



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 12:15 am BST

PDB ID : 8QKP / pdb_00008qkp
EMDB ID : EMD-18469
Title : Asymmetric structure of Satellite Tobacco Necrosis Virus-Like Particle with PS2/3 gRNA
Authors : Javed, A.; Mata, P.C.; Stockley, P.
Deposited on : 2023-09-16
Resolution : 5.26 Å(reported)
Based on initial model : 4bcu

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

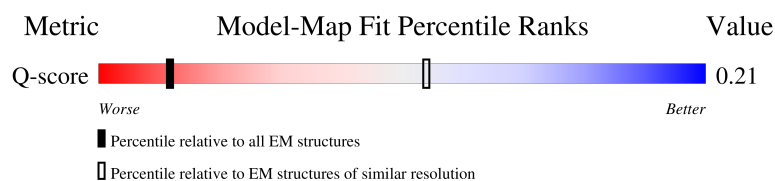
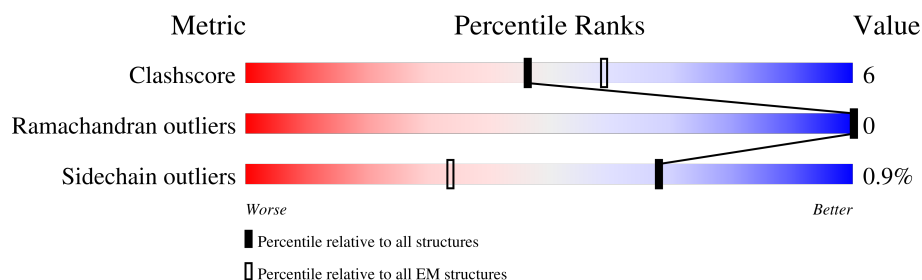
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



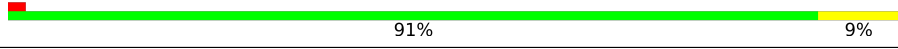
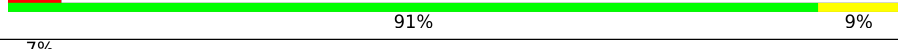
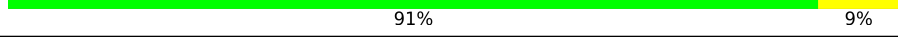
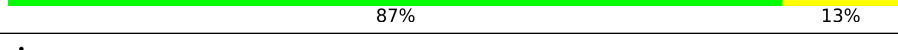
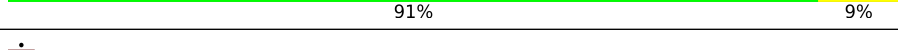
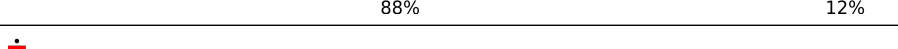
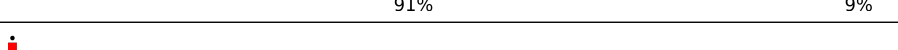
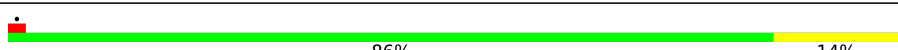
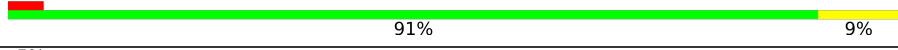
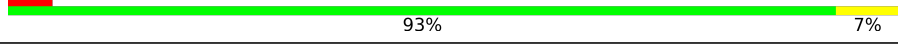
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	593 (4.76 - 5.75)

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

Mol	Chain	Length	Quality of chain
1	0	188	 88% 12%
1	1	188	 85% 15%
1	2	188	 89% 11%
1	3	188	 90% 10%

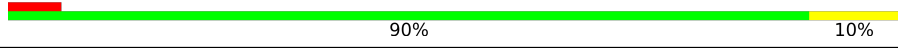
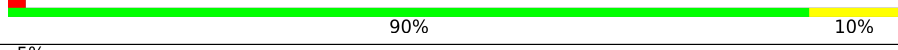
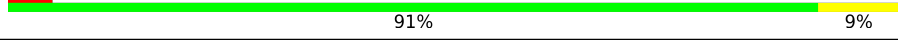
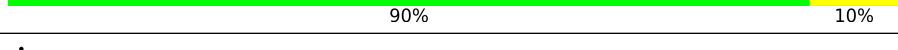
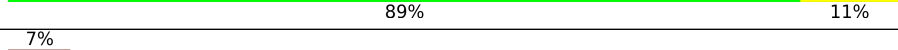
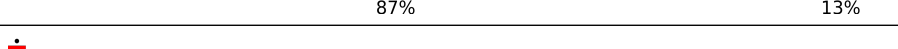
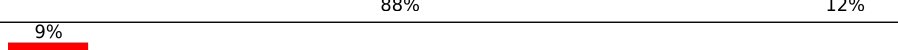
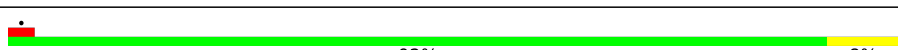
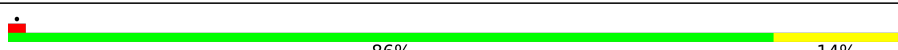
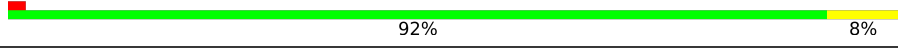
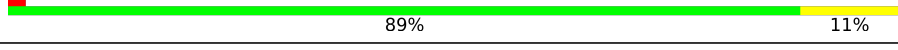
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Mol	Chain	Length	Quality of chain
1	4	188	 89%11%
1	5	188	 89%11%
1	6	188	 91%9%
1	7	188	 89%11%
1	A	188	 6%91%9%
1	B	188	 7%91%9%
1	C	188	 87%13%
1	D	188	 91%9%
1	E	188	 88%12%
1	F	188	 91%9%
1	G	188	 90%10%
1	H	188	 86%14%
1	I	188	 85%15%
1	J	188	 86%14%
1	K	188	 87%13%
1	L	188	 86%14%
1	M	188	 88%12%
1	N	188	 86%14%
1	O	188	 5%87%13%
1	P	188	 90%10%
1	Q	188	 89%11%
1	R	188	 91%9%
1	S	188	 5%93%7%
1	T	188	 88%12%
1	U	188	 6%88%12%

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Mol	Chain	Length	Quality of chain
1	V	188	 91%9%
1	W	188	 88%12%
1	X	188	 6%90%10%
1	Y	188	 90%10%
1	Z	188	 5%91%9%
1	a	188	 88%12%
1	b	188	 90%10%
1	c	188	 89%11%
1	d	188	 7%87%13%
1	e	188	 88%12%
1	f	188	 9%90%10%
1	g	188	 86%14%
1	h	188	 90%10%
1	i	188	 90%10%
1	j	188	 92%8%
1	k	188	 86%14%
1	l	188	 89%11%
1	m	188	 89%11%
1	n	188	 88%12%
1	o	188	 10%88%12%
1	p	188	 90%10%
1	q	188	 92%8%
1	r	188	 89%11%
1	s	188	 89%11%
1	t	188	 89%11%

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Mol	Chain	Length	Quality of chain
1	u	188	
1	v	188	
1	w	188	
1	x	188	
1	y	188	
1	z	188	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SRA	H	2203	-	-	X	-
3	SRA	K	2203	-	-	X	-
3	SRA	L	2206	-	-	X	-
3	SRA	P	202	-	-	X	-
3	SRA	R	2202	-	-	X	-
3	SRA	i	202	-	-	X	-
3	SRA	k	2003	-	-	X	-
3	SRA	t	205	-	-	X	-
4	SSU	4	1002	-	-	X	-
4	SSU	C	2204	-	-	X	-
4	SSU	I	3004	-	-	X	-
4	SSU	K	2204	-	-	X	-
4	SSU	Q	3003	-	-	X	-
4	SSU	T	1002	-	-	X	-
4	SSU	a	203	-	-	X	-
4	SSU	y	203	-	-	X	-
5	G	K	2205	-	-	X	-
5	G	Q	3004	-	-	X	-
5	G	W	2001	-	-	X	-
5	G	b	207	-	-	X	-
5	G	e	202	-	-	X	-
6	C	H	2202	-	-	X	-
6	C	I	3007	-	-	X	-
6	C	W	2002	-	-	X	-
6	C	Y	2002	-	-	X	-
6	C	b	208	-	-	X	-
6	C	r	2002	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 90306 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	B	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	C	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	D	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	E	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	F	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	G	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	H	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	I	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	J	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	K	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	L	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	M	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	N	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	O	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	P	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		
1	Q	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	S	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	T	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	U	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	V	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	W	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	X	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	Y	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	Z	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	a	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	b	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	c	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	d	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	e	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	f	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	g	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	h	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	i	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	j	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	k	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	l	188	Total 1457	C 907	N 268	O 276	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	n	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	o	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	p	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	q	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	r	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	s	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	t	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	u	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	v	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	w	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	x	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	y	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	z	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	0	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	1	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	2	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	3	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	4	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	5	188	Total 1457	C 907	N 268	O 276	S 6	0	0
1	6	188	Total 1457	C 907	N 268	O 276	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	188	Total	C	N	O	S	0	0
			1457	907	268	276	6		

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	2	Total	Ca	0
			2	2	
2	D	1	Total	Ca	0
			1	1	
2	E	2	Total	Ca	0
			2	2	
2	F	3	Total	Ca	0
			3	3	
2	G	2	Total	Ca	0
			2	2	
2	H	2	Total	Ca	0
			2	2	
2	I	1	Total	Ca	0
			1	1	
2	J	1	Total	Ca	0
			1	1	
2	K	1	Total	Ca	0
			1	1	
2	L	2	Total	Ca	0
			2	2	
2	M	2	Total	Ca	0
			2	2	
2	N	2	Total	Ca	0
			2	2	
2	O	2	Total	Ca	0
			2	2	
2	P	1	Total	Ca	0
			1	1	
2	Q	1	Total	Ca	0
			1	1	
2	R	2	Total	Ca	0
			2	2	

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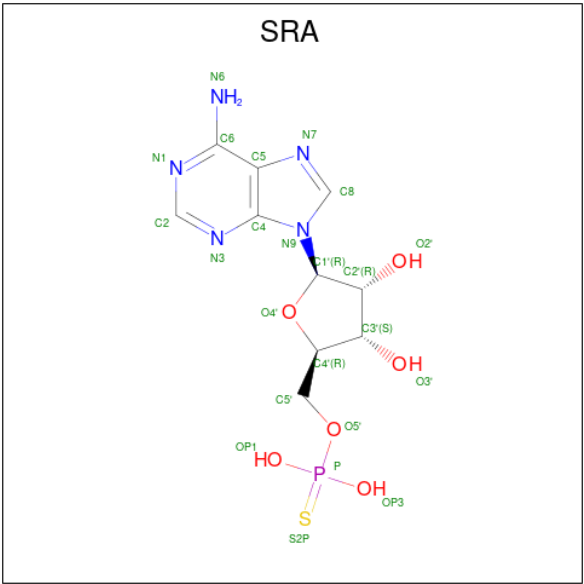
Mol	Chain	Residues	Atoms		AltConf
2	S	2	Total 2	Ca 2	0
2	T	1	Total 1	Ca 1	0
2	U	2	Total 2	Ca 2	0
2	V	2	Total 2	Ca 2	0
2	W	2	Total 2	Ca 2	0
2	X	2	Total 2	Ca 2	0
2	Y	1	Total 1	Ca 1	0
2	Z	1	Total 1	Ca 1	0
2	a	1	Total 1	Ca 1	0
2	b	1	Total 1	Ca 1	0
2	c	1	Total 1	Ca 1	0
2	d	1	Total 1	Ca 1	0
2	e	1	Total 1	Ca 1	0
2	f	1	Total 1	Ca 1	0
2	g	1	Total 1	Ca 1	0
2	h	1	Total 1	Ca 1	0
2	i	1	Total 1	Ca 1	0
2	j	1	Total 1	Ca 1	0
2	k	1	Total 1	Ca 1	0
2	l	1	Total 1	Ca 1	0
2	m	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	n	1	Total 1	Ca 1	0
2	o	1	Total 1	Ca 1	0
2	p	1	Total 1	Ca 1	0
2	q	1	Total 1	Ca 1	0
2	r	1	Total 1	Ca 1	0
2	s	1	Total 1	Ca 1	0
2	t	1	Total 1	Ca 1	0
2	u	1	Total 1	Ca 1	0
2	v	1	Total 1	Ca 1	0
2	w	1	Total 1	Ca 1	0
2	x	1	Total 1	Ca 1	0
2	y	1	Total 1	Ca 1	0
2	z	1	Total 1	Ca 1	0
2	0	3	Total 3	Ca 3	0
2	1	3	Total 3	Ca 3	0
2	2	3	Total 3	Ca 3	0
2	3	3	Total 3	Ca 3	0
2	4	3	Total 3	Ca 3	0
2	5	3	Total 3	Ca 3	0
2	6	3	Total 3	Ca 3	0
2	7	3	Total 3	Ca 3	0

- Molecule 3 is ADENOSINE -5'-THIO-MONOPHOSPHATE (CCD ID: SRA) (formula: C₁₀H₁₄N₅O₆PS).



Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	E	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	F	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	F	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	H	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	H	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	H	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	I	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	I	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	J	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	K	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	L	1	Total	C	N	O	P	0
			22	10	5	6	1	

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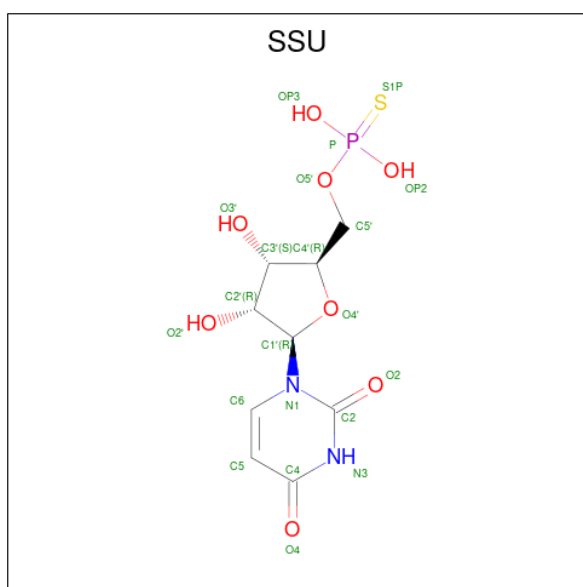
Mol	Chain	Residues	Atoms					AltConf
3	L	1	Total 22	C 10	N 5	O 6	P 1	0
3	L	1	Total 22	C 10	N 5	O 6	P 1	0
3	N	1	Total 22	C 10	N 5	O 6	P 1	0
3	P	1	Total 22	C 10	N 5	O 6	P 1	0
3	Q	1	Total 22	C 10	N 5	O 6	P 1	0
3	R	1	Total 22	C 10	N 5	O 6	P 1	0
3	R	1	Total 22	C 10	N 5	O 6	P 1	0
3	T	1	Total 22	C 10	N 5	O 6	P 1	0
3	W	1	Total 22	C 10	N 5	O 6	P 1	0
3	Y	1	Total 22	C 10	N 5	O 6	P 1	0
3	Y	1	Total 22	C 10	N 5	O 6	P 1	0
3	a	1	Total 22	C 10	N 5	O 6	P 1	0
3	b	1	Total 22	C 10	N 5	O 6	P 1	0
3	b	1	Total 22	C 10	N 5	O 6	P 1	0
3	b	1	Total 22	C 10	N 5	O 6	P 1	0
3	e	1	Total 22	C 10	N 5	O 6	P 1	0
3	g	1	Total 22	C 10	N 5	O 6	P 1	0
3	g	1	Total 22	C 10	N 5	O 6	P 1	0
3	h	1	Total 22	C 10	N 5	O 6	P 1	0
3	i	1	Total 22	C 10	N 5	O 6	P 1	0
3	k	1	Total 22	C 10	N 5	O 6	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
3	k	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	q	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	q	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	r	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	t	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	t	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	w	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	x	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	y	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	z	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	4	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 4 is URIDINE-5'-PHOSPHOROTHIOATE (CCD ID: SSU) (formula: $C_9H_{13}N_2O_8PS$).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	F	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	H	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	H	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	I	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	J	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	K	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	K	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	K	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	L	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	L	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	P	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	P	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	Q	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	R	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	T	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	X	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	X	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	a	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	a	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	b	1	Total	C	N	O	P	0
			20	9	2	8	1	
4	b	1	Total	C	N	O	P	0
			20	9	2	8	1	

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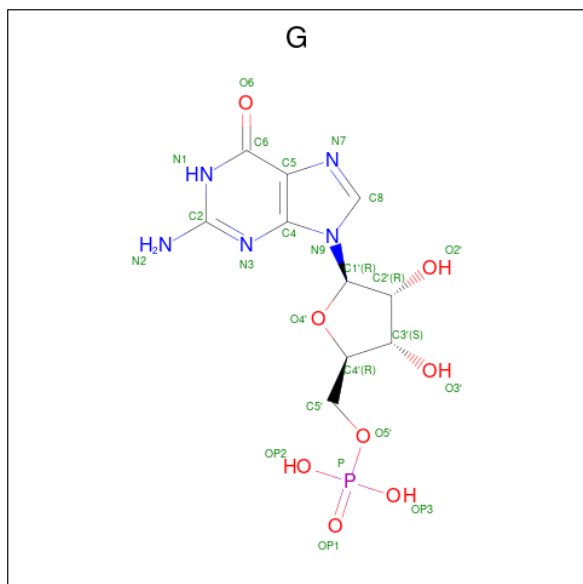
Mol	Chain	Residues	Atoms					AltConf
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4	g	1	Total 20	C 9	N 2	O 8	P 1	0
4	g	1	Total 20	C 9	N 2	O 8	P 1	0
4	h	1	Total 20	C 9	N 2	O 8	P 1	0
4	i	1	Total 20	C 9	N 2	O 8	P 1	0
4	i	1	Total 20	C 9	N 2	O 8	P 1	0
4	q	1	Total 20	C 9	N 2	O 8	P 1	0
4	r	1	Total 20	C 9	N 2	O 8	P 1	0
4	t	1	Total 20	C 9	N 2	O 8	P 1	0
4	t	1	Total 20	C 9	N 2	O 8	P 1	0
4	t	1	Total 20	C 9	N 2	O 8	P 1	0
4	t	1	Total 20	C 9	N 2	O 8	P 1	0
4	v	1	Total 20	C 9	N 2	O 8	P 1	0
4	w	1	Total 20	C 9	N 2	O 8	P 1	0
4	w	1	Total 20	C 9	N 2	O 8	P 1	0
4	y	1	Total 20	C 9	N 2	O 8	P 1	0
4	z	1	Total 20	C 9	N 2	O 8	P 1	0
4	z	1	Total 20	C 9	N 2	O 8	P 1	0
4	2	1	Total 20	C 9	N 2	O 8	P 1	0
4	3	1	Total 20	C 9	N 2	O 8	P 1	0
4	3	1	Total 20	C 9	N 2	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
4	4	1	Total	C	N	O	P	0
			20	9	2	8	1	

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: G) (formula: $C_{10}H_{14}N_5O_8P$).



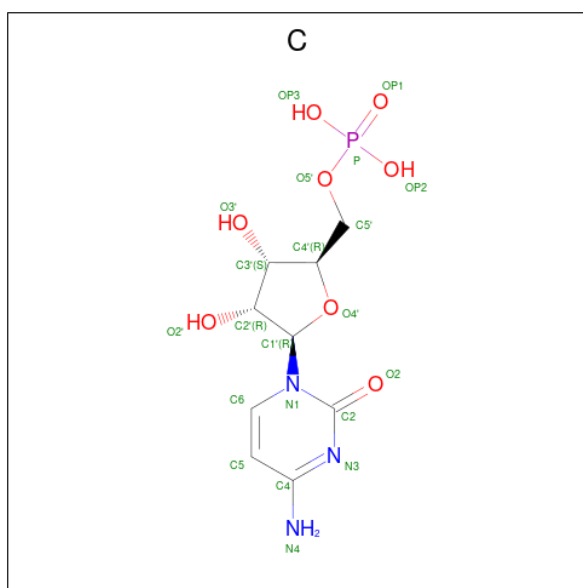
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	H	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	I	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	I	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	K	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	P	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	Q	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	R	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	T	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	W	1	Total	C	N	O	P	0
			23	10	5	7	1	

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Mol	Chain	Residues	Atoms					AltConf
5	Y	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	a	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	b	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	b	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	e	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	g	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	i	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	k	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	q	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	r	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	y	1	Total	C	N	O	P	0
			23	10	5	7	1	
5	4	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 6 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C) (formula: $C_9H_{14}N_3O_8P$).

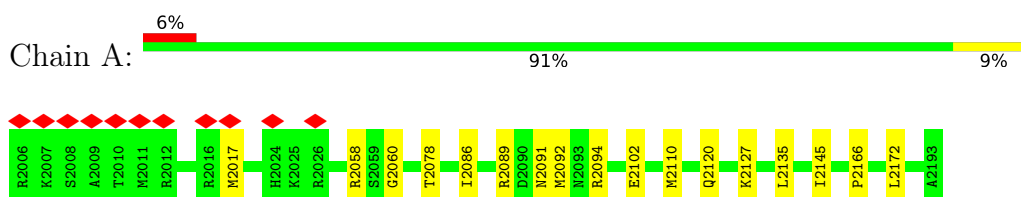


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	E	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	H	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	I	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	I	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	L	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	N	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	W	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	Y	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	b	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	b	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	e	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	g	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	g	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	i	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	k	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	q	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	r	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	r	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	y	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	z	1	Total	C	N	O	P	0
			20	9	3	7	1	
6	2	1	Total	C	N	O	P	0
			20	9	3	7	1	

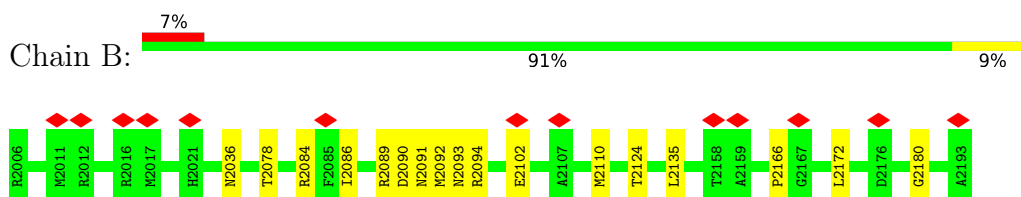
3 Residue-property plots [i](#)

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.

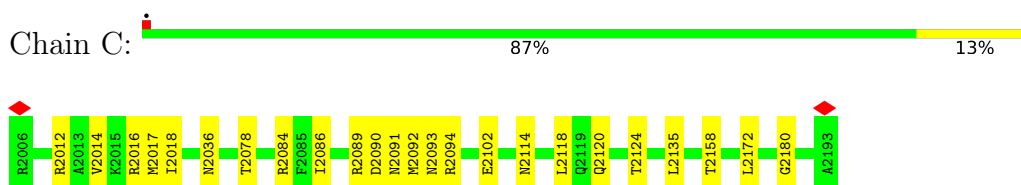
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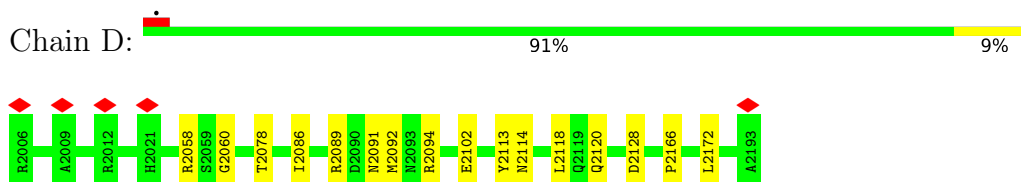
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

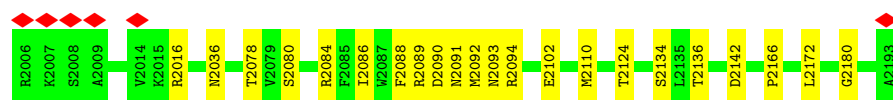


- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

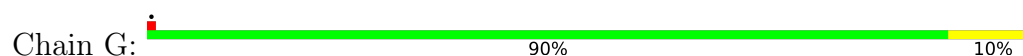




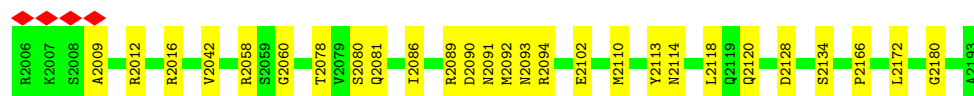
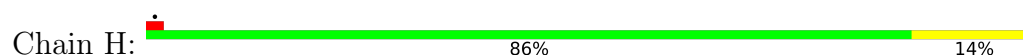
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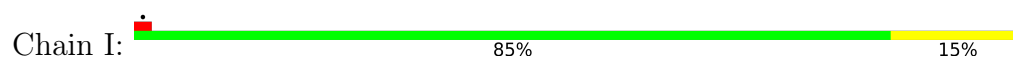
- Molecule 1: Capsid protein



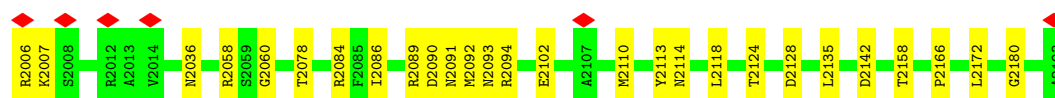
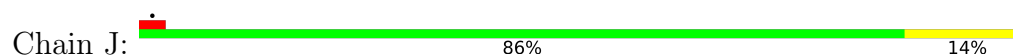
- Molecule 1: Capsid protein



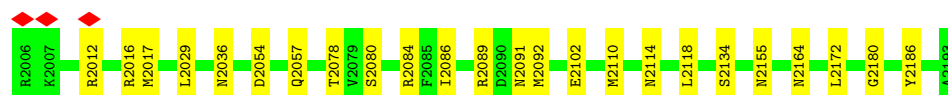
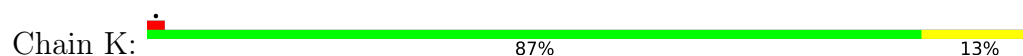
- Molecule 1: Capsid protein



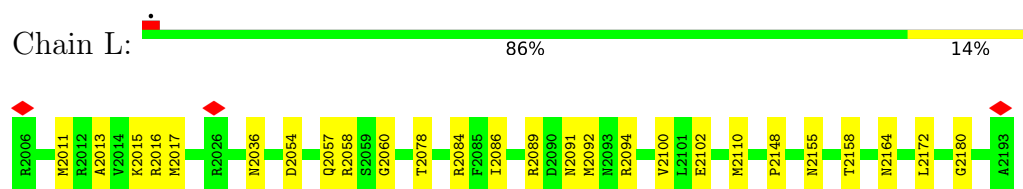
- Molecule 1: Capsid protein



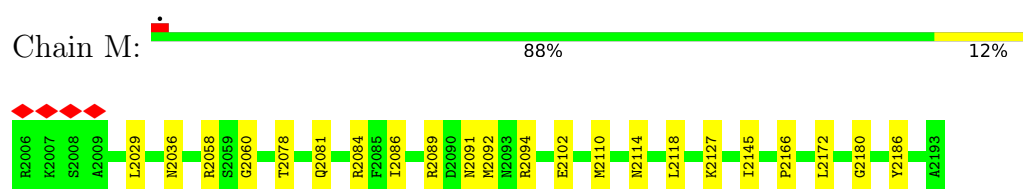
- Molecule 1: Capsid protein



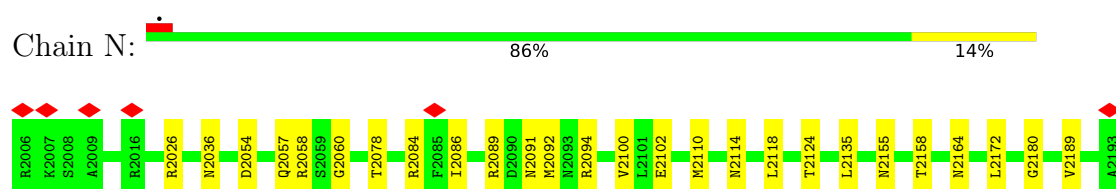
● Molecule 1: Capsid protein



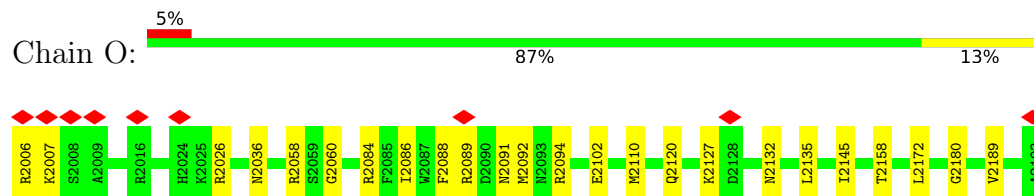
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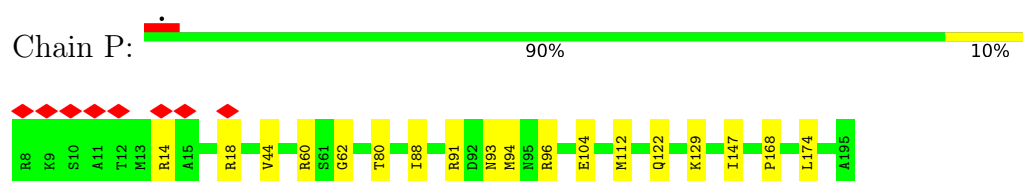
● Molecule 1: Capsid protein



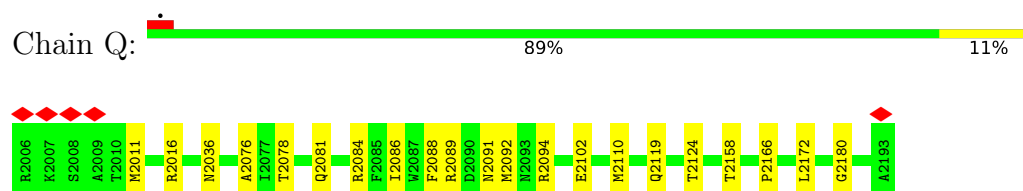
● Molecule 1: Capsid protein



● Molecule 1: Capsid protein

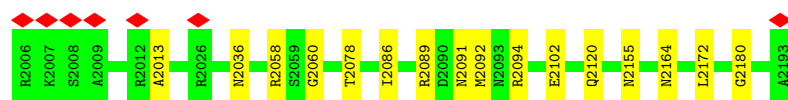


● Molecule 1: Capsid protein

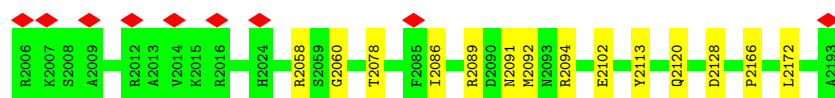


● Molecule 1: Capsid protein

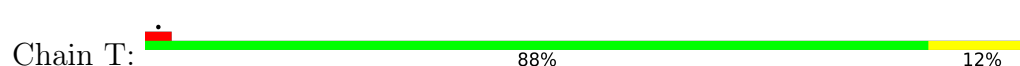




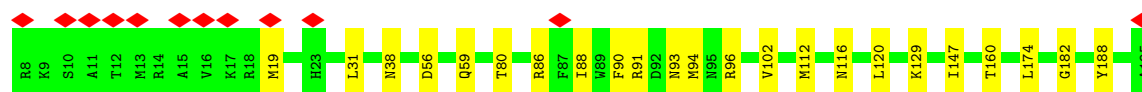
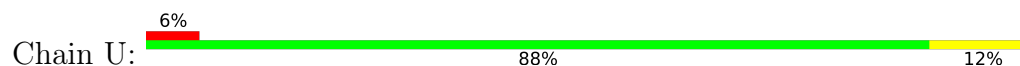
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



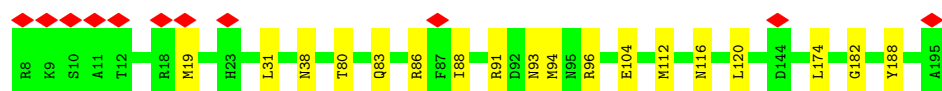
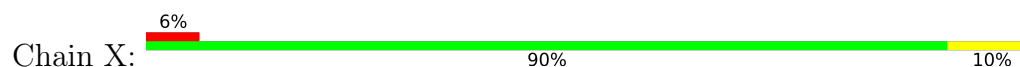
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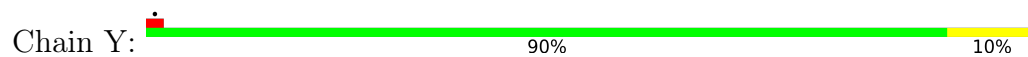
• Molecule 1: Capsid protein



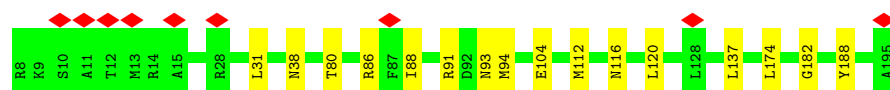
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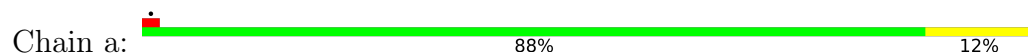
• Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



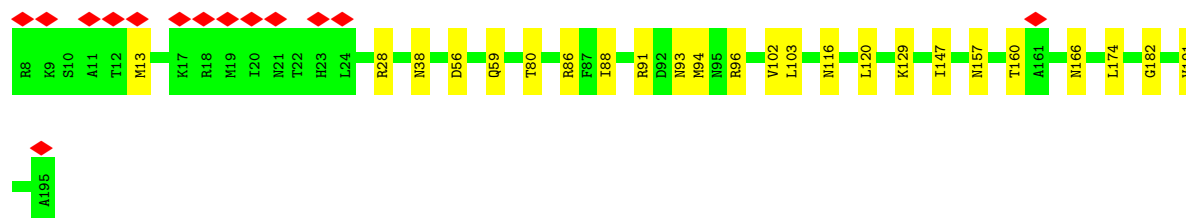
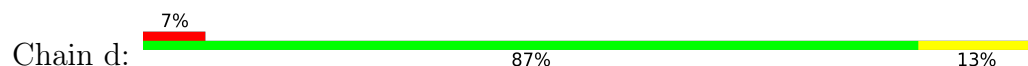
- Molecule 1: Capsid protein



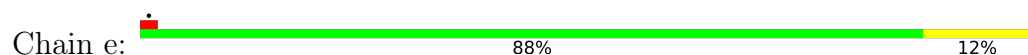
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

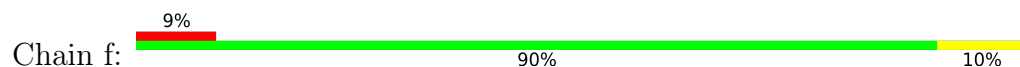


- Molecule 1: Capsid protein

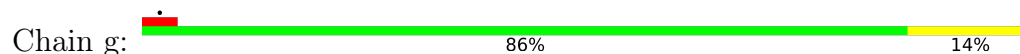




- Molecule 1: Capsid protein



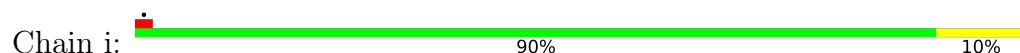
- Molecule 1: Capsid protein



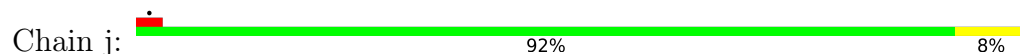
- Molecule 1: Capsid protein



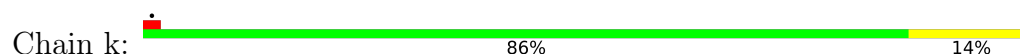
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

Chain l:  89% 11%



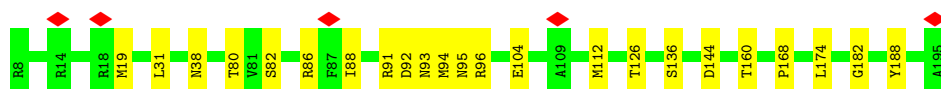
• Molecule 1: Capsid protein

Chain m:  89% 11%



• Molecule 1: Capsid protein

Chain n:  88% 12%



• Molecule 1: Capsid protein

Chain o:  10% 88% 12%



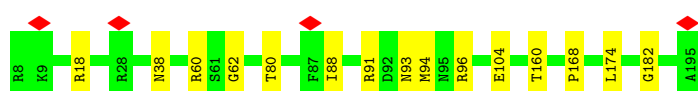
• Molecule 1: Capsid protein

Chain p:  10% 90% 10%

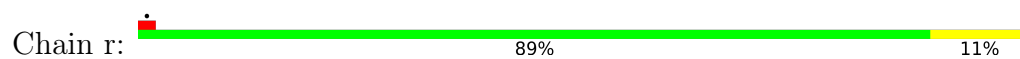


• Molecule 1: Capsid protein

Chain q:  92% 8%



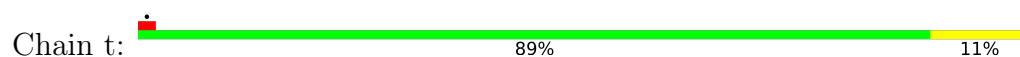
• Molecule 1: Capsid protein



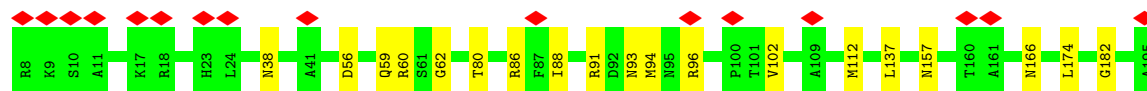
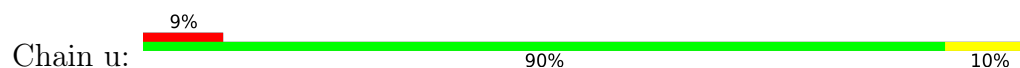
• Molecule 1: Capsid protein



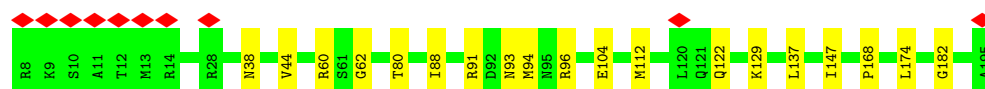
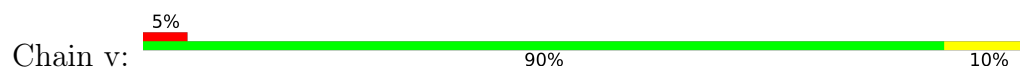
• Molecule 1: Capsid protein



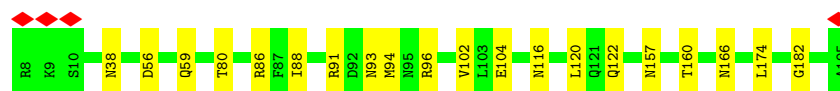
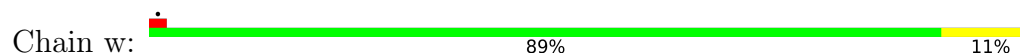
• Molecule 1: Capsid protein



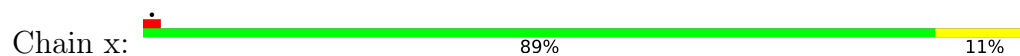
• Molecule 1: Capsid protein



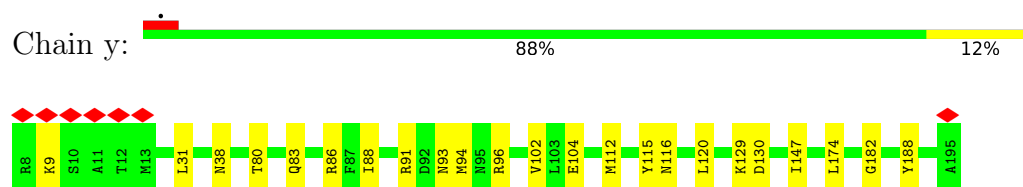
• Molecule 1: Capsid protein



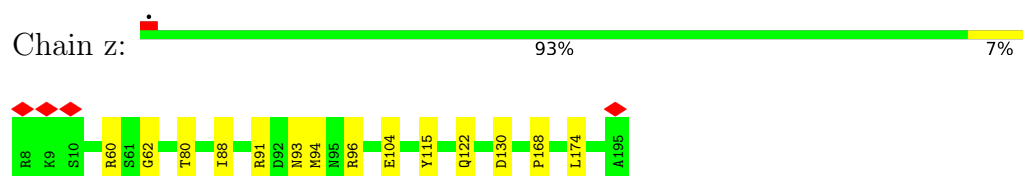
• Molecule 1: Capsid protein



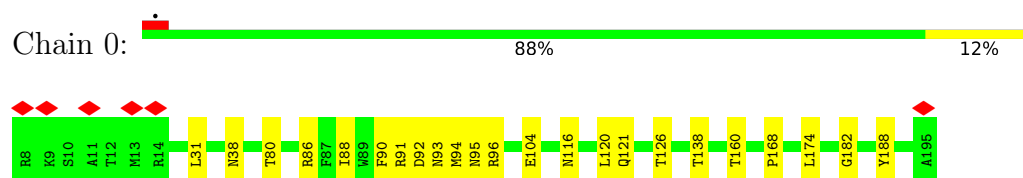
• Molecule 1: Capsid protein



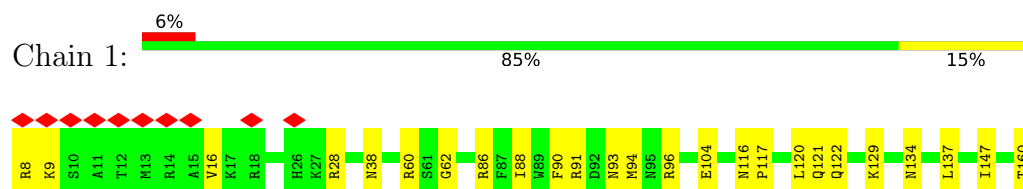
• Molecule 1: Capsid protein



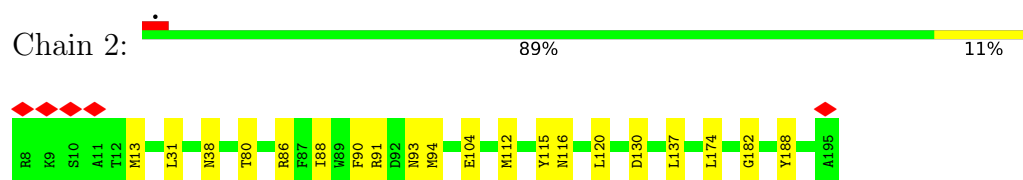
• Molecule 1: Capsid protein



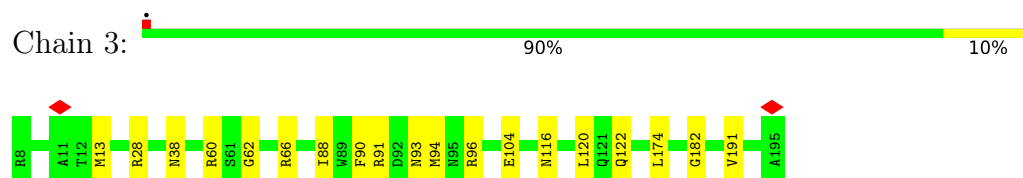
• Molecule 1: Capsid protein



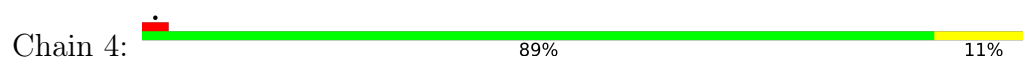
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

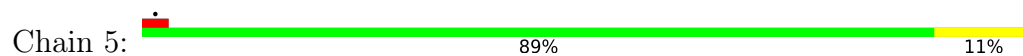


• Molecule 1: Capsid protein

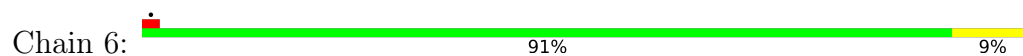




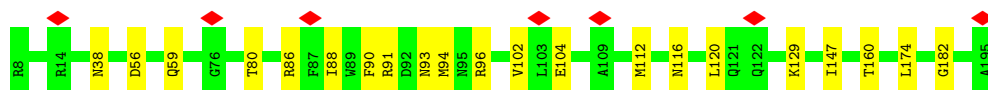
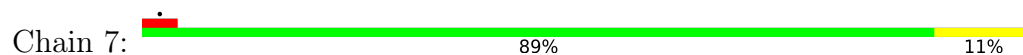
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.759	Depositor
Minimum map value	-0.939	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	268.38, 268.38, 268.38	wwPDB
Map dimensions	252, 252, 252	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SRA, SSU

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	0	0.35	0/1479	0.48	0/2004
1	1	0.35	0/1479	0.48	0/2004
1	2	0.35	0/1479	0.46	0/2004
1	3	0.35	0/1479	0.50	0/2004
1	4	0.35	0/1479	0.47	0/2004
1	5	0.35	0/1479	0.48	0/2004
1	6	0.35	0/1479	0.46	0/2004
1	7	0.35	0/1479	0.46	0/2004
1	A	0.35	0/1479	0.46	0/2004
1	B	0.35	0/1479	0.46	0/2004
1	C	0.36	0/1479	0.49	0/2004
1	D	0.35	0/1479	0.46	0/2004
1	E	0.35	0/1479	0.47	0/2004
1	F	0.35	0/1479	0.46	0/2004
1	G	0.35	0/1479	0.45	0/2004
1	H	0.35	0/1479	0.46	0/2004
1	I	0.36	0/1479	0.48	0/2004
1	J	0.35	0/1479	0.46	0/2004
1	K	0.35	0/1479	0.46	0/2004
1	L	0.35	0/1479	0.46	0/2004
1	M	0.35	0/1479	0.45	0/2004
1	N	0.35	0/1479	0.46	0/2004
1	O	0.35	0/1479	0.47	0/2004
1	P	0.34	0/1479	0.46	0/2004
1	Q	0.35	0/1479	0.47	0/2004
1	R	0.34	0/1479	0.46	0/2004
1	S	0.34	0/1479	0.46	0/2004
1	T	0.35	0/1479	0.47	0/2004
1	U	0.35	0/1479	0.45	0/2004
1	V	0.35	0/1479	0.46	0/2004
1	W	0.35	0/1479	0.45	0/2004
1	X	0.35	0/1479	0.45	0/2004

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.35	0/1479	0.48	0/2004
1	Z	0.35	0/1479	0.45	0/2004
1	a	0.35	0/1479	0.45	0/2004
1	b	0.35	0/1479	0.46	0/2004
1	c	0.35	0/1479	0.47	0/2004
1	d	0.34	0/1479	0.46	0/2004
1	e	0.34	0/1479	0.45	0/2004
1	f	0.35	0/1479	0.45	0/2004
1	g	0.35	0/1479	0.46	0/2004
1	h	0.35	0/1479	0.47	0/2004
1	i	0.35	0/1479	0.46	0/2004
1	j	0.35	0/1479	0.45	0/2004
1	k	0.35	0/1479	0.45	0/2004
1	l	0.35	0/1479	0.47	0/2004
1	m	0.35	0/1479	0.47	0/2004
1	n	0.35	0/1479	0.46	0/2004
1	o	0.35	0/1479	0.46	0/2004
1	p	0.35	0/1479	0.46	0/2004
1	q	0.35	0/1479	0.45	0/2004
1	r	0.35	0/1479	0.48	0/2004
1	s	0.35	0/1479	0.47	0/2004
1	t	0.35	0/1479	0.47	0/2004
1	u	0.35	0/1479	0.47	0/2004
1	v	0.35	0/1479	0.46	0/2004
1	w	0.35	0/1479	0.46	0/2004
1	x	0.35	0/1479	0.47	0/2004
1	y	0.35	0/1479	0.46	0/2004
1	z	0.34	0/1479	0.46	0/2004
All	All	0.35	0/88740	0.46	0/120240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1457	0	1463	16	0
1	1	1457	0	1463	19	0
1	2	1457	0	1463	18	0
1	3	1457	0	1463	14	0
1	4	1457	0	1463	22	0
1	5	1457	0	1463	14	0
1	6	1457	0	1463	12	0
1	7	1457	0	1463	14	0
1	A	1457	0	1463	14	0
1	B	1457	0	1463	13	0
1	C	1457	0	1463	28	0
1	D	1457	0	1463	11	0
1	E	1457	0	1463	17	0
1	F	1457	0	1463	13	0
1	G	1457	0	1463	13	0
1	H	1457	0	1462	33	0
1	I	1457	0	1462	43	0
1	J	1457	0	1463	17	0
1	K	1457	0	1463	28	0
1	L	1457	0	1463	23	0
1	M	1457	0	1463	15	0
1	N	1457	0	1463	17	0
1	O	1457	0	1463	17	0
1	P	1457	0	1463	16	0
1	Q	1457	0	1463	23	0
1	R	1457	0	1463	13	0
1	S	1457	0	1463	10	0
1	T	1457	0	1461	19	0
1	U	1457	0	1463	15	0
1	V	1457	0	1463	11	0
1	W	1457	0	1463	23	0
1	X	1457	0	1463	13	0
1	Y	1457	0	1463	21	0
1	Z	1457	0	1463	11	0
1	a	1457	0	1463	22	0
1	b	1457	0	1461	19	0
1	c	1457	0	1463	14	0
1	d	1457	0	1463	15	0
1	e	1457	0	1461	15	0
1	f	1457	0	1463	12	0
1	g	1457	0	1463	17	0
1	h	1457	0	1463	13	0
1	i	1457	0	1463	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1457	0	1463	10	0
1	k	1457	0	1463	24	0
1	l	1457	0	1463	13	0
1	m	1457	0	1463	14	0
1	n	1457	0	1463	18	0
1	o	1457	0	1463	17	0
1	p	1457	0	1463	14	0
1	q	1457	0	1463	12	0
1	r	1457	0	1463	23	0
1	s	1457	0	1463	15	0
1	t	1457	0	1463	20	0
1	u	1457	0	1463	12	0
1	v	1457	0	1463	12	0
1	w	1457	0	1463	13	0
1	x	1457	0	1463	16	0
1	y	1457	0	1463	23	0
1	z	1457	0	1463	9	0
2	0	3	0	0	0	0
2	1	3	0	0	0	0
2	2	3	0	0	0	0
2	3	3	0	0	0	0
2	4	3	0	0	0	0
2	5	3	0	0	0	0
2	6	3	0	0	0	0
2	7	3	0	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	1	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	c	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	1	0	0	0	0
2	j	1	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	1	0	0	0	0
2	o	1	0	0	0	0
2	p	1	0	0	0	0
2	q	1	0	0	0	0
2	r	1	0	0	0	0
2	s	1	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0
2	v	1	0	0	0	0
2	w	1	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
3	4	22	0	11	4	0
3	C	22	0	11	5	0
3	E	22	0	11	2	0
3	F	44	0	22	7	0
3	H	66	0	33	20	0
3	I	44	0	23	5	0
3	J	22	0	11	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	22	0	11	7	0
3	L	66	0	33	16	0
3	N	22	0	12	1	0
3	P	22	0	11	7	0
3	Q	22	0	11	5	0
3	R	44	0	22	16	0
3	T	22	0	11	6	0
3	W	22	0	11	2	0
3	Y	44	0	22	7	0
3	a	22	0	11	6	0
3	b	66	0	35	8	0
3	e	22	0	11	2	0
3	g	44	0	24	2	0
3	h	22	0	12	1	0
3	i	22	0	11	7	0
3	k	44	0	22	13	0
3	q	44	0	22	10	0
3	r	22	0	12	1	0
3	t	44	0	22	13	0
3	w	22	0	11	6	0
3	x	22	0	12	1	0
3	y	22	0	12	1	0
3	z	22	0	12	1	0
4	2	20	0	10	1	0
4	3	40	0	21	4	0
4	4	20	0	10	10	0
4	C	20	0	10	15	0
4	F	20	0	11	2	0
4	H	40	0	21	3	0
4	I	20	0	10	15	0
4	J	20	0	11	2	0
4	K	60	0	31	15	0
4	L	40	0	21	9	0
4	P	40	0	20	7	0
4	Q	20	0	10	8	0
4	R	20	0	11	2	0
4	T	20	0	8	8	0
4	X	40	0	21	3	0
4	a	40	0	20	12	0
4	b	40	0	20	5	0
4	e	20	0	10	1	0
4	g	40	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	h	20	0	10	1	0
4	i	40	0	20	5	0
4	q	20	0	10	1	0
4	r	20	0	10	1	0
4	t	80	0	41	10	0
4	v	20	0	11	2	0
4	w	40	0	21	3	0
4	y	20	0	10	9	0
4	z	40	0	20	2	0
5	4	23	0	11	5	0
5	C	23	0	11	5	0
5	H	23	0	11	5	0
5	I	46	0	22	9	0
5	K	23	0	11	7	0
5	P	23	0	11	4	0
5	Q	23	0	11	7	0
5	R	23	0	11	5	0
5	T	23	0	11	4	0
5	W	23	0	11	9	0
5	Y	23	0	11	4	0
5	a	23	0	11	5	0
5	b	46	0	22	15	0
5	e	23	0	11	7	0
5	g	23	0	11	5	0
5	i	23	0	11	5	0
5	k	23	0	11	5	0
5	q	23	0	11	5	0
5	r	23	0	11	4	0
5	y	23	0	11	4	0
6	2	20	0	11	5	0
6	C	20	0	11	5	0
6	E	20	0	11	6	0
6	H	20	0	11	15	0
6	I	40	0	22	19	0
6	L	20	0	11	4	0
6	N	20	0	11	4	0
6	W	20	0	11	7	0
6	Y	20	0	11	10	0
6	b	40	0	22	12	0
6	e	20	0	11	5	0
6	g	40	0	22	10	0
6	i	20	0	11	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	k	20	0	11	5	0
6	q	20	0	11	5	0
6	r	40	0	22	18	0
6	y	20	0	11	4	0
6	z	20	0	11	5	0
All	All	90306	0	89200	1094	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 6.

