



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:01 AM UTC

PDB ID : 7OKA / pdb_00007oka
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

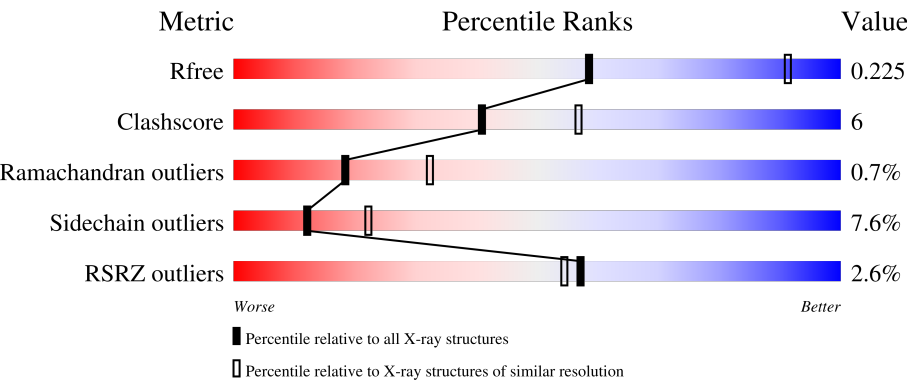
1 Overall quality at a glance i

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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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	% 76% 21% ..
1	B	261	2% 78% 19% ..
1	C	261	3% 75% 21% ..
1	D	261	% 72% 23% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	261	78% 17% ..
1	F	261	69% 24% 5% ..
1	G	261	75% 20% ...
1	H	261	75% 19% ...
1	I	261	82% 15% ..
1	J	261	72% 22% ..
1	K	261	78% 18% ..
1	L	261	75% 20% ..
1	M	261	70% 26% ..
1	N	261	72% 24% ..
1	O	261	76% 20% ...
1	P	261	77% 17% ..
1	Q	261	77% 17% ...
1	R	261	75% 20% ...
1	S	261	75% 19% ..
1	T	261	78% 16% ..
1	U	261	77% 17% ..
1	V	261	73% 21% ...
1	W	261	78% 18% ..
1	X	261	74% 20% ...
1	Y	261	77% 17% ..
1	Z	261	78% 16% ..
1	a	261	73% 22% ..
1	b	261	75% 19% ...
1	c	261	74% 23% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	d	261	3% 72% 23% ...

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

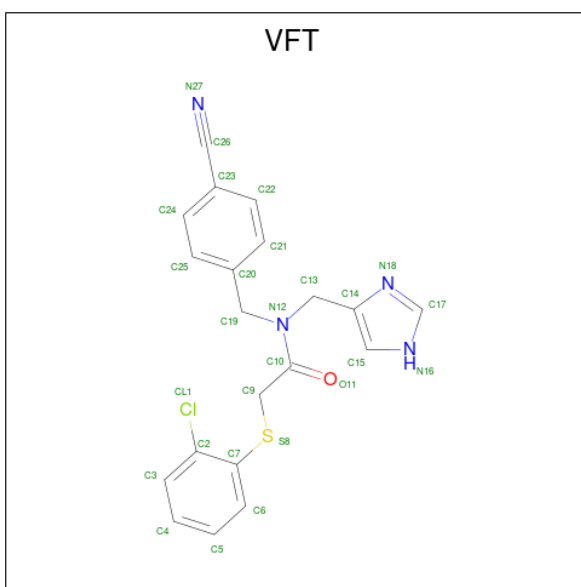
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A6V1E4
E	-2	GLY	-	expression tag	UNP A6V1E4
E	-1	SER	-	expression tag	UNP A6V1E4
E	0	HIS	-	expression tag	UNP A6V1E4
F	-2	GLY	-	expression tag	UNP A6V1E4
F	-1	SER	-	expression tag	UNP A6V1E4
F	0	HIS	-	expression tag	UNP A6V1E4
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

Continued on next page...

Continued from previous page...

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 (CCD ID: VFT) (formula: C₂₀H₁₇ClN₄OS) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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 (CCD ID: CL) (formula: Cl).

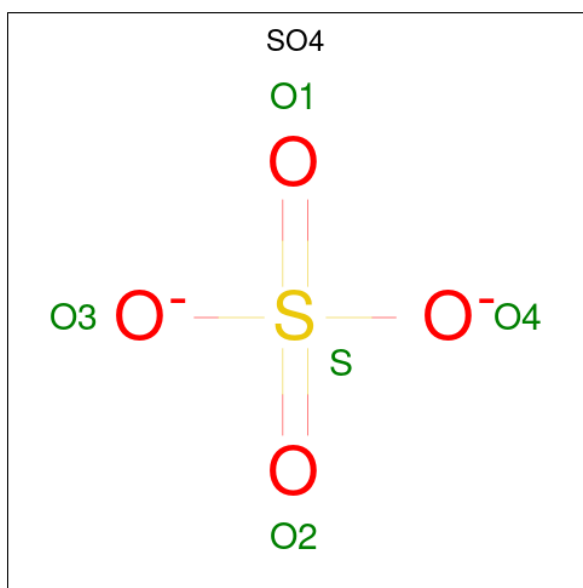
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	2	Total 2	Cl 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

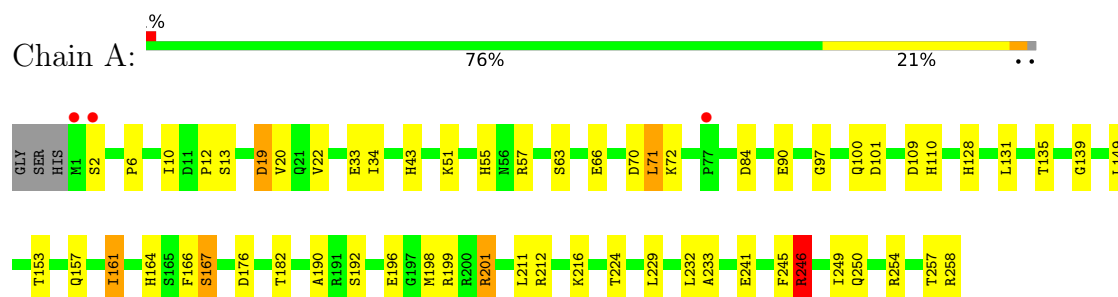
Continued from previous page...

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

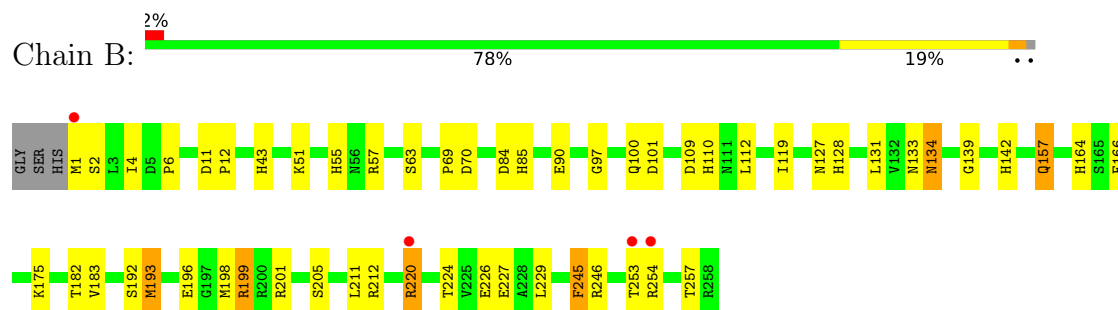
3 Residue-property plots [i](#)

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.

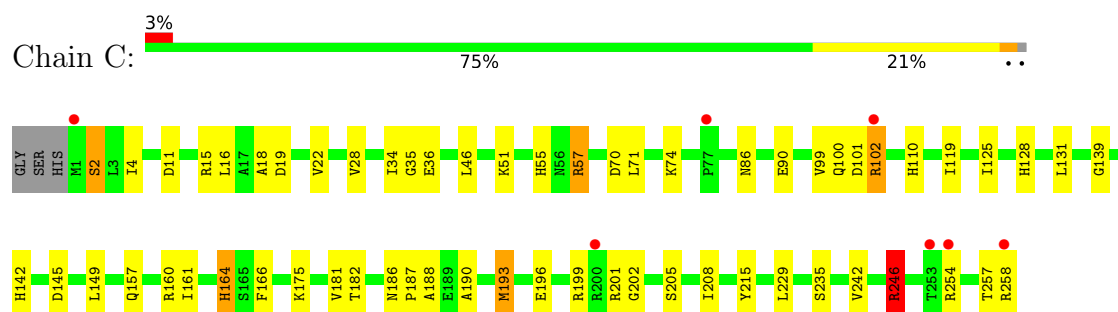
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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

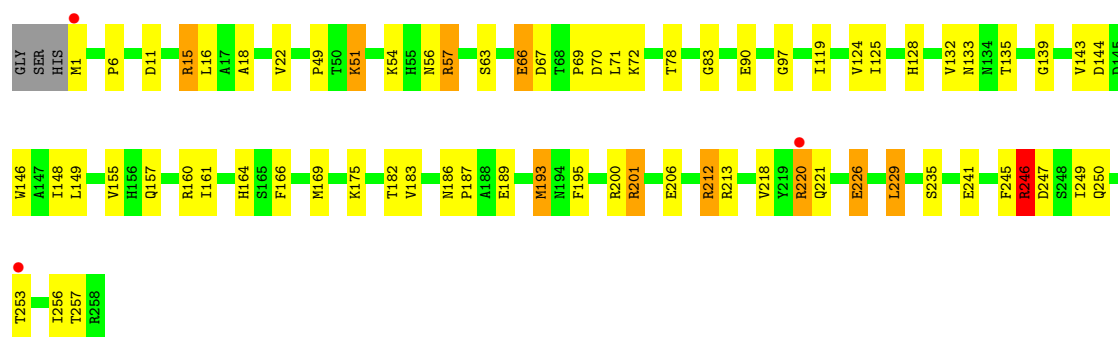


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

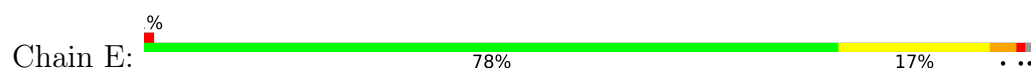


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase





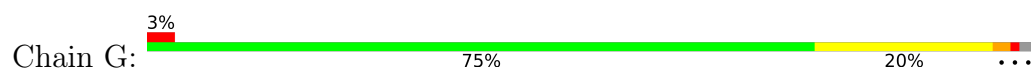
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



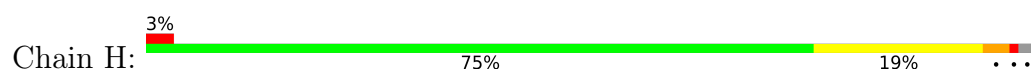
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

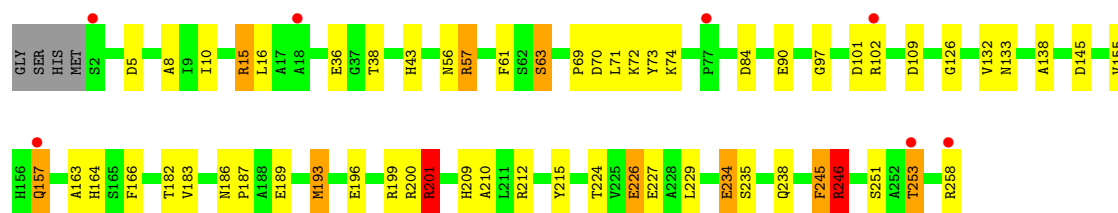


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

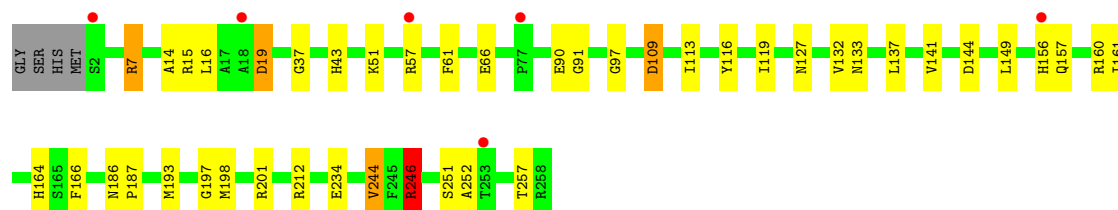
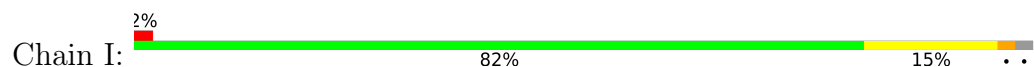


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

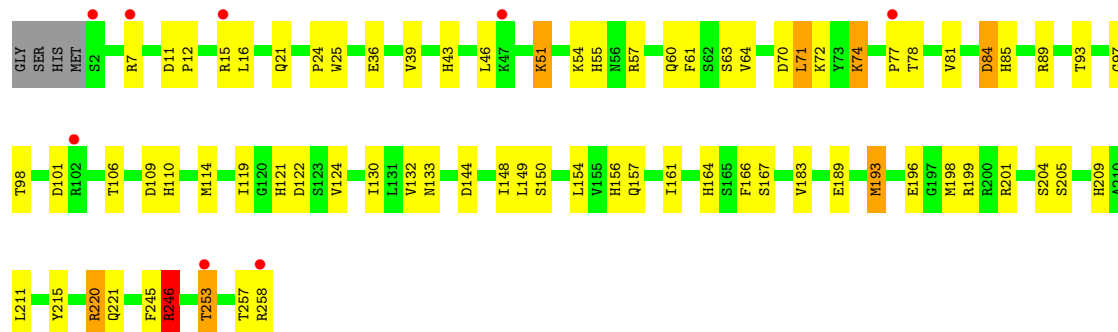




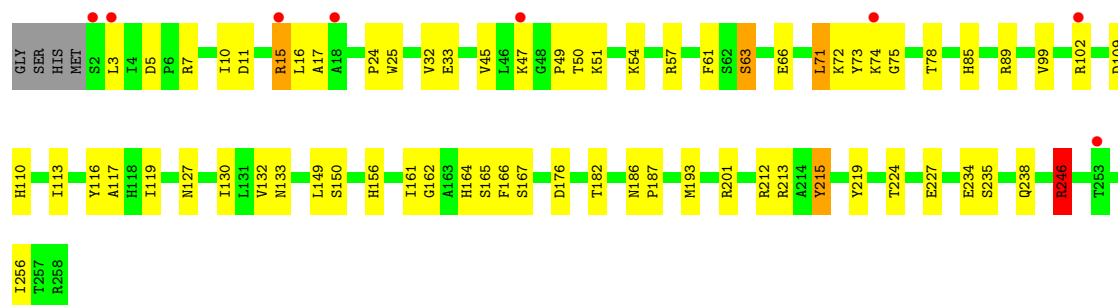
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



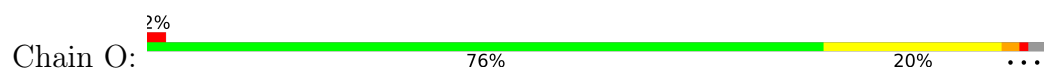
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

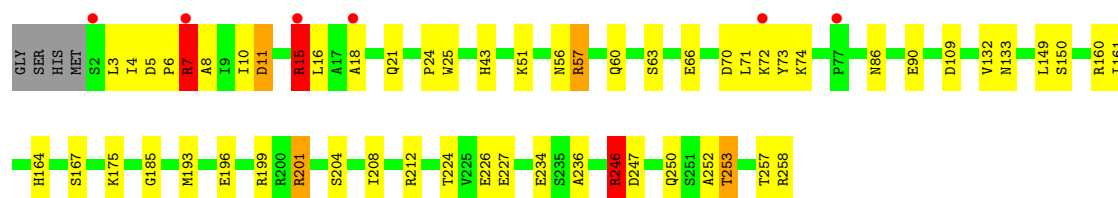


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

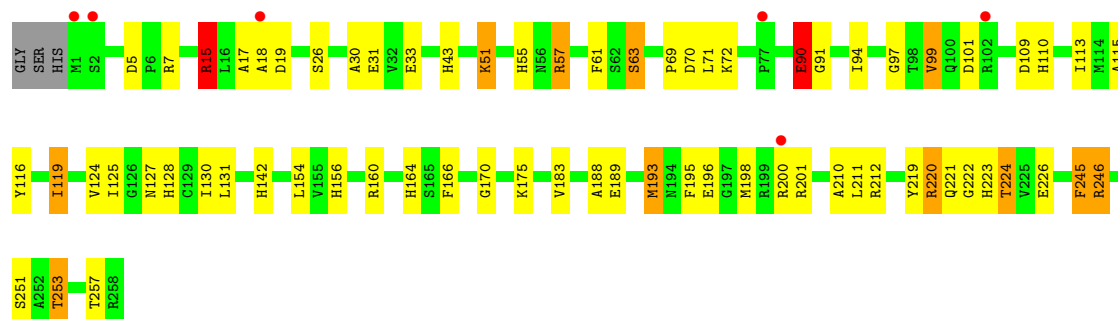


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

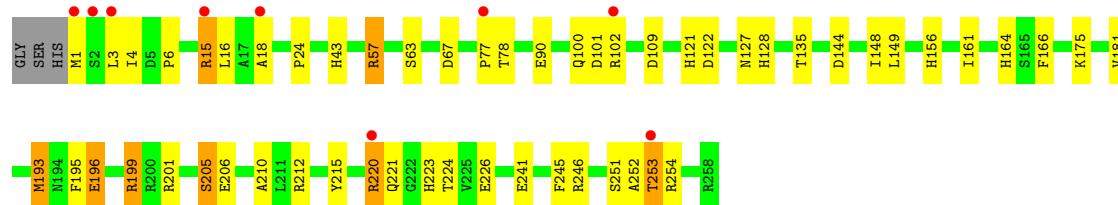
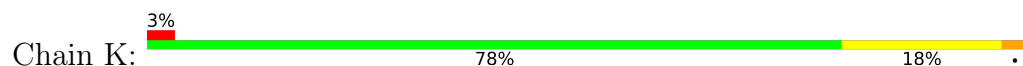




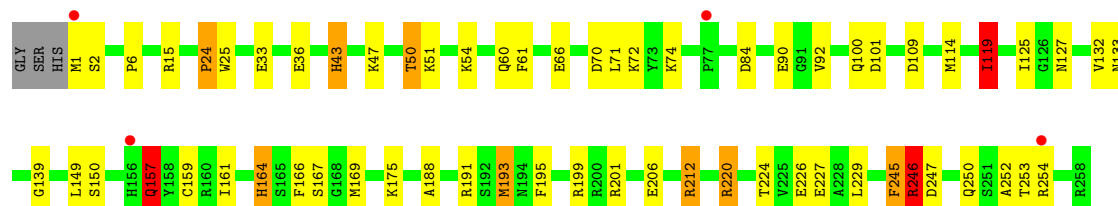
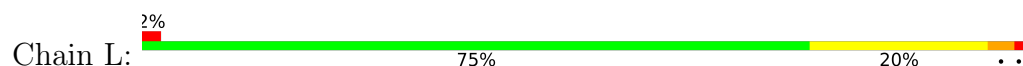
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



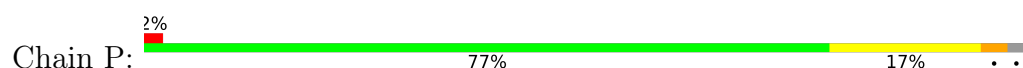
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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

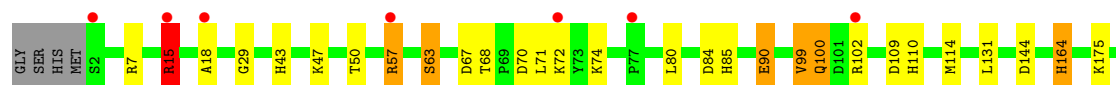
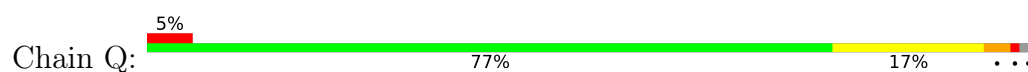


• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

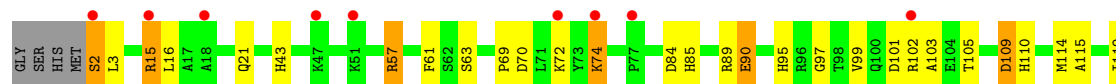
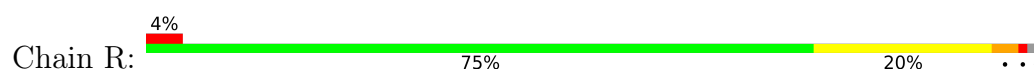




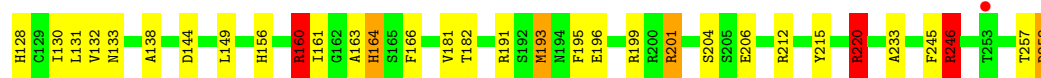
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



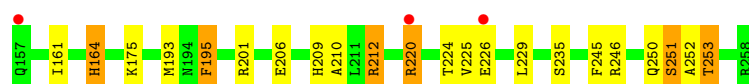
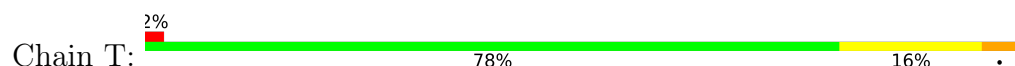
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



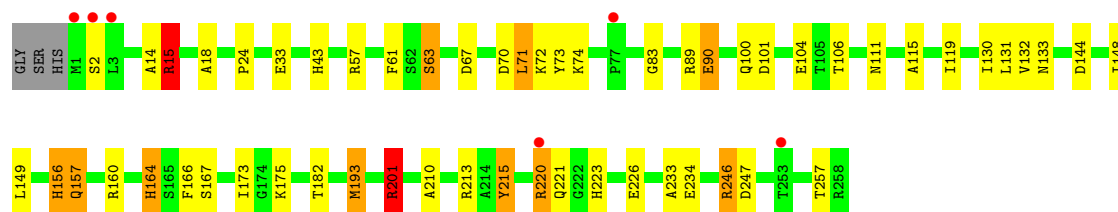
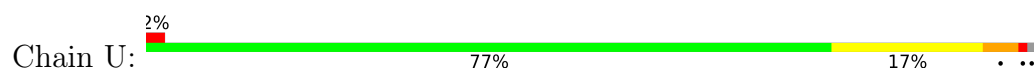
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



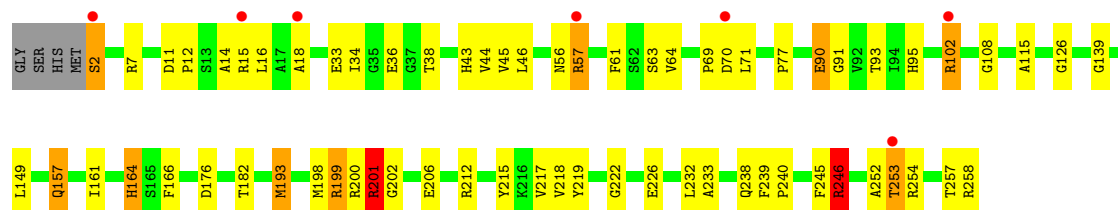
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



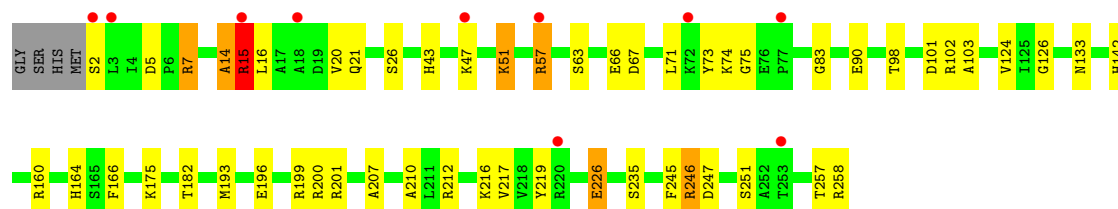
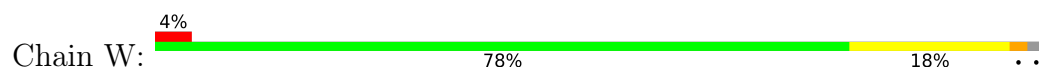
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



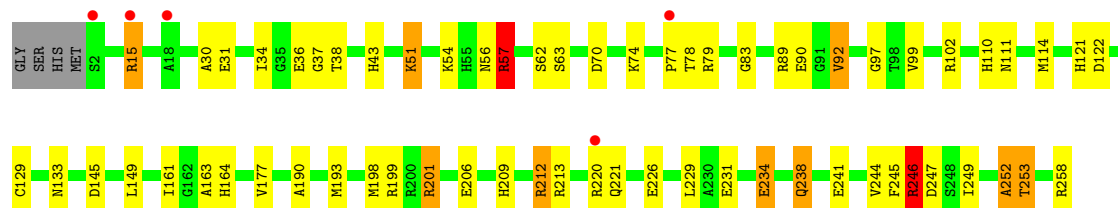
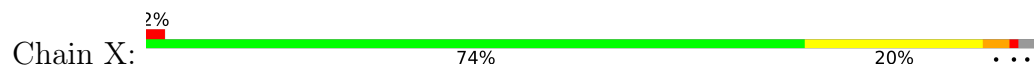
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



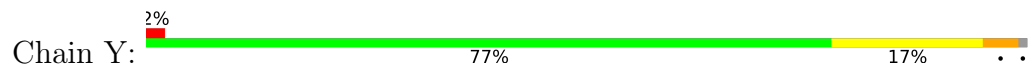
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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

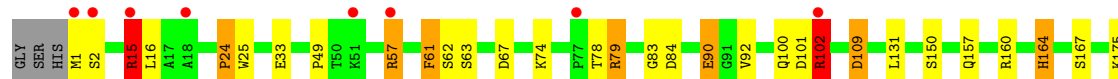
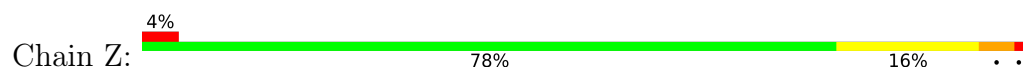


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

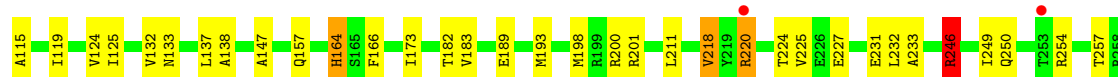
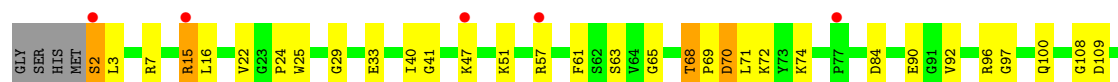




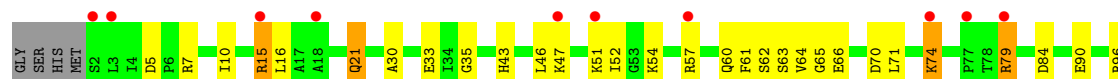
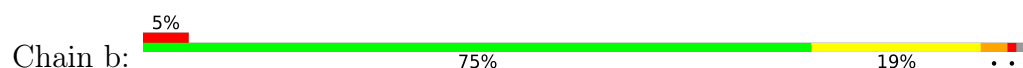
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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



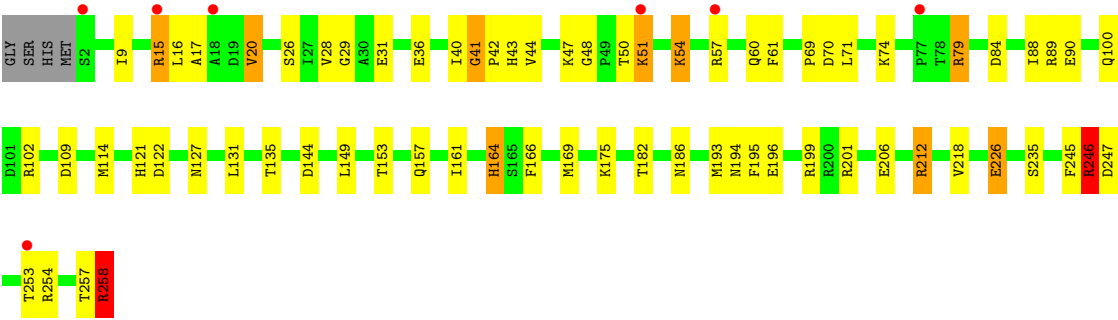
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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



● 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 – 2.74 113.45 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (113.45-2.74) 99.8 (113.45-2.74)	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 (5.01%)	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)	0.34 , 33.5	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	0.95	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.33	11/2045 (0.5%)	1.60	23/2772 (0.8%)
1	B	1.34	15/2056 (0.7%)	1.56	12/2786 (0.4%)
1	C	1.37	15/2047 (0.7%)	1.61	16/2774 (0.6%)
1	D	1.36	16/2025 (0.8%)	1.65	30/2746 (1.1%)
1	E	1.31	8/2016 (0.4%)	1.63	21/2734 (0.8%)
1	F	1.32	8/2036 (0.4%)	1.63	22/2760 (0.8%)
1	G	1.25	5/2008 (0.2%)	1.64	21/2724 (0.8%)
1	H	1.28	4/2008 (0.2%)	1.63	25/2724 (0.9%)
1	I	1.26	4/2008 (0.2%)	1.58	14/2724 (0.5%)
1	J	1.39	17/2027 (0.8%)	1.68	26/2748 (0.9%)
1	K	1.31	10/2016 (0.5%)	1.62	19/2734 (0.7%)
1	L	1.33	11/2016 (0.5%)	1.59	15/2734 (0.5%)
1	M	1.27	3/2008 (0.1%)	1.61	17/2724 (0.6%)
1	N	1.26	5/2008 (0.2%)	1.60	11/2724 (0.4%)
1	O	1.22	3/2008 (0.1%)	1.64	23/2724 (0.8%)
1	P	1.27	7/2008 (0.3%)	1.66	22/2724 (0.8%)
1	Q	1.25	7/2019 (0.3%)	1.64	24/2738 (0.9%)
1	R	1.25	7/2008 (0.3%)	1.62	24/2724 (0.9%)
1	S	1.35	15/2016 (0.7%)	1.65	26/2734 (1.0%)
1	T	1.32	14/2016 (0.7%)	1.68	28/2734 (1.0%)
1	U	1.31	10/2016 (0.5%)	1.62	25/2734 (0.9%)
1	V	1.26	9/2008 (0.4%)	1.63	21/2724 (0.8%)
1	W	1.24	5/2017 (0.2%)	1.66	19/2736 (0.7%)
1	X	1.26	5/2017 (0.2%)	1.64	26/2736 (1.0%)
1	Y	1.24	6/2025 (0.3%)	1.57	17/2746 (0.6%)
1	Z	1.30	7/2025 (0.3%)	1.64	22/2746 (0.8%)
1	a	1.26	10/2017 (0.5%)	1.58	12/2736 (0.4%)
1	b	1.26	4/2017 (0.2%)	1.64	19/2736 (0.7%)
1	c	1.25	6/2025 (0.3%)	1.58	25/2746 (0.9%)
1	d	1.24	5/2017 (0.2%)	1.58	18/2736 (0.7%)
All	All	1.29	252/60583 (0.4%)	1.62	623/82162 (0.8%)

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

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	256	ILE	C-O	-10.20	1.13	1.24
1	c	97	GLY	C-O	9.78	1.32	1.23
1	J	57	ARG	NE-CZ	9.50	1.43	1.33
1	J	164	HIS	CE1-NE2	9.36	1.42	1.32
1	H	164	HIS	CE1-NE2	9.27	1.41	1.32
1	B	110	HIS	CE1-NE2	8.63	1.41	1.32
1	J	210	ALA	C-O	8.59	1.34	1.24
1	C	57	ARG	NE-CZ	8.52	1.42	1.33
1	K	156	HIS	CE1-NE2	8.37	1.41	1.32
1	W	210	ALA	C-O	8.34	1.34	1.24
1	F	10	ILE	C-O	-8.18	1.15	1.24
1	U	220	ARG	NE-CZ	8.09	1.42	1.33
1	C	128	HIS	CE1-NE2	8.05	1.40	1.32
1	J	97	GLY	C-O	7.98	1.31	1.23
1	S	57	ARG	NE-CZ	7.97	1.41	1.33
1	D	57	ARG	NE-CZ	7.90	1.41	1.33
1	T	220	ARG	NE-CZ	7.88	1.41	1.33
1	R	220	ARG	NE-CZ	7.82	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	220	ARG	NE-CZ	7.77	1.41	1.33
1	S	233	ALA	C-O	7.68	1.32	1.24
1	C	229	LEU	C-O	7.67	1.33	1.24
1	B	220	ARG	NE-CZ	7.58	1.41	1.33
1	U	210	ALA	C-O	7.57	1.32	1.24
1	H	138	ALA	C-O	7.54	1.33	1.24
1	A	164	HIS	CE1-NE2	7.53	1.40	1.32
1	Q	220	ARG	NE-CZ	7.51	1.41	1.33
1	S	43	HIS	CE1-NE2	7.50	1.40	1.32
1	B	90	GLU	C-O	-7.39	1.15	1.24
1	X	220	ARG	NE-CZ	7.38	1.41	1.33
1	D	220	ARG	NE-CZ	7.32	1.41	1.33
1	F	128	HIS	CE1-NE2	7.22	1.39	1.32
1	Y	229	LEU	C-O	7.19	1.32	1.24
1	F	164	HIS	CE1-NE2	7.16	1.39	1.32
1	a	220	ARG	NE-CZ	7.11	1.40	1.33
1	E	164	HIS	CE1-NE2	7.03	1.39	1.32
1	Z	220	ARG	NE-CZ	6.92	1.40	1.33
1	U	164	HIS	CE1-NE2	6.85	1.39	1.32
1	b	97	GLY	C-O	6.84	1.29	1.23
1	S	104	GLU	C-O	6.84	1.31	1.23
1	A	57	ARG	NE-CZ	6.83	1.40	1.33
1	L	43	HIS	CE1-NE2	6.83	1.39	1.32
1	C	190	ALA	C-O	-6.81	1.15	1.23
1	B	128	HIS	CE1-NE2	6.78	1.39	1.32
1	A	97	GLY	C-O	6.77	1.29	1.23
1	C	22	VAL	C-O	-6.76	1.16	1.24
1	L	220	ARG	NE-CZ	6.70	1.40	1.33
1	G	174	GLY	C-O	-6.62	1.14	1.23
1	R	256	ILE	C-O	-6.62	1.17	1.24
1	K	220	ARG	NE-CZ	6.61	1.40	1.33
1	B	6	PRO	C-O	-6.60	1.15	1.24
1	B	119	ILE	C-O	-6.59	1.16	1.24
1	d	164	HIS	CE1-NE2	6.59	1.39	1.32
1	V	164	HIS	CE1-NE2	6.57	1.39	1.32
1	T	97	GLY	C-O	6.57	1.30	1.23
1	F	219	TYR	C-O	-6.55	1.14	1.23
1	Z	229	LEU	C-O	6.55	1.31	1.24
1	C	164	HIS	CE1-NE2	6.52	1.39	1.32
1	P	164	HIS	CE1-NE2	6.51	1.39	1.32
1	J	57	ARG	CD-NE	6.48	1.55	1.46
1	T	128	HIS	CE1-NE2	6.47	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	95	HIS	CE1-NE2	6.43	1.39	1.32
1	c	220	ARG	C-O	-6.41	1.15	1.24
1	a	137	LEU	C-O	-6.39	1.16	1.24
1	D	124	VAL	C-O	-6.39	1.17	1.24
1	J	128	HIS	CE1-NE2	6.37	1.39	1.32
1	a	97	GLY	C-O	6.37	1.29	1.23
1	R	210	ALA	C-O	6.36	1.32	1.24
1	L	229	LEU	C-O	6.34	1.31	1.24
1	L	164	HIS	CE1-NE2	6.33	1.38	1.32
1	B	192	SER	CA-CB	-6.32	1.45	1.54
1	R	97	GLY	C-O	6.31	1.29	1.23
1	a	138	ALA	C-O	6.30	1.31	1.24
1	Z	101	ASP	N-CA	6.28	1.50	1.46
1	A	12	PRO	C-O	-6.27	1.16	1.24
1	J	220	ARG	C-O	-6.26	1.14	1.24
1	I	166	PHE	C-O	-6.26	1.17	1.23
1	K	4	ILE	C-O	-6.23	1.18	1.23
1	V	219	TYR	C-O	-6.22	1.15	1.24
1	G	192	SER	CA-CB	-6.22	1.49	1.54
1	D	143	VAL	C-O	-6.22	1.17	1.24
1	T	95	HIS	CE1-NE2	6.20	1.38	1.32
1	U	24	PRO	C-O	-6.20	1.16	1.23
1	B	220	ARG	C-O	-6.19	1.15	1.23
1	Q	244	VAL	C-O	6.17	1.31	1.24
1	X	190	ALA	C-O	-6.14	1.16	1.23
1	T	164	HIS	CE1-NE2	6.14	1.38	1.32
1	J	154	LEU	C-O	6.13	1.31	1.24
1	C	18	ALA	C-O	6.12	1.31	1.24
1	D	6	PRO	C-O	-6.11	1.15	1.24
1	D	22	VAL	C-O	-6.10	1.17	1.24
1	S	12	PRO	C-O	-6.09	1.16	1.24
1	F	124	VAL	C-O	-6.08	1.17	1.24
1	Q	164	HIS	CE1-NE2	6.07	1.38	1.32
1	M	97	GLY	C-O	6.05	1.29	1.23
1	a	164	HIS	CE1-NE2	6.05	1.38	1.32
1	b	221	GLN	N-CA	6.04	1.52	1.46
1	P	220	ARG	NE-CZ	6.03	1.39	1.33
1	K	128	HIS	CE1-NE2	6.03	1.38	1.32
1	I	97	GLY	C-O	6.02	1.29	1.23
1	V	217	VAL	C-O	6.02	1.31	1.24
1	J	101	ASP	C-O	-6.01	1.16	1.24
1	H	97	GLY	C-O	6.01	1.29	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	169	MET	C-O	-5.99	1.16	1.23
1	Z	164	HIS	CE1-NE2	5.93	1.38	1.32
1	A	34	ILE	C-O	-5.92	1.18	1.24
1	K	210	ALA	C-O	5.91	1.31	1.24
1	N	3	LEU	C-O	5.90	1.30	1.24
1	M	71	LEU	C-O	-5.88	1.16	1.24
1	K	24	PRO	C-O	-5.86	1.17	1.23
1	V	201	ARG	NE-CZ	5.86	1.39	1.33
1	I	57	ARG	NE-CZ	5.85	1.39	1.33
1	A	22	VAL	C-O	-5.84	1.18	1.24
1	Q	229	LEU	C-O	5.84	1.30	1.24
1	S	164	HIS	CE1-NE2	5.83	1.38	1.32
1	T	22	VAL	C-O	-5.80	1.18	1.24
1	W	200	ARG	C-O	-5.78	1.16	1.24
1	K	77	PRO	C-O	-5.78	1.16	1.24
1	Y	164	HIS	CE1-NE2	5.78	1.38	1.32
1	d	218	VAL	C-O	-5.77	1.17	1.24
1	D	18	ALA	C-O	5.76	1.30	1.24
1	D	97	GLY	C-O	5.75	1.28	1.23
1	D	226	GLU	C-O	5.74	1.30	1.24
1	U	14	ALA	C-O	-5.74	1.16	1.23
1	V	206	GLU	C-O	5.73	1.30	1.24
1	B	183	VAL	C-O	-5.73	1.18	1.24
1	J	55	HIS	CE1-NE2	5.73	1.38	1.32
1	P	97	GLY	C-O	5.71	1.29	1.23
1	K	18	ALA	C-O	5.71	1.30	1.24
1	E	4	ILE	C-O	-5.70	1.17	1.23
1	D	70	ASP	CG-OD2	5.69	1.36	1.25
1	D	256	ILE	C-O	-5.69	1.18	1.24
1	C	110	HIS	C-O	-5.69	1.16	1.23
1	A	6	PRO	C-O	-5.68	1.17	1.24
1	L	24	PRO	C-O	-5.68	1.16	1.23
1	b	220	ARG	NE-CZ	5.68	1.39	1.33
1	S	163	ALA	C-O	-5.68	1.17	1.23
1	O	57	ARG	NE-CZ	5.67	1.39	1.33
1	U	18	ALA	C-O	5.67	1.30	1.24
1	A	10	ILE	C-O	-5.66	1.18	1.24
1	B	142	HIS	CE1-NE2	5.66	1.38	1.32
1	c	95	HIS	CE1-NE2	5.66	1.38	1.32
1	E	15	ARG	C-O	-5.65	1.17	1.24
1	E	55	HIS	C-O	-5.64	1.16	1.23
1	X	110	HIS	CE1-NE2	5.61	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	18	ALA	C-O	5.60	1.30	1.24
1	Z	220	ARG	C-O	-5.59	1.16	1.24
1	G	6	PRO	C-O	-5.58	1.17	1.24
1	Y	192	SER	CA-CB	-5.57	1.46	1.54
1	D	200	ARG	NE-CZ	5.56	1.39	1.33
1	T	43	HIS	C-O	-5.54	1.16	1.23
1	c	43	HIS	CE1-NE2	5.53	1.38	1.32
1	K	6	PRO	C-O	-5.53	1.17	1.24
1	T	128	HIS	CG-ND1	5.53	1.44	1.38
1	N	164	HIS	CE1-NE2	5.53	1.38	1.32
1	J	128	HIS	CG-ND1	5.53	1.44	1.38
1	T	16	LEU	C-O	-5.52	1.17	1.24
1	E	205	SER	CA-CB	-5.52	1.44	1.53
1	T	42	PRO	C-O	-5.52	1.17	1.23
1	Y	102	ARG	NE-CZ	5.51	1.39	1.33
1	P	229	LEU	C-O	5.51	1.30	1.24
1	L	191	ARG	C-O	-5.50	1.17	1.24
1	D	164	HIS	CE1-NE2	5.49	1.38	1.32
1	T	210	ALA	C-O	5.49	1.30	1.24
1	T	155	VAL	C-O	-5.49	1.18	1.24
1	H	210	ALA	C-O	5.48	1.30	1.24
1	L	50	THR	C-O	-5.48	1.17	1.23
1	P	221	GLN	N-CA	5.47	1.51	1.46
1	C	86	ASN	C-O	-5.47	1.16	1.23
1	J	170	GLY	C-O	-5.47	1.16	1.23
1	a	231	GLU	C-O	5.47	1.30	1.24
1	S	20	VAL	C-O	-5.46	1.17	1.24
1	W	207	ALA	C-O	5.46	1.30	1.24
1	C	57	ARG	CD-NE	5.45	1.53	1.46
1	Z	15	ARG	NE-CZ	5.44	1.39	1.33
1	Y	256	ILE	C-O	-5.44	1.18	1.24
1	S	42	PRO	C-O	-5.43	1.17	1.23
1	G	229	LEU	C-O	5.43	1.30	1.24
1	S	156	HIS	CE1-NE2	5.41	1.38	1.32
1	d	186	ASN	C-O	-5.39	1.20	1.25
1	Q	217	VAL	C-O	5.38	1.29	1.24
1	A	55	HIS	C-O	-5.36	1.16	1.23
1	A	192	SER	CA-CB	-5.36	1.47	1.54
1	R	57	ARG	NE-CZ	5.36	1.39	1.33
1	N	256	ILE	C-O	-5.35	1.18	1.24
1	b	30	ALA	C-O	5.34	1.30	1.23
1	C	110	HIS	CE1-NE2	5.34	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	92	VAL	C-O	-5.33	1.17	1.24
1	V	102	ARG	C-O	-5.33	1.17	1.23
1	a	29	GLY	C-O	5.33	1.31	1.23
1	a	173	ILE	C-O	-5.33	1.18	1.24
1	C	205	SER	CA-CB	-5.33	1.44	1.53
1	C	34	ILE	C-O	-5.32	1.18	1.24
1	D	221	GLN	N-CA	5.32	1.51	1.46
1	J	219	TYR	C-O	-5.31	1.17	1.24
1	E	43	HIS	CE1-NE2	5.30	1.37	1.32
1	U	221	GLN	N-CA	5.30	1.51	1.46
1	Q	186	ASN	C-O	-5.29	1.20	1.24
1	N	3	LEU	N-CA	5.28	1.52	1.46
1	O	236	ALA	C-O	-5.28	1.17	1.24
1	N	116	TYR	C-O	-5.28	1.14	1.24
1	W	219	TYR	C-O	-5.28	1.17	1.23
1	a	92	VAL	C-O	-5.28	1.18	1.24
1	U	223	HIS	C-O	-5.28	1.17	1.23
1	S	110	HIS	CE1-NE2	5.27	1.37	1.32
1	B	85	HIS	CE1-NE2	5.26	1.37	1.32
1	F	12	PRO	C-O	-5.25	1.17	1.24
1	X	238	GLN	C-O	-5.23	1.17	1.24
1	Q	192	SER	CA-CB	-5.23	1.50	1.54
1	K	196	GLU	CD-OE1	5.23	1.35	1.25
1	J	26	SER	C-O	-5.22	1.17	1.23
1	S	92	VAL	C-O	-5.21	1.18	1.24
1	P	206	GLU	C-O	5.20	1.30	1.24
1	a	147	ALA	C-O	-5.20	1.17	1.23
1	C	101	ASP	C-O	-5.20	1.17	1.24
1	W	15	ARG	NE-CZ	5.20	1.38	1.33
1	U	156	HIS	CE1-NE2	5.20	1.37	1.32
1	F	29	GLY	C-O	5.19	1.29	1.23
1	I	198	MET	C-O	5.18	1.30	1.24
1	R	186	ASN	C-O	-5.18	1.19	1.24
1	J	110	HIS	CE1-NE2	5.17	1.37	1.32
1	d	42	PRO	C-O	-5.17	1.17	1.23
1	C	55	HIS	CG-ND1	5.16	1.44	1.38
1	S	91	GLY	C-O	5.16	1.30	1.24
1	R	3	LEU	C-O	5.15	1.30	1.24
1	T	1	MET	N-CA	5.14	1.56	1.46
1	D	155	VAL	C-O	-5.12	1.18	1.24
1	G	256	ILE	C-O	-5.12	1.18	1.24
1	P	121	HIS	CE1-NE2	5.12	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	LEU	C-O	5.11	1.29	1.24
1	F	200	ARG	NE-CZ	5.11	1.38	1.33
1	S	138	ALA	C-O	5.11	1.30	1.24
1	d	88	ILE	C-O	5.11	1.29	1.24
1	S	191	ARG	C-O	-5.10	1.17	1.24
1	J	156	HIS	CE1-NE2	5.09	1.37	1.32
1	B	69	PRO	C-O	-5.09	1.18	1.24
1	T	251	SER	C-O	-5.08	1.17	1.24
1	V	200	ARG	NE-CZ	5.08	1.38	1.33
1	J	94	ILE	C-O	-5.08	1.18	1.24
1	L	6	PRO	C-O	-5.07	1.18	1.24
1	E	143	VAL	C-O	-5.07	1.18	1.24
1	L	159	CYS	C-O	-5.07	1.17	1.23
1	Y	95	HIS	CE1-NE2	5.07	1.37	1.32
1	B	55	HIS	CE1-NE2	5.06	1.37	1.32
1	E	61	PHE	C-O	5.06	1.34	1.24
1	M	209	HIS	CE1-NE2	5.06	1.37	1.32
1	c	221	GLN	N-CA	5.06	1.51	1.46
1	X	220	ARG	C-O	-5.06	1.17	1.23
1	B	70	ASP	CG-OD2	5.05	1.34	1.25
1	A	20	VAL	C-O	-5.05	1.18	1.24
1	D	57	ARG	CD-NE	5.02	1.53	1.46
1	U	156	HIS	CG-ND1	5.02	1.43	1.38
1	V	18	ALA	C-O	5.01	1.29	1.24

