



wwPDB X-ray Structure Validation Summary Report

Oct 18, 2021 – 03:42 pm BST

PDB ID : 7OKA
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 14
Authors : Ryan, M.D.; Parkes, A.L.; Southey, M.; Andersen, O.A.; Zahn, M.; Barker, J.; DeJonge, B.L.M.
Deposited on : 2021-05-17
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

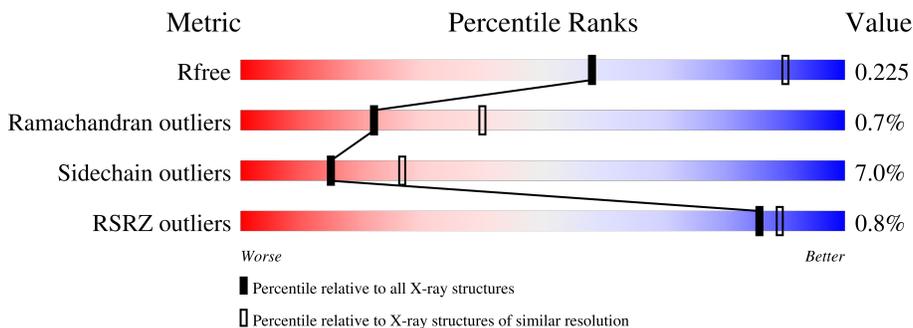
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	261	92% 6% ..
1	B	261	92% 6% ..
1	C	261	93% 5% ..
1	D	261	89% 9% ..
1	E	261	90% 7% ..
1	F	261	88% 8% ..

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Mol	Chain	Length	Quality of chain
1	G	261	3% 93% 5% ..
1	H	261	90% 7% ..
1	I	261	% 92% 6% .
1	J	261	90% 8% ..
1	K	261	90% 8% ..
1	L	261	90% 8% ..
1	M	261	2% 90% 8% ..
1	N	261	% 90% 8% ..
1	O	261	% 91% 7% .
1	P	261	% 92% 5% ..
1	Q	261	2% 90% 6% ..
1	R	261	90% 7% ..
1	S	261	92% 5% ..
1	T	261	90% 8% ..
1	U	261	91% 6% ..
1	V	261	2% 90% 7% ..
1	W	261	6% 91% 7% ..
1	X	261	90% 7% ..
1	Y	261	2% 90% 7% ..
1	Z	261	89% 9% ..
1	a	261	2% 90% 8% .
1	b	261	% 87% 10% ..
1	c	261	% 91% 7% ..
1	d	261	% 89% 8% ..

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	Q	306	-	-	-	X
4	SO4	V	303	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60786 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 Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total 1994	C 1248	N 368	O 371	S 7	0	3	0
1	B	258	Total 2002	C 1253	N 371	O 371	S 7	0	4	0
1	C	258	Total 1996	C 1249	N 371	O 369	S 7	0	3	0
1	D	258	Total 1980	C 1239	N 365	O 369	S 7	0	1	0
1	E	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	F	258	Total 1988	C 1244	N 368	O 369	S 7	0	2	0
1	G	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	H	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	I	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	M	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	N	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	O	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	J	258	Total 1982	C 1240	N 367	O 368	S 7	0	1	0
1	K	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	L	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	P	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	R	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	S	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	T	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	U	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	V	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	W	257	Total	C	N	O	S	0	1	0
			1972	1234	364	368	6			
1	X	257	Total	C	N	O	S	0	1	0
			1972	1234	364	368	6			
1	Y	258	Total	C	N	O	S	0	1	0
			1980	1239	365	369	7			
1	Z	258	Total	C	N	O	S	0	1	0
			1980	1239	365	369	7			
1	a	257	Total	C	N	O	S	0	1	0
			1972	1234	364	368	6			
1	b	257	Total	C	N	O	S	0	1	0
			1972	1234	364	368	6			
1	c	258	Total	C	N	O	S	0	1	0
			1980	1239	365	369	7			
1	d	257	Total	C	N	O	S	0	1	0
			1972	1234	364	368	6			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A6V1E4
A	-1	SER	-	expression tag	UNP A6V1E4
A	0	HIS	-	expression tag	UNP A6V1E4
B	-2	GLY	-	expression tag	UNP A6V1E4
B	-1	SER	-	expression tag	UNP A6V1E4
B	0	HIS	-	expression tag	UNP A6V1E4
C	-2	GLY	-	expression tag	UNP A6V1E4
C	-1	SER	-	expression tag	UNP A6V1E4
C	0	HIS	-	expression tag	UNP A6V1E4
D	-2	GLY	-	expression tag	UNP A6V1E4
D	-1	SER	-	expression tag	UNP A6V1E4

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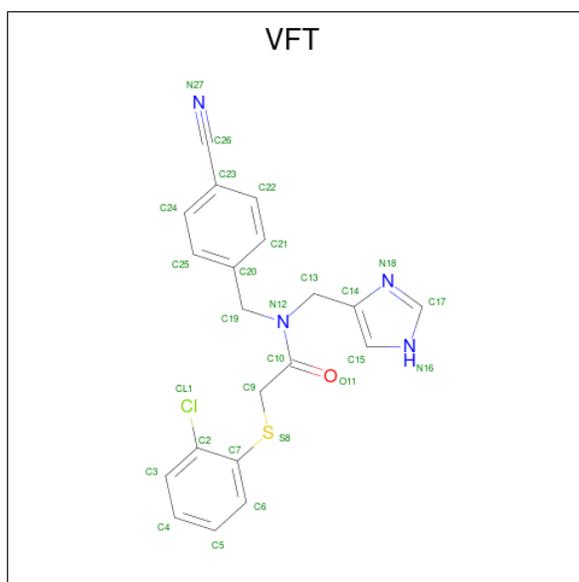
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A6V1E4
E	-2	GLY	-	expression tag	UNP A6V1E4
E	-1	SER	-	expression tag	UNP A6V1E4
E	0	HIS	-	expression tag	UNP A6V1E4
F	-2	GLY	-	expression tag	UNP A6V1E4
F	-1	SER	-	expression tag	UNP A6V1E4
F	0	HIS	-	expression tag	UNP A6V1E4
G	-2	GLY	-	expression tag	UNP A6V1E4
G	-1	SER	-	expression tag	UNP A6V1E4
G	0	HIS	-	expression tag	UNP A6V1E4
H	-2	GLY	-	expression tag	UNP A6V1E4
H	-1	SER	-	expression tag	UNP A6V1E4
H	0	HIS	-	expression tag	UNP A6V1E4
I	-2	GLY	-	expression tag	UNP A6V1E4
I	-1	SER	-	expression tag	UNP A6V1E4
I	0	HIS	-	expression tag	UNP A6V1E4
M	-2	GLY	-	expression tag	UNP A6V1E4
M	-1	SER	-	expression tag	UNP A6V1E4
M	0	HIS	-	expression tag	UNP A6V1E4
N	-2	GLY	-	expression tag	UNP A6V1E4
N	-1	SER	-	expression tag	UNP A6V1E4
N	0	HIS	-	expression tag	UNP A6V1E4
O	-2	GLY	-	expression tag	UNP A6V1E4
O	-1	SER	-	expression tag	UNP A6V1E4
O	0	HIS	-	expression tag	UNP A6V1E4
J	-2	GLY	-	expression tag	UNP A6V1E4
J	-1	SER	-	expression tag	UNP A6V1E4
J	0	HIS	-	expression tag	UNP A6V1E4
K	-2	GLY	-	expression tag	UNP A6V1E4
K	-1	SER	-	expression tag	UNP A6V1E4
K	0	HIS	-	expression tag	UNP A6V1E4
L	-2	GLY	-	expression tag	UNP A6V1E4
L	-1	SER	-	expression tag	UNP A6V1E4
L	0	HIS	-	expression tag	UNP A6V1E4
P	-2	GLY	-	expression tag	UNP A6V1E4
P	-1	SER	-	expression tag	UNP A6V1E4
P	0	HIS	-	expression tag	UNP A6V1E4
Q	-2	GLY	-	expression tag	UNP A6V1E4
Q	-1	SER	-	expression tag	UNP A6V1E4
Q	0	HIS	-	expression tag	UNP A6V1E4
R	-2	GLY	-	expression tag	UNP A6V1E4
R	-1	SER	-	expression tag	UNP A6V1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	HIS	-	expression tag	UNP A6V1E4
S	-2	GLY	-	expression tag	UNP A6V1E4
S	-1	SER	-	expression tag	UNP A6V1E4
S	0	HIS	-	expression tag	UNP A6V1E4
T	-2	GLY	-	expression tag	UNP A6V1E4
T	-1	SER	-	expression tag	UNP A6V1E4
T	0	HIS	-	expression tag	UNP A6V1E4
U	-2	GLY	-	expression tag	UNP A6V1E4
U	-1	SER	-	expression tag	UNP A6V1E4
U	0	HIS	-	expression tag	UNP A6V1E4
V	-2	GLY	-	expression tag	UNP A6V1E4
V	-1	SER	-	expression tag	UNP A6V1E4
V	0	HIS	-	expression tag	UNP A6V1E4
W	-2	GLY	-	expression tag	UNP A6V1E4
W	-1	SER	-	expression tag	UNP A6V1E4
W	0	HIS	-	expression tag	UNP A6V1E4
X	-2	GLY	-	expression tag	UNP A6V1E4
X	-1	SER	-	expression tag	UNP A6V1E4
X	0	HIS	-	expression tag	UNP A6V1E4
Y	-2	GLY	-	expression tag	UNP A6V1E4
Y	-1	SER	-	expression tag	UNP A6V1E4
Y	0	HIS	-	expression tag	UNP A6V1E4
Z	-2	GLY	-	expression tag	UNP A6V1E4
Z	-1	SER	-	expression tag	UNP A6V1E4
Z	0	HIS	-	expression tag	UNP A6V1E4
a	-2	GLY	-	expression tag	UNP A6V1E4
a	-1	SER	-	expression tag	UNP A6V1E4
a	0	HIS	-	expression tag	UNP A6V1E4
b	-2	GLY	-	expression tag	UNP A6V1E4
b	-1	SER	-	expression tag	UNP A6V1E4
b	0	HIS	-	expression tag	UNP A6V1E4
c	-2	GLY	-	expression tag	UNP A6V1E4
c	-1	SER	-	expression tag	UNP A6V1E4
c	0	HIS	-	expression tag	UNP A6V1E4
d	-2	GLY	-	expression tag	UNP A6V1E4
d	-1	SER	-	expression tag	UNP A6V1E4
d	0	HIS	-	expression tag	UNP A6V1E4

- Molecule 2 is 2-(2-chlorophenyl)sulfanyl- {N}-[(4-cyanophenyl)methyl]- {N}-(1 {H}-imidazol-4-ylmethyl)ethanamide (three-letter code: VFT) (formula: C₂₀H₁₇ClN₄OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	Total 33	24	1	6	1	1	0	1
2	B	1	Total 33	24	1	6	1	1	0	1
2	B	1	Total 33	24	1	6	1	1	0	1
2	D	1	Total 33	24	1	6	1	1	0	1
2	E	1	Total 33	24	1	6	1	1	0	1
2	F	1	Total 27	20	1	4	1	1	0	0
2	G	1	Total 33	24	1	6	1	1	0	1
2	G	1	Total 33	24	1	6	1	1	0	1
2	H	1	Total 27	20	1	4	1	1	0	0
2	M	1	Total 27	20	1	4	1	1	0	0
2	N	1	Total 27	20	1	4	1	1	0	0
2	O	1	Total 27	20	1	4	1	1	0	0
2	J	1	Total 33	24	1	6	1	1	0	1
2	K	1	Total 33	24	1	6	1	1	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	L	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	Q	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	Q	1	Total 27	C 20	Cl 1	N 4	O 1	S 1	0	0
2	R	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	S	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	T	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	U	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	W	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	W	1	Total 27	C 20	Cl 1	N 4	O 1	S 1	0	0
2	X	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	Y	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	a	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	a	1	Total 27	C 20	Cl 1	N 4	O 1	S 1	0	0
2	b	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	c	1	Total 33	C 24	Cl 1	N 6	O 1	S 1	0	1
2	c	1	Total 27	C 20	Cl 1	N 4	O 1	S 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

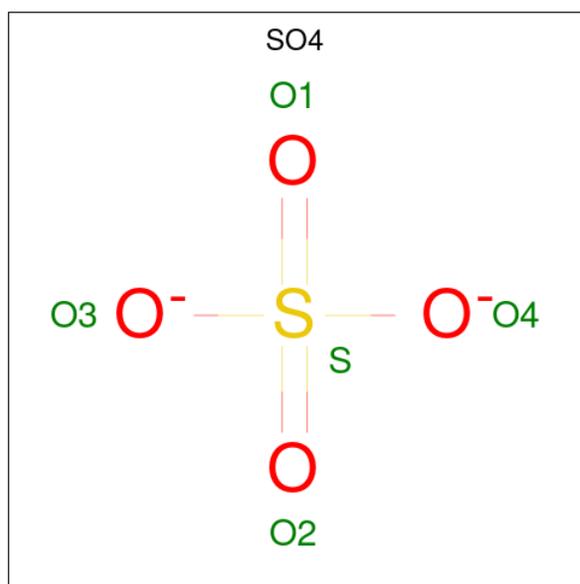
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cl 1 1	0	0
3	E	2	Total Cl 2 2	0	0
3	G	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	M	2	Total Cl 2 2	0	0
3	N	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	Q	1	Total Cl 1 1	0	0
3	S	1	Total Cl 1 1	0	0
3	T	1	Total Cl 1 1	0	0
3	X	2	Total Cl 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	M	1	5	4	1	0	0
4	N	1	5	4	1	0	0
4	N	1	5	4	1	0	0
4	O	1	5	4	1	0	0
4	O	1	5	4	1	0	0
4	J	1	5	4	1	0	0
4	J	1	5	4	1	0	0
4	J	1	5	4	1	0	0
4	K	1	5	4	1	0	0
4	K	1	5	4	1	0	0
4	L	1	5	4	1	0	0
4	L	1	5	4	1	0	0
4	P	1	5	4	1	0	0
4	P	1	5	4	1	0	0
4	P	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	Q	1	5	4	1	0	0
4	R	1	5	4	1	0	0
4	R	1	5	4	1	0	0
4	S	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total 5	O 4	S 1	0	0
4	S	1	Total 5	O 4	S 1	0	0
4	T	1	Total 5	O 4	S 1	0	0
4	T	1	Total 5	O 4	S 1	0	0
4	U	1	Total 5	O 4	S 1	0	0
4	U	1	Total 5	O 4	S 1	0	0
4	U	1	Total 5	O 4	S 1	0	0
4	V	1	Total 5	O 4	S 1	0	0
4	V	1	Total 5	O 4	S 1	0	0
4	V	1	Total 5	O 4	S 1	0	0
4	W	1	Total 5	O 4	S 1	0	0
4	W	1	Total 5	O 4	S 1	0	0
4	X	1	Total 5	O 4	S 1	0	0
4	X	1	Total 5	O 4	S 1	0	0
4	Y	1	Total 5	O 4	S 1	0	0
4	Y	1	Total 5	O 4	S 1	0	0
4	Z	1	Total 5	O 4	S 1	0	0
4	Z	1	Total 5	O 4	S 1	0	0
4	a	1	Total 5	O 4	S 1	0	0
4	a	1	Total 5	O 4	S 1	0	0
4	a	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	b	1	Total	O	S	0	0
			5	4	1		
4	b	1	Total	O	S	0	0
			5	4	1		
4	c	1	Total	O	S	0	0
			5	4	1		
4	c	1	Total	O	S	0	0
			5	4	1		
4	c	1	Total	O	S	0	0
			5	4	1		
4	d	1	Total	O	S	0	0
			5	4	1		
4	d	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	19	Total	O	0	0
			19	19		
5	C	15	Total	O	0	0
			15	15		
5	D	13	Total	O	0	0
			13	13		
5	E	11	Total	O	0	0
			11	11		
5	F	7	Total	O	0	0
			7	7		
5	G	4	Total	O	0	0
			4	4		
5	H	7	Total	O	0	0
			7	7		
5	I	4	Total	O	0	0
			4	4		
5	M	6	Total	O	0	0
			6	6		
5	N	4	Total	O	0	0
			4	4		
5	O	8	Total	O	0	0
			8	8		

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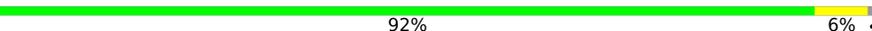
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	10	Total O 10 10	0	0
5	K	7	Total O 7 7	0	0
5	L	8	Total O 8 8	0	0
5	P	5	Total O 5 5	0	0
5	Q	5	Total O 5 5	0	0
5	R	7	Total O 7 7	0	0
5	S	8	Total O 8 8	0	0
5	T	8	Total O 8 8	0	0
5	U	9	Total O 9 9	0	0
5	V	6	Total O 6 6	0	0
5	W	5	Total O 5 5	0	0
5	X	2	Total O 2 2	0	0
5	Y	3	Total O 3 3	0	0
5	Z	4	Total O 4 4	0	0
5	a	6	Total O 6 6	0	0
5	b	6	Total O 6 6	0	0
5	c	7	Total O 7 7	0	0
5	d	5	Total O 5 5	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: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain A: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain B: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain C: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain D: 



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain E: 

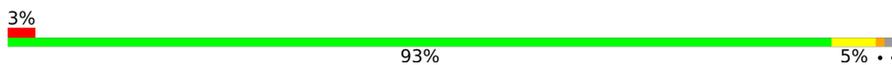


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain F:  88% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain G:  3% 93% 5% ..

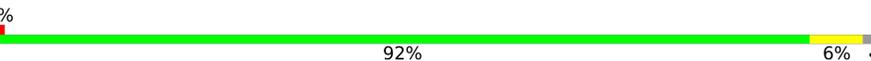


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain H:  90% 7% ..



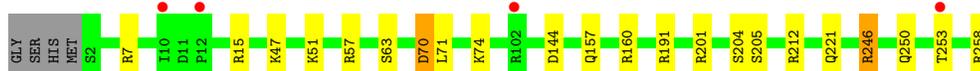
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain I:  % 92% 6% ..



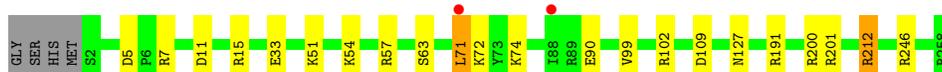
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain M:  2% 90% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain N:  % 90% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain O:  % 91% 7% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J:  90% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain K:  90% 8% ..

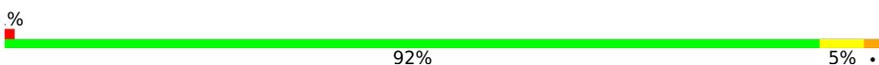


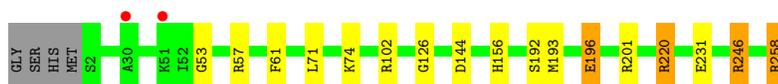
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain L:  90% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain P:  92% 5% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Q:  90% 6% ..

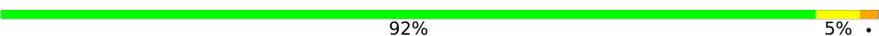


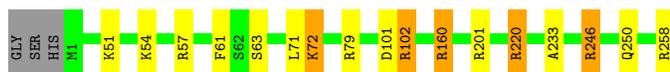
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain R:  90% 7% ..



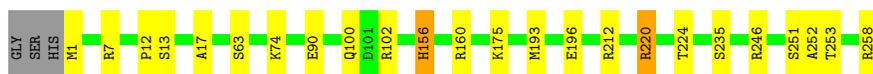
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain S:  92% 5% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain T:  90% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain U:  91% 6% ..

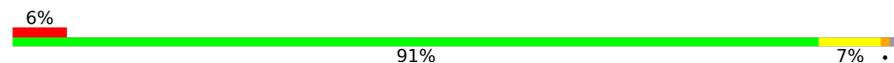


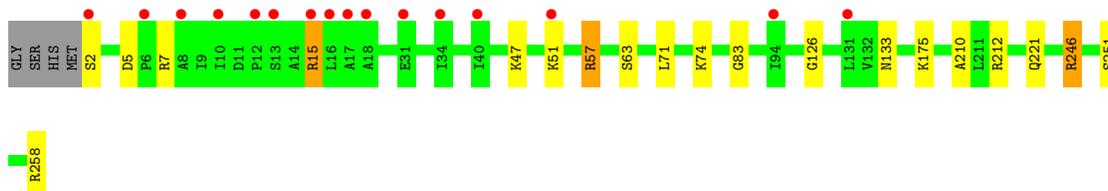
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain V:  2% 90% 7% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain W:  6% 91% 7% ..

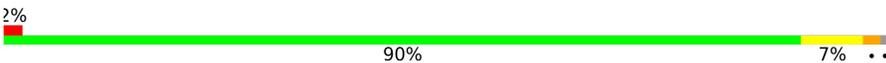


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain X:  90% 7% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Y:  2% 90% 7% ..



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

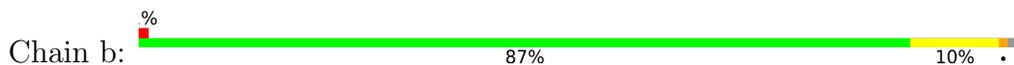
Chain Z:  89% 9% ..



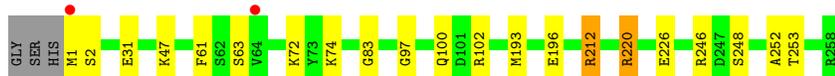
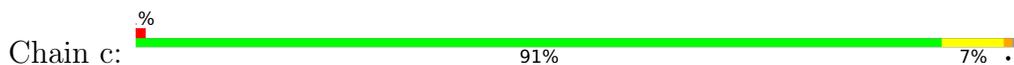
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



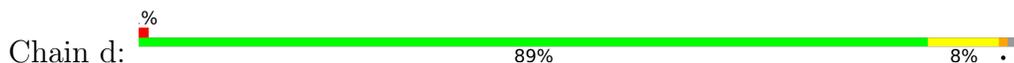
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	377.00Å 377.00Å 263.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.45 – 2.74 113.47 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (113.45-2.74) 99.8 (113.47-2.74)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.225 0.191 , 0.225	Depositor DCC
R_{free} test set	24562 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60786	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VFT, SO4, CL

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	0.91	2/2045 (0.1%)	1.18	9/2772 (0.3%)
1	B	0.94	2/2056 (0.1%)	1.16	7/2786 (0.3%)
1	C	0.96	4/2047 (0.2%)	1.18	7/2774 (0.3%)
1	D	0.98	4/2025 (0.2%)	1.23	15/2746 (0.5%)
1	E	0.94	5/2016 (0.2%)	1.18	8/2734 (0.3%)
1	F	0.97	5/2036 (0.2%)	1.19	9/2760 (0.3%)
1	G	0.88	1/2008 (0.0%)	1.14	4/2724 (0.1%)
1	H	0.90	1/2008 (0.0%)	1.18	7/2724 (0.3%)
1	I	0.88	1/2008 (0.0%)	1.13	6/2724 (0.2%)
1	J	0.97	4/2027 (0.2%)	1.23	12/2748 (0.4%)
1	K	0.94	3/2016 (0.1%)	1.18	7/2734 (0.3%)
1	L	0.95	3/2016 (0.1%)	1.18	6/2734 (0.2%)
1	M	0.89	0/2008	1.16	8/2724 (0.3%)
1	N	0.88	1/2008 (0.0%)	1.15	7/2724 (0.3%)
1	O	0.86	0/2008	1.17	7/2724 (0.3%)
1	P	0.91	4/2008 (0.2%)	1.20	9/2724 (0.3%)
1	Q	0.88	1/2019 (0.0%)	1.19	14/2738 (0.5%)
1	R	0.87	1/2008 (0.0%)	1.17	8/2724 (0.3%)
1	S	0.94	3/2016 (0.1%)	1.25	12/2734 (0.4%)
1	T	0.95	2/2016 (0.1%)	1.21	8/2734 (0.3%)
1	U	0.92	2/2016 (0.1%)	1.23	14/2734 (0.5%)
1	V	0.88	2/2008 (0.1%)	1.16	5/2724 (0.2%)
1	W	0.87	1/2017 (0.0%)	1.16	3/2736 (0.1%)
1	X	0.90	3/2017 (0.1%)	1.18	9/2736 (0.3%)
1	Y	0.90	1/2025 (0.0%)	1.15	7/2746 (0.3%)
1	Z	0.92	5/2025 (0.2%)	1.20	9/2746 (0.3%)
1	a	0.88	1/2017 (0.0%)	1.13	5/2736 (0.2%)
1	b	0.90	2/2017 (0.1%)	1.19	9/2736 (0.3%)
1	c	0.90	5/2025 (0.2%)	1.14	4/2746 (0.1%)
1	d	0.86	0/2017	1.12	6/2736 (0.2%)
All	All	0.91	69/60583 (0.1%)	1.18	241/82162 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	2
1	F	0	3
1	H	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	N	0	1
1	O	0	1
1	R	0	1
1	T	0	2
1	V	0	1
1	X	0	2
1	Z	0	2
1	c	0	1
All	All	0	22

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	196	GLU	CD-OE1	8.76	1.35	1.25
1	F	196	GLU	CD-OE1	8.22	1.34	1.25
1	T	196	GLU	CD-OE1	8.12	1.34	1.25
1	J	57	ARG	NE-CZ	8.04	1.43	1.33
1	D	206	GLU	CD-OE1	7.81	1.34	1.25

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	57	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	R	220	ARG	NE-CZ-NH2	12.65	126.62	120.30
1	Z	220	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	c	220	ARG	NE-CZ-NH2	12.08	126.34	120.30
1	B	220	ARG	NE-CZ-NH2	11.88	126.24	120.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	SER	Peptide
1	C	2	SER	Peptide
1	E	17	ALA	Peptide
1	E	252	ALA	Peptide
1	F	2	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	259/261 (99%)	242 (93%)	17 (7%)	0	100	100
1	B	260/261 (100%)	237 (91%)	21 (8%)	2 (1%)	19	36
1	C	259/261 (99%)	241 (93%)	18 (7%)	0	100	100
1	D	257/261 (98%)	239 (93%)	16 (6%)	2 (1%)	19	36
1	E	256/261 (98%)	240 (94%)	14 (6%)	2 (1%)	19	36
1	F	258/261 (99%)	245 (95%)	11 (4%)	2 (1%)	19	36
1	G	255/261 (98%)	238 (93%)	17 (7%)	0	100	100
1	H	255/261 (98%)	237 (93%)	16 (6%)	2 (1%)	19	36
1	I	255/261 (98%)	241 (94%)	13 (5%)	1 (0%)	34	55
1	J	257/261 (98%)	241 (94%)	13 (5%)	3 (1%)	13	24
1	K	256/261 (98%)	234 (91%)	22 (9%)	0	100	100
1	L	256/261 (98%)	237 (93%)	17 (7%)	2 (1%)	19	36
1	M	255/261 (98%)	233 (91%)	21 (8%)	1 (0%)	34	55
1	N	255/261 (98%)	227 (89%)	26 (10%)	2 (1%)	19	36
1	O	255/261 (98%)	230 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	255/261 (98%)	235 (92%)	18 (7%)	2 (1%)	19	36
1	Q	256/261 (98%)	231 (90%)	22 (9%)	3 (1%)	13	24
1	R	255/261 (98%)	234 (92%)	18 (7%)	3 (1%)	13	24
1	S	256/261 (98%)	236 (92%)	20 (8%)	0	100	100
1	T	256/261 (98%)	240 (94%)	15 (6%)	1 (0%)	34	55
1	U	256/261 (98%)	235 (92%)	19 (7%)	2 (1%)	19	36
1	V	255/261 (98%)	233 (91%)	17 (7%)	5 (2%)	7	13
1	W	256/261 (98%)	233 (91%)	20 (8%)	3 (1%)	13	24
1	X	256/261 (98%)	226 (88%)	26 (10%)	4 (2%)	9	17
1	Y	257/261 (98%)	236 (92%)	19 (7%)	2 (1%)	19	36
1	Z	257/261 (98%)	237 (92%)	18 (7%)	2 (1%)	19	36
1	a	256/261 (98%)	235 (92%)	20 (8%)	1 (0%)	34	55
1	b	256/261 (98%)	236 (92%)	19 (7%)	1 (0%)	34	55
1	c	257/261 (98%)	233 (91%)	23 (9%)	1 (0%)	34	55
1	d	256/261 (98%)	229 (90%)	21 (8%)	6 (2%)	6	10
All	All	7688/7830 (98%)	7071 (92%)	562 (7%)	55 (1%)	22	40

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER
1	J	18	ALA
1	J	224	THR
1	Q	18	ALA
1	R	72	LYS

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	209/208 (100%)	199 (95%)	10 (5%)	25	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	210/208 (101%)	199 (95%)	11 (5%)	23	39
1	C	209/208 (100%)	197 (94%)	12 (6%)	20	36
1	D	207/208 (100%)	189 (91%)	18 (9%)	10	19
1	E	206/208 (99%)	194 (94%)	12 (6%)	20	35
1	F	208/208 (100%)	189 (91%)	19 (9%)	9	17
1	G	205/208 (99%)	192 (94%)	13 (6%)	18	31
1	H	205/208 (99%)	190 (93%)	15 (7%)	14	25
1	I	205/208 (99%)	195 (95%)	10 (5%)	25	43
1	J	207/208 (100%)	194 (94%)	13 (6%)	18	31
1	K	206/208 (99%)	192 (93%)	14 (7%)	16	28
1	L	206/208 (99%)	190 (92%)	16 (8%)	12	22
1	M	205/208 (99%)	189 (92%)	16 (8%)	12	22
1	N	205/208 (99%)	191 (93%)	14 (7%)	16	28
1	O	205/208 (99%)	191 (93%)	14 (7%)	16	28
1	P	205/208 (99%)	194 (95%)	11 (5%)	22	38
1	Q	206/208 (99%)	189 (92%)	17 (8%)	11	20
1	R	205/208 (99%)	190 (93%)	15 (7%)	14	25
1	S	206/208 (99%)	194 (94%)	12 (6%)	20	35
1	T	206/208 (99%)	190 (92%)	16 (8%)	12	22
1	U	206/208 (99%)	193 (94%)	13 (6%)	18	31
1	V	205/208 (99%)	191 (93%)	14 (7%)	16	28
1	W	206/208 (99%)	190 (92%)	16 (8%)	12	22
1	X	206/208 (99%)	195 (95%)	11 (5%)	22	39
1	Y	207/208 (100%)	190 (92%)	17 (8%)	11	21
1	Z	207/208 (100%)	193 (93%)	14 (7%)	16	28
1	a	206/208 (99%)	187 (91%)	19 (9%)	9	17
1	b	206/208 (99%)	186 (90%)	20 (10%)	8	14
1	c	207/208 (100%)	192 (93%)	15 (7%)	14	25
1	d	206/208 (99%)	189 (92%)	17 (8%)	11	20
All	All	6188/6240 (99%)	5754 (93%)	434 (7%)	15	27

5 of 434 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	212	ARG
1	U	160	ARG
1	b	246	ARG
1	R	57	ARG
1	S	250	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	164	HIS
1	a	223	HIS
1	d	223	HIS
1	O	56	ASN
1	O	43	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 143 ligands modelled in this entry, 21 are monoatomic - leaving 122 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VFT	B	301[A]	-	25,29,29	1.06	1 (4%)	31,38,38	1.34	4 (12%)
2	VFT	U	301[A]	-	25,29,29	1.05	1 (4%)	31,38,38	1.54	5 (16%)
4	SO4	Q	305	-	4,4,4	0.28	0	6,6,6	0.17	0
2	VFT	c	301[A]	-	25,29,29	0.89	1 (4%)	31,38,38	1.43	5 (16%)
4	SO4	T	303	-	4,4,4	0.28	0	6,6,6	0.24	0
4	SO4	X	304	-	4,4,4	0.32	0	6,6,6	0.22	0
2	VFT	S	301[A]	-	25,29,29	0.71	0	31,38,38	1.26	3 (9%)
4	SO4	V	301	-	4,4,4	0.37	0	6,6,6	0.30	0
2	VFT	c	301[B]	-	25,29,29	0.87	1 (4%)	31,38,38	1.40	7 (22%)
4	SO4	E	305	-	4,4,4	0.30	0	6,6,6	0.20	0
4	SO4	S	303	-	4,4,4	0.29	0	6,6,6	0.21	0
4	SO4	A	305	-	4,4,4	0.40	0	6,6,6	0.16	0
4	SO4	V	303	-	4,4,4	0.31	0	6,6,6	0.26	0
2	VFT	F	301	-	25,29,29	0.92	2 (8%)	31,38,38	1.26	4 (12%)
2	VFT	S	301[B]	-	25,29,29	0.70	0	31,38,38	1.17	3 (9%)
4	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.33	0
4	SO4	Y	303	-	4,4,4	0.30	0	6,6,6	0.21	0
4	SO4	V	302	-	4,4,4	0.29	0	6,6,6	0.24	0
2	VFT	G	301[B]	-	25,29,29	1.02	2 (8%)	31,38,38	1.10	1 (3%)
2	VFT	W	301[B]	-	25,29,29	0.98	2 (8%)	31,38,38	1.33	5 (16%)
2	VFT	c	302	-	25,29,29	1.06	2 (8%)	31,38,38	1.53	4 (12%)
4	SO4	P	301	-	4,4,4	0.35	0	6,6,6	0.22	0
4	SO4	W	304	-	4,4,4	0.36	0	6,6,6	0.22	0
4	SO4	X	305	-	4,4,4	0.33	0	6,6,6	0.22	0
4	SO4	b	303	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	J	303	-	4,4,4	0.28	0	6,6,6	0.17	0
2	VFT	H	301	-	25,29,29	1.07	3 (12%)	31,38,38	1.57	4 (12%)
2	VFT	R	301[B]	-	25,29,29	1.06	2 (8%)	31,38,38	1.20	5 (16%)
4	SO4	K	302	-	4,4,4	0.26	0	6,6,6	0.28	0
2	VFT	a	302	-	25,29,29	0.82	0	31,38,38	1.52	4 (12%)
4	SO4	S	305	-	4,4,4	0.32	0	6,6,6	0.19	0
2	VFT	M	301	-	25,29,29	0.84	1 (4%)	31,38,38	1.22	2 (6%)
4	SO4	J	304	-	4,4,4	0.34	0	6,6,6	0.22	0
2	VFT	G	301[A]	-	25,29,29	1.02	2 (8%)	31,38,38	1.02	0
2	VFT	W	301[A]	-	25,29,29	0.93	2 (8%)	31,38,38	1.37	4 (12%)
4	SO4	O	304	-	4,4,4	0.30	0	6,6,6	0.24	0
2	VFT	a	301[B]	-	25,29,29	0.89	2 (8%)	31,38,38	1.07	2 (6%)
4	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.21	0
4	SO4	W	303	-	4,4,4	0.37	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	R	302	-	4,4,4	0.31	0	6,6,6	0.25	0
4	SO4	c	305	-	4,4,4	0.29	0	6,6,6	0.26	0
2	VFT	Q	301[B]	-	25,29,29	0.93	1 (4%)	31,38,38	1.00	2 (6%)
4	SO4	L	304	-	4,4,4	0.31	0	6,6,6	0.16	0
4	SO4	I	303	-	4,4,4	0.36	0	6,6,6	0.15	0
2	VFT	R	301[A]	-	25,29,29	0.95	2 (8%)	31,38,38	1.34	5 (16%)
2	VFT	K	301[B]	-	25,29,29	1.26	3 (12%)	31,38,38	1.32	4 (12%)
2	VFT	B	302[B]	-	25,29,29	0.98	1 (4%)	31,38,38	1.30	5 (16%)
2	VFT	D	301[B]	-	25,29,29	0.93	1 (4%)	31,38,38	1.11	2 (6%)
4	SO4	Q	306	-	4,4,4	0.34	0	6,6,6	0.24	0
4	SO4	Z	302	-	4,4,4	0.28	0	6,6,6	0.23	0
4	SO4	G	306	-	4,4,4	0.31	0	6,6,6	0.23	0
2	VFT	J	301[A]	-	25,29,29	0.79	0	31,38,38	1.20	1 (3%)
4	SO4	A	307	-	4,4,4	0.28	0	6,6,6	0.25	0
2	VFT	a	301[A]	-	25,29,29	0.88	2 (8%)	31,38,38	1.11	2 (6%)
4	SO4	O	303	-	4,4,4	0.32	0	6,6,6	0.19	0
4	SO4	D	303	-	4,4,4	0.32	0	6,6,6	0.25	0
2	VFT	L	301[A]	-	25,29,29	0.94	1 (4%)	31,38,38	1.41	2 (6%)
4	SO4	T	304	-	4,4,4	0.36	0	6,6,6	0.24	0
4	SO4	N	303	-	4,4,4	0.27	0	6,6,6	0.25	0
2	VFT	J	301[B]	-	25,29,29	0.73	0	31,38,38	1.19	2 (6%)
4	SO4	P	303	-	4,4,4	0.34	0	6,6,6	0.41	0
4	SO4	d	302	-	4,4,4	0.36	0	6,6,6	0.30	0
4	SO4	a	303	-	4,4,4	0.31	0	6,6,6	0.26	0
2	VFT	Q	301[A]	-	25,29,29	0.95	1 (4%)	31,38,38	1.21	3 (9%)
4	SO4	G	305	-	4,4,4	0.40	0	6,6,6	0.20	0
4	SO4	Y	302	-	4,4,4	0.32	0	6,6,6	0.24	0
2	VFT	E	301[B]	-	25,29,29	0.85	0	31,38,38	1.34	5 (16%)
4	SO4	C	304	-	4,4,4	0.32	0	6,6,6	0.20	0
4	SO4	P	302	-	4,4,4	0.34	0	6,6,6	0.06	0
4	SO4	N	304	-	4,4,4	0.30	0	6,6,6	0.30	0
2	VFT	K	301[A]	-	25,29,29	1.27	3 (12%)	31,38,38	1.40	4 (12%)
2	VFT	L	301[B]	-	25,29,29	0.94	1 (4%)	31,38,38	1.22	2 (6%)
4	SO4	F	303	-	4,4,4	0.35	0	6,6,6	0.18	0
4	SO4	Z	301	-	4,4,4	0.34	0	6,6,6	0.14	0
2	VFT	B	302[A]	-	25,29,29	0.97	1 (4%)	31,38,38	1.36	4 (12%)
2	VFT	D	301[A]	-	25,29,29	0.90	1 (4%)	31,38,38	1.38	2 (6%)
4	SO4	Q	304	-	4,4,4	0.33	0	6,6,6	0.31	0
4	SO4	c	303	-	4,4,4	0.31	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VFT	X	301[B]	-	25,29,29	1.04	2 (8%)	31,38,38	0.97	2 (6%)
4	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.17	0
2	VFT	A	301[A]	-	25,29,29	1.10	2 (8%)	31,38,38	1.20	2 (6%)
2	VFT	G	302[B]	-	25,29,29	0.73	0	31,38,38	1.28	3 (9%)
2	VFT	Q	302	-	25,29,29	1.04	2 (8%)	31,38,38	1.61	6 (19%)
4	SO4	F	302	-	4,4,4	0.25	0	6,6,6	0.22	0
2	VFT	T	301[A]	-	25,29,29	1.19	2 (8%)	31,38,38	1.60	4 (12%)
4	SO4	M	304	-	4,4,4	0.35	0	6,6,6	0.22	0
4	SO4	B	305	-	4,4,4	0.35	0	6,6,6	0.30	0
4	SO4	J	302	-	4,4,4	0.33	0	6,6,6	0.25	0
4	SO4	U	303	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	a	304	-	4,4,4	0.22	0	6,6,6	0.20	0
4	SO4	E	304	-	4,4,4	0.33	0	6,6,6	0.20	0
2	VFT	B	301[B]	-	25,29,29	1.04	1 (4%)	31,38,38	1.17	2 (6%)
2	VFT	O	301	-	25,29,29	1.02	1 (4%)	31,38,38	1.42	4 (12%)
2	VFT	U	301[B]	-	25,29,29	1.06	1 (4%)	31,38,38	1.46	5 (16%)
4	SO4	M	305	-	4,4,4	0.33	0	6,6,6	0.32	0
2	VFT	Y	301[A]	-	25,29,29	0.87	1 (4%)	31,38,38	1.26	4 (12%)
2	VFT	A	301[B]	-	25,29,29	1.10	2 (8%)	31,38,38	1.23	3 (9%)
4	SO4	U	302	-	4,4,4	0.39	0	6,6,6	0.25	0
2	VFT	T	301[B]	-	25,29,29	1.17	2 (8%)	31,38,38	1.47	5 (16%)
4	SO4	U	304	-	4,4,4	0.34	0	6,6,6	0.25	0
4	SO4	K	303	-	4,4,4	0.28	0	6,6,6	0.30	0
2	VFT	E	301[A]	-	25,29,29	0.83	0	31,38,38	1.30	4 (12%)
4	SO4	L	303	-	4,4,4	0.26	0	6,6,6	0.18	0
2	VFT	Y	301[B]	-	25,29,29	0.88	1 (4%)	31,38,38	1.23	4 (12%)
2	VFT	b	301[A]	-	25,29,29	0.86	1 (4%)	31,38,38	1.20	4 (12%)
4	SO4	H	302	-	4,4,4	0.24	0	6,6,6	0.26	0
4	SO4	H	303	-	4,4,4	0.34	0	6,6,6	0.22	0
4	SO4	c	304	-	4,4,4	0.24	0	6,6,6	0.29	0
4	SO4	A	306	-	4,4,4	0.25	0	6,6,6	0.21	0
2	VFT	X	301[A]	-	25,29,29	1.03	2 (8%)	31,38,38	1.12	2 (6%)
2	VFT	N	301	-	25,29,29	1.05	2 (8%)	31,38,38	1.26	4 (12%)
4	SO4	d	301	-	4,4,4	0.32	0	6,6,6	0.20	0
4	SO4	E	306	-	4,4,4	0.40	0	6,6,6	0.24	0
2	VFT	G	302[A]	-	25,29,29	0.72	0	31,38,38	1.31	2 (6%)
4	SO4	C	303	-	4,4,4	0.38	0	6,6,6	0.19	0
2	VFT	W	302	-	25,29,29	1.10	1 (4%)	31,38,38	1.42	5 (16%)
4	SO4	S	304	-	4,4,4	0.27	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	R	303	-	4,4,4	0.35	0	6,6,6	0.22	0
4	SO4	b	302	-	4,4,4	0.28	0	6,6,6	0.22	0
4	SO4	I	302	-	4,4,4	0.29	0	6,6,6	0.26	0
2	VFT	b	301[B]	-	25,29,29	0.91	1 (4%)	31,38,38	1.11	4 (12%)
4	SO4	a	305	-	4,4,4	0.30	0	6,6,6	0.29	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	VFT	A	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	B	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	G	302[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	Q	302	-	-	0/19/19/19	0/3/3/3
2	VFT	R	301[A]	-	-	2/19/19/19	0/3/3/3
2	VFT	K	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	U	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	T	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	B	302[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	D	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	J	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	c	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	B	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	O	301	-	-	0/19/19/19	0/3/3/3
2	VFT	U	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	H	301	-	-	1/19/19/19	0/3/3/3
2	VFT	R	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	Y	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	A	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	S	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	T	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	a	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	a	302	-	-	1/19/19/19	0/3/3/3
2	VFT	E	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	L	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	M	301	-	-	1/19/19/19	0/3/3/3
2	VFT	J	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	c	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	G	301[A]	-	-	3/19/19/19	0/3/3/3
2	VFT	Y	301[B]	-	-	0/19/19/19	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFT	W	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	b	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	Q	301[A]	-	-	2/19/19/19	0/3/3/3
2	VFT	X	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	F	301	-	-	0/19/19/19	0/3/3/3
2	VFT	S	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	a	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	N	301	-	-	0/19/19/19	0/3/3/3
2	VFT	E	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	G	302[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	K	301[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	L	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	W	302	-	-	0/19/19/19	0/3/3/3
2	VFT	B	302[A]	-	-	0/19/19/19	0/3/3/3
2	VFT	D	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	G	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	W	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	Q	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	X	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	b	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	c	302	-	-	0/19/19/19	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301[A]	VFT	C10-N12	3.58	1.42	1.35
2	K	301[B]	VFT	C10-N12	3.58	1.42	1.35
2	B	301[A]	VFT	C10-N12	3.42	1.42	1.35
2	B	301[B]	VFT	C10-N12	3.42	1.42	1.35
2	Q	301[A]	VFT	C10-N12	3.32	1.42	1.35

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	VFT	C14-C13-N12	-5.57	104.22	113.65
2	Q	302	VFT	C14-C13-N12	-5.40	104.50	113.65
2	a	302	VFT	C14-C13-N12	-5.36	104.57	113.65
2	c	302	VFT	C14-C13-N12	-5.33	104.63	113.65
2	D	301[A]	VFT	C14-C13-N12	5.03	122.17	113.65

There are no chirality outliers.