All (1094) 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:H:2016:ARG:CD	3:H:2203:SRA:H5'	1.19	1.60
1:H:2016:ARG:CD	3:H:2203:SRA:C5'	1.87	1.51
1:r:18:ARG:NH2	6:r:2002:C:C4'	1.72	1.49
1:H:2016:ARG:HD3	3:H:2203:SRA:C4'	1.46	1.44
1:R:2013:ALA:HB1	3:R:2202:SRA:OP1	1.21	1.36
1:C:2012:ARG:CD	4:C:2204:SSU:OP3	1.76	1.33
1:H:2016:ARG:HD2	3:H:2203:SRA:C5'	1.48	1.32
1:I:2007:LYS:HE2	4:I:3004:SSU:OP2	1.16	1.29
1:I:2016:ARG:NH2	6:I:3007:C:O2'	1.65	1.28
1:W:18:ARG:NH2	5:W:2001:G:O2'	1.66	1.26
1:I:2007:LYS:CE	4:I:3004:SSU:OP2	1.84	1.24
1:r:18:ARG:NH2	6:r:2002:C:H4'	0.94	1.24
1:H:2016:ARG:HD3	3:H:2203:SRA:C5'	1.55	1.24
1:q:18:ARG:HG2	3:q:204:SRA:OP1	1.35	1.23
1:y:9:LYS:CG	4:y:203:SSU:H5''	1.70	1.22
1:K:2012:ARG:HD2	3:K:2203:SRA:O3'	1.13	1.22
1:R:2013:ALA:CB	3:R:2202:SRA:OP1	1.88	1.18
1:H:2012:ARG:HD2	6:H:2202:C:C4'	1.72	1.18
1:I:2007:LYS:CE	4:I:3004:SSU:P	2.32	1.18
1:b:18:ARG:HD2	5:b:207:G:O3'	1.42	1.17
1:k:18:ARG:HG3	3:k:2003:SRA:OP1	1.42	1.17
1:I:2007:LYS:NZ	4:I:3004:SSU:P	2.17	1.17
1:Y:15:ALA:HA	3:Y:2003:SRA:OP1	1.45	1.17
1:H:2012:ARG:CD	6:H:2202:C:H4'	1.76	1.15
1:T:18:ARG:NE	4:T:1002:SSU:H4'	1.54	1.12
1:i:11:ALA:O	4:i:203:SSU:OP3	1.65	1.12
1:I:2007:LYS:CB	4:I:3004:SSU:H5	1.80	1.11
1:y:9:LYS:HG2	4:y:203:SSU:C5'	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:9:LYS:HG2	4:y:203:SSU:H5''	1.18	1.10
1:a:13:MET:HE3	5:a:204:G:OP1	1.49	1.09
1:H:2016:ARG:CD	3:H:2203:SRA:C4'	2.25	1.07
3:R:2202:SRA:H5'	1:2:13:MET:HE3	1.36	1.07
1:C:2012:ARG:HD2	4:C:2204:SSU:OP3	0.90	1.06
1:r:18:ARG:HH22	6:r:2002:C:C4'	1.48	1.05
1:K:2012:ARG:HB3	4:K:2204:SSU:OP3	1.56	1.04
1:K:2012:ARG:CD	3:K:2203:SRA:O3'	2.06	1.04
1:K:2016:ARG:HB3	5:K:2205:G:OP1	1.59	1.01
1:K:2012:ARG:HD2	4:K:2204:SSU:P	2.02	1.00
1:Y:14:ARG:HD2	6:Y:2002:C:C5'	1.91	1.00
1:I:2007:LYS:HB2	4:I:3004:SSU:C5	1.91	1.00
1:K:2012:ARG:CG	4:K:2204:SSU:OP3	2.11	0.98
1:r:18:ARG:HH21	6:r:2002:C:C4'	1.51	0.97
1:H:2016:ARG:HD3	3:H:2203:SRA:H4'	1.01	0.97
1:C:2016:ARG:HH12	4:C:2204:SSU:P	1.88	0.96
1:q:18:ARG:CG	3:q:204:SRA:OP1	2.13	0.96
1:K:2012:ARG:CB	4:K:2204:SSU:OP3	2.13	0.96
1:W:18:ARG:HE	6:W:2002:C:H5'	1.30	0.96
1:4:15:ALA:HB1	4:4:1002:SSU:H5'	1.48	0.96
1:T:18:ARG:HE	4:T:1002:SSU:H4'	1.12	0.96
1:k:18:ARG:CG	3:k:2003:SRA:OP1	2.13	0.96
1:H:2016:ARG:NH1	6:H:2202:C:H2'	1.80	0.95
1:I:2009:ALA:HB1	6:I:3007:C:OP1	1.65	0.95
1:I:2007:LYS:HE2	4:I:3004:SSU:P	1.99	0.95
1:I:2007:LYS:HB2	4:I:3004:SSU:H5	0.96	0.94
1:y:9:LYS:HG2	4:y:203:SSU:C4'	1.97	0.94
1:q:18:ARG:HG2	3:q:204:SRA:P	2.07	0.94
1:b:18:ARG:HB3	6:b:208:C:OP1	1.66	0.94
1:I:2007:LYS:HZ3	4:I:3004:SSU:P	1.88	0.93
1:a:10:SER:HB2	4:a:203:SSU:C4'	1.97	0.93
1:P:14:ARG:NE	4:P:201:SSU:OP3	2.02	0.92
1:H:2016:ARG:CD	3:H:2203:SRA:H4'	1.93	0.92
1:R:2013:ALA:HB1	3:R:2202:SRA:P	2.09	0.92
1:Q:2016:ARG:NH1	4:Q:3003:SSU:H5'	1.84	0.91
1:Q:2016:ARG:HE	5:Q:3004:G:P	1.94	0.91
1:a:10:SER:HB2	4:a:203:SSU:H4'	1.53	0.90
1:Q:2016:ARG:CZ	4:Q:3003:SSU:H5'	2.03	0.89
1:W:18:ARG:CZ	5:W:2001:G:O2'	2.19	0.89
1:I:2007:LYS:CD	4:I:3004:SSU:OP2	2.22	0.86
1:y:9:LYS:HG3	4:y:203:SSU:H5''	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:10:SER:CB	4:a:203:SSU:H4'	2.07	0.84
5:b:201:G:OP1	1:t:15:ALA:HB1	1.78	0.83
1:H:2016:ARG:NH1	6:H:2202:C:C2'	2.41	0.83
1:C:2016:ARG:NH1	4:C:2204:SSU:OP3	2.12	0.82
1:L:2016:ARG:NH2	3:L:2201:SRA:O2'	2.12	0.82
1:r:18:ARG:HH22	6:r:2002:C:H4'	1.01	0.82
3:R:2202:SRA:C5'	1:2:13:MET:HE3	2.09	0.81
1:C:2016:ARG:HH11	4:C:2204:SSU:H5'	1.44	0.80
1:H:2016:ARG:CZ	6:H:2202:C:O2'	2.29	0.80
1:b:18:ARG:CD	5:b:207:G:O3'	2.28	0.80
1:b:18:ARG:HB3	6:b:208:C:P	2.22	0.79
1:k:83:GLN:HE22	1:k:182:GLY:HA3	1.48	0.79
1:Y:14:ARG:HD2	6:Y:2002:C:H4'	1.64	0.79
1:C:2016:ARG:NH1	4:C:2204:SSU:P	2.56	0.79
1:K:2012:ARG:HG2	4:K:2204:SSU:OP3	1.82	0.79
1:P:18:ARG:NH1	3:P:202:SRA:OP3	2.16	0.78
1:H:2081:GLN:HE22	1:H:2180:GLY:HA3	1.47	0.78
1:Q:2016:ARG:NE	5:Q:3004:G:P	2.56	0.78
1:y:83:GLN:HE22	1:y:182:GLY:HA3	1.48	0.77
1:4:83:GLN:HE22	1:4:182:GLY:HA3	1.49	0.77
1:Y:15:ALA:CA	3:Y:2003:SRA:OP1	2.30	0.77
1:H:2016:ARG:NH1	6:H:2202:C:O2'	2.18	0.77
3:F:203:SRA:H2'	4:F:204:SSU:H6	1.67	0.77
3:b:205:SRA:H2'	4:b:206:SSU:H6	1.67	0.77
3:t:205:SRA:H2'	4:t:206:SSU:H6	1.67	0.77
1:Y:14:ARG:HD2	6:Y:2002:C:H5'	1.67	0.76
3:4:1001:SRA:H2'	4:4:1002:SSU:H6	1.67	0.76
3:Q:3002:SRA:H2'	4:Q:3003:SSU:H6	1.67	0.76
1:W:83:GLN:HE22	1:W:182:GLY:HA3	1.50	0.76
3:J:3002:SRA:H2'	4:J:3003:SSU:H6	1.68	0.76
3:L:2206:SRA:H2'	4:L:2207:SSU:H6	1.67	0.76
3:a:202:SRA:H2'	4:a:203:SSU:H6	1.67	0.76
3:P:202:SRA:H2'	4:P:203:SSU:H6	1.67	0.76
1:X:83:GLN:HE22	1:X:182:GLY:HA3	1.51	0.76
1:4:15:ALA:CB	4:4:1002:SSU:H5'	2.16	0.76
3:H:2204:SRA:H2'	4:K:2201:SSU:H6	1.67	0.76
1:Q:2081:GLN:HE22	1:Q:2180:GLY:HA3	1.51	0.76
3:i:202:SRA:H2'	4:i:203:SSU:H6	1.67	0.76
3:H:2208:SRA:H2'	4:H:2209:SSU:H6	1.67	0.76
3:t:203:SRA:H2'	4:t:204:SSU:H6	1.67	0.76
3:K:2203:SRA:H2'	4:K:2204:SSU:H6	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2201:SRA:H2'	4:L:2202:SSU:H6	1.67	0.75
3:C:2203:SRA:H2'	4:C:2204:SSU:H6	1.67	0.75
1:I:2081:GLN:HE22	1:I:2180:GLY:HA3	1.52	0.75
1:L:2015:LYS:HE3	3:L:2206:SRA:H5''	1.68	0.75
4:X:202:SSU:H6	3:q:205:SRA:H2'	1.67	0.75
3:w:202:SRA:H2'	4:w:203:SSU:H6	1.67	0.74
3:Y:2004:SRA:H2'	4:v:201:SSU:H6	1.67	0.74
1:t:11:ALA:HB1	3:t:205:SRA:O3'	1.86	0.74
1:M:2081:GLN:HE22	1:M:2180:GLY:HA3	1.52	0.74
3:R:2203:SRA:H2'	4:R:2204:SSU:H6	1.67	0.74
3:T:1001:SRA:H2'	4:T:1002:SSU:H6	1.67	0.74
3:k:2004:SRA:H2'	4:3:203:SSU:H6	1.67	0.73
1:x:83:GLN:HE22	1:x:182:GLY:HA3	1.53	0.73
1:b:14:ARG:HD2	4:b:206:SSU:O3'	1.89	0.73
1:Y:14:ARG:HD2	6:Y:2002:C:C4'	2.19	0.72
1:T:18:ARG:HE	4:T:1002:SSU:C4'	1.94	0.72
1:b:18:ARG:NE	5:b:207:G:C3'	2.50	0.70
1:T:18:ARG:NE	4:T:1002:SSU:C4'	2.33	0.69
1:a:10:SER:CB	4:a:203:SSU:C4'	2.68	0.69
1:a:10:SER:OG	4:a:203:SSU:H5''	1.92	0.69
1:g:18:ARG:NH2	6:g:201:C:OP2	2.26	0.69
1:r:18:ARG:NH2	6:r:2002:C:O4'	2.25	0.69
1:a:10:SER:HB2	4:a:203:SSU:O4'	1.92	0.69
1:4:15:ALA:CB	4:4:1002:SSU:C5'	2.71	0.68
1:r:18:ARG:HH21	6:r:2002:C:C3'	2.07	0.68
1:E:2016:ARG:NH2	6:E:3002:C:O2'	2.27	0.67
1:4:15:ALA:HB2	4:4:1002:SSU:H5''	1.76	0.67
1:I:2007:LYS:CD	4:I:3004:SSU:P	2.83	0.67
1:r:18:ARG:HH21	6:r:2002:C:H4'	0.84	0.66
6:E:3002:C:H2'	3:E:3003:SRA:H8	1.78	0.66
3:F:202:SRA:H8	6:r:2002:C:H2'	1.78	0.66
1:H:2012:ARG:HD2	6:H:2202:C:H4'	0.81	0.65
6:H:2202:C:H2'	3:H:2203:SRA:H8	1.78	0.65
3:E:3003:SRA:H2'	3:J:3002:SRA:H8	1.78	0.65
4:K:2202:SSU:H2'	3:K:2203:SRA:H8	1.79	0.65
6:L:2204:C:H2'	3:L:2205:SRA:H8	1.78	0.65
3:b:205:SRA:H8	4:w:201:SSU:H2'	1.78	0.65
6:g:201:C:H2'	3:g:202:SRA:H8	1.78	0.65
3:h:201:SRA:H8	6:i:205:C:H2'	1.78	0.65
6:r:2003:C:H2'	3:r:2004:SRA:H8	1.78	0.65
6:b:202:C:H2'	3:b:203:SRA:H8	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:2002:C:H2'	3:k:2003:SRA:H8	1.78	0.65
3:F:202:SRA:H2'	3:F:203:SRA:H8	1.78	0.65
6:W:2002:C:H2'	3:W:2003:SRA:H8	1.79	0.65
6:q:203:C:H2'	3:q:204:SRA:H8	1.78	0.65
6:z:202:C:H2'	3:z:203:SRA:H8	1.78	0.65
6:C:2206:C:H2'	3:x:201:SRA:H8	1.78	0.65
3:L:2205:SRA:H2'	3:L:2206:SRA:H8	1.78	0.65
1:I:2007:LYS:HZ2	4:I:3004:SSU:P	2.14	0.65
4:P:201:SSU:H2'	3:P:202:SRA:H8	1.79	0.65
1:y:9:LYS:CG	4:y:203:SSU:C5'	2.53	0.65
6:b:208:C:H2'	3:b:209:SRA:H8	1.78	0.65
4:i:201:SSU:H2'	3:i:202:SRA:H8	1.79	0.65
3:q:204:SRA:H2'	3:q:205:SRA:H8	1.79	0.65
3:e:204:SRA:H2'	3:w:202:SRA:H8	1.79	0.64
6:y:201:C:H2'	3:y:202:SRA:H8	1.78	0.64
6:N:2201:C:H2'	3:N:2202:SRA:H8	1.79	0.64
3:T:1001:SRA:H8	4:X:201:SSU:H2'	1.78	0.64
3:C:2203:SRA:N6	3:t:203:SRA:N6	1.94	0.64
6:I:3007:C:H2'	3:I:3008:SRA:H8	1.78	0.64
6:I:3002:C:H2'	3:I:3003:SRA:H8	1.78	0.64
3:Q:3002:SRA:H8	4:3:202:SSU:H2'	1.78	0.64
3:L:2201:SRA:H8	4:g:203:SSU:H2'	1.79	0.64
1:R:2013:ALA:CB	3:R:2202:SRA:P	2.78	0.64
3:R:2202:SRA:H8	6:2:202:C:H2'	1.78	0.64
3:H:2208:SRA:H8	3:I:3008:SRA:H2'	1.78	0.64
1:a:10:SER:CA	4:a:203:SSU:H4'	2.28	0.64
6:g:205:C:H2'	3:g:206:SRA:H8	1.78	0.64
3:H:2203:SRA:H2'	3:H:2204:SRA:H8	1.78	0.63
4:z:201:SSU:H2'	3:4:1001:SRA:H8	1.78	0.63
4:H:2207:SSU:H2'	3:t:205:SRA:H8	1.79	0.63
4:a:201:SSU:H2'	3:a:202:SRA:H8	1.79	0.63
6:e:203:C:H2'	3:e:204:SRA:H8	1.78	0.63
3:k:2003:SRA:H2'	3:k:2004:SRA:H8	1.78	0.63
3:Y:2003:SRA:H2'	3:Y:2004:SRA:H8	1.79	0.63
3:R:2202:SRA:H2'	3:R:2203:SRA:H8	1.79	0.63
3:W:2003:SRA:H2'	3:t:203:SRA:H8	1.78	0.63
6:Y:2002:C:H2'	3:Y:2003:SRA:H8	1.78	0.63
3:C:2203:SRA:H8	4:t:201:SSU:H2'	1.79	0.62
3:L:2206:SRA:N6	3:P:202:SRA:N6	1.94	0.62
3:F:203:SRA:N6	3:i:202:SRA:N6	1.94	0.62
1:t:11:ALA:O	4:t:206:SSU:OP3	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:205:SRA:N6	3:w:202:SRA:N6	1.94	0.61
1:Q:2016:ARG:NE	5:Q:3004:G:OP1	2.32	0.61
1:I:2007:LYS:HD3	4:I:3004:SSU:P	2.40	0.61
1:L:2016:ARG:HH21	4:L:2202:SSU:H5''	1.64	0.61
3:H:2204:SRA:N6	3:L:2201:SRA:N6	1.94	0.61
1:e:18:ARG:NE	5:e:202:G:H4'	1.76	0.61
1:t:150:PRO:HB2	4:t:204:SSU:OP3	2.01	0.60
1:I:2008:SER:OG	3:I:3003:SRA:N6	2.34	0.60
1:J:2006:ARG:HG2	1:J:2007:LYS:HD2	1.82	0.60
3:b:205:SRA:HN62	3:w:202:SRA:C6	2.06	0.60
1:I:2016:ARG:HH22	6:I:3007:C:H4'	1.67	0.60
3:Y:2004:SRA:N6	3:4:1001:SRA:N6	1.94	0.60
3:Q:3002:SRA:N6	3:k:2004:SRA:N6	1.94	0.60
1:L:2011:MET:HG2	3:L:2205:SRA:OP1	2.03	0.59
3:R:2203:SRA:N6	3:a:202:SRA:N6	1.94	0.59
3:H:2208:SRA:N6	3:t:205:SRA:N6	1.94	0.59
1:C:2016:ARG:NH1	4:C:2204:SSU:H5'	2.17	0.59
1:4:15:ALA:HB2	4:4:1002:SSU:C5'	2.33	0.59
1:K:2012:ARG:CD	4:K:2204:SSU:OP3	2.50	0.59
1:G:2089:ARG:NH1	1:G:2091:ASN:OD1	2.36	0.58
1:P:14:ARG:CD	4:P:201:SSU:OP3	2.51	0.58
1:a:91:ARG:NH1	1:a:93:ASN:OD1	2.37	0.58
1:7:91:ARG:NH1	1:7:93:ASN:OD1	2.36	0.58
1:L:2089:ARG:NH1	1:L:2091:ASN:OD1	2.37	0.58
3:T:1001:SRA:N6	3:q:205:SRA:N6	1.94	0.58
1:W:18:ARG:NH2	5:W:2001:G:C2'	2.65	0.58
1:e:91:ARG:NH1	1:e:93:ASN:OD1	2.36	0.58
1:u:91:ARG:NH1	1:u:93:ASN:OD1	2.37	0.58
1:U:91:ARG:NH1	1:U:93:ASN:OD1	2.36	0.58
1:b:18:ARG:NE	5:b:207:G:H3'	2.18	0.58
1:i:91:ARG:NH1	1:i:93:ASN:OD1	2.37	0.58
1:k:91:ARG:NH1	1:k:93:ASN:OD1	2.37	0.58
1:M:2089:ARG:NH1	1:M:2091:ASN:OD1	2.37	0.58
1:T:91:ARG:NH1	1:T:93:ASN:OD1	2.36	0.58
1:I:2016:ARG:NH2	6:I:3007:C:C2'	2.66	0.57
1:K:2016:ARG:CB	5:K:2205:G:OP1	2.44	0.57
1:o:88:ILE:HD12	1:o:174:LEU:HD22	1.86	0.57
1:K:2086:ILE:HD12	1:K:2172:LEU:HD22	1.86	0.57
1:L:2011:MET:HG2	3:L:2205:SRA:H5''	1.84	0.57
1:X:88:ILE:HD12	1:X:174:LEU:HD22	1.87	0.57
1:g:91:ARG:NH1	1:g:93:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:91:ARG:NH1	1:w:93:ASN:OD1	2.37	0.57
1:W:88:ILE:HD12	1:W:174:LEU:HD22	1.86	0.57
1:d:91:ARG:NH1	1:d:93:ASN:OD1	2.36	0.57
1:p:88:ILE:HD12	1:p:174:LEU:HD22	1.86	0.57
1:y:91:ARG:NH1	1:y:93:ASN:OD1	2.38	0.57
3:R:2202:SRA:C5'	1:2:13:MET:CE	2.81	0.57
1:W:91:ARG:NH1	1:W:93:ASN:OD1	2.37	0.57
1:X:91:ARG:NH1	1:X:93:ASN:OD1	2.38	0.57
1:p:91:ARG:NH1	1:p:93:ASN:OD1	2.37	0.57
1:k:88:ILE:HD12	1:k:174:LEU:HD22	1.86	0.57
1:o:91:ARG:NH1	1:o:93:ASN:OD1	2.38	0.57
1:K:2089:ARG:NH1	1:K:2091:ASN:OD1	2.38	0.57
1:a:10:SER:HA	4:a:203:SSU:H4'	1.87	0.57
1:i:88:ILE:HD12	1:i:174:LEU:HD22	1.86	0.57
3:F:203:SRA:C6	3:i:202:SRA:HN62	2.06	0.57
1:f:91:ARG:NH1	1:f:93:ASN:OD1	2.38	0.57
1:3:91:ARG:NH1	1:3:93:ASN:OD1	2.38	0.57
1:O:2086:ILE:HD12	1:O:2172:LEU:HD22	1.87	0.57
1:f:88:ILE:HD12	1:f:174:LEU:HD22	1.87	0.57
1:D:2089:ARG:NH1	1:D:2091:ASN:OD1	2.38	0.57
1:I:2086:ILE:HD12	1:I:2172:LEU:HD22	1.87	0.57
1:Z:88:ILE:HD12	1:Z:174:LEU:HD22	1.87	0.57
1:k:18:ARG:CB	3:k:2003:SRA:OP1	2.53	0.57
1:2:88:ILE:HD12	1:2:174:LEU:HD22	1.86	0.57
1:2:91:ARG:NH1	1:2:93:ASN:OD1	2.37	0.57
1:4:88:ILE:HD12	1:4:174:LEU:HD22	1.87	0.57
1:I:2007:LYS:HD3	4:I:3004:SSU:OP2	2.04	0.56
1:P:91:ARG:NH1	1:P:93:ASN:OD1	2.38	0.56
1:S:2089:ARG:NH1	1:S:2091:ASN:OD1	2.38	0.56
3:T:1001:SRA:HN62	3:q:205:SRA:C6	2.06	0.56
1:z:91:ARG:NH1	1:z:93:ASN:OD1	2.38	0.56
1:4:15:ALA:HB1	4:4:1002:SSU:C5'	2.28	0.56
1:H:2089:ARG:NH1	1:H:2091:ASN:OD1	2.38	0.56
1:M:2086:ILE:HD12	1:M:2172:LEU:HD22	1.86	0.56
1:N:2089:ARG:NH1	1:N:2091:ASN:OD1	2.37	0.56
5:C:2205:G:H2'	6:C:2206:C:H6	1.71	0.56
1:H:2016:ARG:HH12	6:H:2202:C:H2'	1.66	0.56
6:I:3002:C:H6	5:K:2205:G:H2'	1.70	0.56
6:N:2201:C:H6	5:T:1003:G:H2'	1.71	0.56
1:Z:91:ARG:NH1	1:Z:93:ASN:OD1	2.38	0.56
1:j:91:ARG:NH1	1:j:93:ASN:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:201:G:H2'	6:b:202:C:H6	1.70	0.56
5:k:2001:G:H2'	6:k:2002:C:H6	1.71	0.56
1:t:88:ILE:HD12	1:t:174:LEU:HD22	1.87	0.56
1:v:91:ARG:NH1	1:v:93:ASN:OD1	2.39	0.56
1:C:2016:ARG:HH11	4:C:2204:SSU:C5'	2.15	0.56
1:h:91:ARG:NH1	1:h:93:ASN:OD1	2.39	0.56
5:i:204:G:H2'	6:i:205:C:H6	1.70	0.56
1:6:91:ARG:NH1	1:6:93:ASN:OD1	2.38	0.56
1:R:2089:ARG:NH1	1:R:2091:ASN:OD1	2.39	0.56
5:g:204:G:H2'	6:g:205:C:H6	1.71	0.56
1:q:91:ARG:NH1	1:q:93:ASN:OD1	2.38	0.56
5:r:2001:G:H2'	6:r:2002:C:H6	1.71	0.56
6:z:202:C:H6	5:4:1003:G:H2'	1.71	0.56
1:Y:88:ILE:HD12	1:Y:174:LEU:HD22	1.88	0.56
1:Y:91:ARG:NH1	1:Y:93:ASN:OD1	2.39	0.56
1:1:60:ARG:NH1	1:1:62:GLY:O	2.39	0.56
1:4:91:ARG:NH1	1:4:93:ASN:OD1	2.39	0.56
5:Q:3004:G:H2'	6:r:2003:C:H6	1.70	0.56
1:Y:60:ARG:NH1	1:Y:62:GLY:O	2.39	0.56
1:O:2058:ARG:NH1	1:O:2060:GLY:O	2.39	0.56
5:a:204:G:H2'	6:g:201:C:H6	1.70	0.56
5:e:202:G:H2'	6:e:203:C:H6	1.71	0.56
5:q:202:G:H2'	6:q:203:C:H6	1.71	0.56
5:H:2201:G:H2'	6:H:2202:C:H6	1.71	0.56
1:V:91:ARG:NH1	1:V:93:ASN:OD1	2.39	0.56
1:W:15:ALA:HB1	6:W:2002:C:OP1	2.05	0.56
1:y:88:ILE:HD12	1:y:174:LEU:HD22	1.86	0.56
1:0:93:ASN:ND2	1:0:126:THR:HG1	2.04	0.56
5:I:3006:G:H2'	6:I:3007:C:H6	1.71	0.55
5:Y:2001:G:H2'	6:Y:2002:C:H6	1.71	0.55
5:i:204:G:C4	6:i:205:C:C5	2.94	0.55
5:q:202:G:C4	6:q:203:C:C5	2.94	0.55
5:r:2001:G:C4	6:r:2002:C:C5	2.94	0.55
6:I:3002:C:C5	5:K:2205:G:C4	2.95	0.55
1:K:2012:ARG:HD2	4:K:2204:SSU:OP3	2.07	0.55
1:K:2012:ARG:CD	4:K:2204:SSU:P	2.89	0.55
5:b:207:G:C4	6:b:208:C:C5	2.94	0.55
1:m:91:ARG:NH1	1:m:93:ASN:OD1	2.39	0.55
5:I:3006:G:C4	6:I:3007:C:C5	2.94	0.55
5:P:204:G:H2'	6:y:201:C:H6	1.70	0.55
5:R:2201:G:C4	6:2:202:C:C5	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:2001:G:H2'	6:W:2002:C:H6	1.71	0.55
6:E:3002:C:H6	5:I:3005:G:H2'	1.71	0.55
5:W:2001:G:C4	6:W:2002:C:C5	2.94	0.55
1:Y:14:ARG:HD2	6:Y:2002:C:H5''	1.83	0.55
5:b:207:G:H2'	6:b:208:C:H6	1.71	0.55
1:m:88:ILE:HD12	1:m:174:LEU:HD22	1.87	0.55
1:3:88:ILE:HD12	1:3:174:LEU:HD22	1.88	0.55
1:6:88:ILE:HD12	1:6:174:LEU:HD22	1.88	0.55
1:A:2089:ARG:NH1	1:A:2091:ASN:OD1	2.38	0.55
5:R:2201:G:H2'	6:2:202:C:H6	1.71	0.55
5:g:204:G:C4	6:g:205:C:C5	2.94	0.55
1:L:2015:LYS:HD2	3:L:2206:SRA:OP1	2.07	0.55
5:Q:3004:G:C4	6:r:2003:C:C5	2.94	0.55
1:c:91:ARG:NH1	1:c:93:ASN:OD1	2.40	0.55
5:e:202:G:C4	6:e:203:C:C5	2.94	0.55
1:s:91:ARG:NH1	1:s:93:ASN:OD1	2.40	0.55
5:C:2205:G:C4	6:C:2206:C:C5	2.94	0.55
5:H:2201:G:C4	6:H:2202:C:C5	2.94	0.55
5:Y:2001:G:C4	6:Y:2002:C:C5	2.94	0.55
6:E:3002:C:C5	5:I:3005:G:C4	2.95	0.55
1:I:2089:ARG:NH1	1:I:2091:ASN:OD1	2.39	0.55
6:L:2204:C:C5	5:y:204:G:C4	2.94	0.55
1:R:2102:GLU:OE1	1:q:96:ARG:NH2	2.40	0.55
1:b:91:ARG:NH1	1:b:93:ASN:OD1	2.39	0.55
5:k:2001:G:C4	6:k:2002:C:C5	2.94	0.55
1:t:91:ARG:NH1	1:t:93:ASN:OD1	2.40	0.55
1:3:60:ARG:NH1	1:3:62:GLY:O	2.39	0.55
1:D:2094:ARG:NH2	1:j:104:GLU:OE1	2.40	0.55
1:O:2089:ARG:NH1	1:O:2091:ASN:OD1	2.40	0.55
1:S:2094:ARG:NH2	1:V:104:GLU:OE1	2.40	0.55
1:c:88:ILE:HD12	1:c:174:LEU:HD22	1.89	0.55
1:1:91:ARG:NH1	1:1:93:ASN:OD1	2.40	0.55
6:L:2204:C:H6	5:y:204:G:H2'	1.71	0.55
6:z:202:C:C5	5:4:1003:G:C4	2.94	0.55
6:N:2201:C:C5	5:T:1003:G:C4	2.94	0.54
1:P:18:ARG:HH11	3:P:202:SRA:P	2.30	0.54
5:a:204:G:C4	6:g:201:C:C5	2.94	0.54
1:n:91:ARG:NH1	1:n:93:ASN:OD1	2.40	0.54
1:y:9:LYS:HG2	4:y:203:SSU:H4'	1.88	0.54
1:1:88:ILE:HD12	1:1:174:LEU:HD22	1.89	0.54
1:5:91:ARG:NH1	1:5:93:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:60:ARG:NH1	1:6:62:GLY:O	2.41	0.54
1:A:2102:GLU:OE1	1:P:96:ARG:NH2	2.41	0.54
1:B:2089:ARG:NH1	1:B:2091:ASN:OD1	2.41	0.54
1:P:88:ILE:HD12	1:P:174:LEU:HD22	1.90	0.54
1:v:104:GLU:OE1	1:z:96:ARG:NH2	2.40	0.54
1:5:60:ARG:NH1	1:5:62:GLY:O	2.40	0.54
1:7:88:ILE:HD12	1:7:174:LEU:HD22	1.90	0.54
1:C:2114:ASN:O	1:C:2118:LEU:HB2	2.07	0.54
1:H:2094:ARG:NH2	1:b:104:GLU:OE1	2.40	0.54
1:H:2102:GLU:OE1	1:b:96:ARG:NH2	2.41	0.54
1:O:2006:ARG:HG2	1:O:2007:LYS:HD2	1.88	0.54
1:Q:2016:ARG:NH1	4:Q:3003:SSU:OP3	2.41	0.54
1:R:2086:ILE:HD12	1:R:2172:LEU:HD22	1.90	0.54
5:b:201:G:C4	6:b:202:C:C5	2.94	0.54
1:A:2094:ARG:NH2	1:P:104:GLU:OE1	2.41	0.54
1:C:2120:GLN:HG3	1:m:168:PRO:HG2	1.90	0.54
3:J:3002:SRA:N6	3:K:2203:SRA:N6	1.94	0.54
3:T:1001:SRA:C6	3:q:205:SRA:HN62	2.07	0.54
1:c:60:ARG:NH1	1:c:62:GLY:O	2.40	0.54
1:g:88:ILE:HD12	1:g:174:LEU:HD22	1.90	0.54
1:G:2086:ILE:HD12	1:G:2172:LEU:HD22	1.90	0.54
1:J:2089:ARG:NH1	1:J:2091:ASN:OD1	2.41	0.54
1:j:88:ILE:HD12	1:j:174:LEU:HD22	1.89	0.54
1:F:91:ARG:NH1	1:F:93:ASN:OD1	2.41	0.54
1:H:2058:ARG:NH1	1:H:2060:GLY:O	2.41	0.54
1:R:2094:ARG:NH2	1:q:104:GLU:OE1	2.41	0.54
1:h:60:ARG:NH1	1:h:62:GLY:O	2.40	0.54
1:r:91:ARG:NH1	1:r:93:ASN:OD1	2.41	0.54
1:Q:2089:ARG:NH1	1:Q:2091:ASN:OD1	2.41	0.54
1:U:88:ILE:HD12	1:U:174:LEU:HD22	1.89	0.54
1:s:88:ILE:HD12	1:s:174:LEU:HD22	1.89	0.54
1:D:2102:GLU:OE1	1:j:96:ARG:NH2	2.41	0.53
5:P:204:G:C4	6:y:201:C:C5	2.94	0.53
1:k:18:ARG:HG3	3:k:2003:SRA:P	2.47	0.53
1:l:91:ARG:NH1	1:l:93:ASN:OD1	2.41	0.53
1:0:91:ARG:NH1	1:0:93:ASN:OD1	2.41	0.53
1:A:2086:ILE:HD12	1:A:2172:LEU:HD22	1.90	0.53
1:S:2102:GLU:OE1	1:V:96:ARG:NH2	2.41	0.53
1:b:88:ILE:HD12	1:b:174:LEU:HD22	1.89	0.53
1:v:88:ILE:HD12	1:v:174:LEU:HD22	1.90	0.53
1:v:60:ARG:NH1	1:v:62:GLY:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:91:ARG:NH1	1:x:93:ASN:OD1	2.41	0.53
1:L:2086:ILE:HD12	1:L:2172:LEU:HD22	1.90	0.53
1:h:88:ILE:HD12	1:h:174:LEU:HD22	1.88	0.53
1:n:93:ASN:ND2	1:n:126:THR:HG1	2.05	0.53
1:v:96:ARG:NH2	1:z:104:GLU:OE1	2.41	0.53
1:D:2058:ARG:NH1	1:D:2060:GLY:O	2.42	0.53
3:J:3002:SRA:C6	3:K:2203:SRA:HN62	2.06	0.53
1:a:88:ILE:HD12	1:a:174:LEU:HD22	1.90	0.53
1:C:2089:ARG:NH1	1:C:2091:ASN:OD1	2.41	0.53
1:E:2089:ARG:NH1	1:E:2091:ASN:OD1	2.41	0.53
1:S:2086:ILE:HD12	1:S:2172:LEU:HD22	1.90	0.53
1:V:88:ILE:HD12	1:V:174:LEU:HD22	1.89	0.53
1:r:104:GLU:OE1	1:3:96:ARG:NH2	2.42	0.53
1:5:93:ASN:ND2	1:5:126:THR:OG1	2.41	0.53
1:R:2058:ARG:NH1	1:R:2060:GLY:O	2.42	0.53
1:j:60:ARG:NH1	1:j:62:GLY:O	2.41	0.53
1:4:60:ARG:NH1	1:4:62:GLY:O	2.42	0.53
1:N:2086:ILE:HD12	1:N:2172:LEU:HD22	1.91	0.53
1:Y:14:ARG:CD	6:Y:2002:C:H5'	2.38	0.53
1:q:88:ILE:HD12	1:q:174:LEU:HD22	1.90	0.53
1:z:60:ARG:NH1	1:z:62:GLY:O	2.41	0.53
1:G:2166:PRO:HG2	1:p:122:GLN:HG3	1.91	0.53
1:Q:2102:GLU:OE1	1:Y:96:ARG:NH2	2.42	0.53
1:S:2058:ARG:NH1	1:S:2060:GLY:O	2.41	0.53
1:k:60:ARG:NH1	1:k:62:GLY:O	2.42	0.53
1:q:60:ARG:NH1	1:q:62:GLY:O	2.41	0.53
1:w:88:ILE:HD12	1:w:174:LEU:HD22	1.91	0.53
1:D:2086:ILE:HD12	1:D:2172:LEU:HD22	1.90	0.52
1:J:2086:ILE:HD12	1:J:2172:LEU:HD22	1.91	0.52
1:J:2091:ASN:ND2	1:J:2124:THR:OG1	2.41	0.52
1:d:88:ILE:HD12	1:d:174:LEU:HD22	1.91	0.52
1:z:88:ILE:HD12	1:z:174:LEU:HD22	1.90	0.52
1:3:116:ASN:O	1:3:120:LEU:HB2	2.08	0.52
1:H:2086:ILE:HD12	1:H:2172:LEU:HD22	1.91	0.52
1:M:2058:ARG:NH1	1:M:2060:GLY:O	2.42	0.52
1:C:2091:ASN:ND2	1:C:2124:THR:OG1	2.41	0.52
1:F:93:ASN:ND2	1:F:126:THR:OG1	2.43	0.52
1:O:2120:GLN:HG3	1:l:168:PRO:HG2	1.92	0.52
1:n:93:ASN:ND2	1:n:126:THR:OG1	2.43	0.52
1:5:88:ILE:HD12	1:5:174:LEU:HD22	1.92	0.52
1:I:2058:ARG:NH1	1:I:2060:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:88:ILE:HD12	1:T:174:LEU:HD22	1.91	0.52
1:u:60:ARG:NH1	1:u:62:GLY:O	2.43	0.52
1:u:88:ILE:HD12	1:u:174:LEU:HD22	1.90	0.52
1:0:93:ASN:ND2	1:0:126:THR:OG1	2.43	0.52
1:1:8:ARG:HG2	1:1:9:LYS:HD2	1.91	0.52
1:0:168:PRO:HG2	1:1:122:GLN:HG3	1.92	0.52
1:4:122:GLN:HG3	1:5:168:PRO:HG2	1.93	0.52
1:F:104:GLU:OE1	1:h:96:ARG:NH2	2.43	0.51
1:s:60:ARG:NH1	1:s:62:GLY:O	2.43	0.51
1:E:2080:SER:HB2	1:E:2134:SER:HA	1.93	0.51
1:F:88:ILE:HD12	1:F:174:LEU:HD22	1.93	0.51
1:l:93:ASN:ND2	1:l:126:THR:OG1	2.42	0.51
1:r:88:ILE:HD12	1:r:174:LEU:HD22	1.92	0.51
1:r:93:ASN:ND2	1:r:126:THR:OG1	2.43	0.51
1:x:93:ASN:ND2	1:x:126:THR:OG1	2.43	0.51
1:2:31:LEU:HB3	1:2:188:TYR:HB3	1.92	0.51
1:n:104:GLU:OE1	1:6:96:ARG:NH2	2.44	0.51
1:C:2086:ILE:HD12	1:C:2172:LEU:HD22	1.92	0.51
1:C:2016:ARG:NH1	4:C:2204:SSU:C5'	2.73	0.51
1:E:2091:ASN:ND2	1:E:2124:THR:OG1	2.43	0.51
1:Q:2086:ILE:HD12	1:Q:2172:LEU:HD22	1.92	0.51
1:n:168:PRO:HG2	1:6:122:GLN:HG3	1.92	0.51
1:4:96:ARG:NH2	1:5:104:GLU:OE1	2.44	0.51
1:k:18:ARG:HB2	3:k:2003:SRA:OP1	2.10	0.51
1:0:88:ILE:HD12	1:0:174:LEU:HD22	1.92	0.51
1:B:2086:ILE:HD12	1:B:2172:LEU:HD22	1.92	0.51
1:B:2166:PRO:HG2	1:c:122:GLN:HG3	1.92	0.51
1:X:31:LEU:HB3	1:X:188:TYR:HB3	1.93	0.51
1:o:31:LEU:HB3	1:o:188:TYR:HB3	1.93	0.51
1:K:2029:LEU:HB3	1:K:2186:TYR:HB3	1.93	0.51
1:t:122:GLN:HG3	1:x:168:PRO:HG2	1.92	0.51
1:x:88:ILE:HD12	1:x:174:LEU:HD22	1.91	0.51
1:N:2058:ARG:NH1	1:N:2060:GLY:O	2.43	0.51
1:Q:2166:PRO:HG2	1:Y:122:GLN:HG3	1.93	0.51
1:l:88:ILE:HD12	1:l:174:LEU:HD22	1.92	0.51
1:n:82:SER:HB2	1:n:136:SER:HA	1.93	0.51
1:E:2086:ILE:HD12	1:E:2172:LEU:HD22	1.93	0.50
1:I:2094:ARG:NH2	1:J:2102:GLU:OE1	2.44	0.50
1:C:2102:GLU:OE1	1:m:96:ARG:NH2	2.44	0.50
1:F:168:PRO:HG2	1:h:122:GLN:HG3	1.93	0.50
1:I:2016:ARG:HH22	6:I:3007:C:C4'	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:31:LEU:HB3	1:i:188:TYR:HB3	1.93	0.50
1:r:168:PRO:HG2	1:3:122:GLN:HG3	1.93	0.50
1:E:2166:PRO:HG2	1:s:122:GLN:HG3	1.92	0.50
1:O:2094:ARG:NH2	1:l:104:GLU:OE1	2.45	0.50
1:I:2120:GLN:HG3	1:J:2166:PRO:HG2	1.93	0.50
1:W:168:PRO:HG2	1:w:122:GLN:HG3	1.94	0.50
1:n:88:ILE:HD12	1:n:174:LEU:HD22	1.93	0.50
1:E:2102:GLU:OE1	1:s:96:ARG:NH2	2.45	0.50
1:L:2058:ARG:NH1	1:L:2060:GLY:O	2.45	0.50
1:4:15:ALA:CB	4:4:1002:SSU:H5''	2.39	0.50
1:I:2009:ALA:CB	6:I:3007:C:OP1	2.51	0.49
1:W:31:LEU:HB3	1:W:188:TYR:HB3	1.94	0.49
1:I:2014:VAL:HG13	1:K:2017:MET:HE1	1.93	0.49
1:t:11:ALA:HB1	3:t:205:SRA:H4'	1.94	0.49
1:0:104:GLU:OE1	1:1:96:ARG:NH2	2.45	0.49
1:Q:2091:ASN:ND2	1:Q:2124:THR:OG1	2.43	0.49
1:B:2091:ASN:ND2	1:B:2124:THR:OG1	2.44	0.49
1:Z:31:LEU:HB3	1:Z:188:TYR:HB3	1.94	0.49
1:X:19:MET:HE1	1:c:13:MET:HG3	1.95	0.49
1:E:2092:MET:HG2	1:s:94:MET:HG2	1.95	0.49
1:n:96:ARG:NH2	1:6:104:GLU:OE1	2.46	0.49
1:o:19:MET:HE1	1:1:16:VAL:HG13	1.95	0.49
1:c:28:ARG:HG2	1:c:191:VAL:HG22	1.95	0.49
1:f:31:LEU:HB3	1:f:188:TYR:HB3	1.94	0.49
1:m:60:ARG:NH1	1:m:62:GLY:O	2.45	0.49
1:H:2016:ARG:HD2	3:H:2203:SRA:H5'	0.52	0.49
1:K:2016:ARG:HG2	4:K:2204:SSU:O3'	2.13	0.49
1:3:28:ARG:HG2	1:3:191:VAL:HG22	1.94	0.49
1:P:14:ARG:HD3	4:P:201:SSU:H5'	1.94	0.49
1:0:92:ASP:OD2	1:0:95:ASN:ND2	2.46	0.49
1:y:31:LEU:HB3	1:y:188:TYR:HB3	1.93	0.49
1:M:2029:LEU:HB3	1:M:2186:TYR:HB3	1.94	0.48
1:t:104:GLU:OE1	1:x:96:ARG:NH2	2.46	0.48
1:0:94:MET:HG2	1:1:94:MET:HG2	1.95	0.48
1:M:2166:PRO:HG2	1:T:122:GLN:HG3	1.94	0.48
1:e:28:ARG:HG2	1:e:191:VAL:HG22	1.95	0.48
1:H:2012:ARG:HD2	6:H:2202:C:C5'	2.42	0.48
1:O:2092:MET:HG2	1:l:94:MET:HG2	1.95	0.48
1:5:92:ASP:OD2	1:5:95:ASN:ND2	2.46	0.48
3:L:2206:SRA:HN62	3:P:202:SRA:C6	2.07	0.48
1:W:18:ARG:HH21	5:W:2001:G:C3'	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:31:LEU:HB3	1:p:188:TYR:HB3	1.95	0.48
1:t:28:ARG:HG2	1:t:191:VAL:HG22	1.96	0.48
1:6:28:ARG:HG2	1:6:191:VAL:HG22	1.96	0.48
1:B:2102:GLU:OE1	1:c:96:ARG:NH2	2.46	0.48
1:E:2094:ARG:NH2	1:s:104:GLU:OE1	2.47	0.48
1:l:92:ASP:OD2	1:l:95:ASN:ND2	2.46	0.48
1:s:28:ARG:HG2	1:s:191:VAL:HG22	1.96	0.48
1:1:28:ARG:HG2	1:1:191:VAL:HG22	1.96	0.48
1:4:94:MET:HG2	1:5:94:MET:HG2	1.95	0.48
1:T:18:ARG:NH2	4:T:1002:SSU:OP3	2.46	0.48
1:n:94:MET:HG2	1:6:94:MET:HG2	1.96	0.48
1:r:94:MET:HG2	1:3:94:MET:HG2	1.96	0.48
1:t:96:ARG:NH2	1:x:104:GLU:OE1	2.47	0.48
1:B:2090:ASP:OD2	1:B:2093:ASN:ND2	2.46	0.48
1:F:96:ARG:NH2	1:h:104:GLU:OE1	2.47	0.48
1:C:2092:MET:HG2	1:m:94:MET:HG2	1.96	0.48
1:E:2090:ASP:OD2	1:E:2093:ASN:ND2	2.47	0.48
1:B:2092:MET:HG2	1:c:94:MET:HG2	1.95	0.48
1:F:94:MET:HG2	1:h:94:MET:HG2	1.96	0.48
1:H:2080:SER:HB2	1:H:2134:SER:HA	1.96	0.48
1:O:2026:ARG:HG2	1:O:2189:VAL:HG22	1.96	0.48
1:d:28:ARG:HG2	1:d:191:VAL:HG22	1.96	0.48
1:4:28:ARG:HG2	1:4:191:VAL:HG22	1.95	0.48
1:Q:2016:ARG:NH2	4:Q:3003:SSU:OP3	2.45	0.47
1:Q:2092:MET:HG2	1:Y:94:MET:HG2	1.96	0.47
1:y:9:LYS:HB3	4:y:203:SSU:O4'	2.14	0.47
5:a:204:G:H2'	6:g:201:C:C6	2.49	0.47
5:g:204:G:H2'	6:g:205:C:C6	2.50	0.47
1:p:116:ASN:O	1:p:120:LEU:HB2	2.14	0.47
6:z:202:C:C6	5:4:1003:G:H2'	2.49	0.47
1:A:2120:GLN:HG3	1:P:168:PRO:HG2	1.96	0.47
1:H:2166:PRO:HG2	1:b:122:GLN:HG3	1.96	0.47
1:O:2036:ASN:N	1:O:2180:GLY:O	2.48	0.47
1:2:112:MET:HE3	1:2:112:MET:HB3	1.75	0.47
1:I:2092:MET:HG2	1:J:2092:MET:HG2	1.95	0.47
1:Q:2094:ARG:NH2	1:Y:104:GLU:OE1	2.47	0.47
1:T:102:VAL:HG13	1:T:174:LEU:HD11	1.96	0.47
5:i:204:G:H2'	6:i:205:C:C6	2.49	0.47
1:B:2094:ARG:NH2	1:c:104:GLU:OE1	2.47	0.47
6:I:3002:C:C6	5:K:2205:G:H2'	2.49	0.47
1:N:2084:ARG:HE	1:N:2086:ILE:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2203:SRA:HN62	3:a:202:SRA:C6	2.07	0.47
1:S:2166:PRO:HG2	1:V:122:GLN:HG3	1.97	0.47
5:Y:2001:G:H2'	6:Y:2002:C:C6	2.50	0.47
5:b:201:G:H2'	6:b:202:C:C6	2.49	0.47
1:v:122:GLN:HG3	1:z:168:PRO:HG2	1.97	0.47
5:C:2205:G:H2'	6:C:2206:C:C6	2.50	0.47
1:G:2094:ARG:NH2	1:p:104:GLU:OE1	2.48	0.47
1:N:2100:VAL:HG13	1:N:2172:LEU:HD11	1.97	0.47
1:O:2102:GLU:OE1	1:l:96:ARG:NH2	2.48	0.47
1:W:18:ARG:HH21	5:W:2001:G:C2'	2.27	0.47
1:Y:38:ASN:N	1:Y:182:GLY:O	2.48	0.47
1:k:31:LEU:HB3	1:k:188:TYR:HB3	1.95	0.47
1:m:38:ASN:N	1:m:182:GLY:O	2.48	0.47
1:r:96:ARG:NH2	1:3:104:GLU:OE1	2.47	0.47
1:s:38:ASN:N	1:s:182:GLY:O	2.48	0.47
1:t:11:ALA:HB1	3:t:205:SRA:C4'	2.44	0.47
1:t:94:MET:HG2	1:x:94:MET:HG2	1.96	0.47
1:1:38:ASN:N	1:1:182:GLY:O	2.48	0.47
1:A:2166:PRO:HG2	1:P:122:GLN:HG3	1.96	0.47
1:I:2026:ARG:HG2	1:I:2189:VAL:HG22	1.97	0.47
1:K:2114:ASN:O	1:K:2118:LEU:HB2	2.13	0.47
1:V:60:ARG:NH1	1:V:62:GLY:O	2.47	0.47
1:c:38:ASN:N	1:c:182:GLY:O	2.48	0.47
1:k:18:ARG:HB3	3:k:2003:SRA:H5''	1.96	0.47
1:R:2120:GLN:HG3	1:q:168:PRO:HG2	1.97	0.47
1:a:102:VAL:HG13	1:a:174:LEU:HD11	1.96	0.47
1:g:102:VAL:HG13	1:g:174:LEU:HD11	1.97	0.47
1:w:86:ARG:HE	1:w:88:ILE:HD11	1.80	0.47
1:0:96:ARG:NH2	1:1:104:GLU:OE1	2.48	0.47
1:4:104:GLU:OE1	1:5:96:ARG:NH2	2.47	0.47
1:k:88:ILE:HB	1:k:174:LEU:HB3	1.97	0.47
1:n:92:ASP:OD2	1:n:95:ASN:ND2	2.48	0.47
1:t:38:ASN:N	1:t:182:GLY:O	2.48	0.47
1:v:94:MET:HG2	1:z:94:MET:HG2	1.97	0.47
1:H:2113:TYR:OH	1:H:2128:ASP:OD1	2.29	0.46
1:N:2026:ARG:HG2	1:N:2189:VAL:HG22	1.96	0.46
1:U:19:MET:HE1	1:d:13:MET:HG3	1.97	0.46
1:W:96:ARG:NH2	1:w:104:GLU:OE1	2.49	0.46
1:g:8:ARG:HG2	1:g:9:LYS:HD2	1.96	0.46
1:h:38:ASN:N	1:h:182:GLY:O	2.48	0.46
5:k:2001:G:H2'	6:k:2002:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:168:PRO:HG2	1:z:122:GLN:HG3	1.97	0.46
1:4:38:ASN:N	1:4:182:GLY:O	2.48	0.46
1:E:2036:ASN:N	1:E:2180:GLY:O	2.48	0.46
1:H:2092:MET:HG2	1:b:94:MET:HG2	1.98	0.46
1:J:2090:ASP:OD2	1:J:2093:ASN:ND2	2.48	0.46
5:P:204:G:H2'	6:y:201:C:C6	2.50	0.46
1:S:2092:MET:HG2	1:V:94:MET:HG2	1.98	0.46
1:Y:28:ARG:HG2	1:Y:191:VAL:HG22	1.96	0.46
1:g:28:ARG:HG2	1:g:191:VAL:HG22	1.96	0.46
1:i:86:ARG:HE	1:i:88:ILE:HD11	1.81	0.46
1:3:38:ASN:N	1:3:182:GLY:O	2.48	0.46
1:D:2120:GLN:HG3	1:j:168:PRO:HG2	1.98	0.46
1:K:2084:ARG:HE	1:K:2086:ILE:HD11	1.80	0.46
6:N:2201:C:C6	5:T:1003:G:H2'	2.50	0.46
1:S:2120:GLN:HG3	1:V:168:PRO:HG2	1.97	0.46
1:m:28:ARG:HG2	1:m:191:VAL:HG22	1.98	0.46
1:r:18:ARG:HH22	6:r:2002:C:C5'	2.21	0.46
4:y:203:SSU:H2'	5:y:204:G:H8	1.81	0.46
4:C:2204:SSU:H2'	5:C:2205:G:H8	1.81	0.46
1:D:2113:TYR:OH	1:D:2128:ASP:OD1	2.29	0.46
1:I:2102:GLU:OE1	1:J:2094:ARG:NH2	2.48	0.46
5:Q:3004:G:H2'	6:r:2003:C:C6	2.49	0.46
1:i:38:ASN:N	1:i:182:GLY:O	2.49	0.46
1:k:86:ARG:HE	1:k:88:ILE:HD11	1.81	0.46
1:l:38:ASN:N	1:l:182:GLY:O	2.49	0.46
4:4:1002:SSU:H2'	5:4:1003:G:H8	1.81	0.46
1:C:2090:ASP:OD2	1:C:2093:ASN:ND2	2.48	0.46
3:C:2203:SRA:HN62	3:t:203:SRA:C6	2.06	0.46
5:H:2201:G:H8	4:g:207:SSU:H2'	1.81	0.46
1:M:2086:ILE:HB	1:M:2172:LEU:HB3	1.98	0.46
1:Q:2016:ARG:NE	4:Q:3003:SSU:O3'	2.48	0.46
5:R:2201:G:H8	4:2:201:SSU:H2'	1.81	0.46
5:Y:2001:G:H8	4:z:204:SSU:H2'	1.81	0.46
1:b:20:ILE:HD12	1:t:19:MET:HE3	1.97	0.46
1:h:28:ARG:HG2	1:h:191:VAL:HG22	1.96	0.46
4:h:202:SSU:H2'	5:r:2001:G:H8	1.81	0.46
1:x:92:ASP:OD2	1:x:95:ASN:ND2	2.49	0.46
1:2:115:TYR:OH	1:2:130:ASP:OD1	2.29	0.46
4:I:3004:SSU:H2'	5:I:3005:G:H8	1.81	0.46
1:R:2092:MET:HG2	1:q:94:MET:HG2	1.97	0.46
1:X:88:ILE:HB	1:X:174:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:201:SSU:H2'	5:e:202:G:H8	1.81	0.46
1:f:104:GLU:OE1	1:7:96:ARG:NH2	2.49	0.46
1:g:86:ARG:HE	1:g:88:ILE:HD11	1.81	0.46
1:o:88:ILE:HB	1:o:174:LEU:HB3	1.97	0.46
1:6:38:ASN:N	1:6:182:GLY:O	2.48	0.46
1:C:2036:ASN:N	1:C:2180:GLY:O	2.49	0.46
1:D:2092:MET:HG2	1:j:94:MET:HG2	1.97	0.46
1:Z:88:ILE:HB	1:Z:174:LEU:HB3	1.98	0.46
1:i:88:ILE:HB	1:i:174:LEU:HB3	1.98	0.46
1:p:88:ILE:HB	1:p:174:LEU:HB3	1.98	0.46
1:H:2120:GLN:HG3	1:b:168:PRO:HG2	1.97	0.46
1:J:2142:ASP:OD2	1:1:134:ASN:ND2	2.45	0.46
1:Y:112:MET:HB3	1:Y:112:MET:HE3	1.79	0.46
1:a:28:ARG:HG2	1:a:191:VAL:HG22	1.97	0.46
1:c:115:TYR:OH	1:c:130:ASP:OD1	2.31	0.46
1:7:102:VAL:HG13	1:7:174:LEU:HD11	1.98	0.46
1:A:2110:MET:HE3	1:A:2110:MET:HB3	1.79	0.46
1:G:2100:VAL:HG13	1:G:2172:LEU:HD11	1.97	0.46
6:L:2204:C:C6	5:y:204:G:H2'	2.50	0.46
1:2:86:ARG:HE	1:2:88:ILE:HD11	1.81	0.46
4:Q:3003:SSU:H2'	5:Q:3004:G:H8	1.81	0.46
1:f:38:ASN:N	1:f:182:GLY:O	2.49	0.46
1:2:88:ILE:HB	1:2:174:LEU:HB3	1.97	0.46
1:2:116:ASN:O	1:2:120:LEU:HB2	2.16	0.46
1:A:2092:MET:HG2	1:P:94:MET:HG2	1.98	0.45
4:P:203:SSU:H2'	5:P:204:G:H8	1.81	0.45
1:W:88:ILE:HB	1:W:174:LEU:HB3	1.98	0.45
5:b:207:G:H2'	6:b:208:C:C6	2.50	0.45
5:k:2001:G:H8	4:r:2005:SSU:H2'	1.81	0.45
1:r:38:ASN:N	1:r:182:GLY:O	2.49	0.45
5:I:3006:G:H8	4:b:204:SSU:H2'	1.81	0.45
1:K:2036:ASN:N	1:K:2180:GLY:O	2.49	0.45
1:O:2132:ASN:ND2	1:5:144:ASP:OD2	2.45	0.45
4:T:1002:SSU:H2'	5:T:1003:G:H8	1.81	0.45
1:X:38:ASN:N	1:X:182:GLY:O	2.49	0.45
1:Z:86:ARG:HE	1:Z:88:ILE:HD11	1.81	0.45
1:a:86:ARG:HE	1:a:88:ILE:HD11	1.81	0.45
4:b:206:SSU:H2'	5:b:207:G:H8	1.81	0.45
1:l:60:ARG:NH1	1:l:62:GLY:O	2.49	0.45
1:C:2018:ILE:HD12	1:n:19:MET:HE3	1.99	0.45
4:a:203:SSU:H2'	5:a:204:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2013:ALA:CB	4:L:2202:SSU:OP3	2.64	0.45
3:Q:3002:SRA:C6	3:k:2004:SRA:HN62	2.07	0.45
1:U:96:ARG:NH2	1:Z:104:GLU:OE1	2.50	0.45
5:W:2001:G:H8	4:t:202:SSU:H2'	1.81	0.45
1:n:86:ARG:HE	1:n:88:ILE:HD11	1.81	0.45
1:r:115:TYR:OH	1:r:130:ASP:OD2	2.31	0.45
1:s:86:ARG:HE	1:s:88:ILE:HD11	1.82	0.45
1:M:2084:ARG:HE	1:M:2086:ILE:HD11	1.81	0.45
5:e:202:G:H2'	6:e:203:C:C6	2.50	0.45
1:u:102:VAL:HG13	1:u:174:LEU:HD11	1.97	0.45
1:w:116:ASN:O	1:w:120:LEU:HB2	2.17	0.45
3:C:2203:SRA:C4	4:C:2204:SSU:C5	2.95	0.45
4:i:203:SSU:H2'	5:i:204:G:H8	1.81	0.45
3:k:2004:SRA:C4	4:3:203:SSU:C5	2.95	0.45
1:n:38:ASN:N	1:n:182:GLY:O	2.48	0.45
1:o:86:ARG:HE	1:o:88:ILE:HD11	1.82	0.45
5:r:2001:G:H2'	6:r:2002:C:C6	2.50	0.45
1:v:112:MET:HE3	1:v:112:MET:HB3	1.79	0.45
1:2:38:ASN:N	1:2:182:GLY:O	2.50	0.45
1:D:2166:PRO:HG2	1:j:122:GLN:HG3	1.98	0.45
3:F:203:SRA:C4	4:F:204:SSU:C5	2.95	0.45
5:H:2201:G:H2'	6:H:2202:C:C6	2.50	0.45
1:J:2084:ARG:HE	1:J:2086:ILE:HD11	1.82	0.45
3:J:3002:SRA:C4	4:J:3003:SSU:C5	2.95	0.45
1:K:2086:ILE:HB	1:K:2172:LEU:HB3	1.98	0.45
4:L:2202:SSU:H2'	5:g:204:G:H8	1.81	0.45
5:R:2201:G:H2'	6:2:202:C:C6	2.50	0.45
1:W:86:ARG:HE	1:W:88:ILE:HD11	1.82	0.45
3:Y:2004:SRA:C4	4:v:201:SSU:C5	2.95	0.45
3:b:205:SRA:C4	4:b:206:SSU:C5	2.95	0.45
1:y:86:ARG:HE	1:y:88:ILE:HD11	1.82	0.45
1:A:2058:ARG:NH1	1:A:2060:GLY:O	2.49	0.45
1:F:38:ASN:N	1:F:182:GLY:O	2.48	0.45
1:M:2114:ASN:O	1:M:2118:LEU:HB2	2.17	0.45
1:P:60:ARG:NH1	1:P:62:GLY:O	2.49	0.45
3:R:2203:SRA:C4	4:R:2204:SSU:C5	2.95	0.45
5:b:201:G:H8	4:t:206:SSU:H2'	1.81	0.45
1:i:116:ASN:O	1:i:120:LEU:HB2	2.17	0.45
1:r:86:ARG:HE	1:r:88:ILE:HD11	1.82	0.45
3:t:205:SRA:C4	4:t:206:SSU:C5	2.95	0.45
1:5:38:ASN:N	1:5:182:GLY:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:86:ARG:HE	1:5:88:ILE:HD11	1.82	0.45
6:E:3002:C:C6	5:I:3005:G:H2'	2.50	0.45
1:L:2155:ASN:ND2	1:L:2164:ASN:O	2.49	0.45
3:Q:3002:SRA:C4	4:Q:3003:SSU:C5	2.95	0.45
1:U:112:MET:HE3	1:U:112:MET:HB3	1.90	0.45
1:Z:38:ASN:N	1:Z:182:GLY:O	2.49	0.45
3:a:202:SRA:C4	4:a:203:SSU:C5	2.95	0.45
1:c:86:ARG:HE	1:c:88:ILE:HD11	1.82	0.45
1:K:2102:GLU:OE1	1:g:96:ARG:NH2	2.49	0.45
3:K:2203:SRA:C4	4:K:2204:SSU:C5	2.95	0.45
1:N:2110:MET:HE3	1:N:2110:MET:HB3	1.85	0.45
4:X:202:SSU:C5	3:q:205:SRA:C4	2.95	0.45
4:q:201:SSU:H2'	5:q:202:G:H8	1.81	0.45
1:u:157:ASN:ND2	1:u:166:ASN:O	2.49	0.45
1:E:2084:ARG:HE	1:E:2086:ILE:HD11	1.82	0.44
3:R:2203:SRA:H2	3:a:202:SRA:H2	1.56	0.44
1:f:88:ILE:HB	1:f:174:LEU:HB3	1.98	0.44
1:g:137:LEU:HD23	1:g:137:LEU:HA	1.87	0.44
1:k:19:MET:HE2	1:3:13:MET:HE3	1.98	0.44
4:K:2204:SSU:H2'	5:K:2205:G:H8	1.81	0.44
1:U:102:VAL:HG13	1:U:174:LEU:HD11	1.98	0.44
1:o:115:TYR:OH	1:o:130:ASP:OD1	2.29	0.44
1:o:116:ASN:O	1:o:120:LEU:HB2	2.18	0.44
1:w:102:VAL:HG13	1:w:174:LEU:HD11	1.98	0.44
1:w:157:ASN:ND2	1:w:166:ASN:O	2.49	0.44
1:B:2036:ASN:N	1:B:2180:GLY:O	2.48	0.44
1:F:86:ARG:HE	1:F:88:ILE:HD11	1.82	0.44
1:L:2084:ARG:HE	1:L:2086:ILE:HD11	1.83	0.44
3:P:202:SRA:C4	4:P:203:SSU:C5	2.95	0.44
1:T:157:ASN:ND2	1:T:166:ASN:O	2.50	0.44
1:X:86:ARG:HE	1:X:88:ILE:HD11	1.82	0.44
1:h:90:PHE:HE1	1:h:174:LEU:HB2	1.82	0.44
1:y:88:ILE:HB	1:y:174:LEU:HB3	1.99	0.44
1:B:2084:ARG:HE	1:B:2086:ILE:HD11	1.83	0.44
1:C:2084:ARG:HE	1:C:2086:ILE:HD11	1.82	0.44
1:R:2155:ASN:ND2	1:R:2164:ASN:O	2.51	0.44
1:x:86:ARG:HE	1:x:88:ILE:HD11	1.82	0.44
1:4:129:LYS:HG2	1:4:147:ILE:HG12	2.00	0.44
1:G:2036:ASN:N	1:G:2180:GLY:O	2.51	0.44
1:I:2036:ASN:N	1:I:2180:GLY:O	2.48	0.44
5:I:3006:G:H2'	6:I:3007:C:C6	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2058:ARG:NH1	1:J:2060:GLY:O	2.51	0.44
1:W:112:MET:HE3	1:W:112:MET:HB3	1.83	0.44
1:k:38:ASN:N	1:k:182:GLY:O	2.50	0.44
1:o:38:ASN:N	1:o:182:GLY:O	2.49	0.44
5:q:202:G:H2'	6:q:203:C:C6	2.50	0.44
3:H:2204:SRA:C4	4:K:2201:SSU:C5	2.95	0.44
3:L:2201:SRA:C4	4:L:2202:SSU:C5	2.95	0.44
1:N:2135:LEU:HD23	1:N:2135:LEU:HA	1.87	0.44
1:T:38:ASN:N	1:T:182:GLY:O	2.51	0.44
1:Y:90:PHE:HE1	1:Y:174:LEU:HB2	1.83	0.44
1:t:88:ILE:HB	1:t:174:LEU:HB3	2.00	0.44
1:0:86:ARG:HE	1:0:88:ILE:HD11	1.83	0.44
1:7:86:ARG:HE	1:7:88:ILE:HD11	1.82	0.44
1:I:2084:ARG:HE	1:I:2086:ILE:HD11	1.83	0.44
1:L:2100:VAL:HG13	1:L:2172:LEU:HD11	1.98	0.44
1:e:102:VAL:HG13	1:e:174:LEU:HD11	1.99	0.44
1:l:86:ARG:HE	1:l:88:ILE:HD11	1.82	0.44
1:o:112:MET:HE3	1:o:112:MET:HB3	1.79	0.44
3:H:2208:SRA:C4	4:H:2209:SSU:C5	2.95	0.44
1:M:2036:ASN:N	1:M:2180:GLY:O	2.50	0.44
1:N:2155:ASN:ND2	1:N:2164:ASN:O	2.51	0.44
3:T:1001:SRA:C4	4:T:1002:SSU:C5	2.95	0.44
1:W:116:ASN:O	1:W:120:LEU:HB2	2.18	0.44
1:a:88:ILE:HB	1:a:174:LEU:HB3	1.99	0.44
1:d:38:ASN:N	1:d:182:GLY:O	2.51	0.44
3:t:203:SRA:C4	4:t:204:SSU:C5	2.95	0.44
1:F:112:MET:HE3	1:F:112:MET:HB3	1.82	0.44
1:G:2017:MET:HE1	1:T:13:MET:HG3	2.00	0.44
1:I:2114:ASN:O	1:I:2118:LEU:HB2	2.18	0.44
1:L:2148:PRO:HG3	4:L:2207:SSU:O3'	2.18	0.44
1:d:94:MET:HG2	1:i:94:MET:HG2	1.99	0.44
1:e:94:MET:HG2	1:k:94:MET:HG2	2.00	0.44
1:e:96:ARG:NH2	1:k:104:GLU:OE1	2.51	0.44
1:f:86:ARG:HE	1:f:88:ILE:HD11	1.82	0.44
1:k:137:LEU:HD23	1:k:137:LEU:HA	1.89	0.44
1:s:112:MET:HE3	1:s:112:MET:HB3	1.77	0.44
1:u:112:MET:HE3	1:u:112:MET:HB3	1.86	0.44
3:4:1001:SRA:C4	4:4:1002:SSU:C5	2.95	0.44
1:A:2017:MET:HE1	1:o:16:VAL:HG13	1.99	0.43
1:K:2110:MET:HE3	1:K:2110:MET:HB3	1.79	0.43
1:L:2036:ASN:N	1:L:2180:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2110:MET:HE3	1:O:2110:MET:HB3	1.79	0.43
1:U:86:ARG:HE	1:U:88:ILE:HD11	1.83	0.43
1:U:90:PHE:HE1	1:U:174:LEU:HB2	1.83	0.43
3:i:202:SRA:C4	4:i:203:SSU:C5	2.95	0.43
1:C:2012:ARG:HD3	4:C:2204:SSU:OP3	1.99	0.43
3:F:203:SRA:HN62	3:i:202:SRA:C6	2.07	0.43
1:H:2114:ASN:O	1:H:2118:LEU:HB2	2.18	0.43
1:K:2080:SER:HB2	1:K:2134:SER:HA	2.00	0.43
1:M:2092:MET:HG2	1:T:94:MET:HG2	2.01	0.43
1:Q:2084:ARG:HE	1:Q:2086:ILE:HD11	1.81	0.43
1:X:116:ASN:O	1:X:120:LEU:HB2	2.18	0.43
1:d:96:ARG:NH2	1:i:104:GLU:OE1	2.51	0.43
1:u:38:ASN:N	1:u:182:GLY:O	2.51	0.43
1:u:86:ARG:HE	1:u:88:ILE:HD11	1.83	0.43
3:L:2206:SRA:C4	4:L:2207:SSU:C5	2.95	0.43
1:d:102:VAL:HG13	1:d:174:LEU:HD11	1.99	0.43
1:e:88:ILE:HD12	1:e:174:LEU:HD22	2.00	0.43
1:C:2094:ARG:NH2	1:m:104:GLU:OE1	2.50	0.43
1:U:88:ILE:HB	1:U:174:LEU:HB3	2.00	0.43
1:g:38:ASN:N	1:g:182:GLY:O	2.51	0.43
1:g:90:PHE:HE1	1:g:174:LEU:HB2	1.83	0.43
1:m:116:ASN:O	1:m:120:LEU:HB2	2.18	0.43
1:o:94:MET:HG2	1:u:94:MET:HG2	2.00	0.43
3:w:202:SRA:C4	4:w:203:SSU:C5	2.95	0.43
1:y:116:ASN:O	1:y:120:LEU:HB2	2.18	0.43
1:H:2009:ALA:HB1	6:H:2202:C:OP1	2.19	0.43
1:M:2102:GLU:OE1	1:T:96:ARG:NH2	2.52	0.43
1:N:2094:ARG:NH2	1:X:104:GLU:OE1	2.52	0.43
1:o:104:GLU:OE1	1:u:96:ARG:NH2	2.51	0.43
1:w:38:ASN:N	1:w:182:GLY:O	2.52	0.43
1:1:86:ARG:HE	1:1:88:ILE:HD11	1.83	0.43
1:F:19:MET:HE2	1:Q:2011:MET:HE3	2.00	0.43
1:N:2036:ASN:N	1:N:2180:GLY:O	2.51	0.43
5:W:2001:G:H2'	6:W:2002:C:C6	2.50	0.43
1:a:96:ARG:NH2	1:2:104:GLU:OE1	2.52	0.43
1:k:18:ARG:CB	3:k:2003:SRA:H5''	2.48	0.43
1:m:90:PHE:HE1	1:m:174:LEU:HB2	1.84	0.43
1:3:90:PHE:HE1	1:3:174:LEU:HB2	1.83	0.43
1:C:2016:ARG:NH1	4:C:2204:SSU:O5'	2.52	0.43
1:G:2086:ILE:HB	1:G:2172:LEU:HB3	2.00	0.43
1:K:2092:MET:HG2	1:g:94:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2092:MET:HG2	1:y:94:MET:HG2	2.00	0.43
1:N:2102:GLU:OE1	1:X:96:ARG:NH2	2.52	0.43
1:O:2086:ILE:HB	1:O:2172:LEU:HB3	2.01	0.43
1:P:112:MET:HB3	1:P:112:MET:HE3	1.78	0.43
1:a:94:MET:HG2	1:2:94:MET:HG2	1.99	0.43
1:e:38:ASN:N	1:e:182:GLY:O	2.50	0.43
1:o:137:LEU:O	1:0:138:THR:OG1	2.35	0.43
1:I:2016:ARG:NH2	6:I:3007:C:HO2'	2.01	0.43
1:X:112:MET:HB3	1:X:112:MET:HE3	1.81	0.43
1:C:2014:VAL:HG13	1:n:19:MET:HE1	1.99	0.43
1:C:2135:LEU:HD23	1:C:2135:LEU:HA	1.92	0.43
1:G:2088:PHE:HE1	1:G:2172:LEU:HB2	1.84	0.43
1:L:2094:ARG:NH2	1:y:104:GLU:OE1	2.52	0.43
1:O:2084:ARG:HE	1:O:2086:ILE:HD11	1.84	0.43
1:U:129:LYS:HG2	1:U:147:ILE:HG12	2.00	0.43
3:b:205:SRA:H2	3:w:202:SRA:H2	1.56	0.43
1:k:116:ASN:O	1:k:120:LEU:HB2	2.18	0.43
1:p:38:ASN:N	1:p:182:GLY:O	2.48	0.43
1:p:86:ARG:HE	1:p:88:ILE:HD11	1.82	0.43
1:r:15:ALA:HB2	6:r:2002:C:H5''	2.01	0.43
1:s:90:PHE:HE1	1:s:174:LEU:HB2	1.84	0.43
1:u:137:LEU:HD23	1:u:137:LEU:HA	1.88	0.43
1:7:90:PHE:HE1	1:7:174:LEU:HB2	1.84	0.43
1:O:2088:PHE:HE1	1:O:2172:LEU:HB2	1.84	0.43
1:e:88:ILE:HB	1:e:174:LEU:HB3	2.01	0.43
1:f:116:ASN:O	1:f:120:LEU:HB2	2.19	0.43
1:n:31:LEU:HB3	1:n:188:TYR:HB3	2.01	0.43
1:6:86:ARG:HE	1:6:88:ILE:HD11	1.84	0.43
1:G:2092:MET:HG2	1:p:94:MET:HG2	2.01	0.42
1:O:2135:LEU:HD23	1:O:2135:LEU:HA	1.89	0.42
1:b:115:TYR:OH	1:b:130:ASP:OD2	2.29	0.42
1:i:11:ALA:HB1	3:i:202:SRA:H5''	2.01	0.42
1:4:86:ARG:HE	1:4:88:ILE:HD11	1.84	0.42
1:A:2135:LEU:HD23	1:A:2135:LEU:HA	1.89	0.42
1:H:2090:ASP:OD2	1:H:2093:ASN:ND2	2.52	0.42
3:R:2202:SRA:OP1	1:2:13:MET:SD	2.76	0.42
1:U:38:ASN:N	1:U:182:GLY:O	2.51	0.42
1:U:94:MET:HG2	1:Z:94:MET:HG2	2.01	0.42
1:g:56:ASP:H	1:g:59:GLN:HE21	1.68	0.42
1:h:112:MET:HE3	1:h:112:MET:HB3	1.80	0.42
1:w:56:ASP:H	1:w:59:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:PHE:HE1	1:1:174:LEU:HB2	1.83	0.42
1:7:88:ILE:HB	1:7:174:LEU:HB3	2.00	0.42
1:D:2086:ILE:HB	1:D:2172:LEU:HB3	2.02	0.42
1:H:2110:MET:HE3	1:H:2110:MET:HB3	1.82	0.42
1:N:2054:ASP:H	1:N:2057:GLN:HE21	1.66	0.42
1:W:94:MET:HG2	1:w:94:MET:HG2	2.01	0.42
1:Z:116:ASN:O	1:Z:120:LEU:HB2	2.18	0.42
1:e:18:ARG:HE	5:e:202:G:H4'	1.74	0.42
1:e:115:TYR:OH	1:e:130:ASP:OD2	2.34	0.42
1:n:112:MET:HE3	1:n:112:MET:HB3	1.83	0.42
1:t:86:ARG:HE	1:t:88:ILE:HD11	1.83	0.42
1:x:78:ALA:HA	1:x:83:GLN:HE21	1.84	0.42
1:0:38:ASN:N	1:0:182:GLY:O	2.49	0.42
1:L:2017:MET:HE2	1:g:13:MET:HE3	2.00	0.42
1:Y:137:LEU:HD23	1:Y:137:LEU:HA	1.90	0.42
1:c:90:PHE:HE1	1:c:174:LEU:HB2	1.85	0.42
1:d:157:ASN:ND2	1:d:166:ASN:O	2.52	0.42
1:e:46:ASN:HD22	1:e:49:ASN:HD22	1.66	0.42
1:o:129:LYS:HG2	1:o:147:ILE:HG12	2.01	0.42
1:E:2142:ASP:OD2	1:I:2132:ASN:ND2	2.45	0.42
1:G:2155:ASN:OD1	1:p:122:GLN:NE2	2.47	0.42
1:J:2110:MET:HE3	1:J:2110:MET:HB3	1.83	0.42
1:0:90:PHE:HE1	1:0:174:LEU:HB2	1.85	0.42
1:W:18:ARG:NE	6:W:2002:C:H5'	2.14	0.42
1:W:104:GLU:OE1	1:w:96:ARG:NH2	2.53	0.42
1:a:56:ASP:H	1:a:59:GLN:HE21	1.66	0.42
1:h:116:ASN:O	1:h:120:LEU:HB2	2.19	0.42
1:B:2110:MET:HE3	1:B:2110:MET:HB3	1.89	0.42
1:I:2088:PHE:HE1	1:I:2172:LEU:HB2	1.83	0.42
1:L:2102:GLU:OE1	1:y:96:ARG:NH2	2.53	0.42
1:Q:2076:ALA:HA	1:Q:2081:GLN:HE21	1.85	0.42
1:d:86:ARG:HE	1:d:88:ILE:HD11	1.83	0.42
1:d:88:ILE:HB	1:d:174:LEU:HB3	2.02	0.42
1:g:88:ILE:HB	1:g:174:LEU:HB3	2.01	0.42
1:g:129:LYS:HG2	1:g:147:ILE:HG12	2.02	0.42
1:j:88:ILE:HB	1:j:174:LEU:HB3	2.02	0.42
1:k:112:MET:HE3	1:k:112:MET:HB3	1.78	0.42
1:m:88:ILE:HB	1:m:174:LEU:HB3	2.01	0.42
1:x:38:ASN:N	1:x:182:GLY:O	2.50	0.42
1:y:38:ASN:N	1:y:182:GLY:O	2.50	0.42
1:G:2114:ASN:O	1:G:2118:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:56:ASP:H	1:u:59:GLN:HE21	1.67	0.42
1:1:88:ILE:HB	1:1:174:LEU:HB3	2.02	0.42
1:6:90:PHE:HE1	1:6:174:LEU:HB2	1.84	0.42
1:7:38:ASN:N	1:7:182:GLY:O	2.51	0.42
1:A:2017:MET:HE3	1:o:20:ILE:HD12	2.02	0.42
1:E:2136:THR:OG1	1:f:137:LEU:O	2.35	0.42
1:I:2016:ARG:HH22	6:I:3007:C:C3'	2.33	0.42
1:J:2036:ASN:N	1:J:2180:GLY:O	2.48	0.42
1:Z:112:MET:HB3	1:Z:112:MET:HE3	1.79	0.42
1:d:129:LYS:HG2	1:d:147:ILE:HG12	2.02	0.42
1:t:90:PHE:HE1	1:t:174:LEU:HB2	1.85	0.42
1:x:88:ILE:HB	1:x:174:LEU:HB3	2.02	0.42
1:F:90:PHE:HE1	1:F:174:LEU:HB2	1.85	0.41
1:M:2094:ARG:NH2	1:T:104:GLU:OE1	2.53	0.41
1:V:137:LEU:HD23	1:V:137:LEU:HA	1.90	0.41
1:g:92:ASP:OD2	1:g:95:ASN:ND2	2.53	0.41
1:i:112:MET:HB3	1:i:112:MET:HE3	1.77	0.41
1:y:115:TYR:OH	1:y:130:ASP:OD1	2.29	0.41
1:1:129:LYS:HG2	1:1:147:ILE:HG12	2.02	0.41
1:I:2016:ARG:HH21	3:I:3008:SRA:H5'	1.85	0.41
1:L:2013:ALA:HB1	4:L:2202:SSU:H5'	2.02	0.41
1:Q:2036:ASN:N	1:Q:2180:GLY:O	2.49	0.41
3:R:2202:SRA:H5''	1:2:13:MET:CE	2.50	0.41
1:V:115:TYR:OH	1:V:130:ASP:OD2	2.29	0.41
1:W:38:ASN:N	1:W:182:GLY:O	2.50	0.41
1:W:129:LYS:HG2	1:W:147:ILE:HG12	2.03	0.41
1:a:38:ASN:N	1:a:182:GLY:O	2.51	0.41
1:b:88:ILE:HB	1:b:174:LEU:HB3	2.02	0.41
1:e:116:ASN:O	1:e:120:LEU:HB2	2.20	0.41
1:n:88:ILE:HB	1:n:174:LEU:HB3	2.02	0.41
1:r:88:ILE:HB	1:r:174:LEU:HB3	2.02	0.41
1:x:90:PHE:HE1	1:x:174:LEU:HB2	1.86	0.41
1:C:2086:ILE:HB	1:C:2172:LEU:HB3	2.02	0.41
1:I:2086:ILE:HB	1:I:2172:LEU:HB3	2.02	0.41
1:T:56:ASP:H	1:T:59:GLN:HE21	1.68	0.41
1:b:60:ARG:NH1	1:b:62:GLY:O	2.53	0.41
1:t:117:PRO:O	1:t:121:GLN:HB2	2.20	0.41
1:1:116:ASN:O	1:1:120:LEU:HB2	2.21	0.41
1:4:88:ILE:HB	1:4:174:LEU:HB3	2.02	0.41
1:4:112:MET:HB3	1:4:112:MET:HE3	1.77	0.41
1:6:88:ILE:HB	1:6:174:LEU:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:88:ILE:HB	1:T:174:LEU:HB3	2.01	0.41
1:Y:88:ILE:HB	1:Y:174:LEU:HB3	2.02	0.41
1:j:112:MET:HB3	1:j:112:MET:HE3	1.81	0.41
1:C:2016:ARG:HD3	4:C:2204:SSU:C3'	2.17	0.41
3:H:2208:SRA:H2	3:t:205:SRA:H2	1.56	0.41
1:I:2127:LYS:HG2	1:I:2145:ILE:HG12	2.02	0.41
1:L:2054:ASP:H	1:L:2057:GLN:HE21	1.69	0.41
1:d:56:ASP:H	1:d:59:GLN:HE21	1.69	0.41
1:e:104:GLU:OE1	1:k:96:ARG:NH2	2.54	0.41
1:r:112:MET:HB3	1:r:112:MET:HE3	1.83	0.41
1:w:88:ILE:HB	1:w:174:LEU:HB3	2.03	0.41
1:K:2017:MET:HE2	1:K:2017:MET:HB3	1.84	0.41
1:L:2086:ILE:HB	1:L:2172:LEU:HB3	2.03	0.41
1:U:56:ASP:H	1:U:59:GLN:HE21	1.68	0.41
1:V:112:MET:HE3	1:V:112:MET:HB3	1.80	0.41
1:d:103:LEU:HD23	1:d:103:LEU:HA	1.93	0.41
1:f:94:MET:HG2	1:7:94:MET:HG2	2.01	0.41
1:m:115:TYR:OH	1:m:130:ASP:OD2	2.30	0.41
1:z:115:TYR:OH	1:z:130:ASP:OD1	2.29	0.41
1:2:137:LEU:HD23	1:2:137:LEU:HA	1.95	0.41
1:3:66:ARG:NH1	4:3:203:SSU:OP3	2.53	0.41
1:7:129:LYS:HG2	1:7:147:ILE:HG12	2.02	0.41
3:H:2204:SRA:H2	3:L:2201:SRA:H2	1.56	0.41
1:I:2009:ALA:O	6:I:3007:C:OP1	2.38	0.41
1:J:2113:TYR:OH	1:J:2128:ASP:OD2	2.31	0.41
1:K:2155:ASN:ND2	1:K:2164:ASN:O	2.54	0.41
1:T:129:LYS:HG2	1:T:147:ILE:HG12	2.03	0.41
1:h:88:ILE:HB	1:h:174:LEU:HB3	2.02	0.41
1:3:88:ILE:HB	1:3:174:LEU:HB3	2.02	0.41
1:4:90:PHE:HE1	1:4:174:LEU:HB2	1.84	0.41
1:5:88:ILE:HB	1:5:174:LEU:HB3	2.03	0.41
1:E:2086:ILE:HB	1:E:2172:LEU:HB3	2.03	0.41
1:F:88:ILE:HB	1:F:174:LEU:HB3	2.02	0.41
1:N:2091:ASN:ND2	1:N:2124:THR:OG1	2.52	0.41
1:N:2092:MET:HG2	1:X:94:MET:HG2	2.01	0.41
1:e:86:ARG:HE	1:e:88:ILE:HD11	1.86	0.41
1:r:90:PHE:HE1	1:r:174:LEU:HB2	1.85	0.41
1:y:102:VAL:HG13	1:y:174:LEU:HD11	2.03	0.41
1:y:112:MET:HB3	1:y:112:MET:HE3	1.81	0.41
6:I:3002:C:N4	5:K:2205:G:C6	2.89	0.41
1:K:2054:ASP:H	1:K:2057:GLN:HE21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2127:LYS:HG2	1:O:2145:ILE:HG12	2.03	0.41
1:Q:2086:ILE:HB	1:Q:2172:LEU:HB3	2.02	0.41
1:S:2113:TYR:OH	1:S:2128:ASP:OD1	2.29	0.41
1:U:31:LEU:HB3	1:U:188:TYR:HB3	2.02	0.41
1:U:116:ASN:O	1:U:120:LEU:HB2	2.20	0.41
1:W:90:PHE:HE1	1:W:174:LEU:HB2	1.86	0.41
1:d:116:ASN:O	1:d:120:LEU:HB2	2.21	0.41
5:i:204:G:C6	6:i:205:C:N4	2.89	0.41
1:k:129:LYS:HG2	1:k:147:ILE:HG12	2.03	0.41
1:p:56:ASP:H	1:p:59:GLN:HE21	1.69	0.41
1:q:88:ILE:HB	1:q:174:LEU:HB3	2.02	0.41
1:s:117:PRO:O	1:s:121:GLN:HB2	2.21	0.41
1:l:137:LEU:HD23	1:l:137:LEU:HA	1.90	0.41
1:A:2017:MET:HE2	1:A:2017:MET:HB3	1.88	0.41
1:C:2017:MET:HE2	1:x:13:MET:HE3	2.02	0.41
1:E:2110:MET:HE3	1:E:2110:MET:HB3	1.83	0.41
1:a:31:LEU:HB3	1:a:188:TYR:HB3	2.02	0.41
1:a:90:PHE:HE1	1:a:174:LEU:HB2	1.85	0.41
1:l:90:PHE:HE1	1:l:174:LEU:HB2	1.85	0.41
1:t:150:PRO:HG2	4:t:204:SSU:H5'	2.03	0.41
1:v:38:ASN:N	1:v:182:GLY:O	2.54	0.41
6:E:3002:C:N4	5:I:3005:G:C6	2.89	0.40
1:P:88:ILE:HB	1:P:174:LEU:HB3	2.03	0.40
1:P:129:LYS:HG2	1:P:147:ILE:HG12	2.03	0.40
1:R:2036:ASN:N	1:R:2180:GLY:O	2.54	0.40
1:T:86:ARG:HE	1:T:88:ILE:HD11	1.85	0.40
5:b:201:G:C6	6:b:202:C:N4	2.89	0.40
1:l:115:TYR:OH	1:l:130:ASP:OD2	2.30	0.40
1:p:112:MET:HE3	1:p:112:MET:HB3	1.83	0.40
1:s:88:ILE:HB	1:s:174:LEU:HB3	2.03	0.40
1:s:137:LEU:HD23	1:s:137:LEU:HA	1.90	0.40
1:Q:2110:MET:HE3	1:Q:2110:MET:HB3	1.83	0.40
5:R:2201:G:C6	6:2:202:C:N4	2.90	0.40
1:Z:137:LEU:HD23	1:Z:137:LEU:HA	1.89	0.40
1:b:112:MET:HE3	1:b:112:MET:HB3	1.78	0.40
1:i:90:PHE:HE1	1:i:174:LEU:HB2	1.86	0.40
1:m:134:ASN:ND2	1:n:144:ASP:OD1	2.44	0.40
5:q:202:G:C6	6:q:203:C:N4	2.90	0.40
6:z:202:C:N4	5:4:1003:G:C6	2.89	0.40
1:7:56:ASP:H	1:7:59:GLN:HE21	1.68	0.40
1:7:112:MET:HE3	1:7:112:MET:HB3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:ILE:HB	1:B:2172:LEU:HB3	2.02	0.40
1:B:2135:LEU:HD23	1:B:2135:LEU:HA	1.92	0.40
5:C:2205:G:C6	6:C:2206:C:N4	2.89	0.40
1:G:2084:ARG:HE	1:G:2086:ILE:HD11	1.86	0.40
1:J:2114:ASN:O	1:J:2118:LEU:HB2	2.21	0.40
1:M:2127:LYS:HG2	1:M:2145:ILE:HG12	2.02	0.40
1:S:2086:ILE:HB	1:S:2172:LEU:HB3	2.03	0.40
1:a:116:ASN:O	1:a:120:LEU:HB2	2.22	0.40
1:c:117:PRO:O	1:c:121:GLN:HB2	2.21	0.40
1:k:78:ALA:HA	1:k:83:GLN:HE21	1.86	0.40
5:k:2001:G:C6	6:k:2002:C:N4	2.90	0.40
1:p:90:PHE:HE1	1:p:174:LEU:HB2	1.87	0.40
1:y:129:LYS:HG2	1:y:147:ILE:HG12	2.04	0.40
1:0:88:ILE:HB	1:0:174:LEU:HB3	2.03	0.40
1:5:90:PHE:HE1	1:5:174:LEU:HB2	1.87	0.40
1:A:2127:LYS:HG2	1:A:2145:ILE:HG12	2.03	0.40
1:D:2114:ASN:O	1:D:2118:LEU:HB2	2.22	0.40
1:E:2088:PHE:HE1	1:E:2172:LEU:HB2	1.86	0.40
5:H:2201:G:C6	6:H:2202:C:N4	2.90	0.40
1:I:2016:ARG:HH22	6:I:3007:C:C2'	2.33	0.40
1:M:2110:MET:HB3	1:M:2110:MET:HE3	1.82	0.40
1:Q:2088:PHE:HE1	1:Q:2172:LEU:HB2	1.87	0.40
5:e:202:G:C6	6:e:203:C:N4	2.90	0.40
5:g:204:G:C6	6:g:205:C:N4	2.89	0.40
1:q:38:ASN:N	1:q:182:GLY:O	2.55	0.40
1:v:137:LEU:HD23	1:v:137:LEU:HA	1.90	0.40
1:x:137:LEU:HD23	1:x:137:LEU:HA	1.95	0.40
1:0:116:ASN:O	1:0:120:LEU:HB2	2.22	0.40
1:1:117:PRO:O	1:1:121:GLN:HB2	2.21	0.40
1:2:90:PHE:HE1	1:2:174:LEU:HB2	1.87	0.40
1:J:2135:LEU:HD23	1:J:2135:LEU:HA	1.92	0.40
1:L:2110:MET:HB3	1:L:2110:MET:HE3	1.87	0.40
1:N:2086:ILE:HB	1:N:2172:LEU:HB3	2.02	0.40
1:N:2114:ASN:O	1:N:2118:LEU:HB2	2.22	0.40
5:b:207:G:C6	6:b:208:C:N4	2.89	0.40
1:f:96:ARG:NH2	1:7:104:GLU:OE1	2.54	0.40
1:f:129:LYS:HG2	1:f:147:ILE:HG12	2.02	0.40
1:o:137:LEU:HA	1:o:137:LEU:HD23	1.89	0.40
1:v:129:LYS:HG2	1:v:147:ILE:HG12	2.03	0.40
1:0:31:LEU:HB3	1:0:188:TYR:HB3	2.04	0.40
1:7:116:ASN:O	1:7:120:LEU:HB2	2.20	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	0	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	1	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	2	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	3	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	4	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	5	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	6	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	7	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	A	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	B	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	C	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	D	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	E	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	F	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	G	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	H	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	I	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	J	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	K	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	L	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	M	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	N	186/188 (99%)	183 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	P	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	Q	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	R	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	S	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	T	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
1	U	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	V	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	W	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
1	X	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	Y	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	Z	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	a	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	b	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	c	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	d	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	e	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	f	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	g	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	h	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	i	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	j	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	k	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	l	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	m	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	n	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	o	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
1	p	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	q	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	r	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	s	186/188 (99%)	182 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	t	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	u	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	v	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	w	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	x	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
1	y	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	z	186/188 (99%)	182 (98%)	4 (2%)	0	100	100
All	All	11160/11280 (99%)	10921 (98%)	239 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	1	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	2	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	3	160/160 (100%)	160 (100%)	0	100	100
1	4	160/160 (100%)	160 (100%)	0	100	100
1	5	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	6	160/160 (100%)	160 (100%)	0	100	100
1	7	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	A	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	B	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	C	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	D	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	E	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	F	160/160 (100%)	158 (99%)	2 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	H	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	I	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	J	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	K	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	L	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	M	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	N	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	O	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	P	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	Q	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	R	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	S	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	T	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	U	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	V	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	W	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	X	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	Y	160/160 (100%)	160 (100%)	0	100	100
1	Z	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	a	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	b	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	c	160/160 (100%)	160 (100%)	0	100	100
1	d	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	e	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	f	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	g	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	h	160/160 (100%)	160 (100%)	0	100	100
1	i	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	j	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	k	160/160 (100%)	158 (99%)	2 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	m	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	n	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	o	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	p	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	q	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	r	160/160 (100%)	157 (98%)	3 (2%)	50	66
1	s	160/160 (100%)	160 (100%)	0	100	100
1	t	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	u	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	v	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	w	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	x	160/160 (100%)	158 (99%)	2 (1%)	61	72
1	y	160/160 (100%)	159 (99%)	1 (1%)	78	81
1	z	160/160 (100%)	159 (99%)	1 (1%)	78	81
All	All	9600/9600 (100%)	9510 (99%)	90 (1%)	68	77