All (623) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	57	ARG	CB-CA-C	13.29	130.02	110.62
1	Q	57	ARG	CB-CA-C	12.79	131.40	110.16
1	G	57	ARG	CB-CA-C	12.62	129.04	110.62
1	H	57	ARG	CB-CA-C	12.15	128.97	110.62
1	C	57	ARG	CB-CA-C	11.43	128.42	110.14
1	M	57	ARG	CB-CA-C	11.29	128.21	110.14
1	b	57	ARG	CB-CA-C	11.16	128.00	110.14
1	T	225	VAL	N-CA-C	-11.06	102.89	111.62
1	D	57	ARG	CB-CA-C	10.71	127.94	110.16
1	R	57	ARG	CB-CA-C	10.71	127.27	110.14
1	J	70	ASP	CA-CB-CG	10.61	123.21	112.60
1	N	57	ARG	CB-CA-C	10.43	127.30	110.19
1	P	57	ARG	CB-CA-C	10.00	125.55	110.14
1	J	57	ARG	CB-CA-C	9.67	127.20	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	LYS	CB-CA-C	9.61	125.14	110.62
1	C	70	ASP	CA-CB-CG	9.41	122.01	112.60
1	A	57	ARG	CB-CA-C	9.35	124.74	110.62
1	B	257	THR	CA-CB-OG1	-9.33	95.61	109.60
1	U	90	GLU	CB-CA-C	9.30	124.77	109.89
1	V	57	ARG	CB-CA-C	9.14	125.17	110.19
1	Z	246	ARG	CG-CD-NE	-9.03	92.14	112.00
1	I	57	ARG	CB-CA-C	8.92	124.41	110.14
1	V	246	ARG	CB-CG-CD	8.78	131.50	111.30
1	G	67	ASP	CA-CB-CG	8.77	121.37	112.60
1	D	90	GLU	CB-CA-C	8.76	123.90	109.89
1	a	33	GLU	CB-CA-C	8.75	124.19	109.75
1	P	220	ARG	CB-CA-C	8.75	125.37	110.94
1	P	246	ARG	CB-CG-CD	8.73	131.39	111.30
1	O	57	ARG	CB-CA-C	8.65	125.54	109.71
1	K	90	GLU	CB-CG-CD	8.47	127.00	112.60
1	J	57	ARG	CB-CG-CD	8.43	130.69	111.30
1	S	57	ARG	CB-CA-C	8.43	124.95	109.70
1	I	144	ASP	CB-CA-C	8.41	124.99	110.45
1	K	90	GLU	CB-CA-C	8.30	122.11	110.16
1	R	220	ARG	NE-CZ-NH2	8.25	126.62	119.20
1	D	90	GLU	CB-CG-CD	8.23	126.60	112.60
1	O	70	ASP	CA-CB-CG	8.11	120.71	112.60
1	Z	90	GLU	CB-CA-C	8.11	122.42	110.26
1	L	245	PHE	CA-C-O	-8.09	112.50	121.00
1	D	57	ARG	CB-CG-CD	8.09	129.90	111.30
1	Z	220	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	M	246	ARG	CB-CG-CD	7.94	129.55	111.30
1	c	220	ARG	NE-CZ-NH2	7.93	126.34	119.20
1	H	90	GLU	CB-CA-C	7.93	122.58	109.89
1	X	57	ARG	CB-CA-C	7.91	122.56	110.62
1	T	246	ARG	CG-CD-NE	-7.85	94.72	112.00
1	B	220	ARG	NE-CZ-NH2	7.82	126.24	119.20
1	L	246	ARG	CB-CG-CD	7.81	129.27	111.30
1	W	67	ASP	CA-CB-CG	7.76	120.36	112.60
1	b	253	THR	CB-CA-C	-7.73	100.25	111.23
1	T	70	ASP	CA-CB-CG	7.72	120.32	112.60
1	L	90	GLU	CB-CA-C	7.68	122.18	109.89
1	A	70	ASP	CA-CB-CG	7.67	120.27	112.60
1	Q	220	ARG	NE-CZ-NH2	7.65	126.08	119.20
1	Q	246	ARG	CB-CG-CD	7.65	128.90	111.30
1	H	246	ARG	CB-CG-CD	7.64	128.87	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	72	LYS	CB-CA-C	-7.61	97.75	110.68
1	K	144	ASP	CA-CB-CG	7.59	120.19	112.60
1	H	69	PRO	CB-CA-C	-7.55	100.03	111.44
1	T	156	HIS	CB-CA-C	7.55	123.36	109.46
1	U	220	ARG	NE-CZ-NH2	7.55	126.00	119.20
1	D	247	ASP	CA-CB-CG	7.55	120.15	112.60
1	E	19	ASP	CA-CB-CG	-7.54	105.06	112.60
1	J	90	GLU	CB-CA-C	7.50	121.89	109.89
1	d	69	PRO	CA-C-O	-7.49	109.84	118.98
1	A	90	GLU	CB-CA-C	7.47	122.43	109.65
1	F	250	GLN	CB-CG-CD	-7.45	99.93	112.60
1	A	19	ASP	CA-CB-CG	-7.44	105.16	112.60
1	T	220	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	F	245	PHE	CA-C-O	-7.42	113.26	120.90
1	L	70	ASP	CA-CB-CG	7.39	119.99	112.60
1	Y	246	ARG	CB-CG-CD	7.39	128.30	111.30
1	T	90	GLU	CB-CG-CD	7.38	125.15	112.60
1	Y	245	PHE	CA-C-O	-7.38	113.10	120.70
1	c	97	GLY	O-C-N	7.37	128.46	122.71
1	R	245	PHE	CA-C-O	-7.37	113.11	120.70
1	T	156	HIS	CA-CB-CG	7.36	121.16	113.80
1	D	246	ARG	CB-CG-CD	7.35	128.21	111.30
1	X	220	ARG	CB-CA-C	7.32	122.92	111.13
1	H	84	ASP	CA-CB-CG	7.32	119.92	112.60
1	K	15	ARG	CB-CA-C	7.32	121.67	110.62
1	D	206	GLU	CB-CG-CD	7.31	125.03	112.60
1	U	72	LYS	CB-CA-C	-7.25	98.75	110.79
1	A	97	GLY	O-C-N	7.25	128.37	122.71
1	a	220	ARG	CB-CA-C	7.22	122.69	111.28
1	D	57	ARG	N-CA-C	-7.22	96.64	108.41
1	T	90	GLU	CB-CA-C	7.18	121.54	109.84
1	H	226	GLU	N-CA-C	-7.14	103.58	111.36
1	S	57	ARG	CB-CG-CD	7.14	127.72	111.30
1	P	156	HIS	CA-CB-CG	7.13	120.93	113.80
1	I	97	GLY	O-C-N	7.10	128.25	122.71
1	P	220	ARG	N-CA-C	-7.09	104.64	112.72
1	d	246	ARG	CB-CG-CD	7.07	127.57	111.30
1	O	246	ARG	CB-CG-CD	7.07	127.56	111.30
1	D	70	ASP	CA-CB-CG	7.06	119.66	112.60
1	b	246	ARG	CB-CG-CD	7.05	127.50	111.30
1	Z	245	PHE	CA-C-O	-7.01	113.45	120.82
1	Z	160	ARG	CG-CD-NE	-7.00	96.60	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	220	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	P	247	ASP	CA-CB-CG	7.00	119.59	112.60
1	A	33	GLU	CB-CA-C	6.99	122.50	109.71
1	R	257	THR	CA-CB-OG1	-6.99	99.12	109.60
1	W	245	PHE	CA-C-O	-6.98	113.51	120.70
1	E	61	PHE	N-CA-CB	-6.96	103.42	113.65
1	Z	67	ASP	CA-CB-CG	6.95	119.55	112.60
1	H	226	GLU	CB-CG-CD	6.95	124.41	112.60
1	H	73	TYR	CA-C-O	-6.94	112.65	120.43
1	M	101	ASP	CA-CB-CG	6.89	119.49	112.60
1	P	145	ASP	CA-CB-CG	6.89	119.49	112.60
1	b	245	PHE	CA-C-O	-6.87	113.60	120.82
1	d	90	GLU	CB-CA-C	6.86	120.55	110.26
1	V	252	ALA	N-CA-C	-6.85	106.81	114.62
1	W	98	THR	CA-C-O	-6.85	113.37	121.11
1	Z	15	ARG	CA-C-N	6.83	132.42	123.00
1	Z	15	ARG	C-N-CA	6.83	132.42	123.00
1	d	247	ASP	CA-CB-CG	6.80	119.40	112.60
1	U	70	ASP	CA-CB-CG	6.79	119.39	112.60
1	K	246	ARG	CG-CD-NE	-6.78	97.09	112.00
1	X	177	VAL	CA-C-O	6.76	122.91	119.12
1	K	245	PHE	CA-C-O	-6.75	113.26	120.42
1	G	73	TYR	CA-C-O	-6.75	112.87	120.43
1	C	188	ALA	CA-C-O	-6.74	114.21	120.95
1	F	206	GLU	CB-CG-CD	6.74	124.05	112.60
1	b	99	VAL	CA-C-N	6.73	129.97	120.28
1	b	99	VAL	C-N-CA	6.73	129.97	120.28
1	G	201	ARG	CB-CG-CD	6.71	126.74	111.30
1	R	144	ASP	CB-CA-C	6.68	123.14	110.51
1	F	257	THR	CA-C-O	-6.66	113.70	120.96
1	M	57	ARG	CB-CG-CD	6.65	126.60	111.30
1	E	6	PRO	CB-CA-C	-6.64	101.98	111.68
1	G	97	GLY	O-C-N	6.62	127.88	122.71
1	F	90	GLU	CB-CG-CD	6.62	123.86	112.60
1	R	253	THR	CA-C-O	-6.62	115.52	121.67
1	X	246	ARG	CB-CG-CD	6.61	126.51	111.30
1	W	247	ASP	CA-CB-CG	6.60	119.20	112.60
1	b	97	GLY	O-C-N	6.60	127.86	122.71
1	X	97	GLY	O-C-N	6.60	127.86	122.71
1	d	258	ARG	CB-CG-CD	6.58	126.43	111.30
1	S	233	ALA	O-C-N	6.57	128.93	122.09
1	N	246	ARG	CB-CG-CD	6.56	126.40	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	7	ARG	N-CA-C	-6.56	105.24	113.18
1	b	21	GLN	CB-CG-CD	-6.54	101.48	112.60
1	R	70	ASP	CA-CB-CG	6.54	119.14	112.60
1	O	90	GLU	CB-CA-C	6.53	120.49	109.84
1	Q	212	ARG	CA-C-O	-6.52	113.98	120.70
1	c	220	ARG	CD-NE-CZ	6.52	133.53	124.40
1	V	33	GLU	CB-CA-C	6.51	120.99	109.72
1	D	257	THR	CA-C-O	-6.51	113.50	120.92
1	L	90	GLU	CB-CG-CD	6.49	123.63	112.60
1	G	246	ARG	CB-CG-CD	6.47	126.19	111.30
1	Q	220	ARG	CD-NE-CZ	6.47	133.46	124.40
1	T	220	ARG	CB-CA-C	6.46	121.48	111.02
1	d	257	THR	CA-C-O	-6.45	113.83	120.80
1	V	245	PHE	CA-C-O	-6.44	114.26	120.90
1	I	90	GLU	CB-CA-C	6.43	119.43	110.16
1	J	210	ALA	O-C-N	6.43	129.49	122.15
1	Q	67	ASP	CA-CB-CG	6.42	119.02	112.60
1	a	70	ASP	CA-CB-CG	6.41	119.01	112.60
1	Q	100	GLN	CB-CG-CD	6.40	123.49	112.60
1	V	218	VAL	O-C-N	6.39	128.41	121.83
1	P	257	THR	CA-CB-OG1	-6.38	100.02	109.60
1	G	101	ASP	CA-CB-CG	6.38	118.98	112.60
1	F	225	VAL	CA-C-O	-6.38	114.09	120.85
1	D	97	GLY	O-C-N	6.37	127.68	122.71
1	J	257	THR	CA-CB-OG1	-6.37	100.05	109.60
1	F	76	GLU	CB-CA-C	6.37	120.94	109.61
1	E	70	ASP	CA-CB-CG	6.36	118.96	112.60
1	D	70	ASP	CB-CA-C	6.36	119.81	109.90
1	d	70	ASP	N-CA-CB	6.36	119.43	109.83
1	W	246	ARG	CB-CG-CD	6.35	125.89	111.30
1	M	156	HIS	CB-CA-C	6.32	120.21	109.53
1	O	73	TYR	CA-C-O	-6.31	113.41	120.54
1	A	66	GLU	N-CA-CB	-6.31	101.34	110.36
1	G	84	ASP	CA-CB-CG	6.29	118.89	112.60
1	d	206	GLU	CB-CG-CD	6.29	123.29	112.60
1	C	57	ARG	CB-CG-CD	6.29	125.76	111.30
1	R	246	ARG	CB-CG-CD	6.26	125.70	111.30
1	A	51	LYS	CB-CA-C	6.25	120.54	110.16
1	A	257	THR	CA-C-O	-6.22	113.55	120.70
1	Q	220	ARG	CB-CA-C	6.22	121.09	111.02
1	Y	140	HIS	CA-CB-CG	6.22	120.02	113.80
1	Q	57	ARG	CB-CG-CD	6.21	125.59	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	67	ASP	CA-CB-CG	6.21	118.81	112.60
1	J	15	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	L	15	ARG	CB-CA-C	6.20	120.03	111.23
1	J	97	GLY	O-C-N	6.18	128.13	122.81
1	M	245	PHE	CA-C-O	-6.17	114.34	120.70
1	S	72	LYS	CB-CA-C	6.17	121.04	110.79
1	B	245	PHE	CA-C-O	-6.17	114.34	120.82
1	R	90	GLU	CB-CA-C	6.17	119.90	109.84
1	R	220	ARG	CD-NE-CZ	6.16	133.03	124.40
1	E	1	MET	CA-C-N	6.16	133.31	121.54
1	E	1	MET	C-N-CA	6.16	133.31	121.54
1	N	156	HIS	CB-CA-C	6.16	120.18	109.65
1	G	244	VAL	O-C-N	6.15	127.93	121.91
1	C	246	ARG	CB-CG-CD	6.14	125.42	111.30
1	X	70	ASP	CB-CA-C	-6.13	100.64	109.84
1	b	220	ARG	CB-CA-C	6.12	120.98	111.13
1	W	14	ALA	CA-C-O	-6.12	114.77	121.87
1	J	119	ILE	CA-C-N	6.12	125.91	120.10
1	J	119	ILE	C-N-CA	6.12	125.91	120.10
1	R	234	GLU	CA-C-N	6.11	128.75	120.38
1	R	234	GLU	C-N-CA	6.11	128.75	120.38
1	T	67	ASP	CA-CB-CG	6.11	118.71	112.60
1	O	185	GLY	CA-C-O	-6.11	117.69	122.52
1	G	244	VAL	CA-C-N	6.10	128.71	120.65
1	G	244	VAL	C-N-CA	6.10	128.71	120.65
1	L	188	ALA	CA-C-O	-6.10	114.33	121.16
1	U	220	ARG	CB-CA-C	6.09	120.89	111.02
1	U	220	ARG	N-CA-C	-6.09	104.49	112.41
1	I	109	ASP	CA-CB-CG	6.08	118.68	112.60
1	c	90	GLU	CB-CA-C	6.08	119.61	109.89
1	O	71	LEU	CA-C-N	6.07	129.02	120.28
1	O	71	LEU	C-N-CA	6.07	129.02	120.28
1	I	156	HIS	CB-CA-C	6.06	120.70	109.54
1	C	145	ASP	CA-C-O	-6.06	115.13	121.55
1	B	90	GLU	CB-CA-C	6.05	119.34	110.26
1	d	226	GLU	CB-CA-C	6.05	120.95	110.79
1	Q	206	GLU	CB-CG-CD	6.04	122.87	112.60
1	F	244	VAL	O-C-N	6.02	127.71	121.87
1	E	226	GLU	CB-CA-C	6.02	122.22	110.67
1	c	220	ARG	N-CA-C	-6.02	104.59	112.41
1	D	200	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	d	144	ASP	CB-CA-C	6.01	120.85	110.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	144	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	220	ARG	CB-CA-C	6.00	120.67	111.02
1	S	90	GLU	CB-CG-CD	5.99	122.79	112.60
1	Y	67	ASP	CA-C-O	-5.98	115.21	121.55
1	R	74	LYS	CB-CA-C	5.98	122.31	110.42
1	B	97	GLY	O-C-N	5.97	127.94	122.81
1	T	220	ARG	N-CA-C	-5.96	104.66	112.41
1	S	57	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	d	144	ASP	CA-CB-CG	5.95	118.55	112.60
1	c	220	ARG	CB-CA-C	5.94	120.65	111.02
1	S	246	ARG	N-CA-CB	5.94	118.58	109.91
1	S	257	THR	CA-CB-OG1	-5.94	100.69	109.60
1	J	188	ALA	CA-C-O	-5.94	114.51	121.16
1	J	30	ALA	CA-C-O	-5.93	114.50	120.96
1	Y	206	GLU	N-CA-C	-5.92	104.90	111.36
1	U	90	GLU	CB-CG-CD	5.92	122.67	112.60
1	K	206	GLU	CB-CG-CD	5.92	122.66	112.60
1	J	57	ARG	N-CA-C	-5.91	98.78	108.76
1	I	57	ARG	CB-CG-CD	5.90	124.88	111.30
1	T	250	GLN	CA-C-O	-5.90	114.59	120.90
1	D	241	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	161	ILE	CA-C-N	5.88	125.68	120.10
1	A	161	ILE	C-N-CA	5.88	125.68	120.10
1	b	84	ASP	CA-CB-CG	5.87	118.47	112.60
1	H	245	PHE	CA-C-O	-5.87	114.65	120.82
1	L	33	GLU	CB-CA-C	5.87	120.45	109.71
1	V	34	ILE	CA-C-N	5.87	125.68	120.10
1	V	34	ILE	C-N-CA	5.87	125.68	120.10
1	N	109	ASP	CA-CB-CG	5.87	118.47	112.60
1	W	226	GLU	N-CA-CB	5.86	118.74	110.12
1	P	57	ARG	CB-CG-CD	5.86	124.77	111.30
1	S	245	PHE	CA-C-O	-5.85	114.29	120.55
1	H	109	ASP	CA-CB-CG	5.85	118.45	112.60
1	Z	33	GLU	CB-CA-C	5.85	120.41	109.71
1	H	57	ARG	CB-CG-CD	5.84	124.74	111.30
1	Q	247	ASP	CA-CB-CG	5.84	118.44	112.60
1	H	5	ASP	CB-CA-C	5.84	116.80	108.68
1	b	90	GLU	CB-CA-C	5.83	119.01	110.26
1	K	101	ASP	CA-CB-CG	5.83	118.43	112.60
1	V	70	ASP	CA-CB-CG	5.83	118.43	112.60
1	U	201	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	250	GLN	CB-CG-CD	-5.82	102.71	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	196	GLU	N-CA-C	-5.82	104.94	111.28
1	X	212	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	Q	258	ARG	CG-CD-NE	5.81	124.79	112.00
1	V	77	PRO	CB-CA-C	5.80	116.74	111.87
1	V	198	MET	N-CA-C	-5.80	105.04	111.36
1	D	229	LEU	CA-C-N	5.79	128.30	120.65
1	D	229	LEU	C-N-CA	5.79	128.30	120.65
1	J	57	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	X	234	GLU	CA-C-N	5.79	128.35	120.54
1	X	234	GLU	C-N-CA	5.79	128.35	120.54
1	K	135	THR	CA-CB-OG1	-5.79	100.92	109.60
1	H	234	GLU	CA-C-N	5.78	128.30	120.38
1	H	234	GLU	C-N-CA	5.78	128.30	120.38
1	Z	24	PRO	CB-CA-C	-5.78	104.22	111.56
1	C	57	ARG	N-CA-C	-5.78	98.87	108.34
1	P	37	GLY	CA-C-N	5.78	129.47	120.75
1	P	37	GLY	C-N-CA	5.78	129.47	120.75
1	a	246	ARG	CB-CG-CD	5.78	124.58	111.30
1	K	220	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	K	67	ASP	CA-C-O	-5.77	115.27	121.56
1	A	135	THR	CA-CB-OG1	-5.76	100.96	109.60
1	U	173	ILE	N-CA-CB	-5.76	104.25	110.53
1	G	70	ASP	CA-CB-CG	5.75	118.36	112.60
1	Q	257	THR	CA-C-O	-5.75	114.69	120.96
1	T	195	PHE	CA-C-O	-5.75	114.45	120.55
1	C	102	ARG	CB-CA-C	5.75	120.27	111.02
1	K	144	ASP	CB-CA-C	5.74	121.35	110.51
1	A	101	ASP	CB-CA-C	5.74	121.83	110.42
1	V	200	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	J	33	GLU	N-CA-CB	-5.73	101.08	110.42
1	L	246	ARG	N-CA-CB	5.73	118.48	109.94
1	T	19	ASP	CA-CB-CG	-5.72	106.88	112.60
1	T	220	ARG	CD-NE-CZ	5.72	132.41	124.40
1	U	257	THR	CA-C-O	-5.72	115.50	120.88
1	M	93	THR	CA-CB-OG1	5.71	118.17	109.60
1	J	57	ARG	NH1-CZ-NH2	-5.71	111.88	119.30
1	P	245	PHE	CA-C-O	-5.71	115.02	120.90
1	H	69	PRO	CA-C-O	-5.71	110.99	118.86
1	Q	144	ASP	CB-CA-C	5.70	120.30	110.45
1	S	90	GLU	CB-CA-C	5.69	119.38	109.65
1	b	257	THR	CA-CB-OG1	-5.68	101.07	109.60
1	Z	253	THR	CA-C-O	-5.67	116.39	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	209	HIS	N-CA-C	-5.67	105.25	111.82
1	T	225	VAL	O-C-N	5.67	126.34	121.98
1	K	77	PRO	CA-C-N	5.67	131.03	120.95
1	K	77	PRO	C-N-CA	5.67	131.03	120.95
1	J	101	ASP	CA-CB-CG	5.66	118.26	112.60
1	E	257	THR	CA-C-O	-5.66	114.82	121.16
1	O	57	ARG	CB-CG-CD	5.66	124.31	111.30
1	W	15	ARG	CA-C-N	5.66	130.89	122.86
1	W	15	ARG	C-N-CA	5.66	130.89	122.86
1	O	90	GLU	CB-CG-CD	5.65	122.21	112.60
1	E	206	GLU	N-CA-C	-5.64	105.21	111.36
1	T	226	GLU	N-CA-C	-5.64	104.35	111.11
1	X	245	PHE	CA-C-O	-5.63	115.10	120.90
1	C	208	ILE	N-CA-C	-5.62	105.02	110.42
1	F	90	GLU	CB-CA-C	5.62	119.26	109.65
1	S	220	ARG	CG-CD-NE	5.62	124.36	112.00
1	Y	90	GLU	CB-CA-C	5.62	118.68	110.26
1	Z	247	ASP	CB-CA-C	5.61	119.79	110.81
1	c	203	PHE	CA-C-O	-5.61	115.44	121.56
1	Q	245	PHE	CA-C-O	-5.61	114.93	120.70
1	Y	246	ARG	N-CA-CB	5.61	118.14	110.01
1	H	70	ASP	CA-CB-CG	5.60	118.20	112.60
1	U	220	ARG	CD-NE-CZ	5.60	132.24	124.40
1	Z	102	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	S	144	ASP	CB-CA-C	5.60	119.62	109.83
1	D	66	GLU	N-CA-CB	-5.59	102.37	110.36
1	I	257	THR	CA-CB-OG1	-5.59	101.21	109.60
1	b	74	LYS	CB-CA-C	5.58	120.27	111.72
1	H	5	ASP	CA-CB-CG	5.58	118.18	112.60
1	Y	247	ASP	CA-CB-CG	5.58	118.18	112.60
1	Z	15	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	L	206	GLU	CB-CG-CD	5.57	122.08	112.60
1	Q	67	ASP	CA-C-O	-5.57	115.49	121.56
1	H	258	ARG	CA-C-O	5.57	137.71	121.00
1	E	230	ALA	CA-C-O	-5.57	114.97	120.82
1	D	16	LEU	CA-C-O	-5.56	114.35	120.36
1	G	90	GLU	CB-CA-C	5.56	118.57	109.90
1	J	253	THR	CA-CB-OG1	5.56	117.94	109.60
1	E	212	ARG	CA-C-O	-5.55	114.99	120.82
1	Y	156	HIS	CA-CB-CG	5.55	119.35	113.80
1	M	119	ILE	CB-CA-C	5.54	118.02	111.59
1	S	84	ASP	CA-CB-CG	5.54	118.14	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ASP	CB-CA-C	5.54	118.11	109.42
1	Q	211	LEU	N-CA-C	-5.54	105.25	112.23
1	M	144	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	220	ARG	N-CA-C	-5.53	105.84	112.59
1	Y	90	GLU	CB-CG-CD	5.53	122.01	112.60
1	a	220	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	Z	200	ARG	CA-C-O	-5.53	114.69	120.55
1	F	226	GLU	N-CA-CB	5.53	118.24	110.12
1	c	227	GLU	CA-C-N	5.52	127.62	120.44
1	c	227	GLU	C-N-CA	5.52	127.62	120.44
1	V	2	SER	CA-C-N	5.52	129.10	120.82
1	V	2	SER	C-N-CA	5.52	129.10	120.82
1	Y	164	HIS	CA-CB-CG	-5.52	108.28	113.80
1	O	257	THR	CA-CB-OG1	-5.51	101.33	109.60
1	Z	57	ARG	N-CA-C	-5.51	100.20	109.07
1	X	57	ARG	N-CA-CB	-5.51	102.47	110.84
1	F	160	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	a	220	ARG	CD-NE-CZ	5.49	132.08	124.40
1	B	246	ARG	CG-CD-NE	-5.48	99.94	112.00
1	S	19	ASP	CA-CB-CG	-5.48	107.12	112.60
1	D	67	ASP	CA-CB-CG	5.48	118.08	112.60
1	R	57	ARG	N-CA-C	-5.47	99.36	108.34
1	W	90	GLU	CB-CG-CD	5.47	121.90	112.60
1	T	97	GLY	O-C-N	5.47	128.22	122.59
1	F	111	ASN	CA-CB-CG	-5.46	107.14	112.60
1	a	69	PRO	CA-C-O	-5.46	112.31	118.98
1	b	33	GLU	CB-CA-C	5.46	119.70	109.71
1	U	71	LEU	CA-C-N	5.46	127.59	120.28
1	U	71	LEU	C-N-CA	5.46	127.59	120.28
1	B	220	ARG	CD-NE-CZ	5.46	132.04	124.40
1	P	90	GLU	CB-CA-C	5.44	118.60	109.89
1	Y	77	PRO	CA-C-O	-5.44	117.19	121.38
1	O	70	ASP	N-CA-CB	5.44	117.97	109.97
1	E	157	GLN	CB-CG-CD	-5.43	103.36	112.60
1	Q	72	LYS	CB-CA-C	-5.43	99.61	110.42
1	A	245	PHE	CA-C-O	-5.43	115.12	120.82
1	F	144	ASP	CB-CA-C	5.43	119.84	110.45
1	Q	225	VAL	CA-C-O	-5.43	115.42	121.17
1	V	14	ALA	CA-C-O	-5.42	115.91	121.87
1	O	72	LYS	N-CA-CB	-5.41	101.88	110.22
1	F	77	PRO	N-CA-CB	-5.39	99.20	102.81
1	F	66	GLU	CB-CG-CD	5.39	121.76	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	258	ARG	CB-CG-CD	5.38	123.68	111.30
1	c	119	ILE	CB-CA-C	5.38	117.83	111.59
1	X	198	MET	CA-C-N	5.38	127.95	120.63
1	X	198	MET	C-N-CA	5.38	127.95	120.63
1	M	253	THR	CB-CA-C	-5.38	101.48	110.19
1	R	109	ASP	CA-CB-CG	5.38	117.98	112.60
1	S	57	ARG	N-CA-C	-5.38	99.67	108.76
1	C	257	THR	CA-CB-OG1	-5.38	101.54	109.60
1	K	67	ASP	CA-CB-CG	5.37	117.97	112.60
1	G	35	GLY	CA-C-N	5.37	128.73	121.05
1	G	35	GLY	C-N-CA	5.37	128.73	121.05
1	U	73	TYR	CA-C-O	-5.37	114.35	120.58
1	E	145	ASP	CA-CB-CG	5.37	117.97	112.60
1	W	226	GLU	N-CA-C	-5.37	105.43	111.28
1	J	245	PHE	CA-C-O	-5.36	115.19	120.82
1	Y	246	ARG	N-CA-C	-5.36	105.33	111.07
1	A	246	ARG	CB-CG-CD	5.36	123.63	111.30
1	X	201	ARG	N-CA-C	-5.36	106.59	113.02
1	X	252	ALA	N-CA-C	-5.36	107.76	114.56
1	W	219	TYR	CA-C-O	-5.35	113.25	118.97
1	E	206	GLU	CB-CG-CD	5.35	121.69	112.60
1	T	35	GLY	CA-C-N	5.35	128.69	121.05
1	T	35	GLY	C-N-CA	5.35	128.69	121.05
1	A	71	LEU	CA-C-N	5.34	127.44	120.28
1	A	71	LEU	C-N-CA	5.34	127.44	120.28
1	W	257	THR	CB-CA-C	5.34	117.49	110.06
1	I	244	VAL	N-CA-C	-5.34	105.33	110.72
1	Q	90	GLU	CB-CA-C	5.34	117.85	110.16
1	D	245	PHE	CA-C-O	-5.34	115.40	120.90
1	B	97	GLY	CA-C-O	-5.33	116.71	122.47
1	A	190	ALA	CA-C-O	-5.33	115.19	121.16
1	N	57	ARG	N-CA-C	-5.33	99.83	108.52
1	b	160	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	Z	15	ARG	CB-CA-C	5.33	118.34	110.14
1	Q	234	GLU	CB-CG-CD	5.32	121.65	112.60
1	R	257	THR	CA-C-O	-5.32	115.05	120.80
1	b	57	ARG	N-CA-C	-5.32	99.61	108.34
1	c	90	GLU	CB-CG-CD	5.32	121.64	112.60
1	M	154	LEU	CA-C-O	-5.32	114.59	120.38
1	X	212	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	F	205	SER	CB-CA-C	5.31	121.08	109.99
1	F	258	ARG	CG-CD-NE	5.31	123.67	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	47	LYS	CB-CA-C	5.31	118.47	109.50
1	d	246	ARG	N-CA-CB	5.31	117.85	109.94
1	G	71	LEU	CA-C-N	5.30	131.67	121.54
1	G	71	LEU	C-N-CA	5.30	131.67	121.54
1	d	226	GLU	N-CA-C	-5.30	104.93	111.40
1	P	61	PHE	N-CA-CB	-5.30	105.58	114.27
1	Q	15	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	a	220	ARG	N-CA-C	-5.30	104.40	111.87
1	V	93	THR	CA-CB-OG1	5.30	117.55	109.60
1	A	241	GLU	CB-CG-CD	5.29	121.60	112.60
1	T	1	MET	CA-C-N	5.29	128.38	120.87
1	T	1	MET	C-N-CA	5.29	128.38	120.87
1	T	206	GLU	N-CA-C	-5.29	105.60	111.36
1	P	212	ARG	N-CA-C	-5.29	105.43	111.14
1	E	15	ARG	CB-CA-C	5.29	118.60	110.62
1	H	8	ALA	CA-C-O	-5.28	115.71	121.89
1	L	250	GLN	CB-CG-CD	-5.28	103.62	112.60
1	S	220	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	G	258	ARG	CB-CG-CD	5.28	123.45	111.30
1	X	77	PRO	CA-C-N	5.28	131.63	121.54
1	X	77	PRO	C-N-CA	5.28	131.63	121.54
1	Z	225	VAL	CA-C-O	-5.28	115.06	120.71
1	d	245	PHE	CA-C-O	-5.28	115.46	120.90
1	N	57	ARG	CB-CG-CD	5.28	123.44	111.30
1	U	111	ASN	CA-CB-CG	-5.28	107.32	112.60
1	M	144	ASP	CB-CA-C	5.28	122.15	111.60
1	U	213	ARG	N-CA-C	-5.28	105.61	111.36
1	S	101	ASP	CB-CA-C	5.27	120.91	110.42
1	X	90	GLU	CB-CA-C	5.27	118.45	109.80
1	c	67	ASP	CA-C-O	-5.27	115.81	121.56
1	U	15	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	F	234	GLU	CA-C-N	5.27	127.59	120.38
1	F	234	GLU	C-N-CA	5.27	127.59	120.38
1	S	246	ARG	CB-CG-CD	5.27	123.41	111.30
1	H	200	ARG	CB-CA-C	5.26	119.62	110.68
1	V	57	ARG	CB-CG-CD	5.26	123.40	111.30
1	Y	187	PRO	N-CA-CB	5.25	108.38	102.60
1	G	67	ASP	N-CA-CB	5.25	118.27	110.29
1	S	233	ALA	CA-C-N	5.25	127.77	120.63
1	S	233	ALA	C-N-CA	5.25	127.77	120.63
1	T	45	VAL	CA-C-O	-5.25	114.91	120.53
1	T	225	VAL	CB-CA-C	5.25	115.72	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ARG	CB-CA-C	5.24	119.57	111.13
1	Y	257	THR	CA-CB-OG1	-5.24	101.74	109.60
1	E	55	HIS	CA-C-O	-5.24	115.05	121.28
1	R	186	ASN	CB-CA-C	-5.24	103.78	111.01
1	K	78	THR	N-CA-C	5.23	117.08	110.33
1	W	216	LYS	N-CA-C	-5.23	105.58	111.28
1	U	101	ASP	CA-CB-CG	5.22	117.82	112.60
1	I	234	GLU	CA-C-N	5.22	127.28	120.28
1	I	234	GLU	C-N-CA	5.22	127.28	120.28
1	N	213	ARG	N-CA-C	-5.22	105.76	111.82
1	G	252	ALA	N-CA-C	-5.22	107.46	113.88
1	M	84	ASP	CA-C-N	5.22	129.77	122.36
1	M	84	ASP	C-N-CA	5.22	129.77	122.36
1	J	90	GLU	CB-CG-CD	5.22	121.47	112.60
1	c	70	ASP	N-CA-CB	5.22	117.56	109.48
1	U	223	HIS	CA-C-O	-5.21	115.32	121.16
1	O	212	ARG	N-CA-C	-5.21	105.60	111.28
1	P	57	ARG	N-CA-C	-5.21	99.62	108.26
1	c	5	ASP	CB-CA-C	5.21	117.75	109.52
1	c	200	ARG	CA-C-O	-5.21	115.01	120.63
1	c	257	THR	CA-CB-OG1	-5.20	101.80	109.60
1	d	51	LYS	CB-CG-CD	5.20	123.27	111.30
1	P	246	ARG	N-CA-C	-5.20	104.87	111.11
1	U	33	GLU	CB-CA-C	5.20	119.23	109.71
1	Q	255	GLY	CA-C-O	-5.20	117.21	122.56
1	V	70	ASP	CB-CA-C	5.20	118.01	109.90
1	C	86	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	101	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	164	HIS	CA-CB-CG	-5.19	108.61	113.80
1	c	84	ASP	CA-CB-CG	5.19	117.79	112.60
1	E	220	ARG	CB-CG-CD	5.18	123.22	111.30
1	I	14	ALA	CA-C-O	-5.18	115.36	121.16
1	H	101	ASP	CA-CB-CG	5.18	117.78	112.60
1	R	74	LYS	CB-CG-CD	5.18	123.21	111.30
1	c	119	ILE	CA-C-N	5.18	126.08	120.44
1	c	119	ILE	C-N-CA	5.18	126.08	120.44
1	L	66	GLU	CB-CA-C	5.18	120.06	109.76
1	D	229	LEU	O-C-N	5.17	127.60	122.12
1	R	135	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	224	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	H	201	ARG	CB-CG-CD	5.17	123.19	111.30
1	V	257	THR	CA-CB-OG1	-5.17	101.85	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	101	ASP	CA-CB-CG	5.16	117.76	112.60
1	a	200	ARG	CA-C-O	-5.16	115.05	120.63
1	L	119	ILE	N-CA-CB	-5.16	105.91	112.15
1	F	33	GLU	CB-CA-C	5.16	118.72	110.16
1	O	15	ARG	CA-C-N	5.16	130.60	123.07
1	O	15	ARG	C-N-CA	5.16	130.60	123.07
1	O	11	ASP	CB-CA-C	5.16	116.93	109.20
1	b	160	ARG	CB-CG-CD	5.15	123.15	111.30
1	H	226	GLU	N-CA-CB	5.15	117.78	110.16
1	K	241	GLU	CB-CA-C	5.15	119.33	110.79
1	J	226	GLU	CA-C-N	5.14	127.13	120.44
1	J	226	GLU	C-N-CA	5.14	127.13	120.44
1	C	101	ASP	CB-CA-C	5.14	120.66	110.42
1	X	92	VAL	CA-C-O	-5.14	115.26	121.28
1	T	245	PHE	CA-C-O	-5.14	115.42	120.82
1	D	144	ASP	CB-CA-C	5.13	120.21	110.51
1	D	56	ASN	CA-C-O	-5.13	115.23	121.28
1	P	66	GLU	CB-CA-C	5.13	118.98	109.54
1	c	231	GLU	N-CA-C	-5.13	105.69	111.28
1	P	144	ASP	CB-CA-C	5.13	121.01	110.40
1	a	257	THR	CA-CB-OG1	-5.12	101.91	109.60
1	I	246	ARG	N-CA-C	-5.12	105.59	111.07
1	M	77	PRO	N-CA-CB	-5.12	99.41	102.79
1	N	117	ALA	CA-C-O	-5.12	116.24	122.03
1	N	215	TYR	N-CA-C	-5.12	105.61	111.14
1	S	5	ASP	CA-C-O	5.12	125.45	120.23
1	E	78	THR	CA-C-O	-5.12	115.45	121.44
1	F	257	THR	CA-CB-OG1	-5.12	101.92	109.60
1	N	156	HIS	CA-CB-CG	5.12	118.92	113.80
1	N	45	VAL	CA-C-O	-5.12	115.07	120.39
1	S	160	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	X	37	GLY	CA-C-N	5.12	128.93	121.31
1	X	37	GLY	C-N-CA	5.12	128.93	121.31
1	A	57	ARG	CB-CG-CD	5.11	123.06	111.30
1	S	61	PHE	N-CA-CB	-5.11	106.13	113.65
1	U	173	ILE	CA-C-O	-5.11	115.02	120.85
1	O	234	GLU	CA-C-N	5.10	127.12	120.28
1	O	234	GLU	C-N-CA	5.10	127.12	120.28
1	a	70	ASP	N-CA-CB	5.10	117.39	109.48
1	Z	61	PHE	N-CA-CB	-5.10	106.15	113.65
1	D	213	ARG	N-CA-C	-5.10	105.91	111.82
1	U	215	TYR	N-CA-C	-5.10	105.61	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	109	ASP	CA-CB-CG	5.10	117.70	112.60
1	W	66	GLU	CA-C-N	5.10	127.95	120.71
1	W	66	GLU	C-N-CA	5.10	127.95	120.71
1	c	78	THR	CA-C-O	-5.09	115.50	121.46
1	G	172	ALA	CA-C-O	-5.09	114.85	121.11
1	C	90	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	134	ASN	N-CA-CB	-5.09	105.93	114.27
1	B	134	ASN	CA-CB-CG	-5.08	107.52	112.60
1	D	15	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	F	31	GLU	CB-CG-CD	-5.08	103.96	112.60
1	b	51	LYS	N-CA-CB	5.08	118.54	110.16
1	C	102	ARG	N-CA-C	-5.08	106.39	112.59
1	D	69	PRO	CA-C-O	-5.07	112.22	118.81
1	M	97	GLY	O-C-N	5.07	126.67	122.71
1	U	67	ASP	CA-C-O	-5.07	115.61	121.19
1	C	19	ASP	CA-CB-CG	-5.07	107.53	112.60
1	E	2	SER	CA-C-N	5.06	131.21	121.54
1	E	2	SER	C-N-CA	5.06	131.21	121.54
1	K	57	ARG	N-CA-C	-5.06	100.65	108.90
1	S	57	ARG	CD-NE-CZ	5.06	131.48	124.40
1	Z	67	ASP	CA-C-O	-5.06	116.19	121.55
1	R	253	THR	N-CA-CB	-5.06	103.76	111.19
1	U	233	ALA	O-C-N	5.05	127.48	122.12
1	X	244	VAL	O-C-N	5.05	127.03	121.83
1	P	69	PRO	CA-C-O	-5.05	112.82	118.98
1	X	241	GLU	CB-CA-C	5.05	119.18	110.79
1	R	90	GLU	CB-CG-CD	5.05	121.19	112.60
1	Z	109	ASP	CA-CB-CG	5.05	117.65	112.60
1	b	57	ARG	N-CA-CB	-5.04	102.85	110.77
1	c	47	LYS	CB-CA-C	5.04	119.27	109.33
1	O	6	PRO	N-CA-C	5.04	120.23	114.03
1	V	199	ARG	O-C-N	5.04	127.48	122.03
1	Z	246	ARG	N-CA-C	-5.04	105.70	111.14
1	c	17	ALA	CA-C-N	5.04	127.30	120.65
1	c	17	ALA	C-N-CA	5.04	127.30	120.65
1	I	252	ALA	N-CA-C	-5.04	107.30	113.50
1	P	97	GLY	O-C-N	5.04	127.14	122.81
1	O	7	ARG	N-CA-CB	5.04	118.87	110.41
1	P	224	THR	CA-CB-OG1	5.04	117.16	109.60
1	S	128	HIS	CA-C-O	-5.04	114.78	121.08
1	K	199	ARG	O-C-N	5.03	127.46	122.03
1	W	26	SER	CB-CA-C	5.03	117.93	109.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	69	PRO	CB-CA-C	-5.03	103.45	111.04
1	H	57	ARG	N-CA-C	-5.03	99.08	108.02
1	Q	144	ASP	CA-CB-CG	5.03	117.63	112.60
1	Y	156	HIS	CB-CA-C	5.02	118.70	109.46
1	d	15	ARG	CB-CA-C	5.02	117.88	110.14
1	C	246	ARG	N-CA-C	-5.02	105.08	111.11
1	X	206	GLU	CB-CG-CD	5.02	121.14	112.60
1	T	246	ARG	N-CA-CB	5.02	117.29	110.01
1	J	99	VAL	CA-C-N	5.02	127.25	120.38
1	J	99	VAL	C-N-CA	5.02	127.25	120.38
1	J	101	ASP	CA-C-O	-5.02	113.33	120.51
1	E	119	ILE	CB-CA-C	5.01	117.41	111.59
1	H	155	VAL	CA-C-O	-5.01	115.20	120.27
1	L	101	ASP	CA-CB-CG	5.01	117.61	112.60
1	W	101	ASP	CA-CB-CG	5.01	117.61	112.60
1	Y	19	ASP	CA-CB-CG	-5.01	107.59	112.60
1	M	257	THR	CA-CB-OG1	-5.01	102.08	109.60
1	a	257	THR	CA-C-O	-5.01	115.05	120.81
1	d	258	ARG	CG-CD-NE	5.01	123.02	112.00
1	R	2	SER	CA-C-N	5.01	126.95	120.44
1	R	2	SER	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

