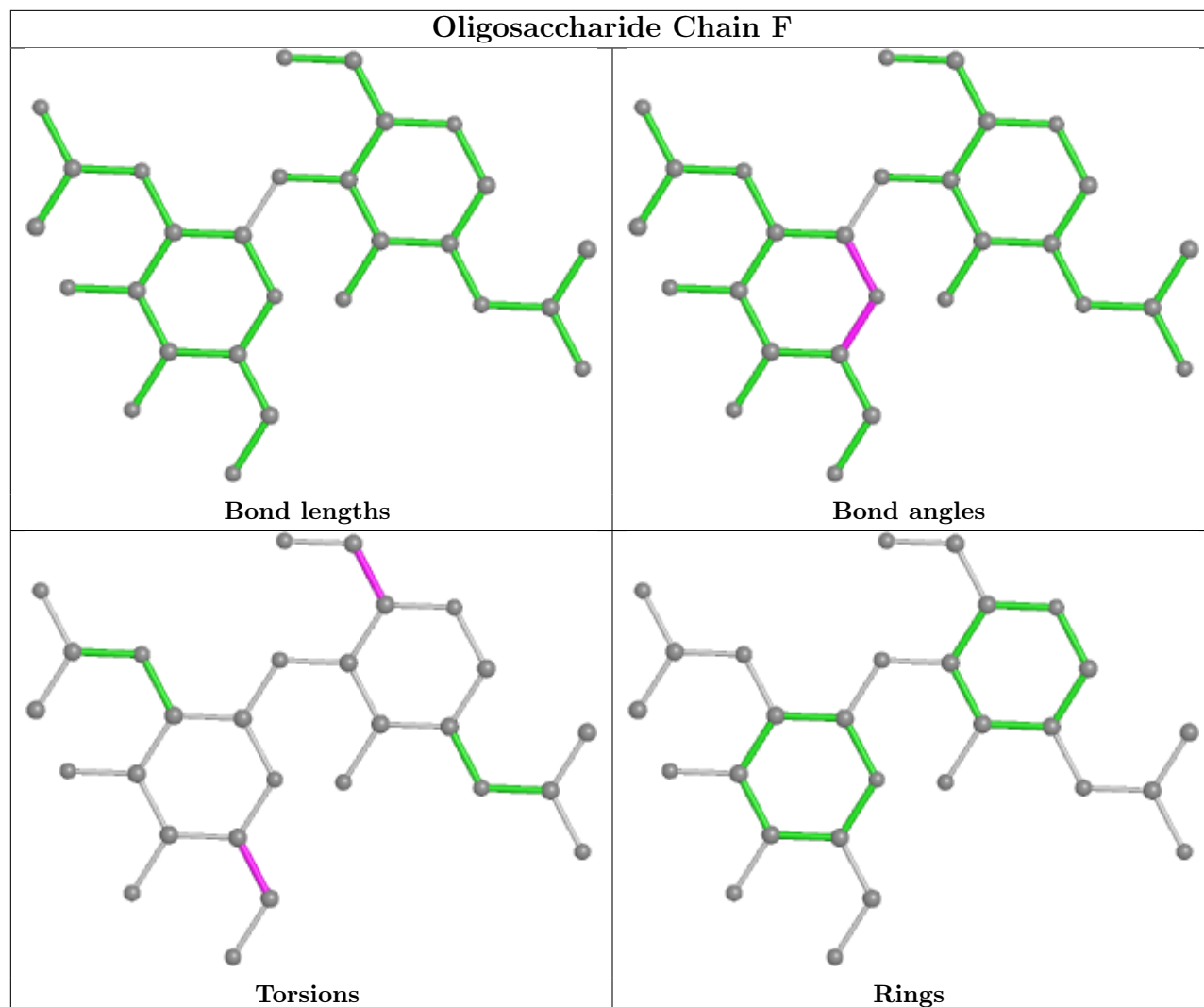
There are no ring outliers.

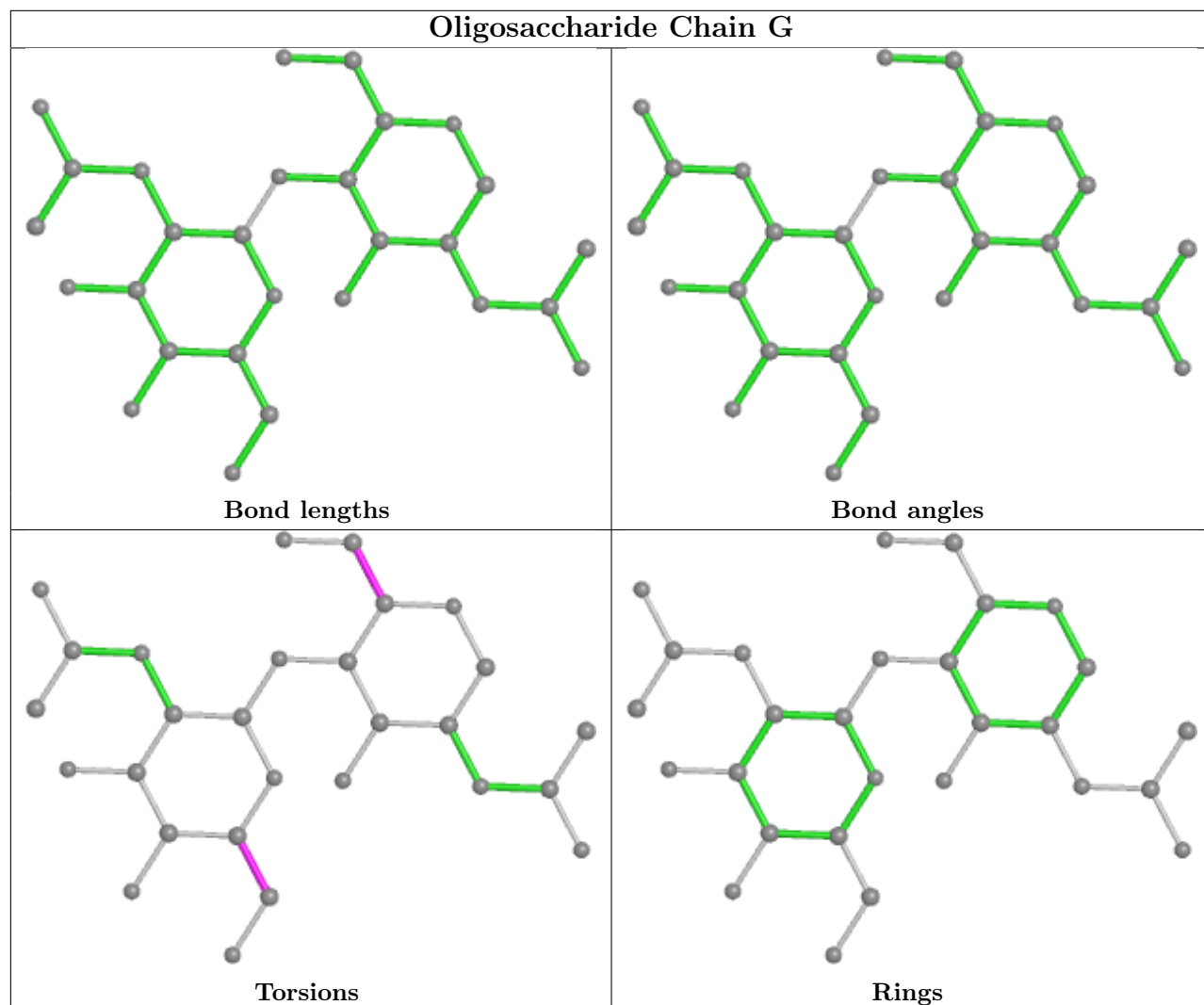
14 monomers are involved in 17 short contacts:

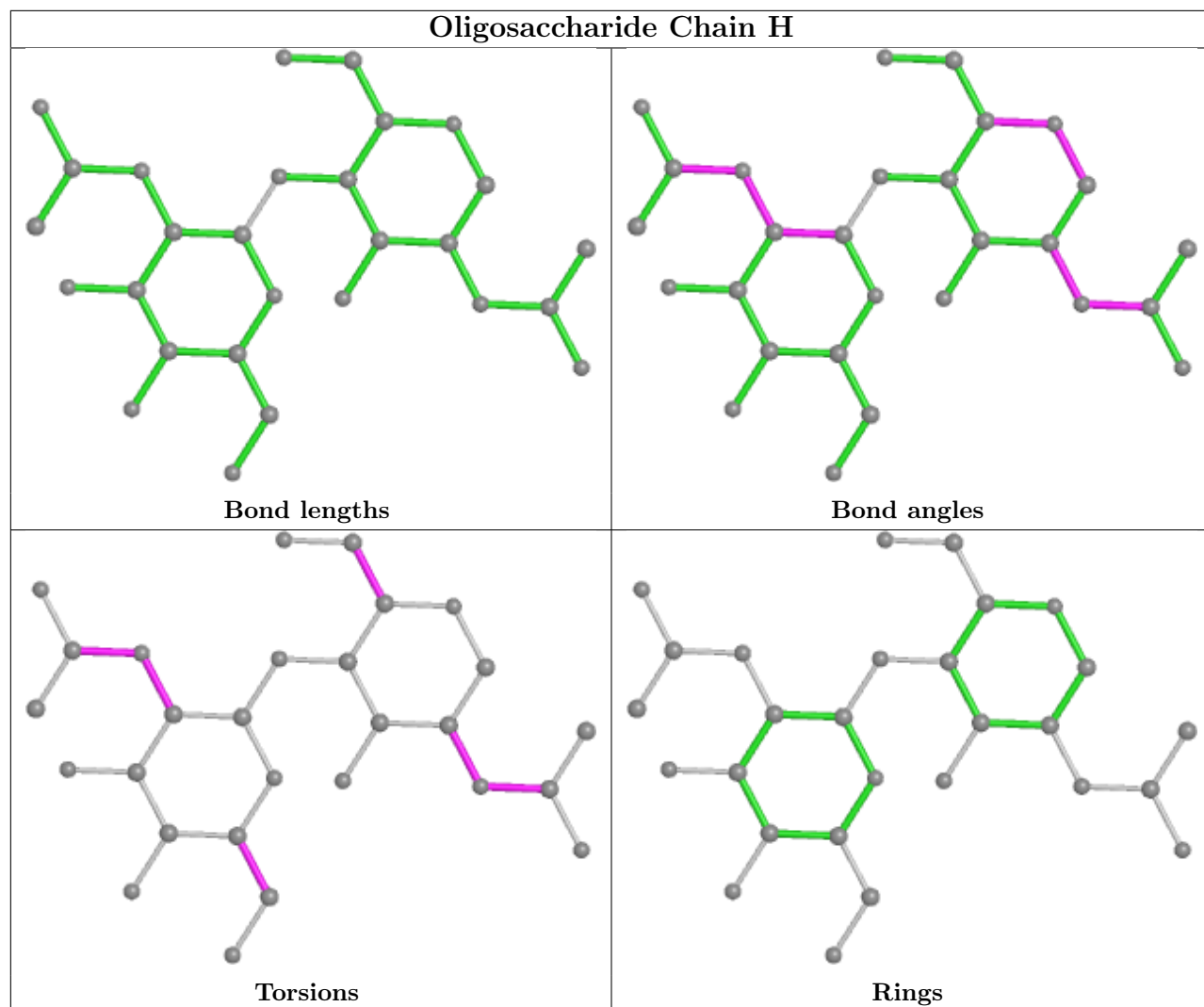
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	N	2	NAG	1	0
3	U	1	NAG	2	0
3	O	1	NAG	1	0
3	T	1	NAG	2	0
3	H	2	NAG	1	0
3	X	1	NAG	1	0
3	D	1	NAG	1	0
3	T	2	NAG	2	0
3	W	1	NAG	3	0
3	N	1	NAG	1	0
3	O	2	NAG	1	0
3	V	1	NAG	1	0
3	Q	1	NAG	3	0

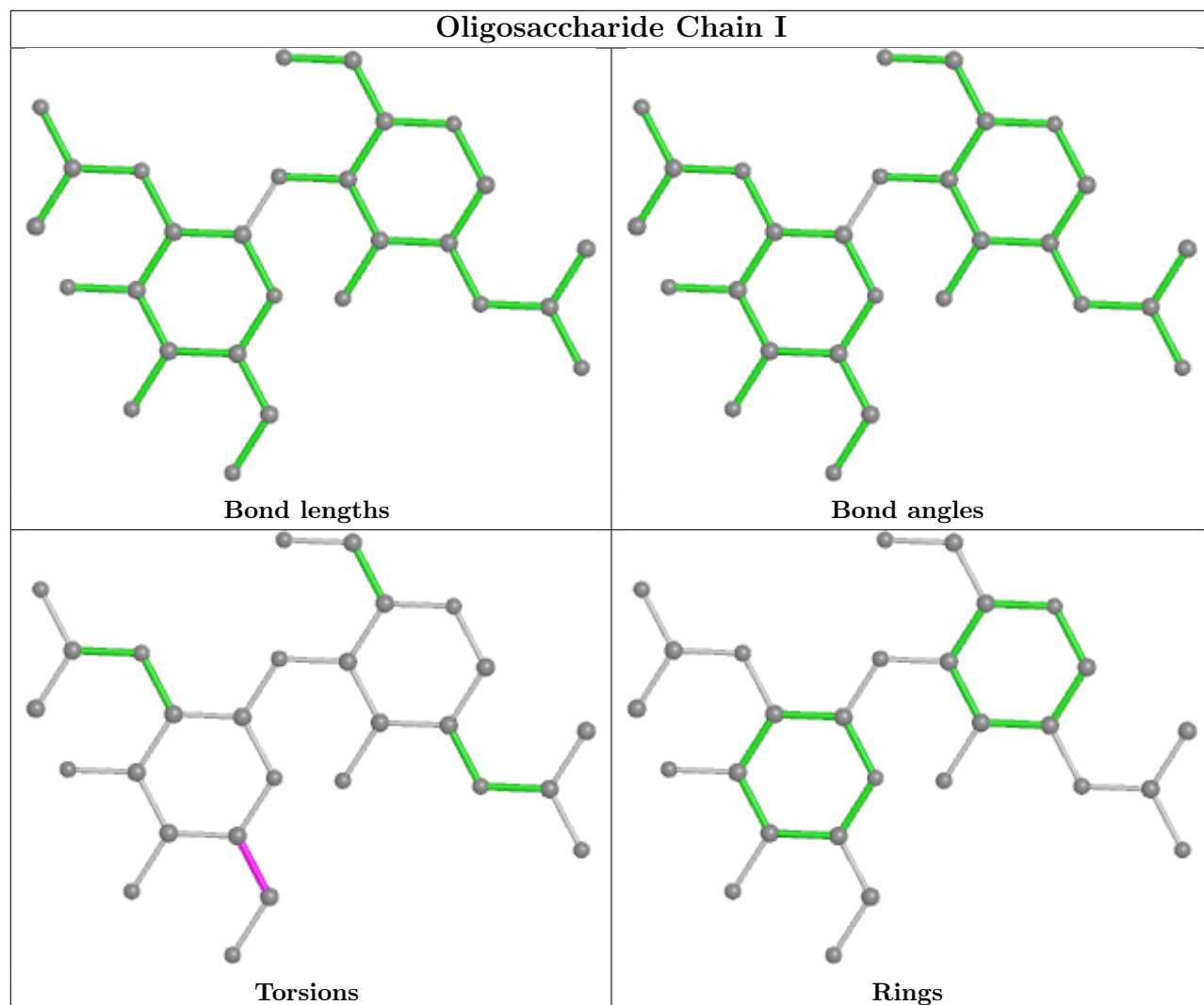
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



