



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 04:49 am GMT

PDB ID : 5FVB
Title : CRYSTAL STRUCTURE OF PHORMIDIUM C-PHYCOERYTHRIN AT PH 5.0
Authors : Kumar, V.; Sonani, R.R.; Sharma, M.; Gupta, G.D.; Madamwar, D.
Deposited on : 2016-02-05
Resolution : 1.93 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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

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:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

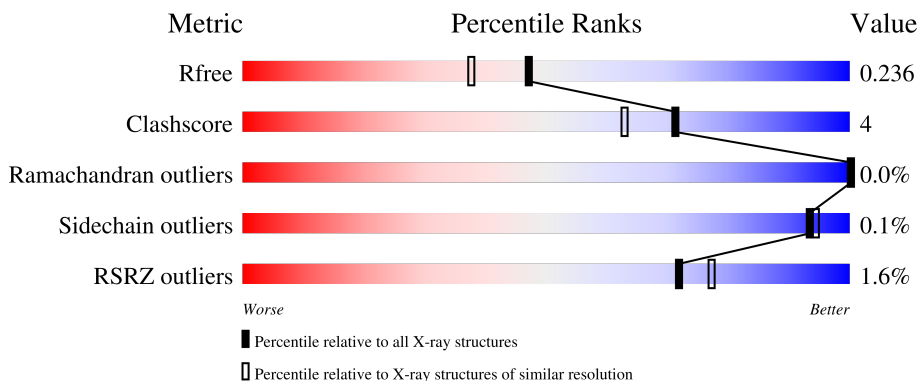
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



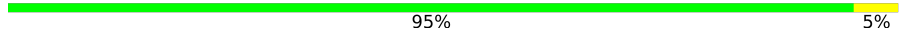
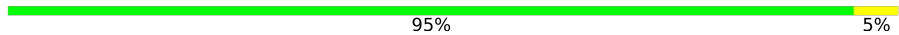
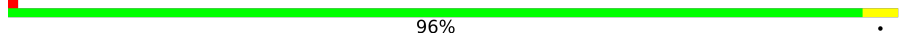
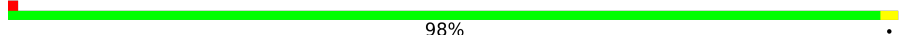
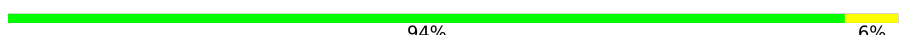
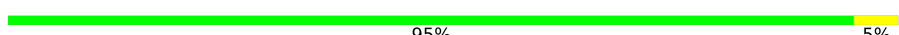





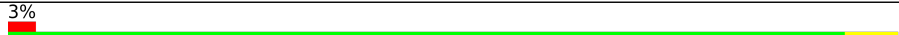

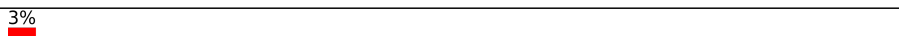
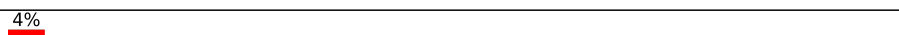
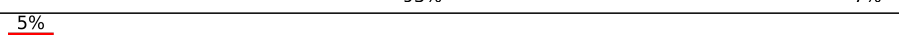
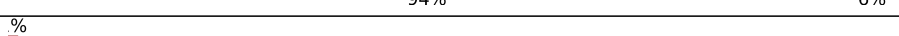
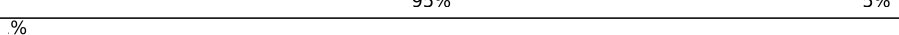
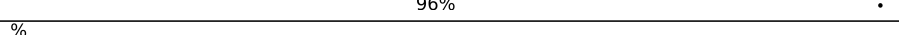
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	
1	C	164	
1	D	164	
1	E	164	

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Mol	Chain	Length	Quality of chain
1	F	164	 95% 5%
1	G	164	 95% 5%
1	H	164	 96% .
1	I	164	 98% .
1	J	164	 94% 6%
1	K	164	 95% 5%
1	L	164	 91% 9%
2	M	184	 97% . .
2	N	184	 94% 6%
2	O	184	 96% .
2	P	184	 96% .
2	Q	184	 94% 6%
2	R	184	 90% 10%
2	S	184	 93% 7%
2	T	184	 93% 7%
2	U	184	 94% 6%
2	V	184	 95% 5%
2	W	184	 96% .
2	X	184	 97% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 C-PHYCOERYTHRIN ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1239	771	218	244	6	0	0	0
1	B	164	1239	771	218	244	6	0	0	0
1	C	164	1239	771	218	244	6	0	0	0
1	D	164	1239	771	218	244	6	0	0	0
1	E	164	1239	771	218	244	6	0	0	0
1	F	164	1239	771	218	244	6	0	0	0
1	G	164	1239	771	218	244	6	0	0	0
1	H	164	1239	771	218	244	6	0	0	0
1	I	164	1239	771	218	244	6	0	0	0
1	J	164	1239	771	218	244	6	0	0	0
1	K	164	1239	771	218	244	6	0	0	0
1	L	164	1239	771	218	244	6	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
A	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
A	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
A	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
B	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
C	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
C	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
D	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
D	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
E	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
E	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
F	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
F	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
G	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
G	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
H	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
H	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
I	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
I	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
J	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
J	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
K	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
K	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
L	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01

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Chain	Residue	Modelled	Actual	Comment	Reference
L	164	SER	-	SEE REMARK 999	UNP A0A0E3W01

- Molecule 2 is a protein called C-PHYCOERYTHRIN BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	184	1347	827	244	263	13	0	0	0
2	N	184	1347	827	244	263	13	0	0	0
2	O	184	1347	827	244	263	13	0	0	0
2	P	184	1347	827	244	263	13	0	0	0
2	Q	184	1347	827	244	263	13	0	0	0
2	R	184	1347	827	244	263	13	0	0	0
2	S	184	1347	827	244	263	13	0	0	0
2	T	184	1347	827	244	263	13	0	0	0
2	U	184	1347	827	244	263	13	0	0	0
2	V	184	1347	827	244	263	13	0	0	0
2	W	184	1347	827	244	263	13	0	0	0
2	X	184	1347	827	244	263	13	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
M	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
M	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
M	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
M	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
M	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
M	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
N	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
N	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

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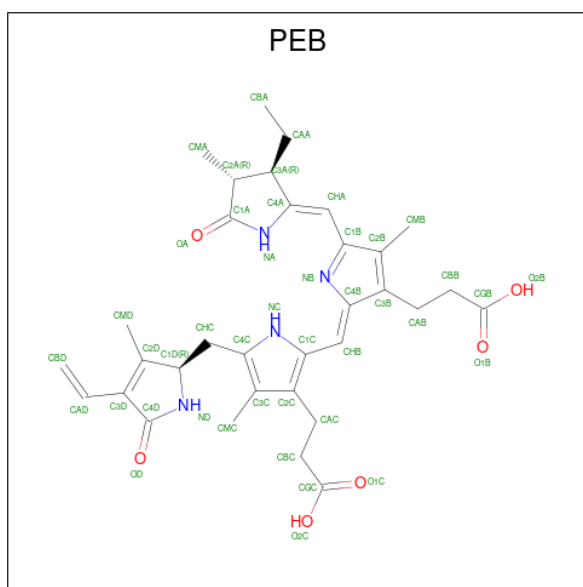
Chain	Residue	Modelled	Actual	Comment	Reference
N	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
N	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
N	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
N	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
N	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
O	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
O	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
O	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
O	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
O	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
O	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
O	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
P	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
P	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
P	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
P	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
P	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
P	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
P	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
Q	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
Q	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
Q	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
Q	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
Q	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
Q	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
Q	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
R	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
R	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
R	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
R	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
R	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
R	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
R	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
S	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
S	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
S	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
S	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
S	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
S	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
S	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
T	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
T	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

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Chain	Residue	Modelled	Actual	Comment	Reference
T	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
T	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
T	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
T	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
T	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
U	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
U	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
U	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
U	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
U	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
U	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
U	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
V	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
V	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
V	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
V	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
V	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
V	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
V	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
W	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
W	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
W	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
W	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
W	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
W	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
W	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
X	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
X	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
X	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
X	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
X	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
X	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
X	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	43	33	4	6	0	0
3	A	1	43	33	4	6	0	0
3	B	1	43	33	4	6	0	0
3	B	1	43	33	4	6	0	0
3	C	1	43	33	4	6	0	0
3	C	1	43	33	4	6	0	0
3	D	1	43	33	4	6	0	0
3	D	1	43	33	4	6	0	0
3	E	1	43	33	4	6	0	0
3	E	1	43	33	4	6	0	0
3	F	1	43	33	4	6	0	0
3	F	1	43	33	4	6	0	0
3	G	1	43	33	4	6	0	0
3	G	1	43	33	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0

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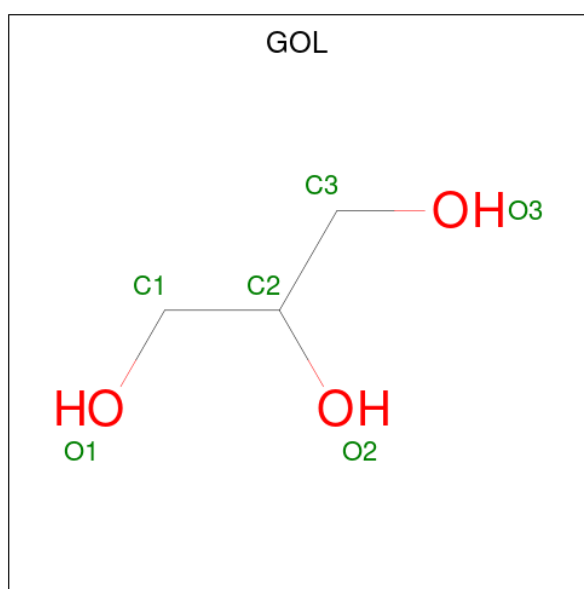
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	P	1	43	33	4	6	0	0
3	Q	1	43	33	4	6	0	0
3	Q	1	43	33	4	6	0	0
3	Q	1	43	33	4	6	0	0
3	R	1	43	33	4	6	0	0
3	R	1	43	33	4	6	0	0
3	R	1	43	33	4	6	0	0
3	S	1	43	33	4	6	0	0
3	S	1	43	33	4	6	0	0
3	S	1	43	33	4	6	0	0
3	T	1	43	33	4	6	0	0
3	T	1	43	33	4	6	0	0
3	T	1	43	33	4	6	0	0
3	U	1	43	33	4	6	0	0
3	U	1	43	33	4	6	0	0
3	U	1	43	33	4	6	0	0
3	V	1	43	33	4	6	0	0
3	V	1	43	33	4	6	0	0
3	V	1	43	33	4	6	0	0
3	W	1	43	33	4	6	0	0
3	W	1	43	33	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total	O	0	0
			241	241		
5	B	219	Total	O	0	0
			219	219		
5	C	227	Total	O	0	0
			227	227		
5	D	193	Total	O	0	0
			193	193		
5	E	185	Total	O	0	0
			185	185		
5	F	188	Total	O	0	0
			188	188		
5	G	217	Total	O	0	0
			217	217		
5	H	186	Total	O	0	0
			186	186		
5	I	183	Total	O	0	0
			183	183		
5	J	243	Total	O	0	0
			243	243		
5	K	217	Total	O	0	0
			217	217		
5	L	223	Total	O	0	0
			223	223		
5	M	247	Total	O	0	0
			247	247		
5	N	227	Total	O	0	0
			227	227		
5	O	246	Total	O	0	0
			246	246		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	200	Total 200	O 200	0	0
5	Q	201	Total 201	O 201	0	0
5	R	170	Total 170	O 170	0	0
5	S	194	Total 194	O 194	0	0
5	T	200	Total 200	O 200	0	0
5	U	193	Total 193	O 193	0	0
5	V	259	Total 259	O 259	0	0
5	W	220	Total 220	O 220	0	0
5	X	243	Total 243	O 243	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain A:  93% 7%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain B:  94% 6%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain C:  94% 6%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain D:  93% 7%



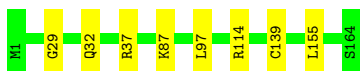
- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain E:  94% 6% 2%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain F:  95% 5%



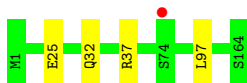
- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT



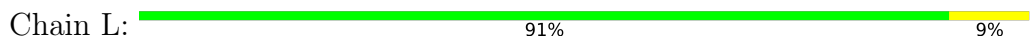
- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

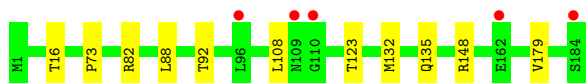
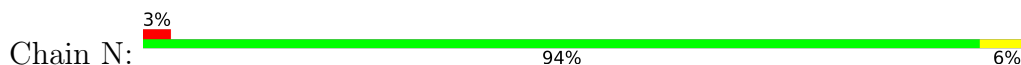


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

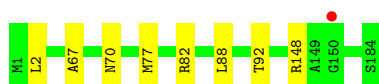




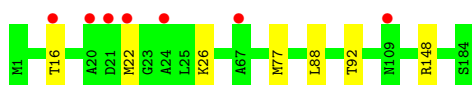
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



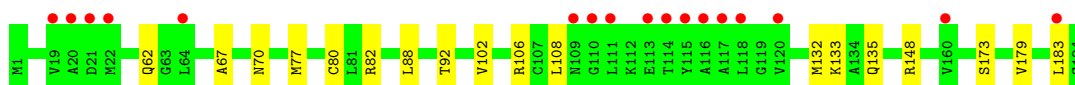
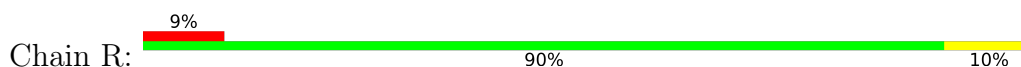
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



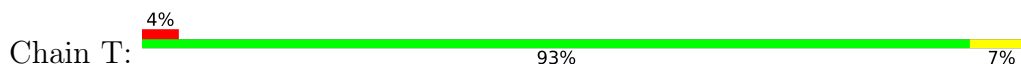
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

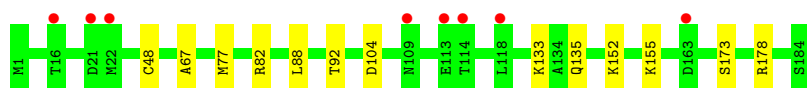


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT





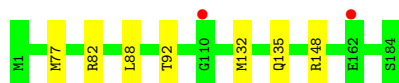
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



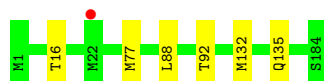
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.17Å 109.15Å 117.68Å 78.71° 82.30° 61.55°	Depositor
Resolution (Å)	38.89 – 1.93 38.89 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.89-1.93) 96.2 (38.89-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.94Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.239 0.182 , 0.236	Depositor DCC
R_{free} test set	17307 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38800	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, PEB, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/1259	0.54	0/1706
1	B	0.39	0/1259	0.54	0/1706
1	C	0.37	0/1259	0.50	0/1706
1	D	0.37	0/1259	0.51	0/1706
1	E	0.36	0/1259	0.50	0/1706
1	F	0.35	0/1259	0.49	0/1706
1	G	0.37	0/1259	0.50	0/1706
1	H	0.36	0/1259	0.50	0/1706
1	I	0.35	0/1259	0.50	0/1706
1	J	0.39	0/1259	0.52	0/1706
1	K	0.40	0/1259	0.51	0/1706
1	L	0.43	0/1259	0.56	0/1706
2	M	0.39	0/1349	0.51	0/1820
2	N	0.35	0/1349	0.48	0/1820
2	O	0.38	0/1349	0.49	0/1820
2	P	0.36	0/1349	0.48	0/1820
2	Q	0.35	0/1349	0.48	0/1820
2	R	0.32	0/1349	0.45	0/1820
2	S	0.34	0/1349	0.47	0/1820
2	T	0.33	0/1349	0.46	0/1820
2	U	0.37	0/1349	0.49	0/1820
2	V	0.40	0/1349	0.52	0/1820
2	W	0.35	0/1349	0.47	0/1820
2	X	0.38	0/1349	0.50	0/1820
All	All	0.37	0/31296	0.50	0/42312

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1239	0	1221	10	0
1	B	1239	0	1221	9	0
1	C	1239	0	1221	8	0
1	D	1239	0	1221	11	0
1	E	1239	0	1221	11	0
1	F	1239	0	1221	9	0
1	G	1239	0	1221	8	0
1	H	1239	0	1221	6	0
1	I	1239	0	1221	3	0
1	J	1239	0	1221	8	0
1	K	1239	0	1221	8	0
1	L	1239	0	1221	10	0
2	M	1347	0	1359	6	0
2	N	1347	0	1359	9	0
2	O	1347	0	1359	7	0
2	P	1347	0	1359	5	0
2	Q	1347	0	1359	9	0
2	R	1347	0	1359	14	0
2	S	1347	0	1359	10	0
2	T	1347	0	1359	9	0
2	U	1347	0	1359	8	0
2	V	1347	0	1359	9	0
2	W	1347	0	1359	6	0
2	X	1347	0	1359	5	0
3	A	86	0	74	3	0
3	B	86	0	74	3	0
3	C	86	0	74	1	0
3	D	86	0	73	1	0
3	E	86	0	74	3	0
3	F	86	0	73	4	0
3	G	86	0	74	3	0
3	H	86	0	73	3	0
3	I	86	0	73	3	0
3	J	86	0	74	5	0
3	K	86	0	74	3	0
3	L	86	0	74	2	0
3	M	129	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	110	7	0
3	O	129	0	110	6	0
3	P	129	0	110	5	0
3	Q	129	0	110	7	0
3	R	129	0	110	9	0
3	S	129	0	110	10	0
3	T	129	0	110	5	0
3	U	129	0	110	8	0
3	V	129	0	110	9	0
3	W	129	0	110	7	0
3	X	129	0	110	6	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	0	0
4	L	6	0	8	0	0
5	A	241	0	0	1	0
5	B	219	0	0	1	0
5	C	227	0	0	1	0
5	D	193	0	0	1	0
5	E	185	0	0	1	0
5	F	188	0	0	3	0
5	G	217	0	0	2	0
5	H	186	0	0	1	0
5	I	183	0	0	0	0
5	J	243	0	0	2	0
5	K	217	0	0	1	0
5	L	223	0	0	3	0
5	M	247	0	0	1	0
5	N	227	0	0	1	0
5	O	246	0	0	0	0
5	P	200	0	0	0	0
5	Q	201	0	0	0	0
5	R	170	0	0	1	0
5	S	194	0	0	1	0
5	T	200	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	193	0	0	1	0
5	V	259	0	0	1	0
5	W	220	0	0	0	0
5	X	243	0	0	0	0
All	All	38800	0	33252	234	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 4.

The worst 5 of 234 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:I:32:GLN:HG3	1:L:32:GLN:HG3	1.39	1.04
1:A:32:GLN:HG3	1:D:32:GLN:HG3	1.40	1.03
1:B:32:GLN:HG3	1:E:32:GLN:HG3	1.49	0.94
1:H:32:GLN:HG3	1:K:32:GLN:HG3	1.48	0.94
1:C:32:GLN:HG3	1:F:32:GLN:HG3	1.53	0.90

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	B	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	25	13
1	C	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	D	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	E	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	F	162/164 (99%)	158 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	H	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	I	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	K	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	L	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	M	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	N	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	25	13
2	O	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	P	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	Q	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	R	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	S	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	T	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	U	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	V	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	W	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	X	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
All	All	4116/4176 (99%)	4026 (98%)	88 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	GLY
2	N	73	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/127 (100%)	127 (100%)	0	100	100
1	B	127/127 (100%)	127 (100%)	0	100	100
1	C	127/127 (100%)	127 (100%)	0	100	100
1	D	127/127 (100%)	127 (100%)	0	100	100
1	E	127/127 (100%)	127 (100%)	0	100	100
1	F	127/127 (100%)	127 (100%)	0	100	100
1	G	127/127 (100%)	127 (100%)	0	100	100
1	H	127/127 (100%)	127 (100%)	0	100	100
1	I	127/127 (100%)	127 (100%)	0	100	100
1	J	127/127 (100%)	126 (99%)	1 (1%)	81	78
1	K	127/127 (100%)	127 (100%)	0	100	100
1	L	127/127 (100%)	126 (99%)	1 (1%)	81	78
2	M	138/138 (100%)	137 (99%)	1 (1%)	84	81
2	N	138/138 (100%)	138 (100%)	0	100	100
2	O	138/138 (100%)	138 (100%)	0	100	100
2	P	138/138 (100%)	138 (100%)	0	100	100
2	Q	138/138 (100%)	138 (100%)	0	100	100
2	R	138/138 (100%)	138 (100%)	0	100	100
2	S	138/138 (100%)	138 (100%)	0	100	100
2	T	138/138 (100%)	138 (100%)	0	100	100
2	U	138/138 (100%)	138 (100%)	0	100	100
2	V	138/138 (100%)	138 (100%)	0	100	100
2	W	138/138 (100%)	138 (100%)	0	100	100
2	X	138/138 (100%)	138 (100%)	0	100	100
All	All	3180/3180 (100%)	3177 (100%)	3 (0%)	93	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	42	GLU
1	L	61	GLN
2	M	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	62	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](#)

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	M	70	2	7,8,9	0.53	0	6,9,11	0.40	0
2	MEN	S	70	2	7,8,9	0.54	0	6,9,11	0.71	0
2	MEN	W	70	2	7,8,9	0.51	0	6,9,11	0.69	0
2	MEN	V	70	2	7,8,9	0.62	0	6,9,11	0.82	0
2	MEN	O	70	2	7,8,9	0.54	0	6,9,11	0.91	0
2	MEN	X	70	2	7,8,9	0.51	0	6,9,11	0.66	0
2	MEN	R	70	2	7,8,9	0.51	0	6,9,11	0.52	0
2	MEN	P	70	2	7,8,9	0.51	0	6,9,11	0.79	0
2	MEN	Q	70	2	7,8,9	0.60	0	6,9,11	0.86	0
2	MEN	T	70	2	7,8,9	0.59	0	6,9,11	0.56	0
2	MEN	U	70	2	7,8,9	0.55	0	6,9,11	0.69	0
2	MEN	N	70	2	7,8,9	0.66	0	6,9,11	0.75	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
2	MEN	M	70	2	-	4/7/8/10	-
2	MEN	S	70	2	-	4/7/8/10	-
2	MEN	W	70	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	V	70	2	-	4/7/8/10	-
2	MEN	O	70	2	-	4/7/8/10	-
2	MEN	X	70	2	-	4/7/8/10	-
2	MEN	R	70	2	-	4/7/8/10	-
2	MEN	P	70	2	-	4/7/8/10	-
2	MEN	Q	70	2	-	4/7/8/10	-
2	MEN	T	70	2	-	5/7/8/10	-
2	MEN	U	70	2	-	4/7/8/10	-
2	MEN	N	70	2	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	70	MEN	C-CA-CB-CG
2	Q	70	MEN	C-CA-CB-CG
2	R	70	MEN	C-CA-CB-CG
2	S	70	MEN	C-CA-CB-CG
2	U	70	MEN	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	70	MEN	1	0
2	O	70	MEN	1	0
2	R	70	MEN	1	0
2	Q	70	MEN	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

71 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	S	203	2	43,46,46	3.37	9 (20%)	45,67,67	1.98	15 (33%)
3	PEB	B	201	1	43,46,46	3.30	8 (18%)	45,67,67	2.34	17 (37%)
3	PEB	L	202	1	43,46,46	3.26	8 (18%)	45,67,67	2.00	14 (31%)
3	PEB	S	202	2	43,46,46	3.38	9 (20%)	45,67,67	2.04	15 (33%)
4	GOL	J	203	-	5,5,5	0.32	0	5,5,5	0.23	0
3	PEB	T	201	2	43,46,46	3.37	9 (20%)	45,67,67	2.08	16 (35%)
3	PEB	R	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.08	14 (31%)
3	PEB	M	203	2	43,46,46	3.38	9 (20%)	45,67,67	2.00	15 (33%)
3	PEB	V	203	2	43,46,46	3.42	11 (25%)	45,67,67	1.96	15 (33%)
3	PEB	B	202	1	43,46,46	3.26	9 (20%)	45,67,67	2.04	15 (33%)
3	PEB	F	202	1	43,46,46	3.42	9 (20%)	45,67,67	1.79	13 (28%)
3	PEB	M	201	2	43,46,46	3.29	9 (20%)	45,67,67	2.28	16 (35%)
3	PEB	W	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.27	19 (42%)
3	PEB	Q	203	2	43,46,46	3.55	10 (23%)	45,67,67	1.91	12 (26%)
3	PEB	X	203	2	43,46,46	3.48	9 (20%)	45,67,67	1.81	14 (31%)
3	PEB	J	202	1	43,46,46	3.28	11 (25%)	45,67,67	1.99	12 (26%)
4	GOL	C	203	-	5,5,5	0.32	0	5,5,5	0.45	0
3	PEB	A	202	1	43,46,46	3.22	10 (23%)	45,67,67	2.06	13 (28%)
3	PEB	U	201	2	43,46,46	3.28	11 (25%)	45,67,67	2.24	14 (31%)
3	PEB	T	202	2	43,46,46	3.31	8 (18%)	45,67,67	2.10	14 (31%)
4	GOL	A	203	-	5,5,5	0.30	0	5,5,5	0.28	0
3	PEB	X	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.35	18 (40%)
3	PEB	H	202	1	43,46,46	3.35	11 (25%)	45,67,67	1.94	12 (26%)
4	GOL	H	203	-	5,5,5	0.38	0	5,5,5	0.21	0
3	PEB	I	201	1	43,46,46	3.41	10 (23%)	45,67,67	2.26	16 (35%)
3	PEB	D	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.98	14 (31%)
3	PEB	G	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.89	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	T	203	2	43,46,46	3.58	12 (27%)	45,67,67	1.94	13 (28%)
3	PEB	U	203	2	43,46,46	3.51	12 (27%)	45,67,67	2.18	18 (40%)
3	PEB	P	201	2	43,46,46	3.25	9 (20%)	45,67,67	2.28	14 (31%)
3	PEB	A	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.47	18 (40%)
3	PEB	C	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.27	16 (35%)
3	PEB	O	202	2	43,46,46	3.42	10 (23%)	45,67,67	1.94	14 (31%)
3	PEB	O	203	2	43,46,46	3.35	8 (18%)	45,67,67	2.09	17 (37%)
3	PEB	W	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.07	17 (37%)
4	GOL	I	203	-	5,5,5	0.34	0	5,5,5	0.54	0
3	PEB	Q	202	2	43,46,46	3.43	9 (20%)	45,67,67	1.98	14 (31%)
3	PEB	N	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.24	18 (40%)
4	GOL	D	203	-	5,5,5	0.30	0	5,5,5	0.42	0
3	PEB	K	202	1	43,46,46	3.29	8 (18%)	45,67,67	1.96	15 (33%)
3	PEB	P	202	2	43,46,46	3.43	9 (20%)	45,67,67	1.91	14 (31%)
3	PEB	S	201	2	43,46,46	3.50	9 (20%)	45,67,67	2.16	18 (40%)
4	GOL	K	203	-	5,5,5	0.26	0	5,5,5	0.34	0
3	PEB	N	202	2	43,46,46	3.48	9 (20%)	45,67,67	1.99	14 (31%)
3	PEB	C	202	1	43,46,46	3.33	10 (23%)	45,67,67	1.91	12 (26%)
3	PEB	R	201	2	43,46,46	3.50	10 (23%)	45,67,67	2.30	16 (35%)
3	PEB	I	202	1	43,46,46	3.36	11 (25%)	45,67,67	1.97	15 (33%)
3	PEB	G	201	1	43,46,46	3.19	9 (20%)	45,67,67	2.41	18 (40%)
4	GOL	E	203	-	5,5,5	0.37	0	5,5,5	0.27	0
3	PEB	D	201	1	43,46,46	3.41	10 (23%)	45,67,67	2.36	17 (37%)
3	PEB	R	203	2	43,46,46	3.45	12 (27%)	45,67,67	2.01	13 (28%)
4	GOL	L	203	-	5,5,5	0.30	0	5,5,5	0.38	0
4	GOL	B	203	-	5,5,5	0.30	0	5,5,5	0.49	0
3	PEB	M	202	2	43,46,46	3.36	10 (23%)	45,67,67	1.94	13 (28%)
3	PEB	U	202	2	43,46,46	3.29	9 (20%)	45,67,67	2.04	15 (33%)
3	PEB	P	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.05	15 (33%)
3	PEB	O	201	2	43,46,46	3.37	9 (20%)	45,67,67	2.28	15 (33%)
3	PEB	V	201	2	43,46,46	3.32	9 (20%)	45,67,67	2.29	16 (35%)
3	PEB	W	202	2	43,46,46	3.29	9 (20%)	45,67,67	1.92	15 (33%)
3	PEB	Q	201	2	43,46,46	3.47	10 (23%)	45,67,67	2.18	16 (35%)
3	PEB	V	202	2	43,46,46	3.40	10 (23%)	45,67,67	1.93	13 (28%)
4	GOL	G	203	-	5,5,5	0.33	0	5,5,5	0.36	0
3	PEB	K	201	1	43,46,46	3.32	11 (25%)	45,67,67	2.37	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	E	202	1	43,46,46	3.32	9 (20%)	45,67,67	1.95	13 (28%)
3	PEB	L	201	1	43,46,46	3.28	9 (20%)	45,67,67	2.48	20 (44%)
3	PEB	X	202	2	43,46,46	3.31	9 (20%)	45,67,67	1.97	16 (35%)
3	PEB	F	201	1	43,46,46	3.26	8 (18%)	45,67,67	2.26	15 (33%)
3	PEB	H	201	1	43,46,46	3.37	9 (20%)	45,67,67	2.42	20 (44%)
3	PEB	N	203	2	43,46,46	3.45	12 (27%)	45,67,67	2.00	17 (37%)
3	PEB	E	201	1	43,46,46	3.46	11 (25%)	45,67,67	2.42	20 (44%)
3	PEB	J	201	1	43,46,46	3.41	9 (20%)	45,67,67	2.43	19 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	S	203	2	-	3/24/74/74	0/4/4/4
3	PEB	B	201	1	-	4/24/74/74	0/4/4/4
3	PEB	L	202	1	-	6/24/74/74	0/4/4/4
3	PEB	S	202	2	-	8/24/74/74	0/4/4/4
4	GOL	J	203	-	-	0/4/4/4	-
3	PEB	T	201	2	-	6/24/74/74	0/4/4/4
3	PEB	R	202	2	-	8/24/74/74	0/4/4/4
3	PEB	M	203	2	-	8/24/74/74	0/4/4/4
3	PEB	V	203	2	-	8/24/74/74	0/4/4/4
3	PEB	B	202	1	-	7/24/74/74	0/4/4/4
3	PEB	F	202	1	-	7/24/74/74	0/4/4/4
3	PEB	M	201	2	-	6/24/74/74	0/4/4/4
3	PEB	W	201	2	-	6/24/74/74	0/4/4/4
3	PEB	Q	203	2	-	6/24/74/74	0/4/4/4
3	PEB	X	203	2	-	4/24/74/74	0/4/4/4
3	PEB	J	202	1	-	6/24/74/74	0/4/4/4
4	GOL	C	203	-	-	0/4/4/4	-
3	PEB	A	202	1	-	7/24/74/74	0/4/4/4
3	PEB	U	201	2	-	4/24/74/74	0/4/4/4
3	PEB	T	202	2	-	8/24/74/74	0/4/4/4
4	GOL	A	203	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	X	201	2	-	6/24/74/74	0/4/4/4
3	PEB	H	202	1	-	7/24/74/74	0/4/4/4
4	GOL	H	203	-	-	2/4/4/4	-
3	PEB	I	201	1	-	4/24/74/74	0/4/4/4
3	PEB	D	202	1	-	8/24/74/74	0/4/4/4
3	PEB	G	202	1	-	6/24/74/74	0/4/4/4
3	PEB	T	203	2	-	4/24/74/74	0/4/4/4
3	PEB	U	203	2	-	8/24/74/74	0/4/4/4
3	PEB	P	201	2	-	4/24/74/74	0/4/4/4
3	PEB	A	201	1	-	4/24/74/74	0/4/4/4
3	PEB	C	201	1	-	4/24/74/74	0/4/4/4
3	PEB	O	202	2	-	8/24/74/74	0/4/4/4
3	PEB	O	203	2	-	8/24/74/74	0/4/4/4
3	PEB	W	203	2	-	8/24/74/74	0/4/4/4
4	GOL	I	203	-	-	2/4/4/4	-
3	PEB	Q	202	2	-	7/24/74/74	0/4/4/4
3	PEB	N	201	2	-	6/24/74/74	0/4/4/4
4	GOL	D	203	-	-	4/4/4/4	-
3	PEB	K	202	1	-	7/24/74/74	0/4/4/4
3	PEB	P	202	2	-	8/24/74/74	0/4/4/4
3	PEB	S	201	2	-	7/24/74/74	0/4/4/4
4	GOL	K	203	-	-	0/4/4/4	-
3	PEB	N	202	2	-	8/24/74/74	0/4/4/4
3	PEB	C	202	1	-	6/24/74/74	0/4/4/4
3	PEB	R	201	2	-	6/24/74/74	0/4/4/4
3	PEB	I	202	1	-	9/24/74/74	0/4/4/4
3	PEB	G	201	1	-	4/24/74/74	0/4/4/4
4	GOL	E	203	-	-	0/4/4/4	-
3	PEB	D	201	1	-	4/24/74/74	0/4/4/4
3	PEB	R	203	2	-	7/24/74/74	0/4/4/4
4	GOL	L	203	-	-	2/4/4/4	-
4	GOL	B	203	-	-	0/4/4/4	-
3	PEB	M	202	2	-	8/24/74/74	0/4/4/4
3	PEB	U	202	2	-	8/24/74/74	0/4/4/4
3	PEB	P	203	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	O	201	2	-	6/24/74/74	0/4/4/4
3	PEB	V	201	2	-	6/24/74/74	0/4/4/4
3	PEB	W	202	2	-	7/24/74/74	0/4/4/4
3	PEB	Q	201	2	-	6/24/74/74	0/4/4/4
3	PEB	V	202	2	-	7/24/74/74	0/4/4/4
4	GOL	G	203	-	-	0/4/4/4	-
3	PEB	K	201	1	-	4/24/74/74	0/4/4/4
3	PEB	E	202	1	-	6/24/74/74	0/4/4/4
3	PEB	L	201	1	-	4/24/74/74	0/4/4/4
3	PEB	X	202	2	-	8/24/74/74	0/4/4/4
3	PEB	F	201	1	-	4/24/74/74	0/4/4/4
3	PEB	H	201	1	-	4/24/74/74	0/4/4/4
3	PEB	N	203	2	-	4/24/74/74	0/4/4/4
3	PEB	E	201	1	-	4/24/74/74	0/4/4/4
3	PEB	J	201	1	-	4/24/74/74	0/4/4/4

The worst 5 of 583 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	203	PEB	CHB-C4B	17.74	1.49	1.35
3	Q	203	PEB	CHB-C4B	17.68	1.49	1.35
3	X	203	PEB	CHB-C4B	17.38	1.49	1.35
3	S	201	PEB	CHB-C4B	17.21	1.49	1.35
3	R	201	PEB	CHB-C4B	17.21	1.49	1.35

The worst 5 of 923 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	201	PEB	OA-C1A-C2A	-6.97	120.63	126.17
3	M	201	PEB	OA-C1A-C2A	-6.52	120.99	126.17
3	A	201	PEB	OA-C1A-C2A	-6.29	121.17	126.17
3	L	201	PEB	OA-C1A-C2A	-6.28	121.18	126.17
3	R	201	PEB	OA-C1A-C2A	-6.25	121.21	126.17

There are no chirality outliers.

5 of 378 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	PEB	NB-C1B-CHA-C4A
3	A	202	PEB	C2B-C1B-CHA-C4A
3	B	201	PEB	C2B-C1B-CHA-C4A
3	B	202	PEB	NB-C1B-CHA-C4A
3	B	202	PEB	C2B-C1B-CHA-C4A

There are no ring outliers.

57 monomers are involved in 121 short contacts:

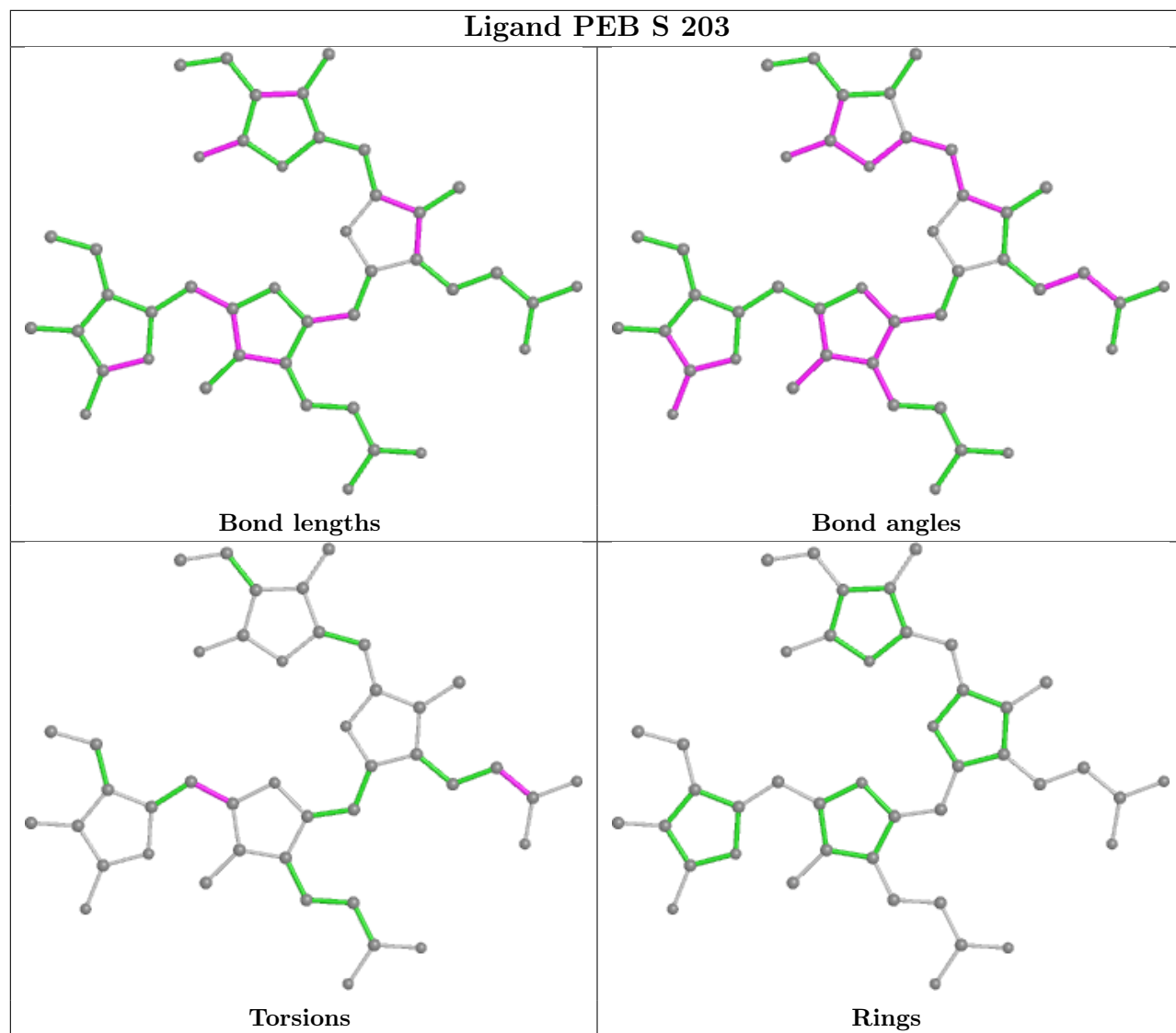
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	203	PEB	5	0
3	B	201	PEB	1	0
3	L	202	PEB	1	0
3	S	202	PEB	4	0
3	T	201	PEB	2	0
3	R	202	PEB	2	0
3	M	203	PEB	3	0
3	V	203	PEB	2	0
3	B	202	PEB	2	0
3	F	202	PEB	3	0
3	M	201	PEB	1	0
3	W	201	PEB	2	0
3	Q	203	PEB	3	0
3	X	203	PEB	2	0
3	J	202	PEB	2	0
4	C	203	GOL	1	0
3	A	202	PEB	1	0
3	U	201	PEB	2	0
3	T	202	PEB	2	0
3	X	201	PEB	1	0
3	I	201	PEB	3	0
3	G	202	PEB	2	0
3	T	203	PEB	1	0
3	U	203	PEB	3	0
3	P	201	PEB	1	0
3	A	201	PEB	2	0
3	O	202	PEB	1	0
3	O	203	PEB	2	0
3	W	203	PEB	3	0
3	Q	202	PEB	2	0
3	N	201	PEB	2	0
3	K	202	PEB	2	0
3	P	202	PEB	1	0

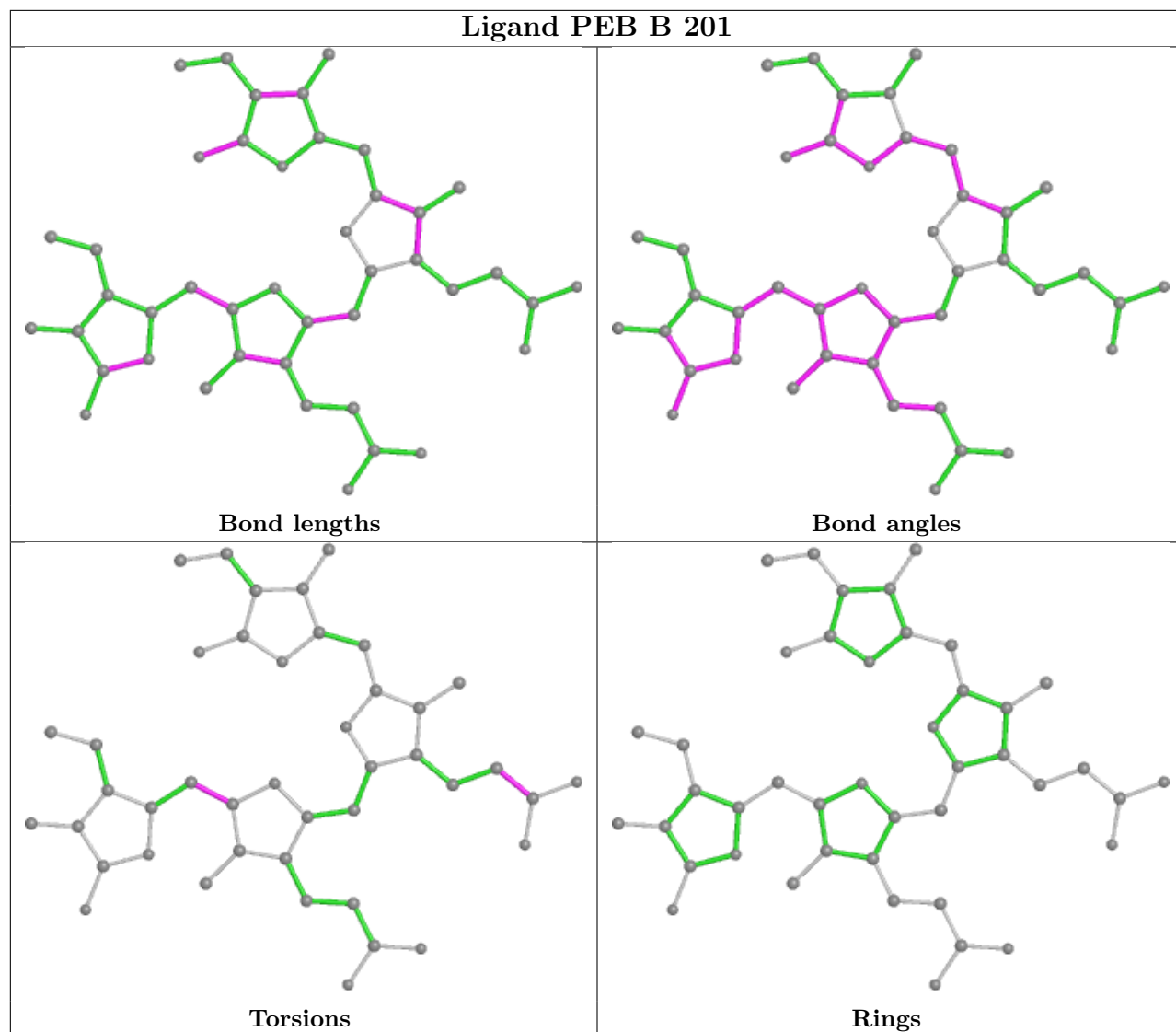
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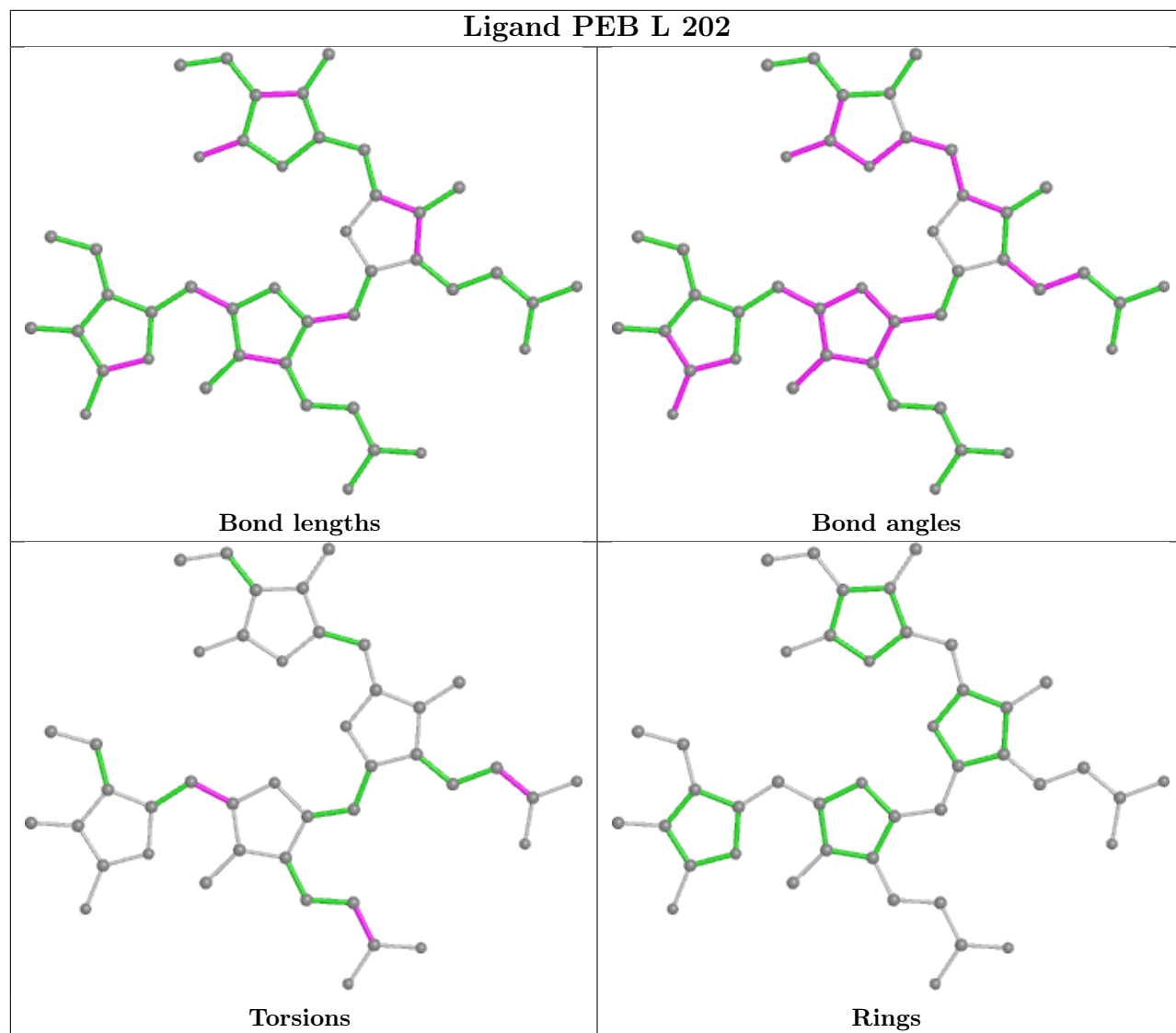
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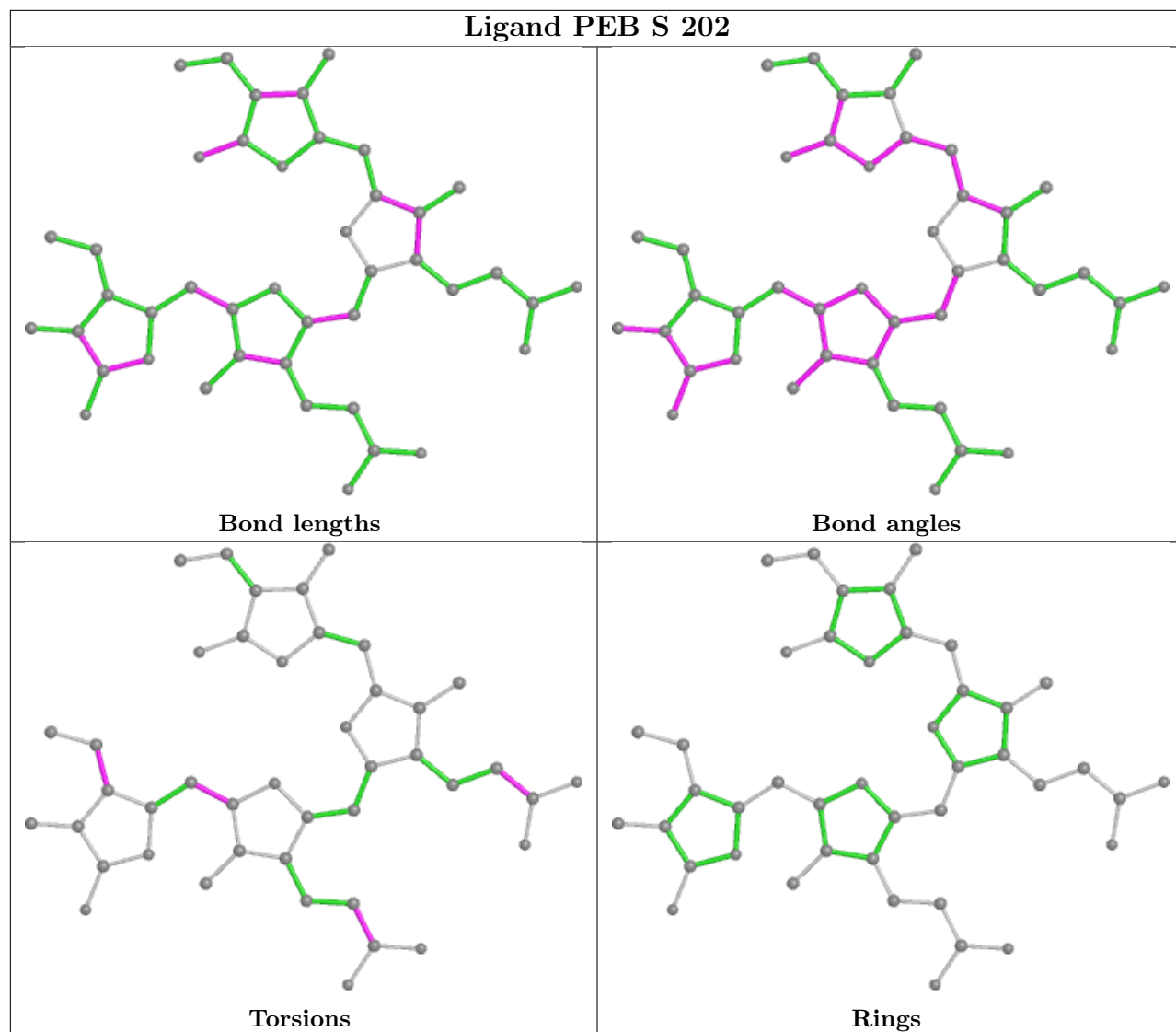
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	201	PEB	1	0
3	N	202	PEB	1	0
3	C	202	PEB	1	0
3	R	201	PEB	4	0
3	G	201	PEB	1	0
4	E	203	GOL	1	0
3	D	201	PEB	1	0
3	R	203	PEB	3	0
3	M	202	PEB	2	0
3	U	202	PEB	3	0
3	P	203	PEB	3	0
3	O	201	PEB	3	0
3	V	201	PEB	4	0
3	W	202	PEB	2	0
3	Q	201	PEB	2	0
3	V	202	PEB	3	0
3	K	201	PEB	1	0
3	L	201	PEB	1	0
3	X	202	PEB	3	0
3	F	201	PEB	1	0
3	H	201	PEB	3	0
3	N	203	PEB	4	0
3	E	201	PEB	3	0
3	J	201	PEB	3	0