All (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	17	ALA	Peptide
1	F	18	ALA	Peptide
1	F	2	SER	Peptide
1	H	253	THR	Peptide
1	J	17	ALA	Peptide
1	K	252	ALA	Peptide
1	L	252	ALA	Peptide
1	N	71	LEU	Peptide
1	O	252	ALA	Peptide
1	R	252	ALA	Peptide
1	T	17	ALA	Peptide
1	T	252	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	V	253	THR	Peptide
1	X	252	ALA	Peptide
1	X	30	ALA	Peptide
1	Z	2	SER	Peptide
1	Z	252	ALA	Peptide
1	c	252	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1994	0	1974	23	0
1	B	2002	0	1987	23	0
1	C	1996	0	1981	33	0
1	D	1980	0	1955	20	0
1	E	1974	0	1947	18	0
1	F	1988	0	1968	40	0
1	G	1966	0	1935	28	0
1	H	1966	0	1935	25	0
1	I	1966	0	1935	19	0
1	J	1982	0	1960	28	0
1	K	1974	0	1947	20	0
1	L	1974	0	1947	29	0
1	M	1966	0	1935	33	0
1	N	1966	0	1935	33	0
1	O	1966	0	1935	31	0
1	P	1966	0	1935	29	0
1	Q	1974	0	1948	22	0
1	R	1966	0	1935	26	0
1	S	1974	0	1947	37	0
1	T	1974	0	1947	17	0
1	U	1974	0	1947	24	0
1	V	1966	0	1935	33	0
1	W	1972	0	1943	18	0
1	X	1972	0	1943	30	0
1	Y	1980	0	1955	33	0
1	Z	1980	0	1955	27	0
1	a	1972	0	1943	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	1972	0	1943	35	0
1	c	1980	0	1955	25	0
1	d	1972	0	1943	34	0
2	A	33	0	0	0	0
2	B	66	0	0	0	0
2	D	33	0	0	0	0
2	E	33	0	0	0	0
2	F	27	0	0	0	0
2	G	66	0	0	2	0
2	H	27	0	0	0	0
2	J	33	0	0	0	0
2	K	33	0	0	0	0
2	L	33	0	0	0	0
2	M	27	0	0	0	0
2	N	27	0	0	0	0
2	O	27	0	0	0	0
2	Q	60	0	0	0	0
2	R	33	0	0	1	0
2	S	33	0	0	0	0
2	T	33	0	0	0	0
2	U	33	0	0	0	0
2	W	60	0	0	0	0
2	X	33	0	0	0	0
2	Y	33	0	0	0	0
2	a	60	0	0	2	0
2	b	33	0	0	2	0
2	c	60	0	0	0	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	M	2	0	0	1	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	1	0
3	T	1	0	0	0	0
3	X	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	15	0	0	0	0
4	F	10	0	0	0	0
4	G	15	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	0	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	10	0	0	0	0
4	M	10	0	0	0	0
4	N	10	0	0	0	0
4	O	10	0	0	0	0
4	P	15	0	0	0	0
4	Q	15	0	0	0	0
4	R	10	0	0	0	0
4	S	15	0	0	0	0
4	T	10	0	0	0	0
4	U	15	0	0	0	0
4	V	15	0	0	0	0
4	W	10	0	0	0	0
4	X	10	0	0	0	0
4	Y	10	0	0	0	0
4	Z	10	0	0	0	0
4	a	15	0	0	0	0
4	b	10	0	0	0	0
4	c	15	0	0	0	0
4	d	10	0	0	0	0
5	A	11	0	0	0	0
5	B	19	0	0	1	0
5	C	15	0	0	1	0
5	D	13	0	0	1	0
5	E	11	0	0	0	0
5	F	7	0	0	1	0
5	G	4	0	0	0	0
5	H	7	0	0	1	0
5	I	4	0	0	0	0
5	J	10	0	0	1	0
5	K	7	0	0	0	0
5	L	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	6	0	0	0	0
5	N	4	0	0	1	0
5	O	8	0	0	0	0
5	P	5	0	0	0	0
5	Q	5	0	0	1	0
5	R	7	0	0	0	0
5	S	8	0	0	0	0
5	T	8	0	0	0	0
5	U	9	0	0	0	0
5	V	6	0	0	0	0
5	W	5	0	0	1	0
5	X	2	0	0	0	0
5	Y	3	0	0	0	0
5	Z	4	0	0	1	0
5	a	6	0	0	0	0
5	b	6	0	0	0	0
5	c	7	0	0	0	0
5	d	5	0	0	1	0
All	All	60786	0	58450	774	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (774) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201[B]:ARG:HG3	1:B:201[B]:ARG:HH11	0.98	1.14
1:A:201[A]:ARG:HG2	1:A:201[A]:ARG:HH11	1.11	1.12
1:W:15:ARG:NH2	1:W:15:ARG:HB2	1.84	0.92
1:S:220:ARG:NH2	3:S:302:CL:CL	2.41	0.91
1:U:246:ARG:HG2	1:U:246:ARG:HH11	1.38	0.88
1:R:196:GLU:OE2	1:R:199:ARG:NH1	2.06	0.87
1:b:157[A]:GLN:NE2	2:b:301[A]:VFT:N18	2.24	0.86
1:a:246:ARG:HH11	1:a:246:ARG:HG2	1.39	0.86
1:W:15:ARG:HB2	1:W:15:ARG:CZ	2.05	0.86
1:N:246:ARG:HG2	1:N:246:ARG:HH11	1.40	0.85
1:B:201[B]:ARG:HG3	1:B:201[B]:ARG:NH1	1.73	0.85
1:F:246[B]:ARG:HH21	1:F:246[B]:ARG:CG	1.91	0.84
1:b:201:ARG:HG2	1:b:201:ARG:HH11	1.42	0.83
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.42	0.83
1:Z:253:THR:HG22	1:Z:253:THR:O	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:157[A]:GLN:NE2	2:a:301[A]:VFT:C17	2.42	0.83
1:F:246[A]:ARG:HH11	1:F:246[A]:ARG:HG2	1.44	0.82
1:A:201[A]:ARG:HG2	1:A:201[A]:ARG:NH1	1.84	0.81
1:I:246:ARG:HG2	1:I:246:ARG:HH11	1.43	0.81
1:G:254:ARG:HB2	1:G:254:ARG:HH21	1.45	0.80
1:F:235:SER:HB2	5:F:403:HOH:O	1.82	0.79
1:H:201:ARG:HG2	1:H:201:ARG:HH11	1.47	0.79
1:J:246:ARG:HG2	1:J:246:ARG:HH11	1.48	0.78
1:Z:253:THR:O	1:Z:253:THR:CG2	2.30	0.78
1:S:201:ARG:HH11	1:S:201:ARG:HG2	1.48	0.78
1:X:164:HIS:HE1	1:X:201:ARG:HG3	1.46	0.78
1:G:199:ARG:HG2	1:G:199:ARG:HH21	1.48	0.77
1:F:246[B]:ARG:HH21	1:F:246[B]:ARG:HG3	1.48	0.77
1:H:196:GLU:OE2	1:H:199:ARG:NH1	2.17	0.77
1:a:246:ARG:HH11	1:a:246:ARG:CG	1.98	0.76
1:C:246:ARG:HH11	1:C:246:ARG:HG2	1.49	0.75
1:Q:201:ARG:HG2	1:Q:201:ARG:HH11	1.51	0.75
1:b:160:ARG:HH21	1:b:160:ARG:HG3	1.50	0.74
1:b:258:ARG:CG	1:b:258:ARG:HH11	2.00	0.74
1:D:201:ARG:HH11	1:D:201:ARG:HG2	1.53	0.74
1:P:157:GLN:NE2	2:R:301[A]:VFT:N18	2.37	0.73
1:H:235:SER:HB2	5:H:405:HOH:O	1.88	0.72
1:R:246:ARG:HH11	1:R:246:ARG:HG2	1.52	0.72
1:P:201:ARG:HG3	1:P:201:ARG:HH11	1.53	0.72
1:B:196:GLU:OE2	1:B:199:ARG:NH1	2.21	0.72
1:O:253:THR:HG23	1:O:253:THR:O	1.90	0.72
1:J:246:ARG:HH11	1:J:246:ARG:CG	2.02	0.72
1:A:246:ARG:HH11	1:A:246:ARG:CG	2.04	0.71
1:F:246[B]:ARG:HG3	1:F:246[B]:ARG:NH2	2.03	0.71
1:S:246:ARG:HG2	1:S:246:ARG:HH11	1.55	0.71
1:N:246:ARG:HH11	1:N:246:ARG:CG	2.02	0.71
1:O:196:GLU:OE2	1:O:199:ARG:NH2	2.23	0.70
1:a:224:THR:OG1	1:a:227:GLU:HG3	1.91	0.70
1:Q:43:HIS:CE1	1:R:43:HIS:HD2	2.09	0.70
1:C:246:ARG:HH11	1:C:246:ARG:CG	2.05	0.70
1:X:15:ARG:HB2	1:X:15:ARG:NH2	2.08	0.69
1:a:157[A]:GLN:HE22	2:a:301[A]:VFT:C17	2.06	0.69
1:b:196:GLU:OE1	1:b:199:ARG:NH1	2.26	0.69
1:D:193:MET:HE2	1:D:193:MET:HA	1.75	0.69
1:a:164:HIS:HE1	1:a:201:ARG:HG3	1.57	0.69
1:W:43:HIS:CE1	1:X:43:HIS:HD2	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246[A]:ARG:NH1	1:F:247:ASP:OD1	2.27	0.68
1:V:43:HIS:HD2	1:X:43:HIS:NE2	1.91	0.68
1:X:164:HIS:CE1	1:X:201:ARG:HG3	2.28	0.67
1:F:181:VAL:HG22	1:F:193:MET:CE	2.25	0.67
1:O:246:ARG:HG2	1:O:246:ARG:HH11	1.57	0.67
1:I:246:ARG:HH11	1:I:246:ARG:CG	2.08	0.67
1:R:253:THR:HG23	1:R:253:THR:O	1.94	0.67
1:L:224:THR:OG1	1:L:227:GLU:HG3	1.95	0.67
1:H:43:HIS:CE1	1:I:43:HIS:HD2	2.13	0.67
1:U:246:ARG:HH11	1:U:246:ARG:CG	2.09	0.66
1:S:43:HIS:ND1	1:U:43:HIS:CE1	2.63	0.66
1:W:15:ARG:C	1:W:16:LEU:HD12	2.21	0.66
1:P:196:GLU:OE2	1:P:199:ARG:NH1	2.29	0.65
1:d:196:GLU:OE2	1:d:199:ARG:NH1	2.21	0.65
1:E:246:ARG:HD2	1:E:246:ARG:C	2.22	0.65
1:V:246:ARG:HH11	1:V:246:ARG:CG	2.10	0.65
1:R:253:THR:O	1:R:253:THR:CG2	2.45	0.65
1:W:164:HIS:HE1	1:W:201:ARG:HD2	1.62	0.65
1:T:164:HIS:HE1	1:T:201:ARG:HG3	1.62	0.64
1:W:196:GLU:OE2	1:W:199:ARG:NH1	2.30	0.64
1:O:246:ARG:HH11	1:O:246:ARG:CG	2.11	0.64
1:I:164:HIS:HE1	1:I:201:ARG:HG3	1.63	0.64
1:V:246:ARG:NH1	1:V:246:ARG:HB3	2.13	0.63
1:Y:254:ARG:HH21	1:Y:254:ARG:HB2	1.64	0.63
1:Y:1:MET:O	1:Y:1:MET:CE	2.47	0.62
1:A:201[A]:ARG:HH11	1:A:201[A]:ARG:CG	2.00	0.62
1:P:246:ARG:CG	1:P:246:ARG:HH11	2.12	0.62
1:O:253:THR:O	1:O:253:THR:CG2	2.47	0.62
1:a:164:HIS:CE1	1:a:201:ARG:HG3	2.33	0.62
1:X:253:THR:O	1:X:253:THR:CG2	2.47	0.62
1:R:164:HIS:HE1	1:R:201:ARG:HG3	1.63	0.62
1:F:246[A]:ARG:HH11	1:F:246[A]:ARG:CG	2.12	0.61
1:b:201:ARG:HG2	1:b:201:ARG:NH1	2.15	0.61
1:A:196:GLU:OE1	1:A:199:ARG:NH1	2.33	0.61
1:K:196:GLU:OE2	1:K:199:ARG:NH2	2.22	0.61
1:D:235:SER:HB2	5:D:404:HOH:O	1.99	0.61
1:c:164:HIS:HE1	1:c:201:ARG:HG3	1.65	0.61
1:F:235:SER:HB3	1:F:242:VAL:HG11	1.82	0.61
1:S:246:ARG:HH11	1:S:246:ARG:CG	2.14	0.61
1:S:196:GLU:OE1	1:S:199:ARG:NH2	2.33	0.60
1:F:246[B]:ARG:HH21	1:F:246[B]:ARG:CB	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:GLU:O	1:H:238:GLN:HG3	2.01	0.60
1:V:201:ARG:HG3	1:V:201:ARG:HH11	1.66	0.60
1:d:164:HIS:HE1	1:d:201:ARG:HG3	1.66	0.60
1:M:246:ARG:HH11	1:M:246:ARG:HG2	1.67	0.60
1:X:253:THR:O	1:X:253:THR:HG23	2.01	0.60
1:Y:201:ARG:HG2	1:Y:201:ARG:HH11	1.66	0.60
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.02	0.60
1:O:15:ARG:NH2	1:O:15:ARG:HB2	2.17	0.60
1:T:164:HIS:CE1	1:T:201:ARG:HG3	2.37	0.59
1:b:246:ARG:HG2	1:b:246:ARG:HH11	1.67	0.59
1:A:229:LEU:HD21	1:A:249:ILE:HG22	1.84	0.59
1:M:246:ARG:HH11	1:M:246:ARG:CG	2.15	0.59
1:H:224:THR:OG1	1:H:227:GLU:HG3	2.03	0.59
1:M:16:LEU:N	1:M:16:LEU:HD12	2.17	0.59
1:N:15:ARG:C	1:N:16:LEU:HD12	2.28	0.59
1:N:176:ASP:OD2	1:L:254:ARG:NH1	2.35	0.59
1:a:198:MET:HE2	1:a:211:LEU:HD13	1.85	0.59
1:C:149:LEU:HD21	1:C:161:ILE:HG21	1.83	0.58
1:Q:43:HIS:CE1	1:R:43:HIS:CD2	2.90	0.58
1:U:15:ARG:HH21	1:U:15:ARG:HB2	1.68	0.58
1:C:196:GLU:OE2	1:C:199:ARG:NH1	2.36	0.58
1:H:193:MET:HE3	1:H:215:TYR:HD2	1.68	0.58
1:M:36:GLU:HB3	1:M:54:LYS:HD3	1.84	0.58
1:P:246:ARG:HB3	1:P:246:ARG:NH1	2.17	0.58
1:B:57:ARG:NH1	5:B:401:HOH:O	2.29	0.58
1:G:254:ARG:HH21	1:G:254:ARG:CB	2.15	0.58
1:Y:16:LEU:N	1:Y:16:LEU:HD12	2.19	0.58
1:F:246[B]:ARG:HH21	1:F:246[B]:ARG:HB2	1.69	0.58
1:O:4:ILE:HG22	1:O:4:ILE:O	2.04	0.57
1:J:63:SER:HB3	1:L:60:GLN:HE21	1.68	0.57
1:N:10:ILE:HG22	1:N:11:ASP:O	2.04	0.57
1:Y:183:VAL:HA	1:Y:189:GLU:O	2.05	0.57
1:Z:196:GLU:OE2	1:Z:199:ARG:NH2	2.32	0.57
1:X:15:ARG:HB2	1:X:15:ARG:CZ	2.35	0.57
1:F:246[B]:ARG:CG	1:F:246[B]:ARG:NH2	2.59	0.57
1:O:224:THR:OG1	1:O:227:GLU:HG3	2.04	0.57
1:b:258:ARG:HH11	1:b:258:ARG:HG2	1.67	0.57
1:Q:195:PHE:HZ	1:Q:212:ARG:HG3	1.70	0.57
1:X:246:ARG:NH1	1:X:247:ASP:OD1	2.37	0.57
1:M:60:GLN:HE21	1:N:63:SER:HB3	1.69	0.56
1:T:5:ASP:OD2	1:T:7:ARG:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:24:PRO:HB2	1:a:25:TRP:CD2	2.40	0.56
1:V:193:MET:HE3	1:V:215:TYR:HD2	1.71	0.56
1:W:43:HIS:CE1	1:X:43:HIS:CD2	2.92	0.56
1:J:200[B]:ARG:NH1	5:J:401:HOH:O	2.29	0.56
1:S:220:ARG:HH21	1:S:220:ARG:HG3	1.70	0.56
1:I:164:HIS:CE1	1:I:201:ARG:HG3	2.39	0.56
1:M:198:MET:HE2	1:M:211:LEU:HD13	1.87	0.56
1:B:201[B]:ARG:NH1	1:B:201[B]:ARG:CG	2.58	0.56
1:M:196:GLU:OE2	1:M:199:ARG:NH2	2.36	0.55
1:C:157[B]:GLN:H	1:C:157[B]:GLN:NE2	2.05	0.55
1:G:246:ARG:NH1	1:G:246:ARG:HB3	2.21	0.55
1:Y:1:MET:O	1:Y:1:MET:HE2	2.06	0.55
1:K:181:VAL:HG22	1:K:193:MET:CE	2.36	0.55
1:R:246:ARG:HH11	1:R:246:ARG:CG	2.18	0.55
1:C:235:SER:HB2	5:C:407:HOH:O	2.05	0.55
1:W:235:SER:HB2	5:W:402:HOH:O	2.05	0.55
1:a:157[B]:GLN:H	1:a:157[B]:GLN:CD	2.14	0.55
1:d:15:ARG:C	1:d:16:LEU:HD12	2.32	0.55
1:S:131:LEU:N	1:S:131:LEU:HD12	2.21	0.55
1:c:199:ARG:HG2	1:c:199:ARG:HH21	1.71	0.55
1:a:24:PRO:HB2	1:a:25:TRP:CE3	2.41	0.55
1:B:139:GLY:O	1:B:157[A]:GLN:HA	2.07	0.55
1:J:131:LEU:N	1:J:131:LEU:HD12	2.21	0.55
1:Z:16:LEU:HD12	1:Z:16:LEU:N	2.22	0.55
1:G:15:ARG:C	1:G:16:LEU:HD12	2.32	0.55
1:J:223:HIS:C	1:J:224:THR:O	2.48	0.54
1:c:85:HIS:O	1:c:110:HIS:HA	2.07	0.54
1:C:254:ARG:HH11	1:V:176:ASP:CG	2.14	0.54
1:Q:195:PHE:CZ	1:Q:212:ARG:HG3	2.43	0.54
1:L:150:SER:HB2	1:L:167:SER:O	2.07	0.54
1:C:157[B]:GLN:H	1:C:157[B]:GLN:HE21	1.53	0.54
1:C:199:ARG:O	1:C:202:GLY:N	2.35	0.54
1:I:16:LEU:HD12	1:I:16:LEU:N	2.23	0.54
1:Y:176:ASP:OD1	1:d:254:ARG:HD2	2.06	0.54
1:A:246:ARG:CG	1:A:246:ARG:NH1	2.66	0.54
1:G:60:GLN:HE21	1:H:63:SER:HB3	1.71	0.54
1:N:24:PRO:HB2	1:N:25:TRP:CD2	2.43	0.54
1:Y:15:ARG:HH21	1:Y:15:ARG:HB2	1.72	0.54
1:d:258:ARG:HH11	1:d:258:ARG:HB2	1.73	0.54
1:R:164:HIS:CE1	1:R:201:ARG:HG3	2.42	0.54
1:U:246:ARG:HG2	1:U:246:ARG:NH1	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:16:LEU:HD23	1:d:20:VAL:HG11	1.90	0.54
1:B:254:ARG:HB2	1:B:254:ARG:HH21	1.73	0.54
1:N:132:VAL:HG12	1:N:133:ASN:N	2.23	0.54
1:c:113:ILE:HD13	1:c:119:ILE:CD1	2.37	0.54
1:F:193:MET:HE3	1:F:215:TYR:HD2	1.74	0.53
1:P:60:GLN:HE21	1:Q:63:SER:HB3	1.72	0.53
1:H:246:ARG:HH11	1:H:246:ARG:CG	2.20	0.53
1:G:246:ARG:NH1	1:G:247:ASP:OD1	2.36	0.53
1:J:198:MET:HE2	1:J:211:LEU:HD13	1.90	0.53
1:b:79:ARG:HB2	1:b:79:ARG:CZ	2.38	0.53
1:M:164:HIS:CE1	1:M:201:ARG:HG3	2.44	0.53
1:N:85:HIS:O	1:N:110:HIS:HA	2.08	0.53
1:A:149:LEU:HD21	1:A:161:ILE:HG21	1.90	0.53
1:N:235:SER:HB2	5:N:402:HOH:O	2.08	0.53
1:b:160:ARG:HH21	1:b:160:ARG:CG	2.21	0.53
1:b:246:ARG:HH11	1:b:246:ARG:CG	2.21	0.53
1:c:164:HIS:CE1	1:c:201:ARG:HG3	2.42	0.53
1:B:164:HIS:HE1	1:B:201[B]:ARG:HG2	1.73	0.53
1:J:43:HIS:CE1	1:K:43:HIS:ND1	2.76	0.53
1:J:196:GLU:OE1	1:J:196:GLU:HA	2.07	0.53
1:Q:246:ARG:HH11	1:Q:246:ARG:CG	2.21	0.53
1:V:199:ARG:O	1:V:202:GLY:N	2.36	0.53
1:Z:15:ARG:HB3	1:Z:15:ARG:HH21	1.73	0.53
1:Z:235:SER:HB2	5:Z:401:HOH:O	2.08	0.53
1:W:164:HIS:HE1	1:W:201:ARG:CD	2.21	0.53
1:V:164:HIS:CE1	1:V:201:ARG:HG2	2.45	0.52
1:L:246:ARG:HH11	1:L:246:ARG:CG	2.23	0.52
1:T:149:LEU:HD21	1:T:161:ILE:HG21	1.90	0.52
1:T:195:PHE:HZ	1:T:212:ARG:HG3	1.75	0.52
1:V:246:ARG:CG	1:V:246:ARG:NH1	2.71	0.52
1:H:193:MET:HE1	1:H:245:PHE:CE1	2.45	0.52
1:O:164:HIS:HE1	1:O:201:ARG:HG2	1.73	0.52
1:U:90:GLU:O	1:U:115:ALA:HA	2.09	0.52
1:d:60:GLN:OE1	1:d:60:GLN:N	2.38	0.52
1:Y:246:ARG:HH11	1:Y:246:ARG:CG	2.22	0.52
1:O:246:ARG:NH1	1:O:247:ASP:OD1	2.39	0.52
1:L:24:PRO:HB2	1:L:25:TRP:CE3	2.45	0.52
1:M:84:ASP:O	1:M:109:ASP:HA	2.10	0.52
1:N:150:SER:HB2	1:N:167:SER:O	2.08	0.52
1:b:16:LEU:N	1:b:16:LEU:HD12	2.25	0.52
1:d:149:LEU:HD21	1:d:161:ILE:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ILE:HD13	1:F:119:ILE:HD11	1.91	0.51
1:O:149:LEU:HD21	1:O:161:ILE:HG21	1.92	0.51
1:B:84:ASP:O	1:B:109:ASP:HA	2.09	0.51
1:N:49:PRO:HD2	1:N:78:THR:O	2.10	0.51
1:Y:246:ARG:HH11	1:Y:246:ARG:HG2	1.75	0.51
1:M:220:ARG:NH1	3:M:302:CL:CL	2.76	0.51
1:S:164:HIS:CE1	1:S:201:ARG:HG3	2.45	0.51
1:c:16:LEU:N	1:c:16:LEU:HD12	2.26	0.51
1:W:166:PHE:O	1:W:182:THR:HA	2.10	0.51
1:X:145:ASP:O	1:X:163:ALA:HA	2.10	0.51
1:T:60:GLN:HG3	1:T:61:PHE:CE2	2.46	0.51
1:M:43:HIS:HD2	1:O:43:HIS:CD2	2.29	0.51
1:Q:246:ARG:NH1	1:Q:246:ARG:HB3	2.26	0.51
1:S:166:PHE:CD1	1:S:166:PHE:C	2.88	0.51
1:O:250:GLN:O	1:O:253:THR:HG22	2.11	0.51
1:S:258:ARG:HG3	1:S:258:ARG:HH11	1.76	0.51
1:d:164:HIS:CE1	1:d:201:ARG:HG3	2.46	0.51
1:C:199:ARG:HG2	1:C:199:ARG:HH21	1.75	0.51
1:O:150:SER:HB2	1:O:167:SER:O	2.10	0.51
1:L:47:LYS:O	1:L:50:THR:OG1	2.22	0.51
1:Y:15:ARG:C	1:Y:16:LEU:HD12	2.36	0.51
1:C:246:ARG:CG	1:C:246:ARG:NH1	2.70	0.51
1:G:65:GLY:O	1:G:96:ARG:HD3	2.11	0.51
1:M:15:ARG:C	1:M:16:LEU:HD12	2.36	0.51
1:X:246:ARG:HG2	1:X:246:ARG:HH11	1.75	0.51
1:a:218:VAL:HG21	1:a:249:ILE:CD1	2.41	0.51
1:I:109:ASP:O	1:I:127:ASN:HA	2.11	0.51
1:X:38:THR:HA	1:X:56:ASN:O	2.11	0.51
1:J:15:ARG:CB	1:J:15:ARG:HH21	2.24	0.50
1:S:43:HIS:CE1	1:T:43:HIS:ND1	2.79	0.50
1:d:89:ARG:HB2	1:d:114:MET:HA	1.93	0.50
1:F:139:GLY:O	1:F:157[A]:GLN:HA	2.11	0.50
1:N:238:GLN:HB3	1:K:205:SER:HB3	1.92	0.50
1:M:24:PRO:HB2	1:M:25:TRP:CD2	2.47	0.50
1:b:35:GLY:N	1:b:52:ILE:O	2.39	0.50
1:J:90:GLU:O	1:J:115:ALA:HA	2.12	0.50
1:P:246:ARG:CG	1:P:246:ARG:NH1	2.75	0.50
1:L:119:ILE:HD13	1:L:125:ILE:HD11	1.92	0.50
1:Z:102:ARG:HH21	1:Z:102:ARG:HB3	1.76	0.50
1:d:246:ARG:HH11	1:d:246:ARG:CG	2.24	0.50
1:C:164:HIS:CE1	1:C:201:ARG:HG3	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:THR:HG23	1:E:253:THR:O	2.12	0.50
1:N:73:TYR:CE2	1:N:75:GLY:HA2	2.47	0.50
1:b:131:LEU:N	1:b:131:LEU:HD12	2.27	0.50
1:H:132:VAL:HG12	1:H:133:ASN:N	2.27	0.50
1:N:113:ILE:HD13	1:N:119:ILE:CD1	2.42	0.50
1:N:176:ASP:CG	1:L:254:ARG:HH11	2.20	0.50
1:O:246:ARG:CG	1:O:246:ARG:NH1	2.72	0.50
1:P:43:HIS:HD2	1:R:43:HIS:CD2	2.30	0.50
1:F:89:ARG:HB2	1:F:114:MET:HA	1.93	0.49
1:W:142:HIS:HB2	1:W:160:ARG:HG2	1.94	0.49
1:J:193:MET:HE1	1:J:245:PHE:CE1	2.48	0.49
1:S:201:ARG:HG2	1:S:201:ARG:NH1	2.20	0.49
1:U:132:VAL:O	1:U:133:ASN:C	2.55	0.49
1:U:149:LEU:HA	1:U:167:SER:OG	2.12	0.49
1:Z:164:HIS:HE1	1:Z:201:ARG:HG3	1.77	0.49
1:G:246:ARG:HH11	1:G:246:ARG:CG	2.25	0.49
2:G:301[A]:VFT:C17	1:H:157:GLN:OE1	2.60	0.49
1:M:16:LEU:N	1:M:16:LEU:CD1	2.75	0.49
1:X:234:GLU:O	1:X:238:GLN:HG3	2.12	0.49
1:O:15:ARG:C	1:O:16:LEU:HD12	2.38	0.49
1:H:246:ARG:HB3	1:H:246:ARG:NH1	2.26	0.49
1:O:164:HIS:CE1	1:O:201:ARG:HG2	2.48	0.49
1:K:43:HIS:CE1	1:L:43:HIS:ND1	2.81	0.49
1:K:193:MET:HE3	1:K:215:TYR:HD2	1.78	0.49
1:K:195:PHE:HZ	1:K:212:ARG:HG3	1.77	0.49
1:d:60:GLN:H	1:d:60:GLN:CD	2.19	0.49
1:N:176:ASP:OD1	1:L:254:ARG:HD2	2.12	0.49
1:X:246:ARG:HH11	1:X:246:ARG:CG	2.25	0.49
1:c:234:GLU:O	1:c:238:GLN:HG3	2.13	0.49
1:J:131:LEU:N	1:J:131:LEU:CD1	2.75	0.49
1:F:199:ARG:HG2	1:F:199:ARG:HH21	1.77	0.49
1:Z:15:ARG:CZ	1:Z:15:ARG:HB2	2.43	0.49
1:F:113:ILE:HD13	1:F:119:ILE:CD1	2.43	0.49
1:I:149:LEU:HD21	1:I:161:ILE:HG21	1.94	0.49
1:S:121:HIS:O	1:S:122:ASP:HB2	2.13	0.49
1:Z:150:SER:HB2	1:Z:167:SER:O	2.12	0.49
1:C:235:SER:HB3	1:C:242:VAL:HG11	1.94	0.49
1:P:201:ARG:HG3	1:P:201:ARG:NH1	2.25	0.49
1:Y:117:ALA:HA	1:Y:135:THR:O	2.12	0.49
1:C:119:ILE:HD13	1:C:125:ILE:CD1	2.42	0.48
1:N:246:ARG:CG	1:N:246:ARG:NH1	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:109:ASP:O	1:S:127:ASN:HA	2.13	0.48
1:c:24:PRO:HB2	1:c:25:TRP:CD2	2.47	0.48
1:N:16:LEU:O	1:N:17:ALA:C	2.56	0.48
1:O:204:SER:O	1:O:208:ILE:HG13	2.13	0.48
1:J:61:PHE:HA	1:L:61:PHE:CZ	2.48	0.48
1:V:164:HIS:HE1	1:V:201:ARG:HG2	1.77	0.48
1:X:111:ASN:OD1	1:X:129:CYS:HB2	2.13	0.48
1:Z:157[B]:GLN:H	1:Z:157[B]:GLN:CD	2.20	0.48
1:c:43:HIS:CE1	1:d:43:HIS:ND1	2.81	0.48
1:D:149:LEU:HD21	1:D:161:ILE:HG21	1.95	0.48
1:N:113:ILE:HD13	1:N:119:ILE:HD11	1.95	0.48
1:J:69:PRO:HG2	1:L:114:MET:HE2	1.95	0.48
1:V:246:ARG:HH11	1:V:246:ARG:HG2	1.78	0.48
1:V:246:ARG:NH1	1:V:246:ARG:CB	2.77	0.48
1:Y:246:ARG:NH1	1:Y:247:ASP:OD1	2.46	0.48
1:a:65:GLY:O	1:a:96:ARG:NH1	2.44	0.48
1:M:193:MET:HE3	1:M:215:TYR:HD2	1.77	0.48
1:L:149:LEU:HD21	1:L:161:ILE:HG21	1.96	0.48
1:W:14:ALA:O	1:W:15:ARG:HG3	2.13	0.48
1:b:160:ARG:CG	1:b:160:ARG:NH2	2.76	0.48
1:G:212:ARG:NH1	1:U:234:GLU:OE1	2.46	0.48
1:H:196:GLU:CD	1:H:199:ARG:HH11	2.21	0.48
1:T:43:HIS:CE1	1:U:43:HIS:ND1	2.81	0.48
1:a:68:THR:HG23	1:a:70:ASP:H	1.79	0.48
1:b:46:LEU:HA	1:b:64:VAL:O	2.13	0.48
1:G:91:GLY:HA3	1:G:116:TYR:CE1	2.49	0.48
1:G:254:ARG:HB2	1:G:254:ARG:NH2	2.23	0.48
1:d:246:ARG:HH11	1:d:246:ARG:HG2	1.78	0.48
1:M:183:VAL:HA	1:M:189:GLU:O	2.13	0.48
1:Q:199:ARG:HG2	1:Q:199:ARG:HH21	1.78	0.48
1:R:195:PHE:HZ	1:R:212:ARG:HG3	1.78	0.48
1:X:34:ILE:CG2	1:X:38:THR:HG21	2.44	0.48
1:Y:119:ILE:HD12	1:Y:125:ILE:HD11	1.94	0.48
1:G:234:GLU:O	1:G:238:GLN:HG3	2.13	0.48
1:K:109:ASP:O	1:K:127:ASN:HA	2.14	0.48
1:P:42:PRO:O	1:P:44:VAL:HG23	2.14	0.48
1:X:57:ARG:NH1	1:X:57:ARG:HG3	2.27	0.48
1:Z:24:PRO:HB2	1:Z:25:TRP:CE3	2.48	0.48
1:C:246:ARG:NH1	1:C:246:ARG:HB3	2.29	0.48
1:D:195:PHE:HZ	1:D:212:ARG:HG3	1.78	0.48
1:D:218:VAL:HG21	1:D:249:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:ARG:CB	1:G:254:ARG:NH2	2.77	0.48
1:L:166:PHE:CD1	1:L:166:PHE:C	2.92	0.48
1:Z:195:PHE:CZ	1:Z:212:ARG:HG3	2.49	0.48
1:D:166:PHE:O	1:D:182:THR:HA	2.14	0.48
1:P:16:LEU:HD12	1:P:16:LEU:N	2.29	0.48
1:b:15:ARG:HA	1:b:15:ARG:HD3	1.71	0.48
1:b:157[A]:GLN:NE2	2:b:301[A]:VFT:C17	2.77	0.48
1:b:258:ARG:HH11	1:b:258:ARG:HG3	1.78	0.48
1:J:130:ILE:C	1:J:131:LEU:HD12	2.38	0.47
1:K:149:LEU:HD21	1:K:161:ILE:HG21	1.95	0.47
1:K:254:ARG:HH21	1:K:254:ARG:HB2	1.79	0.47
1:U:15:ARG:HH21	1:U:15:ARG:CB	2.26	0.47
1:U:246:ARG:NH1	1:U:247:ASP:OD1	2.47	0.47
1:B:193:MET:HE1	1:B:245:PHE:CE1	2.49	0.47
1:a:166:PHE:O	1:a:182:THR:HA	2.14	0.47
1:a:183:VAL:HA	1:a:189:GLU:O	2.14	0.47
1:B:166:PHE:O	1:B:182:THR:HA	2.13	0.47
1:N:166:PHE:CD1	1:N:166:PHE:C	2.92	0.47
1:O:16:LEU:HD12	1:O:16:LEU:N	2.29	0.47
1:W:16:LEU:HD12	1:W:16:LEU:N	2.29	0.47
1:Z:15:ARG:CB	1:Z:15:ARG:NH2	2.77	0.47
1:C:164:HIS:HE1	1:C:201:ARG:HG3	1.80	0.47
1:H:15:ARG:C	1:H:16:LEU:HD12	2.39	0.47
1:N:166:PHE:HB3	1:N:182:THR:HG22	1.97	0.47
1:S:43:HIS:ND1	1:U:43:HIS:HE1	2.12	0.47
1:P:166:PHE:HB3	1:P:182:THR:HG22	1.95	0.47
1:O:24:PRO:HB2	1:O:25:TRP:CD2	2.48	0.47
1:Q:15:ARG:HB2	1:Q:15:ARG:HH21	1.78	0.47
1:d:48:GLY:HA2	1:d:50:THR:OG1	2.15	0.47
1:G:164:HIS:HE1	1:G:201:ARG:HG3	1.80	0.47
1:T:60:GLN:HE21	1:U:63:SER:HB3	1.79	0.47
1:U:193:MET:HE3	1:U:215:TYR:HD2	1.80	0.47
1:Y:16:LEU:N	1:Y:16:LEU:CD1	2.78	0.47
1:F:19:ASP:OD1	1:F:19:ASP:N	2.44	0.47
1:N:162:GLY:O	1:N:165:SER:HB3	2.15	0.47
1:K:164:HIS:HE1	1:K:201:ARG:HG3	1.80	0.47
1:a:15:ARG:C	1:a:16:LEU:HD12	2.39	0.47
1:M:21:GLN:HB2	1:M:39:VAL:HG13	1.97	0.47
1:P:22:VAL:HA	1:P:40:ILE:HB	1.97	0.47
1:P:258:ARG:HH11	1:P:258:ARG:CG	2.28	0.47
1:Q:164:HIS:CE1	1:Q:201:ARG:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:MET:HE3	1:C:215:TYR:HD2	1.81	0.47
1:F:24:PRO:HB2	1:F:25:TRP:CD2	2.49	0.47
1:H:201:ARG:HG2	1:H:201:ARG:NH1	2.23	0.46
1:O:5:ASP:O	1:O:8:ALA:HB3	2.15	0.46
1:S:131:LEU:N	1:S:131:LEU:CD1	2.78	0.46
1:S:166:PHE:O	1:S:182:THR:HA	2.15	0.46
1:D:229:LEU:HD21	1:D:249:ILE:HG22	1.97	0.46
1:H:183:VAL:HA	1:H:189:GLU:O	2.16	0.46
1:J:19:ASP:OD1	1:J:19:ASP:N	2.49	0.46
1:d:40:ILE:O	1:d:41:GLY:O	2.33	0.46
1:A:153:THR:OG1	1:A:167:SER:OG	2.33	0.46
1:C:181:VAL:HG22	1:C:193:MET:CE	2.45	0.46
1:E:201:ARG:HA	1:E:201:ARG:NE	2.30	0.46
1:M:89:ARG:HB2	1:M:114:MET:HA	1.97	0.46
1:Y:1:MET:O	1:Y:1:MET:HG3	2.15	0.46
1:c:199:ARG:HG2	1:c:199:ARG:NH2	2.31	0.46
1:G:193:MET:HE1	1:G:245:PHE:CE1	2.51	0.46
1:H:166:PHE:O	1:H:182:THR:HA	2.15	0.46
1:K:15:ARG:C	1:K:16:LEU:HD12	2.40	0.46
1:b:104:GLU:HG2	1:b:106:THR:OG1	2.16	0.46
1:D:166:PHE:HB3	1:D:182:THR:HG22	1.97	0.46
1:E:225:VAL:HG11	1:E:253:THR:HG21	1.98	0.46
1:L:193:MET:HE1	1:L:245:PHE:CE1	2.51	0.46
1:P:224:THR:OG1	1:P:227:GLU:HG3	2.16	0.46
1:V:38:THR:HA	1:V:56:ASN:O	2.16	0.46
1:Z:15:ARG:C	1:Z:16:LEU:HD12	2.41	0.46
1:a:84:ASP:O	1:a:109:ASP:HA	2.15	0.46
1:F:254:ARG:NH1	1:P:160:ARG:HD2	2.31	0.46
1:O:132:VAL:HG12	1:O:133:ASN:N	2.31	0.46
1:L:109:ASP:O	1:L:127:ASN:HA	2.16	0.46
1:P:43:HIS:HD2	1:R:43:HIS:NE2	2.12	0.46
1:S:195:PHE:HZ	1:S:212:ARG:HG3	1.80	0.46
1:U:104:GLU:HG2	1:U:106:THR:OG1	2.16	0.46
1:X:209:HIS:O	1:X:213:ARG:HG3	2.16	0.46
1:Y:5:ASP:OD1	1:Y:7:ARG:HB2	2.16	0.46
1:Y:234:GLU:OE1	1:c:212:ARG:HD2	2.16	0.46
1:Z:79:ARG:HB2	1:Z:79:ARG:CZ	2.45	0.46
1:C:16:LEU:CD1	1:C:16:LEU:N	2.79	0.46
1:E:102:ARG:O	1:E:103:ALA:HB3	2.15	0.46
1:O:246:ARG:NH1	1:O:246:ARG:HB3	2.31	0.46
1:X:57:ARG:HG3	1:X:57:ARG:HH11	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:199:ARG:HG2	1:X:199:ARG:HH21	1.81	0.46
1:S:130:ILE:C	1:S:131:LEU:HD12	2.41	0.46
1:a:2:SER:OG	1:a:3:LEU:N	2.45	0.46
1:c:183:VAL:HA	1:c:189:GLU:O	2.15	0.46
1:B:11:ASP:CG	1:B:12:PRO:HD2	2.41	0.46
1:V:46:LEU:HA	1:V:64:VAL:O	2.16	0.46
1:X:36:GLU:O	1:X:54:LYS:HA	2.16	0.46
1:d:79:ARG:HB2	1:d:79:ARG:CZ	2.46	0.46
1:F:54:LYS:O	1:F:84:ASP:HA	2.16	0.45
1:F:160:ARG:HH21	1:F:160:ARG:CG	2.29	0.45
1:Y:19:ASP:N	1:Y:19:ASP:OD1	2.41	0.45
1:b:43:HIS:ND1	1:d:43:HIS:CE1	2.84	0.45
1:b:149:LEU:HD21	1:b:161:ILE:HG21	1.98	0.45
1:N:149:LEU:HD21	1:N:161:ILE:HG21	1.99	0.45
1:J:113:ILE:HD13	1:J:119:ILE:HD11	1.98	0.45
1:L:139:GLY:O	1:L:157:GLN:HA	2.16	0.45
1:S:181:VAL:HA	1:S:193:MET:HE2	1.98	0.45
1:V:90:GLU:H	1:V:90:GLU:HG2	1.14	0.45
1:W:51:LYS:HE2	1:W:51:LYS:HB3	1.90	0.45
1:D:183:VAL:HA	1:D:189:GLU:O	2.15	0.45
1:K:121:HIS:O	1:K:122:ASP:HB2	2.16	0.45
1:b:258:ARG:CG	1:b:258:ARG:NH1	2.68	0.45
1:B:164:HIS:CE1	1:B:201[A]:ARG:HG3	2.52	0.45
1:E:131:LEU:N	1:E:131:LEU:HD12	2.31	0.45
1:O:10:ILE:HG22	1:O:11:ASP:H	1.81	0.45
1:J:195:PHE:HZ	1:J:212:ARG:HG3	1.81	0.45
1:L:164:HIS:CE1	1:L:201:ARG:HG3	2.51	0.45
1:L:246:ARG:NH1	1:L:246:ARG:HB3	2.31	0.45
1:T:195:PHE:CZ	1:T:212:ARG:HG3	2.51	0.45
1:c:80:LEU:HD12	1:c:105:THR:O	2.16	0.45
1:M:121:HIS:O	1:M:122:ASP:HB2	2.16	0.45
1:S:19:ASP:OD1	1:S:19:ASP:N	2.45	0.45
1:Y:68:THR:HG23	1:Y:70:ASP:H	1.81	0.45
1:b:199:ARG:HB3	1:b:199:ARG:CZ	2.47	0.45
1:d:235:SER:HB2	5:d:401:HOH:O	2.17	0.45
1:M:72:LYS:O	1:M:74:LYS:HE2	2.16	0.45
1:P:246:ARG:HH11	1:P:246:ARG:HG2	1.80	0.45
1:W:102:ARG:O	1:W:103:ALA:HB3	2.15	0.45
1:c:132:VAL:HG12	1:c:133:ASN:H	1.82	0.45
1:L:119:ILE:HD13	1:L:125:ILE:CD1	2.47	0.45
1:Q:131:LEU:N	1:Q:131:LEU:HD12	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:150:SER:HB2	1:R:167:SER:O	2.17	0.45
1:W:73:TYR:CE2	1:W:75:GLY:HA2	2.51	0.45
1:a:16:LEU:HD12	1:a:16:LEU:N	2.32	0.45
1:D:195:PHE:CZ	1:D:212:ARG:HG3	2.51	0.45
1:M:55:HIS:O	1:M:85:HIS:HA	2.17	0.45
1:M:149:LEU:HD21	1:M:161:ILE:HG21	1.98	0.45
1:L:199:ARG:HG2	1:L:199:ARG:HH21	1.82	0.45
1:Y:51:LYS:NZ	1:Y:79:ARG:HD2	2.32	0.45
1:A:166:PHE:O	1:A:182:THR:HA	2.17	0.45
1:C:131:LEU:HD12	1:C:131:LEU:N	2.31	0.45
1:J:91:GLY:HA3	1:J:116:TYR:CE1	2.52	0.45
1:J:119:ILE:HD13	1:J:125:ILE:CD1	2.47	0.45
1:d:131:LEU:N	1:d:131:LEU:CD1	2.80	0.45
1:C:166:PHE:CD1	1:C:166:PHE:C	2.95	0.44
1:H:186:ASN:HA	1:H:187:PRO:HA	1.76	0.44
1:b:132:VAL:HG12	1:b:133:ASN:N	2.31	0.44
1:c:166:PHE:O	1:c:182:THR:HA	2.18	0.44
1:C:15:ARG:C	1:C:16:LEU:HD12	2.42	0.44
1:b:132:VAL:O	1:b:133:ASN:C	2.60	0.44
1:d:121:HIS:O	1:d:122:ASP:HB2	2.16	0.44
1:D:246:ARG:HB3	1:D:246:ARG:NH1	2.32	0.44
1:S:61:PHE:HA	1:U:61:PHE:CZ	2.53	0.44
1:V:139:GLY:O	1:V:157:GLN:HA	2.16	0.44
1:P:246:ARG:NH1	1:P:246:ARG:CB	2.81	0.44
1:Q:68:THR:HG23	1:Q:70:ASP:N	2.32	0.44
1:Z:16:LEU:N	1:Z:16:LEU:CD1	2.79	0.44
1:G:199:ARG:HH21	1:G:199:ARG:CG	2.25	0.44
1:K:253:THR:HG23	1:K:253:THR:O	2.17	0.44
1:Q:200[B]:ARG:NH2	5:Q:401:HOH:O	2.50	0.44
1:V:90:GLU:HG3	1:V:115:ALA:HB2	1.99	0.44
1:X:89:ARG:HB2	1:X:114:MET:HA	1.98	0.44
1:a:68:THR:HG23	1:a:70:ASP:N	2.33	0.44
1:d:131:LEU:N	1:d:131:LEU:HD12	2.32	0.44
1:P:61:PHE:HA	1:R:61:PHE:CZ	2.53	0.44
1:R:102:ARG:O	1:R:103:ALA:HB3	2.17	0.44
1:Y:176:ASP:CG	1:d:254:ARG:HH11	2.25	0.44
1:d:109:ASP:O	1:d:127:ASN:HA	2.18	0.44
1:M:148:ILE:O	1:M:166:PHE:HA	2.17	0.44
1:Q:85:HIS:O	1:Q:110:HIS:HA	2.18	0.44
1:b:130:ILE:C	1:b:131:LEU:HD12	2.42	0.44
1:L:195:PHE:CZ	1:L:212:ARG:HG3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:110:HIS:O	1:P:128:HIS:HA	2.18	0.44
1:R:195:PHE:CZ	1:R:212:ARG:HG3	2.53	0.44
1:X:62:SER:HA	1:X:92:VAL:O	2.17	0.44
1:c:166:PHE:CD1	1:c:166:PHE:C	2.95	0.44
1:d:166:PHE:O	1:d:182:THR:HA	2.18	0.44
1:D:119:ILE:HD13	1:D:125:ILE:CD1	2.48	0.44
1:G:199:ARG:HG2	1:G:199:ARG:NH2	2.24	0.44
1:M:106:THR:HB	1:M:124:VAL:HG13	2.00	0.44
1:N:224:THR:OG1	1:N:227:GLU:HG3	2.18	0.44
1:K:166:PHE:CD1	1:K:166:PHE:C	2.96	0.44
1:L:246:ARG:HH11	1:L:246:ARG:HG2	1.83	0.44
1:Q:68:THR:HG23	1:Q:70:ASP:H	1.82	0.44
1:S:258:ARG:HG3	1:S:258:ARG:NH1	2.33	0.44
1:V:15:ARG:C	1:V:16:LEU:HD12	2.43	0.44
1:B:166:PHE:CD1	1:B:166:PHE:C	2.96	0.43
1:C:16:LEU:N	1:C:16:LEU:HD12	2.33	0.43
1:C:35:GLY:O	1:C:36:GLU:C	2.60	0.43
1:C:254:ARG:NH1	1:V:176:ASP:OD2	2.50	0.43
1:G:42:PRO:O	1:G:44:VAL:HG23	2.18	0.43
1:I:246:ARG:CG	1:I:246:ARG:NH1	2.75	0.43
1:R:166:PHE:HB3	1:R:182:THR:HG22	2.00	0.43
1:S:132:VAL:HG12	1:S:133:ASN:N	2.32	0.43
1:Y:89:ARG:HB2	1:Y:114:MET:HA	2.00	0.43
1:U:246:ARG:CG	1:U:246:ARG:NH1	2.76	0.43
1:Y:166:PHE:O	1:Y:182:THR:HA	2.18	0.43
1:a:132:VAL:HG12	1:a:133:ASN:N	2.33	0.43
1:A:43:HIS:CE1	1:B:43:HIS:ND1	2.86	0.43
1:E:19:ASP:OD1	1:E:19:ASP:C	2.58	0.43
1:F:181:VAL:HA	1:F:193:MET:HE2	2.00	0.43
1:O:3:LEU:HD22	1:O:21:GLN:HG2	2.01	0.43
1:R:109:ASP:O	1:R:127:ASN:HA	2.18	0.43
1:D:132:VAL:HG12	1:D:133:ASN:N	2.33	0.43
1:R:90:GLU:O	1:R:115:ALA:HA	2.18	0.43
1:Y:1:MET:O	1:Y:1:MET:CG	2.67	0.43
1:Y:131:LEU:CD1	1:Y:131:LEU:N	2.82	0.43
1:c:132:VAL:HG12	1:c:133:ASN:N	2.33	0.43
1:H:132:VAL:HG12	1:H:133:ASN:H	1.83	0.43
1:T:84:ASP:O	1:T:109:ASP:HA	2.18	0.43
1:W:15:ARG:HB2	1:W:15:ARG:HH21	1.72	0.43
1:Y:61:PHE:HA	1:a:61:PHE:CZ	2.52	0.43
1:b:60:GLN:H	1:b:60:GLN:CD	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:65:GLY:O	1:b:96:ARG:HG3	2.18	0.43
1:c:229:LEU:HD23	1:c:229:LEU:HA	1.88	0.43
1:A:216:LYS:HE2	3:A:304:CL:CL	2.55	0.43
1:A:254:ARG:HH21	1:A:254:ARG:HB2	1.83	0.43
1:B:133:ASN:O	1:B:134:ASN:HB2	2.17	0.43
1:C:186:ASN:HA	1:C:187:PRO:HA	1.76	0.43
1:O:60:GLN:H	1:O:60:GLN:CD	2.27	0.43
1:S:193:MET:HE3	1:S:215:TYR:HD2	1.83	0.43
1:U:148:ILE:O	1:U:166:PHE:HA	2.18	0.43
1:X:121:HIS:O	1:X:122:ASP:HB2	2.18	0.43
1:c:47:LYS:HD2	1:c:66:GLU:OE2	2.19	0.43
1:d:89:ARG:HD2	1:d:89:ARG:HA	1.86	0.43
1:O:132:VAL:HG12	1:O:133:ASN:H	1.83	0.43
1:Q:114:MET:HE2	1:R:69:PRO:HG2	1.99	0.43
1:S:258:ARG:HH11	1:S:258:ARG:CG	2.30	0.43
1:V:239:PHE:HA	1:V:240:PRO:HD2	1.91	0.43
1:Y:24:PRO:HB2	1:Y:25:TRP:CD2	2.53	0.43
1:G:55:HIS:O	1:G:85:HIS:HA	2.18	0.43
1:O:56:ASN:HD21	1:O:86:ASN:HD22	1.67	0.43
1:K:181:VAL:HA	1:K:193:MET:HE2	2.01	0.43
1:S:69:PRO:HB3	1:U:89:ARG:NH1	2.33	0.43
1:T:1:MET:HE2	1:T:1:MET:HA	2.01	0.43
1:T:19:ASP:N	1:T:19:ASP:OD1	2.46	0.43
1:T:109:ASP:O	1:T:127:ASN:HA	2.19	0.43
1:Z:84:ASP:O	1:Z:109:ASP:HA	2.18	0.43
1:A:232:LEU:O	1:A:233:ALA:C	2.61	0.43
1:B:205:SER:HB2	1:V:238:GLN:HB3	2.00	0.43
1:D:49:PRO:HD2	1:D:78:THR:O	2.19	0.43
1:E:234:GLU:OE2	1:H:209:HIS:HA	2.19	0.43
1:S:149:LEU:HD21	1:S:161:ILE:HG21	2.01	0.43
1:S:160:ARG:CG	1:S:160:ARG:HH21	2.32	0.43
1:V:7:ARG:HE	1:V:7:ARG:HB2	1.65	0.43
1:Z:131:LEU:HD12	1:Z:131:LEU:N	2.34	0.43
1:b:258:ARG:HG3	1:b:258:ARG:NH1	2.33	0.43
1:c:239:PHE:O	1:c:240:PRO:C	2.62	0.43
1:d:54:LYS:O	1:d:84:ASP:HA	2.19	0.43
1:A:198:MET:HE2	1:A:211:LEU:HD13	2.00	0.43
1:C:142:HIS:HB2	1:C:160[A]:ARG:HG2	2.01	0.43
1:E:54:LYS:O	1:E:84:ASP:HA	2.18	0.43
1:E:164:HIS:CE1	1:E:201:ARG:HG2	2.53	0.43
1:F:160:ARG:HH21	1:F:160:ARG:HG3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:HIS:HB2	1:G:160:ARG:HG2	2.01	0.43
1:I:137:LEU:HD22	1:I:141:VAL:HG11	2.00	0.43
1:Q:229:LEU:HD21	1:Q:249:ILE:HG22	2.01	0.43
1:T:253:THR:O	1:T:253:THR:CG2	2.67	0.43
1:G:86:ASN:OD1	1:G:111:ASN:HB2	2.18	0.42
1:G:201:ARG:CG	1:G:201:ARG:HH11	2.32	0.42
1:N:132:VAL:CG1	1:N:133:ASN:N	2.81	0.42
1:Q:84:ASP:O	1:Q:109:ASP:HA	2.19	0.42
1:X:51:LYS:HE3	1:X:51:LYS:HB3	1.62	0.42
1:E:195:PHE:HZ	1:E:212:ARG:HG3	1.84	0.42
1:F:246[B]:ARG:HG2	1:F:247:ASP:N	2.34	0.42
1:G:196:GLU:OE2	1:G:199:ARG:NH1	2.53	0.42
1:M:61:PHE:CZ	1:N:61:PHE:HA	2.53	0.42
1:Q:99:VAL:O	1:Q:100:GLN:C	2.62	0.42
1:Q:199:ARG:HG2	1:Q:199:ARG:NH2	2.33	0.42
1:R:199:ARG:HG2	1:R:199:ARG:HH21	1.84	0.42
1:a:132:VAL:O	1:a:133:ASN:C	2.62	0.42
1:A:84:ASP:O	1:A:109:ASP:HA	2.19	0.42
1:E:166:PHE:O	1:E:182:THR:HA	2.20	0.42
1:F:127:ASN:O	1:F:145:ASP:HA	2.19	0.42
1:F:166:PHE:O	1:F:182:THR:HA	2.19	0.42
1:J:5:ASP:OD1	1:J:7:ARG:HB2	2.18	0.42
1:J:124:VAL:O	1:J:142:HIS:HA	2.20	0.42
1:R:89:ARG:HB2	1:R:114:MET:HA	2.00	0.42
1:S:5:ASP:CG	1:S:6:PRO:HD2	2.45	0.42
1:S:30:ALA:O	1:S:31:GLU:HB2	2.18	0.42
1:Y:15:ARG:HB2	1:Y:15:ARG:NH2	2.34	0.42
1:Z:234:GLU:O	1:Z:238:GLN:HG3	2.19	0.42
1:a:166:PHE:HB3	1:a:182:THR:HG22	2.00	0.42
1:C:131:LEU:N	1:C:131:LEU:CD1	2.83	0.42
1:M:85:HIS:O	1:M:110:HIS:HA	2.19	0.42
1:Y:116:TYR:O	1:Y:117:ALA:C	2.62	0.42
1:Z:193:MET:HE1	1:Z:245:PHE:CE1	2.54	0.42
1:F:90:GLU:O	1:F:115:ALA:HA	2.20	0.42
1:H:61:PHE:CZ	1:I:61:PHE:HA	2.55	0.42
1:I:7:ARG:HE	1:I:7:ARG:HB2	1.61	0.42
1:N:215:TYR:CE2	1:N:219:TYR:CD2	3.07	0.42
1:Q:50:THR:HA	1:Q:80:LEU:O	2.19	0.42
1:A:131:LEU:HD12	1:A:131:LEU:N	2.34	0.42
1:R:15:ARG:C	1:R:16:LEU:HD12	2.44	0.42
1:V:232:LEU:O	1:V:233:ALA:C	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:232:LEU:O	1:a:233:ALA:C	2.62	0.42
1:A:100:GLN:OE1	1:A:100:GLN:N	2.42	0.42
1:A:139:GLY:O	1:A:157[B]:GLN:HA	2.20	0.42
1:E:195:PHE:CZ	1:E:212:ARG:HG3	2.54	0.42
1:F:72:LYS:HE2	1:F:100:GLN:HG3	2.01	0.42
1:N:89:ARG:HD2	1:N:89:ARG:HA	1.81	0.42
1:U:166:PHE:O	1:U:182:THR:HA	2.19	0.42
1:V:166:PHE:HB3	1:V:182:THR:HG22	2.01	0.42
1:C:28:VAL:HG22	1:C:46:LEU:HD12	2.02	0.42
1:D:186:ASN:HA	1:D:187:PRO:HA	1.84	0.42
1:U:130:ILE:C	1:U:131:LEU:HD12	2.45	0.42
1:U:164:HIS:CE1	1:U:201:ARG:HG3	2.55	0.42
1:V:44:VAL:HG12	1:V:45:VAL:N	2.34	0.42
1:F:214:ALA:HB1	1:F:245:PHE:CE2	2.55	0.42
1:S:51:LYS:HB2	1:S:51:LYS:HE2	1.56	0.42
1:V:61:PHE:O	1:V:91:GLY:HA2	2.20	0.42
1:d:26:SER:HA	1:d:44:VAL:O	2.20	0.42
1:B:109:ASP:O	1:B:127:ASN:HA	2.19	0.41
1:D:148:ILE:O	1:D:166:PHE:HA	2.20	0.41
1:F:51:LYS:HB3	1:F:51:LYS:HE2	1.73	0.41
1:M:11:ASP:HA	1:M:12:PRO:HD3	1.95	0.41
1:J:183:VAL:HA	1:J:189:GLU:O	2.19	0.41
1:L:195:PHE:HZ	1:L:212:ARG:HG3	1.84	0.41
1:S:220:ARG:HH21	1:S:220:ARG:CG	2.32	0.41
1:S:246:ARG:CG	1:S:246:ARG:NH1	2.79	0.41
1:V:43:HIS:HD2	1:X:43:HIS:CD2	2.37	0.41
1:Z:62:SER:HA	1:Z:92:VAL:O	2.20	0.41
1:d:28:VAL:HG12	1:d:28:VAL:O	2.20	0.41
1:d:135:THR:HA	1:d:153:THR:O	2.20	0.41
1:B:131:LEU:N	1:B:131:LEU:HD12	2.36	0.41
1:C:139:GLY:O	1:C:157[A]:GLN:HA	2.20	0.41
1:F:254:ARG:NH1	1:P:176:ASP:OD2	2.53	0.41
1:H:229:LEU:HD23	1:H:229:LEU:HA	1.85	0.41
1:I:19:ASP:OD1	1:I:37:GLY:N	2.53	0.41
1:I:186:ASN:OD1	1:I:186:ASN:C	2.62	0.41
1:P:258:ARG:NH1	1:P:258:ARG:HG2	2.35	0.41
1:A:110:HIS:O	1:A:128:HIS:HA	2.19	0.41
1:D:193:MET:HA	1:D:193:MET:CE	2.48	0.41
1:M:46:LEU:CD2	1:M:64:VAL:HB	2.50	0.41
1:P:74:LYS:HD2	1:P:74:LYS:N	2.36	0.41
1:R:215:TYR:CE2	1:R:219:TYR:CD2	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:11:ASP:O	1:V:12:PRO:C	2.62	0.41
1:a:40:ILE:HG22	1:a:41:GLY:O	2.20	0.41
1:C:160[B]:ARG:HG3	1:V:254:ARG:HH11	1.85	0.41
1:C:181:VAL:HA	1:C:193:MET:HE2	2.02	0.41
1:F:89:ARG:HD2	1:F:89:ARG:HA	1.80	0.41
1:O:56:ASN:ND2	1:O:86:ASN:HD22	2.17	0.41
1:T:229:LEU:HA	1:T:229:LEU:HD23	1.80	0.41
1:A:19:ASP:N	1:A:19:ASP:OD1	2.50	0.41
1:C:166:PHE:O	1:C:182:THR:HA	2.21	0.41
1:F:139:GLY:O	1:F:157[B]:GLN:HA	2.20	0.41
1:F:229:LEU:HD23	1:F:229:LEU:HA	1.91	0.41
1:N:166:PHE:O	1:N:182:THR:HA	2.21	0.41
1:J:109:ASP:O	1:J:127:ASN:HA	2.20	0.41
1:K:221:GLN:OE1	1:K:223:HIS:HE1	2.03	0.41
1:V:201:ARG:HG3	1:V:201:ARG:NH1	2.34	0.41
1:a:90:GLU:O	1:a:115:ALA:HA	2.20	0.41
1:a:96:ARG:CZ	1:a:96:ARG:CB	2.98	0.41
1:E:135:THR:HA	1:E:153:THR:O	2.20	0.41
1:F:121:HIS:O	1:F:122:ASP:HB2	2.21	0.41
1:G:132:VAL:HG12	1:G:133:ASN:N	2.35	0.41
1:I:186:ASN:HA	1:I:187:PRO:HA	1.86	0.41
1:d:195:PHE:CZ	1:d:212:ARG:HG3	2.55	0.41
1:F:46:LEU:HD23	1:F:64:VAL:HB	2.02	0.41
1:G:26:SER:HA	1:G:44:VAL:O	2.20	0.41
1:I:197:GLY:O	1:I:201:ARG:HG2	2.20	0.41
1:M:149:LEU:N	1:M:149:LEU:HD23	2.36	0.41
1:P:90:GLU:O	1:P:115:ALA:HA	2.20	0.41
1:Y:61:PHE:CZ	1:Z:61:PHE:HA	2.56	0.41
1:Z:49:PRO:HD2	1:Z:78:THR:O	2.21	0.41
1:d:195:PHE:HZ	1:d:212:ARG:HG3	1.85	0.41
1:F:132:VAL:O	1:F:133:ASN:C	2.63	0.41
1:N:186:ASN:HA	1:N:187:PRO:HA	1.87	0.41
1:N:234:GLU:O	1:N:238:GLN:HG3	2.20	0.41
1:T:15:ARG:C	1:T:16:LEU:HD12	2.45	0.41
1:V:16:LEU:HD12	1:V:16:LEU:N	2.36	0.41
1:V:149:LEU:HD21	1:V:161:ILE:HG21	2.03	0.41
1:Y:198:MET:HE2	1:Y:211:LEU:HD13	2.03	0.41
1:A:176:ASP:OD1	1:a:254:ARG:HD2	2.20	0.41
1:D:139:GLY:O	1:D:157[A]:GLN:HA	2.21	0.41
1:G:149:LEU:HD21	1:G:161:ILE:HG21	2.02	0.41
1:M:150:SER:HB2	1:M:167:SER:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:ARG:HE	1:O:7:ARG:HB2	1.42	0.41
1:L:132:VAL:O	1:L:133:ASN:C	2.63	0.41
1:R:85:HIS:O	1:R:110:HIS:HA	2.21	0.41
1:U:156:HIS:O	1:U:157:GLN:C	2.64	0.41
1:X:149:LEU:HD21	1:X:161:ILE:HG21	2.02	0.41
1:X:229:LEU:HD21	1:X:249:ILE:HG22	2.02	0.41
1:Z:183:VAL:HA	1:Z:189:GLU:O	2.20	0.41
1:a:96:ARG:CZ	1:a:96:ARG:HB2	2.50	0.41
1:d:40:ILE:C	1:d:41:GLY:O	2.64	0.41
1:M:78:THR:HG21	1:M:98:THR:HA	2.02	0.41
1:K:16:LEU:HD12	1:K:16:LEU:N	2.36	0.41
1:K:148:ILE:O	1:K:166:PHE:HA	2.21	0.41
1:P:150:SER:HB2	1:P:167:SER:O	2.21	0.41
1:c:149:LEU:HD21	1:c:161:ILE:HG21	2.03	0.41
1:B:164:HIS:CE1	1:B:201[B]:ARG:HG2	2.55	0.40
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.87	0.40
1:I:113:ILE:HD13	1:I:119:ILE:HD11	2.03	0.40
1:M:132:VAL:HG12	1:M:133:ASN:N	2.36	0.40
1:K:164:HIS:CE1	1:K:201:ARG:HG3	2.57	0.40
1:P:166:PHE:O	1:P:182:THR:HA	2.21	0.40
1:Z:15:ARG:HB3	1:Z:15:ARG:NH2	2.35	0.40
1:Z:15:ARG:HB2	1:Z:15:ARG:NH2	2.36	0.40
1:b:145:ASP:O	1:b:163:ALA:HA	2.21	0.40
1:E:104:GLU:HG2	1:E:106:THR:OG1	2.22	0.40
1:E:186:ASN:HA	1:E:187:PRO:HA	1.84	0.40
1:H:38:THR:HA	1:H:56:ASN:O	2.21	0.40
1:H:145:ASP:O	1:H:163:ALA:HA	2.21	0.40
1:I:91:GLY:HA3	1:I:116:TYR:CE1	2.56	0.40
1:M:51:LYS:HB2	1:M:81:VAL:HG22	2.04	0.40
1:J:51:LYS:HB2	1:J:51:LYS:HE2	1.91	0.40
1:J:220:ARG:C	1:J:221:GLN:HG3	2.47	0.40
1:R:95:HIS:O	1:R:105:THR:OG1	2.36	0.40
1:S:212:ARG:HH12	1:X:231:GLU:CD	2.29	0.40
1:V:16:LEU:N	1:V:16:LEU:CD1	2.83	0.40
1:c:26:SER:HA	1:c:44:VAL:O	2.20	0.40
1:E:139:GLY:O	1:E:157:GLN:HA	2.21	0.40
1:P:149:LEU:HD21	1:P:161:ILE:HG21	2.03	0.40
1:W:7:ARG:HE	1:W:7:ARG:HB2	1.55	0.40
1:Y:131:LEU:N	1:Y:131:LEU:HD12	2.37	0.40
1:a:22:VAL:HA	1:a:40:ILE:HB	2.04	0.40
1:b:186:ASN:OD1	1:b:186:ASN:C	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:GLY:HA3	1:E:116:TYR:CE1	2.57	0.40
1:G:90:GLU:O	1:G:115:ALA:HA	2.21	0.40
1:I:132:VAL:HG12	1:I:133:ASN:N	2.37	0.40
1:J:166:PHE:CD1	1:J:166:PHE:C	2.99	0.40
1:L:54:LYS:O	1:L:84:ASP:HA	2.21	0.40
1:S:204:SER:HB2	1:S:206:GLU:OE1	2.22	0.40
1:b:61:PHE:CZ	1:c:61:PHE:HA	2.56	0.40
1:b:131:LEU:N	1:b:131:LEU:CD1	2.84	0.40
1:b:225:VAL:HG11	1:b:253:THR:HG21	2.03	0.40
1:d:60:GLN:HG3	1:d:61:PHE:CE2	2.57	0.40
1:B:198:MET:HE2	1:B:211:LEU:HD13	2.04	0.40
1:D:128:HIS:O	1:D:146:TRP:HA	2.22	0.40
1:F:91:GLY:HA3	1:F:116:TYR:CE1	2.57	0.40
1:N:32:VAL:HA	1:N:50:THR:O	2.21	0.40
1:O:247:ASP:O	1:O:250:GLN:HB3	2.22	0.40
1:L:246:ARG:CG	1:L:246:ARG:NH1	2.84	0.40
1:L:246:ARG:NH1	1:L:247:ASP:OD1	2.51	0.40
1:P:106:THR:O	1:P:124:VAL:HA	2.21	0.40
1:c:156:HIS:CD2	1:c:157[B]:GLN:OE1	2.74	0.40
1:c:253:THR:O	1:c:254:ARG:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	16	29
1	C	259/261 (99%)	241 (93%)	18 (7%)	0	100	100
1	D	257/261 (98%)	239 (93%)	16 (6%)	2 (1%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	256/261 (98%)	240 (94%)	14 (6%)	2 (1%)	16	29
1	F	258/261 (99%)	245 (95%)	11 (4%)	2 (1%)	16	29
1	G	255/261 (98%)	238 (93%)	17 (7%)	0	100	100
1	H	255/261 (98%)	237 (93%)	16 (6%)	2 (1%)	16	29
1	I	255/261 (98%)	241 (94%)	13 (5%)	1 (0%)	30	47
1	J	257/261 (98%)	241 (94%)	13 (5%)	3 (1%)	10	19
1	K	256/261 (98%)	234 (91%)	22 (9%)	0	100	100
1	L	256/261 (98%)	237 (93%)	17 (7%)	2 (1%)	16	29
1	M	255/261 (98%)	233 (91%)	21 (8%)	1 (0%)	30	47
1	N	255/261 (98%)	227 (89%)	26 (10%)	2 (1%)	16	29
1	O	255/261 (98%)	230 (90%)	25 (10%)	0	100	100
1	P	255/261 (98%)	235 (92%)	18 (7%)	2 (1%)	16	29
1	Q	256/261 (98%)	231 (90%)	22 (9%)	3 (1%)	10	19
1	R	255/261 (98%)	234 (92%)	18 (7%)	3 (1%)	10	19
1	S	256/261 (98%)	236 (92%)	20 (8%)	0	100	100
1	T	256/261 (98%)	240 (94%)	15 (6%)	1 (0%)	30	47
1	U	256/261 (98%)	235 (92%)	19 (7%)	2 (1%)	16	29
1	V	255/261 (98%)	233 (91%)	17 (7%)	5 (2%)	6	10
1	W	256/261 (98%)	233 (91%)	20 (8%)	3 (1%)	10	19
1	X	256/261 (98%)	226 (88%)	26 (10%)	4 (2%)	7	13
1	Y	257/261 (98%)	236 (92%)	19 (7%)	2 (1%)	16	29
1	Z	257/261 (98%)	237 (92%)	18 (7%)	2 (1%)	16	29
1	a	256/261 (98%)	235 (92%)	20 (8%)	1 (0%)	30	47
1	b	256/261 (98%)	236 (92%)	19 (7%)	1 (0%)	30	47
1	c	257/261 (98%)	233 (91%)	23 (9%)	1 (0%)	30	47
1	d	256/261 (98%)	229 (90%)	21 (8%)	6 (2%)	5	8
All	All	7688/7830 (98%)	7071 (92%)	562 (7%)	55 (1%)	18	32