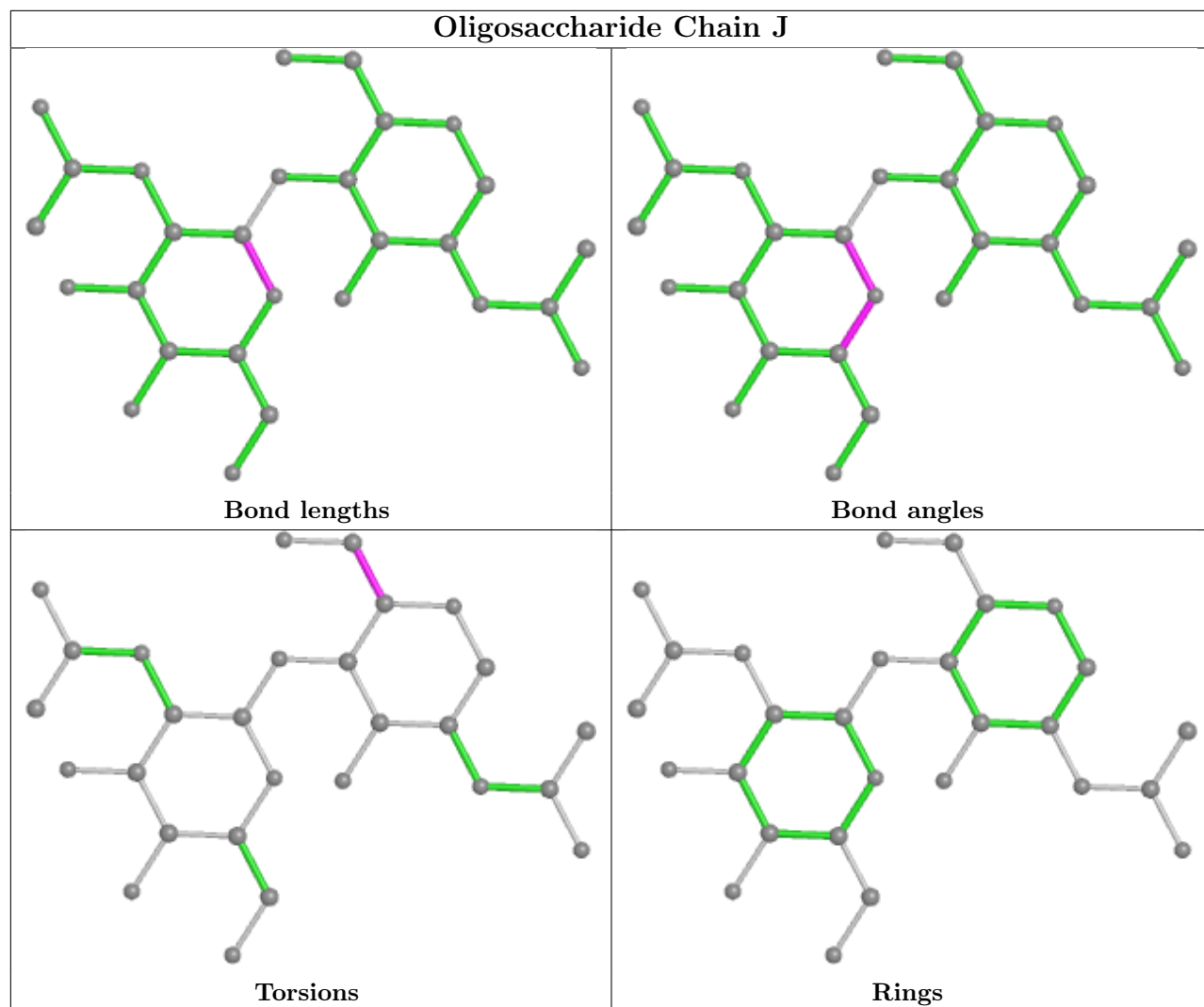


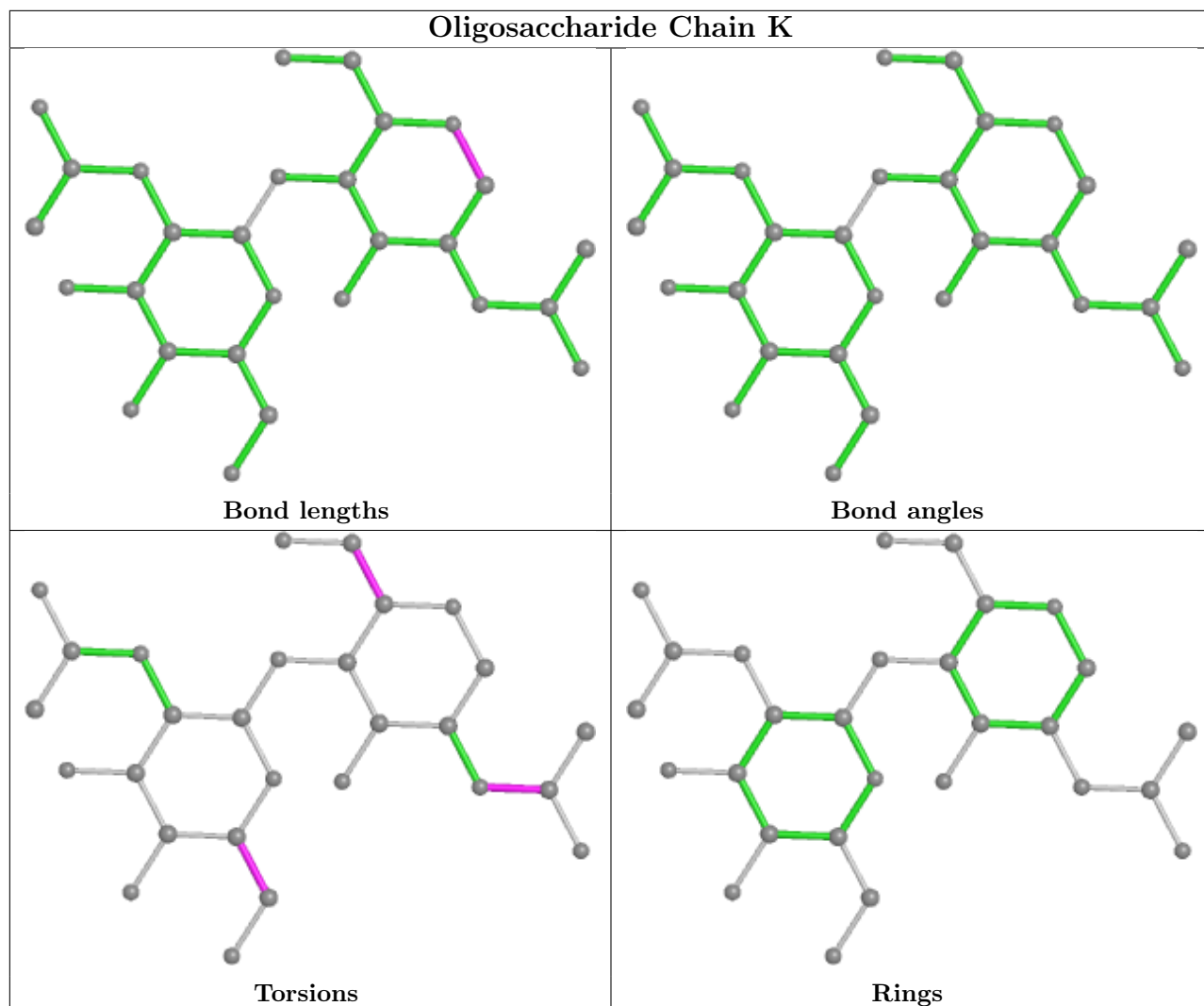


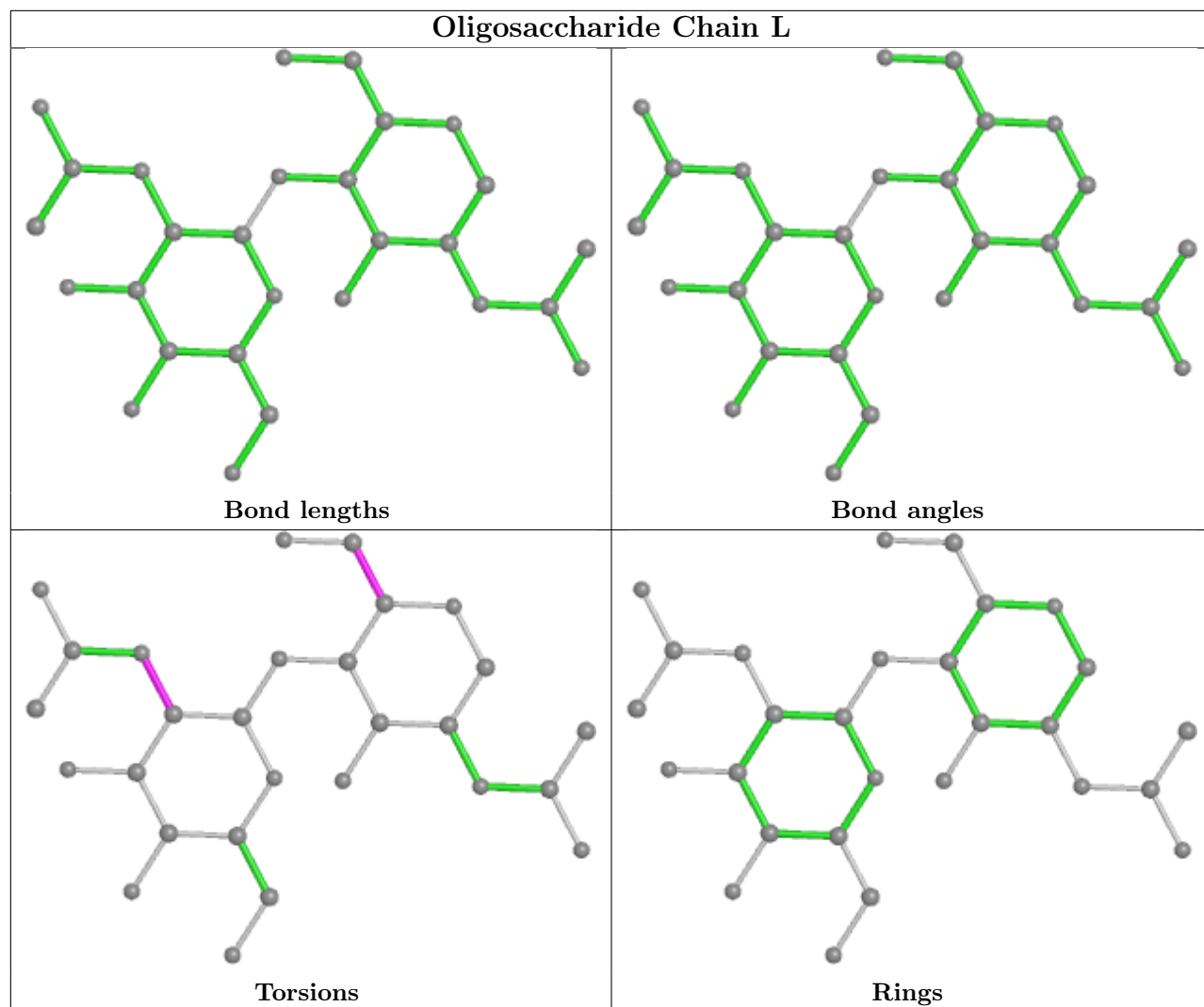


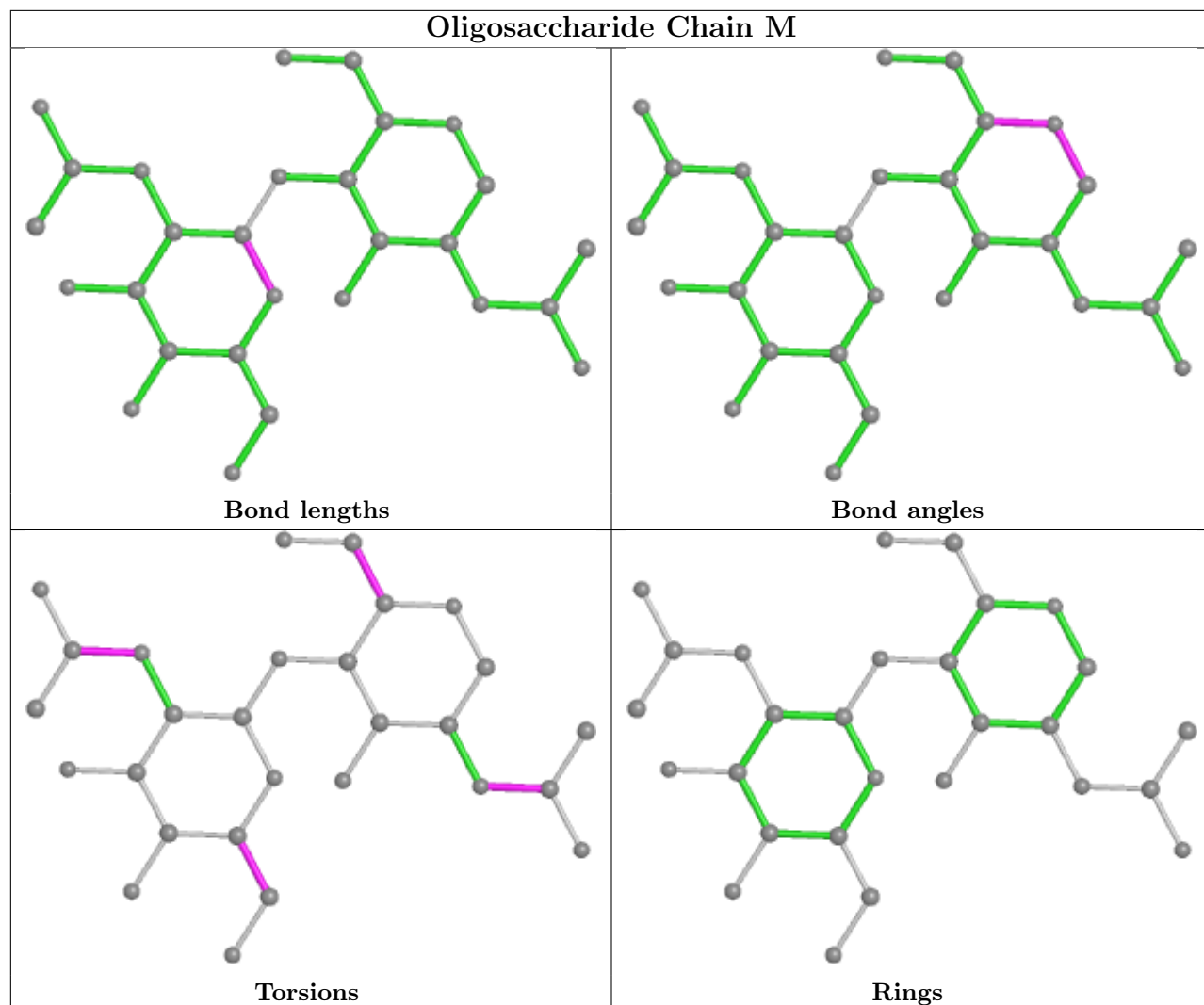


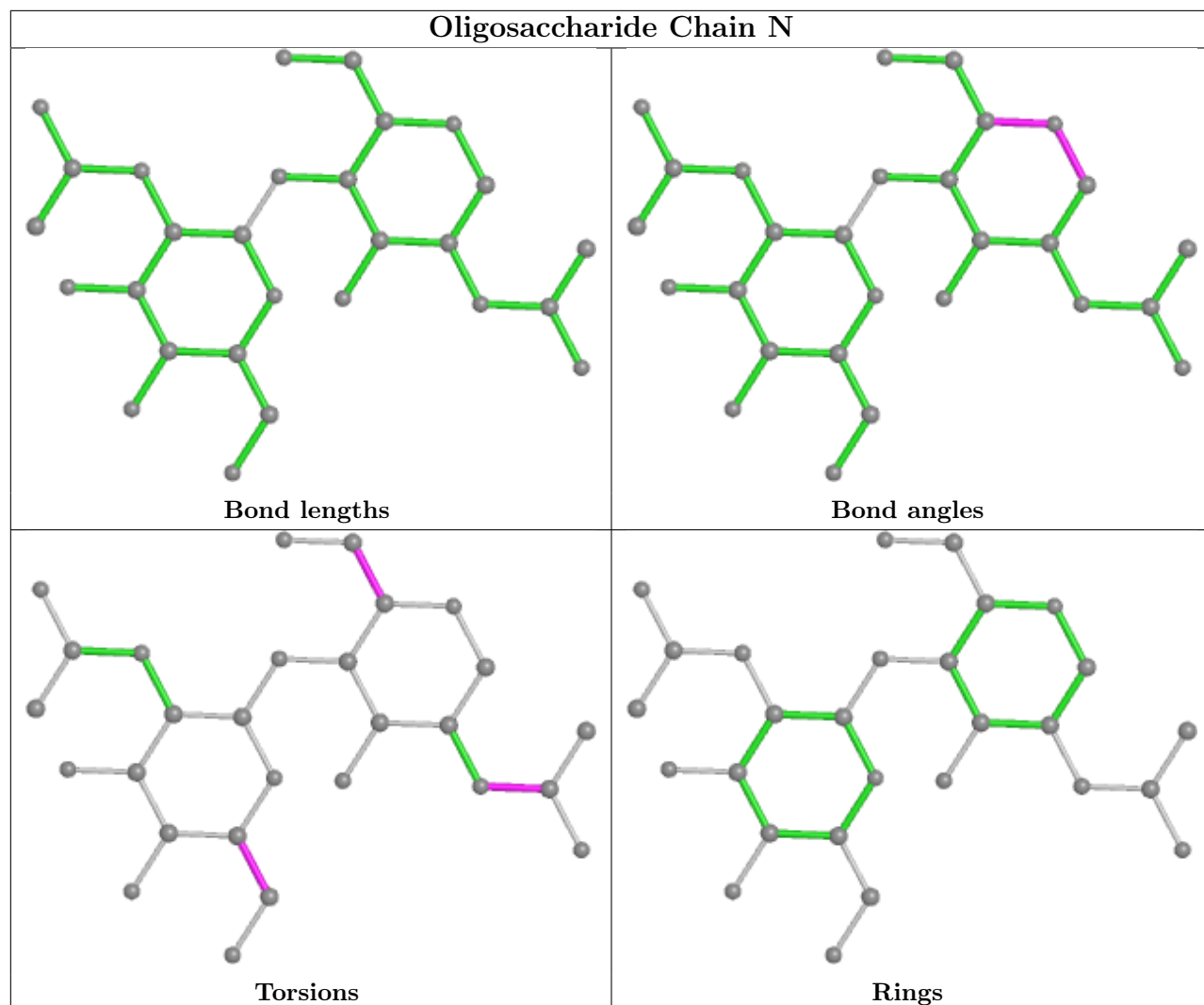


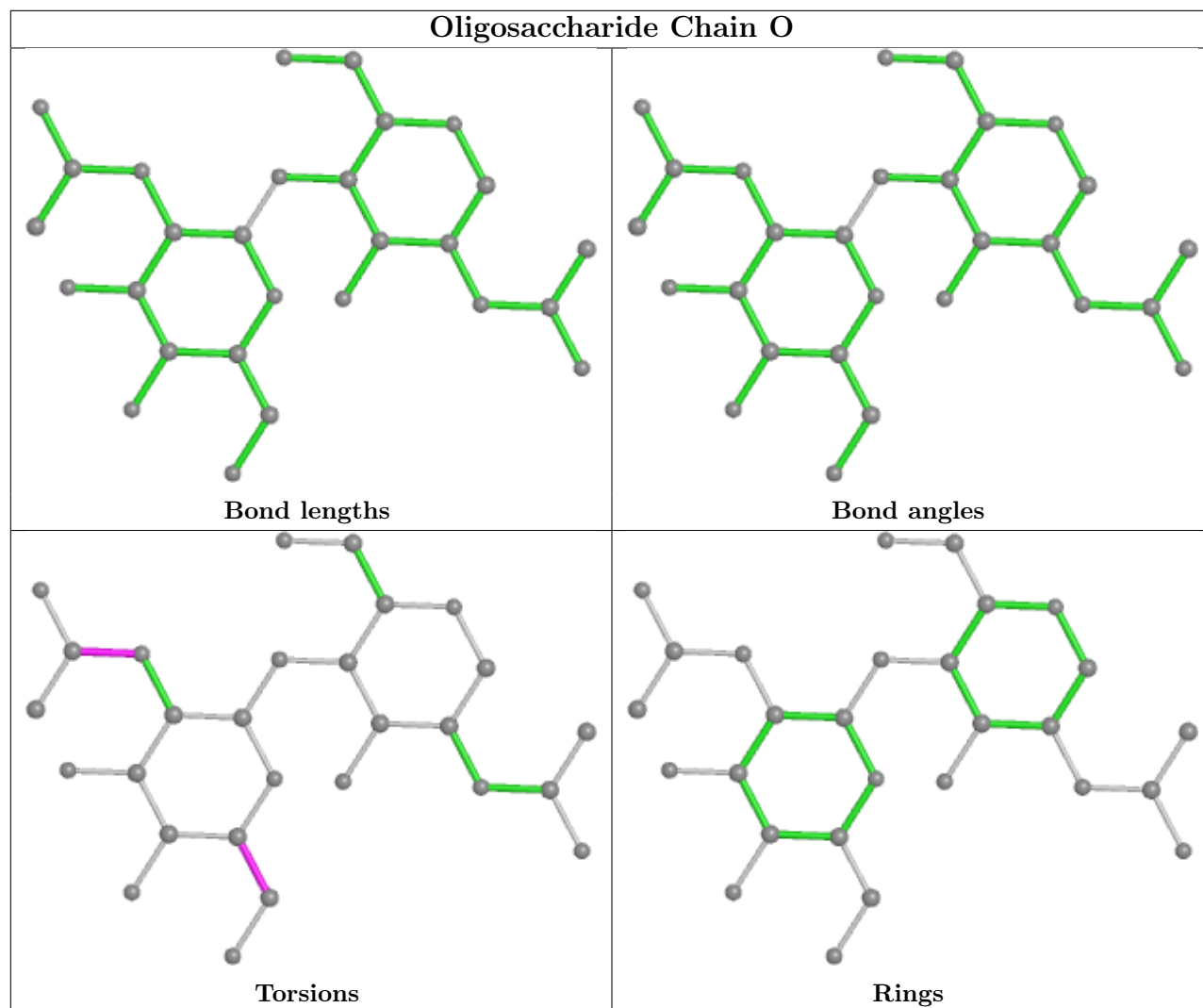


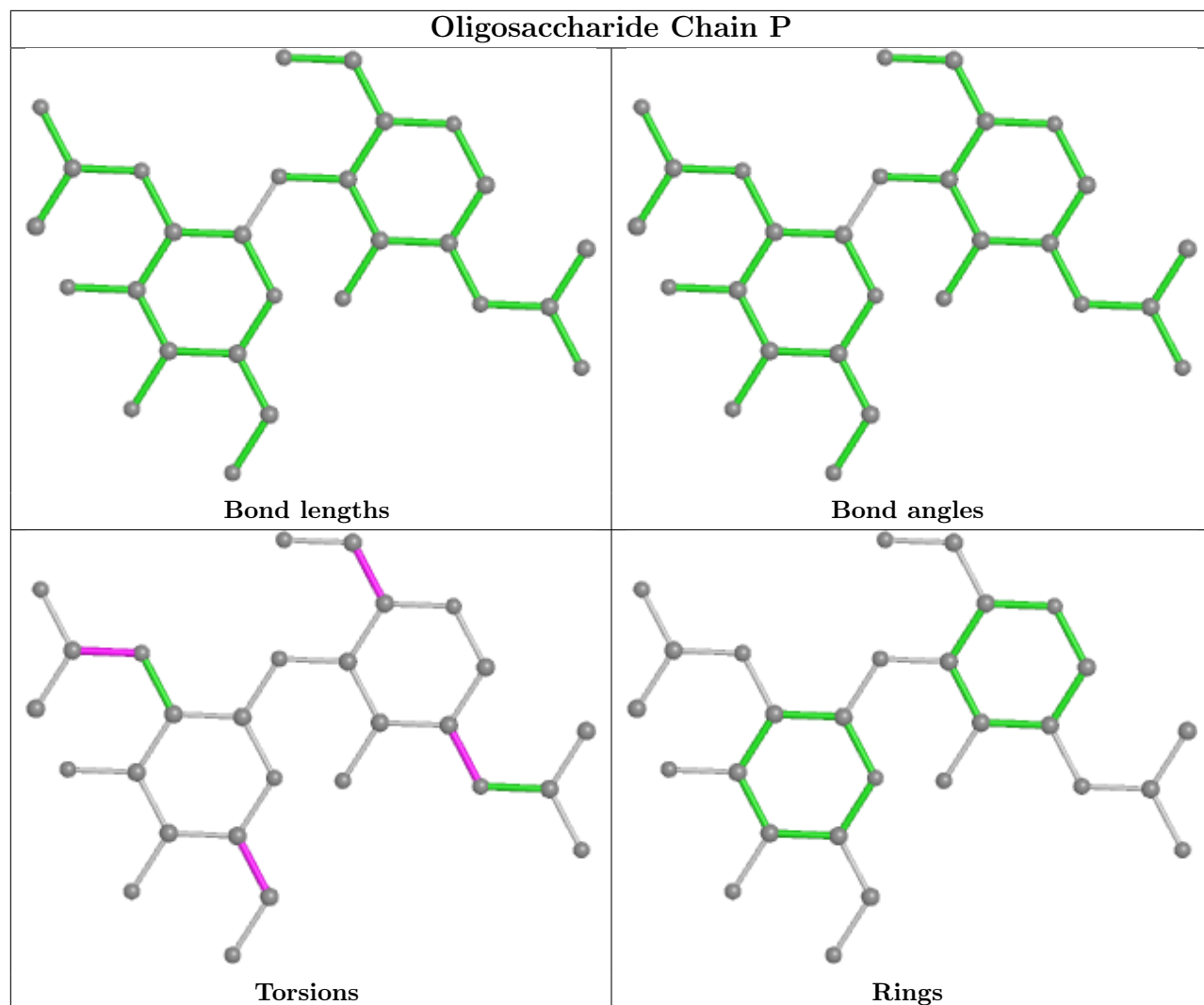


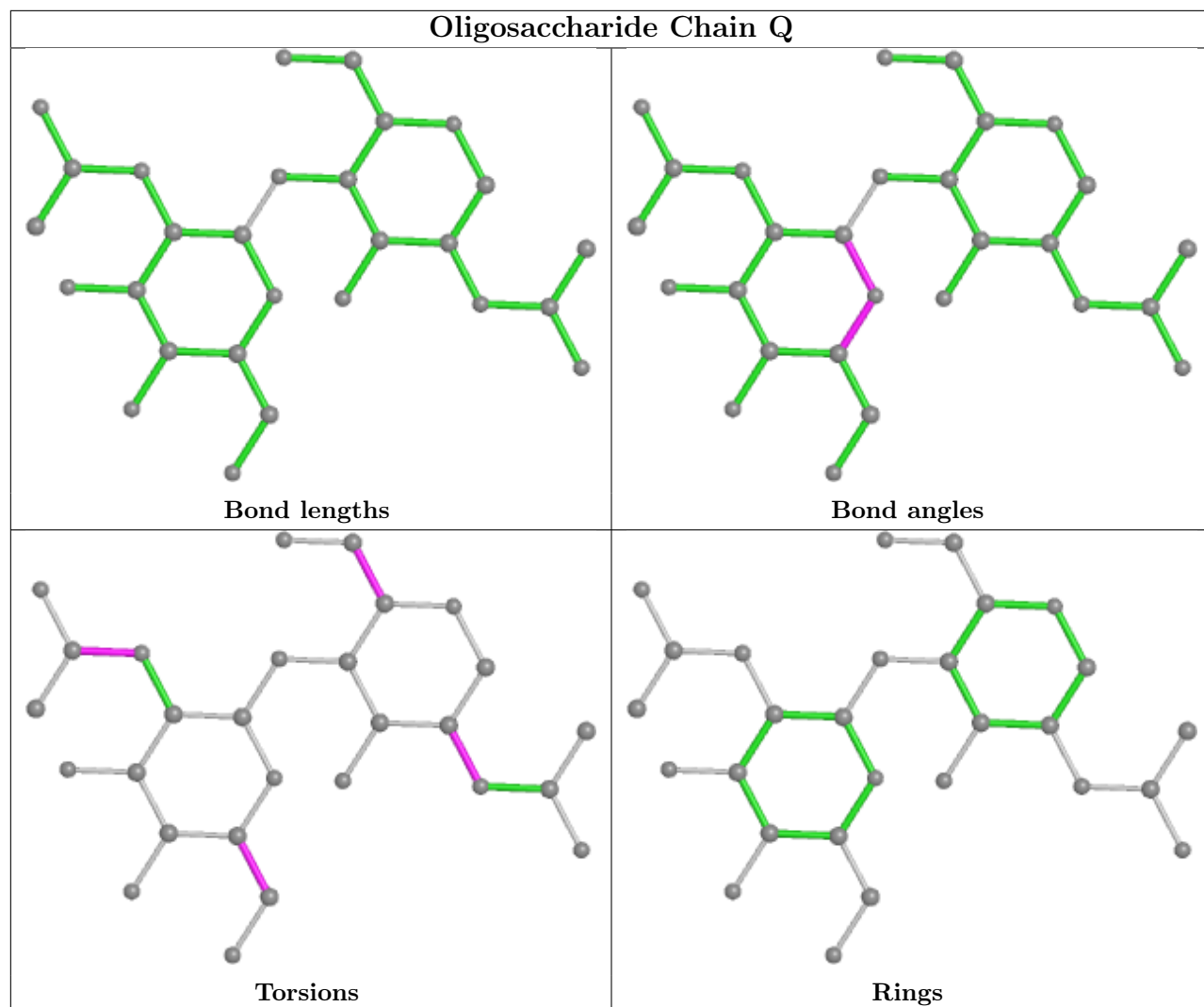




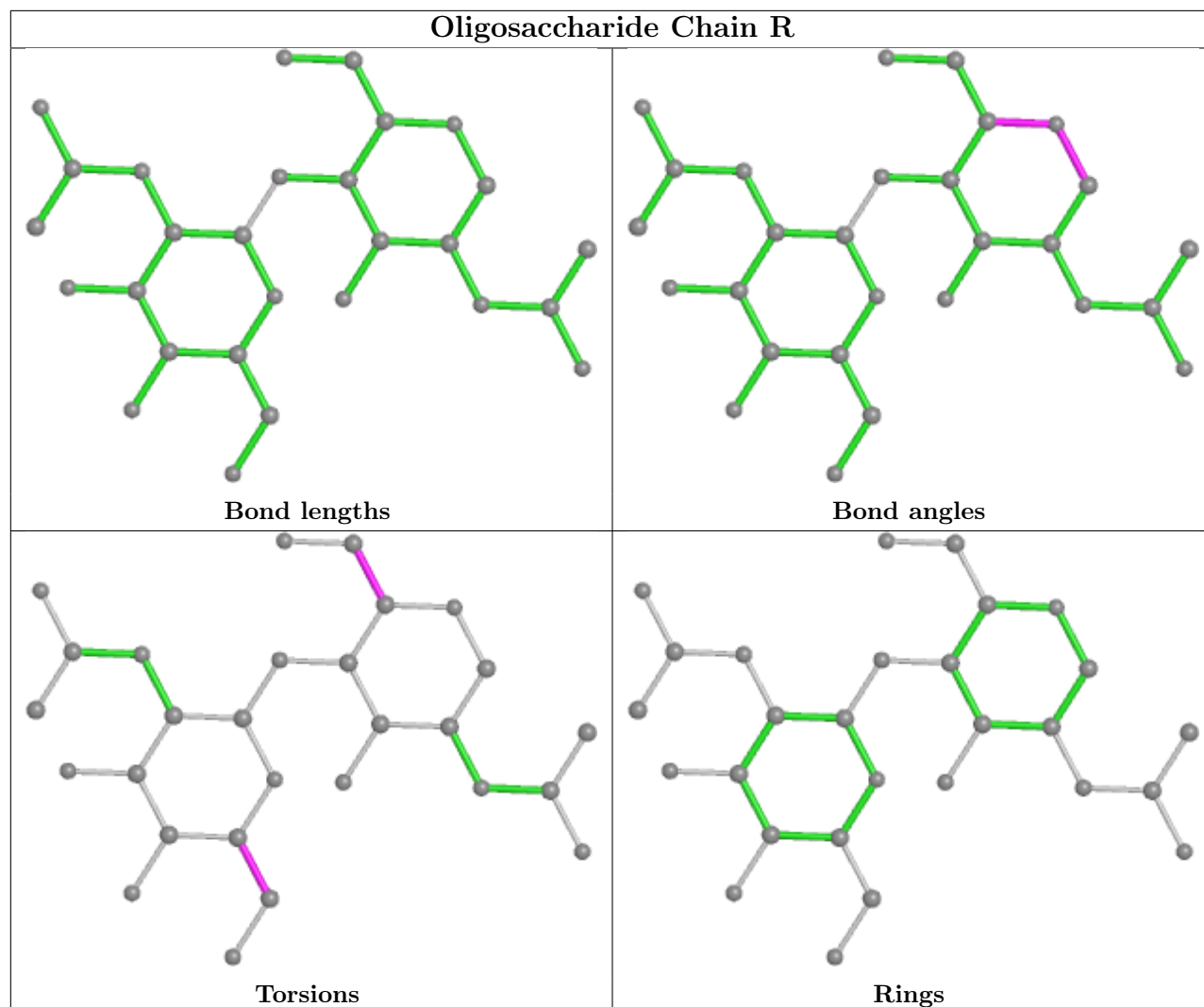


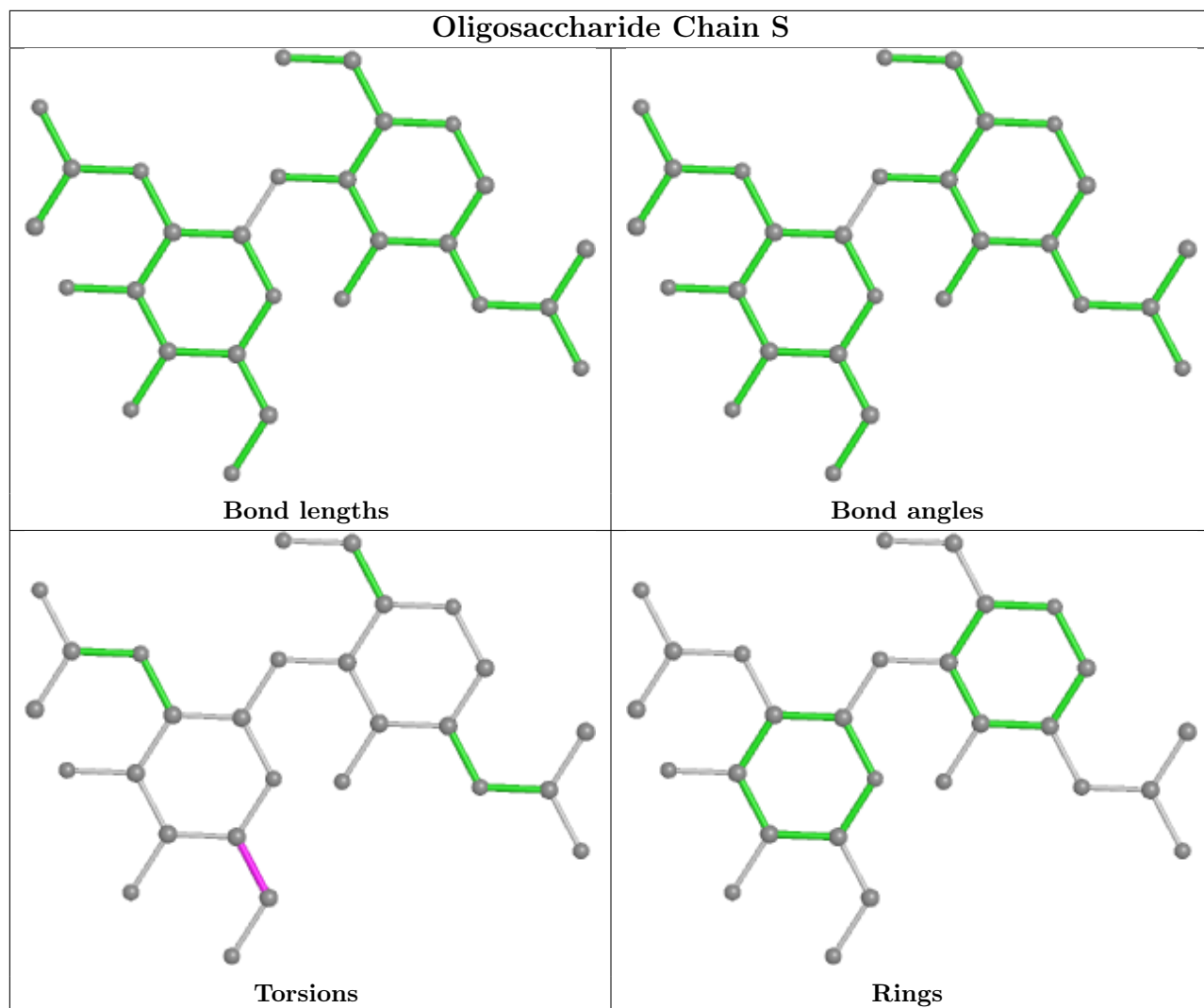


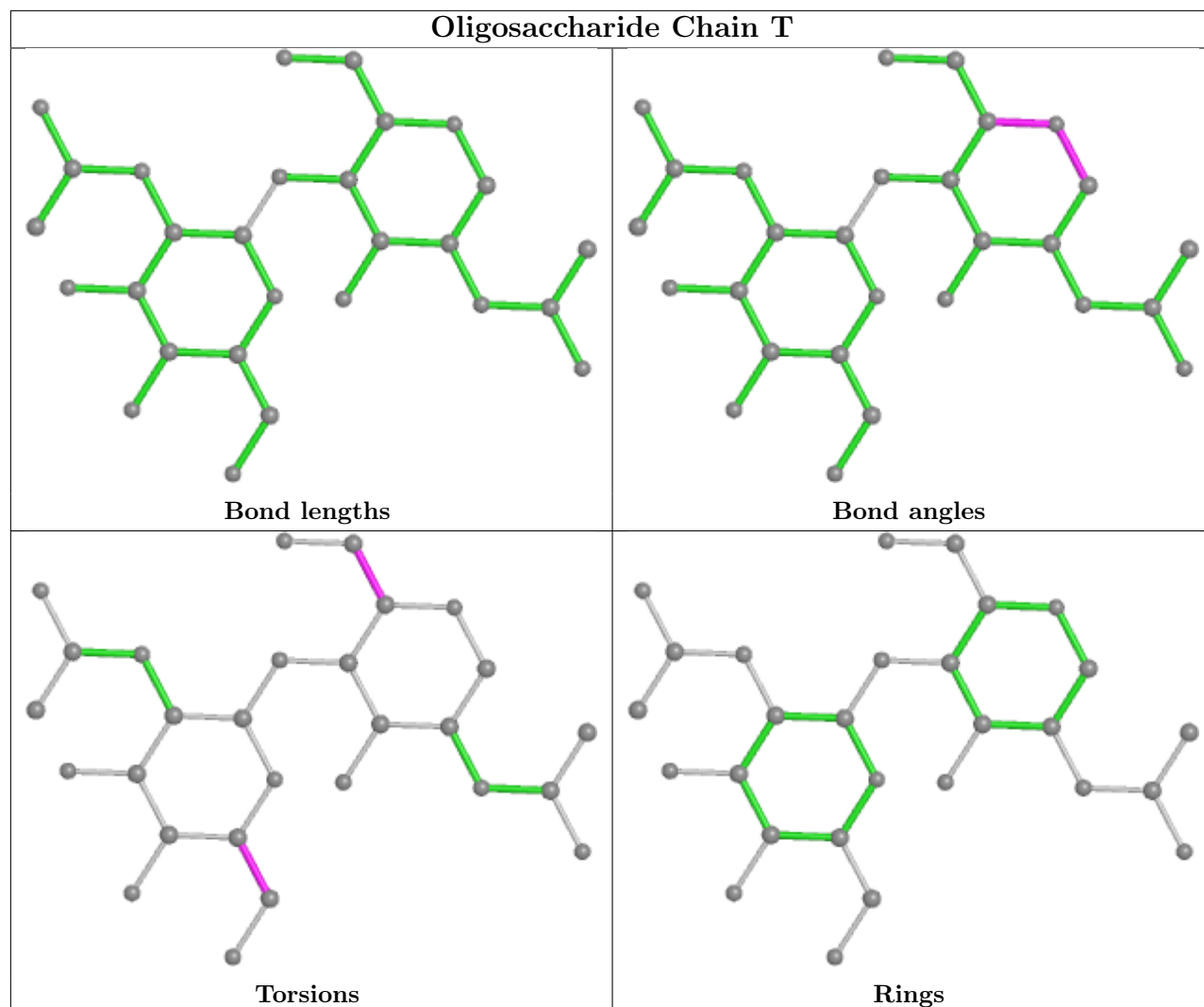


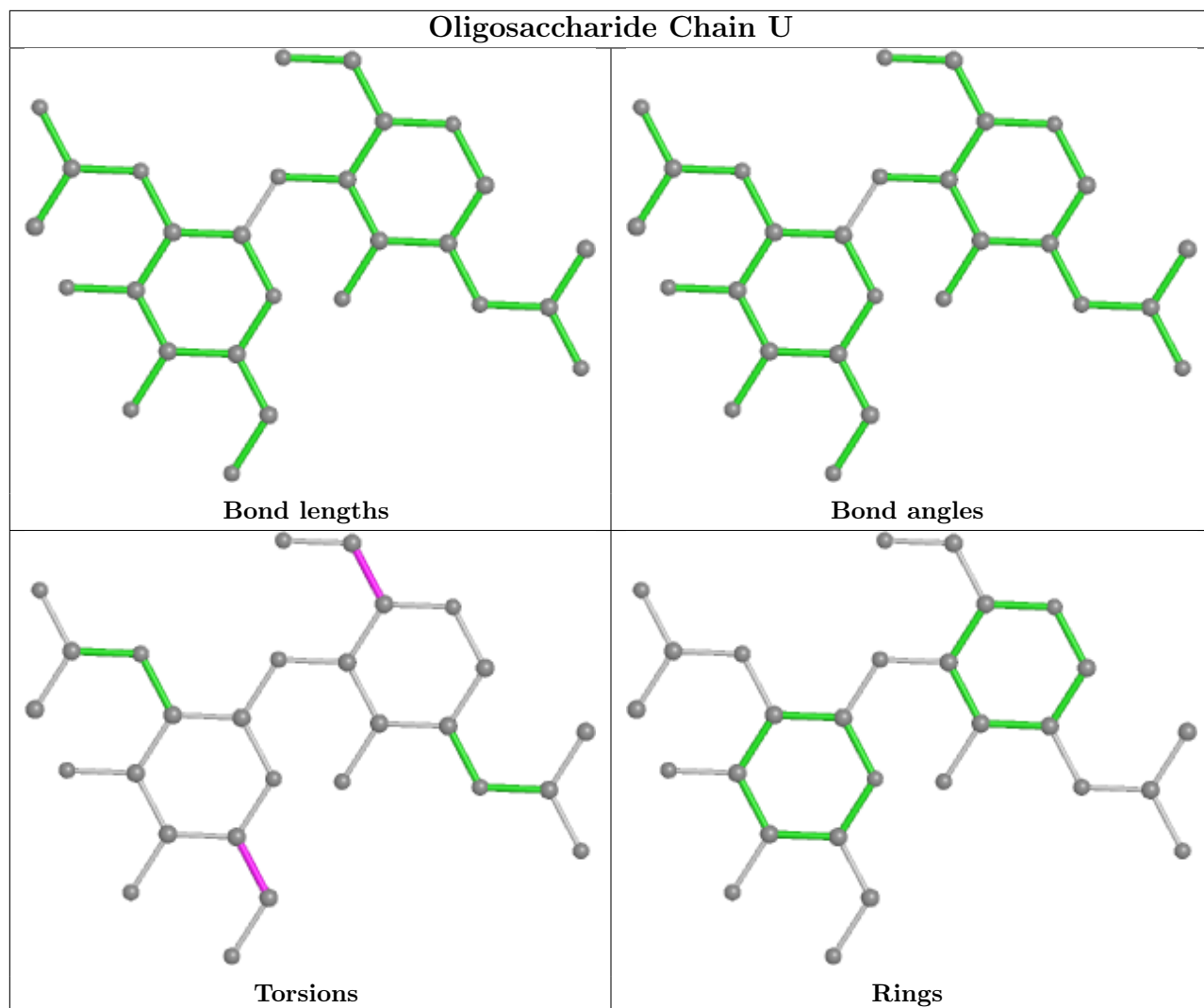


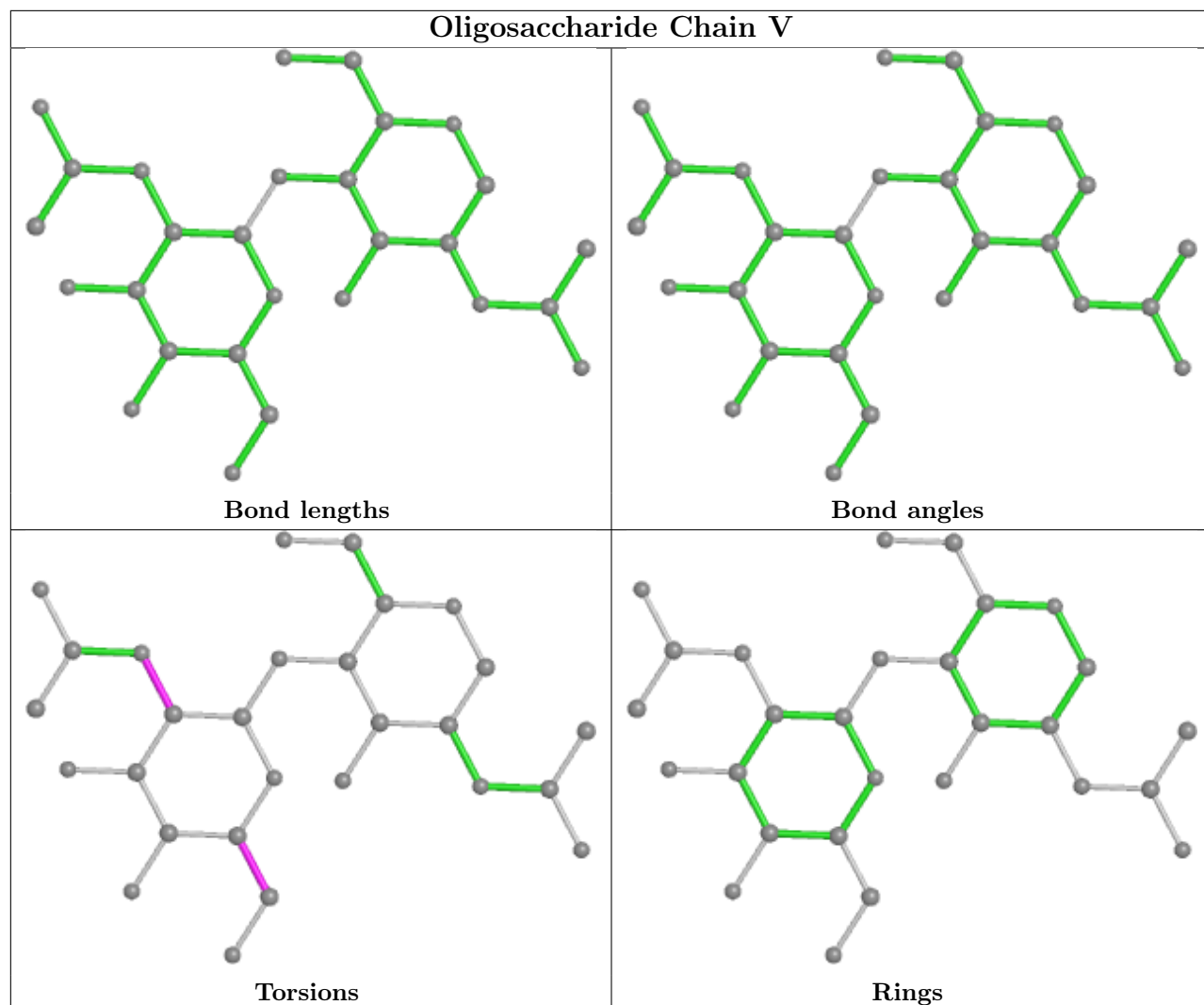


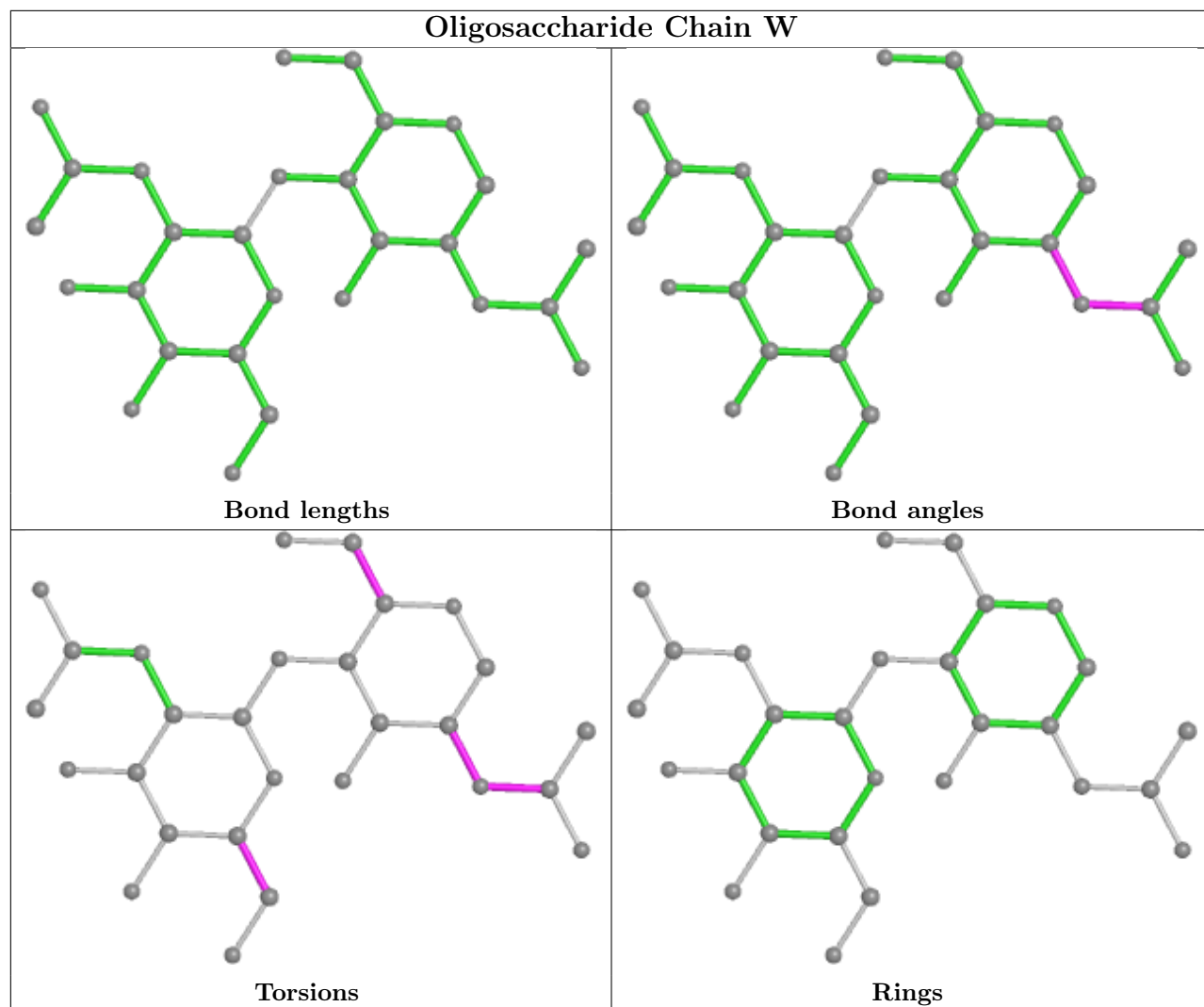


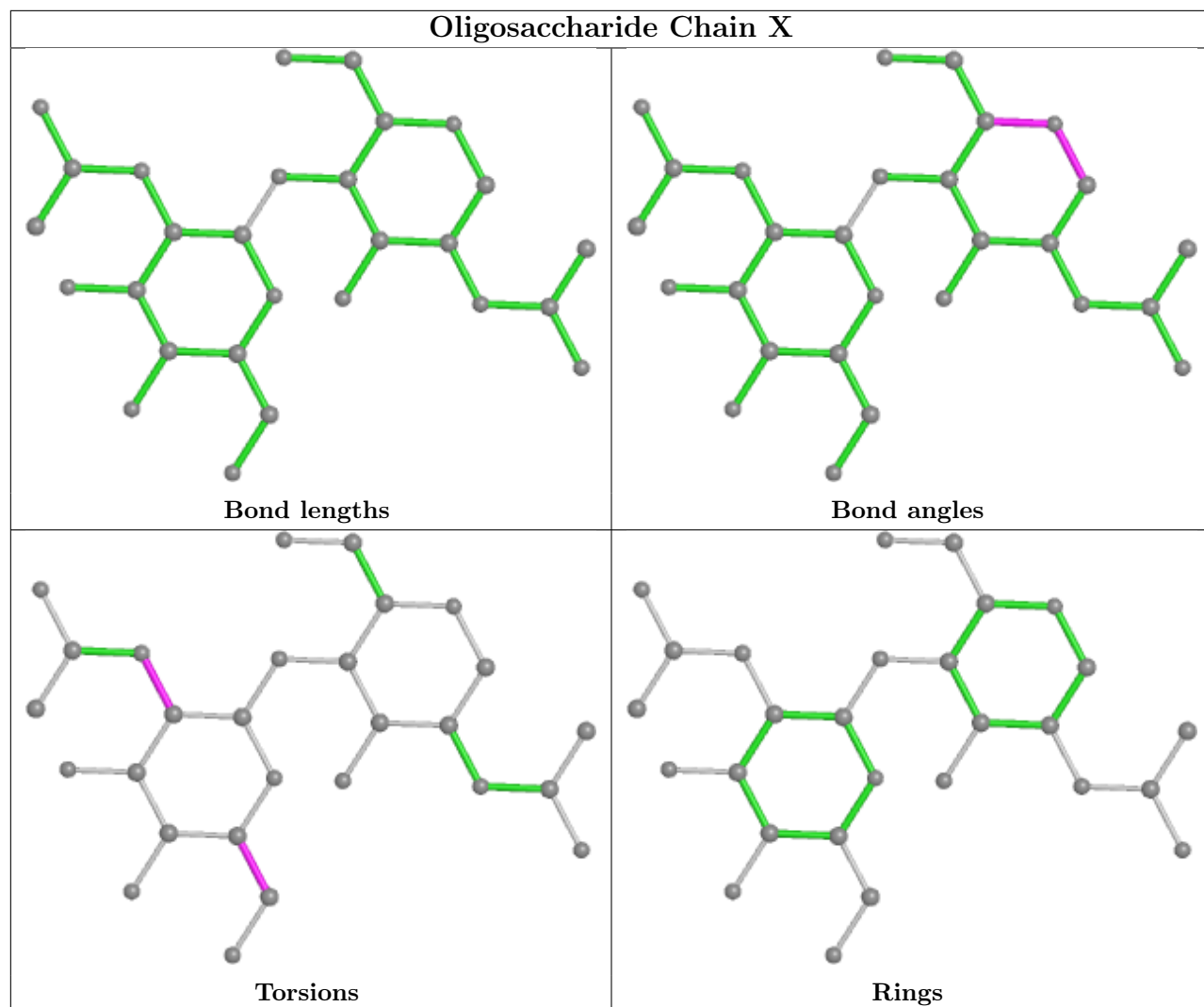


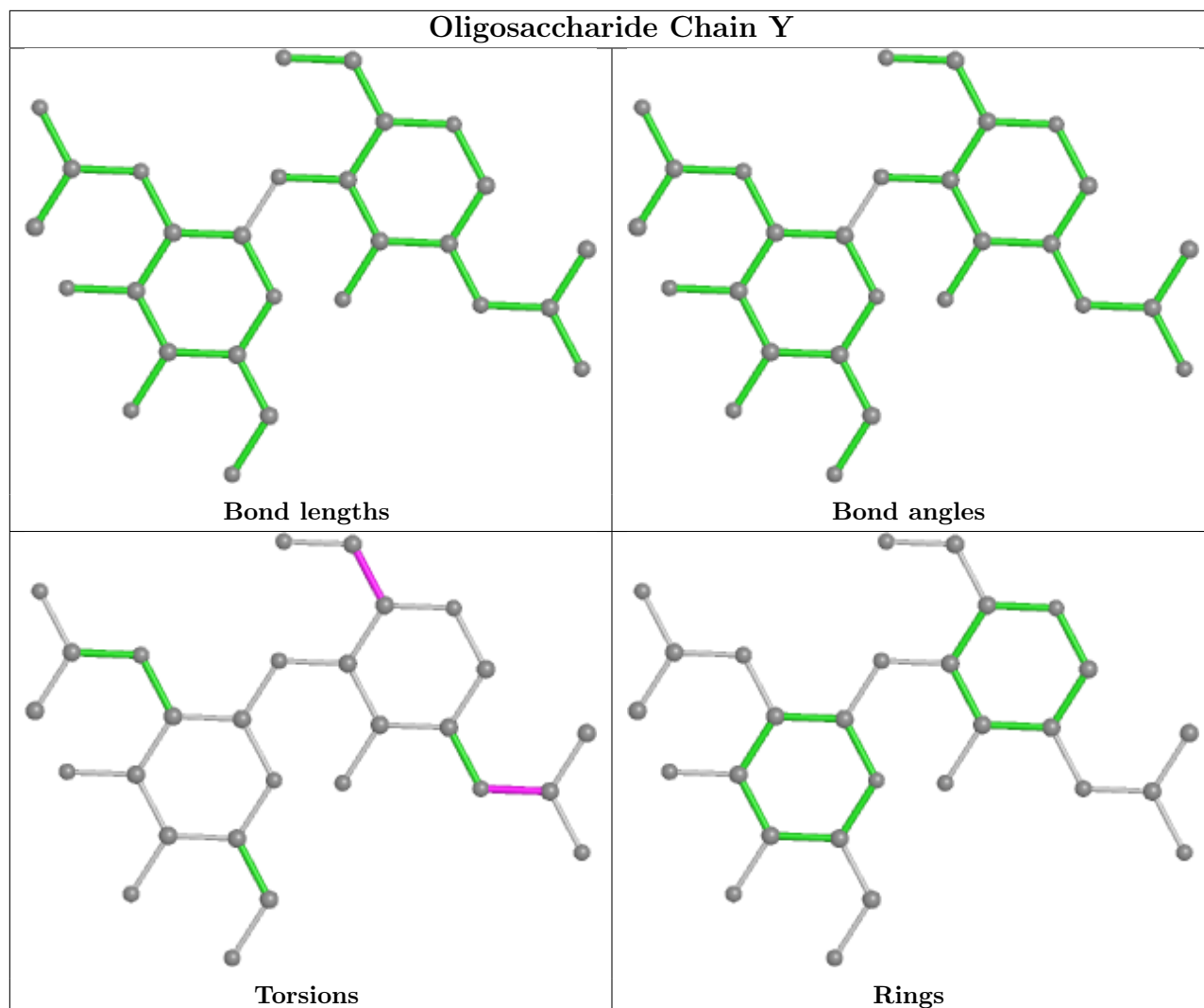












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	$\# Z  > 2$
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	A	1303	1	14,14,15	0.48	0	17,19,21	0.59	0
4	NAG	B	1308	1	14,14,15	0.69	1 (7%)	17,19,21	0.57	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	C	1307	1	14,14,15	0.97	2 (14%)	17,19,21	0.80	1 (5%)
4	NAG	C	1305	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	B	1301	1	14,14,15	0.17	0	17,19,21	0.56	0