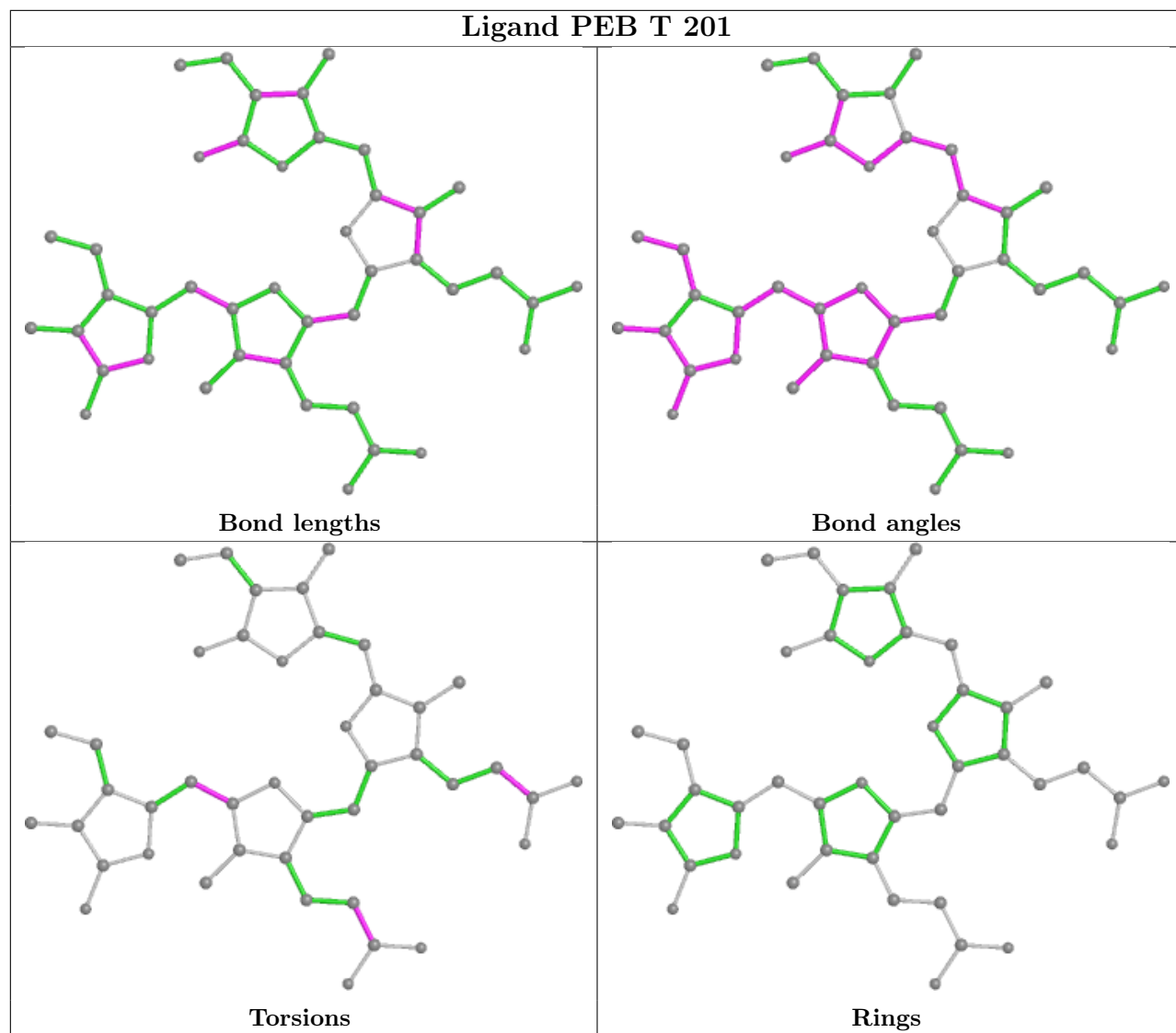
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