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER
1	J	18	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	224	THR
1	Q	18	ALA
1	R	72	LYS
1	V	36	GLU
1	X	31	GLU
1	F	18	ALA
1	M	157	GLN
1	N	72	LYS
1	P	53	GLY
1	P	126	GLY
1	Q	29	GLY
1	U	83	GLY
1	V	222	GLY
1	X	78	THR
1	X	83	GLY
1	Z	83	GLY
1	d	17	ALA
1	d	29	GLY
1	d	41	GLY
1	B	157[A]	GLN
1	B	157[B]	GLN
1	E	3	LEU
1	L	157	GLN
1	R	204	SER
1	T	224	THR
1	U	157	GLN
1	X	133	ASN
1	b	126	GLY
1	d	31	GLU
1	F	36	GLU
1	H	36	GLU
1	I	157	GLN
1	W	83	GLY
1	W	126	GLY
1	W	133	ASN
1	d	36	GLU
1	L	36	GLU
1	Q	180	TYR
1	V	157	GLN
1	d	194	ASN
1	D	72	LYS
1	H	126	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	126	GLY
1	Z	222	GLY
1	V	108	GLY
1	N	5	ASP
1	a	108	GLY
1	J	222	GLY
1	V	126	GLY
1	Y	23	GLY
1	Y	83	GLY
1	c	83	GLY
1	D	83	GLY

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%)	23	42
1	B	210/208 (101%)	197 (94%)	13 (6%)	16	30
1	C	209/208 (100%)	195 (93%)	14 (7%)	15	27
1	D	207/208 (100%)	187 (90%)	20 (10%)	8	15
1	E	206/208 (99%)	194 (94%)	12 (6%)	18	33
1	F	208/208 (100%)	185 (89%)	23 (11%)	6	11
1	G	205/208 (99%)	190 (93%)	15 (7%)	13	24
1	H	205/208 (99%)	189 (92%)	16 (8%)	11	21
1	I	205/208 (99%)	194 (95%)	11 (5%)	20	36
1	J	207/208 (100%)	192 (93%)	15 (7%)	13	24
1	K	206/208 (99%)	192 (93%)	14 (7%)	14	27
1	L	206/208 (99%)	190 (92%)	16 (8%)	11	21
1	M	205/208 (99%)	190 (93%)	15 (7%)	13	24
1	N	205/208 (99%)	187 (91%)	18 (9%)	9	17
1	O	205/208 (99%)	190 (93%)	15 (7%)	13	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	205/208 (99%)	194 (95%)	11 (5%)	20	36
1	Q	206/208 (99%)	187 (91%)	19 (9%)	8	16
1	R	205/208 (99%)	188 (92%)	17 (8%)	10	19
1	S	206/208 (99%)	192 (93%)	14 (7%)	14	27
1	T	206/208 (99%)	191 (93%)	15 (7%)	13	24
1	U	206/208 (99%)	191 (93%)	15 (7%)	13	24
1	V	205/208 (99%)	192 (94%)	13 (6%)	16	29
1	W	206/208 (99%)	185 (90%)	21 (10%)	7	13
1	X	206/208 (99%)	192 (93%)	14 (7%)	14	27
1	Y	207/208 (100%)	192 (93%)	15 (7%)	13	24
1	Z	207/208 (100%)	193 (93%)	14 (7%)	14	27
1	a	206/208 (99%)	185 (90%)	21 (10%)	7	13
1	b	206/208 (99%)	182 (88%)	24 (12%)	5	9
1	c	207/208 (100%)	193 (93%)	14 (7%)	14	27
1	d	206/208 (99%)	186 (90%)	20 (10%)	8	15
All	All	6188/6240 (99%)	5714 (92%)	474 (8%)	12	21

All (474) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	63	SER
1	A	71	LEU
1	A	72	LYS
1	A	167	SER
1	A	201[A]	ARG
1	A	201[B]	ARG
1	A	212	ARG
1	A	246	ARG
1	A	258	ARG
1	B	1	MET
1	B	2	SER
1	B	4	ILE
1	B	51	LYS
1	B	63	SER
1	B	100	GLN
1	B	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	193	MET
1	B	199	ARG
1	B	212	ARG
1	B	220	ARG
1	B	226	GLU
1	B	253	THR
1	C	2	SER
1	C	4	ILE
1	C	11	ASP
1	C	51	LYS
1	C	57	ARG
1	C	71	LEU
1	C	74	LYS
1	C	99	VAL
1	C	100	GLN
1	C	102	ARG
1	C	175	LYS
1	C	193	MET
1	C	246	ARG
1	C	258	ARG
1	D	1	MET
1	D	15	ARG
1	D	51	LYS
1	D	54	LYS
1	D	57	ARG
1	D	63	SER
1	D	66	GLU
1	D	71	LEU
1	D	135	THR
1	D	160	ARG
1	D	169	MET
1	D	175	LYS
1	D	193	MET
1	D	201	ARG
1	D	212	ARG
1	D	220	ARG
1	D	226	GLU
1	D	246	ARG
1	D	250	GLN
1	D	253	THR
1	E	1	MET
1	E	2	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	51	LYS
1	E	63	SER
1	E	74	LYS
1	E	100	GLN
1	E	175	LYS
1	E	201	ARG
1	E	212	ARG
1	E	226	GLU
1	E	253	THR
1	E	258	ARG
1	F	1	MET
1	F	2	SER
1	F	4	ILE
1	F	15	ARG
1	F	36	GLU
1	F	63	SER
1	F	66	GLU
1	F	70	ASP
1	F	71	LEU
1	F	72	LYS
1	F	74	LYS
1	F	90	GLU
1	F	100	GLN
1	F	160	ARG
1	F	193	MET
1	F	205	SER
1	F	221	GLN
1	F	226	GLU
1	F	235	SER
1	F	246[A]	ARG
1	F	246[B]	ARG
1	F	253	THR
1	F	258	ARG
1	G	7	ARG
1	G	51	LYS
1	G	57	ARG
1	G	63	SER
1	G	67	ASP
1	G	71	LEU
1	G	72	LYS
1	G	74	LYS
1	G	90	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	102	ARG
1	G	193	MET
1	G	201	ARG
1	G	220	ARG
1	G	246	ARG
1	G	253	THR
1	H	10	ILE
1	H	15	ARG
1	H	57	ARG
1	H	63	SER
1	H	71	LEU
1	H	72	LYS
1	H	74	LYS
1	H	102	ARG
1	H	157	GLN
1	H	193	MET
1	H	201	ARG
1	H	212	ARG
1	H	226	GLU
1	H	246	ARG
1	H	251	SER
1	H	253	THR
1	I	7	ARG
1	I	15	ARG
1	I	19	ASP
1	I	51	LYS
1	I	66	GLU
1	I	160	ARG
1	I	193	MET
1	I	212	ARG
1	I	244	VAL
1	I	246	ARG
1	I	251	SER
1	M	7	ARG
1	M	51	LYS
1	M	63	SER
1	M	70	ASP
1	M	71	LEU
1	M	74	LYS
1	M	130	ILE
1	M	193	MET
1	M	204	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	205	SER
1	M	220	ARG
1	M	221	GLN
1	M	246	ARG
1	M	253	THR
1	M	258	ARG
1	N	7	ARG
1	N	15	ARG
1	N	33	GLU
1	N	47	LYS
1	N	51	LYS
1	N	54	LYS
1	N	63	SER
1	N	66	GLU
1	N	71	LEU
1	N	74	LYS
1	N	99	VAL
1	N	102	ARG
1	N	127	ASN
1	N	130	ILE
1	N	193	MET
1	N	201	ARG
1	N	212	ARG
1	N	246	ARG
1	O	7	ARG
1	O	15	ARG
1	O	51	LYS
1	O	57	ARG
1	O	63	SER
1	O	66	GLU
1	O	74	LYS
1	O	160	ARG
1	O	175	LYS
1	O	193	MET
1	O	201	ARG
1	O	226	GLU
1	O	246	ARG
1	O	253	THR
1	O	258	ARG
1	J	15	ARG
1	J	31	GLU
1	J	51	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	57	ARG
1	J	63	SER
1	J	71	LEU
1	J	90	GLU
1	J	99	VAL
1	J	160	ARG
1	J	175	LYS
1	J	193	MET
1	J	201	ARG
1	J	246	ARG
1	J	251	SER
1	J	253	THR
1	K	1	MET
1	K	3	LEU
1	K	57	ARG
1	K	63	SER
1	K	100	GLN
1	K	102	ARG
1	K	175	LYS
1	K	193	MET
1	K	205	SER
1	K	220	ARG
1	K	224	THR
1	K	226	GLU
1	K	251	SER
1	K	253	THR
1	L	1	MET
1	L	2	SER
1	L	51	LYS
1	L	71	LEU
1	L	72	LYS
1	L	74	LYS
1	L	100	GLN
1	L	119	ILE
1	L	157	GLN
1	L	175	LYS
1	L	193	MET
1	L	212	ARG
1	L	220	ARG
1	L	226	GLU
1	L	246	ARG
1	L	253	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	7	ARG
1	P	57	ARG
1	P	71	LEU
1	P	74	LYS
1	P	193	MET
1	P	196	GLU
1	P	201	ARG
1	P	220	ARG
1	P	240	PRO
1	P	246	ARG
1	P	258	ARG
1	Q	7	ARG
1	Q	15	ARG
1	Q	47	LYS
1	Q	57	ARG
1	Q	63	SER
1	Q	71	LEU
1	Q	74	LYS
1	Q	90	GLU
1	Q	99	VAL
1	Q	102	ARG
1	Q	175	LYS
1	Q	193	MET
1	Q	201	ARG
1	Q	205	SER
1	Q	212	ARG
1	Q	220	ARG
1	Q	226	GLU
1	Q	246	ARG
1	Q	250	GLN
1	R	2	SER
1	R	15	ARG
1	R	21	GLN
1	R	57	ARG
1	R	63	SER
1	R	74	LYS
1	R	84	ASP
1	R	99	VAL
1	R	119	ILE
1	R	193	MET
1	R	205	SER
1	R	220	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	226	GLU
1	R	246	ARG
1	R	250	GLN
1	R	251	SER
1	R	253	THR
1	S	51	LYS
1	S	54	LYS
1	S	63	SER
1	S	71	LEU
1	S	72	LYS
1	S	74	LYS
1	S	90	GLU
1	S	102	ARG
1	S	160	ARG
1	S	193	MET
1	S	201	ARG
1	S	220	ARG
1	S	246	ARG
1	S	258	ARG
1	T	1	MET
1	T	13	SER
1	T	54	LYS
1	T	63	SER
1	T	74	LYS
1	T	100	GLN
1	T	102	ARG
1	T	156	HIS
1	T	175	LYS
1	T	193	MET
1	T	212	ARG
1	T	220	ARG
1	T	235	SER
1	T	251	SER
1	T	253	THR
1	U	2	SER
1	U	15	ARG
1	U	57	ARG
1	U	63	SER
1	U	71	LEU
1	U	74	LYS
1	U	100	GLN
1	U	119	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	160	ARG
1	U	175	LYS
1	U	193	MET
1	U	201	ARG
1	U	220	ARG
1	U	226	GLU
1	U	246	ARG
1	V	2	SER
1	V	57	ARG
1	V	63	SER
1	V	71	LEU
1	V	90	GLU
1	V	102	ARG
1	V	193	MET
1	V	201	ARG
1	V	212	ARG
1	V	226	GLU
1	V	246	ARG
1	V	253	THR
1	V	258	ARG
1	W	2	SER
1	W	5	ASP
1	W	7	ARG
1	W	15	ARG
1	W	20	VAL
1	W	21	GLN
1	W	47	LYS
1	W	51	LYS
1	W	57	ARG
1	W	63	SER
1	W	71	LEU
1	W	74	LYS
1	W	124	VAL
1	W	175	LYS
1	W	193	MET
1	W	212	ARG
1	W	217	VAL
1	W	226	GLU
1	W	246	ARG
1	W	251	SER
1	W	258	ARG
1	X	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	51	LYS
1	X	57	ARG
1	X	63	SER
1	X	74	LYS
1	X	79	ARG
1	X	99	VAL
1	X	102	ARG
1	X	193	MET
1	X	212	ARG
1	X	221	GLN
1	X	226	GLU
1	X	246	ARG
1	X	253	THR
1	Y	1	MET
1	Y	7	ARG
1	Y	13	SER
1	Y	15	ARG
1	Y	51	LYS
1	Y	68	THR
1	Y	71	LEU
1	Y	74	LYS
1	Y	79	ARG
1	Y	90	GLU
1	Y	193	MET
1	Y	201	ARG
1	Y	212	ARG
1	Y	246	ARG
1	Y	258	ARG
1	Z	1	MET
1	Z	15	ARG
1	Z	57	ARG
1	Z	63	SER
1	Z	74	LYS
1	Z	79	ARG
1	Z	90	GLU
1	Z	100	GLN
1	Z	102	ARG
1	Z	175	LYS
1	Z	193	MET
1	Z	212	ARG
1	Z	226	GLU
1	Z	253	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	2	SER
1	a	7	ARG
1	a	15	ARG
1	a	47	LYS
1	a	51	LYS
1	a	57	ARG
1	a	63	SER
1	a	68	THR
1	a	71	LEU
1	a	72	LYS
1	a	74	LYS
1	a	100	GLN
1	a	119	ILE
1	a	124	VAL
1	a	125	ILE
1	a	193	MET
1	a	218	VAL
1	a	220	ARG
1	a	225	VAL
1	a	246	ARG
1	a	250	GLN
1	b	5	ASP
1	b	7	ARG
1	b	10	ILE
1	b	15	ARG
1	b	21	GLN
1	b	47	LYS
1	b	54	LYS
1	b	62	SER
1	b	63	SER
1	b	66	GLU
1	b	70	ASP
1	b	71	LEU
1	b	74	LYS
1	b	79	ARG
1	b	160	ARG
1	b	175	LYS
1	b	193	MET
1	b	199	ARG
1	b	201	ARG
1	b	212	ARG
1	b	220	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	246	ARG
1	b	250	GLN
1	b	258	ARG
1	c	1	MET
1	c	2	SER
1	c	47	LYS
1	c	63	SER
1	c	72	LYS
1	c	74	LYS
1	c	100	GLN
1	c	102	ARG
1	c	193	MET
1	c	220	ARG
1	c	226	GLU
1	c	246	ARG
1	c	248	SER
1	c	253	THR
1	d	9	ILE
1	d	20	VAL
1	d	51	LYS
1	d	54	LYS
1	d	57	ARG
1	d	71	LEU
1	d	74	LYS
1	d	79	ARG
1	d	100	GLN
1	d	102	ARG
1	d	157[A]	GLN
1	d	157[B]	GLN
1	d	169	MET
1	d	175	LYS
1	d	193	MET
1	d	212	ARG
1	d	226	GLU
1	d	246	ARG
1	d	253	THR
1	d	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	HIS
1	C	156	HIS
1	D	142	HIS
1	E	164	HIS
1	F	164	HIS
1	F	223	HIS
1	G	43	HIS
1	G	164	HIS
1	G	223	HIS
1	H	55	HIS
1	H	85	HIS
1	H	95	HIS
1	H	156	HIS
1	H	164	HIS
1	I	43	HIS
1	I	164	HIS
1	I	209	HIS
1	M	43	HIS
1	M	55	HIS
1	M	156	HIS
1	M	164	HIS
1	N	85	HIS
1	N	128	HIS
1	N	142	HIS
1	N	164	HIS
1	O	43	HIS
1	O	56	ASN
1	O	128	HIS
1	O	134	ASN
1	O	164	HIS
1	J	156	HIS
1	J	157	GLN
1	J	164	HIS
1	J	194	ASN
1	K	164	HIS
1	K	221	GLN
1	K	223	HIS
1	L	85	HIS
1	L	128	HIS
1	L	134	ASN
1	L	164	HIS
1	L	221	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	223	HIS
1	P	43	HIS
1	P	157	GLN
1	Q	128	HIS
1	Q	134	ASN
1	Q	156	HIS
1	Q	164	HIS
1	R	43	HIS
1	R	156	HIS
1	R	164	HIS
1	R	194	ASN
1	R	221	GLN
1	R	223	HIS
1	S	128	HIS
1	S	156	HIS
1	S	157	GLN
1	S	164	HIS
1	S	250	GLN
1	T	55	HIS
1	T	157	GLN
1	T	164	HIS
1	U	128	HIS
1	U	134	ASN
1	U	164	HIS
1	V	43	HIS
1	V	157	GLN
1	V	164	HIS
1	W	128	HIS
1	W	164	HIS
1	X	43	HIS
1	X	85	HIS
1	X	95	HIS
1	X	164	HIS
1	X	250	GLN
1	Y	128	HIS
1	Y	134	ASN
1	Y	156	HIS
1	Y	164	HIS
1	Z	164	HIS
1	a	142	HIS
1	a	164	HIS
1	b	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	134	ASN
1	b	164	HIS
1	c	128	HIS
1	c	164	HIS
1	d	110	HIS
1	d	164	HIS
1	d	223	HIS
1	d	250	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	R	301[B]	-	29,29,29	0.97	2 (6%)	35,38,38	1.09	4 (11%)
4	SO4	Q	306	-	4,4,4	0.29	0	6,6,6	0.24	0
2	VFT	Q	301[A]	-	29,29,29	0.99	1 (3%)	35,38,38	1.20	4 (11%)
2	VFT	T	301[B]	-	29,29,29	1.16	2 (6%)	35,38,38	1.42	6 (17%)
2	VFT	A	301[A]	-	29,29,29	1.06	2 (6%)	35,38,38	1.18	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	K	303	-	4,4,4	0.18	0	6,6,6	0.29	0
4	SO4	P	303	-	4,4,4	0.34	0	6,6,6	0.37	0
2	VFT	D	301[B]	-	29,29,29	0.90	1 (3%)	35,38,38	1.01	2 (5%)
4	SO4	V	302	-	4,4,4	0.22	0	6,6,6	0.23	0
4	SO4	A	306	-	4,4,4	0.16	0	6,6,6	0.20	0
2	VFT	O	301	-	29,29,29	1.03	1 (3%)	35,38,38	1.30	4 (11%)
4	SO4	T	303	-	4,4,4	0.23	0	6,6,6	0.24	0
4	SO4	V	301	-	4,4,4	0.38	0	6,6,6	0.26	0
2	VFT	R	301[A]	-	29,29,29	0.96	2 (6%)	35,38,38	1.30	5 (14%)
4	SO4	c	303	-	4,4,4	0.33	0	6,6,6	0.16	0
4	SO4	J	303	-	4,4,4	0.31	0	6,6,6	0.17	0
4	SO4	W	303	-	4,4,4	0.39	0	6,6,6	0.19	0
2	VFT	H	301	-	29,29,29	1.03	3 (10%)	35,38,38	1.42	4 (11%)
2	VFT	a	302	-	29,29,29	0.88	0	35,38,38	1.34	5 (14%)
2	VFT	A	301[B]	-	29,29,29	1.08	2 (6%)	35,38,38	1.19	3 (8%)
2	VFT	T	301[A]	-	29,29,29	1.23	2 (6%)	35,38,38	1.59	5 (14%)
4	SO4	B	305	-	4,4,4	0.33	0	6,6,6	0.26	0
2	VFT	U	301[B]	-	29,29,29	1.05	2 (6%)	35,38,38	1.43	6 (17%)
4	SO4	R	302	-	4,4,4	0.31	0	6,6,6	0.19	0
4	SO4	F	302	-	4,4,4	0.19	0	6,6,6	0.22	0
2	VFT	D	301[A]	-	29,29,29	0.94	1 (3%)	35,38,38	1.34	3 (8%)
4	SO4	N	304	-	4,4,4	0.32	0	6,6,6	0.23	0
2	VFT	c	301[B]	-	29,29,29	0.87	2 (6%)	35,38,38	1.29	6 (17%)
2	VFT	b	301[B]	-	29,29,29	0.87	1 (3%)	35,38,38	1.02	3 (8%)
4	SO4	U	304	-	4,4,4	0.33	0	6,6,6	0.26	0
4	SO4	M	304	-	4,4,4	0.39	0	6,6,6	0.16	0
4	SO4	I	302	-	4,4,4	0.22	0	6,6,6	0.27	0
4	SO4	U	302	-	4,4,4	0.41	0	6,6,6	0.23	0
4	SO4	I	303	-	4,4,4	0.33	0	6,6,6	0.16	0
4	SO4	E	304	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	W	304	-	4,4,4	0.33	0	6,6,6	0.24	0
4	SO4	V	303	-	4,4,4	0.26	0	6,6,6	0.25	0
2	VFT	K	301[B]	-	29,29,29	1.24	3 (10%)	35,38,38	1.28	5 (14%)
4	SO4	E	305	-	4,4,4	0.27	0	6,6,6	0.21	0
2	VFT	B	302[B]	-	29,29,29	0.95	1 (3%)	35,38,38	1.25	4 (11%)
2	VFT	U	301[A]	-	29,29,29	1.04	2 (6%)	35,38,38	1.52	5 (14%)
4	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.21	0
4	SO4	N	303	-	4,4,4	0.24	0	6,6,6	0.25	0
2	VFT	G	302[A]	-	29,29,29	0.76	0	35,38,38	1.28	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	b	303	-	4,4,4	0.29	0	6,6,6	0.18	0
2	VFT	c	301[A]	-	29,29,29	0.88	2 (6%)	35,38,38	1.39	6 (17%)
2	VFT	b	301[A]	-	29,29,29	0.87	1 (3%)	35,38,38	1.18	4 (11%)
4	SO4	O	304	-	4,4,4	0.26	0	6,6,6	0.25	0
2	VFT	W	301[B]	-	29,29,29	0.93	2 (6%)	35,38,38	1.25	4 (11%)
2	VFT	E	301[B]	-	29,29,29	0.84	0	35,38,38	1.20	5 (14%)
4	SO4	R	303	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	H	303	-	4,4,4	0.32	0	6,6,6	0.22	0
2	VFT	K	301[A]	-	29,29,29	1.23	3 (10%)	35,38,38	1.42	5 (14%)
2	VFT	B	302[A]	-	29,29,29	0.96	1 (3%)	35,38,38	1.37	4 (11%)
4	SO4	d	301	-	4,4,4	0.33	0	6,6,6	0.23	0
2	VFT	G	302[B]	-	29,29,29	0.71	0	35,38,38	1.21	3 (8%)
4	SO4	X	305	-	4,4,4	0.30	0	6,6,6	0.23	0
2	VFT	L	301[B]	-	29,29,29	0.92	1 (3%)	35,38,38	1.10	2 (5%)
4	SO4	c	304	-	4,4,4	0.21	0	6,6,6	0.29	0
4	SO4	D	304	-	4,4,4	0.38	0	6,6,6	0.30	0
4	SO4	L	303	-	4,4,4	0.28	0	6,6,6	0.15	0
4	SO4	Y	302	-	4,4,4	0.26	0	6,6,6	0.26	0
2	VFT	W	301[A]	-	29,29,29	0.94	2 (6%)	35,38,38	1.35	4 (11%)
4	SO4	Z	302	-	4,4,4	0.30	0	6,6,6	0.23	0
2	VFT	E	301[A]	-	29,29,29	0.85	0	35,38,38	1.28	5 (14%)
2	VFT	J	301[B]	-	29,29,29	0.83	1 (3%)	35,38,38	1.13	2 (5%)
4	SO4	G	305	-	4,4,4	0.39	0	6,6,6	0.23	0
4	SO4	Q	305	-	4,4,4	0.26	0	6,6,6	0.18	0
2	VFT	Y	301[B]	-	29,29,29	0.86	1 (3%)	35,38,38	1.18	5 (14%)
2	VFT	N	301	-	29,29,29	1.06	2 (6%)	35,38,38	1.13	3 (8%)
4	SO4	E	306	-	4,4,4	0.37	0	6,6,6	0.25	0
4	SO4	H	302	-	4,4,4	0.21	0	6,6,6	0.26	0
4	SO4	b	302	-	4,4,4	0.23	0	6,6,6	0.23	0
4	SO4	T	304	-	4,4,4	0.35	0	6,6,6	0.25	0
2	VFT	L	301[A]	-	29,29,29	0.99	2 (6%)	35,38,38	1.39	4 (11%)
4	SO4	D	303	-	4,4,4	0.33	0	6,6,6	0.23	0
2	VFT	G	301[B]	-	29,29,29	0.98	2 (6%)	35,38,38	1.00	0
2	VFT	X	301[B]	-	29,29,29	1.00	3 (10%)	35,38,38	0.93	2 (5%)
2	VFT	c	302	-	29,29,29	0.99	2 (6%)	35,38,38	1.36	6 (17%)
2	VFT	F	301	-	29,29,29	0.96	3 (10%)	35,38,38	1.17	5 (14%)
4	SO4	L	304	-	4,4,4	0.34	0	6,6,6	0.16	0
2	VFT	J	301[A]	-	29,29,29	0.76	1 (3%)	35,38,38	1.21	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	J	304	-	4,4,4	0.28	0	6,6,6	0.21	0
4	SO4	P	302	-	4,4,4	0.33	0	6,6,6	0.09	0
4	SO4	J	302	-	4,4,4	0.39	0	6,6,6	0.29	0
2	VFT	Y	301[A]	-	29,29,29	0.87	1 (3%)	35,38,38	1.24	5 (14%)
4	SO4	G	306	-	4,4,4	0.33	0	6,6,6	0.19	0
4	SO4	M	305	-	4,4,4	0.36	0	6,6,6	0.34	0
4	SO4	P	301	-	4,4,4	0.36	0	6,6,6	0.20	0
4	SO4	F	303	-	4,4,4	0.31	0	6,6,6	0.18	0
2	VFT	S	301[B]	-	29,29,29	0.73	0	35,38,38	1.08	2 (5%)
2	VFT	a	301[B]	-	29,29,29	0.85	1 (3%)	35,38,38	0.95	2 (5%)
4	SO4	A	307	-	4,4,4	0.35	0	6,6,6	0.24	0
4	SO4	a	303	-	4,4,4	0.26	0	6,6,6	0.26	0
4	SO4	U	303	-	4,4,4	0.31	0	6,6,6	0.13	0
2	VFT	Q	302	-	29,29,29	1.04	2 (6%)	35,38,38	1.41	6 (17%)
2	VFT	G	301[A]	-	29,29,29	0.99	2 (6%)	35,38,38	1.03	1 (2%)
2	VFT	X	301[A]	-	29,29,29	1.02	3 (10%)	35,38,38	1.10	2 (5%)
4	SO4	S	305	-	4,4,4	0.34	0	6,6,6	0.19	0
2	VFT	W	302	-	29,29,29	1.08	2 (6%)	35,38,38	1.35	7 (20%)
4	SO4	G	304	-	4,4,4	0.25	0	6,6,6	0.18	0
2	VFT	B	301[B]	-	29,29,29	1.05	1 (3%)	35,38,38	1.13	3 (8%)
4	SO4	X	304	-	4,4,4	0.33	0	6,6,6	0.21	0
2	VFT	M	301	-	29,29,29	0.86	1 (3%)	35,38,38	1.06	2 (5%)
4	SO4	Q	304	-	4,4,4	0.36	0	6,6,6	0.25	0
4	SO4	O	303	-	4,4,4	0.28	0	6,6,6	0.21	0
4	SO4	A	305	-	4,4,4	0.41	0	6,6,6	0.13	0
4	SO4	S	303	-	4,4,4	0.30	0	6,6,6	0.21	0
4	SO4	C	303	-	4,4,4	0.29	0	6,6,6	0.20	0
4	SO4	K	302	-	4,4,4	0.18	0	6,6,6	0.27	0
2	VFT	S	301[A]	-	29,29,29	0.75	0	35,38,38	1.25	3 (8%)
2	VFT	a	301[A]	-	29,29,29	0.86	1 (3%)	35,38,38	1.10	2 (5%)
4	SO4	d	302	-	4,4,4	0.39	0	6,6,6	0.26	0
4	SO4	S	304	-	4,4,4	0.25	0	6,6,6	0.30	0
2	VFT	Q	301[B]	-	29,29,29	0.97	1 (3%)	35,38,38	0.96	3 (8%)
4	SO4	a	304	-	4,4,4	0.24	0	6,6,6	0.20	0
2	VFT	B	301[A]	-	29,29,29	1.07	1 (3%)	35,38,38	1.37	5 (14%)
4	SO4	c	305	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	a	305	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SO4	Y	303	-	4,4,4	0.23	0	6,6,6	0.21	0
4	SO4	C	304	-	4,4,4	0.31	0	6,6,6	0.21	0
4	SO4	Z	301	-	4,4,4	0.36	0	6,6,6	0.16	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[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	R	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	Q	302	-	-	0/19/19/19	0/3/3/3
2	VFT	W	301[A]	-	-	2/19/19/19	0/3/3/3
2	VFT	E	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	J	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	G	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	Q	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	T	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	W	302	-	-	1/19/19/19	0/3/3/3
2	VFT	A	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	B	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	Y	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	N	301	-	-	0/19/19/19	0/3/3/3
2	VFT	M	301	-	-	0/19/19/19	0/3/3/3
2	VFT	D	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	K	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	B	302[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	U	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	O	301	-	-	0/19/19/19	0/3/3/3
2	VFT	G	302[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	c	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	b	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	W	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	S	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	L	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	a	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	E	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	R	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	X	301[B]	-	-	1/19/19/19	0/3/3/3
2	VFT	c	302	-	-	0/19/19/19	0/3/3/3
2	VFT	F	301	-	-	0/19/19/19	0/3/3/3
2	VFT	Q	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	J	301[A]	-	-	2/19/19/19	0/3/3/3
2	VFT	H	301	-	-	0/19/19/19	0/3/3/3
2	VFT	a	302	-	-	0/19/19/19	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFT	A	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	T	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	B	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	Y	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	U	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	D	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	K	301[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	B	302[A]	-	-	1/19/19/19	0/3/3/3
2	VFT	c	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	G	302[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	b	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	S	301[B]	-	-	0/19/19/19	0/3/3/3
2	VFT	L	301[B]	-	-	0/19/19/19	0/3/3/3

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301[A]	VFT	C10-N12	3.80	1.42	1.35
2	K	301[B]	VFT	C10-N12	3.80	1.42	1.35
2	B	301[A]	VFT	C10-N12	3.62	1.42	1.35
2	B	301[B]	VFT	C10-N12	3.62	1.42	1.35
2	Q	301[A]	VFT	C10-N12	3.52	1.42	1.35
2	Q	301[B]	VFT	C10-N12	3.52	1.42	1.35
2	U	301[A]	VFT	C10-N12	3.26	1.41	1.35
2	U	301[B]	VFT	C10-N12	3.26	1.41	1.35
2	T	301[A]	VFT	C10-N12	3.25	1.41	1.35
2	T	301[B]	VFT	C10-N12	3.25	1.41	1.35
2	N	301	VFT	C10-N12	3.22	1.41	1.35
2	O	301	VFT	C19-N12	-3.18	1.42	1.46
2	L	301[A]	VFT	C10-N12	3.16	1.41	1.35
2	L	301[B]	VFT	C10-N12	3.16	1.41	1.35
2	B	302[A]	VFT	C19-N12	-3.12	1.42	1.46
2	B	302[B]	VFT	C19-N12	-3.12	1.42	1.46
2	G	301[A]	VFT	C10-N12	3.09	1.41	1.35
2	G	301[B]	VFT	C10-N12	3.09	1.41	1.35
2	A	301[A]	VFT	C10-N12	3.00	1.41	1.35
2	A	301[B]	VFT	C10-N12	3.00	1.41	1.35
2	W	301[A]	VFT	C10-N12	2.87	1.40	1.35
2	W	301[B]	VFT	C10-N12	2.87	1.40	1.35
2	Q	302	VFT	C19-N12	-2.86	1.42	1.46
2	X	301[A]	VFT	C10-N12	2.80	1.40	1.35
2	X	301[B]	VFT	C10-N12	2.80	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	302	VFT	C19-N12	-2.73	1.42	1.46
2	H	301	VFT	C19-C20	-2.59	1.46	1.51
2	M	301	VFT	C19-N12	-2.54	1.43	1.46
2	Q	302	VFT	C10-N12	2.52	1.40	1.35
2	c	302	VFT	C19-N12	-2.52	1.43	1.46
2	R	301[A]	VFT	C10-N12	2.50	1.40	1.35
2	R	301[B]	VFT	C10-N12	2.50	1.40	1.35
2	F	301	VFT	C19-N12	-2.49	1.43	1.46
2	H	301	VFT	C10-N12	2.49	1.40	1.35
2	c	302	VFT	C7-S8	-2.49	1.73	1.77
2	T	301[A]	VFT	C19-N12	-2.46	1.43	1.46
2	T	301[B]	VFT	C19-N12	-2.46	1.43	1.46
2	R	301[A]	VFT	C19-N12	-2.42	1.43	1.46
2	R	301[B]	VFT	C19-N12	-2.42	1.43	1.46
2	a	301[A]	VFT	C10-N12	2.39	1.39	1.35
2	a	301[B]	VFT	C10-N12	2.39	1.39	1.35
2	G	301[A]	VFT	C19-N12	-2.38	1.43	1.46
2	G	301[B]	VFT	C19-N12	-2.38	1.43	1.46
2	K	301[A]	VFT	C2-CL1	-2.38	1.68	1.73
2	K	301[B]	VFT	C2-CL1	-2.38	1.68	1.73
2	D	301[A]	VFT	C10-N12	2.33	1.39	1.35
2	D	301[B]	VFT	C10-N12	2.33	1.39	1.35
2	K	301[A]	VFT	C19-C20	-2.31	1.47	1.51
2	K	301[B]	VFT	C19-C20	-2.31	1.47	1.51
2	A	301[A]	VFT	C19-N12	-2.30	1.43	1.46
2	A	301[B]	VFT	C19-N12	-2.30	1.43	1.46
2	c	301[A]	VFT	C10-N12	2.29	1.39	1.35
2	c	301[B]	VFT	C10-N12	2.29	1.39	1.35
2	N	301	VFT	C19-C20	-2.27	1.47	1.51
2	Y	301[A]	VFT	C10-N12	2.20	1.39	1.35
2	Y	301[B]	VFT	C10-N12	2.20	1.39	1.35
2	b	301[A]	VFT	C10-N12	2.17	1.39	1.35
2	b	301[B]	VFT	C10-N12	2.17	1.39	1.35
2	F	301	VFT	C9-C10	-2.11	1.48	1.51
2	W	302	VFT	C10-N12	2.09	1.39	1.35
2	W	301[A]	VFT	C19-C20	-2.07	1.47	1.51
2	W	301[B]	VFT	C19-C20	-2.07	1.47	1.51
2	U	301[A]	VFT	C23-C26	-2.07	1.40	1.44
2	U	301[B]	VFT	C23-C26	-2.07	1.40	1.44
2	c	301[A]	VFT	C23-C26	-2.07	1.40	1.44
2	c	301[B]	VFT	C23-C26	-2.07	1.40	1.44
2	F	301	VFT	C19-C20	-2.06	1.47	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	301[A]	VFT	C2-CL1	-2.05	1.68	1.73
2	X	301[B]	VFT	C2-CL1	-2.05	1.68	1.73
2	H	301	VFT	C19-N12	-2.05	1.43	1.46
2	X	301[A]	VFT	C23-C26	-2.02	1.40	1.44
2	X	301[B]	VFT	C23-C26	-2.02	1.40	1.44
2	J	301[A]	VFT	C10-N12	2.01	1.39	1.35
2	J	301[B]	VFT	C10-N12	2.01	1.39	1.35
2	L	301[A]	VFT	C13-N12	2.01	1.48	1.45