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2078	THR
1	B	2078	THR
1	C	2078	THR
1	C	2158	THR
1	D	2078	THR
1	E	2078	THR
1	F	80	THR
1	F	160	THR
1	G	2078	THR
1	G	2099	THR
1	G	2158	THR
1	H	2042	VAL
1	H	2078	THR
1	I	2078	THR
1	I	2158	THR
1	J	2078	THR
1	J	2158	THR

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Mol	Chain	Res	Type
1	K	2078	THR
1	L	2078	THR
1	L	2158	THR
1	M	2078	THR
1	N	2078	THR
1	N	2158	THR
1	O	2158	THR
1	P	44	VAL
1	P	80	THR
1	Q	2078	THR
1	Q	2119	GLN
1	Q	2158	THR
1	R	2078	THR
1	S	2078	THR
1	T	80	THR
1	T	160	THR
1	U	80	THR
1	U	160	THR
1	V	44	VAL
1	V	80	THR
1	W	80	THR
1	X	80	THR
1	Z	80	THR
1	a	80	THR
1	b	80	THR
1	b	160	THR
1	d	80	THR
1	d	160	THR
1	e	80	THR
1	e	160	THR
1	f	80	THR
1	f	160	THR
1	g	80	THR
1	g	160	THR
1	i	80	THR
1	i	160	THR
1	j	44	VAL
1	j	80	THR
1	j	160	THR
1	k	80	THR
1	k	160	THR
1	l	80	THR

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Mol	Chain	Res	Type
1	l	160	THR
1	m	160	THR
1	n	80	THR
1	n	160	THR
1	o	80	THR
1	p	80	THR
1	q	80	THR
1	q	160	THR
1	r	80	THR
1	r	121	GLN
1	r	160	THR
1	t	80	THR
1	u	80	THR
1	v	44	VAL
1	v	80	THR
1	w	80	THR
1	w	160	THR
1	x	80	THR
1	x	160	THR
1	y	80	THR
1	z	80	THR
1	0	80	THR
1	0	121	GLN
1	0	160	THR
1	1	160	THR
1	2	80	THR
1	5	80	THR
1	5	121	GLN
1	5	160	THR
1	7	80	THR
1	7	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (236) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2047	ASN
1	A	2057	GLN
1	A	2114	ASN
1	B	2019	ASN
1	B	2024	HIS
1	B	2057	GLN
1	B	2071	HIS

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Mol	Chain	Res	Type
1	B	2119	GLN
1	B	2146	ASN
1	C	2057	GLN
1	C	2071	HIS
1	C	2114	ASN
1	D	2019	ASN
1	D	2057	GLN
1	D	2071	HIS
1	D	2114	ASN
1	D	2153	ASN
1	E	2019	ASN
1	E	2057	GLN
1	E	2071	HIS
1	E	2119	GLN
1	F	21	ASN
1	F	59	GLN
1	F	73	HIS
1	F	116	ASN
1	F	121	GLN
1	F	155	ASN
1	G	2044	ASN
1	G	2047	ASN
1	G	2057	GLN
1	H	2047	ASN
1	H	2057	GLN
1	H	2081	GLN
1	I	2047	ASN
1	I	2057	GLN
1	I	2068	HIS
1	I	2081	GLN
1	I	2105	ASN
1	I	2119	GLN
1	J	2057	GLN
1	J	2071	HIS
1	J	2105	ASN
1	J	2114	ASN
1	K	2057	GLN
1	K	2105	ASN
1	L	2047	ASN
1	L	2057	GLN
1	L	2068	HIS
1	L	2071	HIS

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Mol	Chain	Res	Type
1	M	2057	GLN
1	M	2081	GLN
1	M	2105	ASN
1	N	2047	ASN
1	N	2057	GLN
1	N	2068	HIS
1	N	2071	HIS
1	O	2019	ASN
1	O	2024	HIS
1	O	2047	ASN
1	O	2057	GLN
1	O	2068	HIS
1	O	2114	ASN
1	P	49	ASN
1	P	59	GLN
1	P	116	ASN
1	Q	2024	HIS
1	Q	2044	ASN
1	Q	2047	ASN
1	Q	2057	GLN
1	Q	2071	HIS
1	Q	2081	GLN
1	Q	2153	ASN
1	R	2047	ASN
1	R	2057	GLN
1	R	2114	ASN
1	S	2057	GLN
1	S	2071	HIS
1	S	2114	ASN
1	T	26	HIS
1	T	46	ASN
1	T	49	ASN
1	T	59	GLN
1	T	70	HIS
1	T	73	HIS
1	U	46	ASN
1	U	49	ASN
1	U	59	GLN
1	V	49	ASN
1	V	59	GLN
1	V	116	ASN
1	W	59	GLN

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Mol	Chain	Res	Type
1	W	83	GLN
1	W	107	ASN
1	X	21	ASN
1	X	59	GLN
1	X	83	GLN
1	X	107	ASN
1	Y	49	ASN
1	Y	59	GLN
1	Y	70	HIS
1	Y	107	ASN
1	Y	121	GLN
1	Z	59	GLN
1	Z	107	ASN
1	a	59	GLN
1	a	73	HIS
1	b	49	ASN
1	b	59	GLN
1	b	70	HIS
1	b	73	HIS
1	b	116	ASN
1	c	49	ASN
1	c	59	GLN
1	c	70	HIS
1	c	73	HIS
1	c	107	ASN
1	c	116	ASN
1	c	155	ASN
1	d	46	ASN
1	d	49	ASN
1	d	59	GLN
1	d	70	HIS
1	d	73	HIS
1	e	46	ASN
1	e	59	GLN
1	e	70	HIS
1	f	59	GLN
1	f	107	ASN
1	g	59	GLN
1	g	73	HIS
1	h	49	ASN
1	h	59	GLN
1	h	70	HIS

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Mol	Chain	Res	Type
1	h	107	ASN
1	h	121	GLN
1	i	59	GLN
1	i	107	ASN
1	j	49	ASN
1	j	59	GLN
1	j	73	HIS
1	j	116	ASN
1	k	59	GLN
1	k	83	GLN
1	k	107	ASN
1	l	59	GLN
1	l	73	HIS
1	l	116	ASN
1	l	155	ASN
1	m	49	ASN
1	m	59	GLN
1	m	107	ASN
1	m	166	ASN
1	n	21	ASN
1	n	26	HIS
1	n	46	ASN
1	n	49	ASN
1	n	59	GLN
1	n	73	HIS
1	n	121	GLN
1	o	59	GLN
1	o	107	ASN
1	p	59	GLN
1	p	107	ASN
1	q	49	ASN
1	q	59	GLN
1	q	73	HIS
1	q	116	ASN
1	r	59	GLN
1	r	73	HIS
1	r	155	ASN
1	s	49	ASN
1	s	59	GLN
1	s	70	HIS
1	s	116	ASN
1	t	49	ASN

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Mol	Chain	Res	Type
1	t	59	GLN
1	t	107	ASN
1	u	26	HIS
1	u	49	ASN
1	u	59	GLN
1	u	70	HIS
1	u	73	HIS
1	v	49	ASN
1	v	59	GLN
1	v	73	HIS
1	v	116	ASN
1	w	59	GLN
1	w	70	HIS
1	w	73	HIS
1	x	26	HIS
1	x	59	GLN
1	x	73	HIS
1	x	83	GLN
1	x	116	ASN
1	x	121	GLN
1	x	155	ASN
1	y	59	GLN
1	y	83	GLN
1	z	49	ASN
1	z	59	GLN
1	z	73	HIS
1	z	116	ASN
1	0	26	HIS
1	0	59	GLN
1	0	73	HIS
1	0	107	ASN
1	0	116	ASN
1	0	155	ASN
1	1	49	ASN
1	1	59	GLN
1	1	107	ASN
1	2	26	HIS
1	2	59	GLN
1	2	107	ASN
1	3	49	ASN
1	3	59	GLN
1	3	70	HIS

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Mol	Chain	Res	Type
1	3	166	ASN
1	4	49	ASN
1	4	59	GLN
1	4	70	HIS
1	4	83	GLN
1	4	116	ASN
1	4	121	GLN
1	4	134	ASN
1	4	155	ASN
1	5	59	GLN
1	5	73	HIS
1	5	116	ASN
1	6	49	ASN
1	6	59	GLN
1	6	116	ASN
1	6	134	ASN
1	6	155	ASN
1	7	49	ASN
1	7	59	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 224 ligands modelled in this entry, 92 are monoatomic - leaving 132 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	$\# Z > 2$
6	C	I	3002	3	18,21,22	0.95	1 (5%)	26,30,33	0.60	0
6	C	g	201	3	18,21,22	0.94	1 (5%)	26,30,33	0.60	0
4	SSU	q	201	5	19,21,22	1.01	1 (5%)	25,30,33	0.77	0
3	SRA	R	2203	3,4	22,24,25	0.45	0	30,35,38	0.62	0
3	SRA	e	204	6,3	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	4	1001	3,4	22,24,25	0.45	0	30,35,38	0.65	0
5	G	q	202	4	22,25,26	0.49	0	33,37,40	0.59	0
6	C	q	203	3	18,21,22	1.09	1 (5%)	26,30,33	0.62	0
3	SRA	w	202	3,4	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	H	2209	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
5	G	r	2001	4	22,25,26	0.50	0	33,37,40	0.60	0
4	SSU	z	204	5	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
4	SSU	P	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
4	SSU	R	2204	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
6	C	L	2204	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
5	G	b	207	4	22,25,26	0.49	0	33,37,40	0.61	0
5	G	g	204	4	22,25,26	0.49	0	33,37,40	0.60	0
3	SRA	t	205	3,4	22,24,25	0.45	0	30,35,38	0.65	0
4	SSU	I	3004	5	19,21,22	0.99	1 (5%)	25,30,33	0.77	0
6	C	b	202	3	18,21,22	0.94	1 (5%)	26,30,33	0.61	0
5	G	H	2201	4	22,25,26	0.50	0	33,37,40	0.60	0
6	C	r	2002	3	18,21,22	1.09	1 (5%)	26,30,33	0.62	0
4	SSU	3	202	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
6	C	I	3007	3	18,21,22	1.09	1 (5%)	26,30,33	0.62	0
3	SRA	g	202	6	22,24,25	0.45	0	30,35,38	0.63	0
3	SRA	x	201	6	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	N	2202	6	22,24,25	0.44	0	30,35,38	0.63	0
5	G	I	3006	4	22,25,26	0.50	0	33,37,40	0.60	0
4	SSU	P	203	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0
5	G	i	204	4	22,25,26	0.49	0	33,37,40	0.60	0
6	C	y	201	3	18,21,22	0.94	1 (5%)	26,30,33	0.60	0
3	SRA	H	2203	6,3	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	K	2202	3	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
4	SSU	X	202	3	19,21,22	1.00	1 (5%)	25,30,33	0.78	0
3	SRA	Y	2004	3,4	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	C	2204	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SSU	2	201	5	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
6	C	C	2206	3	18,21,22	0.95	1 (5%)	26,30,33	0.61	0
6	C	i	205	3	18,21,22	0.94	1 (5%)	26,30,33	0.61	0
4	SSU	v	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
3	SRA	I	3008	6,3	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	L	2202	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0
3	SRA	a	202	3,4	22,24,25	0.45	0	30,35,38	0.65	0
6	C	Y	2002	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
3	SRA	W	2003	6,3	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	r	2004	6	22,24,25	0.44	0	30,35,38	0.64	0
5	G	b	201	4	22,25,26	0.49	0	33,37,40	0.60	0
4	SSU	a	203	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0
4	SSU	w	201	3	19,21,22	0.99	1 (5%)	25,30,33	0.77	0
4	SSU	t	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
3	SRA	z	203	6	22,24,25	0.45	0	30,35,38	0.63	0
4	SSU	b	206	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0
5	G	W	2001	4	22,25,26	0.50	0	33,37,40	0.60	0
3	SRA	R	2202	6,3	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	H	2204	3,4	22,24,25	0.45	0	30,35,38	0.63	0
3	SRA	T	1001	3,4	22,24,25	0.45	0	30,35,38	0.64	0
3	SRA	L	2205	6,3	22,24,25	0.44	0	30,35,38	0.63	0
6	C	z	202	3	18,21,22	0.95	1 (5%)	26,30,33	0.61	0
6	C	2	202	3	18,21,22	1.08	1 (5%)	26,30,33	0.63	0
6	C	r	2003	3	18,21,22	0.94	1 (5%)	26,30,33	0.60	0
5	G	Q	3004	4	22,25,26	0.50	0	33,37,40	0.60	0
6	C	e	203	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
5	G	K	2205	4	22,25,26	0.49	0	33,37,40	0.60	0
4	SSU	4	1002	3,5	19,21,22	1.00	1 (5%)	25,30,33	0.75	0
4	SSU	y	203	5	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
4	SSU	J	3003	3	19,21,22	0.98	1 (5%)	25,30,33	0.77	0
4	SSU	Q	3003	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.74	0
3	SRA	F	202	6,3	22,24,25	0.44	0	30,35,38	0.63	0
6	C	H	2202	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
3	SRA	Q	3002	3,4	22,24,25	0.45	0	30,35,38	0.65	0
5	G	4	1003	4	22,25,26	0.50	0	33,37,40	0.61	0
3	SRA	K	2203	3,4	22,24,25	0.46	0	30,35,38	0.64	0
4	SSU	e	201	5	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
4	SSU	i	203	3,5	19,21,22	1.00	1 (5%)	25,30,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SRA	q	204	6,3	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	H	2207	3	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
6	C	b	208	3	18,21,22	0.95	1 (5%)	26,30,33	0.60	0
4	SSU	a	201	3	19,21,22	1.01	1 (5%)	25,30,33	0.76	0
3	SRA	Y	2003	6,3	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	q	205	3,4	22,24,25	0.45	0	30,35,38	0.63	0
5	G	I	3005	4	22,25,26	0.49	0	33,37,40	0.59	0
3	SRA	E	3003	6,3	22,24,25	0.43	0	30,35,38	0.64	0
3	SRA	L	2201	3,4	22,24,25	0.45	0	30,35,38	0.64	0
4	SSU	i	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
5	G	P	204	4	22,25,26	0.49	0	33,37,40	0.60	0
4	SSU	g	207	5	19,21,22	1.01	1 (5%)	25,30,33	0.77	0
4	SSU	z	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
5	G	a	204	4	22,25,26	0.49	0	33,37,40	0.61	0
3	SRA	t	203	3,4	22,24,25	0.45	0	30,35,38	0.63	0
3	SRA	I	3003	6	22,24,25	0.45	0	30,35,38	0.64	0
6	C	k	2002	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
3	SRA	C	2203	3,4	22,24,25	0.44	0	30,35,38	0.65	0
4	SSU	K	2201	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
4	SSU	T	1002	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.75	0
4	SSU	t	206	3,5	19,21,22	1.00	1 (5%)	25,30,33	0.75	0
4	SSU	w	203	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
5	G	C	2205	4	22,25,26	0.50	0	33,37,40	0.60	0
4	SSU	K	2204	3,5	19,21,22	0.99	1 (5%)	25,30,33	0.76	0
4	SSU	F	204	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
3	SRA	k	2004	3,4	22,24,25	0.44	0	30,35,38	0.63	0
5	G	T	1003	4	22,25,26	0.50	0	33,37,40	0.60	0
3	SRA	i	202	3,4	22,24,25	0.45	0	30,35,38	0.65	0
6	C	E	3002	3	18,21,22	1.09	1 (5%)	26,30,33	0.63	0
6	C	N	2201	3	18,21,22	0.94	1 (5%)	26,30,33	0.60	0
3	SRA	b	205	3,4	22,24,25	0.45	0	30,35,38	0.65	0
3	SRA	h	201	6	22,24,25	0.45	0	30,35,38	0.63	0
6	C	W	2002	3	18,21,22	1.08	1 (5%)	26,30,33	0.62	0
3	SRA	P	202	3,4	22,24,25	0.45	0	30,35,38	0.65	0
3	SRA	H	2208	3,4	22,24,25	0.44	0	30,35,38	0.63	0
5	G	k	2001	4	22,25,26	0.49	0	33,37,40	0.60	0
3	SRA	F	203	3,4	22,24,25	0.44	0	30,35,38	0.63	0
3	SRA	g	206	6	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	t	202	5	19,21,22	1.00	1 (5%)	25,30,33	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	G	y	204	4	22,25,26	0.50	0	33,37,40	0.60	0
3	SRA	b	209	6	22,24,25	0.44	0	30,35,38	0.63	0
4	SSU	h	202	5	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
4	SSU	g	203	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
4	SSU	r	2005	5	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
3	SRA	L	2206	3,4	22,24,25	0.45	0	30,35,38	0.62	0
4	SSU	t	204	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
3	SRA	y	202	6	22,24,25	0.45	0	30,35,38	0.63	0
5	G	Y	2001	4	22,25,26	0.50	0	33,37,40	0.60	0
4	SSU	3	203	3	19,21,22	0.99	1 (5%)	25,30,33	0.78	0
3	SRA	b	203	6	22,24,25	0.45	0	30,35,38	0.63	0
4	SSU	X	201	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
4	SSU	b	204	5	19,21,22	1.00	1 (5%)	25,30,33	0.76	0
5	G	e	202	4	22,25,26	0.49	0	33,37,40	0.61	0
6	C	g	205	3	18,21,22	0.94	1 (5%)	26,30,33	0.61	0
4	SSU	L	2207	3	19,21,22	1.00	1 (5%)	25,30,33	0.77	0
5	G	R	2201	4	22,25,26	0.50	0	33,37,40	0.60	0
3	SRA	J	3002	3,4	22,24,25	0.43	0	30,35,38	0.63	0
3	SRA	k	2003	6,3	22,24,25	0.44	0	30,35,38	0.63	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
6	C	I	3002	3	-	0/7/25/26	0/2/2/2
6	C	g	201	3	-	0/7/25/26	0/2/2/2
4	SSU	q	201	5	-	0/7/25/26	0/2/2/2
3	SRA	R	2203	3,4	-	0/7/25/26	0/3/3/3
3	SRA	e	204	6,3	-	0/7/25/26	0/3/3/3
3	SRA	4	1001	3,4	-	0/7/25/26	0/3/3/3
5	G	q	202	4	-	0/7/25/26	0/3/3/3
6	C	q	203	3	-	0/7/25/26	0/2/2/2
3	SRA	w	202	3,4	-	0/7/25/26	0/3/3/3
4	SSU	H	2209	3	-	0/7/25/26	0/2/2/2
5	G	r	2001	4	-	0/7/25/26	0/3/3/3
4	SSU	z	204	5	-	0/7/25/26	0/2/2/2
4	SSU	P	201	3	-	0/7/25/26	0/2/2/2
4	SSU	R	2204	3	-	0/7/25/26	0/2/2/2
6	C	L	2204	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G	b	207	4	-	0/7/25/26	0/3/3/3
5	G	g	204	4	-	0/7/25/26	0/3/3/3
3	SRA	t	205	3,4	-	0/7/25/26	0/3/3/3
4	SSU	I	3004	5	-	0/7/25/26	0/2/2/2
6	C	b	202	3	-	0/7/25/26	0/2/2/2
5	G	H	2201	4	-	0/7/25/26	0/3/3/3
6	C	r	2002	3	-	0/7/25/26	0/2/2/2
4	SSU	3	202	3	-	0/7/25/26	0/2/2/2
6	C	I	3007	3	-	0/7/25/26	0/2/2/2
3	SRA	g	202	6	-	0/7/25/26	0/3/3/3
3	SRA	x	201	6	-	0/7/25/26	0/3/3/3
3	SRA	N	2202	6	-	0/7/25/26	0/3/3/3
5	G	I	3006	4	-	0/7/25/26	0/3/3/3
4	SSU	P	203	3,5	-	0/7/25/26	0/2/2/2
5	G	i	204	4	-	0/7/25/26	0/3/3/3
6	C	y	201	3	-	0/7/25/26	0/2/2/2
3	SRA	H	2203	6,3	-	0/7/25/26	0/3/3/3
4	SSU	K	2202	3	-	0/7/25/26	0/2/2/2
4	SSU	X	202	3	-	0/7/25/26	0/2/2/2
3	SRA	Y	2004	3,4	-	0/7/25/26	0/3/3/3
4	SSU	C	2204	3,5	-	0/7/25/26	0/2/2/2
4	SSU	2	201	5	-	0/7/25/26	0/2/2/2
6	C	C	2206	3	-	0/7/25/26	0/2/2/2
6	C	i	205	3	-	0/7/25/26	0/2/2/2
4	SSU	v	201	3	-	0/7/25/26	0/2/2/2
3	SRA	I	3008	6,3	-	0/7/25/26	0/3/3/3
4	SSU	L	2202	3,5	-	0/7/25/26	0/2/2/2
3	SRA	a	202	3,4	-	0/7/25/26	0/3/3/3
6	C	Y	2002	3	-	0/7/25/26	0/2/2/2
3	SRA	W	2003	6,3	-	0/7/25/26	0/3/3/3
3	SRA	r	2004	6	-	0/7/25/26	0/3/3/3
5	G	b	201	4	-	0/7/25/26	0/3/3/3
4	SSU	a	203	3,5	-	0/7/25/26	0/2/2/2
4	SSU	w	201	3	-	0/7/25/26	0/2/2/2
4	SSU	t	201	3	-	0/7/25/26	0/2/2/2
3	SRA	z	203	6	-	0/7/25/26	0/3/3/3
4	SSU	b	206	3,5	-	0/7/25/26	0/2/2/2
5	G	W	2001	4	-	0/7/25/26	0/3/3/3
3	SRA	R	2202	6,3	-	0/7/25/26	0/3/3/3
3	SRA	H	2204	3,4	-	0/7/25/26	0/3/3/3
3	SRA	T	1001	3,4	-	0/7/25/26	0/3/3/3
3	SRA	L	2205	6,3	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C	z	202	3	-	0/7/25/26	0/2/2/2
6	C	2	202	3	-	0/7/25/26	0/2/2/2
6	C	r	2003	3	-	0/7/25/26	0/2/2/2
5	G	Q	3004	4	-	0/7/25/26	0/3/3/3
6	C	e	203	3	-	0/7/25/26	0/2/2/2
5	G	K	2205	4	-	0/7/25/26	0/3/3/3
4	SSU	4	1002	3,5	-	0/7/25/26	0/2/2/2
4	SSU	y	203	5	-	0/7/25/26	0/2/2/2
4	SSU	J	3003	3	-	0/7/25/26	0/2/2/2
4	SSU	Q	3003	3,5	-	0/7/25/26	0/2/2/2
3	SRA	F	202	6,3	-	0/7/25/26	0/3/3/3
6	C	H	2202	3	-	0/7/25/26	0/2/2/2
3	SRA	Q	3002	3,4	-	0/7/25/26	0/3/3/3
5	G	4	1003	4	-	0/7/25/26	0/3/3/3
3	SRA	K	2203	3,4	-	0/7/25/26	0/3/3/3
4	SSU	e	201	5	-	0/7/25/26	0/2/2/2
4	SSU	i	203	3,5	-	0/7/25/26	0/2/2/2
3	SRA	q	204	6,3	-	0/7/25/26	0/3/3/3
4	SSU	H	2207	3	-	0/7/25/26	0/2/2/2
6	C	b	208	3	-	0/7/25/26	0/2/2/2
4	SSU	a	201	3	-	0/7/25/26	0/2/2/2
3	SRA	Y	2003	6,3	-	0/7/25/26	0/3/3/3
3	SRA	q	205	3,4	-	0/7/25/26	0/3/3/3
5	G	I	3005	4	-	0/7/25/26	0/3/3/3
3	SRA	E	3003	6,3	-	0/7/25/26	0/3/3/3
3	SRA	L	2201	3,4	-	0/7/25/26	0/3/3/3
4	SSU	i	201	3	-	0/7/25/26	0/2/2/2
5	G	P	204	4	-	0/7/25/26	0/3/3/3
4	SSU	g	207	5	-	0/7/25/26	0/2/2/2
4	SSU	z	201	3	-	0/7/25/26	0/2/2/2
5	G	a	204	4	-	0/7/25/26	0/3/3/3
3	SRA	t	203	3,4	-	0/7/25/26	0/3/3/3
3	SRA	I	3003	6	-	0/7/25/26	0/3/3/3
6	C	k	2002	3	-	0/7/25/26	0/2/2/2
3	SRA	C	2203	3,4	-	0/7/25/26	0/3/3/3
4	SSU	K	2201	3	-	0/7/25/26	0/2/2/2
4	SSU	T	1002	3,5	-	0/7/25/26	0/2/2/2
4	SSU	t	206	3,5	-	0/7/25/26	0/2/2/2
4	SSU	w	203	3	-	0/7/25/26	0/2/2/2
5	G	C	2205	4	-	0/7/25/26	0/3/3/3
4	SSU	K	2204	3,5	-	0/7/25/26	0/2/2/2
4	SSU	F	204	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRA	k	2004	3,4	-	0/7/25/26	0/3/3/3
5	G	T	1003	4	-	0/7/25/26	0/3/3/3
3	SRA	i	202	3,4	-	0/7/25/26	0/3/3/3
6	C	E	3002	3	-	0/7/25/26	0/2/2/2
6	C	N	2201	3	-	0/7/25/26	0/2/2/2
3	SRA	b	205	3,4	-	0/7/25/26	0/3/3/3
3	SRA	h	201	6	-	0/7/25/26	0/3/3/3
6	C	W	2002	3	-	0/7/25/26	0/2/2/2
3	SRA	P	202	3,4	-	0/7/25/26	0/3/3/3
3	SRA	H	2208	3,4	-	0/7/25/26	0/3/3/3
5	G	k	2001	4	-	0/7/25/26	0/3/3/3
3	SRA	F	203	3,4	-	0/7/25/26	0/3/3/3
3	SRA	g	206	6	-	0/7/25/26	0/3/3/3
4	SSU	t	202	5	-	0/7/25/26	0/2/2/2
5	G	y	204	4	-	0/7/25/26	0/3/3/3
3	SRA	b	209	6	-	0/7/25/26	0/3/3/3
4	SSU	h	202	5	-	0/7/25/26	0/2/2/2
4	SSU	g	203	3	-	0/7/25/26	0/2/2/2
4	SSU	r	2005	5	-	0/7/25/26	0/2/2/2
3	SRA	L	2206	3,4	-	0/7/25/26	0/3/3/3
4	SSU	t	204	3	-	0/7/25/26	0/2/2/2
3	SRA	y	202	6	-	0/7/25/26	0/3/3/3
5	G	Y	2001	4	-	0/7/25/26	0/3/3/3
4	SSU	3	203	3	-	0/7/25/26	0/2/2/2
3	SRA	b	203	6	-	0/7/25/26	0/3/3/3
4	SSU	X	201	3	-	0/7/25/26	0/2/2/2
4	SSU	b	204	5	-	0/7/25/26	0/2/2/2
5	G	e	202	4	-	0/7/25/26	0/3/3/3
6	C	g	205	3	-	0/7/25/26	0/2/2/2
4	SSU	L	2207	3	-	0/7/25/26	0/2/2/2
5	G	R	2201	4	-	0/7/25/26	0/3/3/3
3	SRA	J	3002	3,4	-	0/7/25/26	0/3/3/3
3	SRA	k	2003	6,3	-	0/7/25/26	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3002	C	C1'-N1	4.29	1.60	1.47
6	I	3007	C	C1'-N1	4.29	1.60	1.47
6	r	2002	C	C1'-N1	4.29	1.60	1.47
6	q	203	C	C1'-N1	4.28	1.60	1.47
6	e	203	C	C1'-N1	4.28	1.59	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	2002	C	C1'-N1	4.26	1.59	1.47
6	H	2202	C	C1'-N1	4.26	1.59	1.47
6	W	2002	C	C1'-N1	4.26	1.59	1.47
6	L	2204	C	C1'-N1	4.26	1.59	1.47
6	k	2002	C	C1'-N1	4.26	1.59	1.47
6	2	202	C	C1'-N1	4.24	1.59	1.47
4	a	201	SSU	C1'-N1	4.03	1.59	1.47
4	q	201	SSU	C1'-N1	4.02	1.59	1.47
4	e	201	SSU	C1'-N1	4.02	1.59	1.47
4	g	207	SSU	C1'-N1	4.02	1.59	1.47
4	w	203	SSU	C1'-N1	4.01	1.59	1.47
4	X	202	SSU	C1'-N1	4.00	1.59	1.47
4	v	201	SSU	C1'-N1	4.00	1.59	1.47
4	z	204	SSU	C1'-N1	4.00	1.59	1.47
4	t	204	SSU	C1'-N1	3.99	1.59	1.47
4	g	203	SSU	C1'-N1	3.99	1.59	1.47
4	b	204	SSU	C1'-N1	3.99	1.59	1.47
4	h	202	SSU	C1'-N1	3.99	1.59	1.47
4	t	202	SSU	C1'-N1	3.99	1.59	1.47
4	K	2202	SSU	C1'-N1	3.99	1.59	1.47
4	R	2204	SSU	C1'-N1	3.99	1.59	1.47
4	3	202	SSU	C1'-N1	3.99	1.59	1.47
4	r	2005	SSU	C1'-N1	3.98	1.59	1.47
4	L	2207	SSU	C1'-N1	3.98	1.59	1.47
4	X	201	SSU	C1'-N1	3.98	1.59	1.47
4	P	201	SSU	C1'-N1	3.98	1.59	1.47
4	H	2207	SSU	C1'-N1	3.98	1.59	1.47
4	i	201	SSU	C1'-N1	3.98	1.59	1.47
4	z	201	SSU	C1'-N1	3.98	1.59	1.47
4	t	201	SSU	C1'-N1	3.97	1.59	1.47
4	K	2201	SSU	C1'-N1	3.97	1.59	1.47
4	y	203	SSU	C1'-N1	3.97	1.59	1.47
4	I	3004	SSU	C1'-N1	3.97	1.59	1.47
4	F	204	SSU	C1'-N1	3.97	1.59	1.47
4	H	2209	SSU	C1'-N1	3.97	1.59	1.47
4	3	203	SSU	C1'-N1	3.97	1.59	1.47
4	w	201	SSU	C1'-N1	3.96	1.59	1.47
4	i	203	SSU	C1'-N1	3.96	1.59	1.47
4	t	206	SSU	C1'-N1	3.96	1.59	1.47
4	2	201	SSU	C1'-N1	3.96	1.59	1.47
4	P	203	SSU	C1'-N1	3.95	1.59	1.47
4	4	1002	SSU	C1'-N1	3.95	1.59	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2204	SSU	C1'-N1	3.93	1.59	1.47
4	L	2202	SSU	C1'-N1	3.92	1.58	1.47
4	a	203	SSU	C1'-N1	3.92	1.58	1.47
4	K	2204	SSU	C1'-N1	3.92	1.58	1.47
4	b	206	SSU	C1'-N1	3.92	1.58	1.47
4	J	3003	SSU	C1'-N1	3.91	1.58	1.47
4	T	1002	SSU	C1'-N1	3.91	1.58	1.47
4	Q	3003	SSU	C1'-N1	3.90	1.58	1.47
6	I	3002	C	C1'-N1	3.63	1.58	1.47
6	z	202	C	C1'-N1	3.62	1.58	1.47
6	r	2003	C	C1'-N1	3.62	1.58	1.47
6	b	208	C	C1'-N1	3.62	1.58	1.47
6	g	205	C	C1'-N1	3.61	1.58	1.47
6	C	2206	C	C1'-N1	3.61	1.58	1.47
6	y	201	C	C1'-N1	3.61	1.58	1.47
6	b	202	C	C1'-N1	3.61	1.58	1.47
6	i	205	C	C1'-N1	3.61	1.58	1.47
6	N	2201	C	C1'-N1	3.59	1.58	1.47
6	g	201	C	C1'-N1	3.57	1.57	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