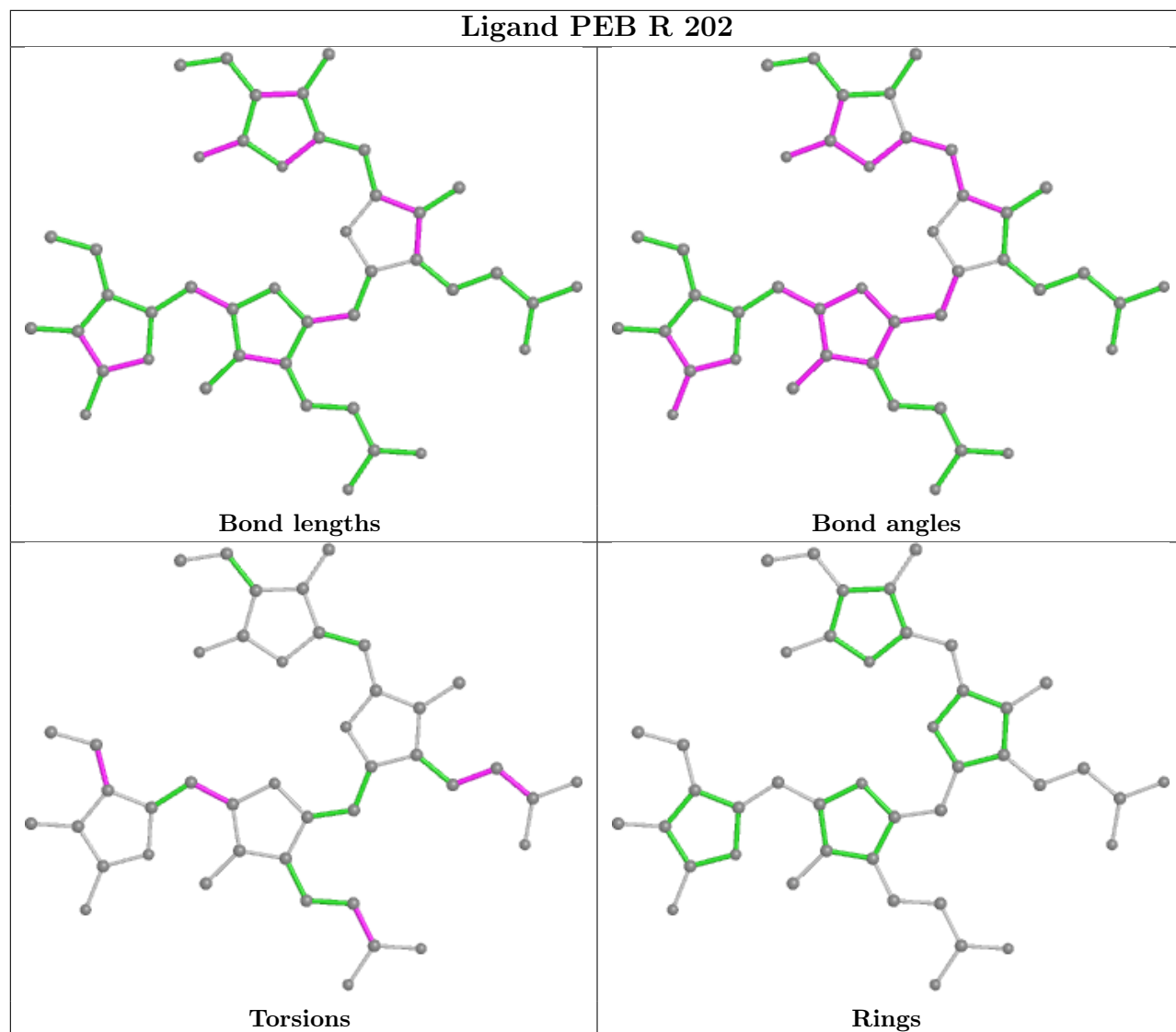


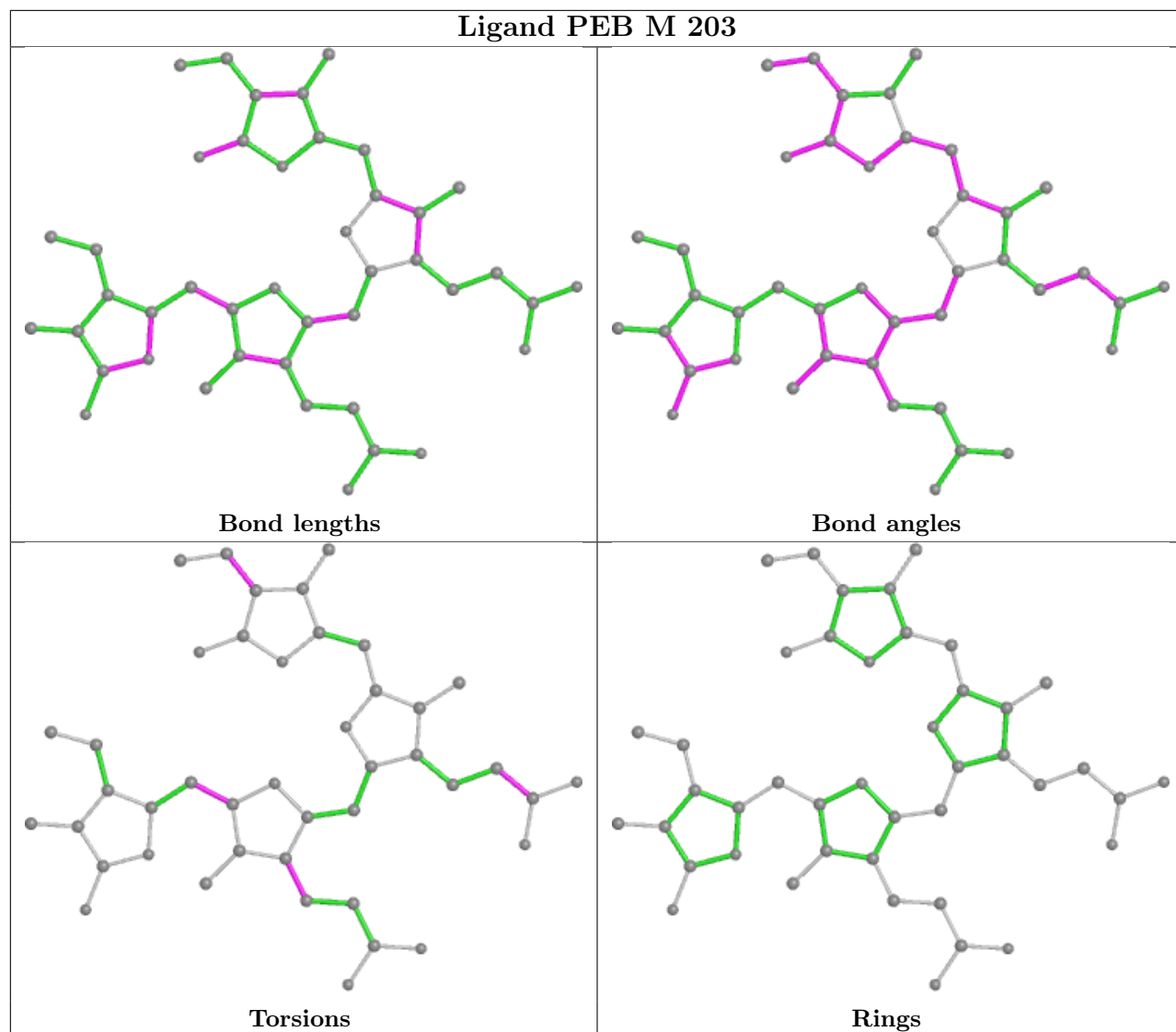


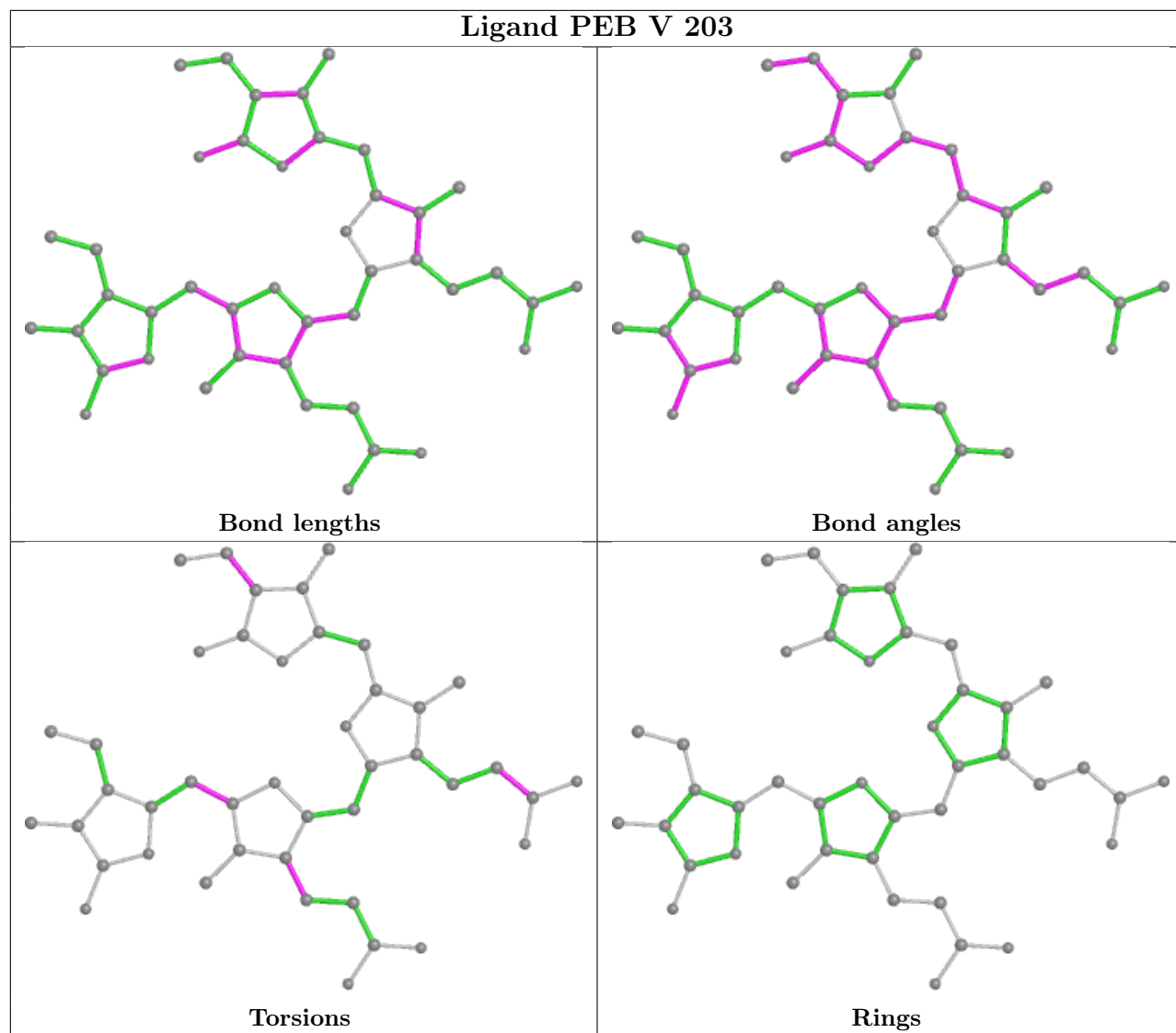


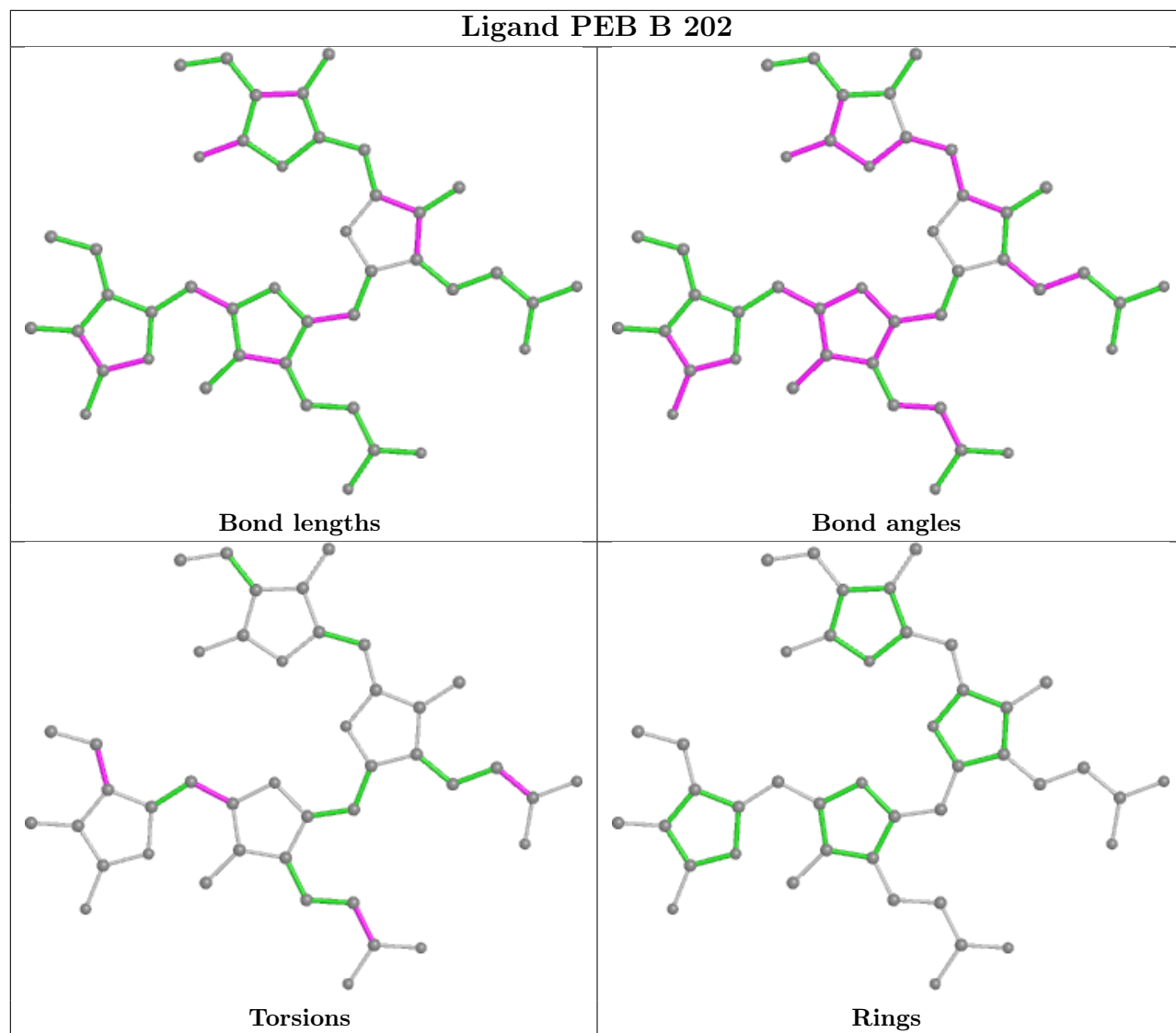


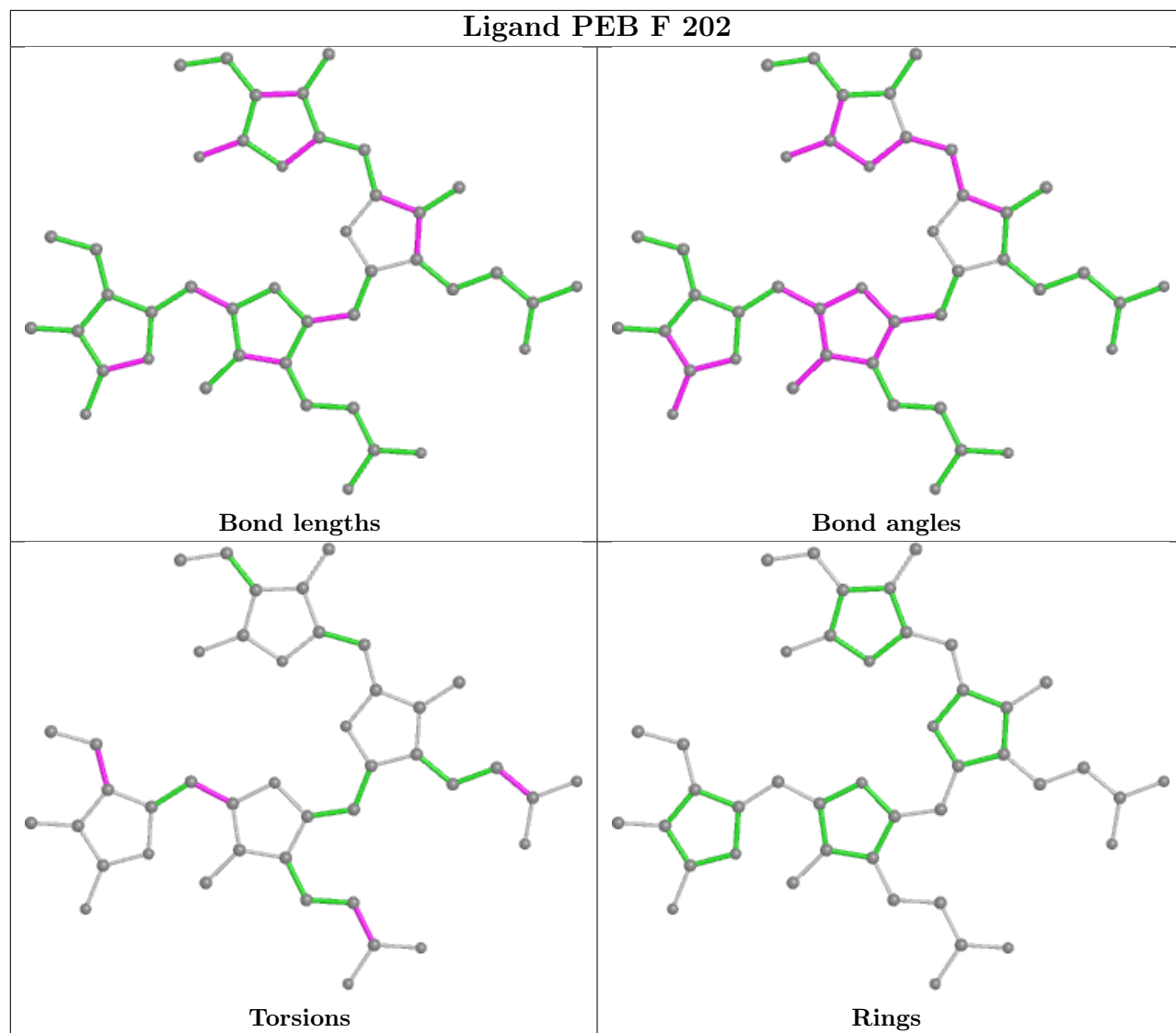


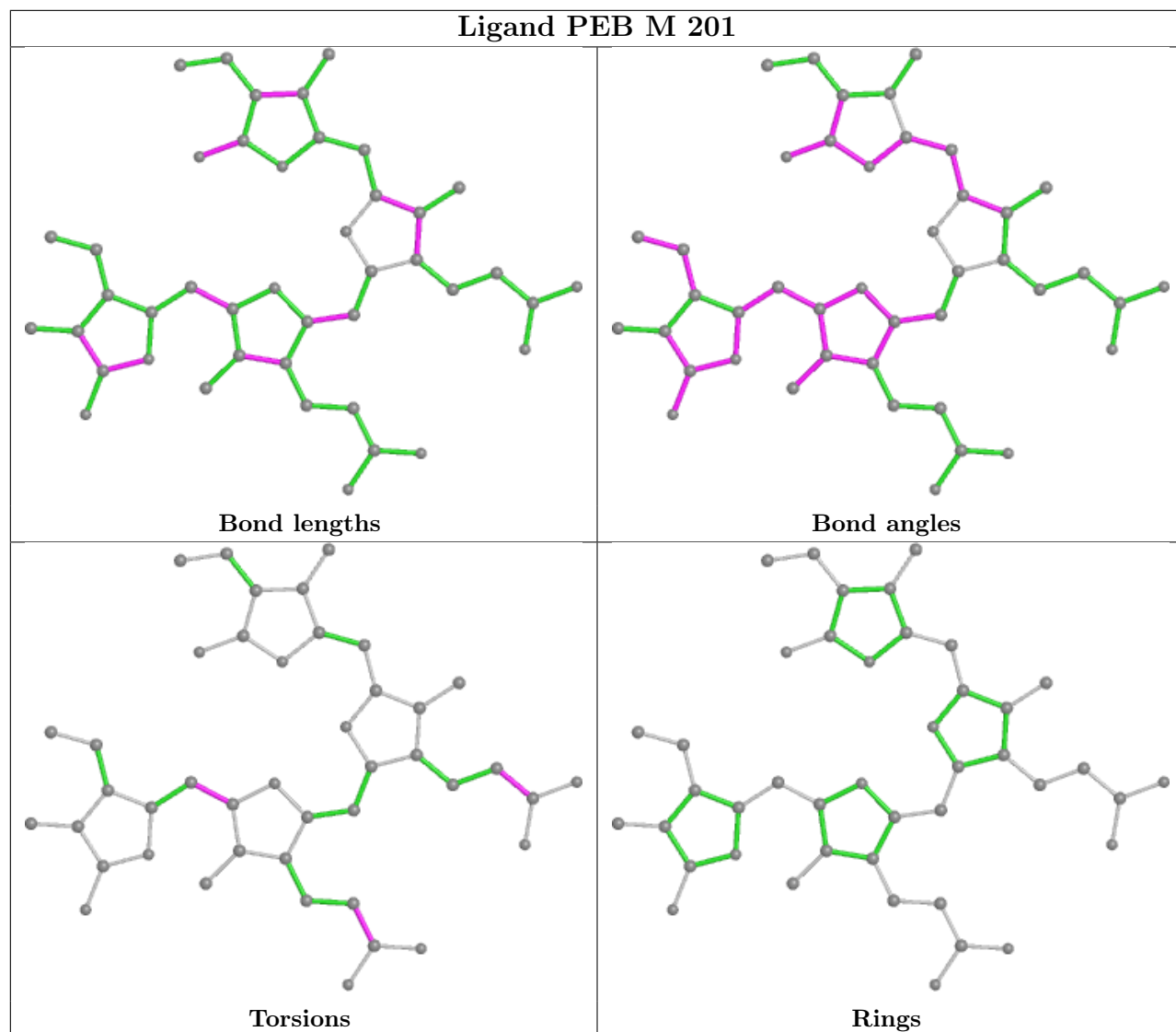


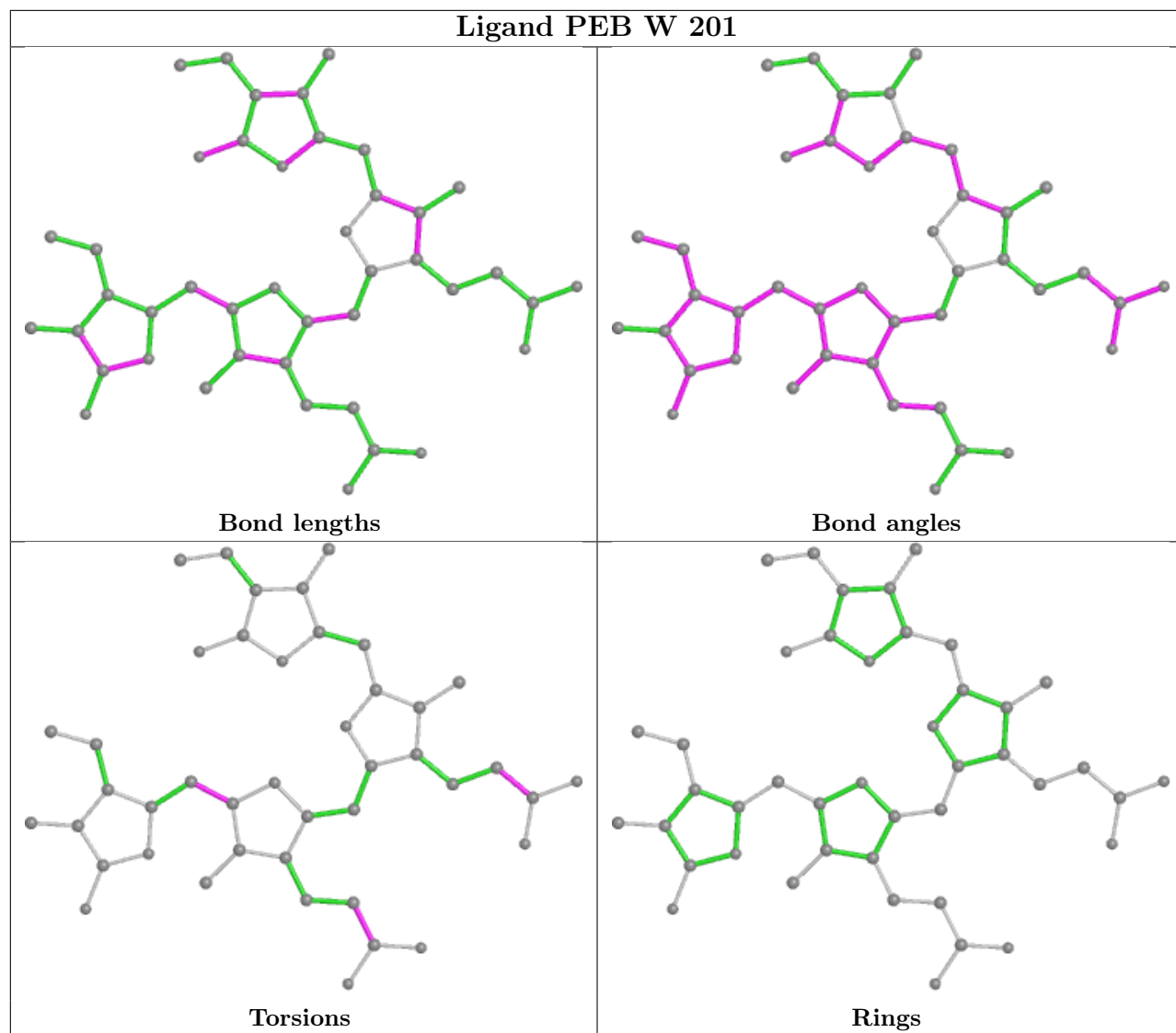


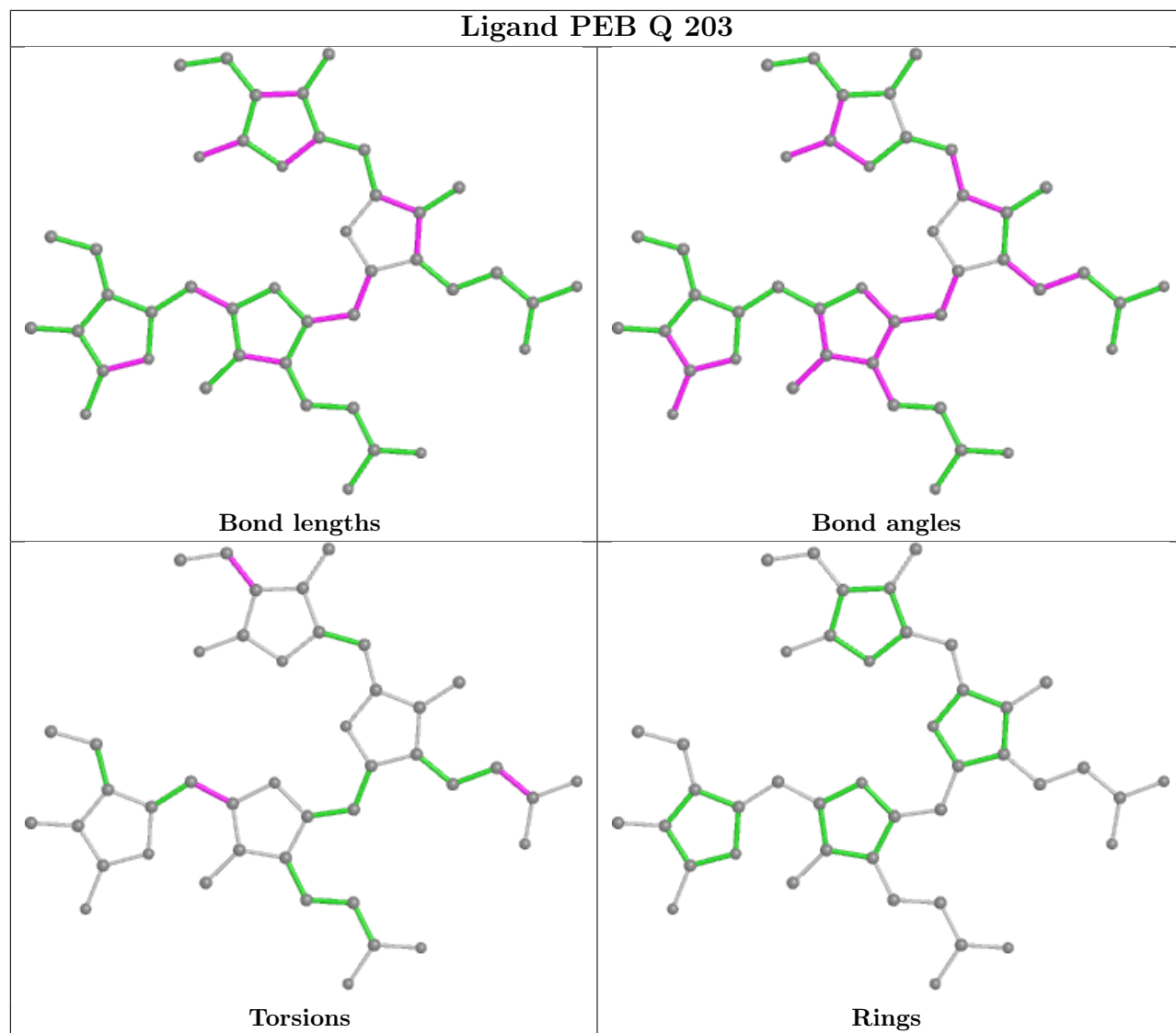


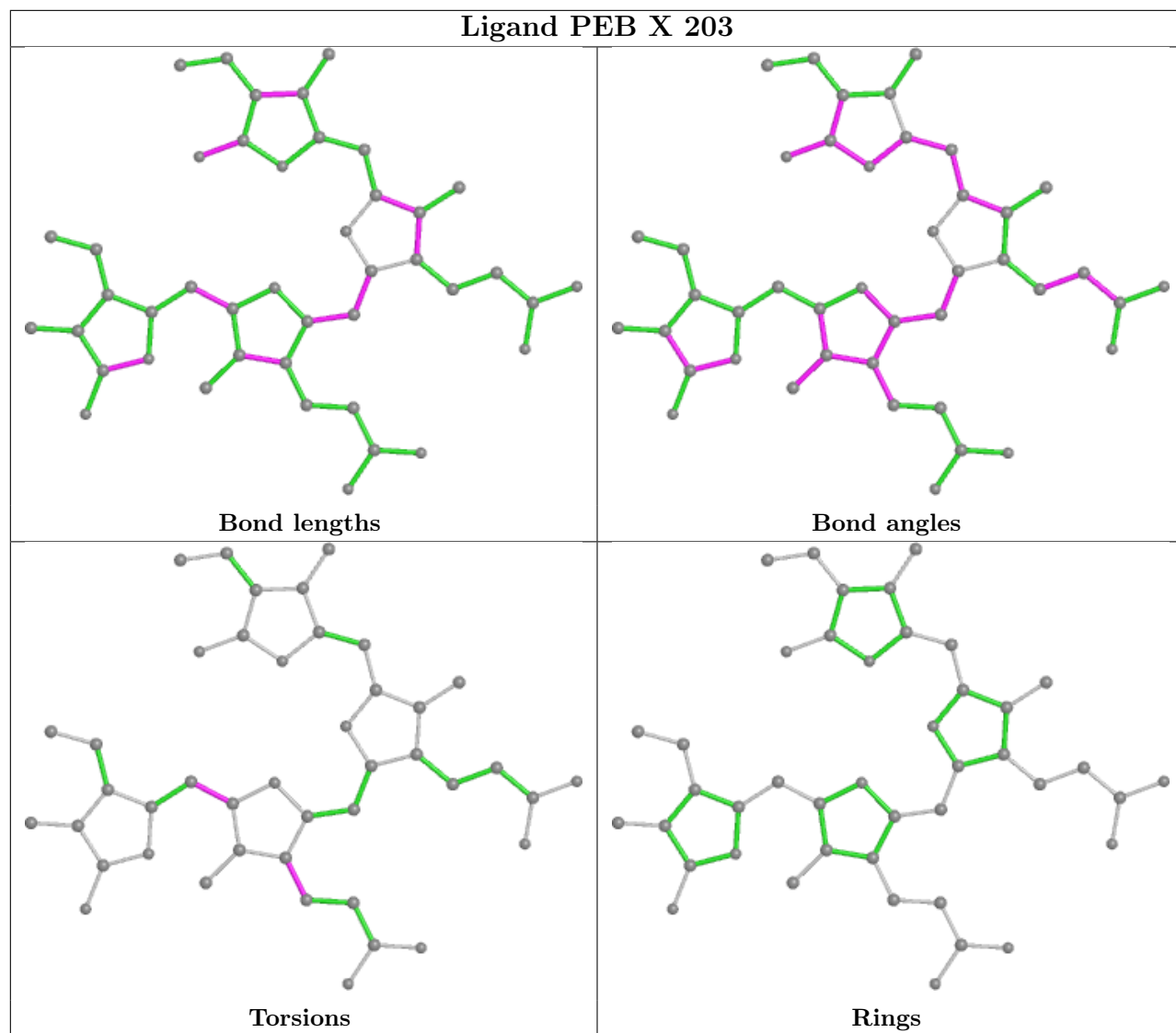


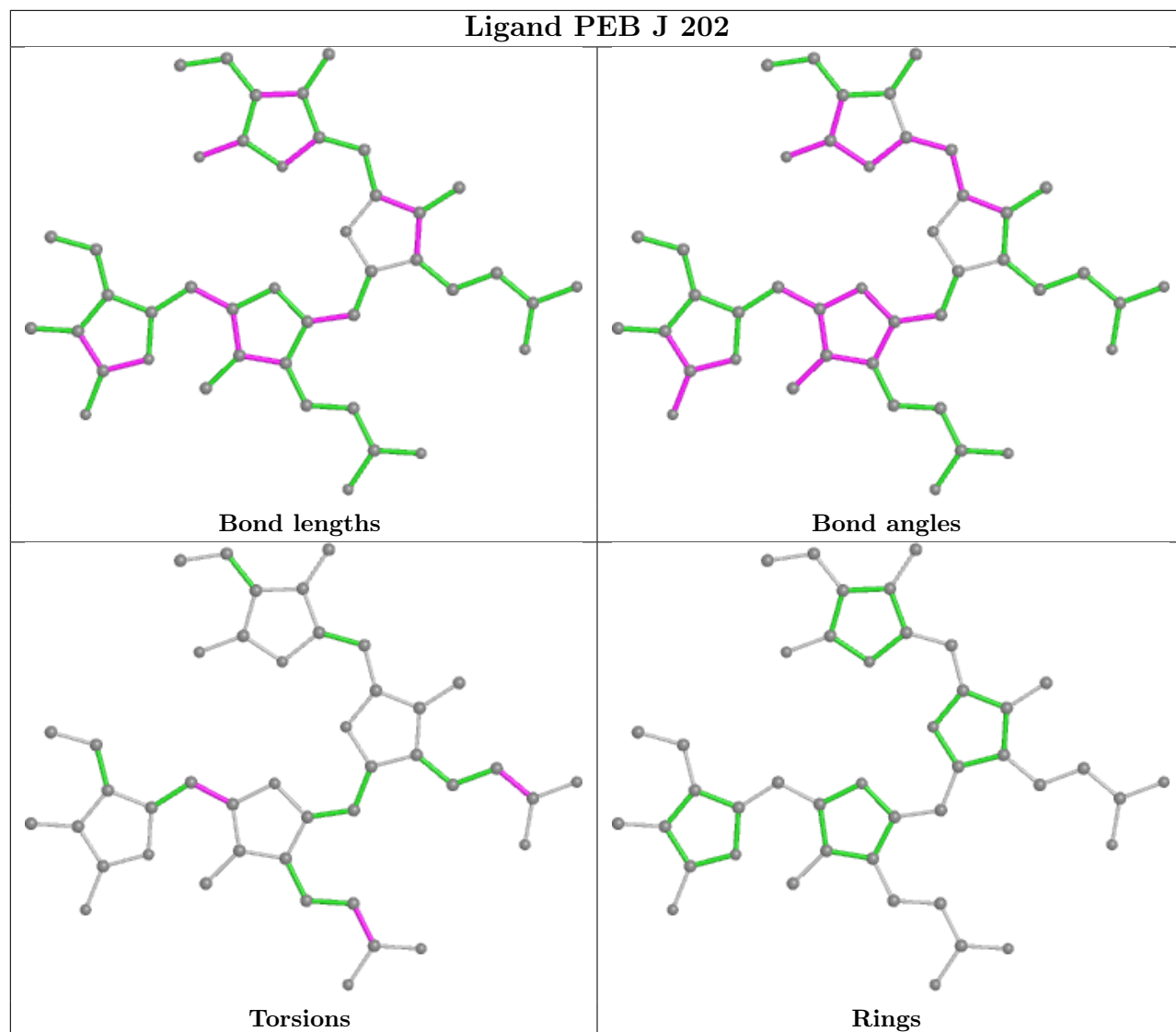


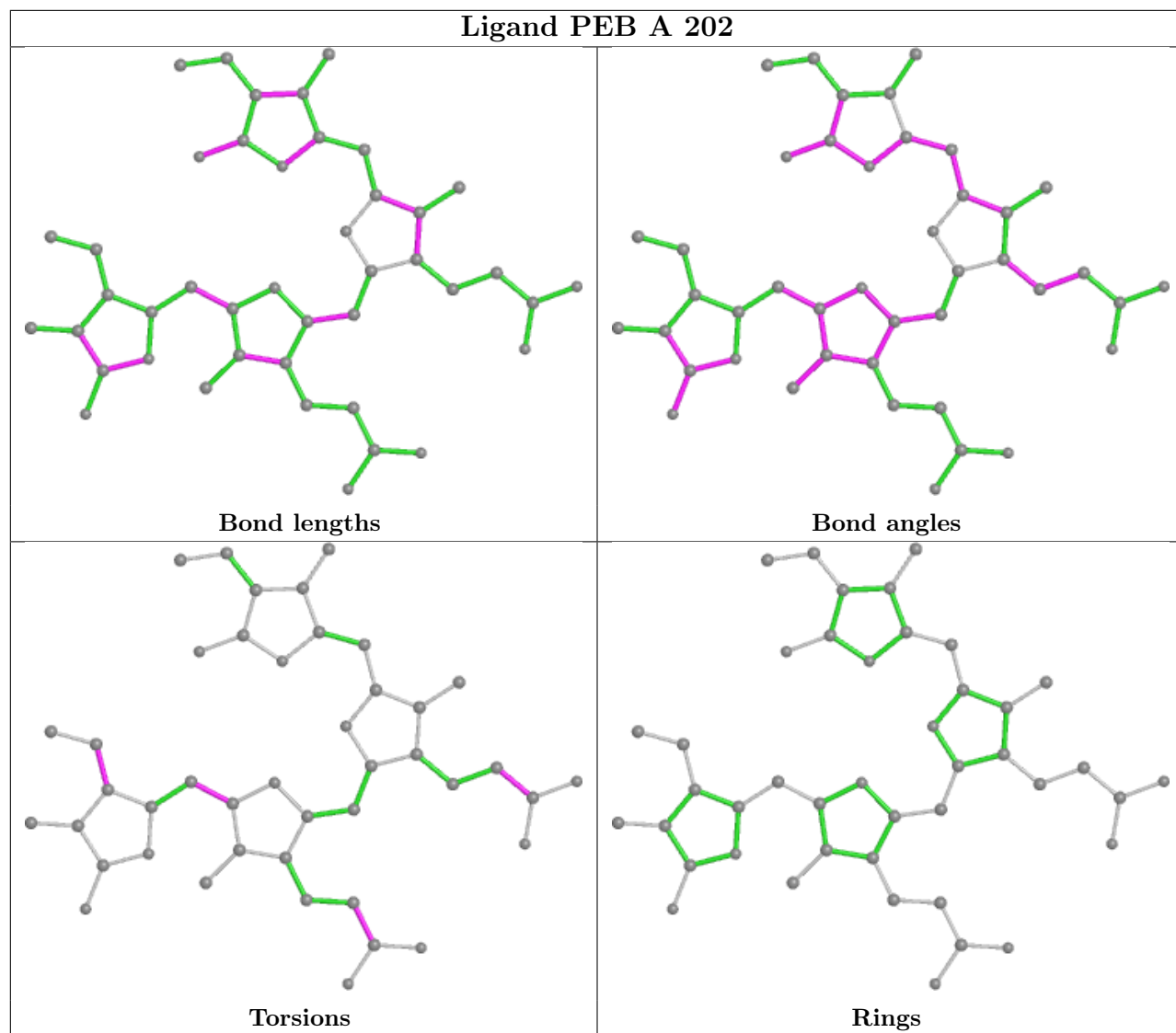


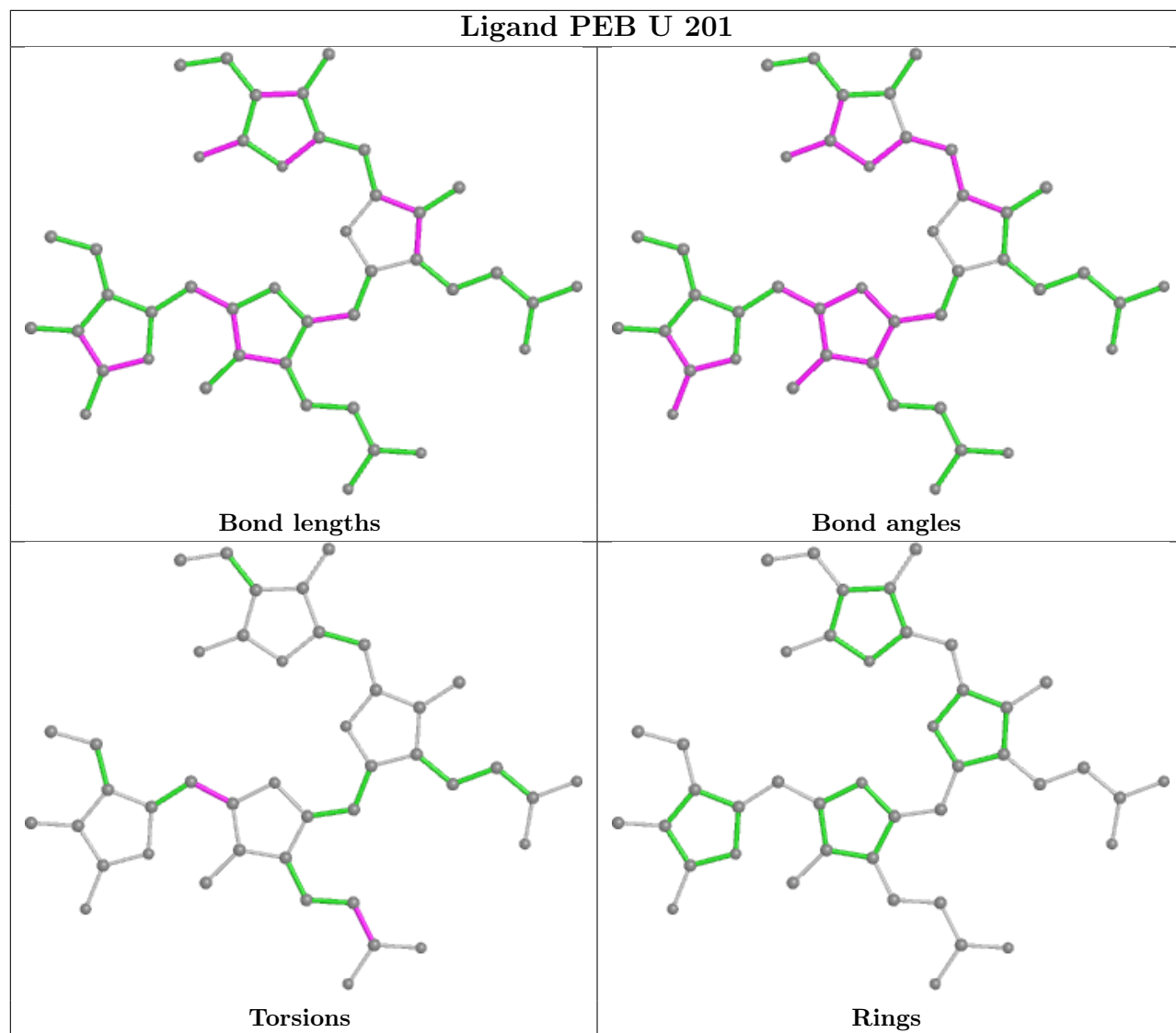


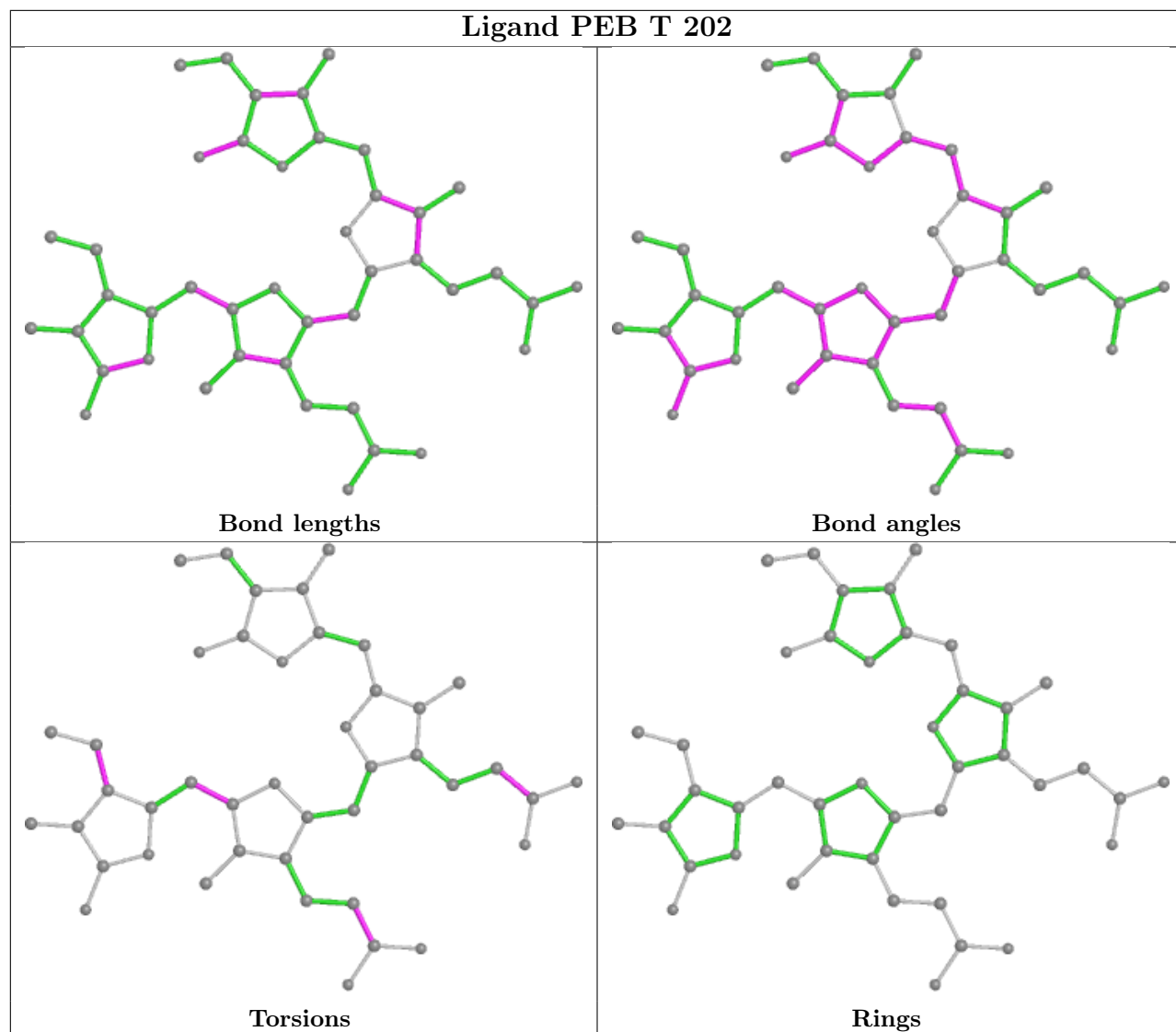


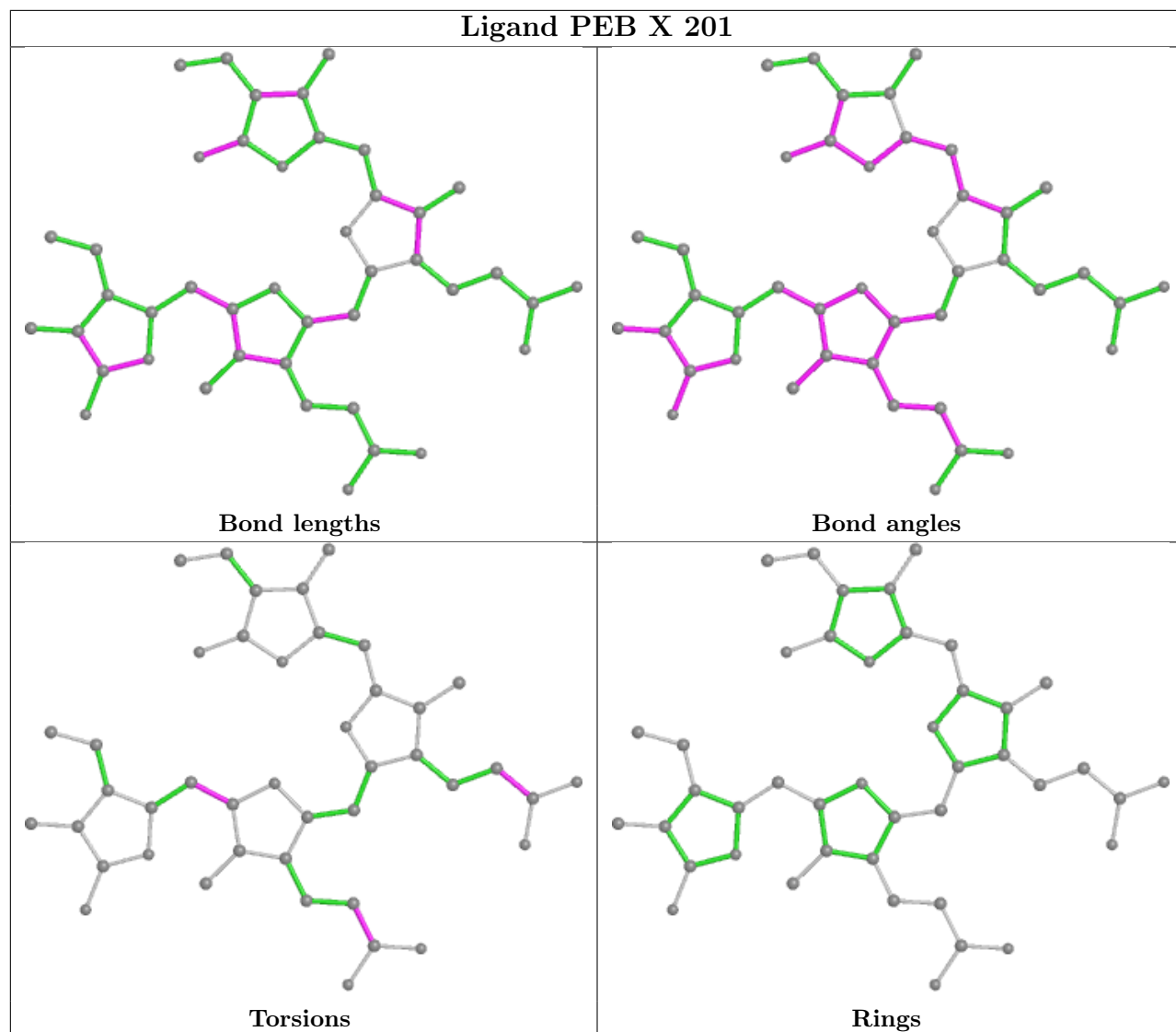


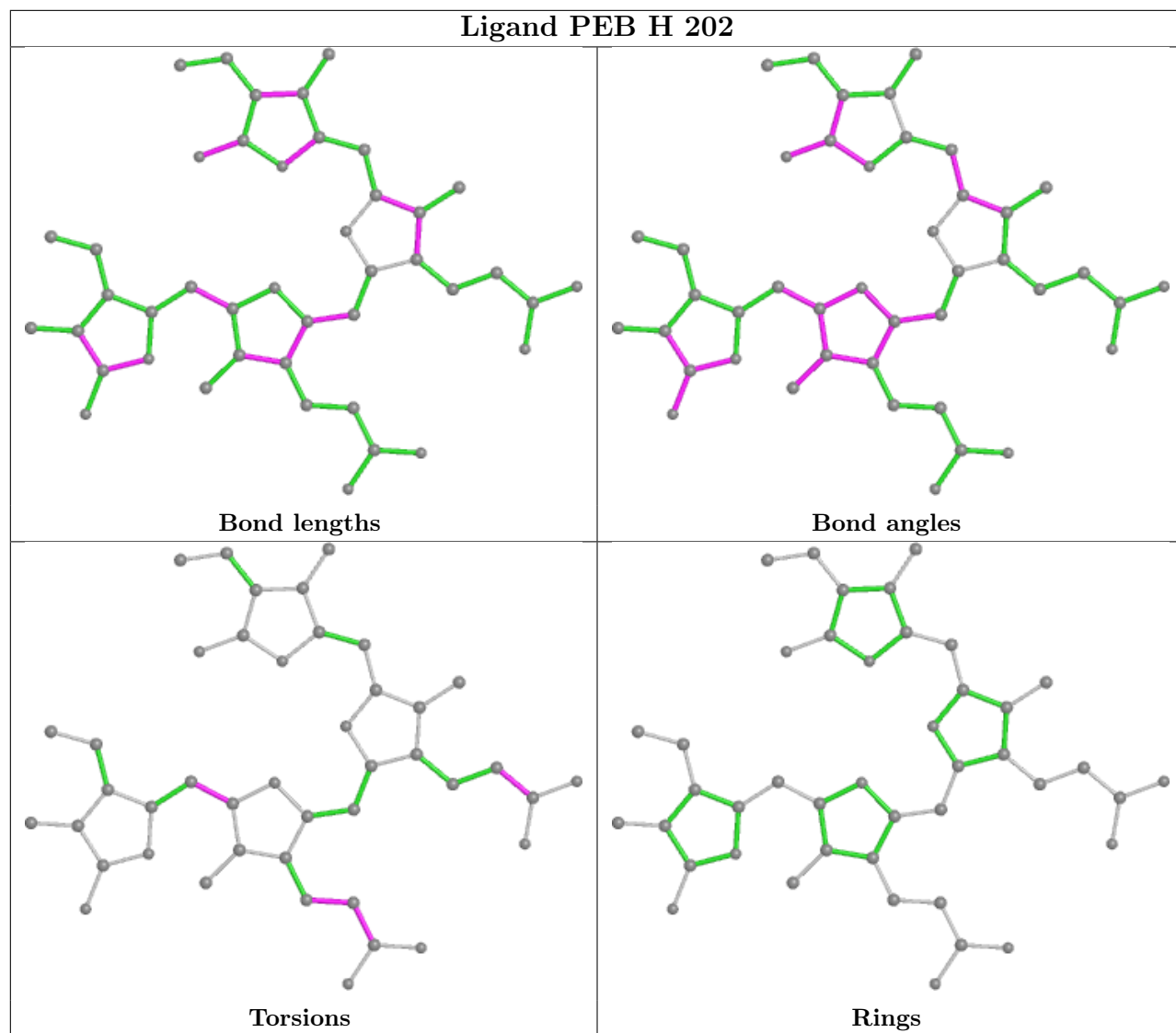


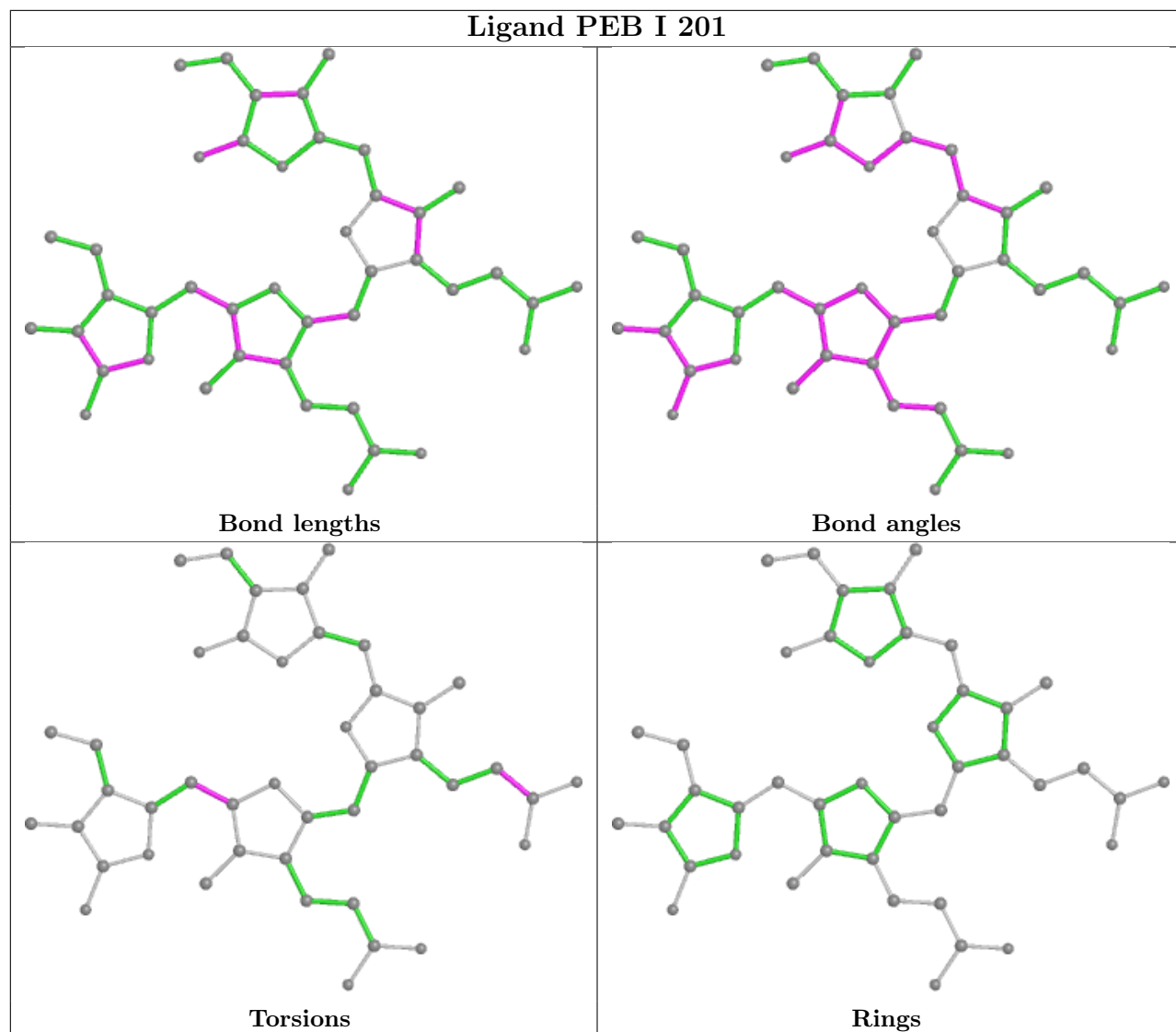


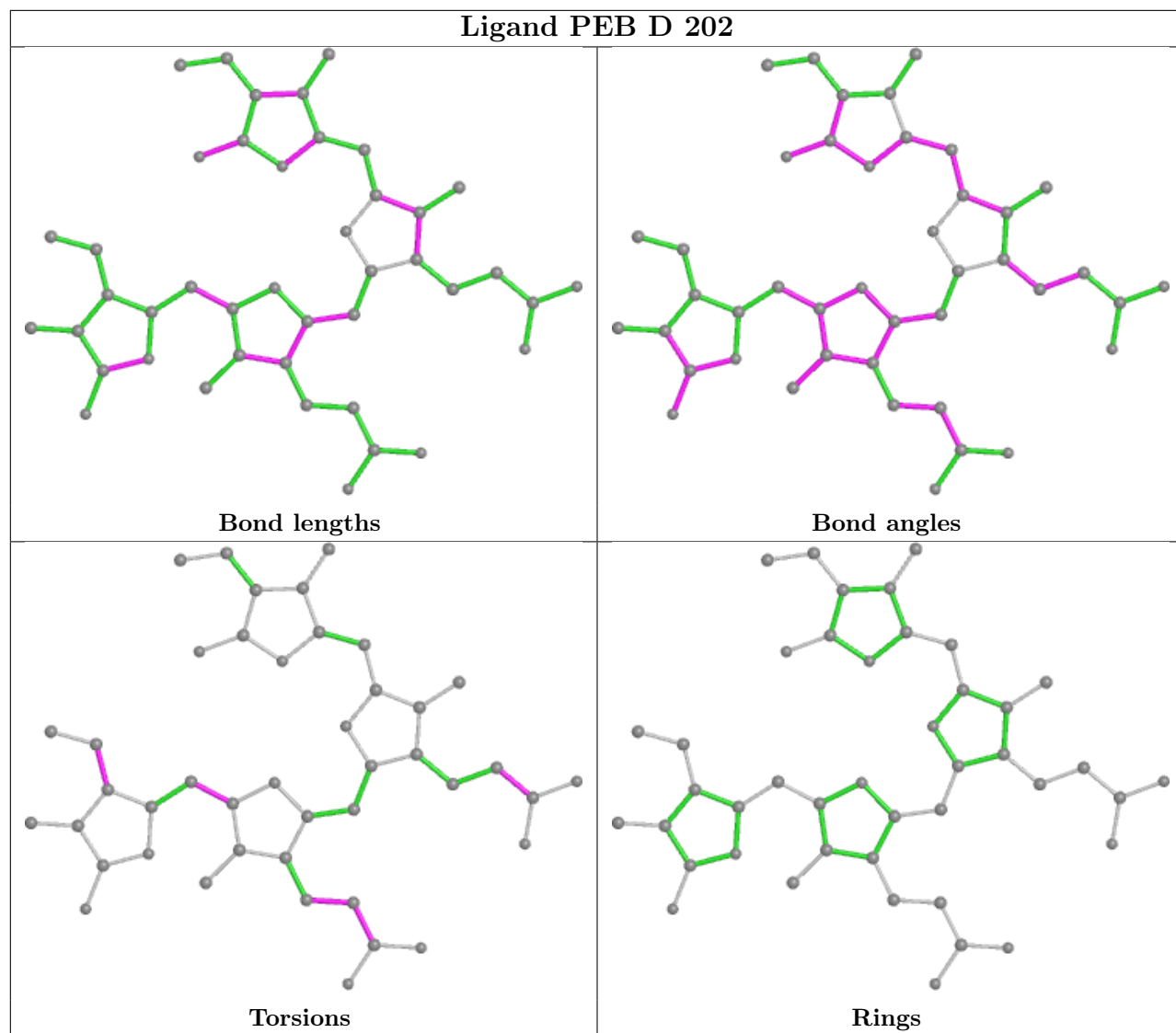


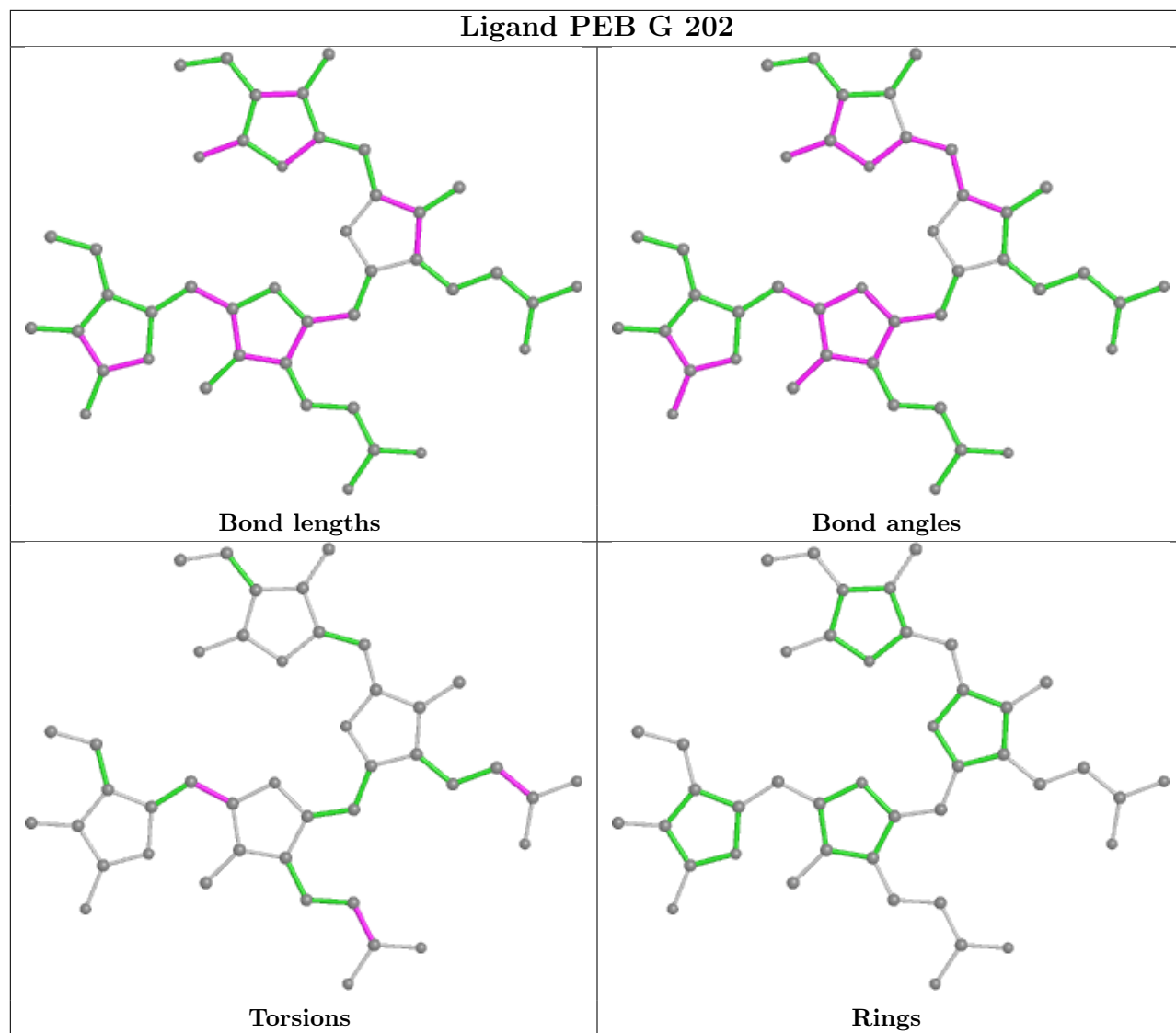


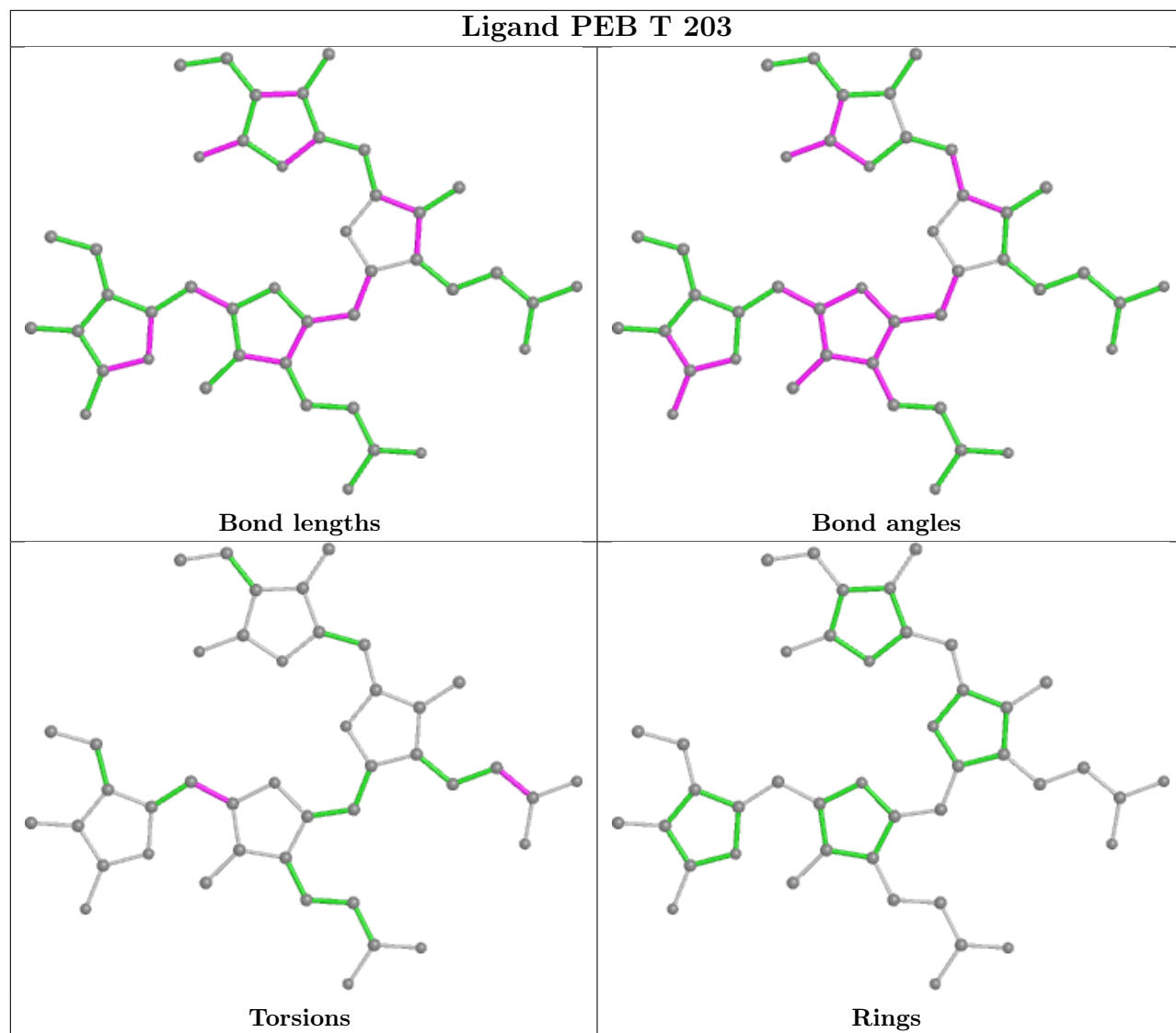


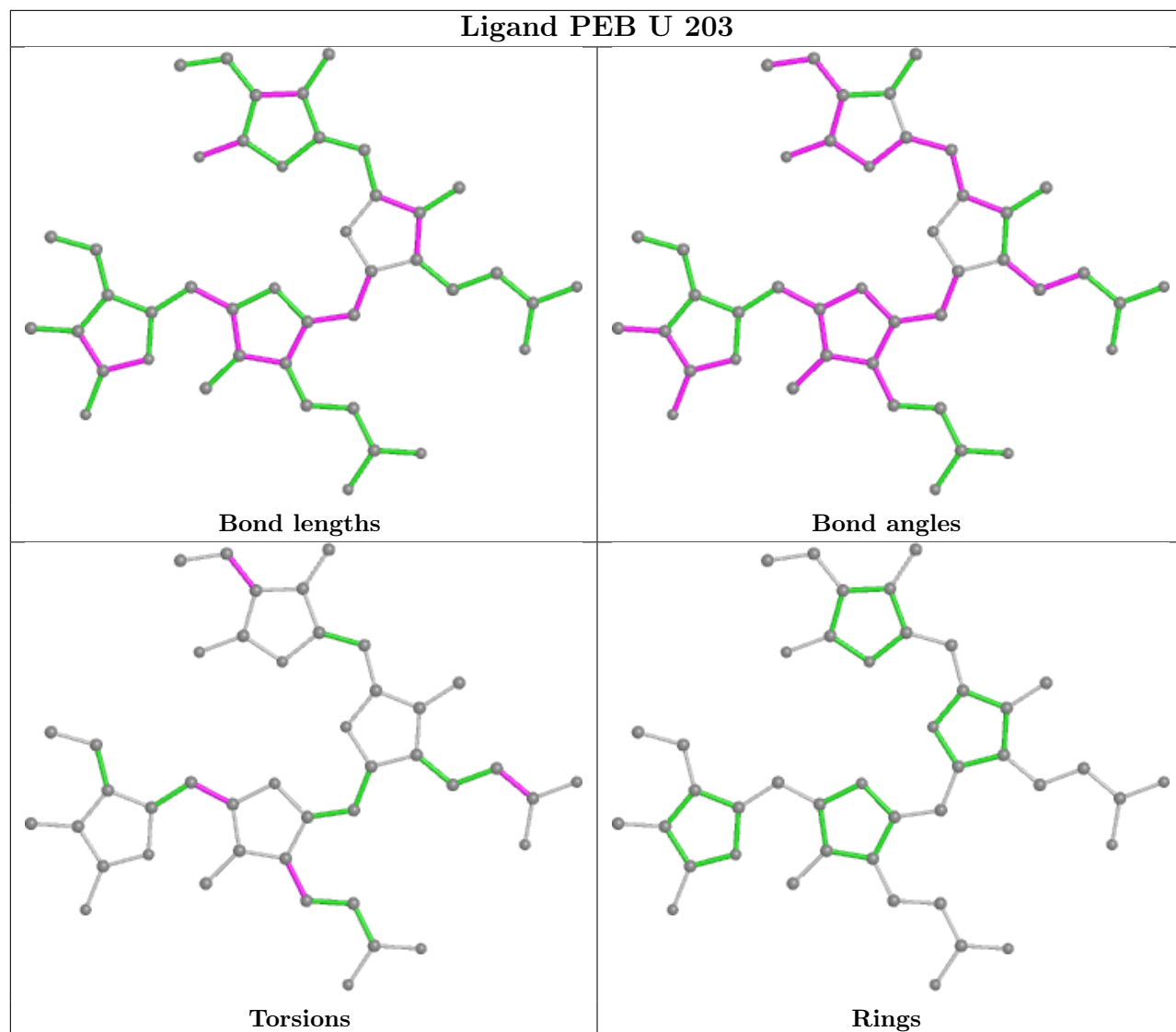


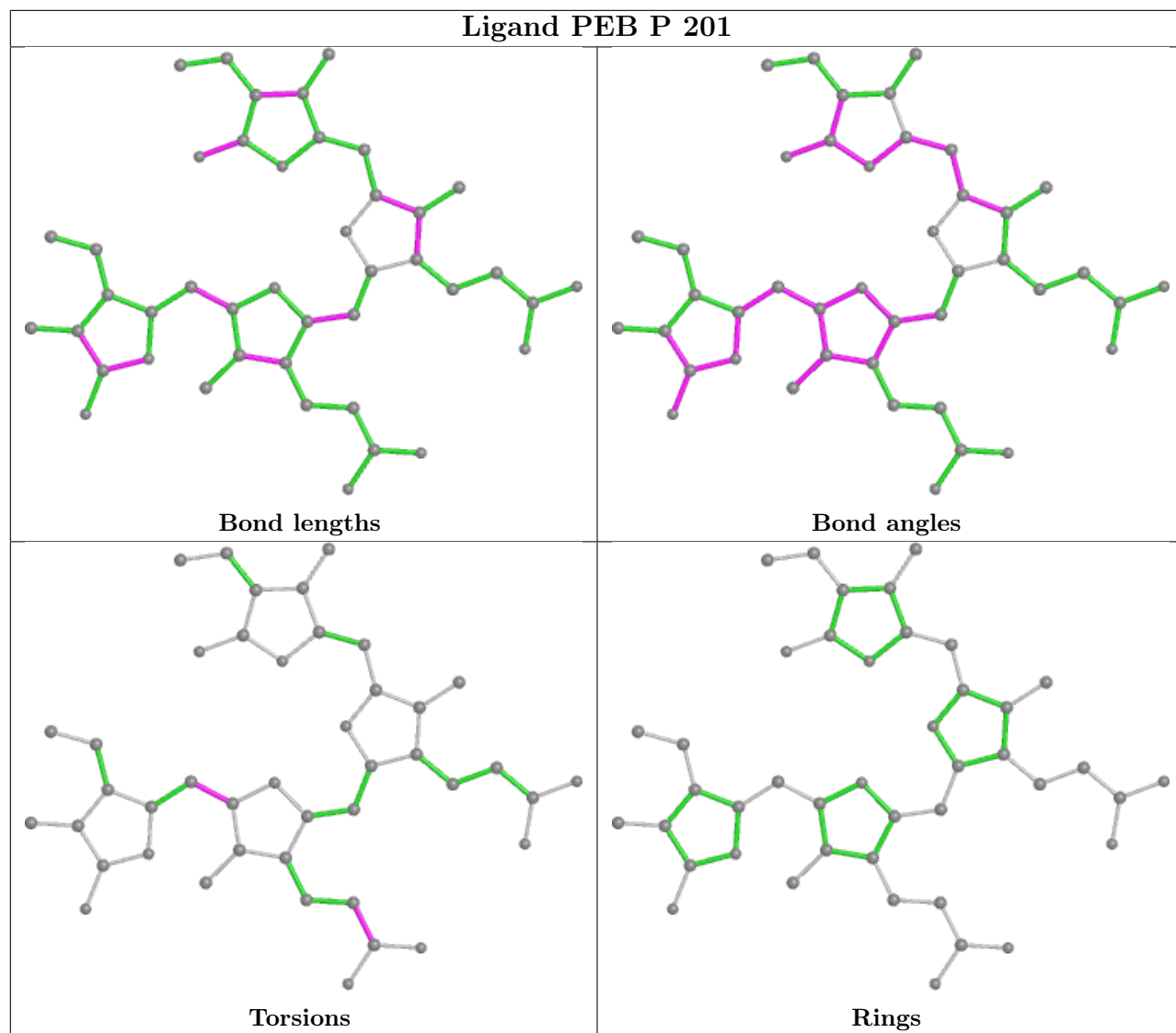


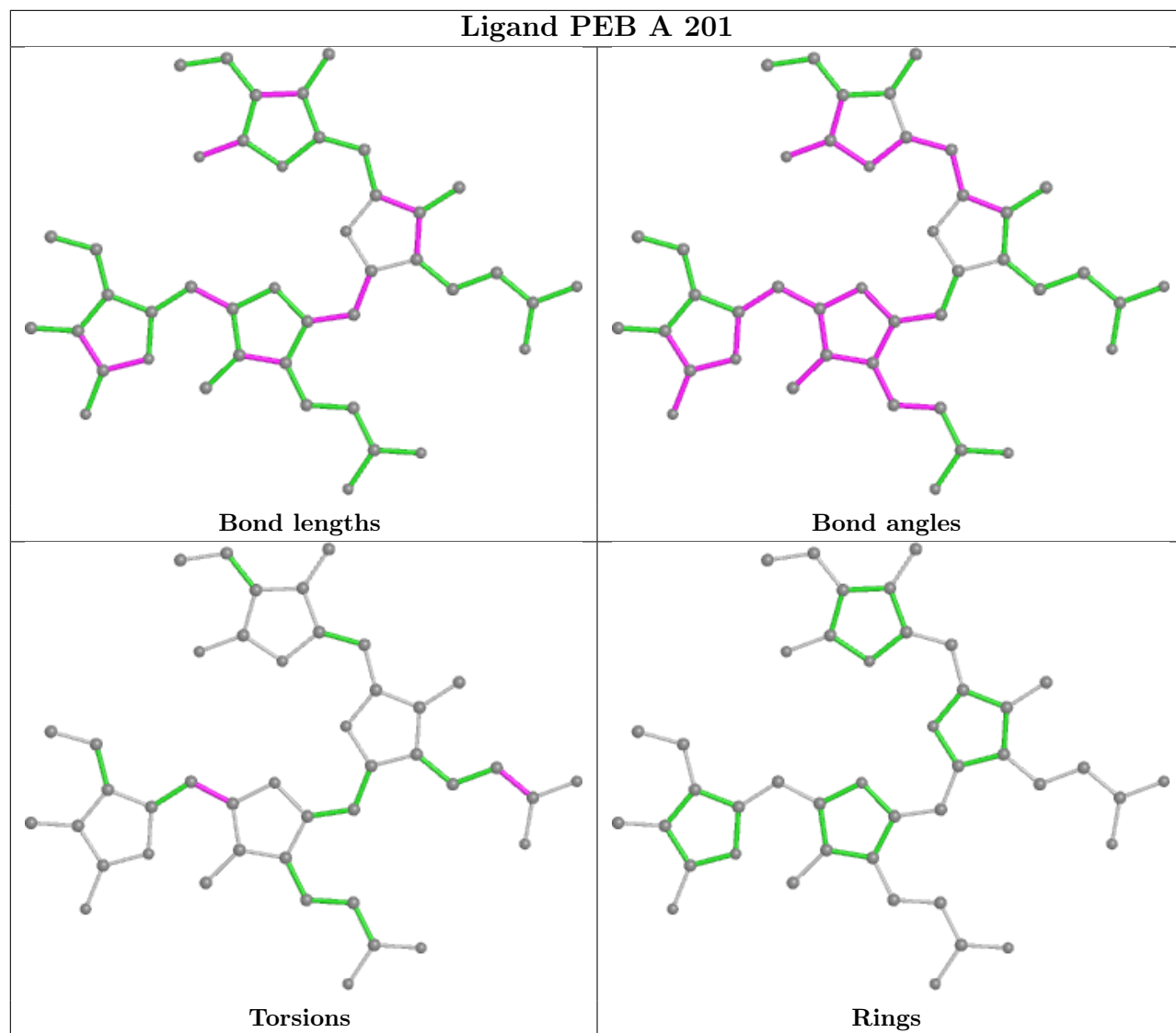


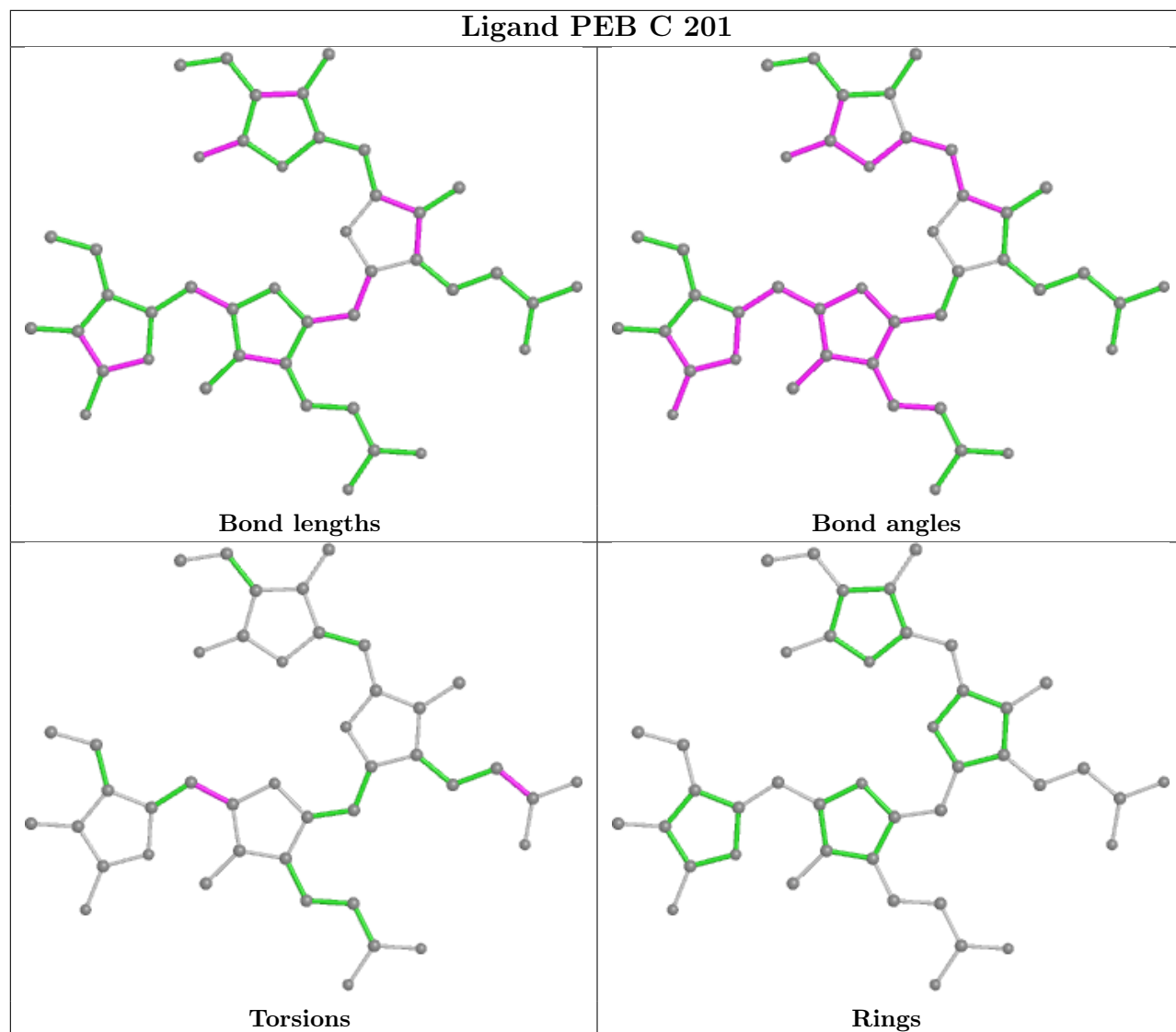


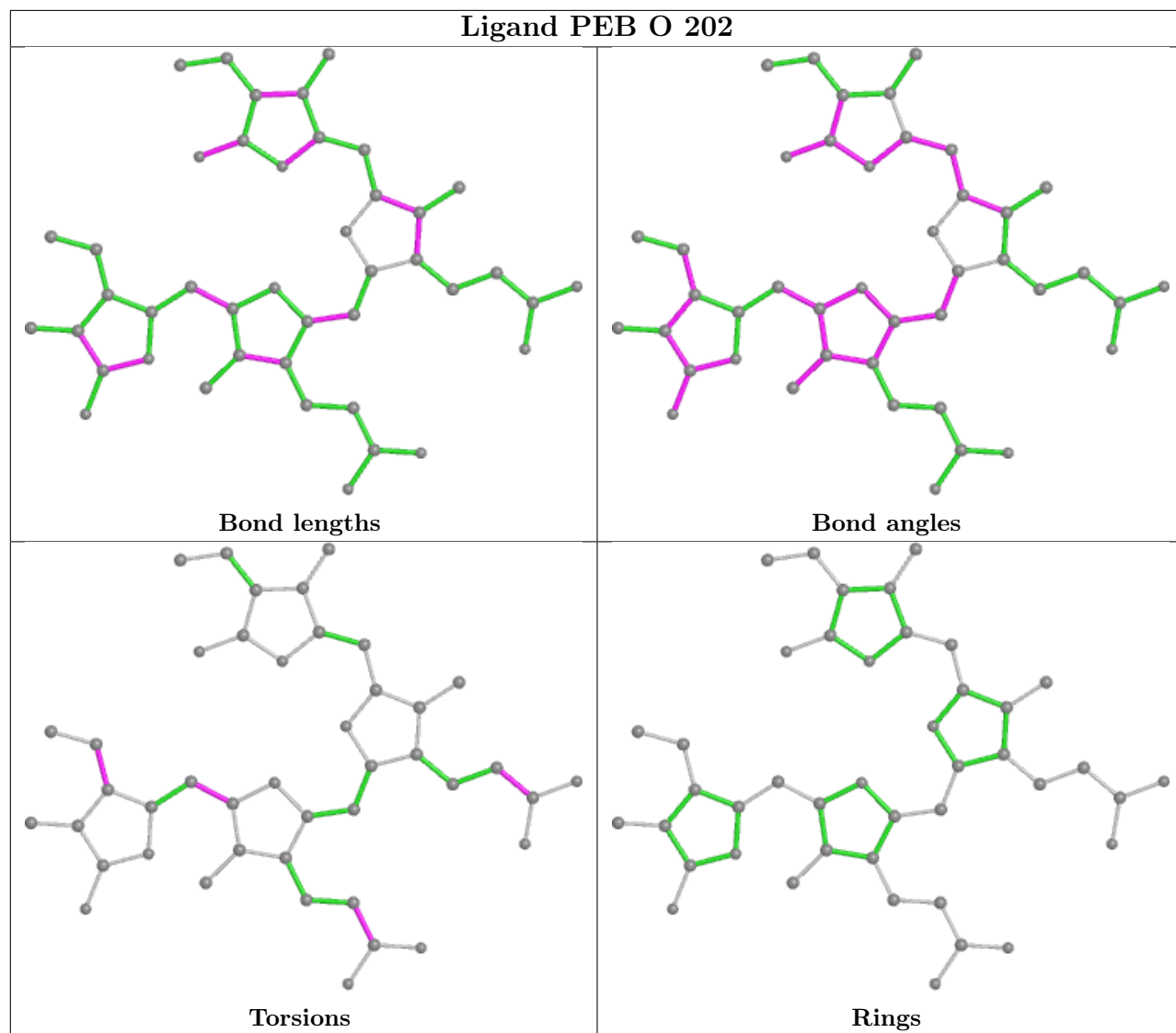


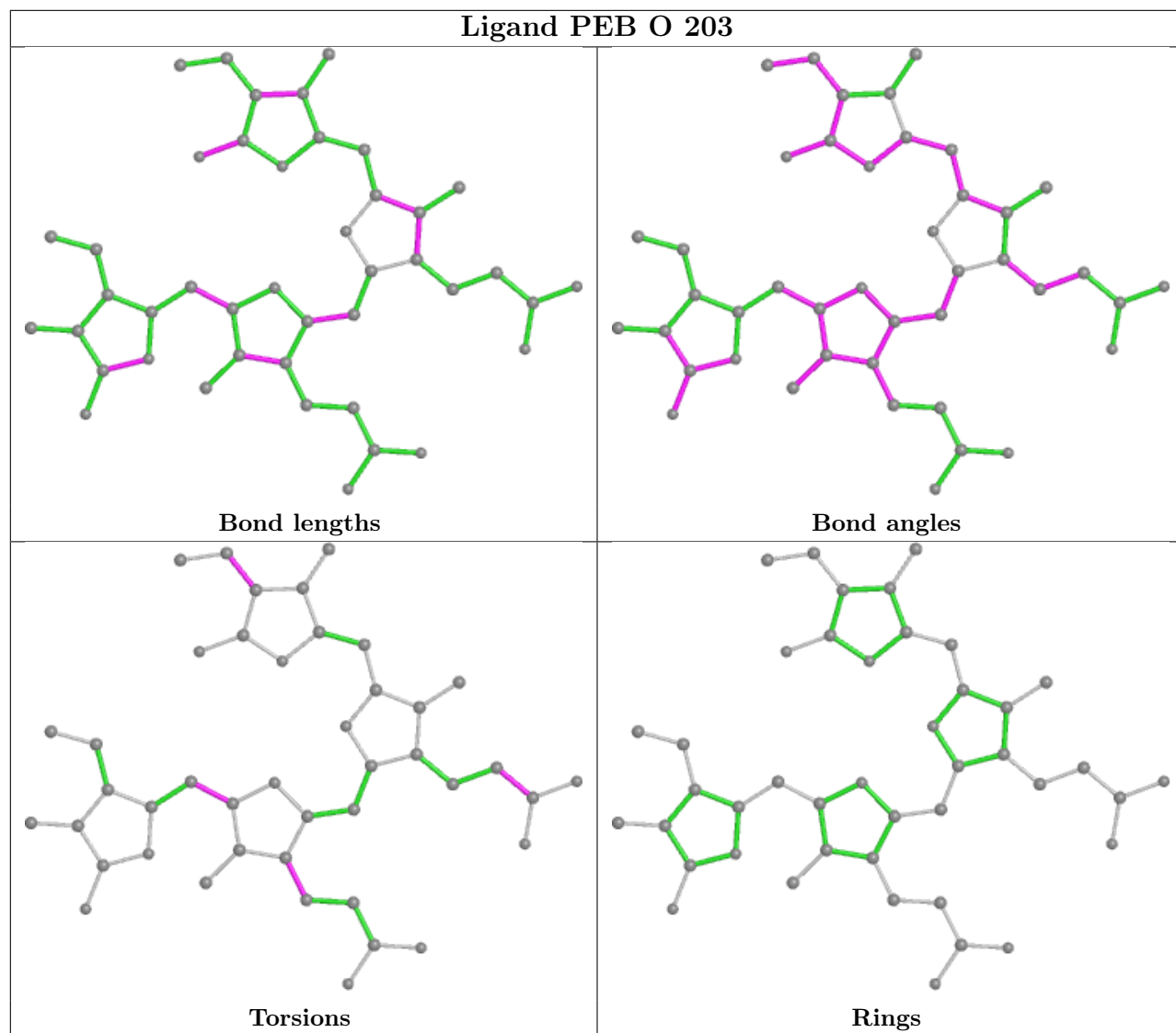


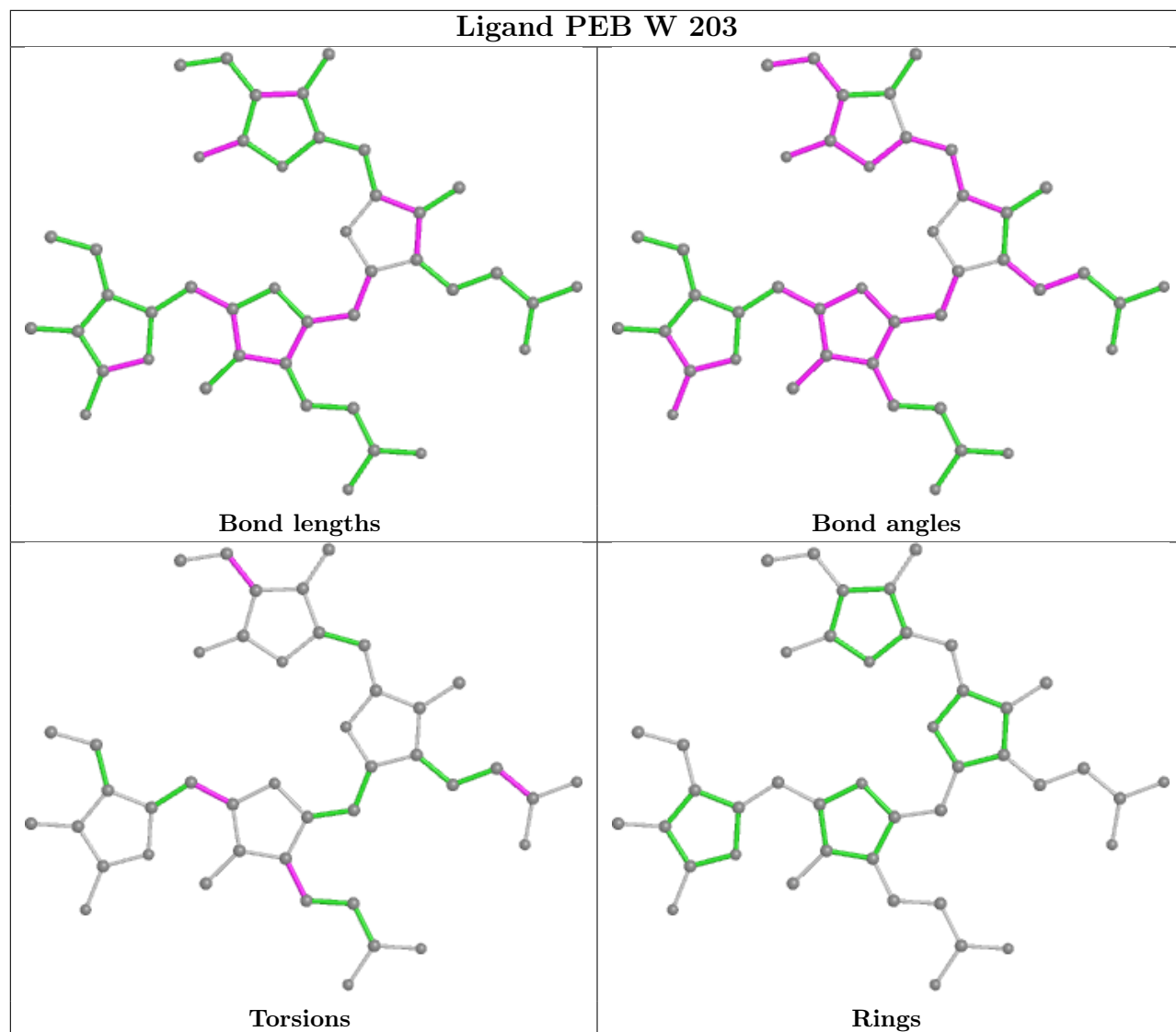


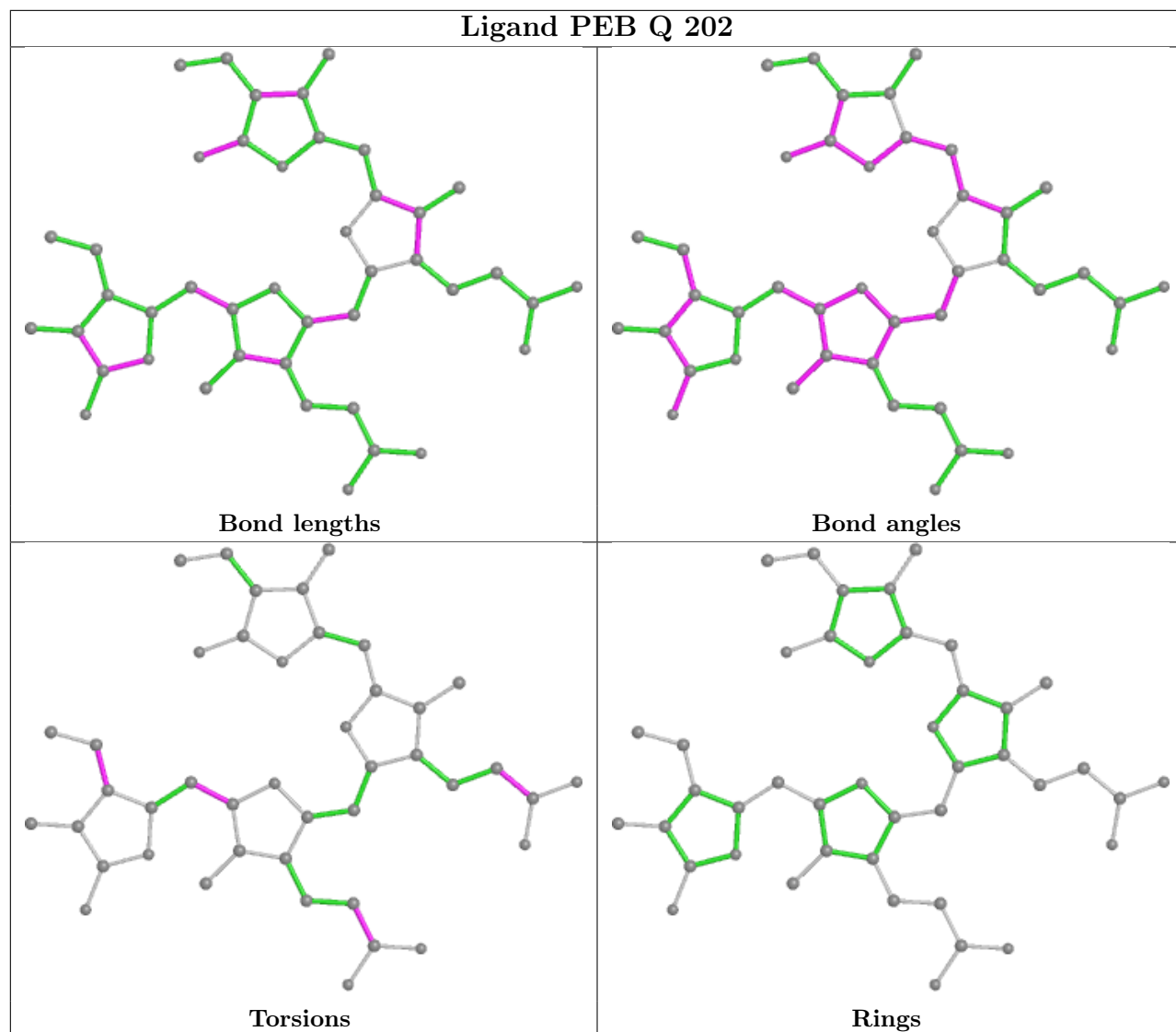


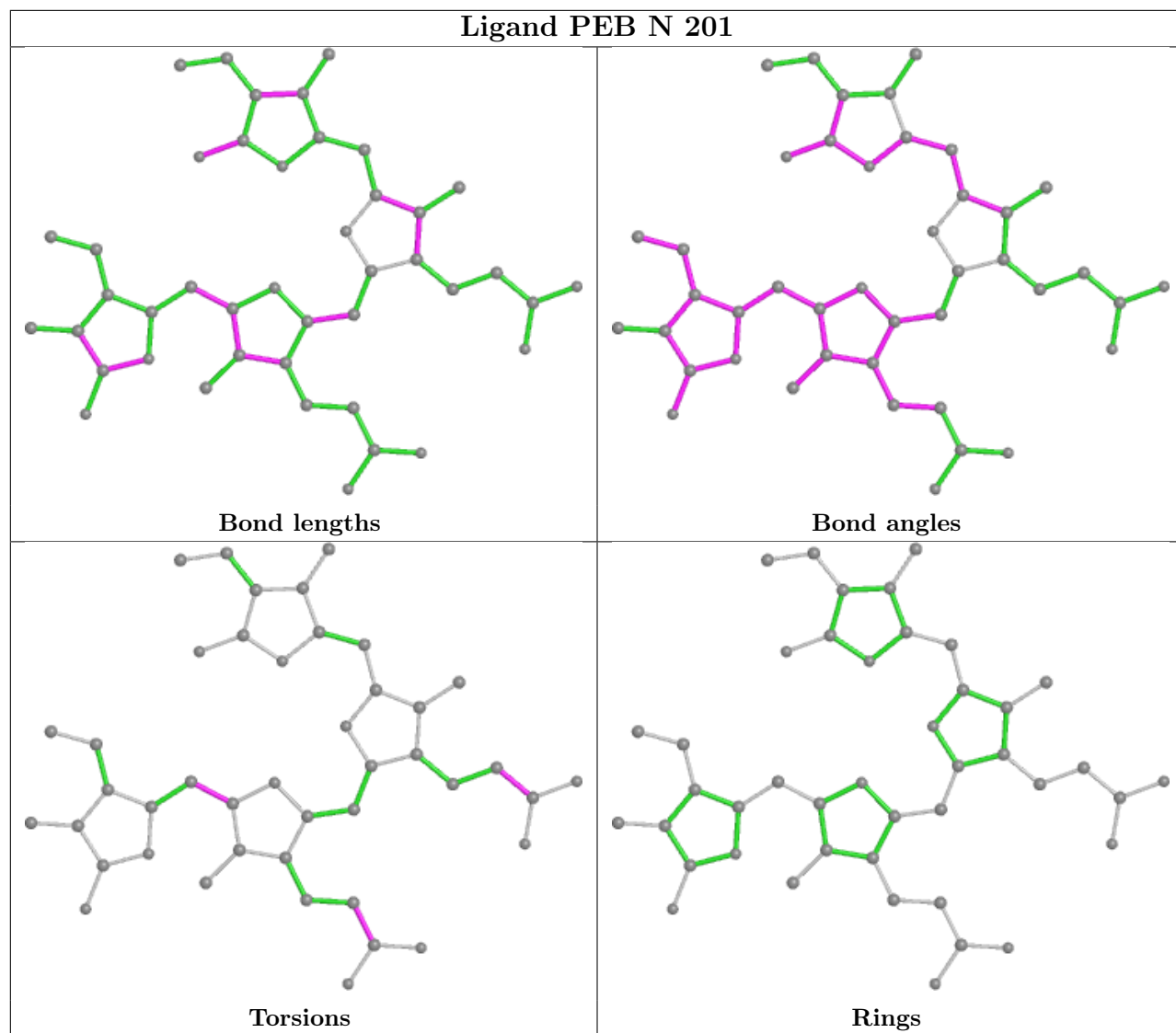


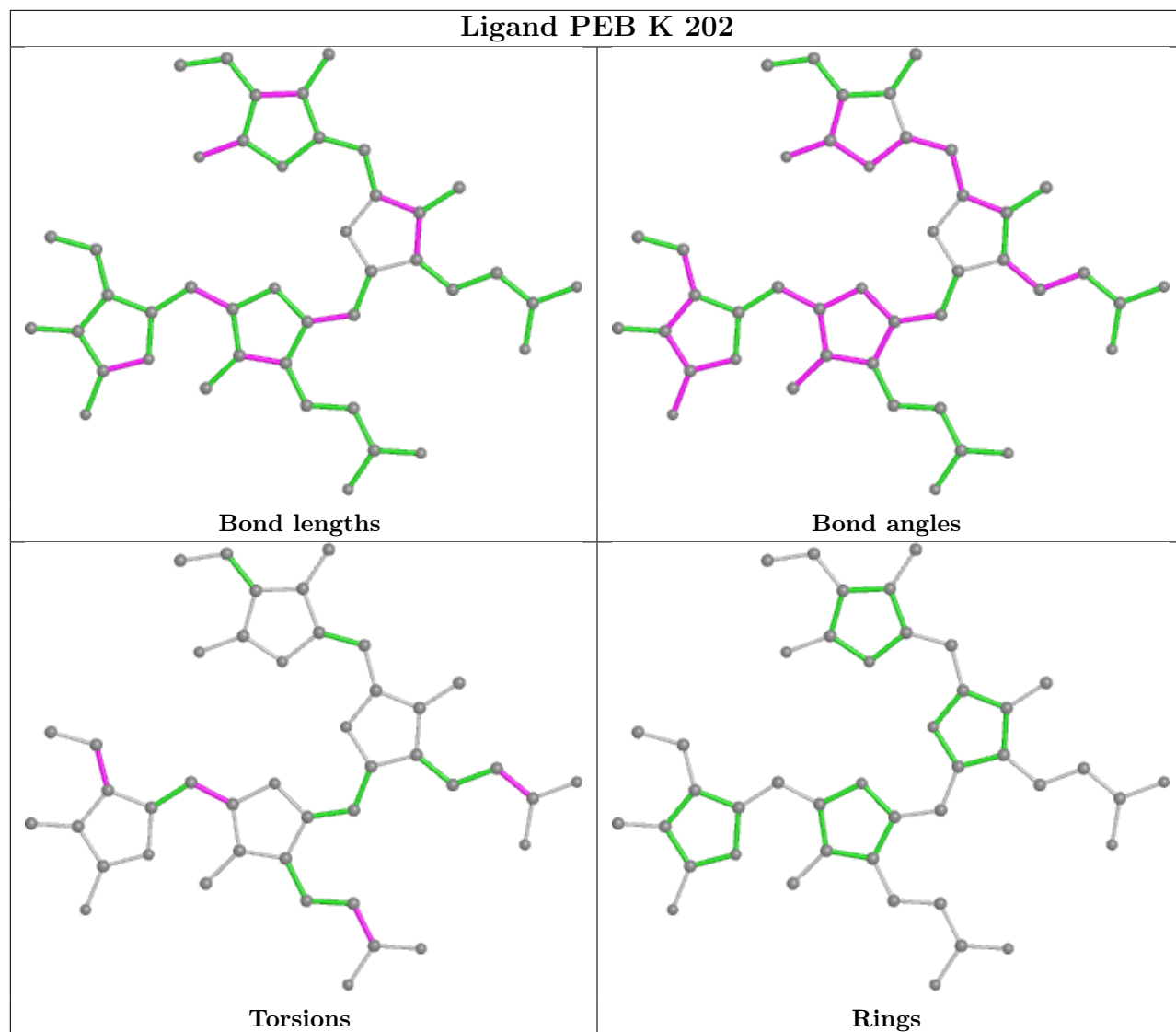


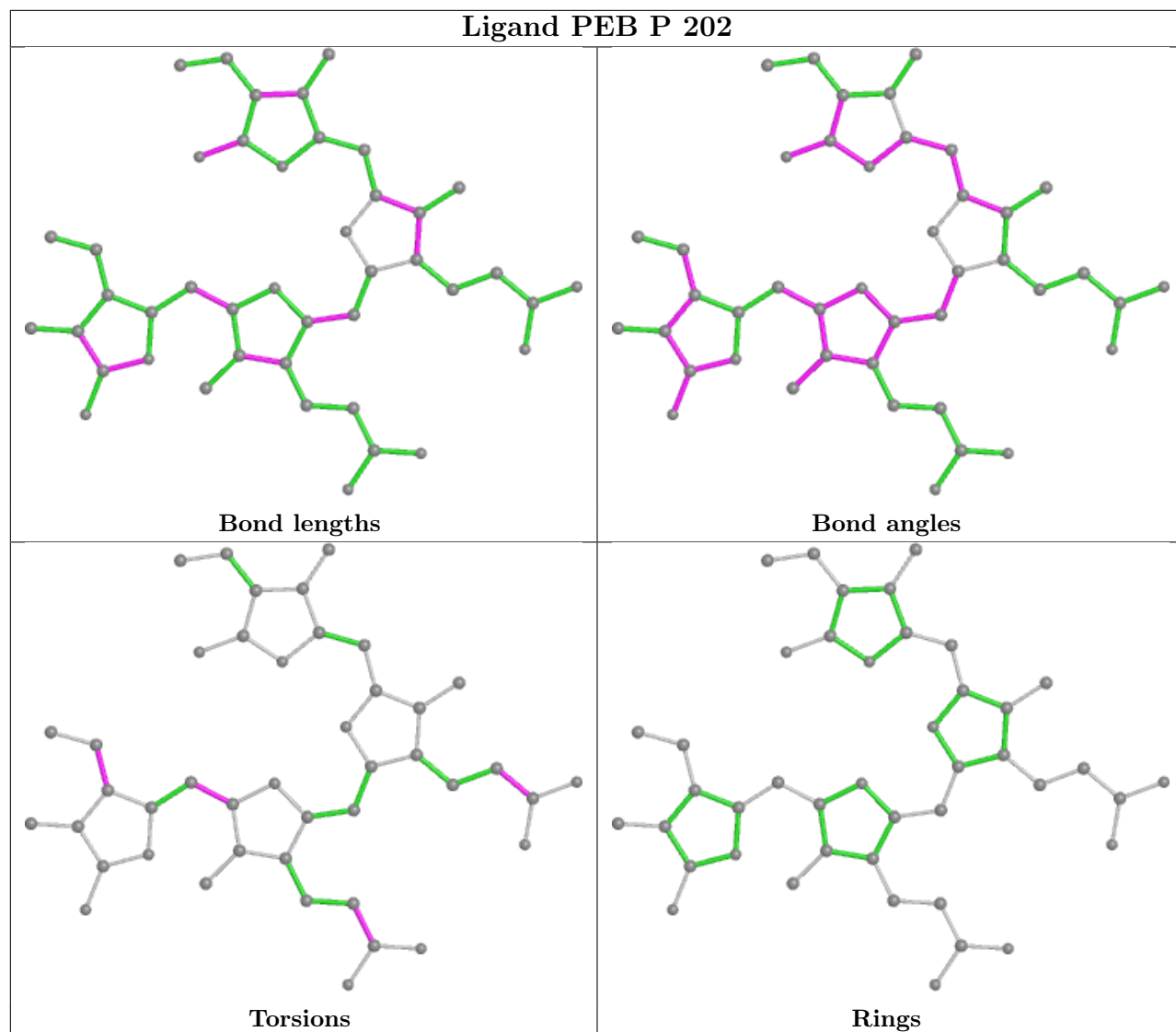


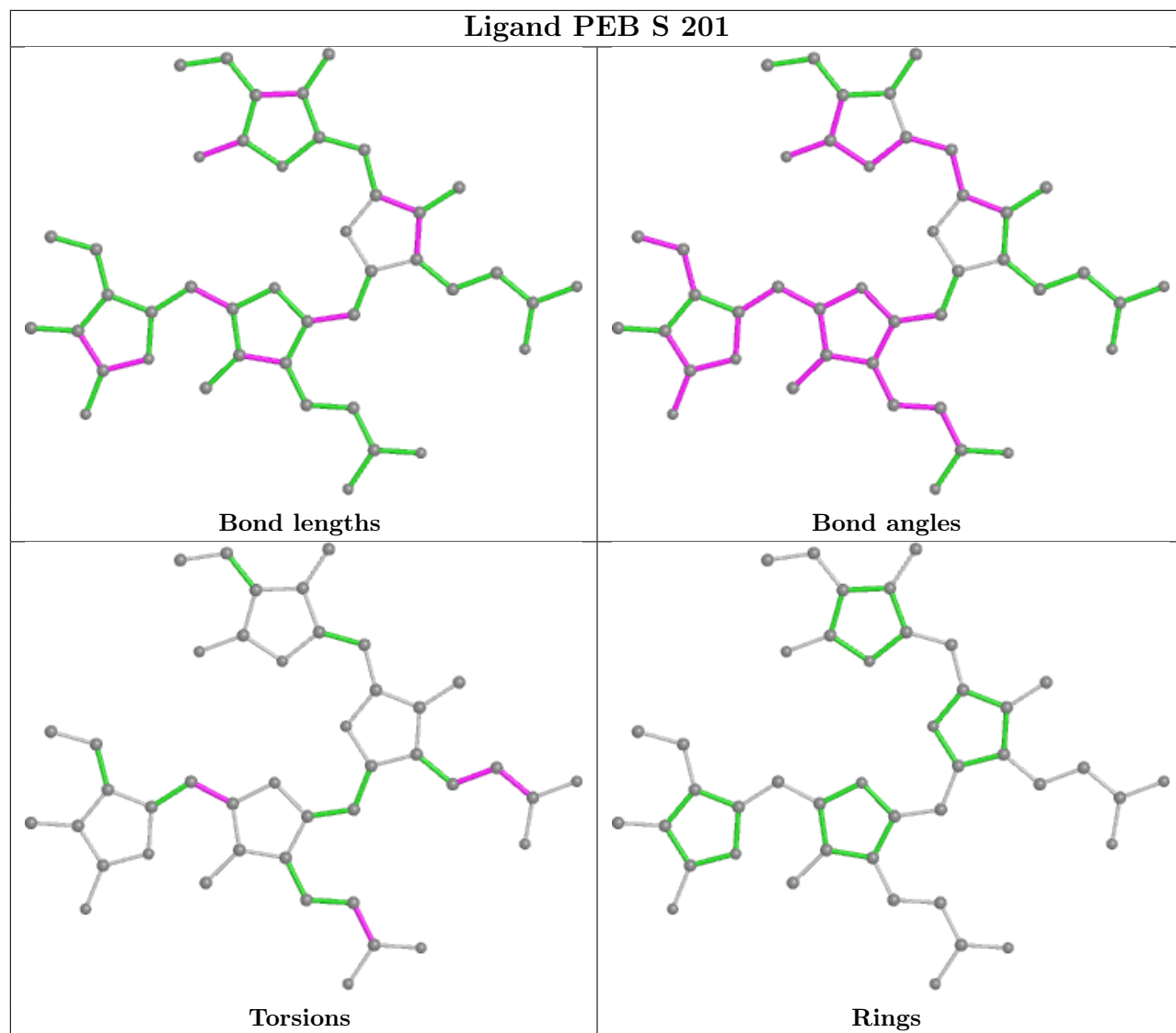


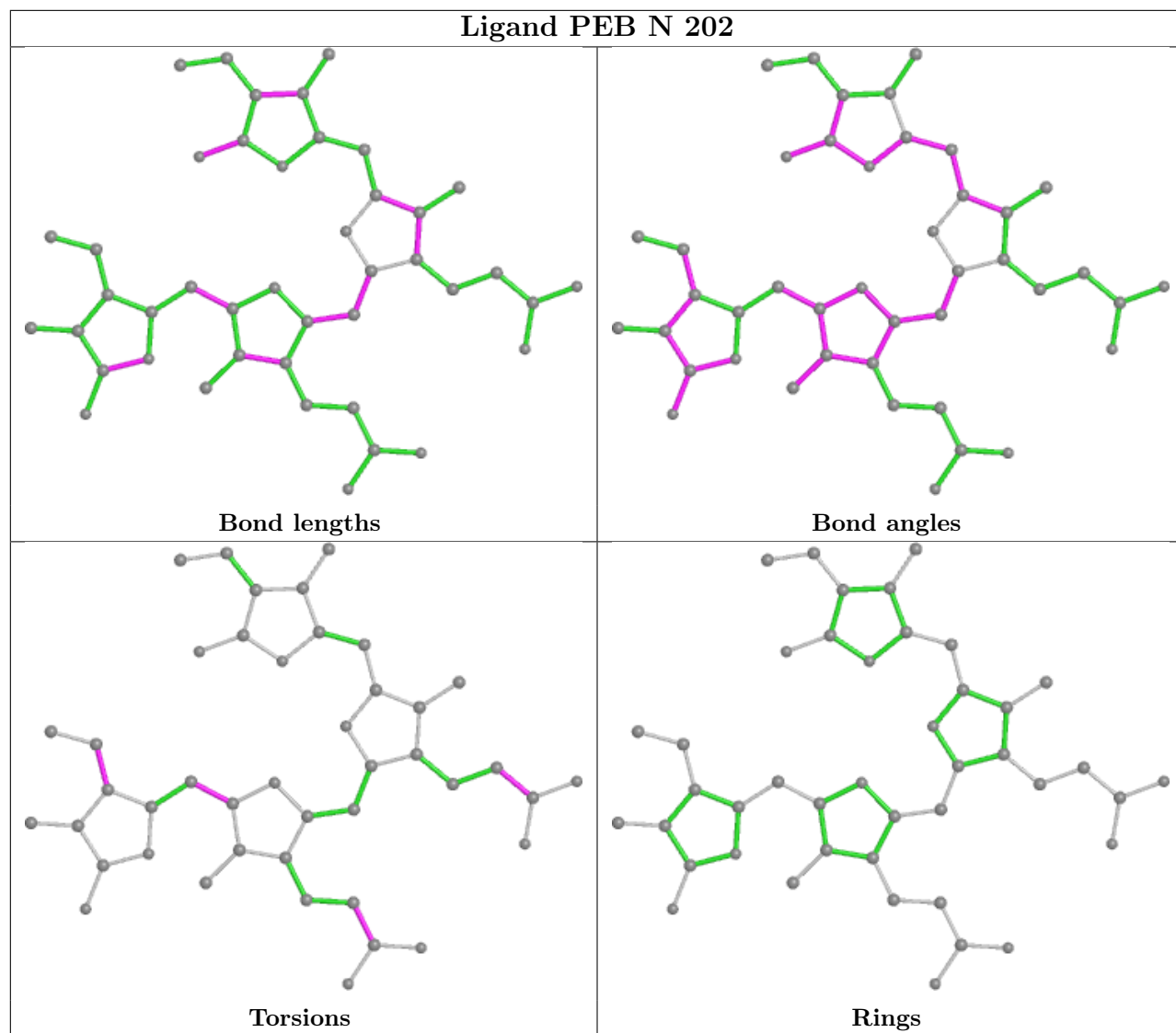


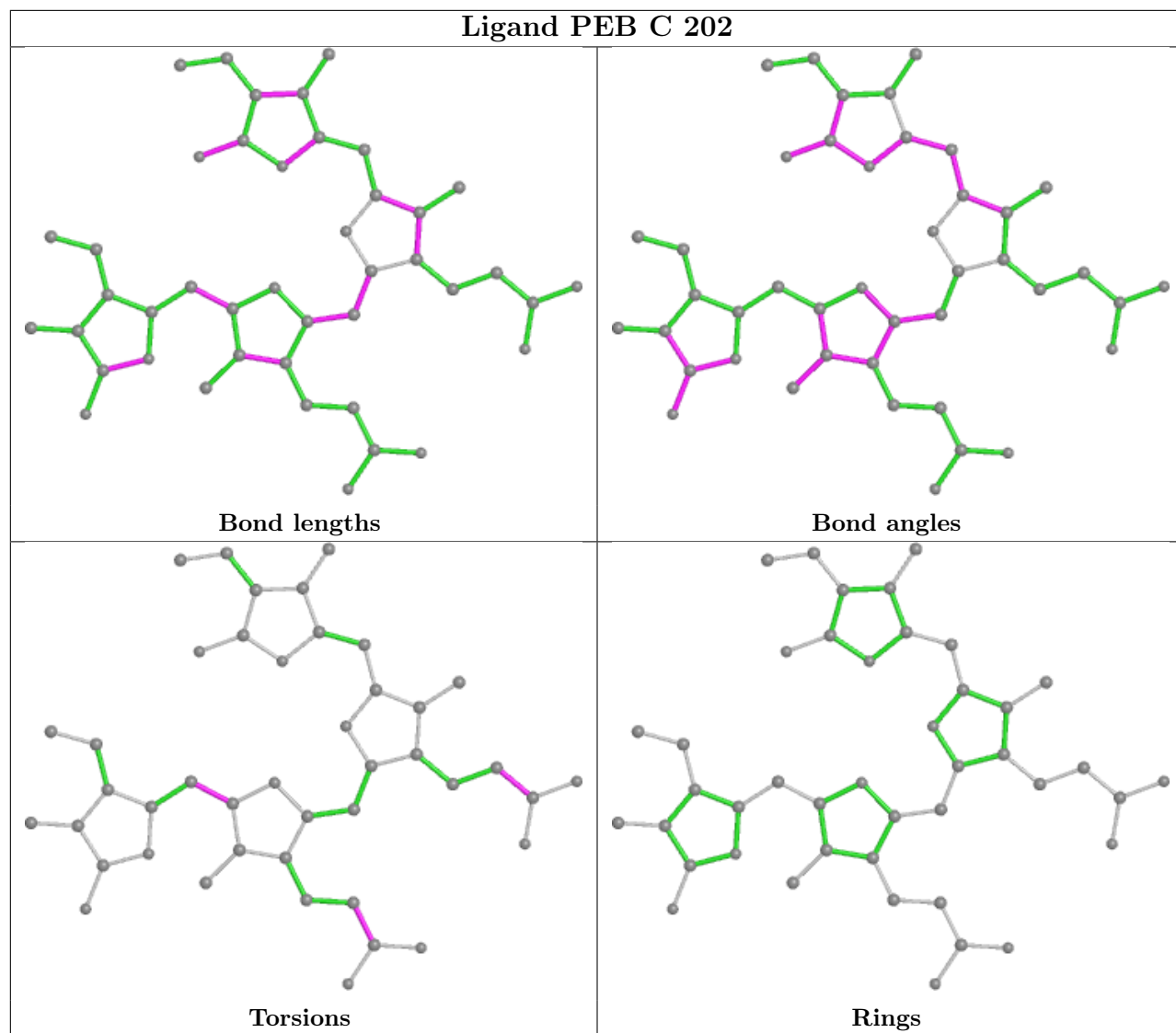


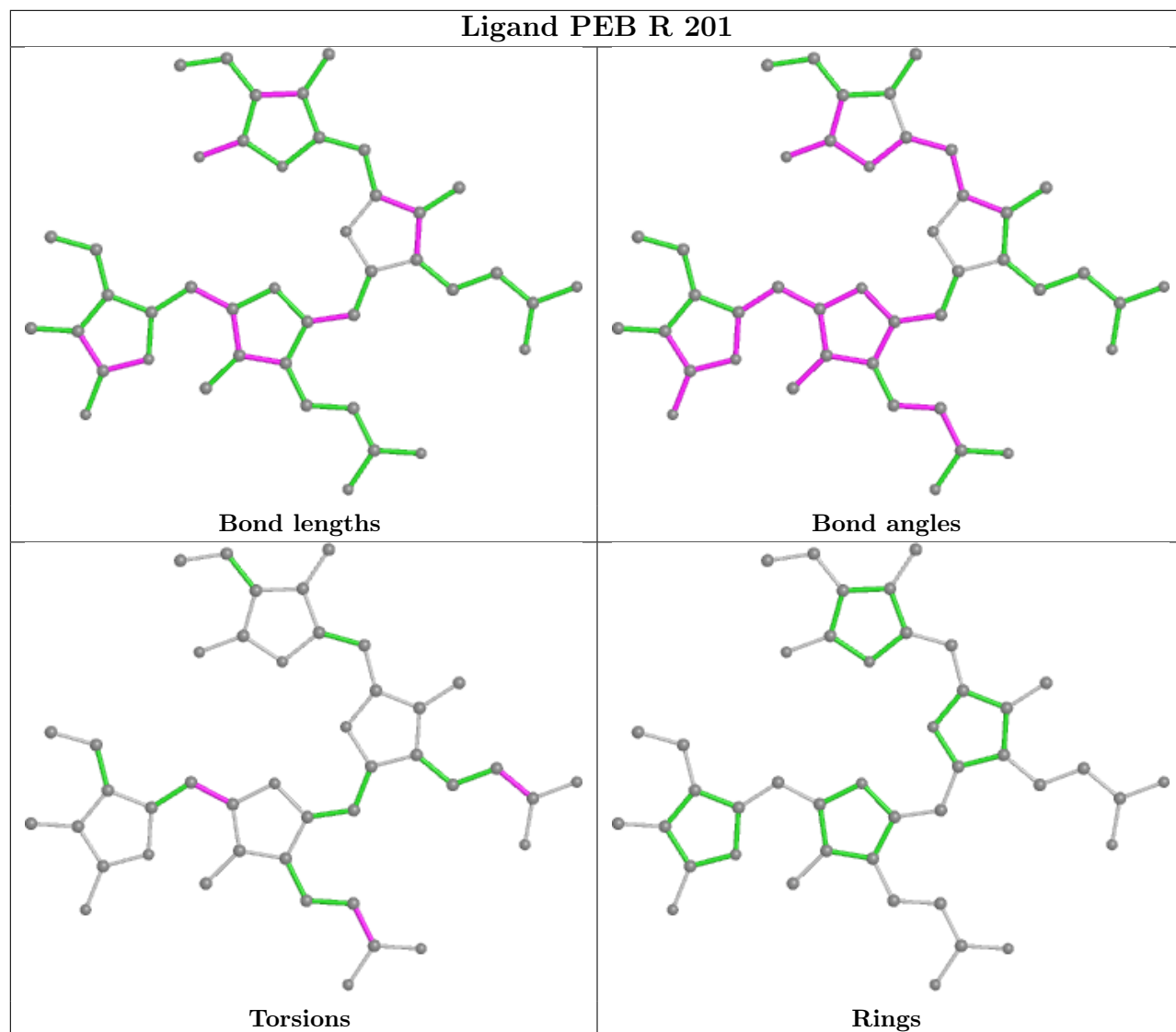


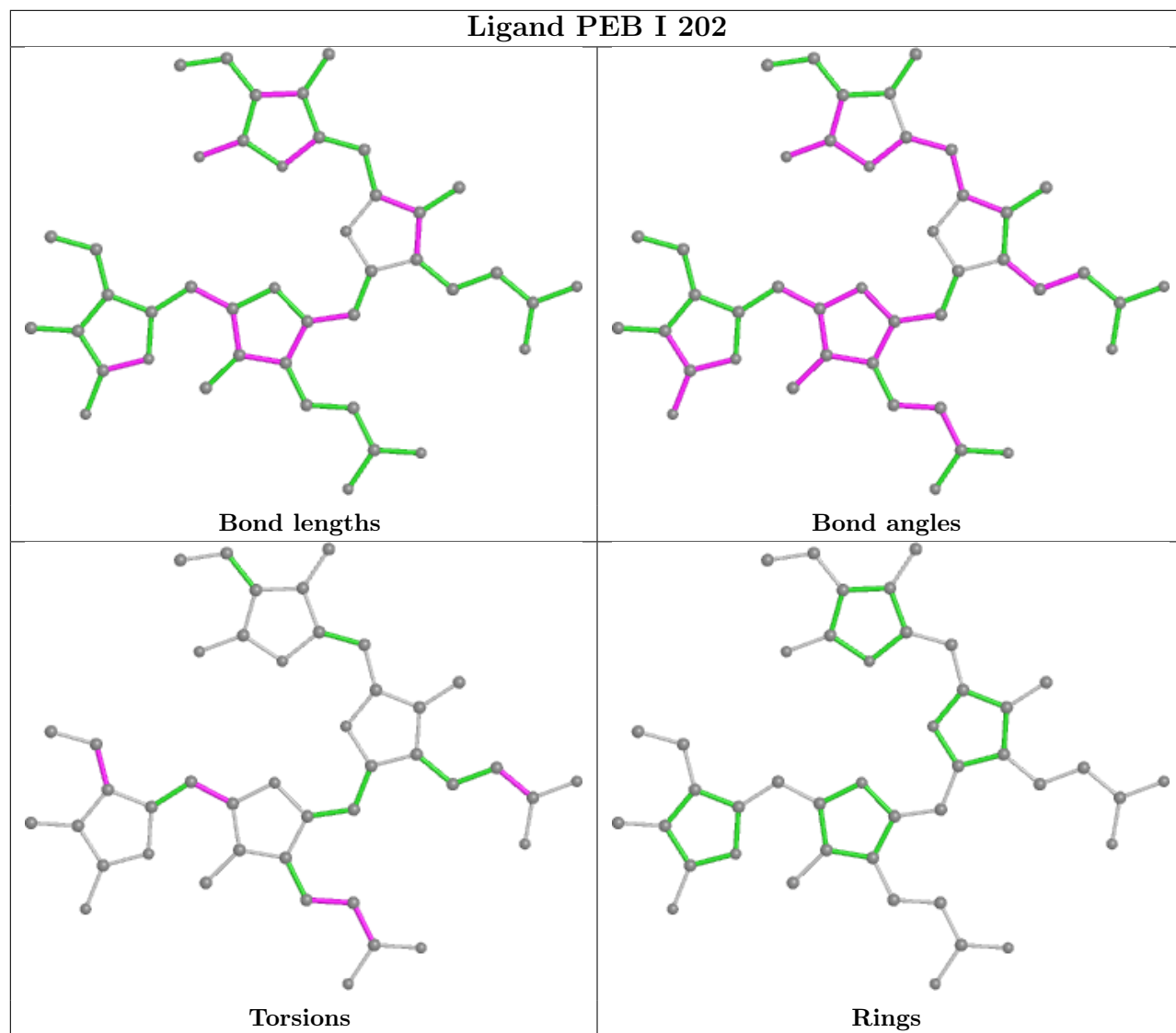


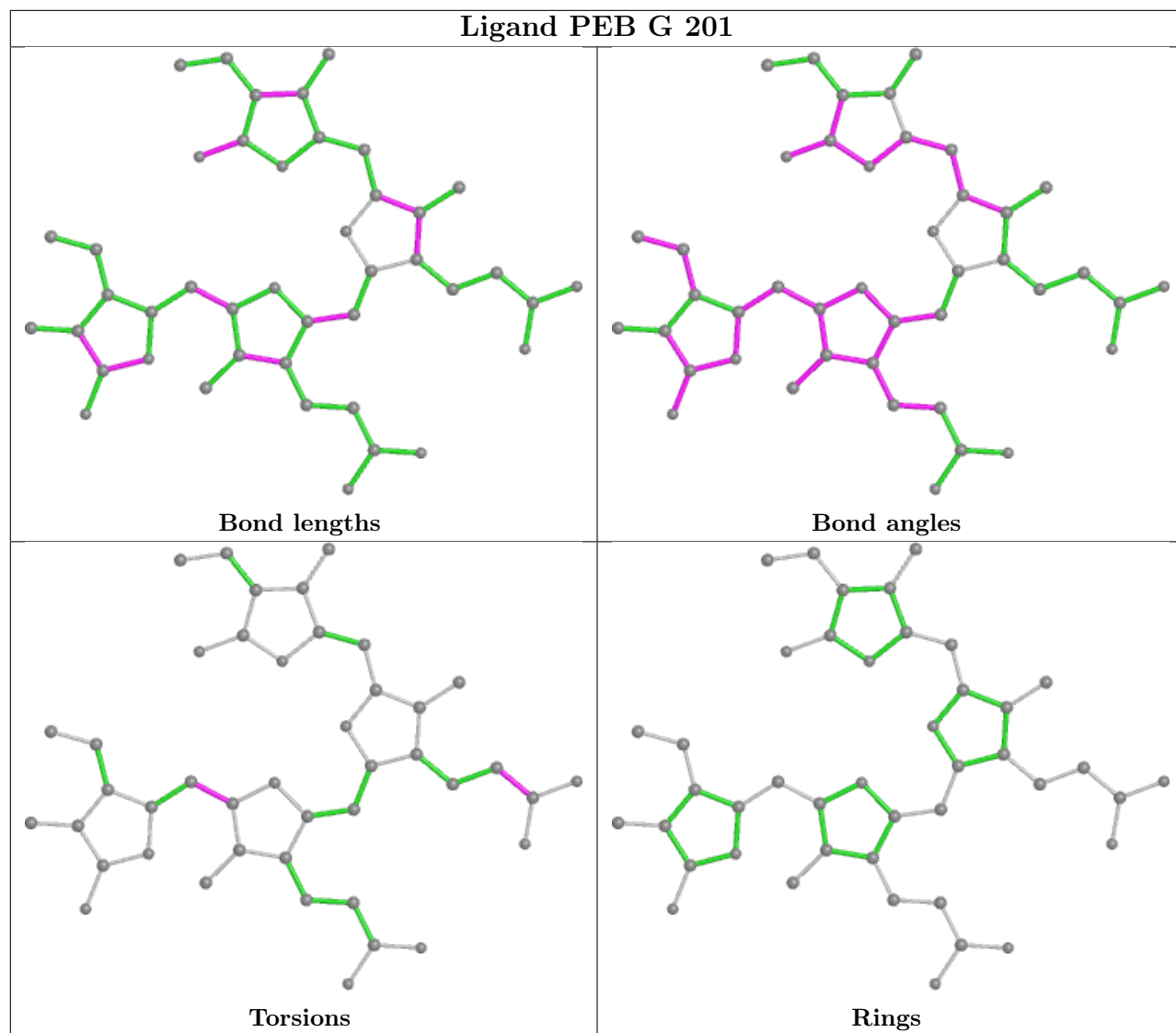


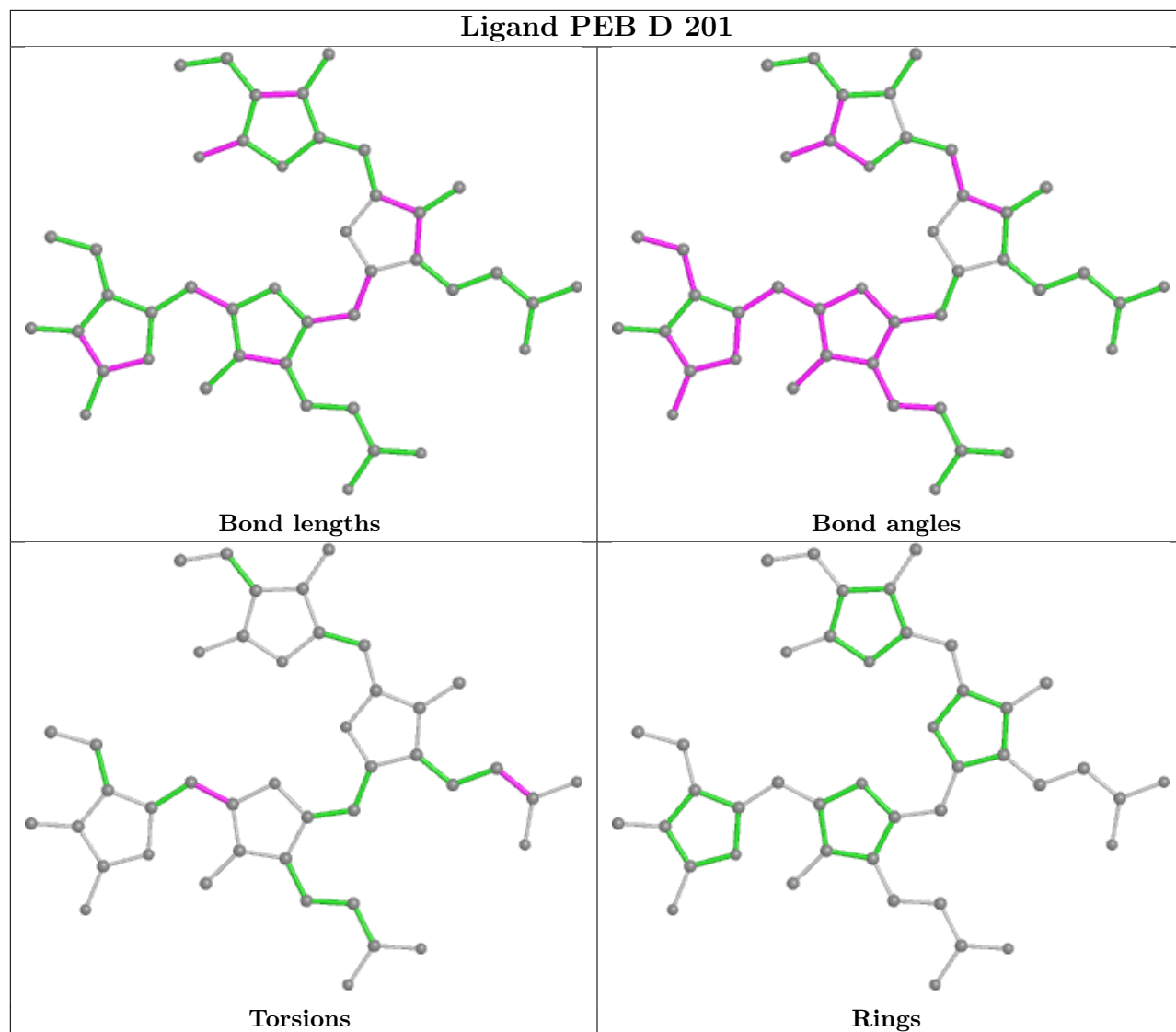


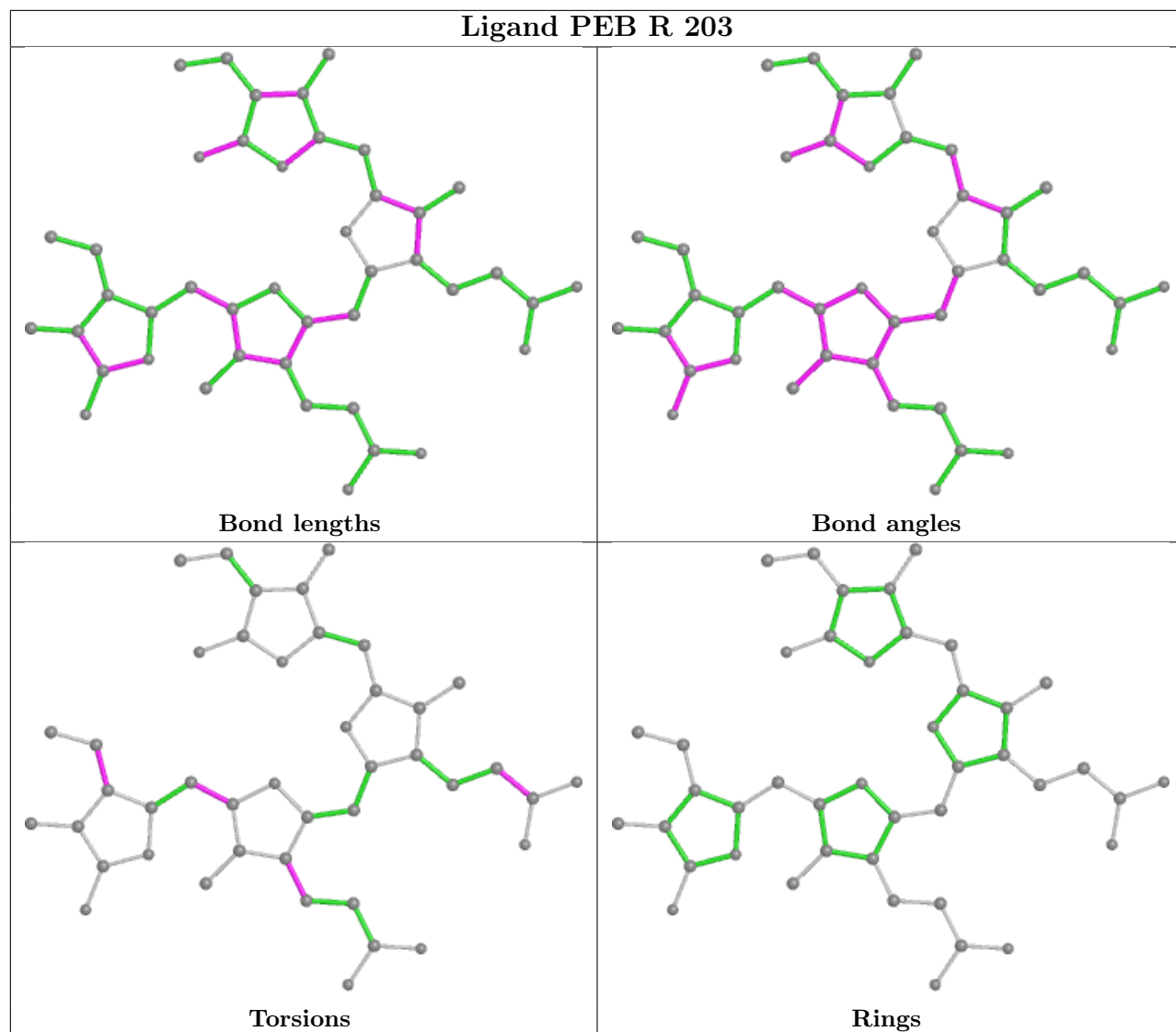


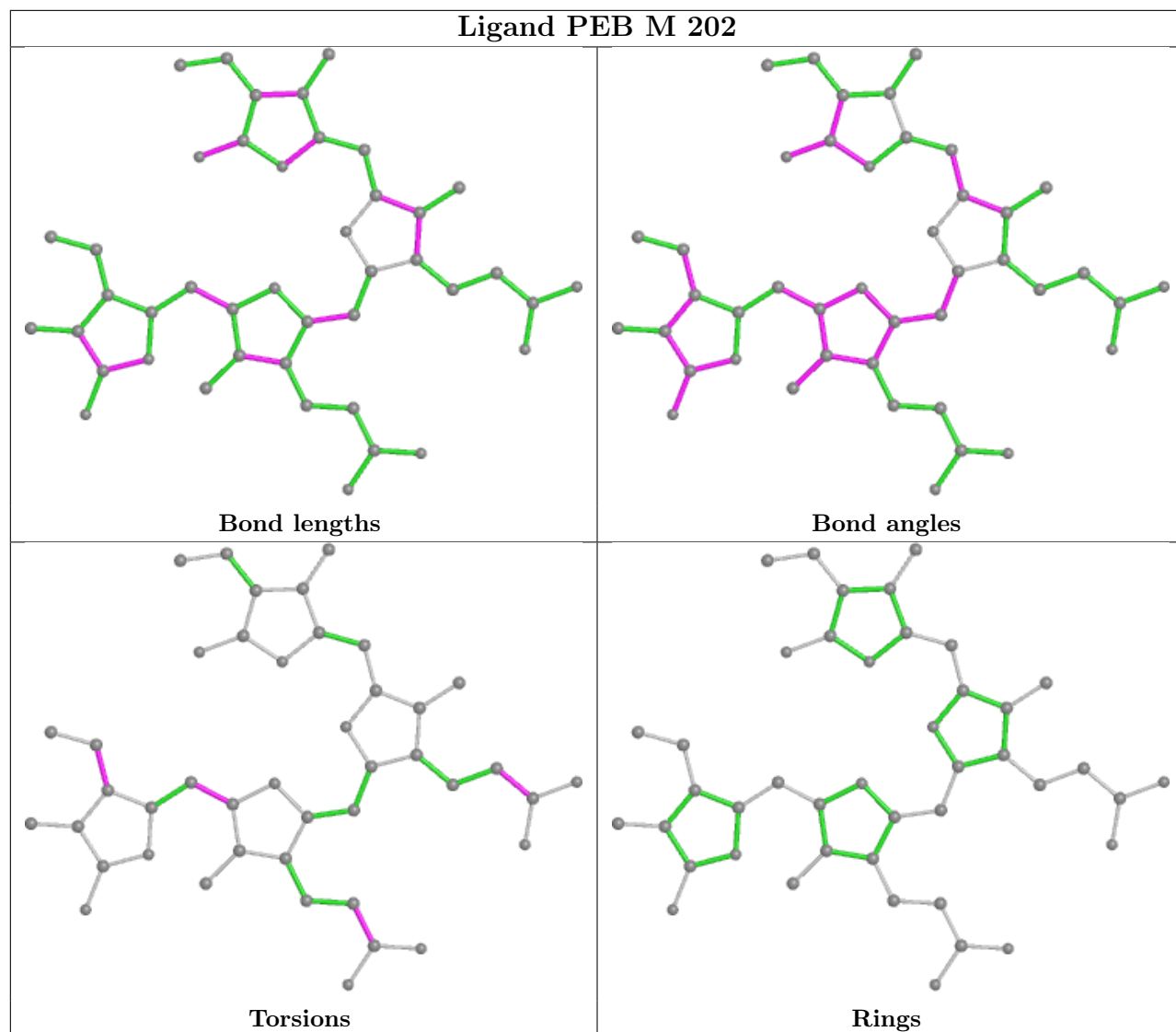


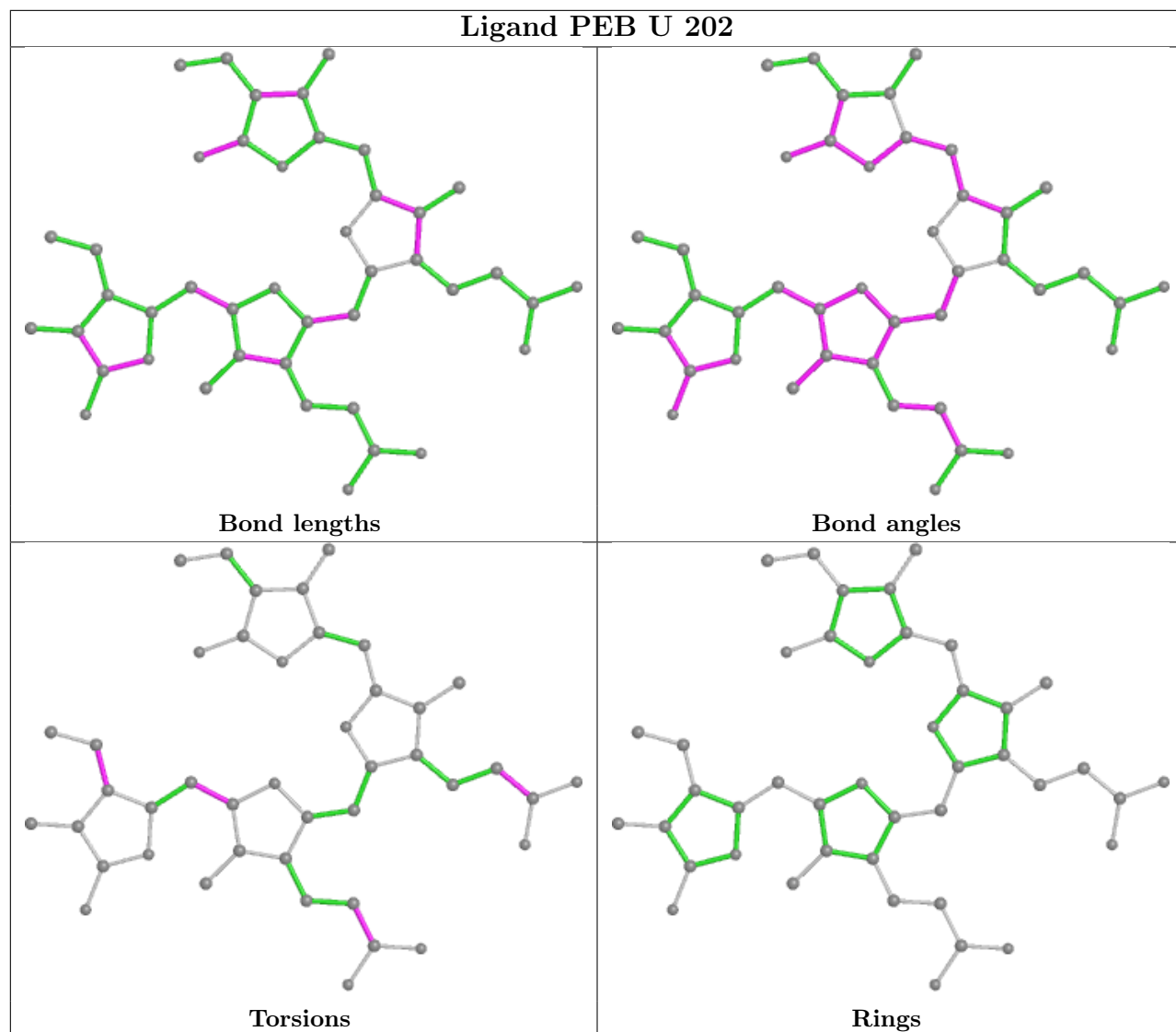


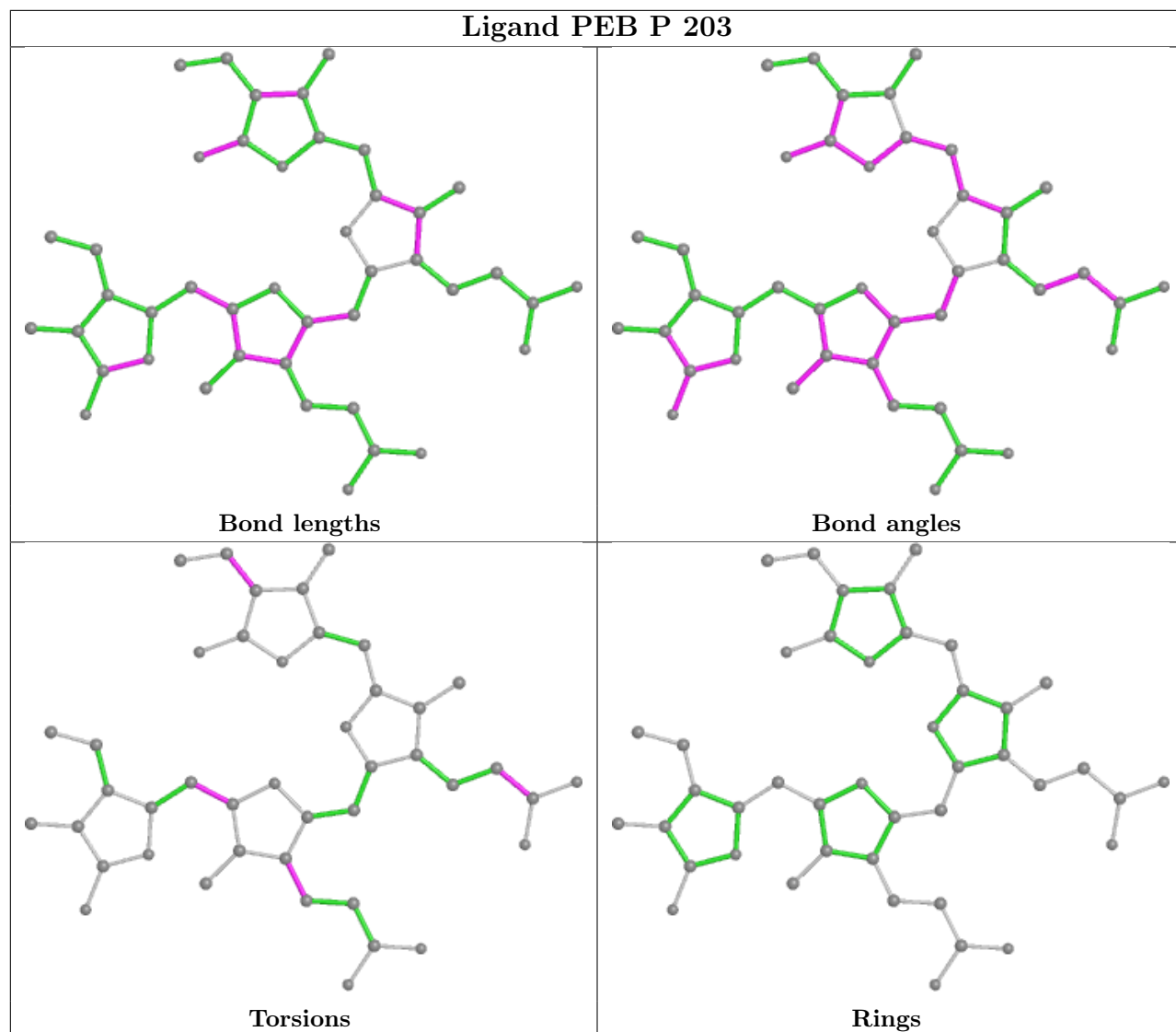


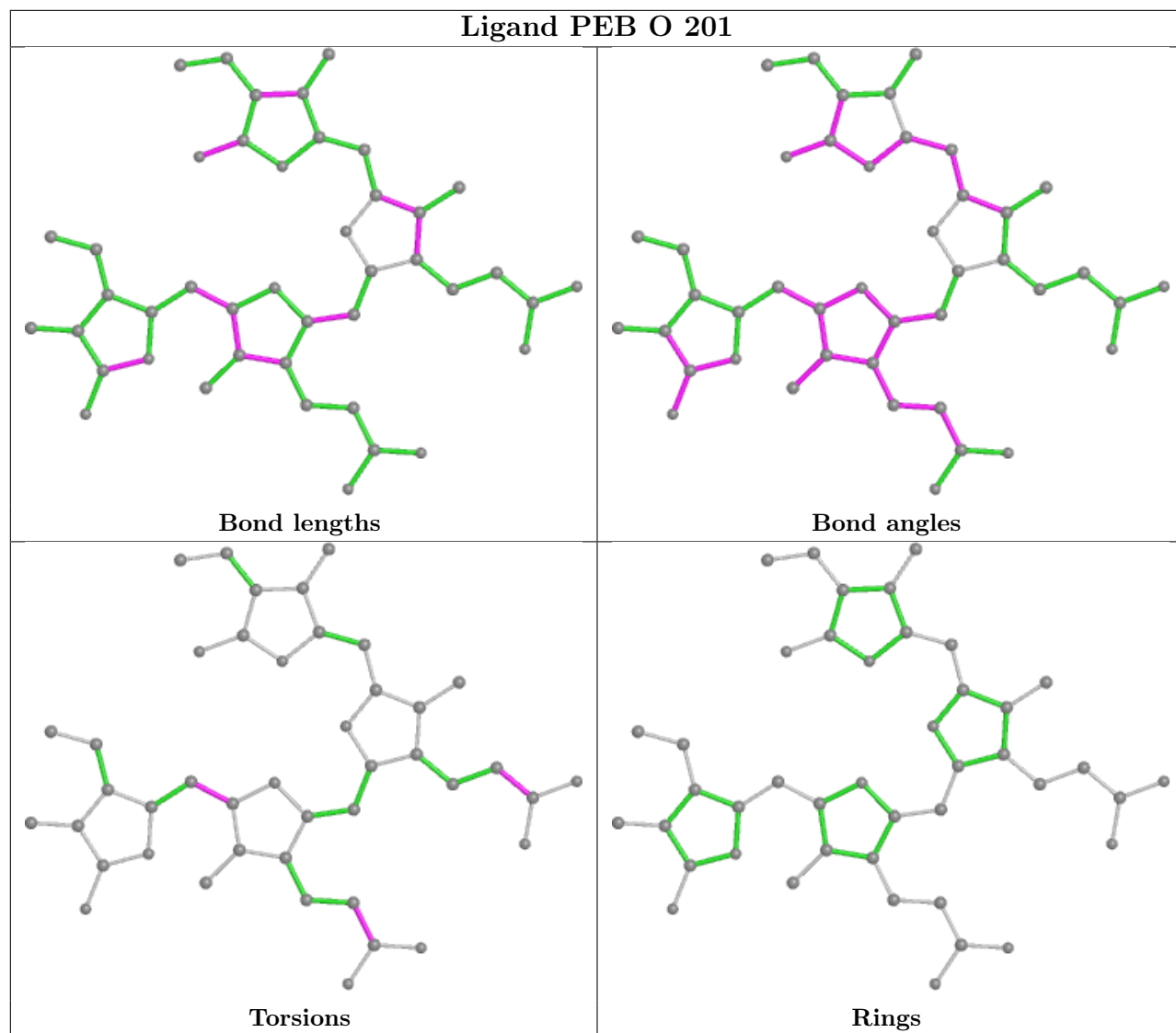


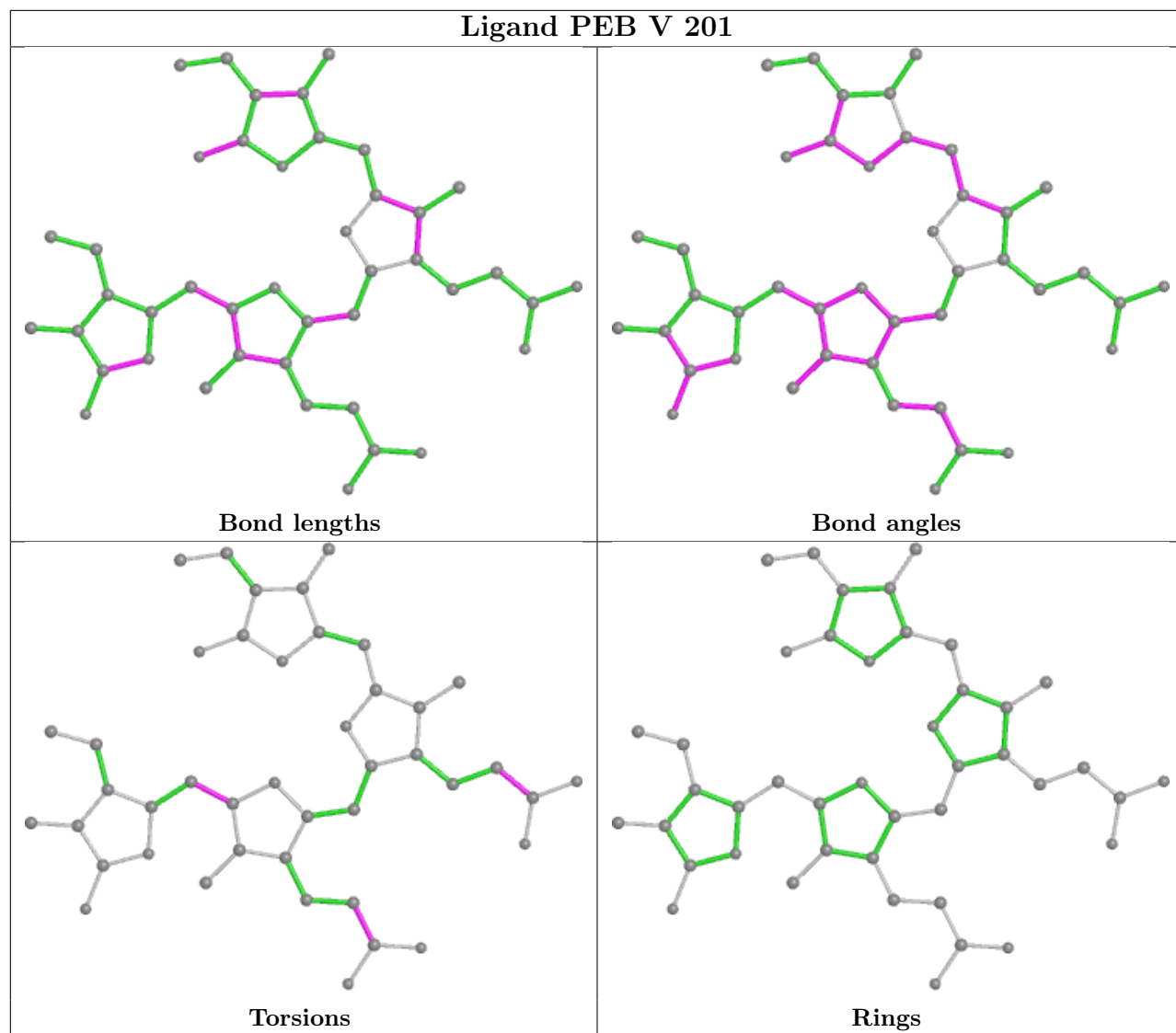


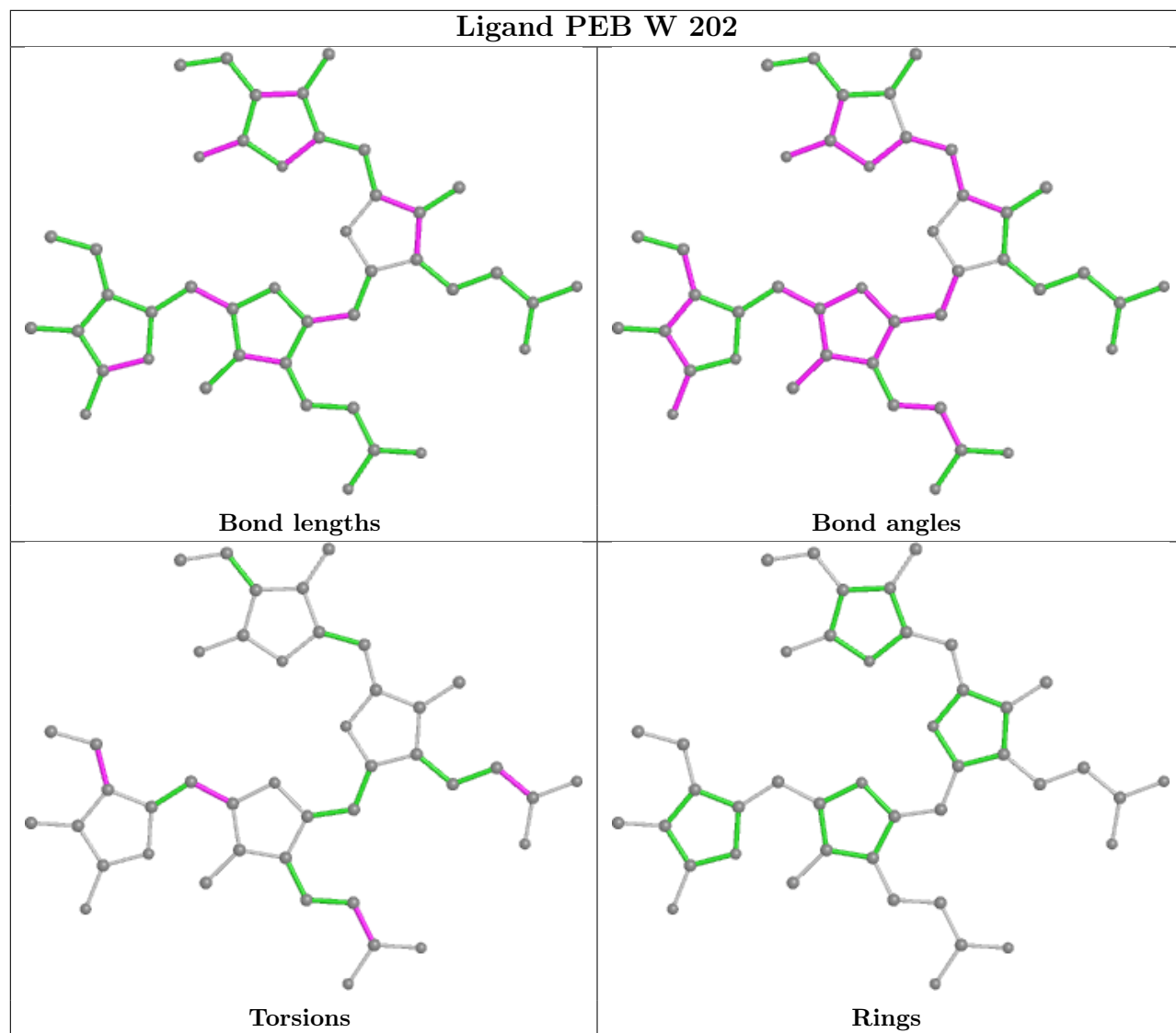


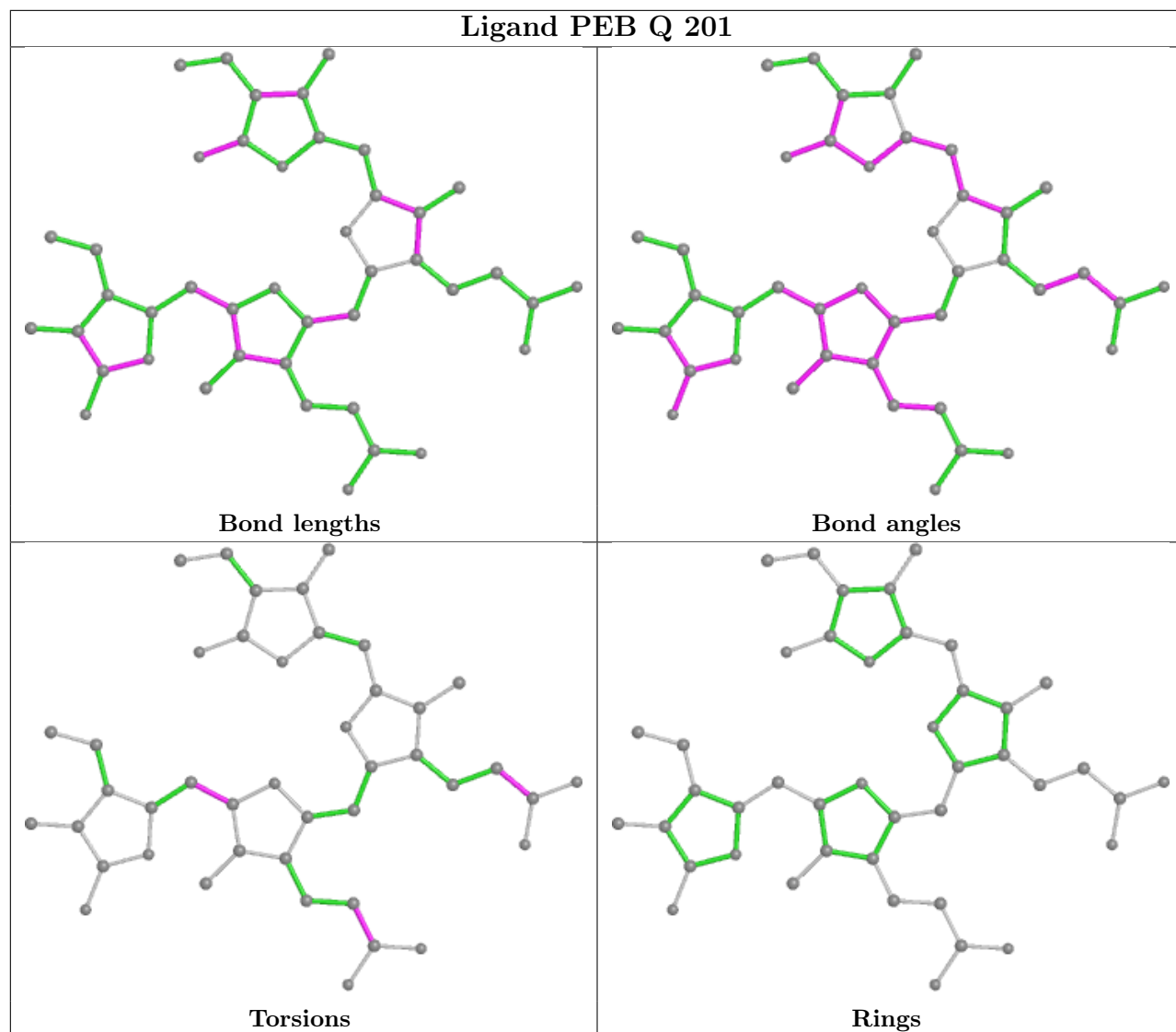


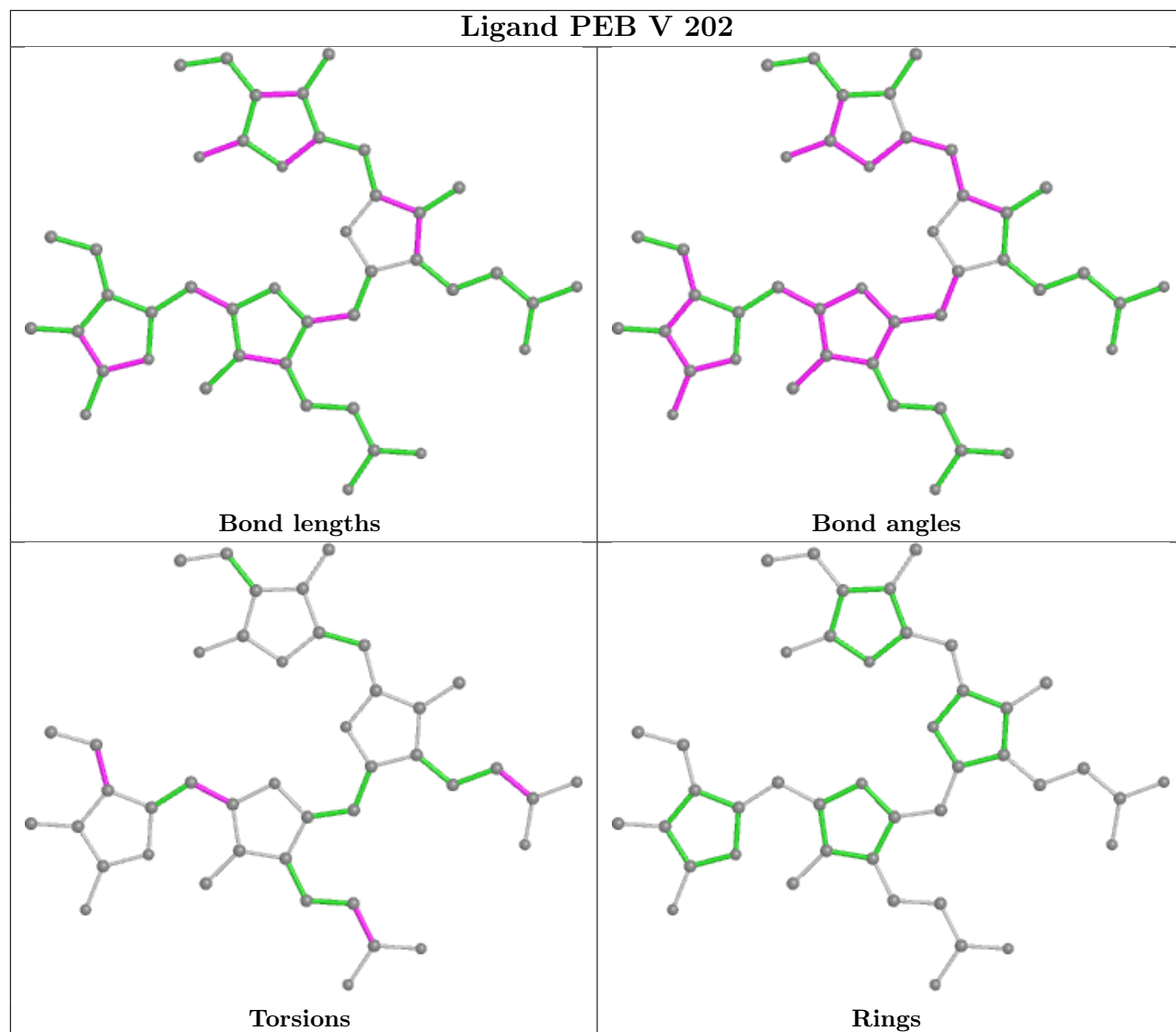


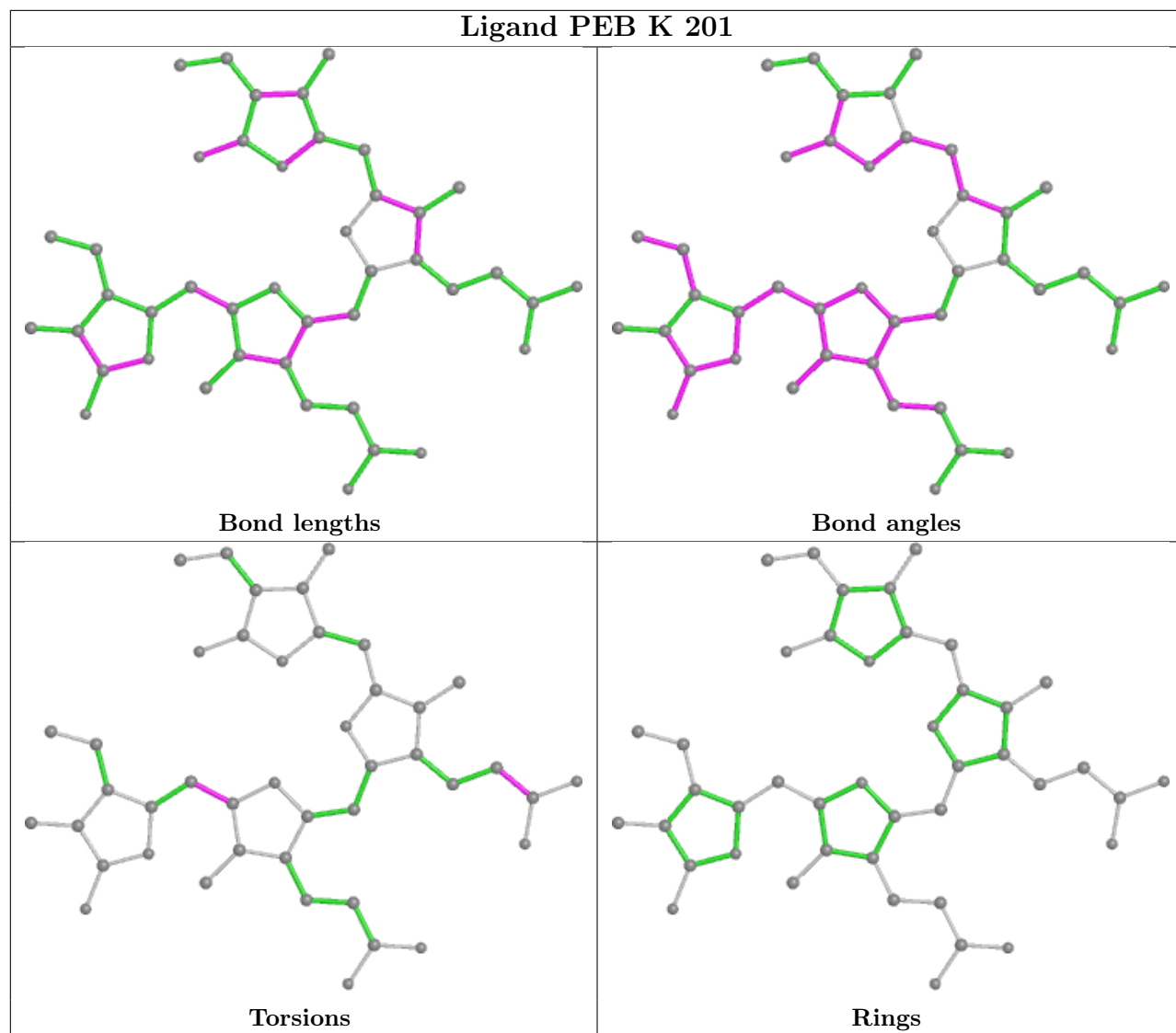


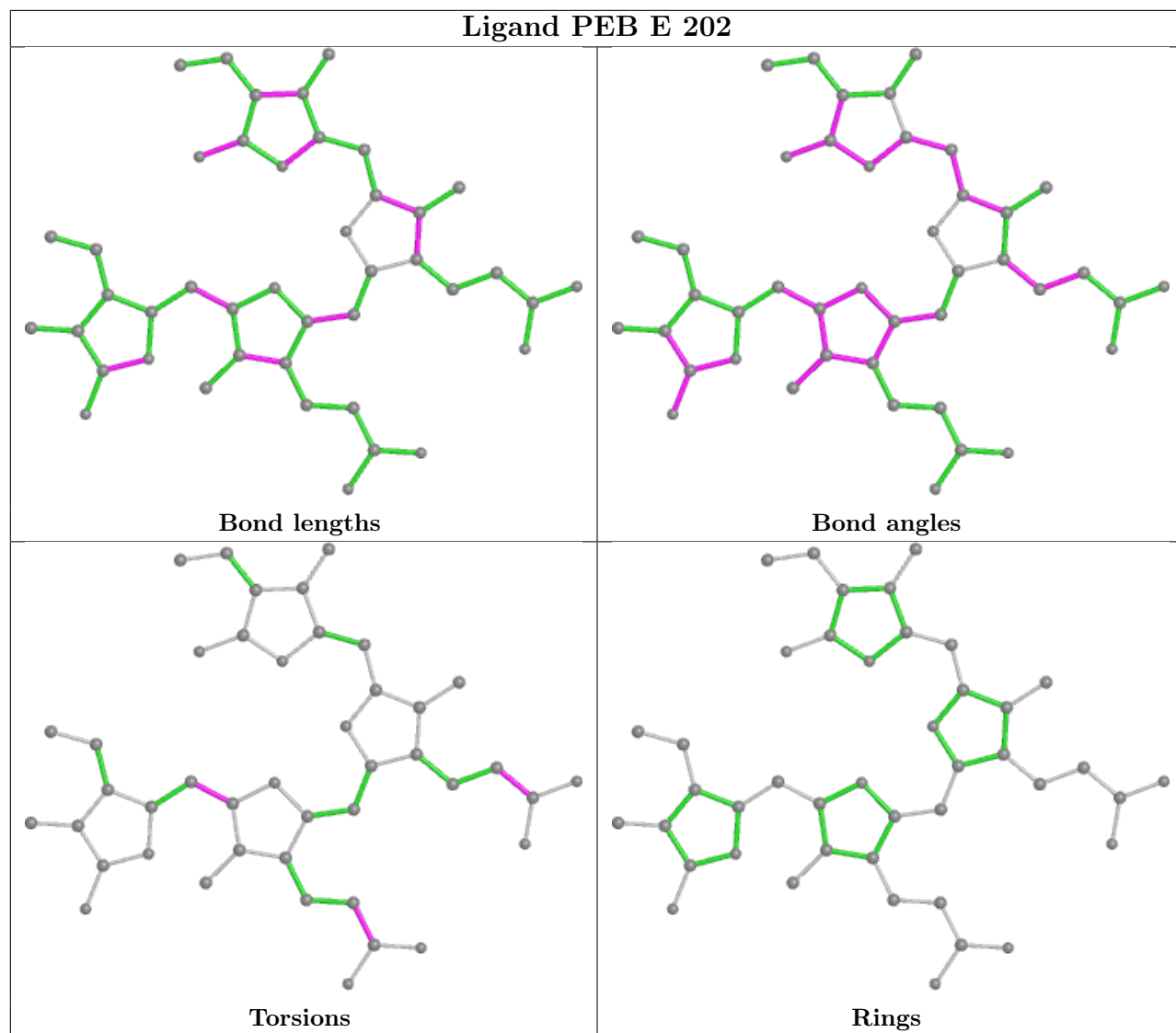


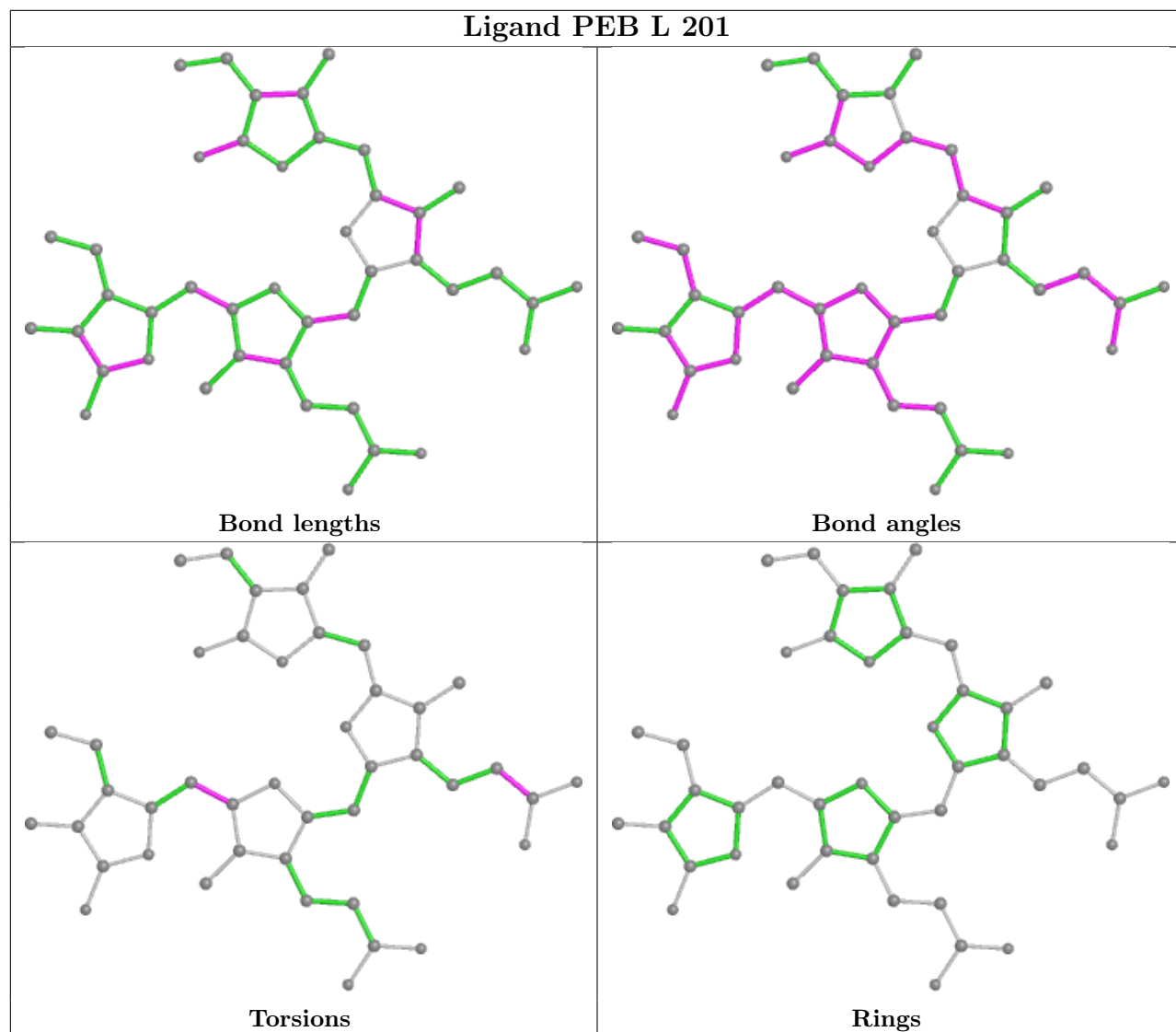


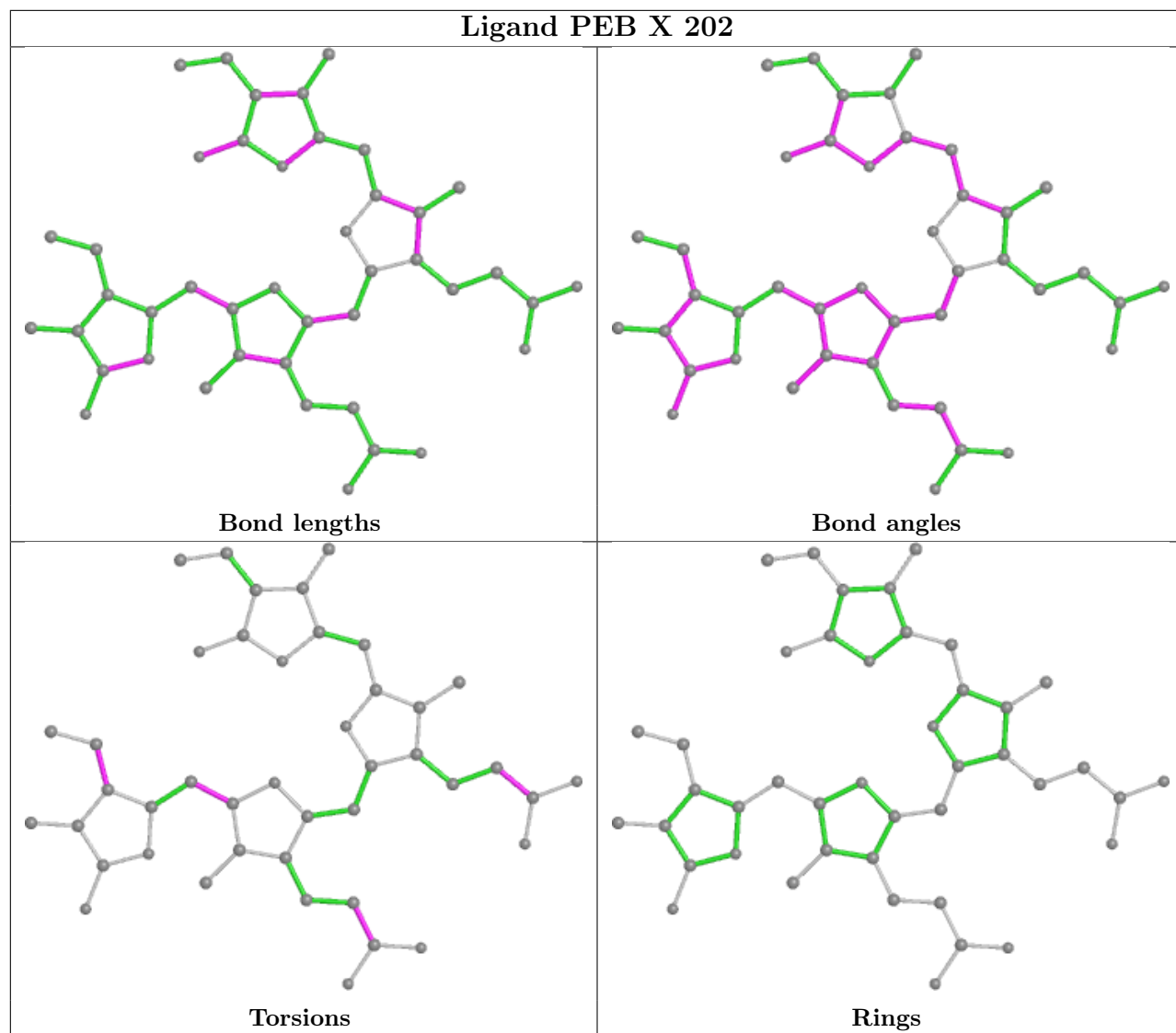


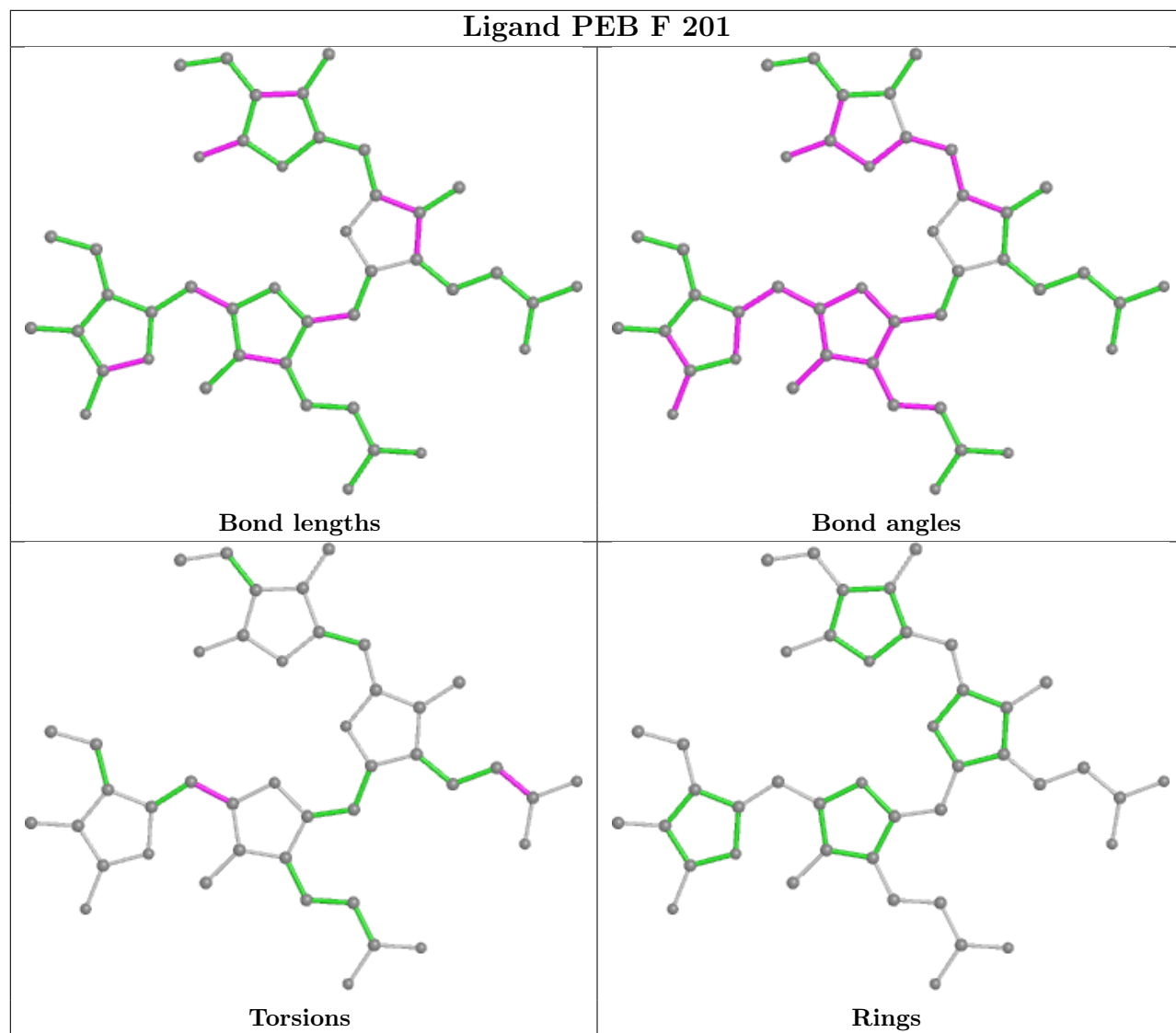


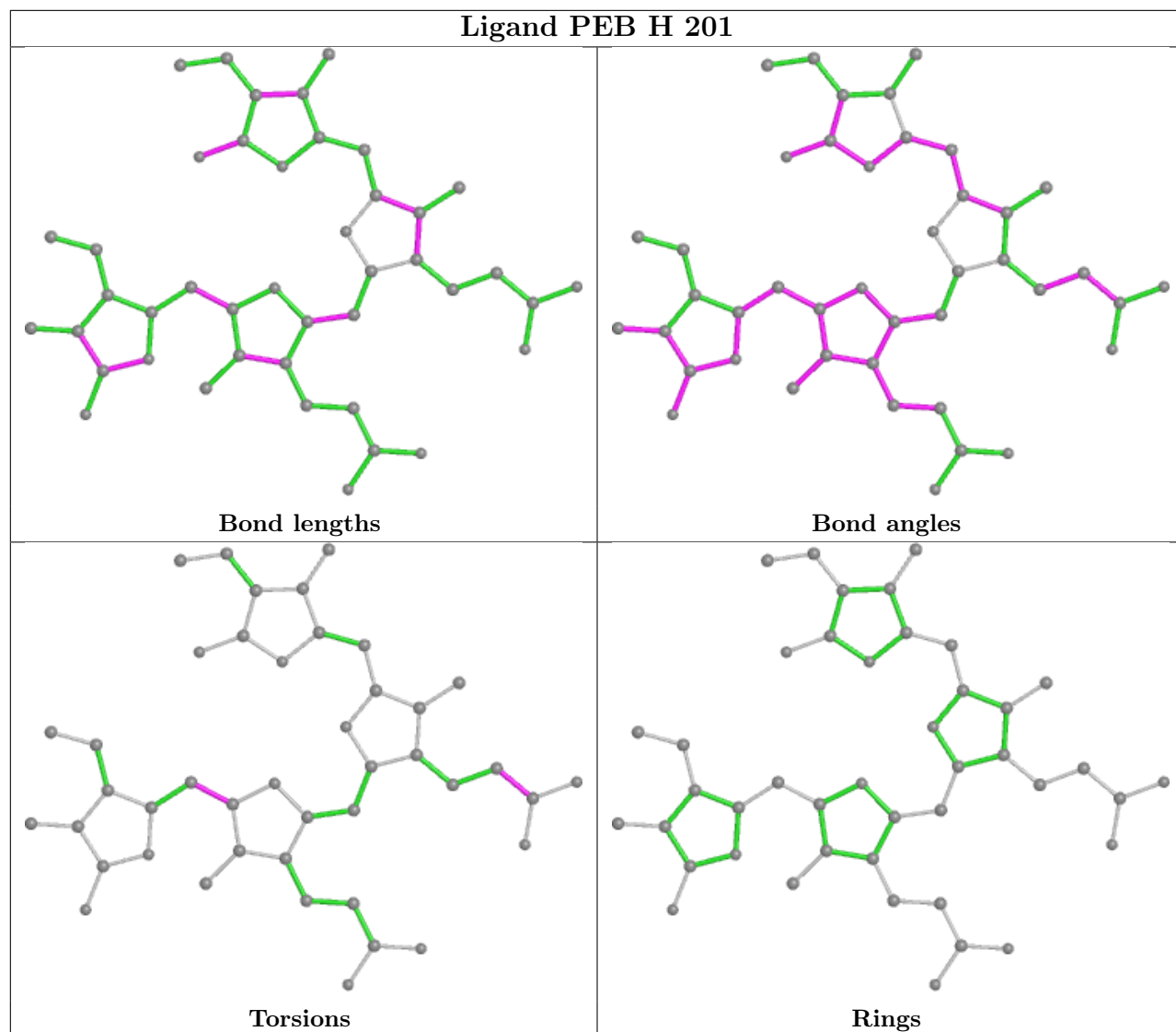


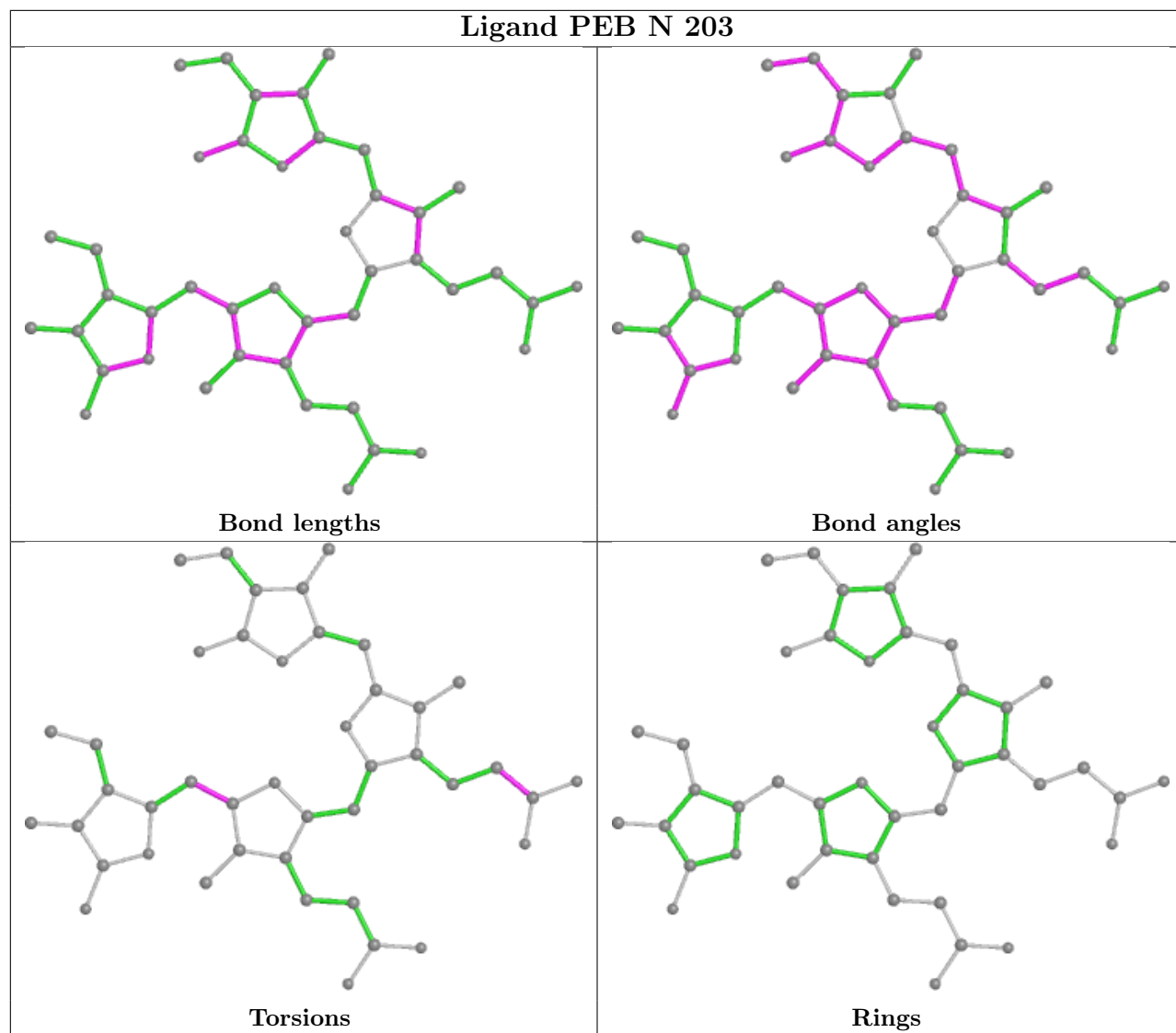


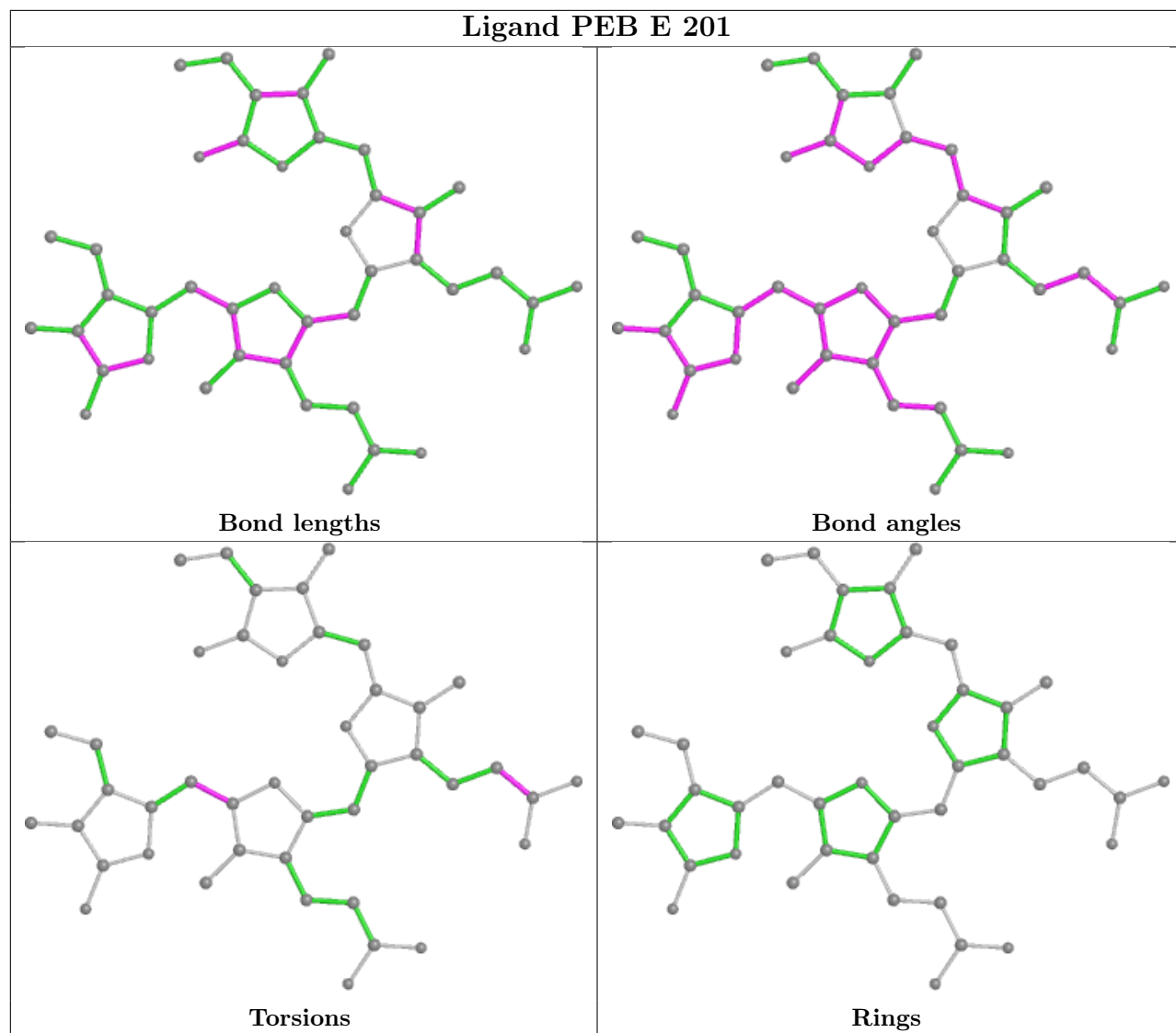


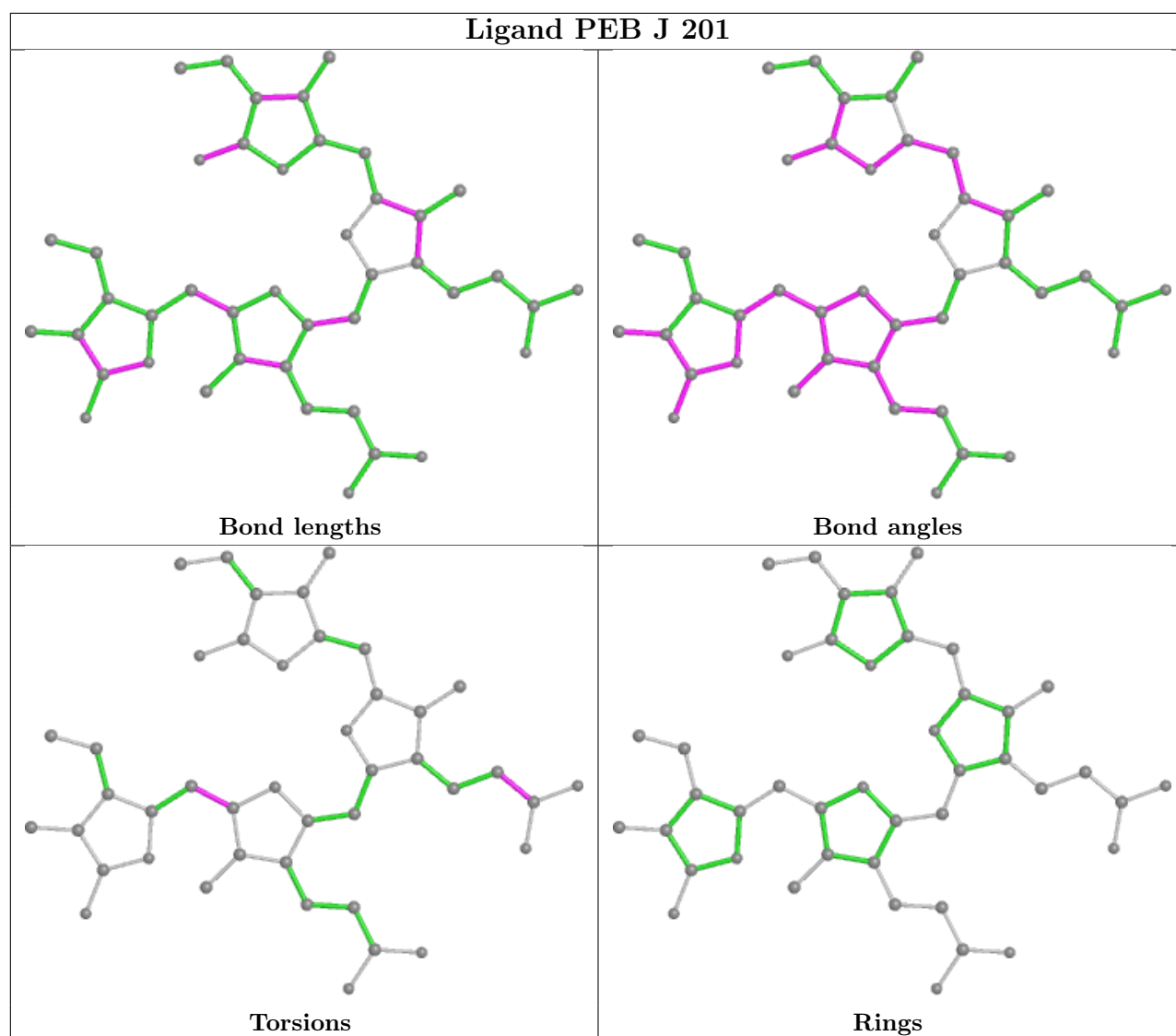












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.15	0 100 100	7, 12, 23, 32	0