4	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	C	1301	1	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
4	NAG	C	1306	1	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	E	702	2	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	B	1309	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	B	1306	1	14,14,15	0.92	1 (7%)	17,19,21	1.41	1 (5%)
4	NAG	E	701	2	14,14,15	0.92	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	E	703	2	14,14,15	0.58	0	17,19,21	1.30	1 (5%)
4	NAG	B	1302	1	14,14,15	0.75	1 (7%)	17,19,21	0.53	0
4	NAG	A	1302	1	14,14,15	0.42	0	17,19,21	0.59	0
4	NAG	C	1302	1	14,14,15	0.44	0	17,19,21	0.64	0
4	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	1304	1	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	C	1303	1	14,14,15	0.32	0	17,19,21	0.82	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
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	702	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	E	701	2	-	1/6/23/26	0/1/1/1
4	NAG	E	703	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1306	NAG	O5-C1	3.32	1.49	1.43
4	E	701	NAG	O5-C1	2.67	1.48	1.43
4	B	1302	NAG	O5-C1	2.66	1.48	1.43
4	C	1307	NAG	O5-C1	2.66	1.48	1.43
4	C	1307	NAG	C1-C2	2.34	1.55	1.52
4	B	1308	NAG	O5-C1	-2.27	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1306	NAG	C1-O5-C5	5.49	119.63	112.19
4	E	703	NAG	C2-N2-C7	4.40	129.16	122.90
4	C	1301	NAG	C1-O5-C5	3.74	117.26	112.19
4	C	1303	NAG	C1-O5-C5	2.90	116.12	112.19
4	C	1307	NAG	C1-O5-C5	2.64	115.76	112.19
4	E	701	NAG	C1-O5-C5	2.61	115.72	112.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	E	703	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	E	702	NAG	C8-C7-N2-C2
4	E	702	NAG	O7-C7-N2-C2
4	E	703	NAG	C8-C7-N2-C2
4	E	703	NAG	O7-C7-N2-C2
4	B	1304	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	E	703	NAG	C4-C5-C6-O6
4	A	1301	NAG	C1-C2-N2-C7
4	C	1306	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

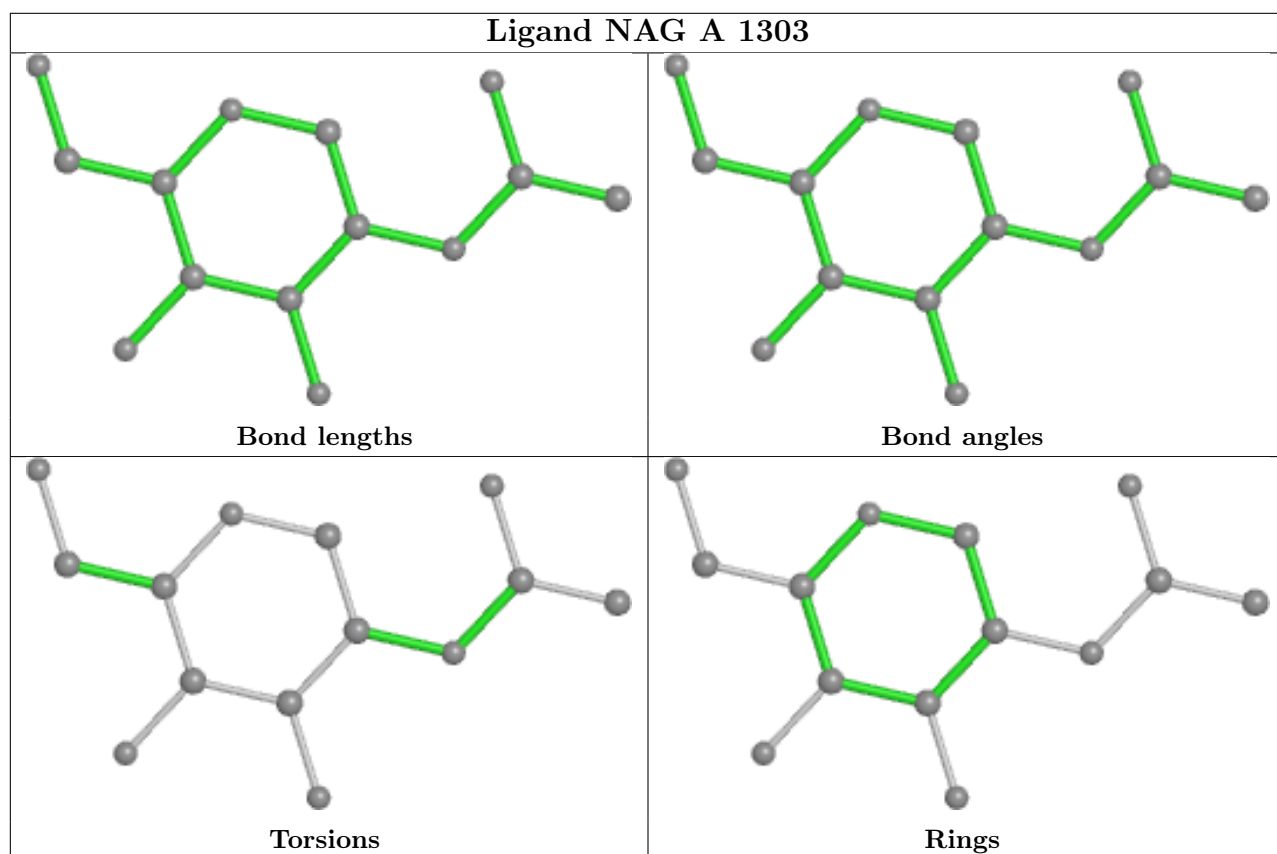
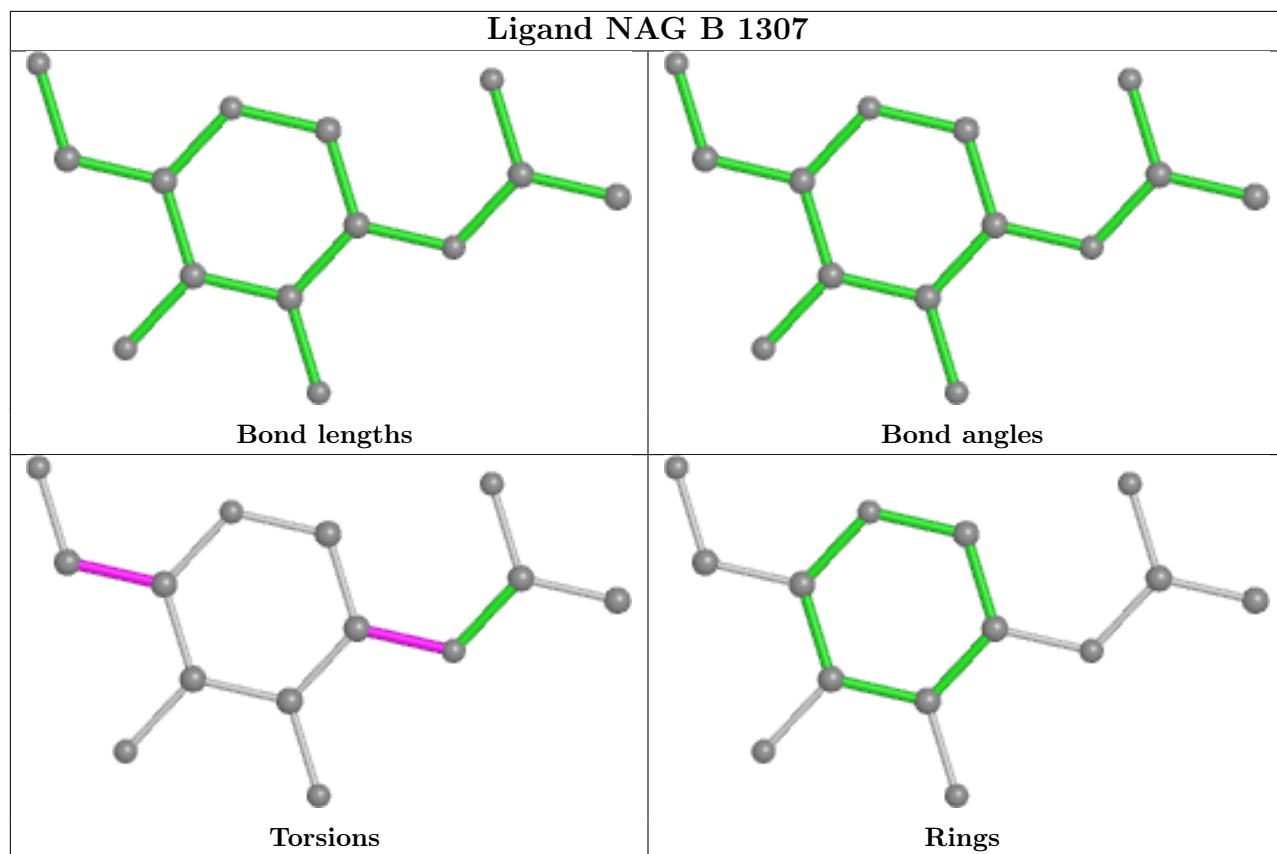
Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	E	703	NAG	C3-C2-N2-C7
4	B	1309	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7

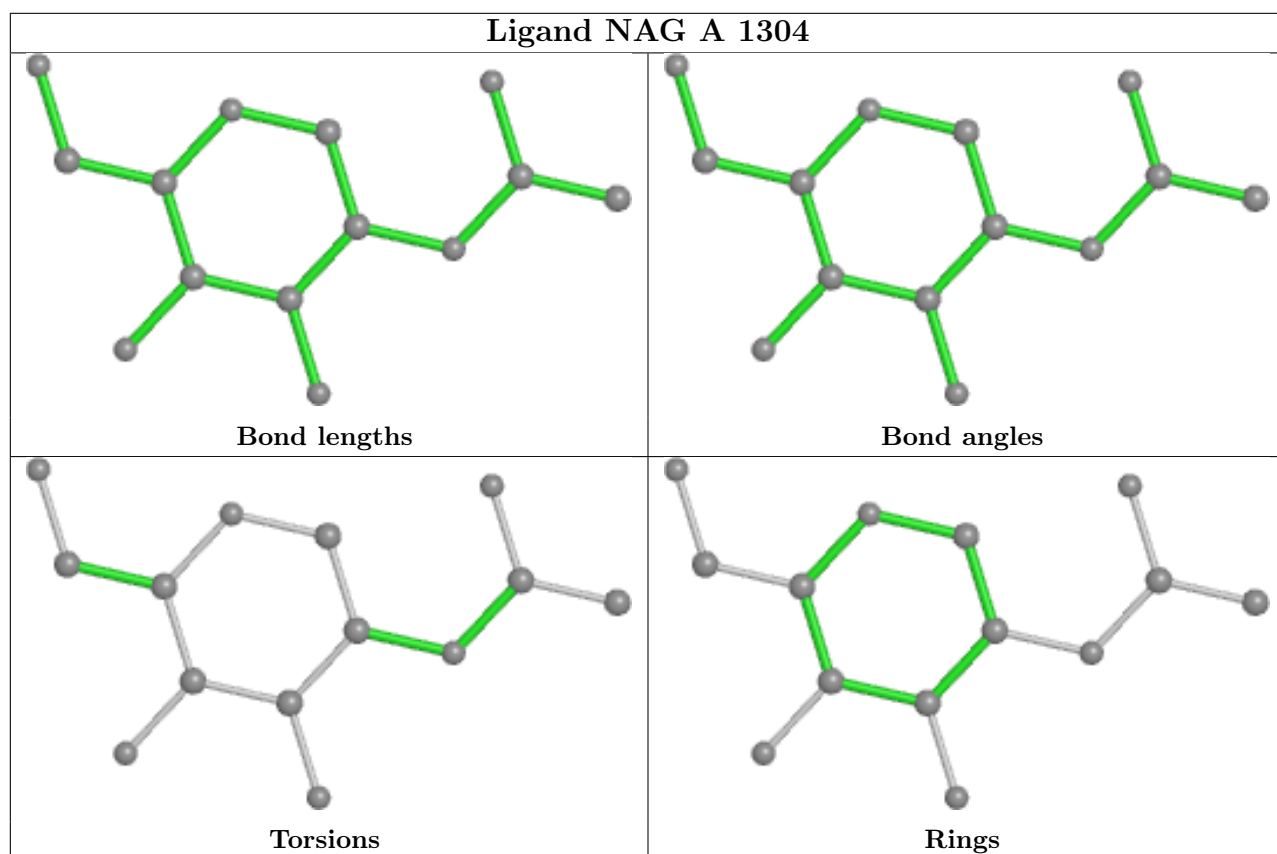
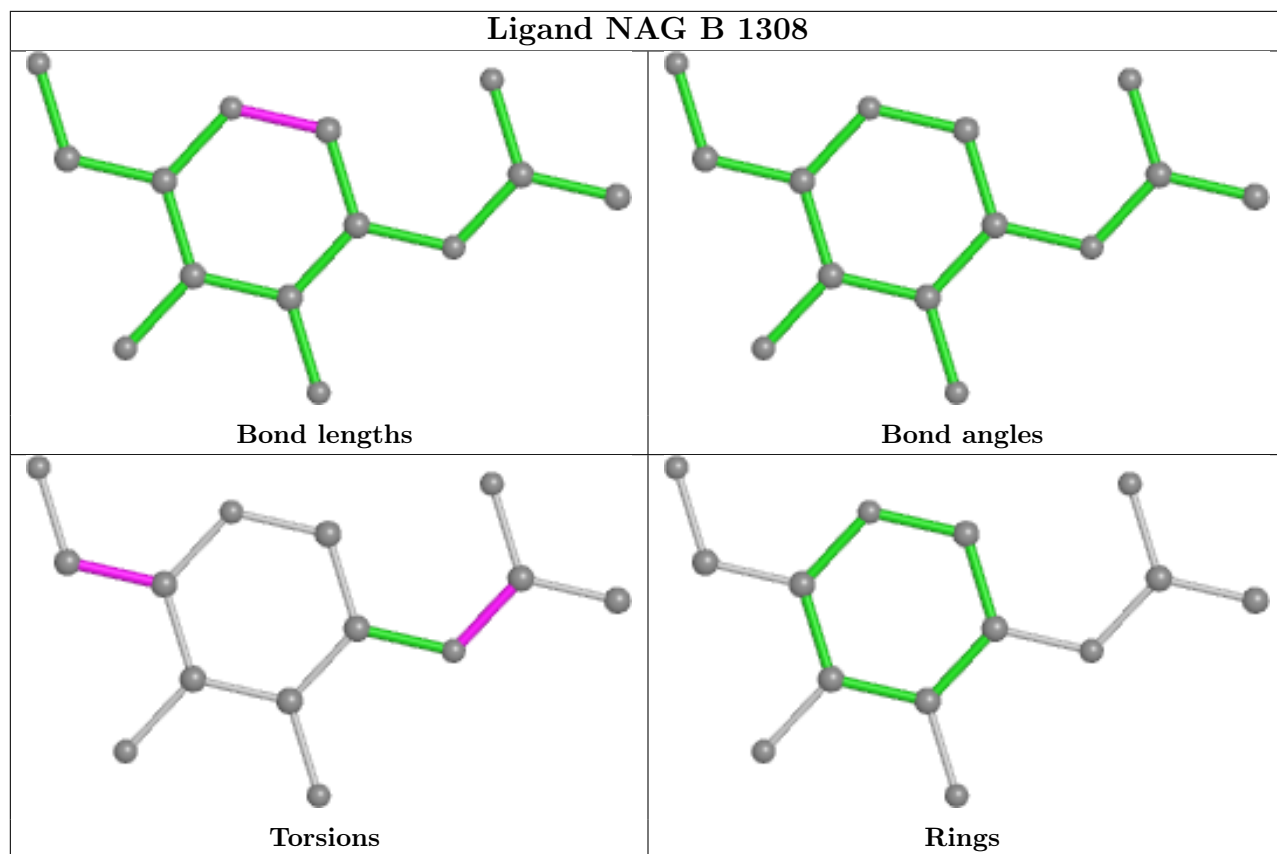
There are no ring outliers.

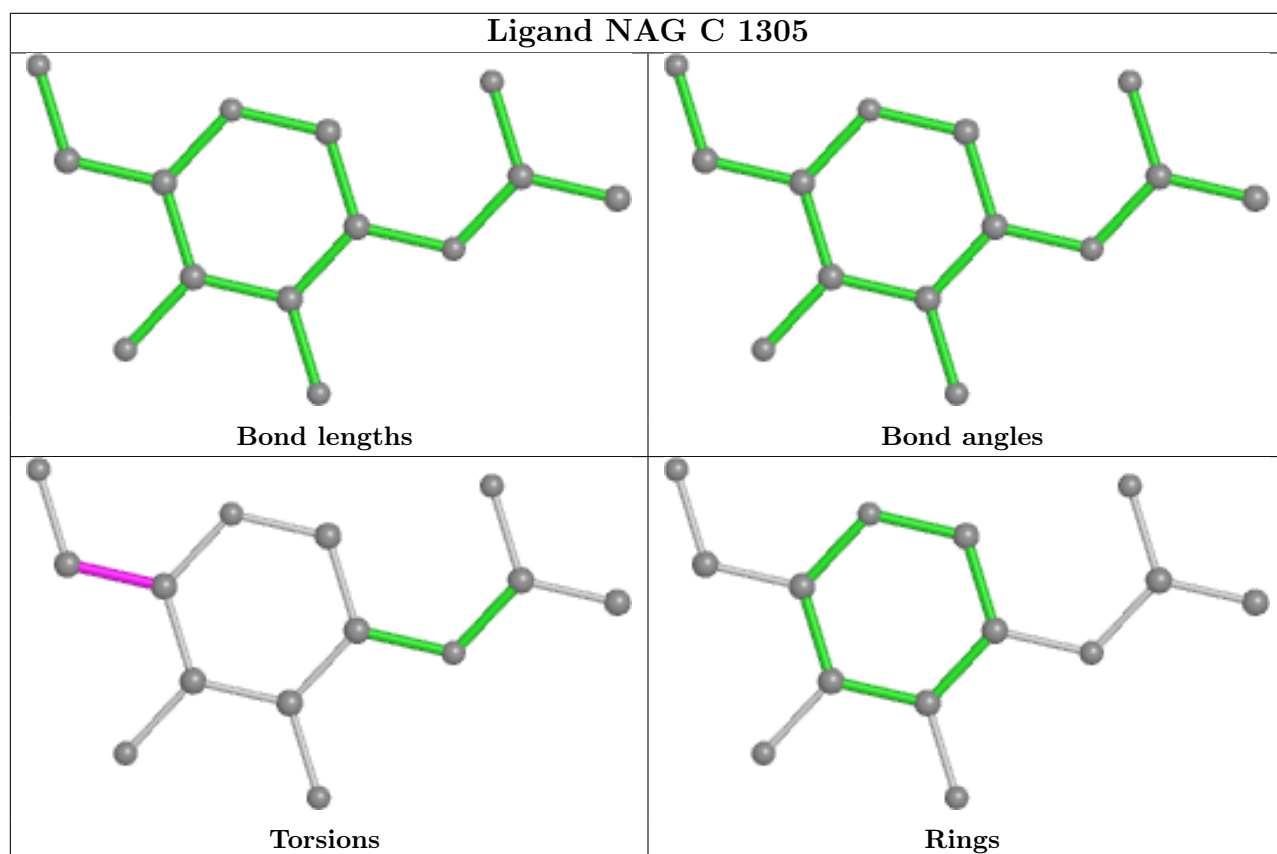
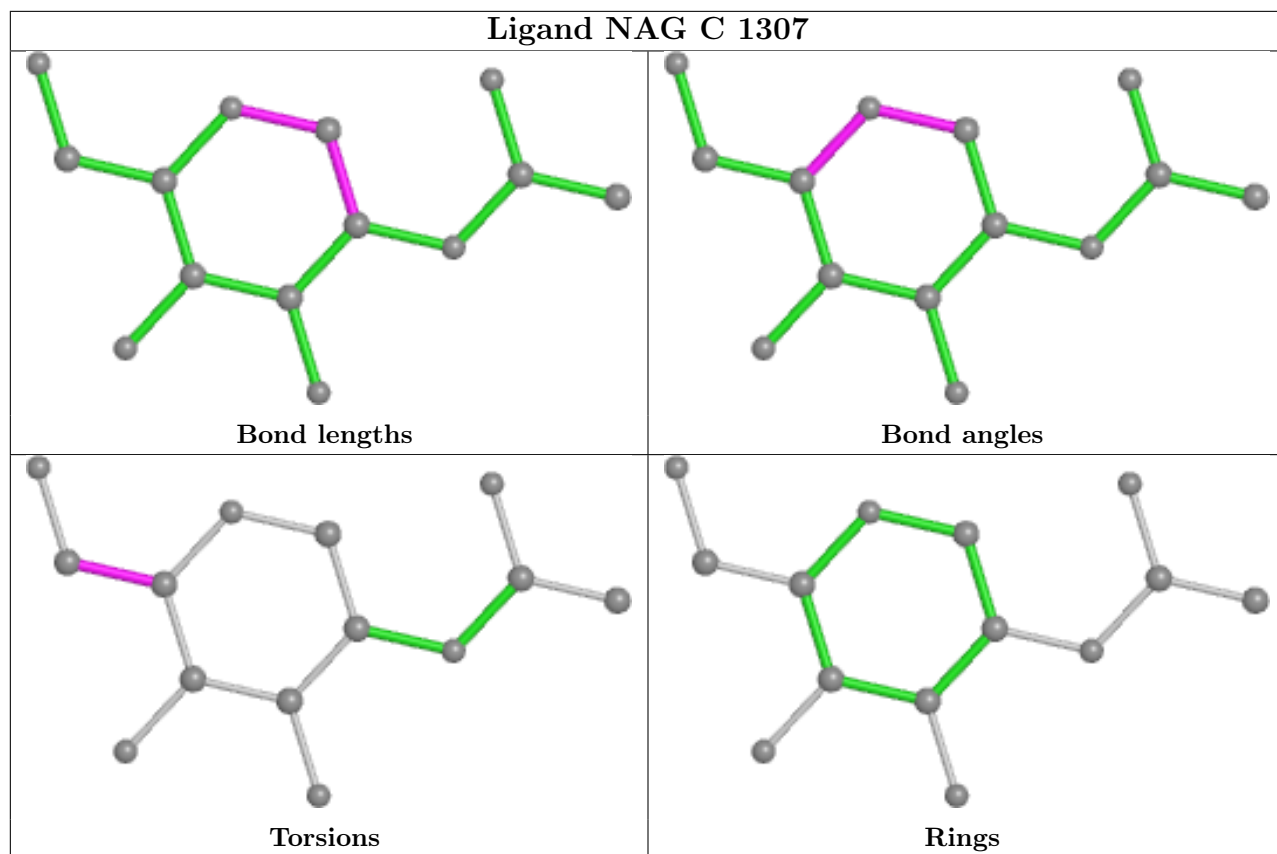
7 monomers are involved in 13 short contacts:

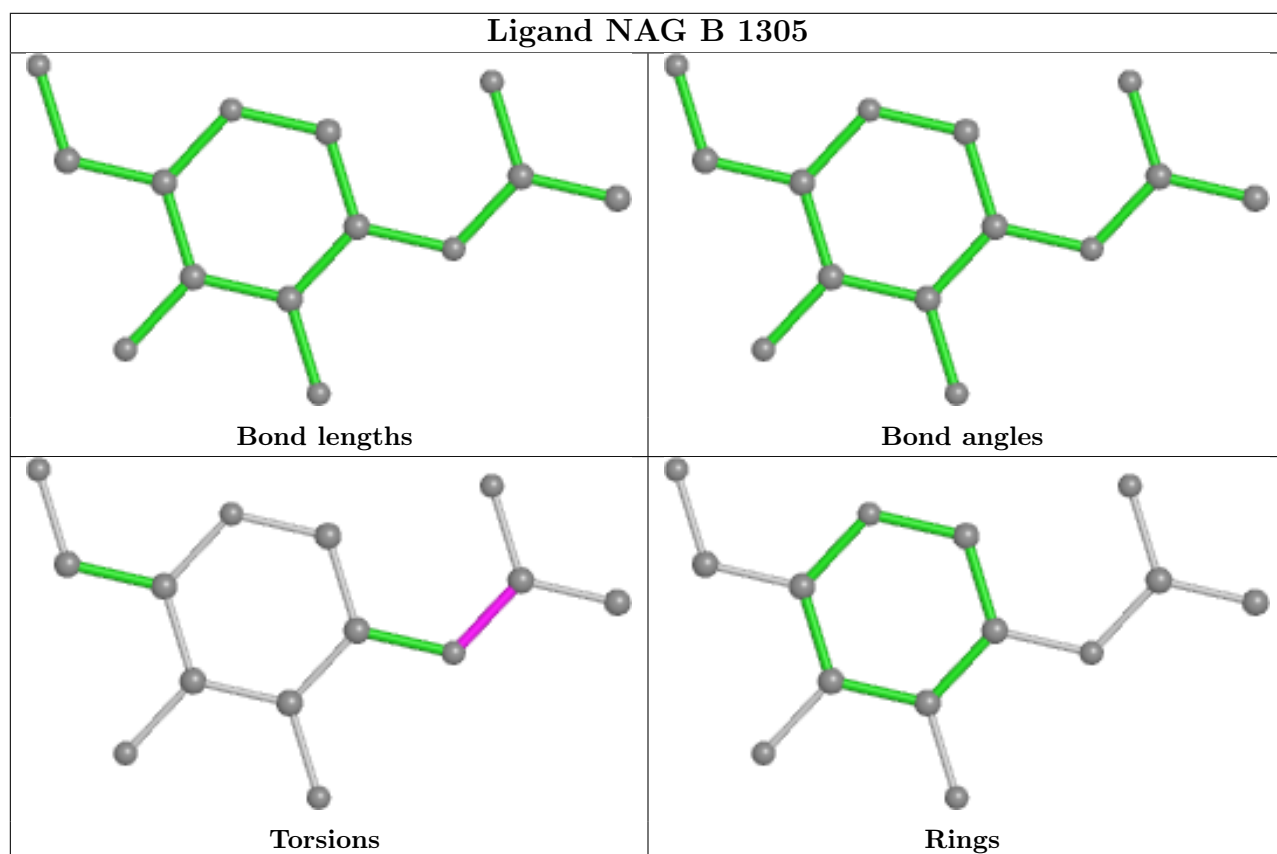
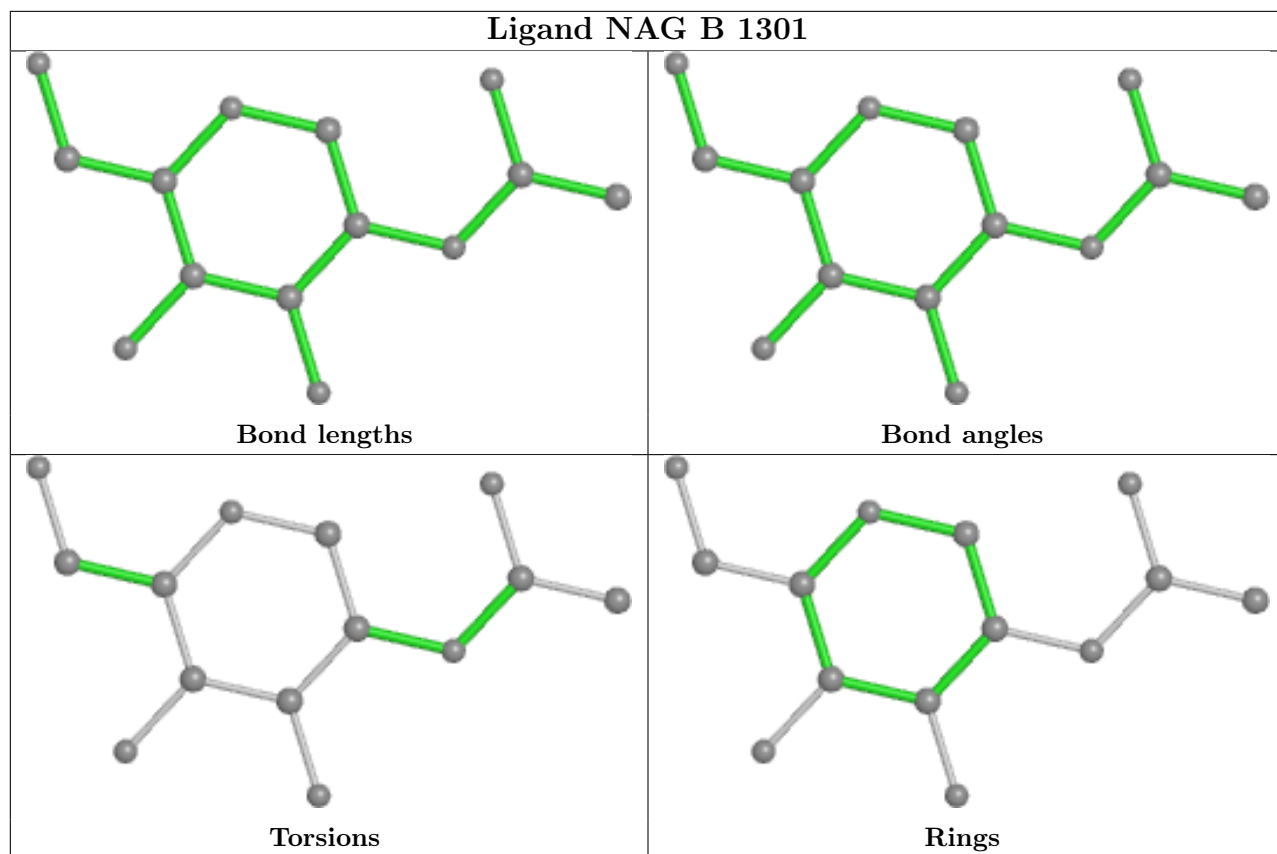
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	NAG	1	0
4	C	1307	NAG	2	0
4	C	1305	NAG	2	0
4	B	1303	NAG	1	0
4	E	701	NAG	2	0
4	E	703	NAG	3	0
4	C	1303	NAG	2	0

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

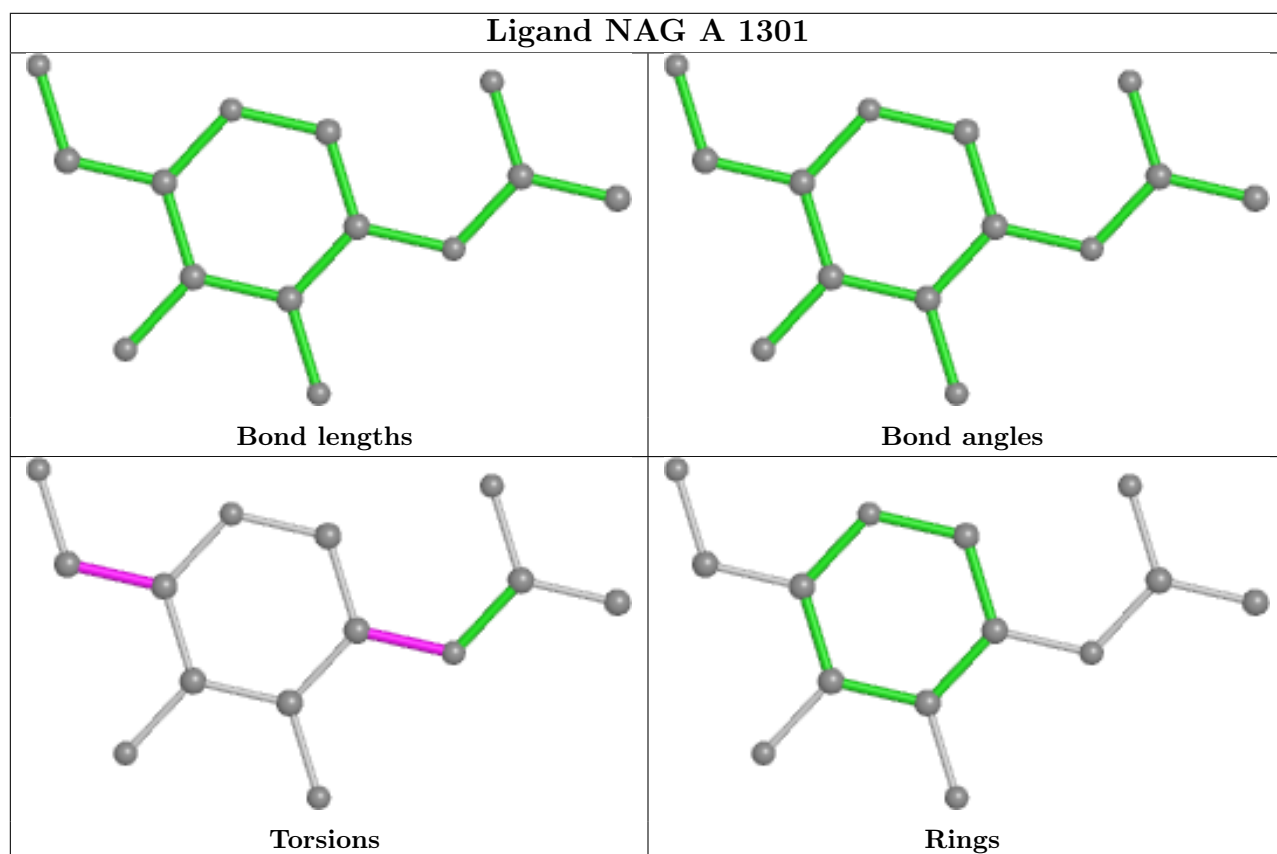
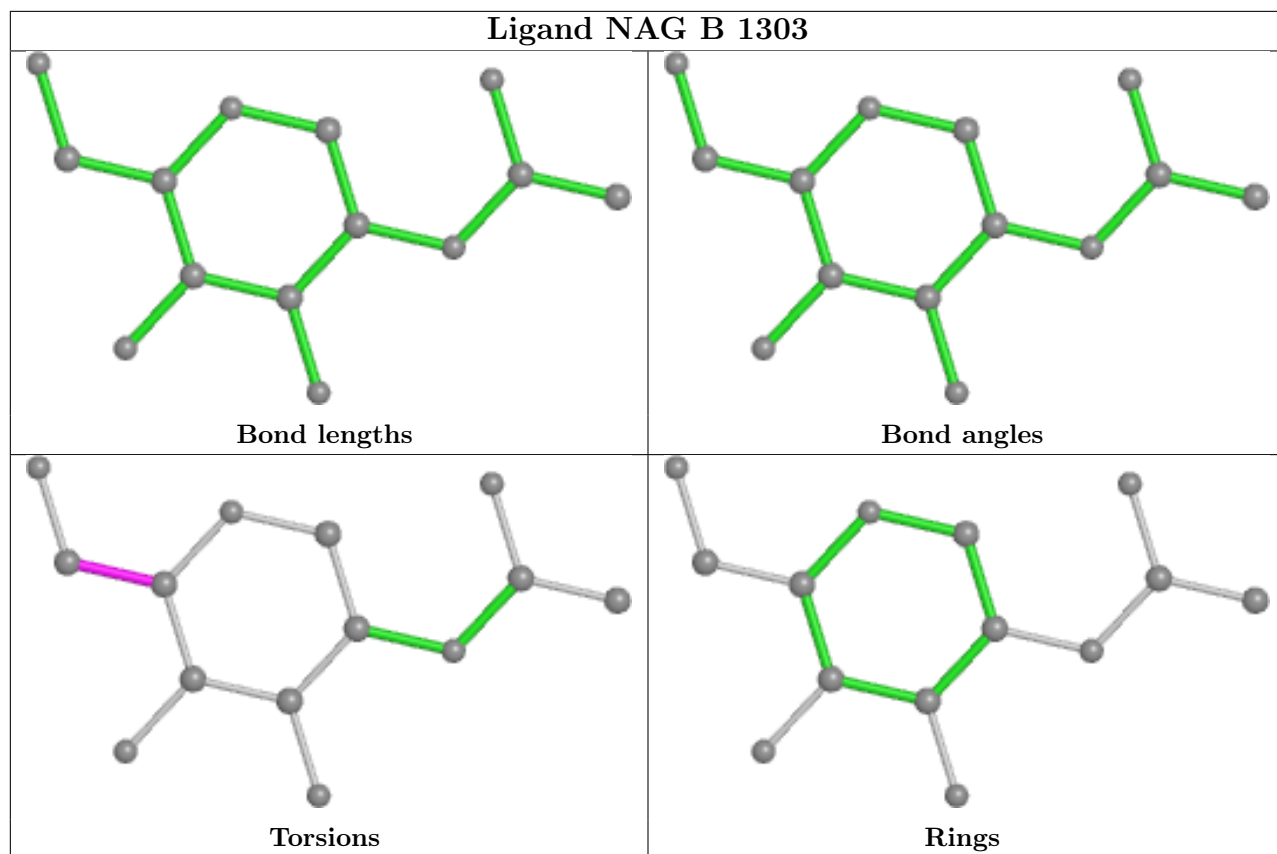


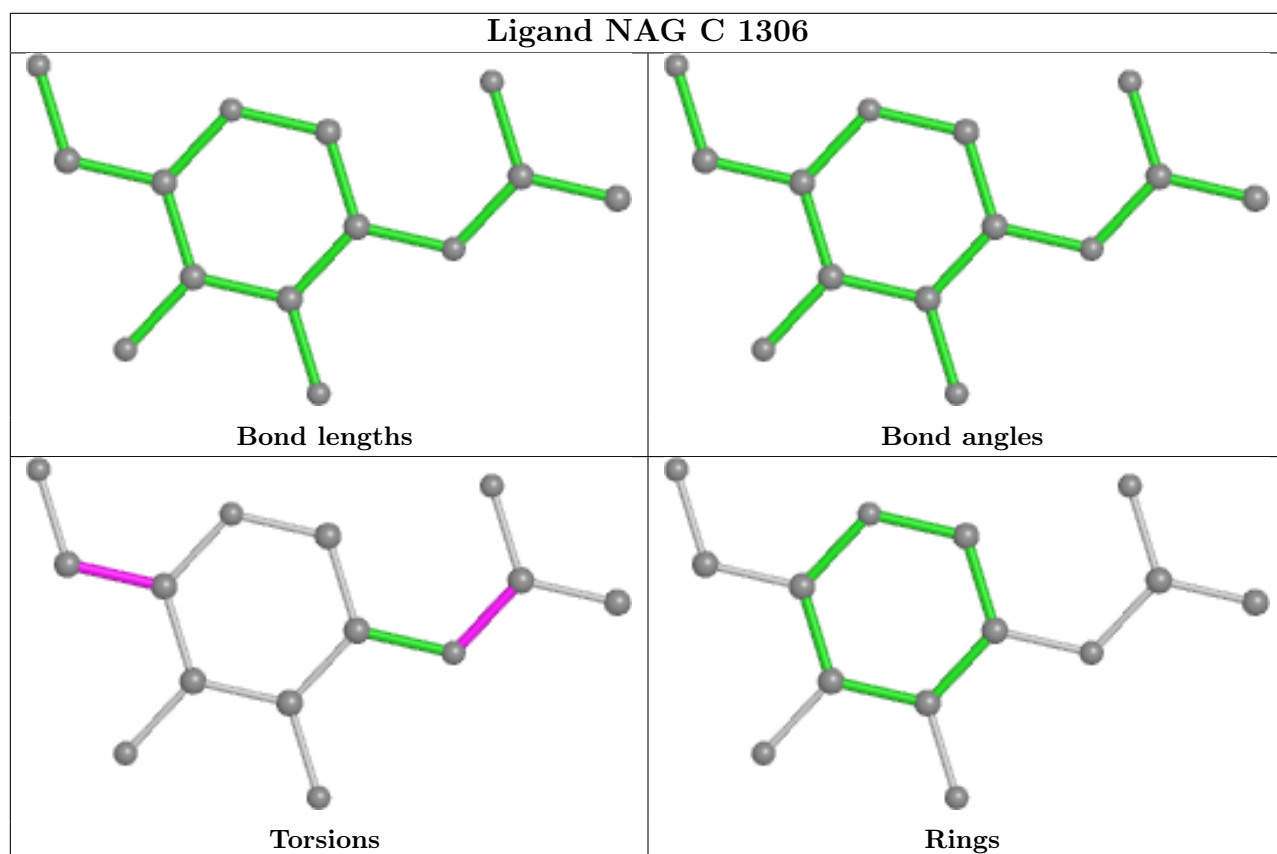
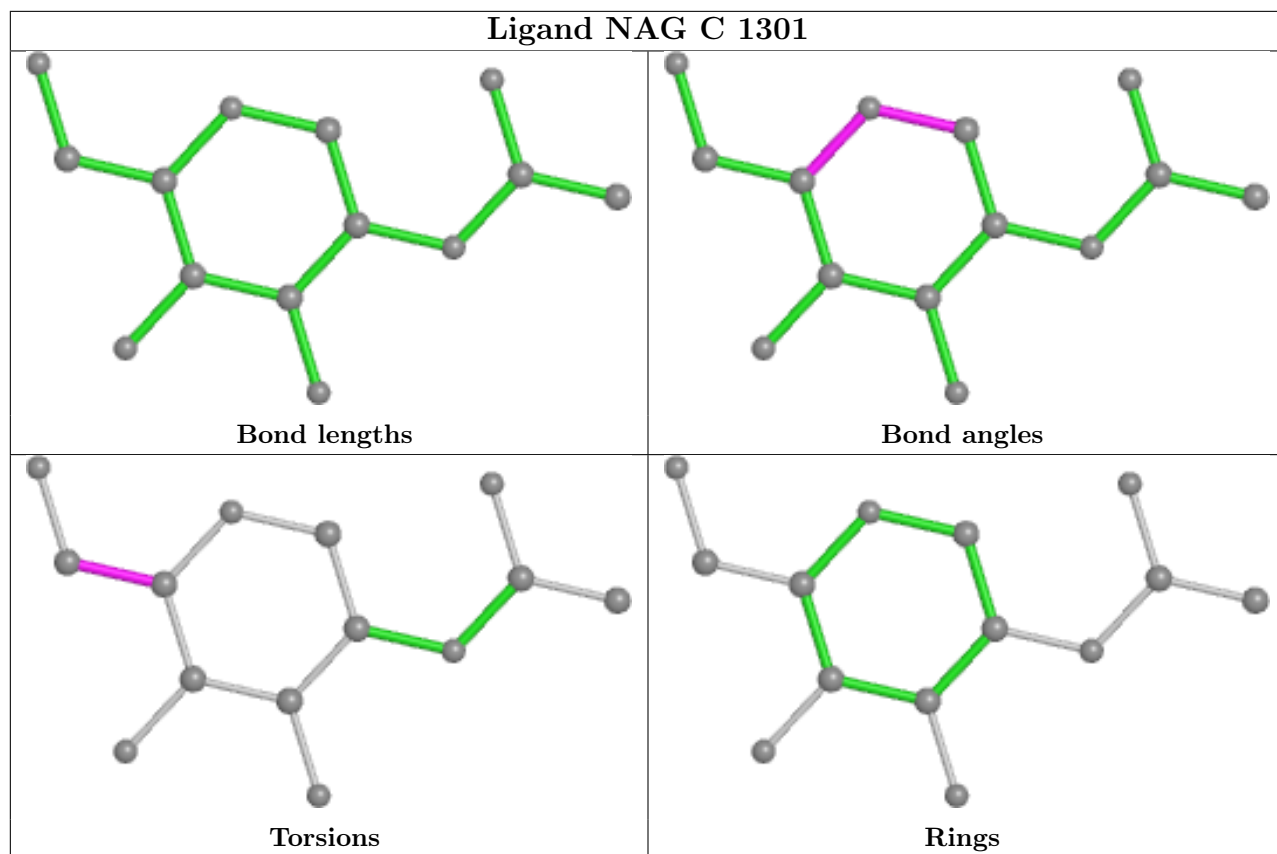


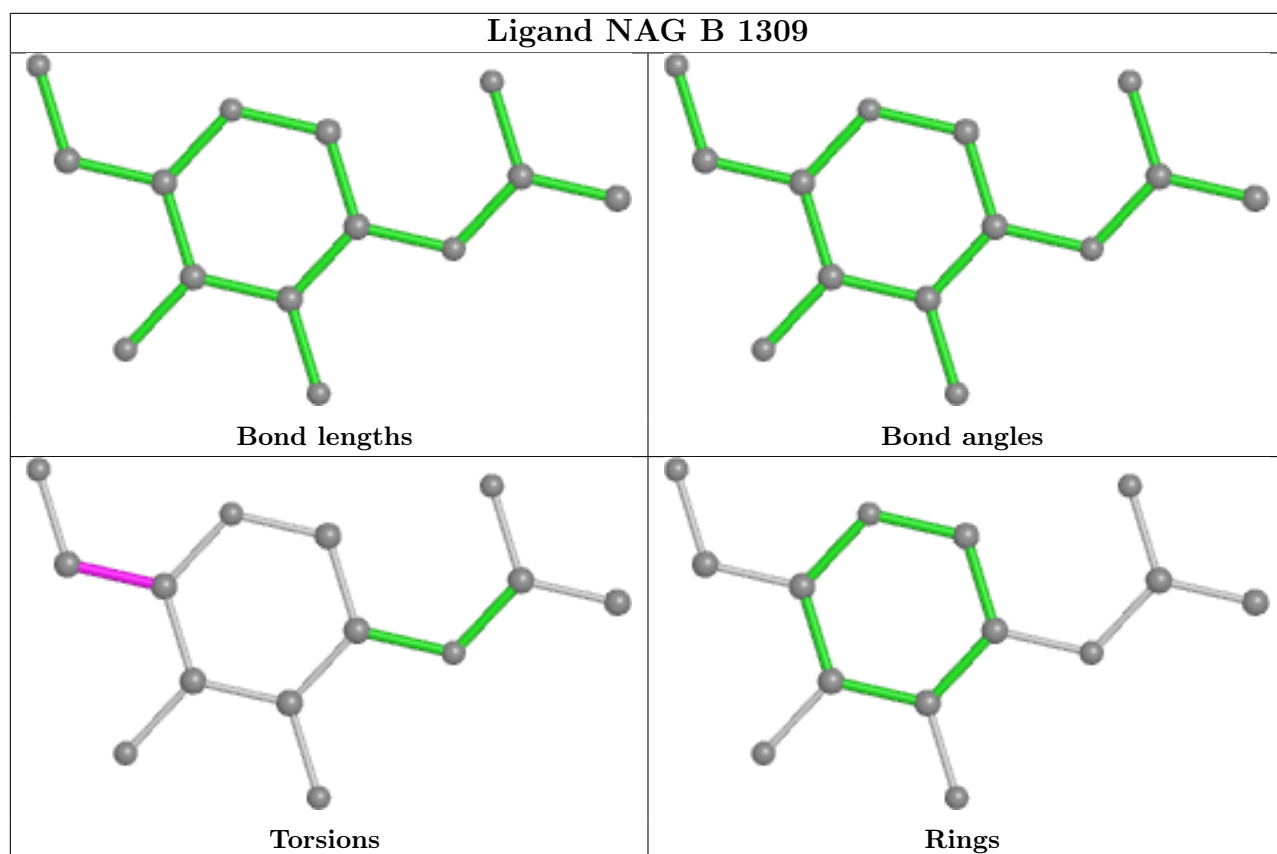
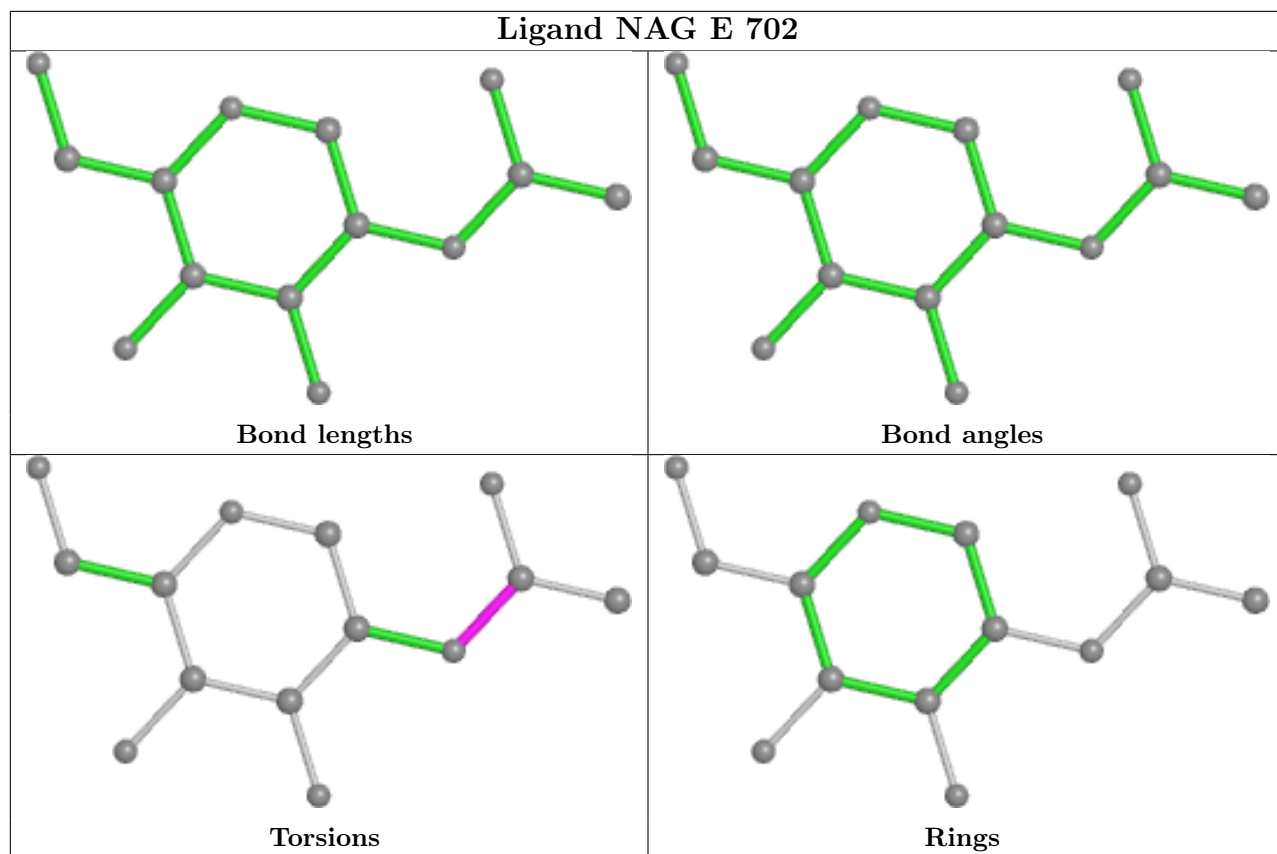