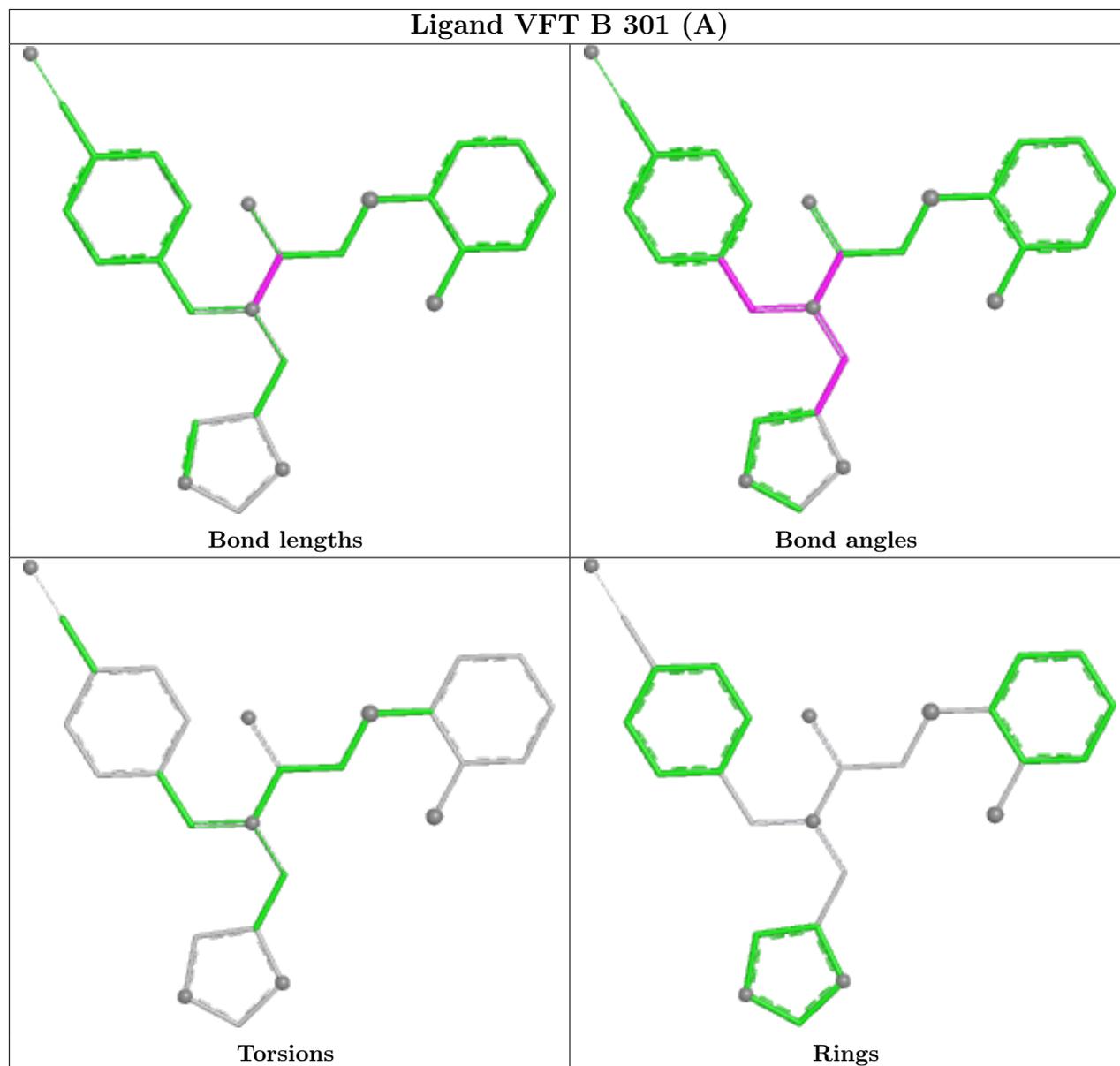
5 of 23 torsion outliers are listed below:

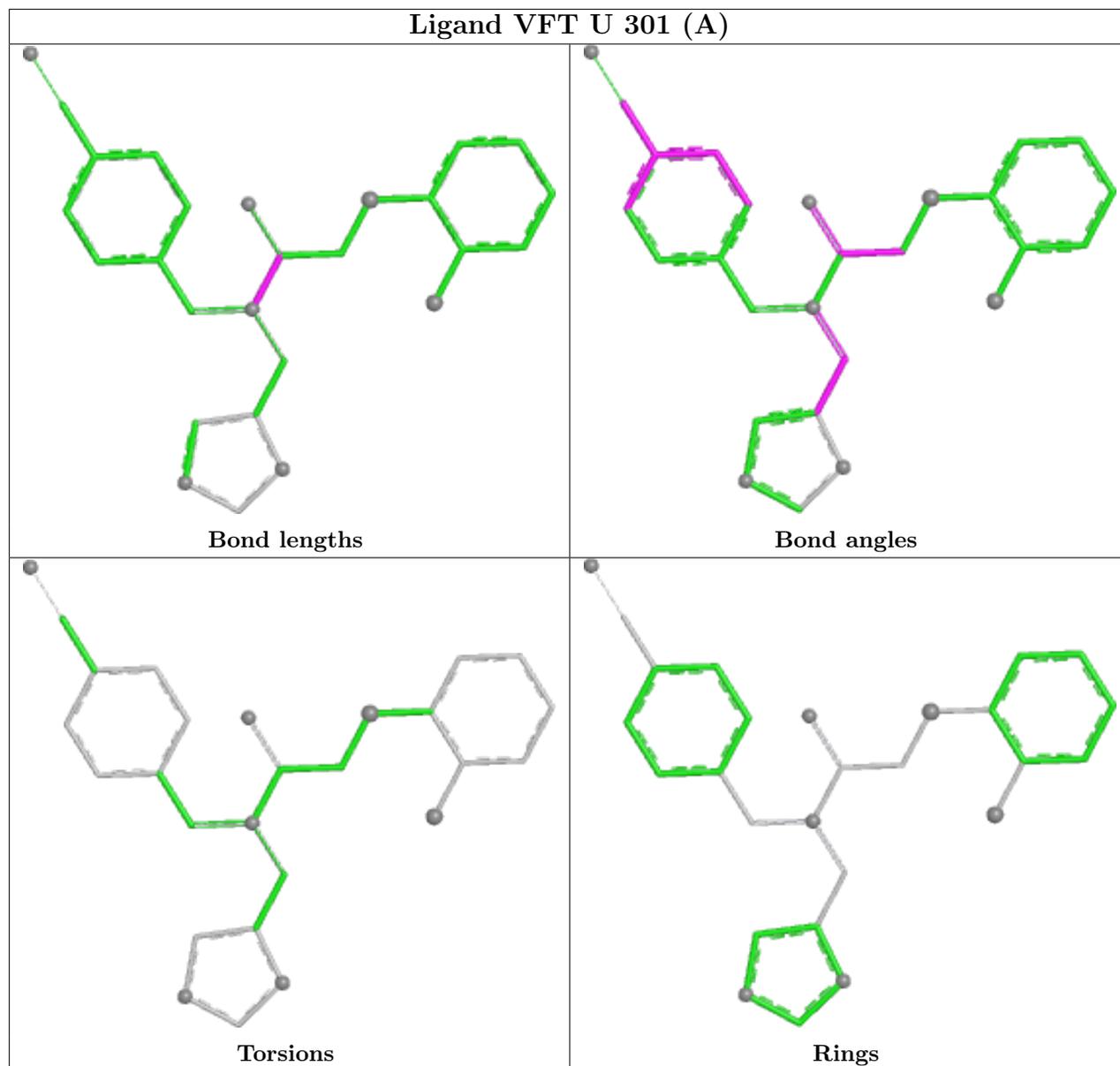
Mol	Chain	Res	Type	Atoms
2	E	301[B]	VFT	N12-C13-C14-N18
2	M	301	VFT	N12-C13-C14-N18
2	T	301[B]	VFT	N12-C13-C14-N18
2	U	301[B]	VFT	N12-C13-C14-N18
2	a	302	VFT	N12-C13-C14-N18

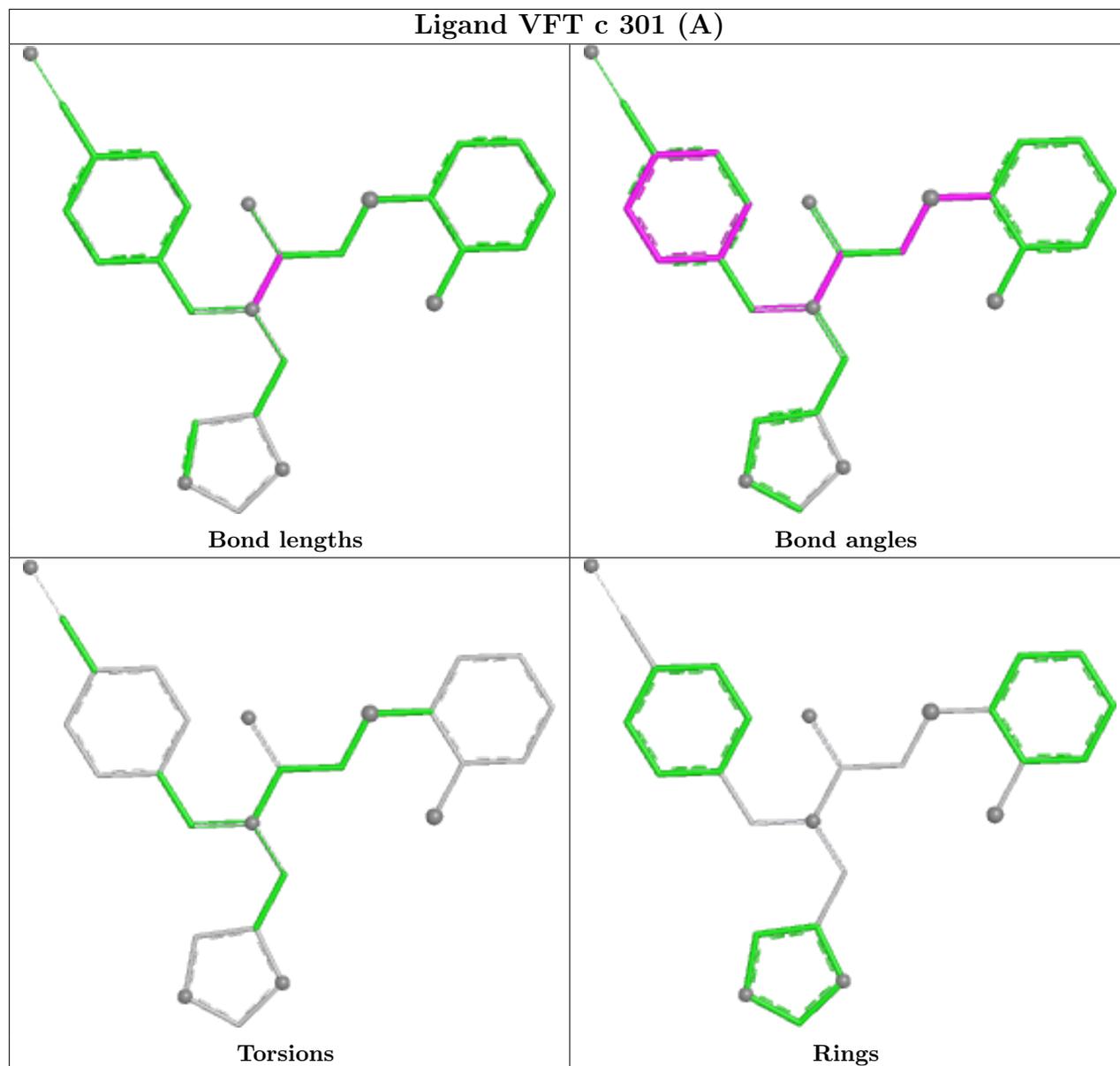
There are no ring outliers.

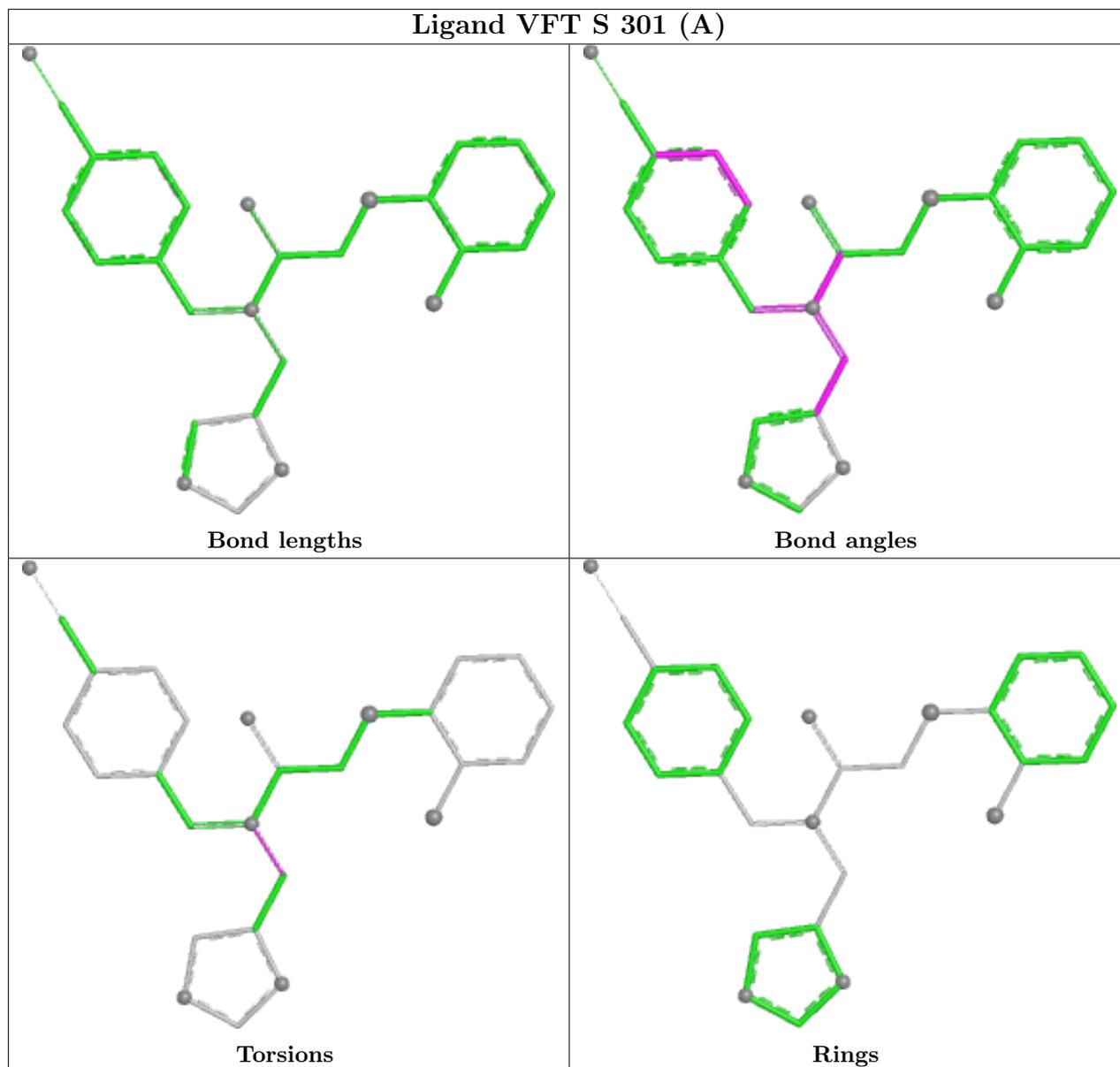
No monomer is involved in short contacts.

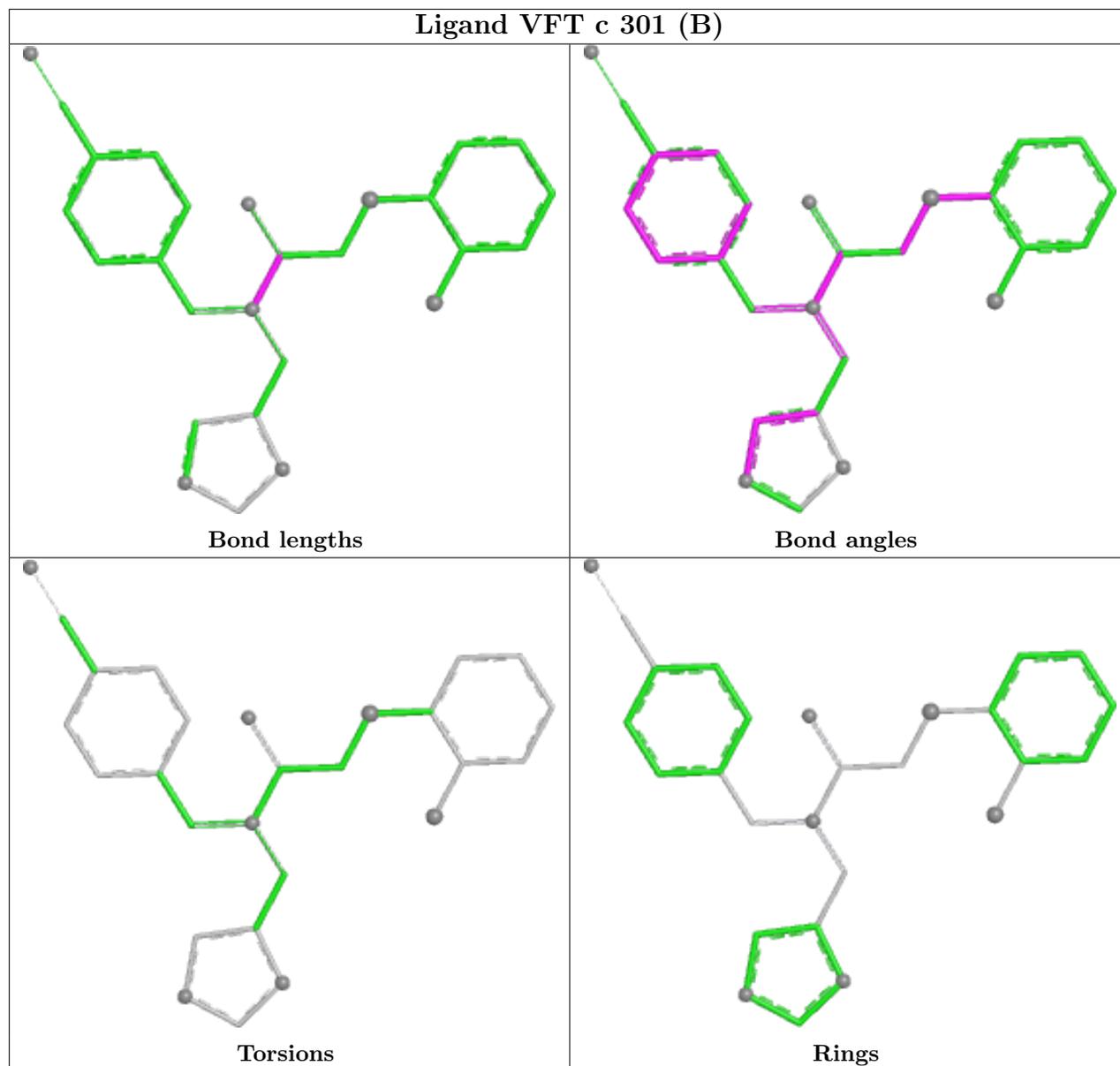
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