132 monomers are involved in 401 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	3002	C	5	0
6	g	201	C	5	0
4	q	201	SSU	1	0
3	R	2203	SRA	6	0
3	e	204	SRA	2	0
3	4	1001	SRA	4	0
5	q	202	G	5	0
6	q	203	C	5	0
3	w	202	SRA	6	0
4	H	2209	SSU	2	0
5	r	2001	G	4	0
4	z	204	SSU	1	0
4	P	201	SSU	4	0
4	R	2204	SSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	2204	C	4	0
5	b	207	G	9	0
5	g	204	G	5	0
3	t	205	SRA	8	0
4	I	3004	SSU	15	0
6	b	202	C	5	0
5	H	2201	G	5	0
6	r	2002	C	14	0
4	3	202	SSU	1	0
6	I	3007	C	14	0
3	g	202	SRA	1	0
3	x	201	SRA	1	0
3	N	2202	SRA	1	0
5	I	3006	G	4	0
4	P	203	SSU	3	0
5	i	204	G	5	0
6	y	201	C	4	0
3	H	2203	SRA	11	0
4	K	2202	SSU	1	0
4	X	202	SSU	2	0
3	Y	2004	SRA	4	0
4	C	2204	SSU	15	0
4	2	201	SSU	1	0
6	C	2206	C	5	0
6	i	205	C	5	0
4	v	201	SSU	2	0
3	I	3008	SRA	3	0
4	L	2202	SSU	6	0
3	a	202	SRA	6	0
6	Y	2002	C	10	0
3	W	2003	SRA	2	0
3	r	2004	SRA	1	0
5	b	201	G	6	0
4	a	203	SSU	11	0
4	w	201	SSU	1	0
4	t	201	SSU	1	0
3	z	203	SRA	1	0
4	b	206	SSU	4	0
5	W	2001	G	9	0
3	R	2202	SRA	11	0
3	H	2204	SRA	5	0
3	T	1001	SRA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	2205	SRA	4	0
6	z	202	C	5	0
6	2	202	C	5	0
6	r	2003	C	4	0
5	Q	3004	G	7	0
6	e	203	C	5	0
5	K	2205	G	7	0
4	4	1002	SSU	10	0
4	y	203	SSU	9	0
4	J	3003	SSU	2	0
4	Q	3003	SSU	8	0
3	F	202	SRA	2	0
6	H	2202	C	15	0
3	Q	3002	SRA	5	0
5	4	1003	G	5	0
3	K	2203	SRA	7	0
4	e	201	SSU	1	0
4	i	203	SSU	4	0
3	q	204	SRA	5	0
4	H	2207	SSU	1	0
6	b	208	C	7	0
4	a	201	SSU	1	0
3	Y	2003	SRA	4	0
3	q	205	SRA	6	0
5	I	3005	G	5	0
3	E	3003	SRA	2	0
3	L	2201	SRA	6	0
4	i	201	SSU	1	0
5	P	204	G	4	0
4	g	207	SSU	1	0
4	z	201	SSU	1	0
5	a	204	G	5	0
3	t	203	SRA	5	0
3	I	3003	SRA	2	0
6	k	2002	C	5	0
3	C	2203	SRA	5	0
4	K	2201	SSU	2	0
4	T	1002	SSU	8	0
4	t	206	SSU	4	0
4	w	203	SSU	2	0
5	C	2205	G	5	0
4	K	2204	SSU	12	0

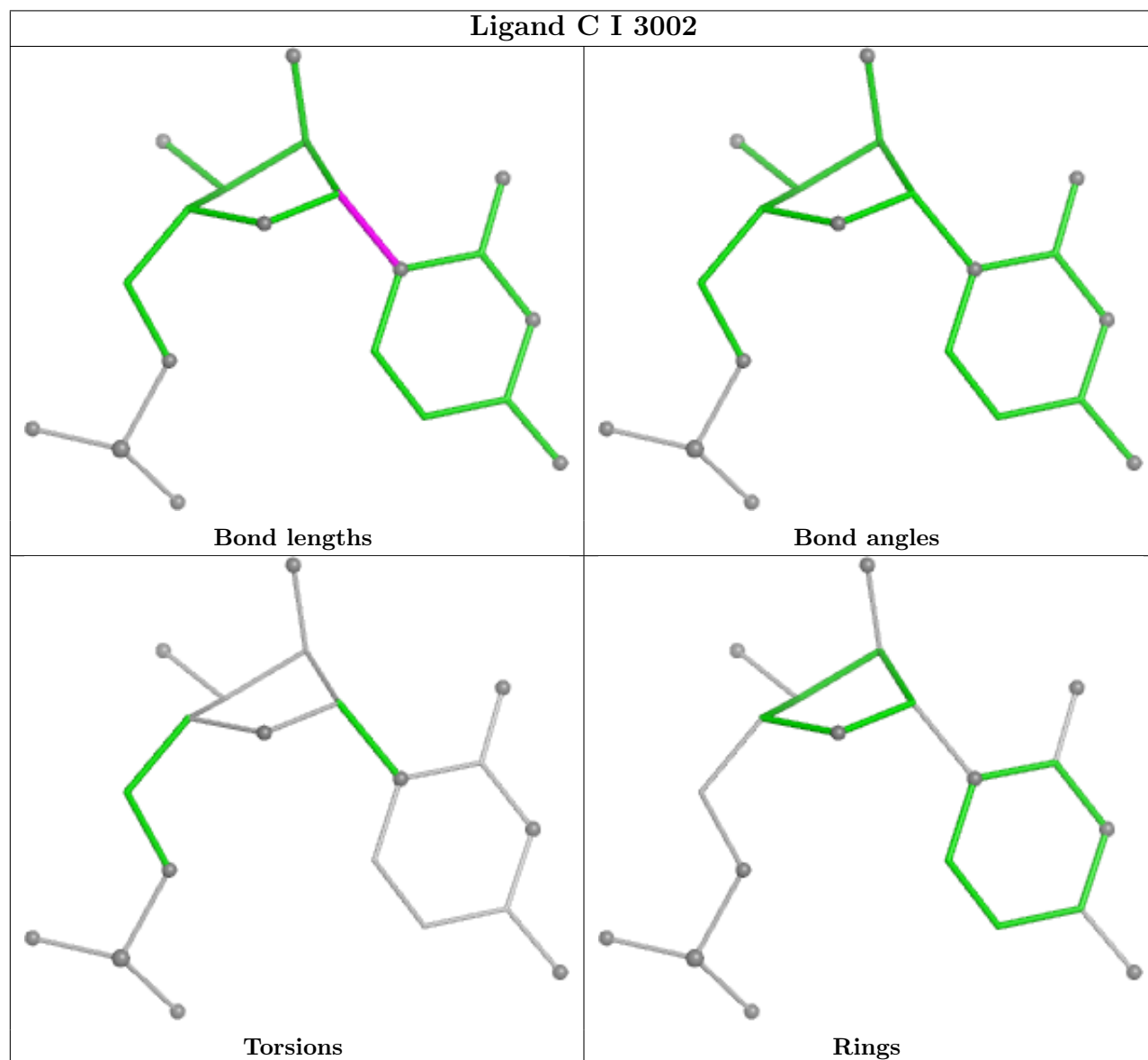
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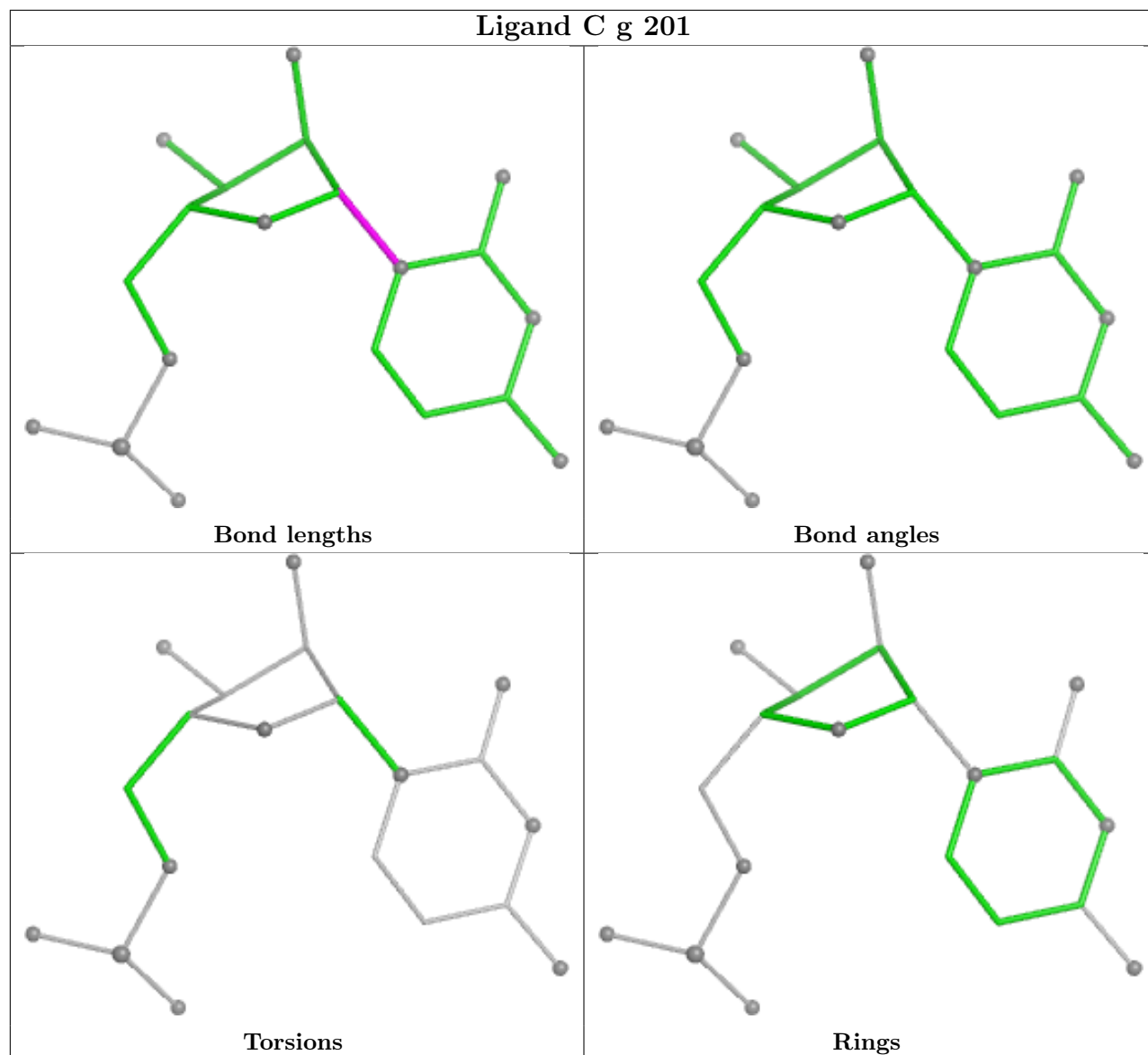
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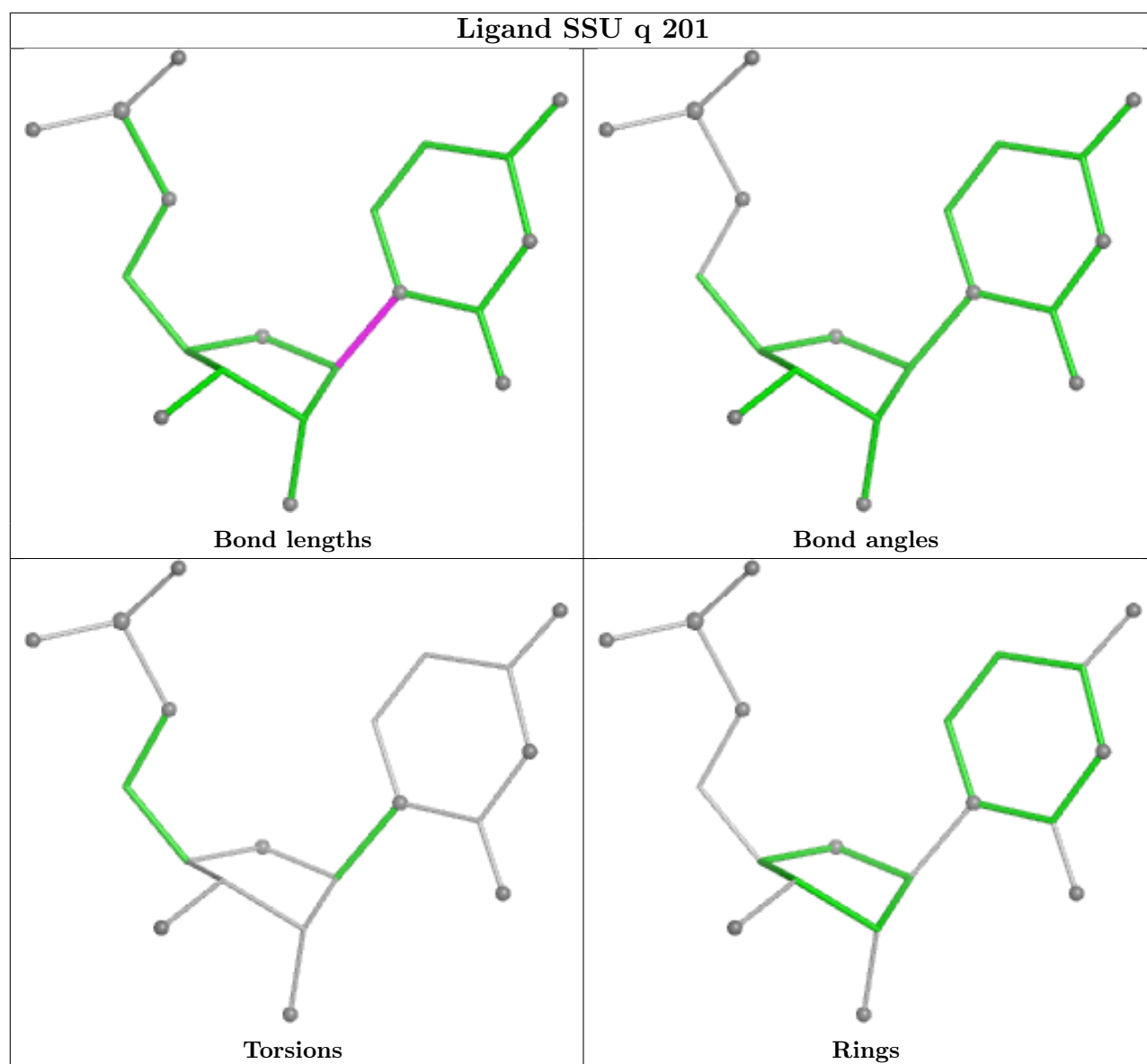
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	204	SSU	2	0
3	k	2004	SRA	5	0
5	T	1003	G	4	0
3	i	202	SRA	7	0
6	E	3002	C	6	0
6	N	2201	C	4	0
3	b	205	SRA	6	0
3	h	201	SRA	1	0
6	W	2002	C	7	0
3	P	202	SRA	7	0
3	H	2208	SRA	5	0
5	k	2001	G	5	0
3	F	203	SRA	6	0
3	g	206	SRA	1	0
4	t	202	SSU	1	0
5	y	204	G	4	0
3	b	209	SRA	1	0
4	h	202	SSU	1	0
4	g	203	SSU	1	0
4	r	2005	SSU	1	0
3	L	2206	SRA	7	0
4	t	204	SSU	4	0
3	y	202	SRA	1	0
5	Y	2001	G	4	0
4	3	203	SSU	3	0
3	b	203	SRA	1	0
4	X	201	SSU	1	0
4	b	204	SSU	1	0
5	e	202	G	7	0
6	g	205	C	5	0
4	L	2207	SSU	3	0
5	R	2201	G	5	0
3	J	3002	SRA	5	0
3	k	2003	SRA	9	0

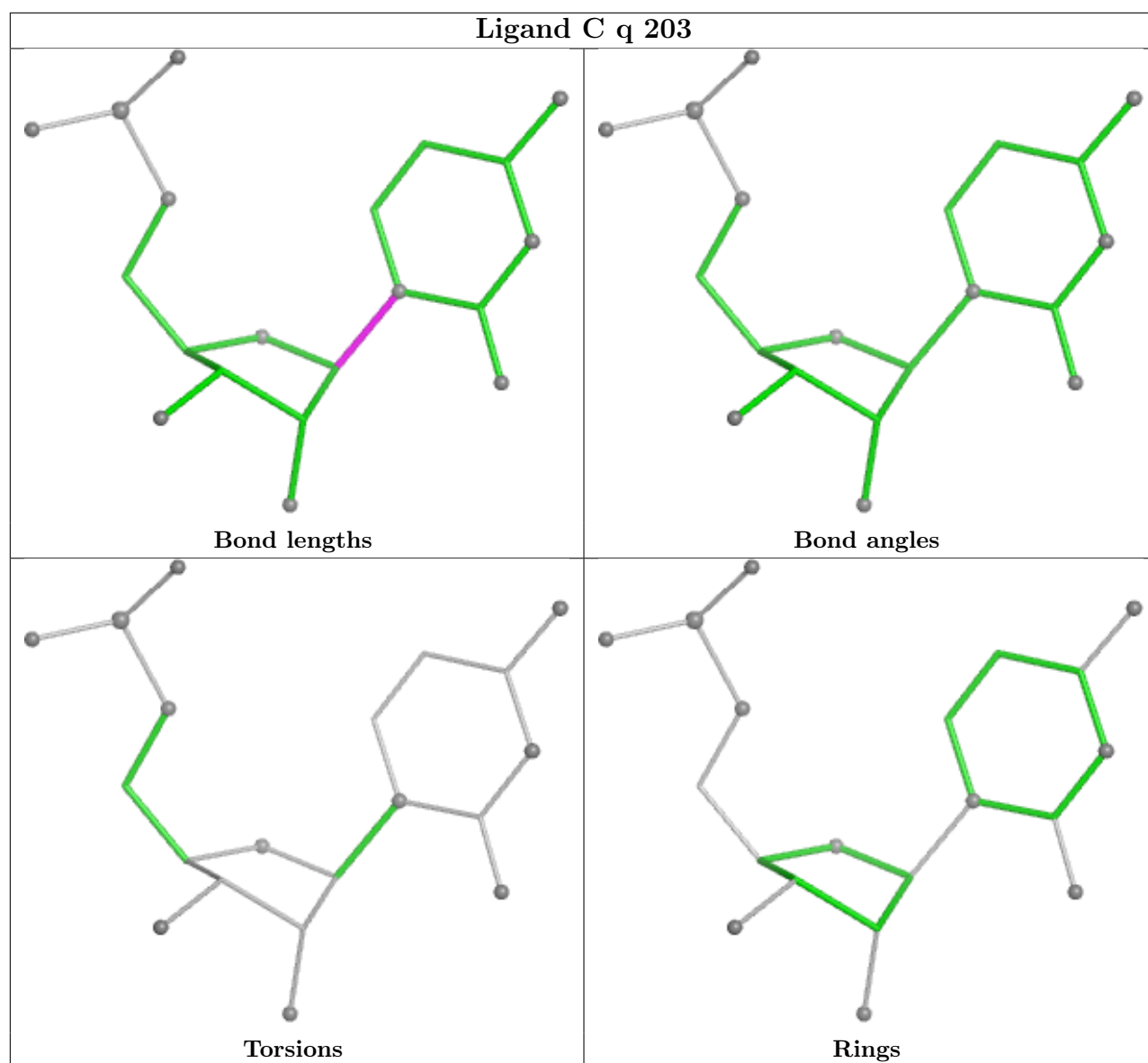
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

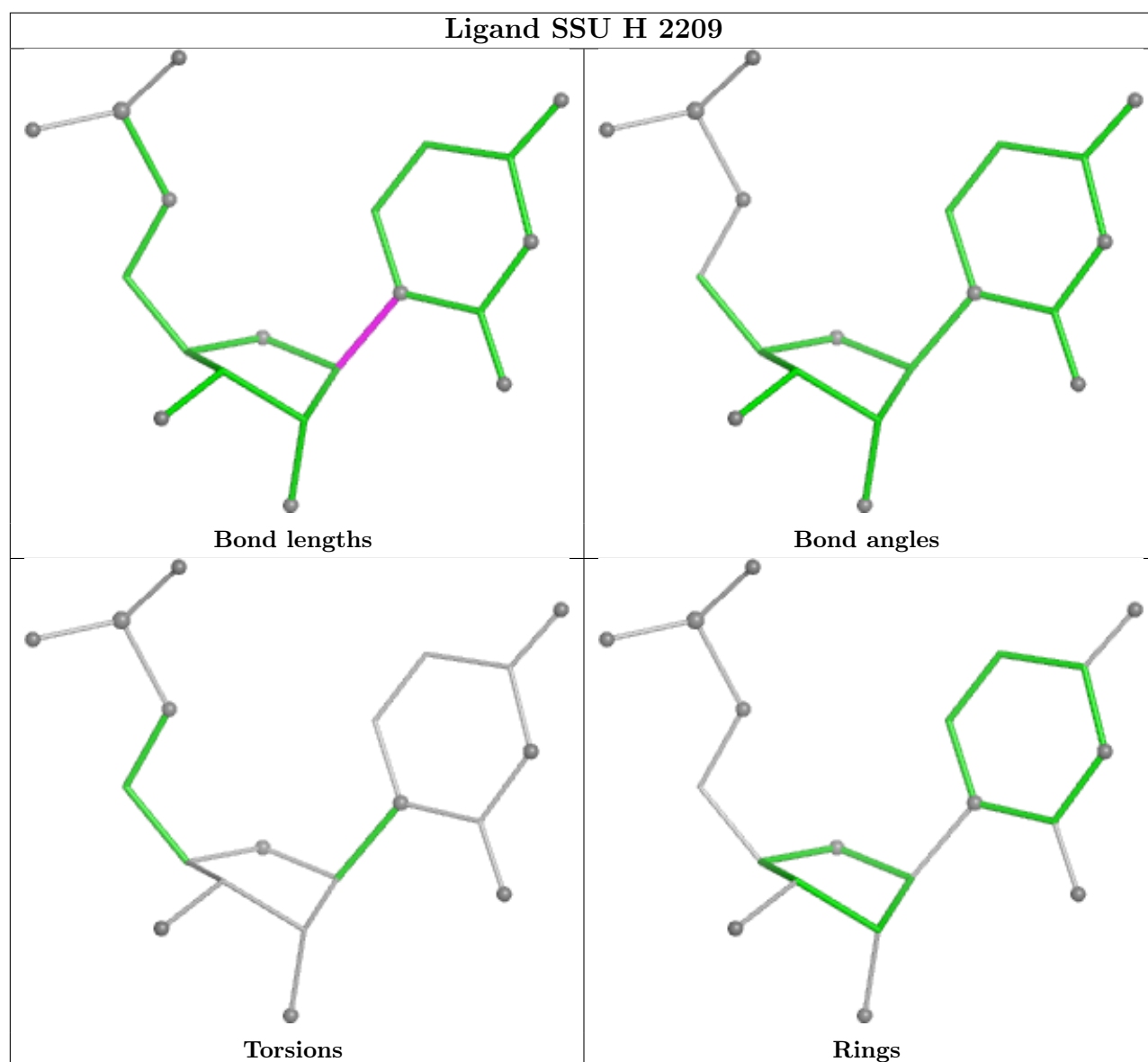
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