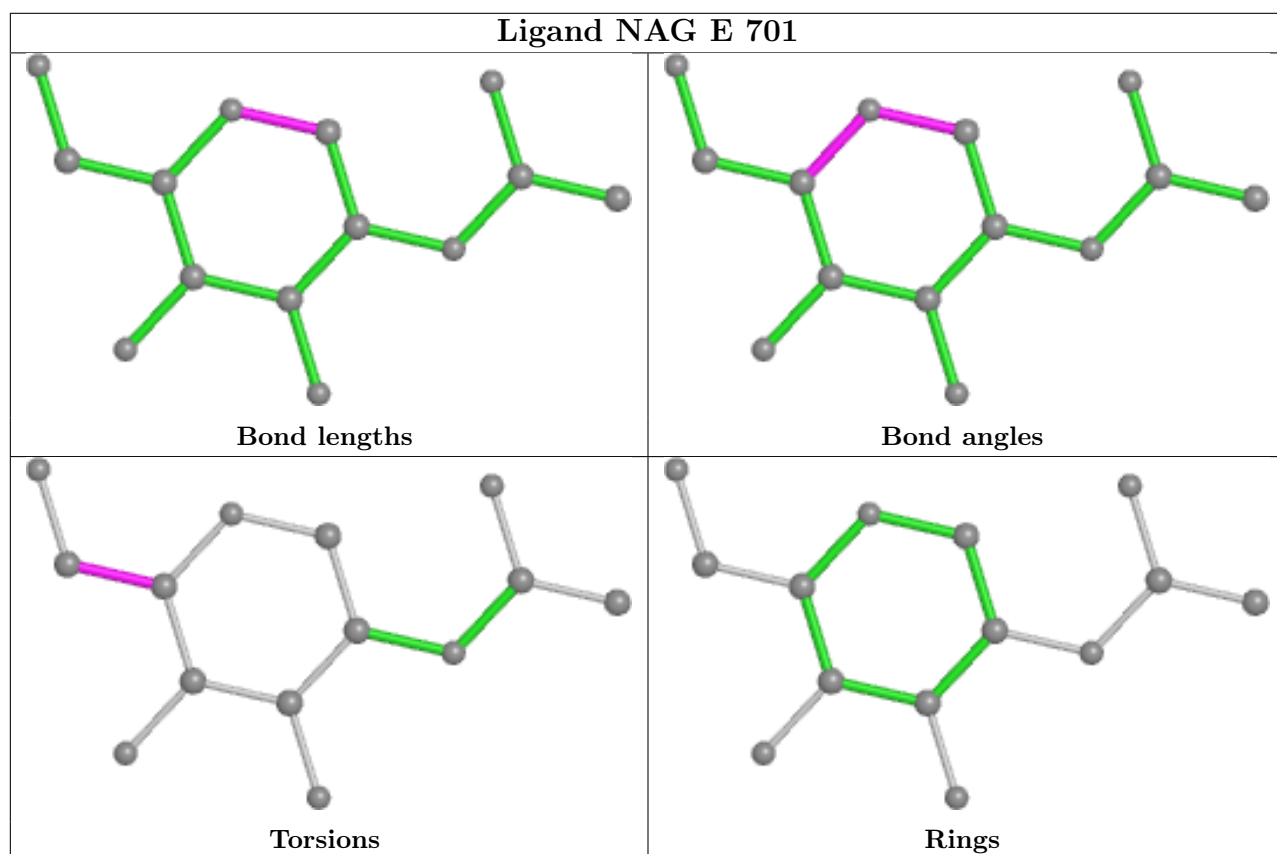
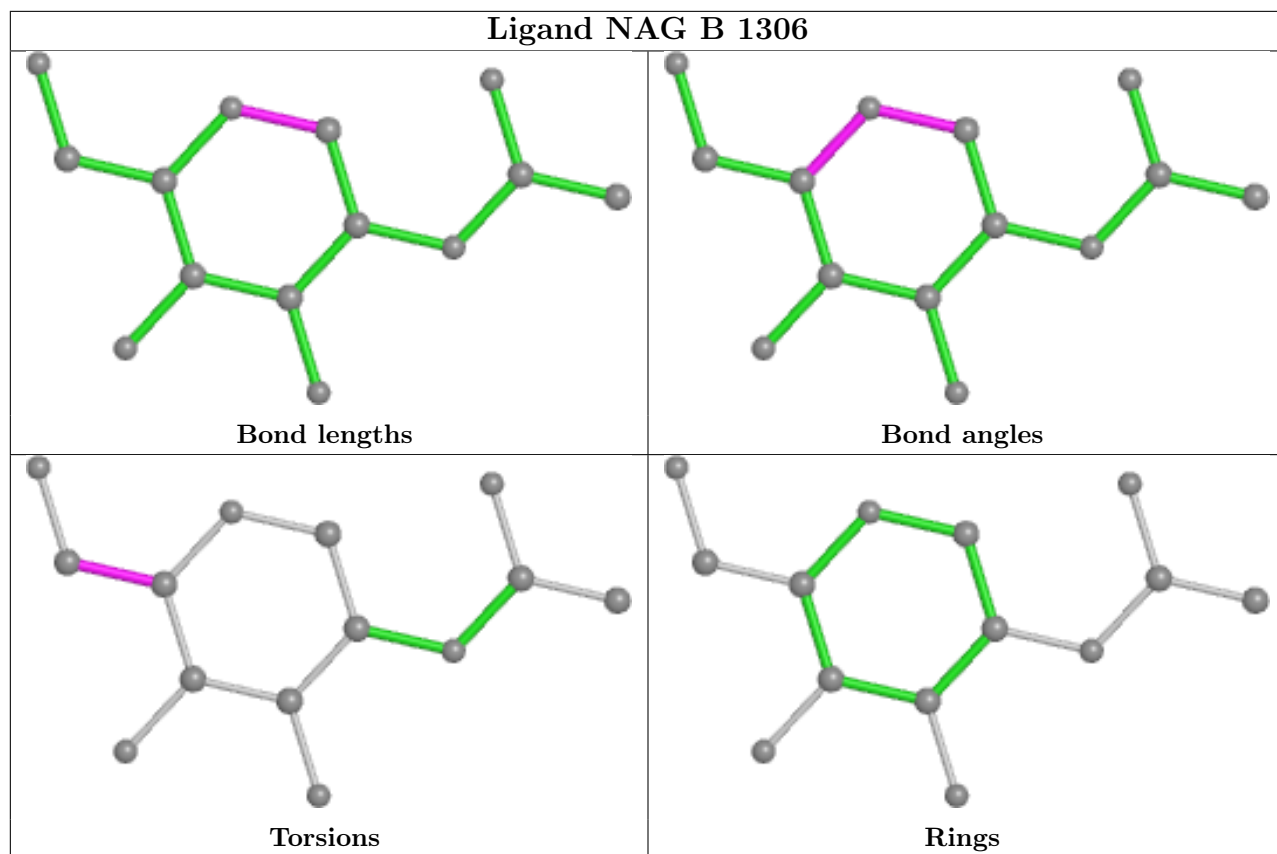


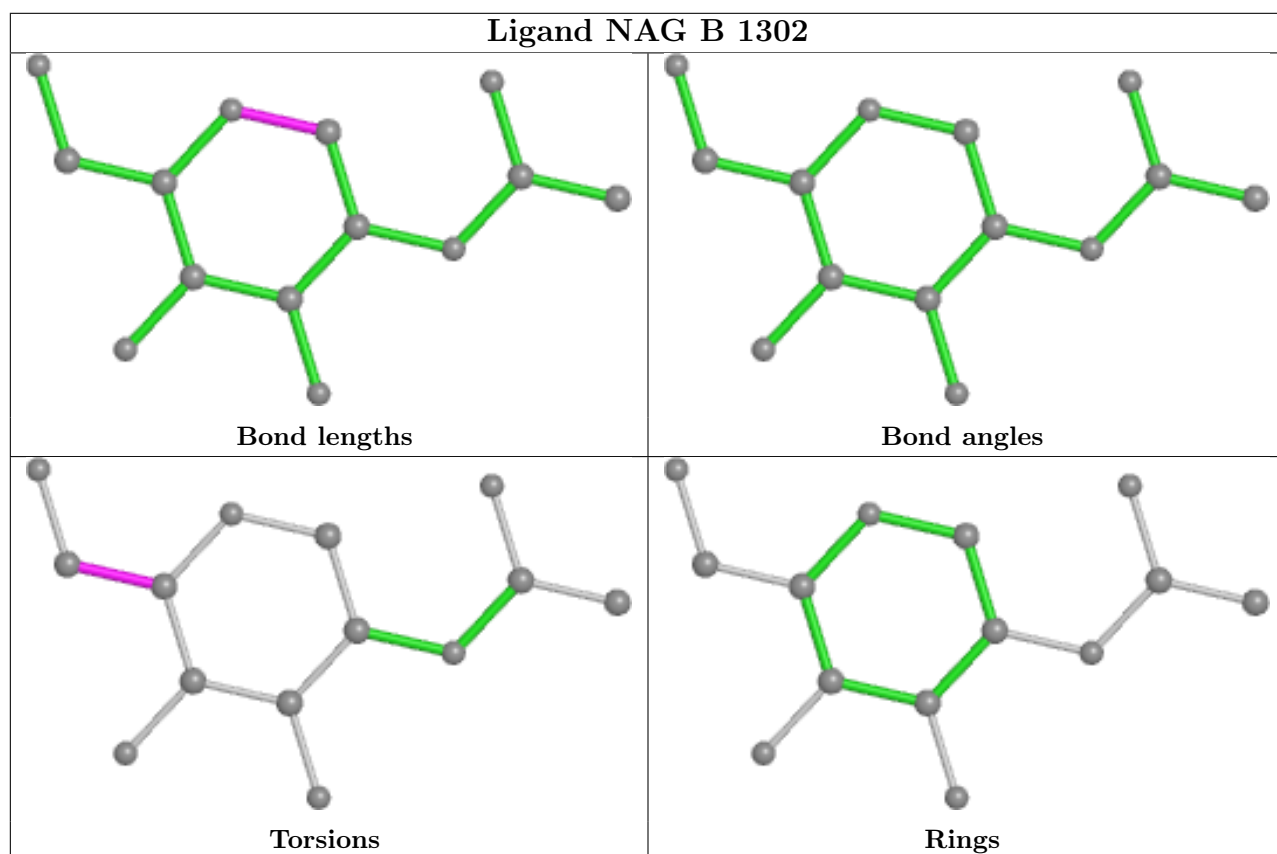
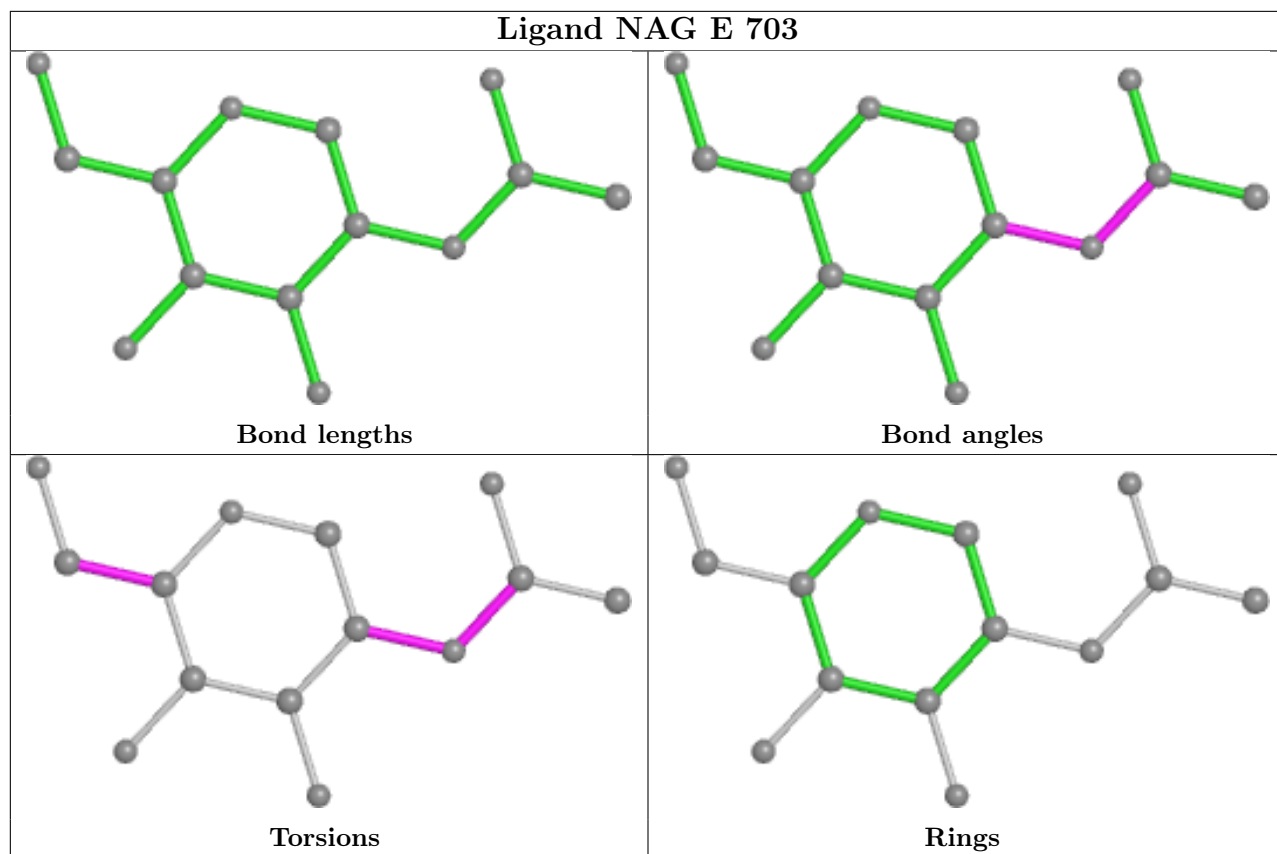


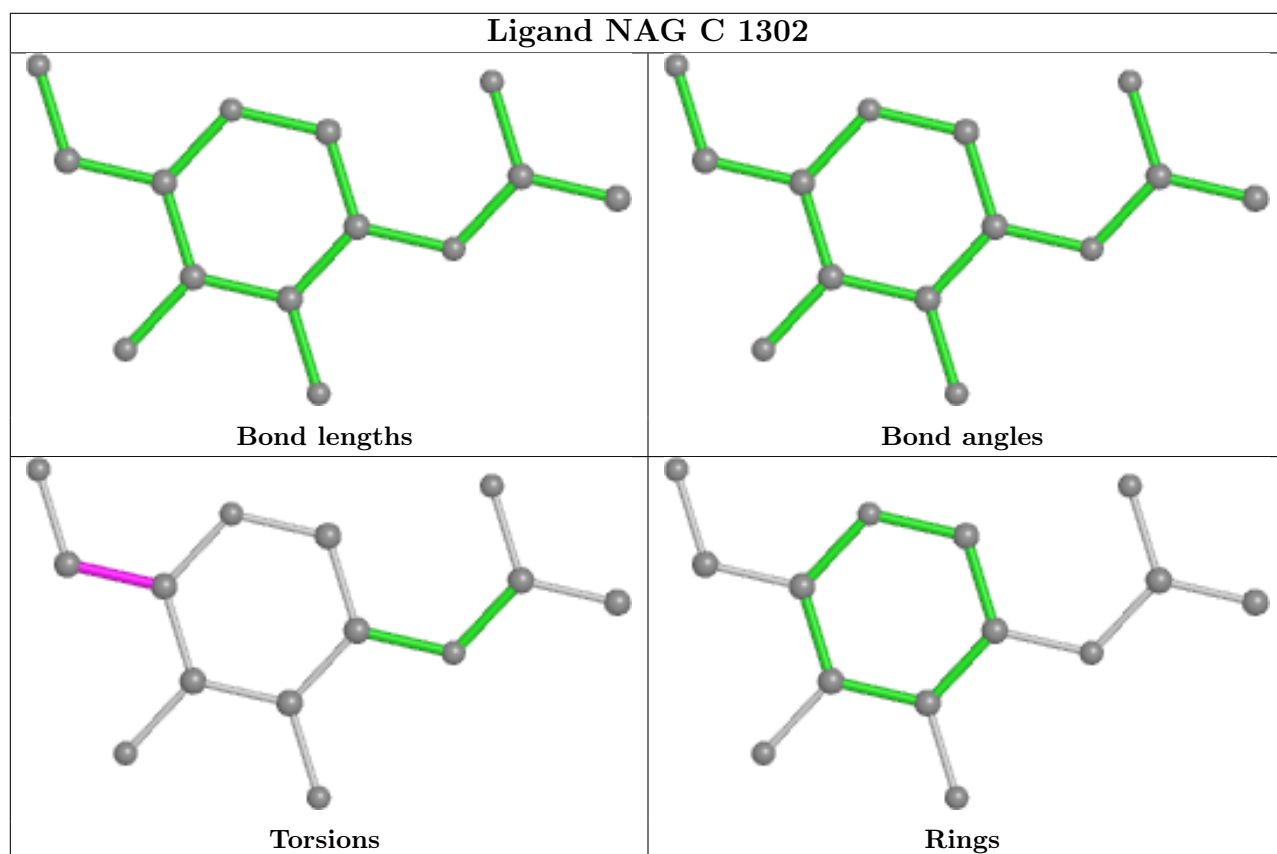
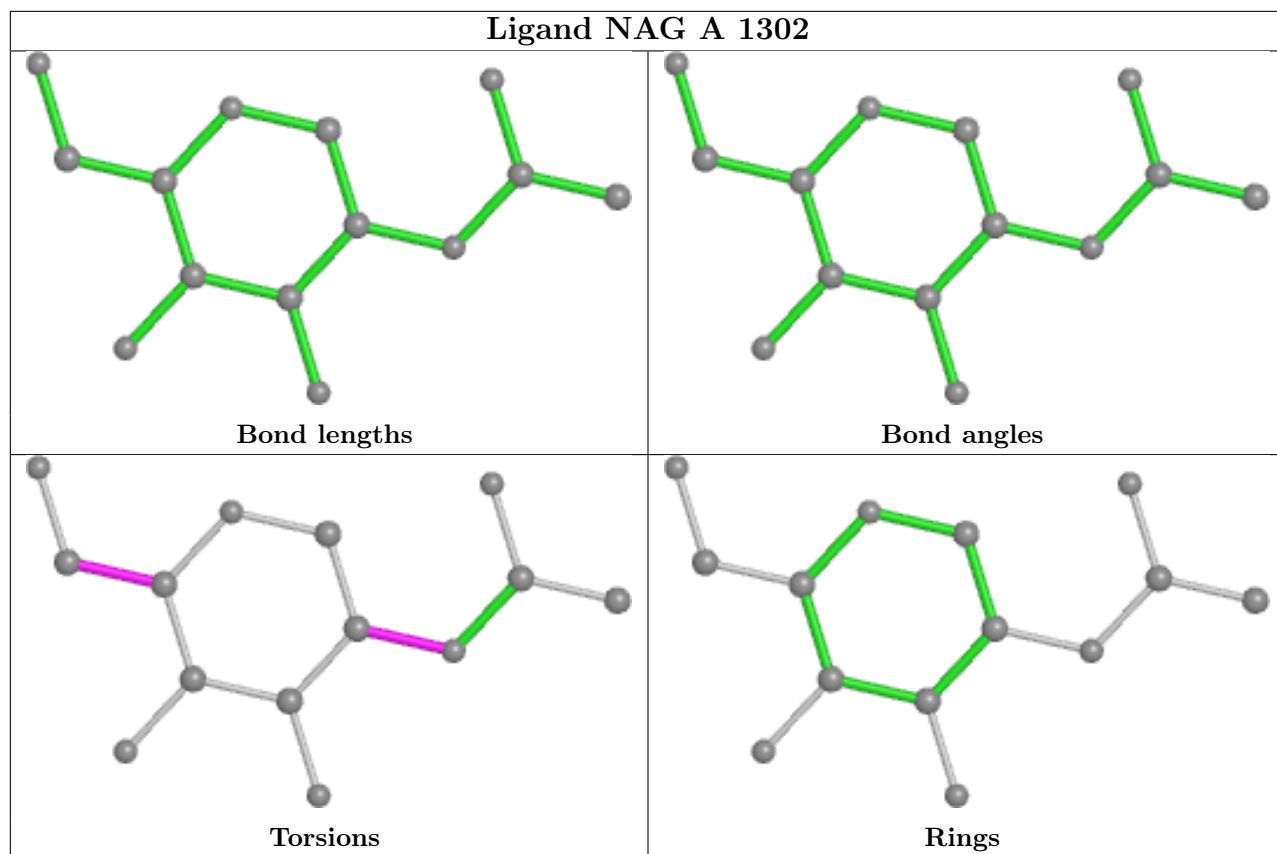