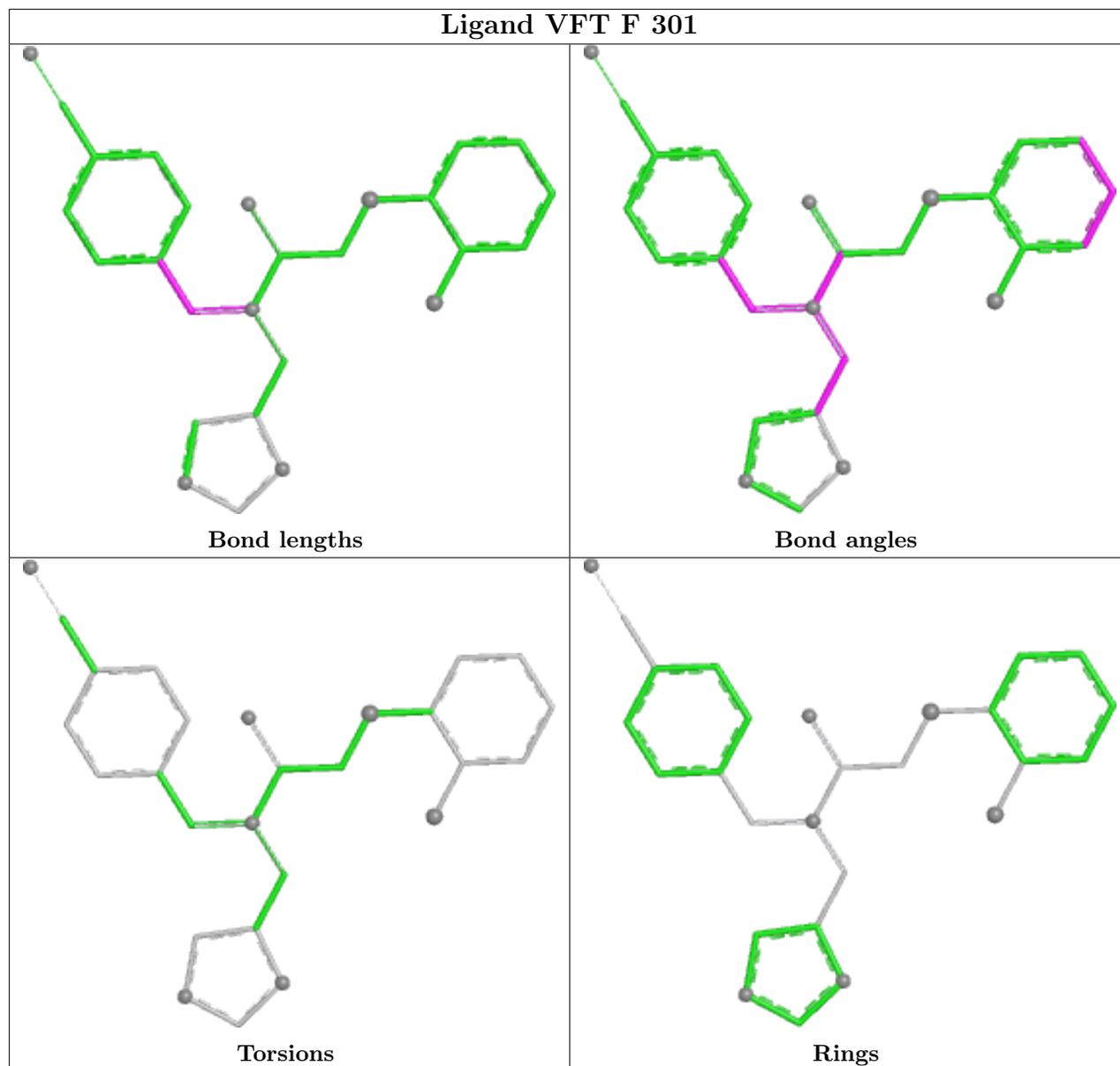


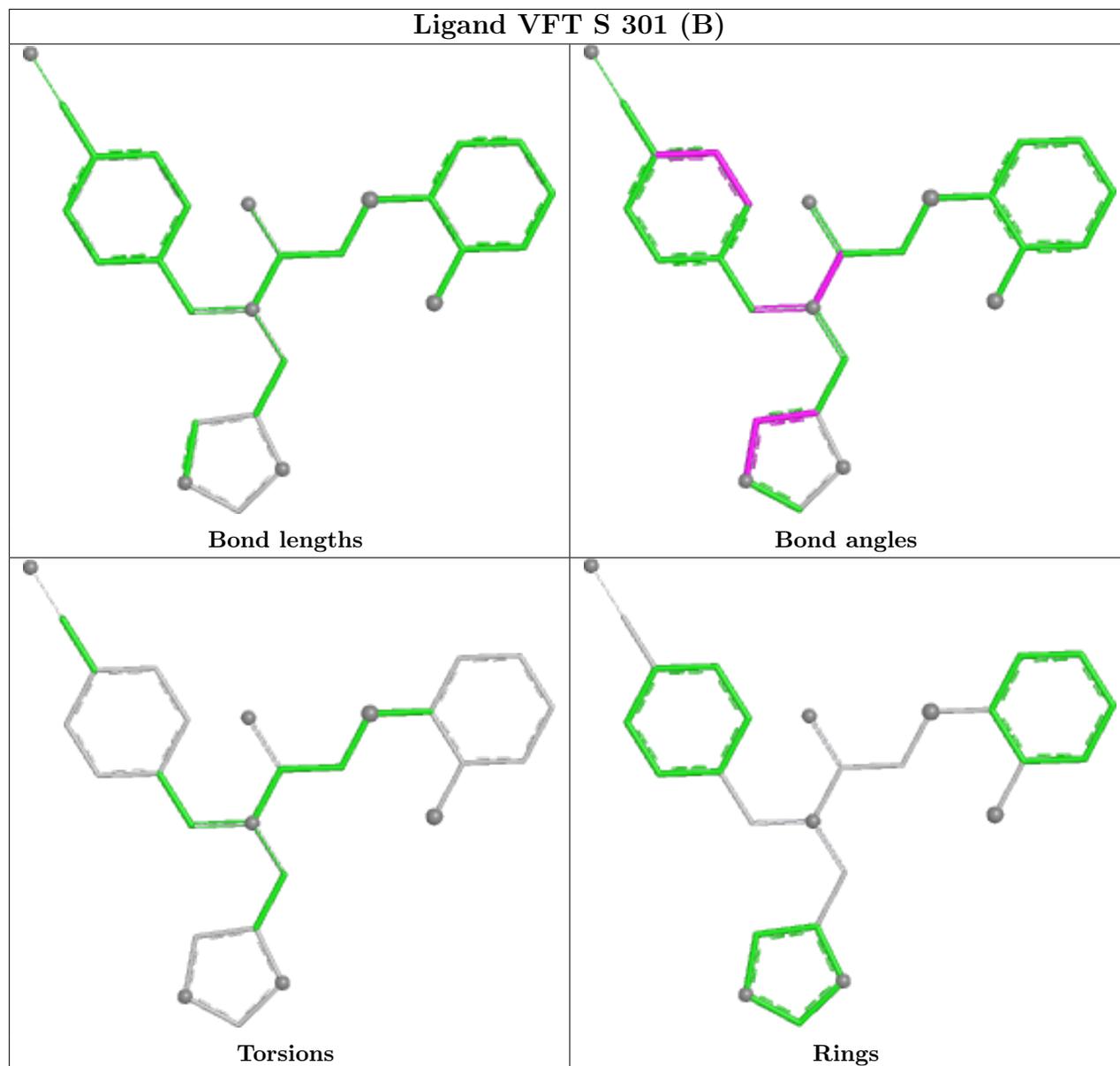


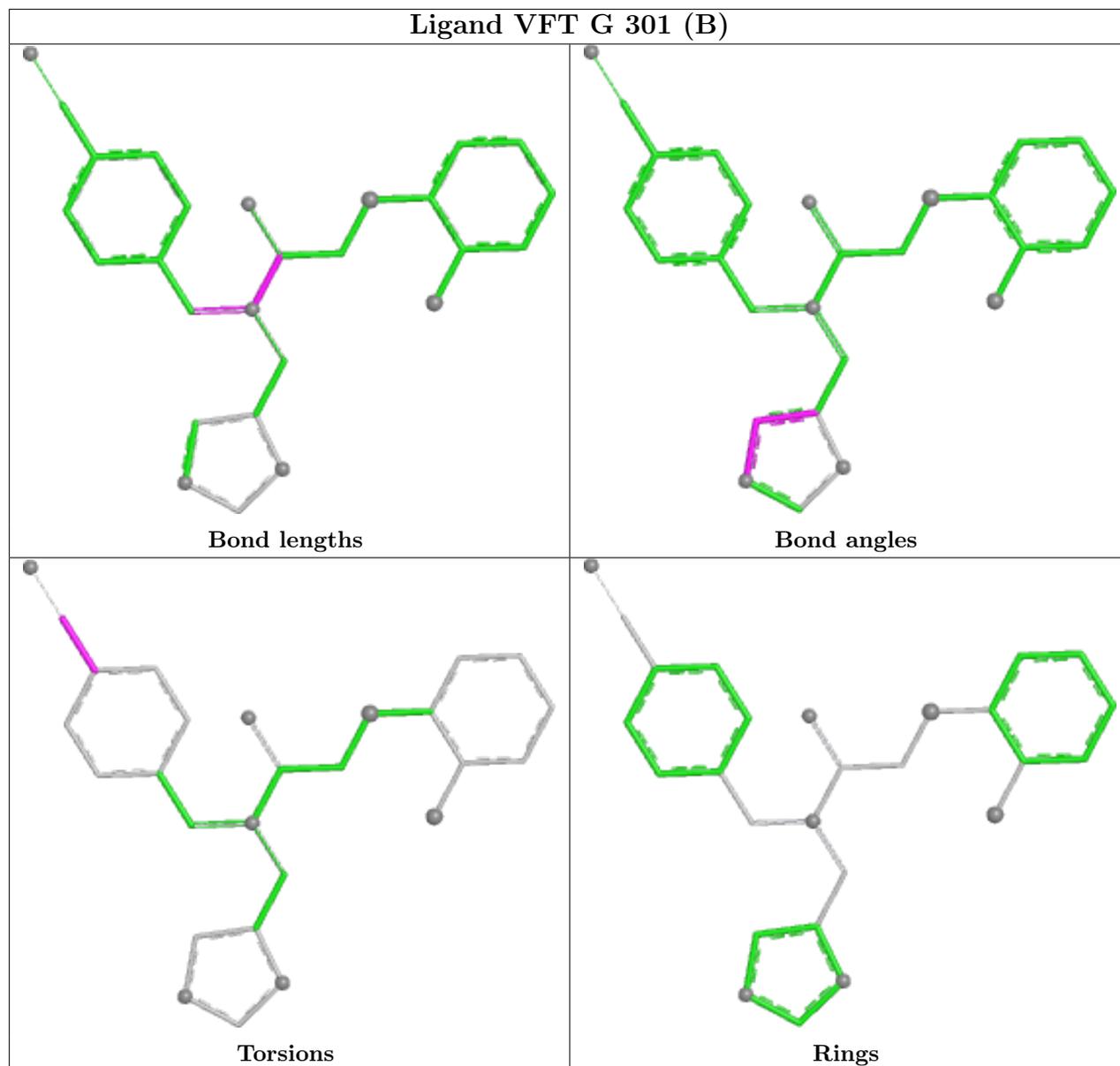


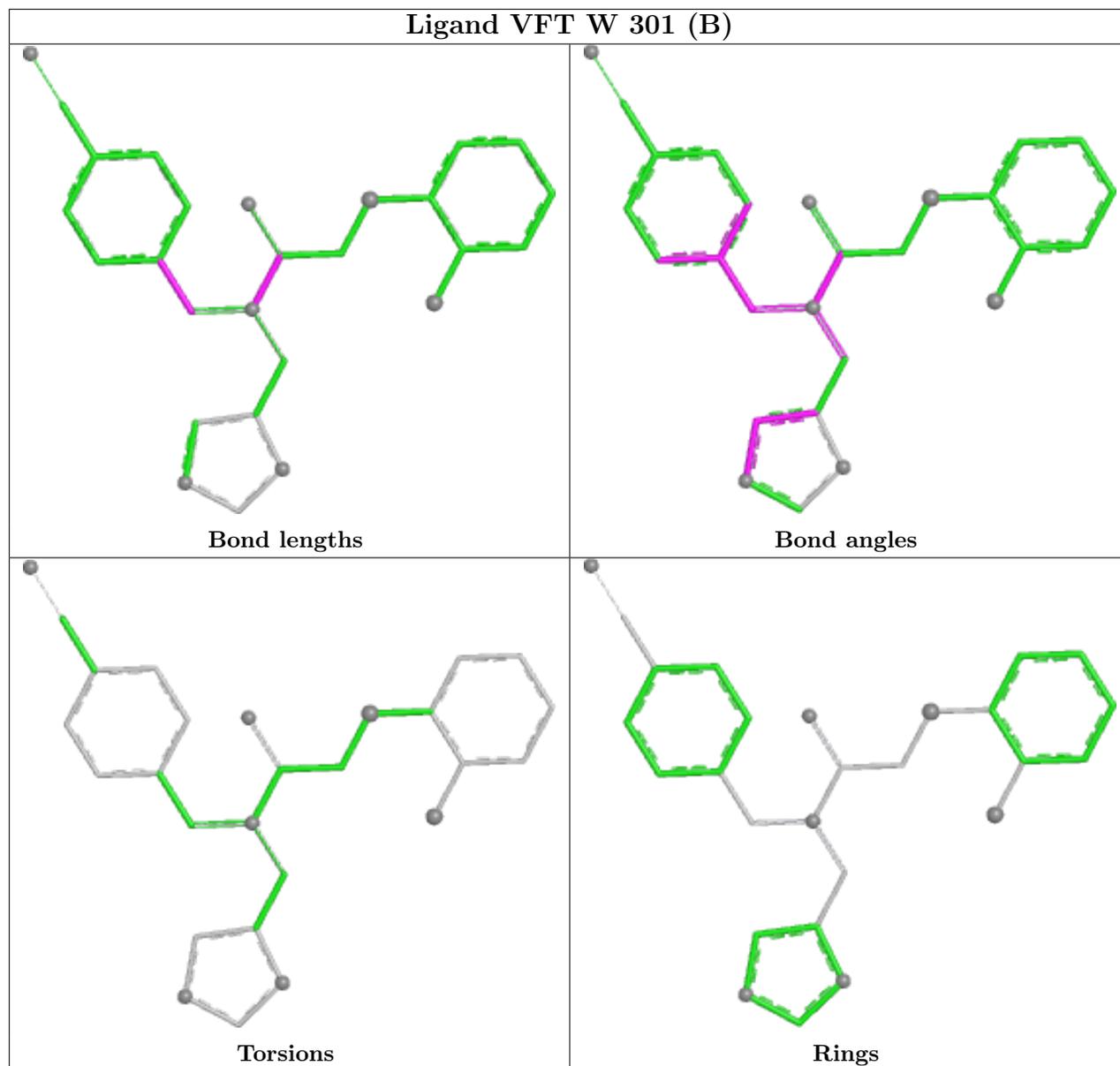


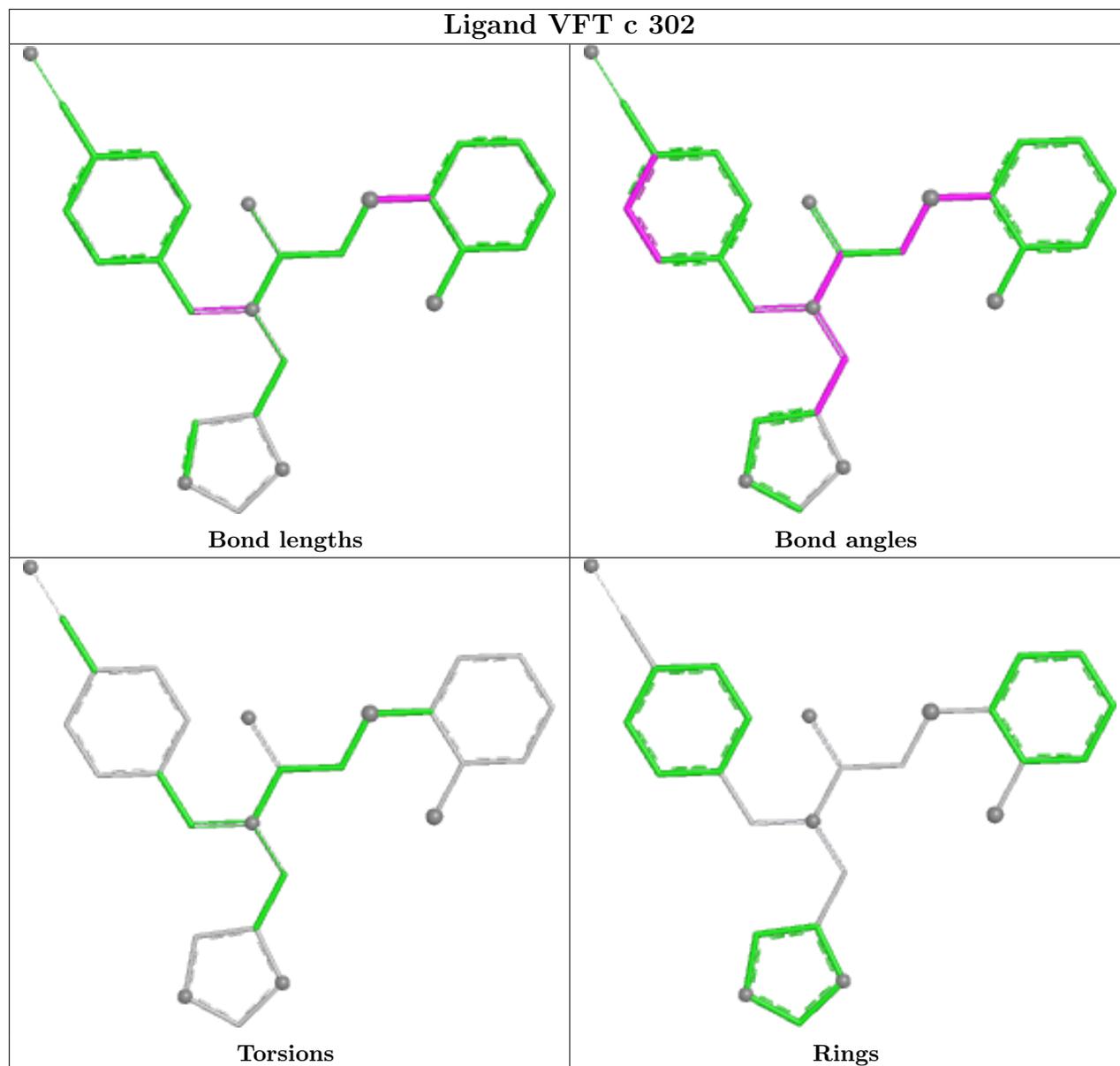


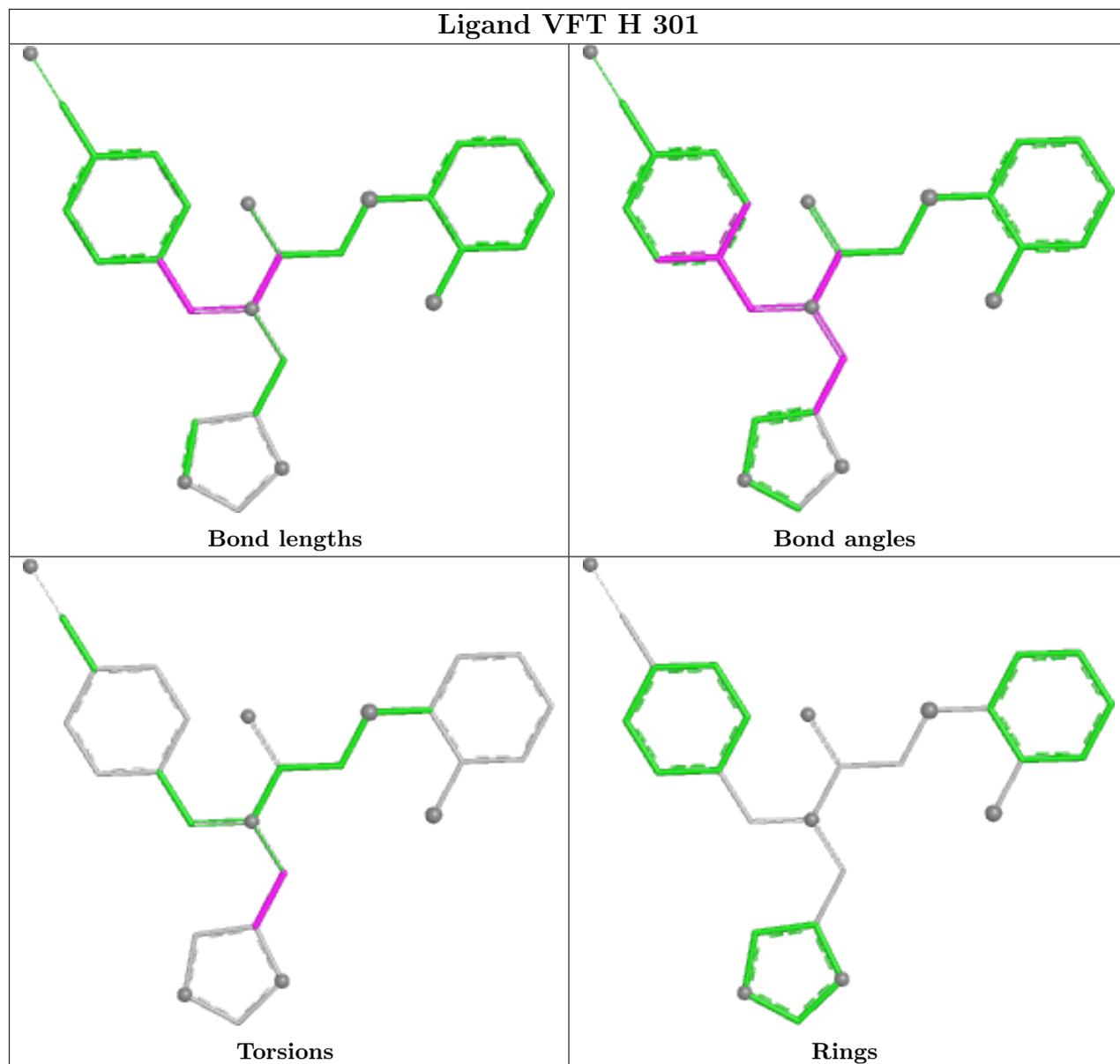


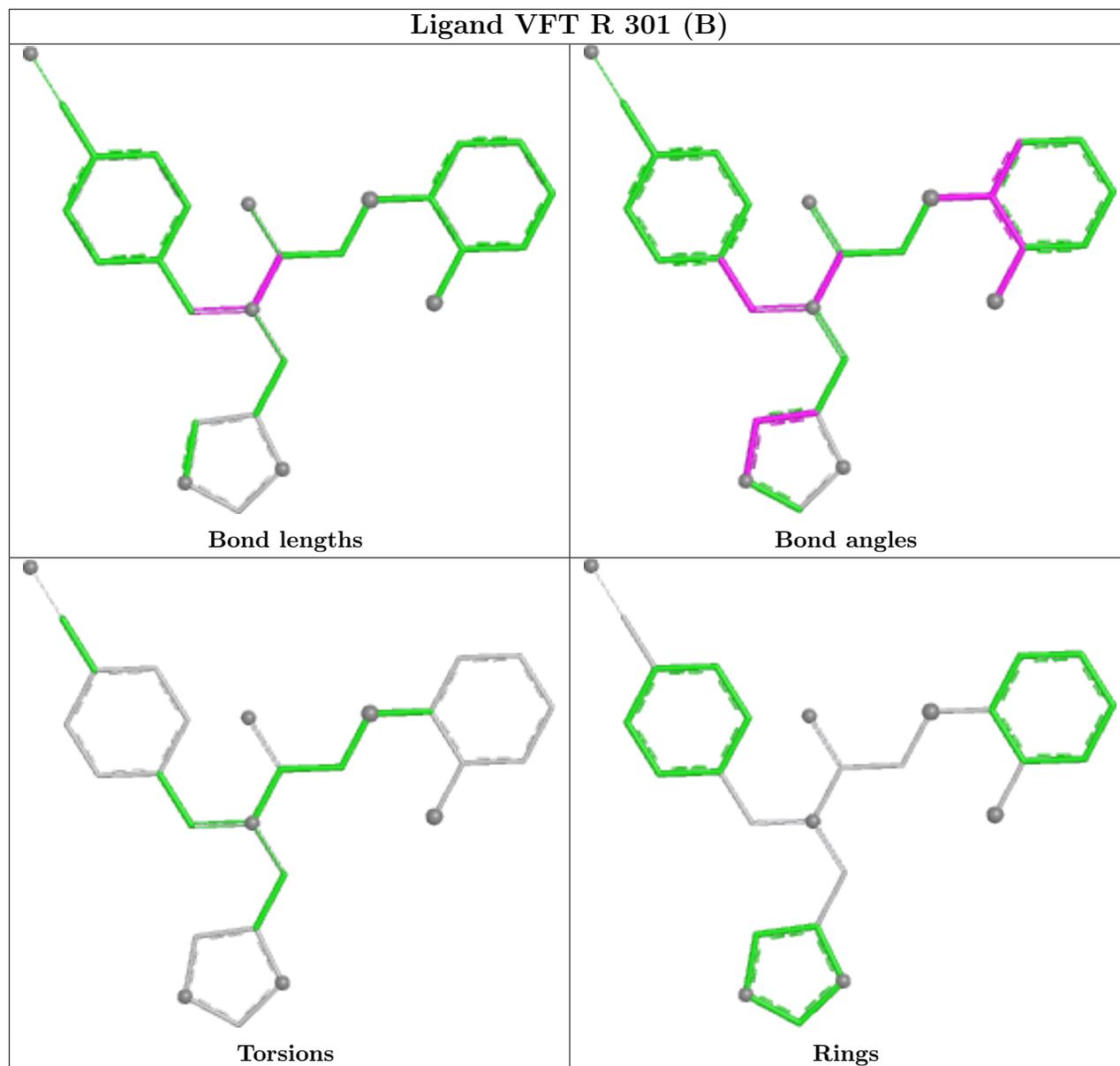


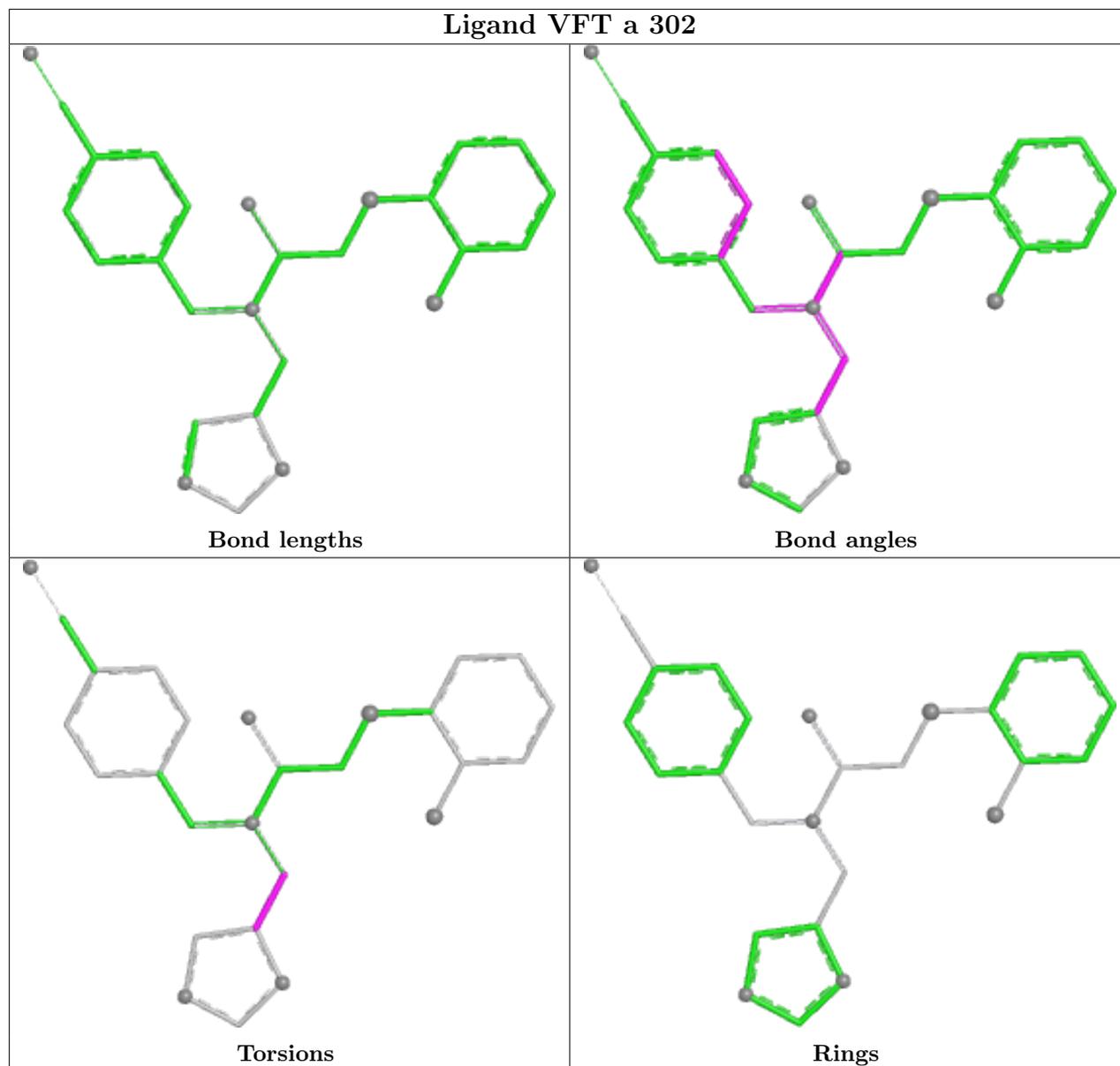


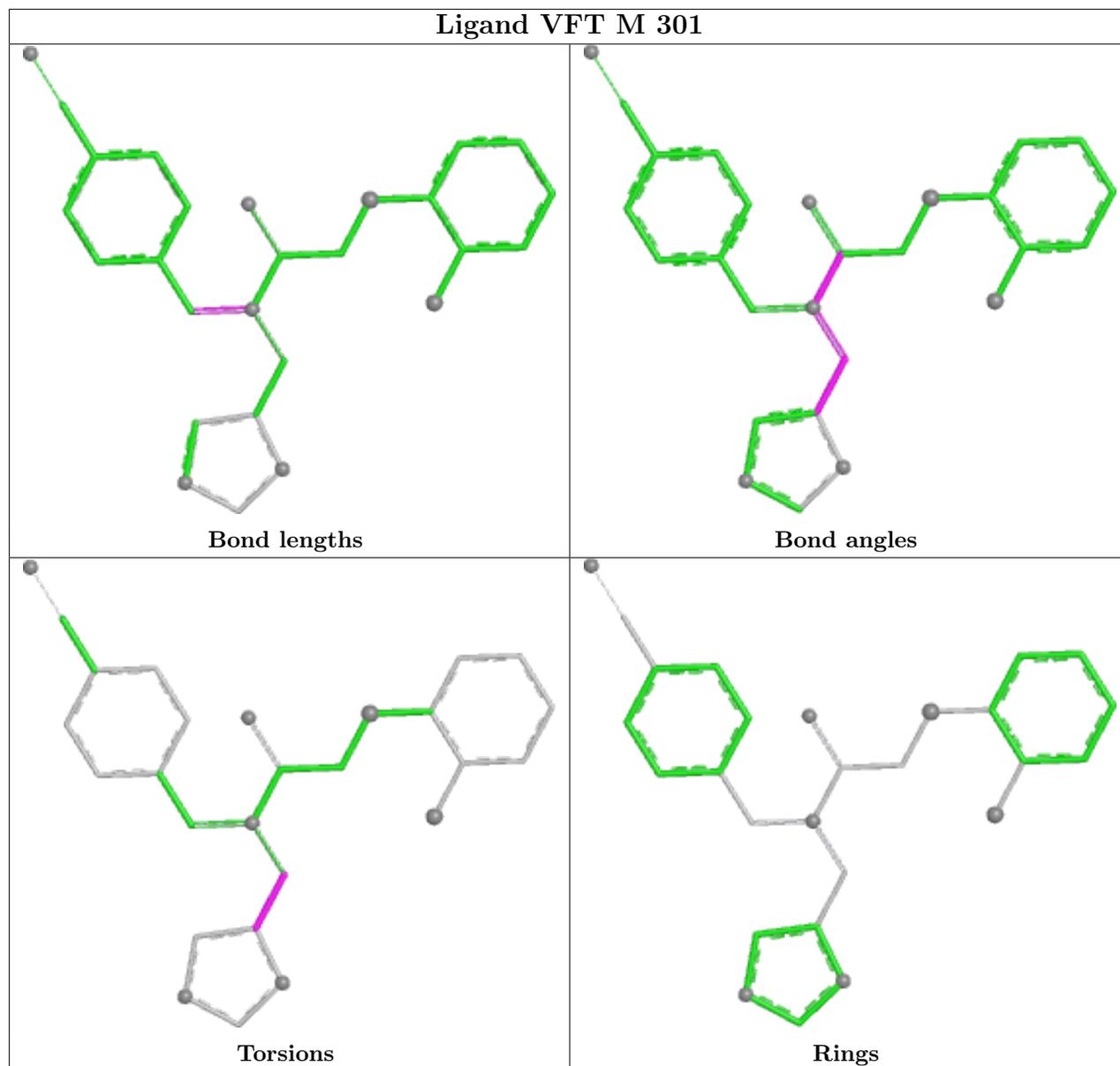


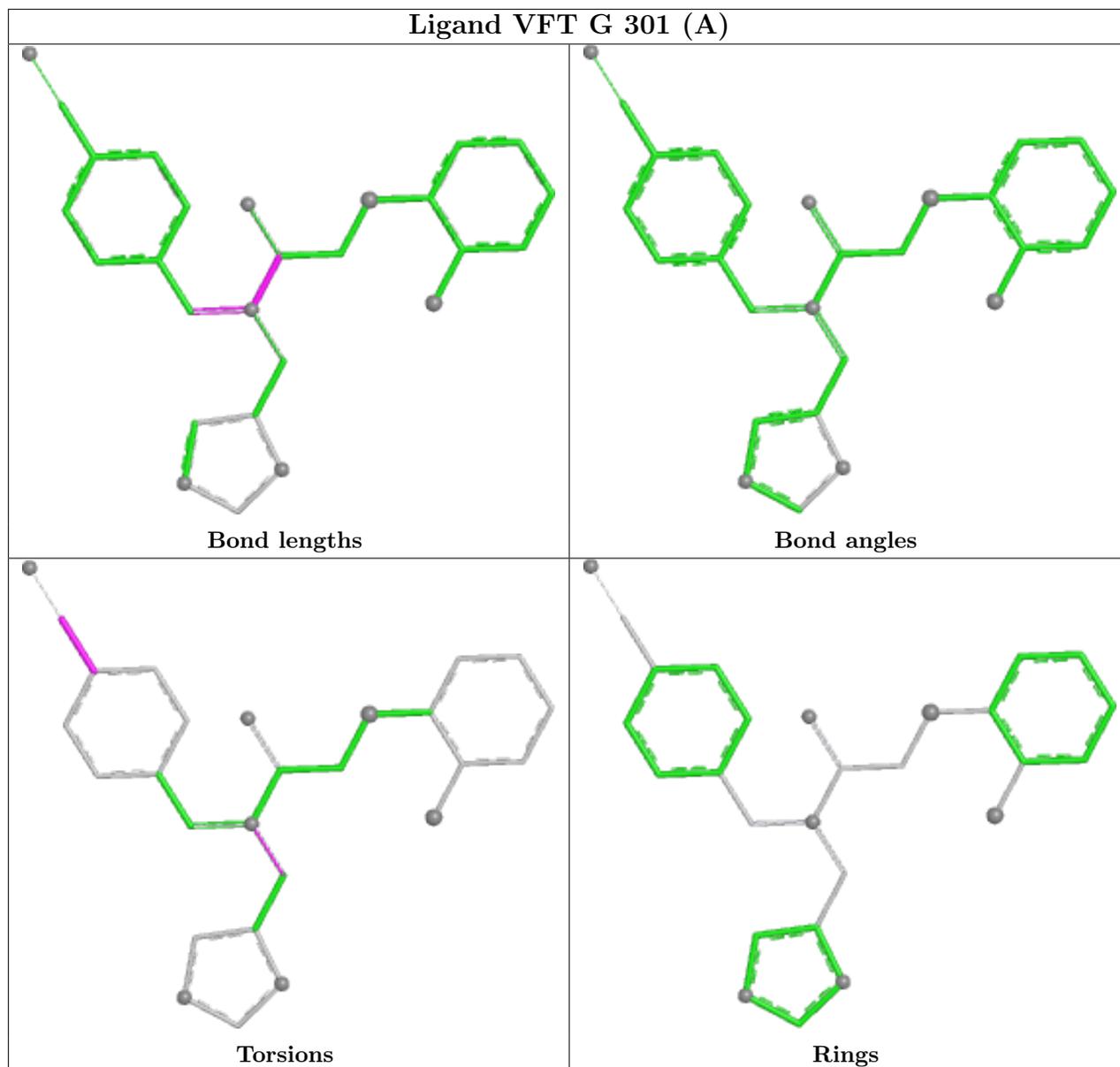


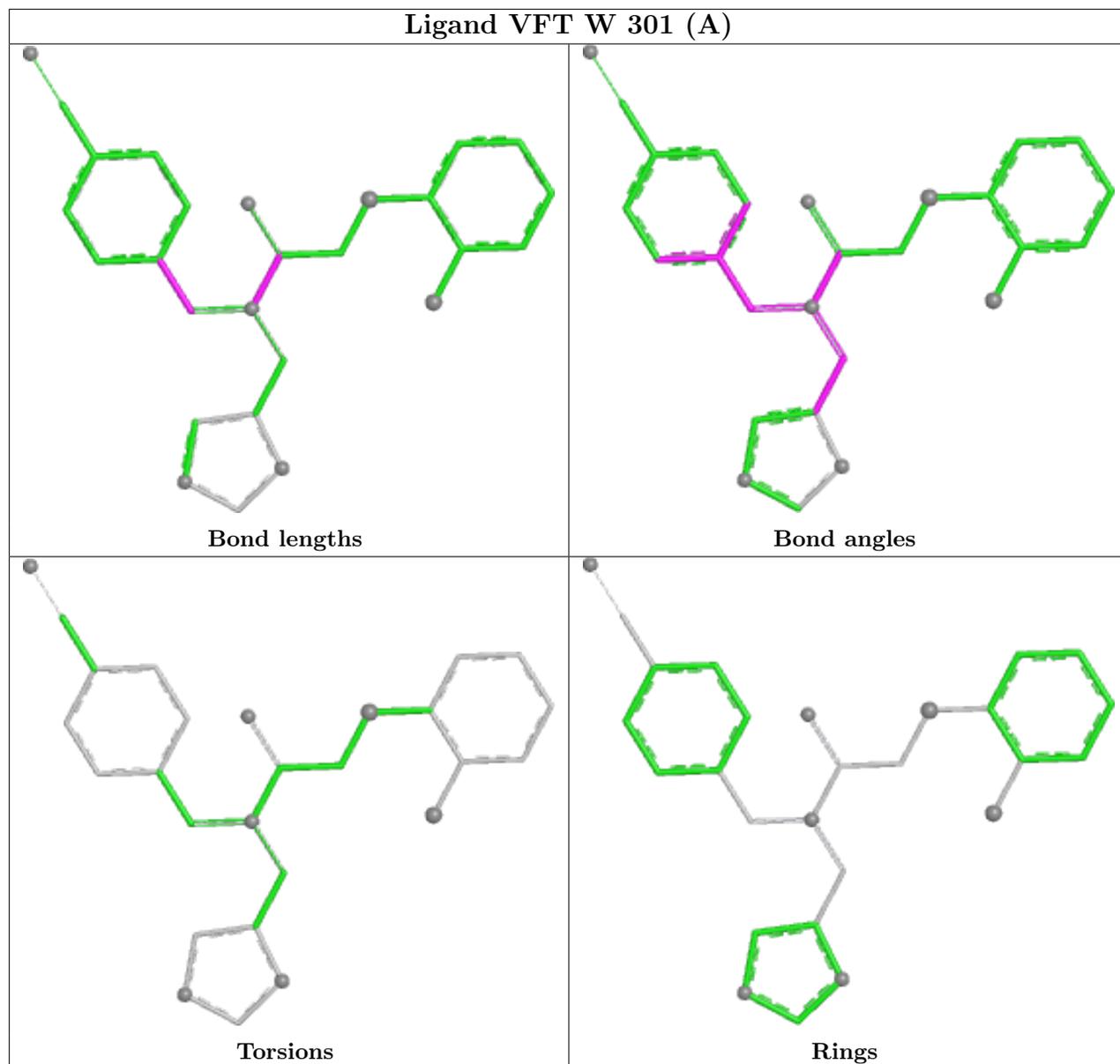


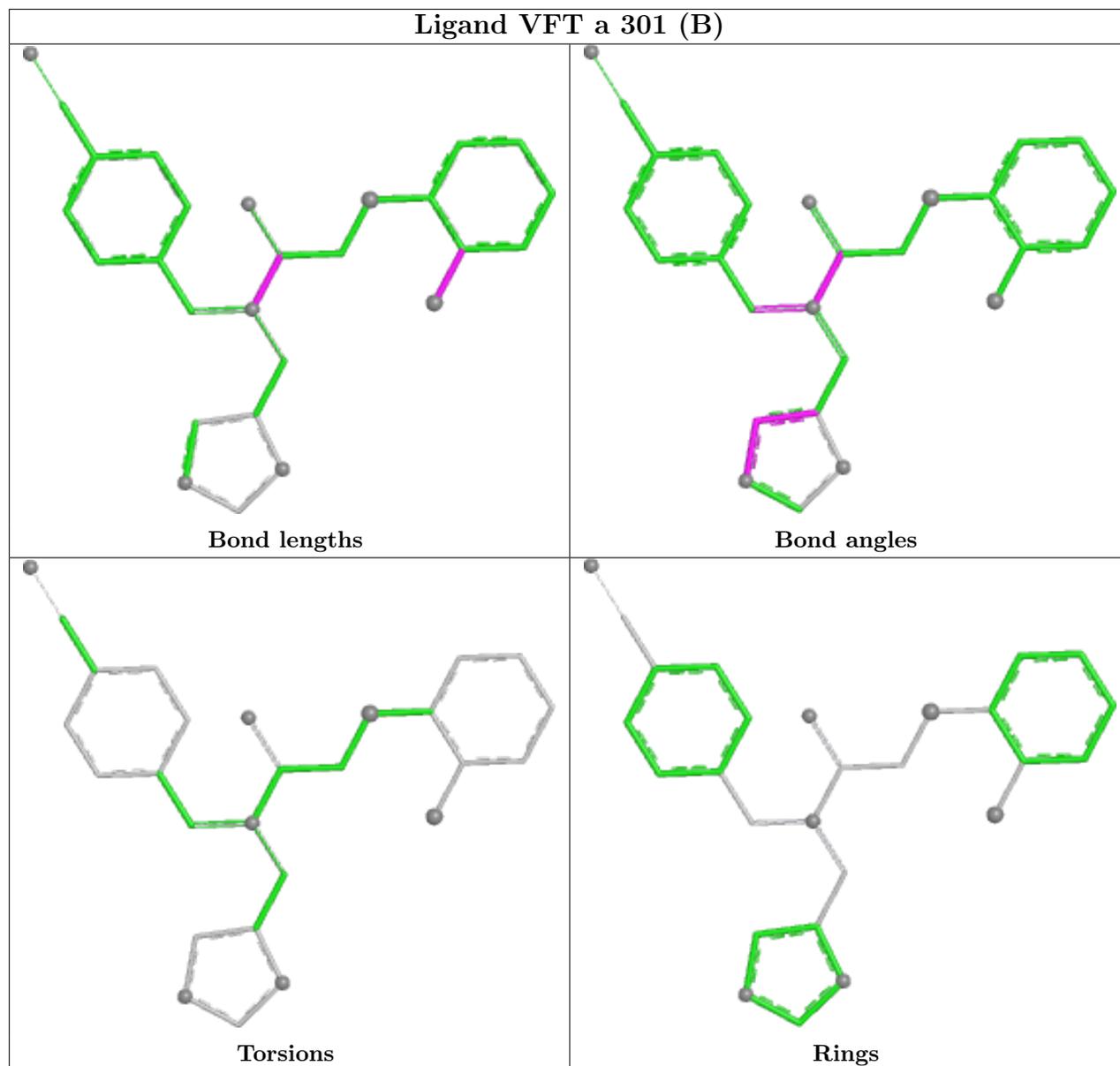


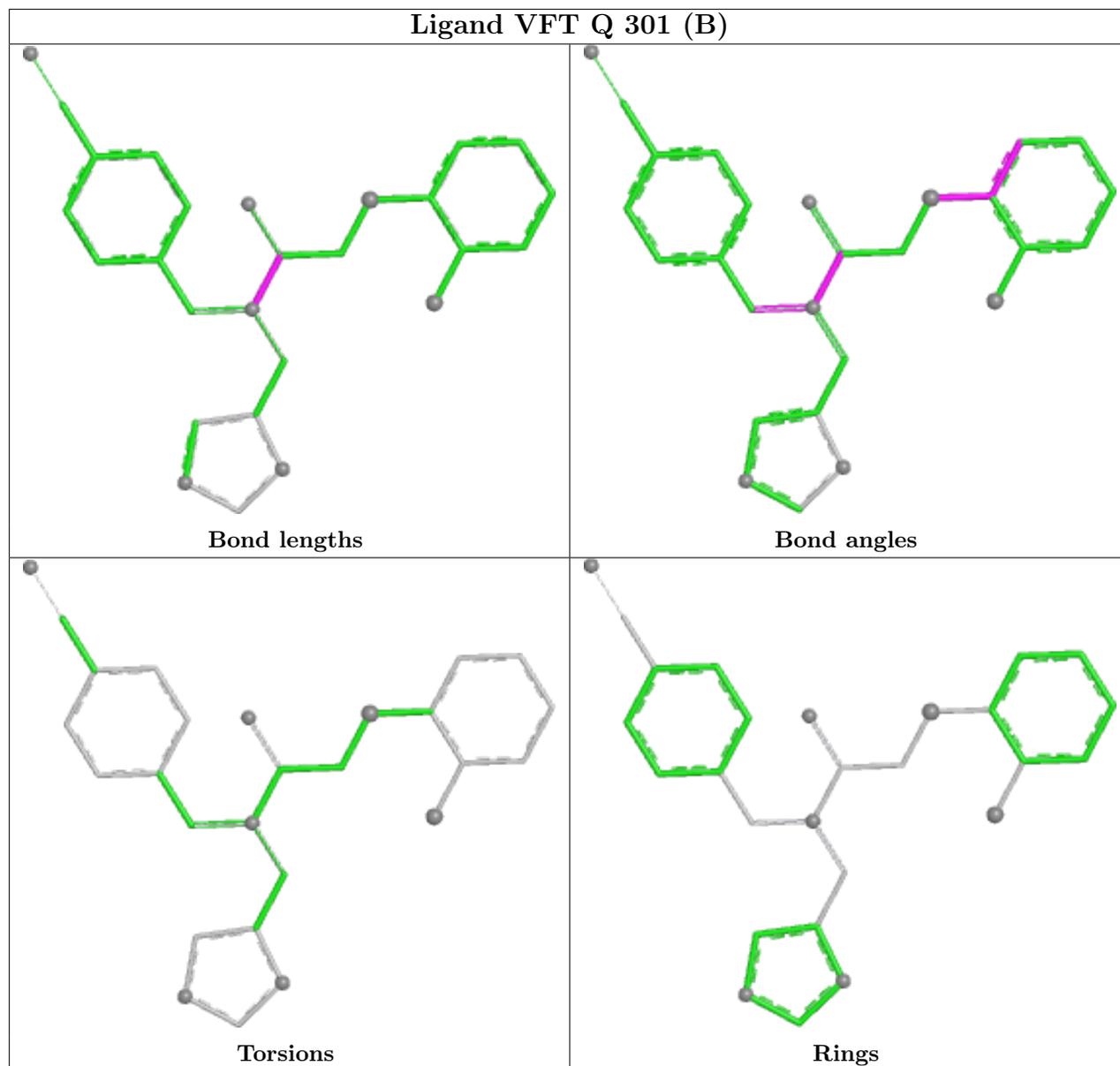


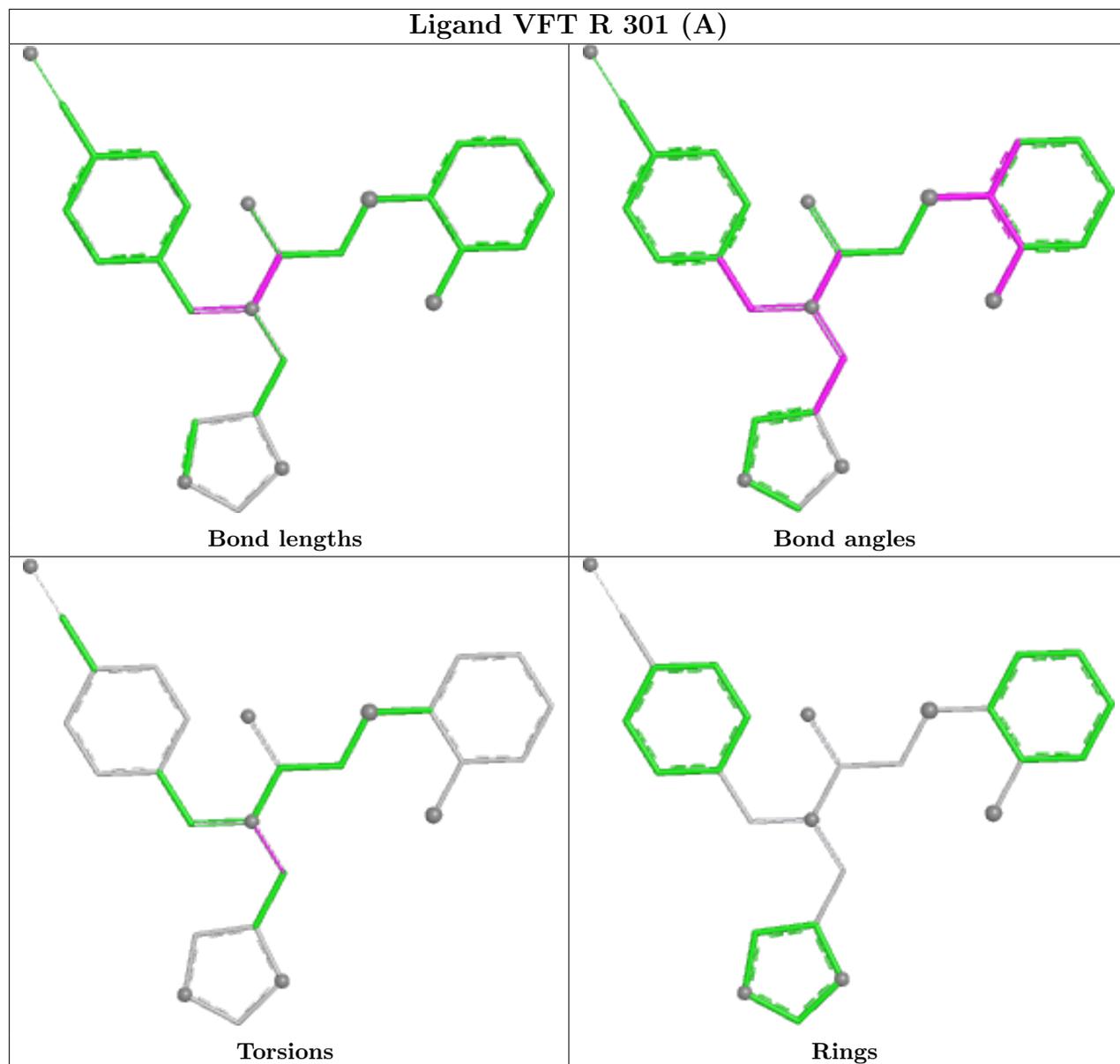


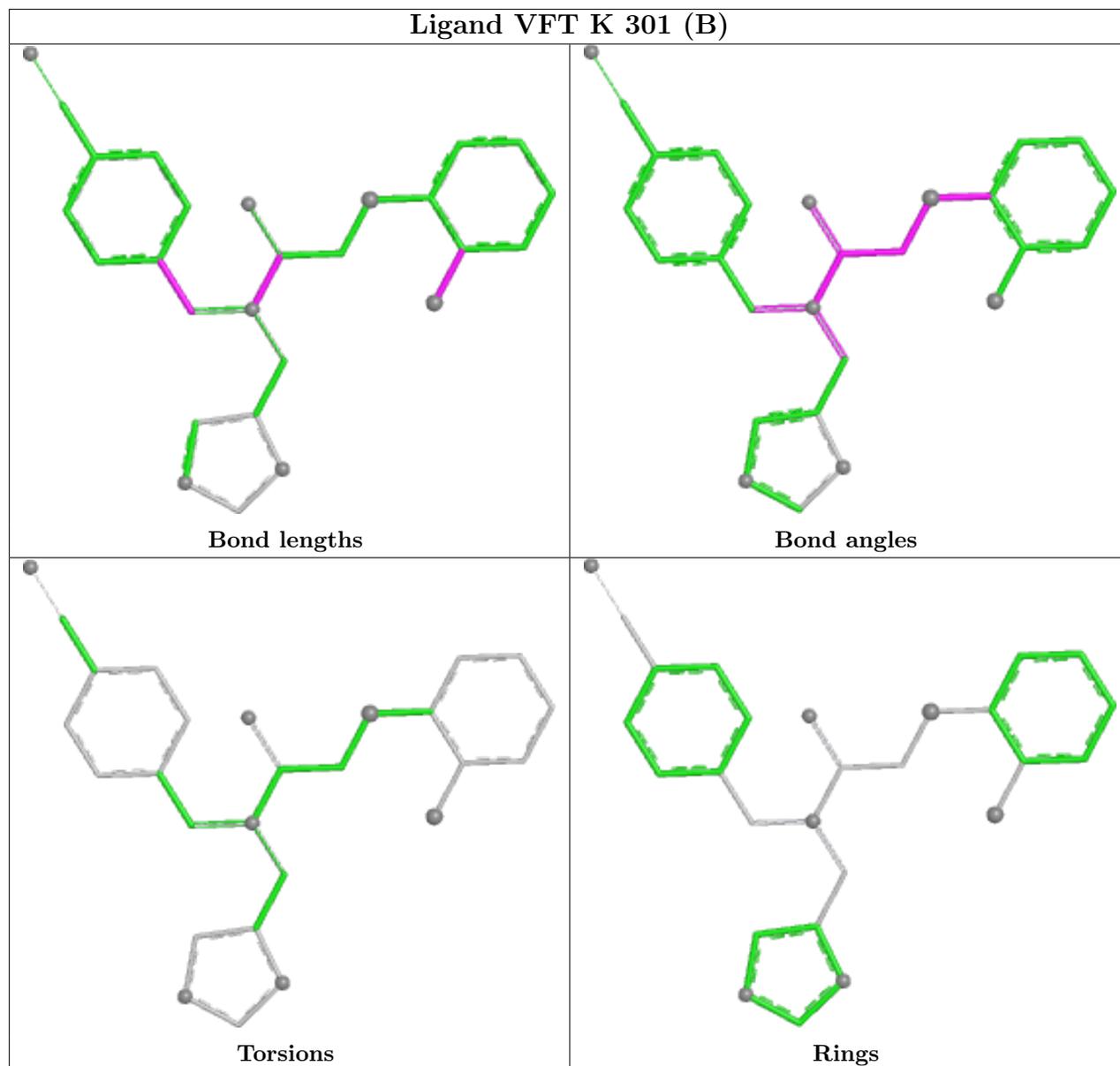


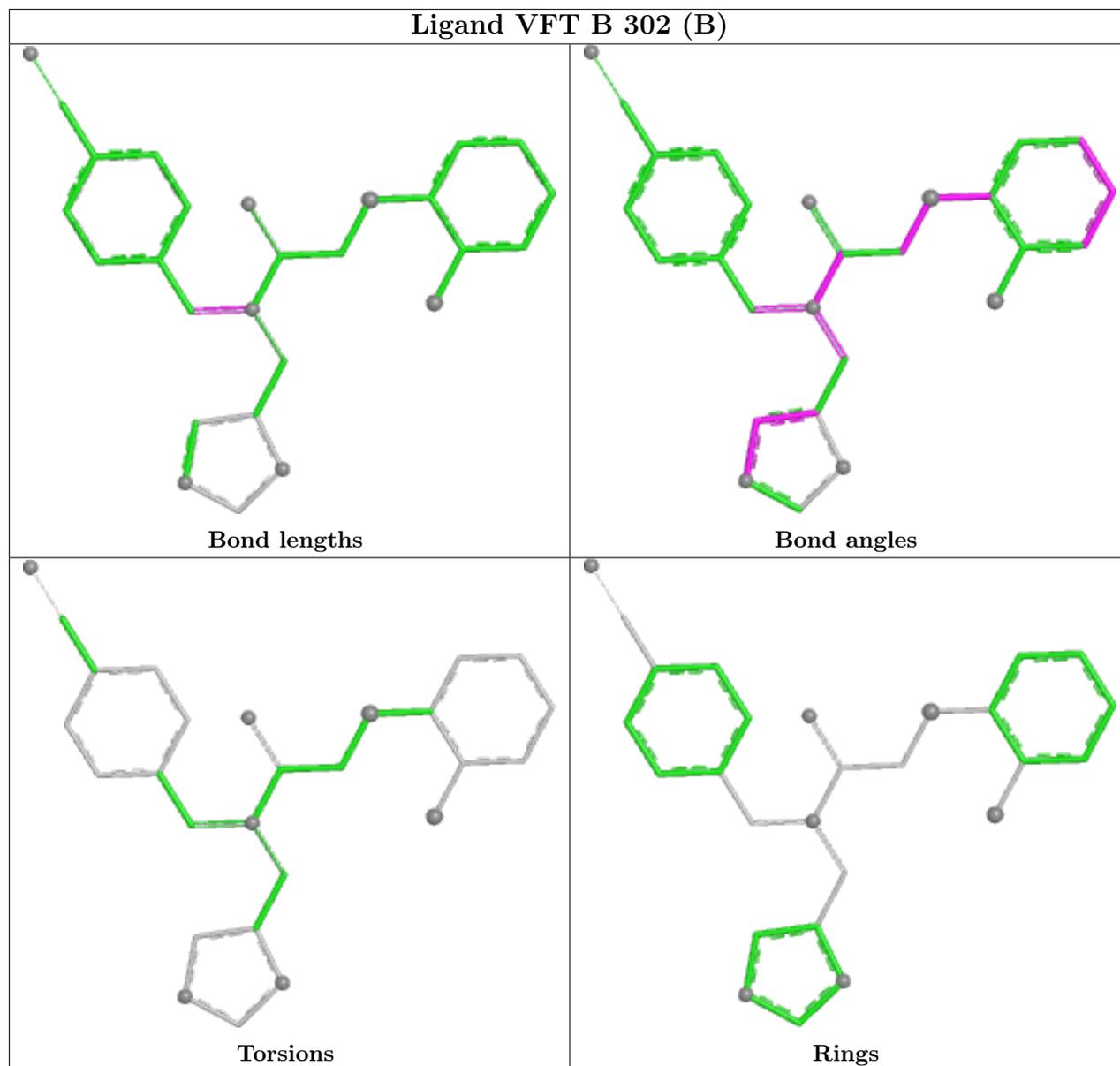


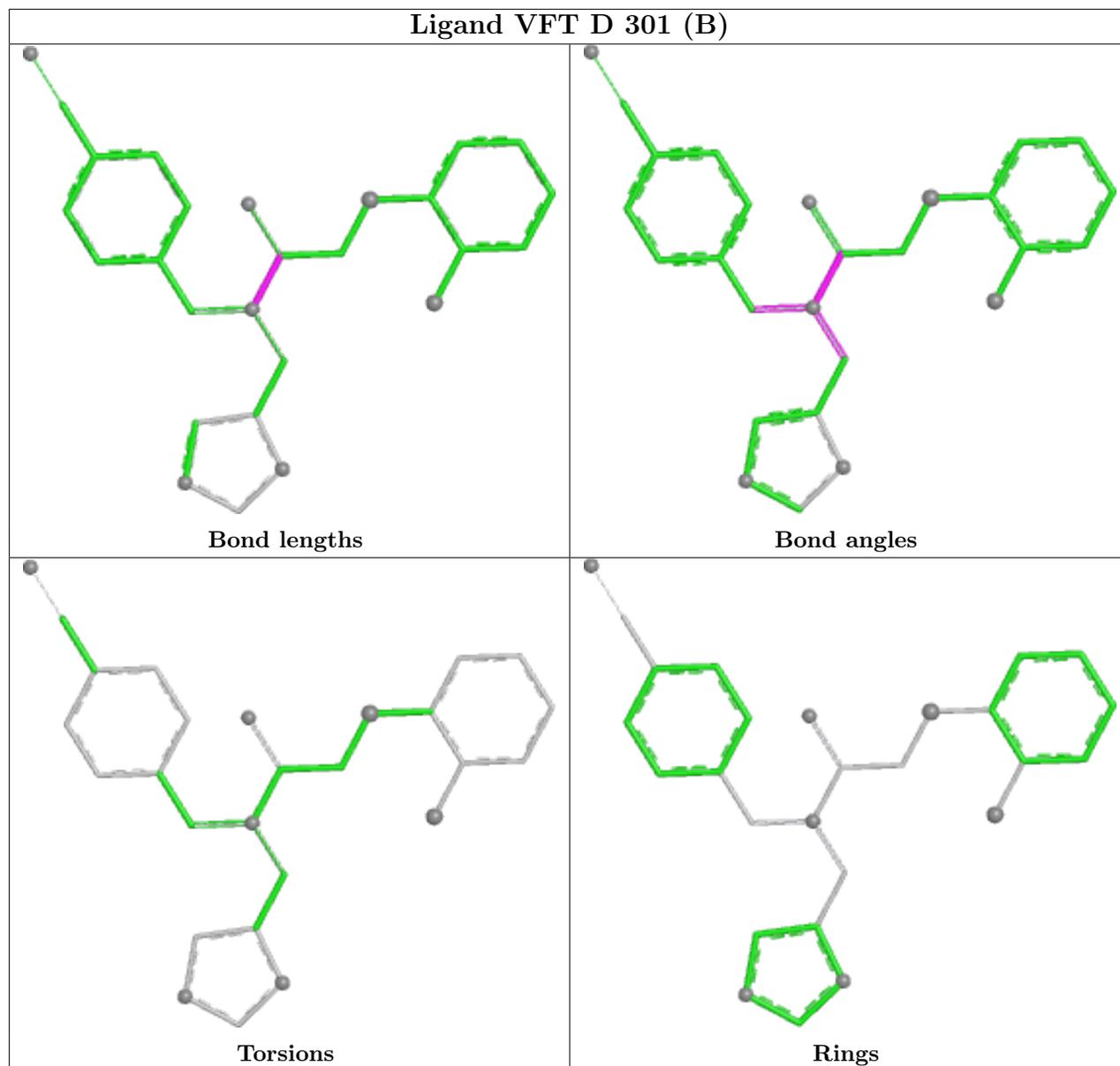


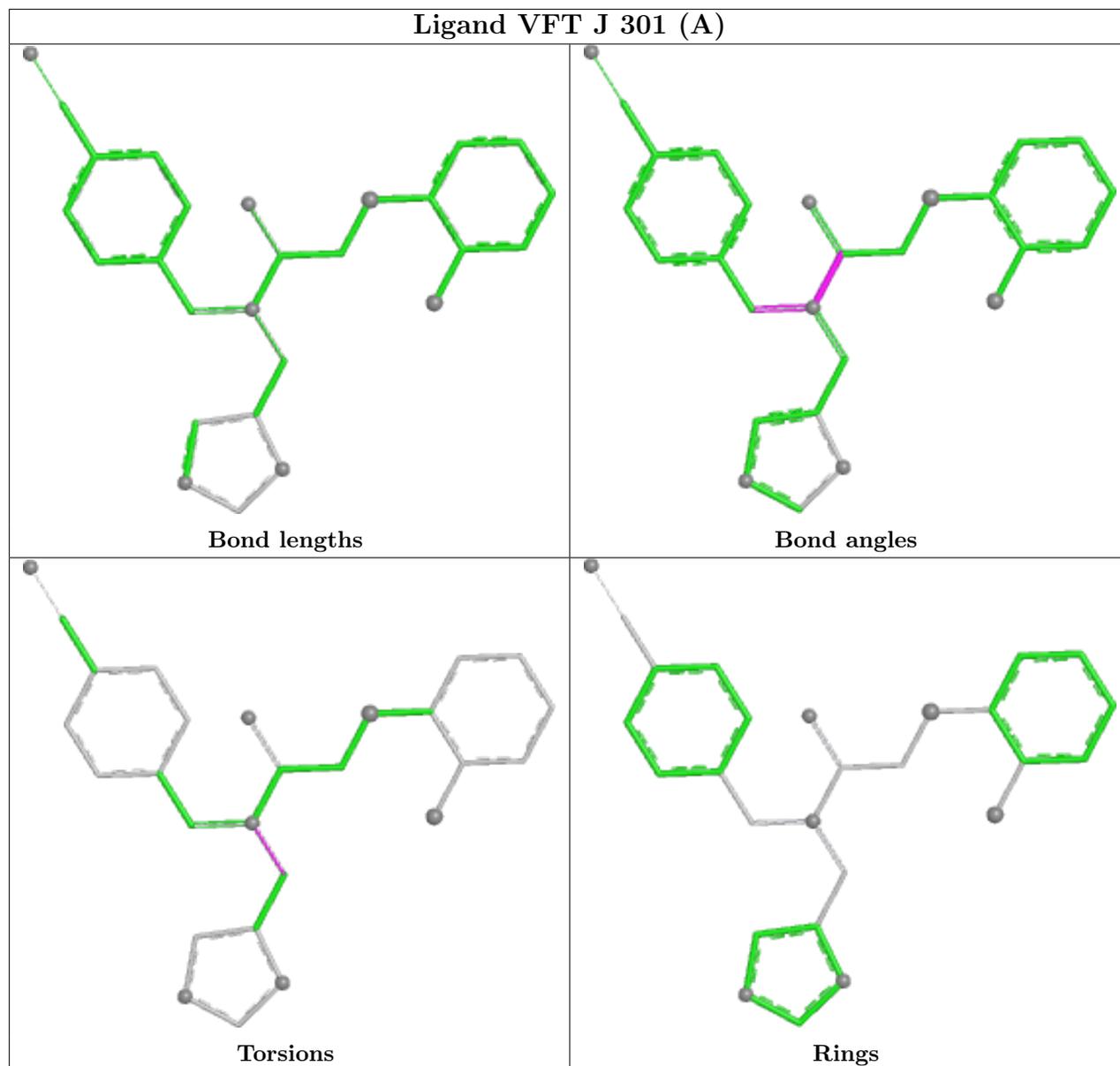


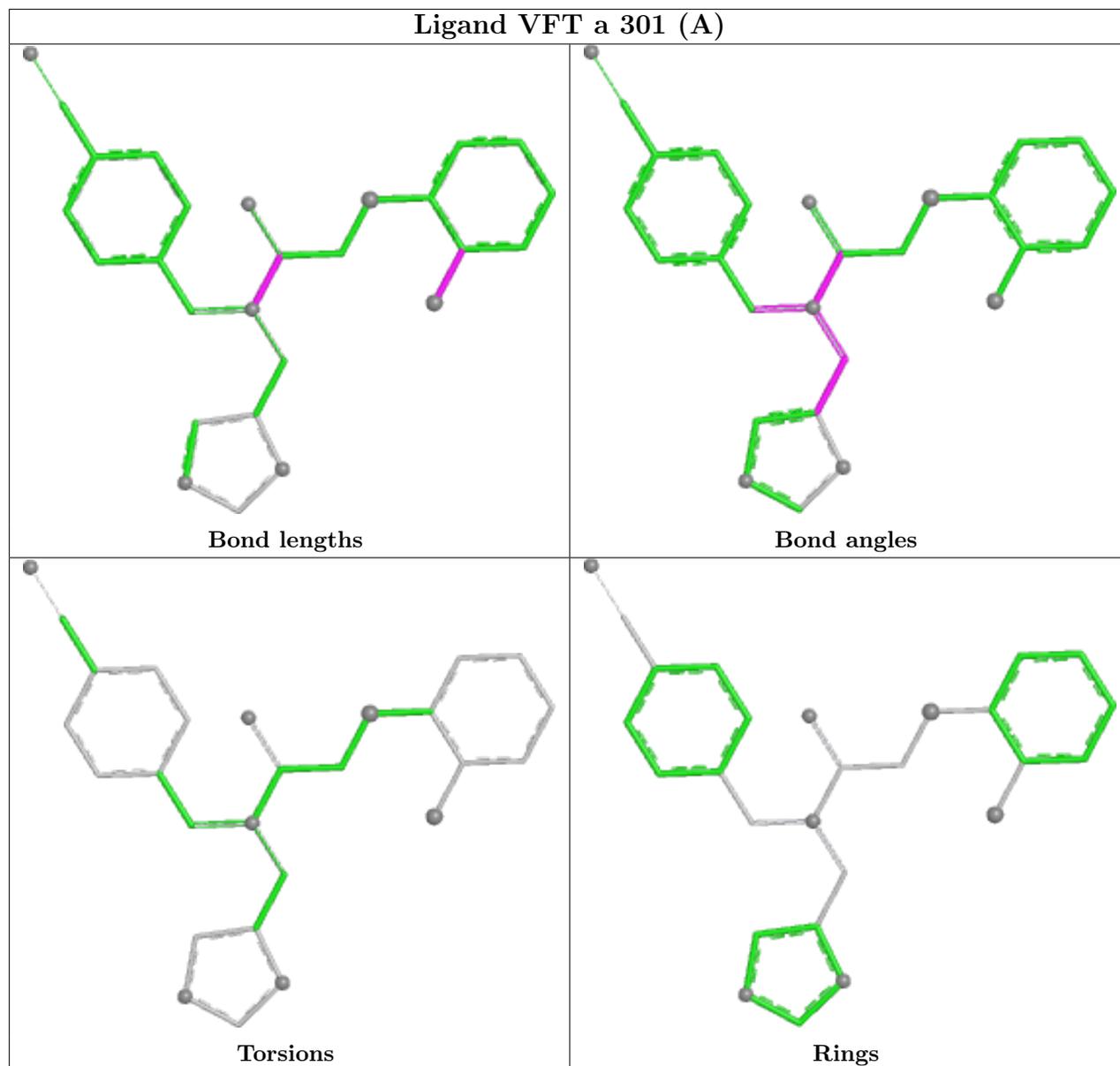


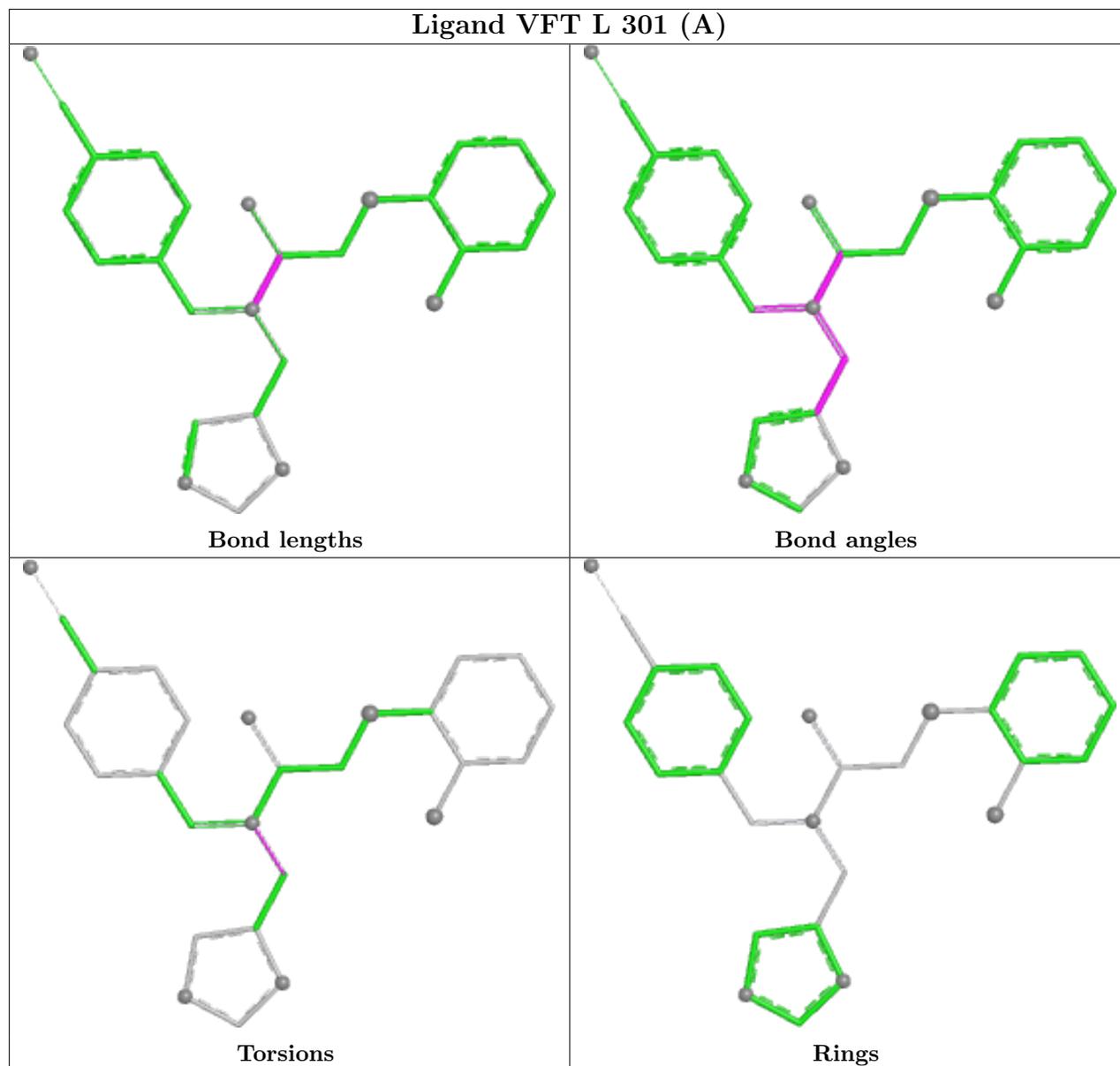


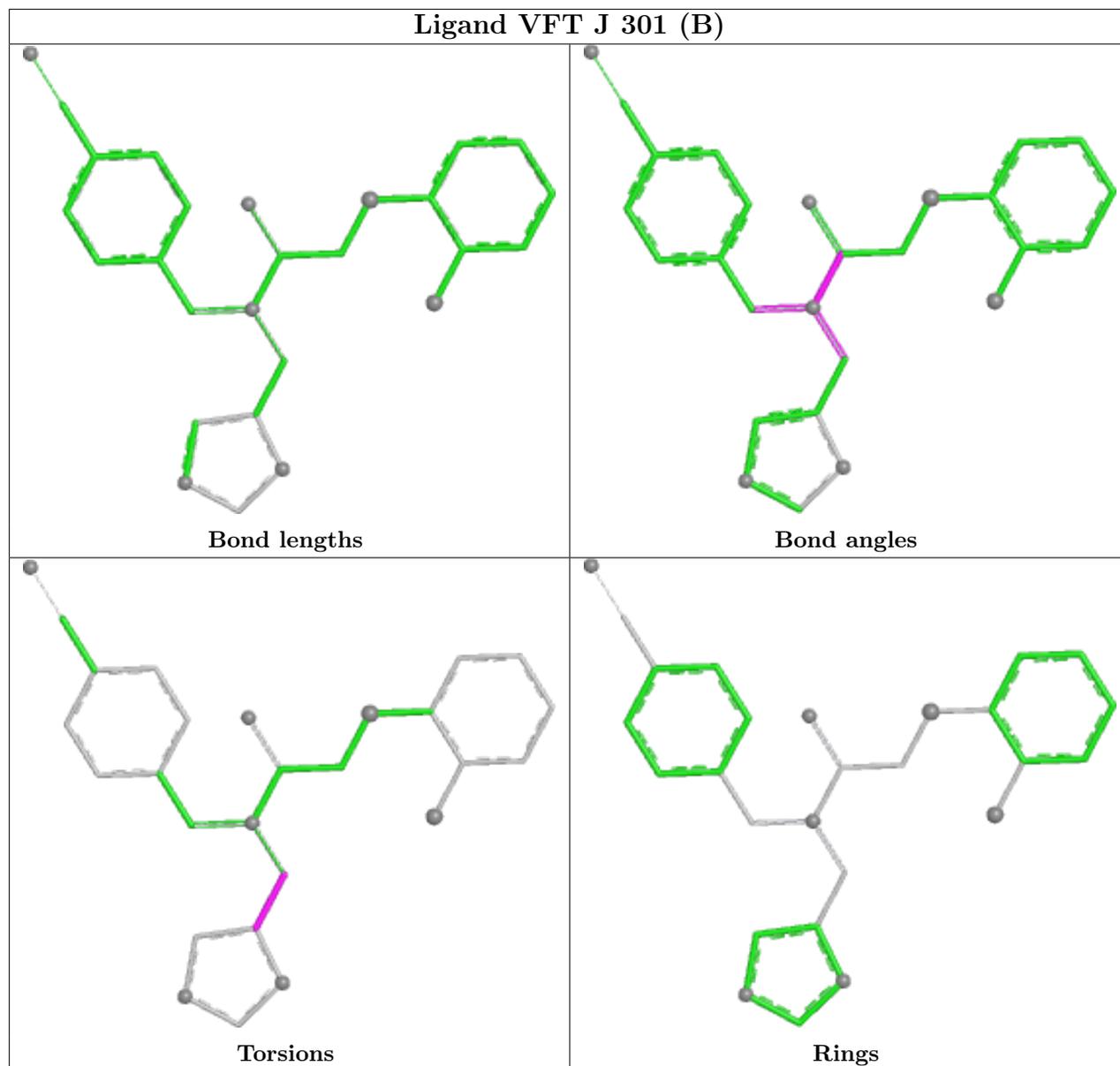


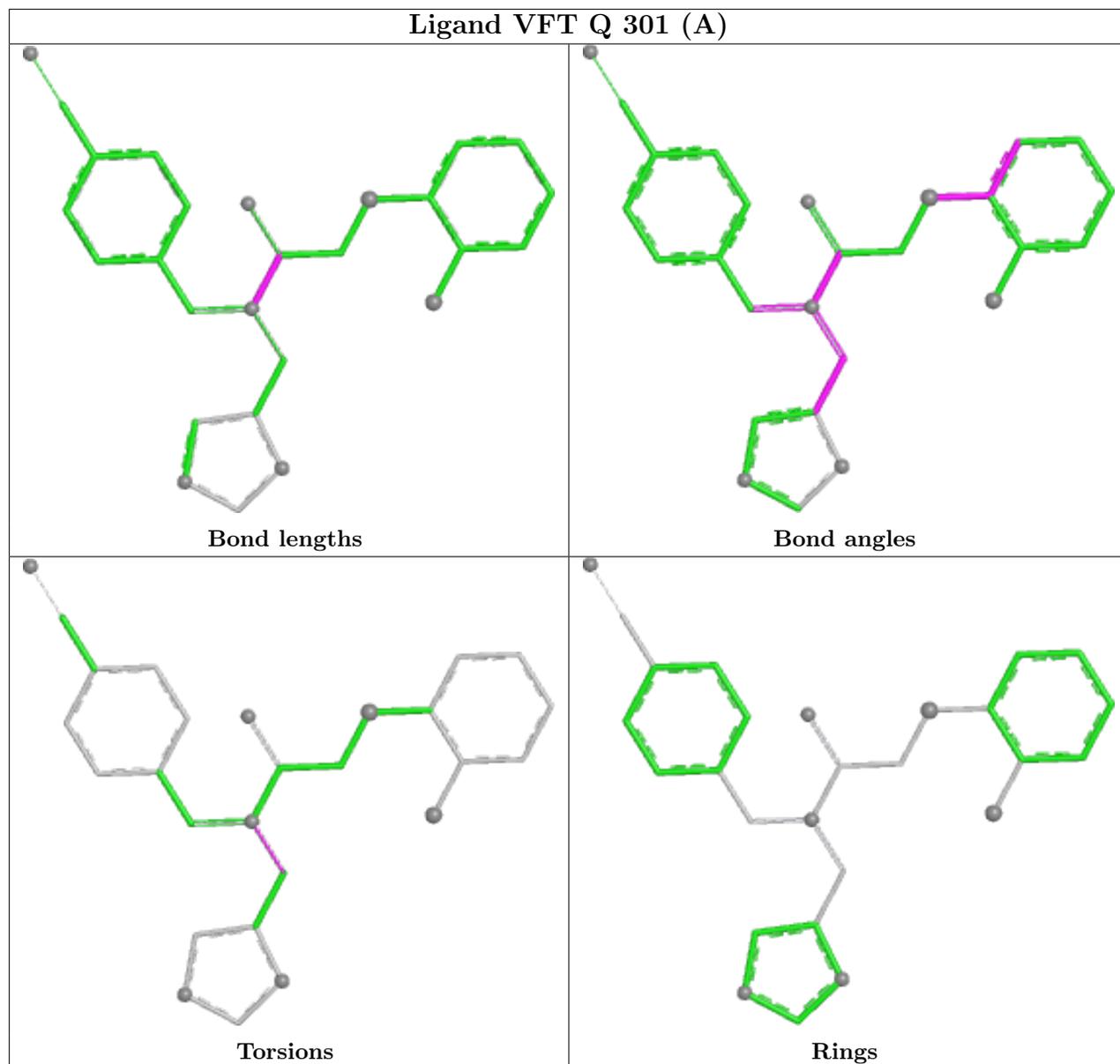


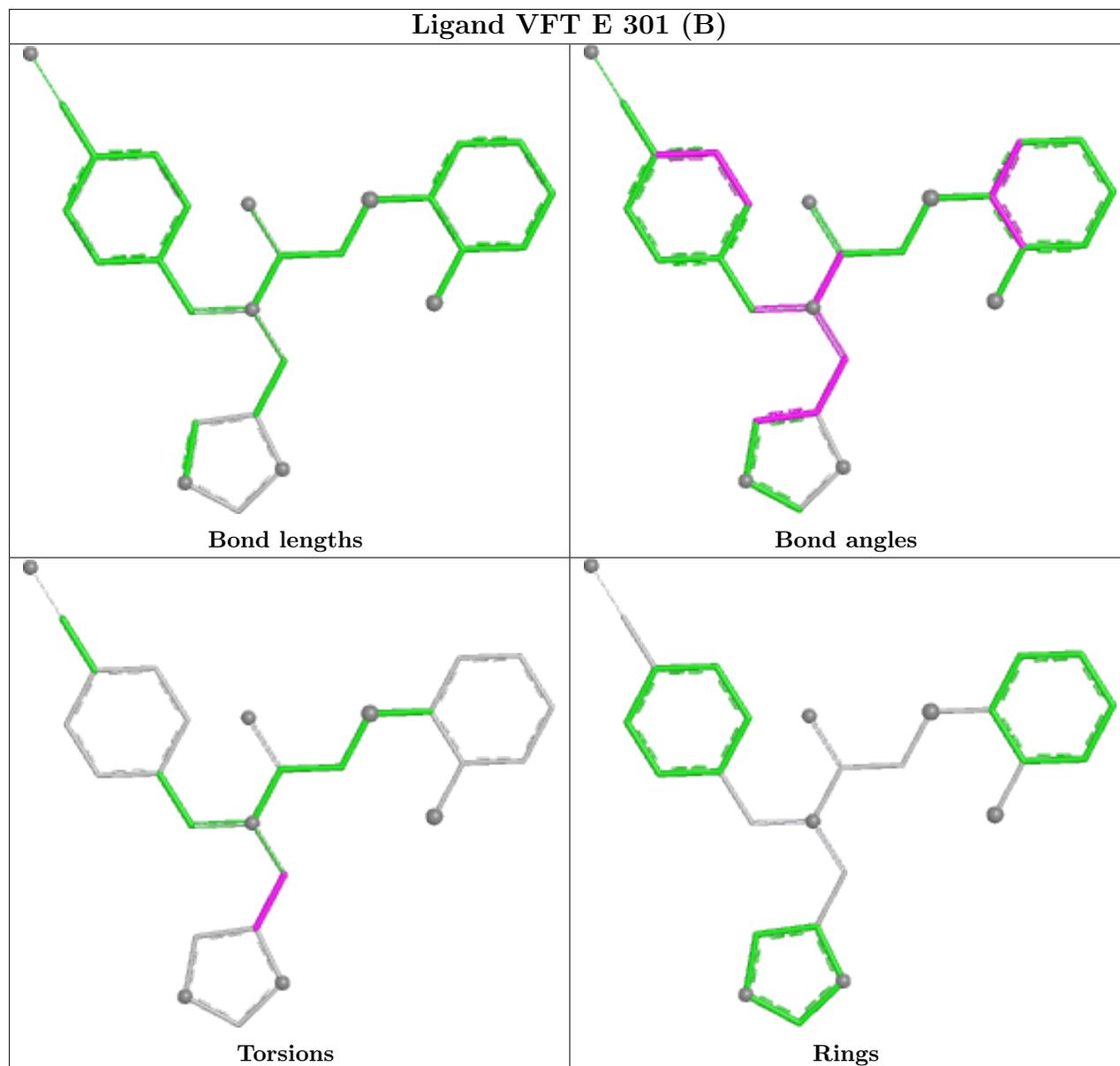


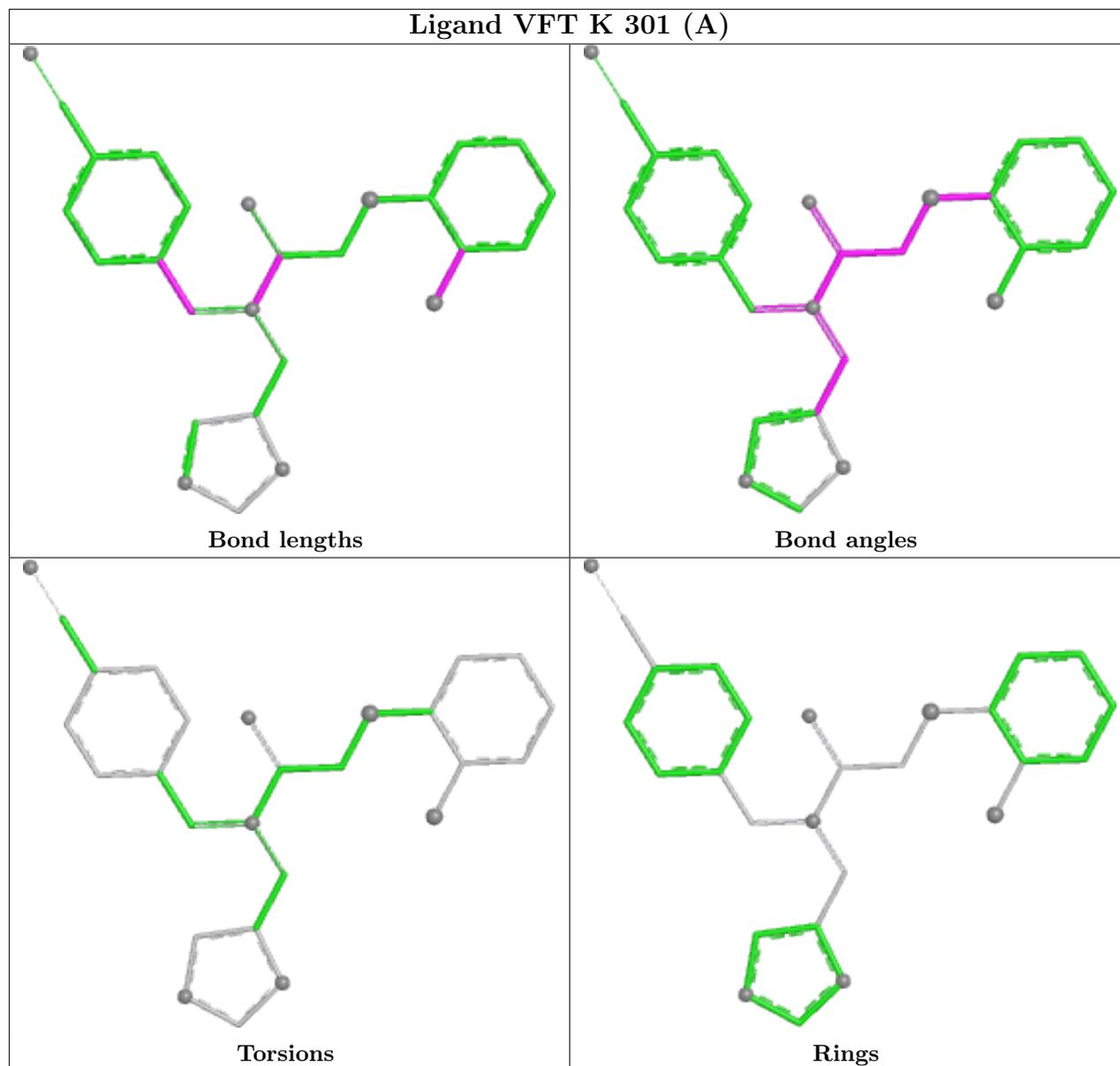


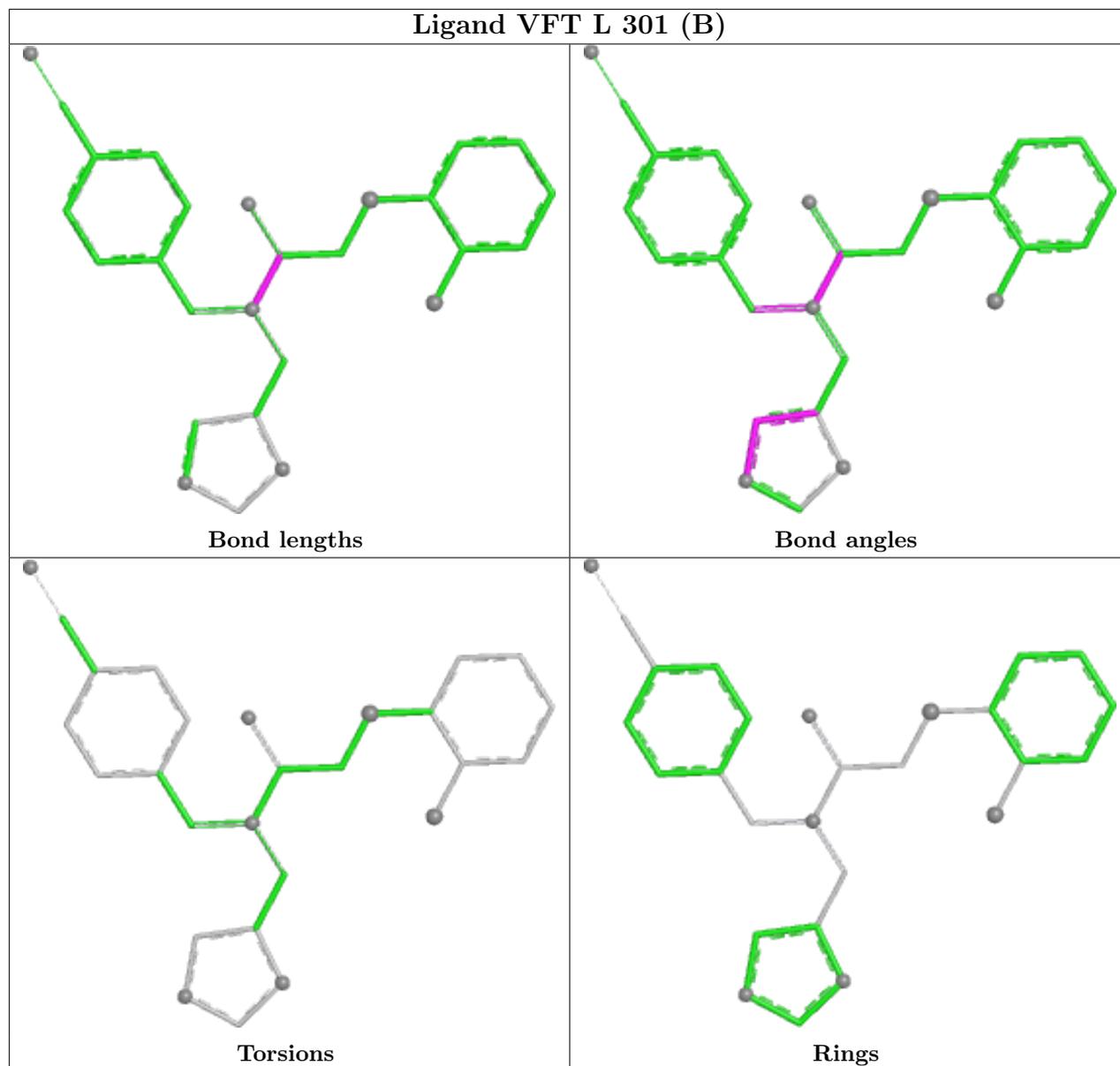


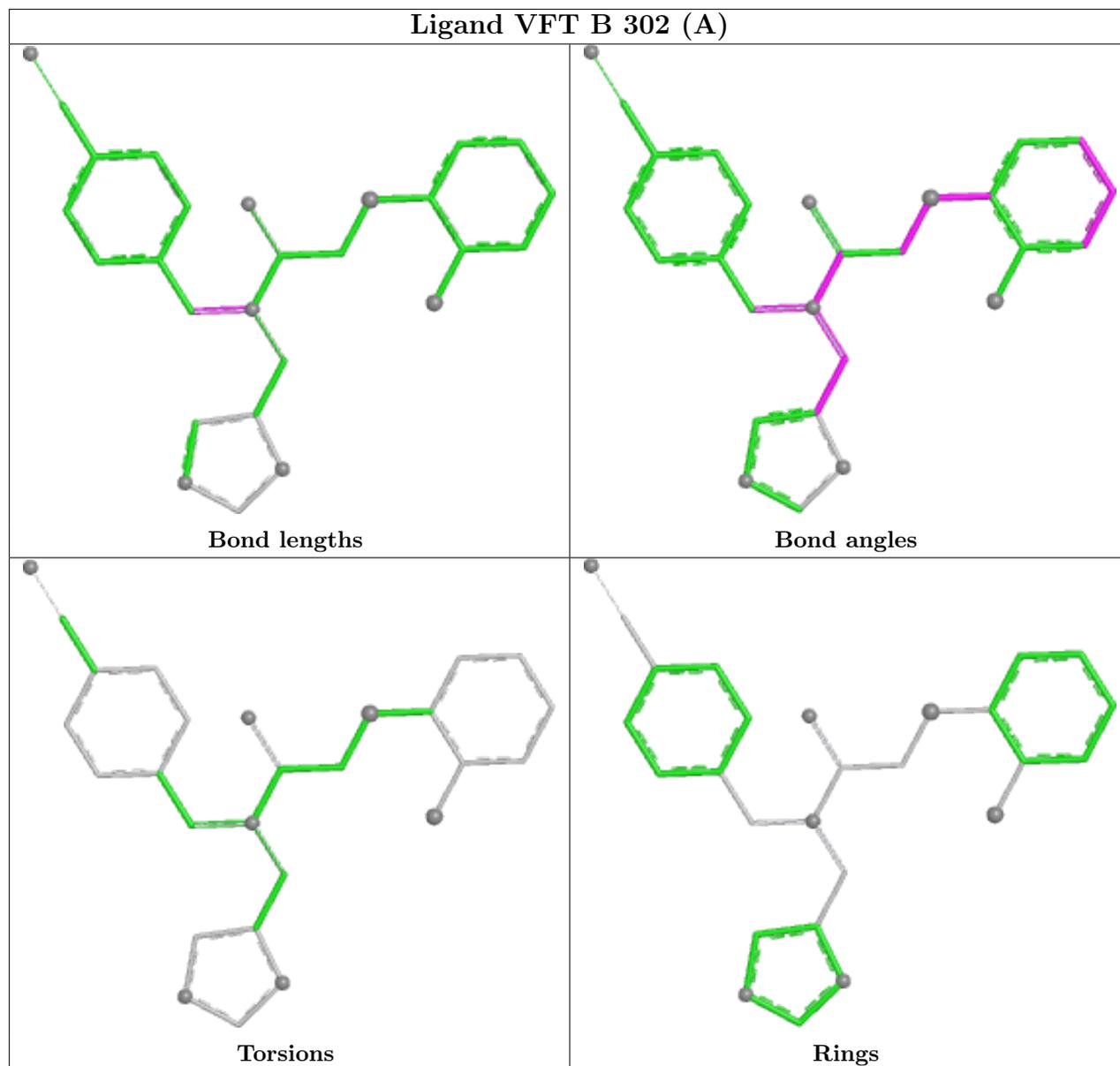


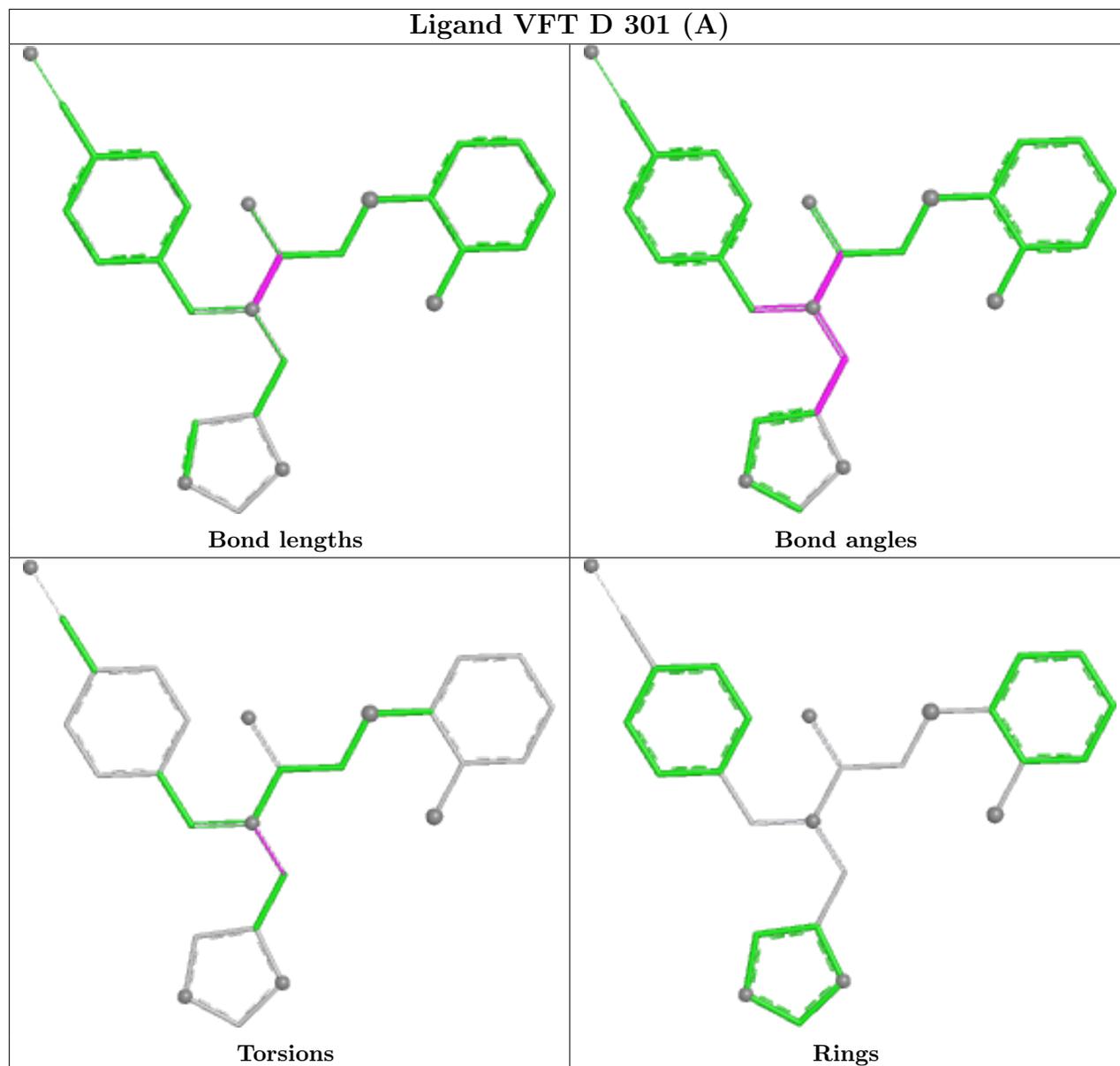


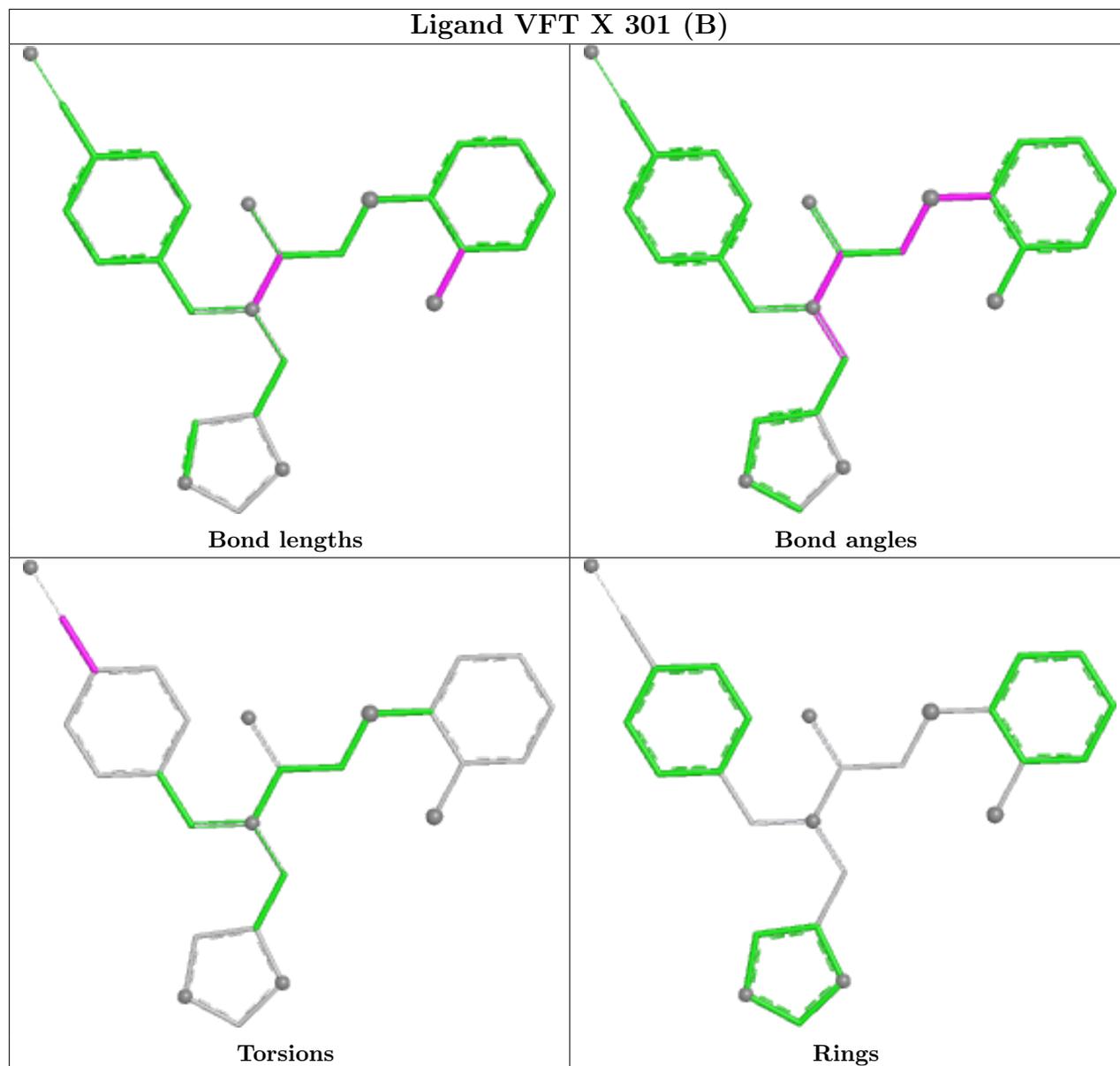


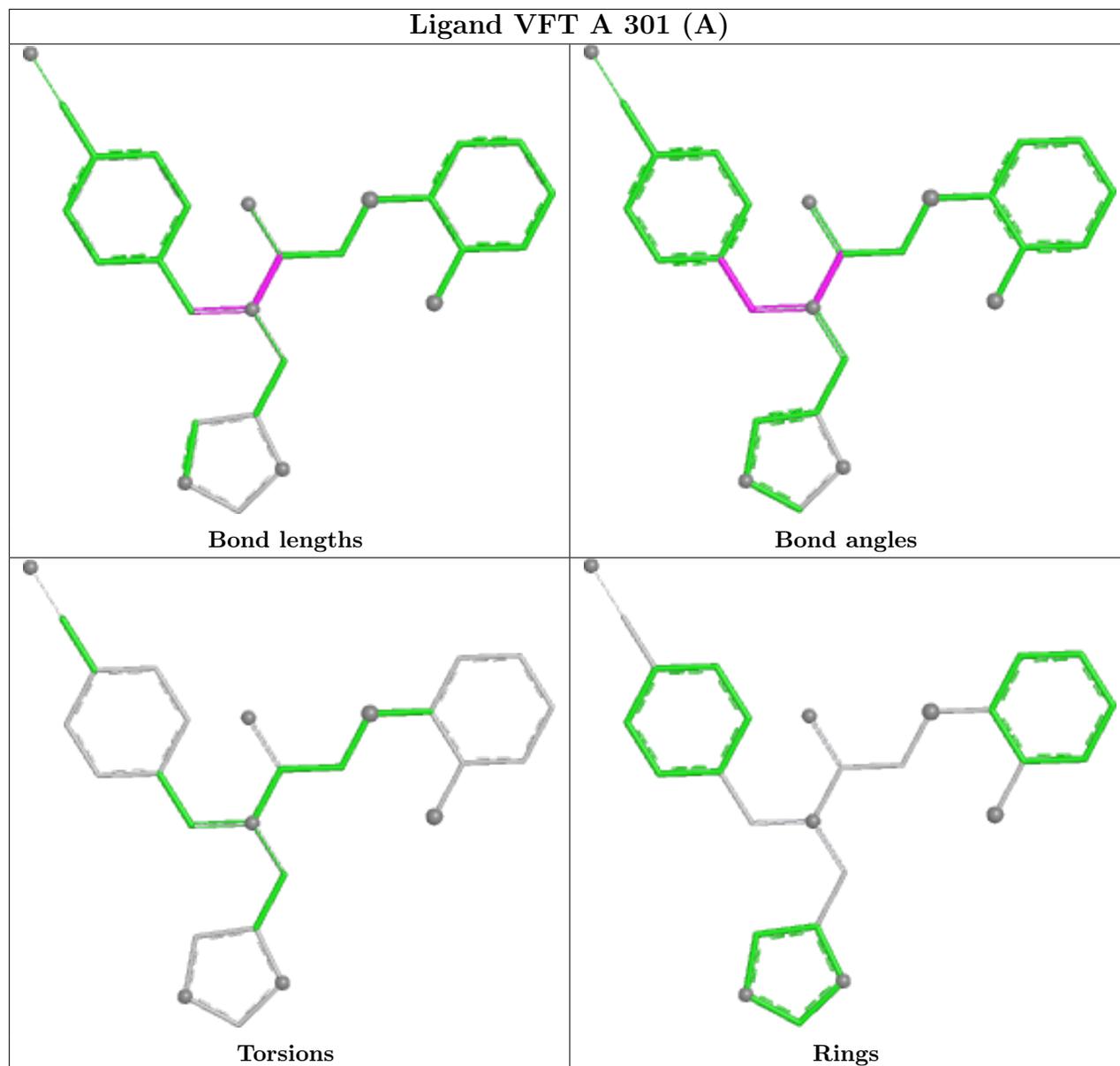


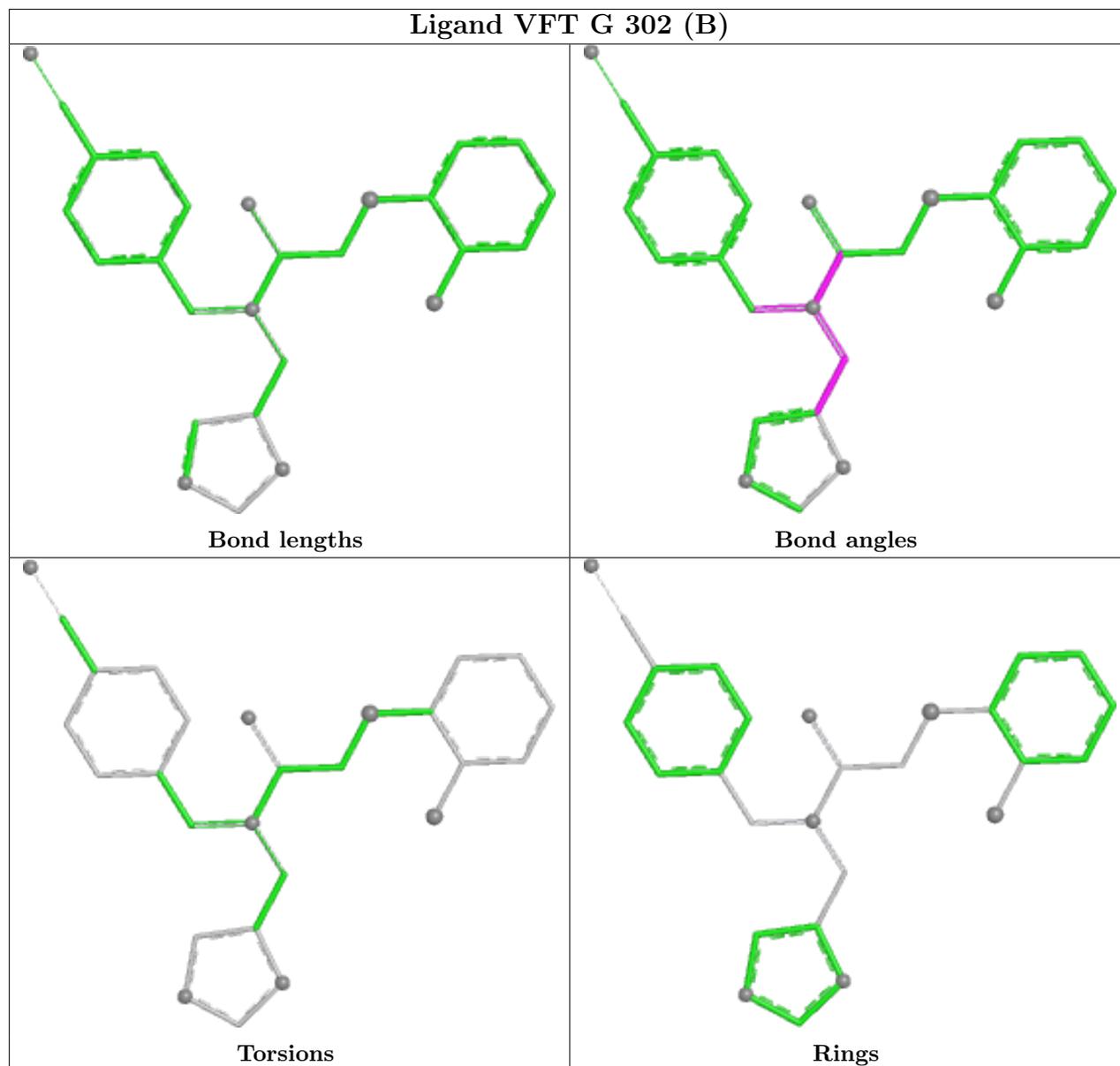