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[A]	VFT	C14-C13-N12	5.35	122.17	112.46
2	L	301[A]	VFT	C14-C13-N12	5.25	122.00	112.46
2	T	301[A]	VFT	C14-C13-N12	5.19	121.89	112.46
2	H	301	VFT	C14-C13-N12	-4.54	104.22	112.46
2	Q	301[A]	VFT	C14-C13-N12	4.41	120.47	112.46
2	Q	302	VFT	C14-C13-N12	-4.38	104.50	112.46
2	a	302	VFT	C14-C13-N12	-4.34	104.57	112.46
2	B	302[A]	VFT	C14-C13-N12	4.31	120.29	112.46
2	c	302	VFT	C14-C13-N12	-4.31	104.63	112.46
2	U	301[A]	VFT	C14-C13-N12	3.99	119.70	112.46
2	G	302[A]	VFT	C14-C13-N12	3.98	119.69	112.46
2	B	301[A]	VFT	C14-C13-N12	3.97	119.67	112.46
2	R	301[A]	VFT	C14-C13-N12	3.96	119.65	112.46
2	U	301[A]	VFT	C24-C23-C26	-3.74	113.88	119.97
2	U	301[B]	VFT	C24-C23-C26	-3.74	113.88	119.97
2	K	301[A]	VFT	C14-C13-N12	3.68	119.14	112.46
2	X	301[A]	VFT	C14-C13-N12	3.60	119.01	112.46
2	E	301[A]	VFT	C14-C13-N12	3.60	118.99	112.46
2	K	301[A]	VFT	O11-C10-C9	-3.46	114.31	121.19
2	K	301[B]	VFT	O11-C10-C9	-3.46	114.31	121.19
2	M	301	VFT	C14-C13-N12	-3.44	106.20	112.46
2	S	301[A]	VFT	C14-C13-N12	3.41	118.65	112.46
2	b	301[A]	VFT	C14-C13-N12	3.40	118.64	112.46
2	O	301	VFT	C13-N12-C10	3.32	130.55	120.81
2	D	301[A]	VFT	C19-N12-C10	-3.25	113.15	121.78
2	D	301[B]	VFT	C19-N12-C10	-3.25	113.15	121.78
2	Y	301[A]	VFT	C14-C13-N12	3.24	118.34	112.46
2	W	301[A]	VFT	C14-C13-N12	3.20	118.28	112.46
2	J	301[A]	VFT	C19-N12-C10	-3.08	113.60	121.78
2	J	301[B]	VFT	C19-N12-C10	-3.08	113.60	121.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	302[A]	VFT	C19-N12-C10	-3.07	113.63	121.78
2	G	302[B]	VFT	C19-N12-C10	-3.07	113.63	121.78
2	W	301[A]	VFT	C19-N12-C10	-3.03	113.75	121.78
2	W	301[B]	VFT	C19-N12-C10	-3.03	113.75	121.78
2	c	301[A]	VFT	C19-N12-C10	-3.01	113.80	121.78
2	c	301[B]	VFT	C19-N12-C10	-3.01	113.80	121.78
2	A	301[A]	VFT	C19-N12-C10	-3.00	113.81	121.78
2	A	301[B]	VFT	C19-N12-C10	-3.00	113.81	121.78
2	B	301[A]	VFT	C20-C19-N12	-2.99	108.45	113.15
2	B	301[B]	VFT	C20-C19-N12	-2.99	108.45	113.15
2	A	301[B]	VFT	C13-N12-C10	2.98	129.55	120.81
2	a	301[A]	VFT	C14-C13-N12	2.98	117.87	112.46
2	N	301	VFT	C14-C13-N12	-2.98	107.06	112.46
2	G	302[B]	VFT	C14-C13-N12	2.94	117.81	112.46
2	W	302	VFT	C13-N12-C10	2.92	129.35	120.81
2	Y	301[B]	VFT	C13-N12-C10	2.89	129.26	120.81
2	T	301[A]	VFT	C19-N12-C10	-2.87	114.16	121.78
2	T	301[B]	VFT	C19-N12-C10	-2.87	114.16	121.78
2	H	301	VFT	C20-C19-N12	-2.85	108.67	113.15
2	A	301[A]	VFT	C20-C19-N12	-2.83	108.70	113.15
2	A	301[B]	VFT	C20-C19-N12	-2.83	108.70	113.15
2	W	301[A]	VFT	C20-C19-N12	-2.83	108.71	113.15
2	W	301[B]	VFT	C20-C19-N12	-2.83	108.71	113.15
2	T	301[B]	VFT	C14-C13-N12	2.83	117.59	112.46
2	O	301	VFT	C14-C13-N12	-2.82	107.33	112.46
2	Q	302	VFT	C9-S8-C7	2.80	107.07	102.27
2	U	301[A]	VFT	O11-C10-C9	-2.76	115.69	121.19
2	U	301[B]	VFT	O11-C10-C9	-2.76	115.69	121.19
2	B	301[A]	VFT	C19-N12-C13	2.73	121.16	116.65
2	S	301[A]	VFT	C21-C22-C23	-2.69	116.92	120.35
2	S	301[B]	VFT	C21-C22-C23	-2.69	116.92	120.35
2	K	301[A]	VFT	C9-S8-C7	2.68	106.85	102.27
2	K	301[B]	VFT	C9-S8-C7	2.68	106.85	102.27
2	c	301[A]	VFT	C24-C23-C22	2.66	123.55	118.96
2	c	301[B]	VFT	C24-C23-C22	2.66	123.55	118.96
2	S	301[A]	VFT	C19-N12-C10	-2.66	114.70	121.78
2	S	301[B]	VFT	C19-N12-C10	-2.66	114.70	121.78
2	F	301	VFT	C5-C4-C3	-2.65	116.97	120.24
2	a	302	VFT	C19-N12-C10	-2.63	114.79	121.78
2	T	301[A]	VFT	C19-C20-C21	-2.63	115.91	120.75
2	T	301[B]	VFT	C19-C20-C21	-2.63	115.91	120.75
2	Q	302	VFT	C13-N12-C10	2.62	128.48	120.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	301[A]	VFT	C19-N12-C10	-2.62	114.83	121.78
2	R	301[B]	VFT	C19-N12-C10	-2.62	114.83	121.78
2	c	302	VFT	C9-S8-C7	2.62	106.75	102.27
2	T	301[B]	VFT	C13-N12-C10	2.61	128.46	120.81
2	c	301[A]	VFT	C9-S8-C7	2.61	106.74	102.27
2	c	301[B]	VFT	C9-S8-C7	2.61	106.74	102.27
2	L	301[A]	VFT	C19-N12-C10	-2.60	114.88	121.78
2	L	301[B]	VFT	C19-N12-C10	-2.60	114.88	121.78
2	B	302[A]	VFT	C5-C4-C3	-2.58	117.06	120.24
2	B	302[B]	VFT	C5-C4-C3	-2.58	117.06	120.24
2	N	301	VFT	C13-N12-C10	2.57	128.35	120.81
2	H	301	VFT	C25-C20-C21	2.57	122.06	118.23
2	U	301[A]	VFT	C22-C23-C26	2.57	124.16	119.97
2	U	301[B]	VFT	C22-C23-C26	2.57	124.16	119.97
2	O	301	VFT	C19-N12-C10	-2.56	114.99	121.78
2	K	301[A]	VFT	C19-N12-C13	2.53	120.83	116.65
2	Y	301[A]	VFT	C19-N12-C10	-2.53	115.06	121.78
2	Y	301[B]	VFT	C19-N12-C10	-2.53	115.06	121.78
2	K	301[B]	VFT	C13-N12-C10	2.53	128.22	120.81
2	E	301[B]	VFT	C13-N12-C10	2.53	128.21	120.81
2	B	302[B]	VFT	C13-N12-C10	2.51	128.15	120.81
2	c	301[A]	VFT	C14-C13-N12	2.50	117.00	112.46
2	c	301[A]	VFT	C25-C20-C21	2.49	121.94	118.23
2	c	301[B]	VFT	C25-C20-C21	2.49	121.94	118.23
2	R	301[A]	VFT	C7-C2-CL1	-2.47	115.43	119.72
2	R	301[B]	VFT	C7-C2-CL1	-2.47	115.43	119.72
2	B	301[A]	VFT	C19-N12-C10	-2.47	115.23	121.78
2	B	301[B]	VFT	C19-N12-C10	-2.47	115.23	121.78
2	c	301[A]	VFT	C25-C24-C23	-2.46	117.21	120.35
2	c	301[B]	VFT	C25-C24-C23	-2.46	117.21	120.35
2	G	302[B]	VFT	C13-N12-C10	2.45	127.98	120.81
2	J	301[B]	VFT	C13-N12-C10	2.42	127.89	120.81
2	E	301[A]	VFT	C6-C7-C2	2.41	120.69	117.55
2	E	301[B]	VFT	C6-C7-C2	2.41	120.69	117.55
2	R	301[A]	VFT	C6-C7-S8	2.40	127.30	121.48
2	R	301[B]	VFT	C6-C7-S8	2.40	127.30	121.48
2	T	301[A]	VFT	O11-C10-N12	2.40	126.39	122.12
2	T	301[B]	VFT	O11-C10-N12	2.40	126.39	122.12
2	F	301	VFT	C19-N12-C10	-2.39	115.42	121.78
2	a	302	VFT	C13-N12-C10	2.39	127.80	120.81
2	W	301[B]	VFT	C13-N12-C10	2.38	127.79	120.81
2	E	301[A]	VFT	C19-N12-C10	-2.38	115.45	121.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301[B]	VFT	C19-N12-C10	-2.38	115.45	121.78
2	Q	302	VFT	O11-C10-N12	2.38	126.36	122.12
2	W	301[A]	VFT	C25-C20-C21	2.38	121.77	118.23
2	W	301[B]	VFT	C25-C20-C21	2.38	121.77	118.23
2	D	301[A]	VFT	C19-N12-C13	2.37	120.58	116.65
2	F	301	VFT	C20-C19-N12	-2.36	109.44	113.15
2	B	302[A]	VFT	C19-N12-C10	-2.36	115.52	121.78
2	B	302[B]	VFT	C19-N12-C10	-2.36	115.52	121.78
2	D	301[B]	VFT	C13-N12-C10	2.35	127.69	120.81
2	W	302	VFT	O11-C10-N12	2.31	126.23	122.12
2	R	301[A]	VFT	C20-C19-N12	-2.29	109.56	113.15
2	R	301[B]	VFT	C20-C19-N12	-2.29	109.56	113.15
2	X	301[B]	VFT	C13-N12-C10	2.28	127.49	120.81
2	c	301[B]	VFT	C13-N12-C10	2.28	127.48	120.81
2	a	301[A]	VFT	C19-N12-C10	-2.27	115.74	121.78
2	a	301[B]	VFT	C19-N12-C10	-2.27	115.74	121.78
2	W	302	VFT	C25-C20-C21	2.26	121.60	118.23
2	b	301[A]	VFT	C19-N12-C10	-2.25	115.81	121.78
2	b	301[B]	VFT	C19-N12-C10	-2.25	115.81	121.78
2	E	301[A]	VFT	C21-C22-C23	-2.24	117.48	120.35
2	E	301[B]	VFT	C21-C22-C23	-2.24	117.48	120.35
2	U	301[B]	VFT	C14-C13-N12	2.24	116.52	112.46
2	A	301[A]	VFT	C14-C13-N12	2.23	116.52	112.46
2	Y	301[B]	VFT	C14-C13-N12	2.23	116.51	112.46
2	c	302	VFT	C19-N12-C10	-2.22	115.88	121.78
2	H	301	VFT	C13-N12-C10	2.21	127.27	120.81
2	U	301[B]	VFT	C13-N12-C10	2.20	127.27	120.81
2	N	301	VFT	O11-C10-N12	2.19	126.03	122.12
2	Y	301[A]	VFT	C22-C23-C26	2.18	123.53	119.97
2	Y	301[B]	VFT	C22-C23-C26	2.18	123.53	119.97
2	J	301[A]	VFT	C19-N12-C13	2.18	120.25	116.65
2	K	301[A]	VFT	C19-N12-C10	-2.18	116.00	121.78
2	K	301[B]	VFT	C19-N12-C10	-2.18	116.00	121.78
2	E	301[A]	VFT	C19-N12-C13	2.17	120.25	116.65
2	Y	301[A]	VFT	C19-N12-C13	2.17	120.24	116.65
2	b	301[A]	VFT	C24-C23-C26	-2.17	116.44	119.97
2	b	301[B]	VFT	C24-C23-C26	-2.17	116.44	119.97
2	B	301[A]	VFT	O11-C10-C9	-2.17	116.87	121.19
2	B	301[B]	VFT	O11-C10-C9	-2.17	116.87	121.19
2	M	301	VFT	C13-N12-C10	2.17	127.16	120.81
2	W	302	VFT	C14-C13-N12	-2.16	108.53	112.46
2	G	301[A]	VFT	C14-C13-N12	2.16	116.38	112.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301[A]	VFT	C14-C13-N12	2.15	116.36	112.46
2	U	301[A]	VFT	C21-C22-C23	-2.14	117.61	120.35
2	U	301[B]	VFT	C21-C22-C23	-2.14	117.61	120.35
2	Y	301[A]	VFT	C24-C23-C26	-2.14	116.49	119.97
2	Y	301[B]	VFT	C24-C23-C26	-2.14	116.49	119.97
2	c	302	VFT	C13-N12-C10	2.14	127.08	120.81
2	W	302	VFT	C9-S8-C7	2.14	105.93	102.27
2	E	301[B]	VFT	C13-C14-C15	-2.13	126.23	129.90
2	b	301[A]	VFT	C6-C7-C2	2.13	120.33	117.55
2	b	301[B]	VFT	C6-C7-C2	2.13	120.33	117.55
2	Q	301[A]	VFT	C19-N12-C10	-2.13	116.13	121.78
2	Q	301[B]	VFT	C19-N12-C10	-2.13	116.13	121.78
2	Q	302	VFT	C19-N12-C10	-2.12	116.16	121.78
2	O	301	VFT	C25-C20-C21	2.12	121.38	118.23
2	X	301[A]	VFT	C9-S8-C7	2.11	105.89	102.27
2	X	301[B]	VFT	C9-S8-C7	2.11	105.89	102.27
2	Q	302	VFT	C19-C20-C21	-2.11	116.86	120.75
2	Q	301[B]	VFT	C14-C13-N12	2.09	116.25	112.46
2	L	301[A]	VFT	C19-N12-C13	2.09	120.10	116.65
2	W	302	VFT	C4-C5-C6	2.08	122.81	120.24
2	a	302	VFT	C4-C5-C6	2.08	122.81	120.24
2	a	302	VFT	C22-C21-C20	-2.08	118.27	121.00
2	F	301	VFT	C14-C13-N12	-2.06	108.71	112.46
2	a	301[B]	VFT	C13-N12-C10	2.06	126.84	120.81
2	W	302	VFT	C19-N12-C13	-2.05	113.25	116.65
2	c	302	VFT	C22-C21-C20	-2.05	118.30	121.00
2	c	302	VFT	C25-C24-C23	-2.05	117.74	120.35
2	Q	301[A]	VFT	C19-N12-C13	2.02	119.99	116.65
2	L	301[A]	VFT	C24-C23-C22	2.02	122.43	118.96
2	L	301[B]	VFT	C24-C23-C22	2.02	122.43	118.96
2	B	302[A]	VFT	C20-C19-N12	-2.01	109.99	113.15
2	B	302[B]	VFT	C20-C19-N12	-2.01	109.99	113.15
2	T	301[A]	VFT	C22-C23-C26	-2.01	116.70	119.97
2	T	301[B]	VFT	C22-C23-C26	-2.01	116.70	119.97
2	Q	301[A]	VFT	C6-C7-S8	2.01	126.34	121.48
2	Q	301[B]	VFT	C6-C7-S8	2.01	126.34	121.48
2	F	301	VFT	C13-N12-C10	2.00	126.68	120.81
2	K	301[B]	VFT	C14-C13-N12	2.00	116.10	112.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	301[A]	VFT	C14-C13-N12-C10
2	S	301[A]	VFT	C14-C13-N12-C10
2	E	301[A]	VFT	C14-C13-N12-C10
2	G	301[A]	VFT	C14-C13-N12-C10
2	J	301[A]	VFT	C14-C13-N12-C10
2	Q	301[A]	VFT	C14-C13-N12-C10
2	A	301[A]	VFT	C14-C13-N12-C10
2	c	301[A]	VFT	C14-C13-N12-C10
2	L	301[A]	VFT	C14-C13-N12-C10
2	D	301[A]	VFT	C14-C13-N12-C10
2	W	301[A]	VFT	C14-C13-N12-C10
2	B	302[A]	VFT	C14-C13-N12-C10
2	K	301[A]	VFT	C14-C13-N12-C10
2	Y	301[A]	VFT	C14-C13-N12-C10
2	b	301[A]	VFT	C14-C13-N12-C10
2	T	301[A]	VFT	C14-C13-N12-C10
2	U	301[A]	VFT	C14-C13-N12-C10
2	B	301[A]	VFT	C14-C13-N12-C10
2	G	302[A]	VFT	C14-C13-N12-C10
2	a	301[A]	VFT	C14-C13-N12-C10
2	G	301[A]	VFT	C24-C23-C26-N27
2	G	301[B]	VFT	C24-C23-C26-N27
2	X	301[A]	VFT	C22-C23-C26-N27
2	X	301[B]	VFT	C22-C23-C26-N27
2	J	301[A]	VFT	C24-C23-C26-N27
2	J	301[B]	VFT	C24-C23-C26-N27
2	W	301[A]	VFT	C24-C23-C26-N27
2	W	301[B]	VFT	C24-C23-C26-N27
2	W	302	VFT	C24-C23-C26-N27

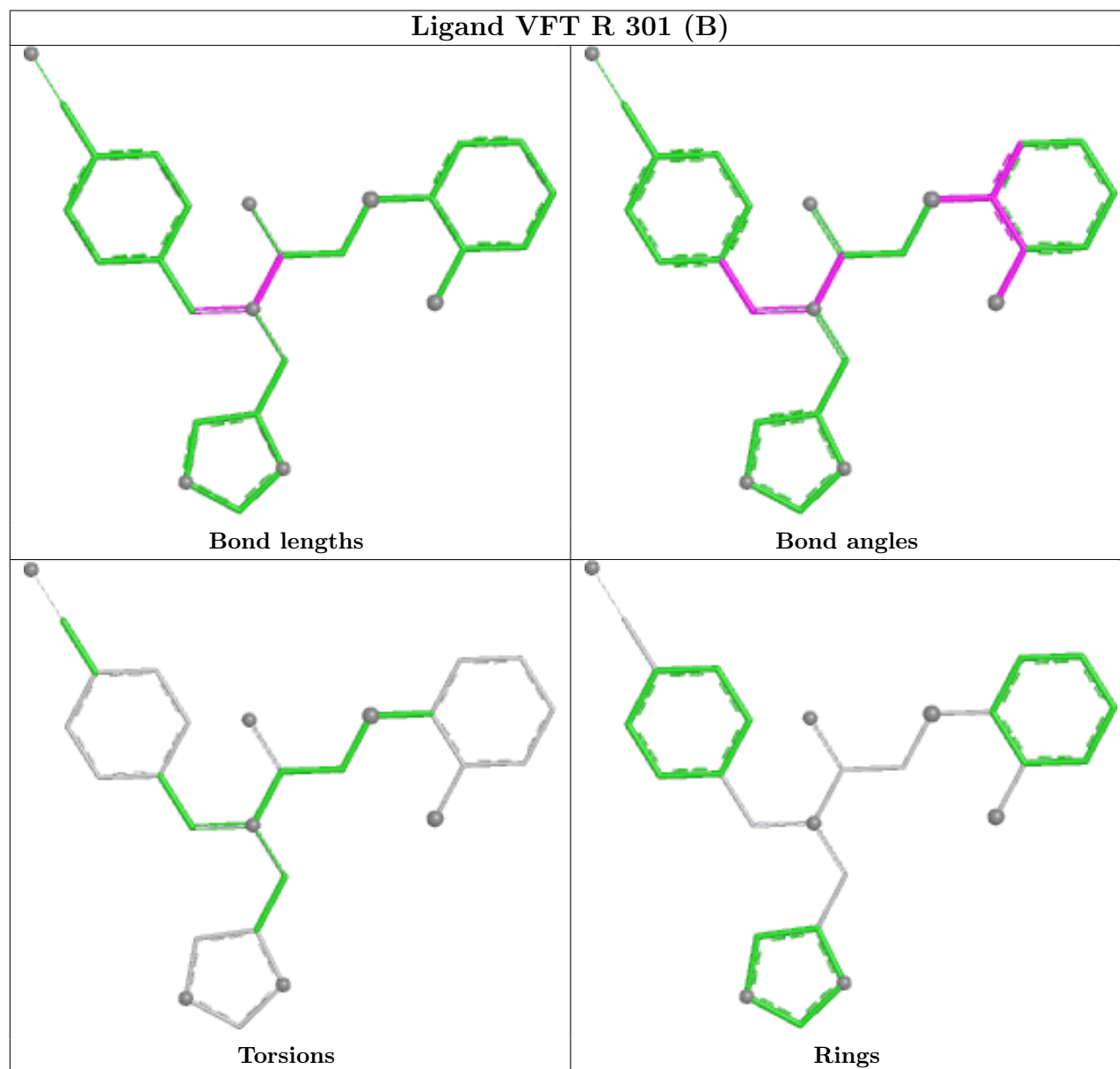
There are no ring outliers.

4 monomers are involved in 7 short contacts:

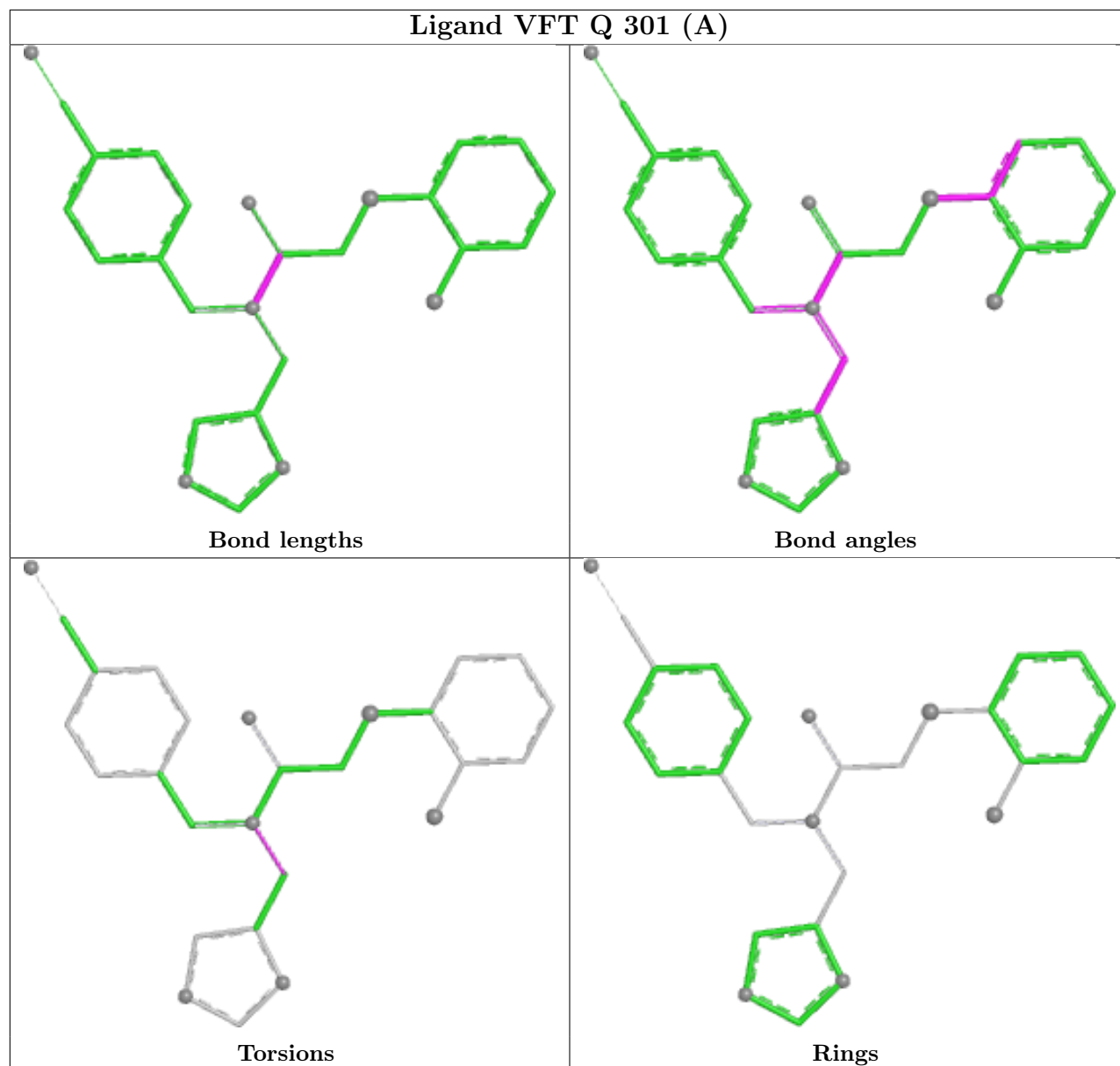
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	301[A]	VFT	1	0
2	b	301[A]	VFT	2	0
2	G	301[A]	VFT	2	0
2	a	301[A]	VFT	2	0

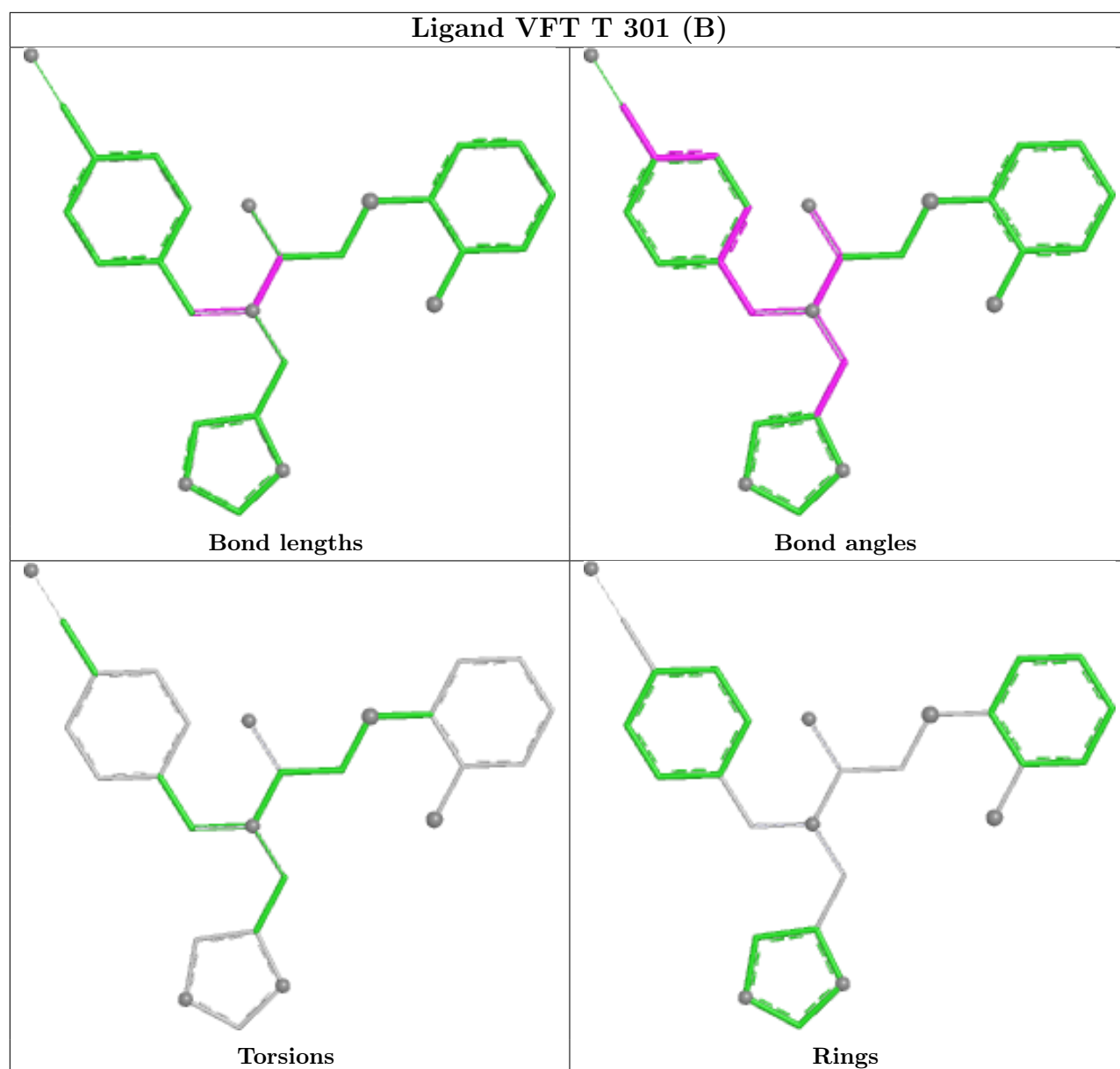
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

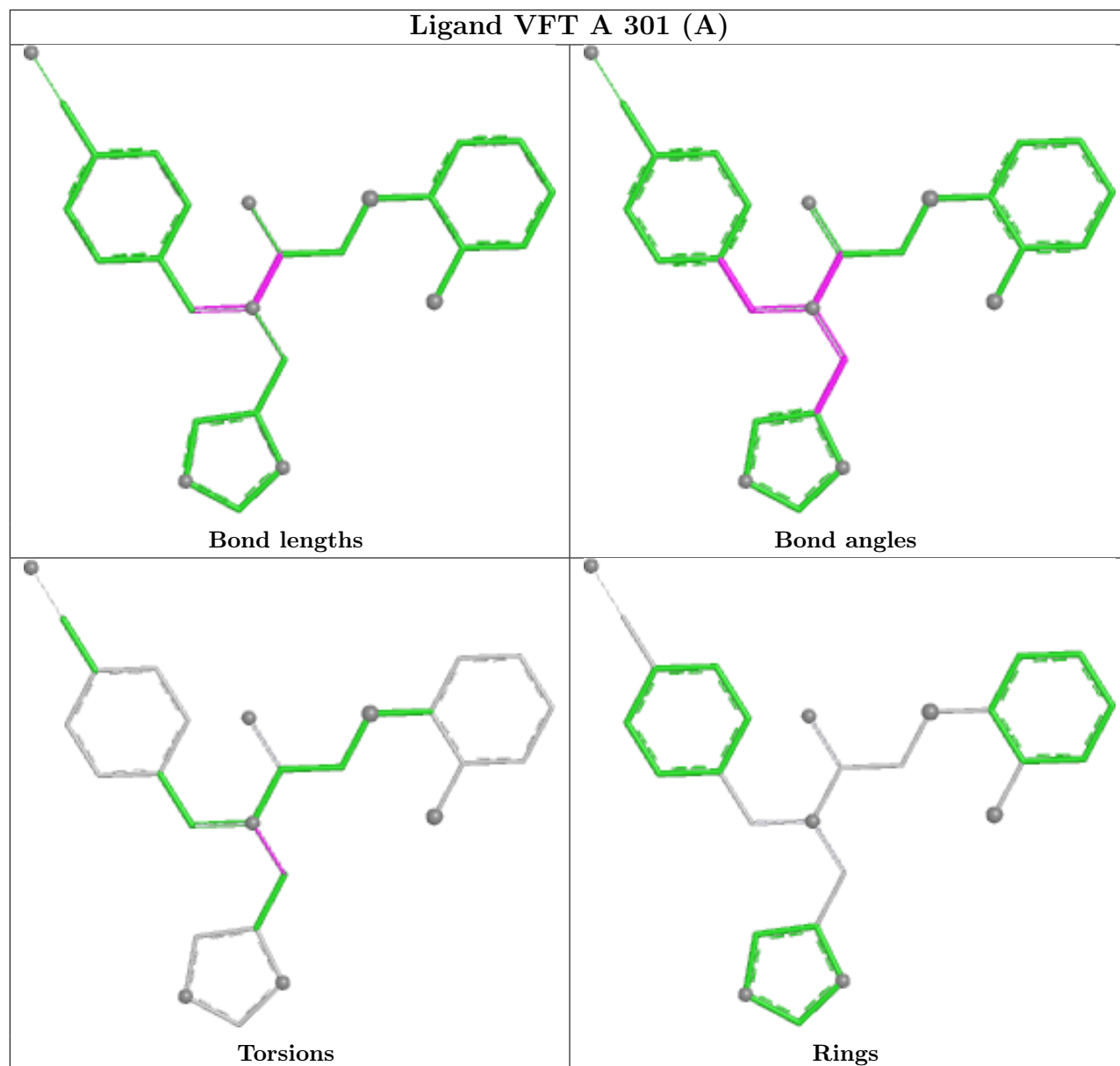


Ligand VFT Q 301 (A)

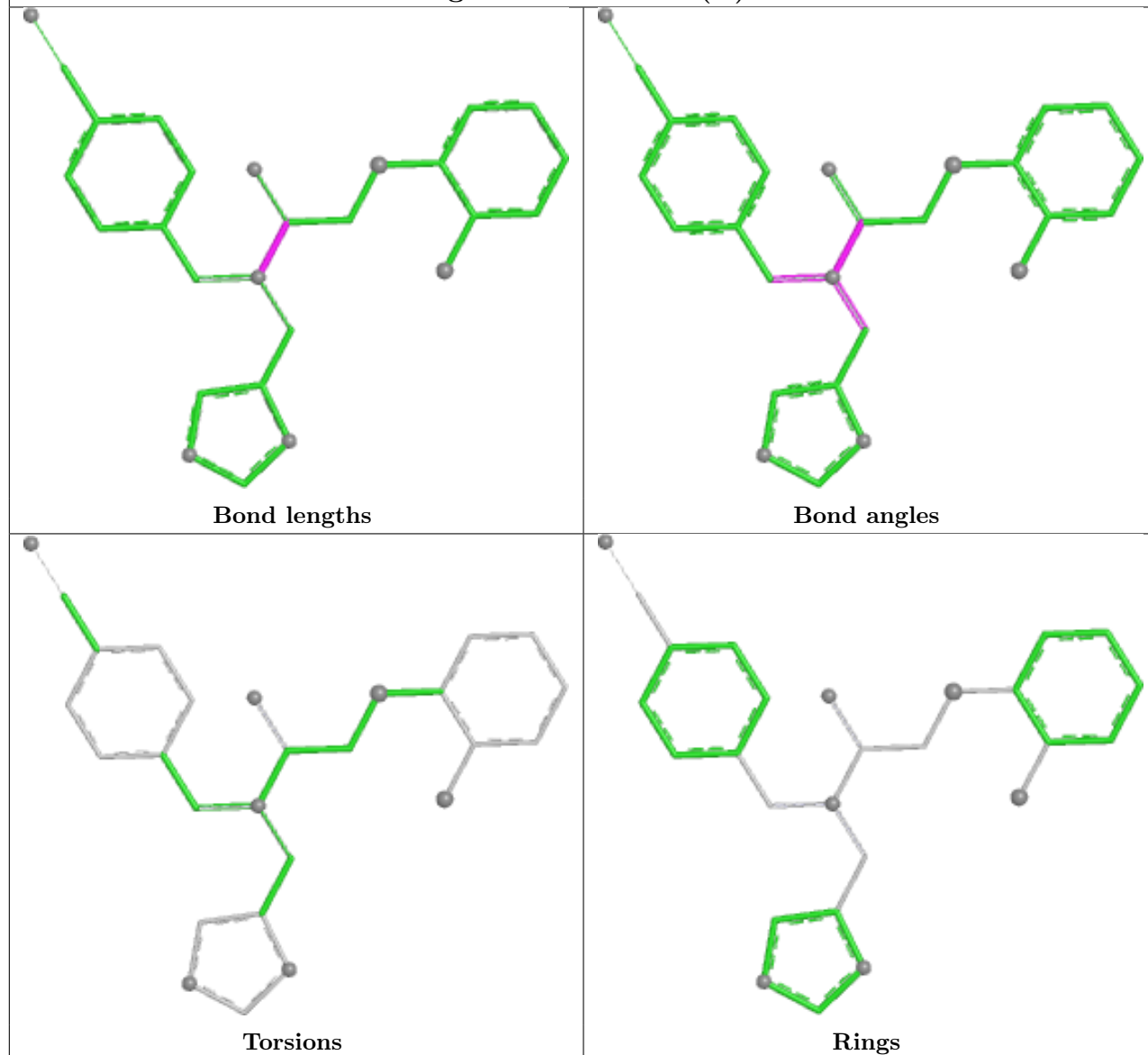


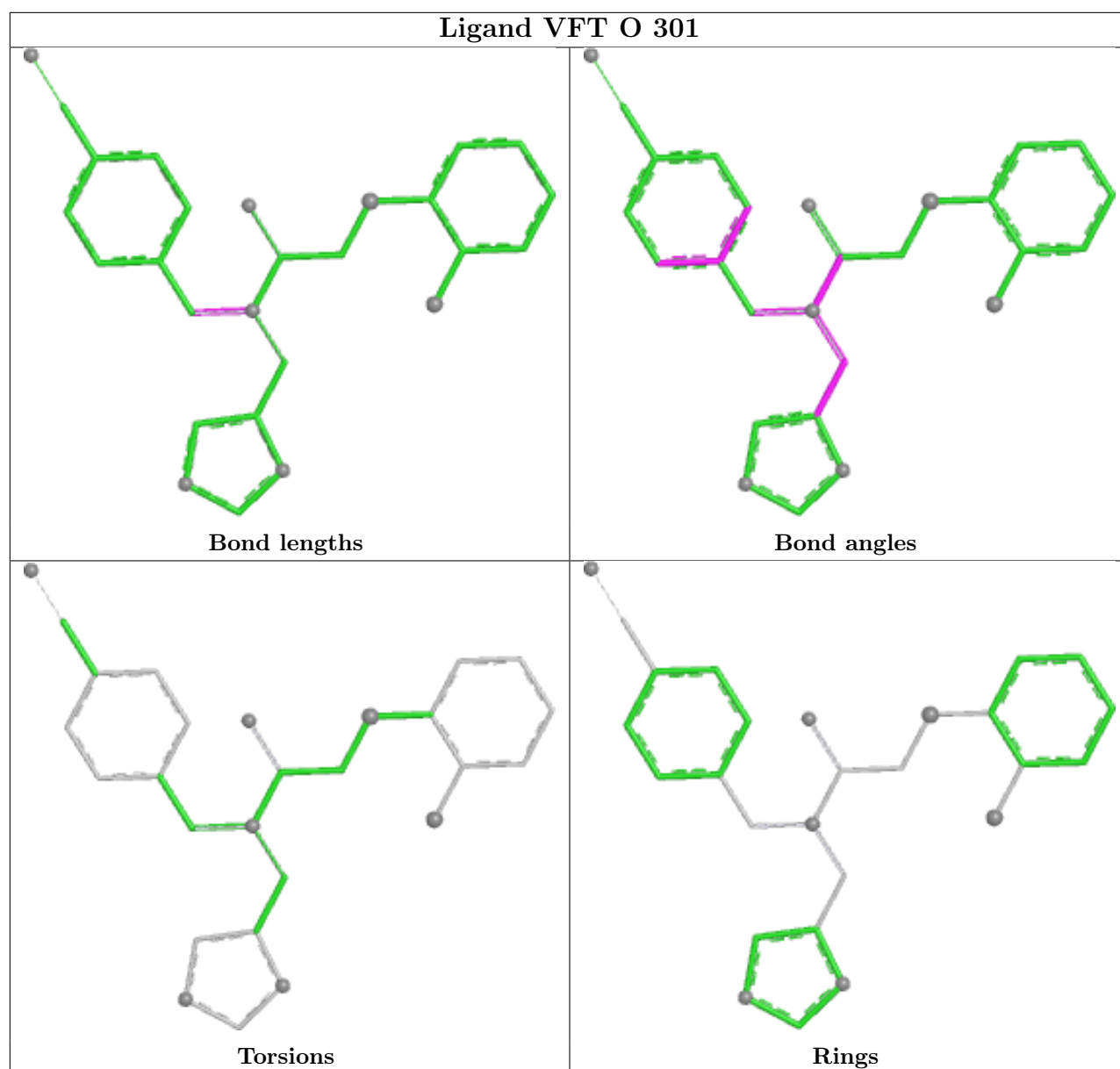


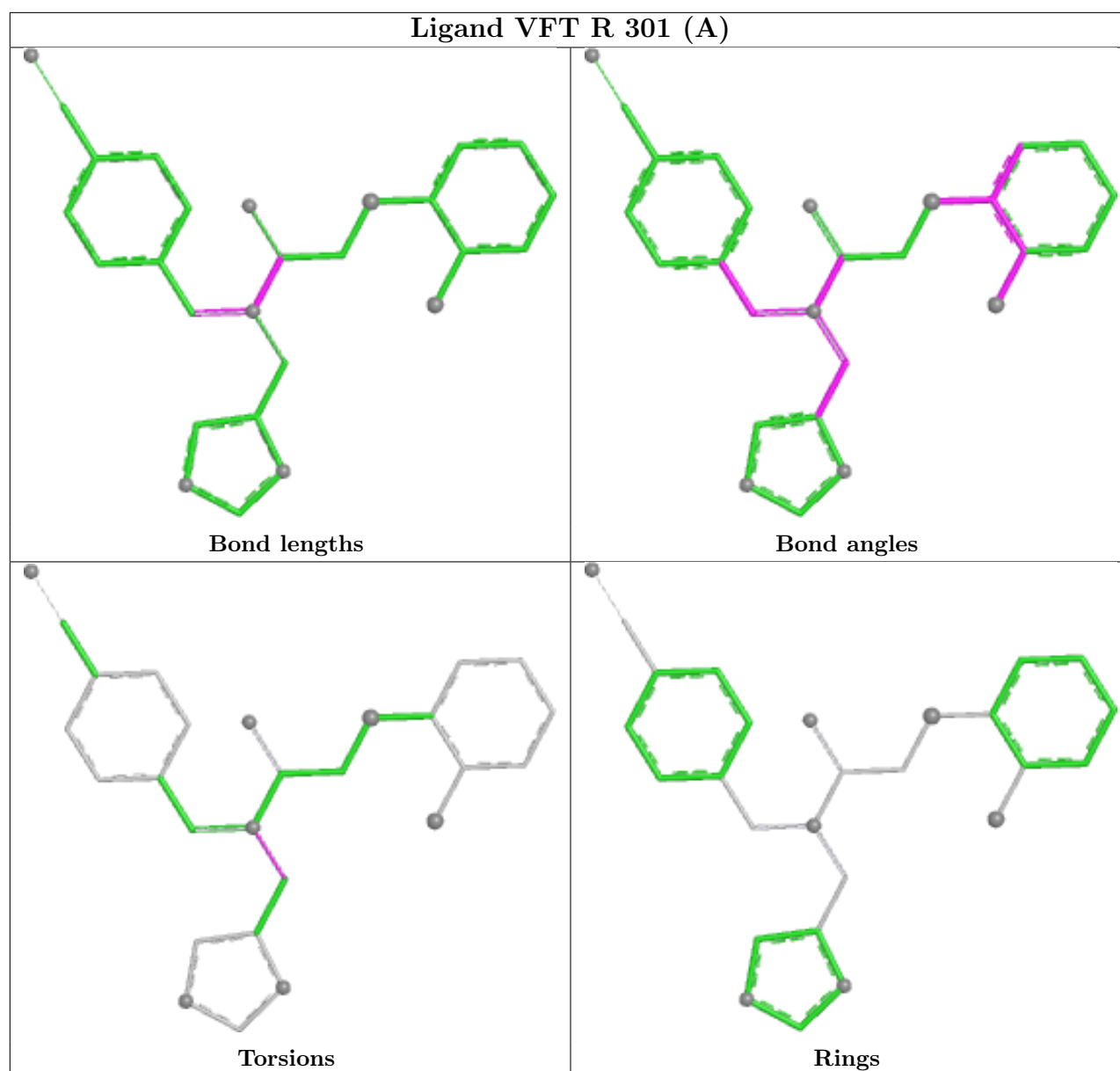
Ligand VFT A 301 (A)

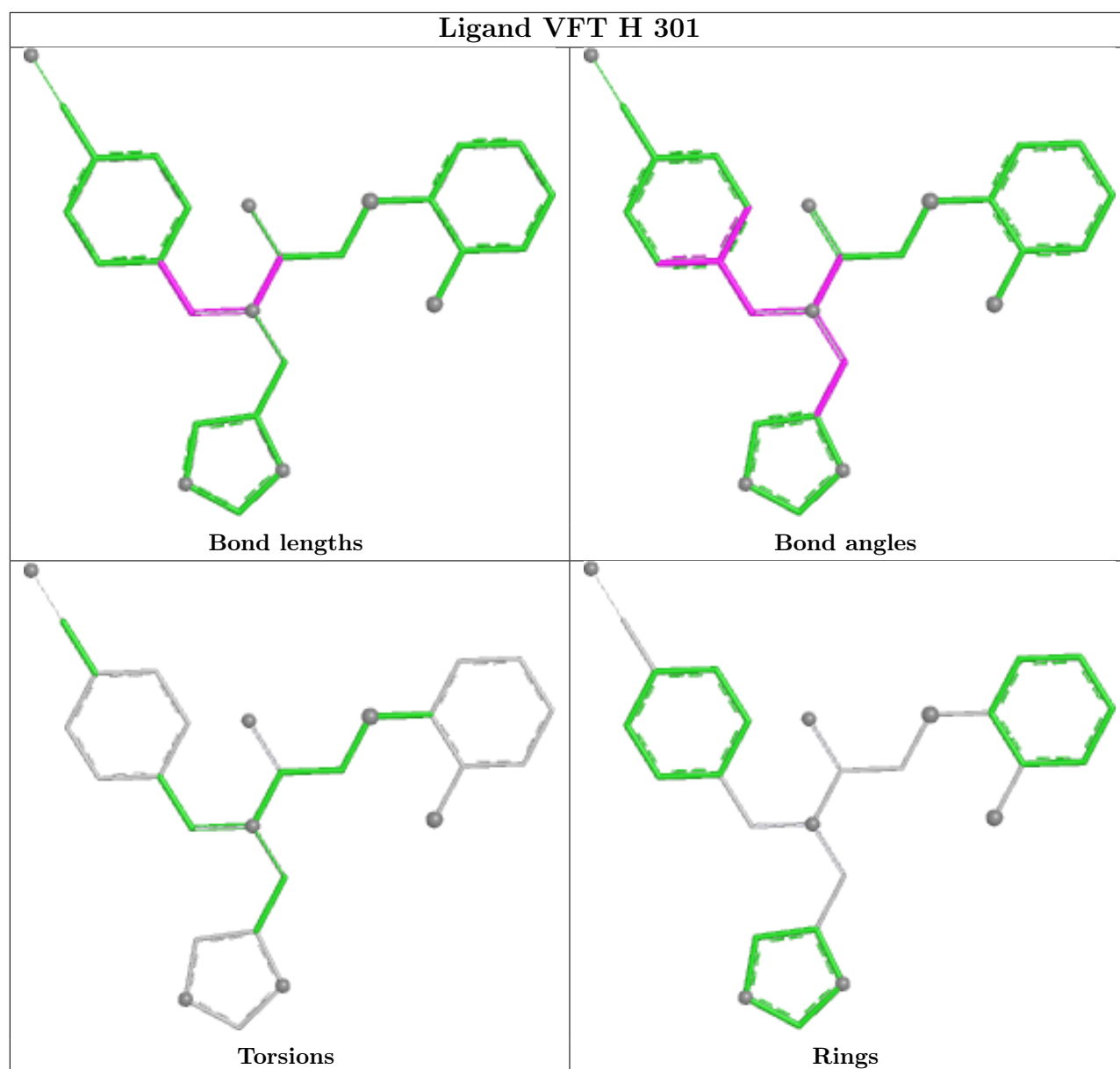


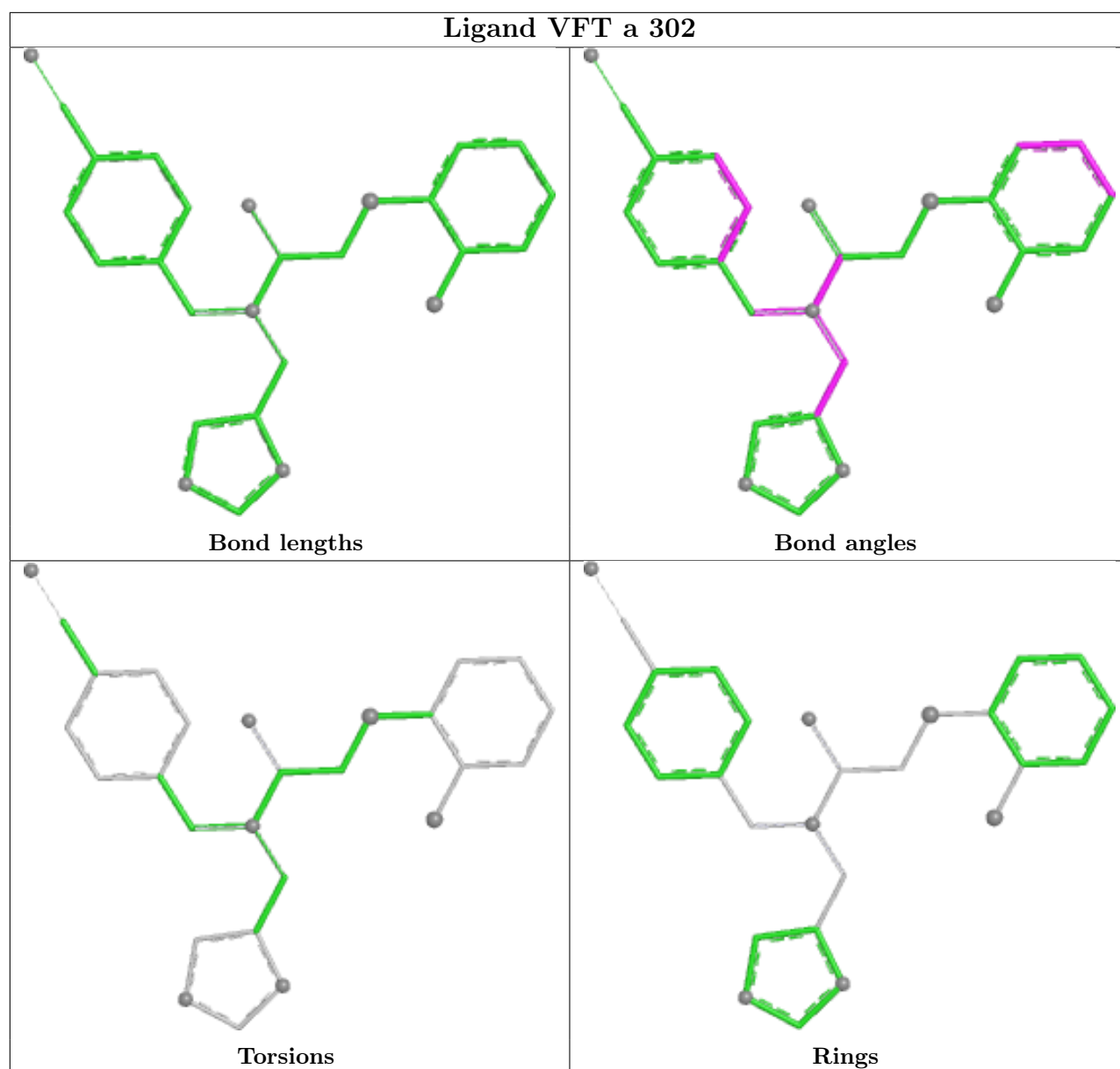
Ligand VFT D 301 (B)