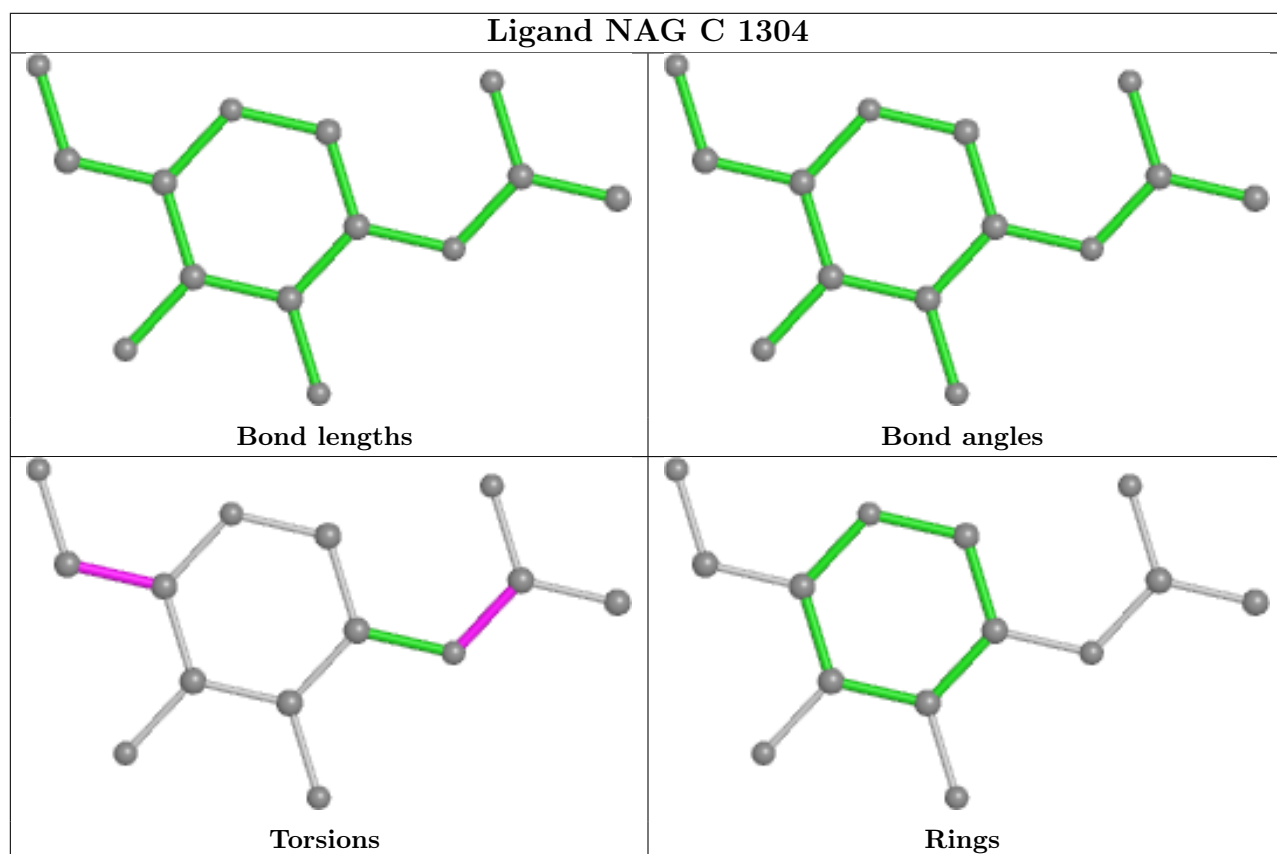
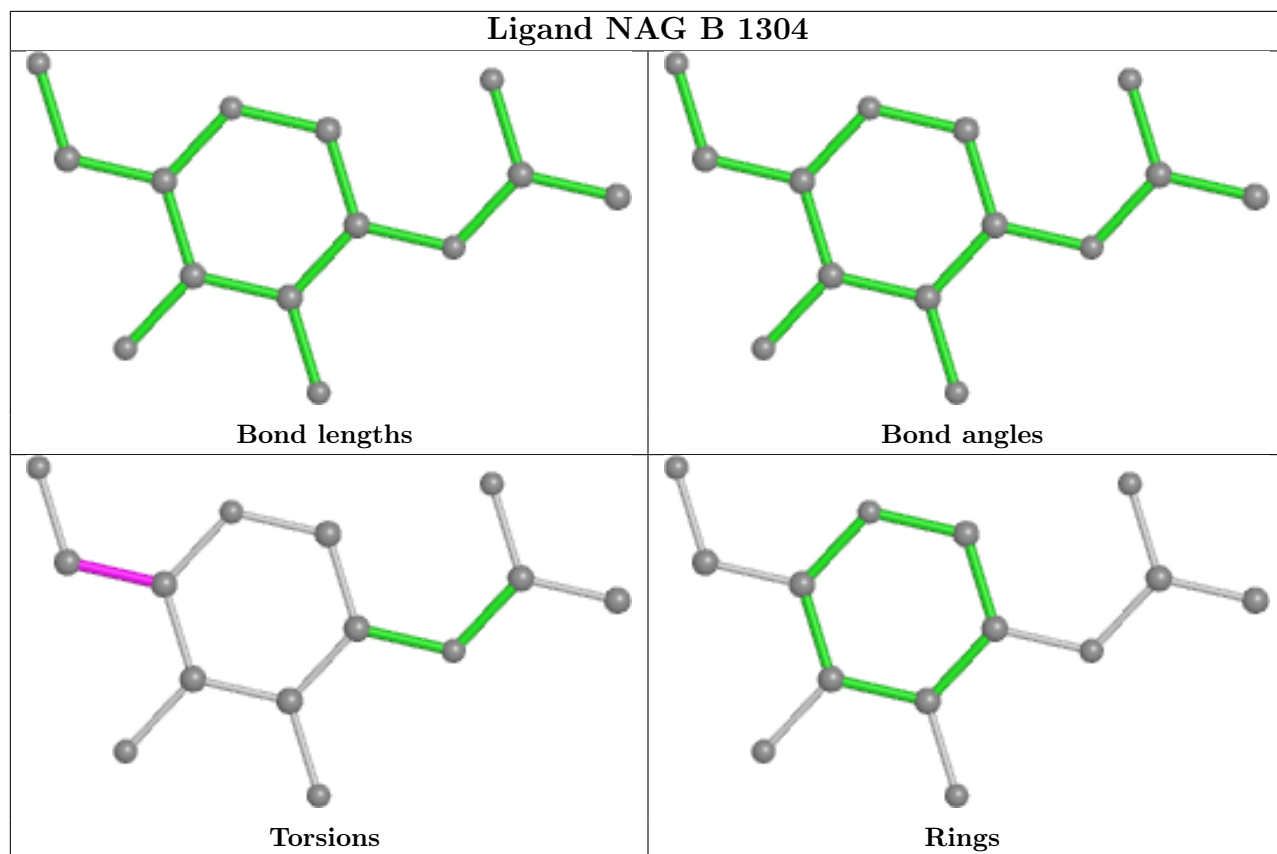


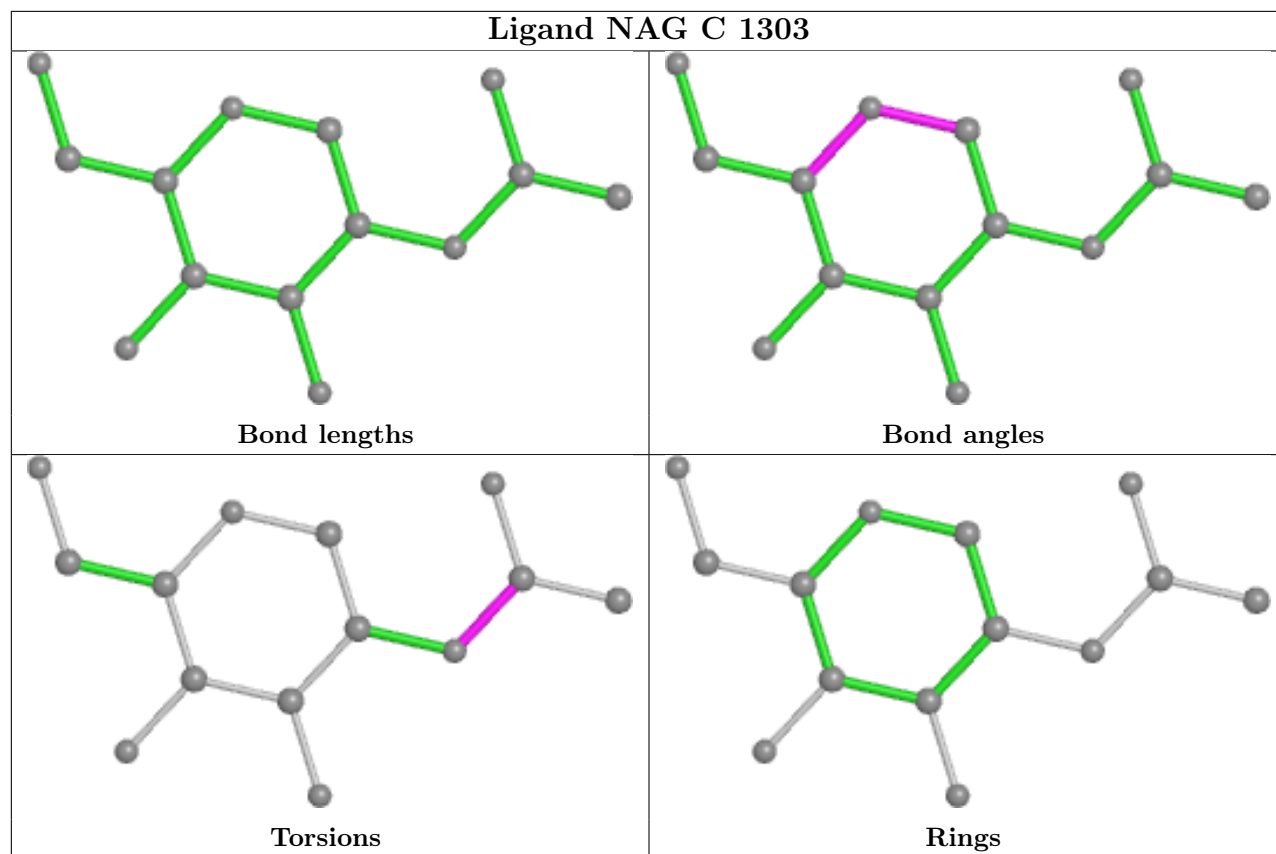












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



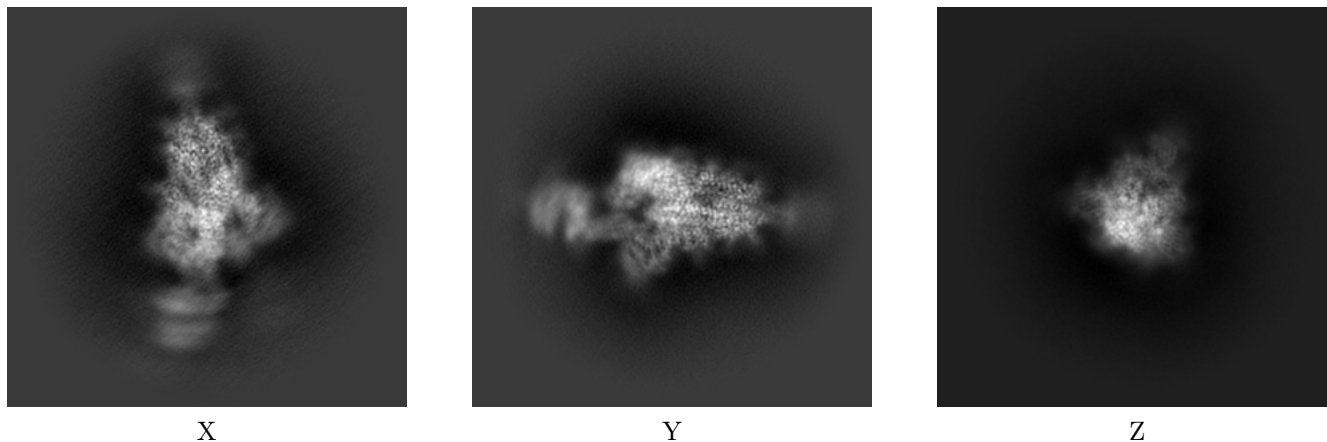
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34729. These allow visual inspection of the internal detail of the map and identification of artifacts.

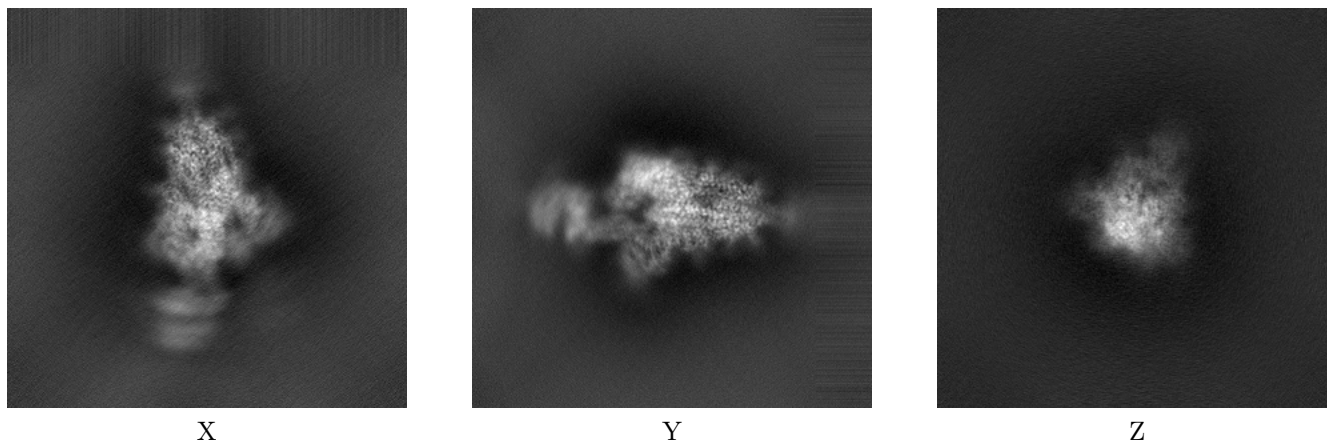
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



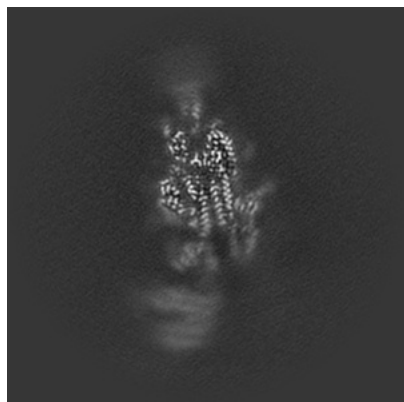
#### 6.1.2 Raw map



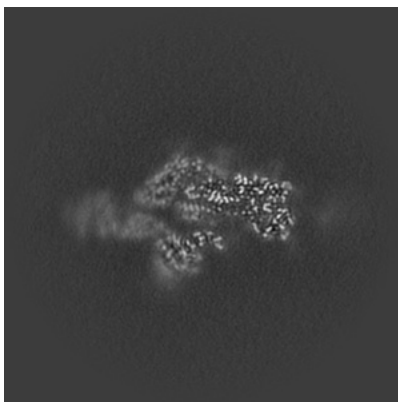
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

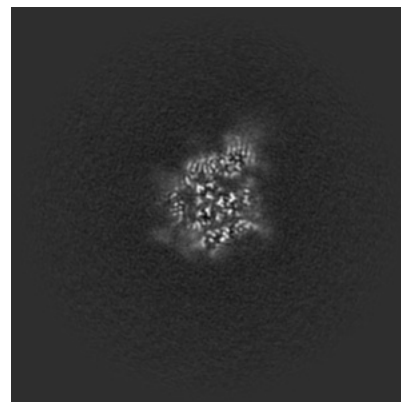
### 6.2.1 Primary map



X Index: 224

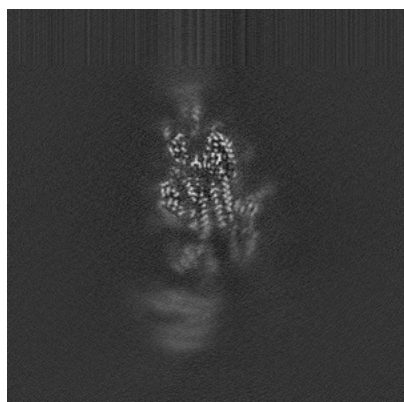


Y Index: 224

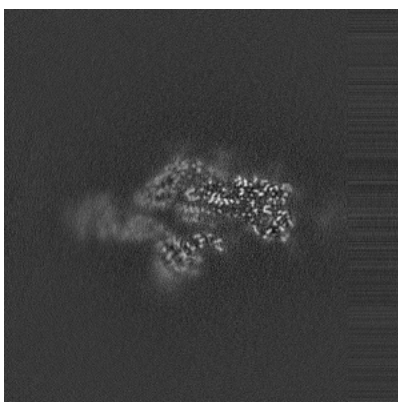


Z Index: 224

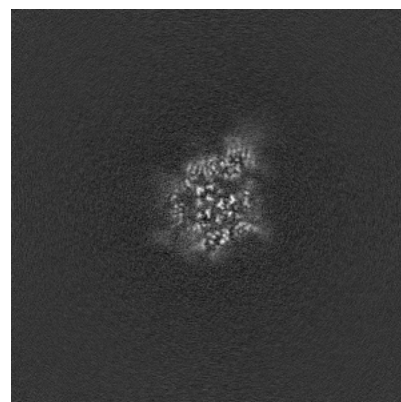
### 6.2.2 Raw map



X Index: 224



Y Index: 224

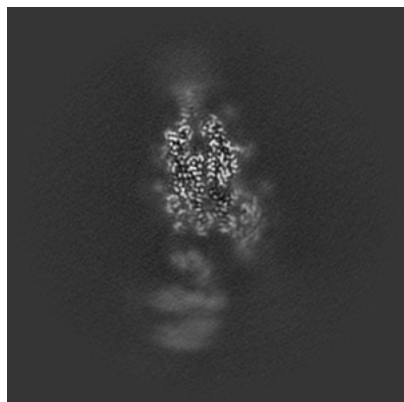


Z Index: 224

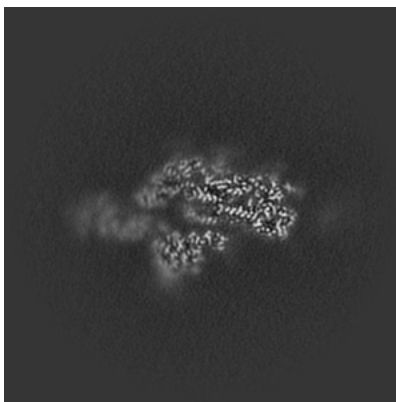
The images above show central slices of the map in three orthogonal directions.

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

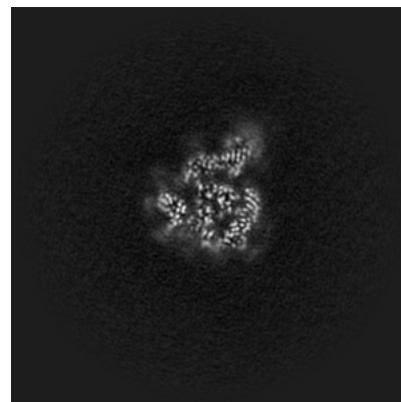
### 6.3.1 Primary map



X Index: 216

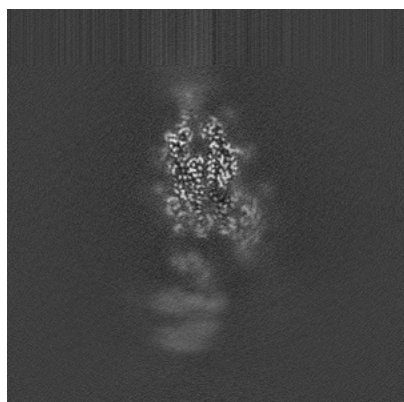


Y Index: 228

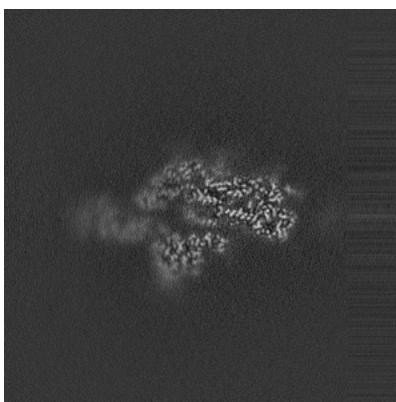


Z Index: 218

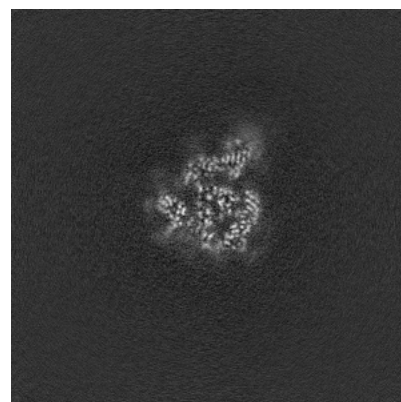
### 6.3.2 Raw map



X Index: 216



Y Index: 228

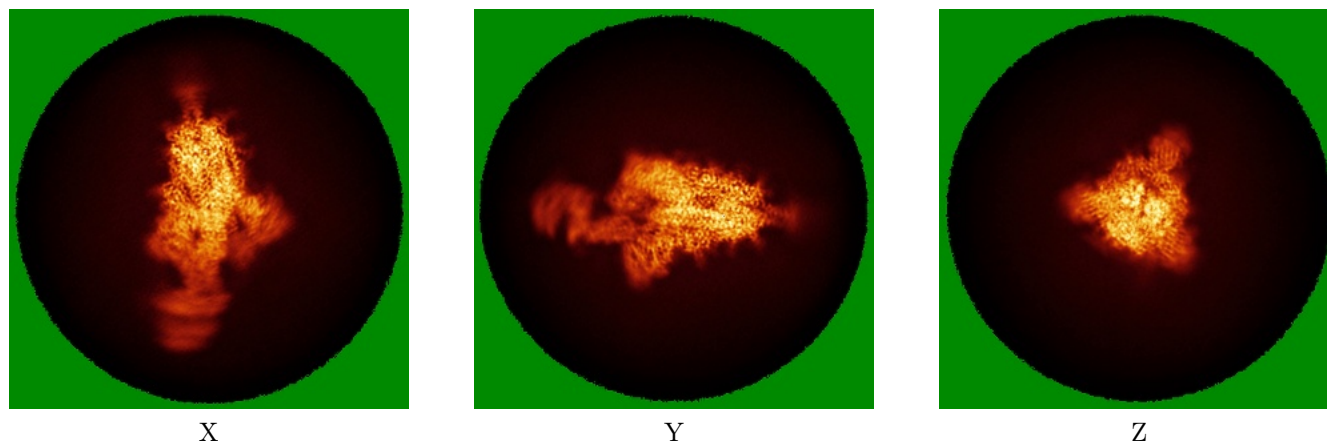


Z Index: 218

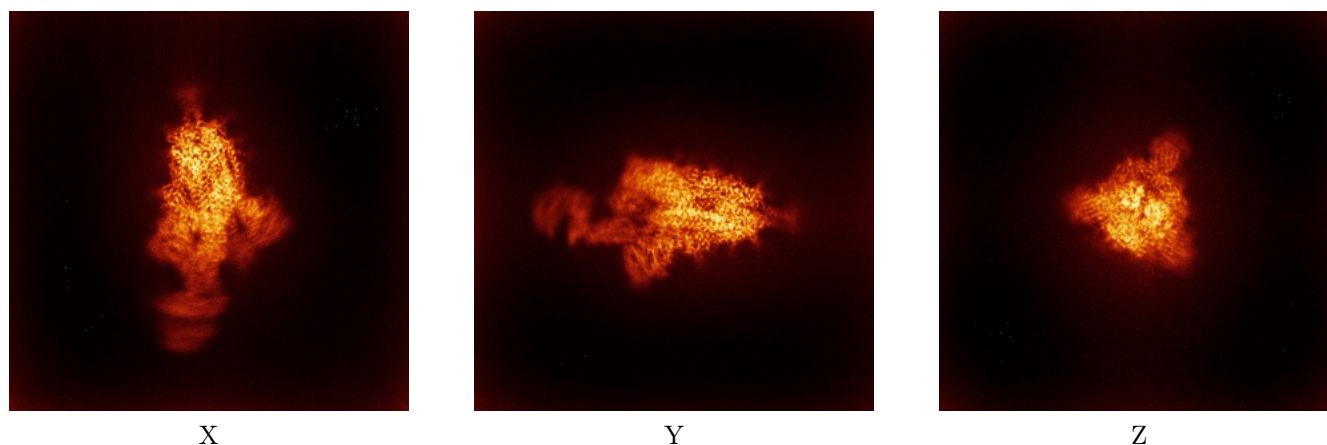
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