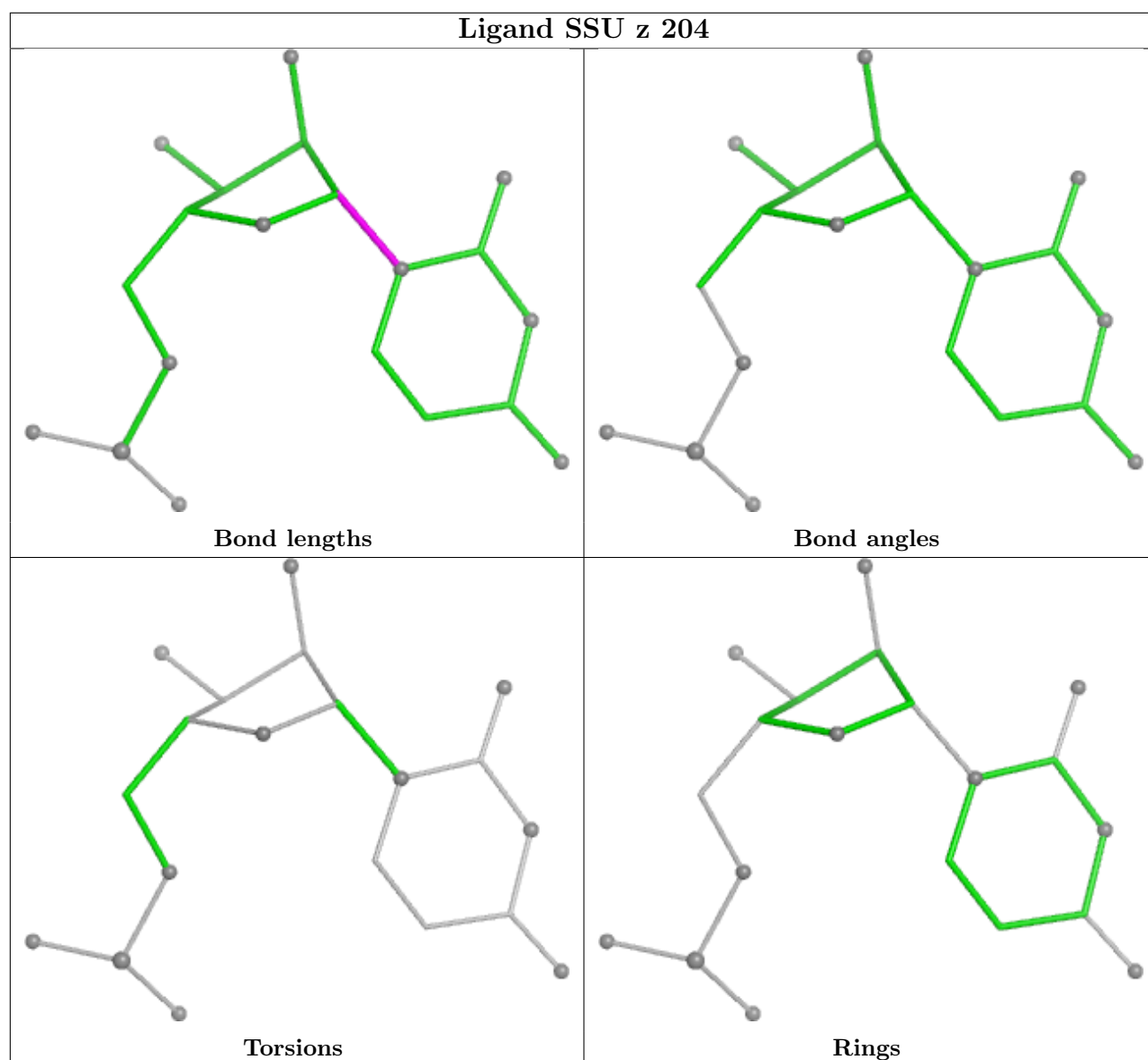


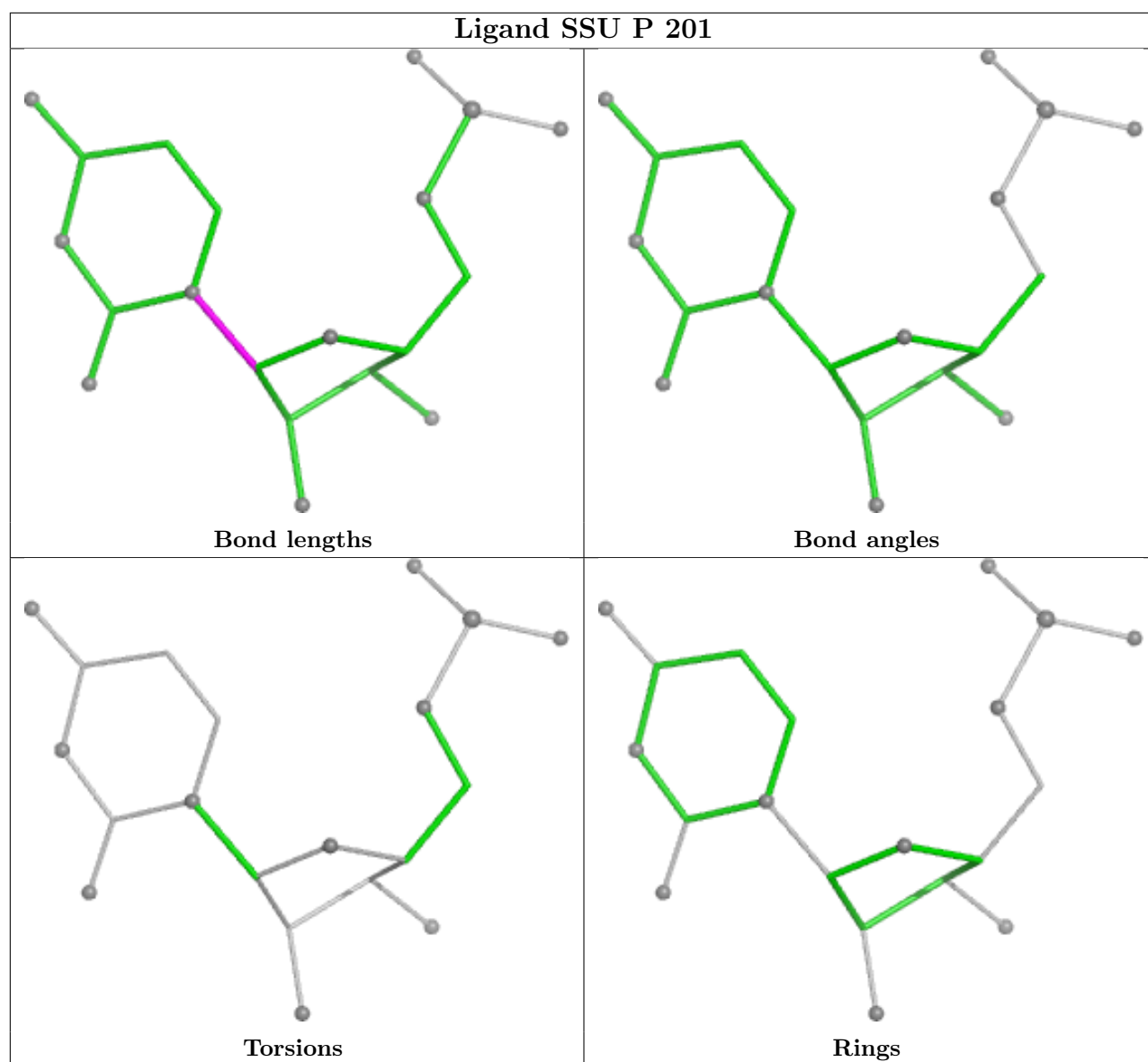


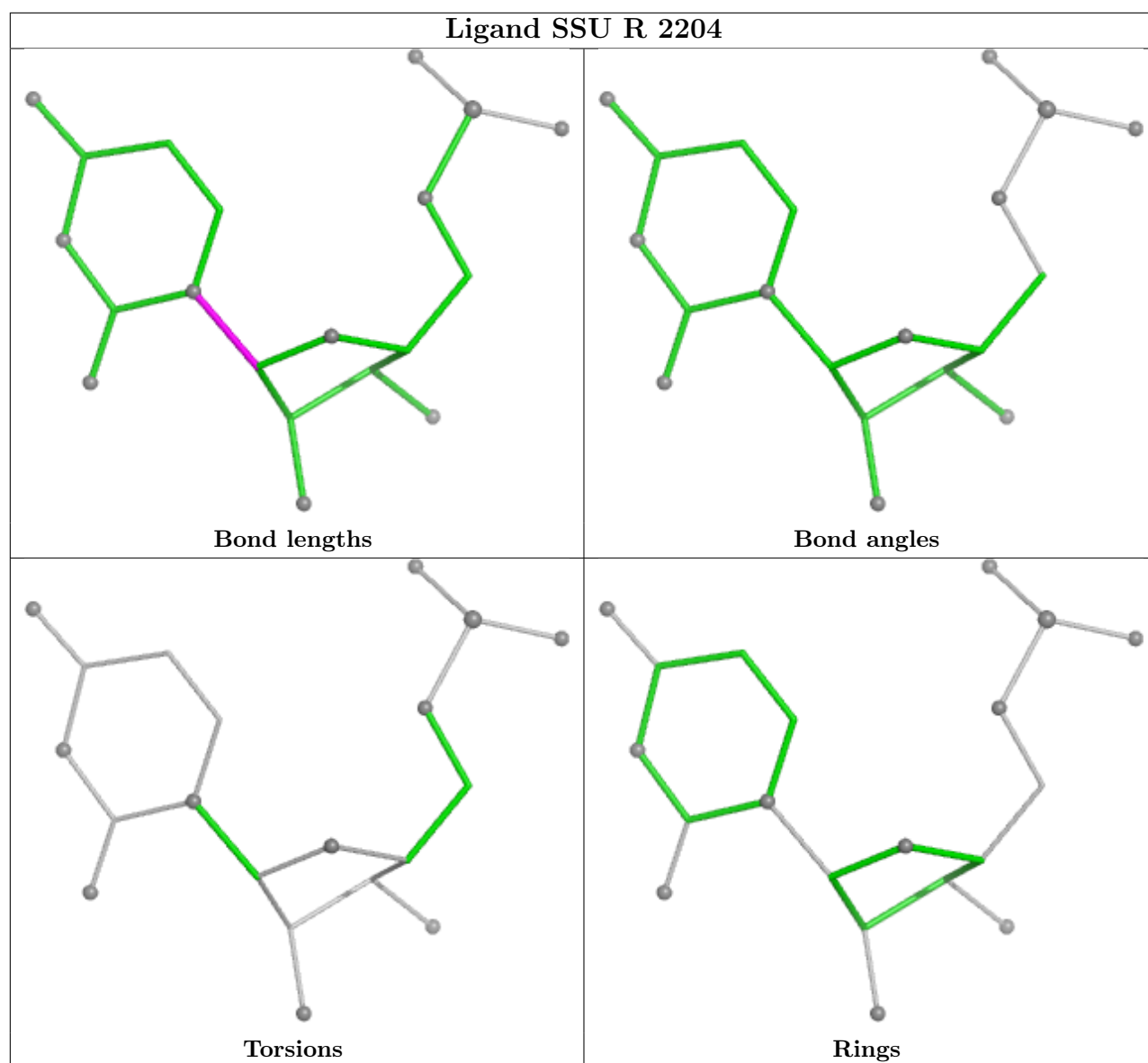


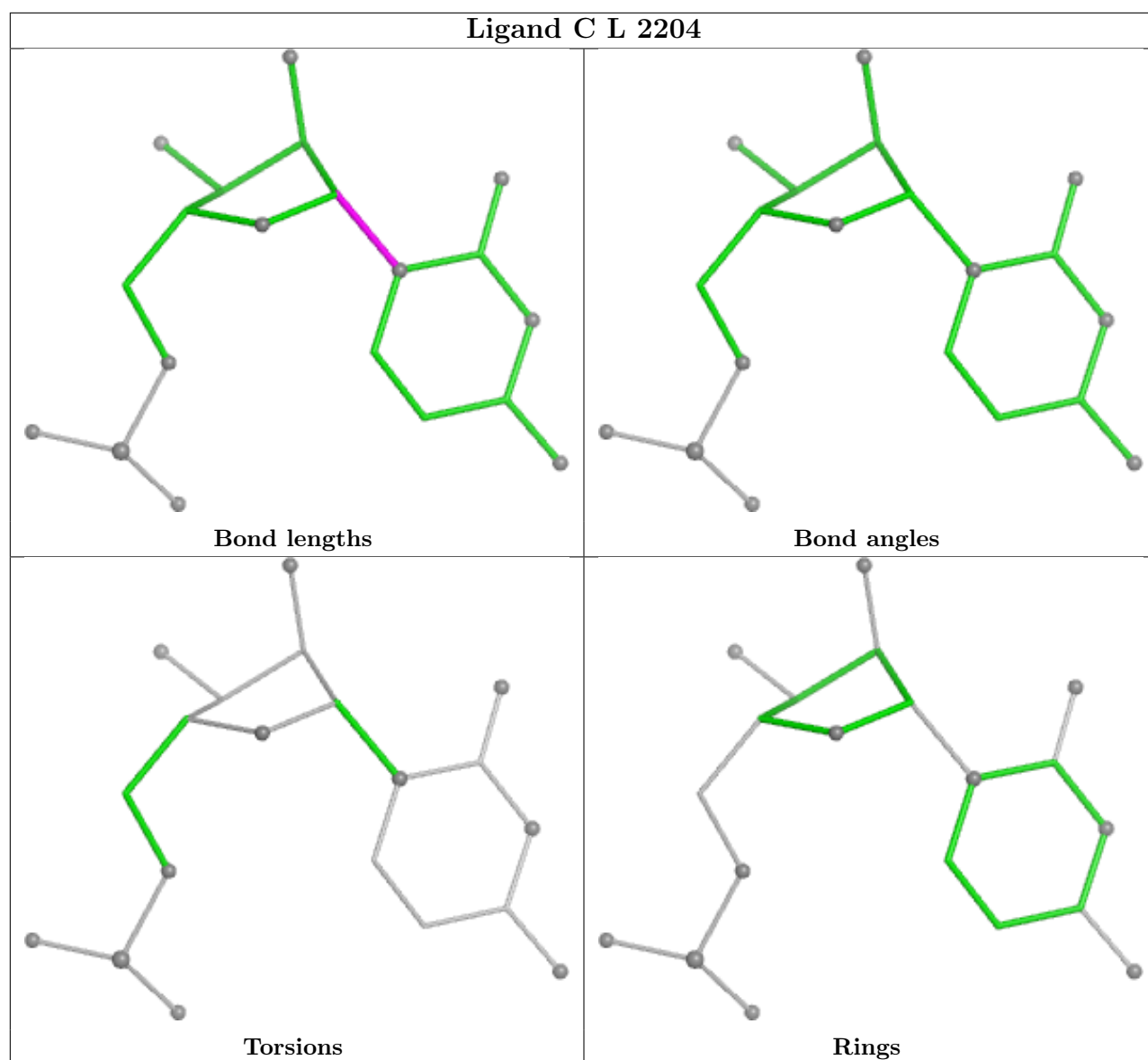


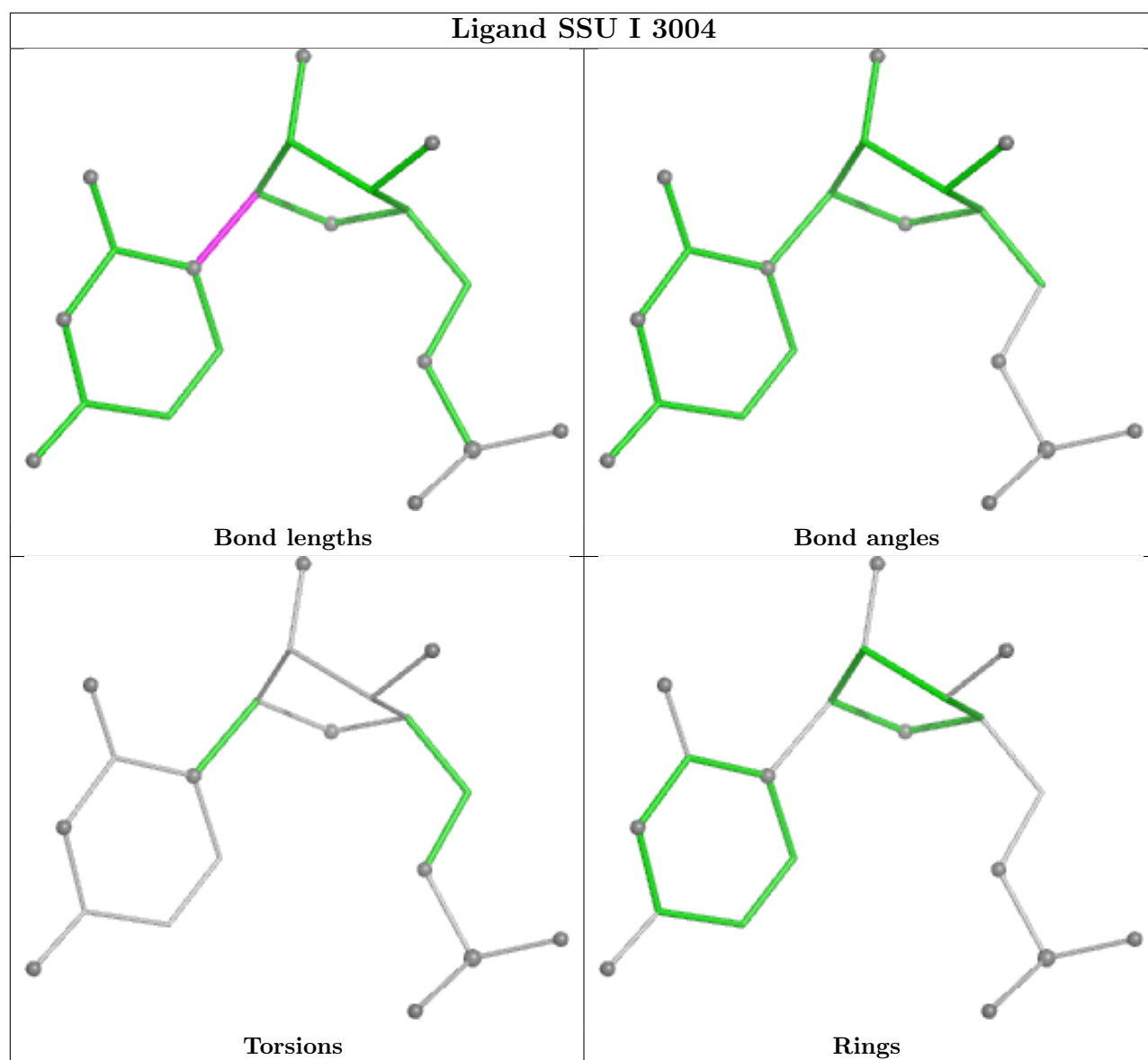


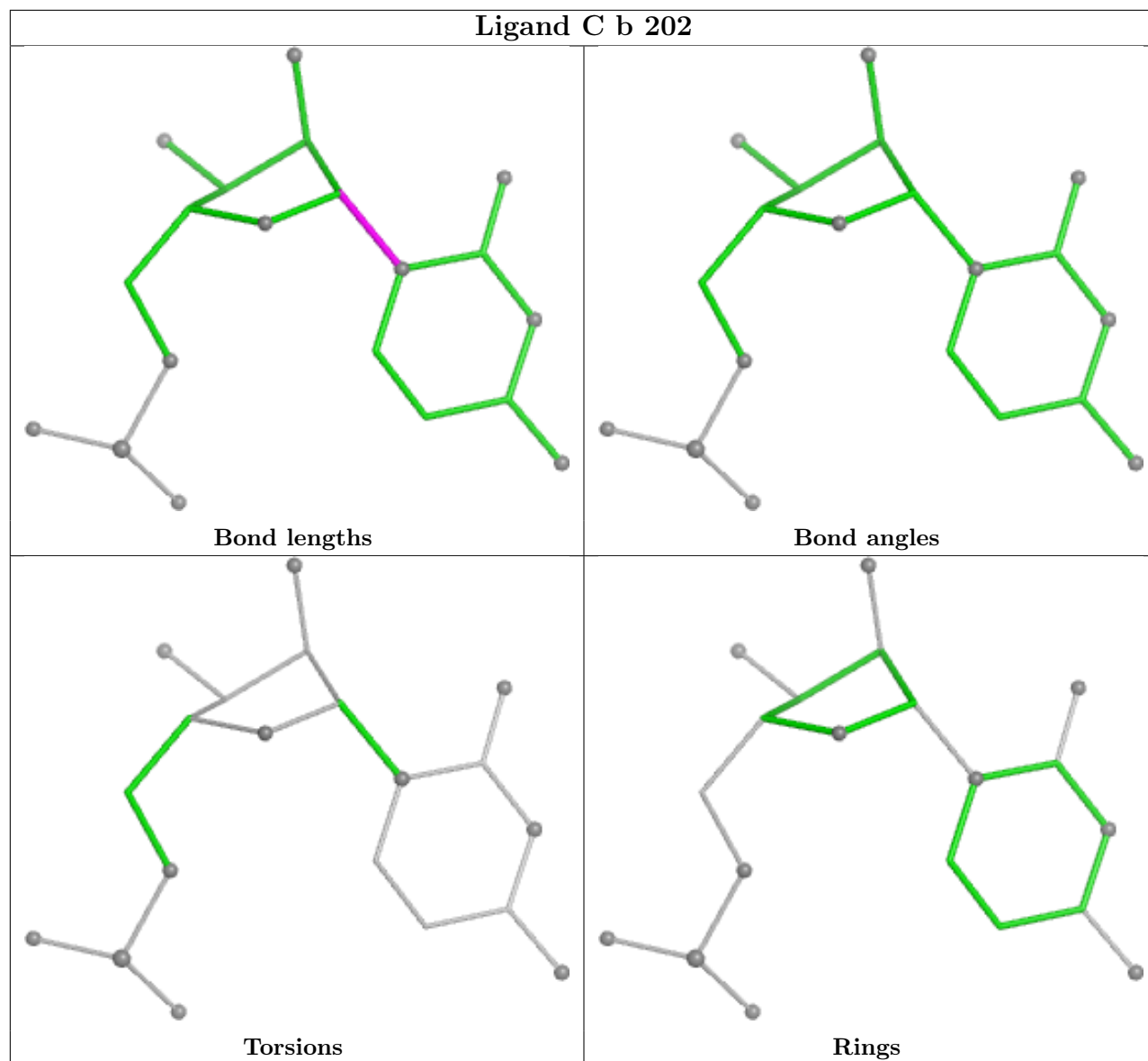


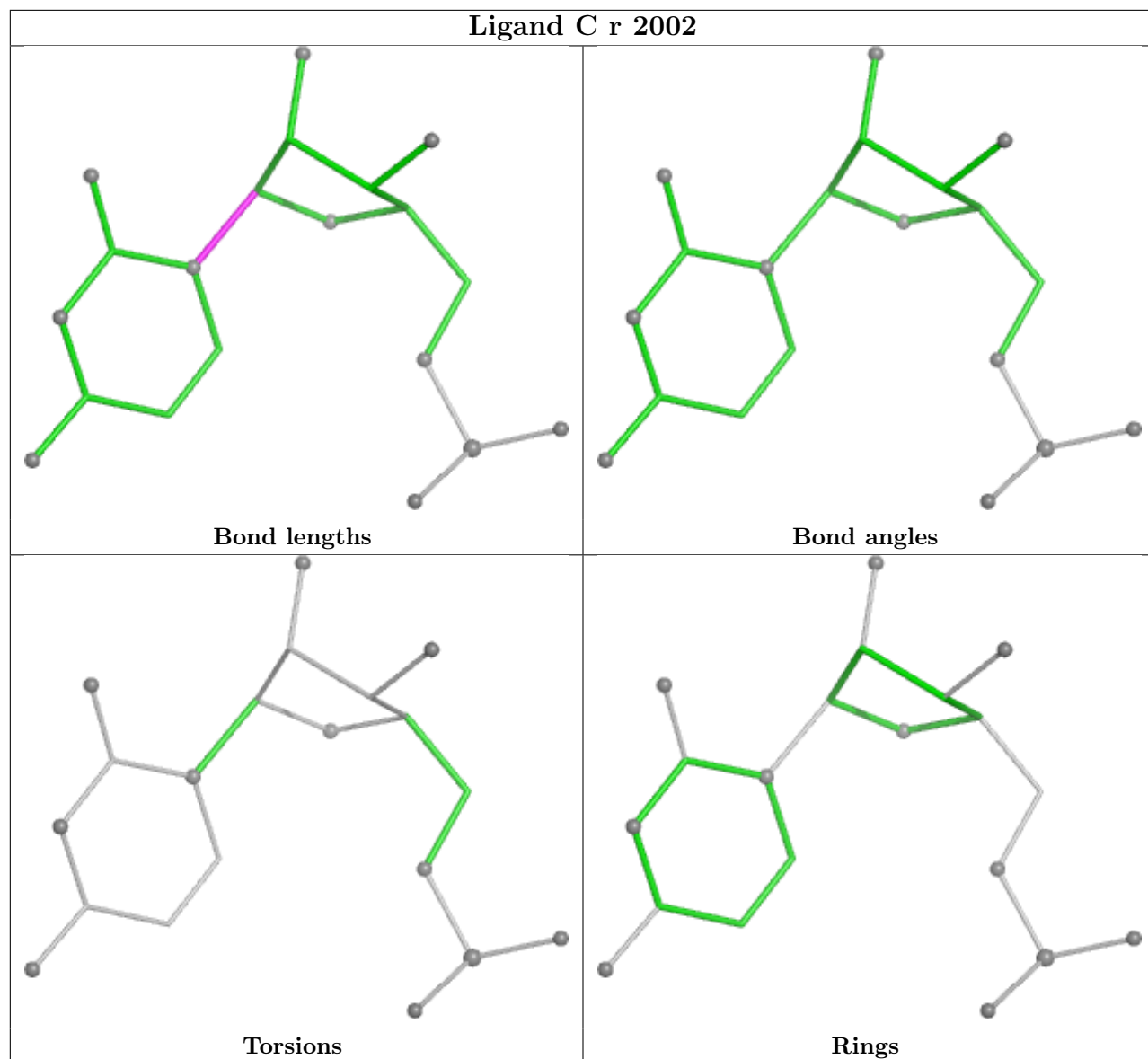


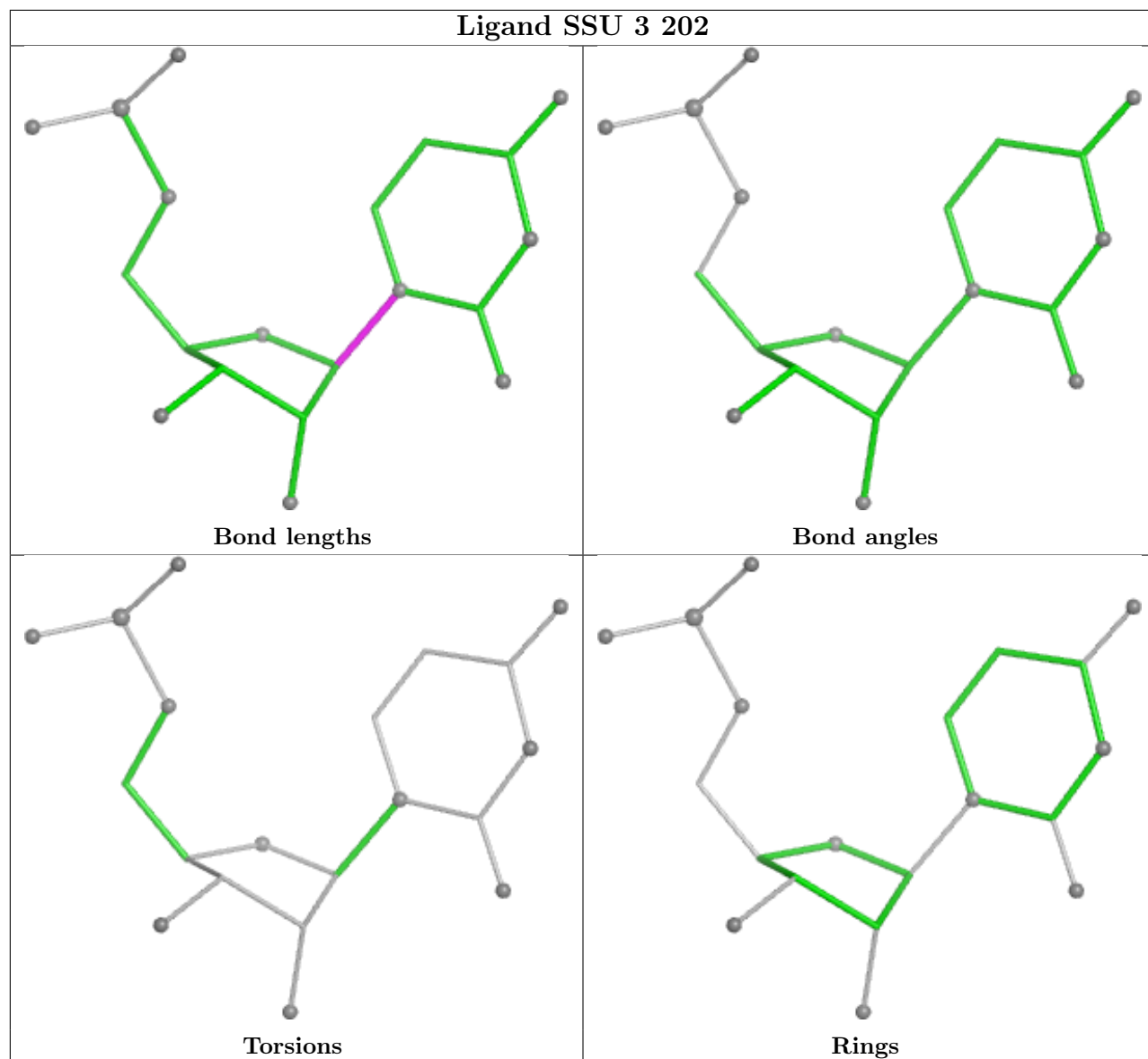


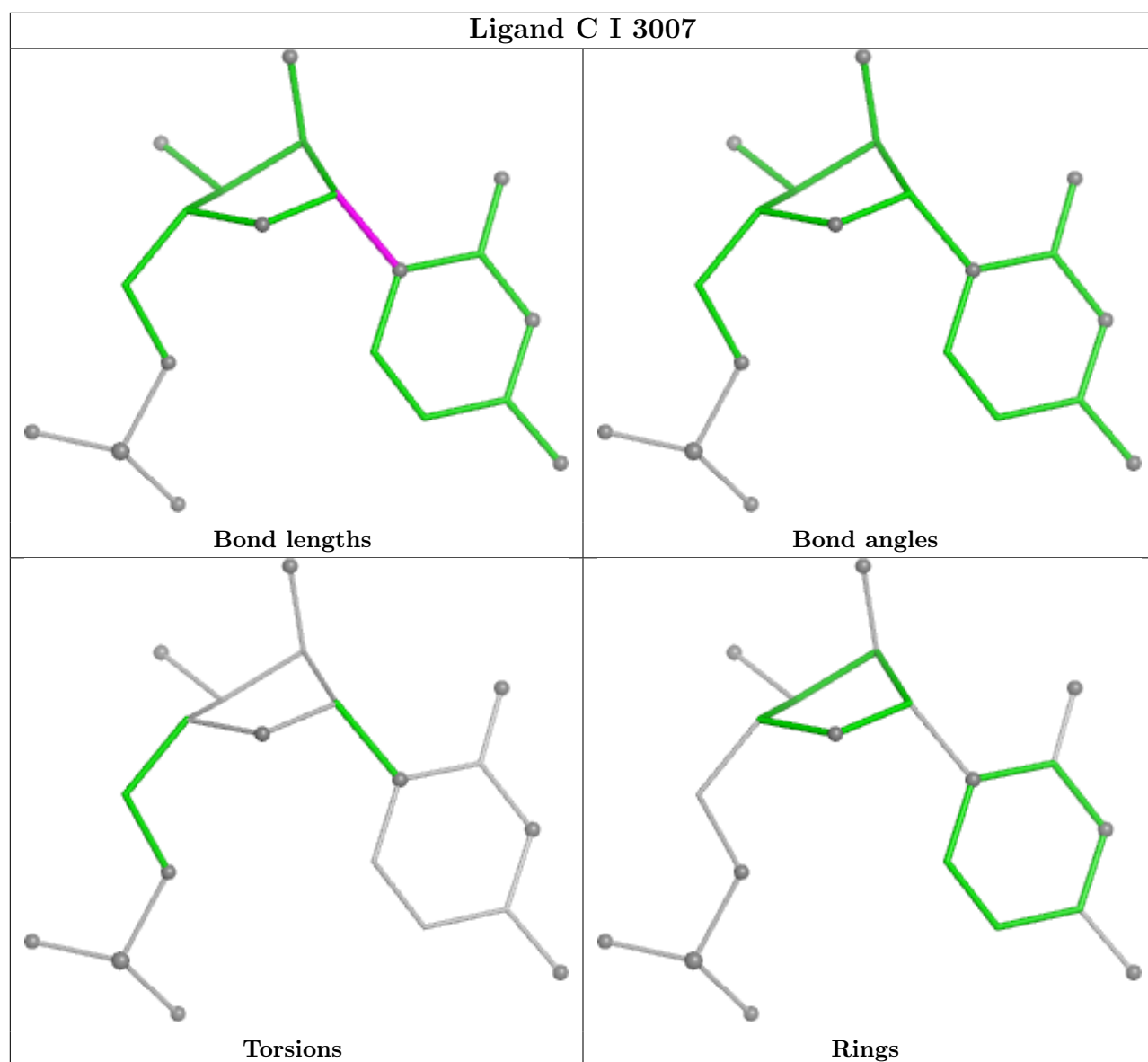


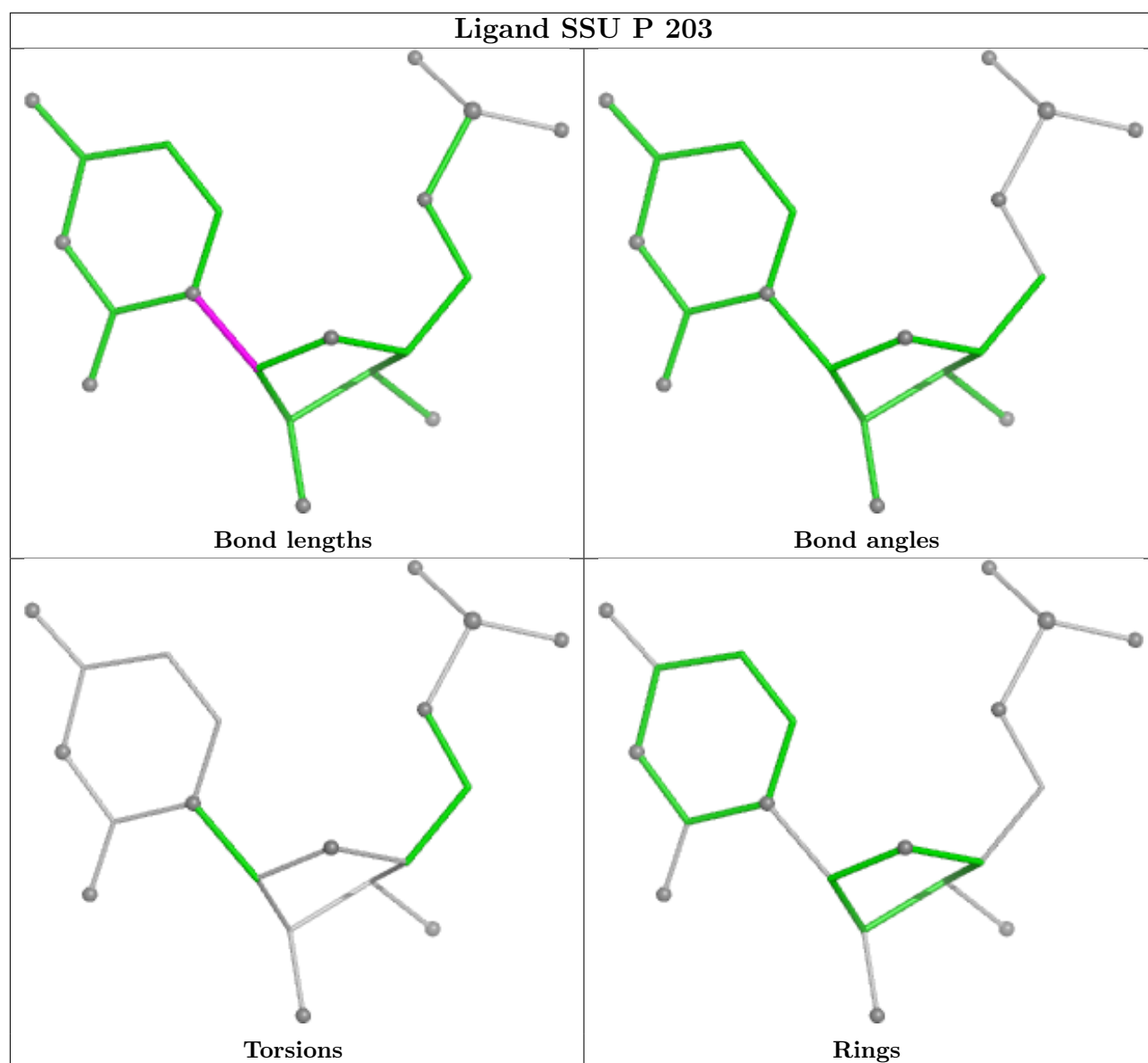


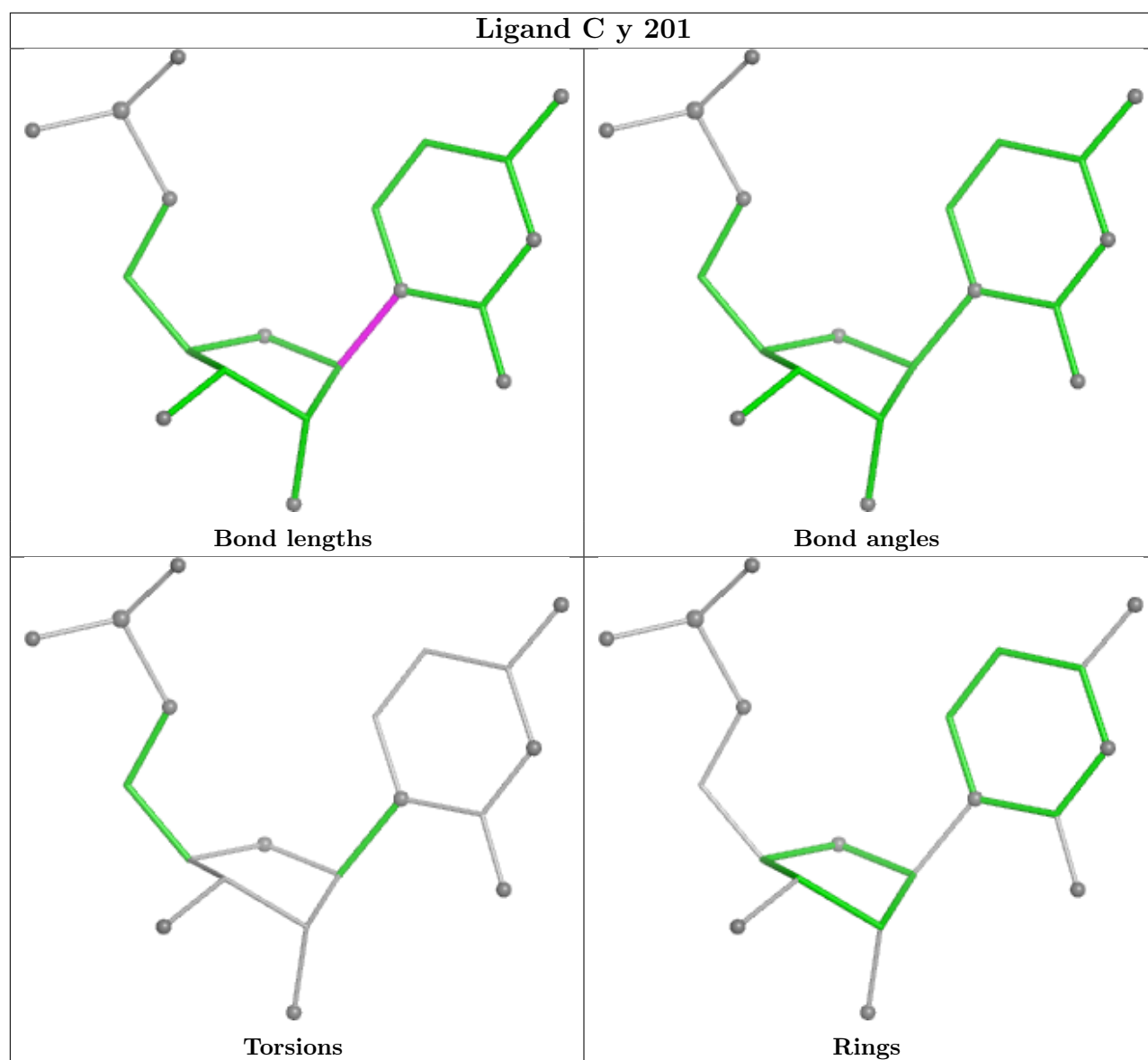


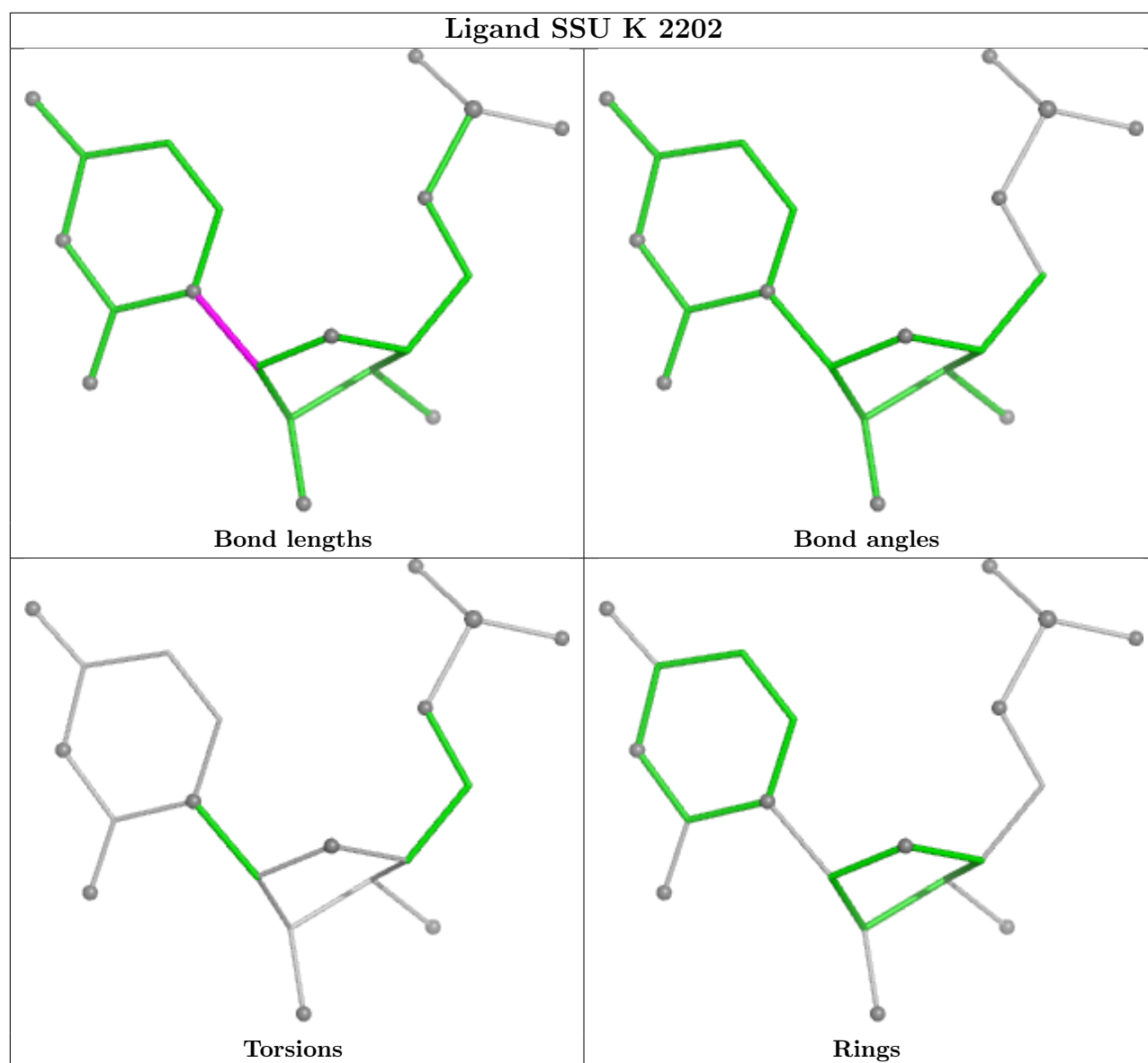


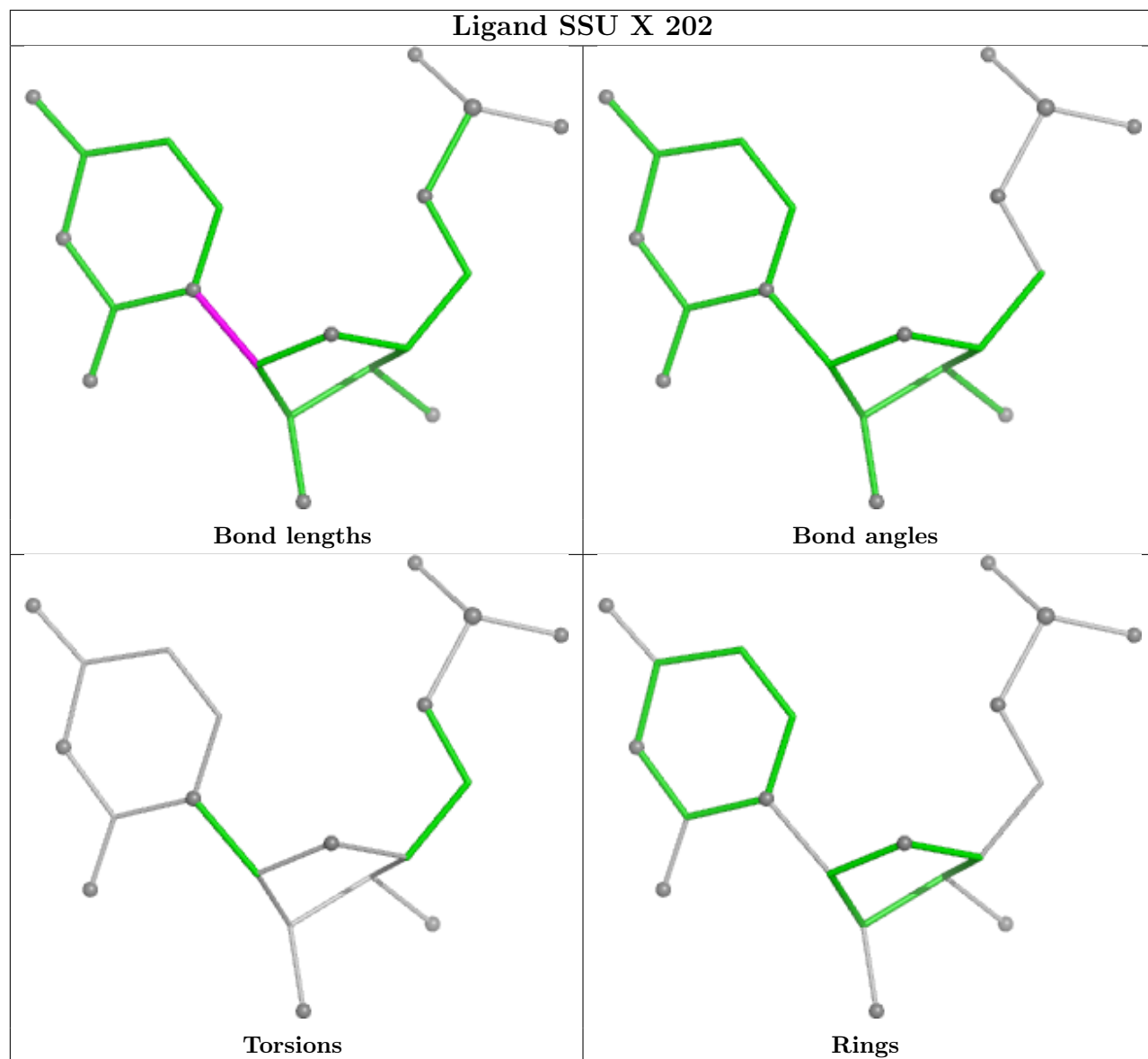


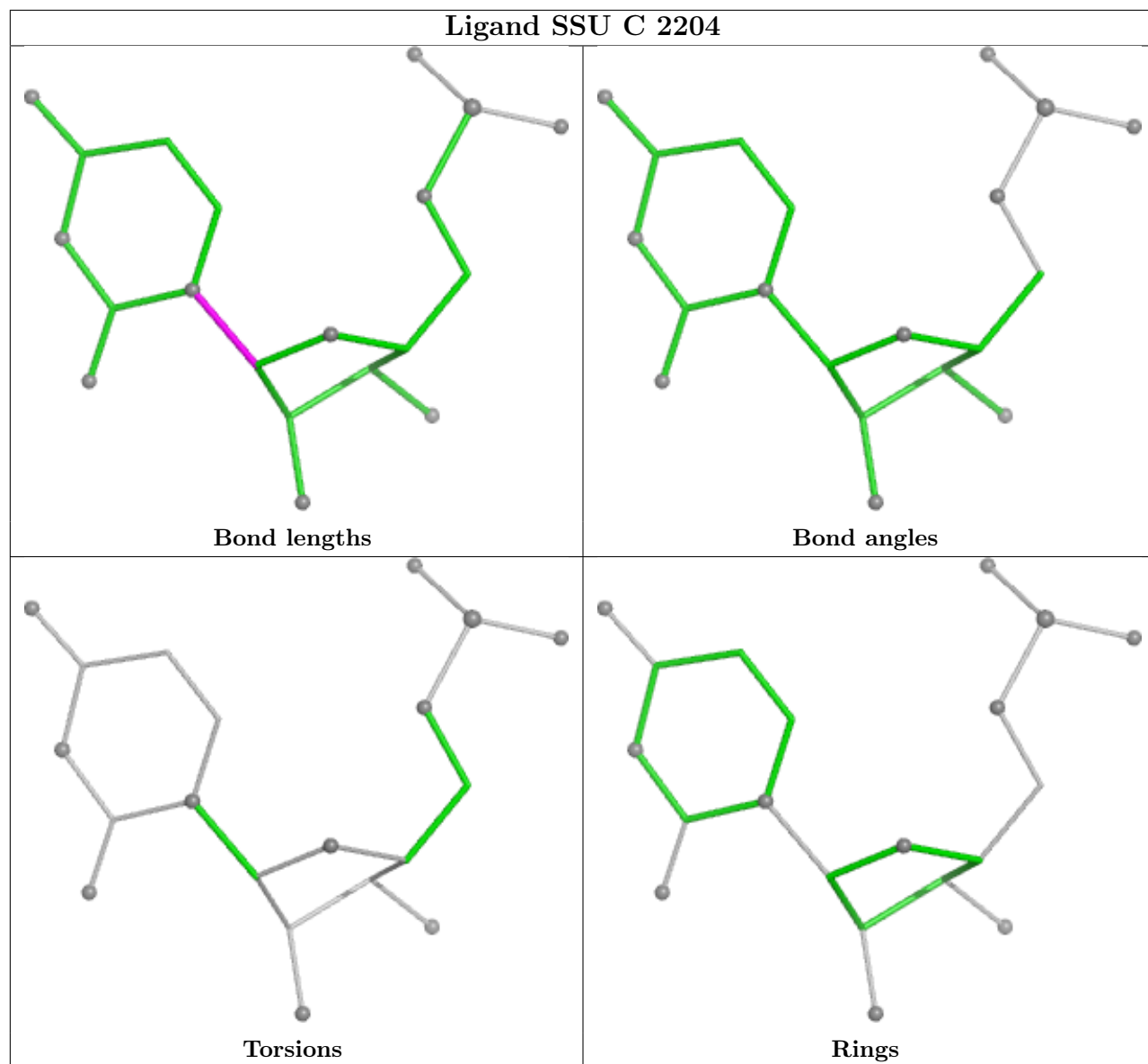


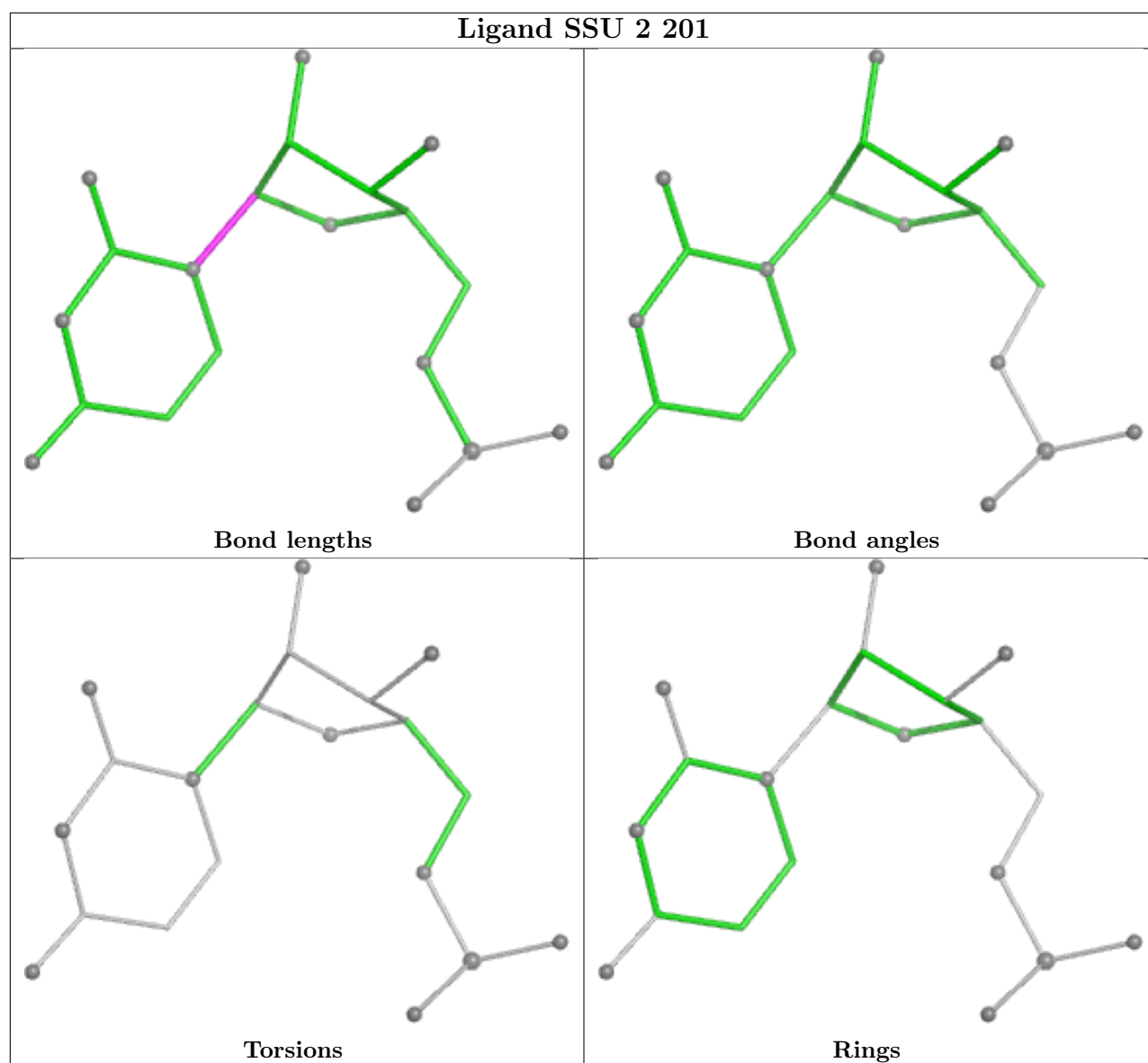




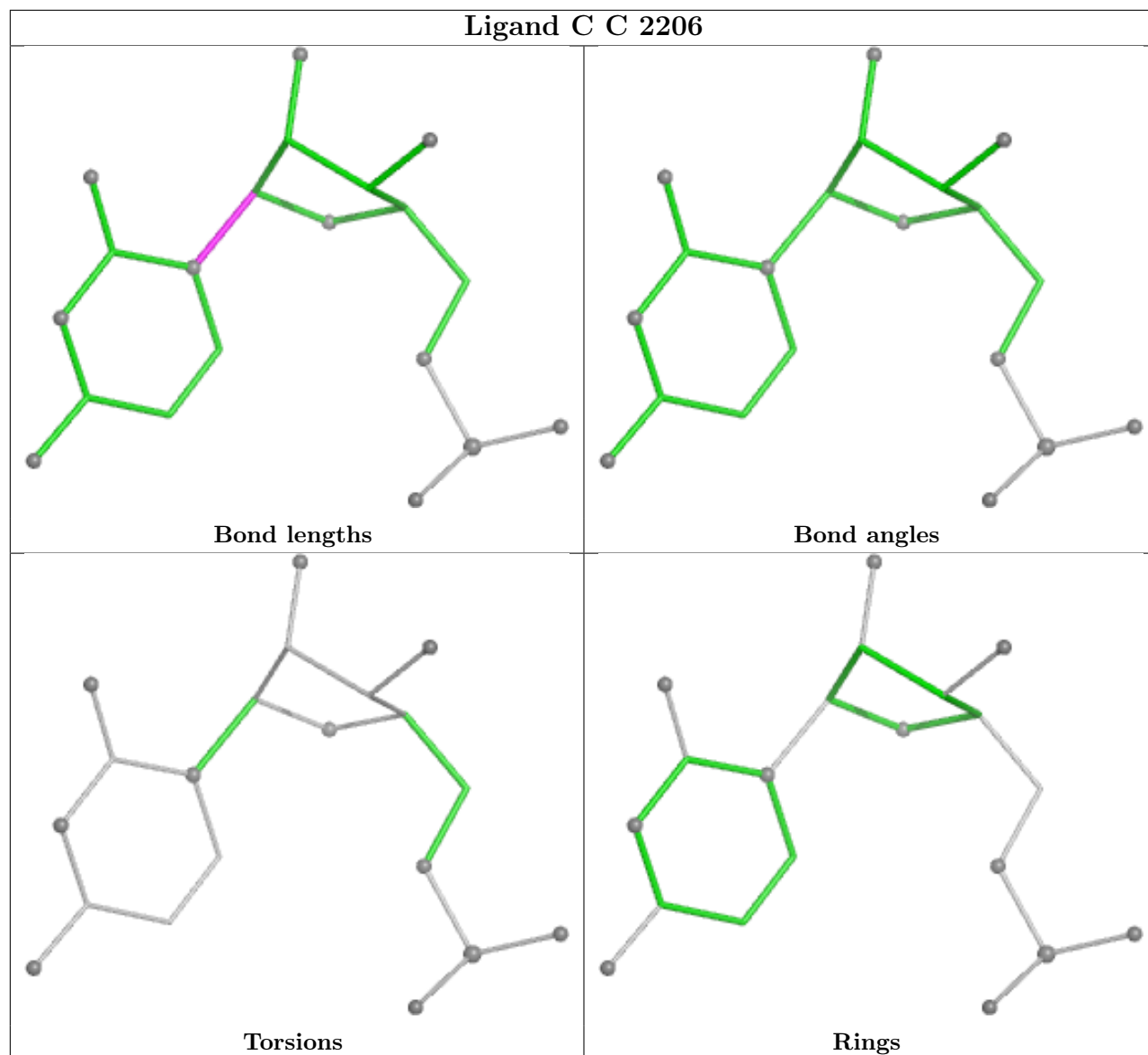




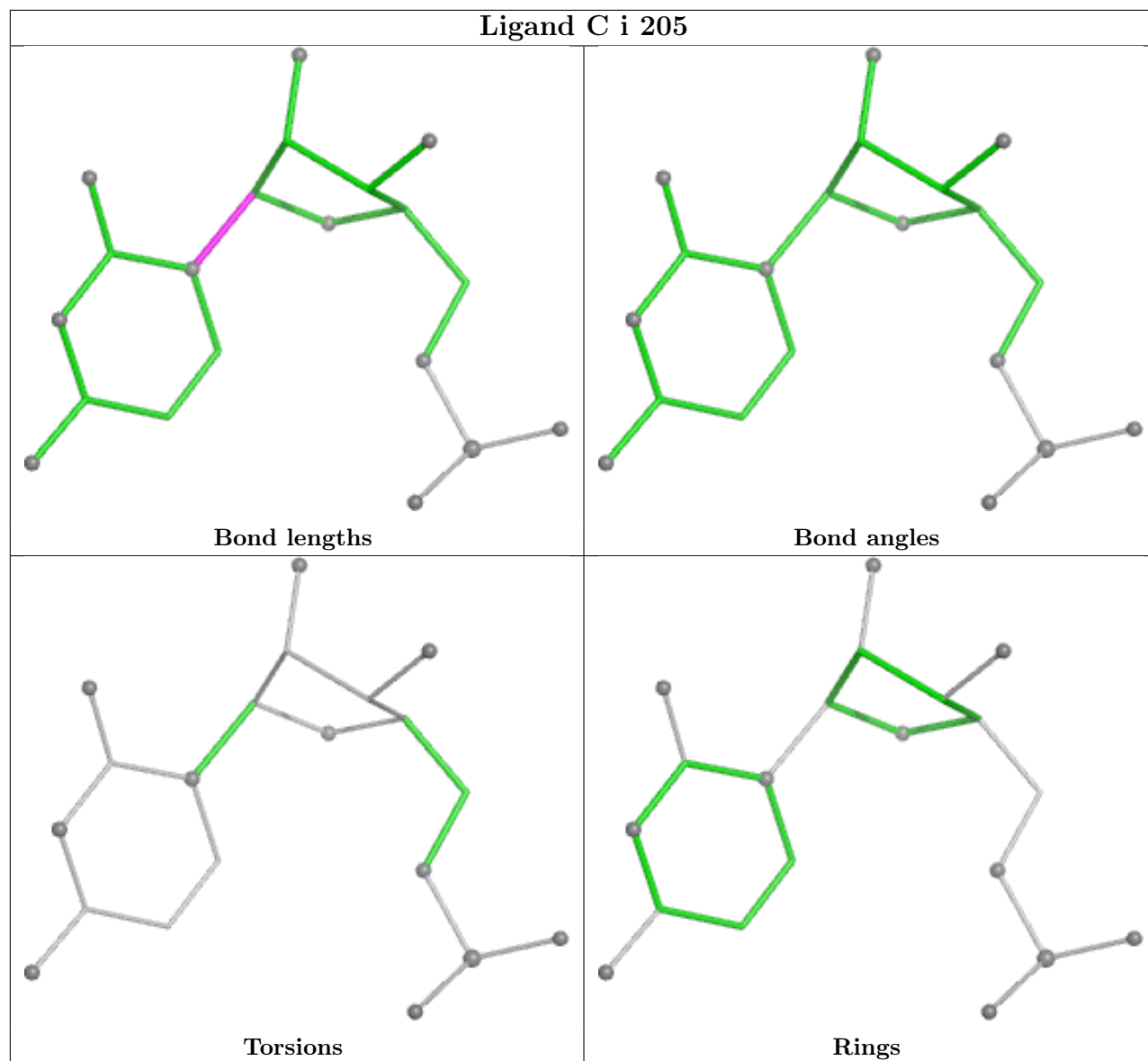


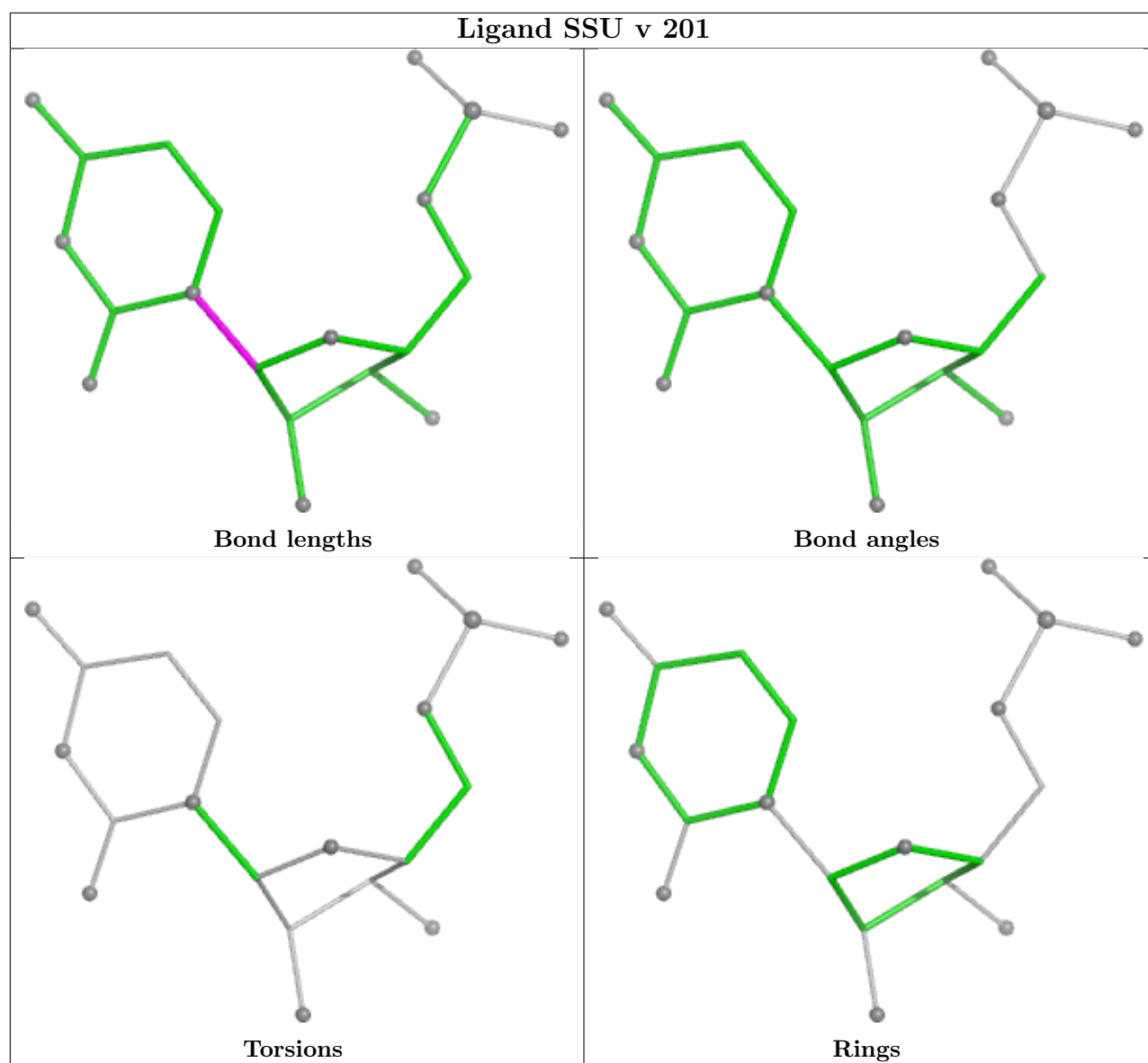


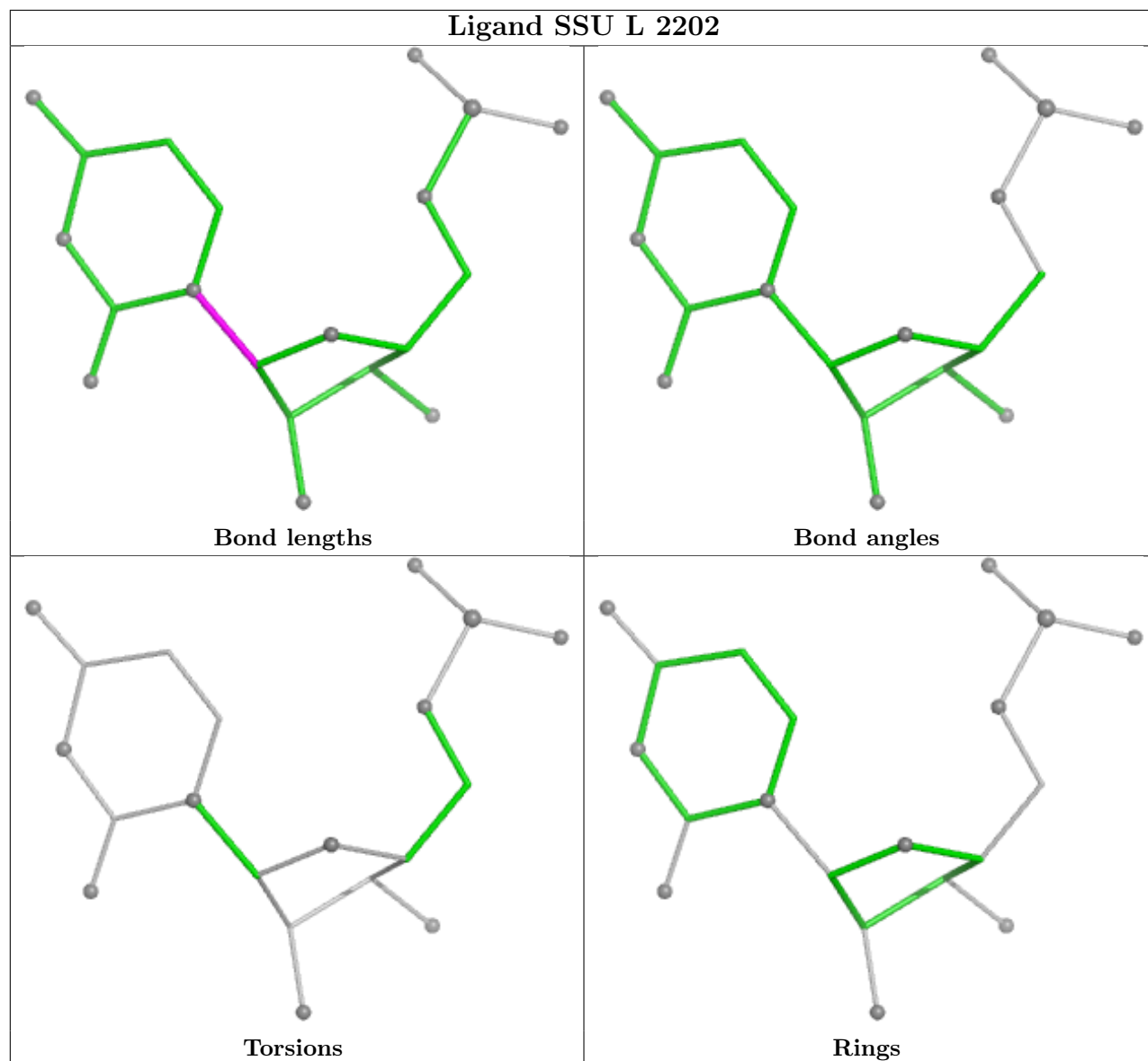
Ligand C C 2206

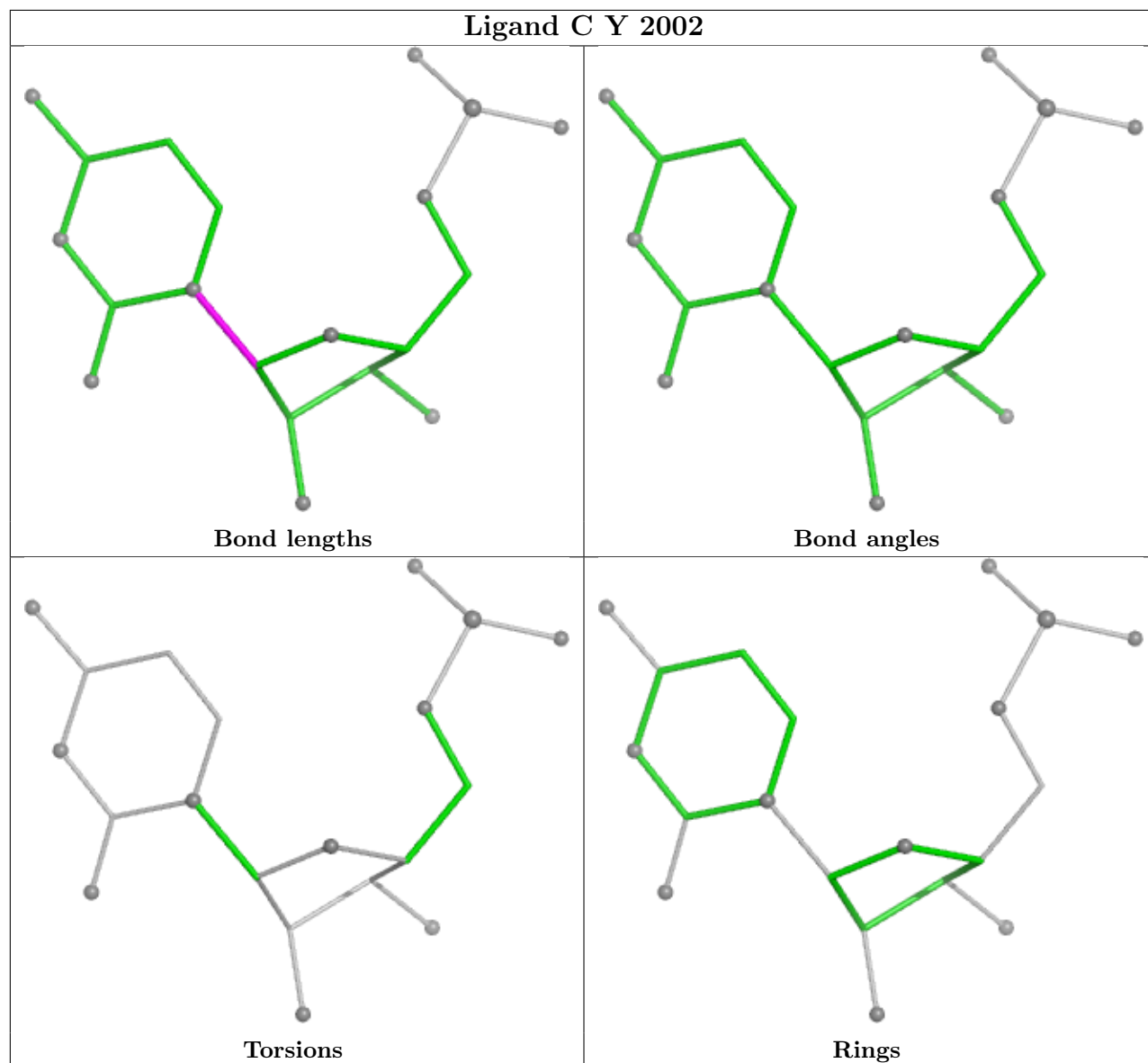


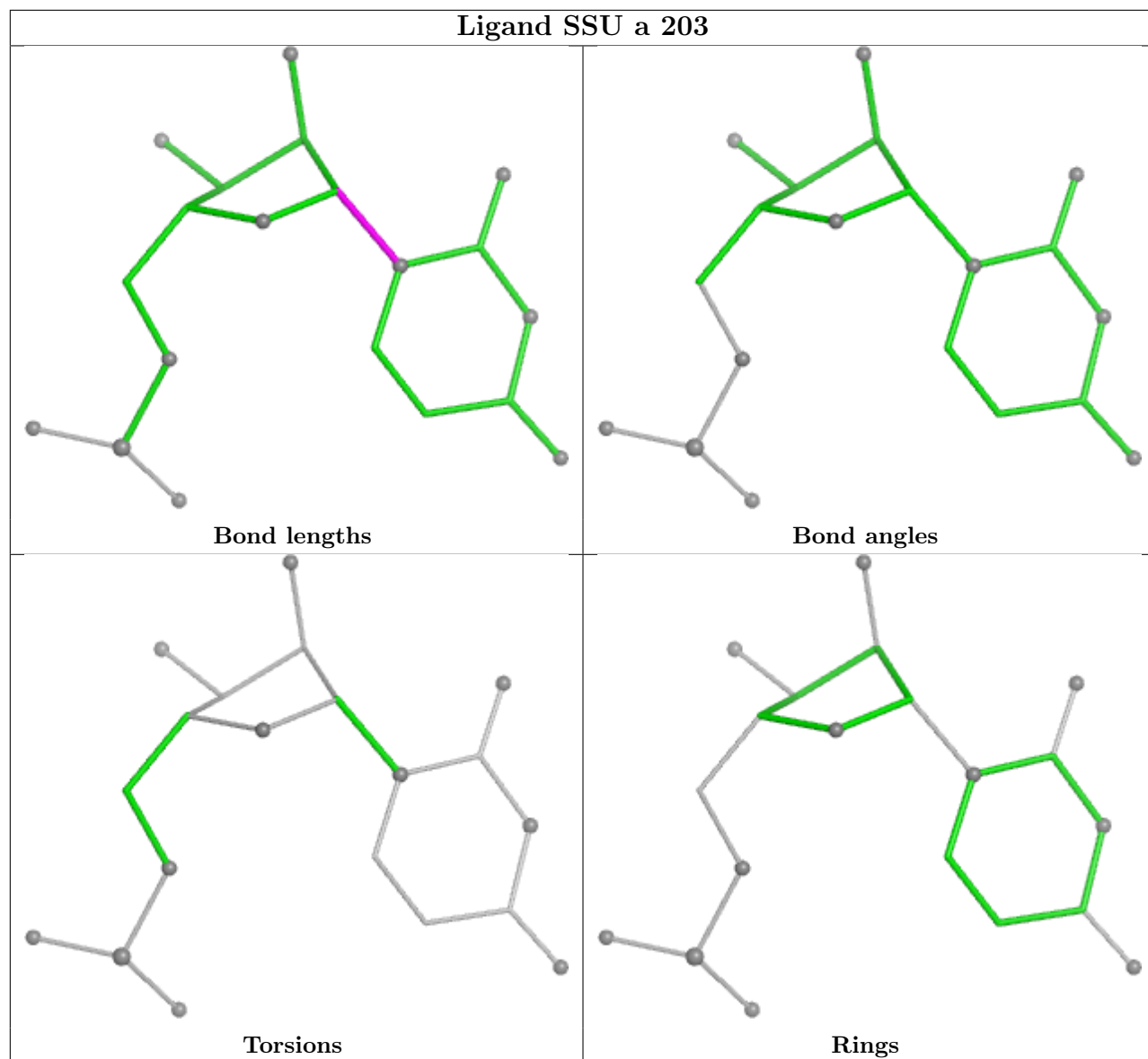
Ligand C i 205

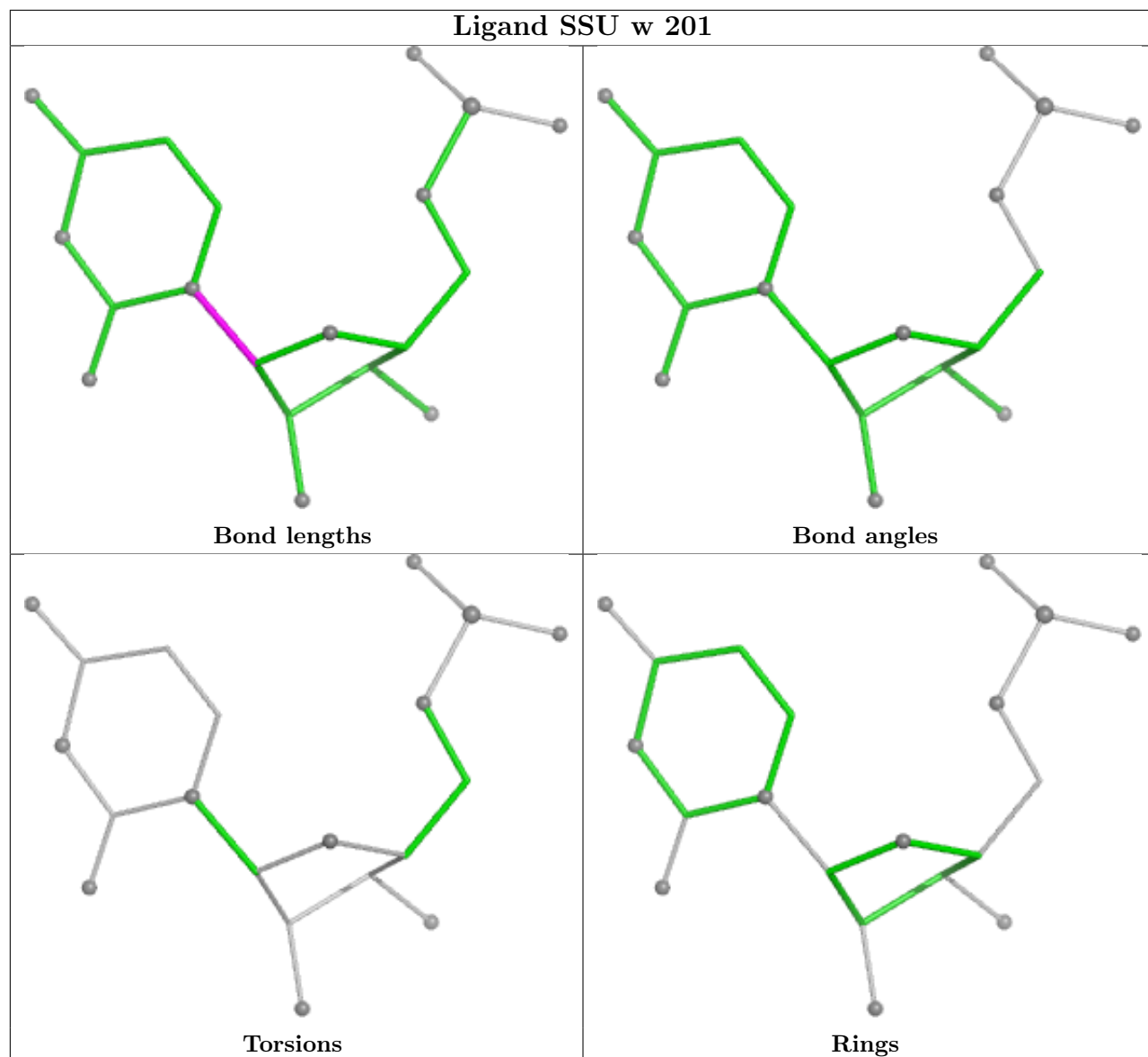


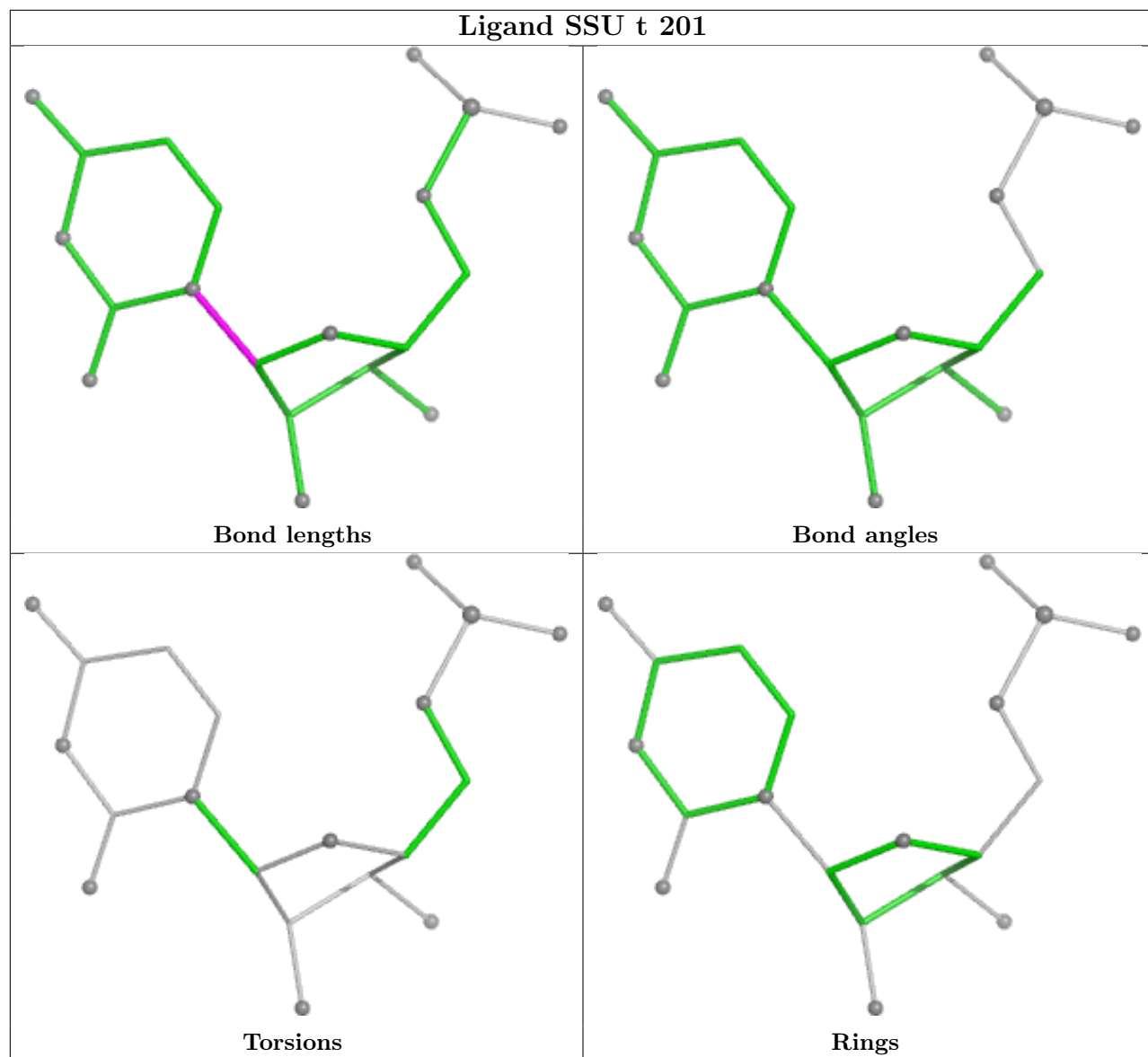


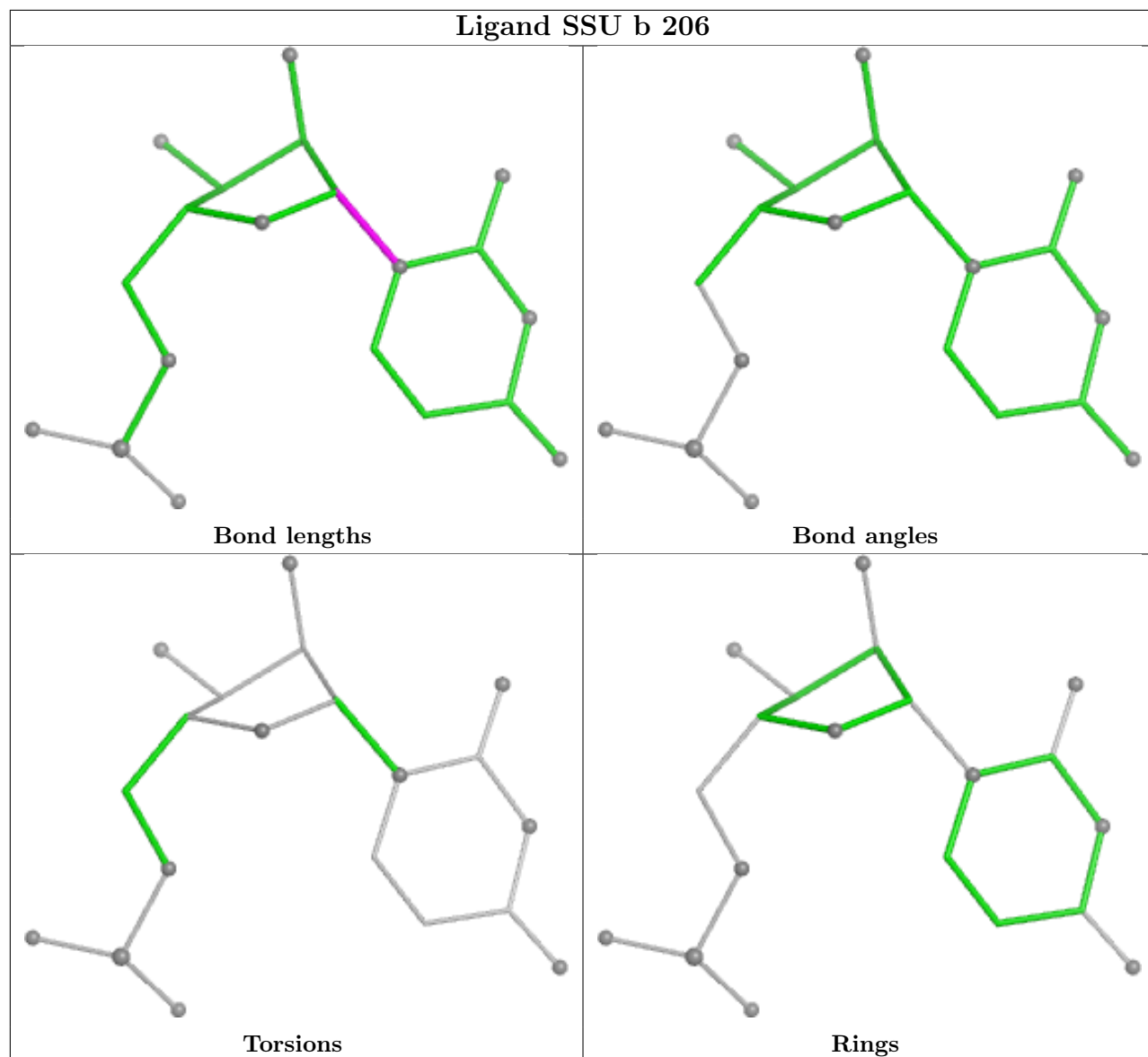


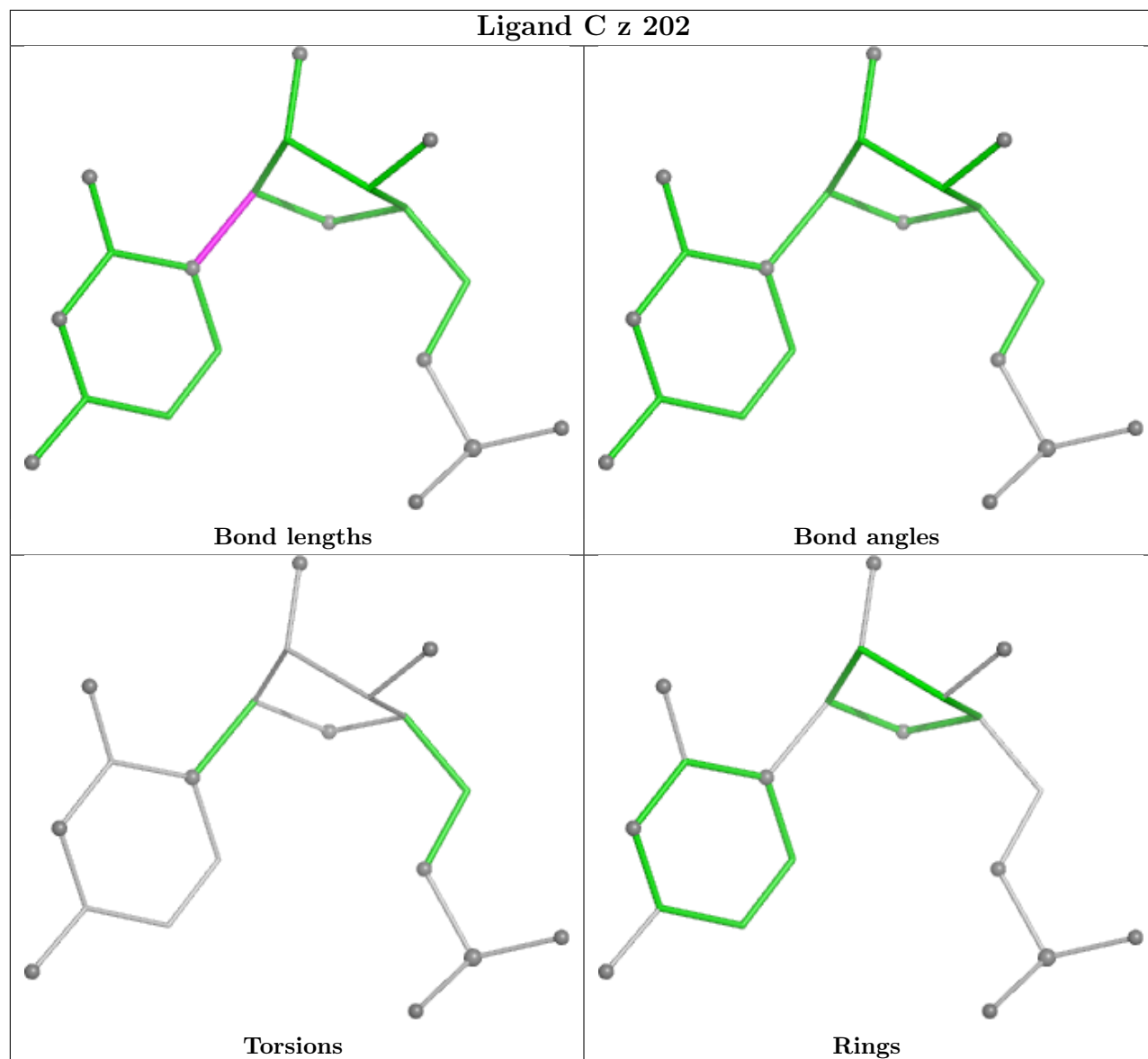


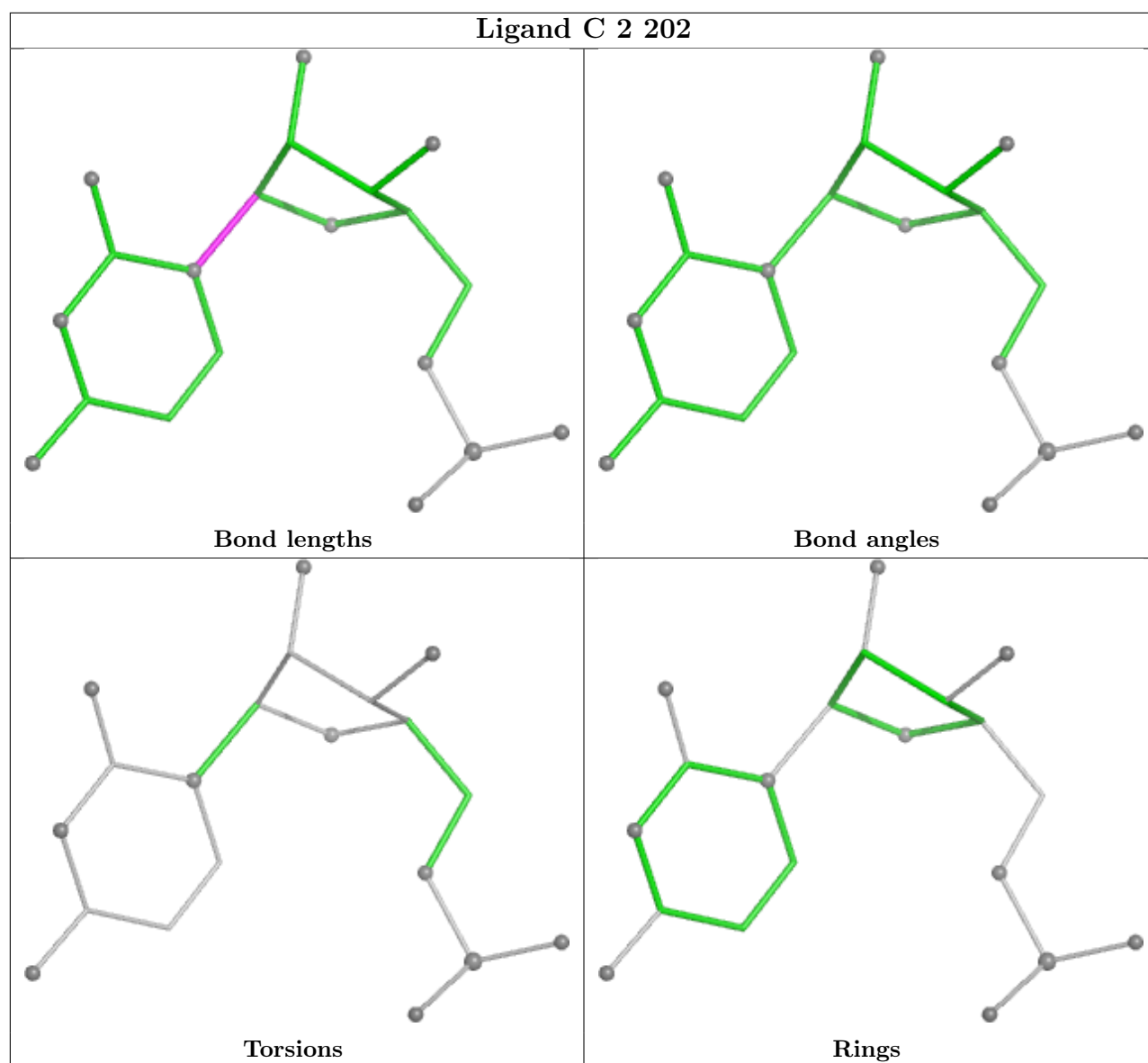


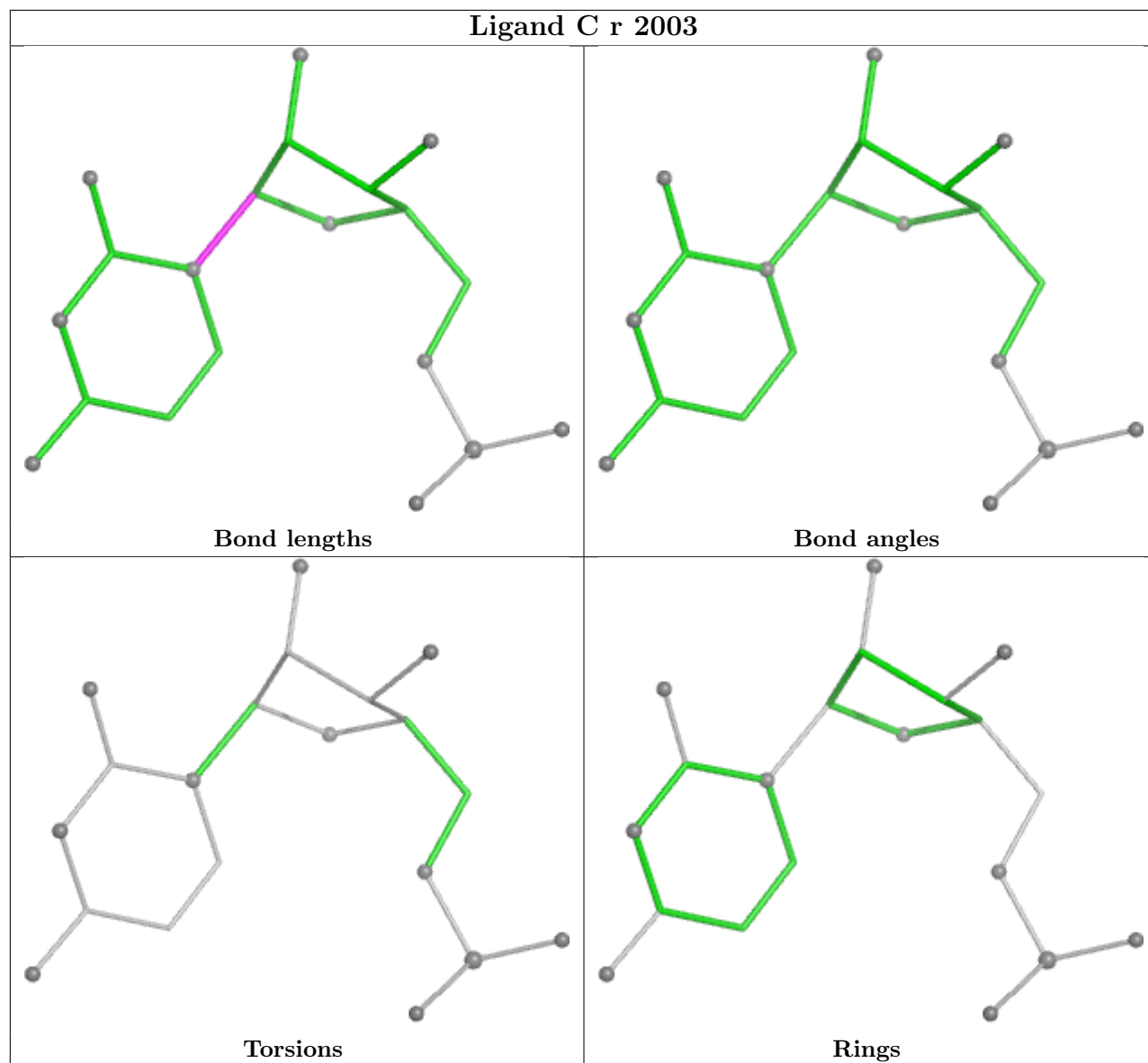


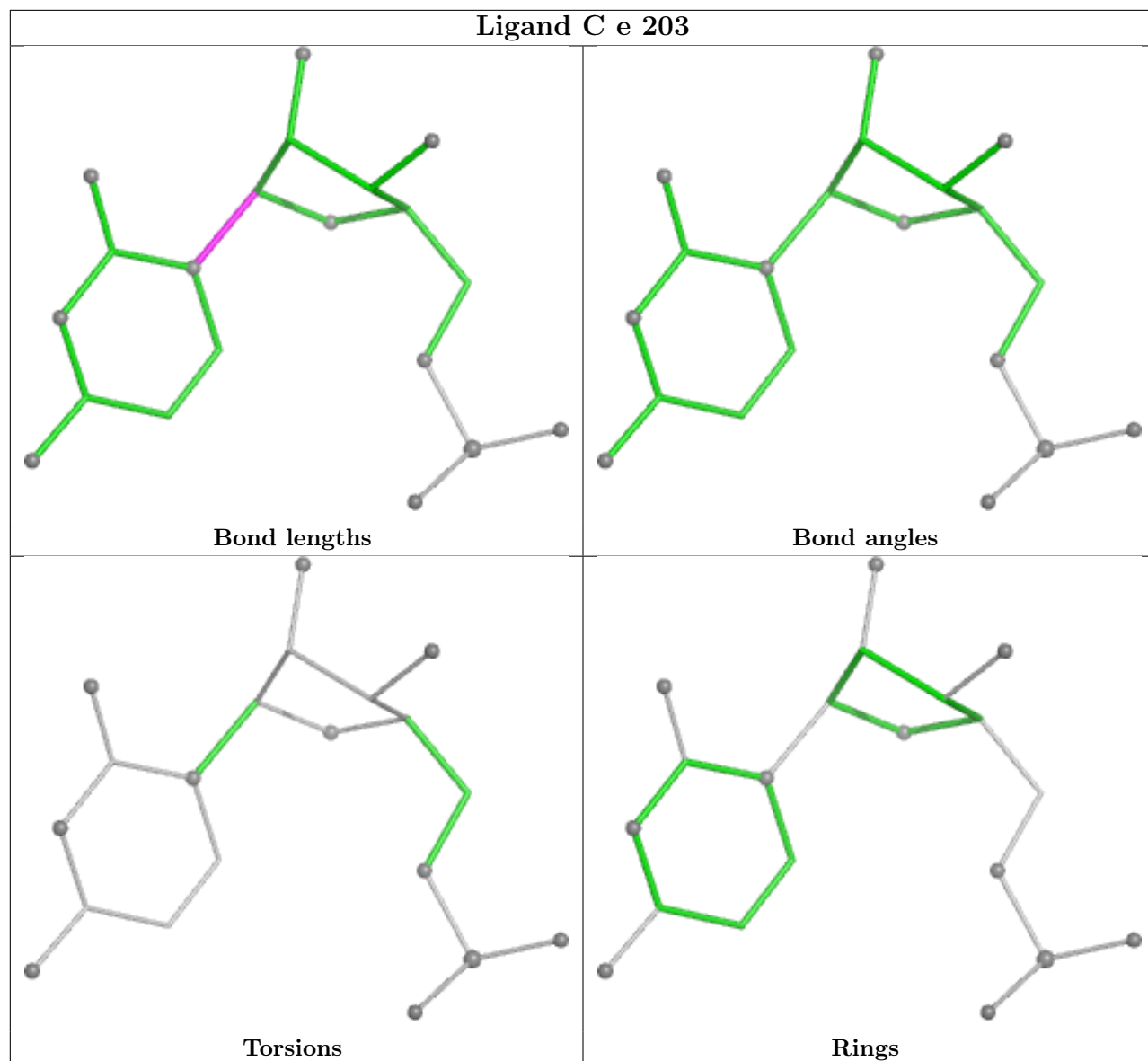


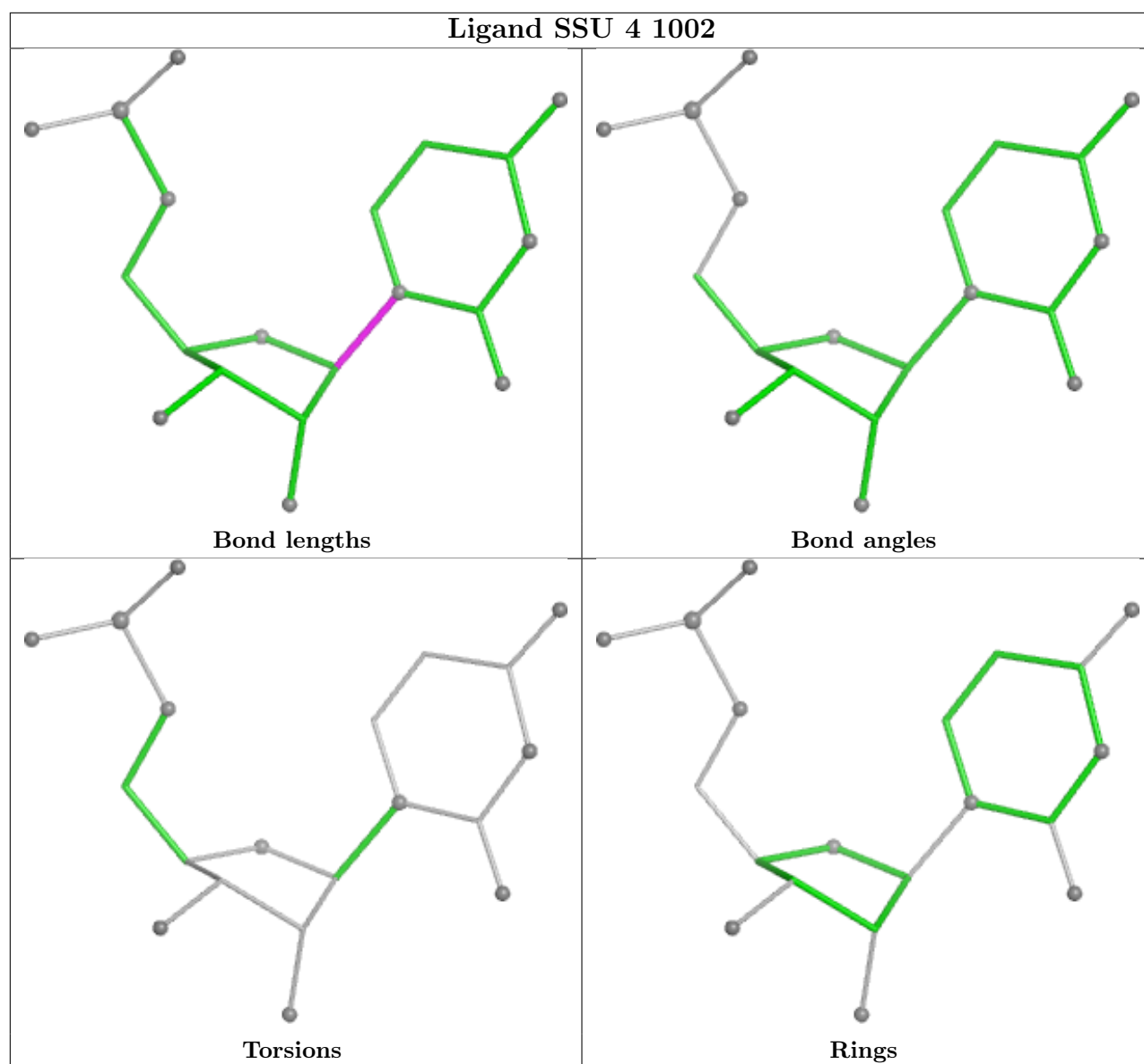


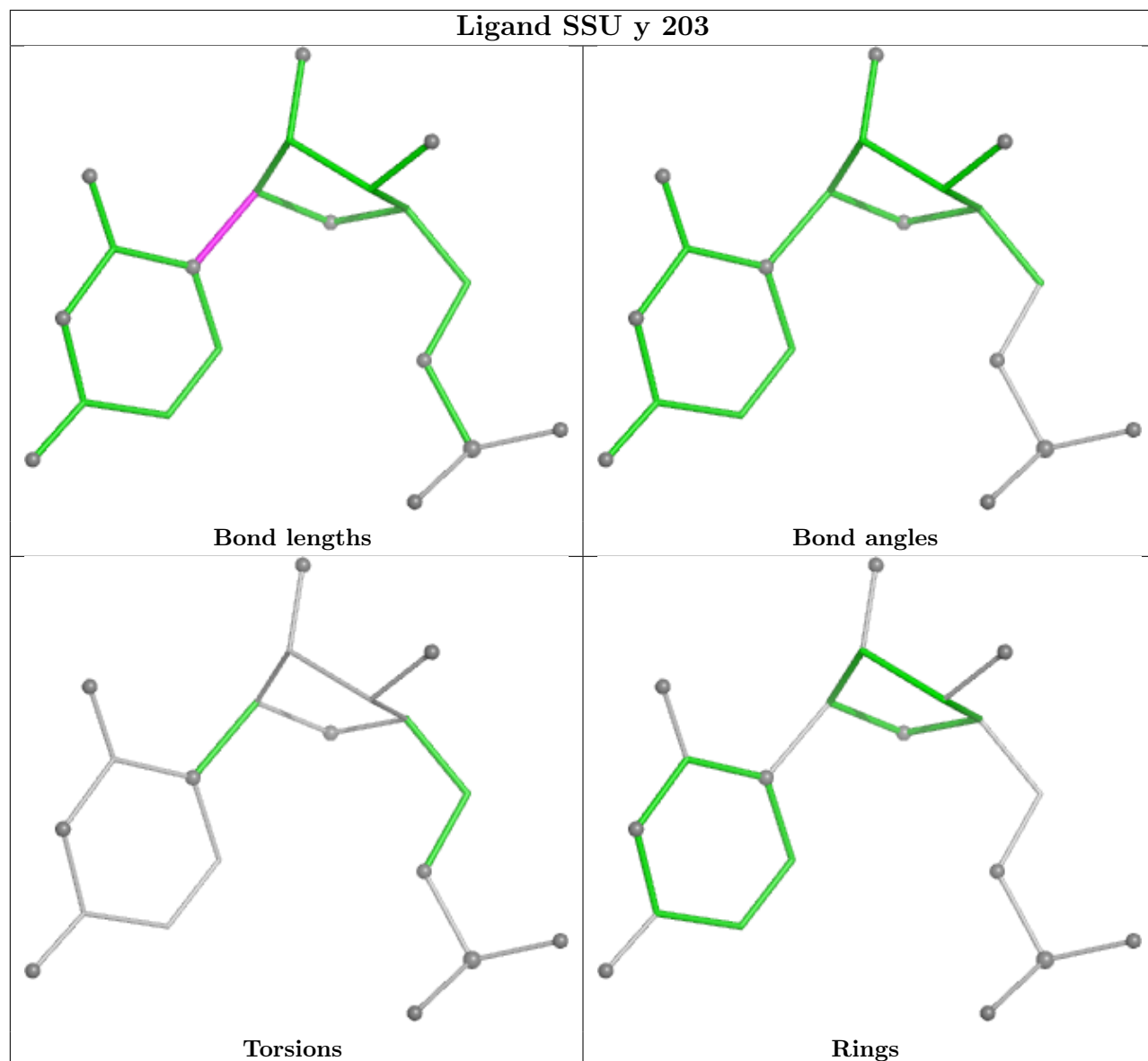


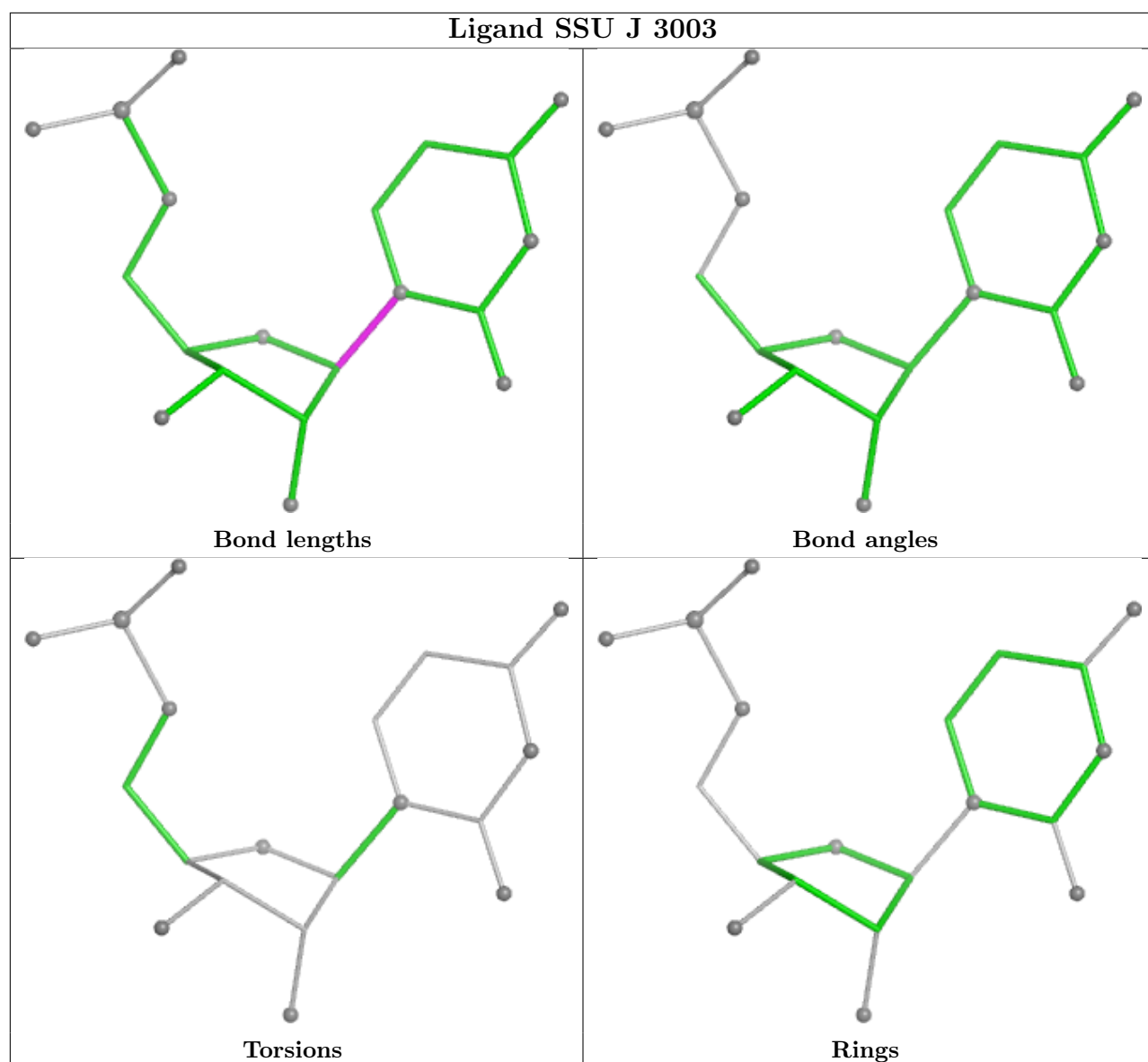


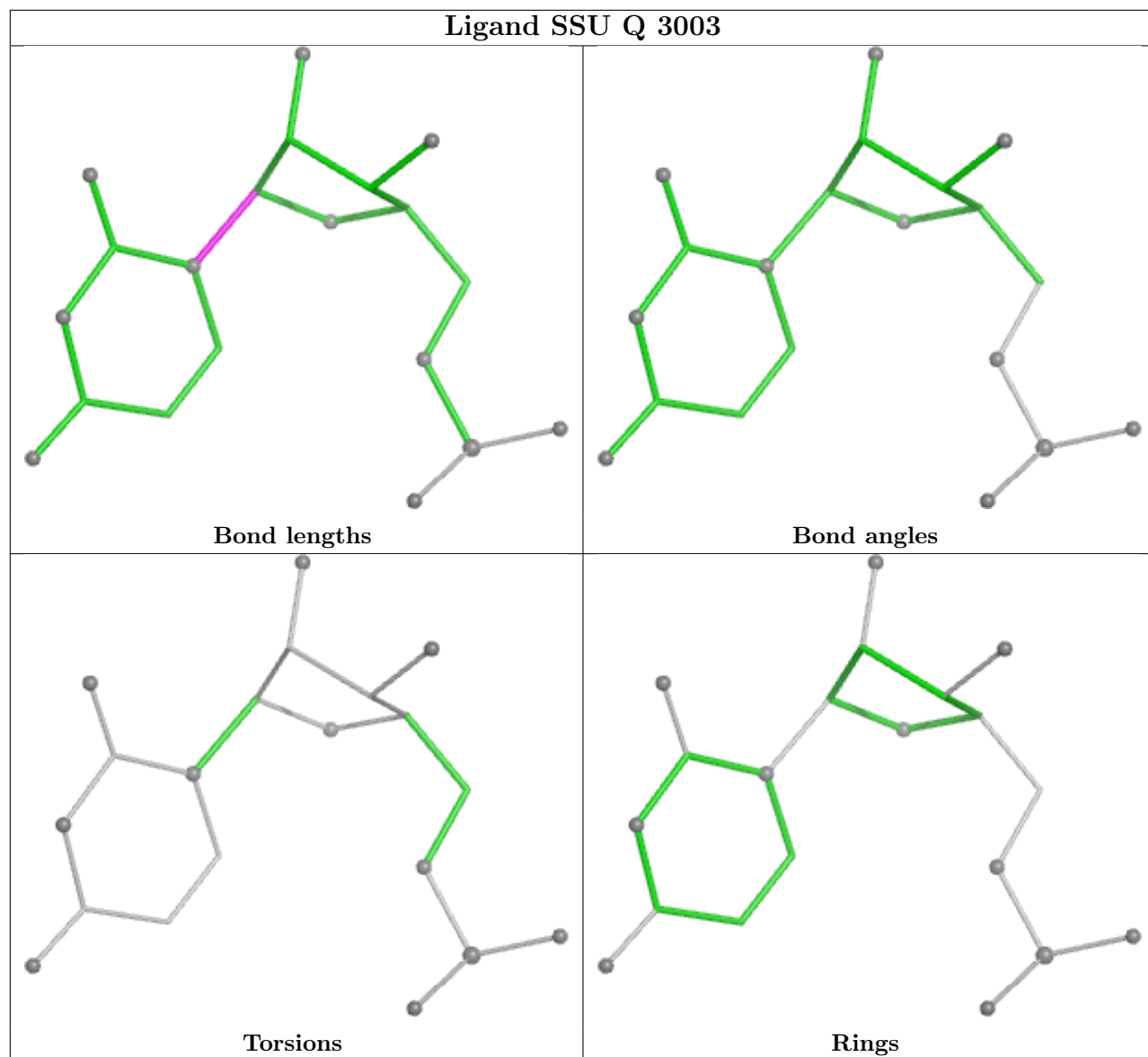


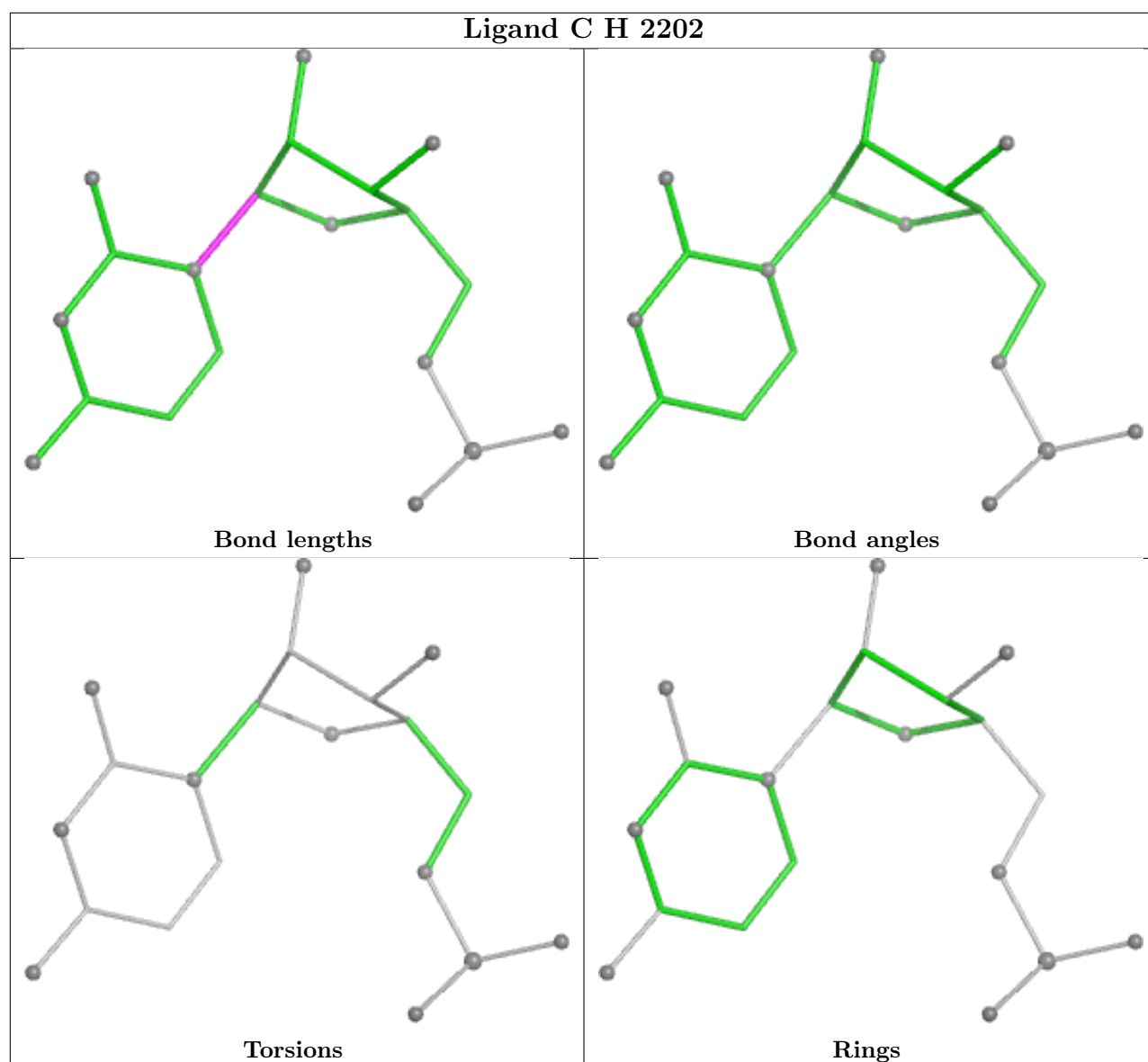


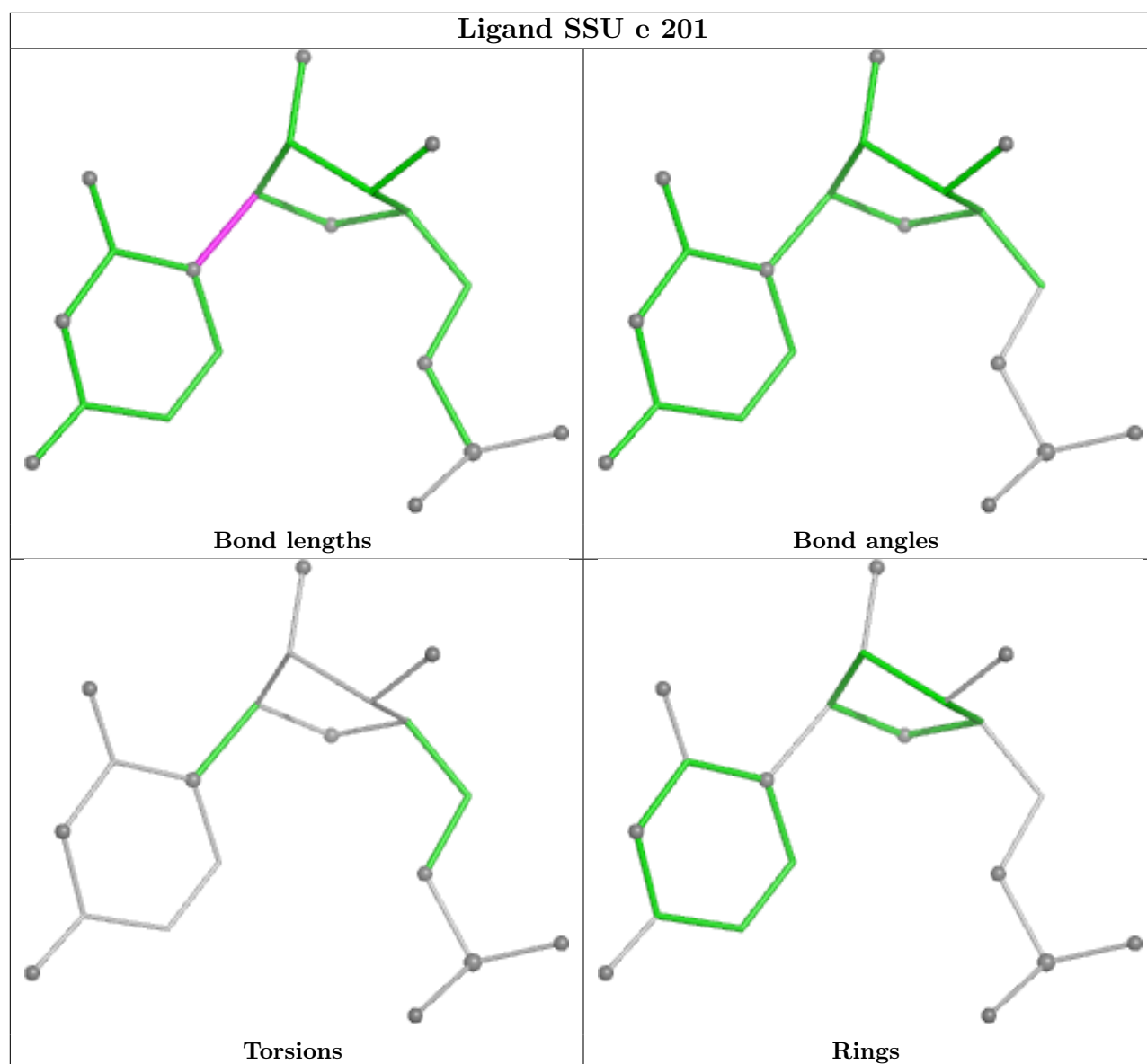


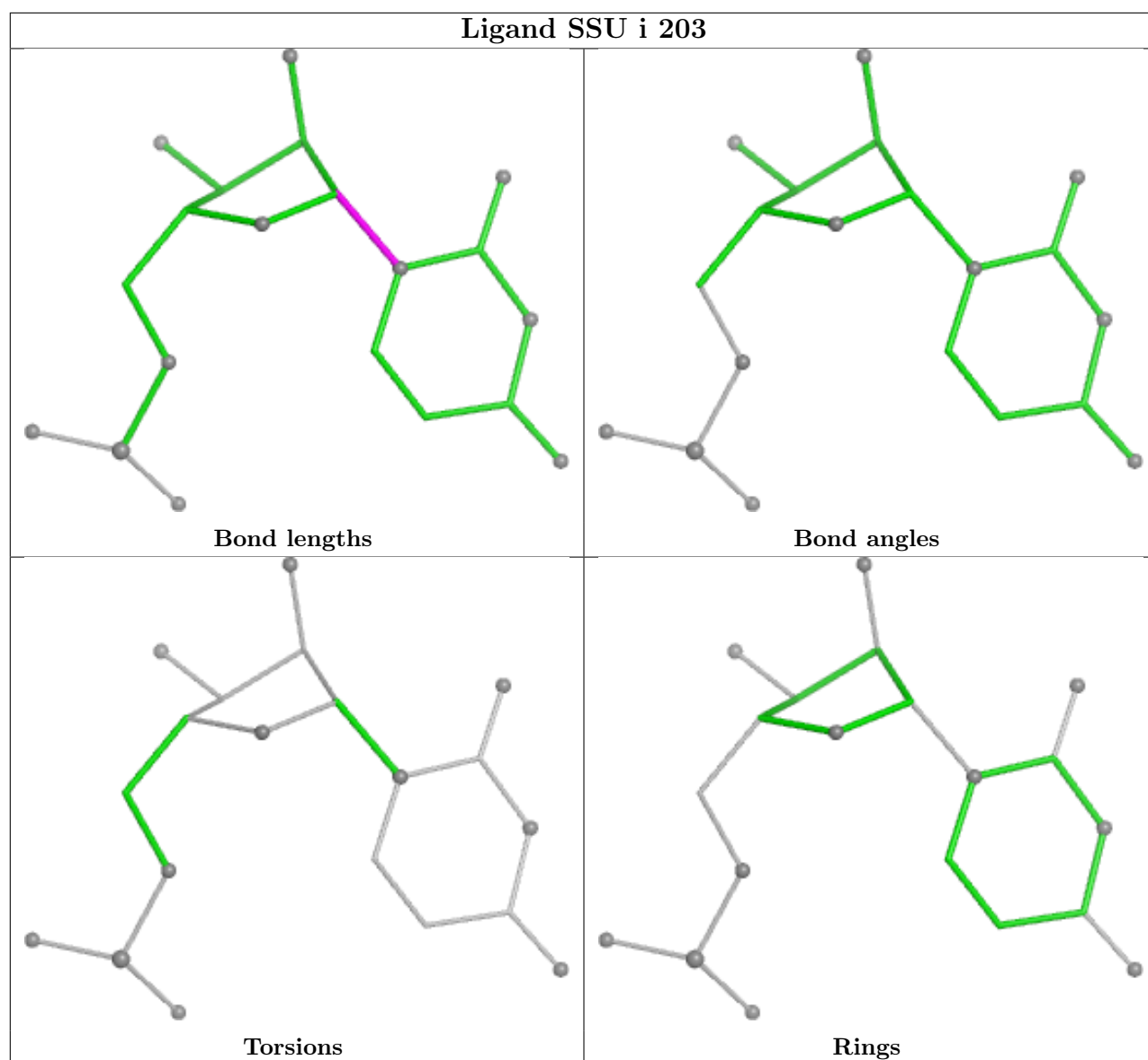


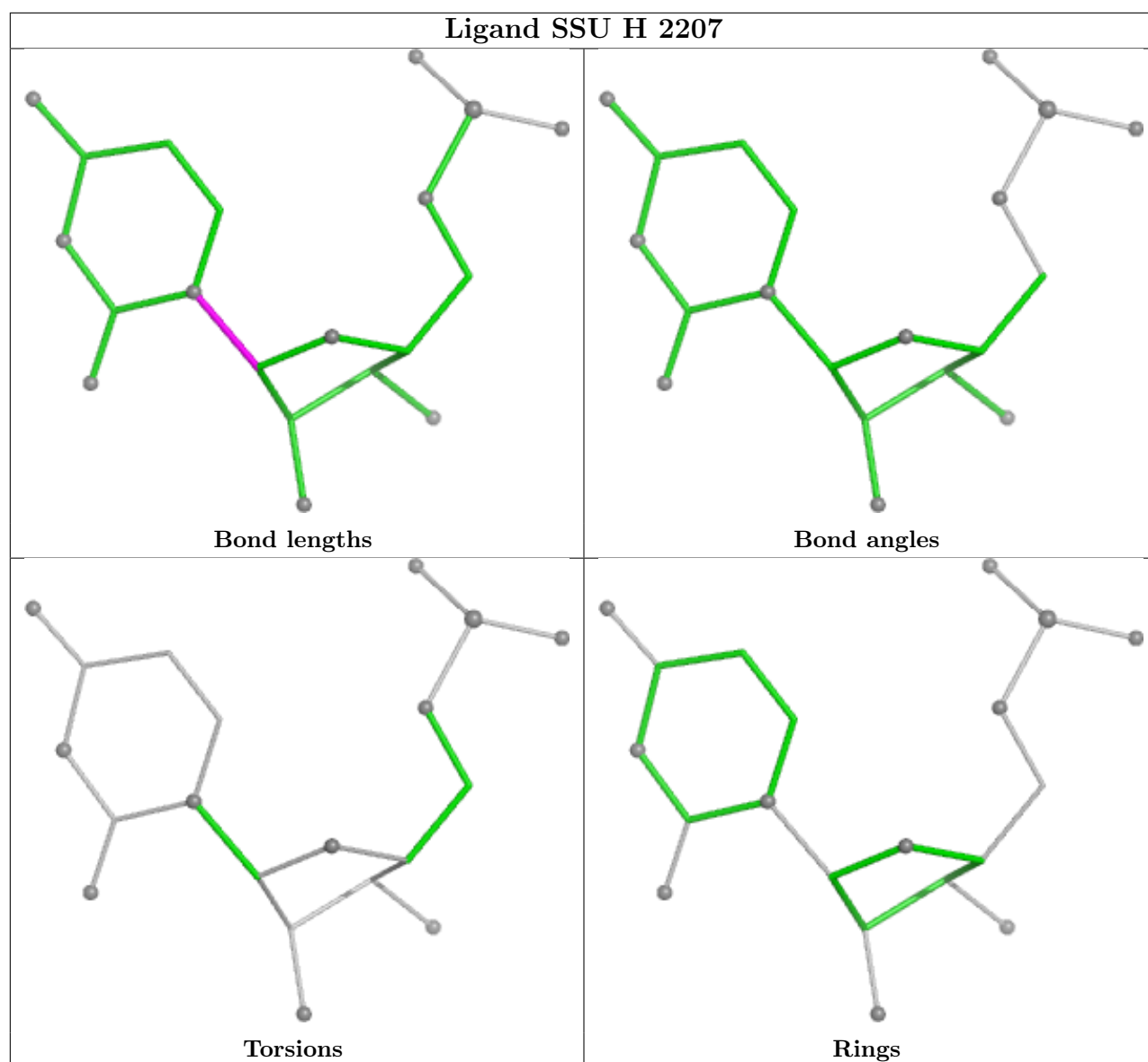


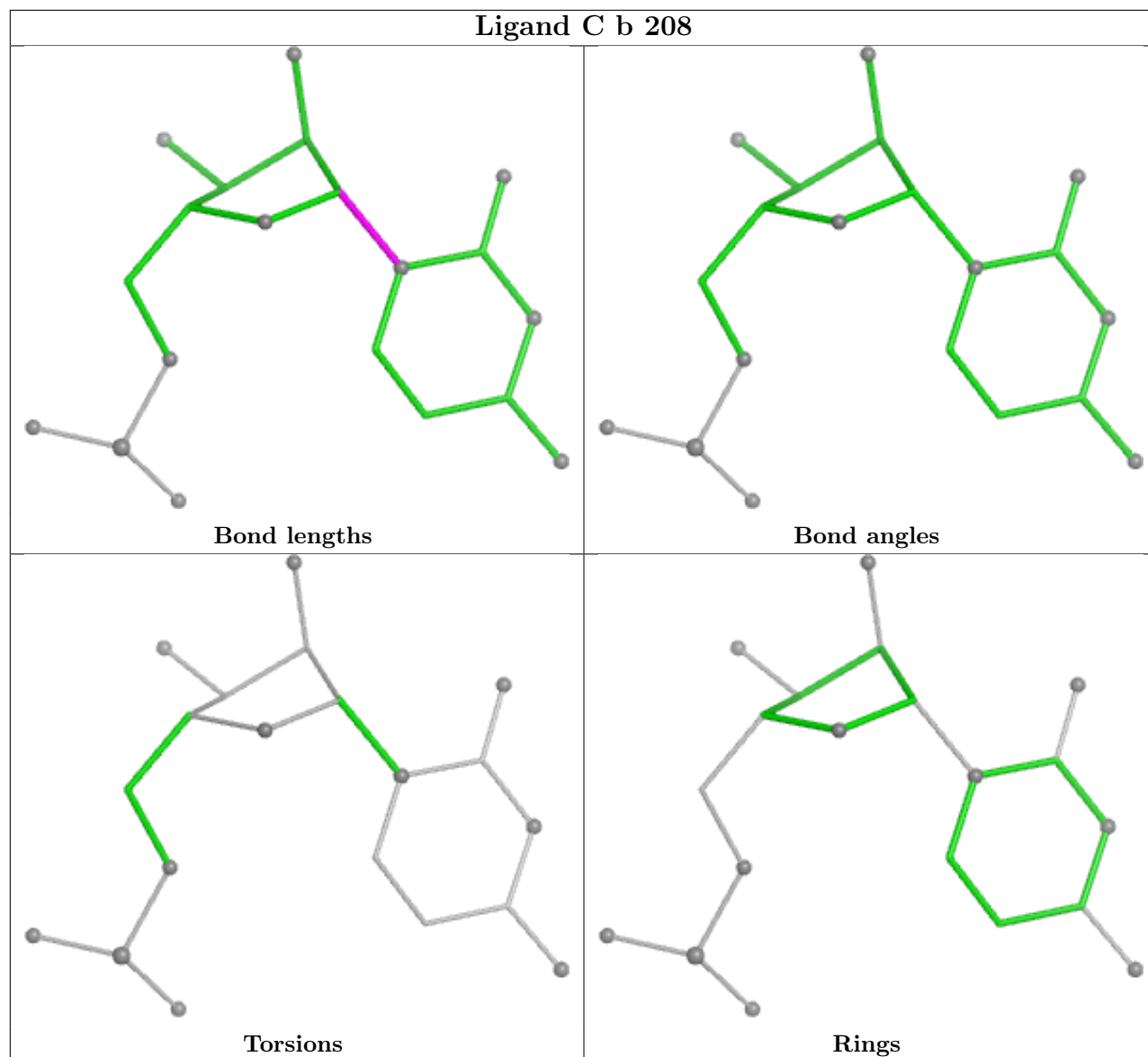


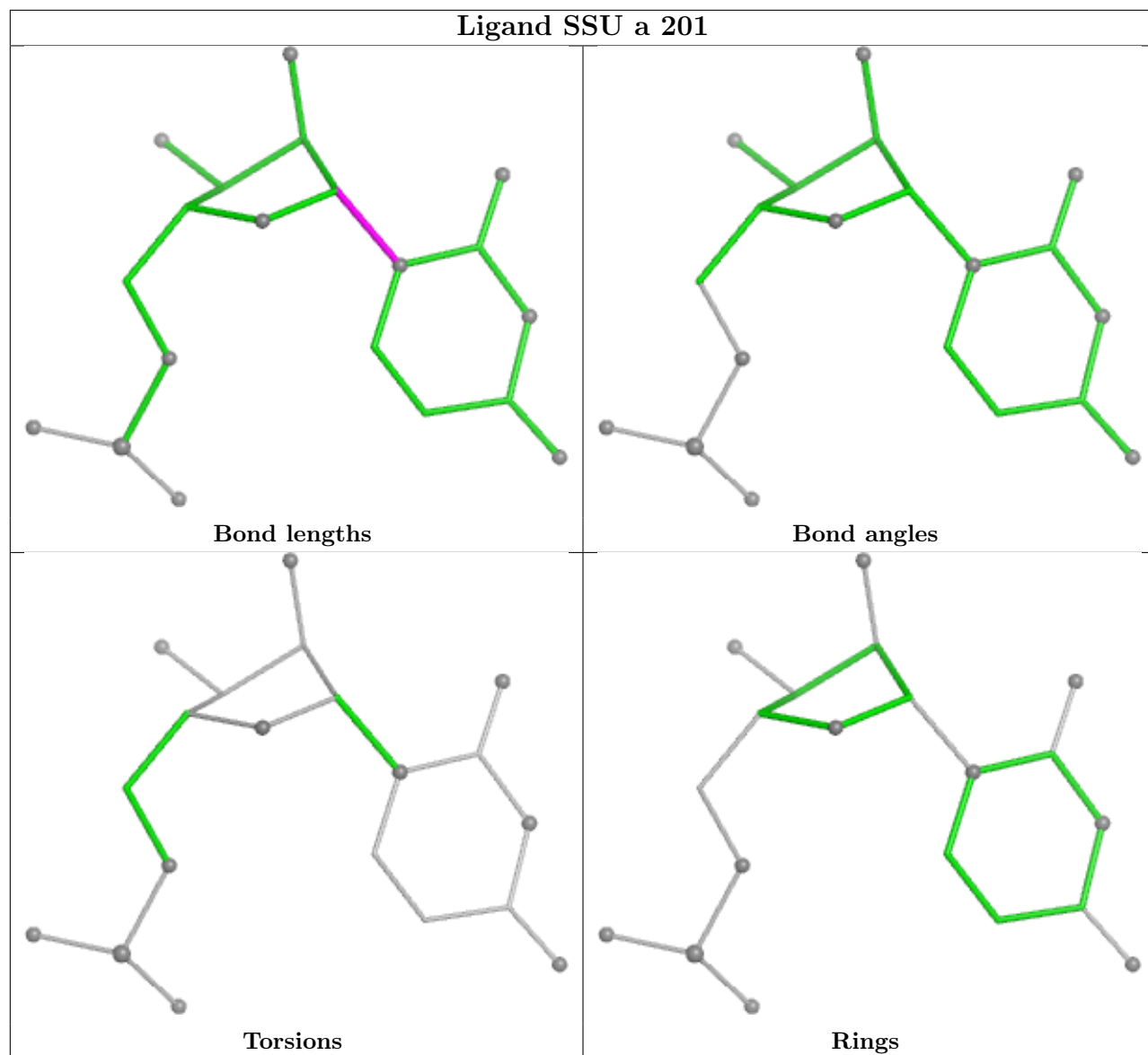


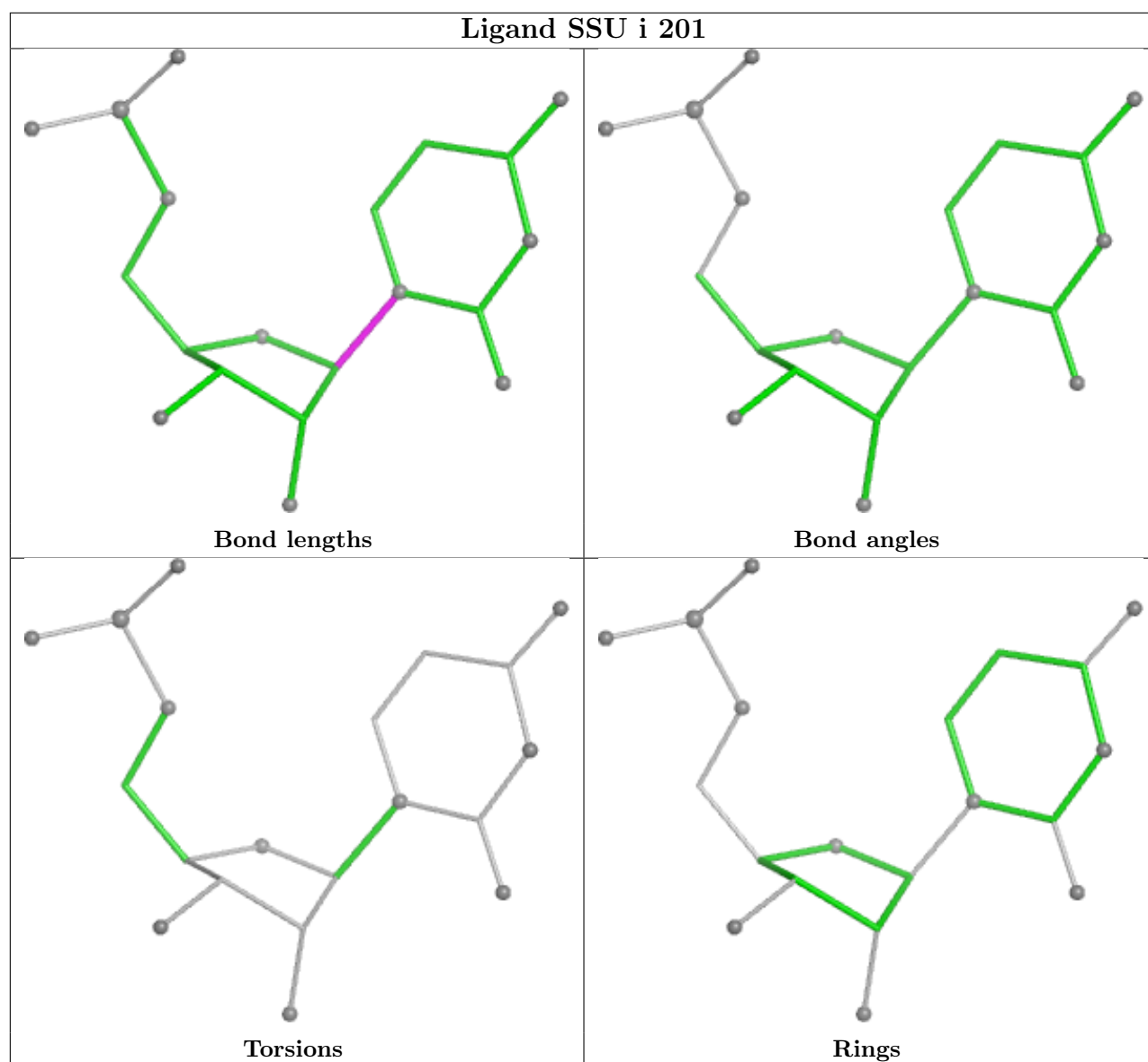


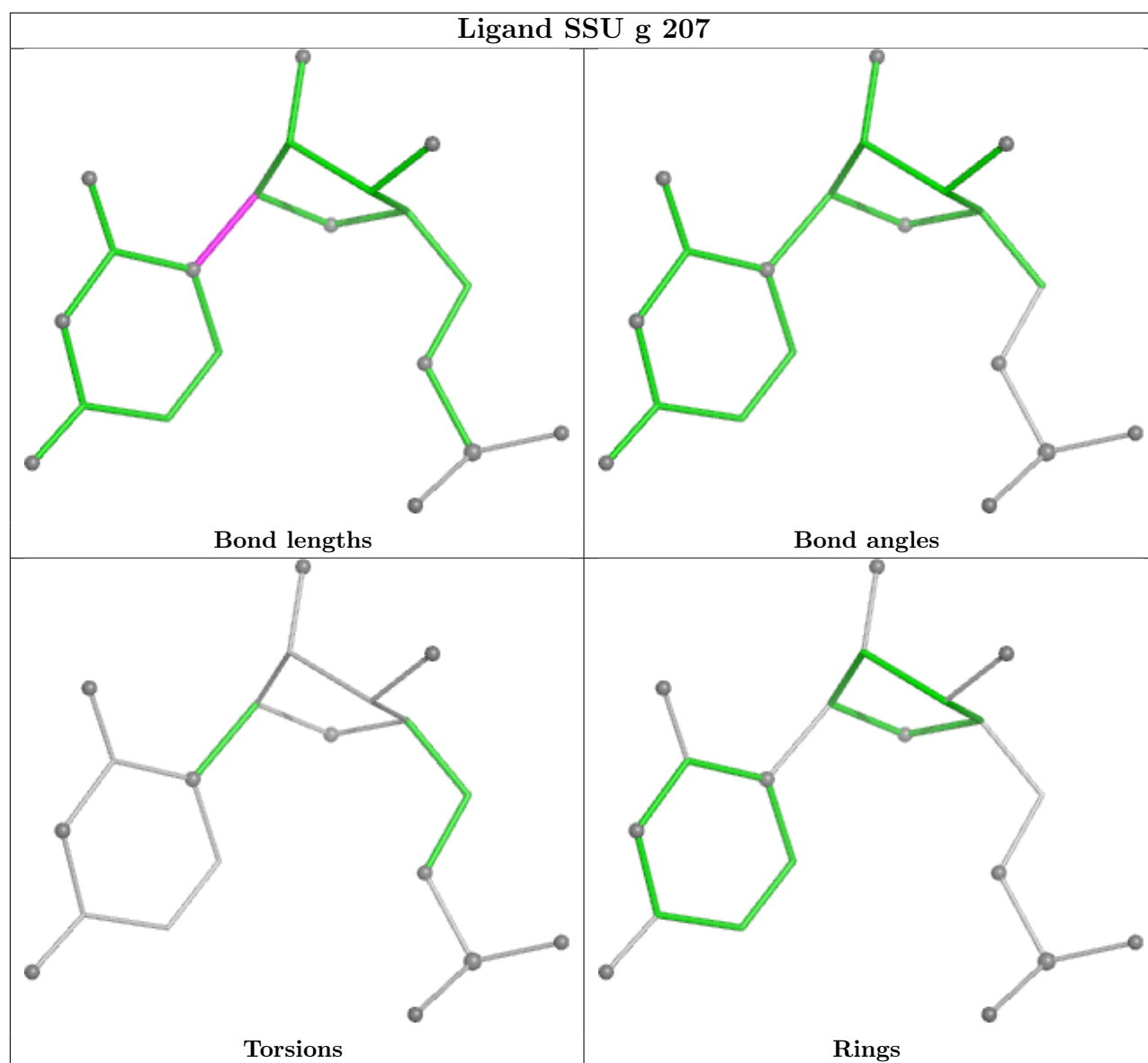


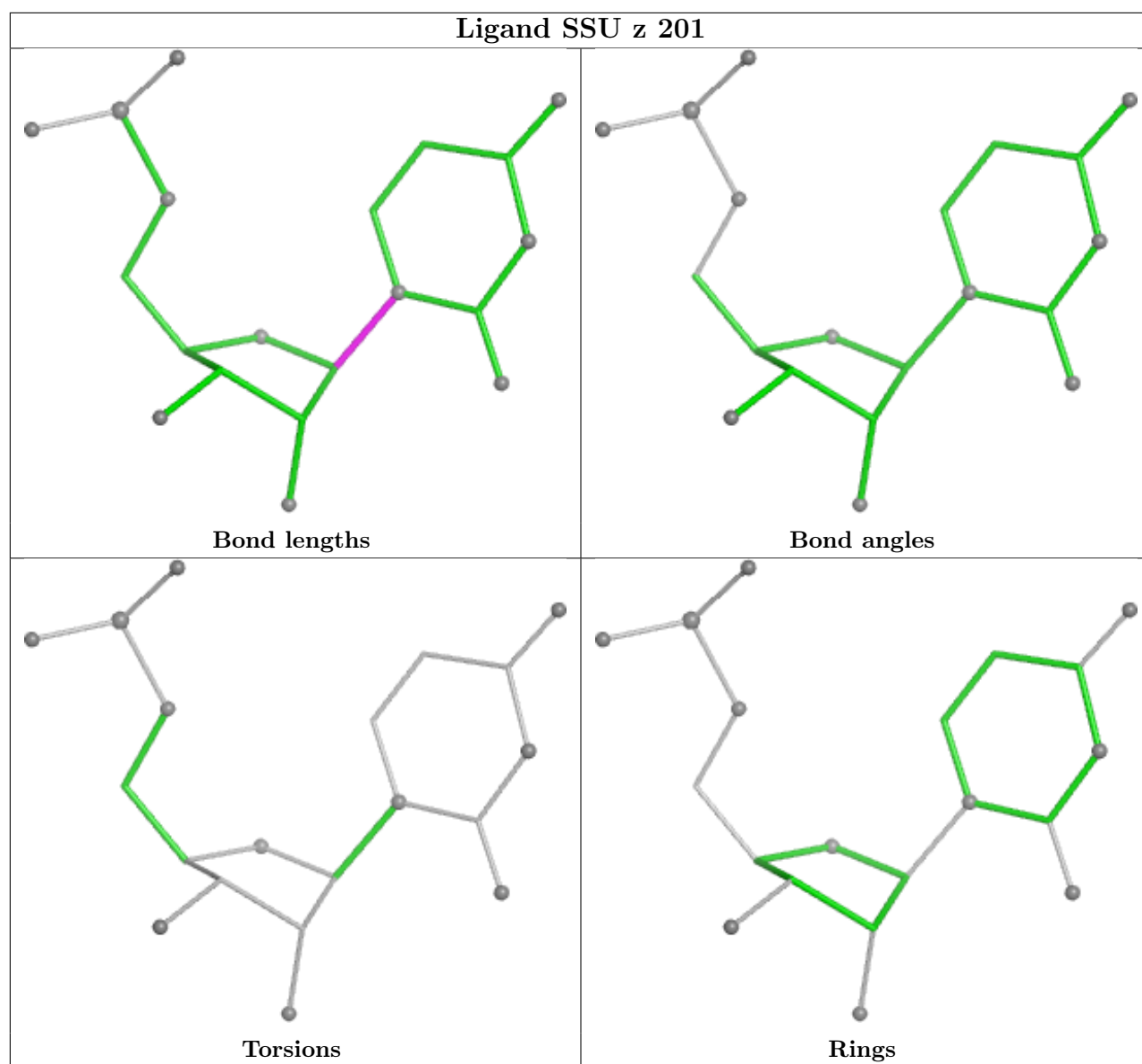


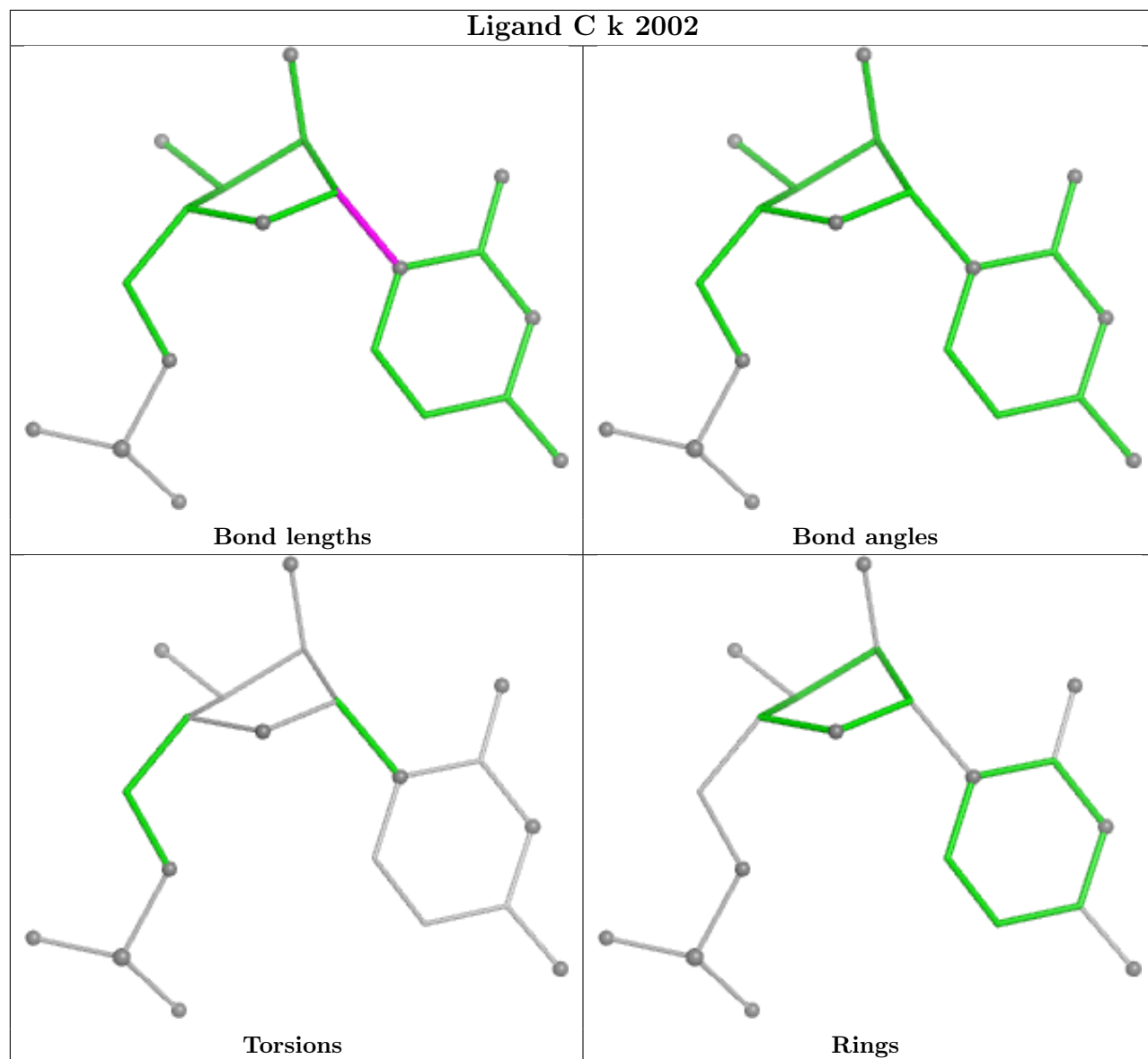