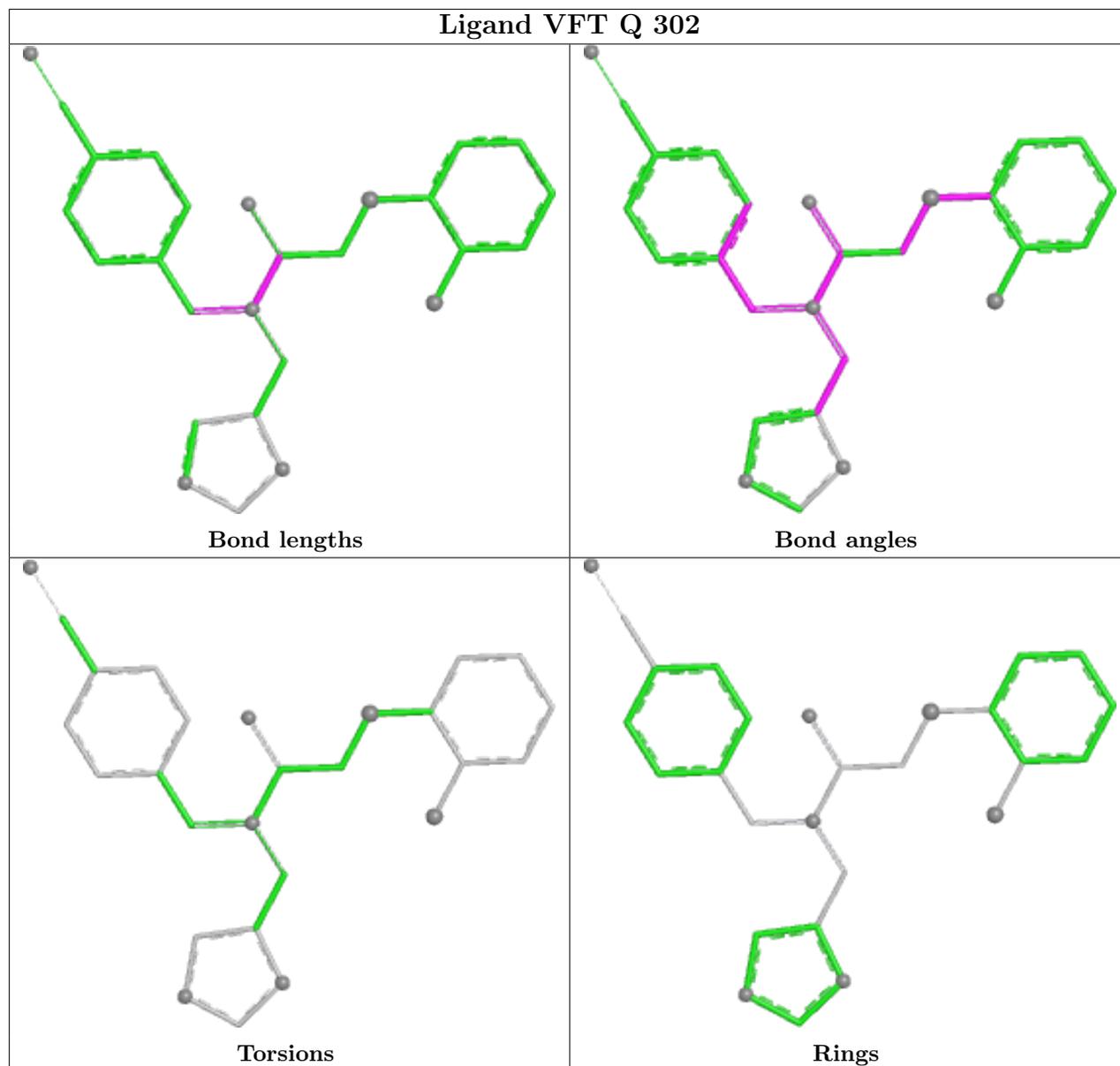


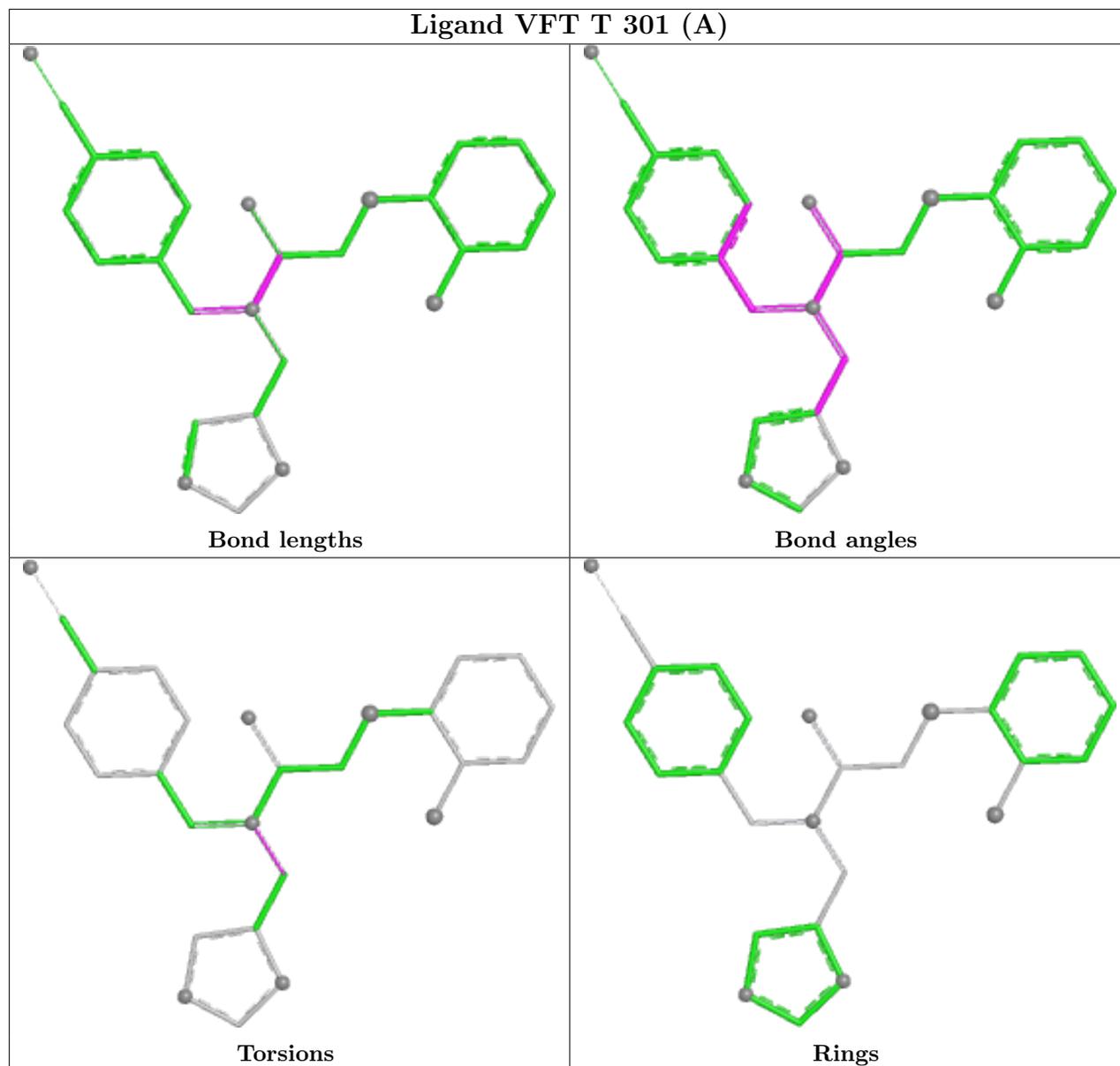


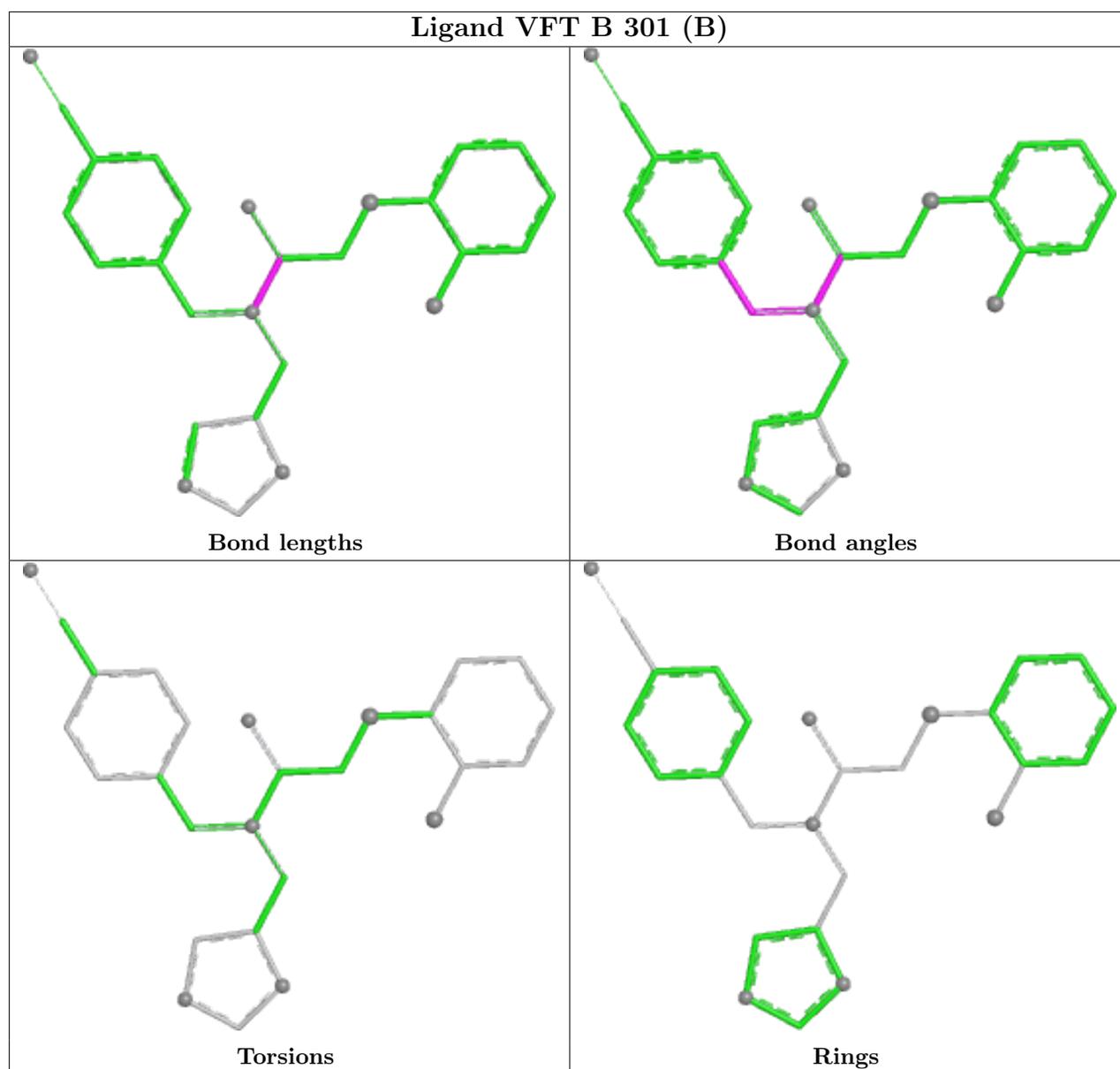


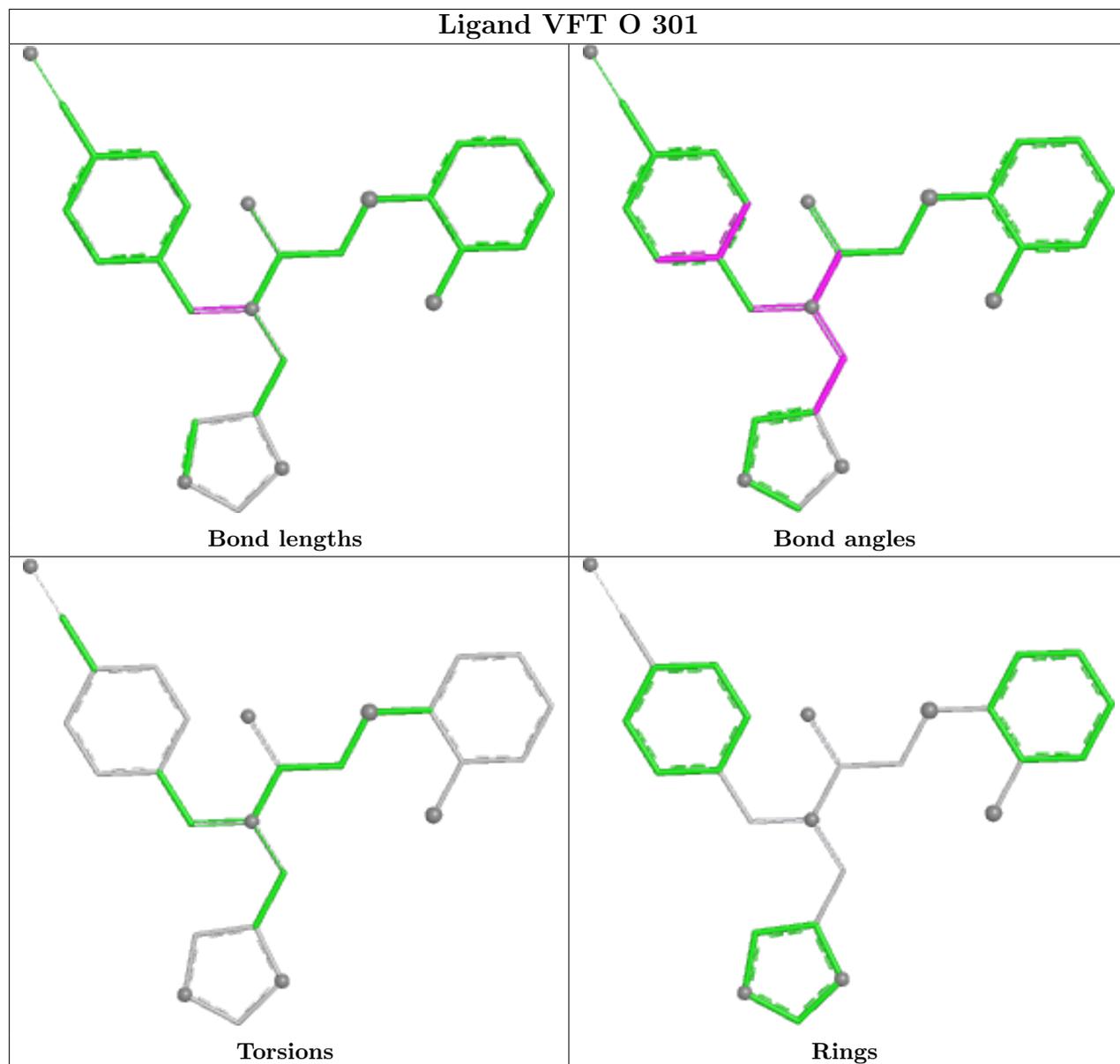


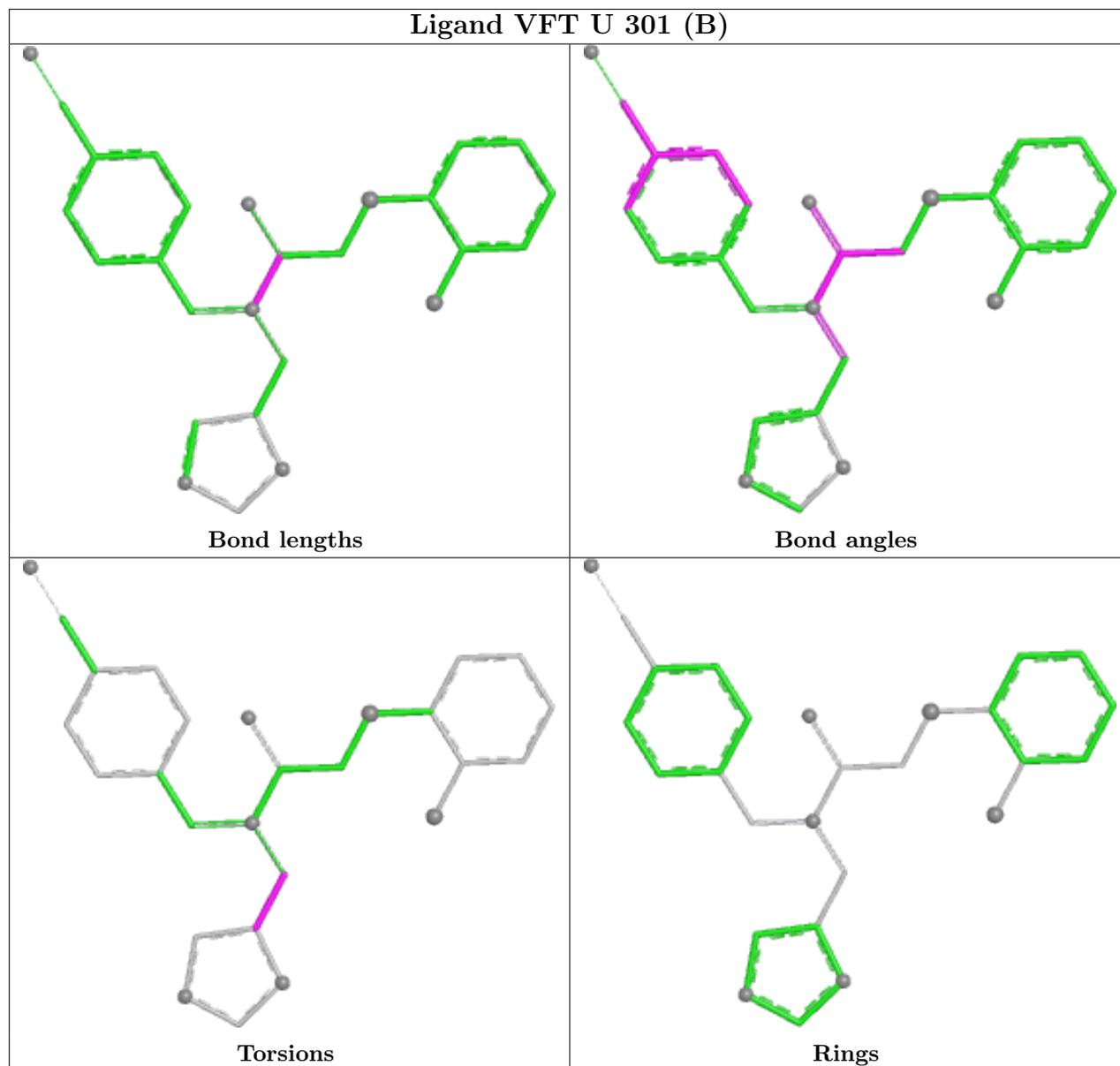


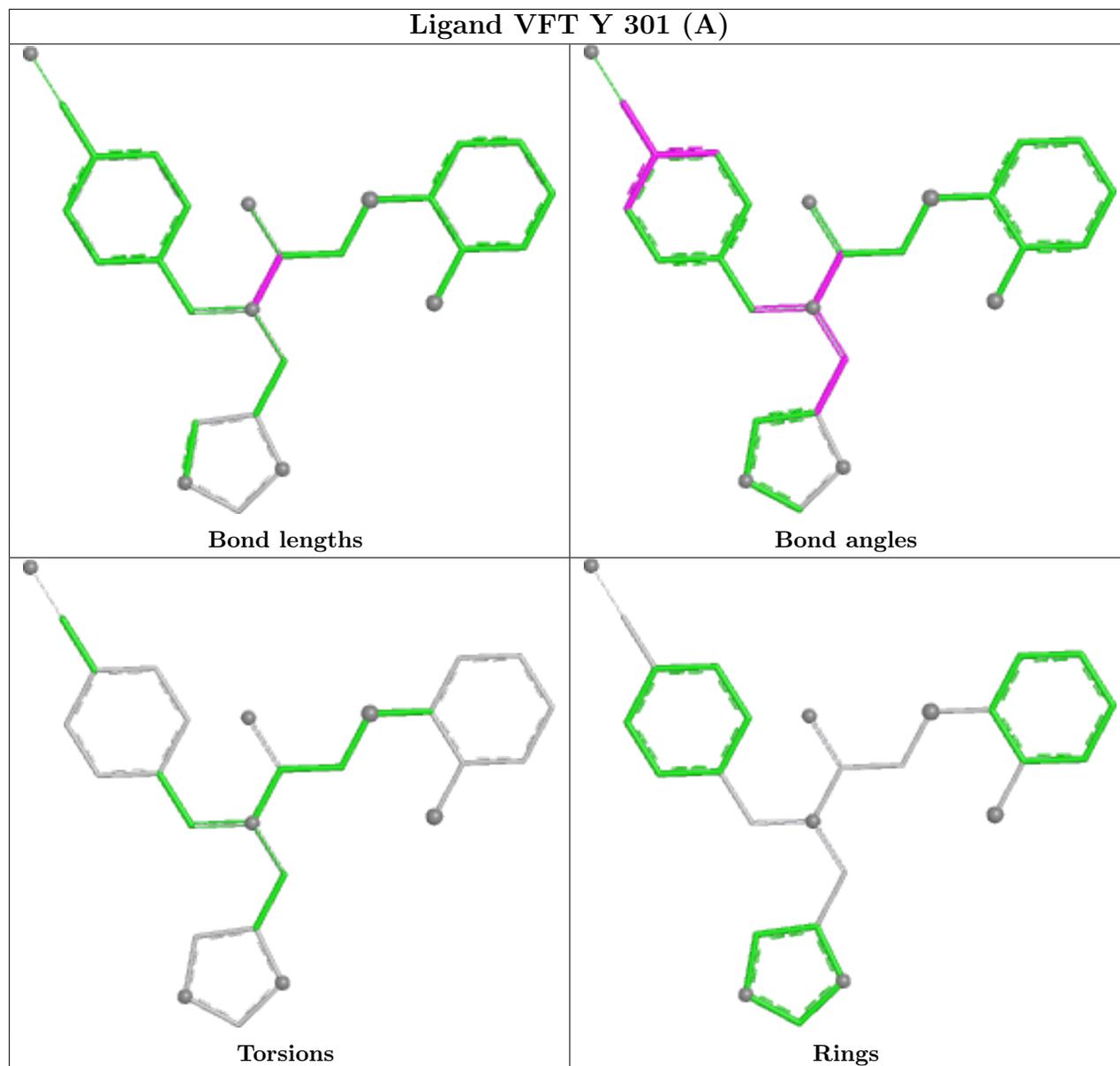


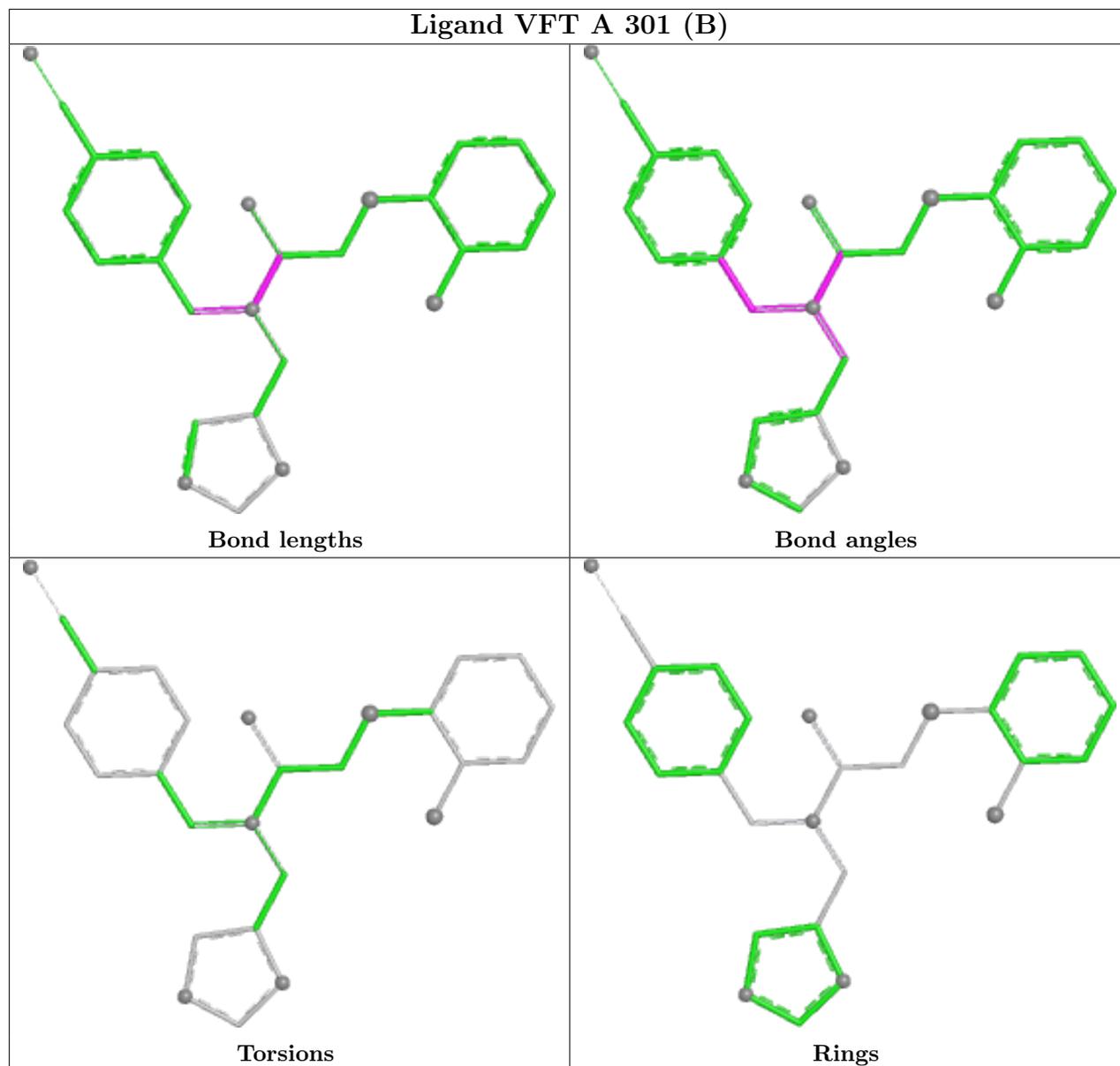


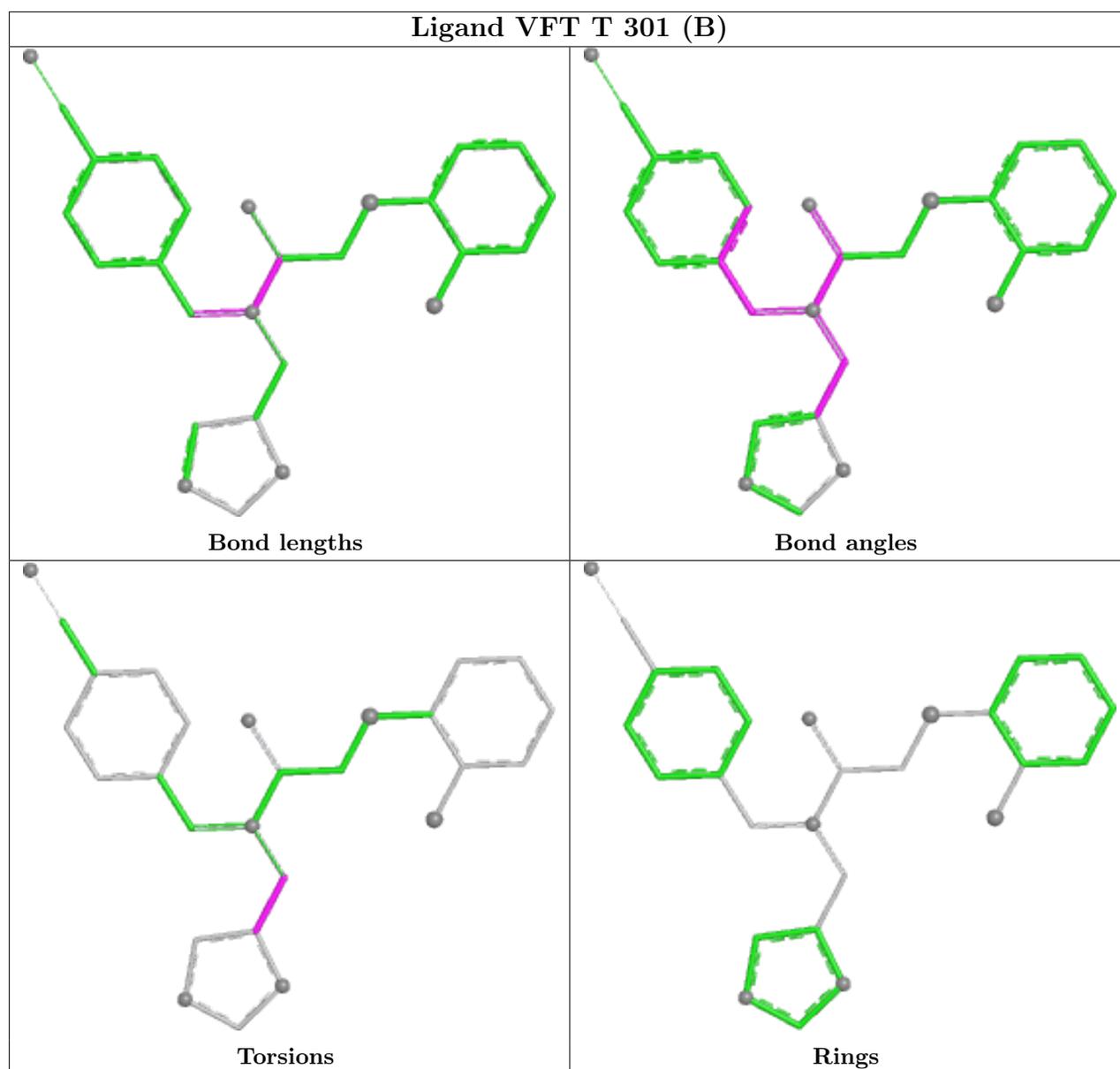


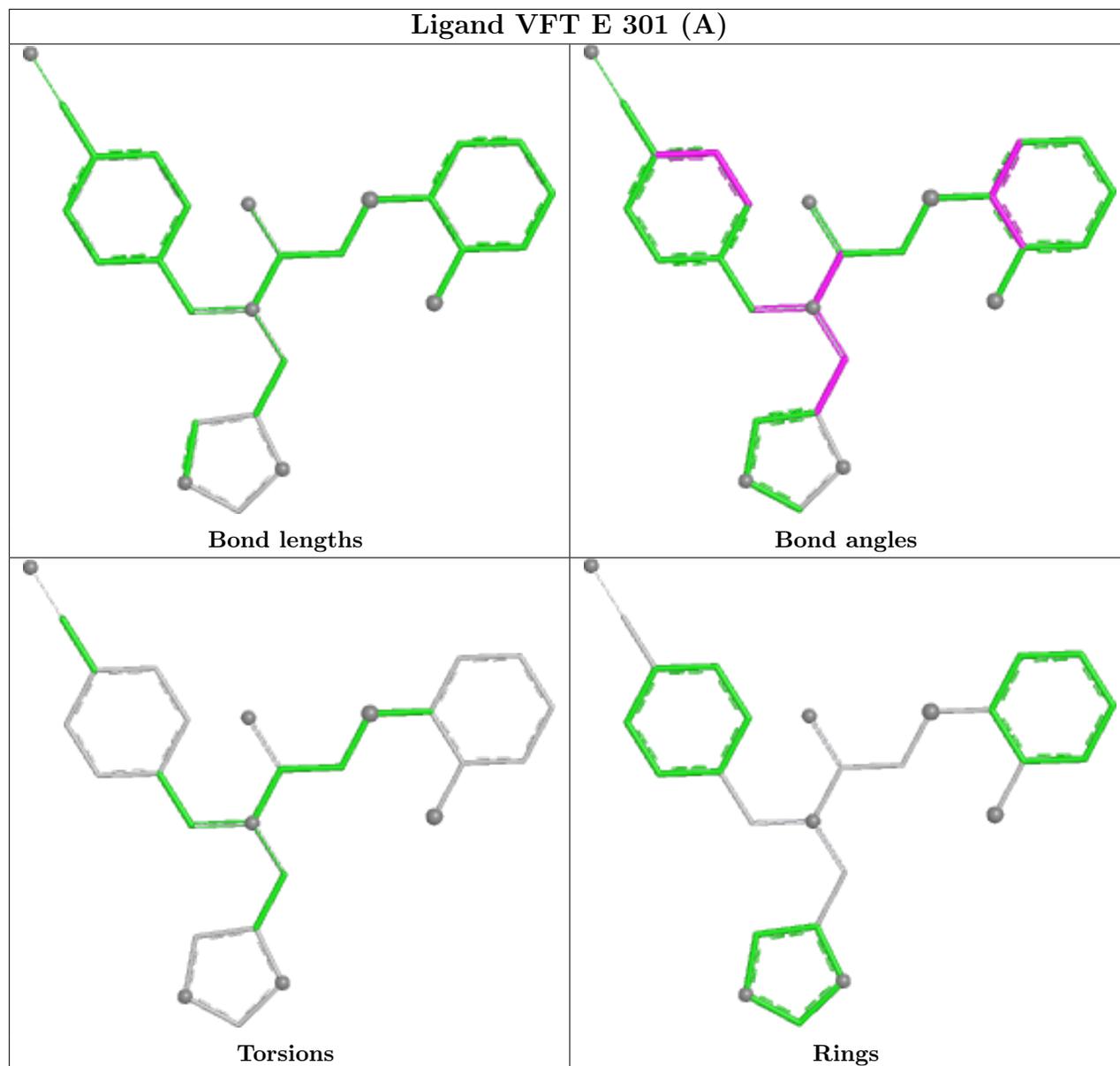


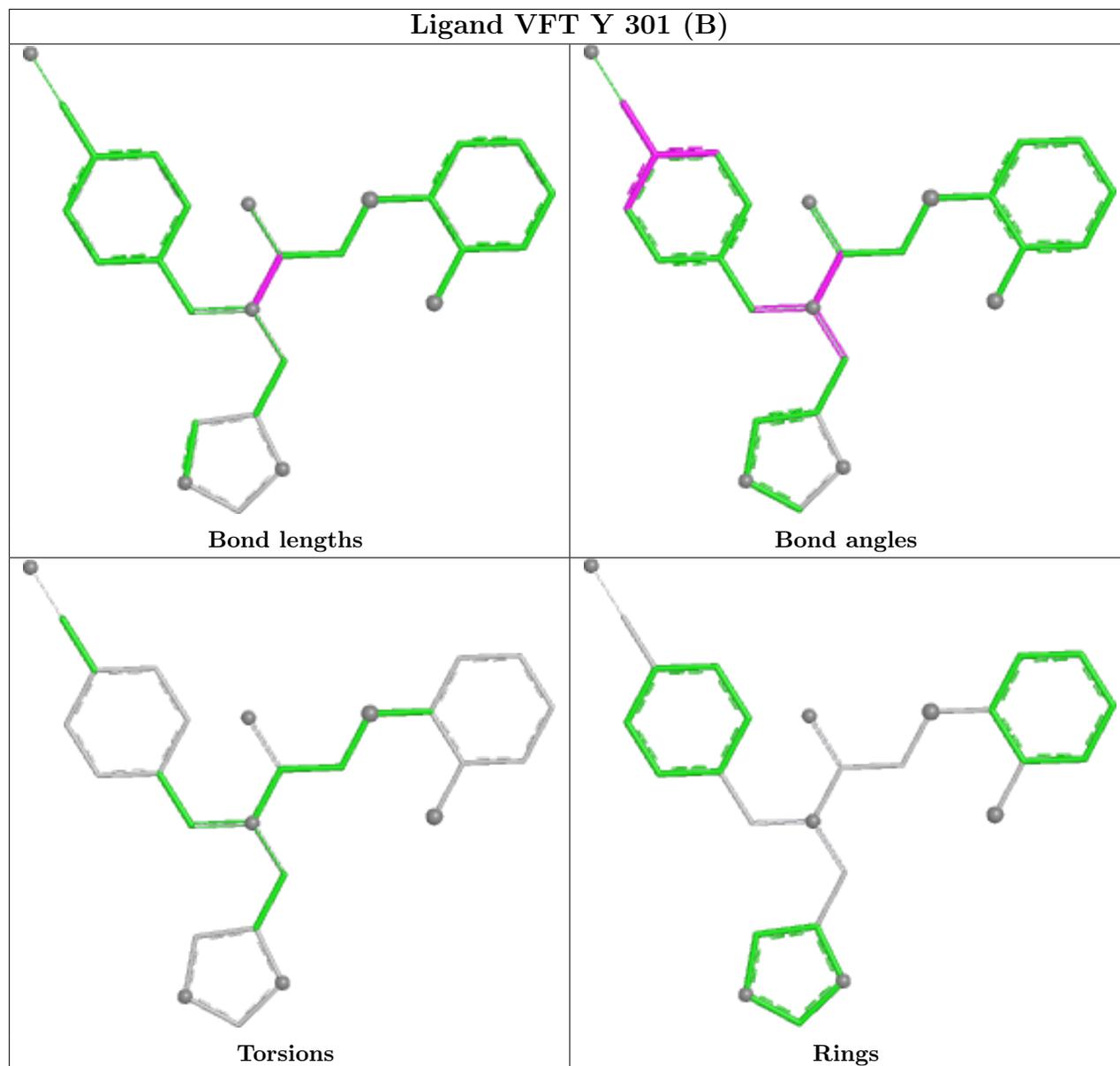


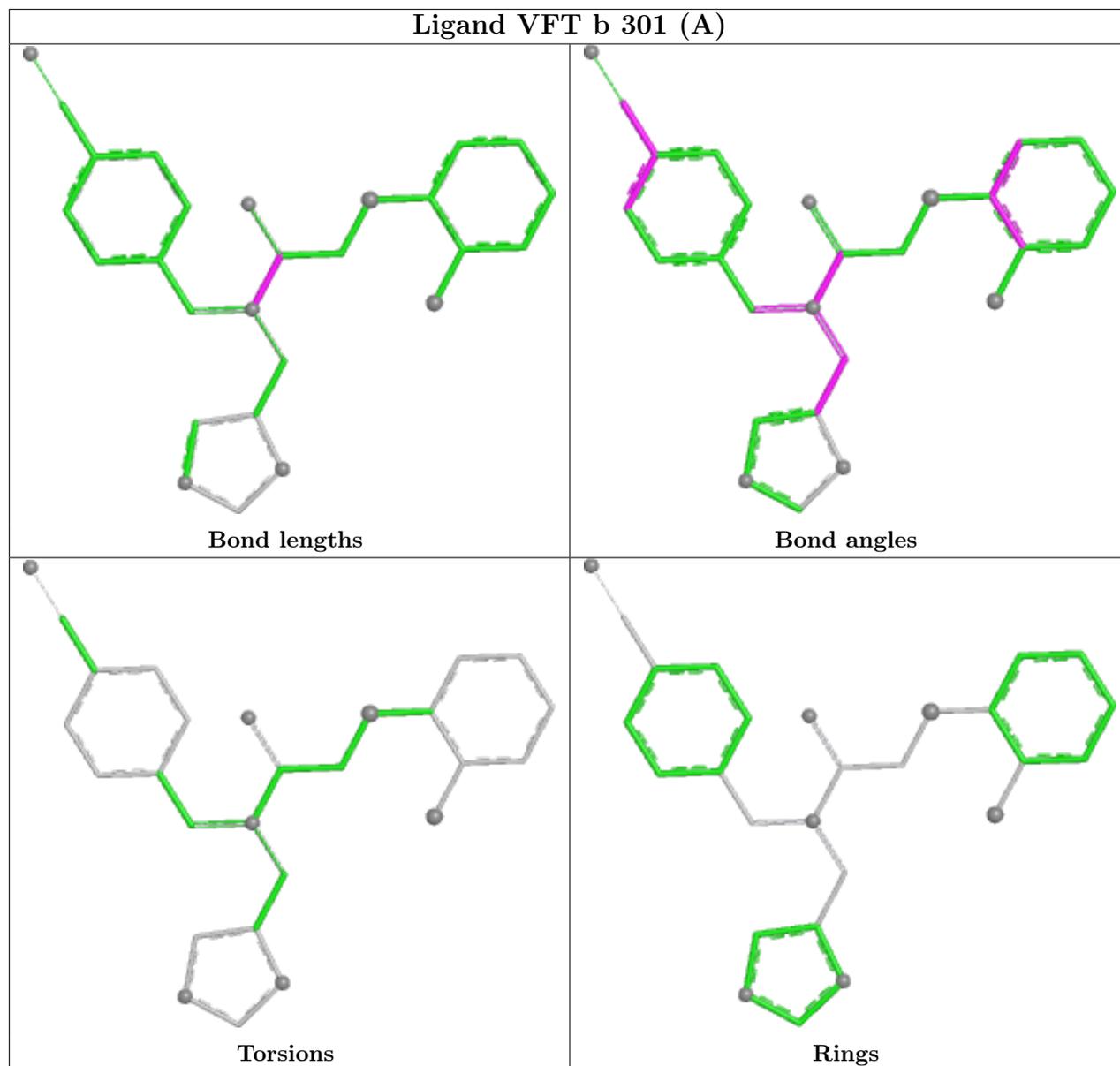


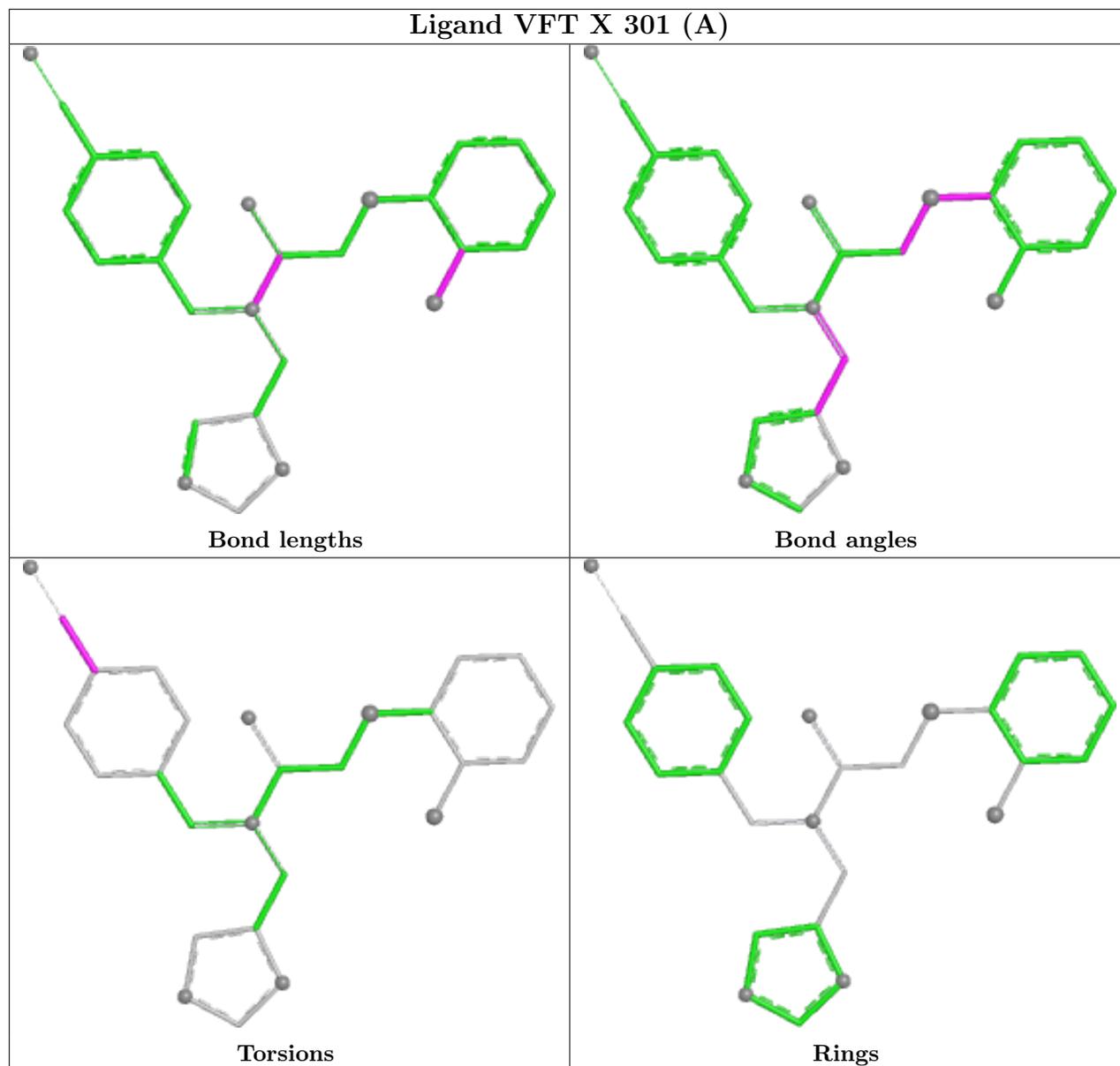


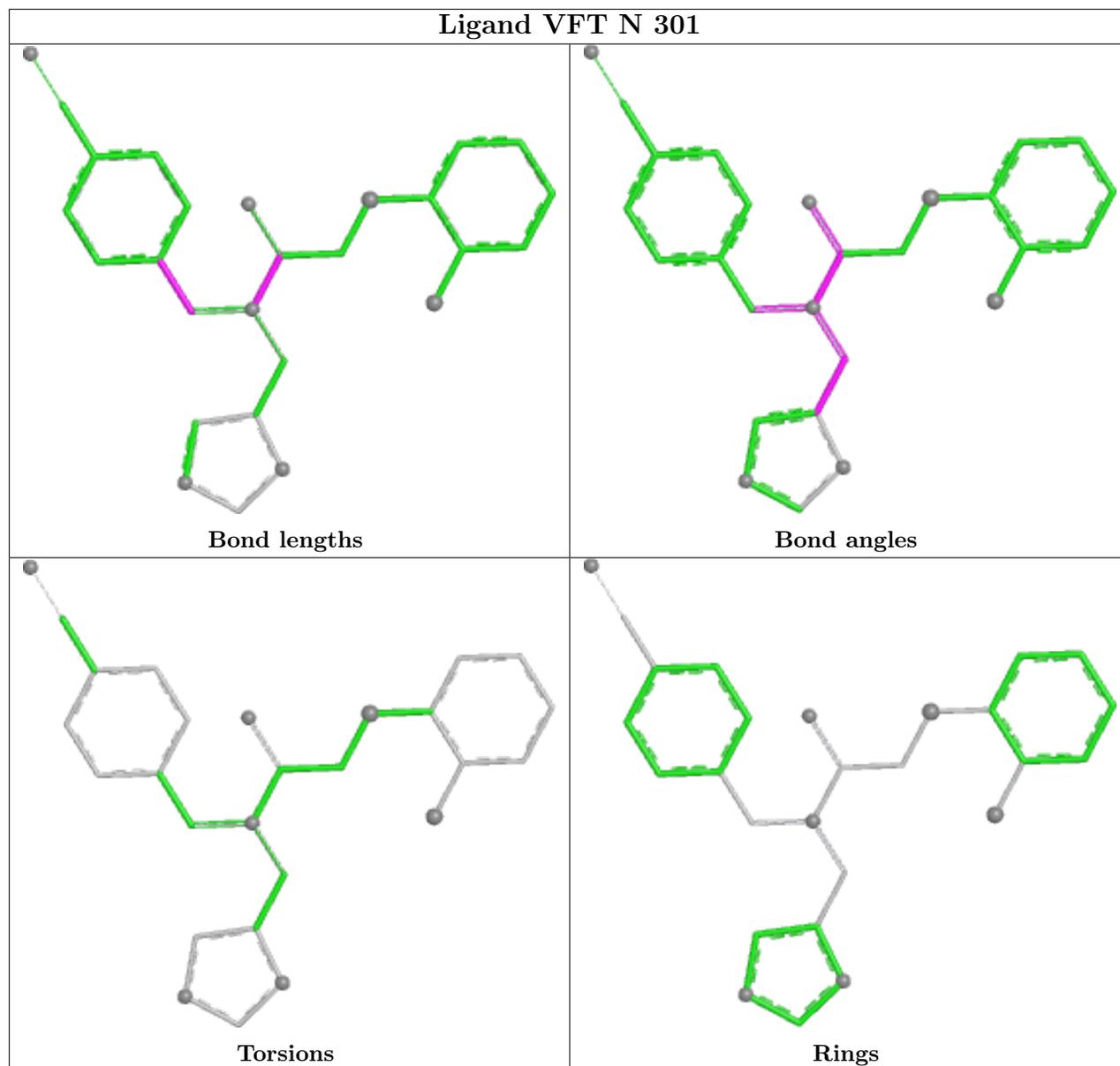


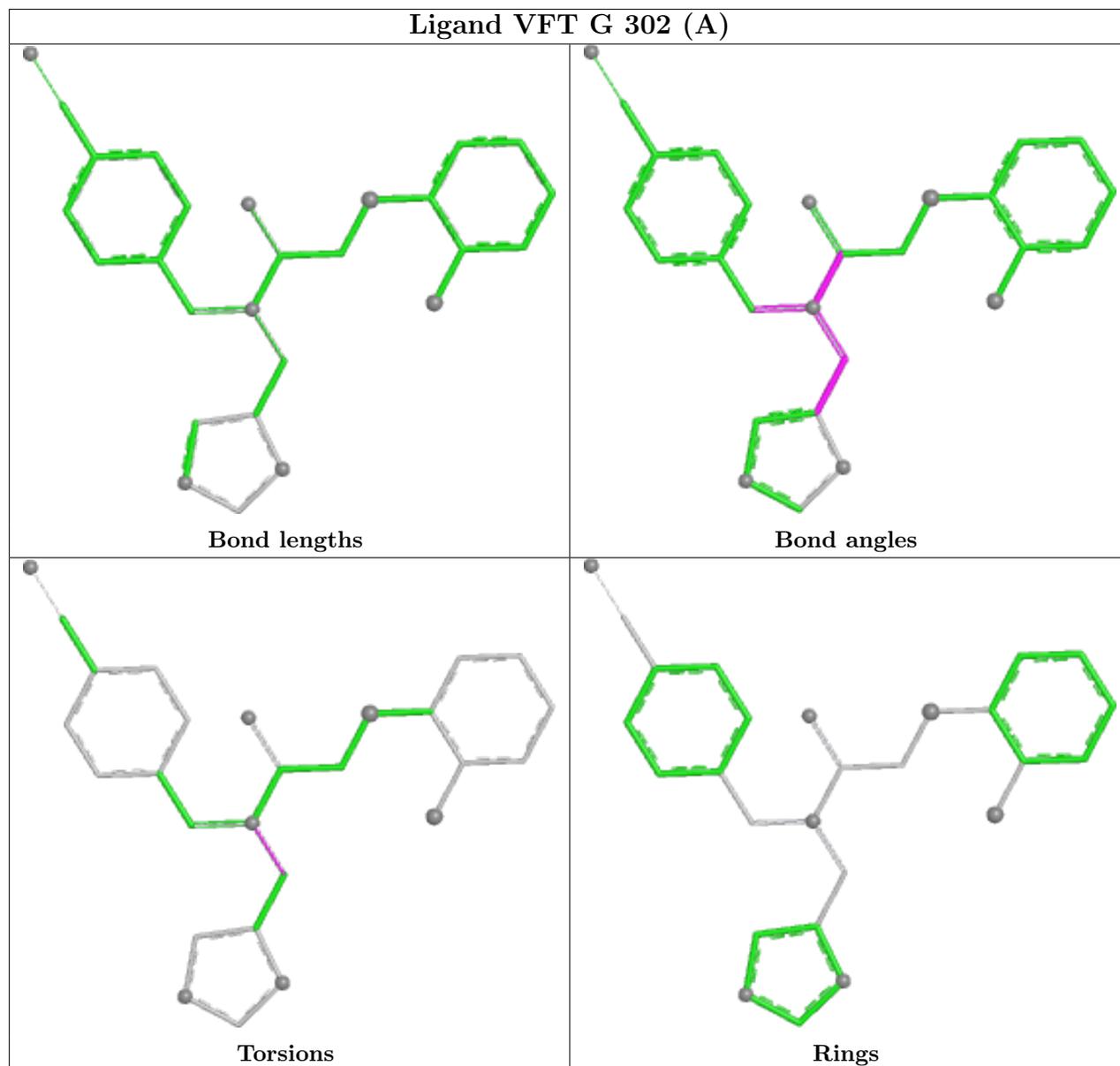


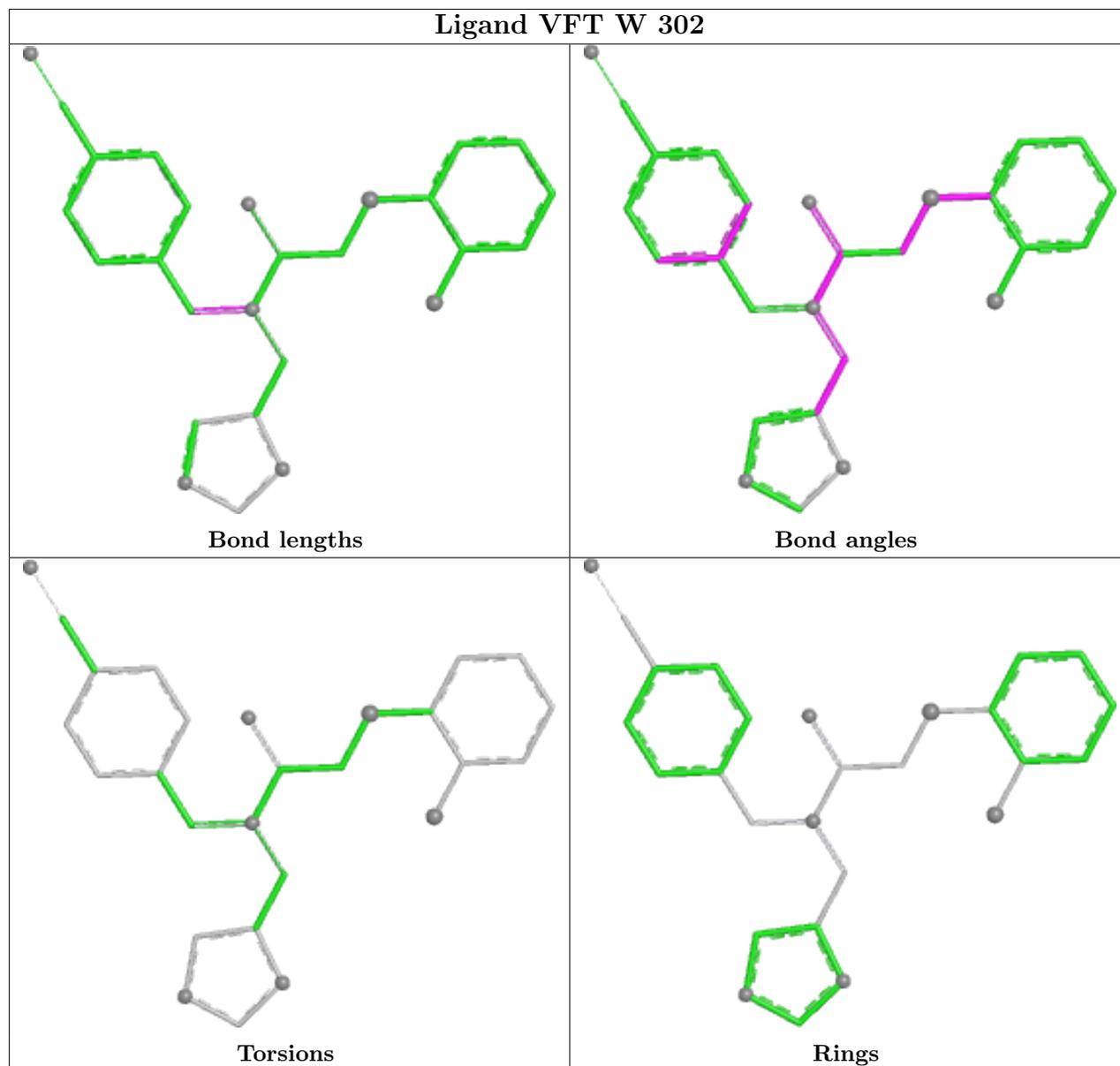


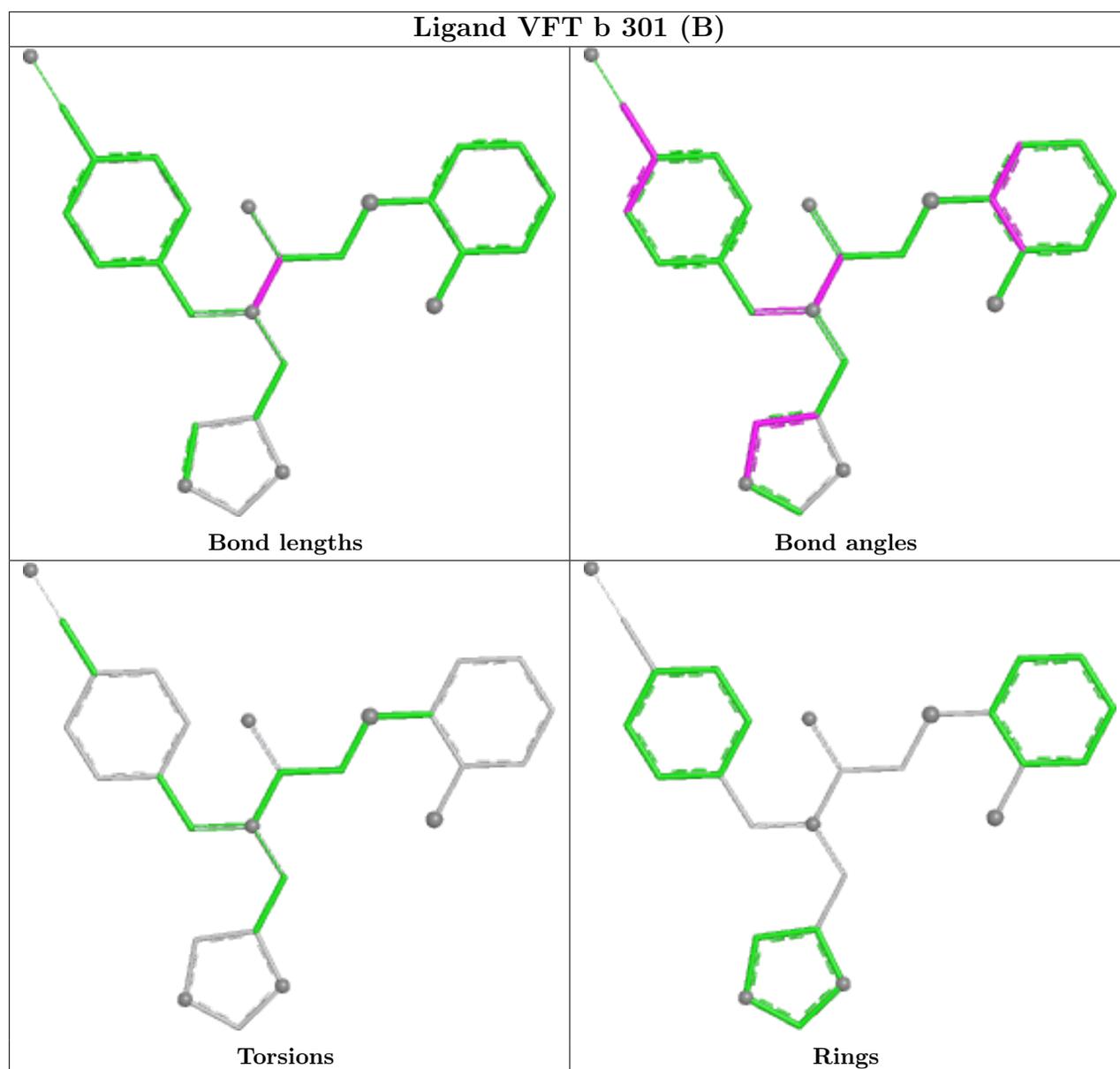












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 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	258/261 (98%)	0.52	0 100 100	31, 42, 70, 121	0
1	B	258/261 (98%)	0.48	0 100 100	32, 42, 66, 102	0
1	C	258/261 (98%)	0.49	0 100 100	31, 42, 66, 109	0
1	D	258/261 (98%)	0.50	0 100 100	30, 41, 64, 102	0
1	E	258/261 (98%)	0.52	1 (0%) 92 95	30, 41, 66, 121	0
1	F	258/261 (98%)	0.44	0 100 100	30, 42, 68, 106	0
1	G	257/261 (98%)	0.76	7 (2%) 54 61	37, 54, 83, 95	0
1	H	257/261 (98%)	0.53	0 100 100	36, 53, 84, 97	0
1	I	257/261 (98%)	0.62	2 (0%) 86 89	36, 52, 83, 105	0
1	J	258/261 (98%)	0.49	0 100 100	30, 43, 68, 103	0