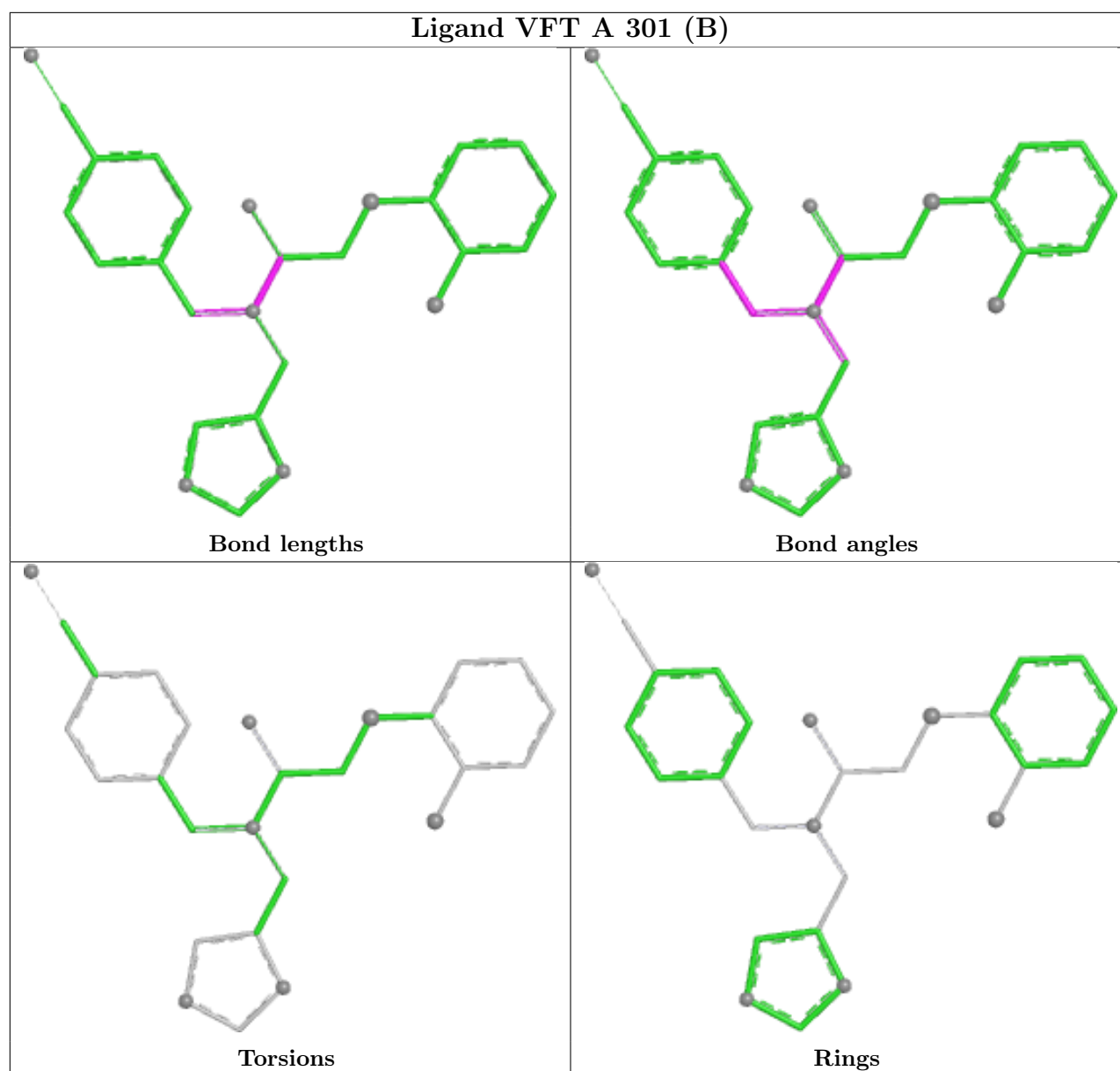


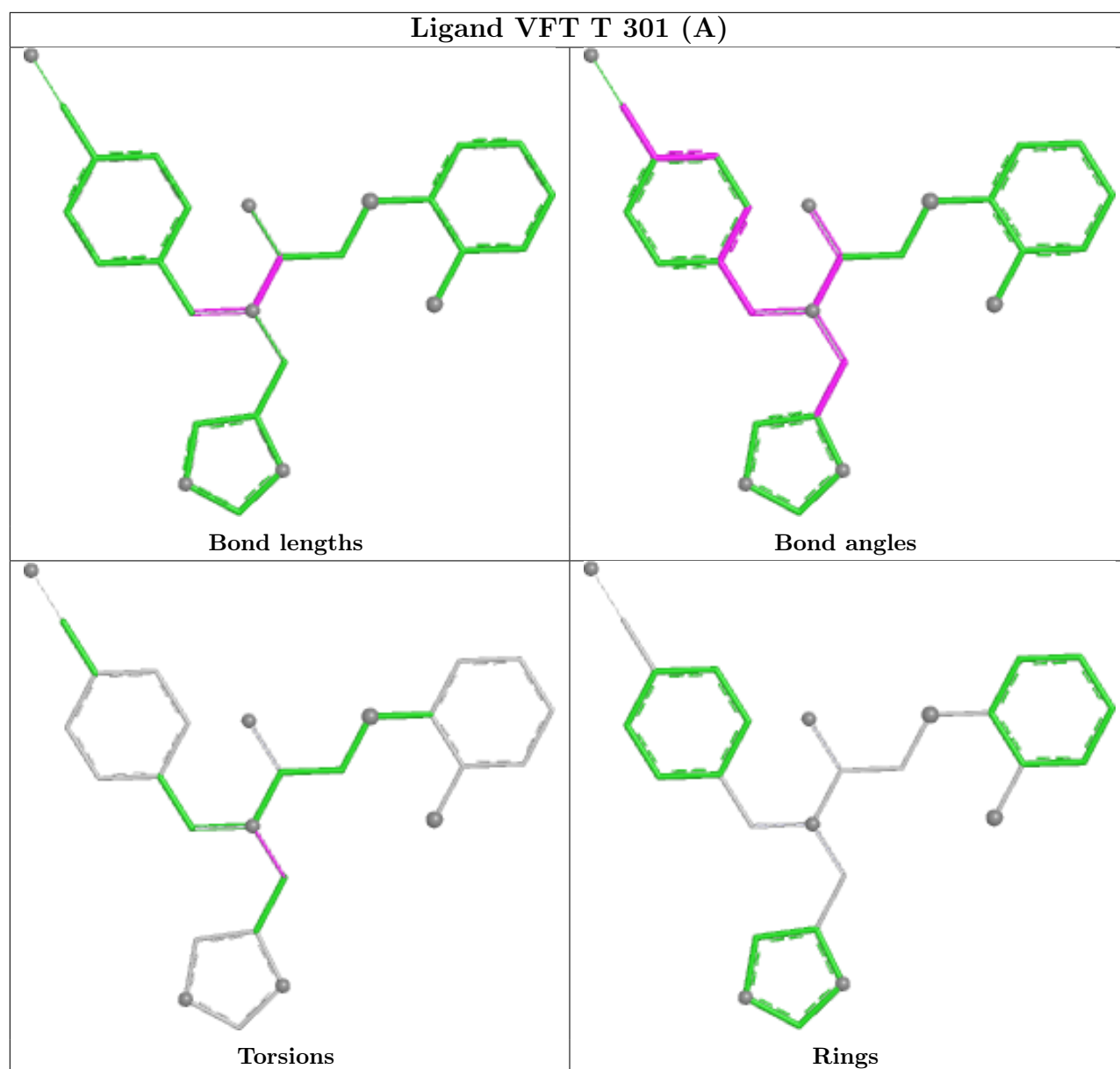




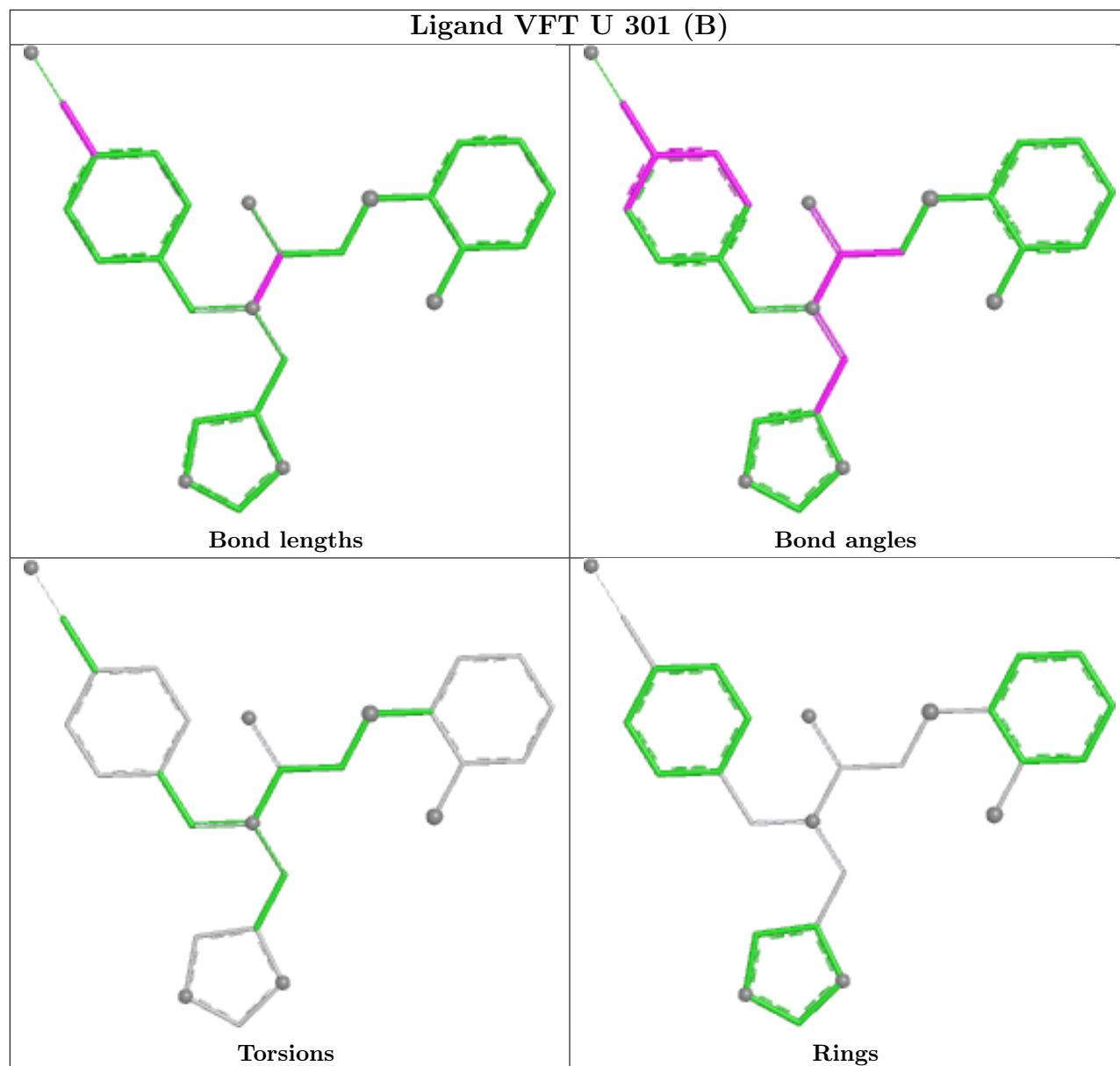


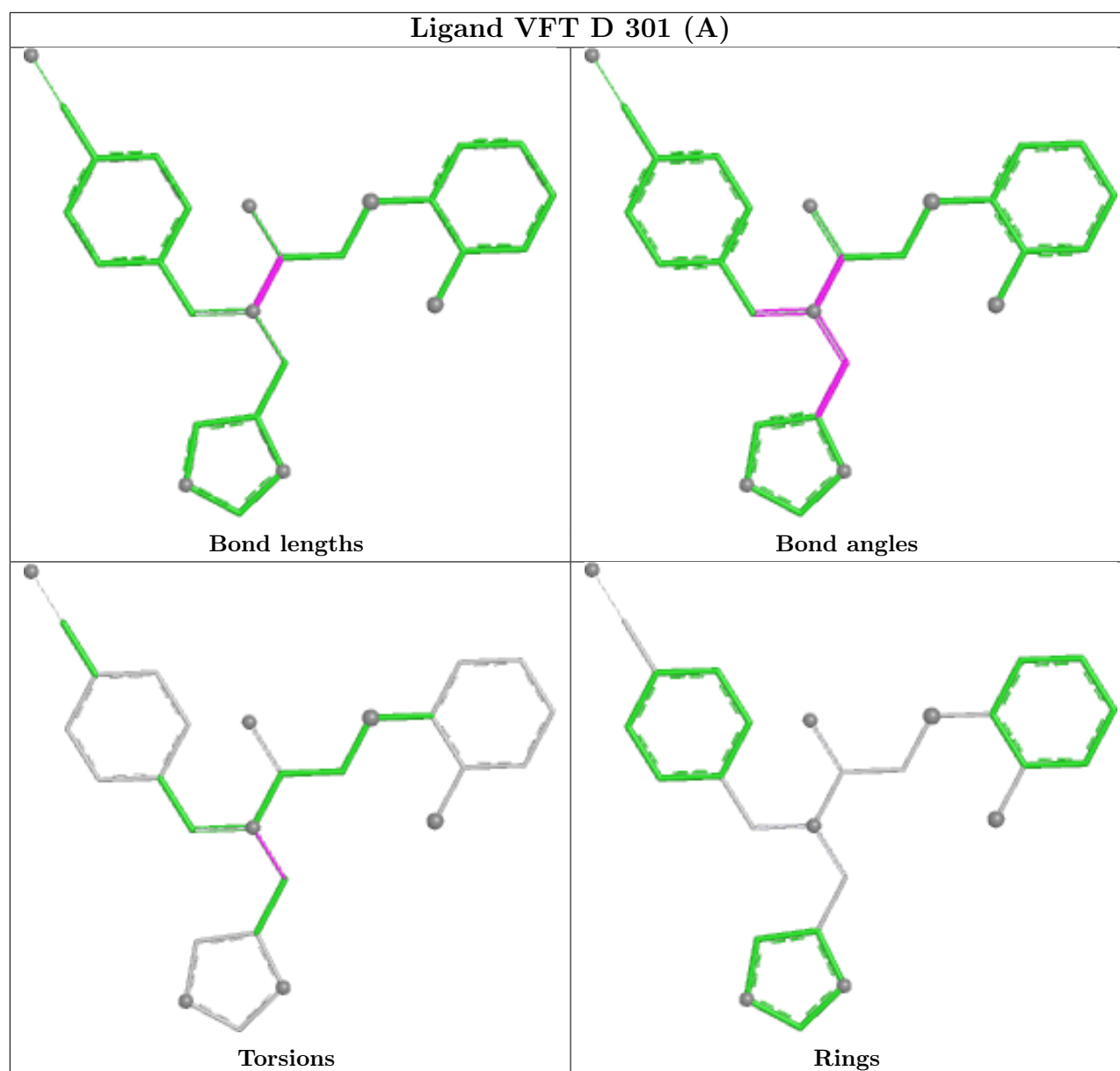


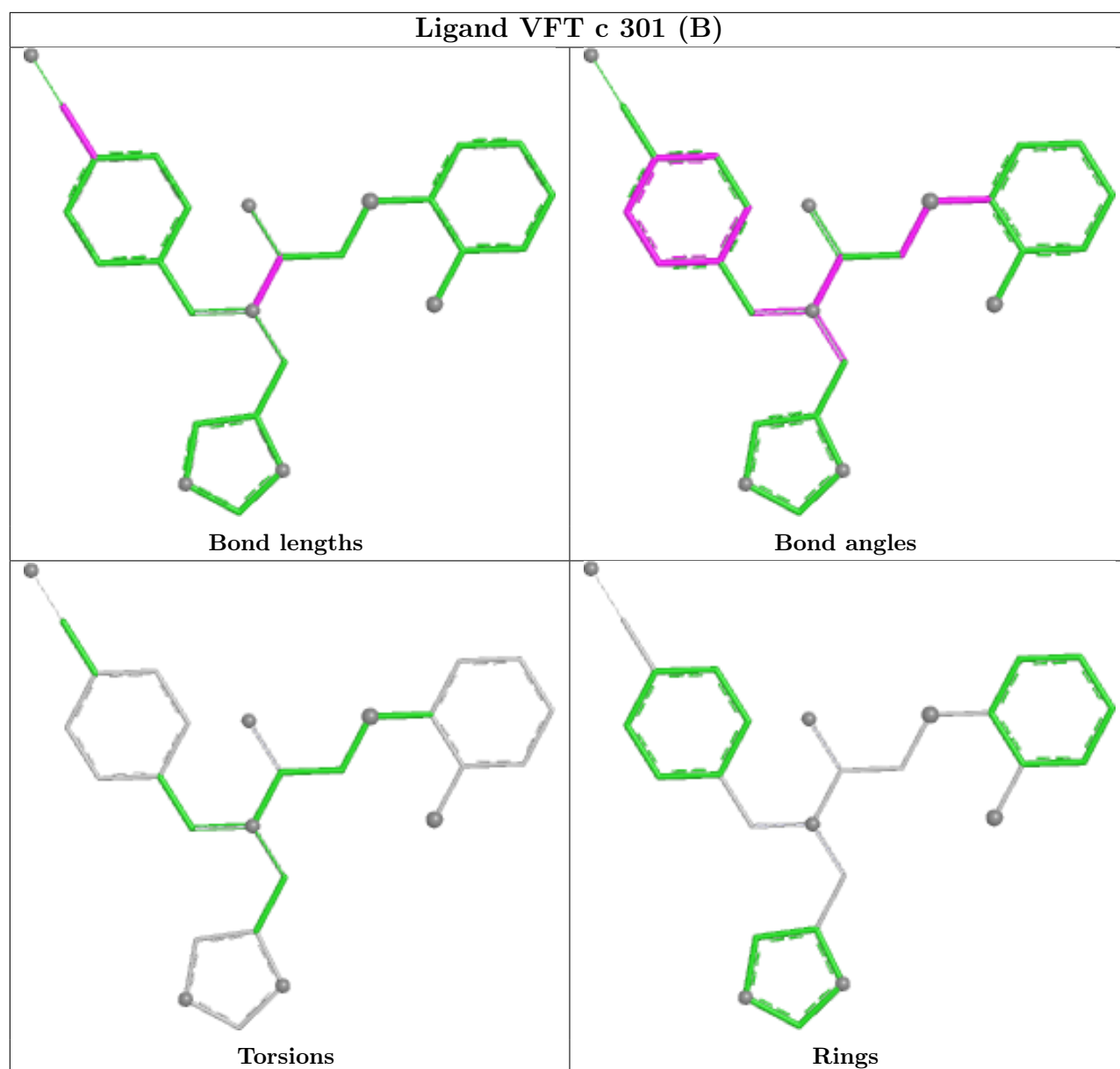


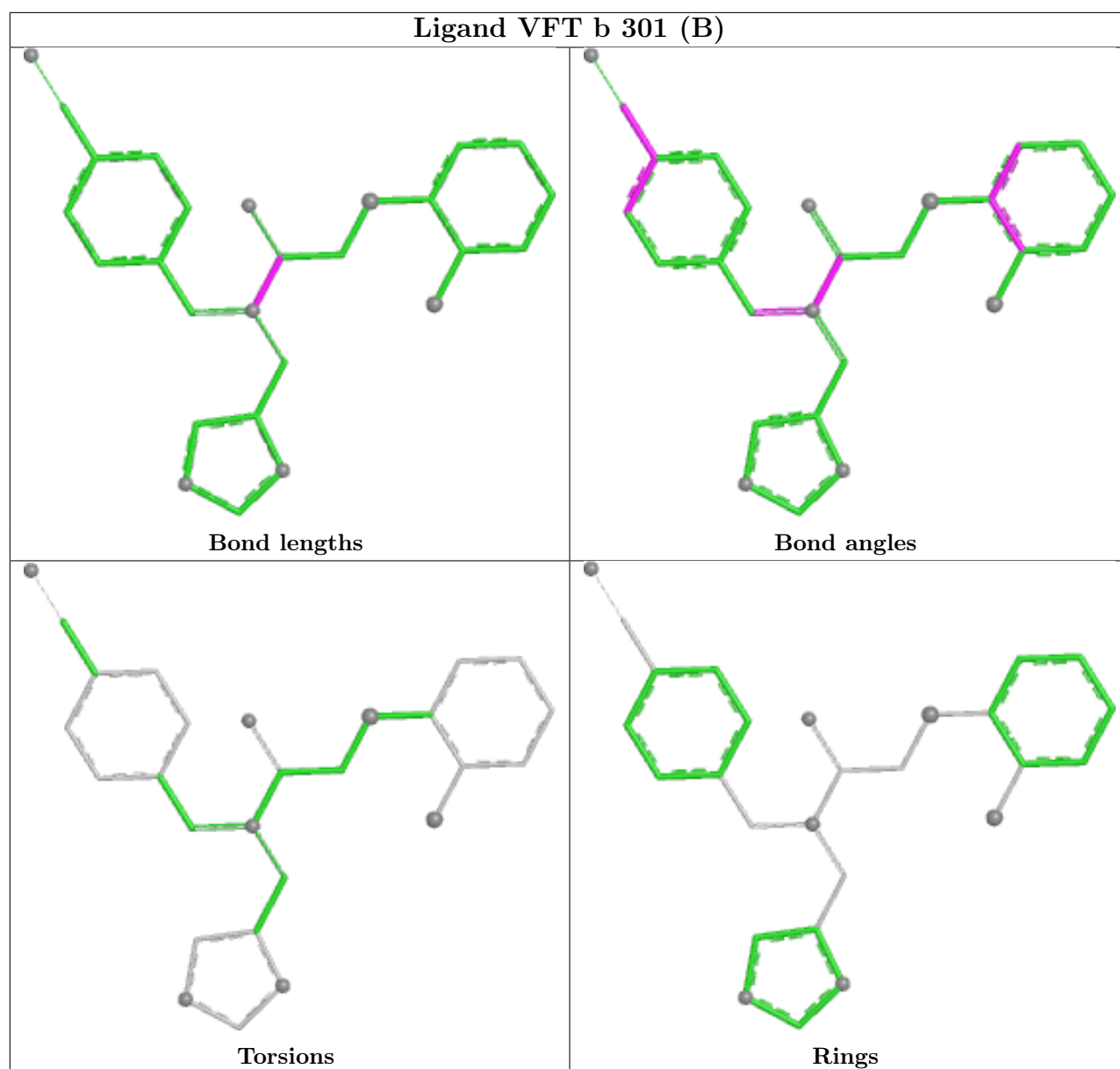


Ligand VFT U 301 (B)

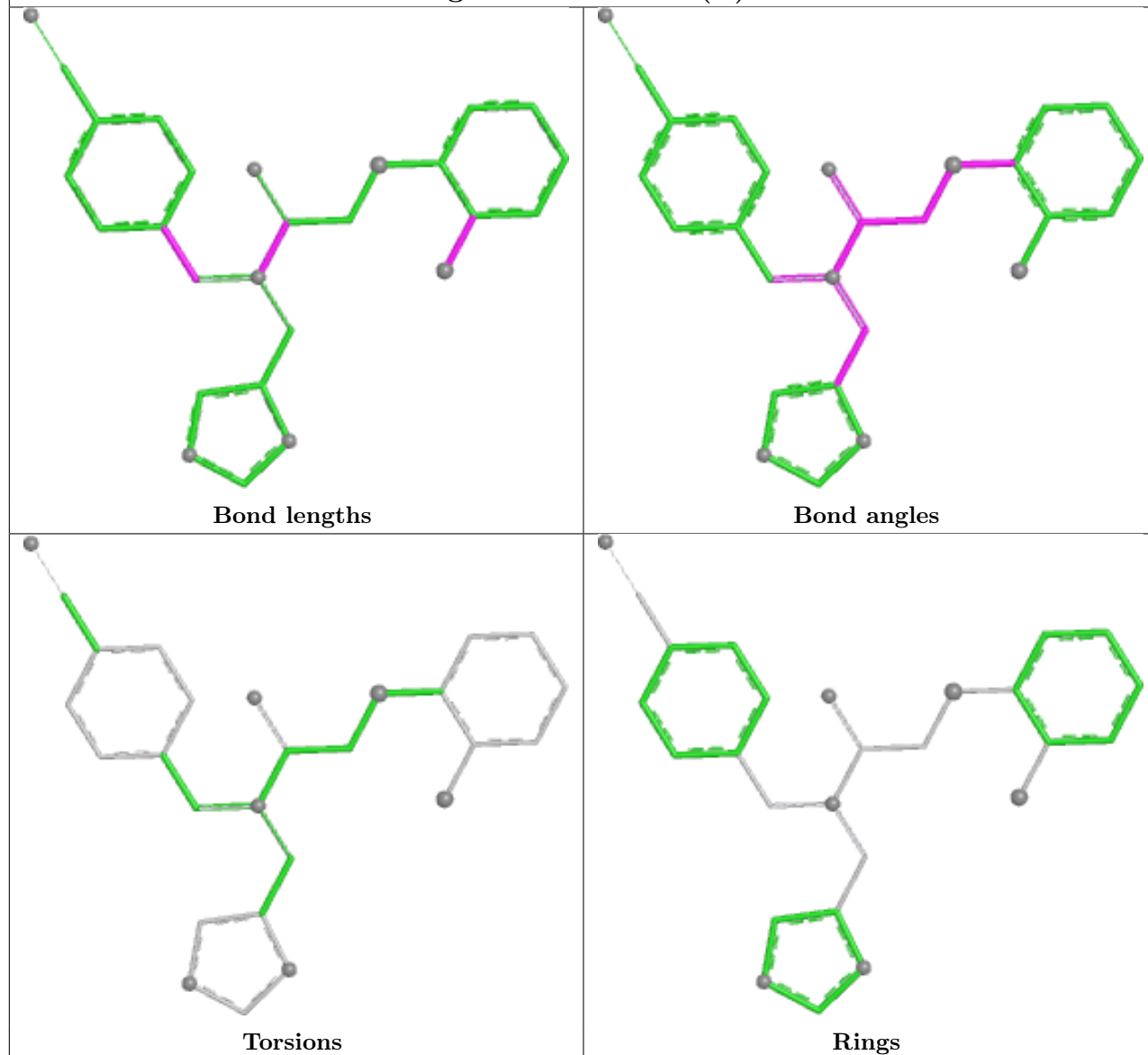


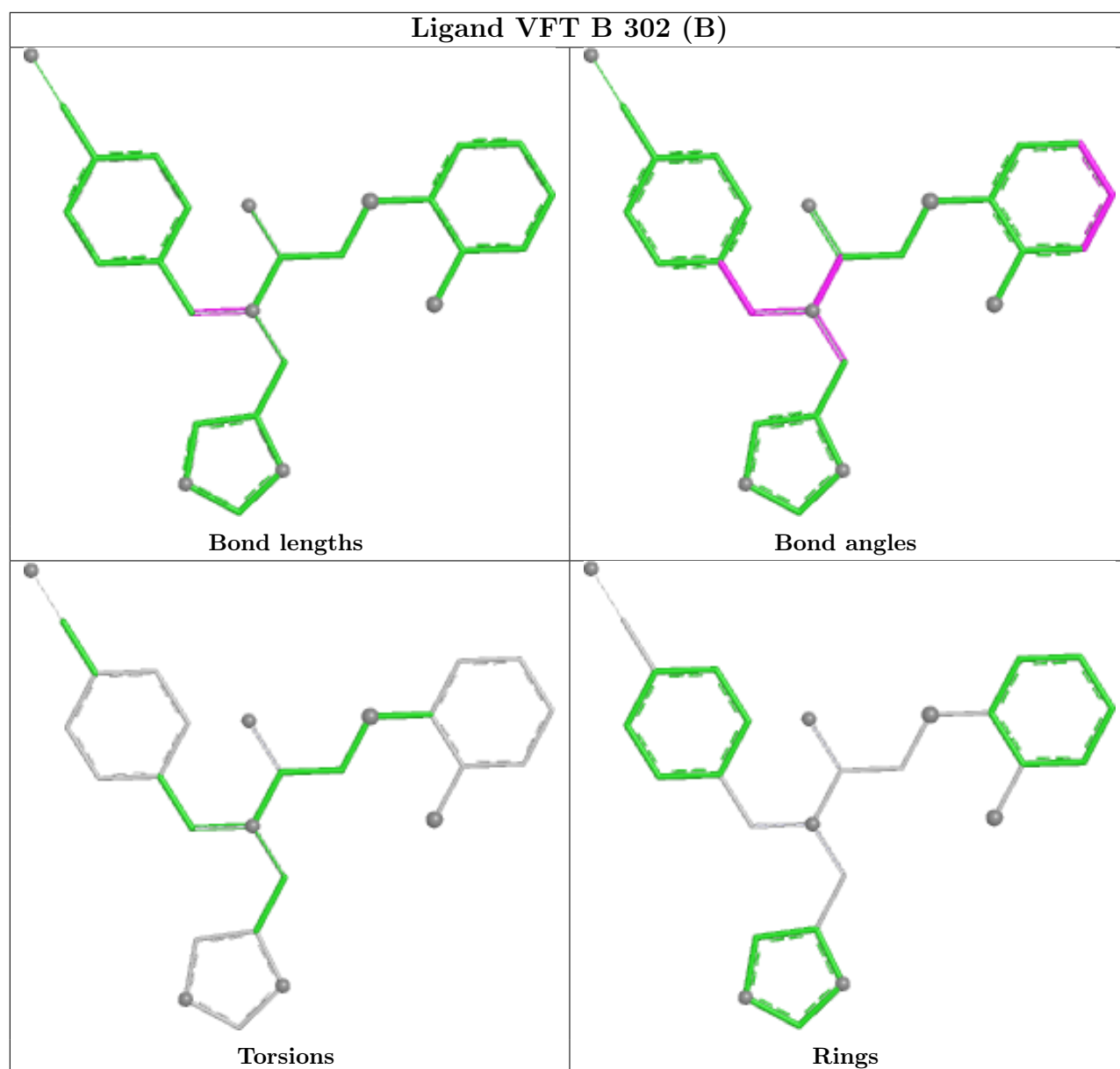


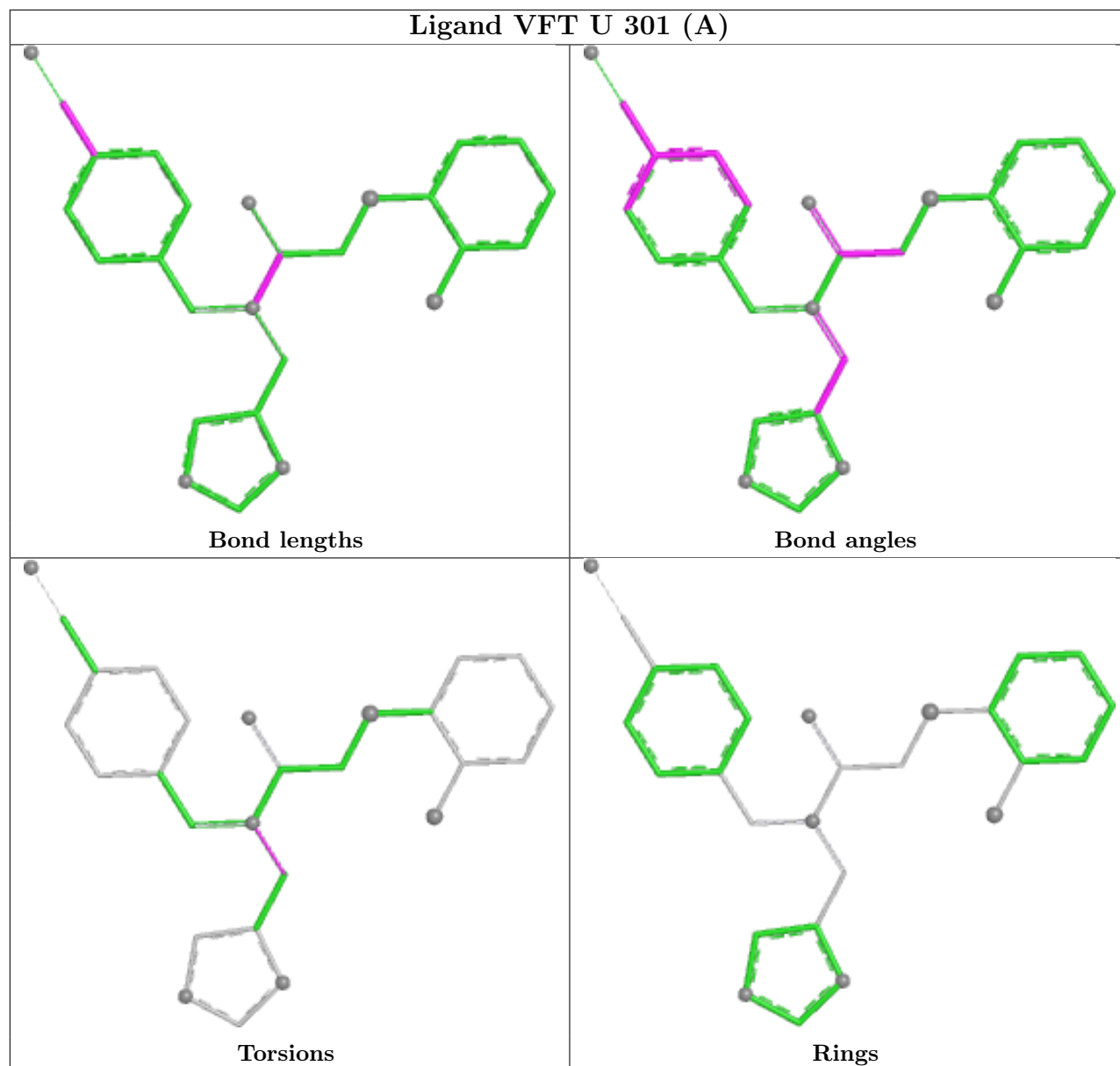




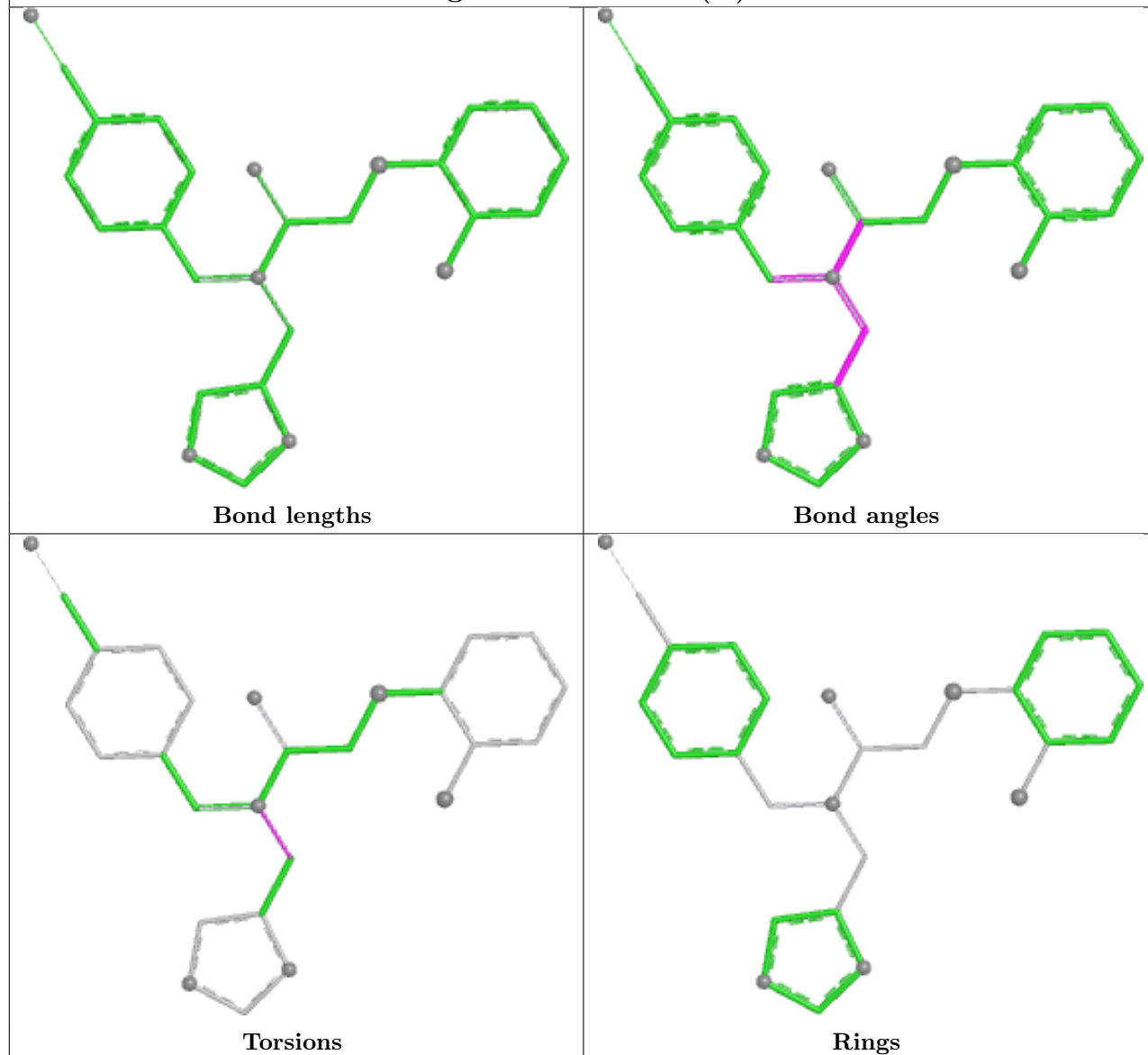
Ligand VFT K 301 (B)

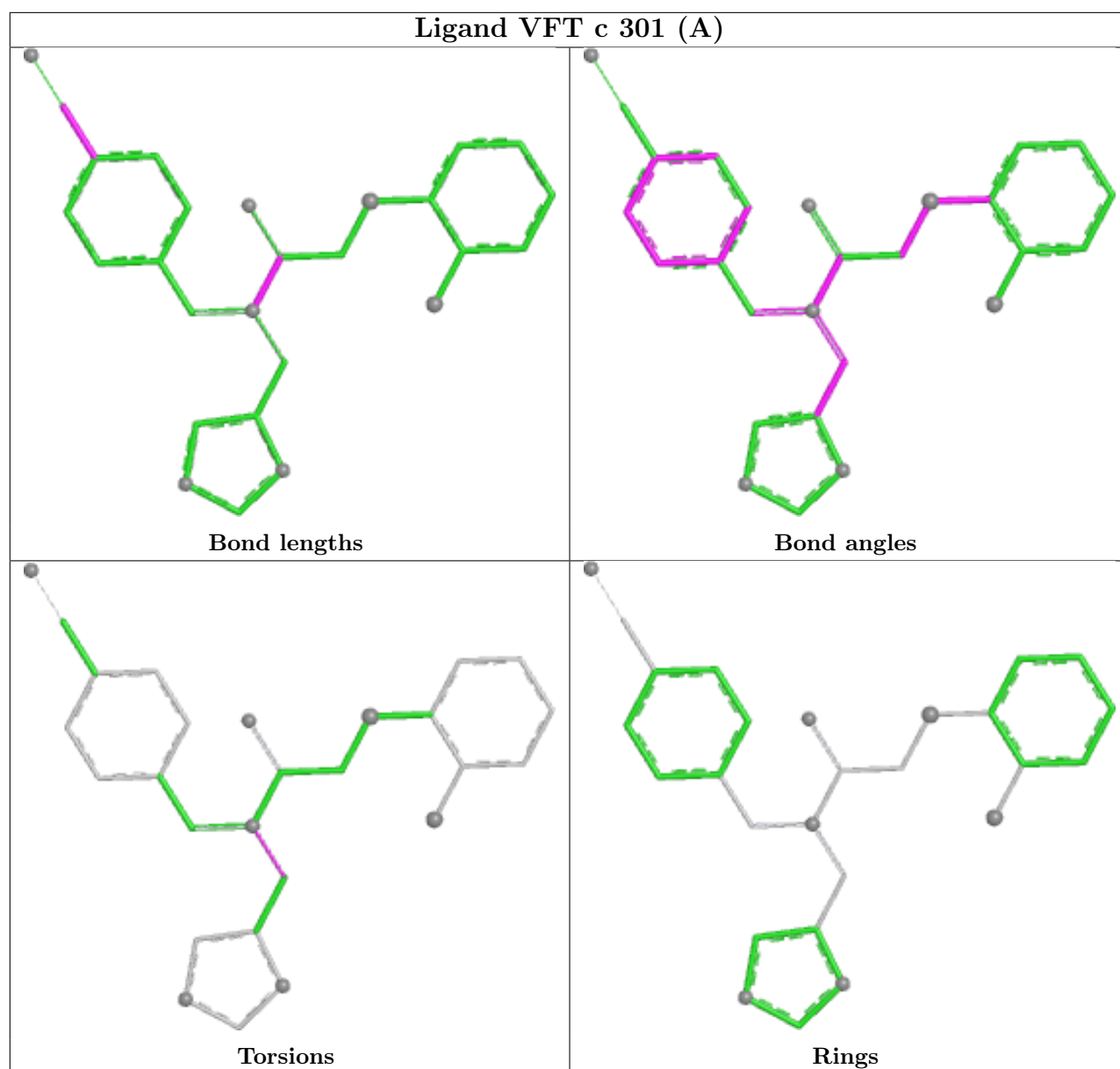


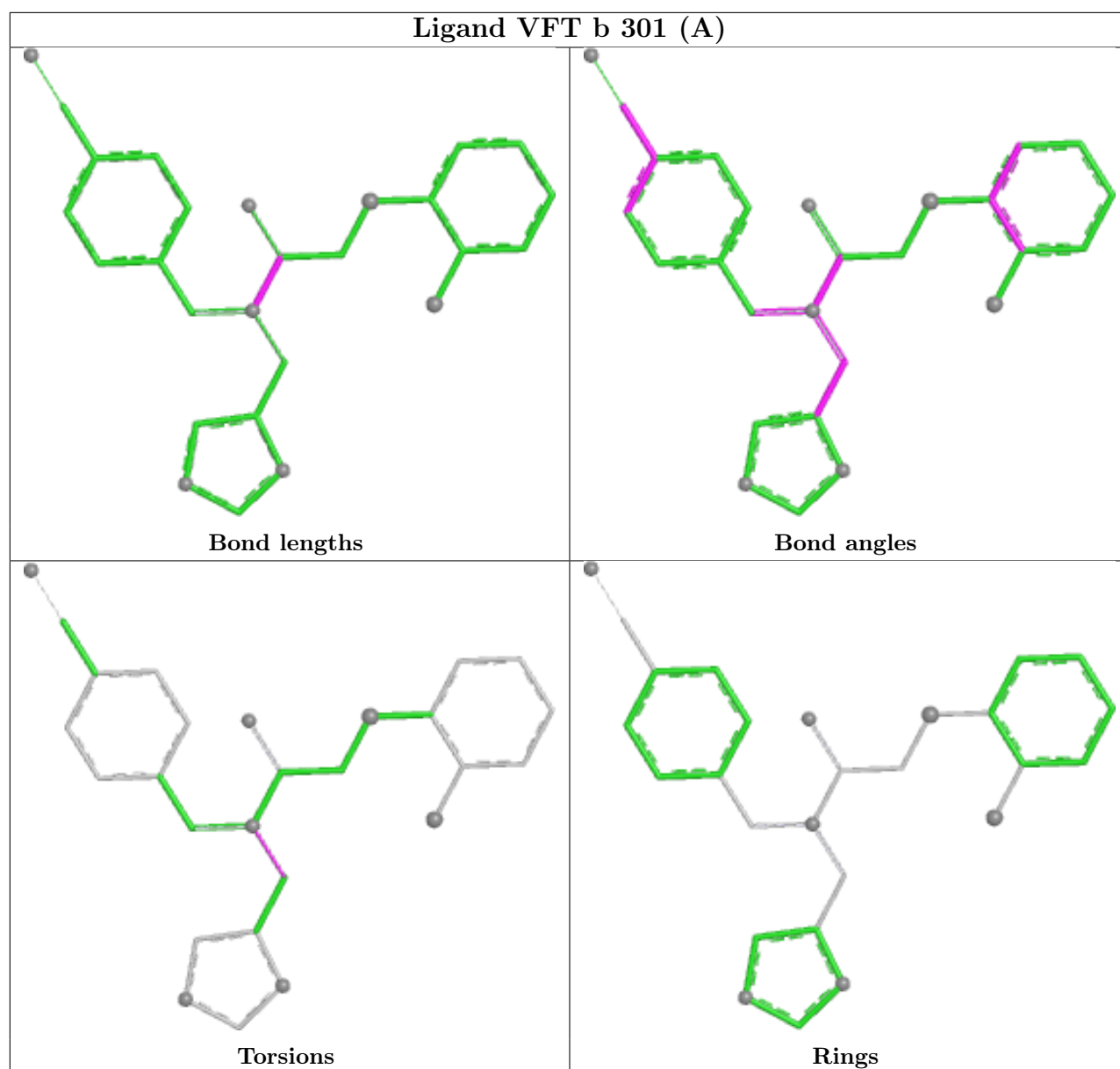




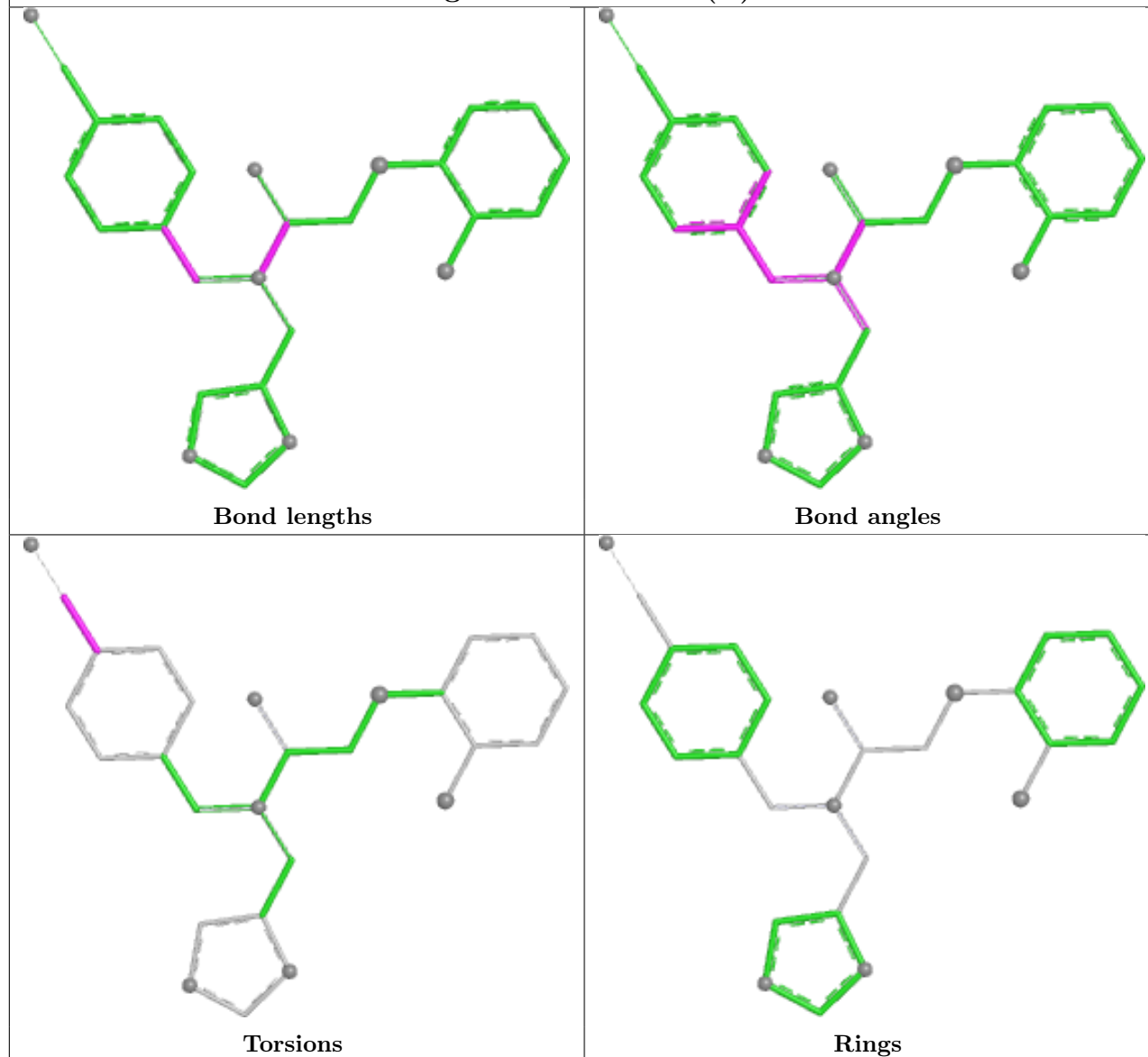
Ligand VFT G 302 (A)