1	B	164/164 (100%)	-0.10	0 100 100	10, 14, 24, 29	0
1	C	164/164 (100%)	-0.08	0 100 100	11, 18, 29, 37	0
1	D	164/164 (100%)	0.12	0 100 100	9, 18, 30, 35	0
1	E	164/164 (100%)	0.13	3 (1%) 68 74	10, 19, 33, 39	0
1	F	164/164 (100%)	0.16	0 100 100	15, 21, 27, 34	0
1	G	164/164 (100%)	-0.07	0 100 100	10, 17, 26, 32	0
1	H	164/164 (100%)	0.06	1 (0%) 89 92	11, 18, 28, 34	0
1	I	164/164 (100%)	0.21	1 (0%) 89 92	11, 20, 34, 44	0
1	J	164/164 (100%)	-0.20	0 100 100	8, 14, 26, 33	0
1	K	164/164 (100%)	0.02	0 100 100	10, 16, 26, 32	0
1	L	164/164 (100%)	-0.17	0 100 100	8, 13, 22, 29	0
2	M	183/184 (99%)	-0.12	1 (0%) 91 93	8, 14, 25, 41	0
2	N	183/184 (99%)	0.04	5 (2%) 54 61	12, 19, 33, 45	0
2	O	183/184 (99%)	-0.15	1 (0%) 91 93	10, 17, 27, 37	0
2	P	183/184 (99%)	0.13	7 (3%) 40 48	9, 18, 32, 50	0
2	Q	183/184 (99%)	0.05	5 (2%) 54 61	10, 18, 30, 44	0
2	R	183/184 (99%)	0.56	17 (9%) 8 13	16, 25, 38, 54	0
2	S	183/184 (99%)	0.05	5 (2%) 54 61	10, 18, 29, 45	0
2	T	183/184 (99%)	0.17	8 (4%) 34 41	12, 21, 33, 44	0
2	U	183/184 (99%)	0.20	10 (5%) 25 31	9, 18, 35, 52	0
2	V	183/184 (99%)	-0.14	1 (0%) 91 93	9, 15, 25, 37	0
2	W	183/184 (99%)	0.02	2 (1%) 80 84	11, 18, 30, 44	0
2	X	183/184 (99%)	-0.10	1 (0%) 91 93	9, 15, 26, 39	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4164/4176 (99%)	0.03	68 (1%) 72 77	7, 17, 31, 54	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	150	GLY	4.0
2	R	183	LEU	3.9
2	U	24	ALA	3.6
2	R	110	GLY	3.6
2	U	21	ASP	3.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	P	70	9/10	0.94	0.13	15,17,21,21	0
2	MEN	S	70	9/10	0.94	0.10	17,18,21,21	0
2	MEN	N	70	9/10	0.95	0.10	15,17,19,19	0
2	MEN	O	70	9/10	0.95	0.08	12,14,17,19	0
2	MEN	U	70	9/10	0.95	0.09	14,17,19,20	0
2	MEN	Q	70	9/10	0.96	0.08	13,15,17,19	0
2	MEN	T	70	9/10	0.96	0.11	18,21,24,25	0
2	MEN	R	70	9/10	0.96	0.11	23,24,28,29	0
2	MEN	X	70	9/10	0.96	0.08	13,14,17,18	0
2	MEN	V	70	9/10	0.97	0.10	10,14,18,20	0
2	MEN	W	70	9/10	0.97	0.09	10,13,15,17	0
2	MEN	M	70	9/10	0.97	0.08	12,13,15,17	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	203	6/6	0.73	0.20	21,24,29,32	0
4	GOL	C	203	6/6	0.79	0.13	30,32,34,38	0
4	GOL	H	203	6/6	0.81	0.16	25,34,42,42	0
4	GOL	J	203	6/6	0.81	0.16	25,28,29,40	0
4	GOL	K	203	6/6	0.82	0.22	26,31,32,35	0
4	GOL	E	203	6/6	0.85	0.20	20,23,26,40	0
3	PEB	Q	202	43/43	0.85	0.15	11,19,31,39	0
4	GOL	D	203	6/6	0.86	0.16	21,23,26,38	0
4	GOL	B	203	6/6	0.86	0.14	27,28,30,33	0
4	GOL	G	203	6/6	0.86	0.11	21,25,28,32	0