1	K	258/261 (98%)	0.41	0 100 100	31, 45, 72, 123	0
1	L	258/261 (98%)	0.48	0 100 100	33, 44, 68, 113	0
1	M	257/261 (98%)	0.75	4 (1%) 72 78	35, 55, 86, 100	0
1	N	257/261 (98%)	0.52	2 (0%) 86 89	37, 53, 84, 102	0
1	O	257/261 (98%)	0.59	2 (0%) 86 89	36, 54, 85, 104	0
1	P	257/261 (98%)	0.52	2 (0%) 86 89	37, 54, 84, 105	0
1	Q	257/261 (98%)	0.62	4 (1%) 72 78	36, 56, 88, 109	0
1	R	257/261 (98%)	0.48	0 100 100	36, 54, 83, 106	0
1	S	258/261 (98%)	0.46	0 100 100	32, 43, 70, 107	0
1	T	258/261 (98%)	0.43	0 100 100	32, 42, 67, 99	0
1	U	258/261 (98%)	0.50	0 100 100	31, 43, 69, 108	0
1	V	257/261 (98%)	0.52	6 (2%) 60 67	37, 55, 84, 100	0
1	W	257/261 (98%)	0.76	16 (6%) 20 23	37, 54, 87, 104	0
1	X	257/261 (98%)	0.50	0 100 100	37, 53, 84, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	258/261 (98%)	0.70	4 (1%) 72 78	35, 53, 85, 133	0
1	Z	258/261 (98%)	0.52	0 100 100	36, 52, 84, 123	0
1	a	257/261 (98%)	0.54	5 (1%) 66 73	36, 54, 84, 101	0
1	b	257/261 (98%)	0.56	3 (1%) 79 83	36, 53, 87, 110	0
1	c	258/261 (98%)	0.55	2 (0%) 86 89	35, 53, 88, 141	0
1	d	257/261 (98%)	0.66	3 (1%) 79 83	36, 55, 86, 104	0
All	All	7725/7830 (98%)	0.55	63 (0%) 86 89	30, 49, 83, 141	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	18	ALA	4.7
1	c	1	MET	4.1
1	W	15	ARG	3.9
1	M	253	THR	3.4
1	Q	15	ARG	3.4