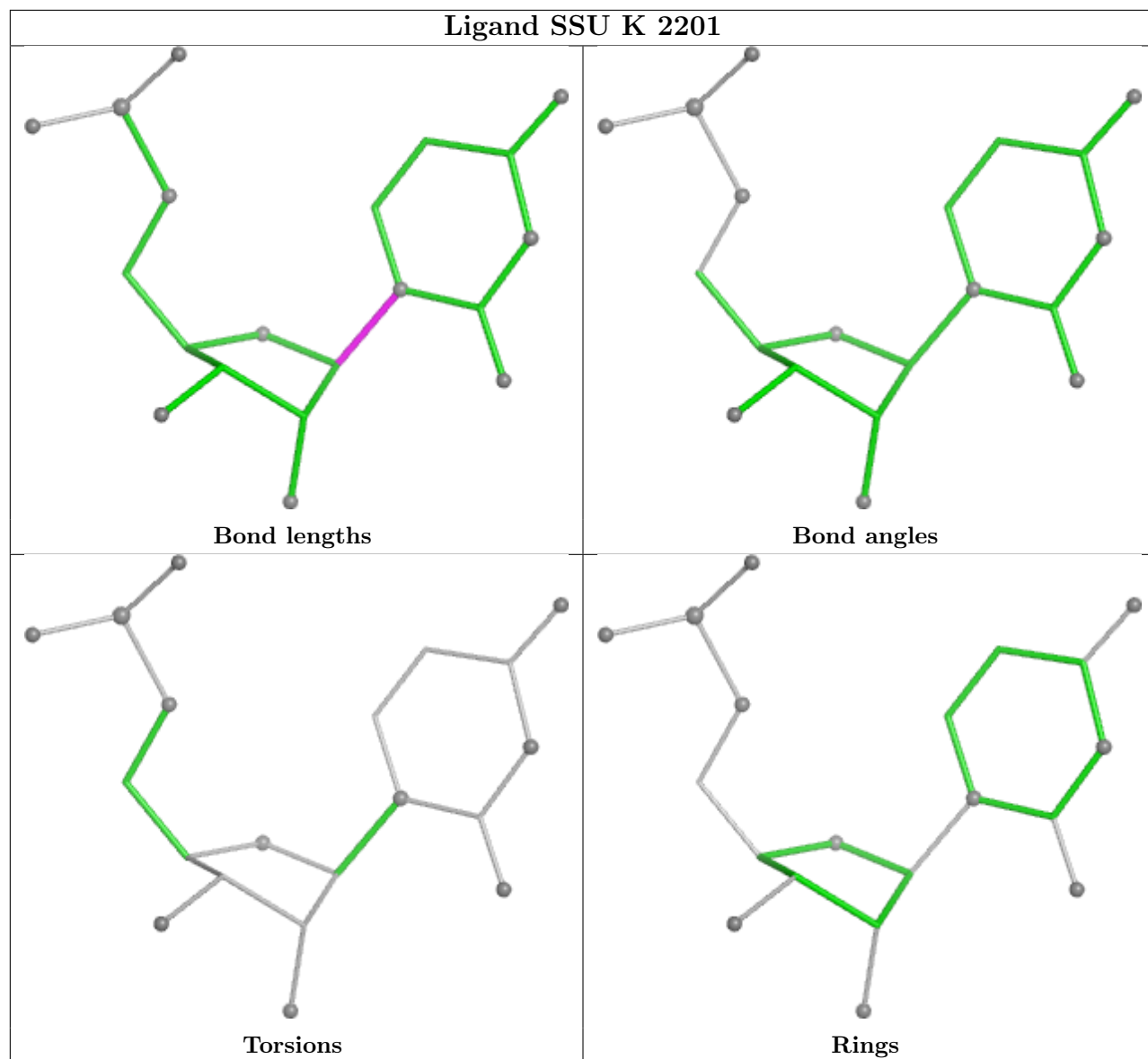


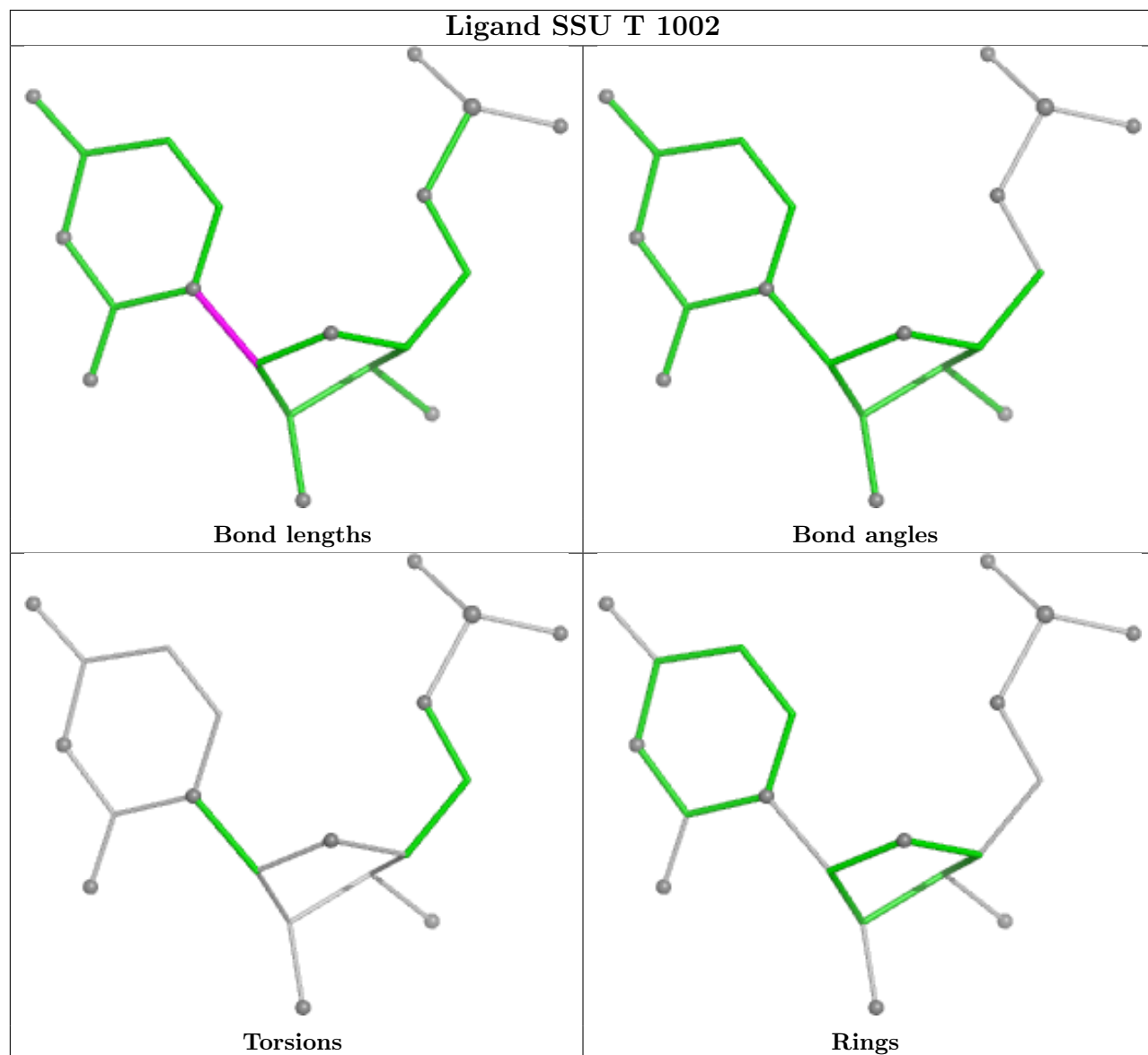


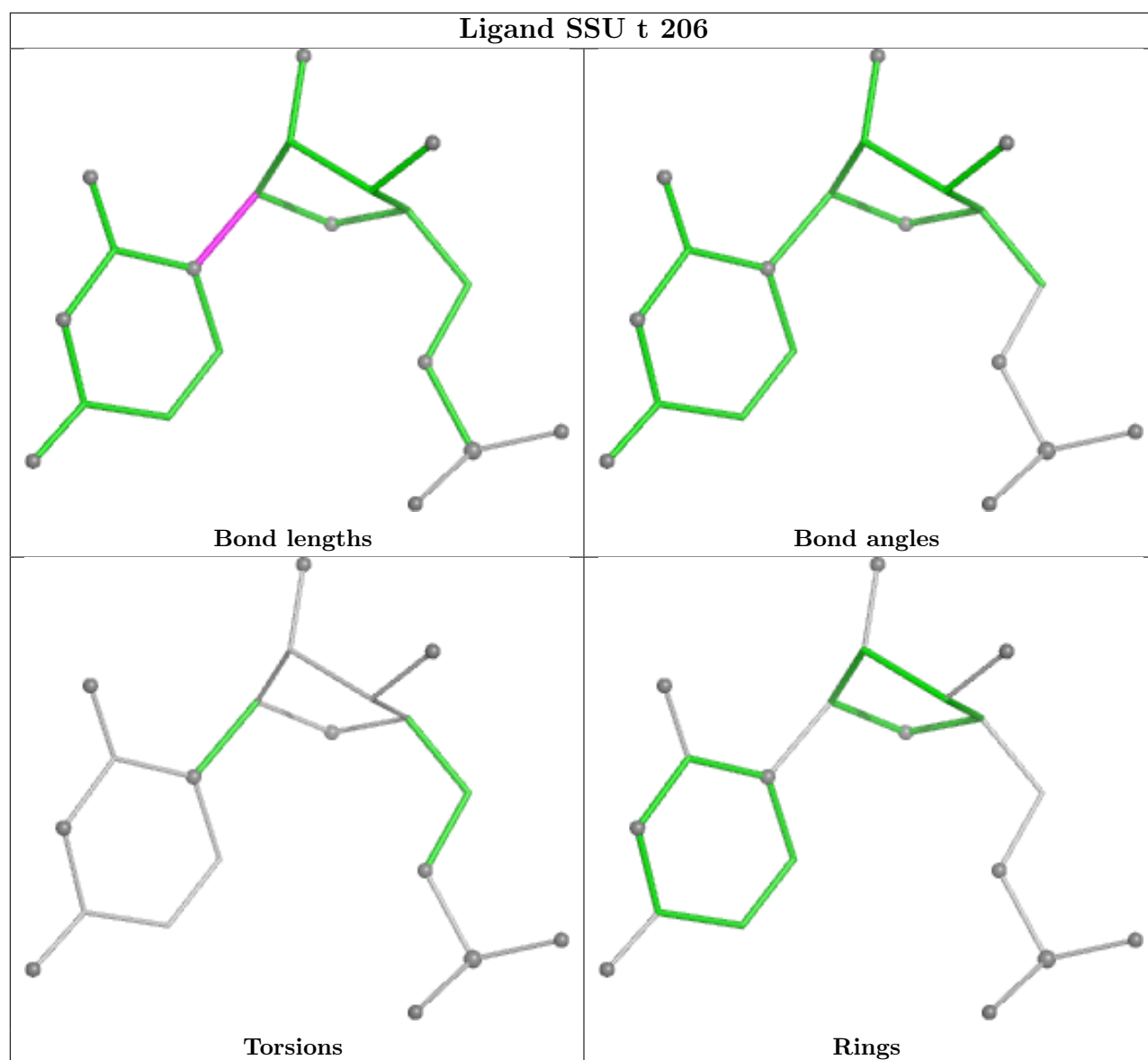


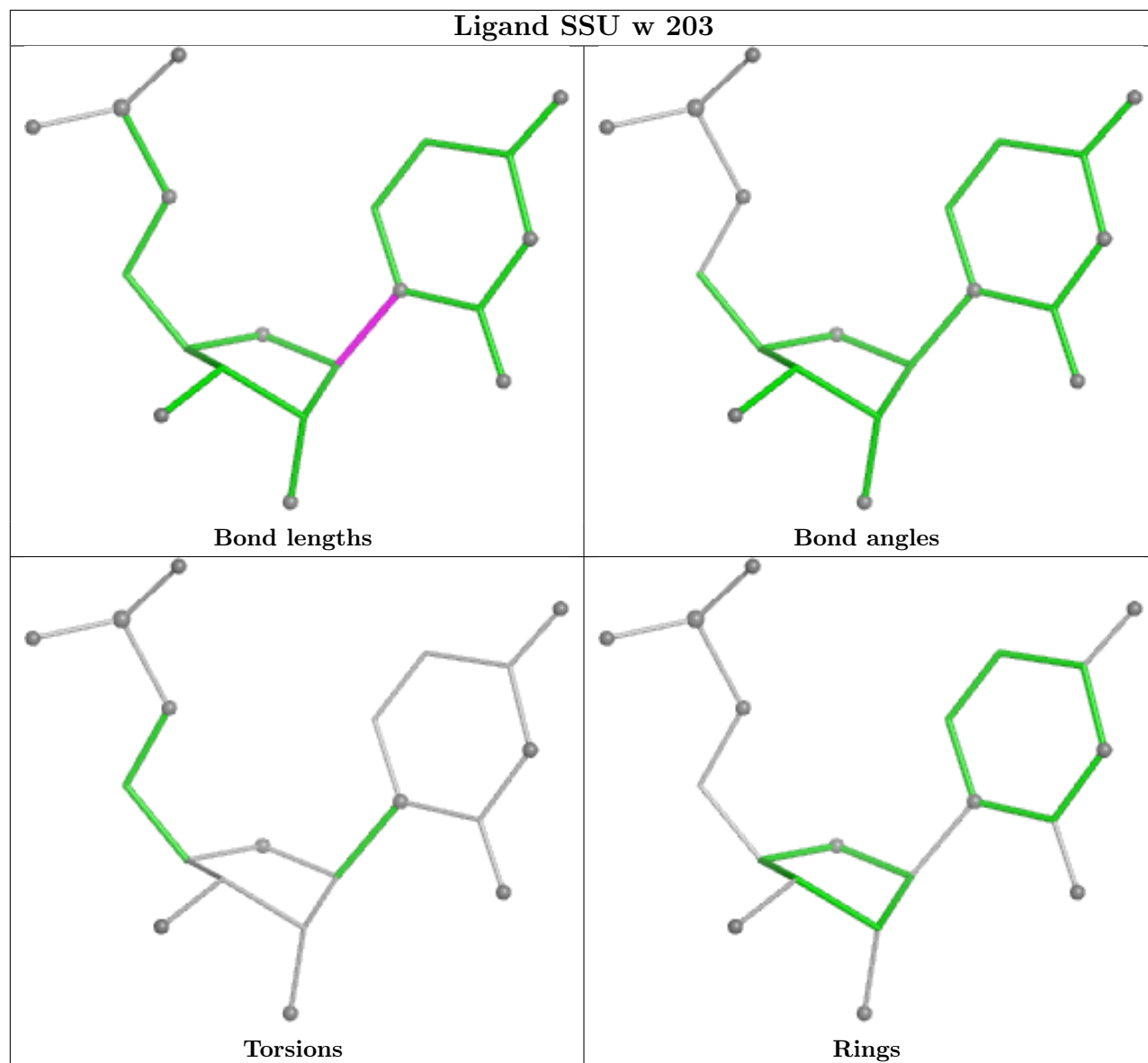


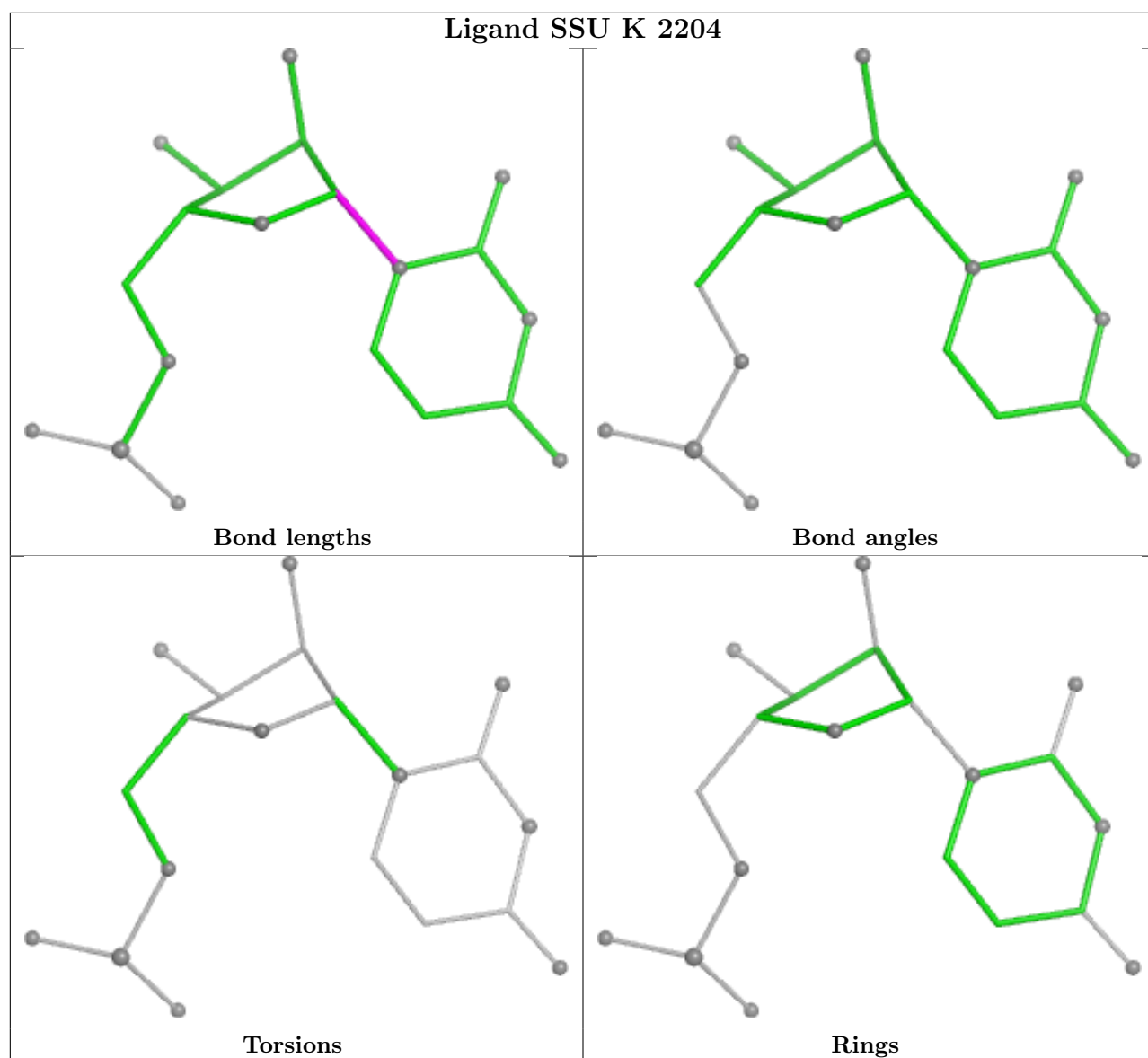


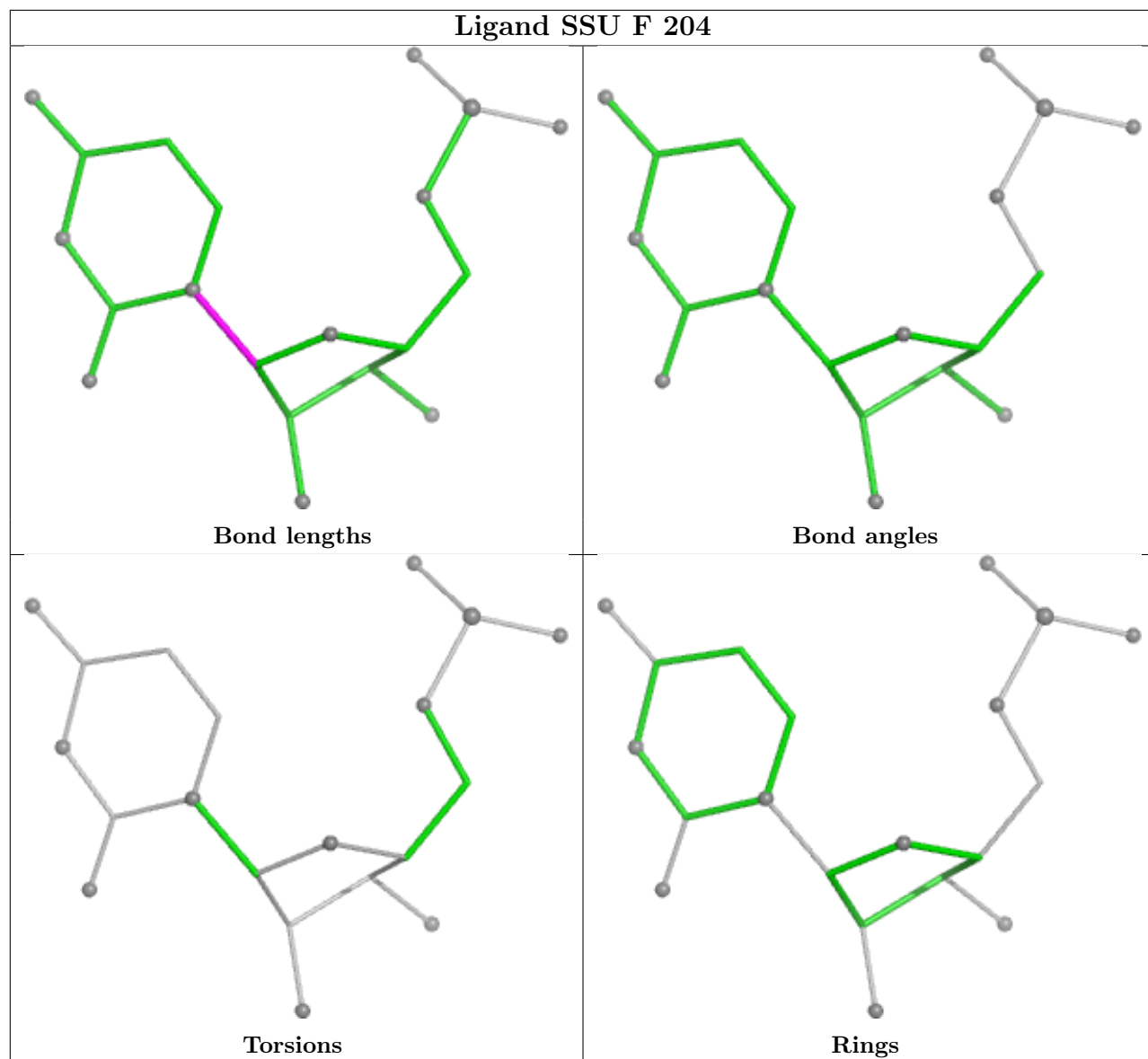


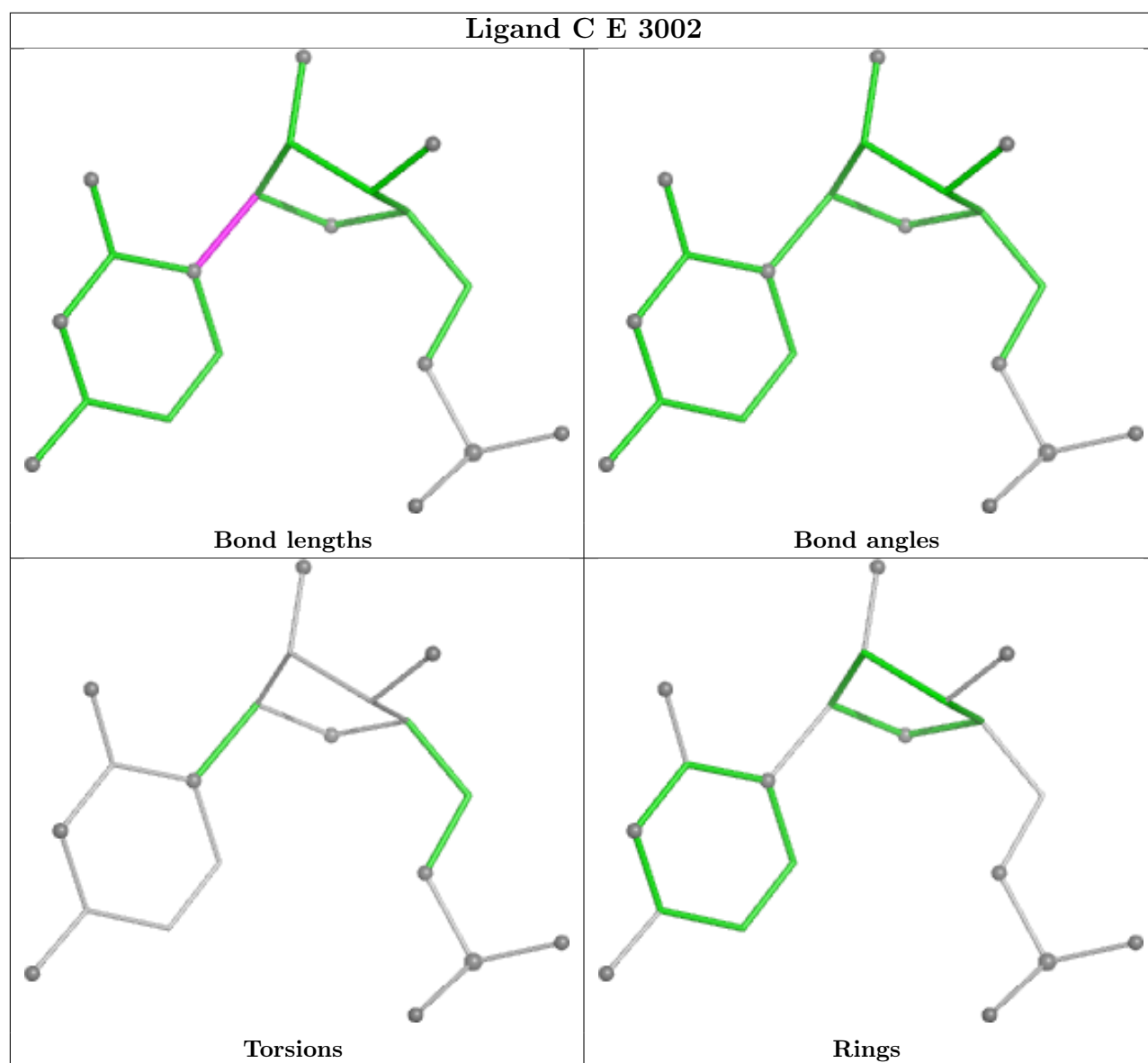


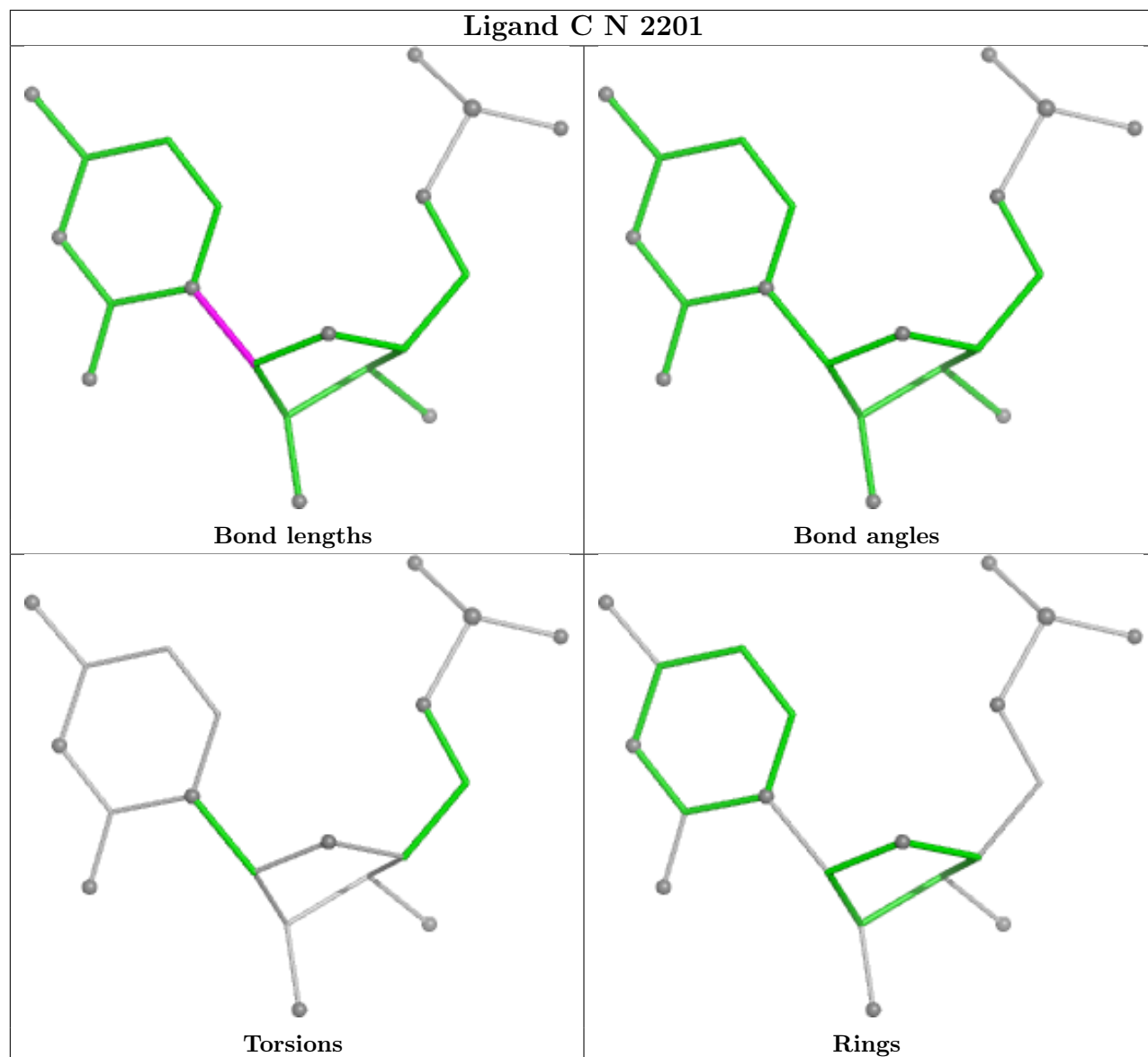


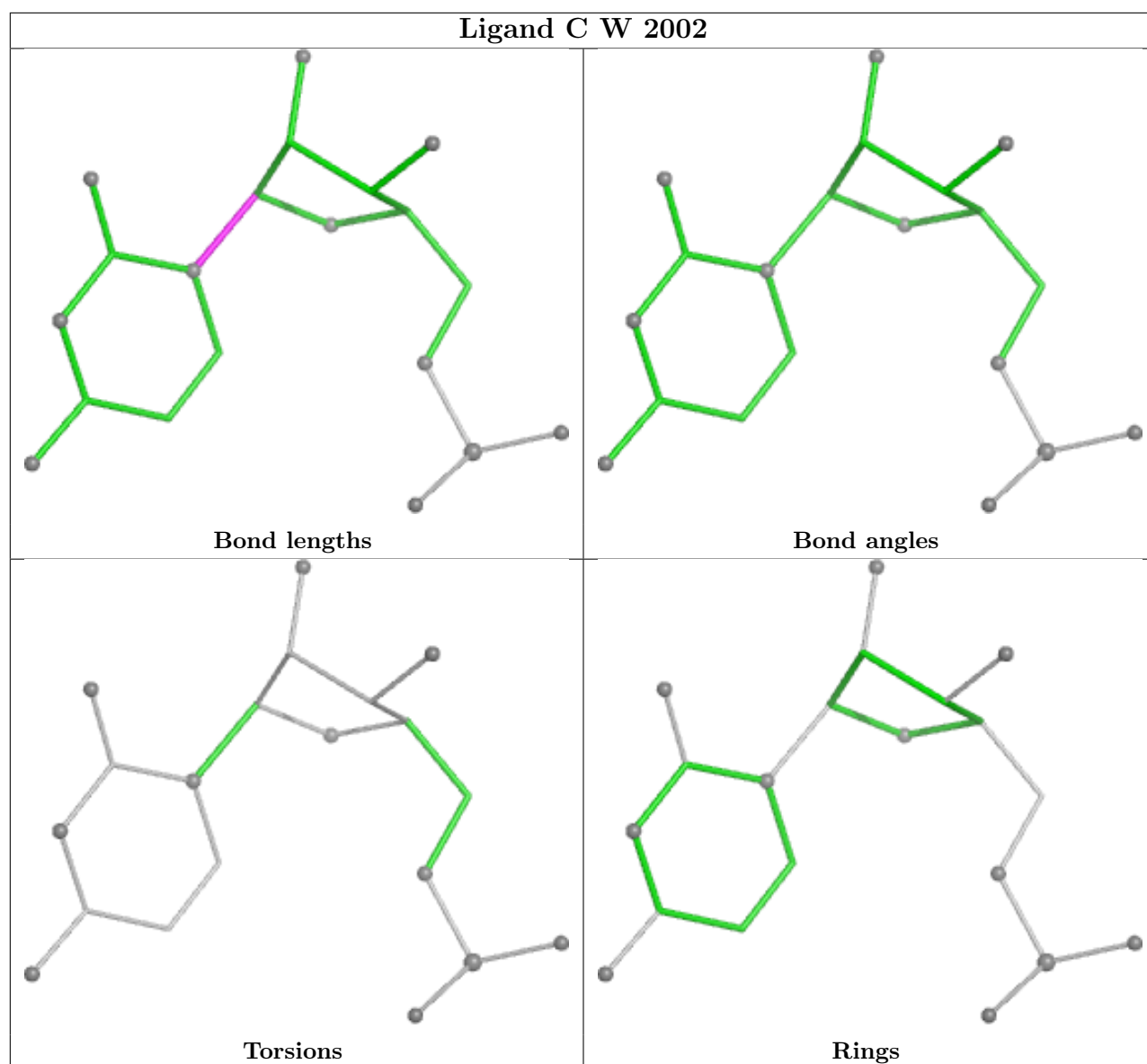


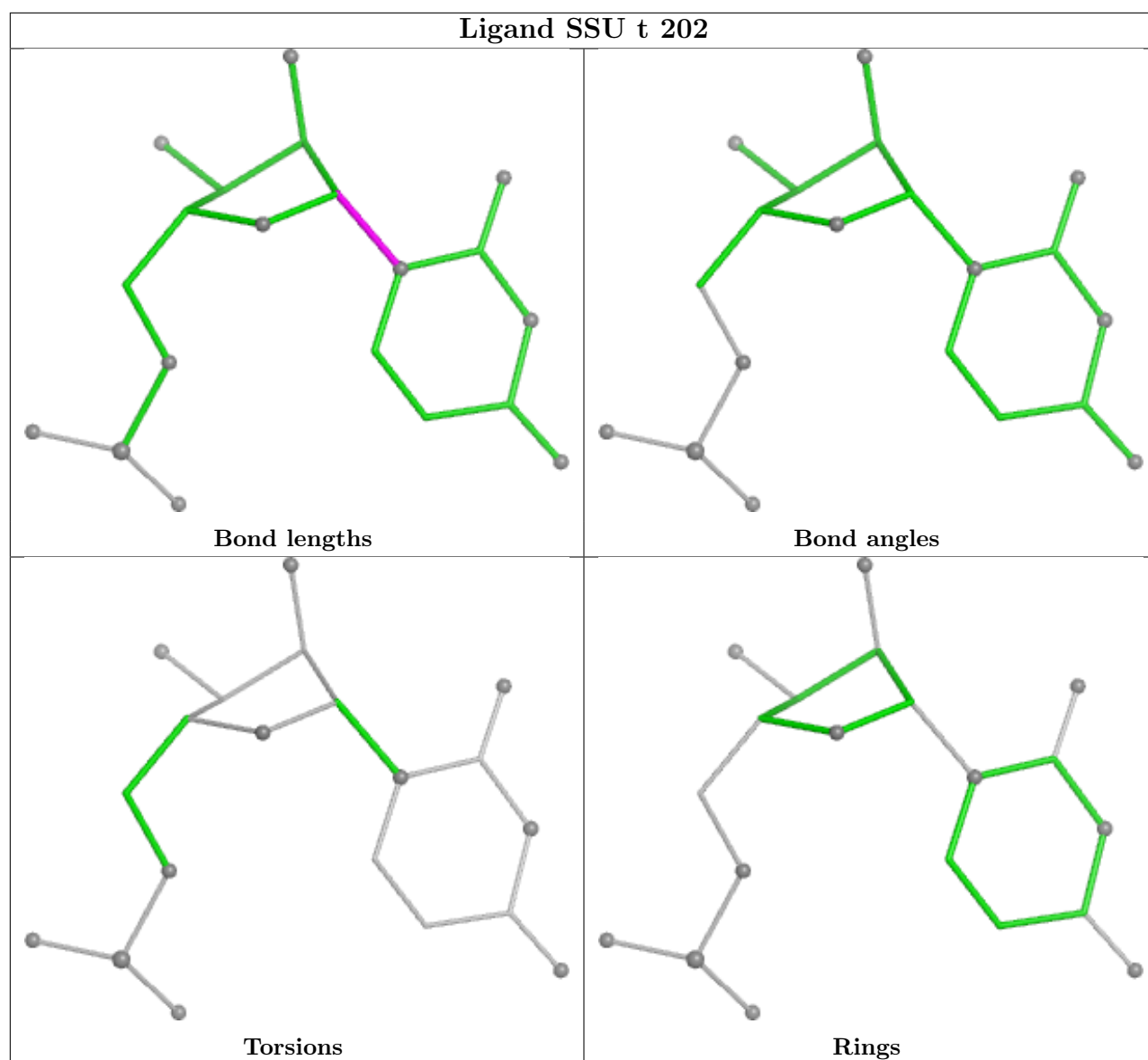


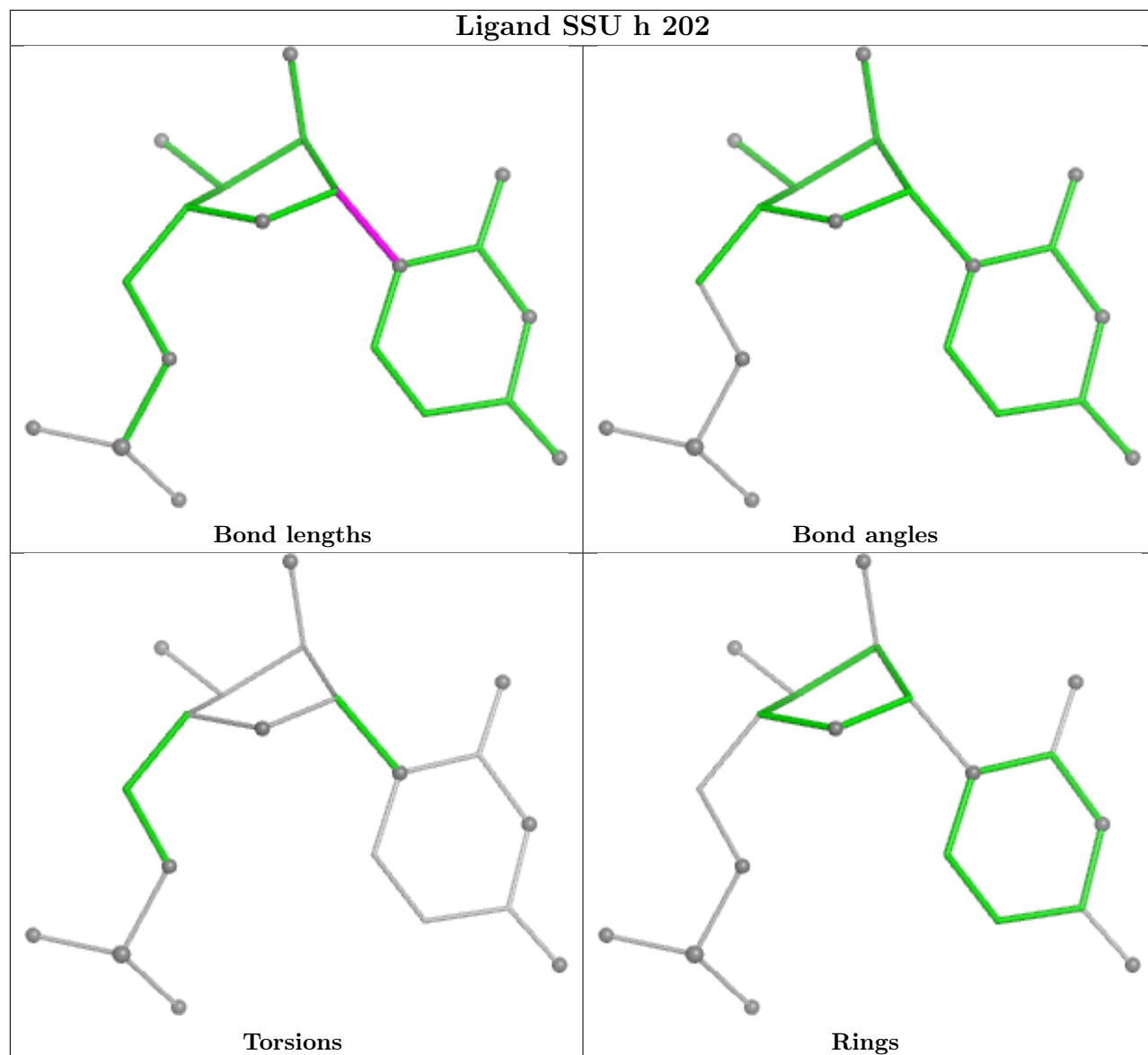


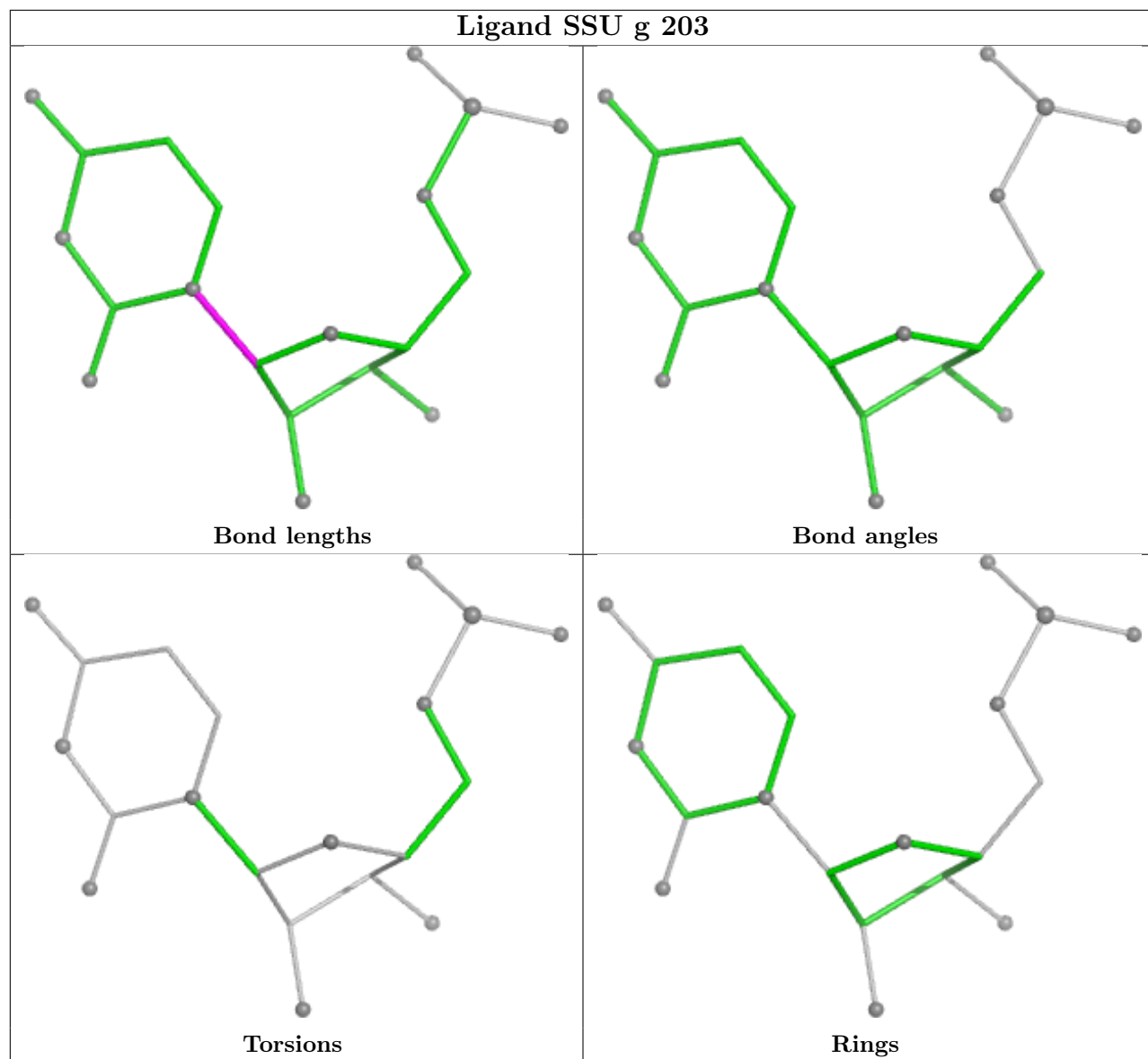


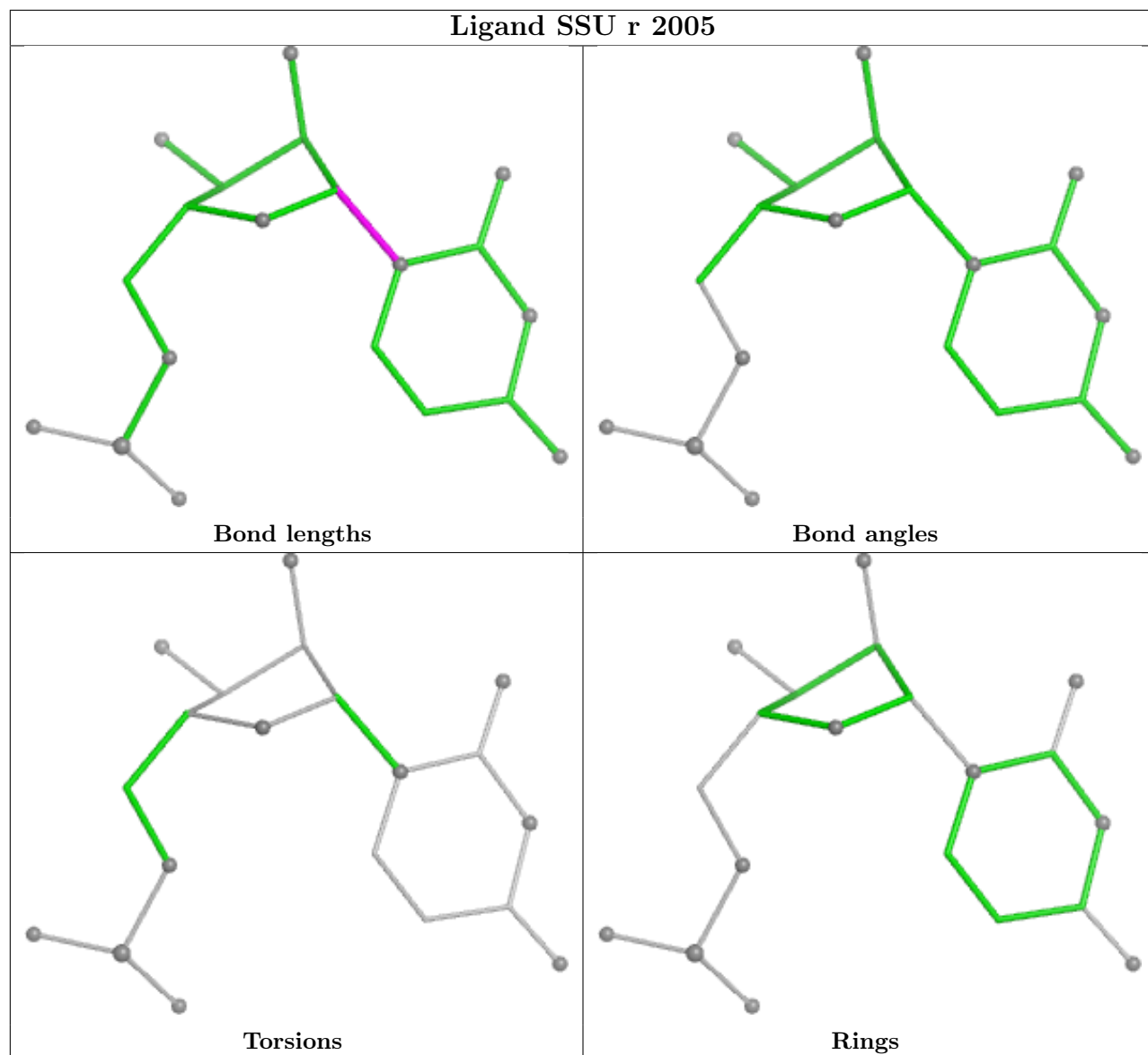


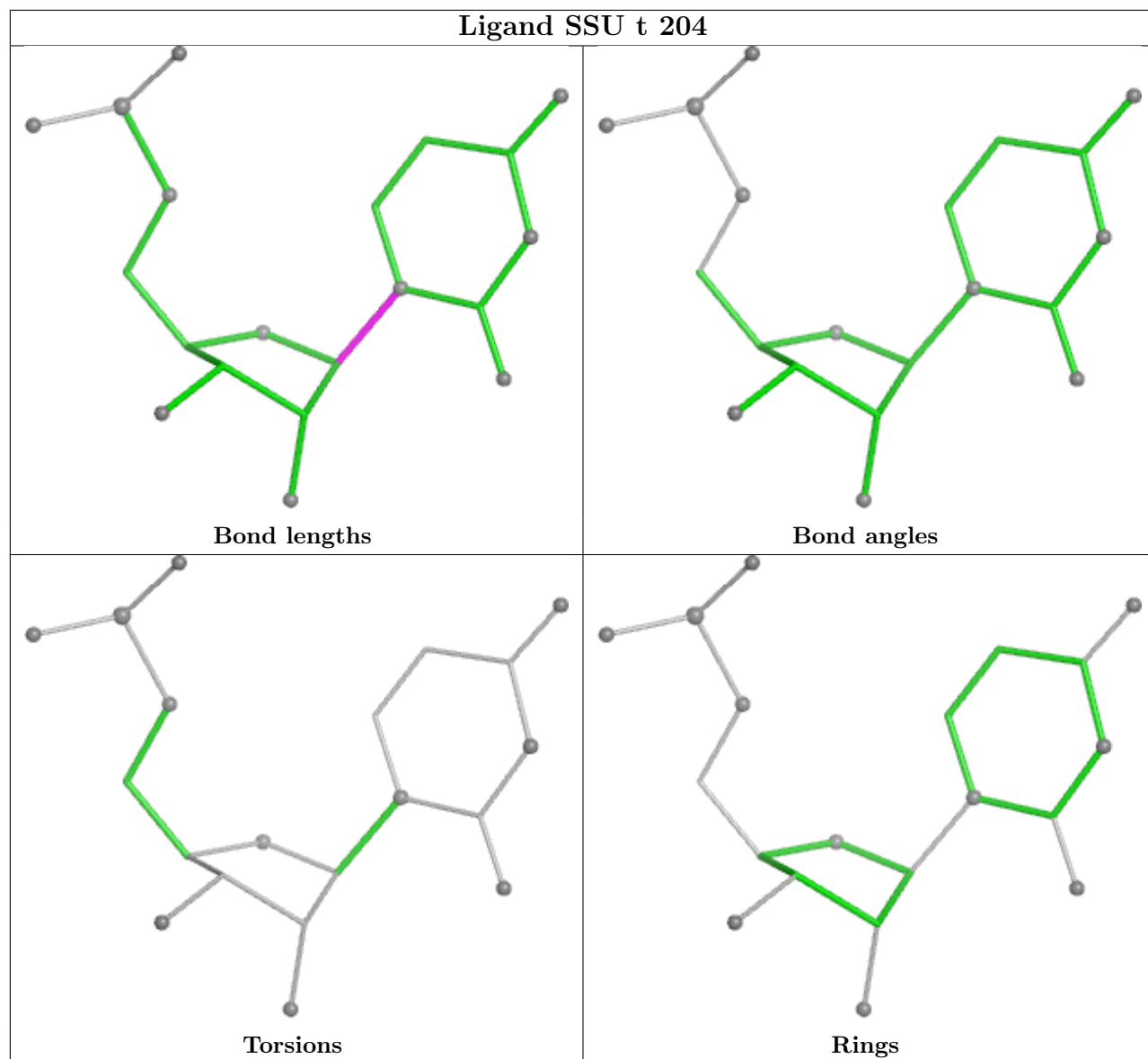


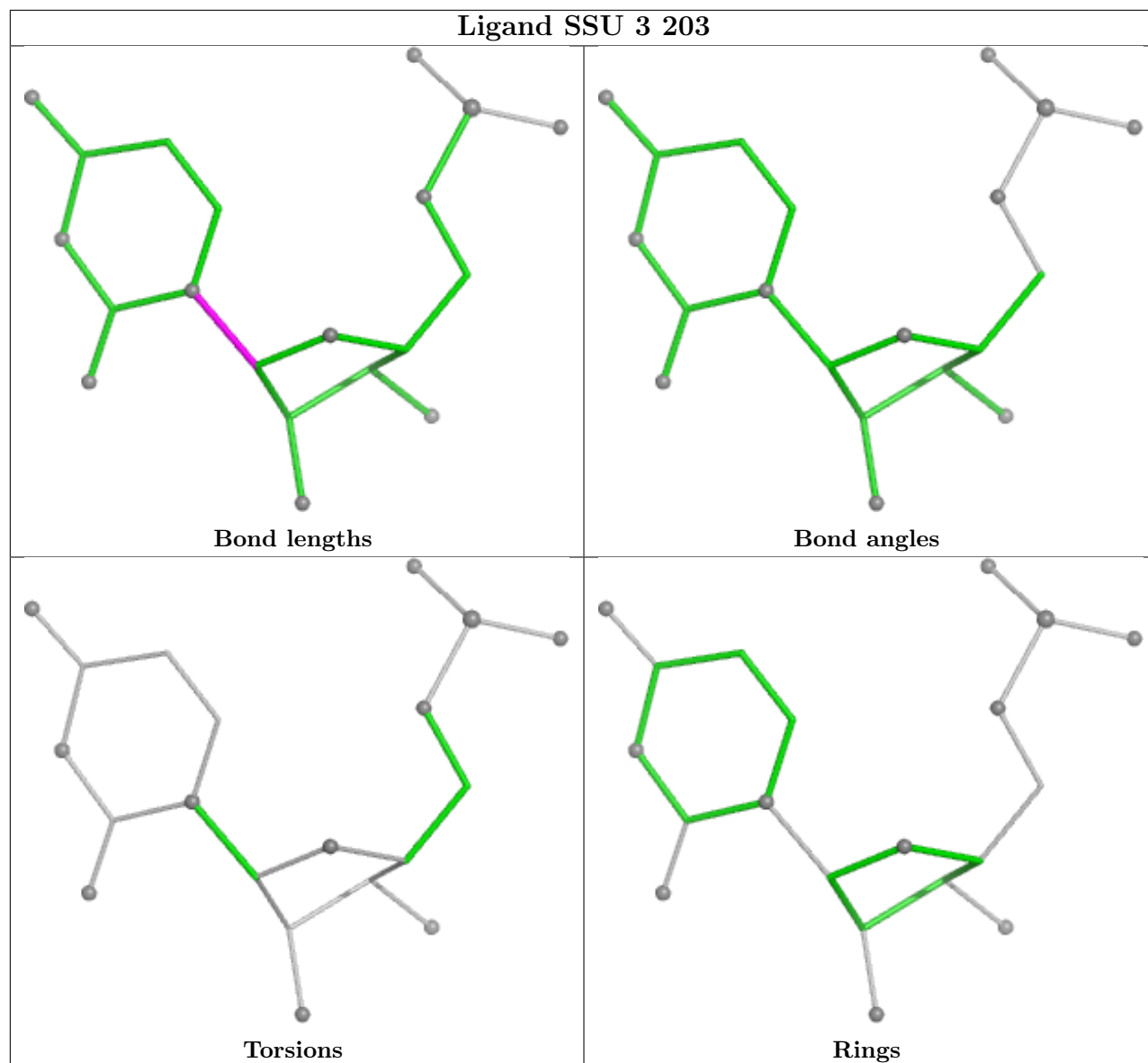


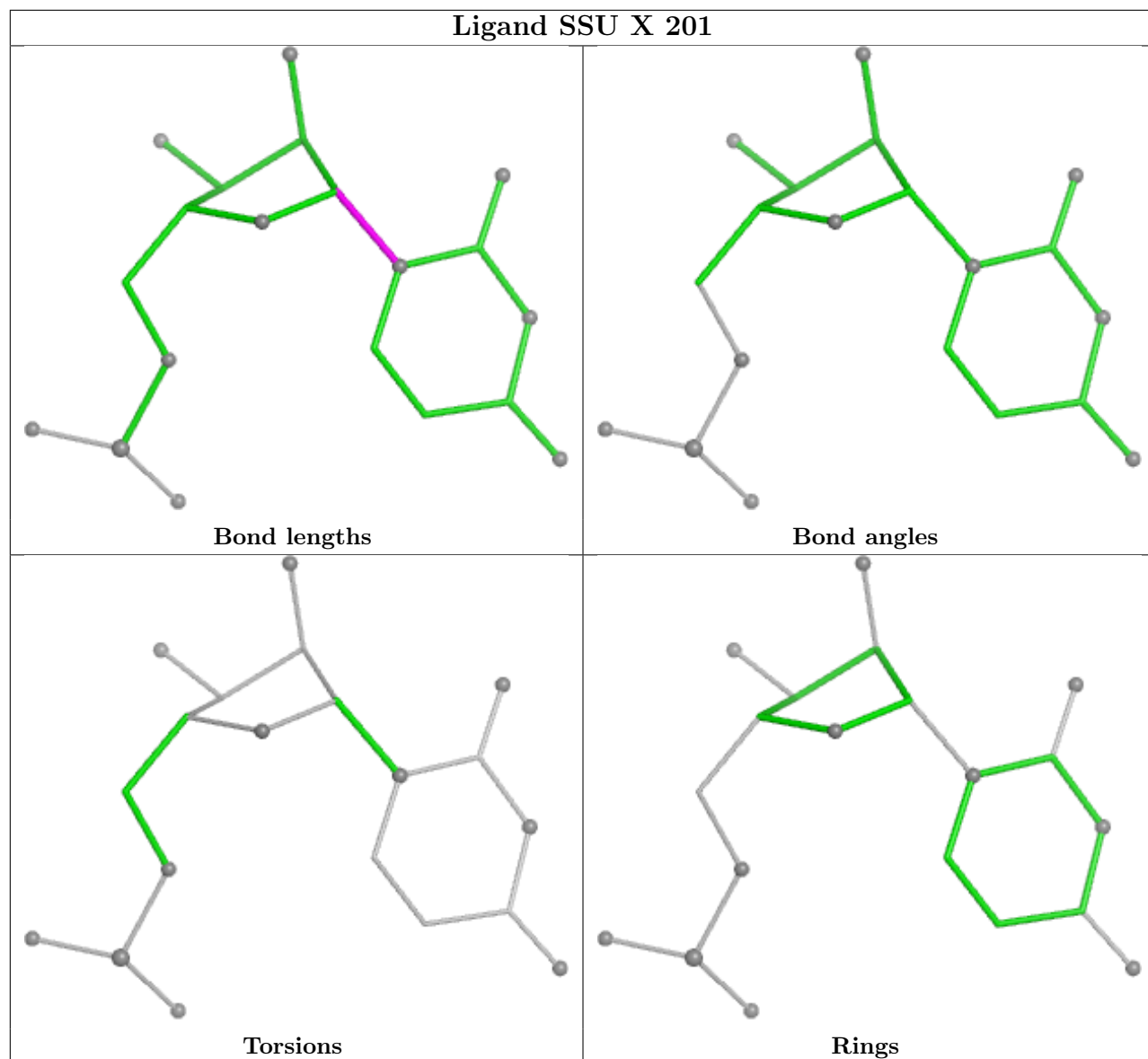


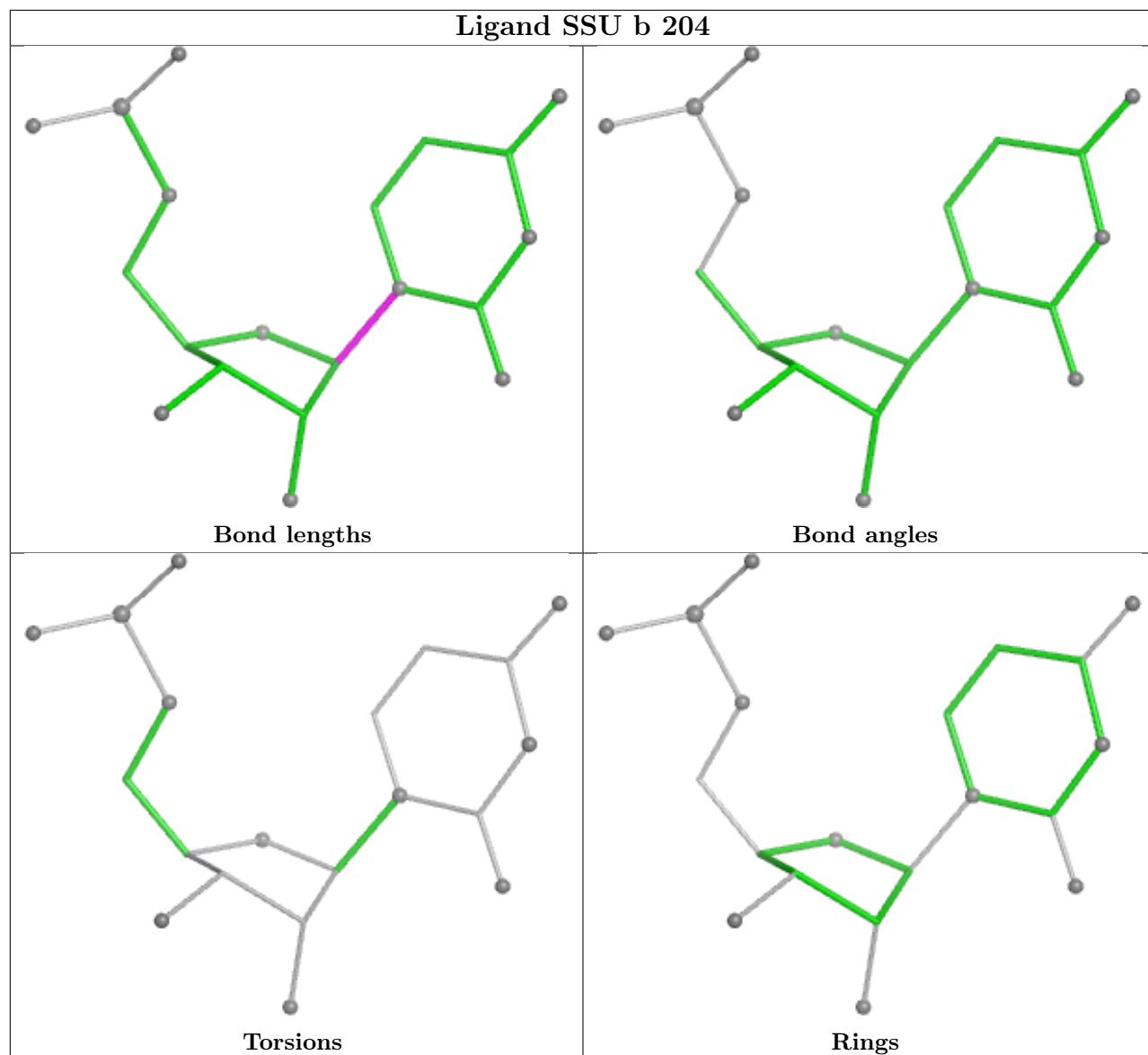


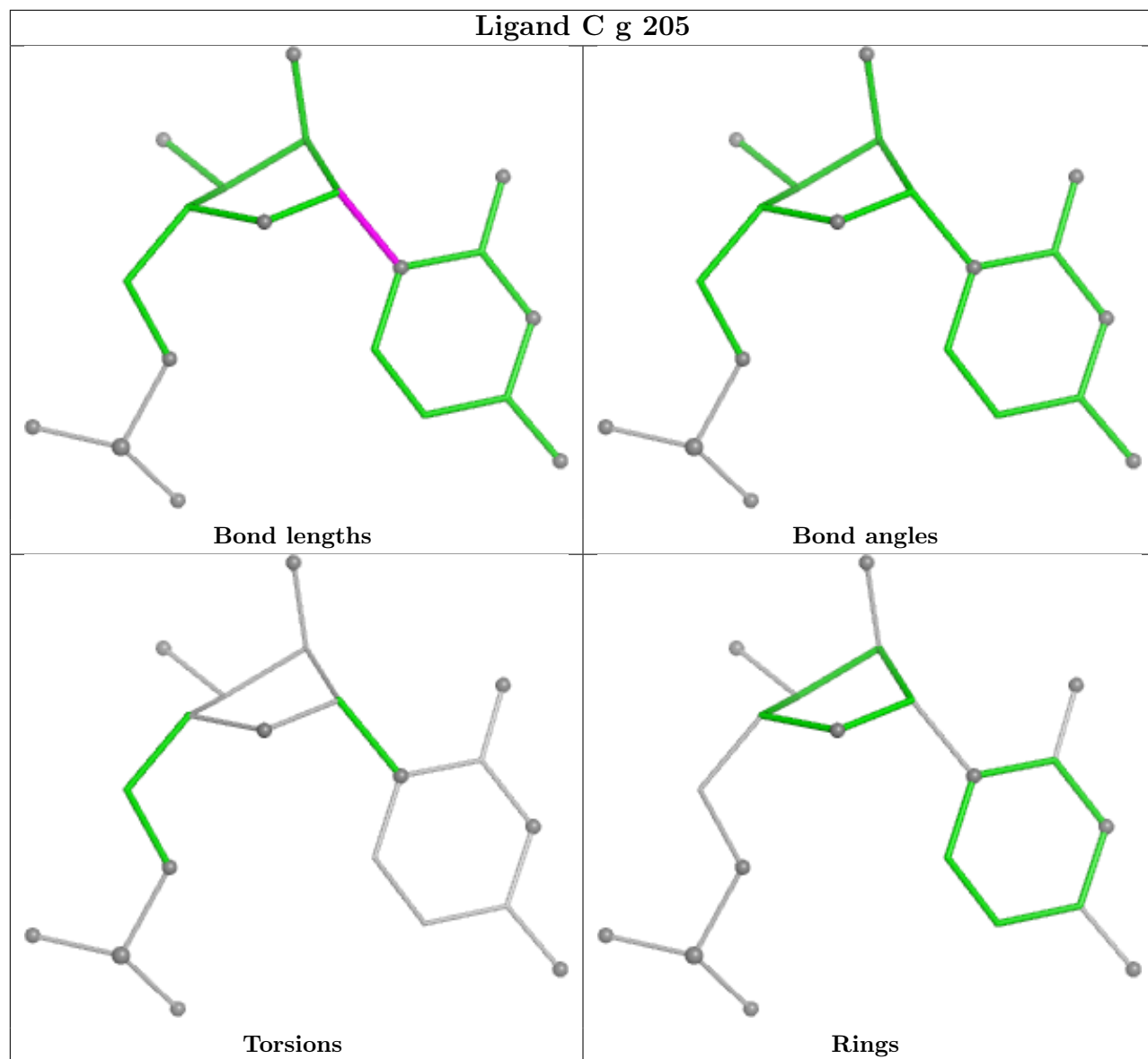


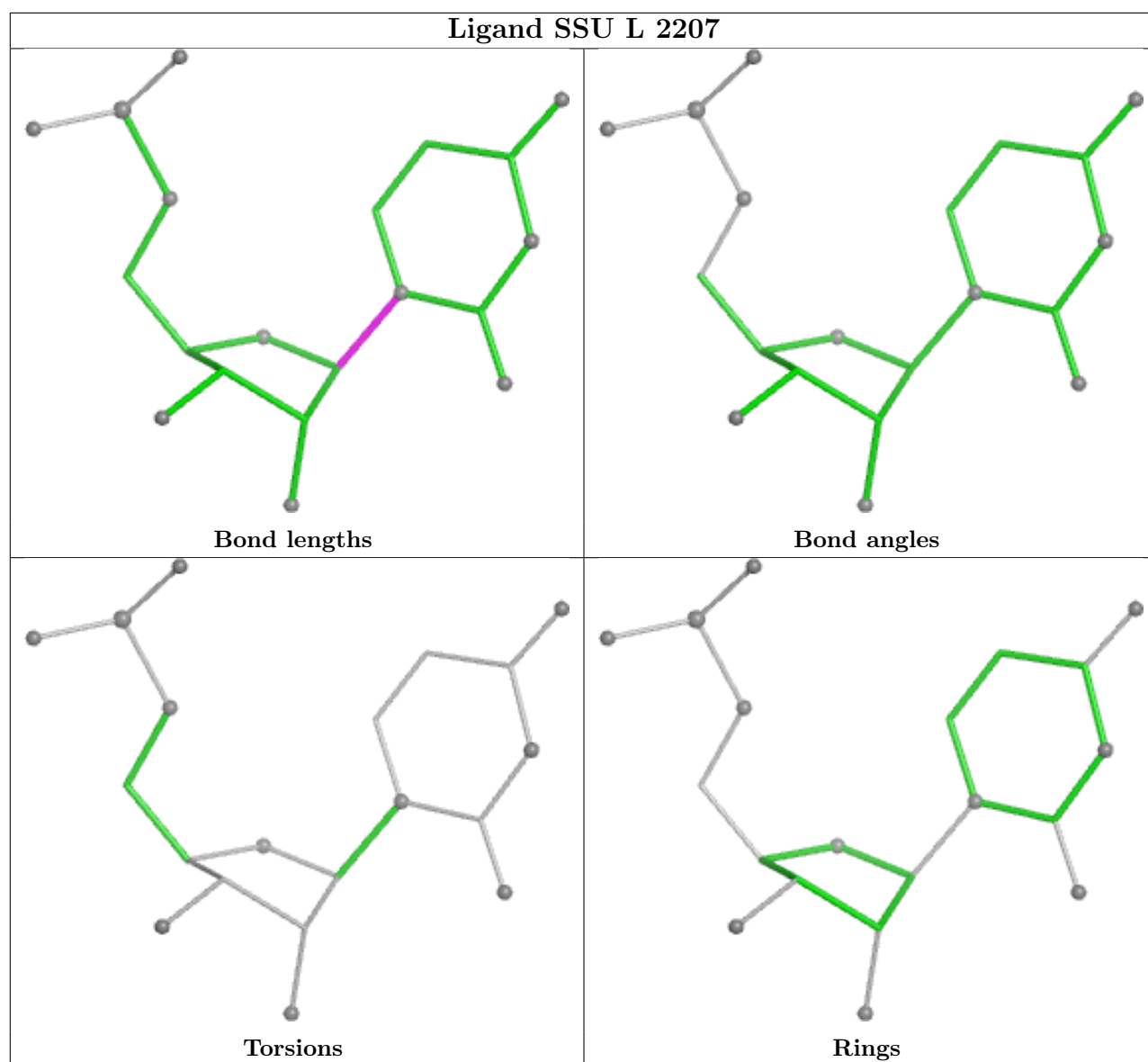












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

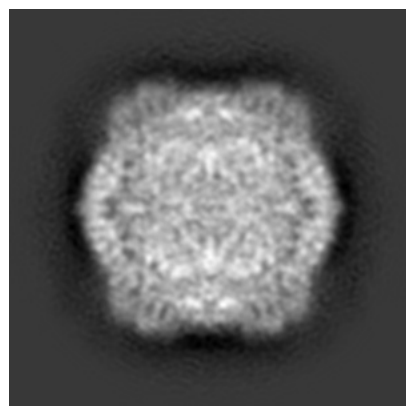
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18469. These allow visual inspection of the internal detail of the map and identification of artifacts.

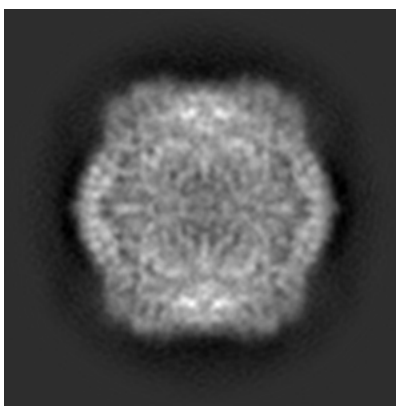
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

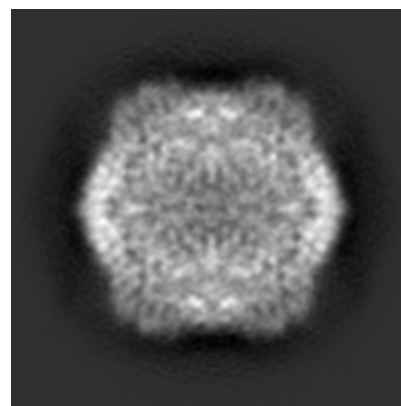
6.1.1 Primary map



X

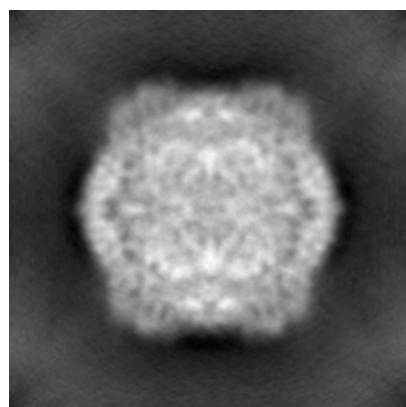


Y

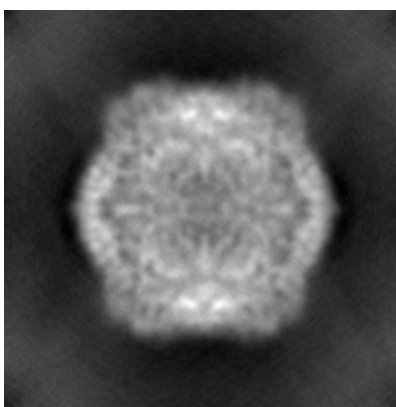


Z

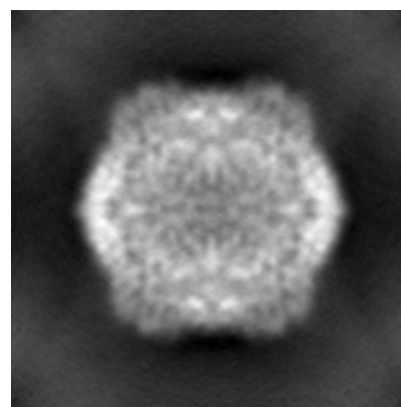
6.1.2 Raw map



X



Y

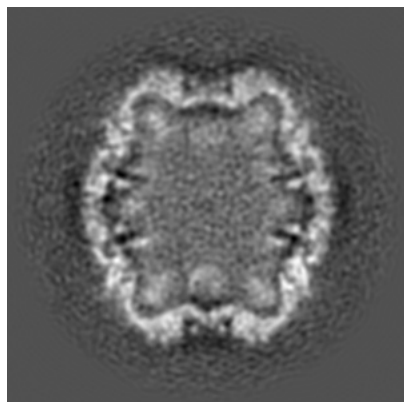


Z

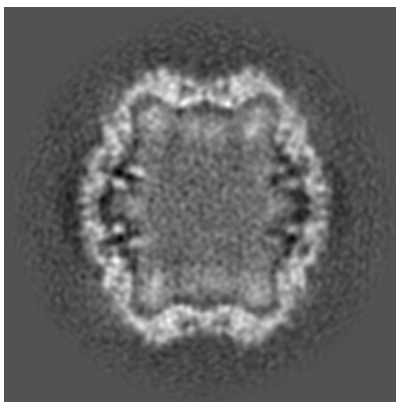
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

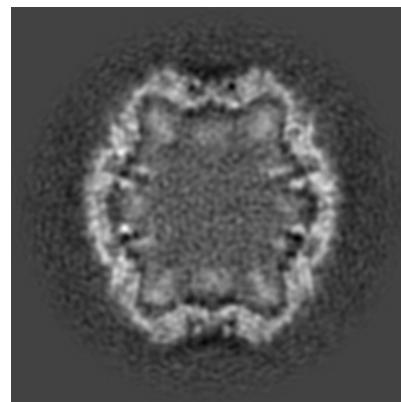
6.2.1 Primary map



X Index: 126

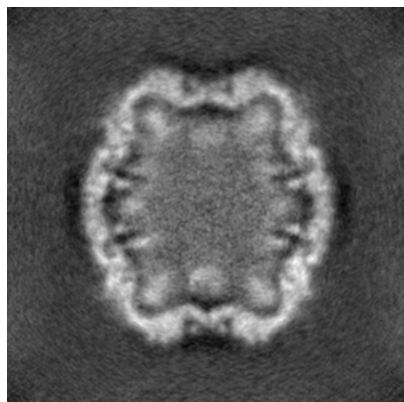


Y Index: 126

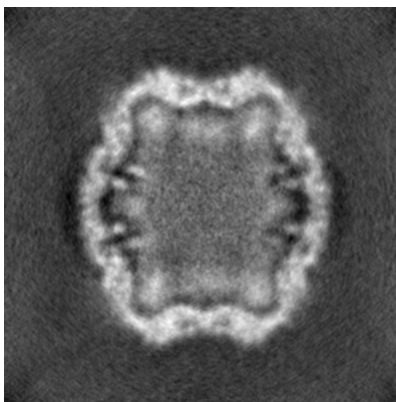


Z Index: 126

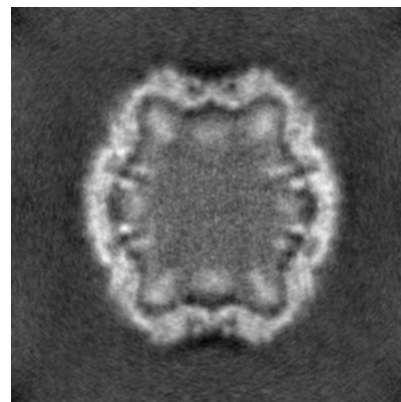
6.2.2 Raw map



X Index: 126



Y Index: 126

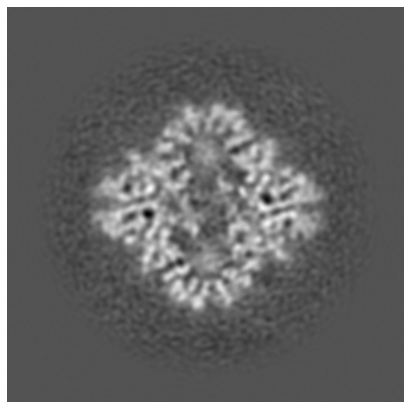