3	PEB	W	202	43/43	0.87	0.14	15,22,31,34	0
3	PEB	I	201	43/43	0.87	0.13	17,25,30,36	0
3	PEB	F	202	43/43	0.88	0.19	20,28,31,36	0
3	PEB	R	202	43/43	0.88	0.17	16,24,30,39	0
3	PEB	I	202	43/43	0.88	0.16	20,30,36,40	0
3	PEB	R	201	43/43	0.89	0.17	19,26,34,42	0
3	PEB	T	202	43/43	0.89	0.15	11,21,32,34	0
3	PEB	D	202	43/43	0.90	0.16	18,30,36,39	0
3	PEB	E	202	43/43	0.90	0.14	18,28,32,36	0
3	PEB	D	201	43/43	0.90	0.12	15,20,26,36	0
3	PEB	H	202	43/43	0.90	0.15	19,28,36,42	0
3	PEB	E	201	43/43	0.91	0.13	19,23,30,43	0
3	PEB	R	203	43/43	0.91	0.13	15,23,31,38	0
3	PEB	N	202	43/43	0.91	0.12	14,22,26,29	0
4	GOL	I	203	6/6	0.91	0.12	24,28,30,31	0
3	PEB	T	203	43/43	0.91	0.12	15,21,30,33	0
3	PEB	V	202	43/43	0.91	0.12	9,17,25,34	0
4	GOL	L	203	6/6	0.91	0.10	21,22,29,31	0
3	PEB	F	201	43/43	0.92	0.12	14,19,22,25	0
3	PEB	O	202	43/43	0.92	0.12	14,21,33,41	0
3	PEB	M	202	43/43	0.92	0.12	11,17,25,34	0
3	PEB	X	202	43/43	0.92	0.11	12,17,24,31	0
3	PEB	Q	203	43/43	0.92	0.12	12,17,23,26	0
3	PEB	P	201	43/43	0.93	0.12	11,17,30,37	0
3	PEB	S	201	43/43	0.93	0.12	13,18,26,36	0
3	PEB	T	201	43/43	0.93	0.12	18,22,30,35	0
3	PEB	Q	201	43/43	0.93	0.10	12,17,27,30	0
3	PEB	C	201	43/43	0.93	0.11	11,19,25,32	0
3	PEB	U	202	43/43	0.93	0.11	8,15,23,27	0
3	PEB	V	201	43/43	0.93	0.11	10,15,24,37	0
3	PEB	J	201	43/43	0.93	0.11	12,16,21,26	0

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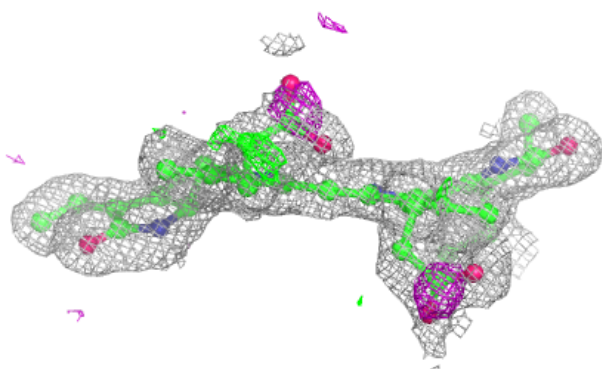
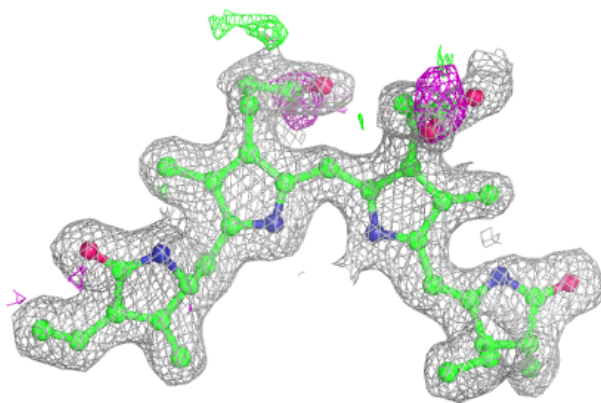
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEB	N	203	43/43	0.93	0.14	14,20,26,30	0
3	PEB	W	203	43/43	0.93	0.12	12,17,21,25	0
3	PEB	M	201	43/43	0.93	0.12	9,14,23,29	0
3	PEB	P	202	43/43	0.94	0.11	10,16,22,29	0
3	PEB	P	203	43/43	0.94	0.10	8,13,21,29	0
3	PEB	V	203	43/43	0.94	0.12	10,15,18,27	0
3	PEB	W	201	43/43	0.94	0.10	11,15,23,28	0
3	PEB	K	201	43/43	0.94	0.10	10,16,21,27	0
3	PEB	K	202	43/43	0.94	0.10	10,16,22,28	0
3	PEB	X	201	43/43	0.94	0.11	8,13,24,31	0
3	PEB	G	202	43/43	0.94	0.13	11,21,25,29	0
3	PEB	X	203	43/43	0.94	0.12	10,14,22,28	0
3	PEB	H	201	43/43	0.94	0.11	13,19,25,34	0
3	PEB	M	203	43/43	0.94	0.11	9,14,22,32	0
3	PEB	B	201	43/43	0.94	0.10	10,14,22,29	0
3	PEB	A	201	43/43	0.94	0.10	8,13,17,25	0
3	PEB	S	202	43/43	0.94	0.12	11,17,25,37	0
3	PEB	S	203	43/43	0.94	0.09	10,16,21,26	0
3	PEB	O	201	43/43	0.94	0.10	10,16,26,32	0
3	PEB	C	202	43/43	0.94	0.13	10,16,23,27	0
3	PEB	O	203	43/43	0.94	0.14	12,16,22,27	0
3	PEB	U	201	43/43	0.94	0.11	10,16,26,31	0
3	PEB	G	201	43/43	0.94	0.10	12,17,22,29	0