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

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

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
3	CL	B	303	1/1	0.71	0.14	70,70,70,70	0
4	SO4	A	307	5/5	0.75	0.28	64,73,93,95	5
4	SO4	D	304	5/5	0.75	0.30	53,72,80,92	5
4	SO4	U	304	5/5	0.76	0.36	83,85,92,94	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	V	303	5/5	0.77	0.46	62,79,90,107	5
4	SO4	Y	303	5/5	0.77	0.40	68,75,93,99	5
4	SO4	Q	306	5/5	0.78	0.40	69,81,92,102	5
3	CL	C	301	1/1	0.78	0.11	69,69,69,69	0
3	CL	E	302	1/1	0.79	0.14	71,71,71,71	0
3	CL	C	302	1/1	0.80	0.10	82,82,82,82	0
4	SO4	Z	302	5/5	0.80	0.37	66,74,91,95	5
4	SO4	d	302	5/5	0.80	0.40	63,67,85,96	5
4	SO4	B	305	5/5	0.81	0.28	64,66,87,94	5
4	SO4	M	305	5/5	0.81	0.34	64,76,90,93	5
4	SO4	b	303	5/5	0.82	0.38	71,75,91,99	5
4	SO4	N	304	5/5	0.82	0.37	67,74,91,99	5
4	SO4	J	304	5/5	0.83	0.35	60,77,84,91	5
3	CL	M	303	1/1	0.83	0.09	65,65,65,65	0
4	SO4	a	305	5/5	0.83	0.27	68,80,85,93	5
3	CL	D	302	1/1	0.83	0.09	68,68,68,68	0
3	CL	M	302	1/1	0.83	0.14	65,65,65,65	0
3	CL	E	303	1/1	0.84	0.13	69,69,69,69	0
4	SO4	S	305	5/5	0.84	0.28	61,69,82,92	5
4	SO4	c	305	5/5	0.84	0.31	60,69,79,81	5
3	CL	T	302	1/1	0.84	0.13	66,66,66,66	0
4	SO4	K	303	5/5	0.85	0.35	57,61,83,90	5
3	CL	A	304	1/1	0.85	0.08	75,75,75,75	0
3	CL	A	302	1/1	0.85	0.10	71,71,71,71	0
4	SO4	U	303	5/5	0.85	0.22	100,100,110,113	0
4	SO4	T	304	5/5	0.86	0.35	69,70,81,91	5
4	SO4	X	305	5/5	0.86	0.39	70,76,87,90	5
3	CL	X	303	1/1	0.86	0.17	66,66,66,66	0
4	SO4	G	306	5/5	0.86	0.37	65,74,86,88	5
4	SO4	R	303	5/5	0.87	0.31	74,77,94,101	5
3	CL	G	303	1/1	0.87	0.11	66,66,66,66	0
3	CL	O	302	1/1	0.87	0.12	66,66,66,66	0
4	SO4	L	304	5/5	0.87	0.35	68,72,79,80	5
4	SO4	P	303	5/5	0.87	0.28	73,75,79,79	5
4	SO4	O	304	5/5	0.87	0.38	67,79,93,105	5
4	SO4	W	304	5/5	0.87	0.38	72,73,87,91	5
4	SO4	H	303	5/5	0.88	0.33	67,77,85,92	5
3	CL	I	301	1/1	0.89	0.07	65,65,65,65	0
4	SO4	P	302	5/5	0.89	0.19	101,104,110,114	0
4	SO4	J	303	5/5	0.90	0.24	85,99,117,117	0
4	SO4	F	303	5/5	0.90	0.36	62,65,80,84	5
4	SO4	E	306	5/5	0.90	0.36	67,72,90,94	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	L	302	1/1	0.91	0.11	67,67,67,67	0
4	SO4	H	302	5/5	0.91	0.23	59,67,95,98	0
4	SO4	J	302	5/5	0.91	0.23	66,78,90,101	0
2	VFT	c	301[A]	27/27	0.92	0.24	37,49,57,62	6
2	VFT	c	301[B]	27/27	0.92	0.24	44,53,66,70	6
3	CL	Q	303	1/1	0.92	0.12	74,74,74,74	0
2	VFT	Y	301[A]	27/27	0.92	0.27	36,43,63,67	6
3	CL	A	303	1/1	0.92	0.08	79,79,79,79	0
2	VFT	Y	301[B]	27/27	0.92	0.27	36,54,64,67	6
4	SO4	c	304	5/5	0.92	0.16	75,76,98,114	0
4	SO4	I	303	5/5	0.92	0.35	64,74,81,83	5
3	CL	N	302	1/1	0.92	0.12	64,64,64,64	0
4	SO4	C	304	5/5	0.93	0.39	64,74,81,97	5
4	SO4	P	301	5/5	0.93	0.23	61,82,86,103	0
4	SO4	Z	301	5/5	0.93	0.26	72,75,95,106	0
2	VFT	W	301[B]	27/27	0.93	0.25	42,48,59,62	6
4	SO4	E	305	5/5	0.93	0.22	59,86,98,107	0
4	SO4	V	301	5/5	0.93	0.26	80,85,99,112	0
4	SO4	K	302	5/5	0.93	0.26	70,78,96,115	0
2	VFT	W	301[A]	27/27	0.93	0.25	32,45,54,57	6
4	SO4	X	304	5/5	0.93	0.23	64,67,90,104	0
2	VFT	L	301[A]	27/27	0.94	0.28	26,38,44,45	6
4	SO4	C	303	5/5	0.94	0.22	68,77,84,98	0
2	VFT	L	301[B]	27/27	0.94	0.28	36,40,57,63	6
4	SO4	D	303	5/5	0.94	0.22	63,67,85,107	0
2	VFT	R	301[A]	27/27	0.94	0.25	35,47,55,57	6
2	VFT	R	301[B]	27/27	0.94	0.25	41,50,75,78	6
2	VFT	U	301[A]	27/27	0.94	0.26	27,37,46,47	6
2	VFT	U	301[B]	27/27	0.94	0.26	33,42,56,59	6
4	SO4	G	305	5/5	0.94	0.25	77,82,91,93	0
2	VFT	B	301[A]	27/27	0.94	0.26	27,37,44,47	6
2	VFT	B	301[B]	27/27	0.94	0.26	32,40,60,64	6
2	VFT	D	301[A]	27/27	0.94	0.24	25,36,39,46	6
2	VFT	D	301[B]	27/27	0.94	0.24	34,37,64,68	6
2	VFT	a	301[A]	27/27	0.94	0.26	33,49,57,58	6
4	SO4	Y	302	5/5	0.94	0.27	69,72,102,105	0
2	VFT	a	301[B]	27/27	0.94	0.26	37,52,65,69	6
2	VFT	b	301[A]	27/27	0.94	0.30	30,41,53,61	6
2	VFT	b	301[B]	27/27	0.94	0.30	37,46,69,71	6
4	SO4	a	304	5/5	0.94	0.16	71,72,90,96	0
2	VFT	G	302[A]	27/27	0.94	0.30	34,45,61,63	6
2	VFT	G	302[B]	27/27	0.94	0.30	40,55,63,69	6

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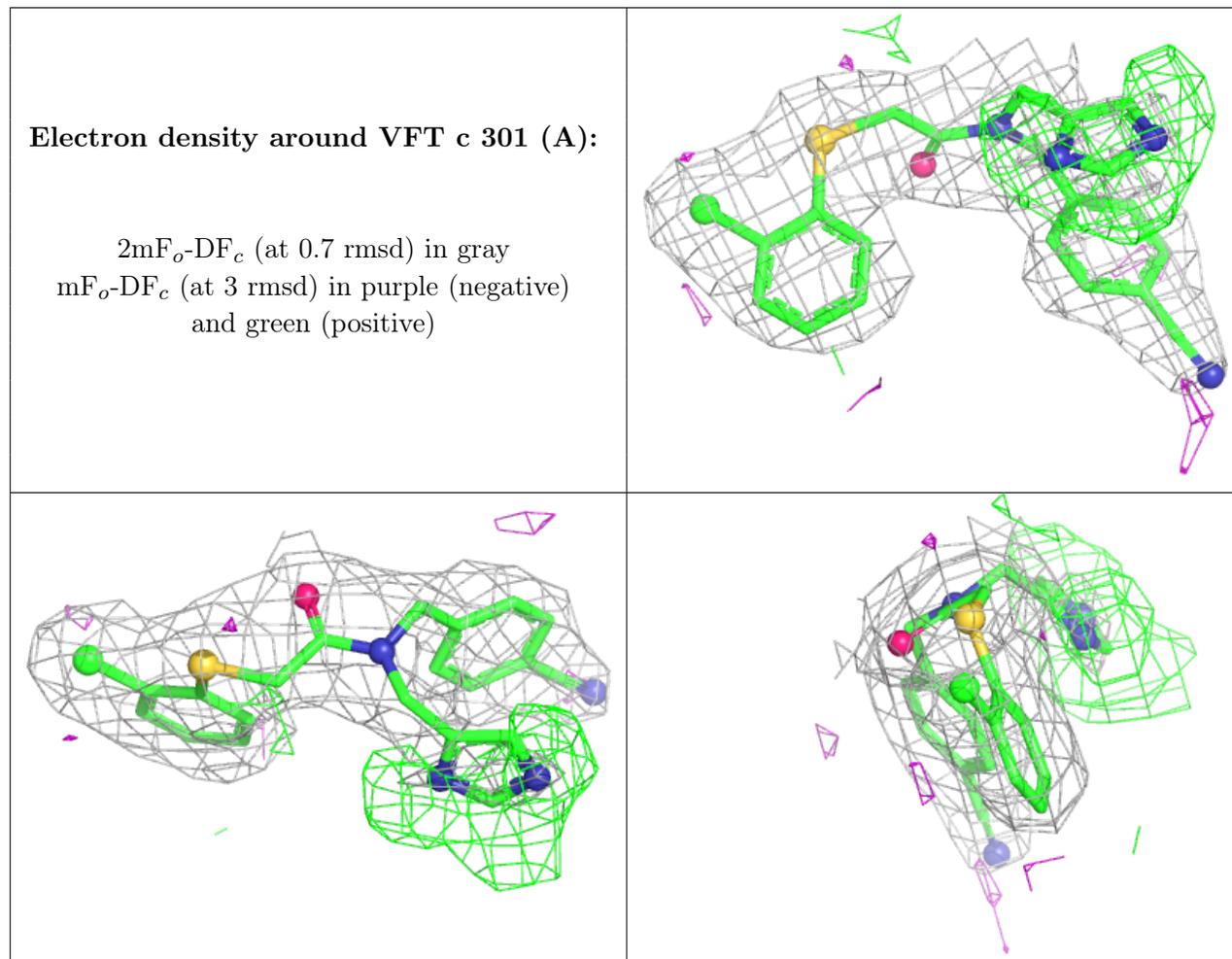
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	VFT	J	301[A]	27/27	0.94	0.26	25,38,41,48	6
4	SO4	A	305	5/5	0.94	0.24	78,79,92,101	0
4	SO4	d	301	5/5	0.94	0.21	67,69,101,104	0
2	VFT	J	301[B]	27/27	0.94	0.26	35,39,58,63	6
2	VFT	S	301[B]	27/27	0.95	0.28	33,39,62,67	6
4	SO4	S	303	5/5	0.95	0.26	68,81,101,107	0
4	SO4	S	304	5/5	0.95	0.18	48,51,64,67	5
4	SO4	I	302	5/5	0.95	0.20	61,76,87,98	0
2	VFT	T	301[A]	27/27	0.95	0.26	33,40,45,47	6
4	SO4	U	302	5/5	0.95	0.20	65,71,87,99	0
4	SO4	M	304	5/5	0.95	0.21	75,81,92,94	0
2	VFT	T	301[B]	27/27	0.95	0.26	33,41,45,47	6
4	SO4	N	303	5/5	0.95	0.22	66,72,90,99	0
4	SO4	V	302	5/5	0.95	0.13	73,77,95,100	0
2	VFT	E	301[A]	27/27	0.95	0.23	27,37,46,50	6
2	VFT	E	301[B]	27/27	0.95	0.23	33,41,57,63	6
2	VFT	Q	301[A]	27/27	0.95	0.28	37,46,55,67	6
2	VFT	Q	301[B]	27/27	0.95	0.28	38,49,64,67	6
2	VFT	X	301[A]	27/27	0.95	0.26	31,45,51,60	6
2	VFT	X	301[B]	27/27	0.95	0.26	43,47,65,72	6
4	SO4	F	302	5/5	0.95	0.18	65,72,85,89	0
4	SO4	L	303	5/5	0.95	0.20	62,66,96,97	0
4	SO4	a	303	5/5	0.95	0.26	66,84,96,107	0
2	VFT	G	301[A]	27/27	0.95	0.27	33,46,51,52	6
4	SO4	G	304	5/5	0.95	0.14	53,60,69,71	5
3	CL	S	302	1/1	0.95	0.06	83,83,83,83	0
4	SO4	c	303	5/5	0.95	0.27	72,78,89,92	0
2	VFT	G	301[B]	27/27	0.95	0.27	39,49,62,66	6
4	SO4	Q	304	5/5	0.95	0.22	63,76,88,94	0
4	SO4	Q	305	5/5	0.95	0.09	83,88,108,113	0
2	VFT	S	301[A]	27/27	0.95	0.28	29,38,42,46	6
2	VFT	a	302	27/27	0.96	0.30	44,48,84,88	0
4	SO4	T	303	5/5	0.96	0.23	70,71,88,97	0
2	VFT	A	301[A]	27/27	0.96	0.25	29,37,46,49	6
4	SO4	O	303	5/5	0.96	0.22	72,74,92,94	0
2	VFT	A	301[B]	27/27	0.96	0.25	29,44,59,64	6
2	VFT	K	301[A]	27/27	0.96	0.25	30,38,43,46	6
4	SO4	E	304	5/5	0.96	0.23	45,49,58,69	5
4	SO4	b	302	5/5	0.96	0.20	73,80,92,97	0
2	VFT	K	301[B]	27/27	0.96	0.25	36,39,57,59	6
4	SO4	R	302	5/5	0.96	0.20	70,80,88,103	0
4	SO4	W	303	5/5	0.96	0.21	74,79,87,87	0

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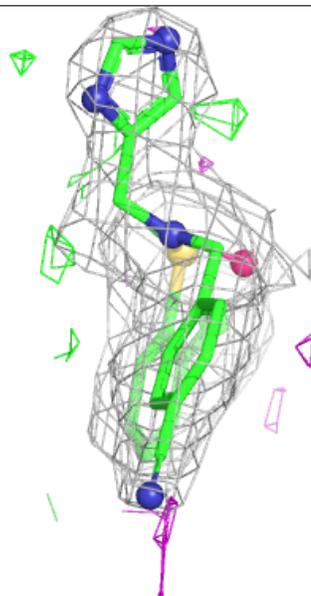
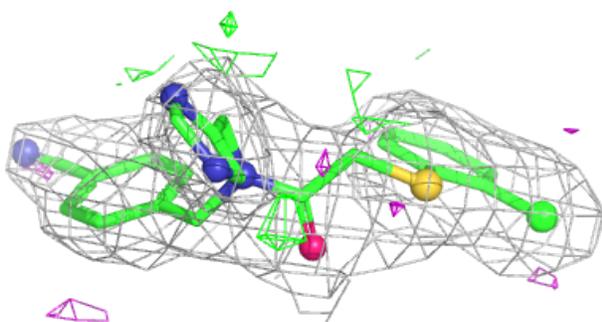
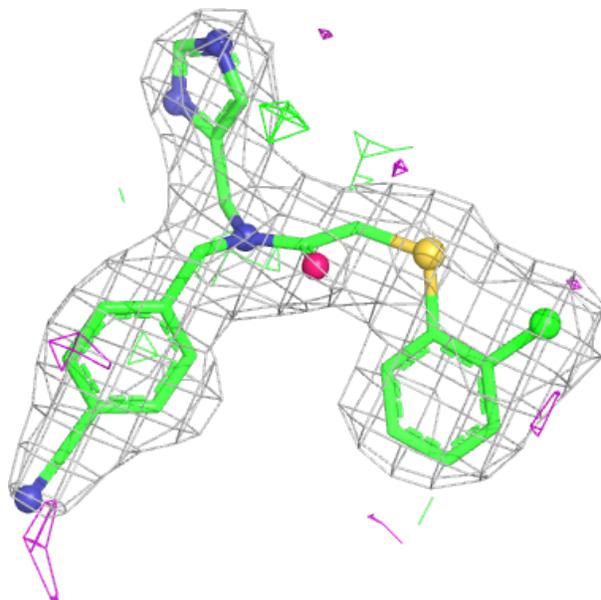
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	VFT	B	302[A]	27/27	0.96	0.26	34,38,42,44	6
4	SO4	B	304	5/5	0.96	0.18	60,62,88,95	0
2	VFT	B	302[B]	27/27	0.96	0.26	34,36,39,44	6
2	VFT	N	301	27/27	0.97	0.24	36,49,83,99	0
2	VFT	Q	302	27/27	0.97	0.25	41,50,84,96	0
4	SO4	A	306	5/5	0.97	0.20	50,54,59,62	5
2	VFT	O	301	27/27	0.97	0.29	38,51,78,89	0
2	VFT	M	301	27/27	0.97	0.29	36,49,96,97	0
2	VFT	W	302	27/27	0.97	0.27	44,52,89,94	0
2	VFT	H	301	27/27	0.98	0.23	38,48,85,91	0
2	VFT	c	302	27/27	0.98	0.27	40,48,85,90	0
2	VFT	F	301	27/27	0.98	0.26	33,41,77,84	0
3	CL	X	302	1/1	0.98	0.11	66,66,66,66	0

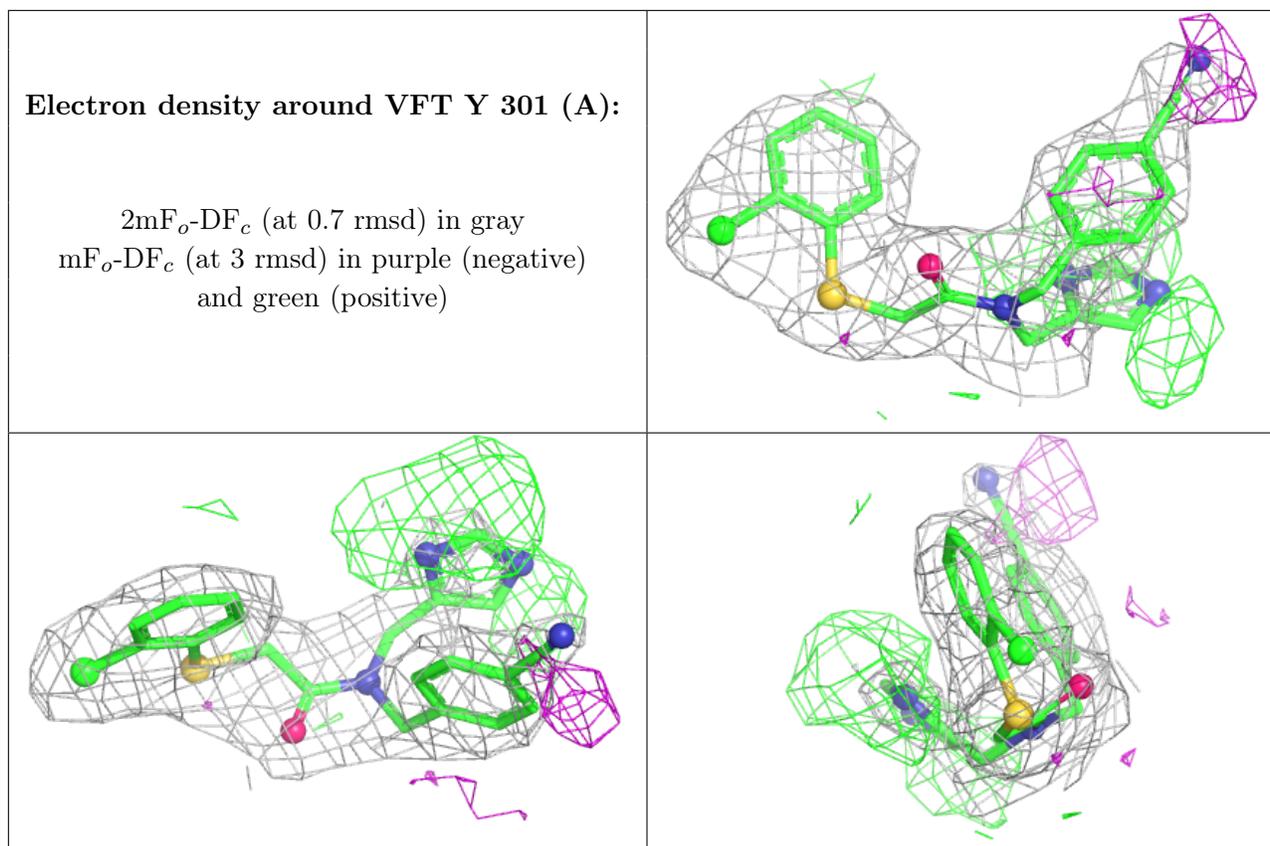
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around VFT c 301 (B):

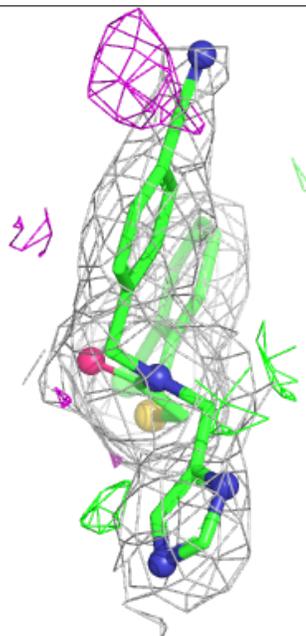
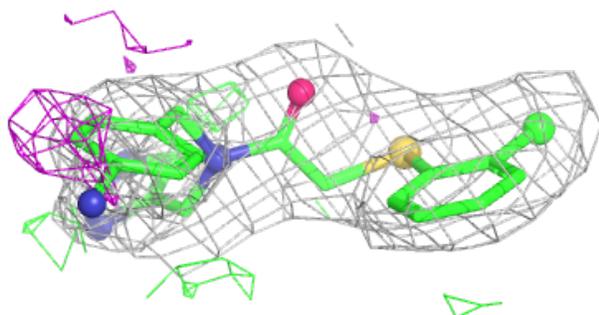
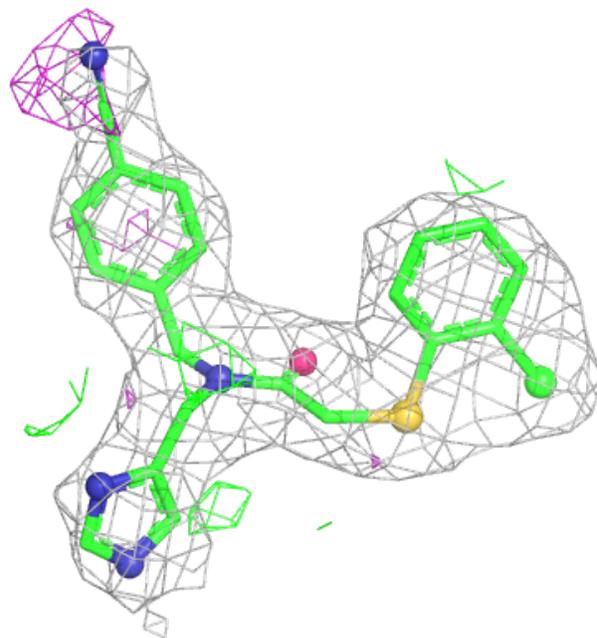
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





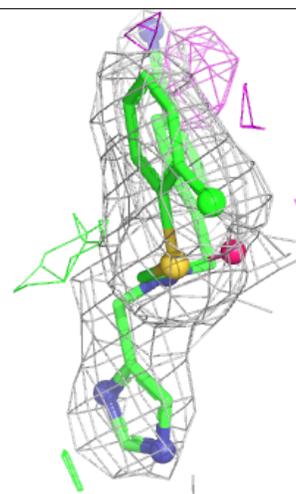
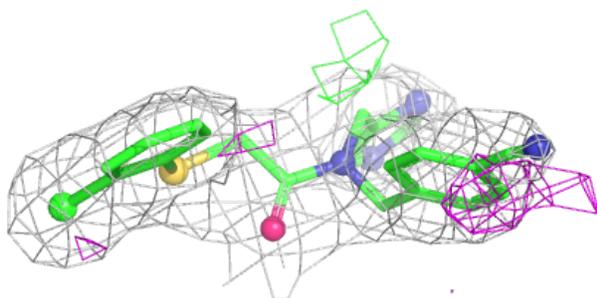
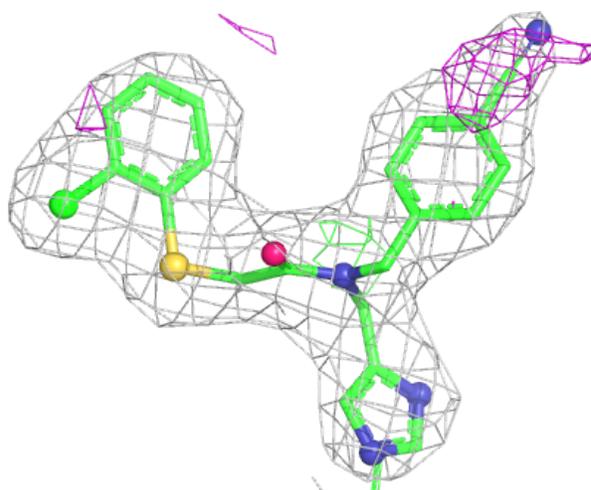
Electron density around VFT Y 301 (B):

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



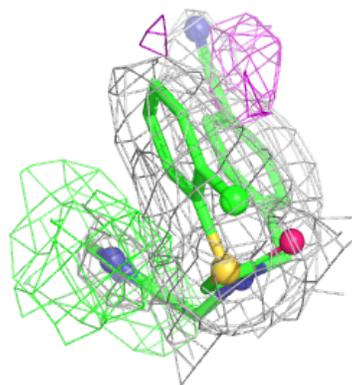
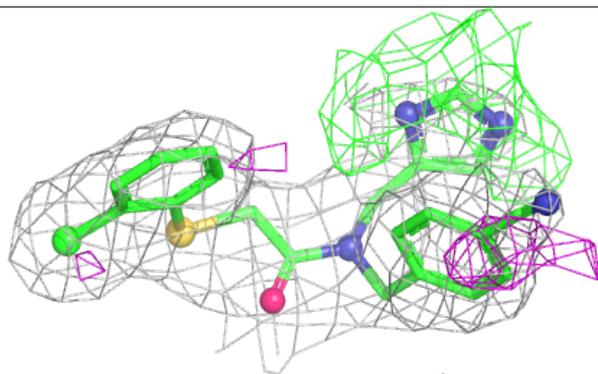
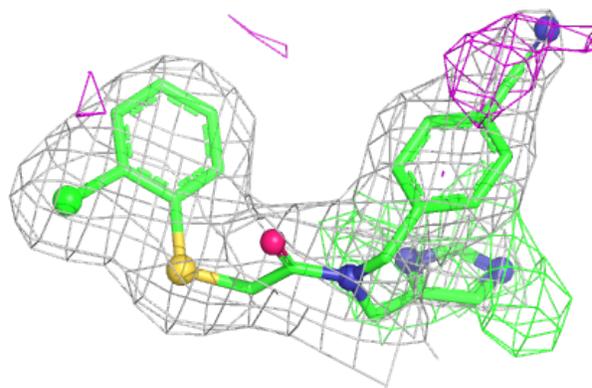
Electron density around VFT W 301 (B):

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

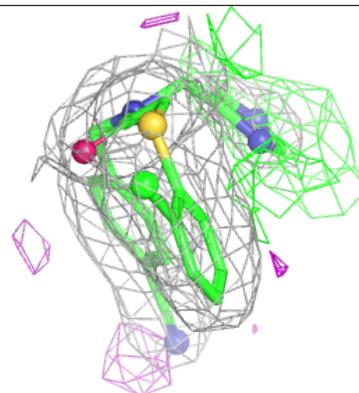
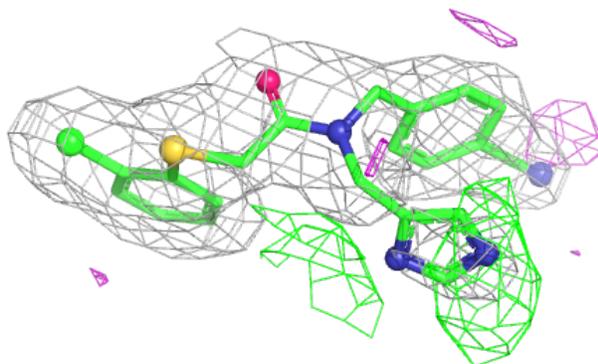
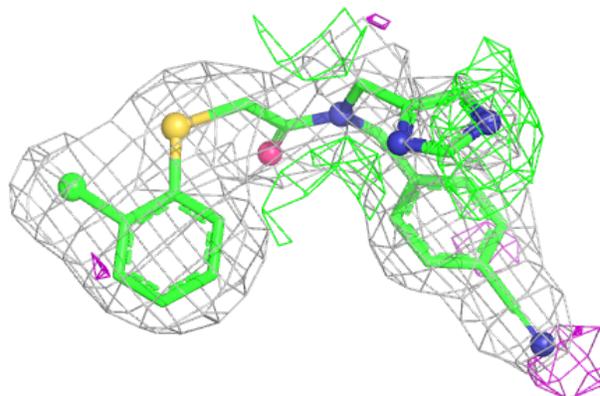


Electron density around VFT W 301 (A):

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

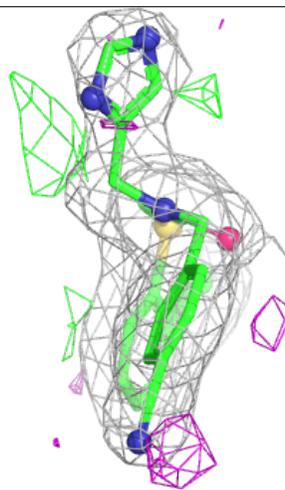
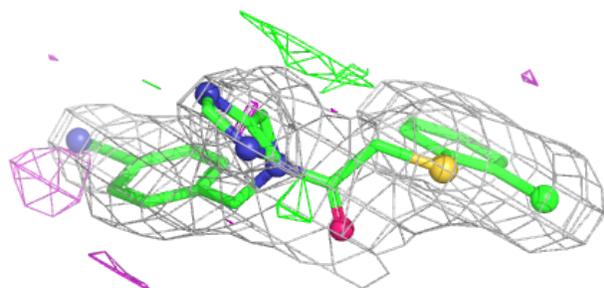
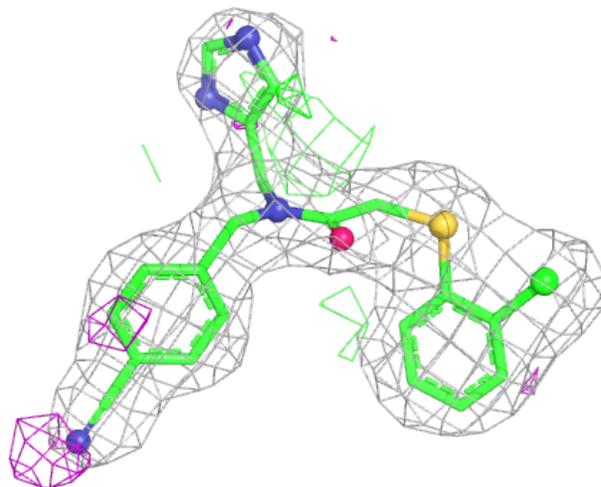
**Electron density around VFT L 301 (A):**

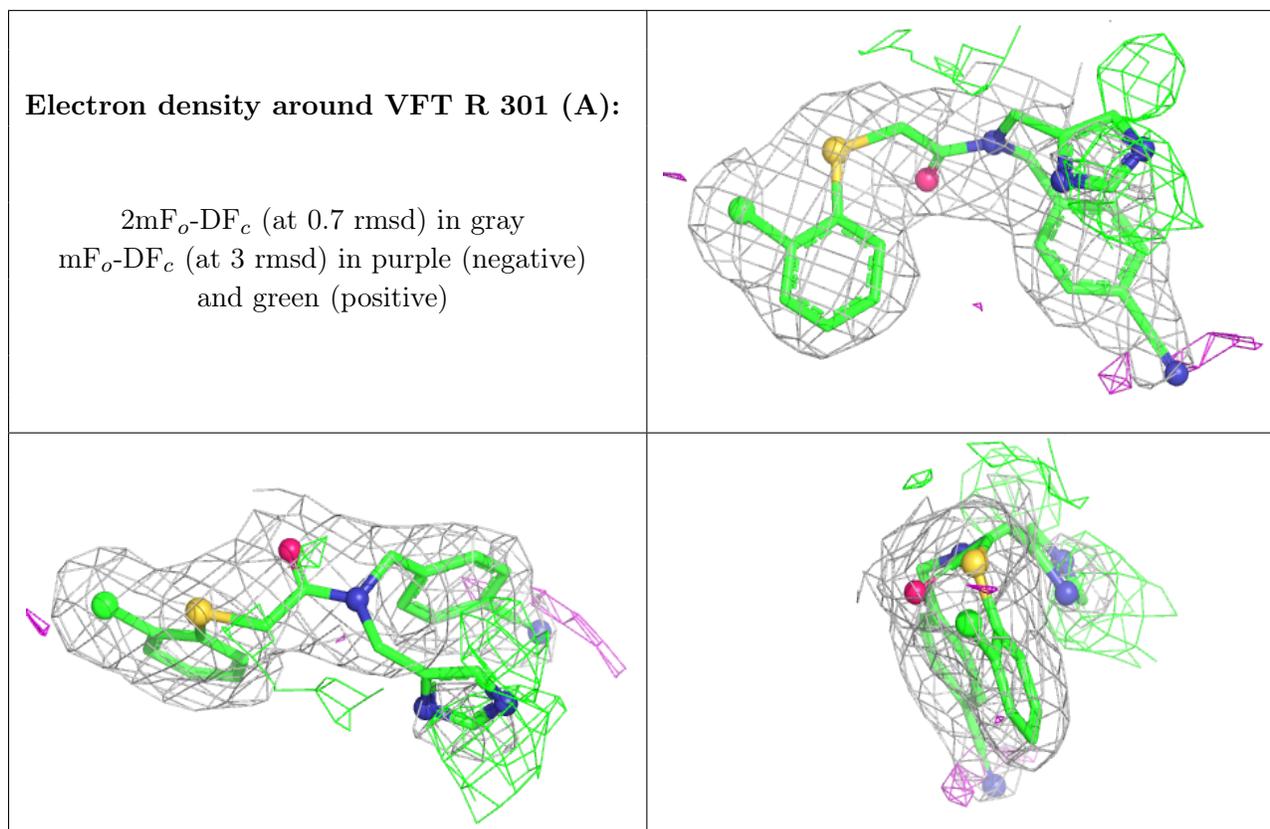
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VFT L 301 (B):

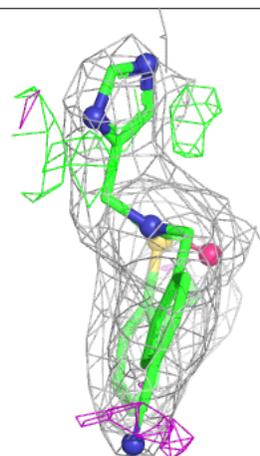
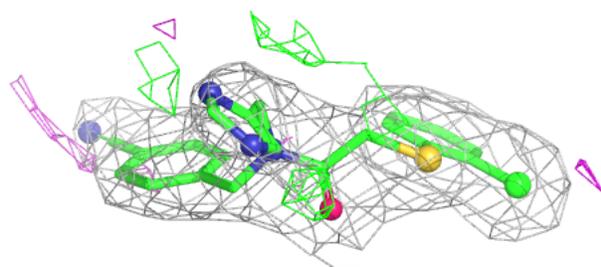
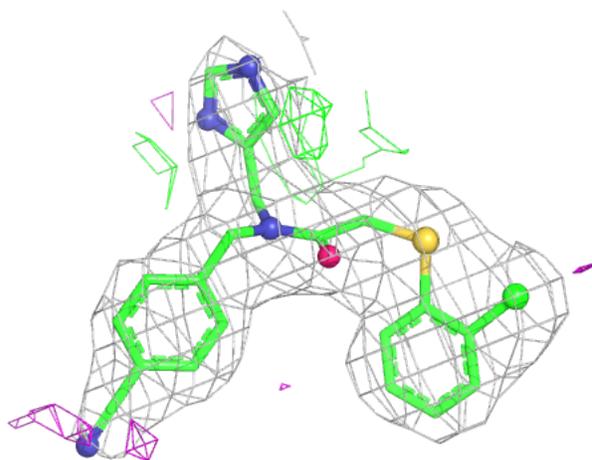
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

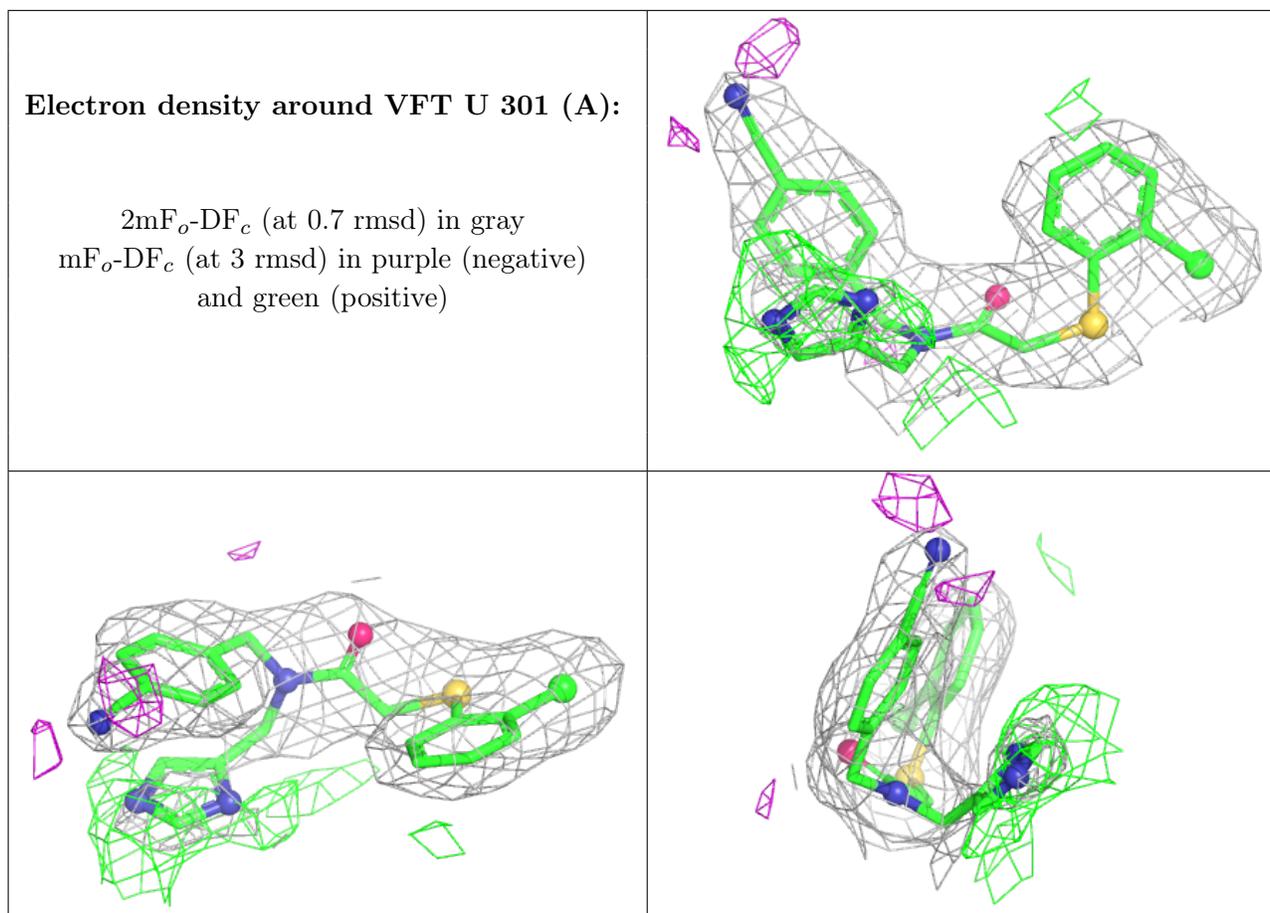




Electron density around VFT R 301 (B):