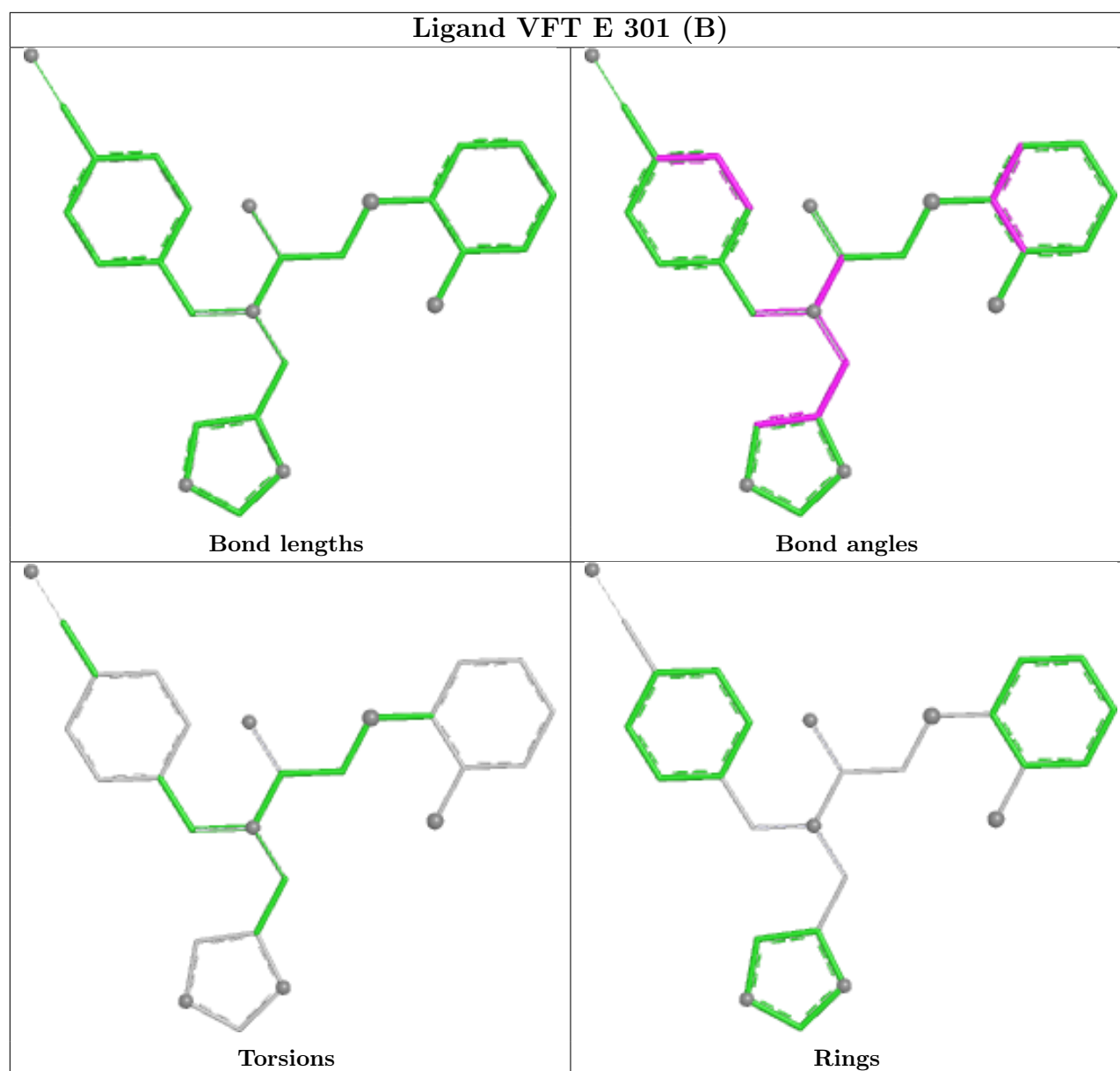




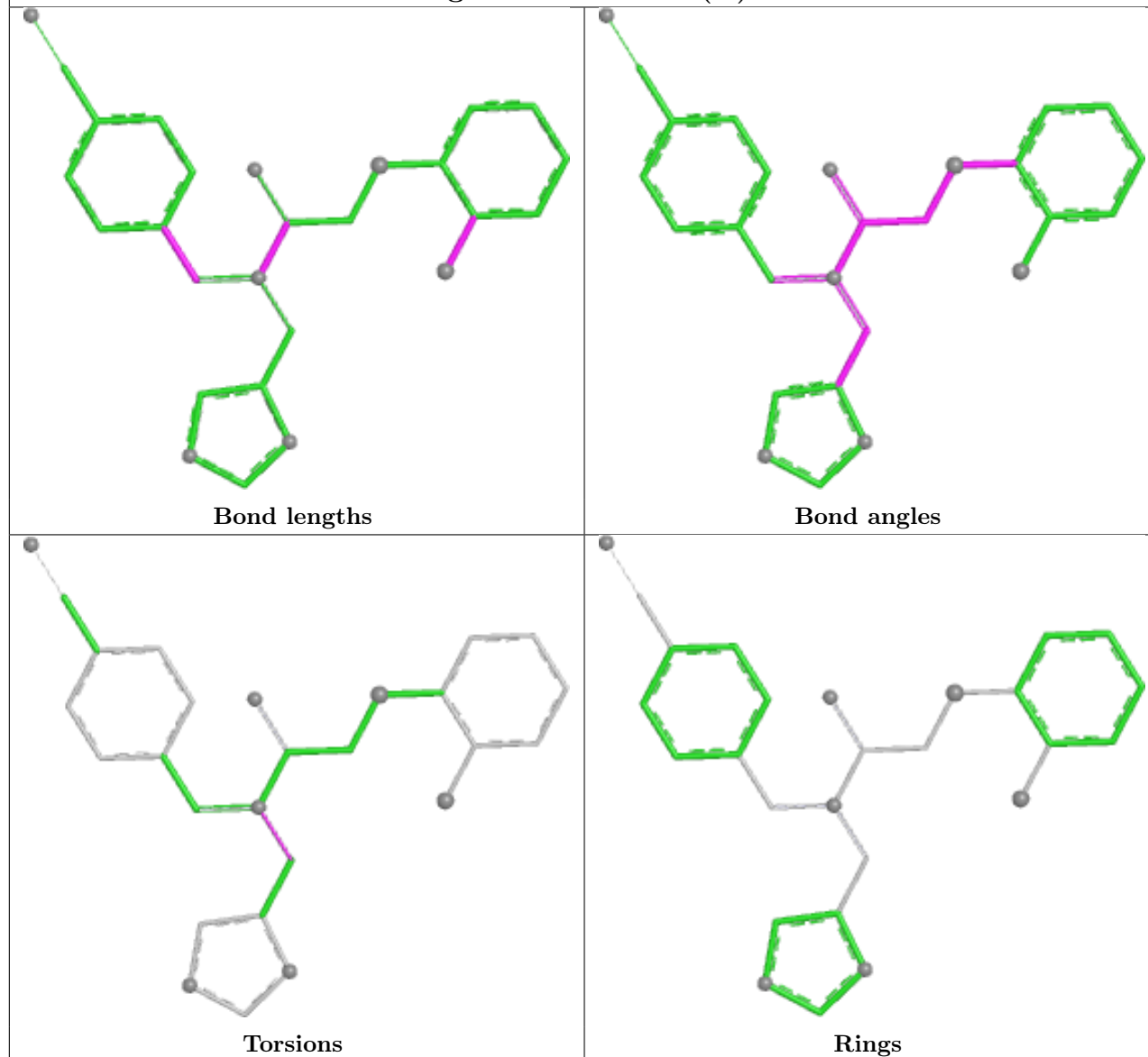


Ligand VFT W 301 (B)

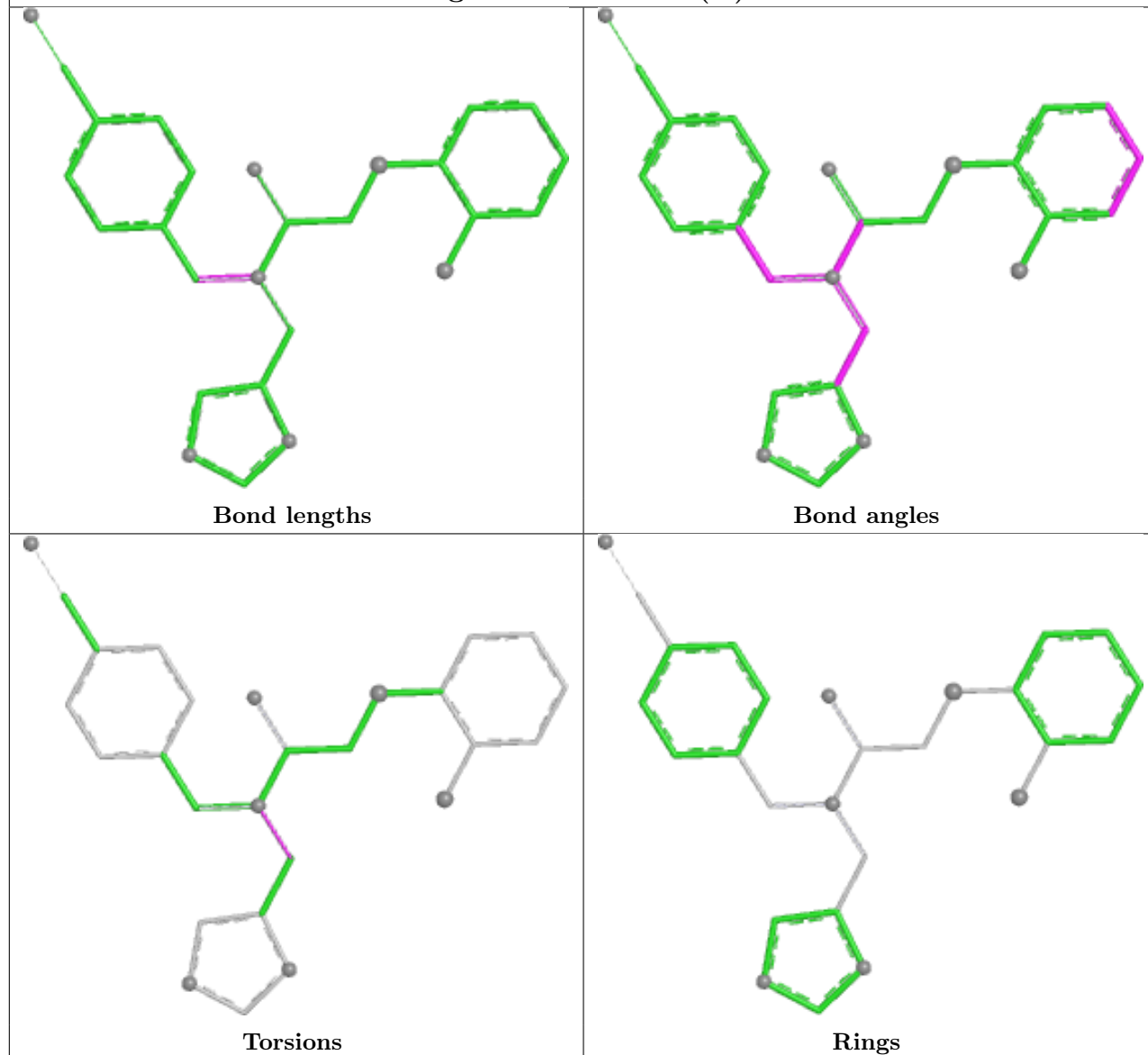




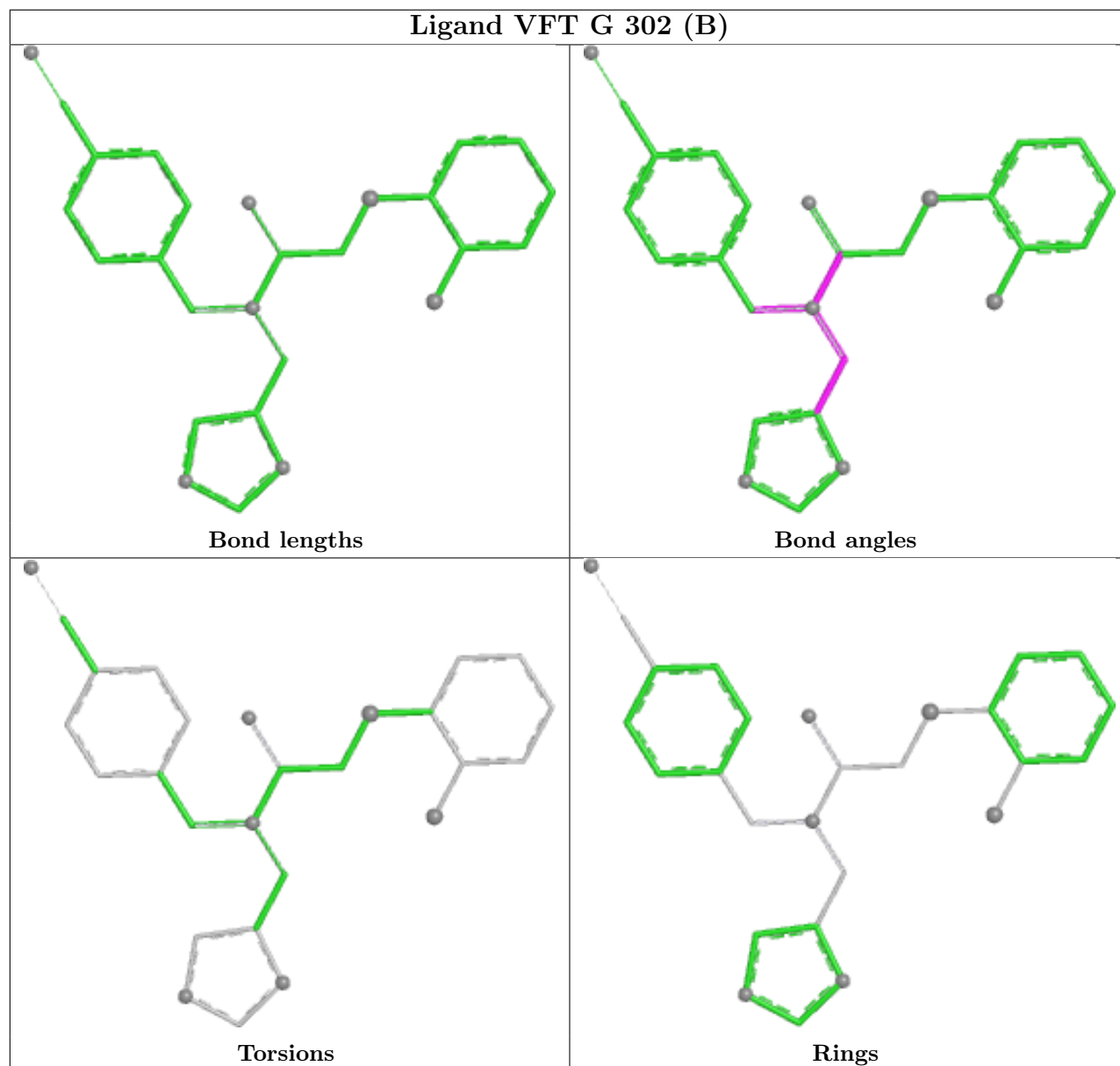
Ligand VFT K 301 (A)

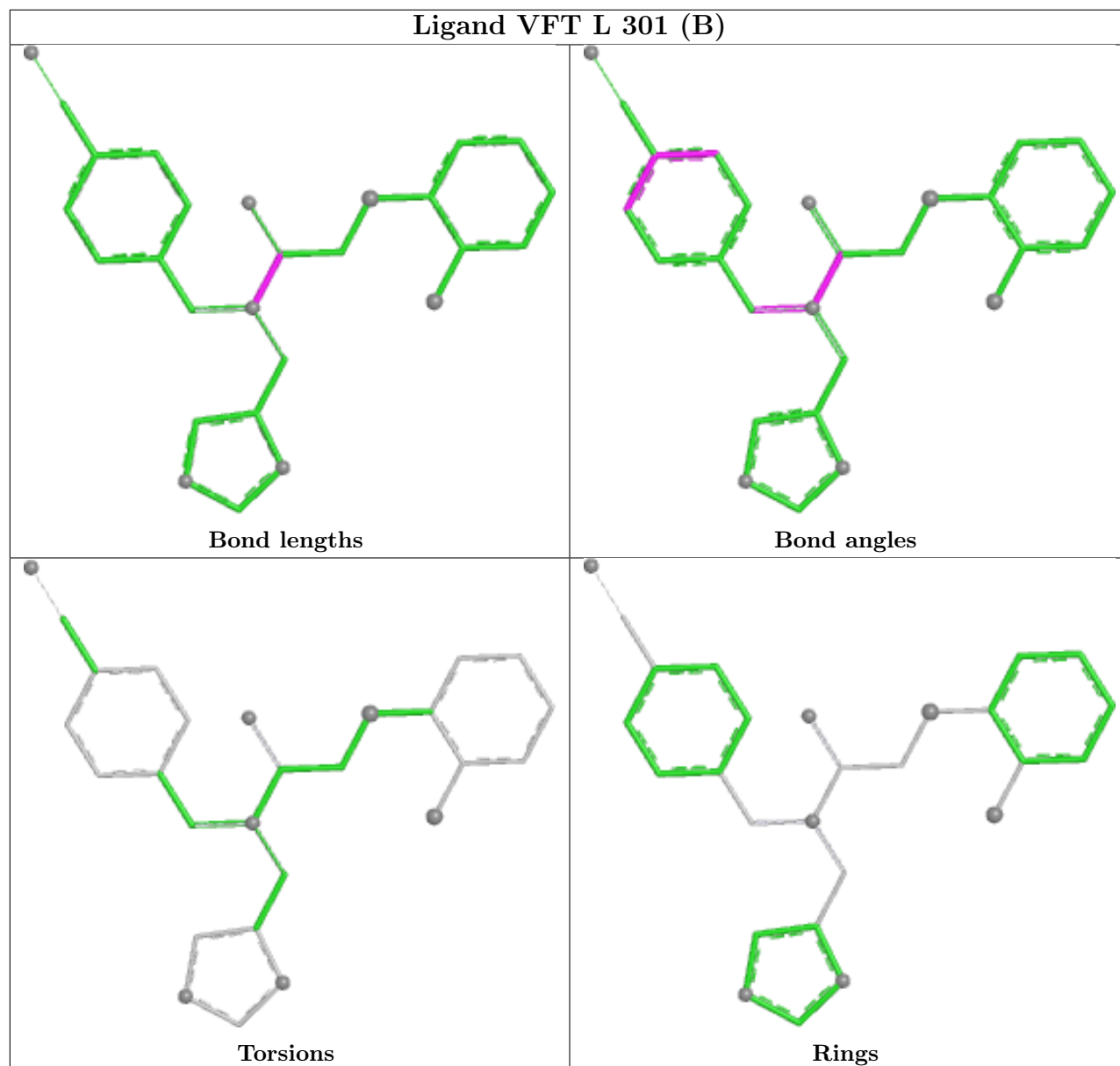


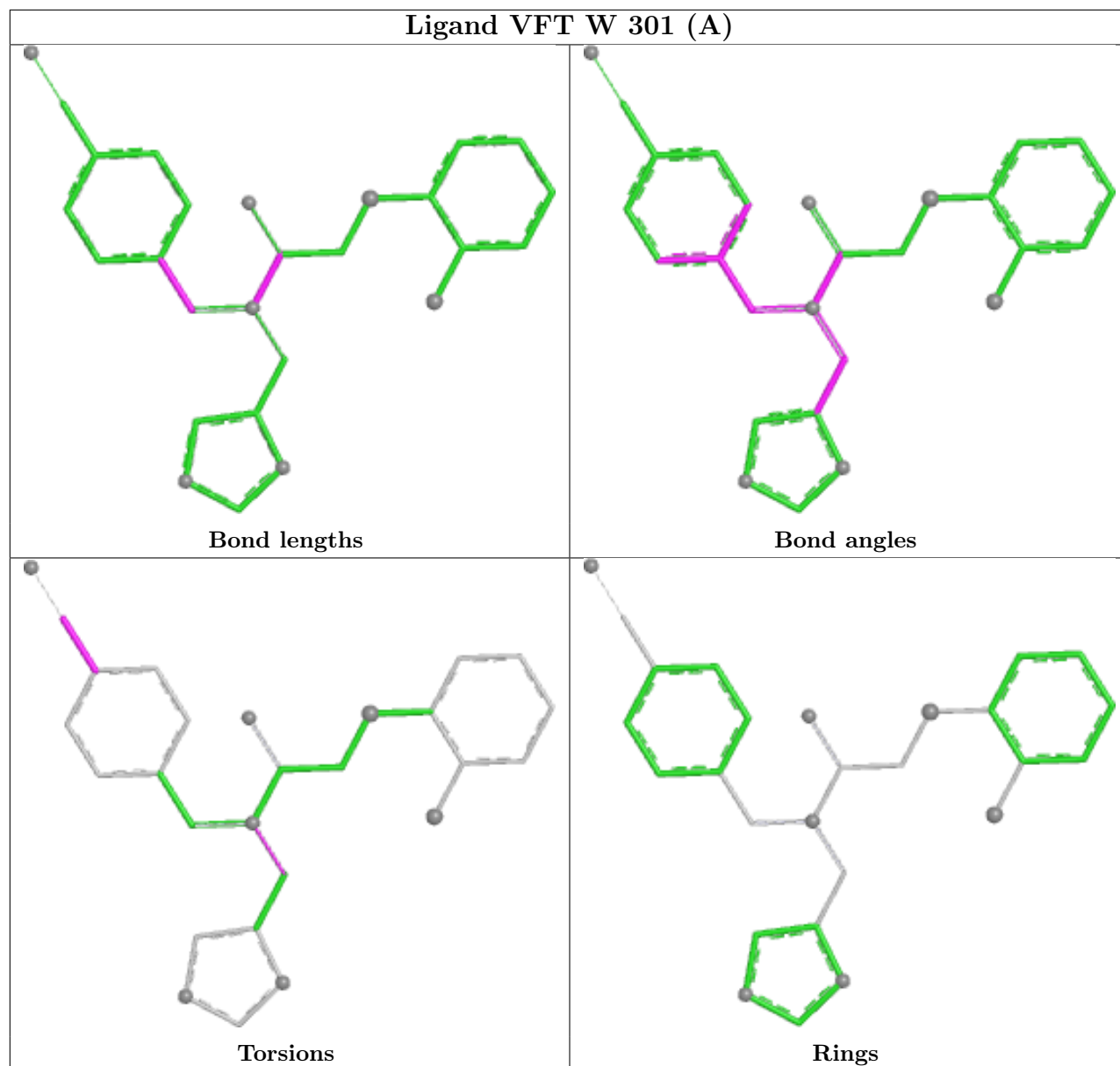
Ligand VFT B 302 (A)

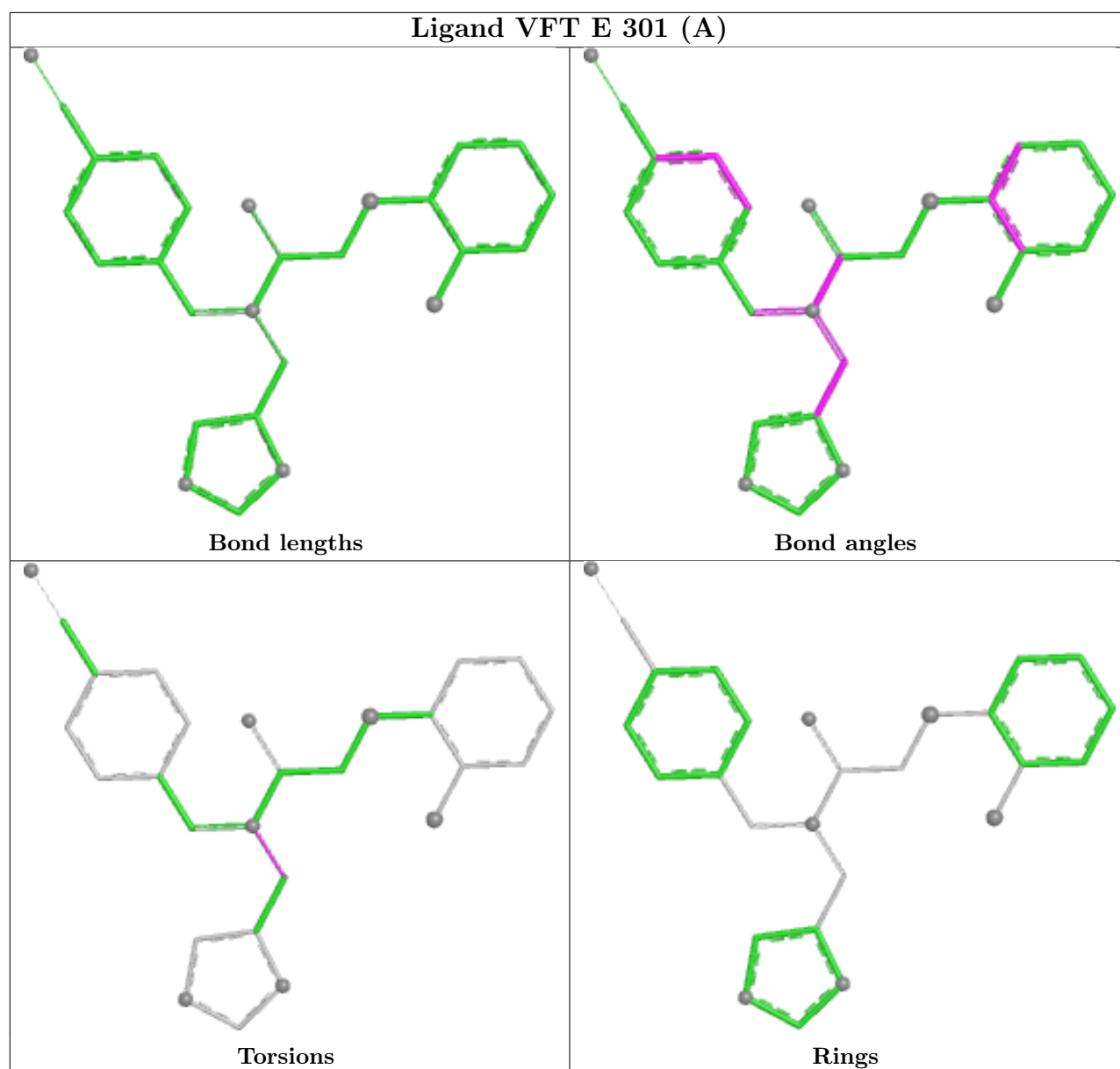


Ligand VFT G 302 (B)

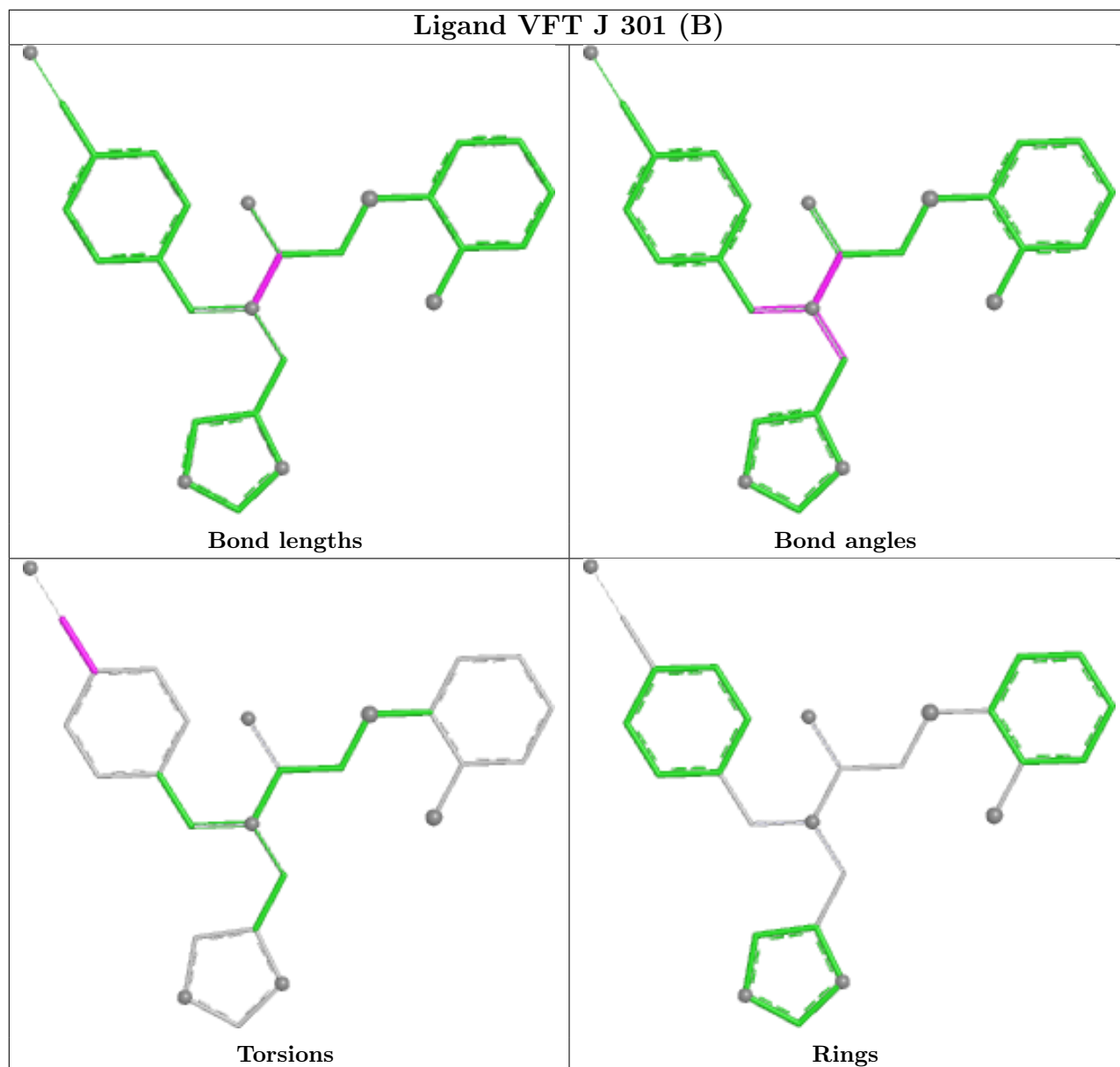




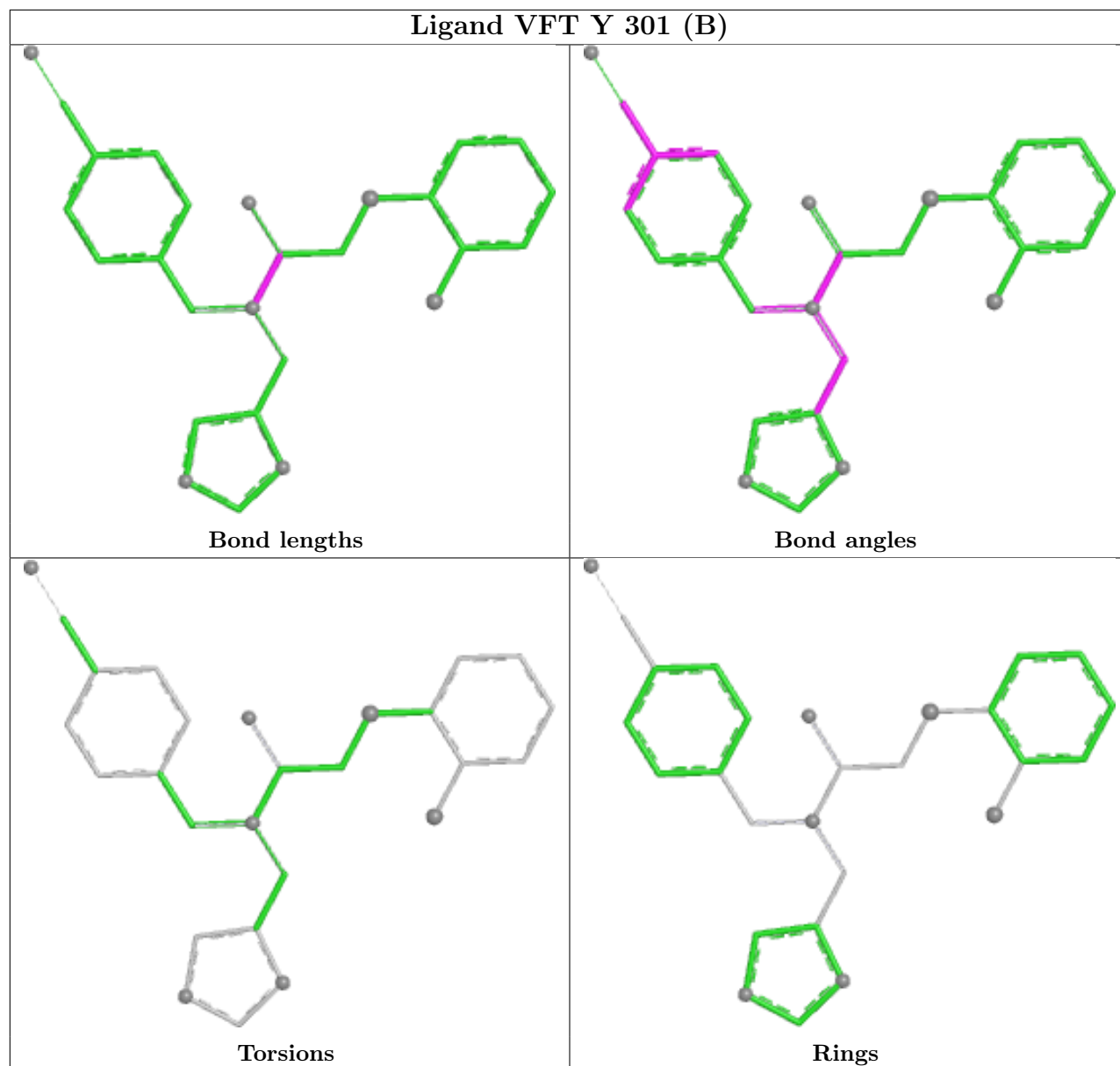


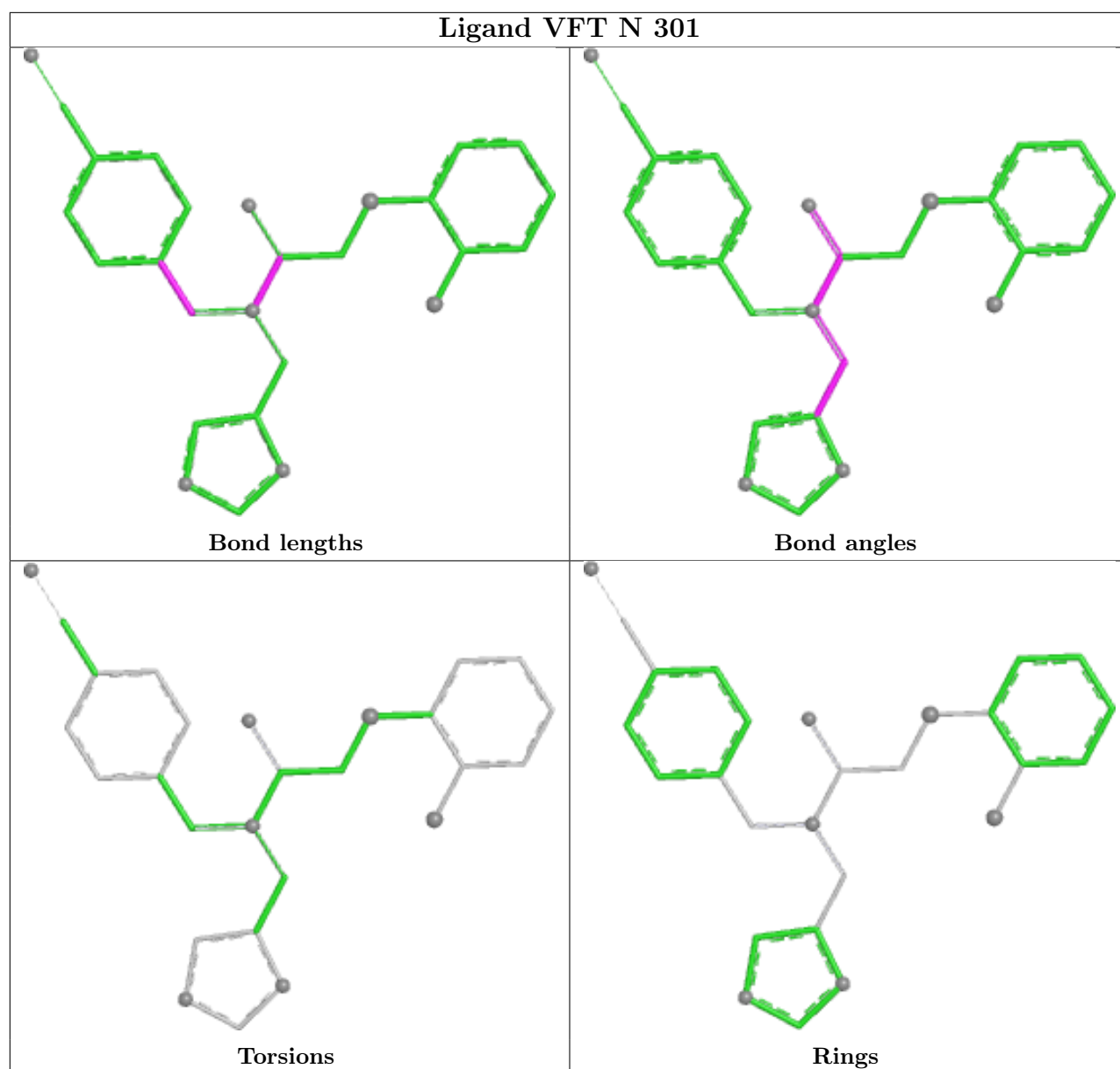


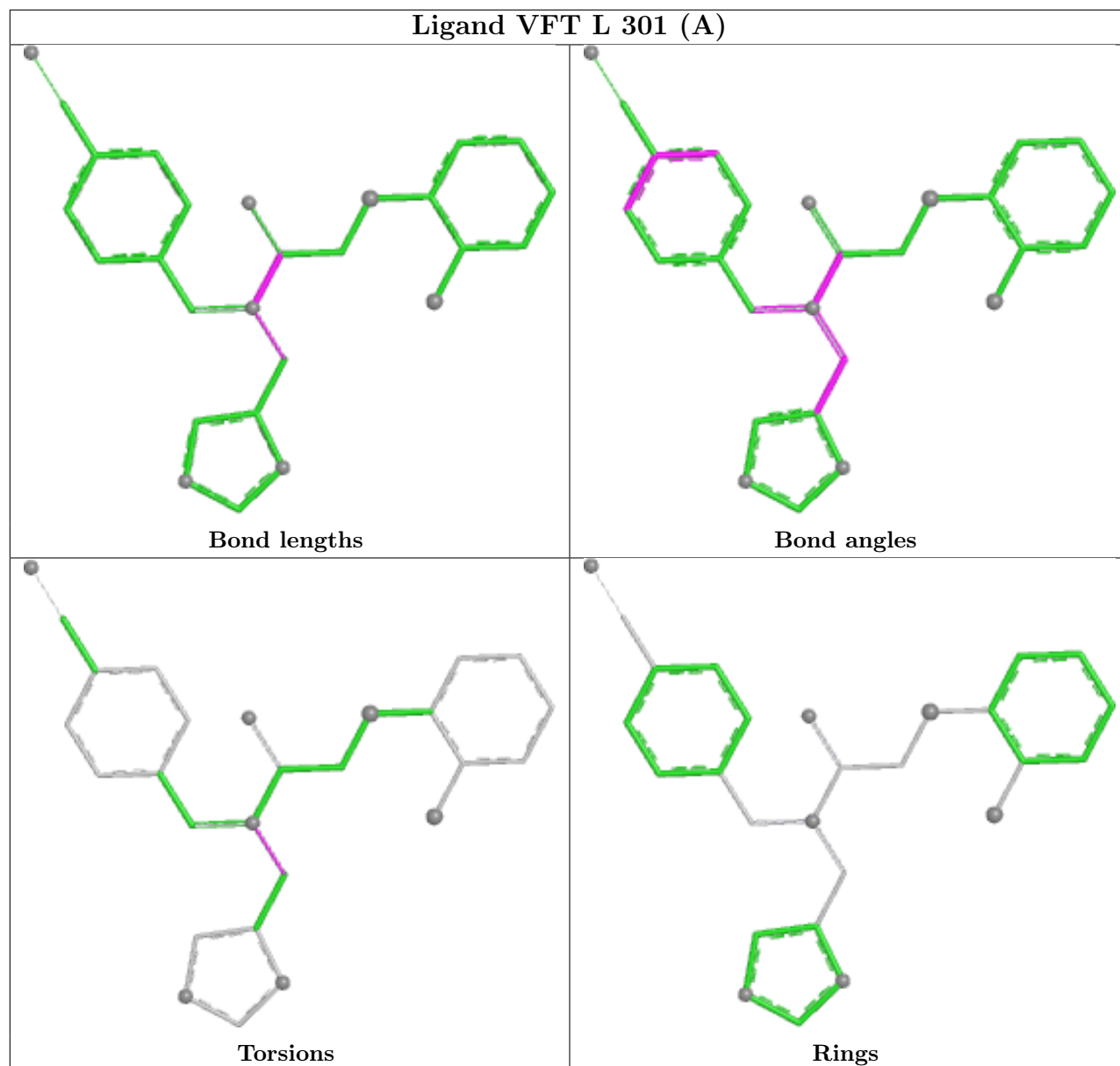
Ligand VFT J 301 (B)



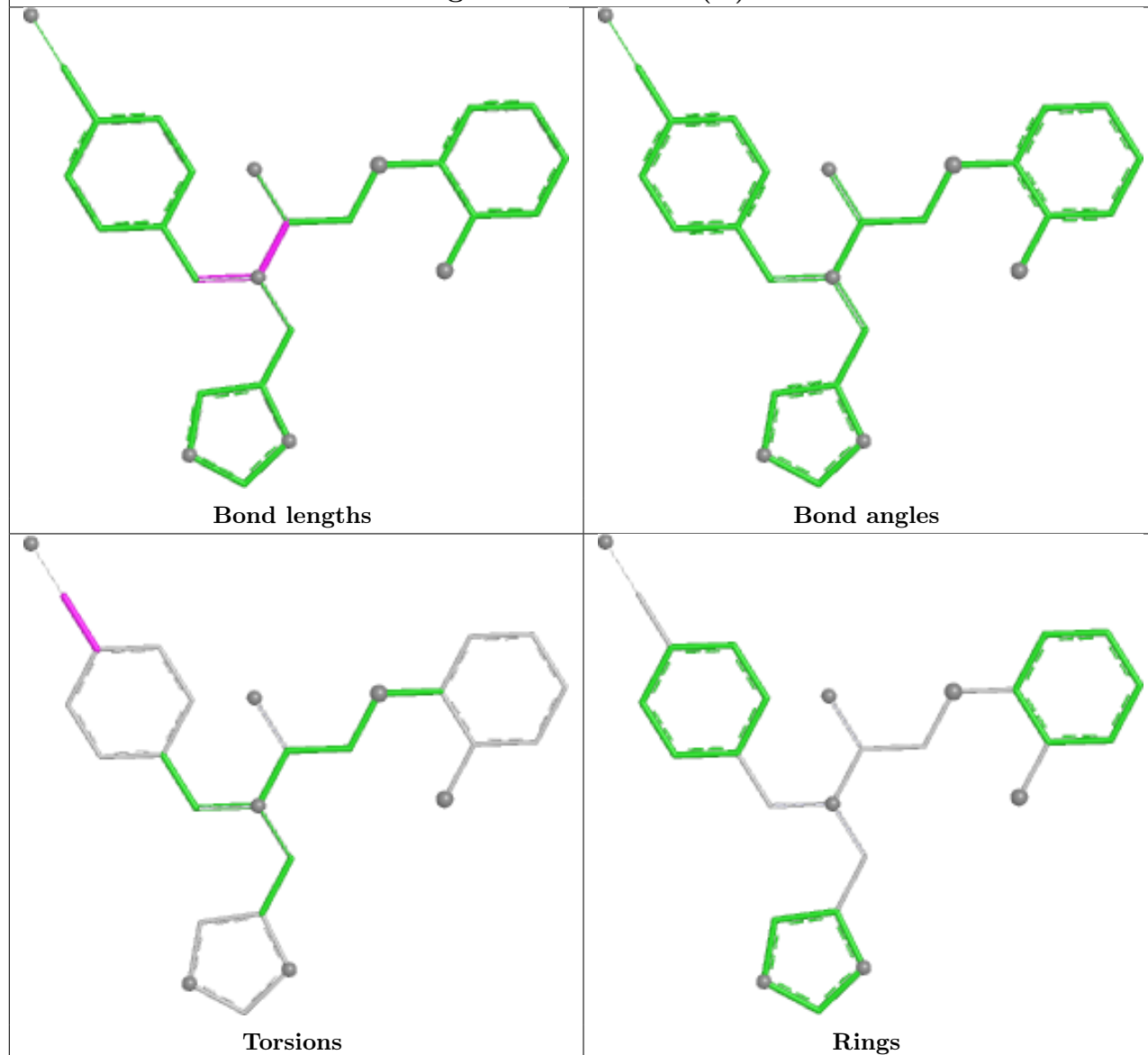
Ligand VFT Y 301 (B)



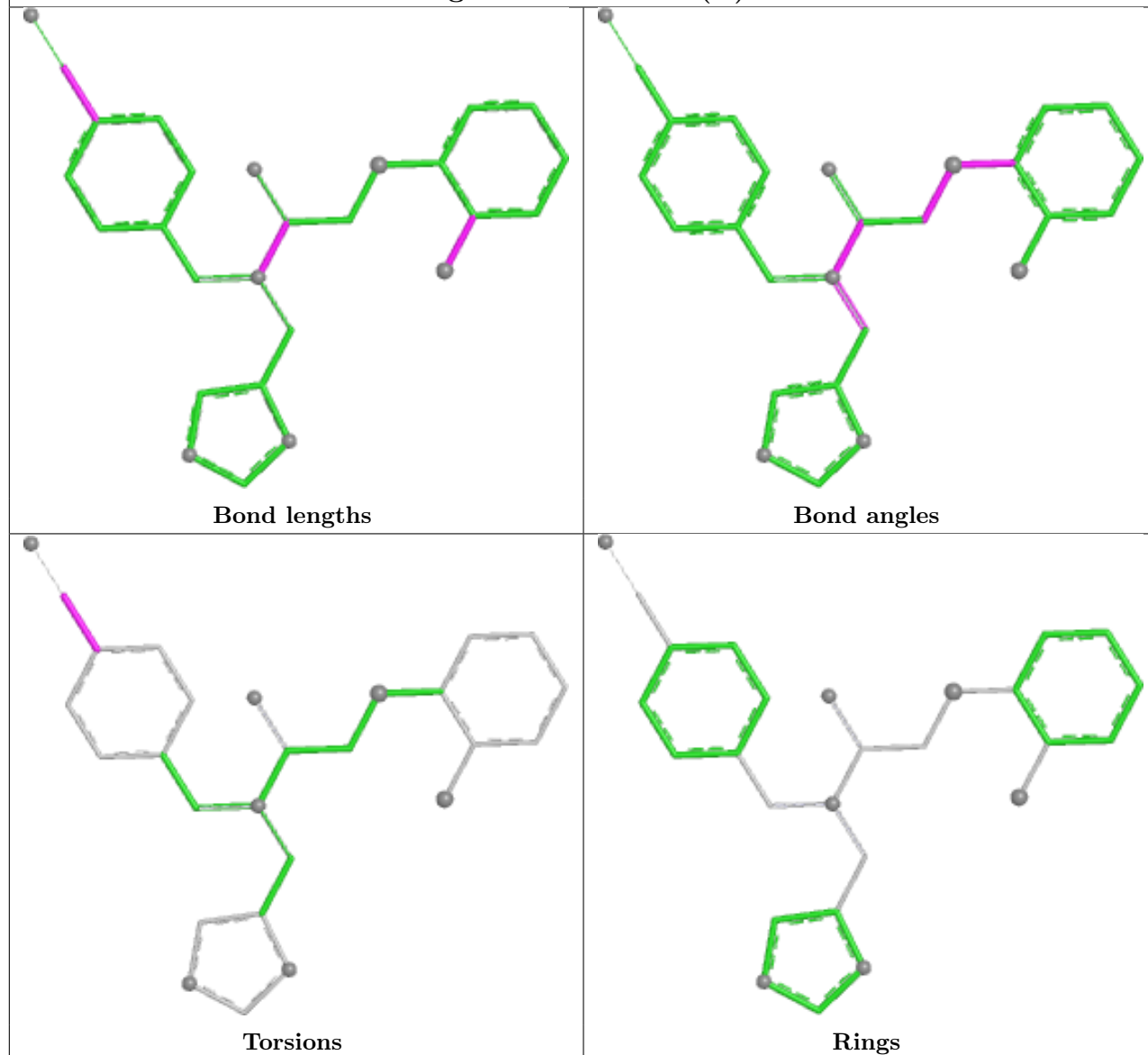


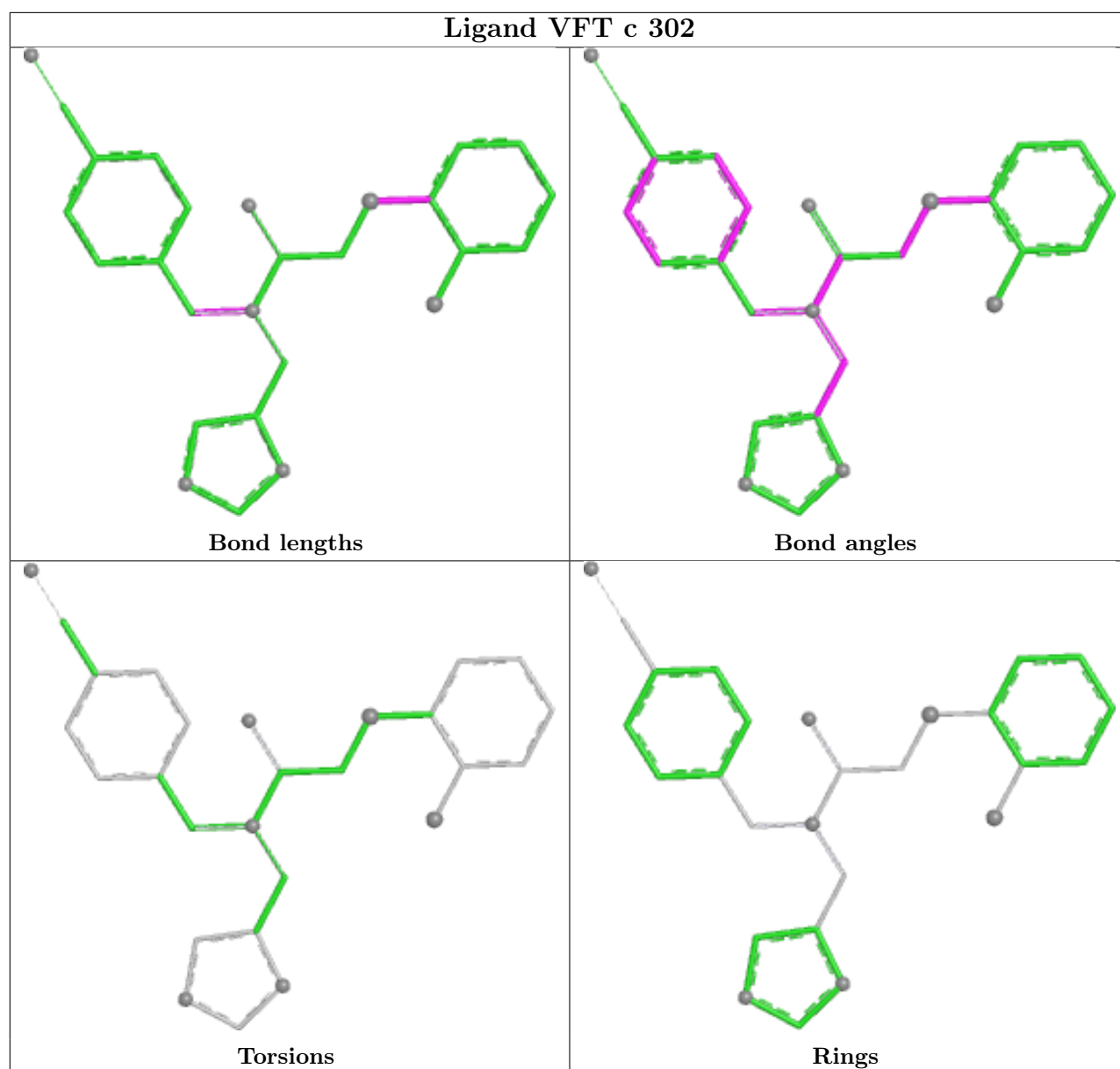


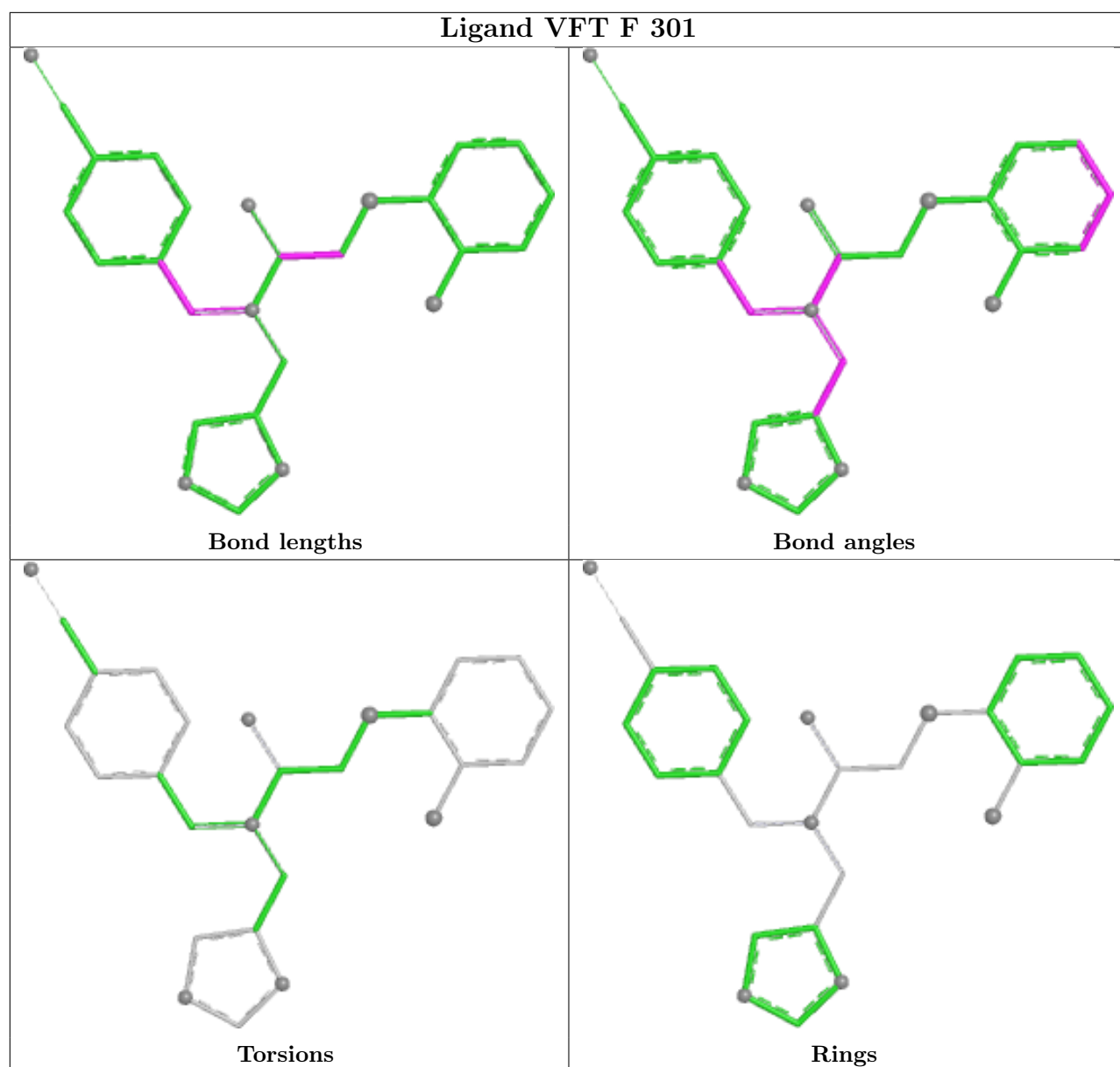
Ligand VFT G 301 (B)