Z Index: 126

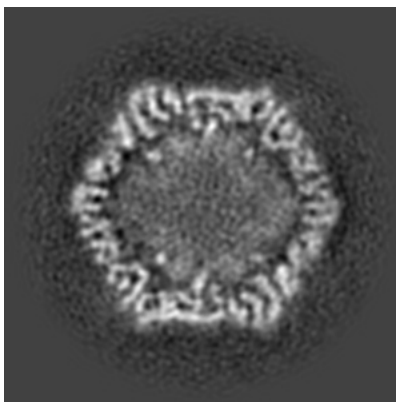
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

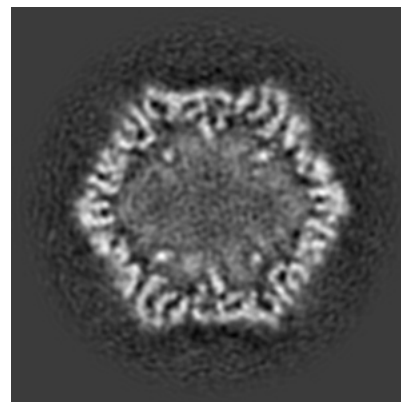
6.3.1 Primary map



X Index: 68

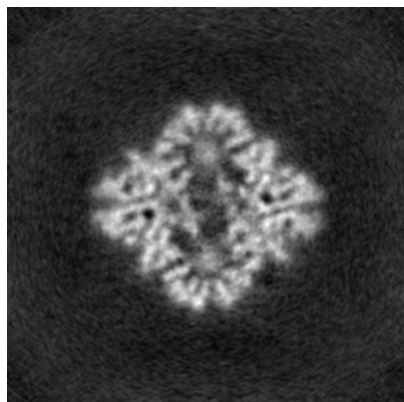


Y Index: 150

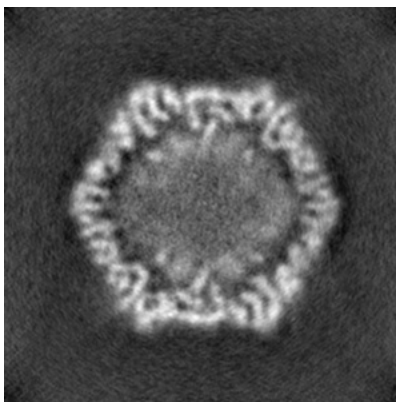


Z Index: 102

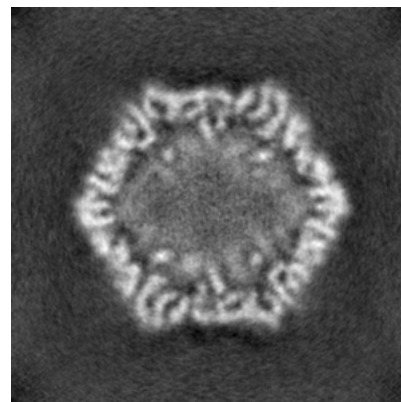
6.3.2 Raw map



X Index: 68



Y Index: 149

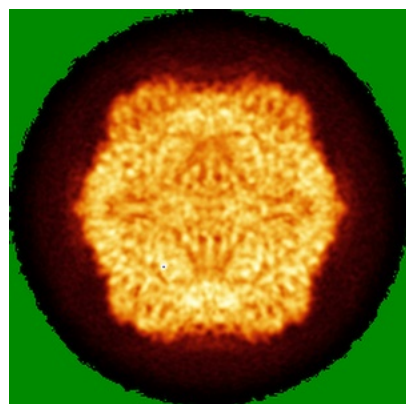


Z Index: 102

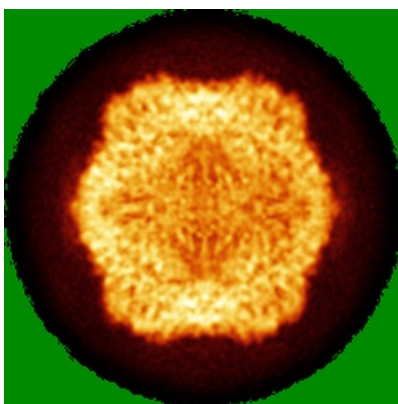
The images above show the largest variance slices of the map in three orthogonal directions.

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

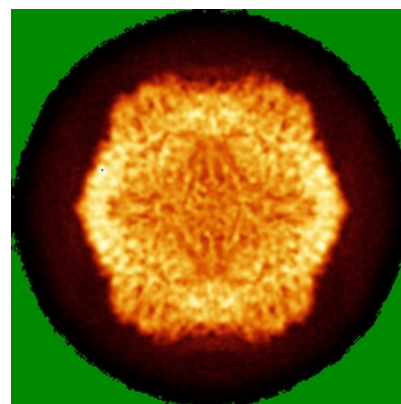
6.4.1 Primary map



X

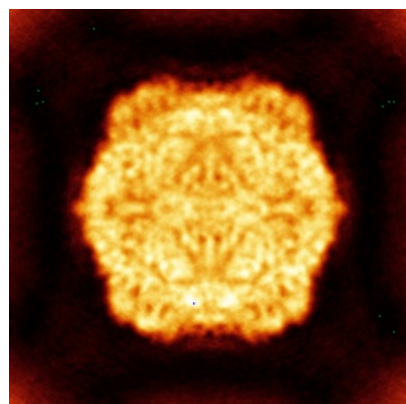


Y

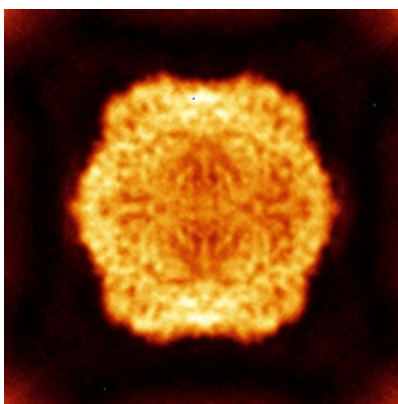


Z

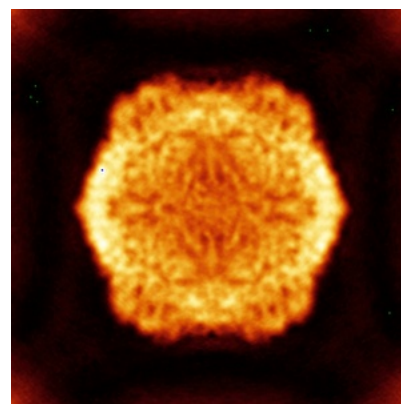
6.4.2 Raw map



X



Y

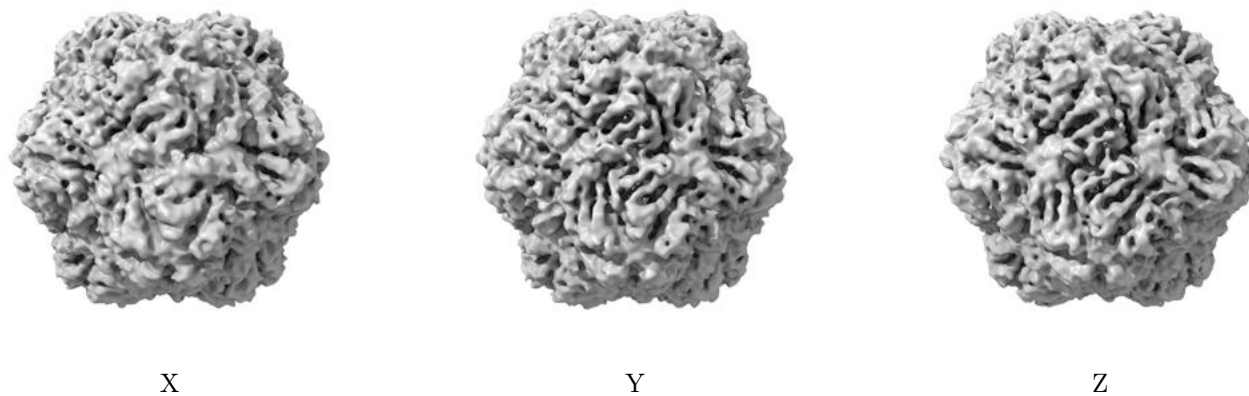


Z

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

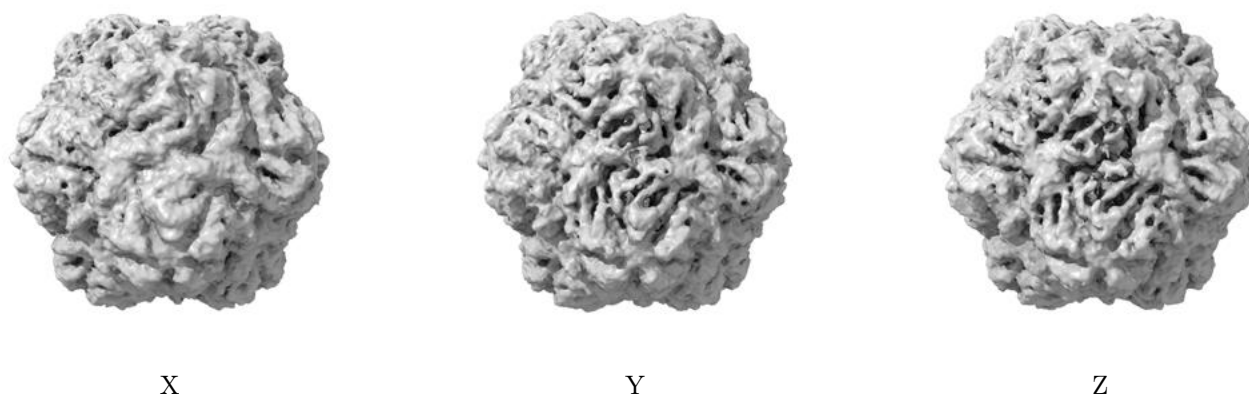
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

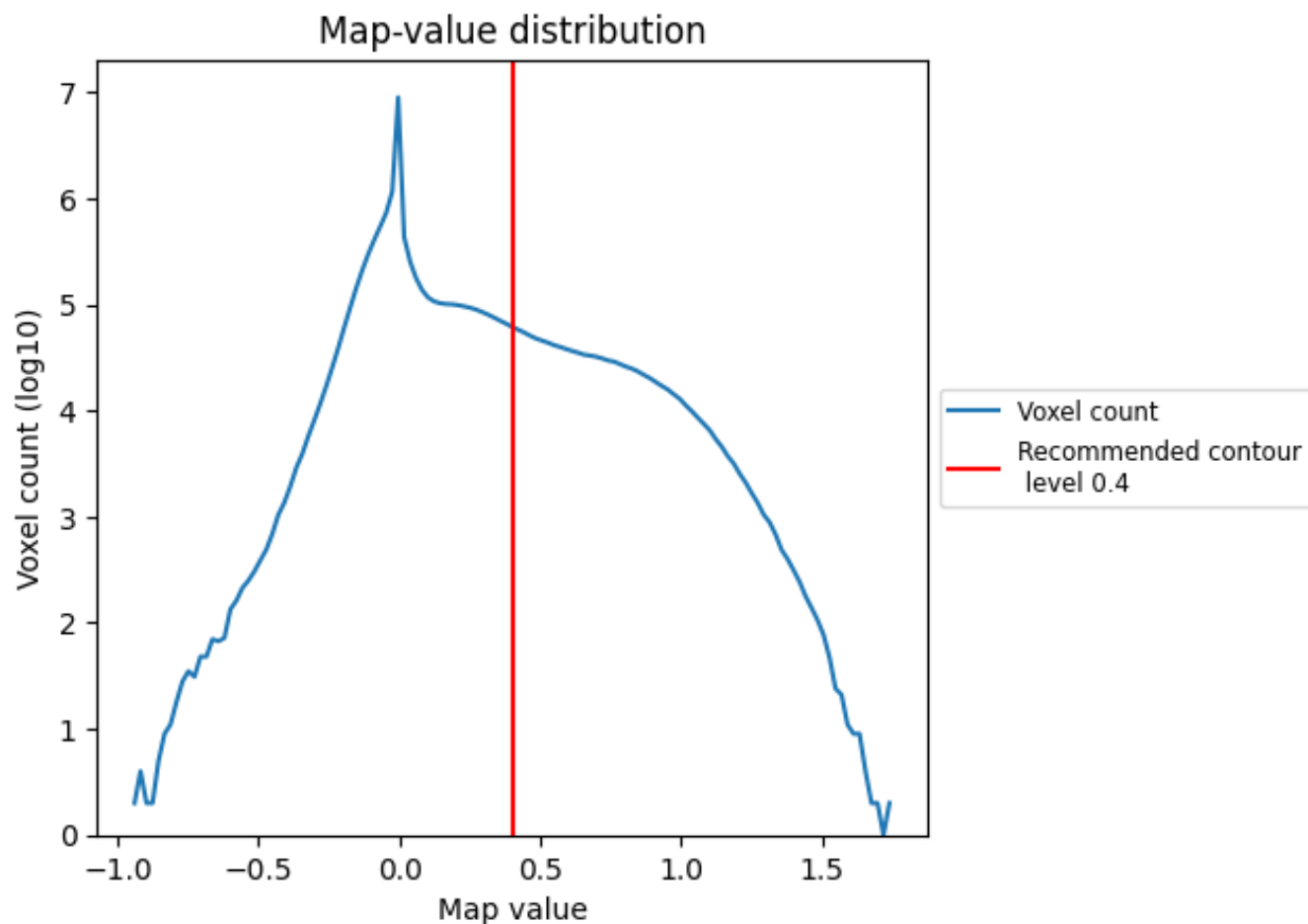
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

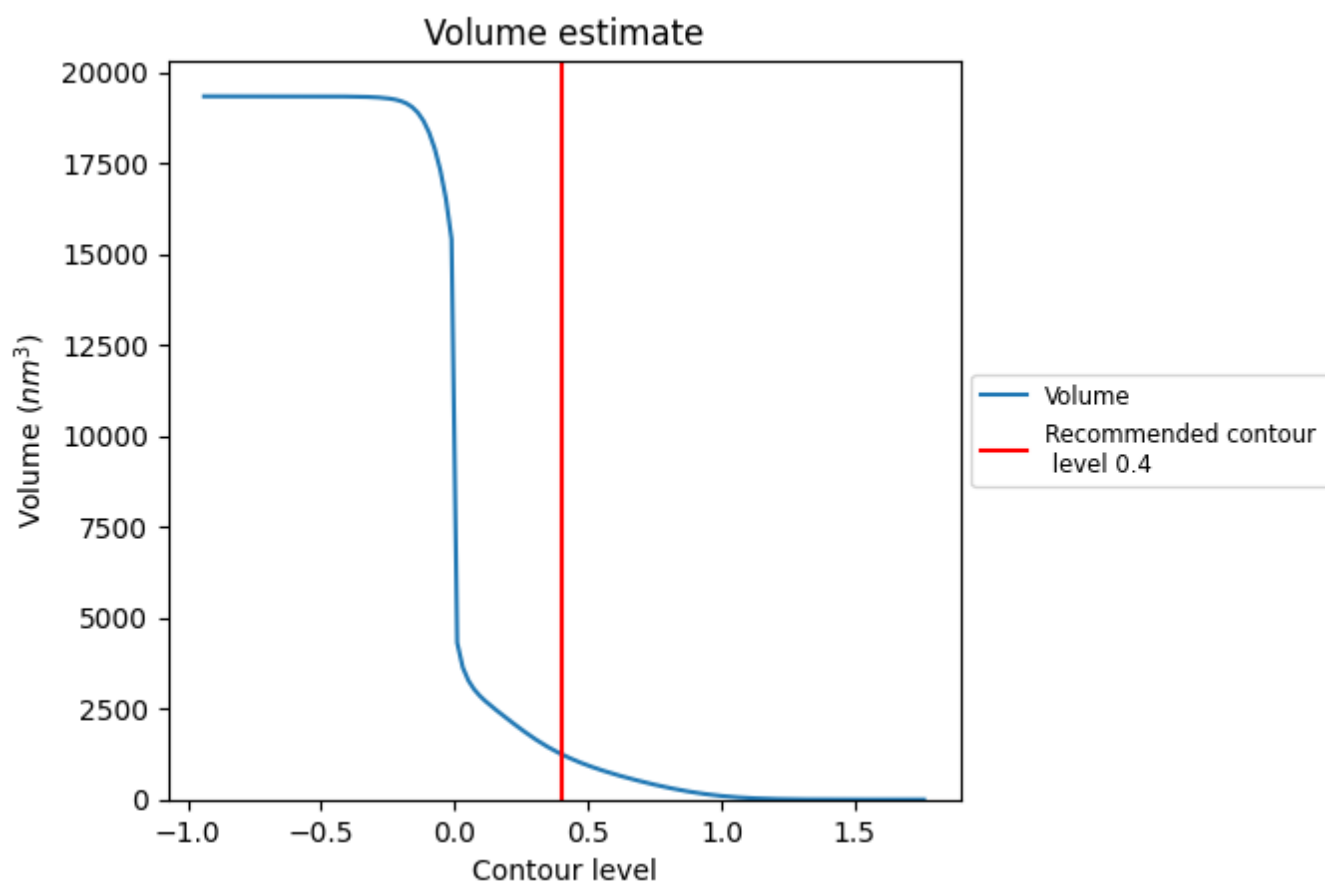
This section contains the results of statistical analysis of the map.

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.

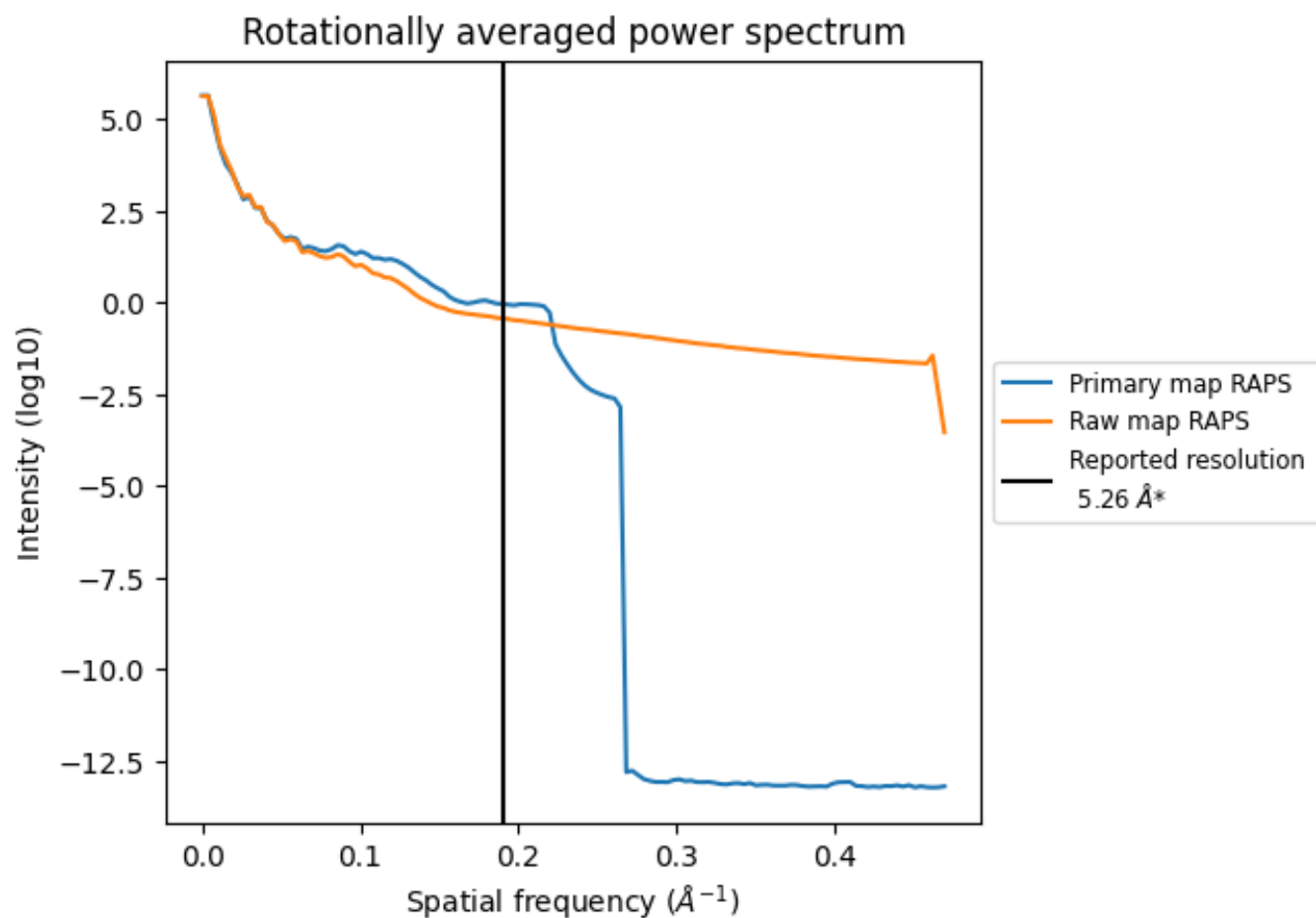
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1249 nm³; this corresponds to an approximate mass of 1128 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

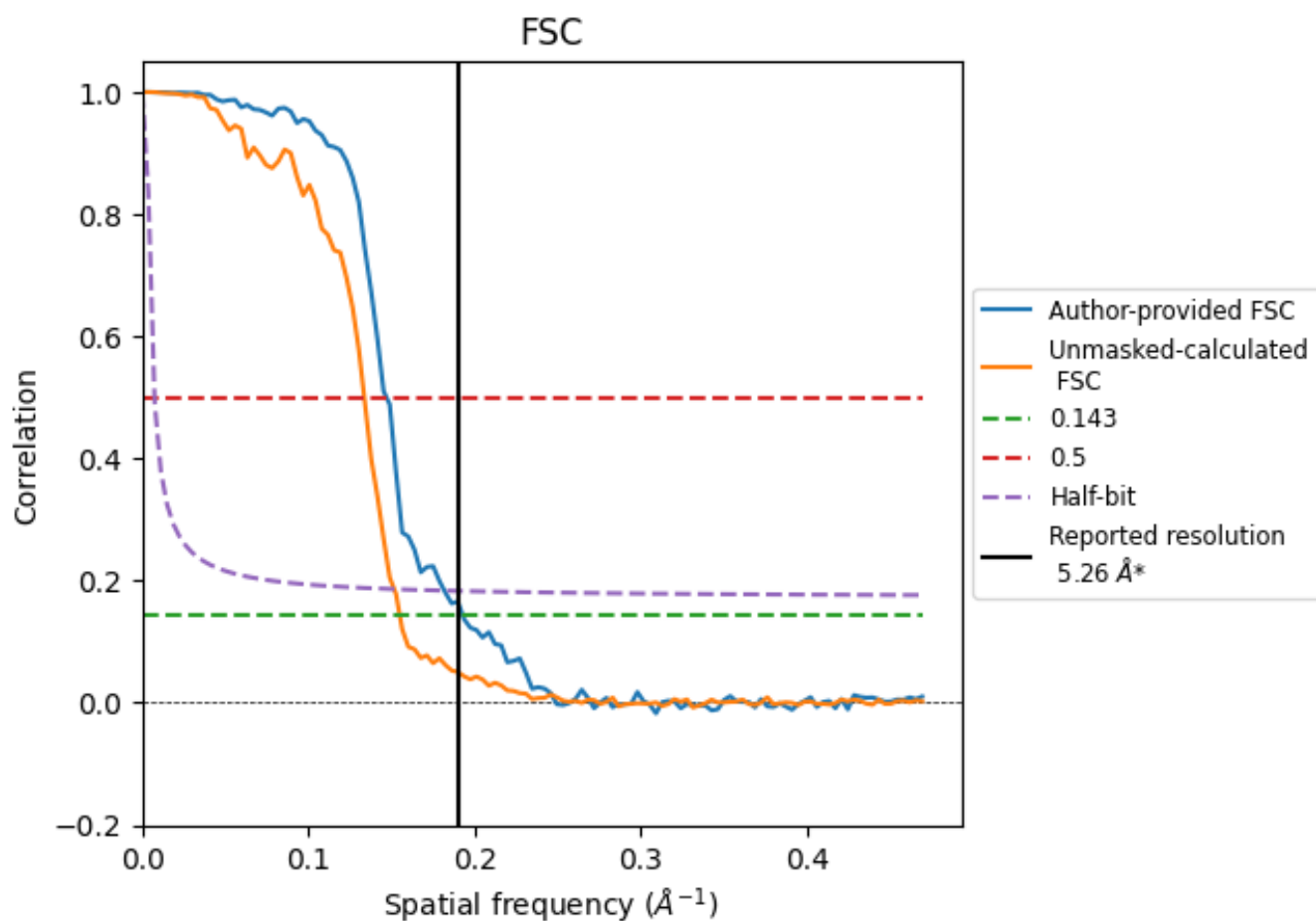


*Reported resolution corresponds to spatial frequency of 0.190 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.190 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

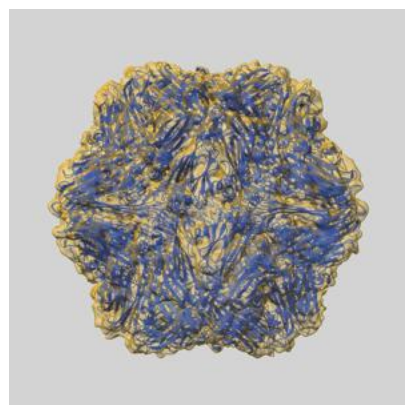
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.26	-	-