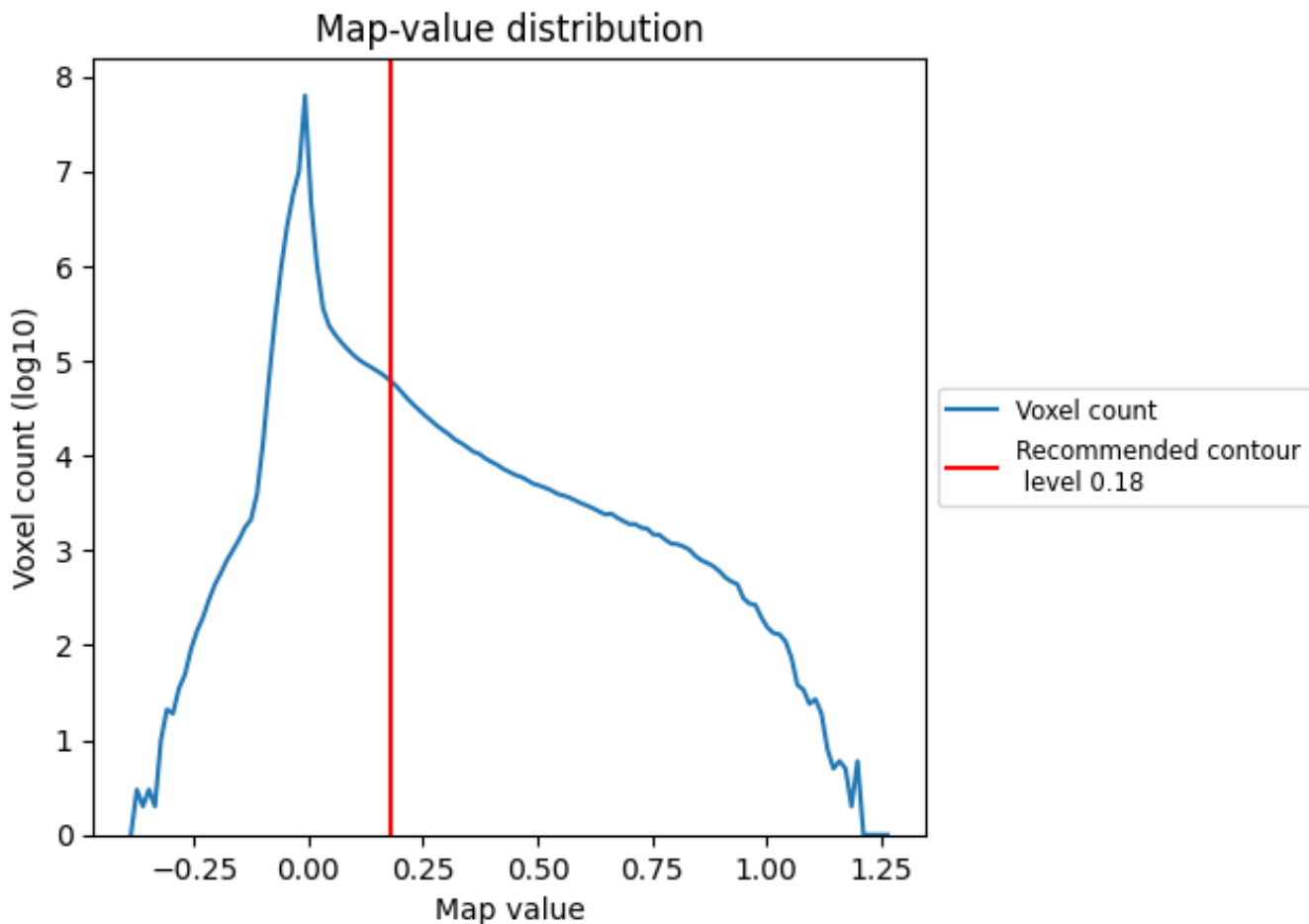
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

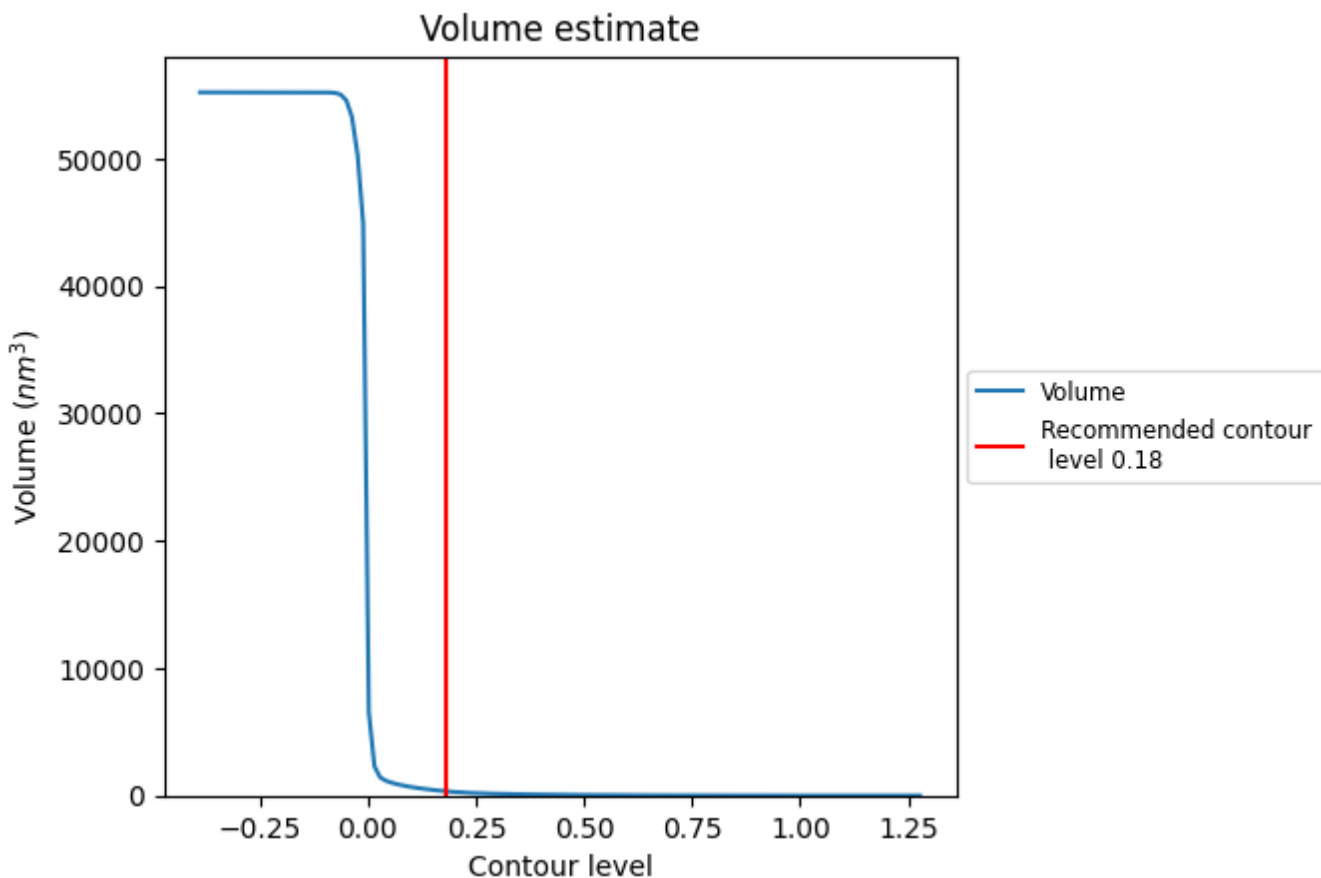
### 7.1 Map-value distribution [i](#)



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.



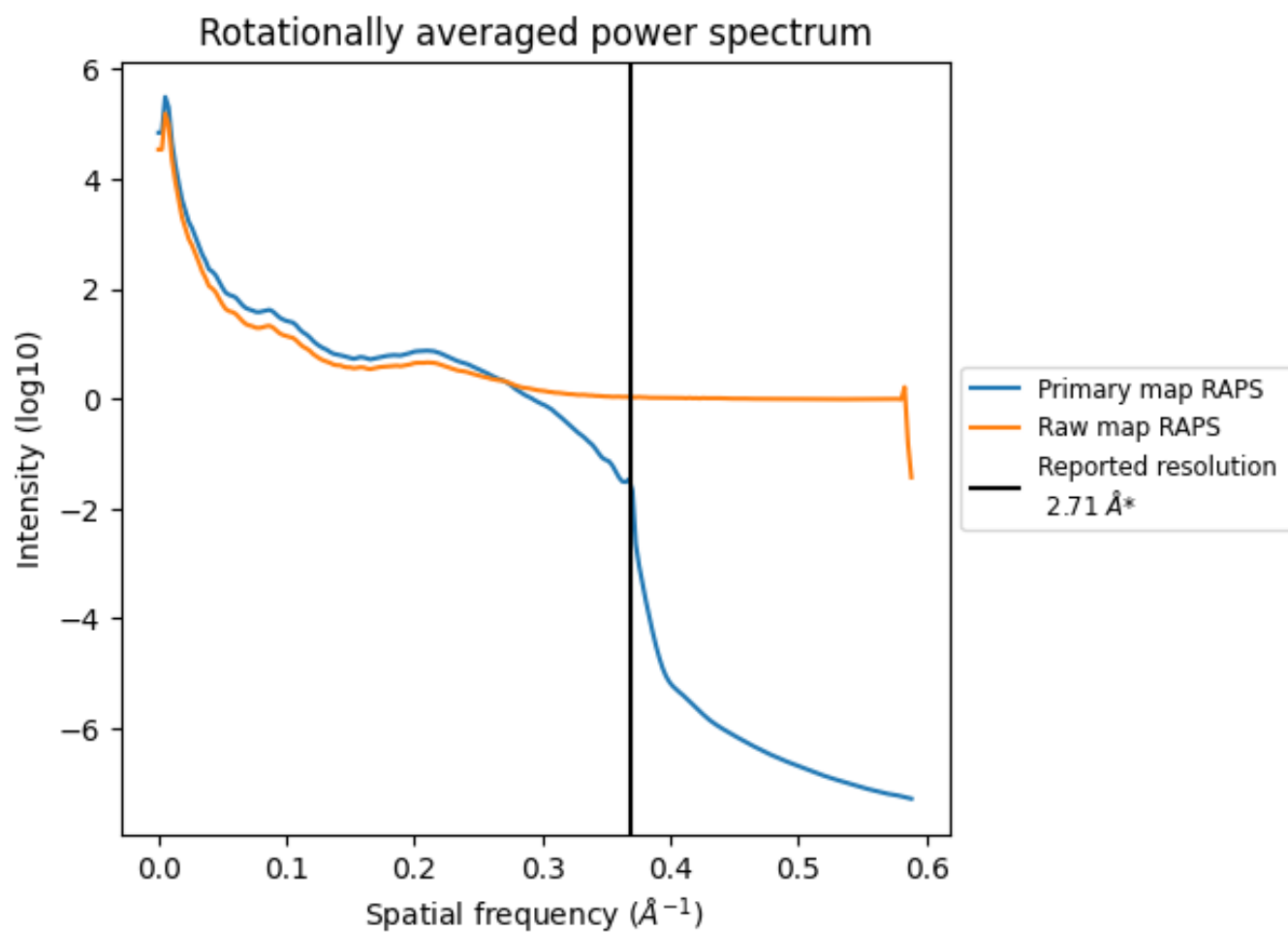
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 340  $\text{nm}^3$ ; this corresponds to an approximate mass of 307 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



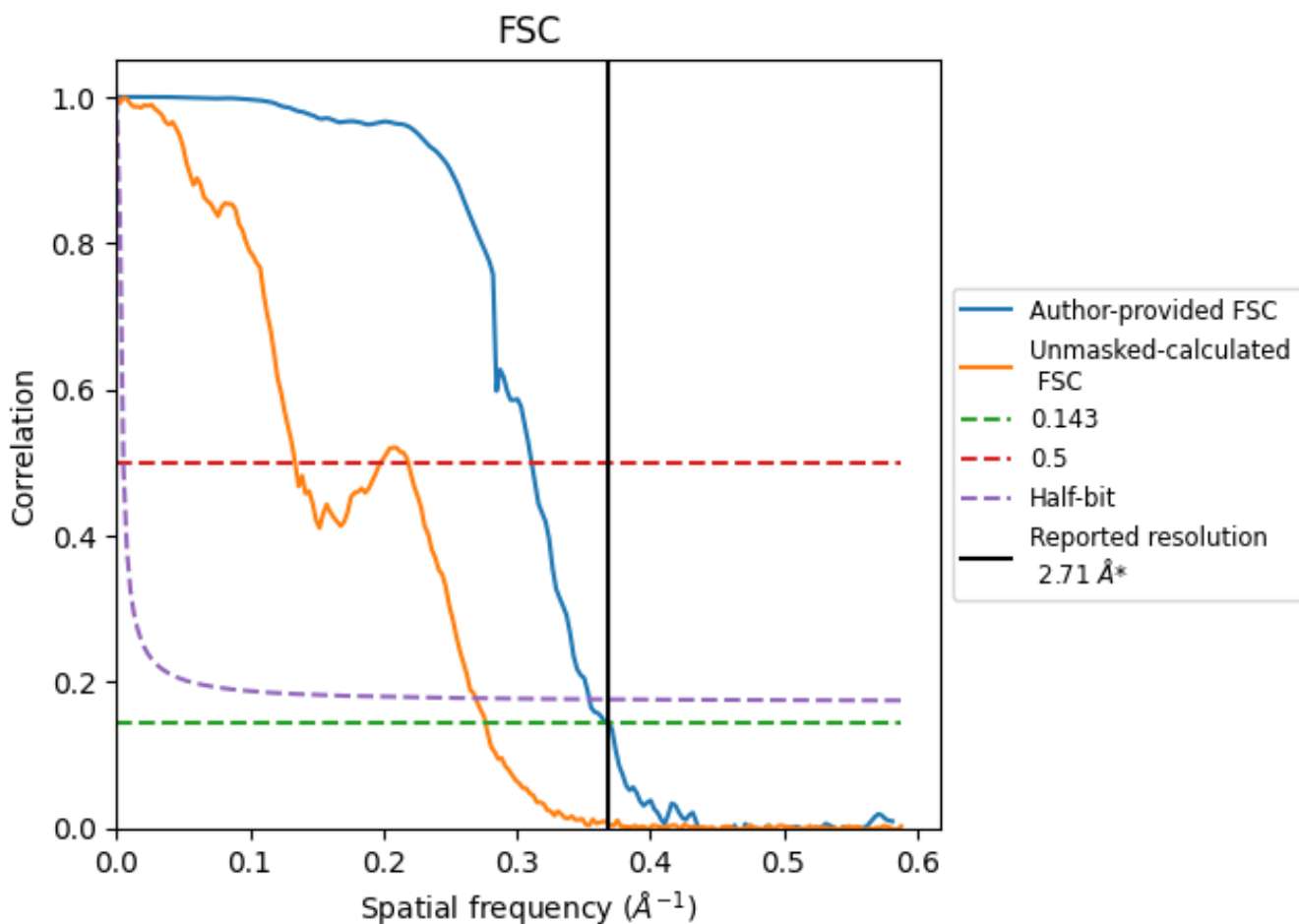
\*Reported resolution corresponds to spatial frequency of 0.369 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.369 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

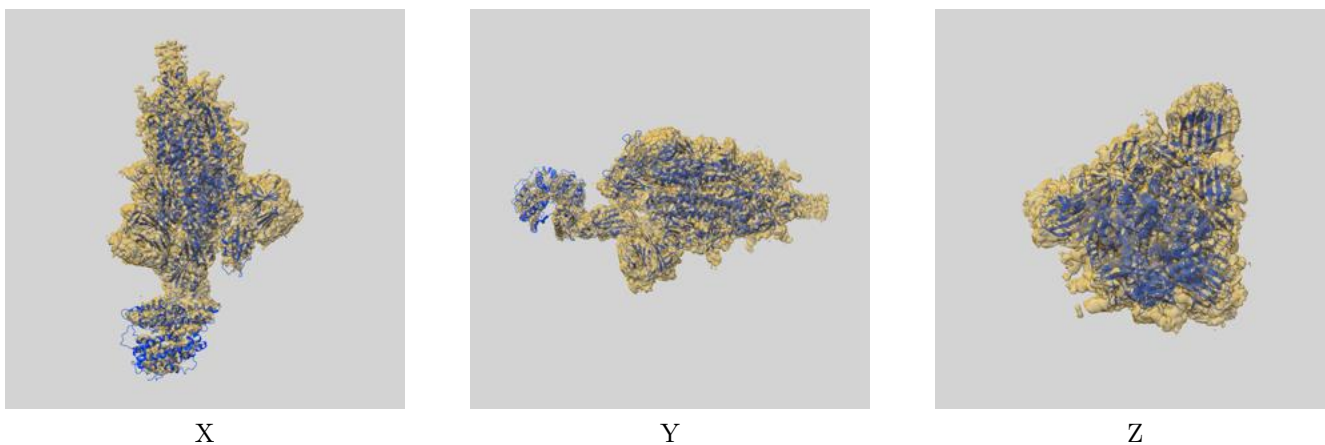
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.21	2.82
Unmasked-calculated*	3.61	7.47	3.71

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.71 by more than 10 %

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

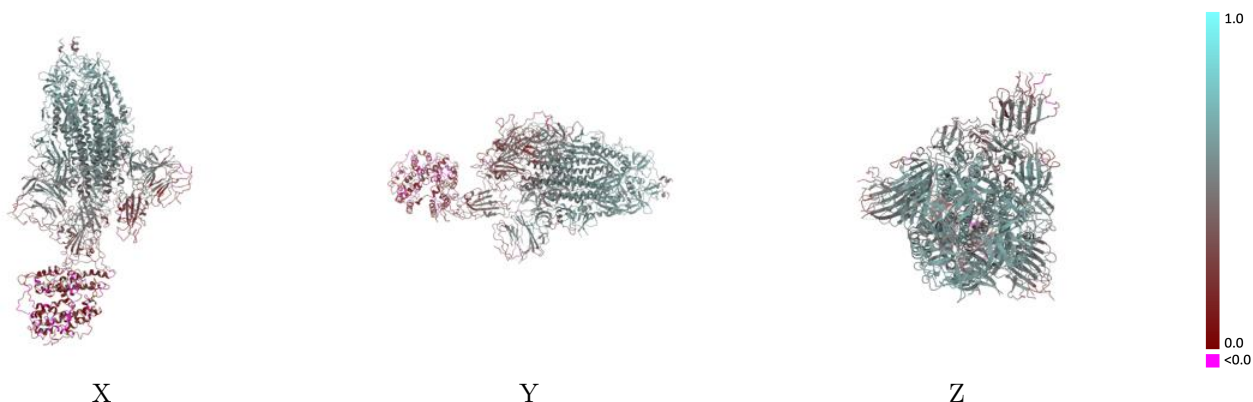
This section contains information regarding the fit between EMDB map EMD-34729 and PDB model 8HFZ. Per-residue inclusion information can be found in section 3 on page 9.

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



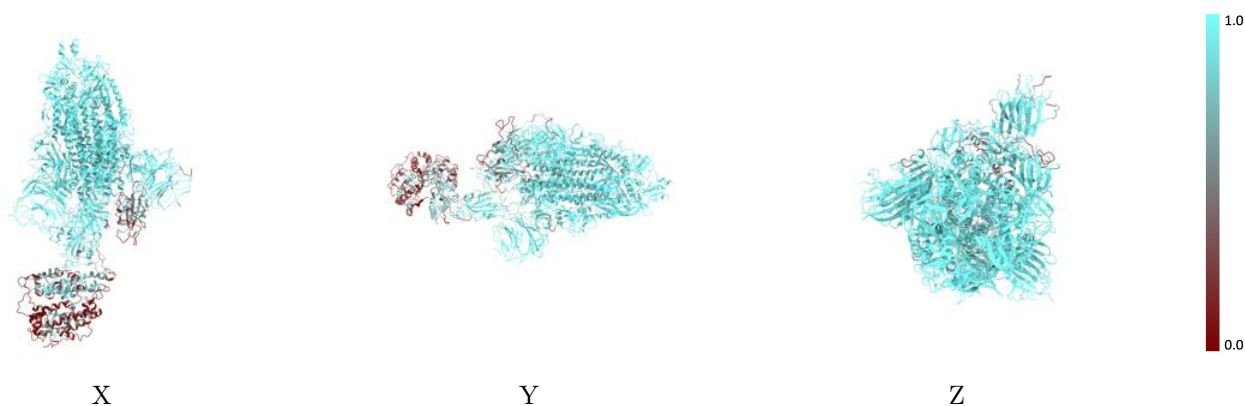
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



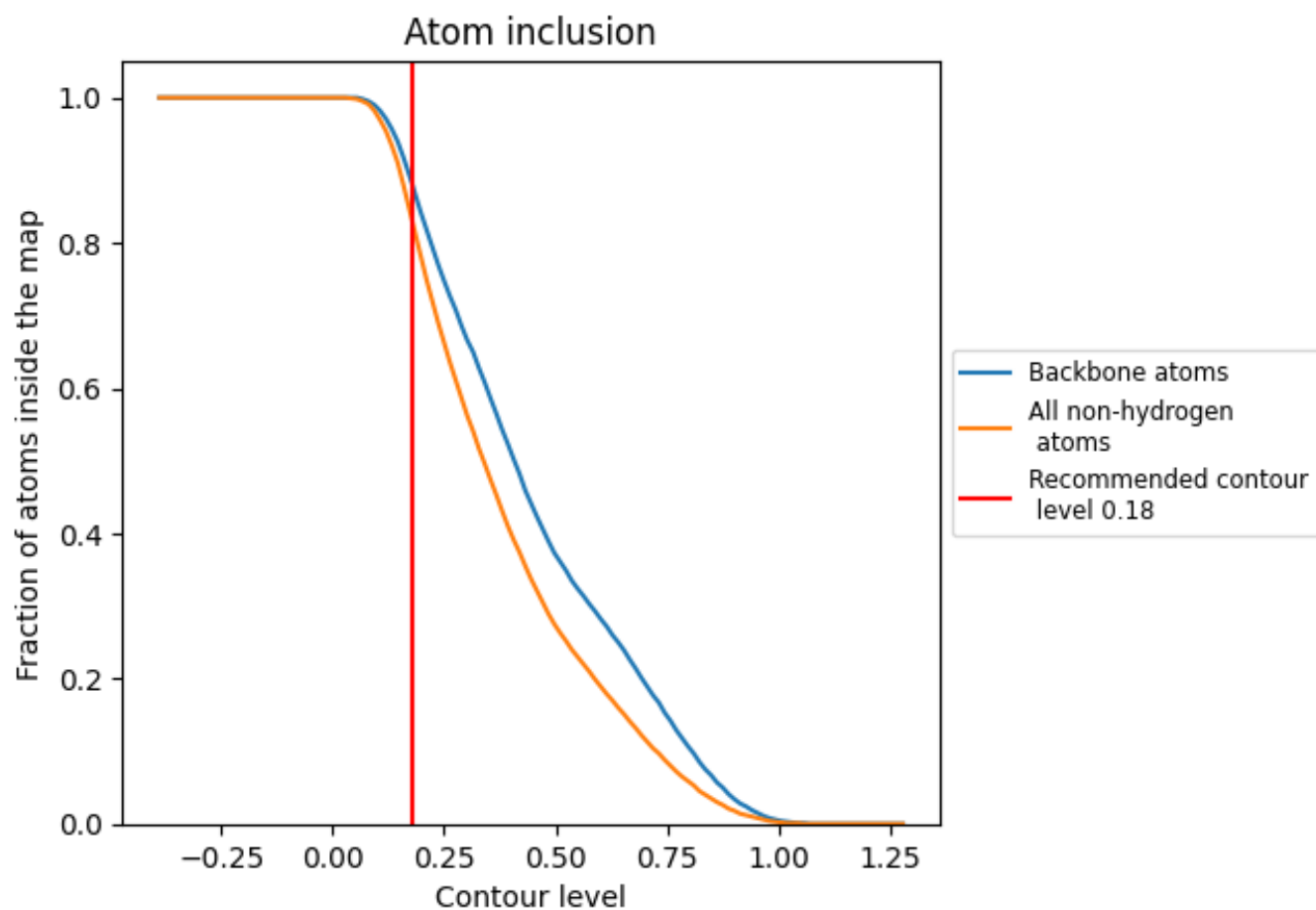
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.4230
A	 0.9470	 0.4790
B	 0.8650	 0.4720
C	 0.9380	 0.4820
D	 0.5710	 0.2690
E	 0.3690	 0.1490
F	 0.8570	 0.3850
G	 0.9290	 0.4010
H	 0.8570	 0.3760
I	 0.9640	 0.4840
J	 0.7140	 0.3400
K	 0.8930	 0.4390
L	 0.8570	 0.3900
M	 0.7140	 0.1930
N	 0.8930	 0.5100
O	 0.8210	 0.4490
P	 0.3210	 0.1800
Q	 0.9290	 0.4790
R	 0.8210	 0.4180
S	 0.7500	 0.4120
T	 0.8930	 0.4360
U	 0.8930	 0.3760
V	 0.6430	 0.3900
W	 0.9290	 0.4230
X	 0.8930	 0.4170
Y	 0.0000	 0.3270