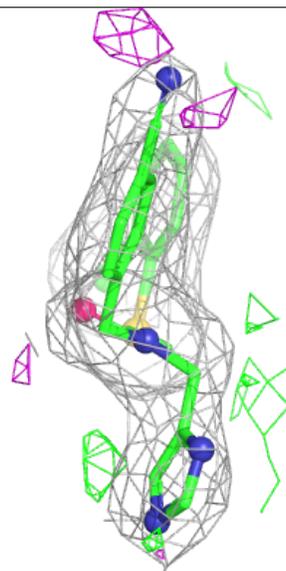
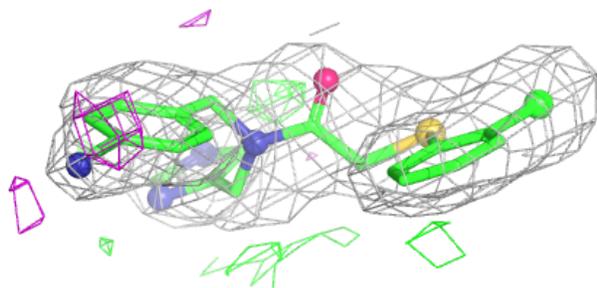
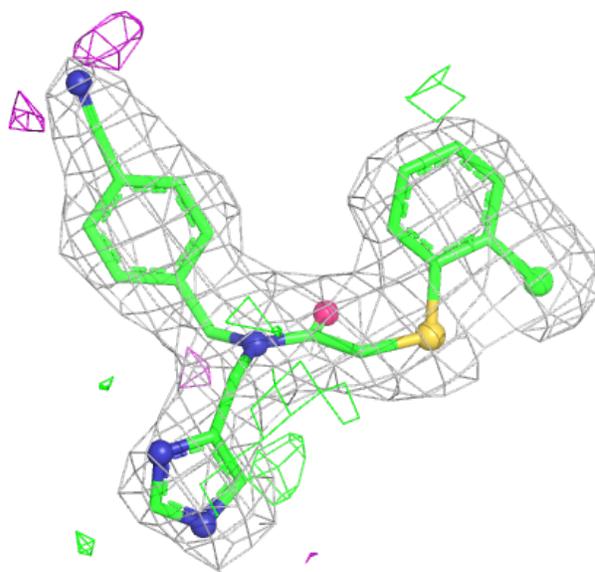
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





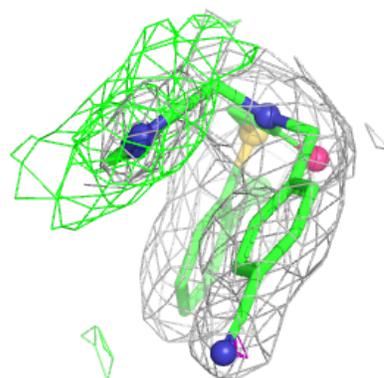
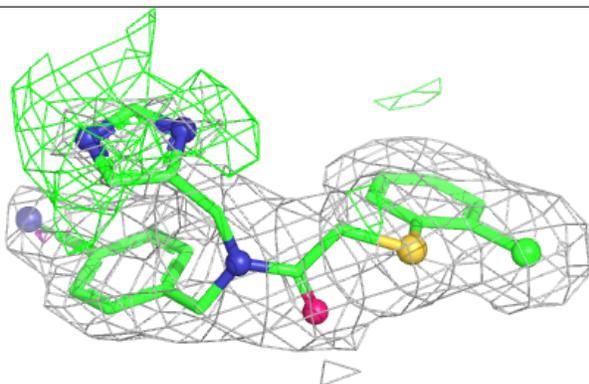
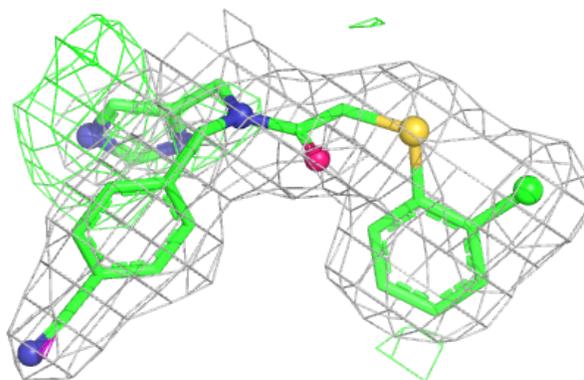
Electron density around VFT U 301 (B):

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



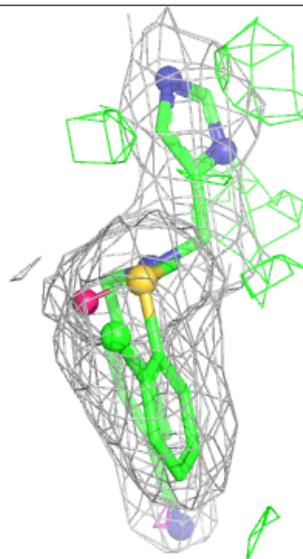
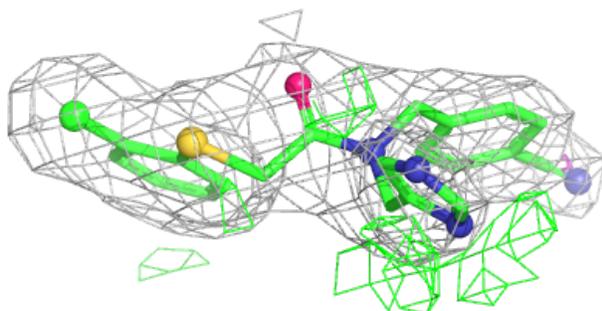
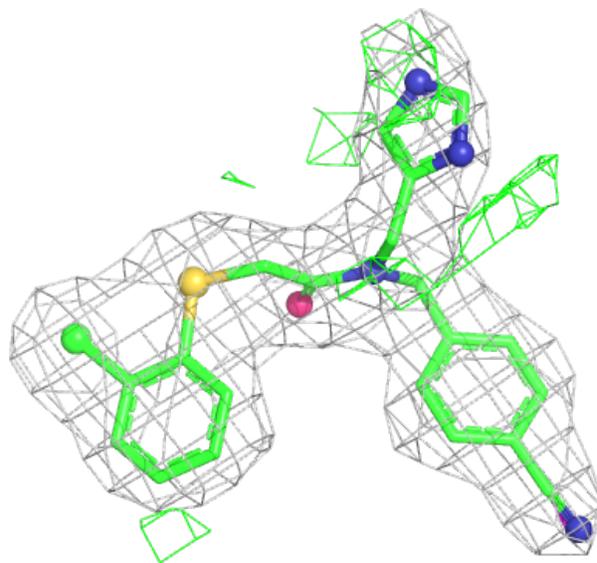
Electron density around VFT B 301 (A):

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



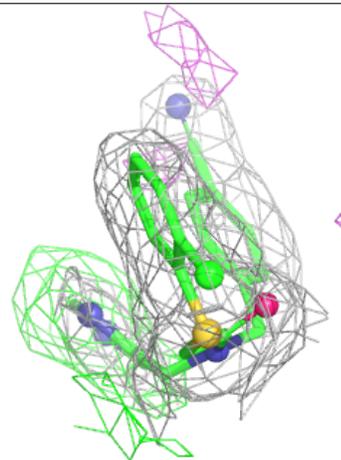
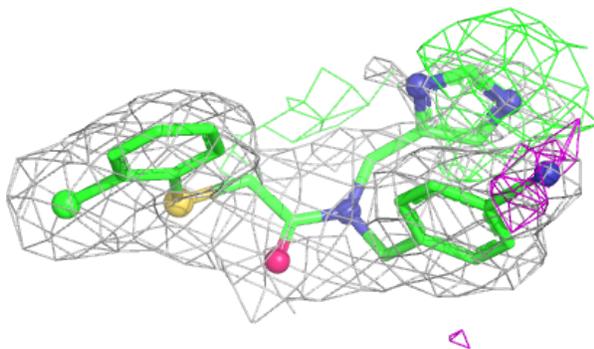
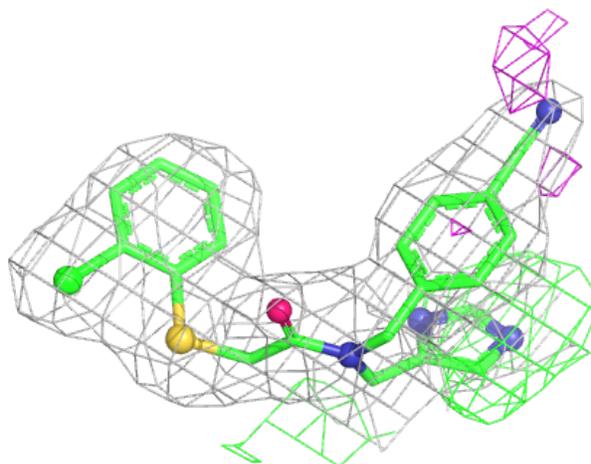
Electron density around VFT B 301 (B):

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and green (positive)



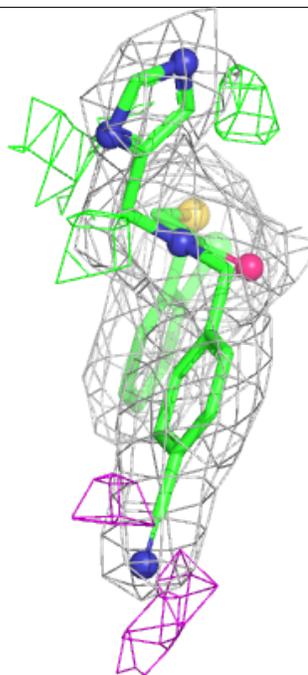
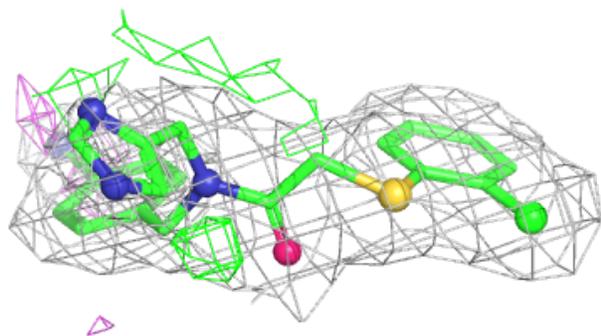
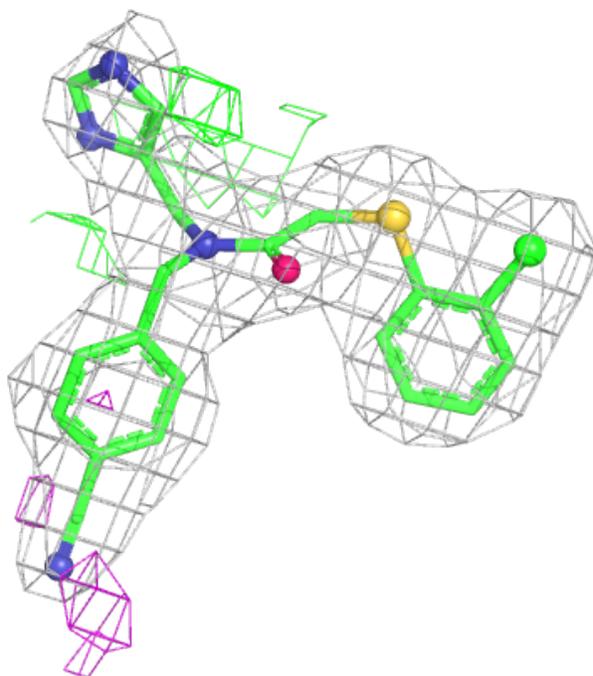
Electron density around VFT D 301 (A):

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



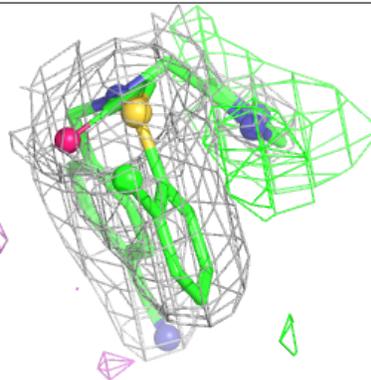
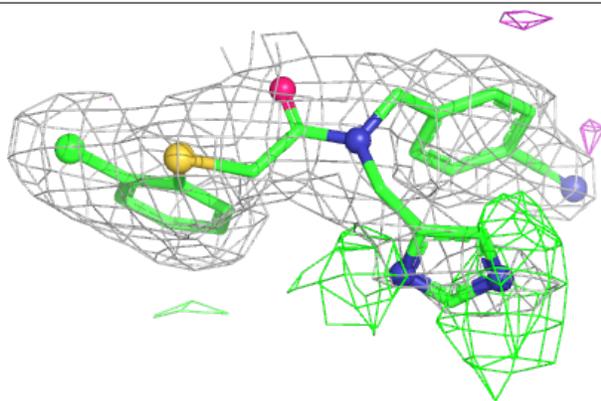
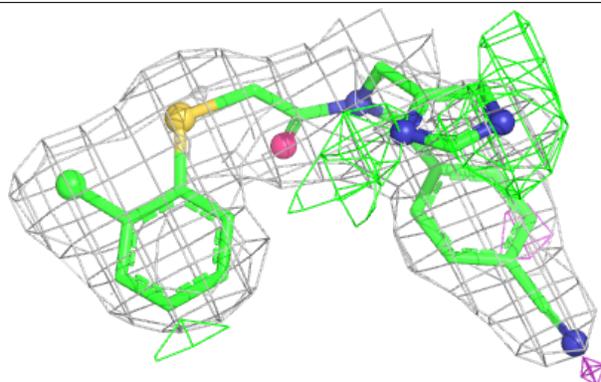
Electron density around VFT D 301 (B):

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



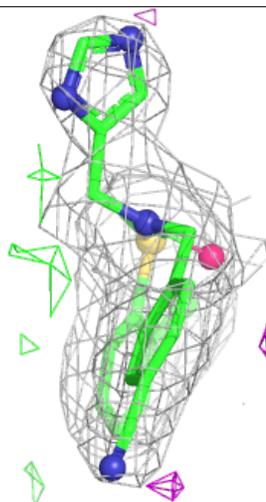
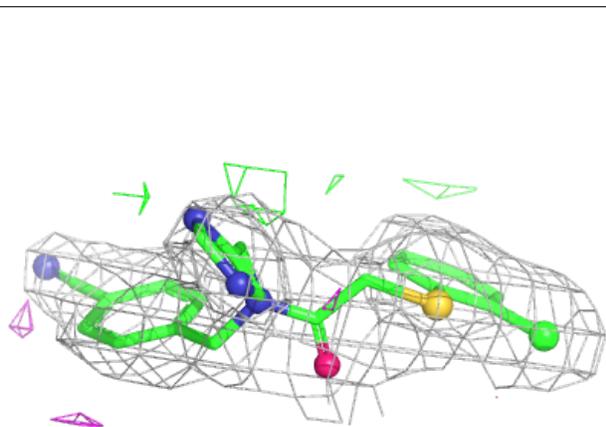
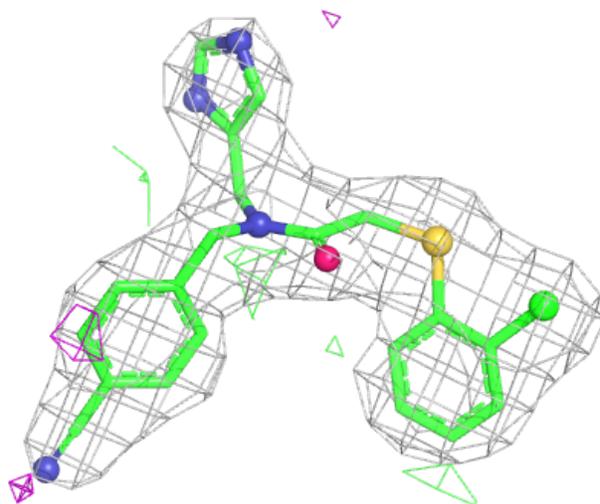
Electron density around VFT a 301 (A):

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



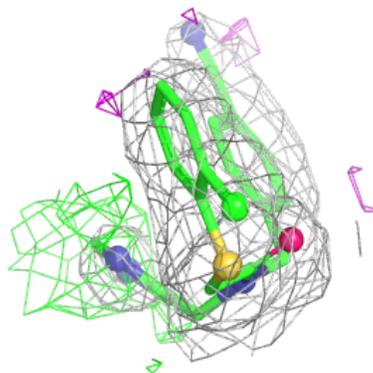
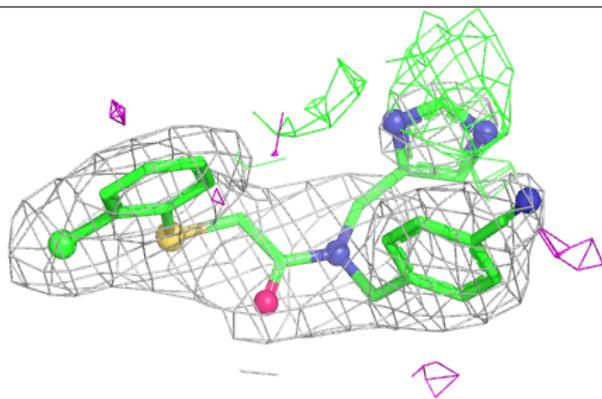
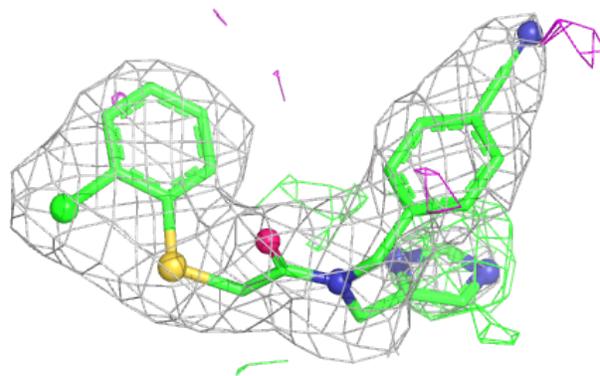
Electron density around VFT a 301 (B):

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



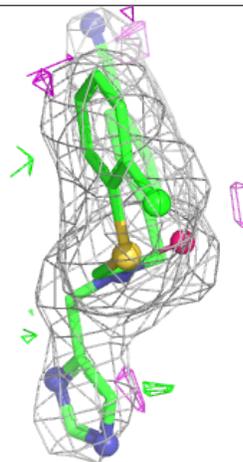
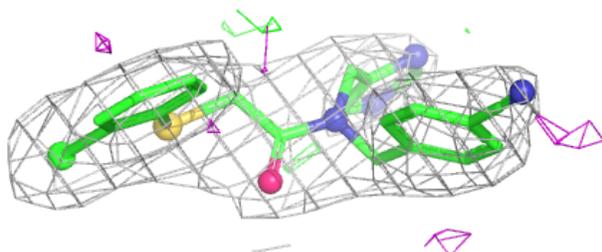
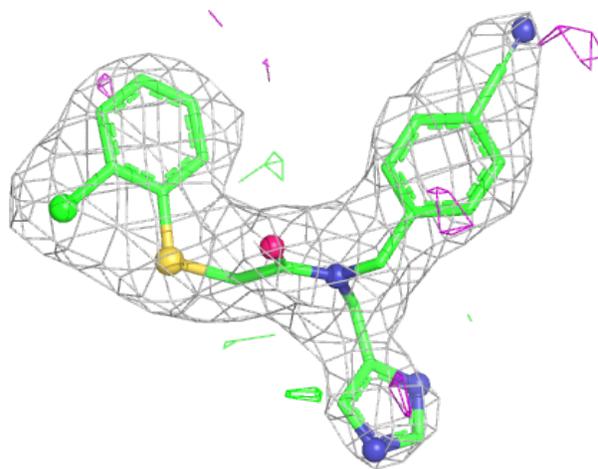
Electron density around VFT b 301 (A):

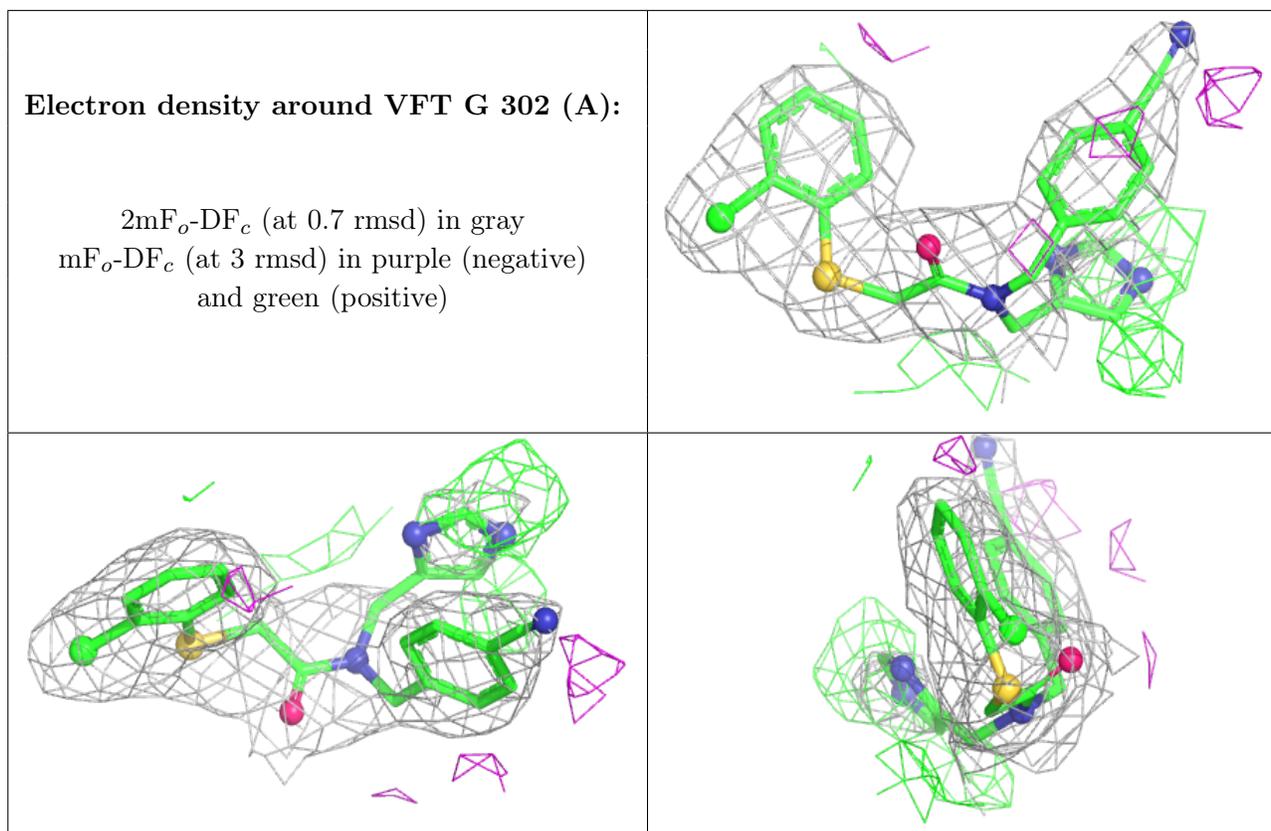
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VFT b 301 (B):

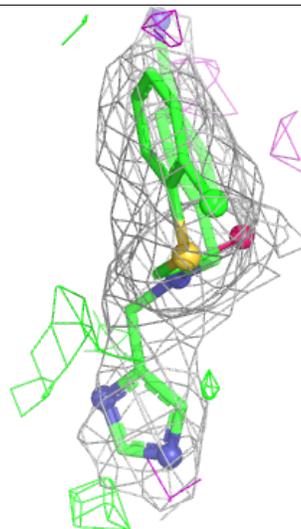
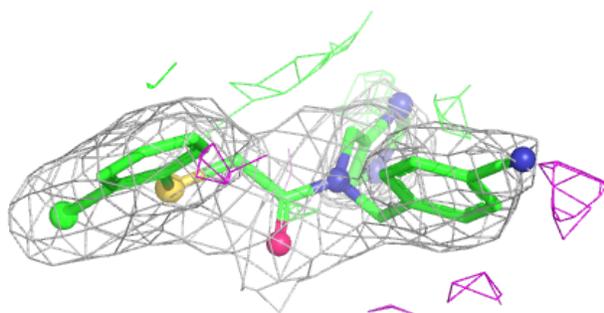
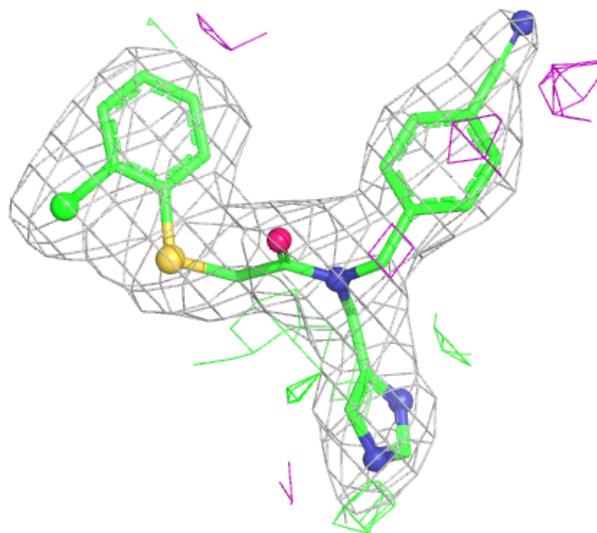
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





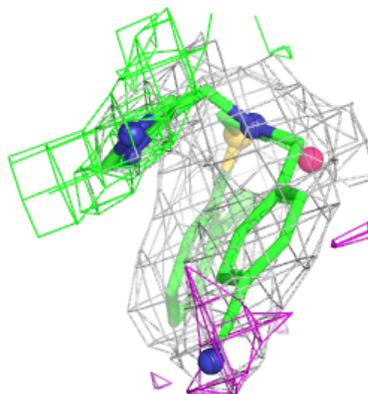
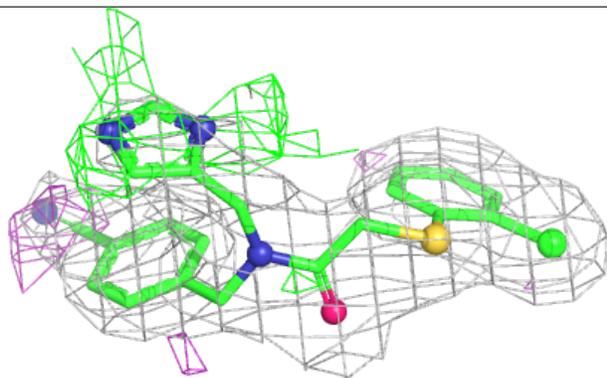
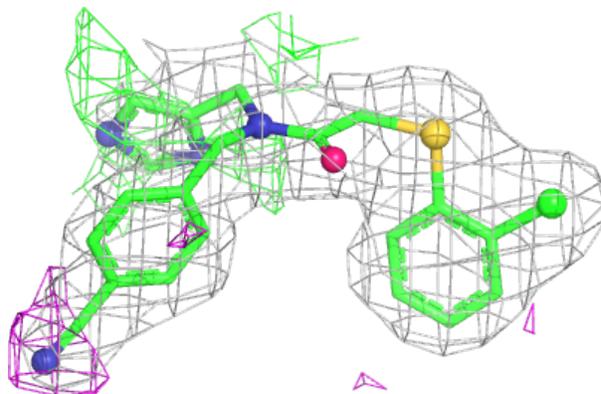
Electron density around VFT G 302 (B):

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



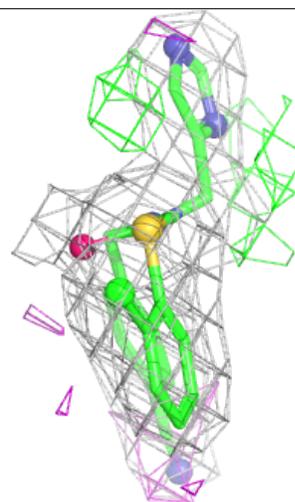
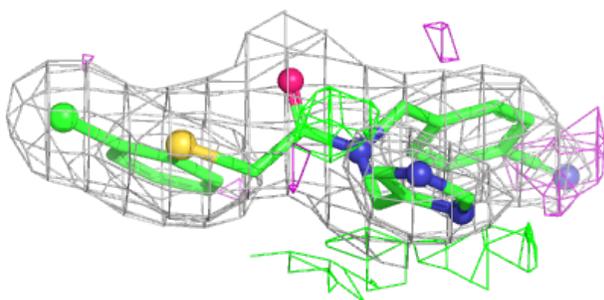
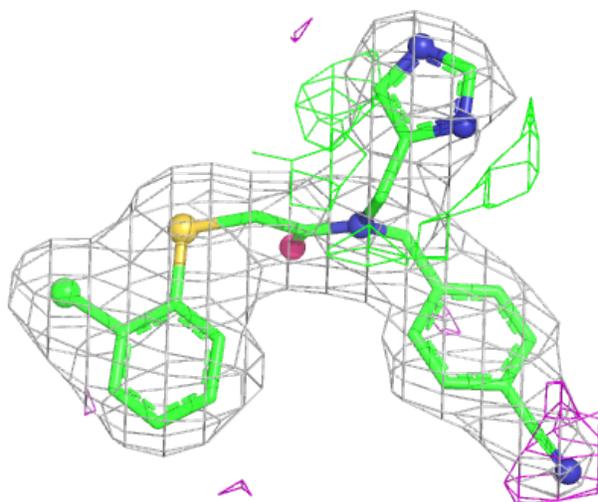
Electron density around VFT J 301 (A):

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



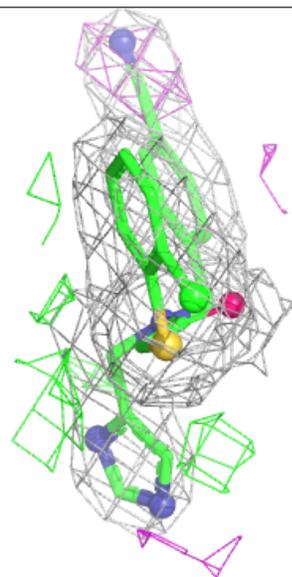
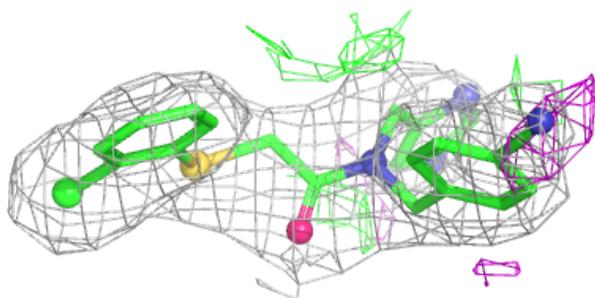
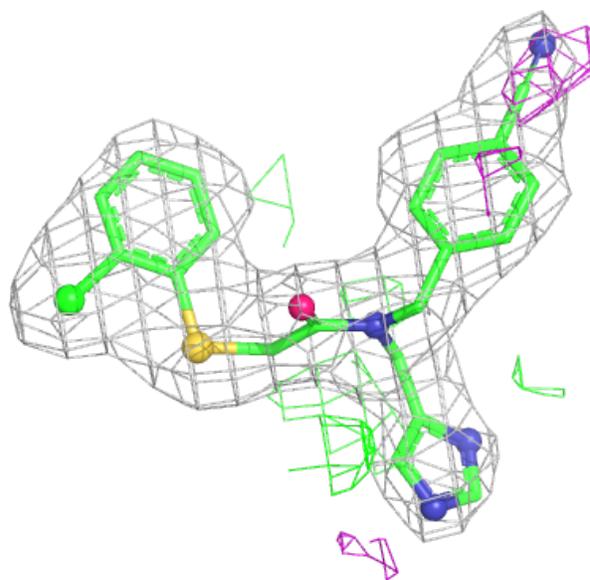
Electron density around VFT J 301 (B):

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



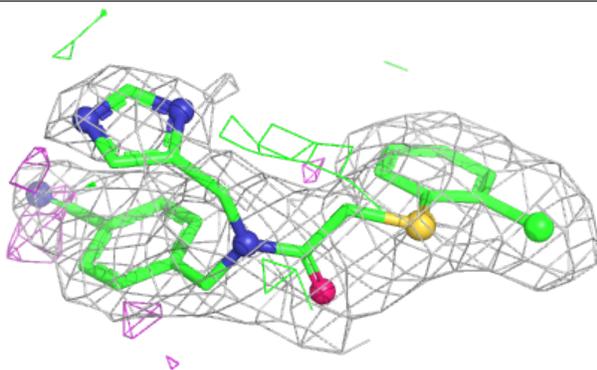
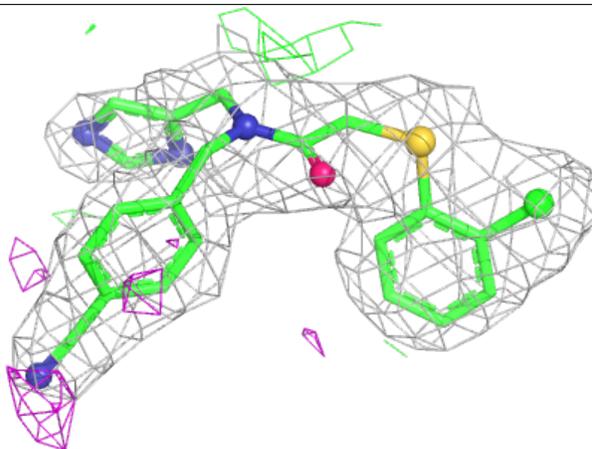
Electron density around VFT S 301 (B):

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



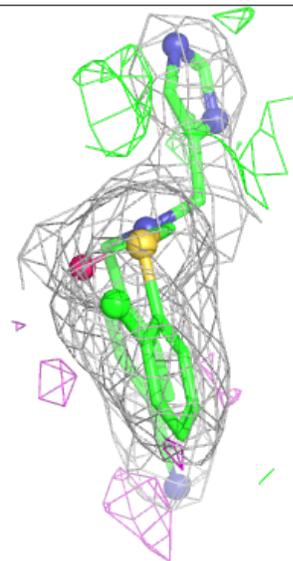
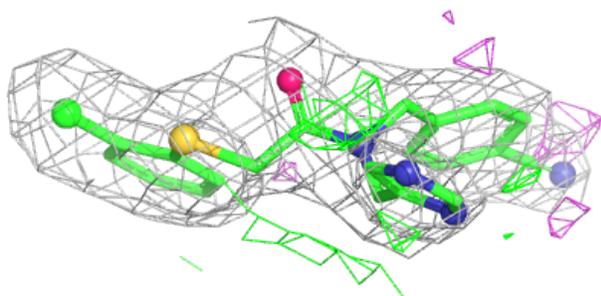
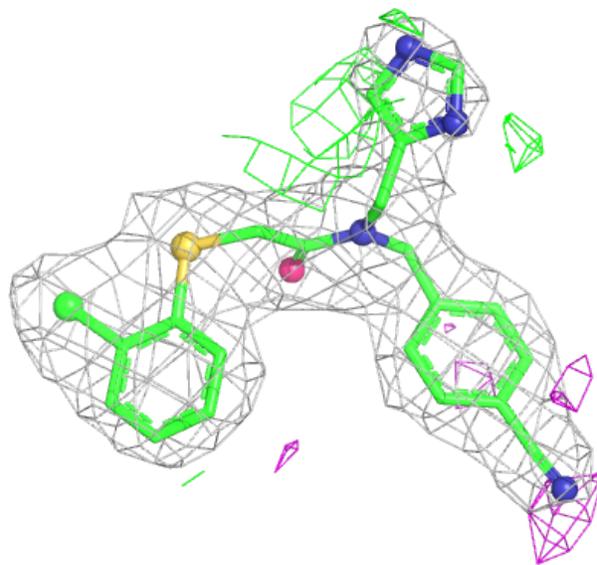
Electron density around VFT T 301 (A):

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



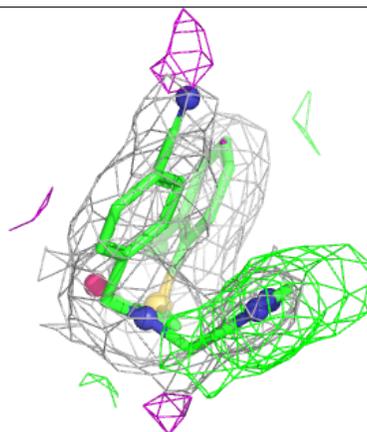
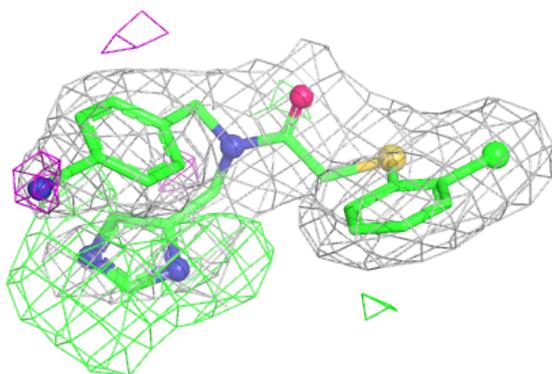
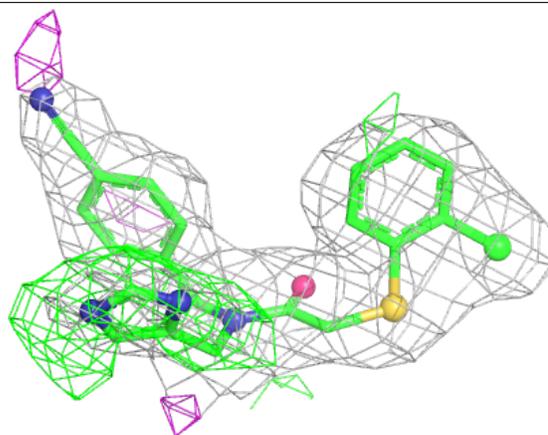
Electron density around VFT T 301 (B):

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



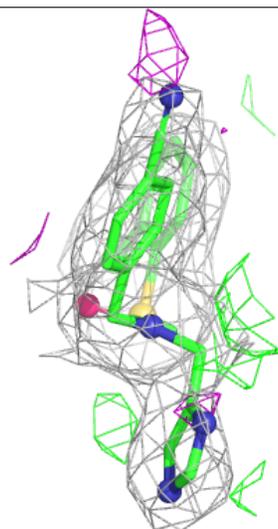
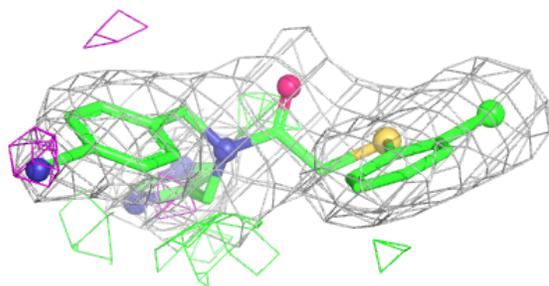
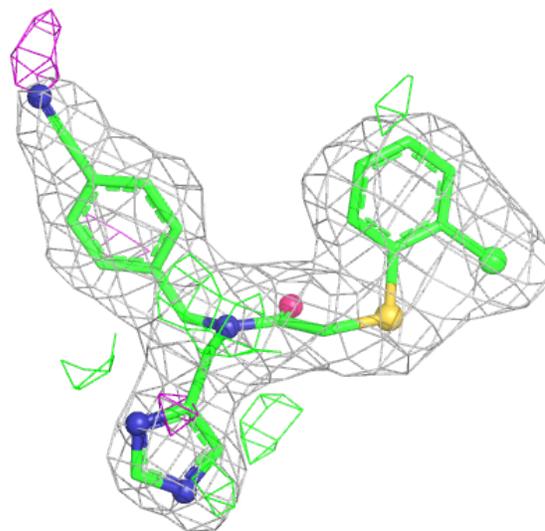
Electron density around VFT E 301 (A):

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



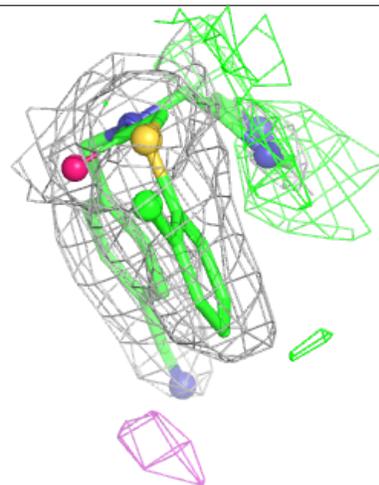
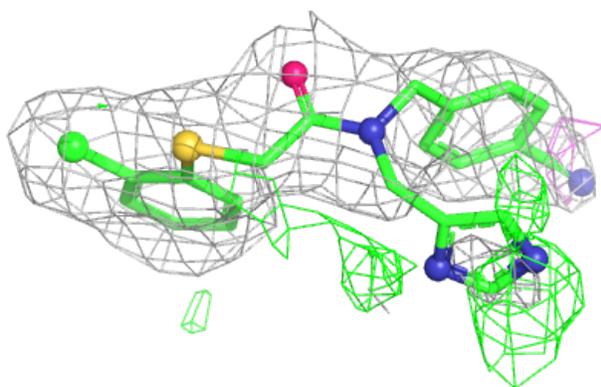
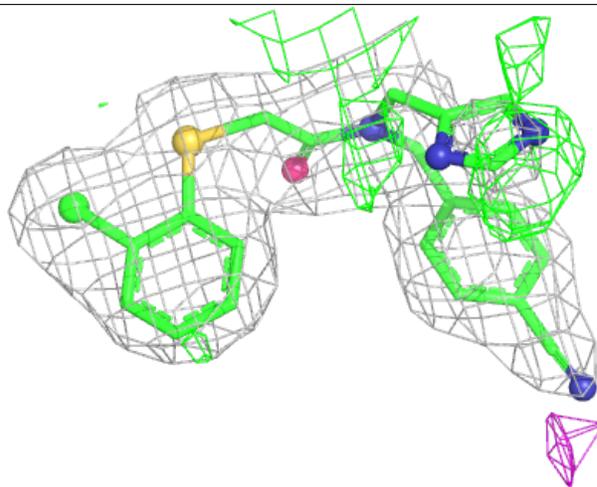
Electron density around VFT E 301 (B):

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



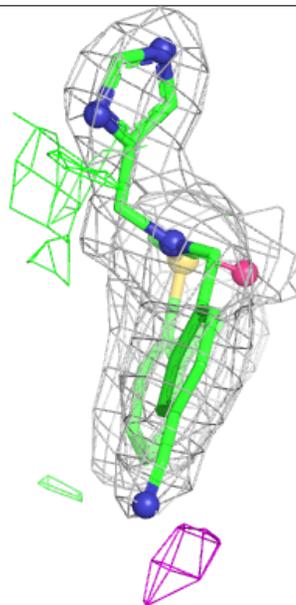
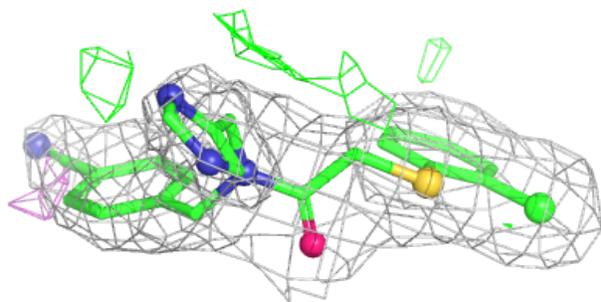
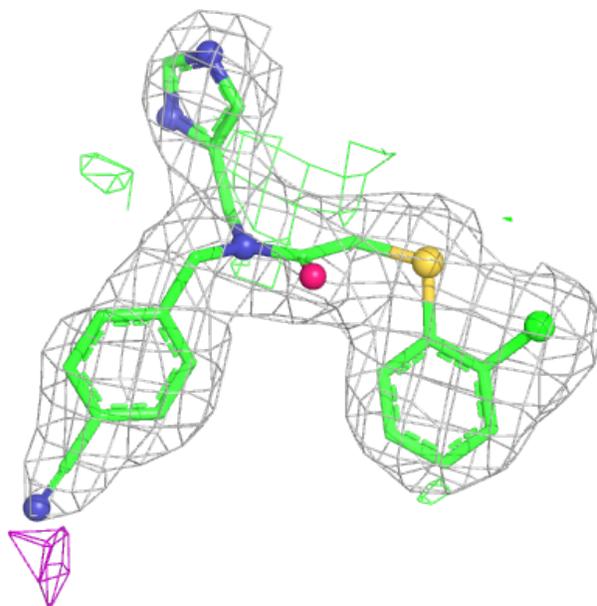
Electron density around VFT Q 301 (A):

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



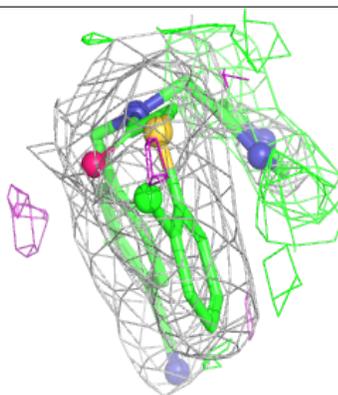
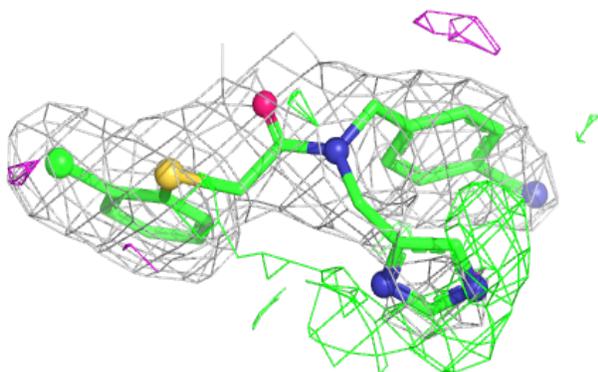
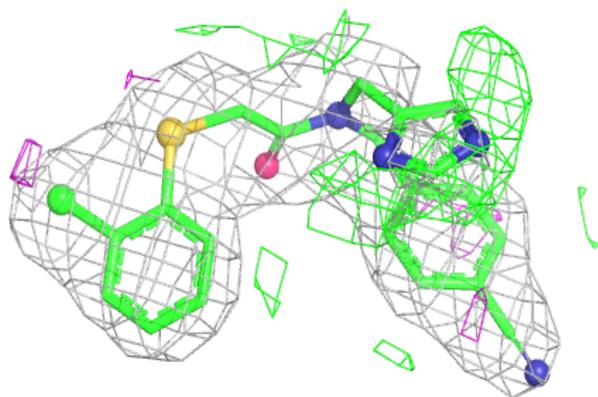
Electron density around VFT Q 301 (B):