3	PEB	N	201	43/43	0.95	0.10	12,17,23,31	0
3	PEB	L	201	43/43	0.95	0.09	9,13,16,25	0
3	PEB	J	202	43/43	0.95	0.12	8,14,19,24	0
3	PEB	U	203	43/43	0.95	0.09	8,14,21,30	0
3	PEB	B	202	43/43	0.95	0.09	9,16,24,28	0
3	PEB	A	202	43/43	0.95	0.09	10,15,18,19	0
3	PEB	L	202	43/43	0.96	0.09	6,12,16,19	0

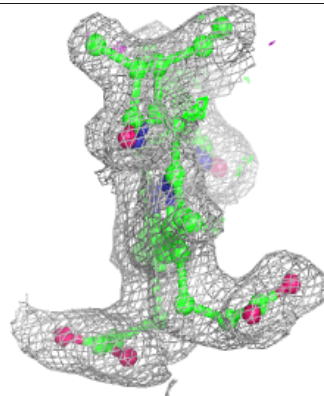
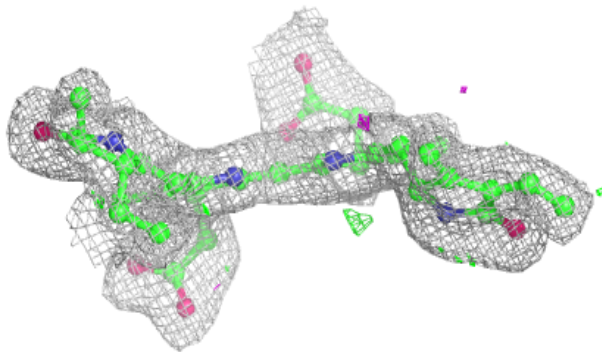
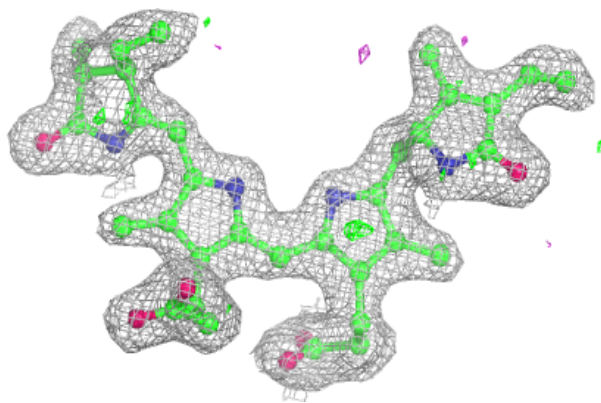
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEB Q 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

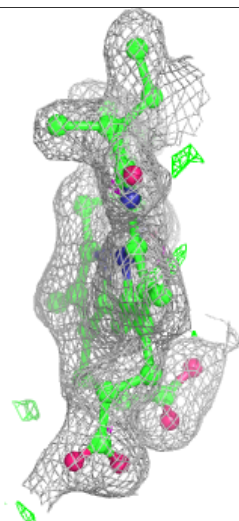
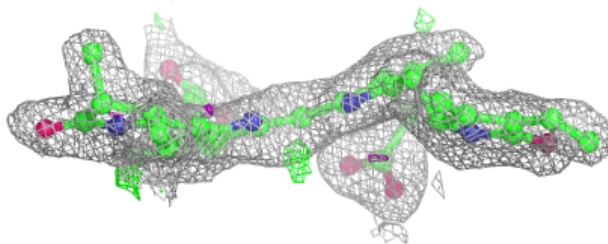
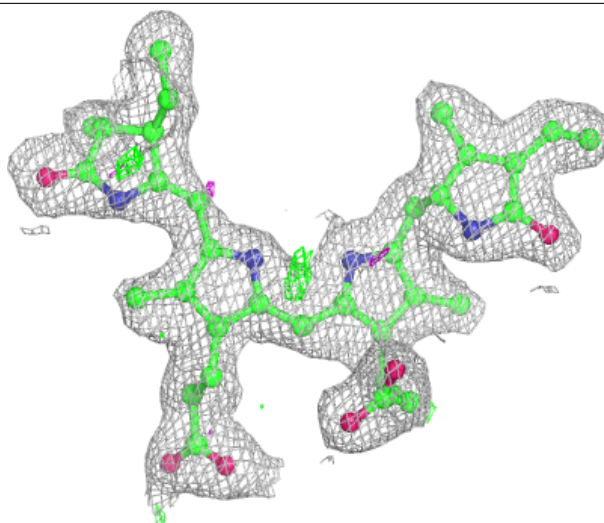
**Electron density around PEB W 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



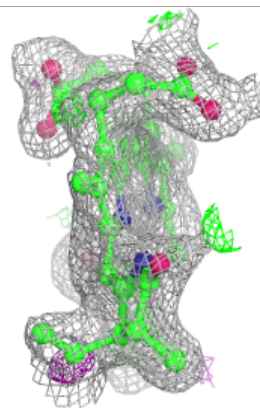
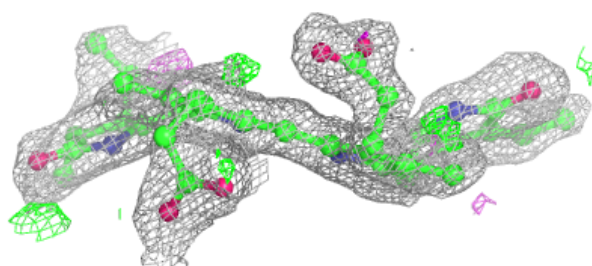
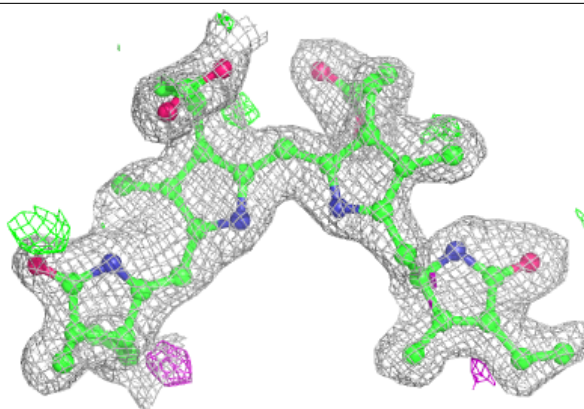
Electron density around PEB I 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

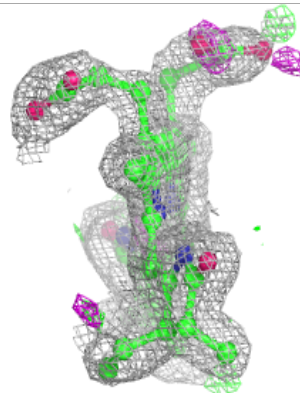
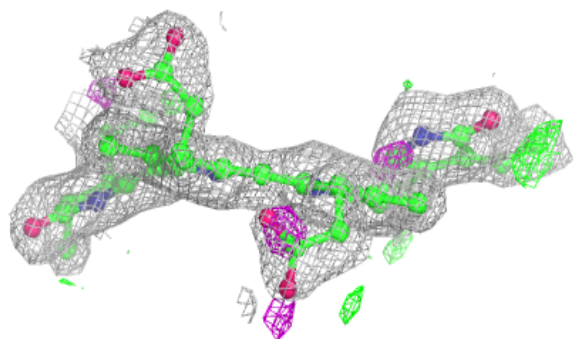
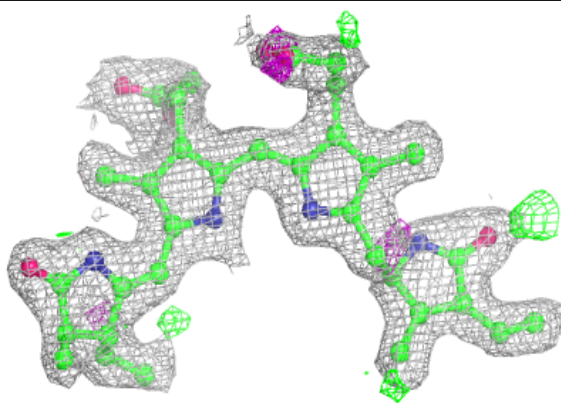


Electron density around PEB F 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

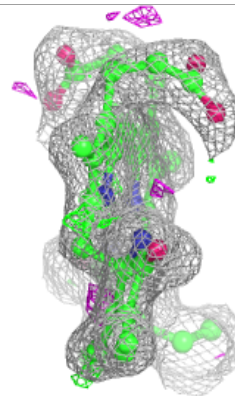
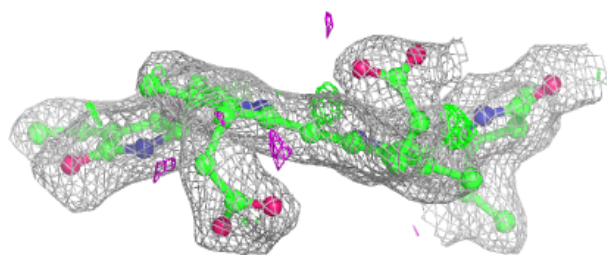
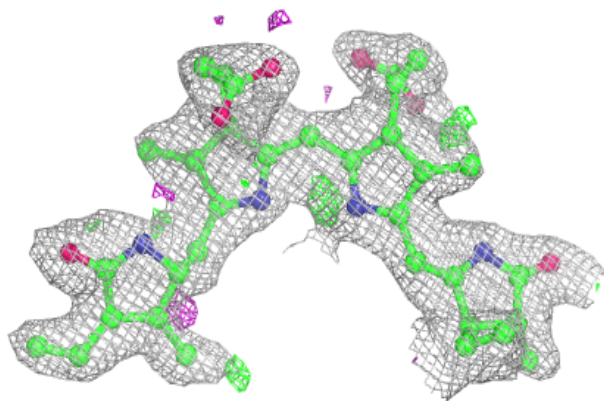
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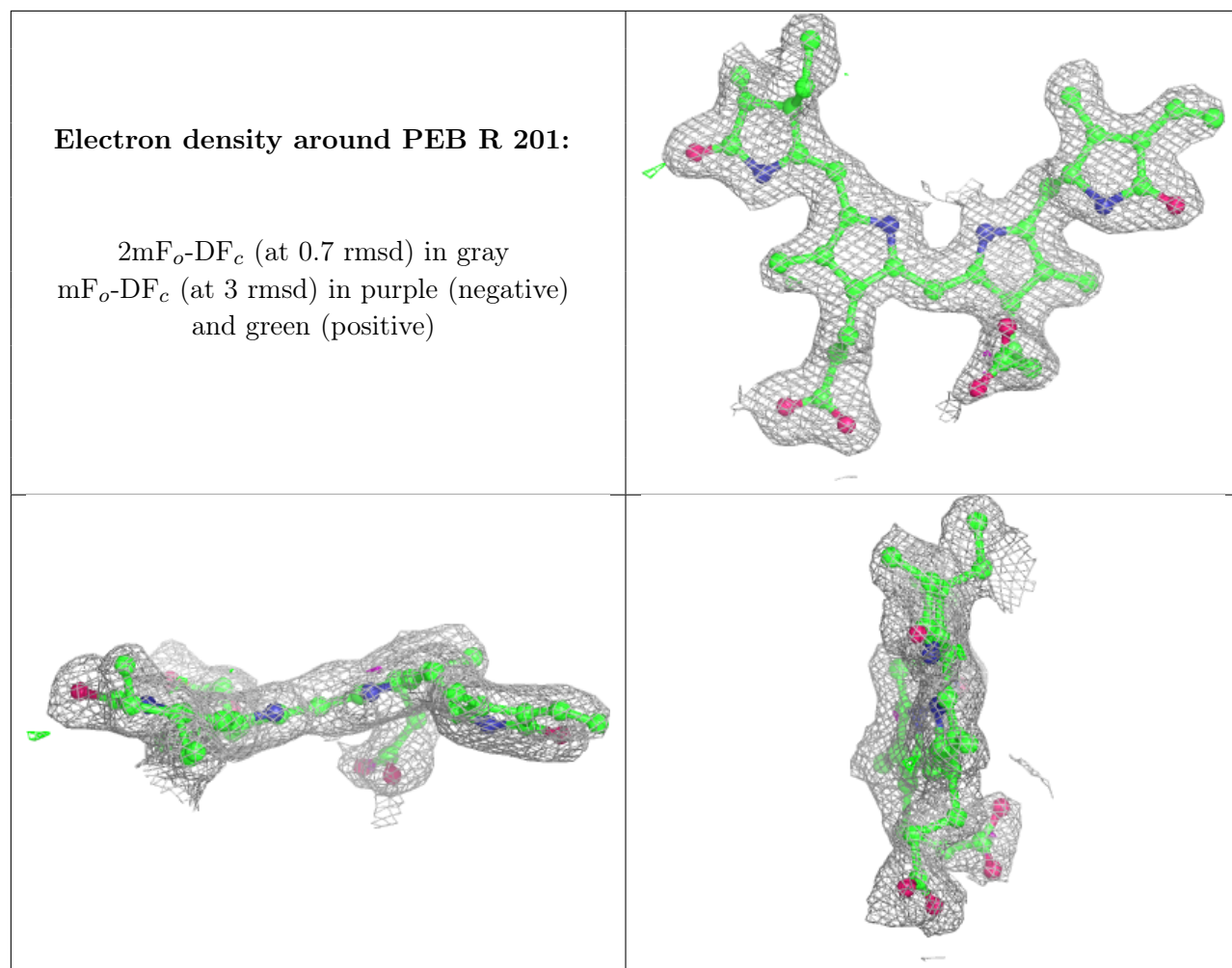
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB I 202:

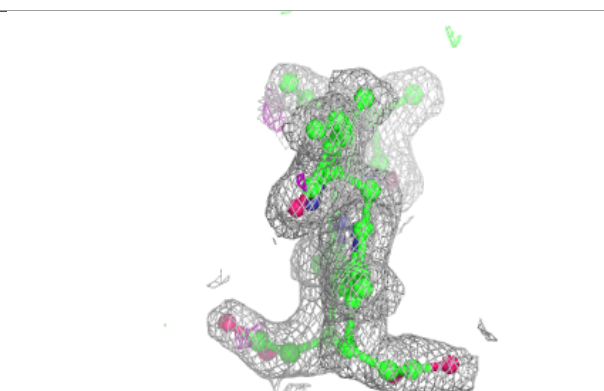
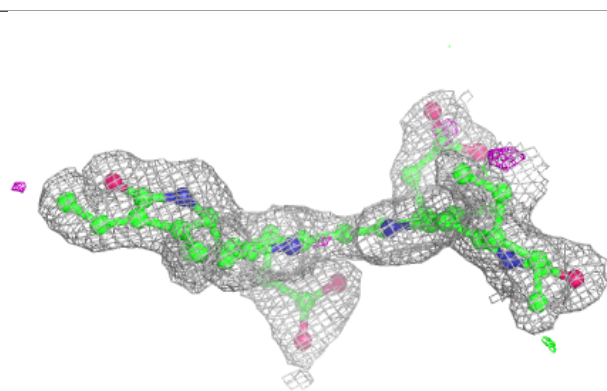
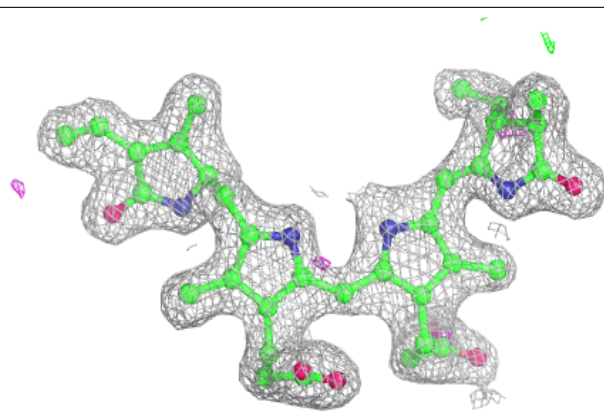
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



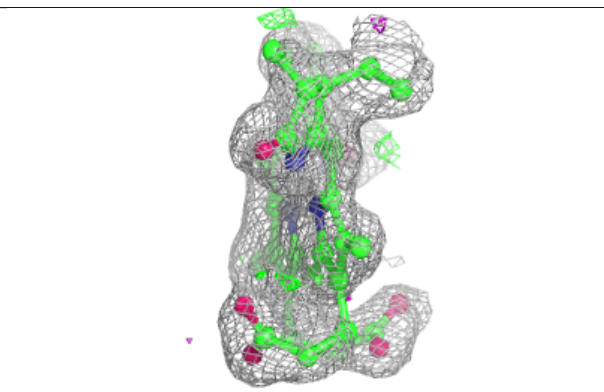
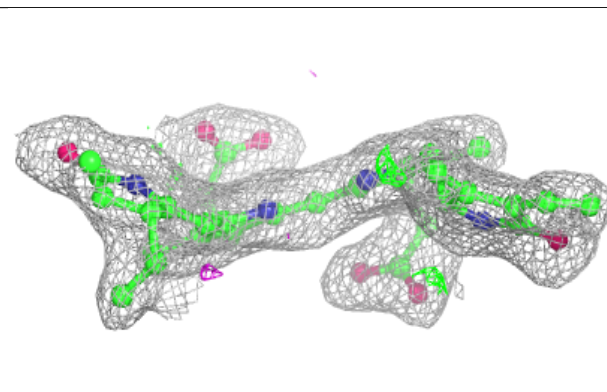
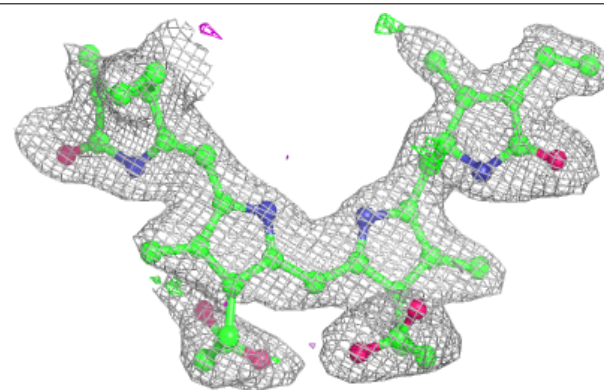


Electron density around PEB T 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

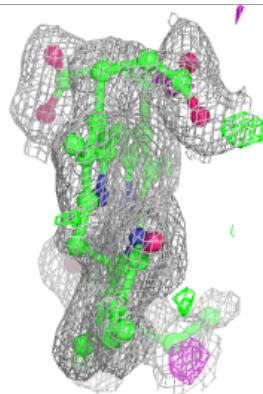
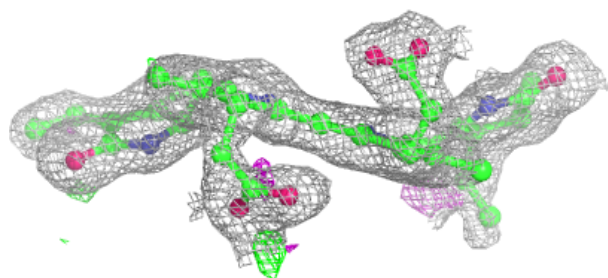
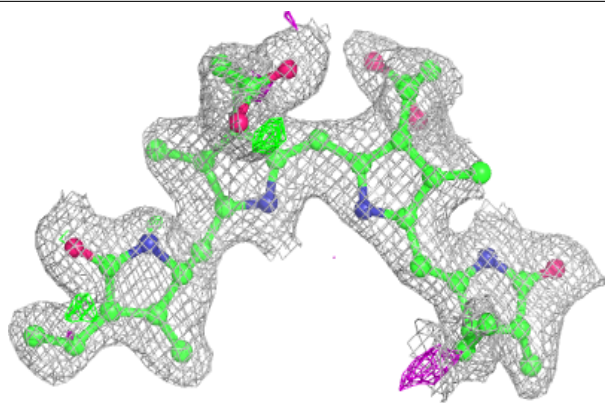
**Electron density around PEB D 202:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



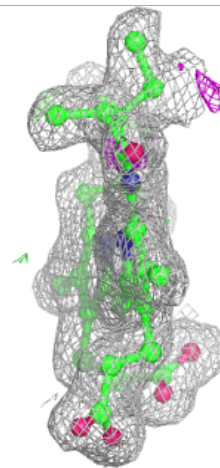
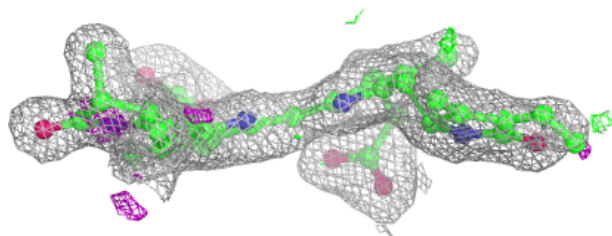
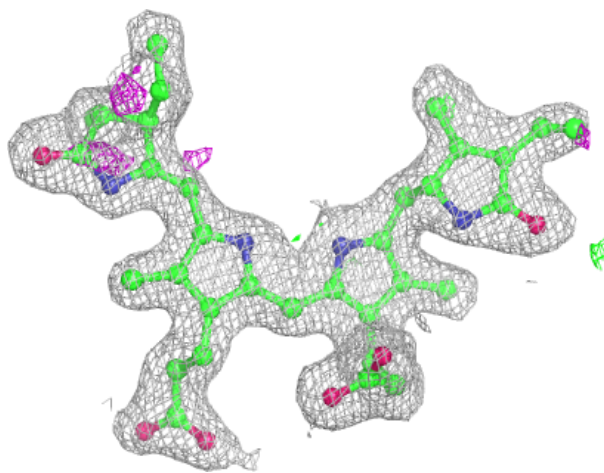
Electron density around PEB E 202:

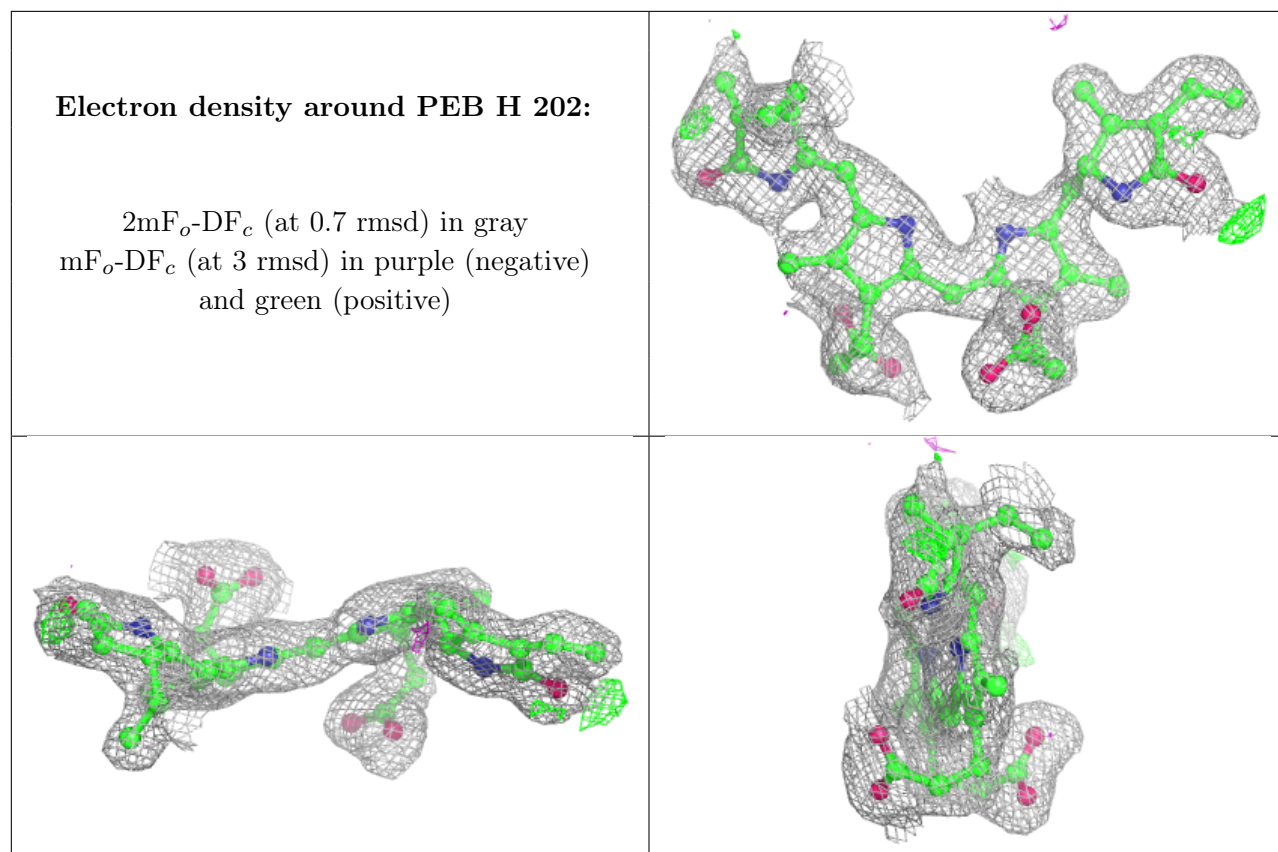
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB D 201:

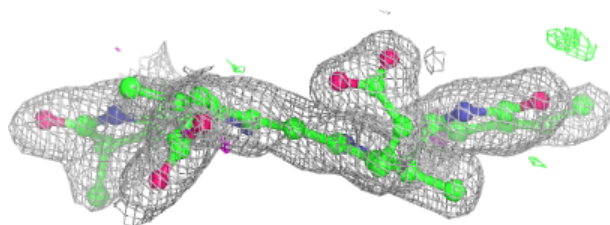
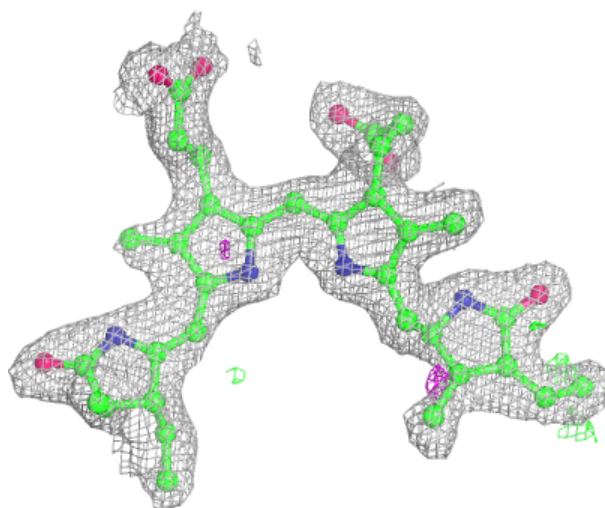
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