Author-provided FSC curve	5.18	6.80	5.50
Unmasked-calculated*	6.45	7.48	6.60

*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 6.45 differs from the reported value 5.26 by more than 10 %

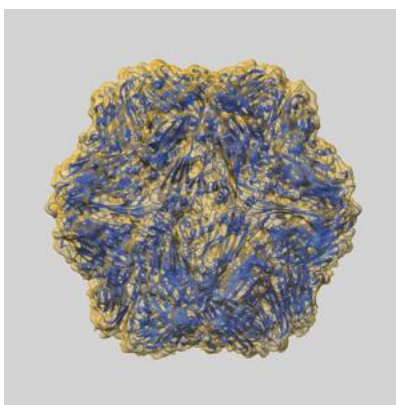
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18469 and PDB model 8QKP. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

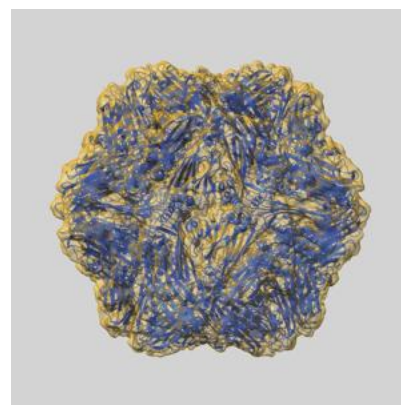
9.1 Map-model overlay [i](#)



X



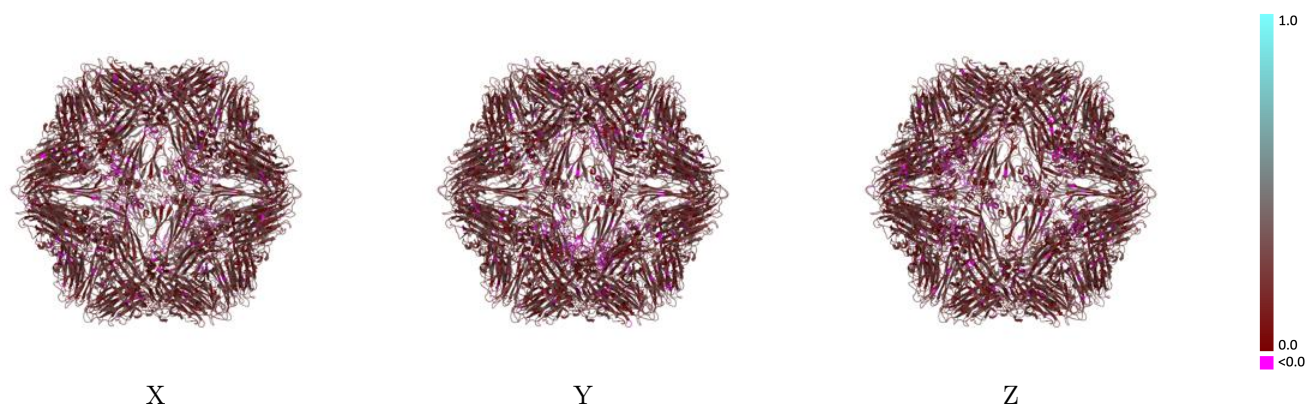
Y



Z

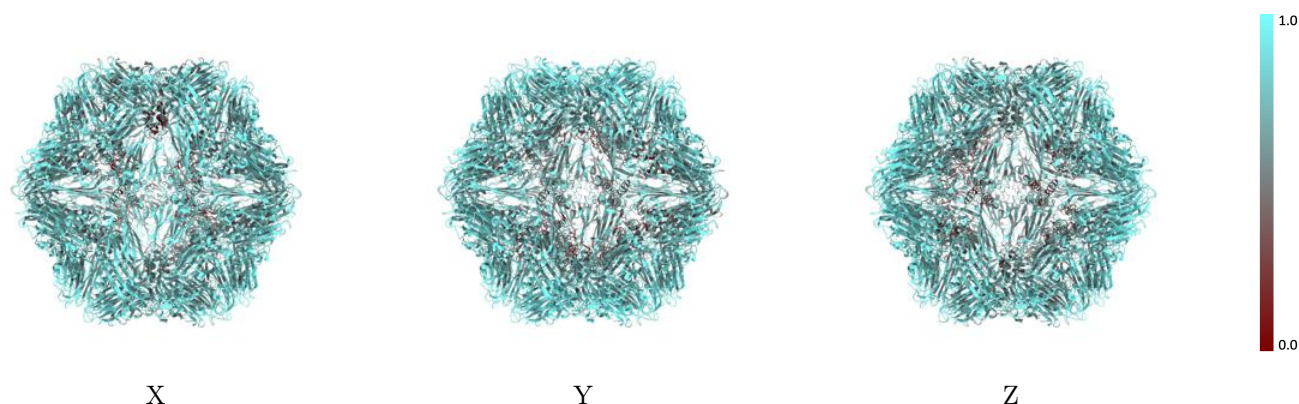
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



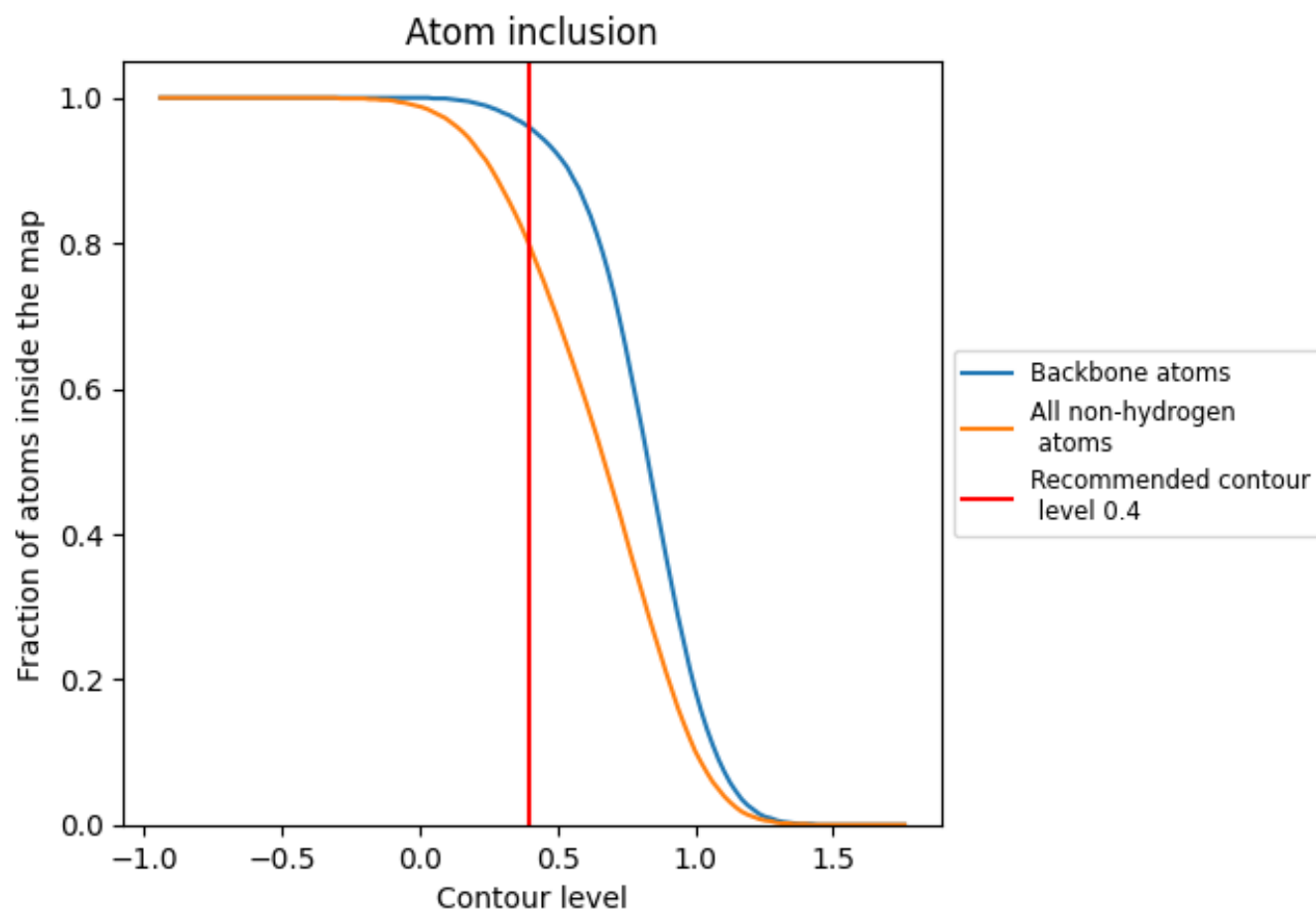
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.2100
0	 0.7800	 0.2090
1	 0.8010	 0.2070
2	 0.8410	 0.2080
3	 0.8520	 0.2150
4	 0.7830	 0.2030
5	 0.8050	 0.2060
6	 0.7440	 0.2270
7	 0.7290	 0.2110
A	 0.7350	 0.2090
B	 0.7280	 0.2090
C	 0.7970	 0.2100
D	 0.8090	 0.2160
E	 0.8090	 0.2020
F	 0.8580	 0.2100
G	 0.8400	 0.2260
H	 0.8350	 0.2010
I	 0.8140	 0.2000
J	 0.8560	 0.2080
K	 0.8350	 0.2030
L	 0.8460	 0.1970
M	 0.8630	 0.2120
N	 0.8210	 0.2130
O	 0.7890	 0.2140
P	 0.7970	 0.2060
Q	 0.8590	 0.2030
R	 0.7800	 0.2160
S	 0.7730	 0.2110
T	 0.8210	 0.2170
U	 0.7920	 0.2050
V	 0.8030	 0.2050
W	 0.8230	 0.2180
X	 0.7580	 0.2110
Y	 0.8260	 0.1990
Z	 0.7700	 0.2020



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Chain	Atom inclusion	Q-score
a	 0.8340	 0.2030
b	 0.7780	 0.1960
c	 0.7300	 0.2220
d	 0.7370	 0.2020
e	 0.8350	 0.2180
f	 0.7030	 0.2100
g	 0.8250	 0.2080
h	 0.8310	 0.2010
i	 0.8080	 0.2070
j	 0.8110	 0.2210
k	 0.7710	 0.2130
l	 0.7690	 0.2160
m	 0.8300	 0.2190
n	 0.7440	 0.2330
o	 0.6780	 0.2000
p	 0.7940	 0.2220
q	 0.7960	 0.2060
r	 0.8280	 0.2110
s	 0.7840	 0.2110
t	 0.8100	 0.2060
u	 0.6690	 0.1980
v	 0.8110	 0.2020
w	 0.7630	 0.2120
x	 0.7860	 0.2310
y	 0.8000	 0.2000
z	 0.8270	 0.2140