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



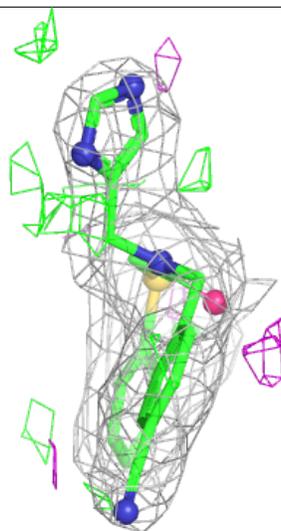
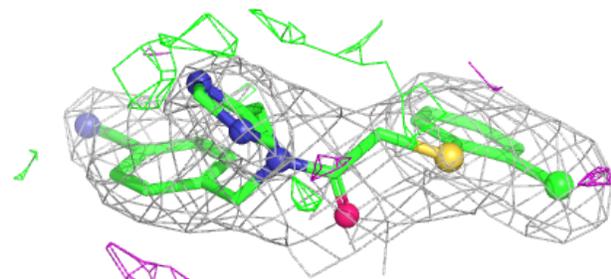
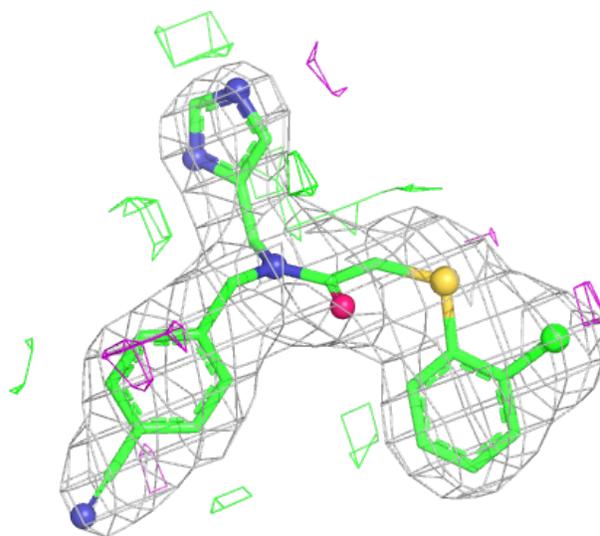
Electron density around VFT X 301 (A):

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



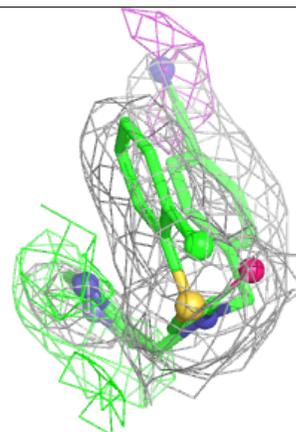
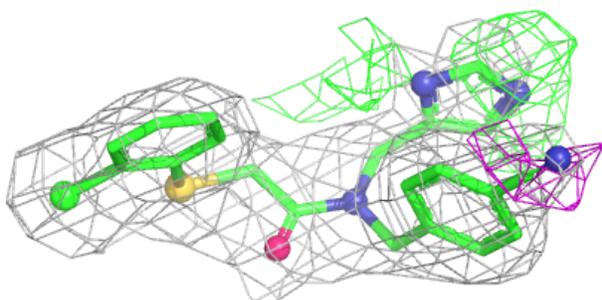
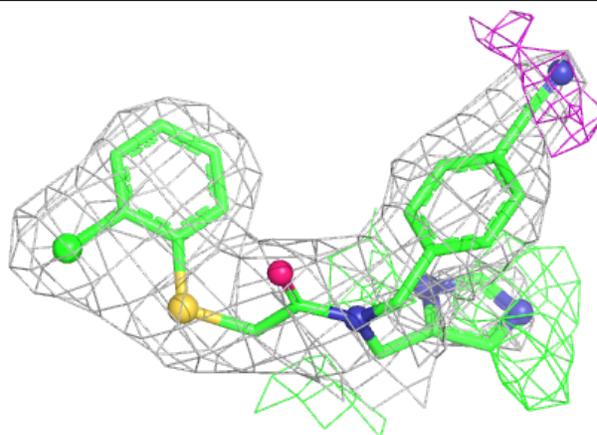
Electron density around VFT X 301 (B):

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



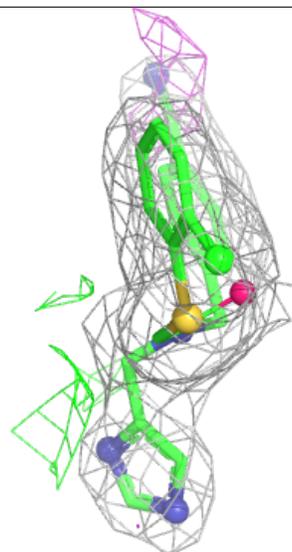
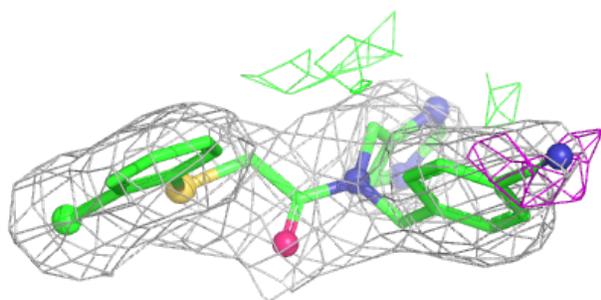
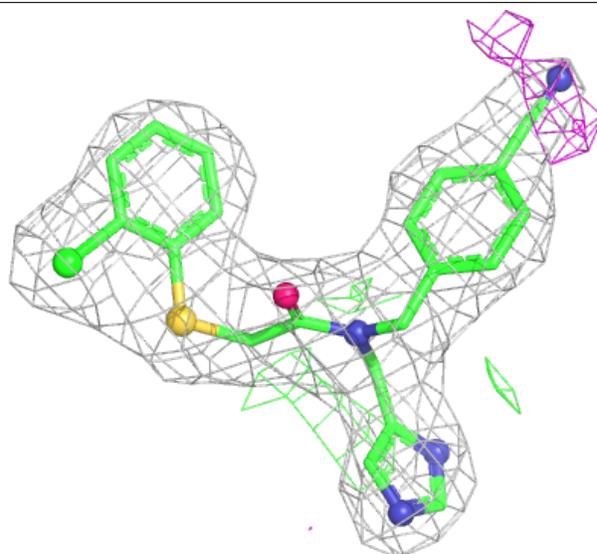
Electron density around VFT G 301 (A):

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



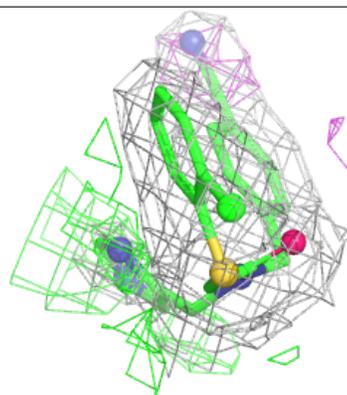
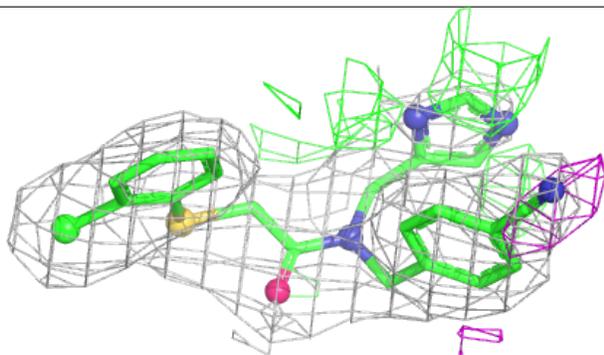
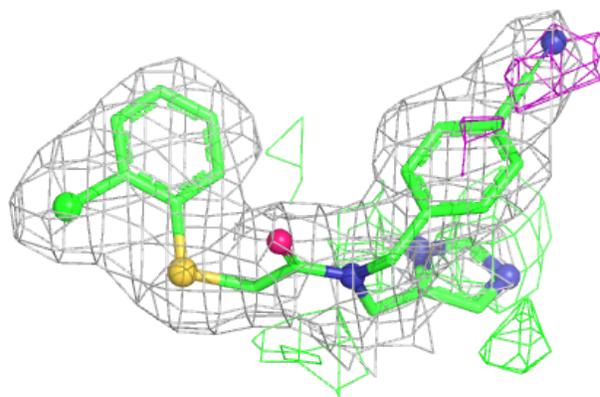
Electron density around VFT G 301 (B):

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



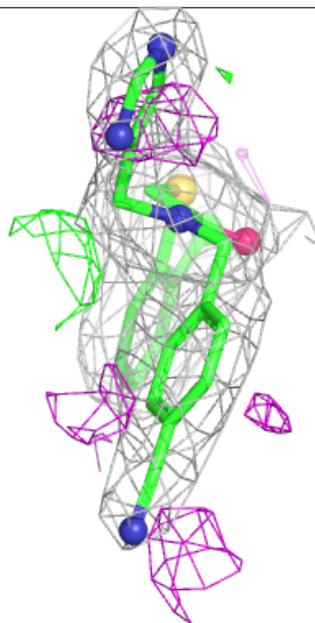
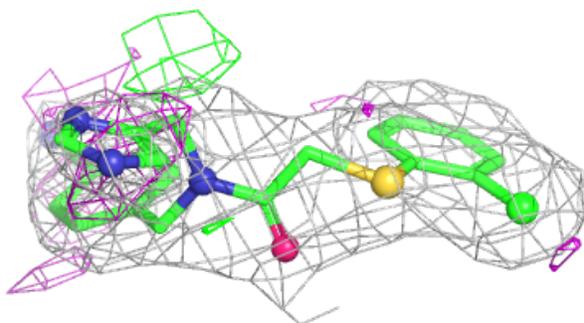
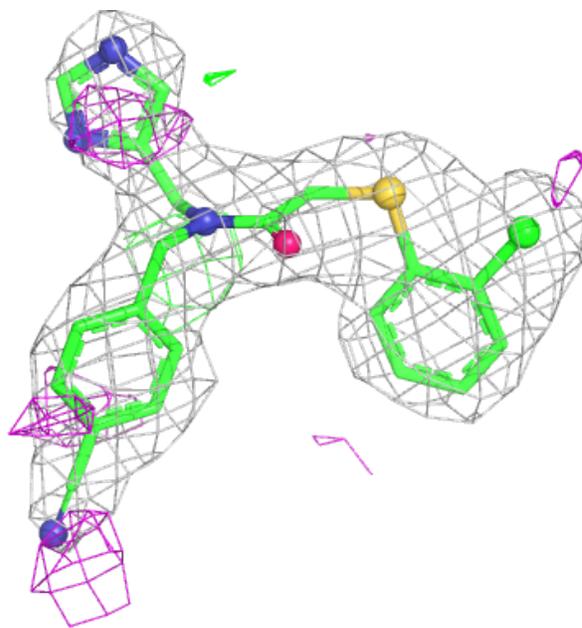
Electron density around VFT S 301 (A):

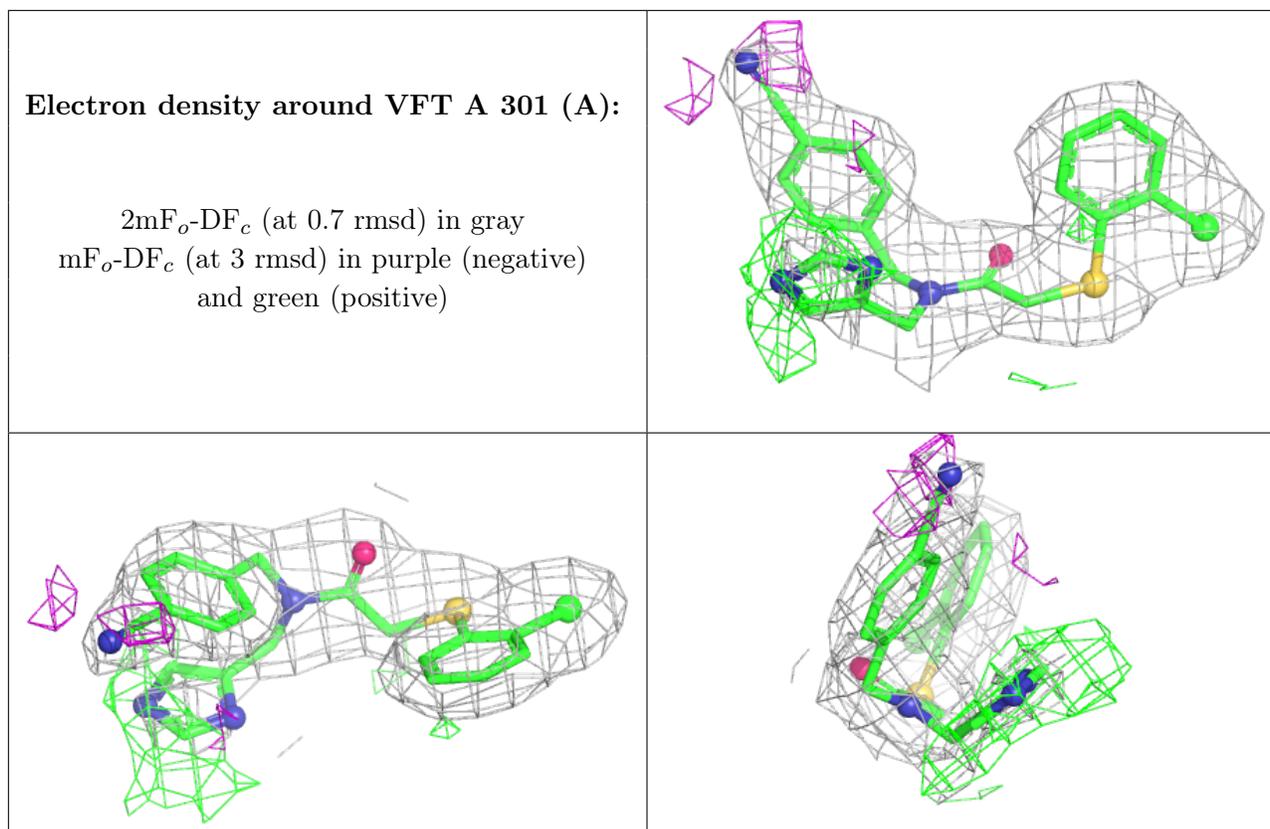
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VFT a 302:

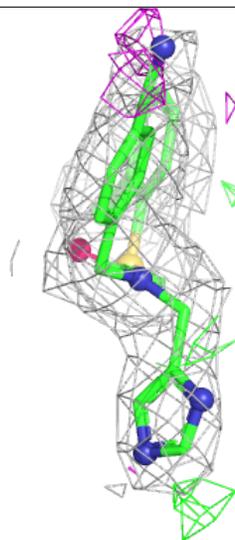
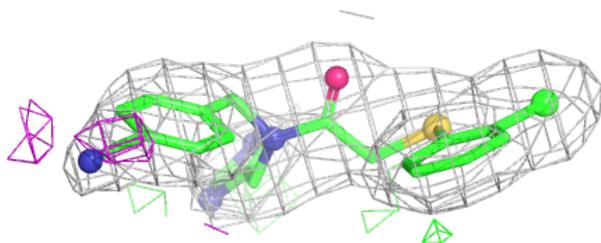
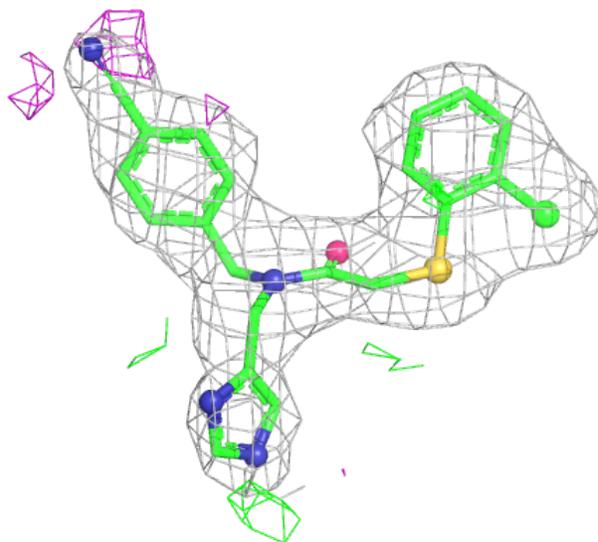
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





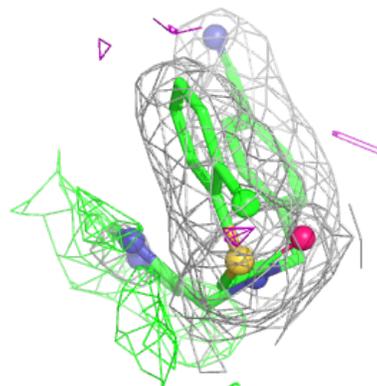
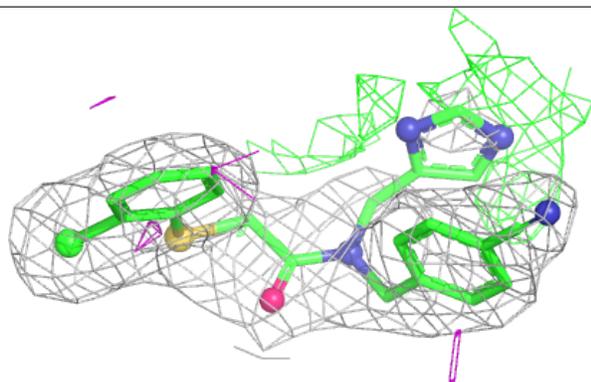
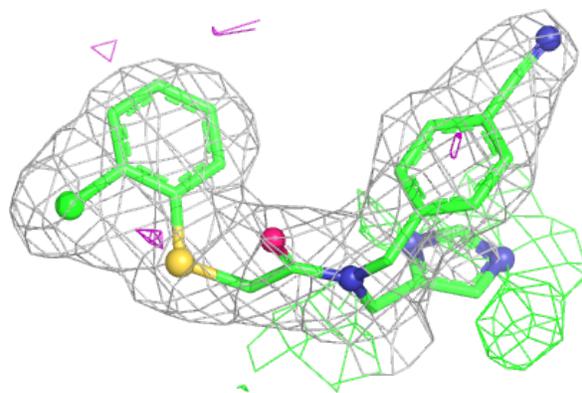
Electron density around VFT A 301 (B):

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



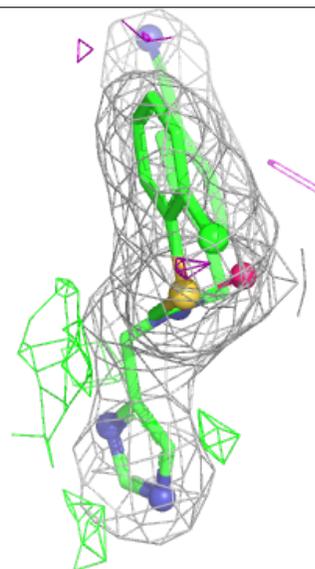
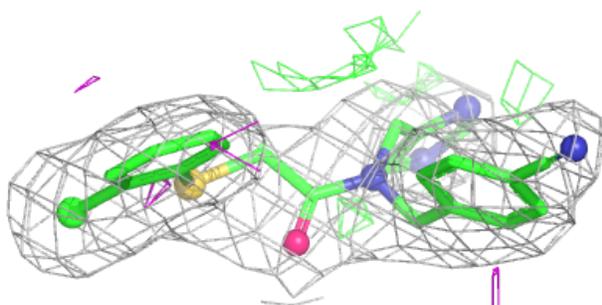
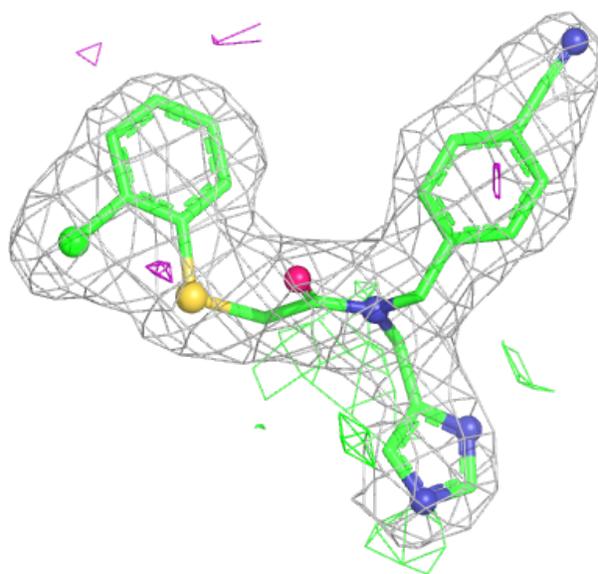
Electron density around VFT K 301 (A):

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



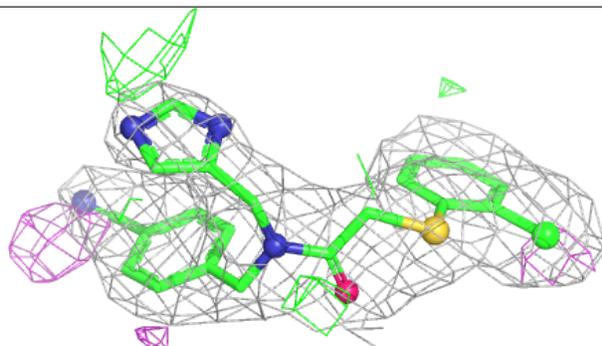
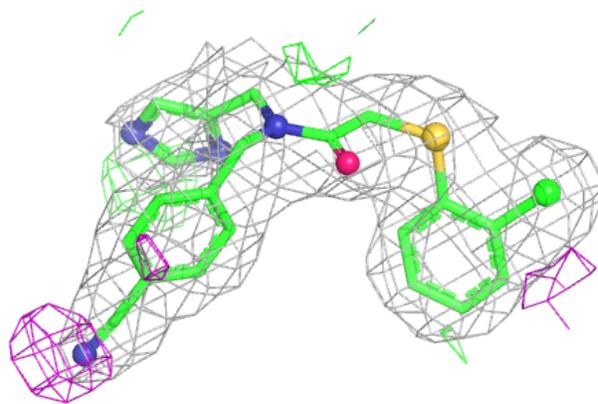
Electron density around VFT K 301 (B):

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



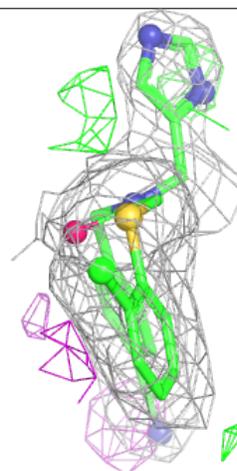
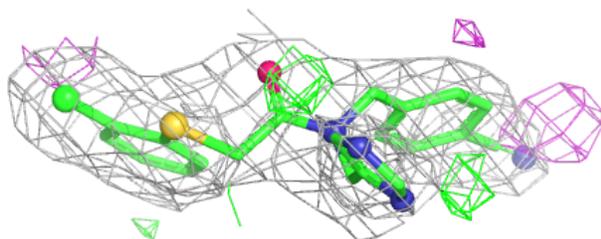
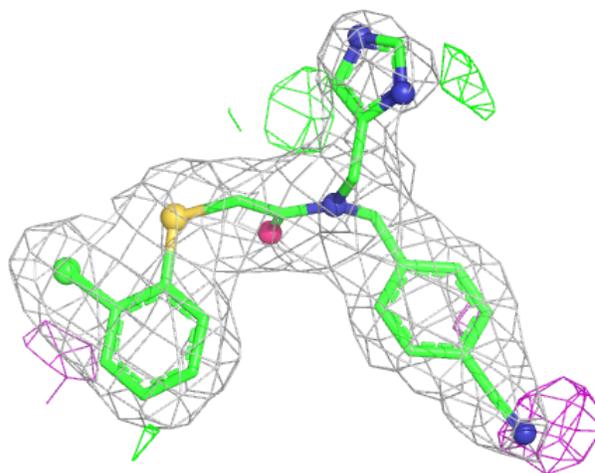
Electron density around VFT B 302 (A):

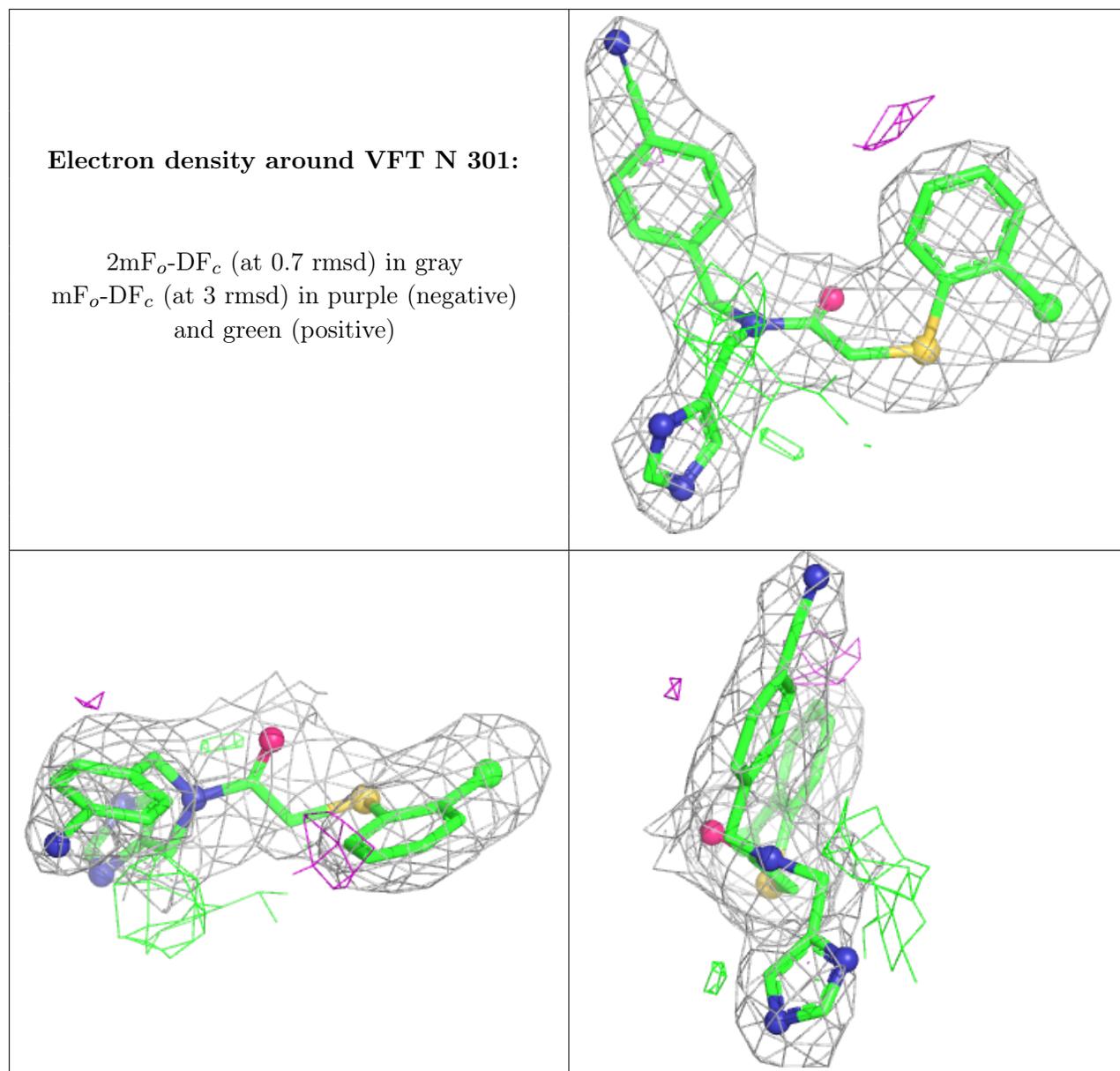
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VFT B 302 (B):

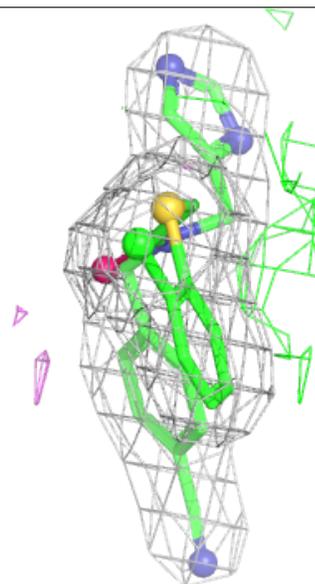
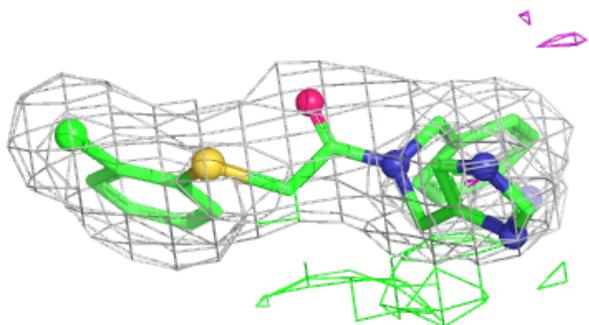
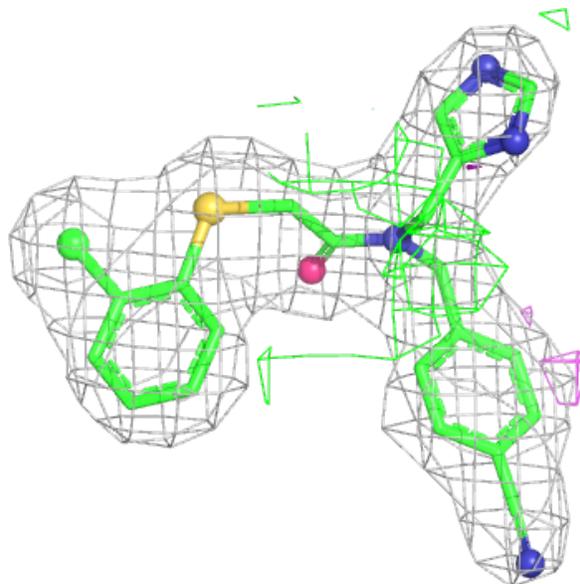
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





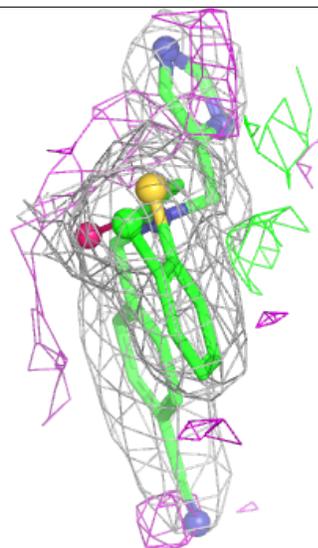
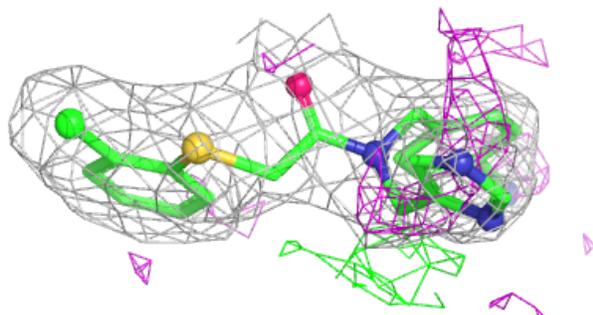
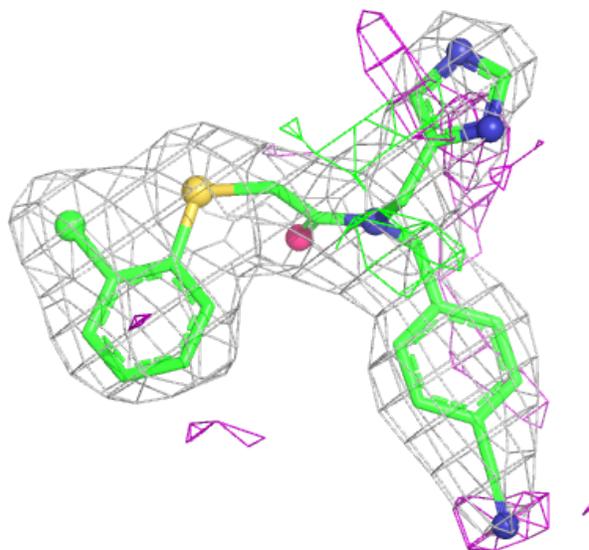
Electron density around VFT Q 302:

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



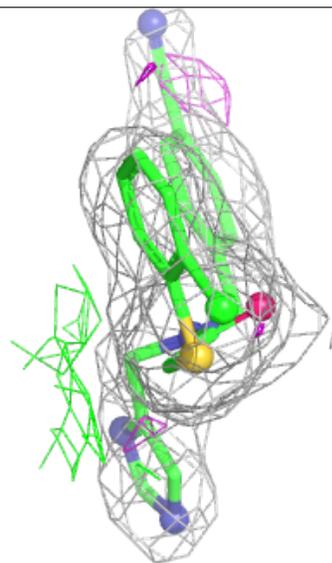
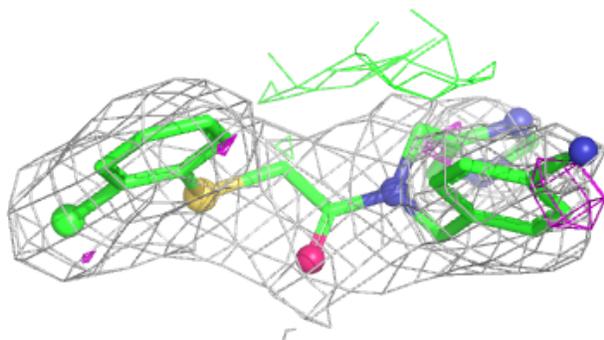
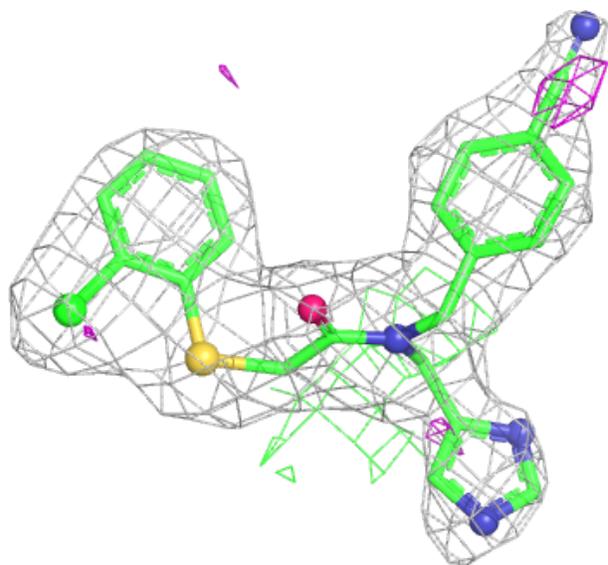
Electron density around VFT O 301:

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



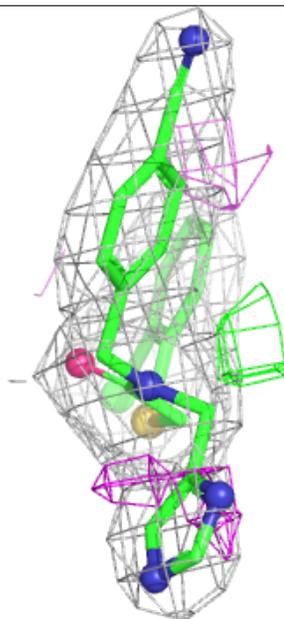
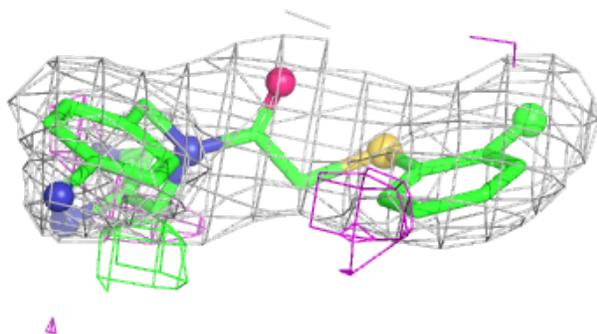
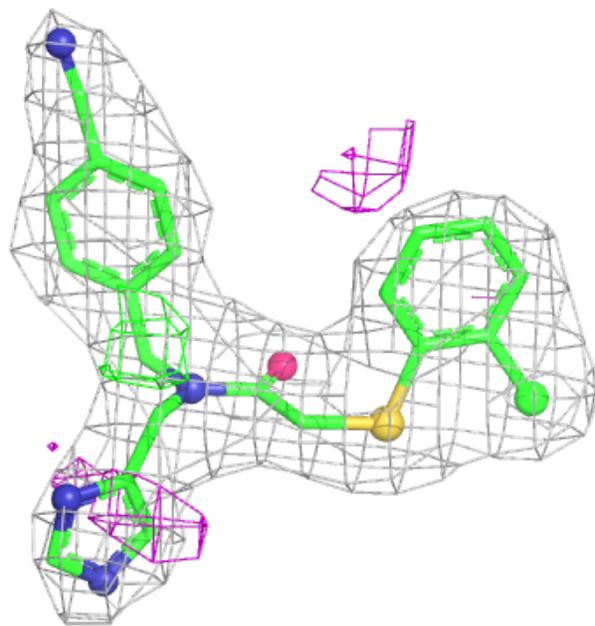
Electron density around VFT M 301:

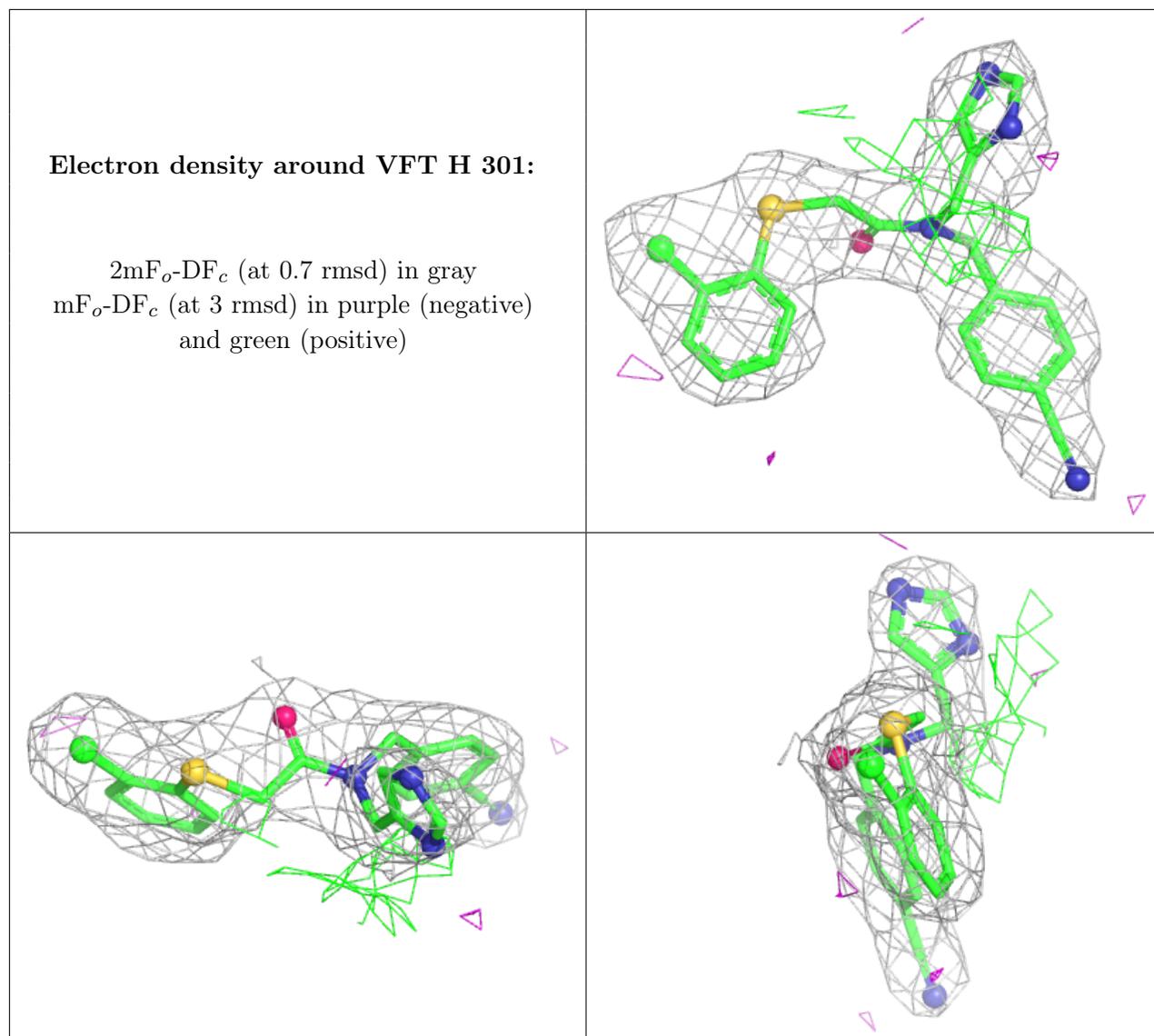
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VFT W 302:

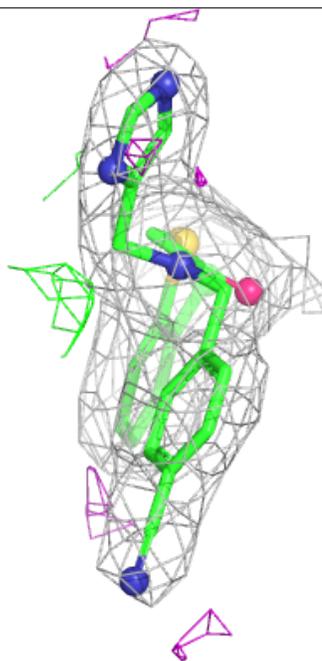
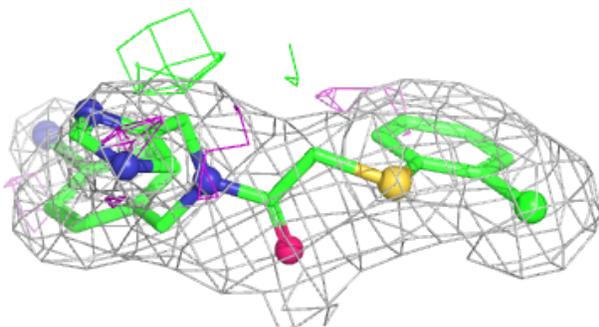
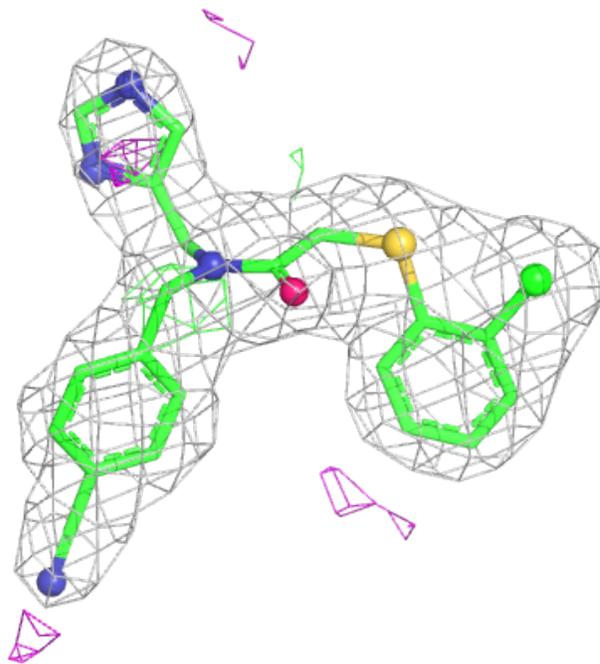
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

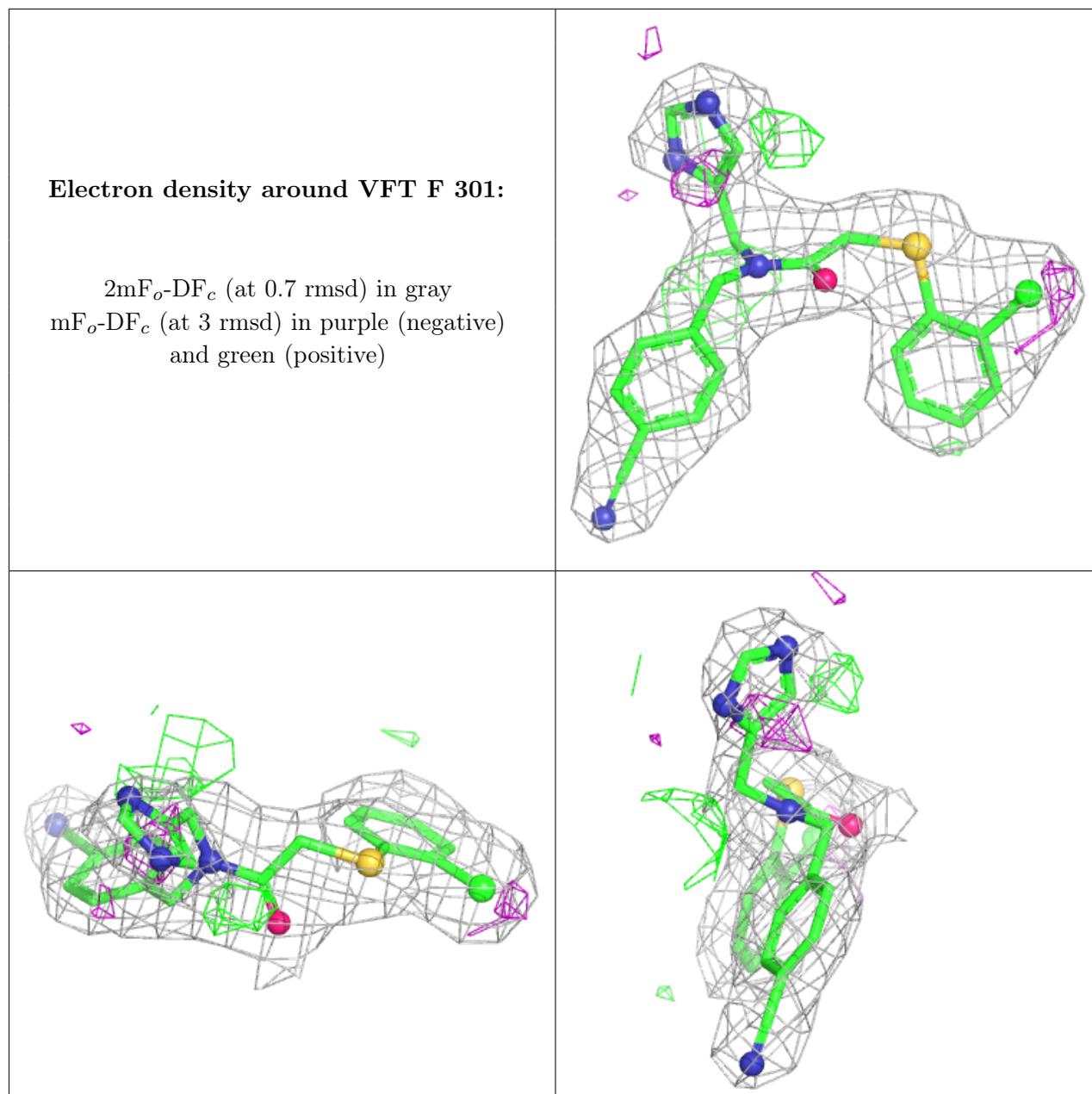




Electron density around VFT c 302:

$2mF_o-DF_c$ (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.