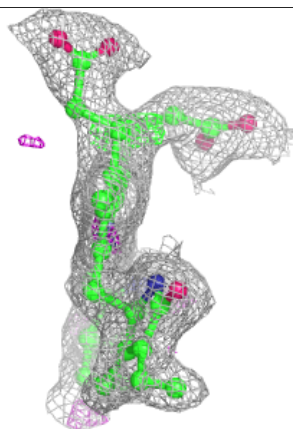
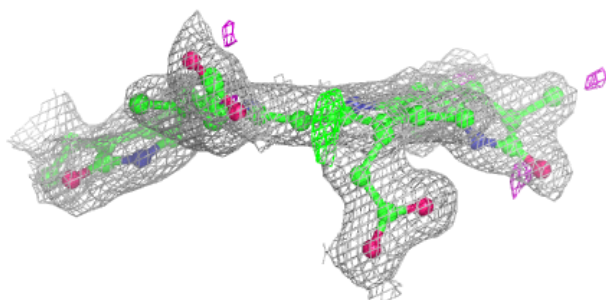
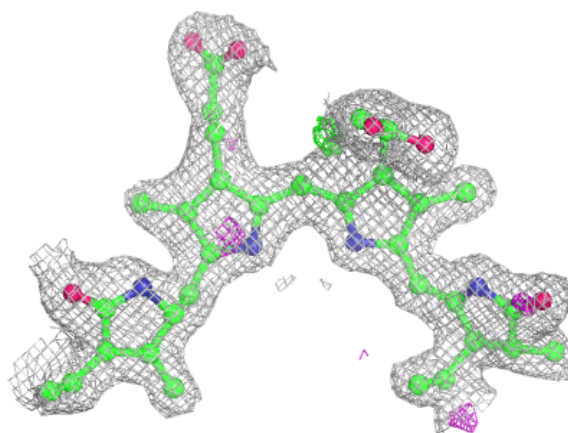
Electron density around PEB E 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

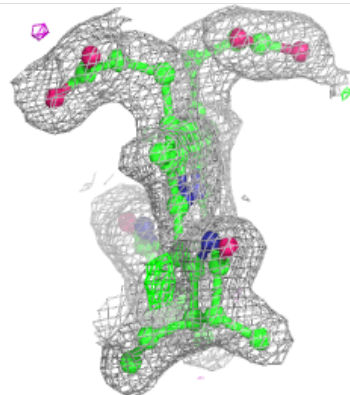
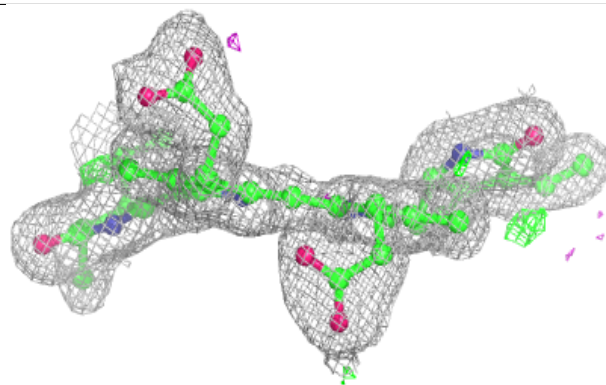
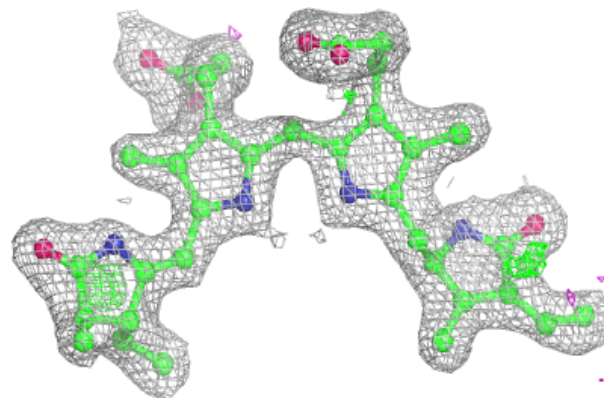


Electron density around PEB R 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

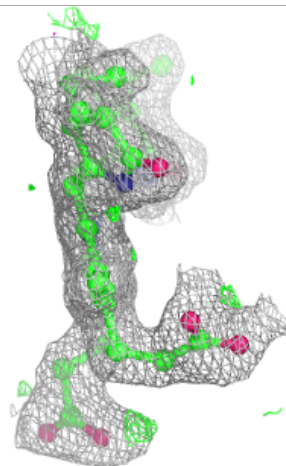
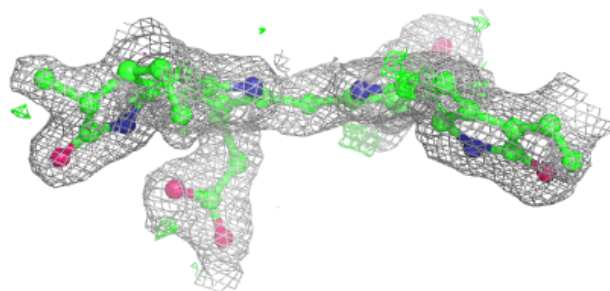
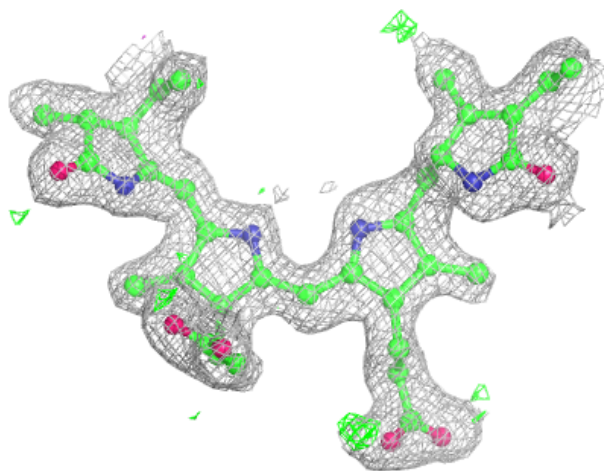
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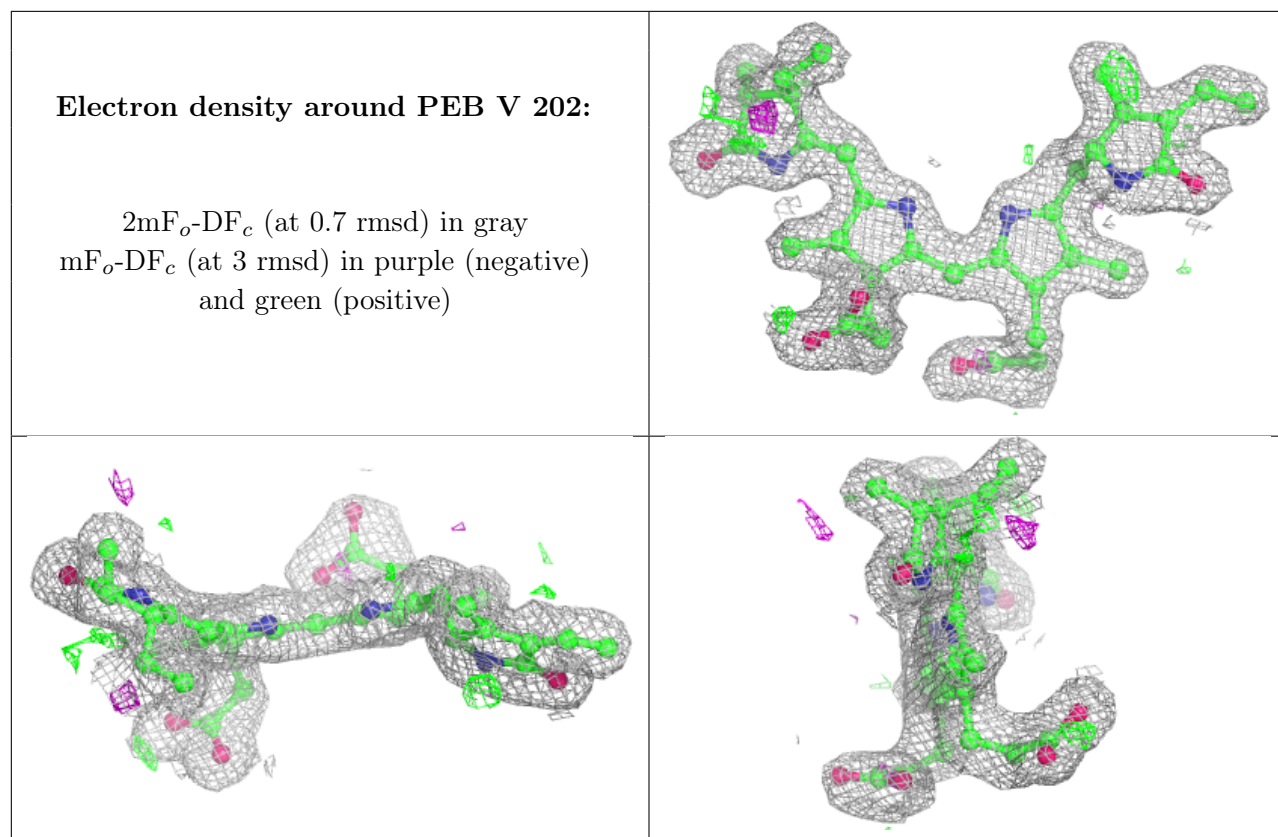
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and green (positive)



Electron density around PEB T 203:

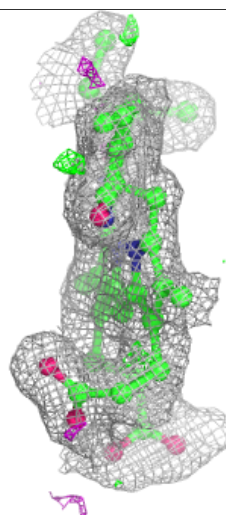
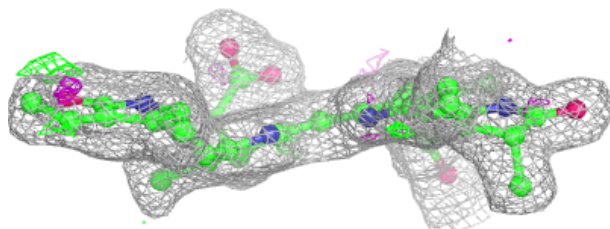
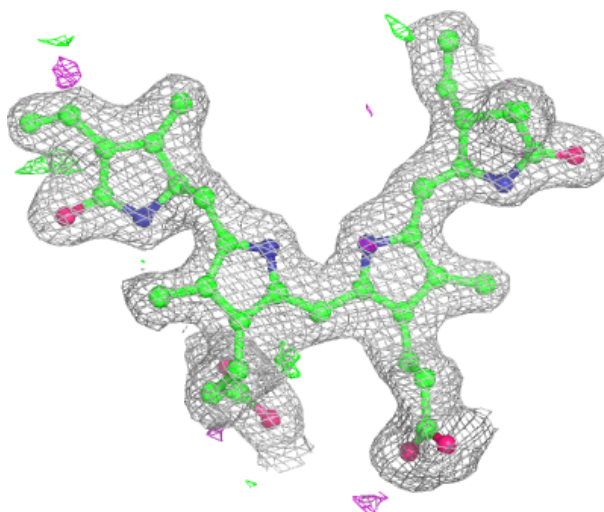
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and green (positive)





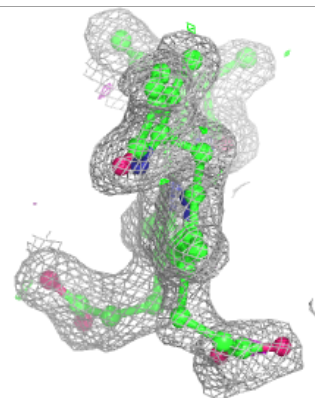
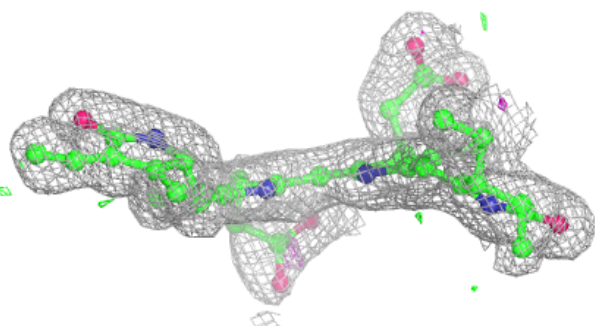
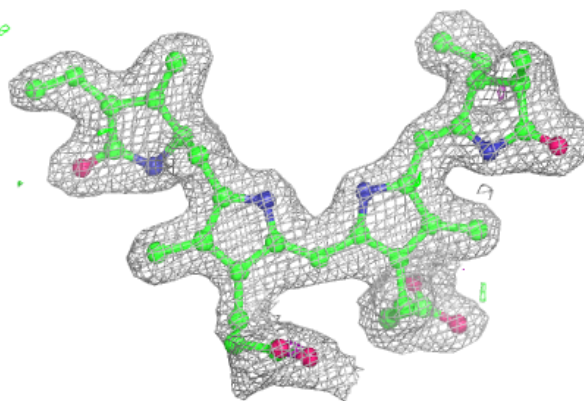
Electron density around PEB F 201:

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and green (positive)

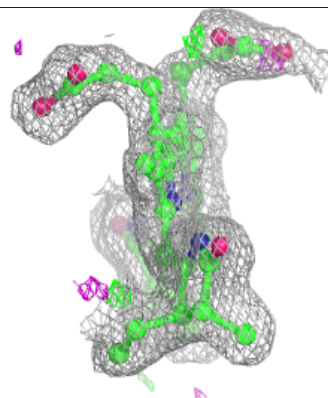
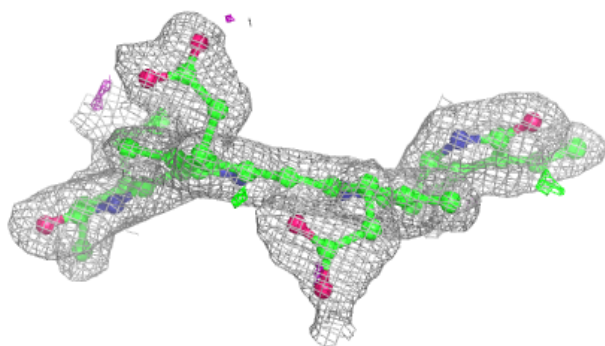
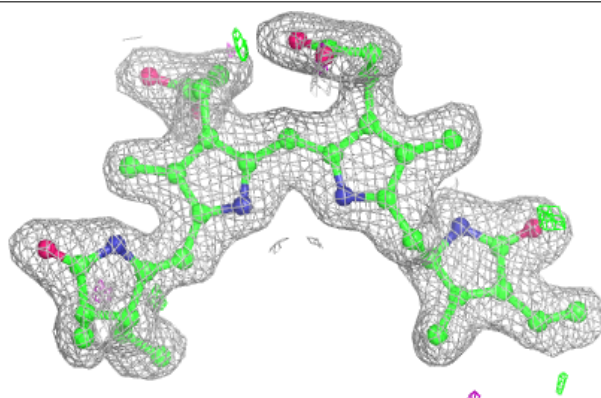


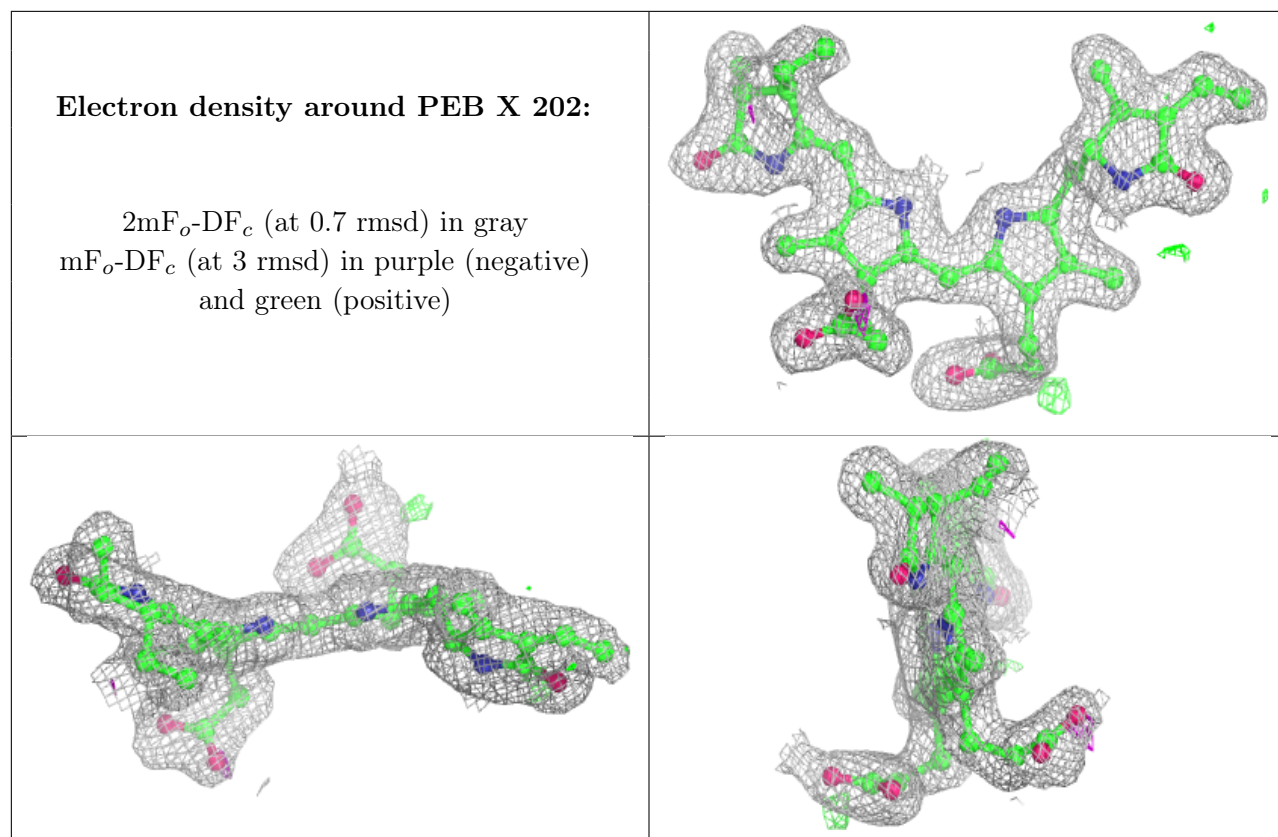
Electron density around PEB O 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PEB M 202:**

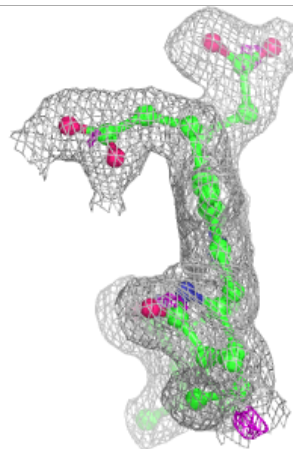
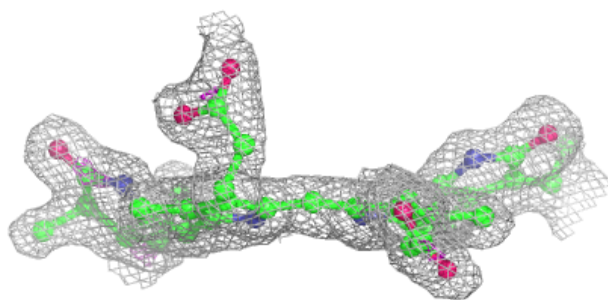
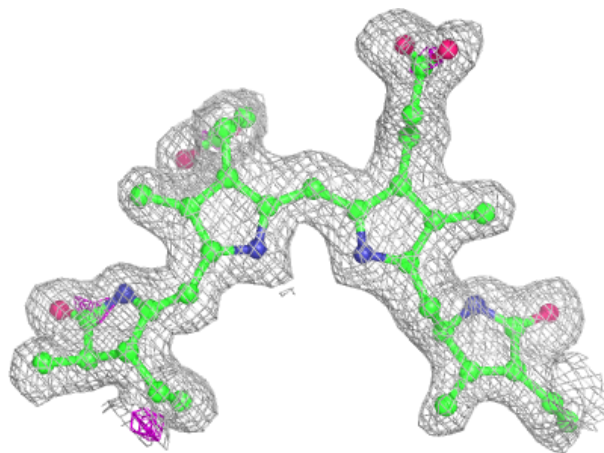
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





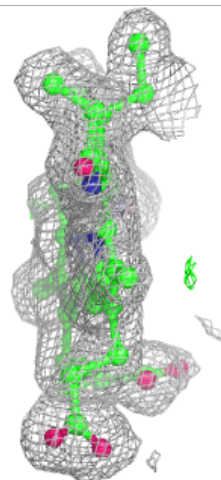
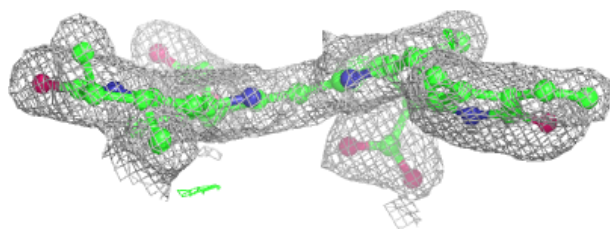
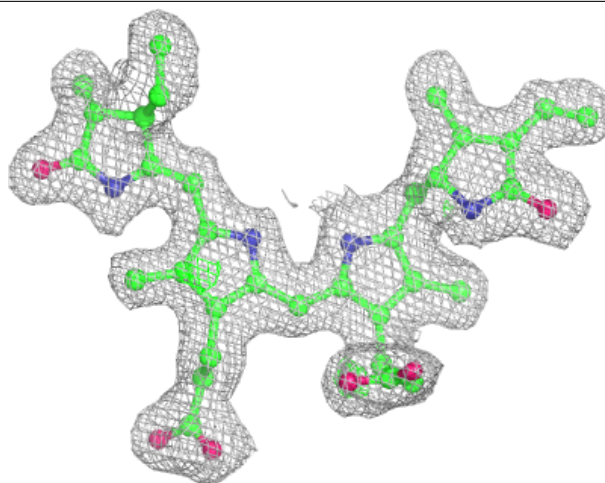
Electron density around PEB Q 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



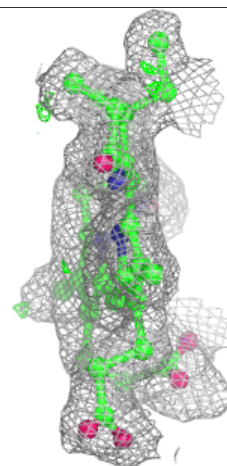
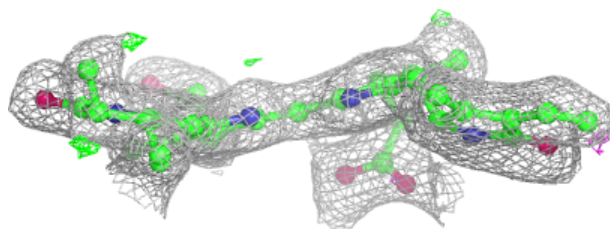
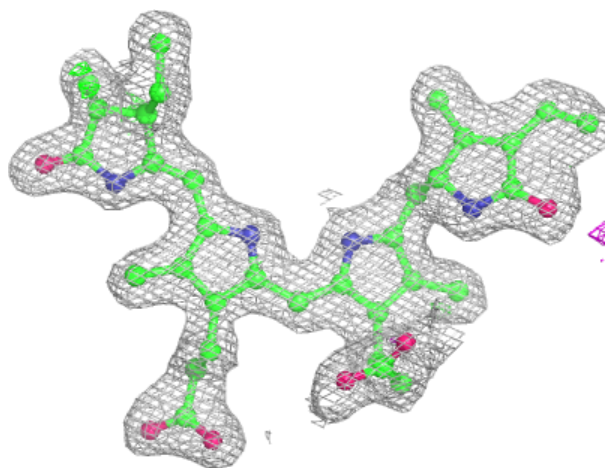
Electron density around PEB P 201:

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and green (positive)



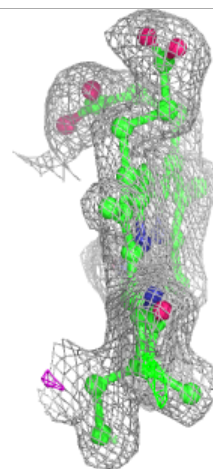
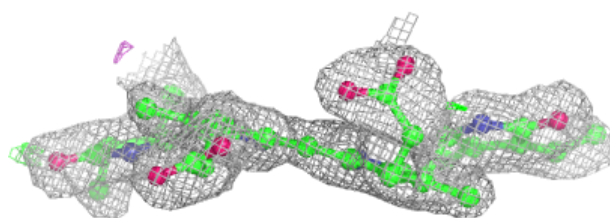
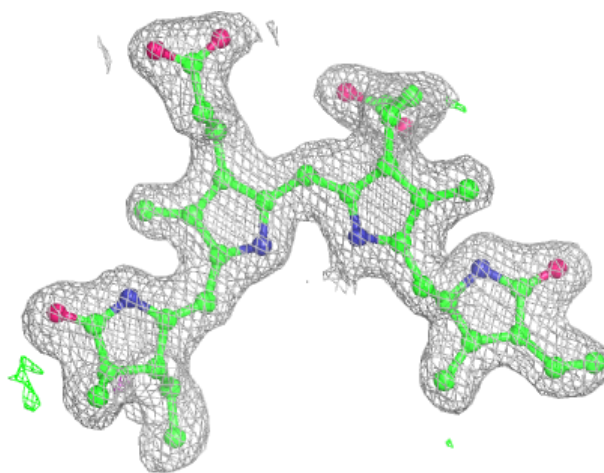
Electron density around PEB S 201:

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and green (positive)



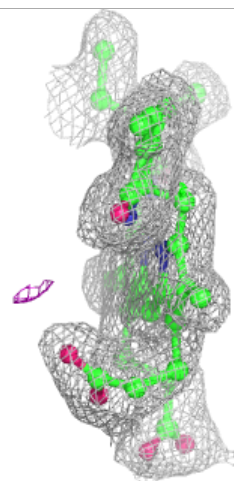
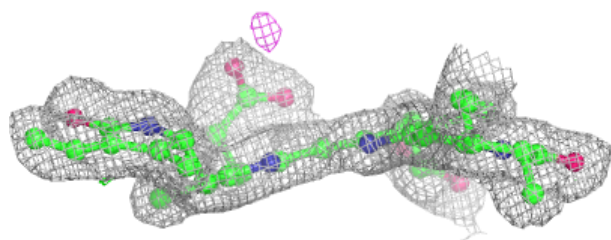
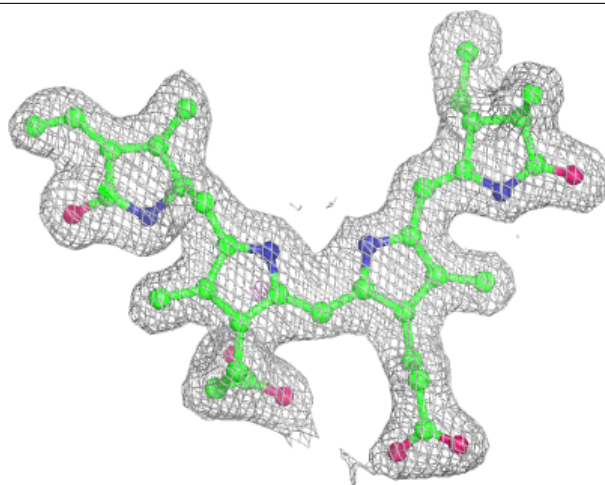
Electron density around PEB T 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



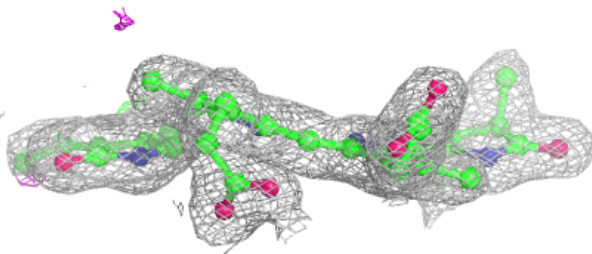
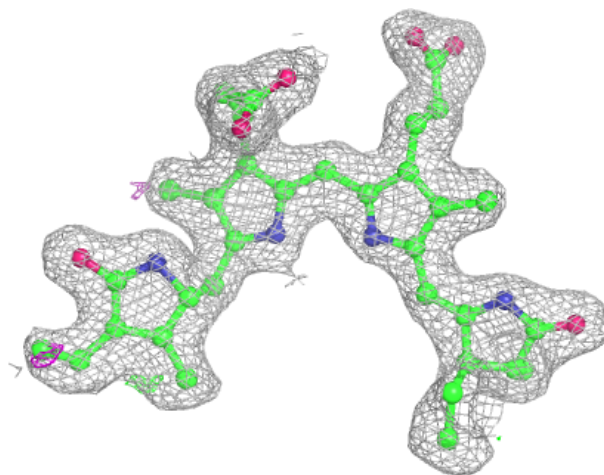
Electron density around PEB Q 201:

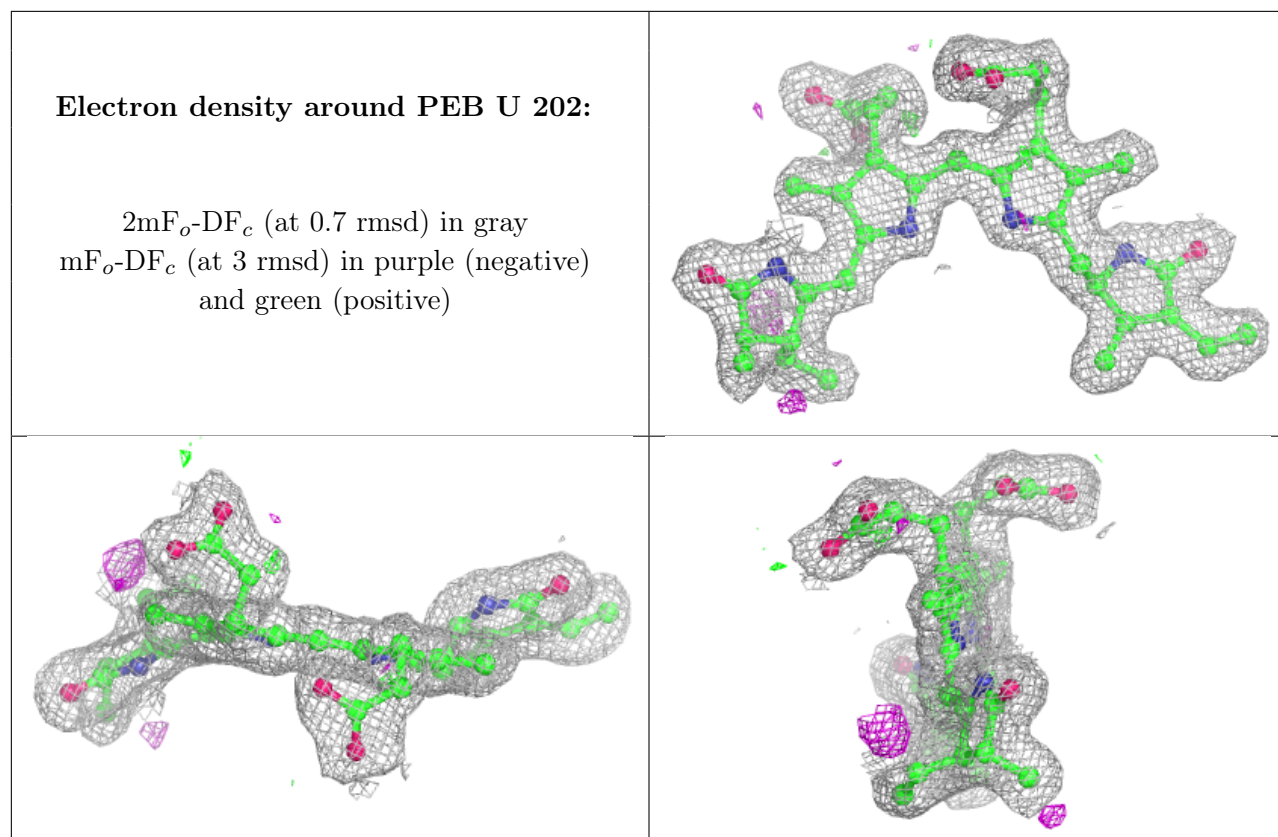
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB C 201:

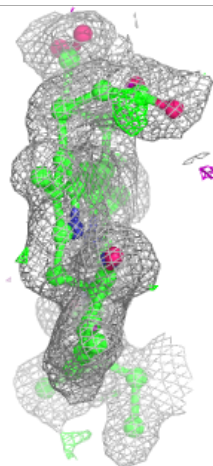
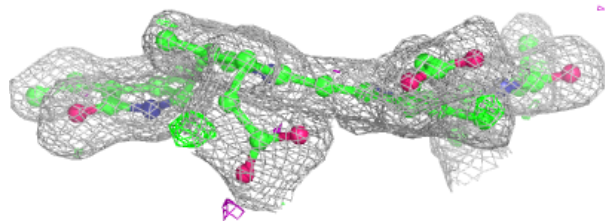
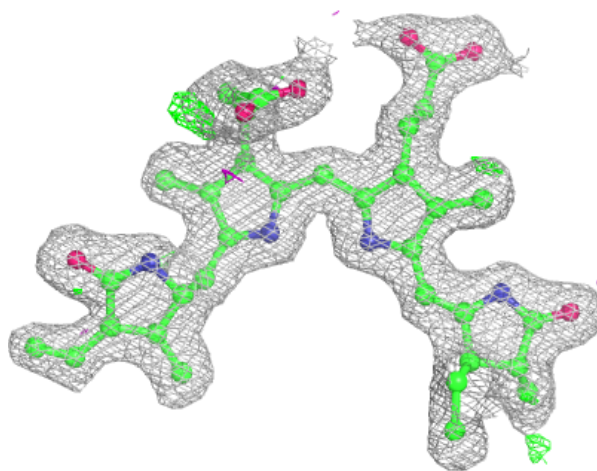
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





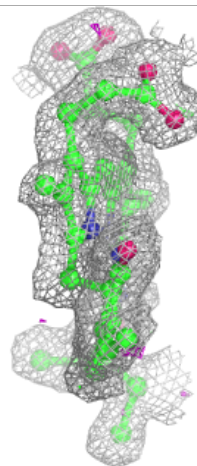
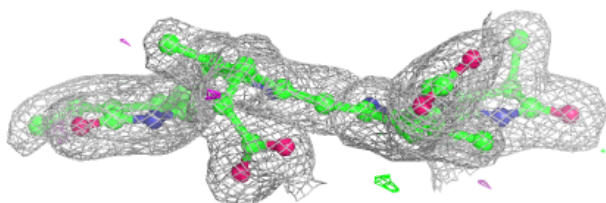
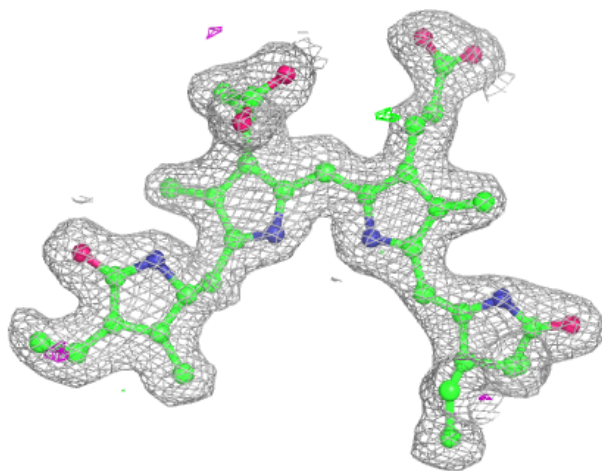
Electron density around PEB V 201:

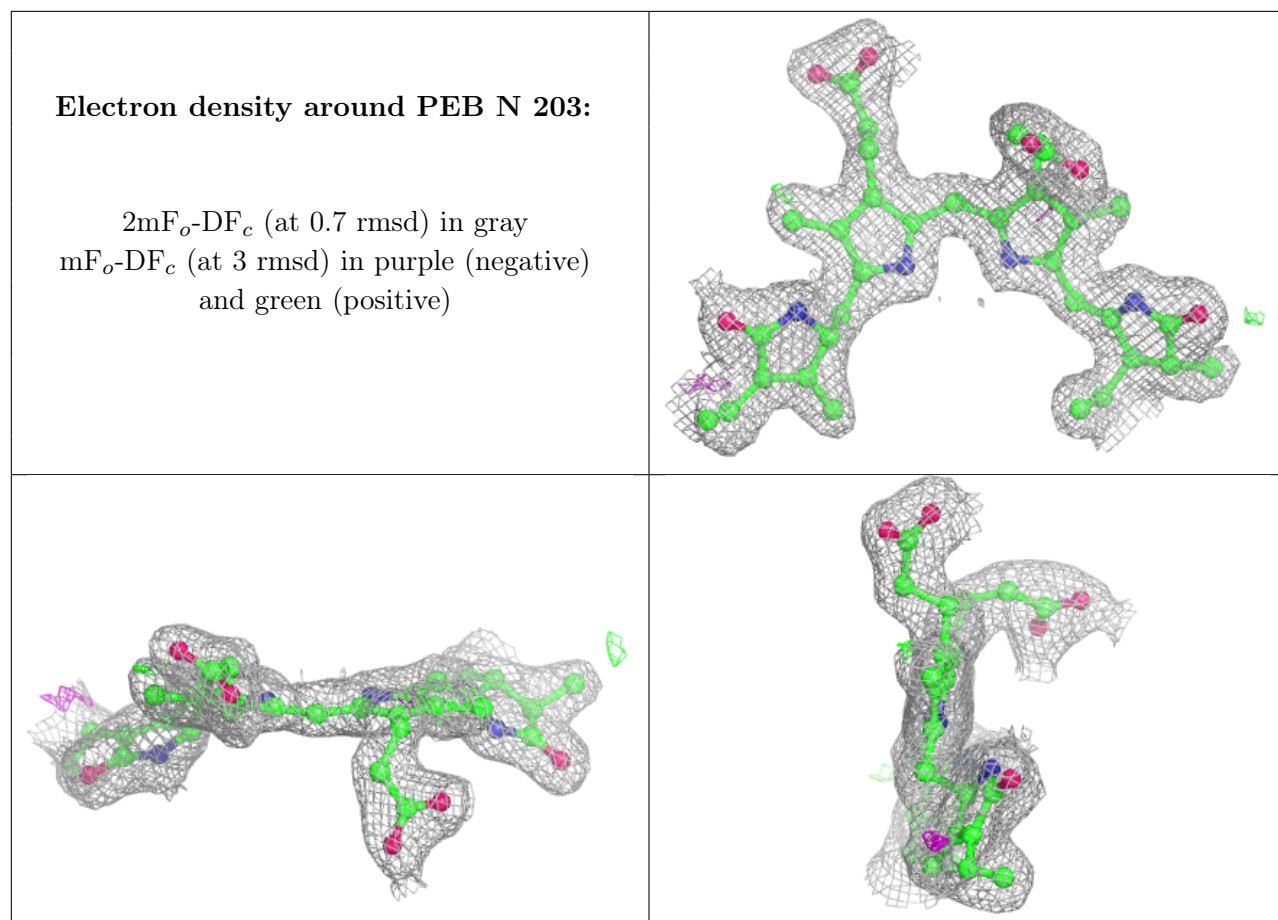
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB J 201:

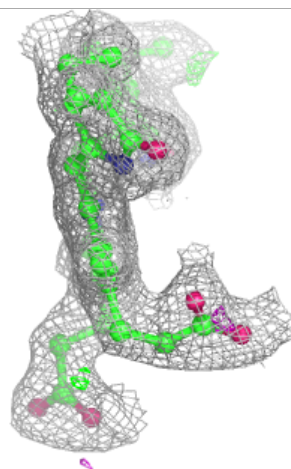
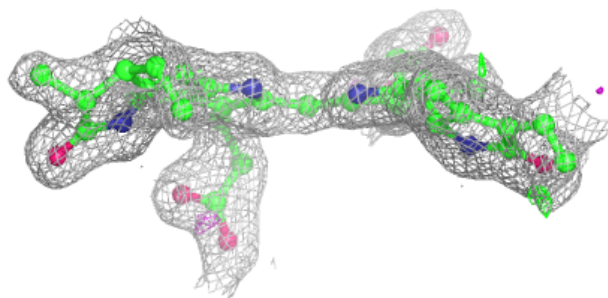
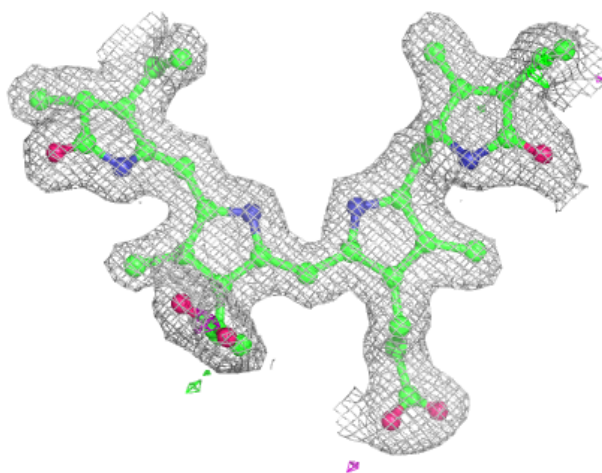
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





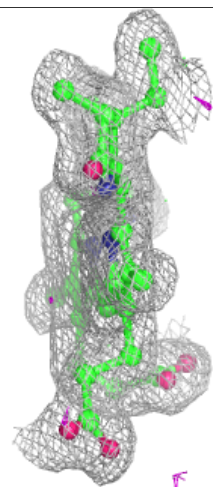
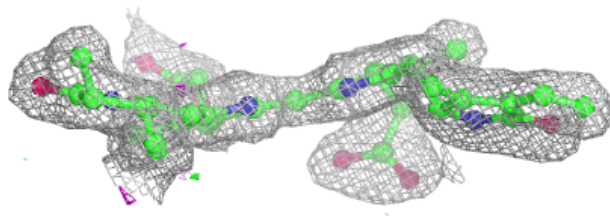
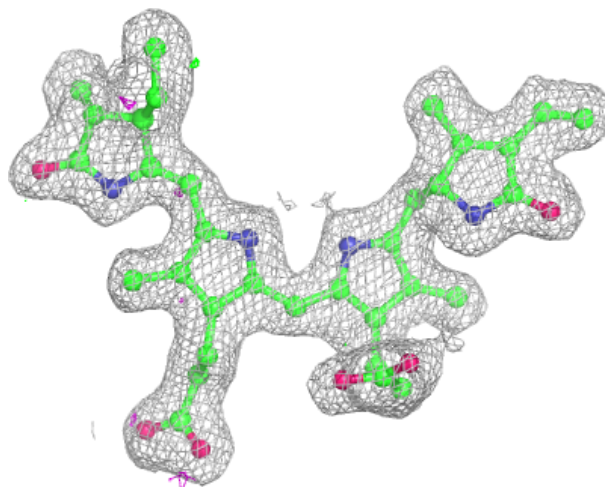
Electron density around PEB W 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



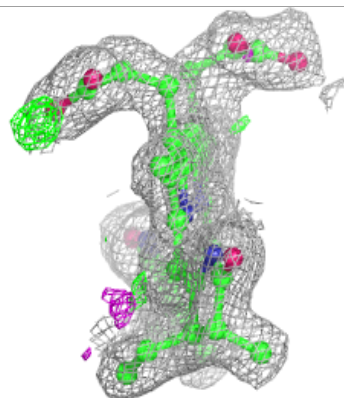
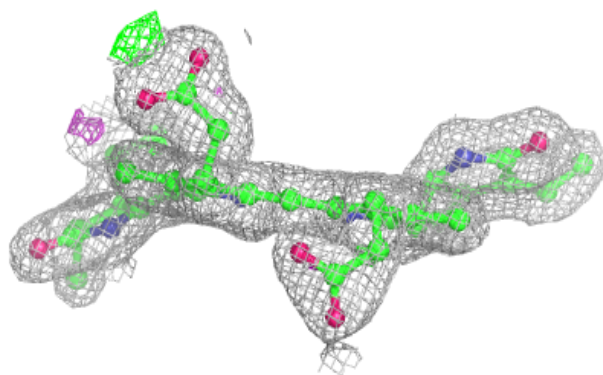
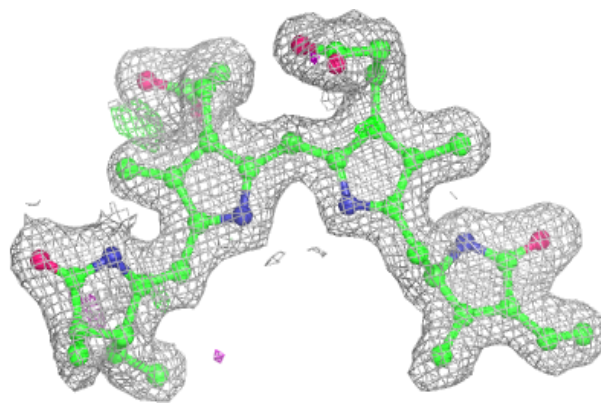
Electron density around PEB M 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



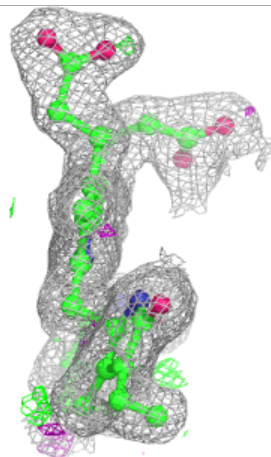
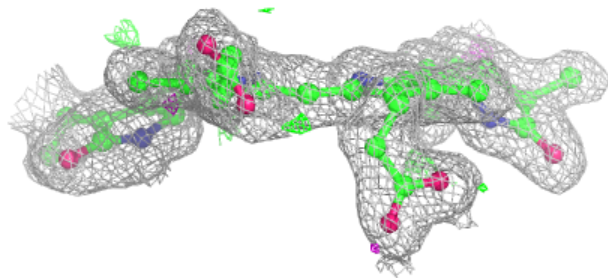
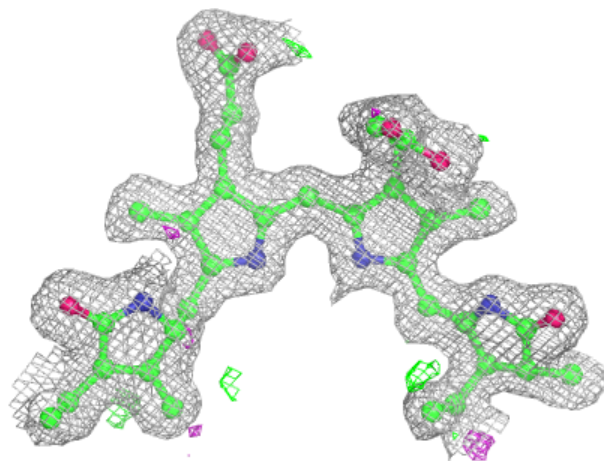
Electron density around PEB P 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



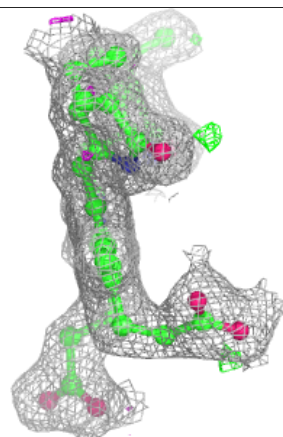
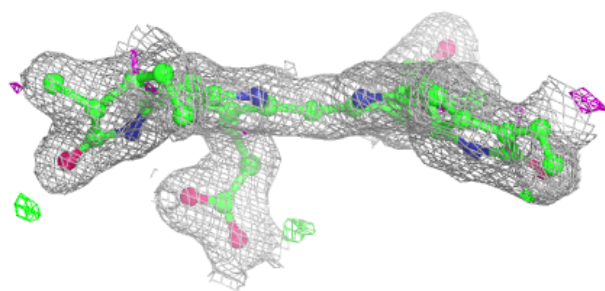
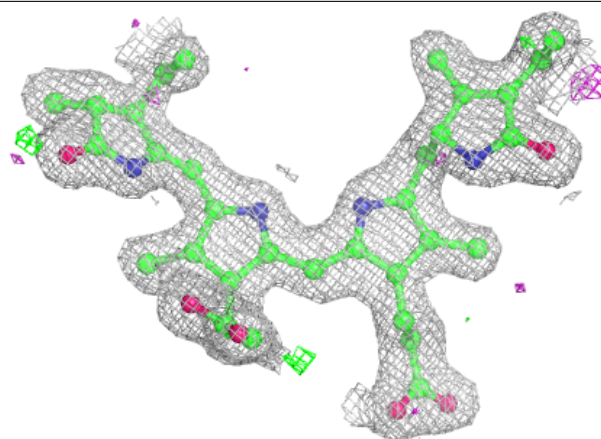
Electron density around PEB P 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



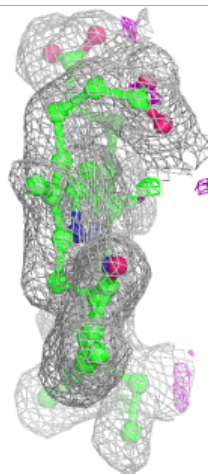
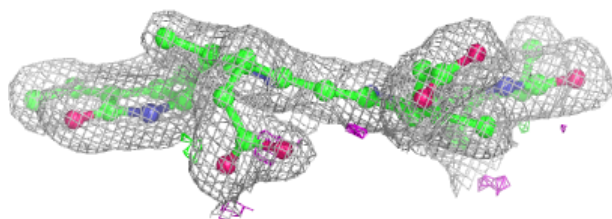
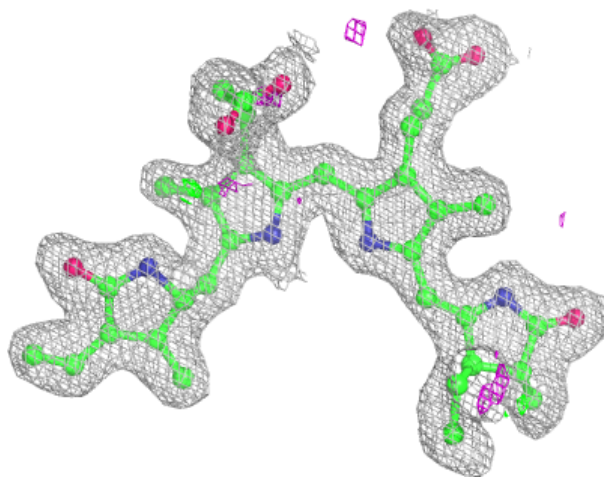
Electron density around PEB V 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



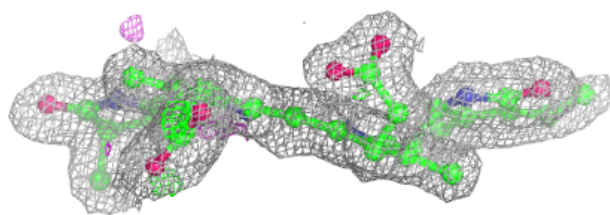
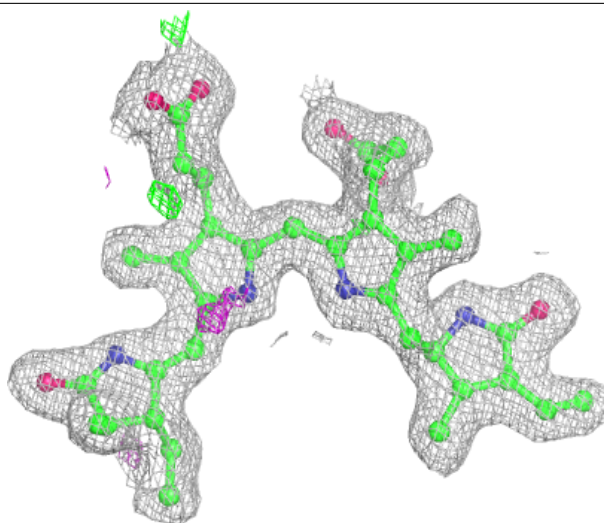
Electron density around PEB W 201:

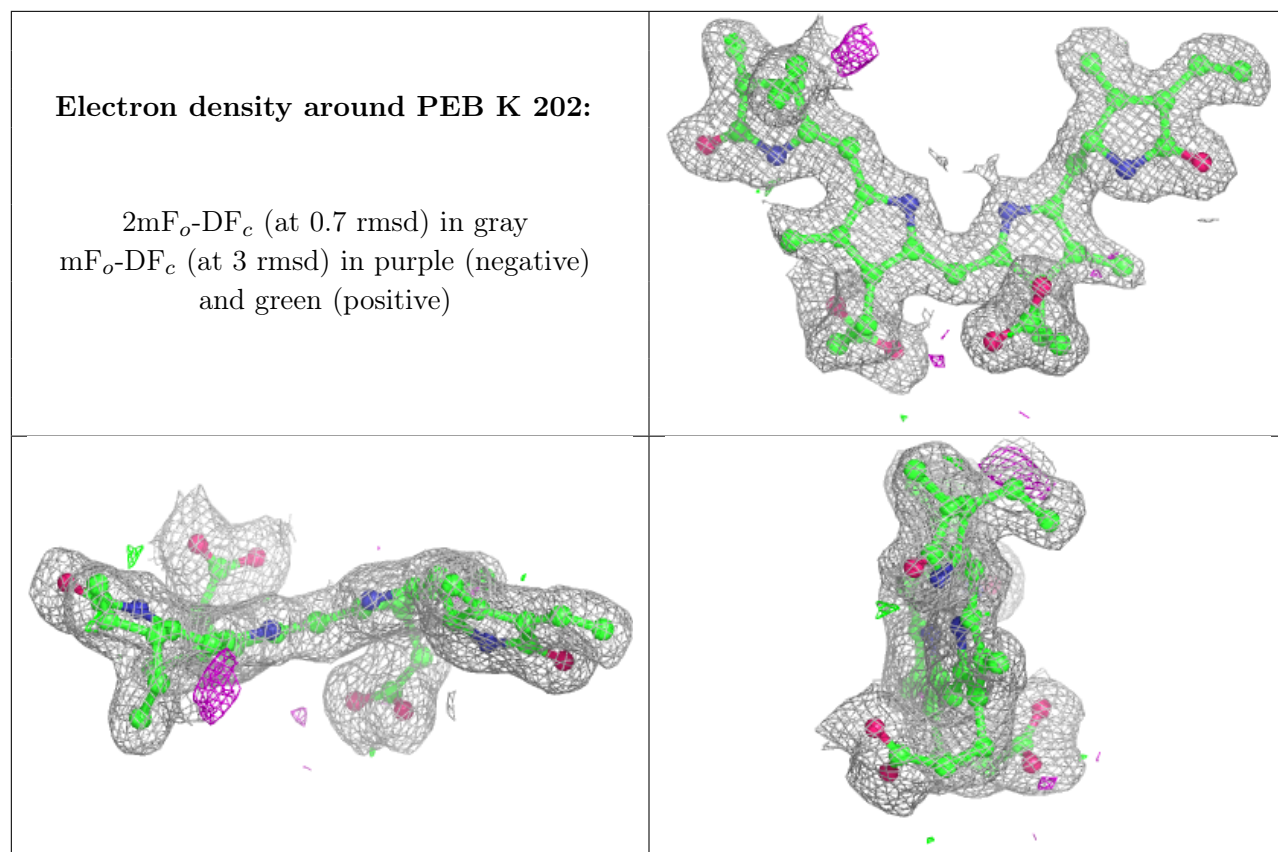
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB K 201:

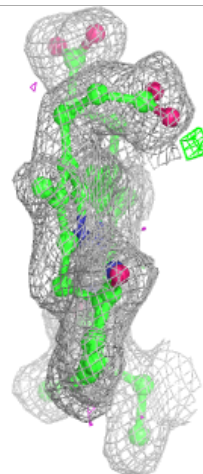
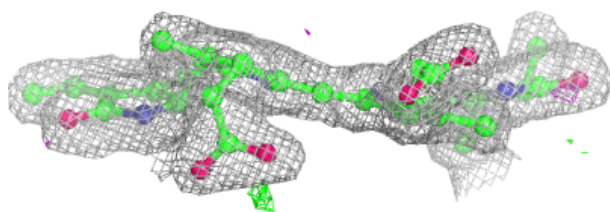
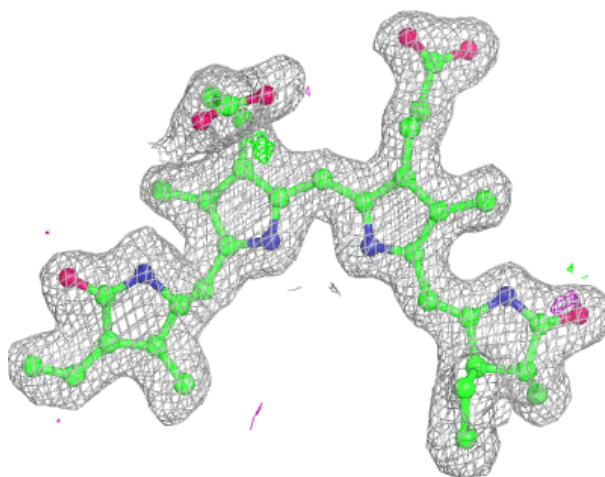
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

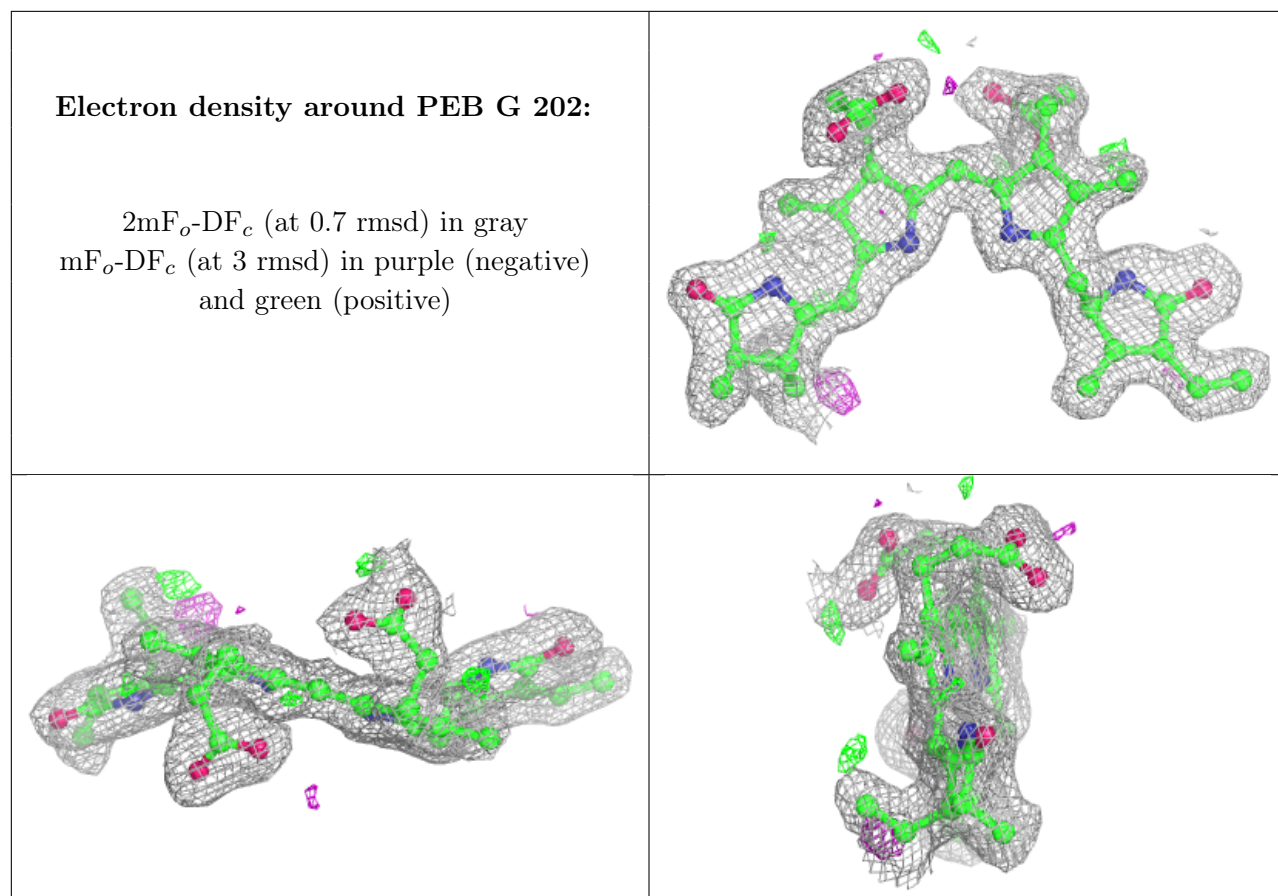




Electron density around PEB X 201:

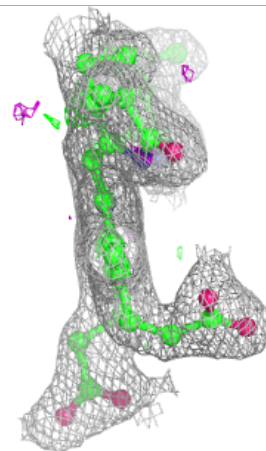
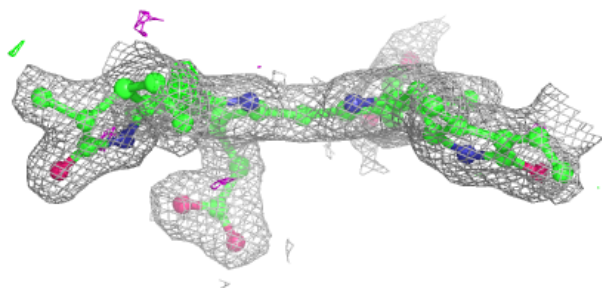
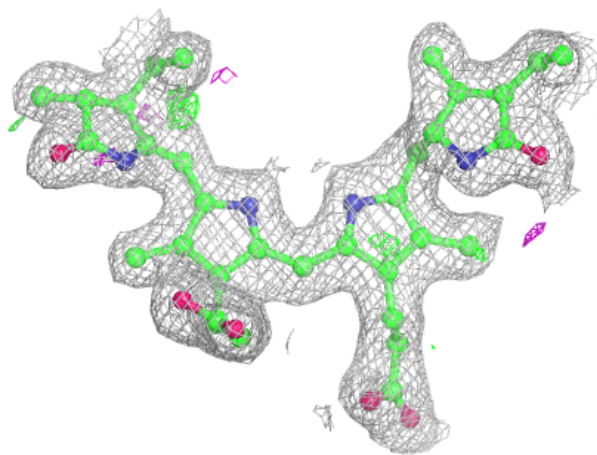
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

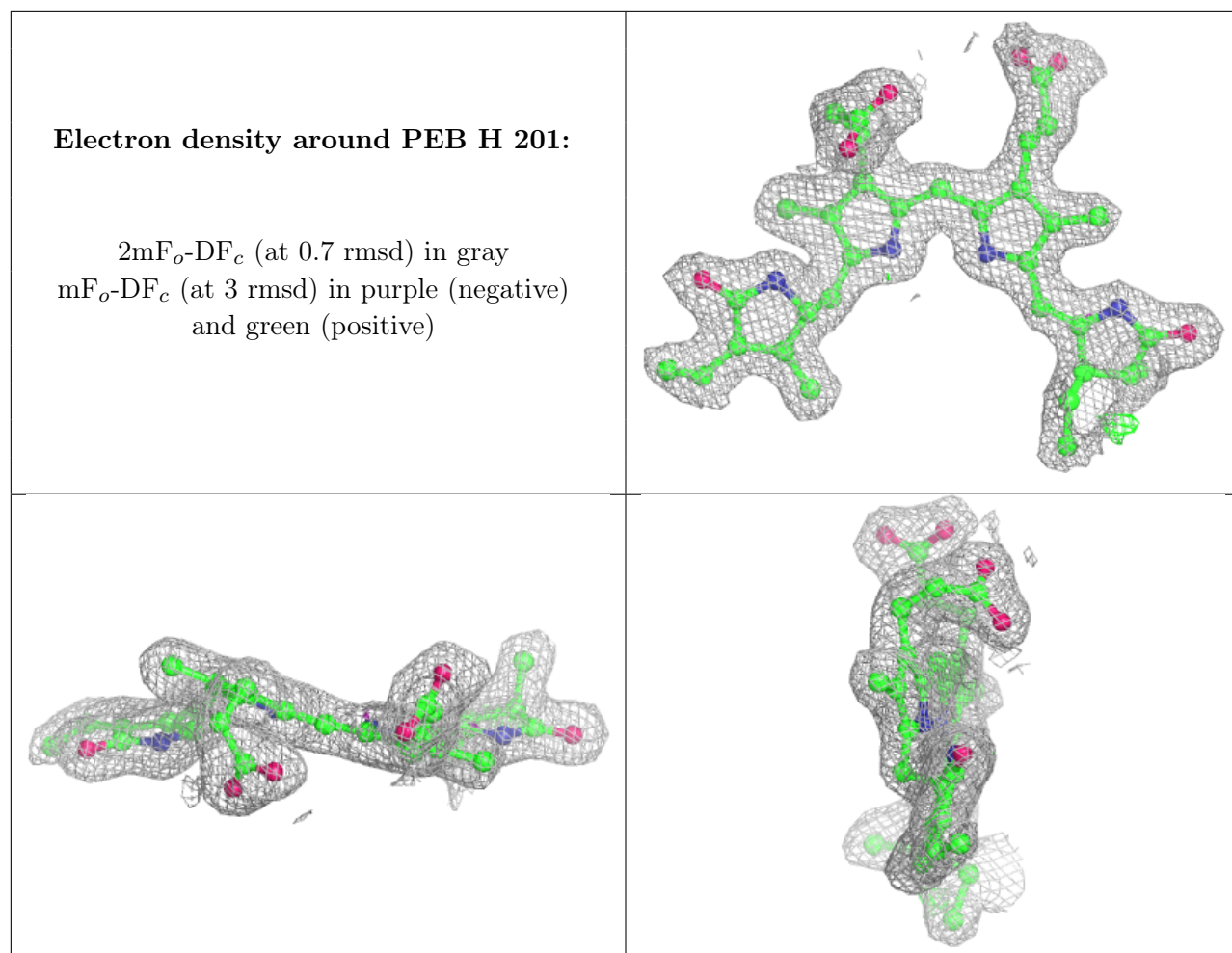




Electron density around PEB X 203:

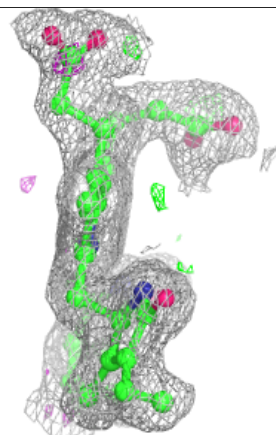
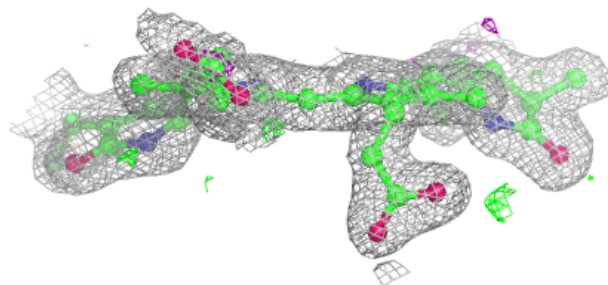
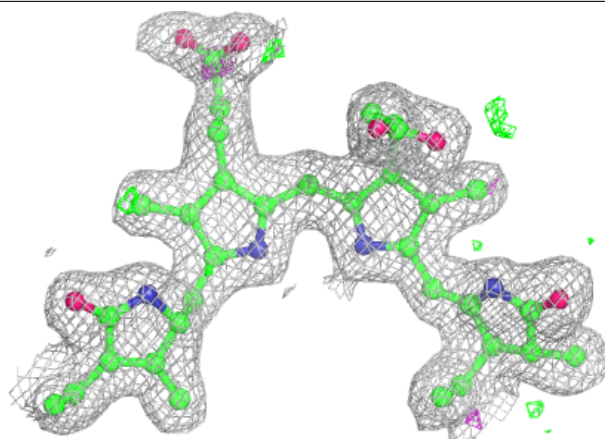
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





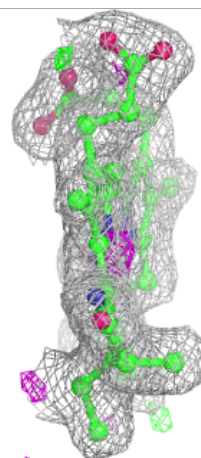
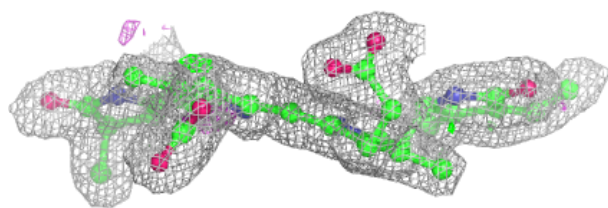
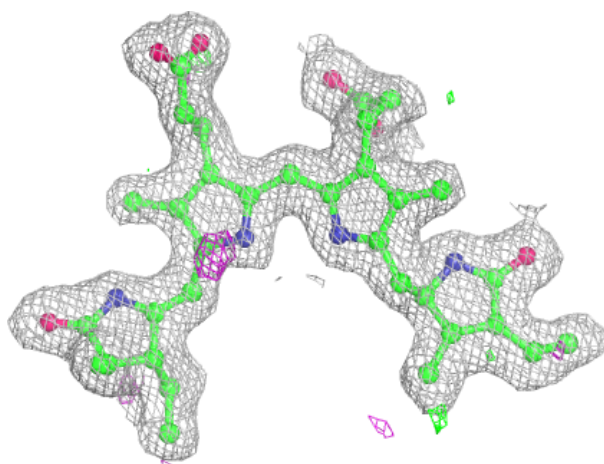
Electron density around PEB M 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



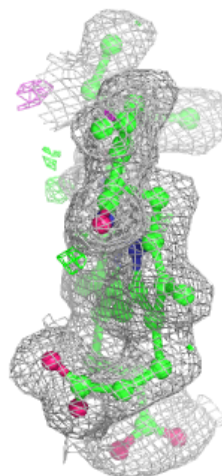
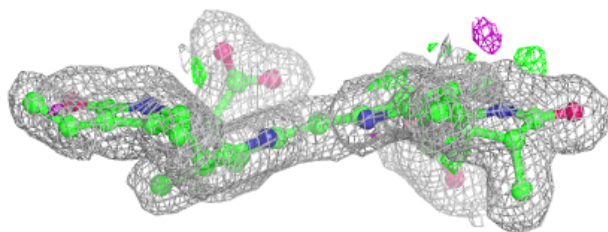
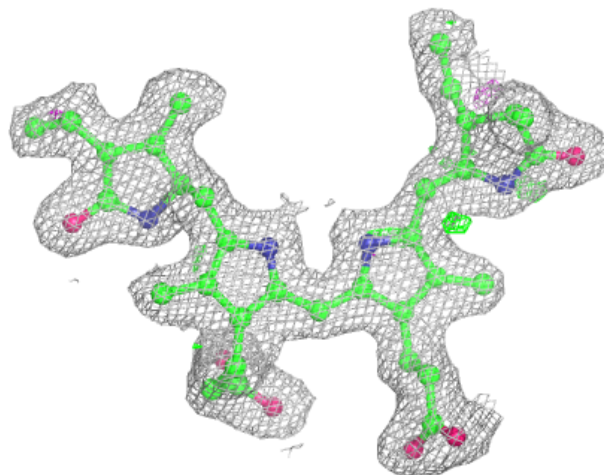
Electron density around PEB B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



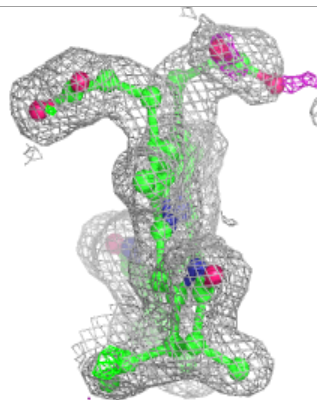
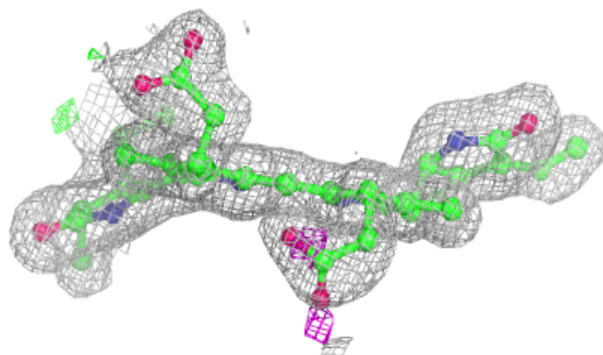
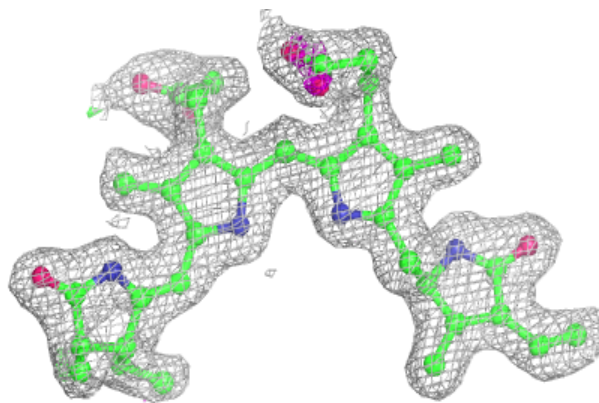
Electron density around PEB A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

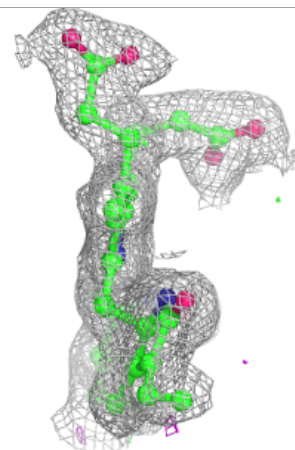
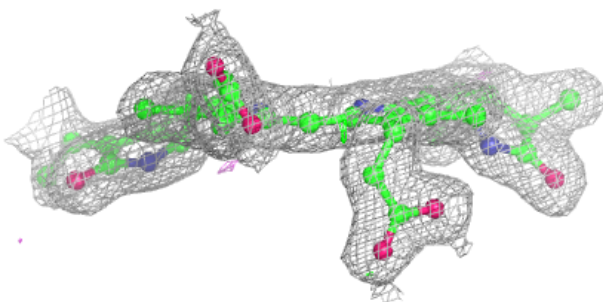
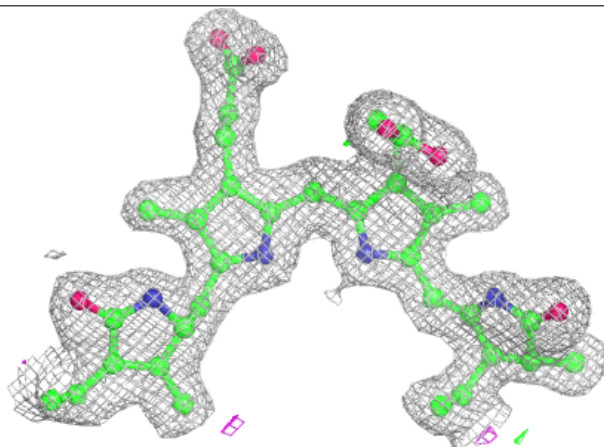


Electron density around PEB S 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

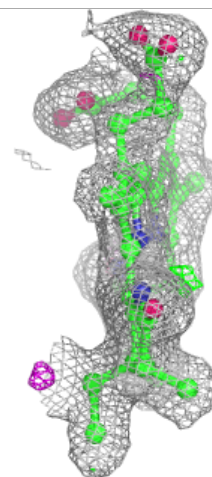
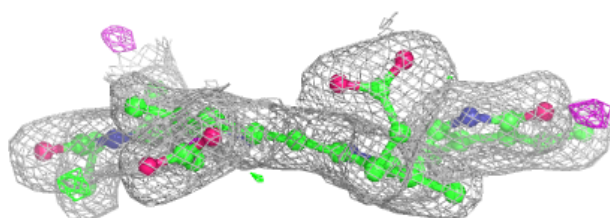
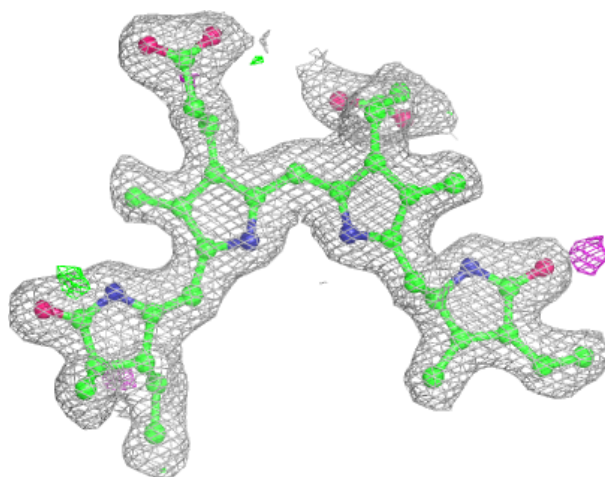
**Electron density around PEB S 203:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



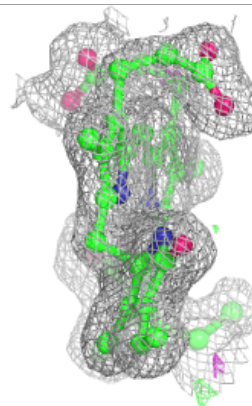
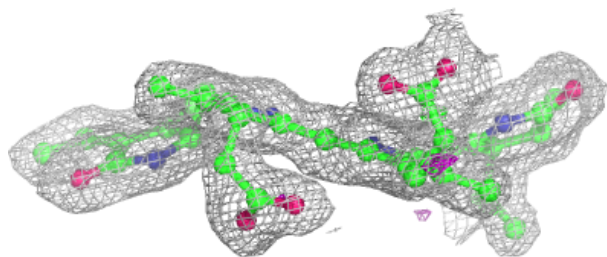
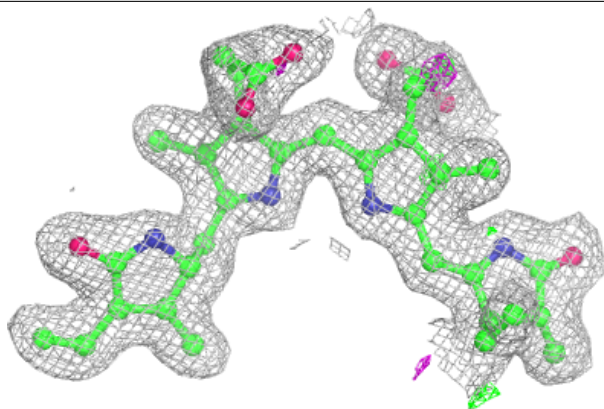
Electron density around PEB O 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



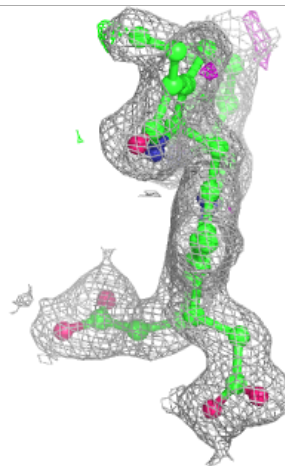
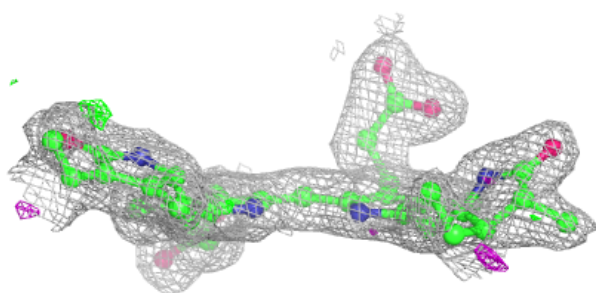
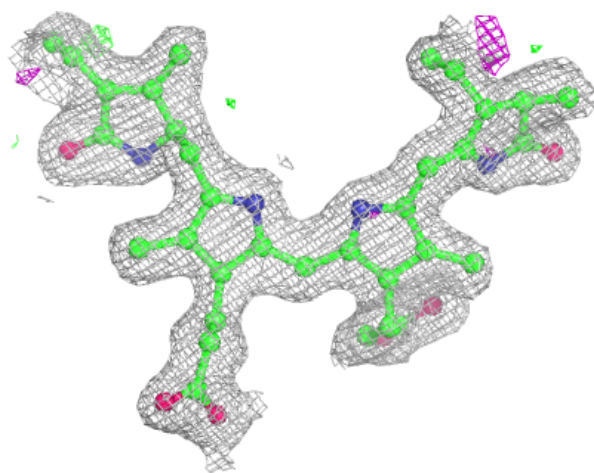
Electron density around PEB C 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



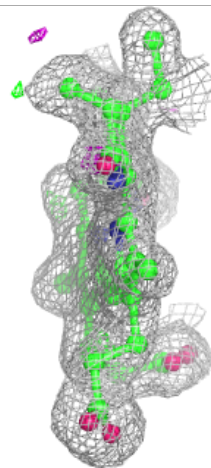
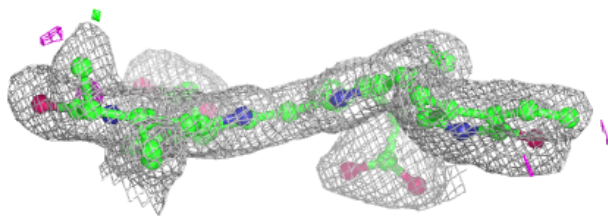
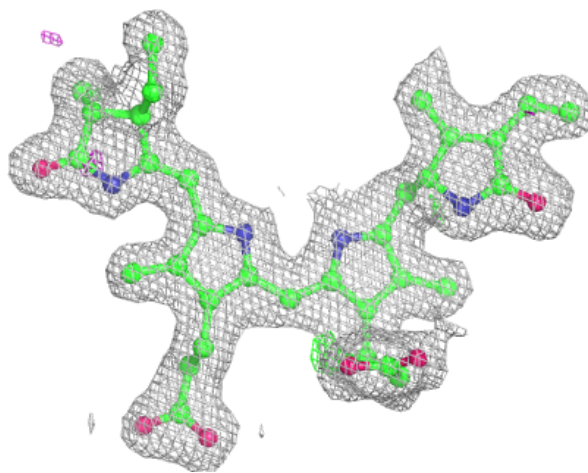
Electron density around PEB O 203:

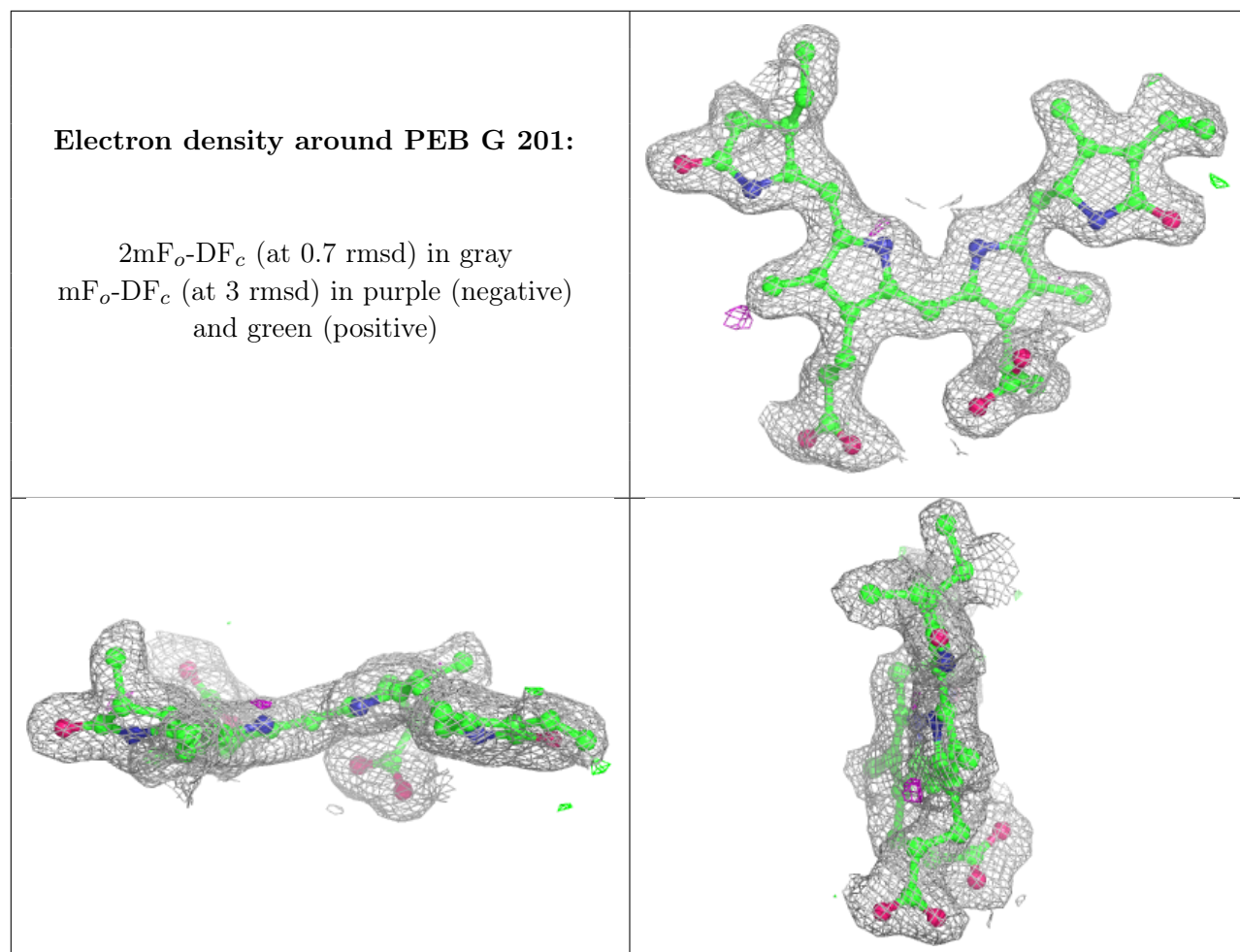
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEB U 201:

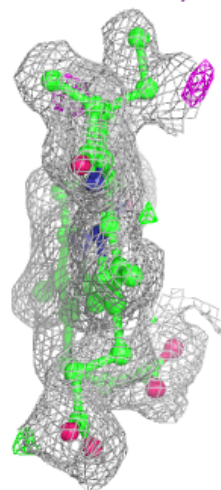
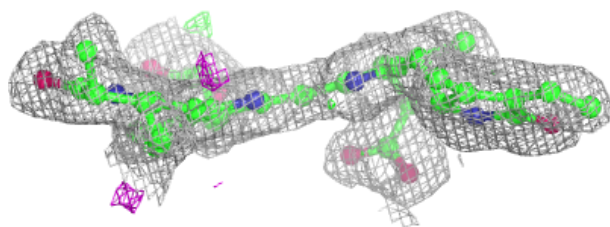
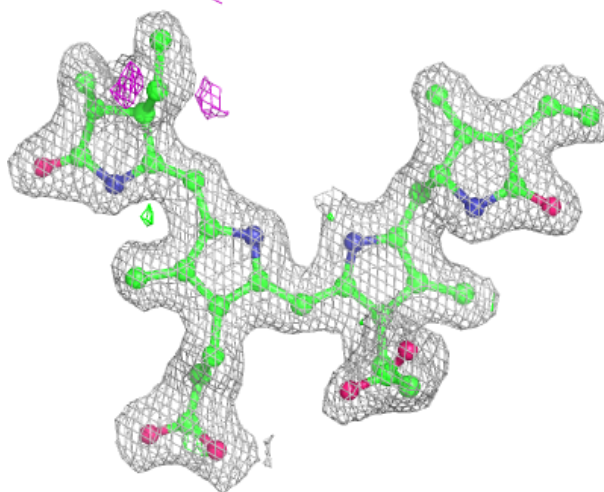
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





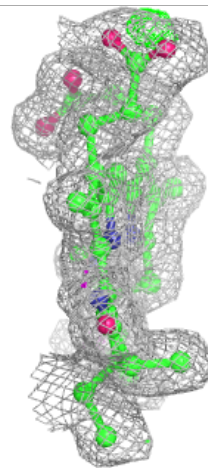
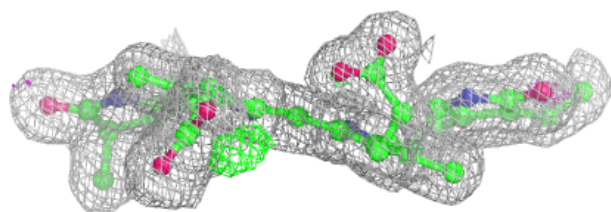
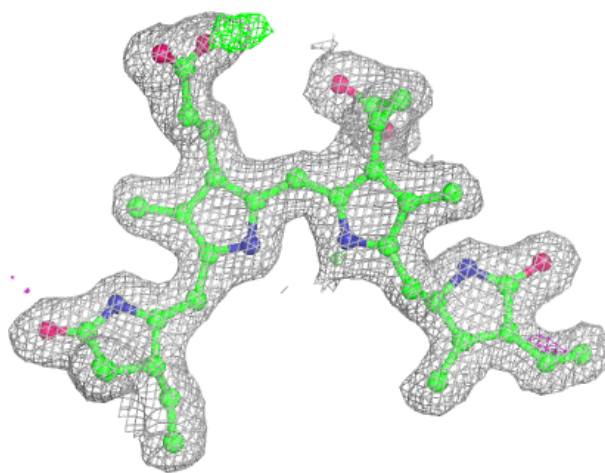
Electron density around PEB N 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



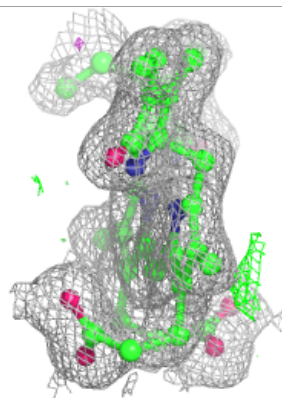
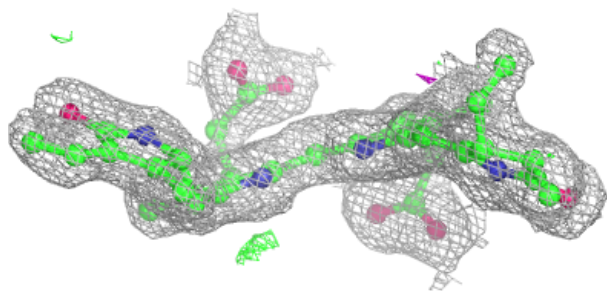
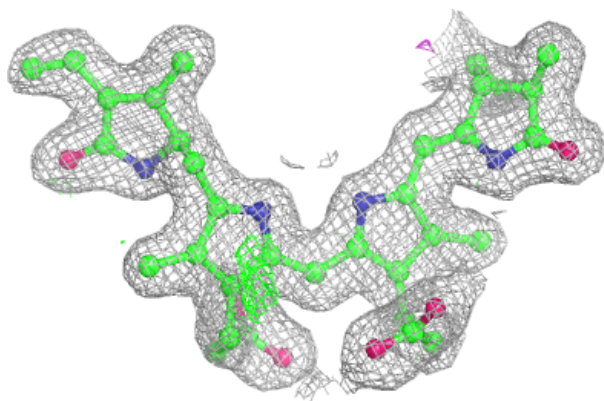
Electron density around PEB L 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

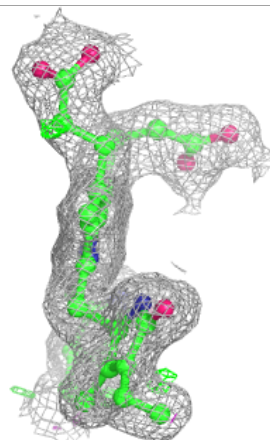
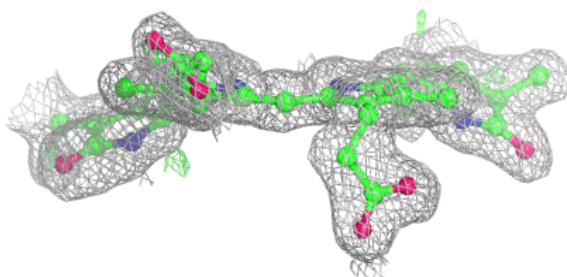
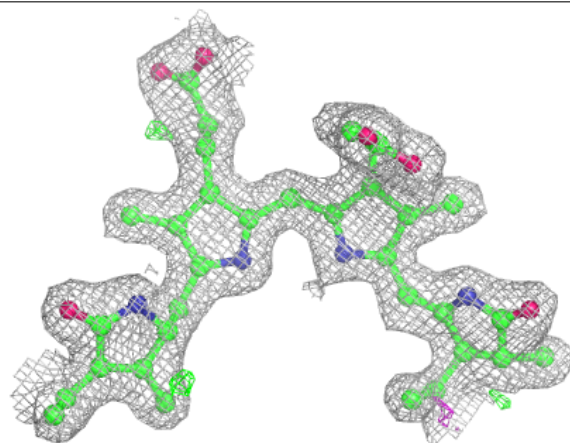


Electron density around PEB J 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

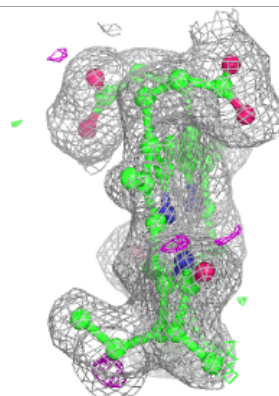
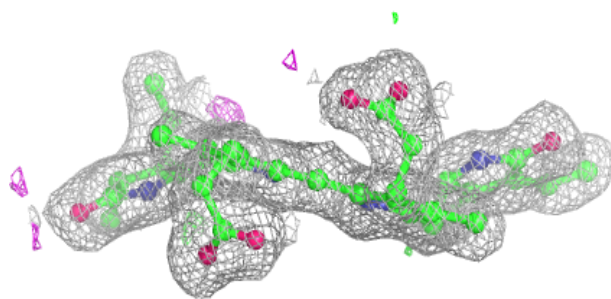
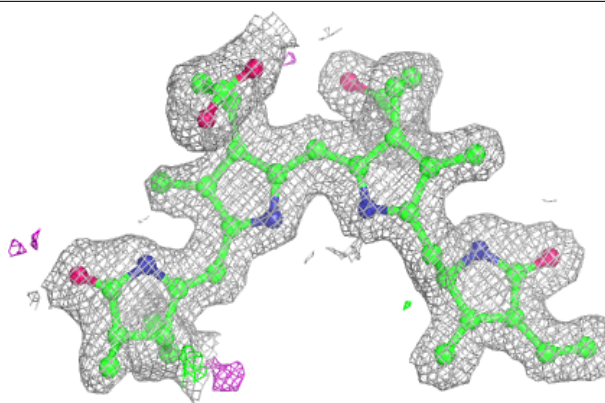
**Electron density around PEB U 203:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

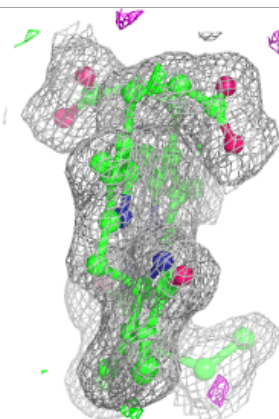
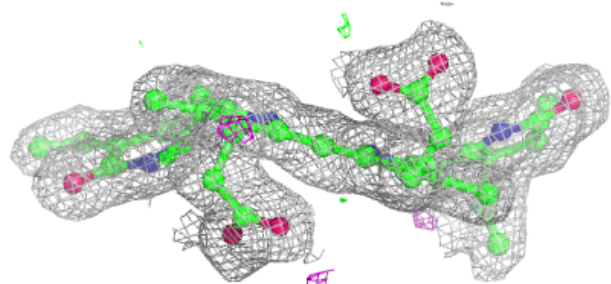
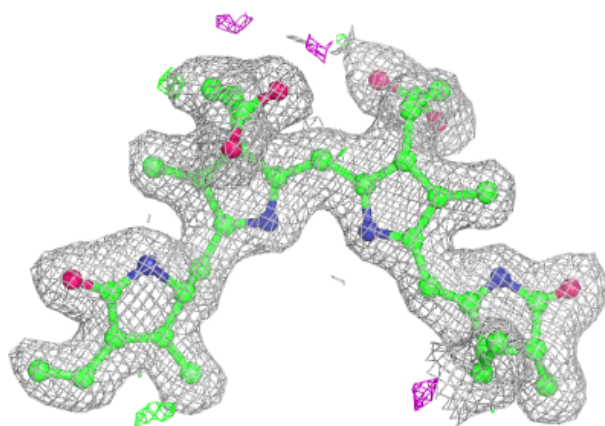


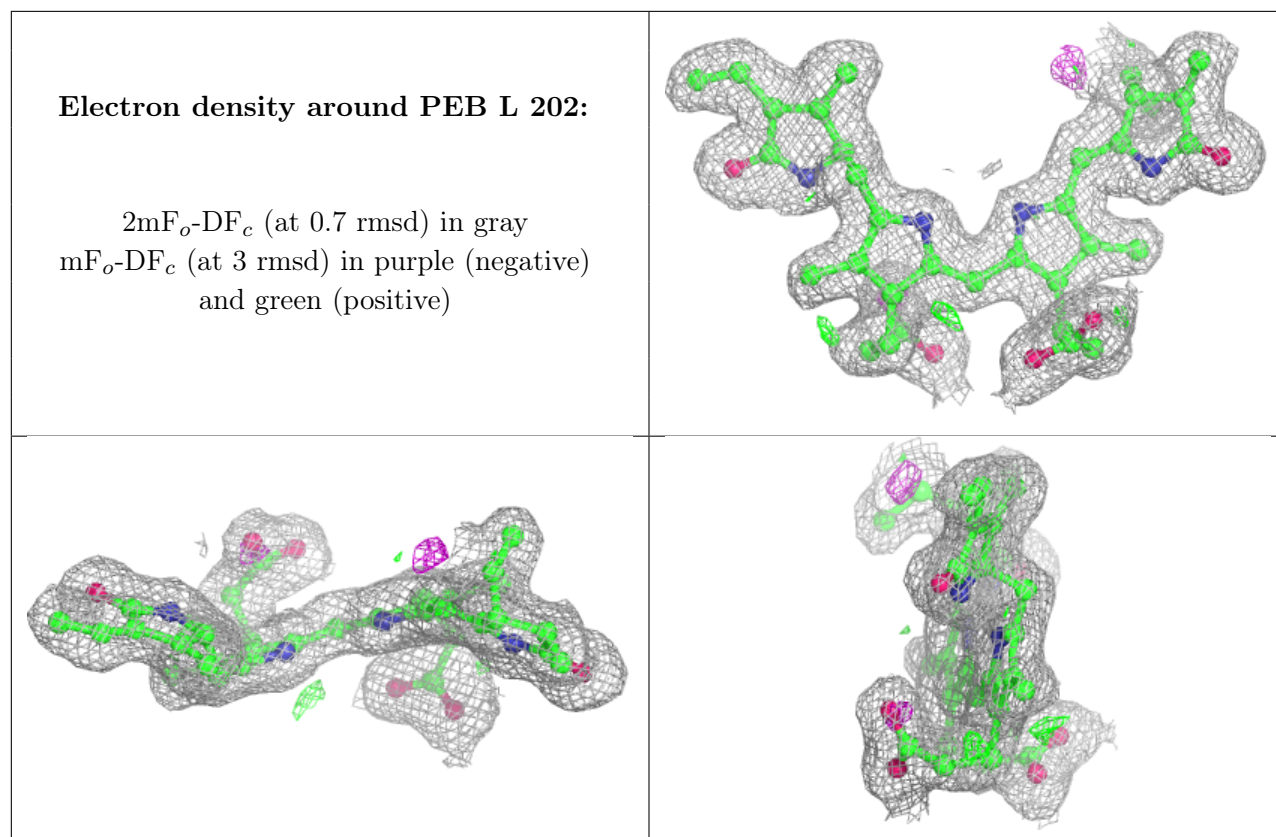
Electron density around PEB B 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PEB A 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.