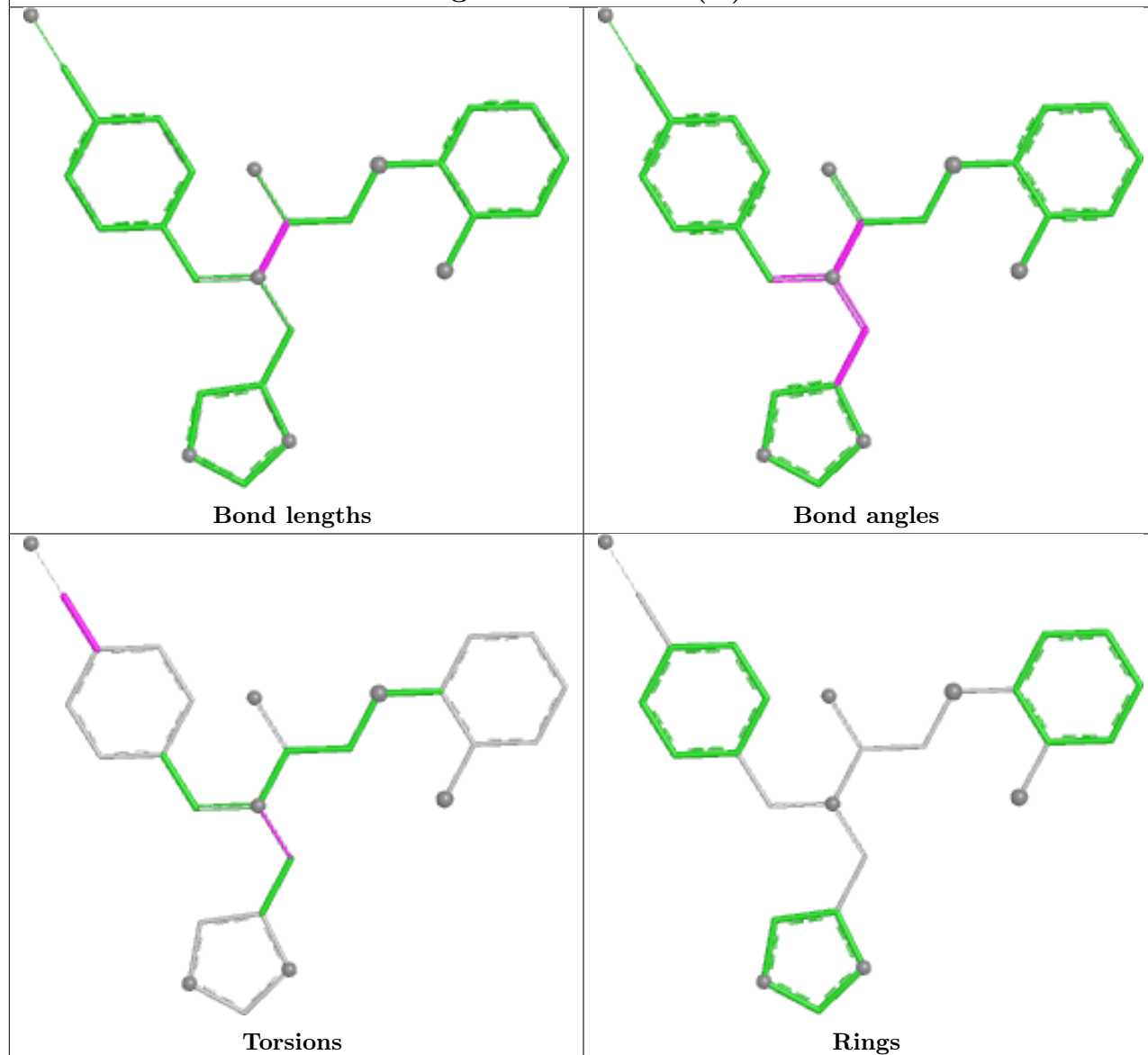
Ligand VFT X 301 (B)



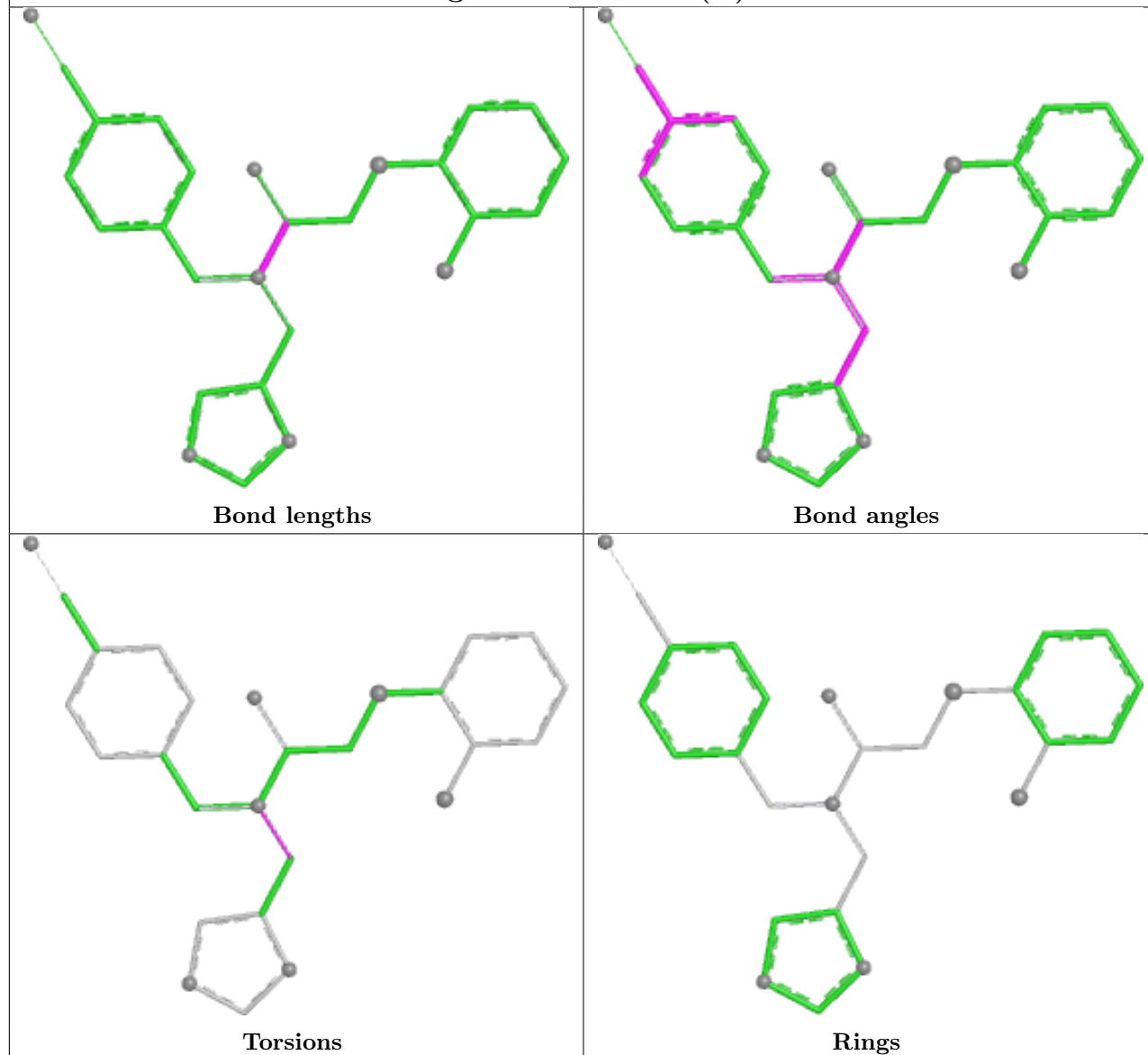


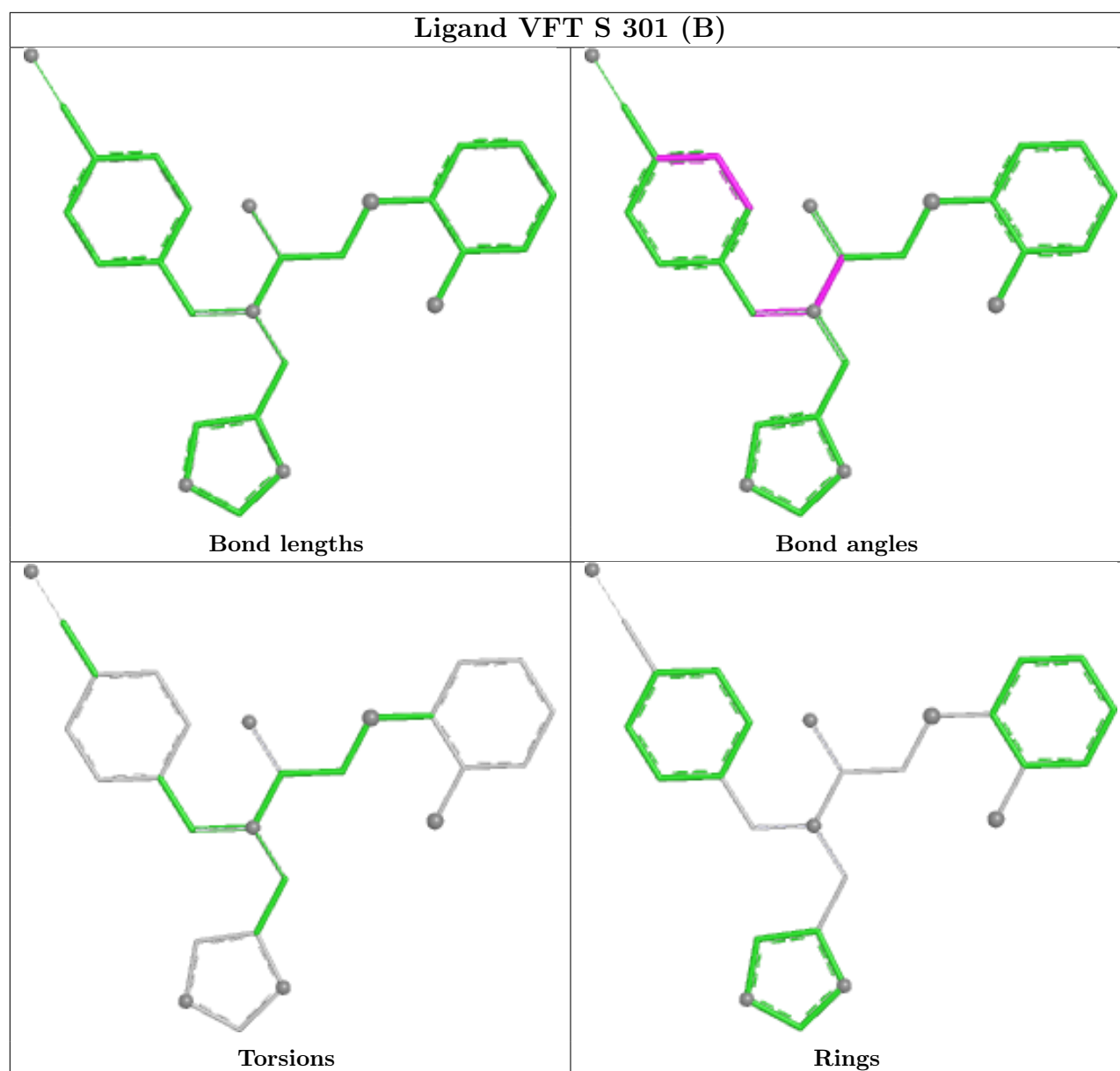


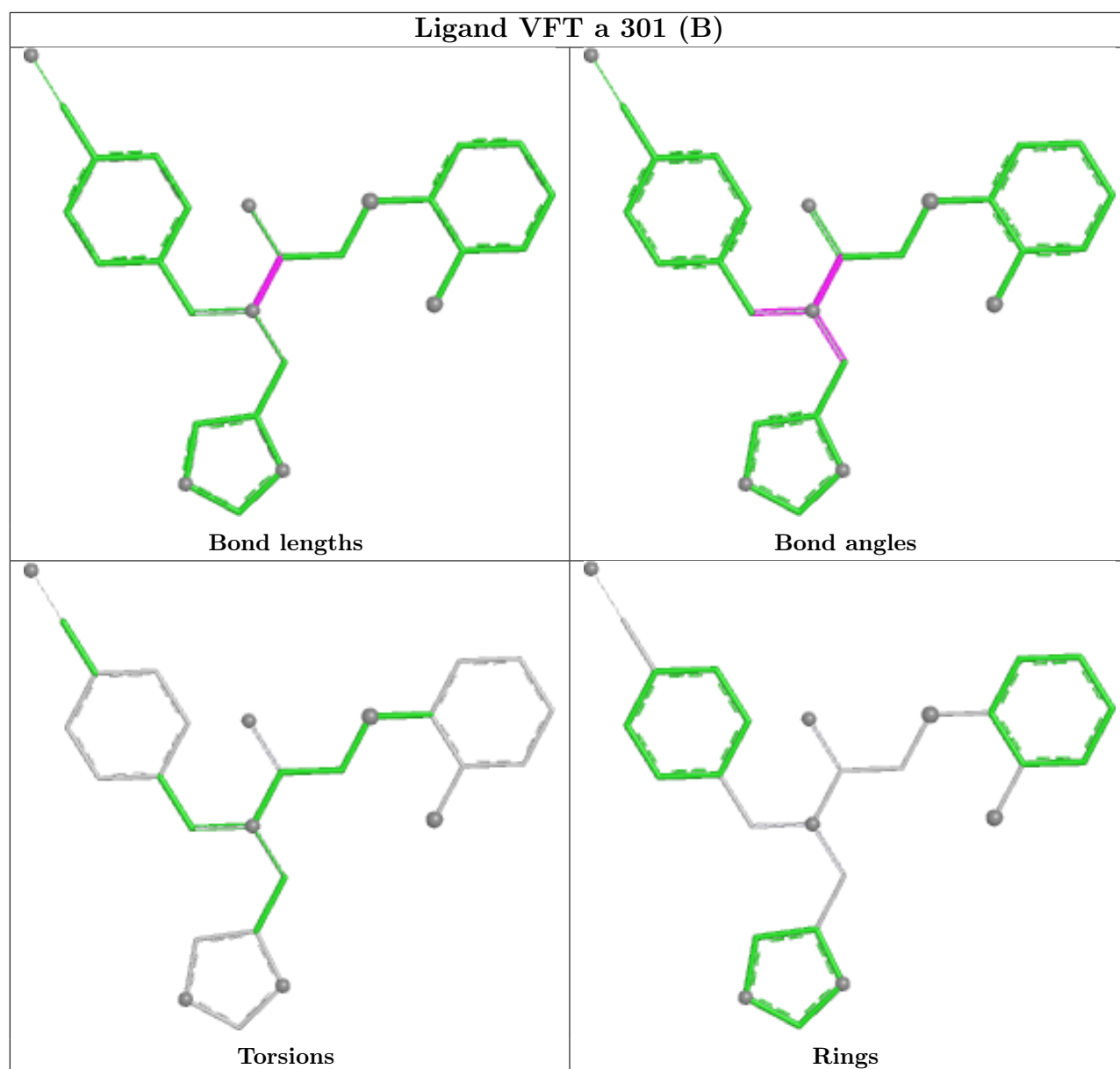
Ligand VFT J 301 (A)

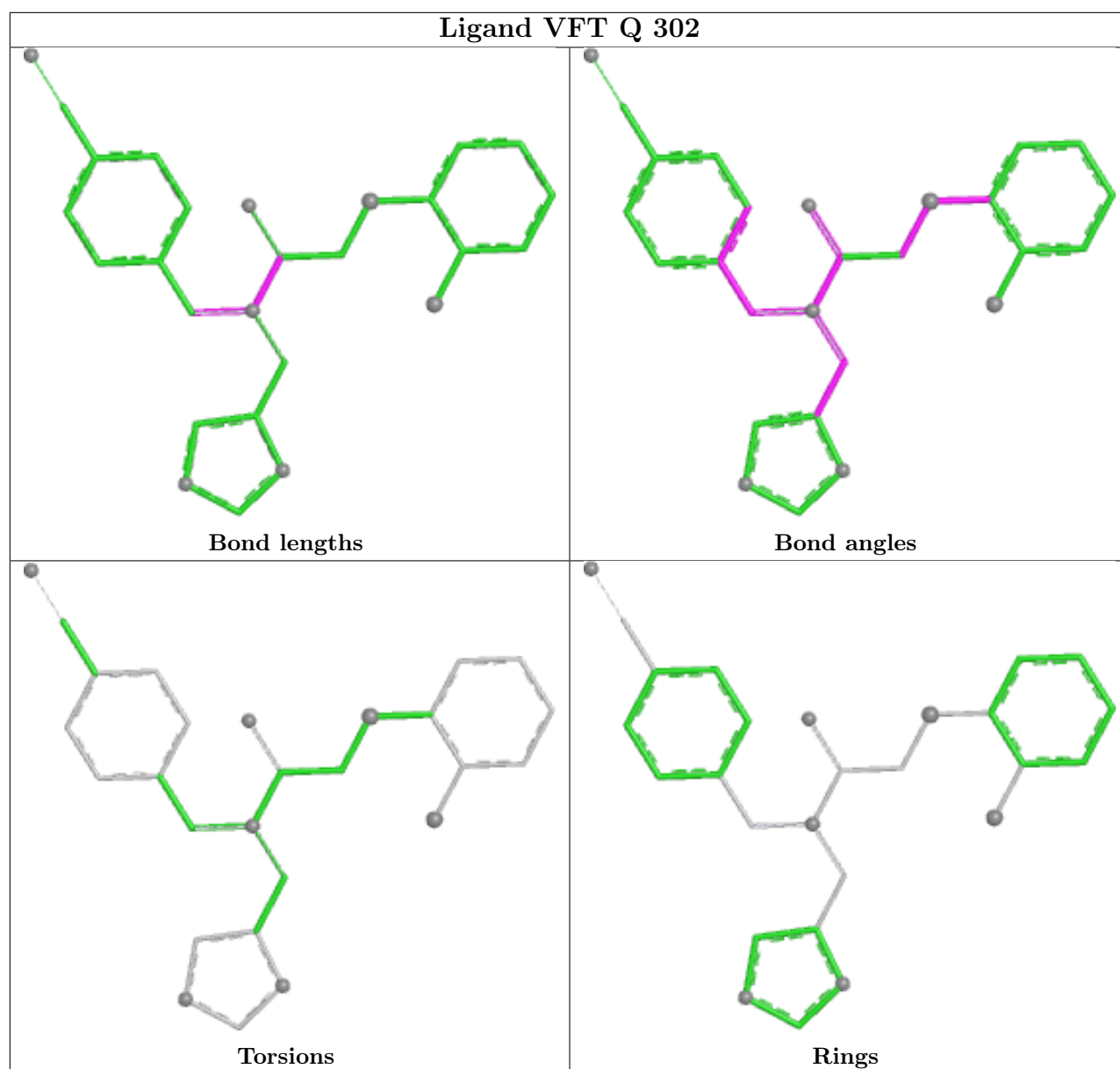


Ligand VFT Y 301 (A)

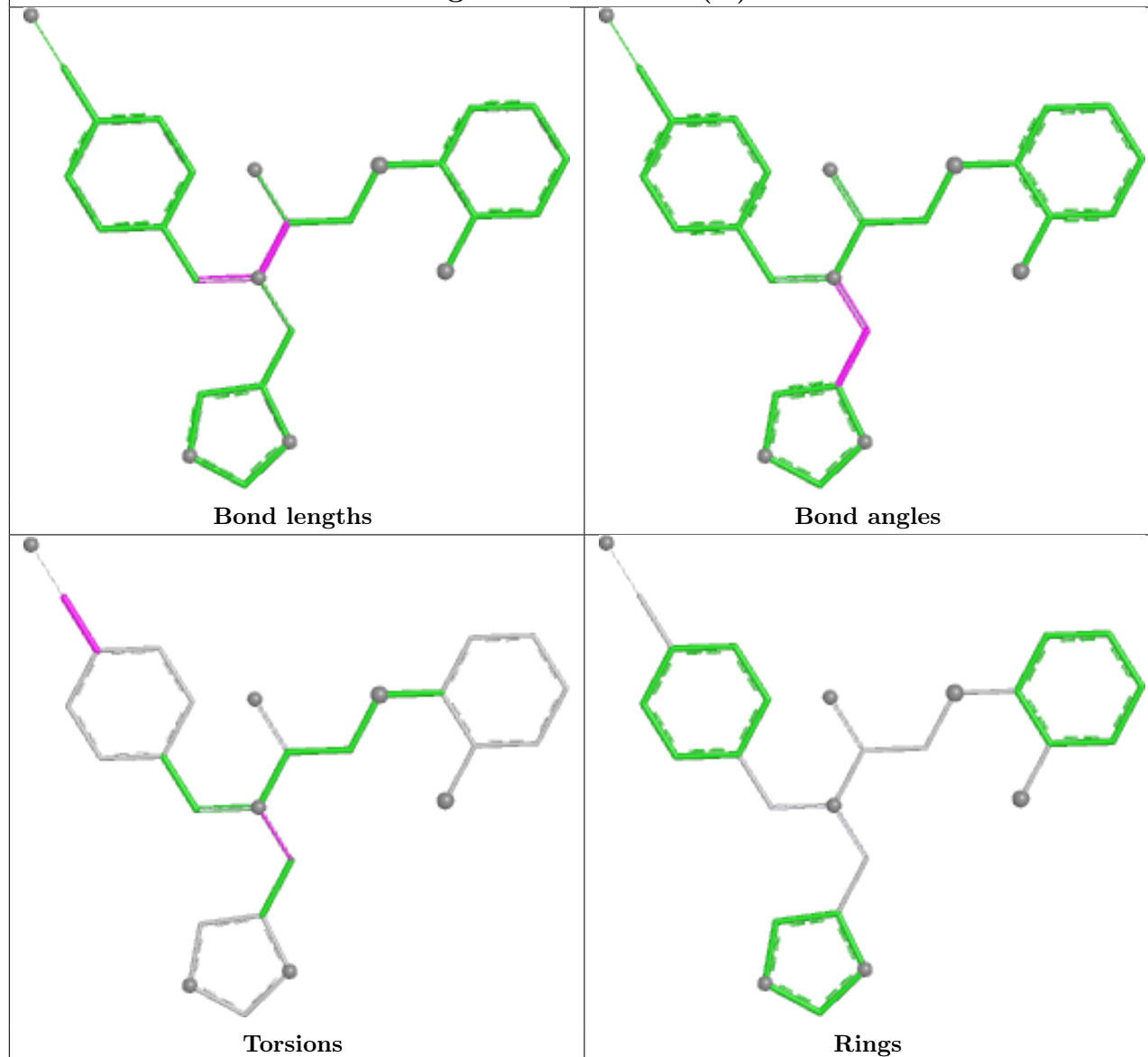


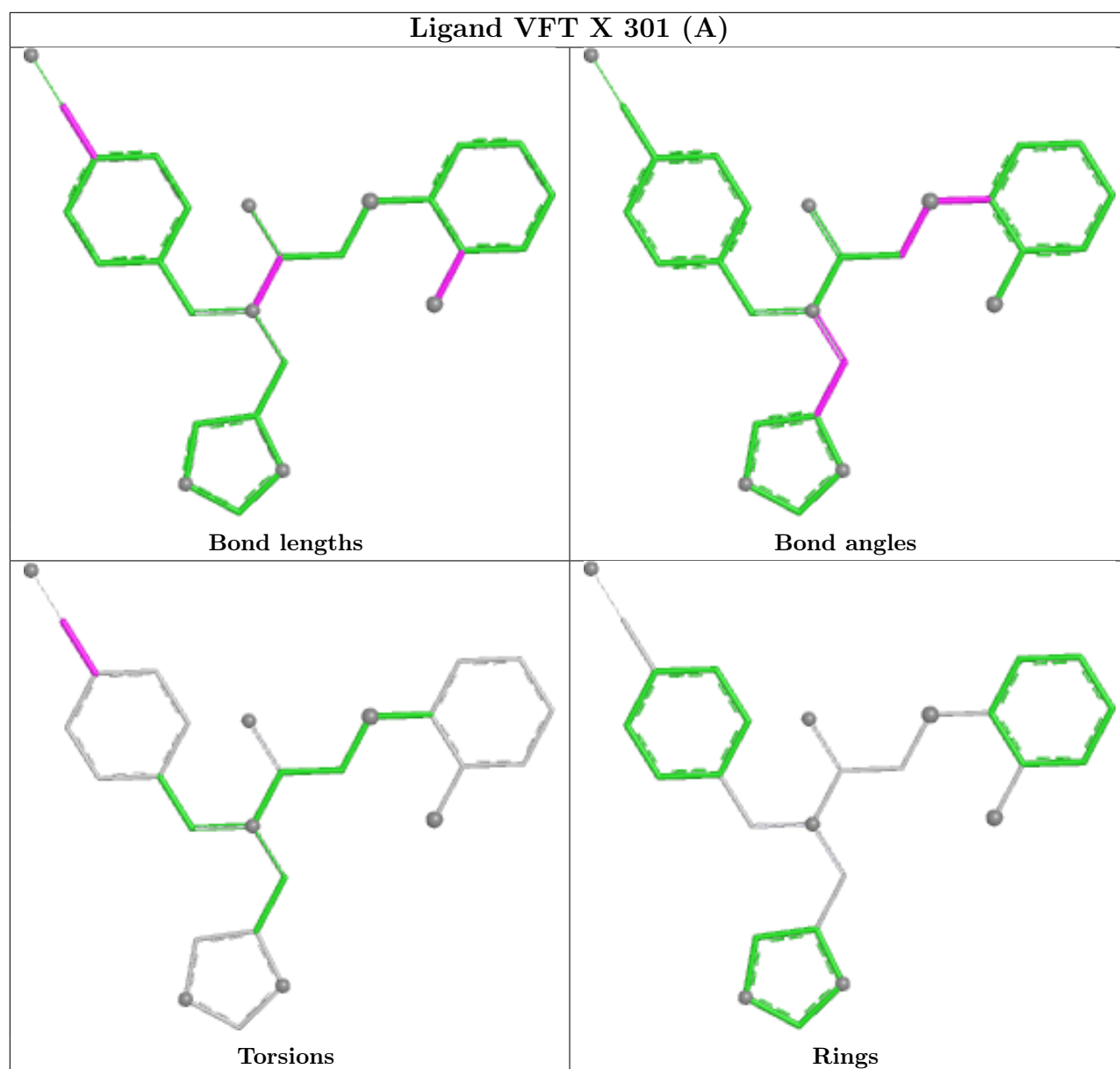


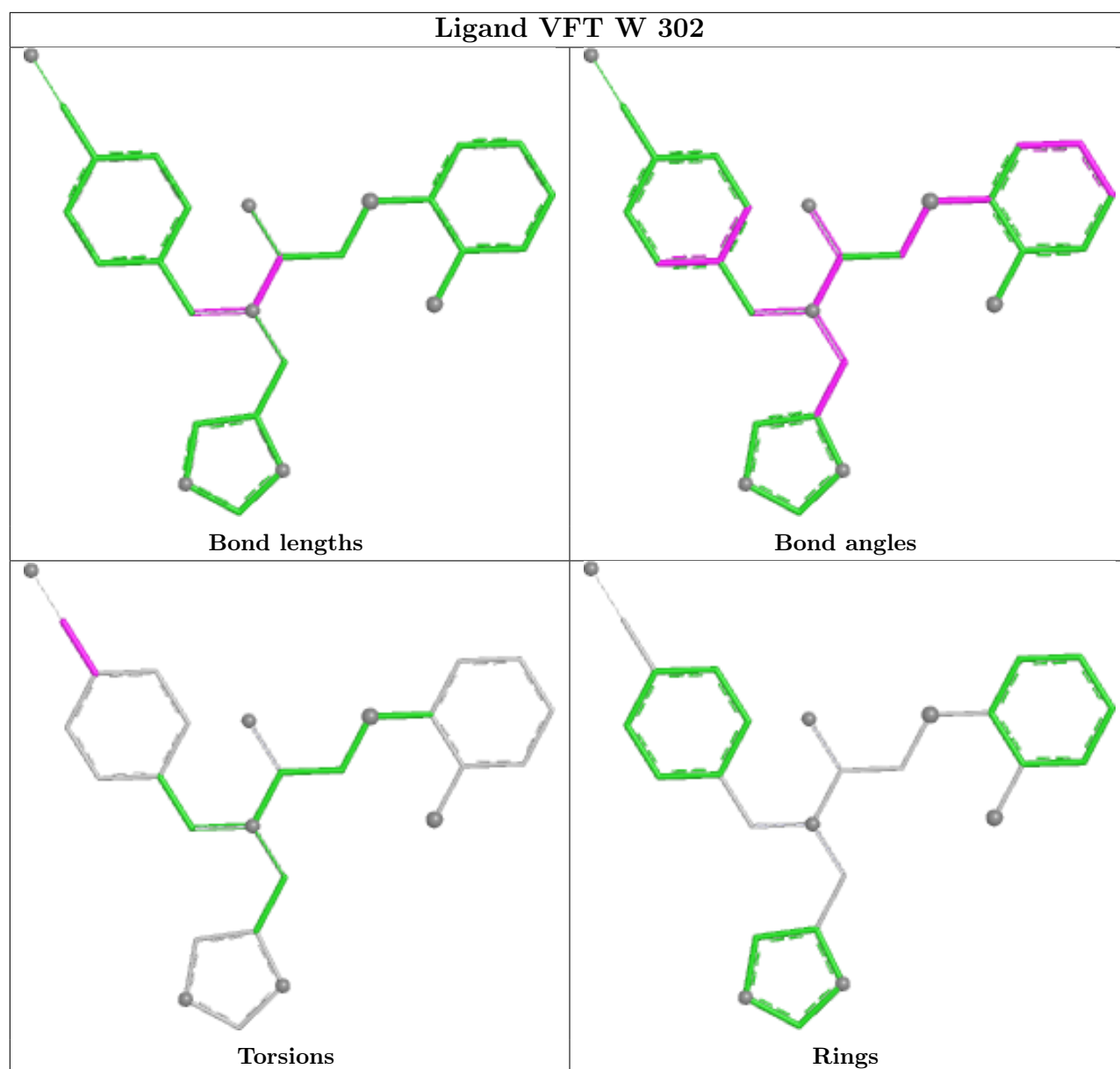




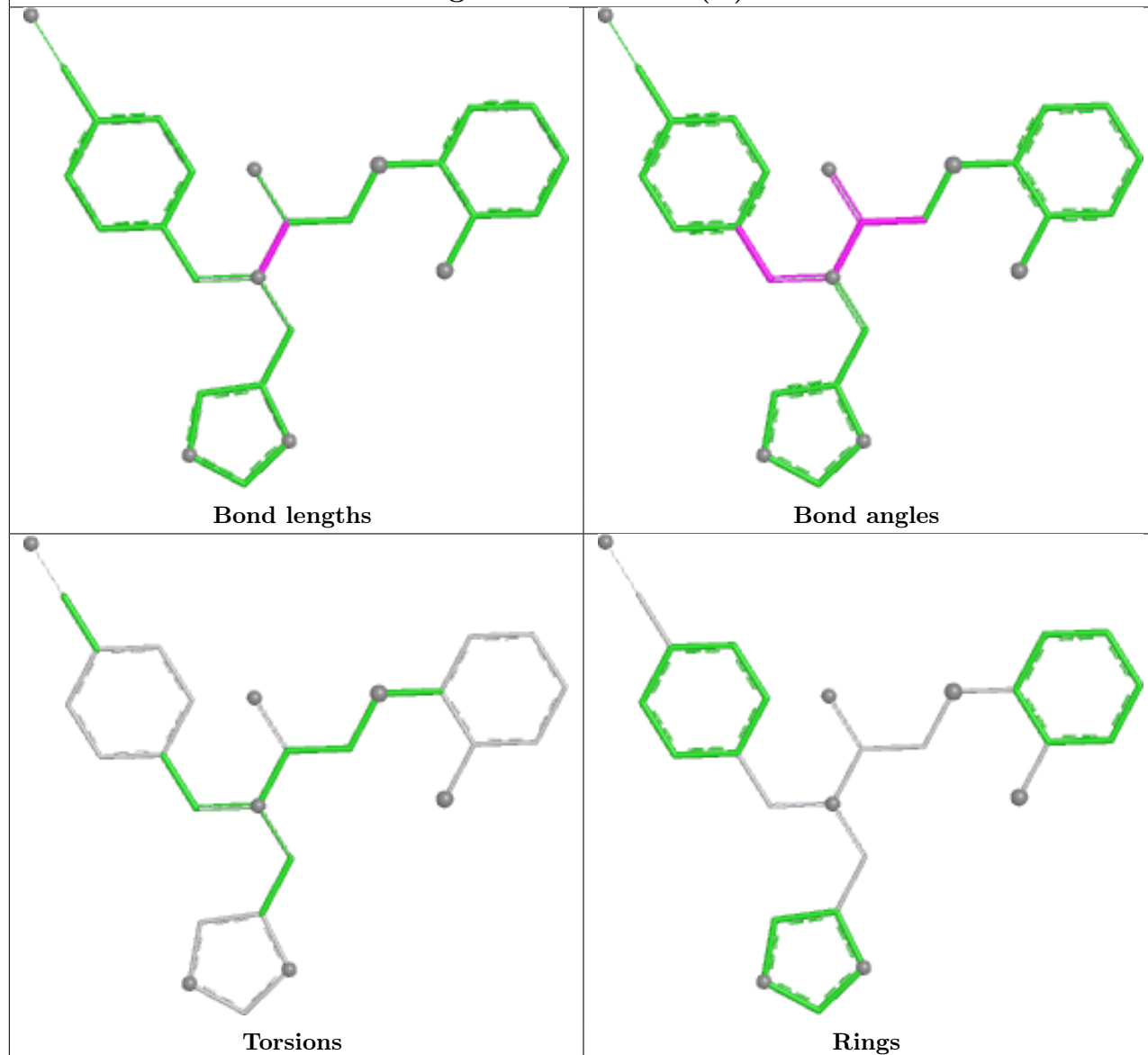
Ligand VFT G 301 (A)

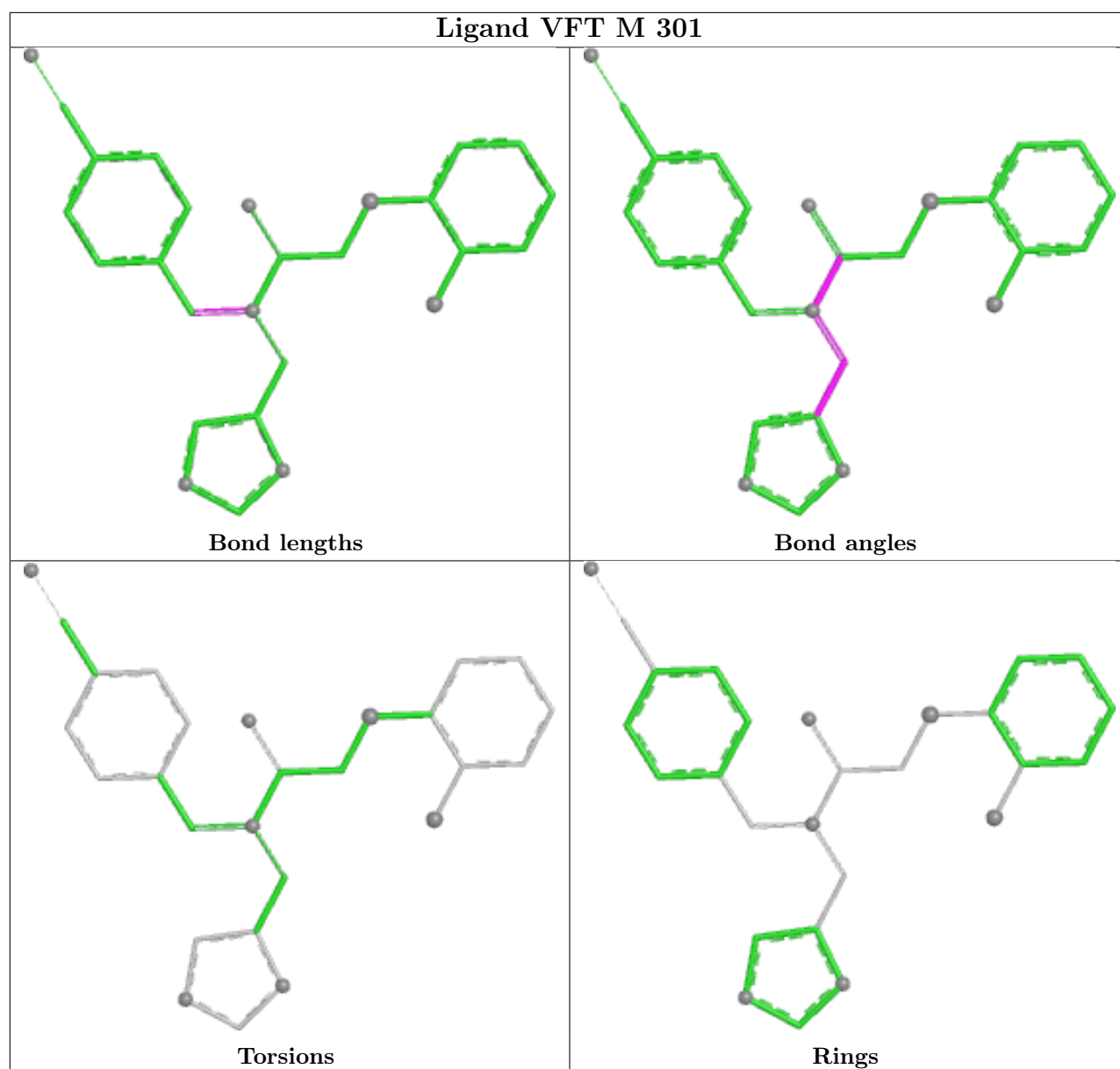


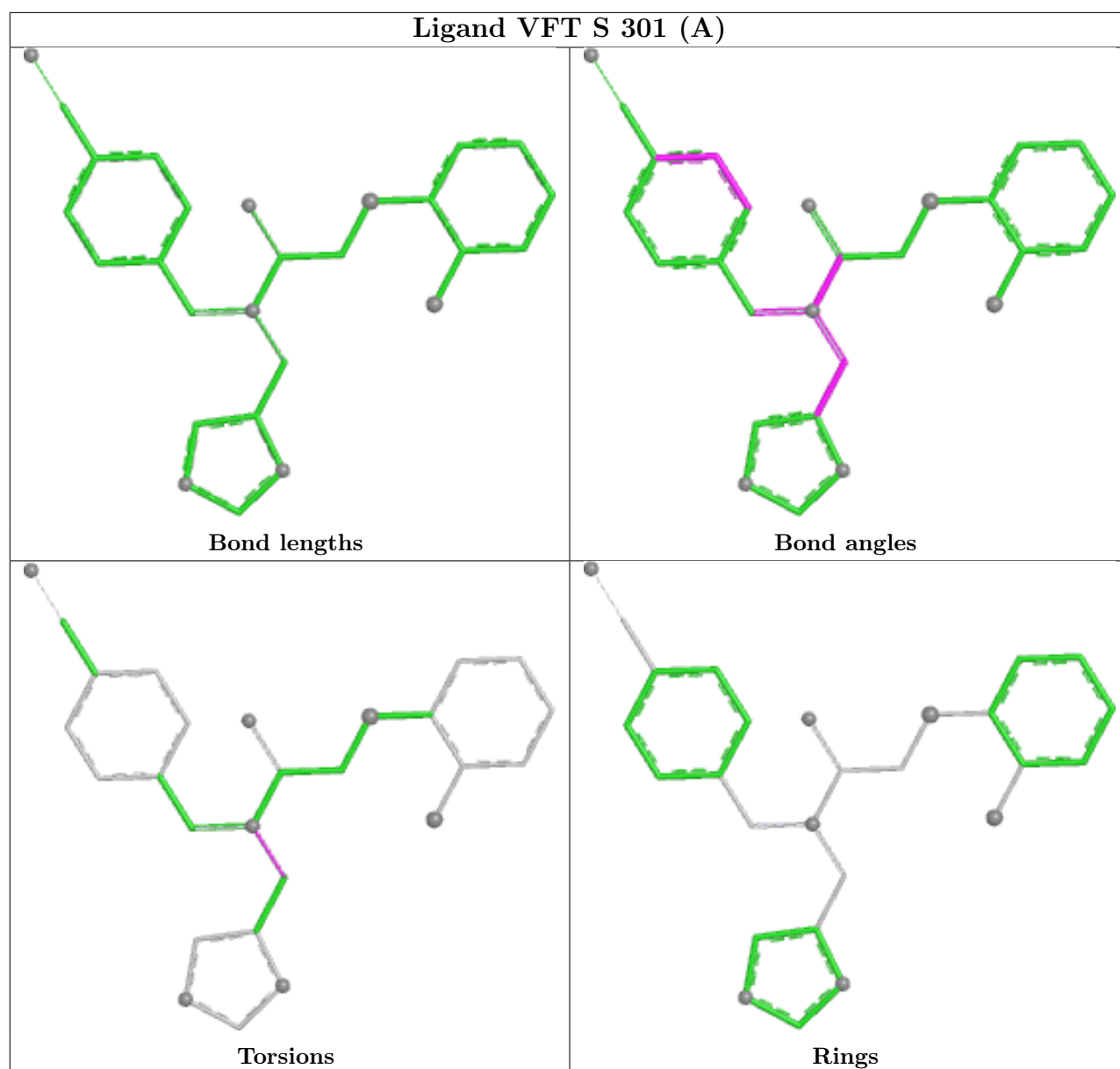


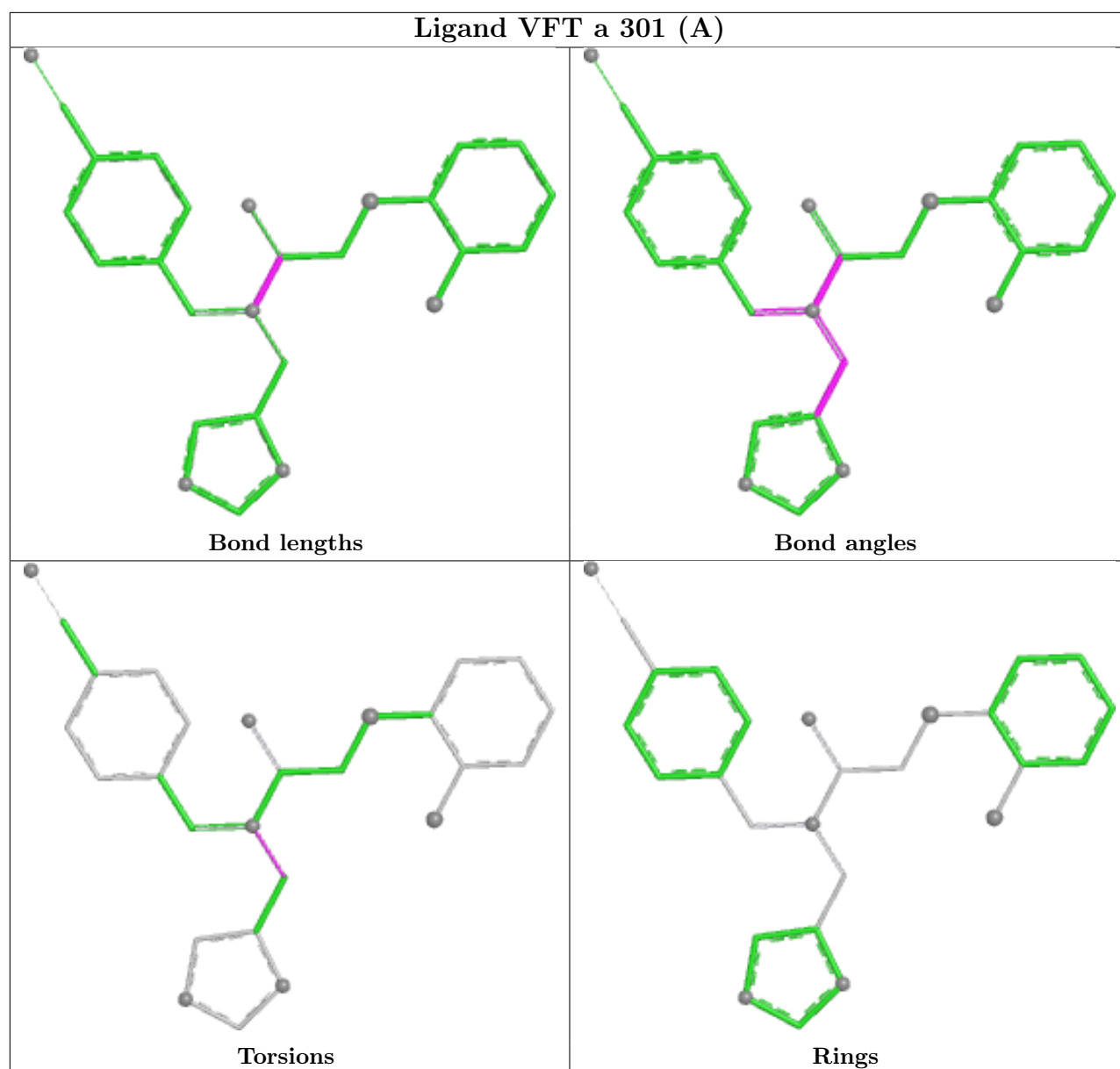


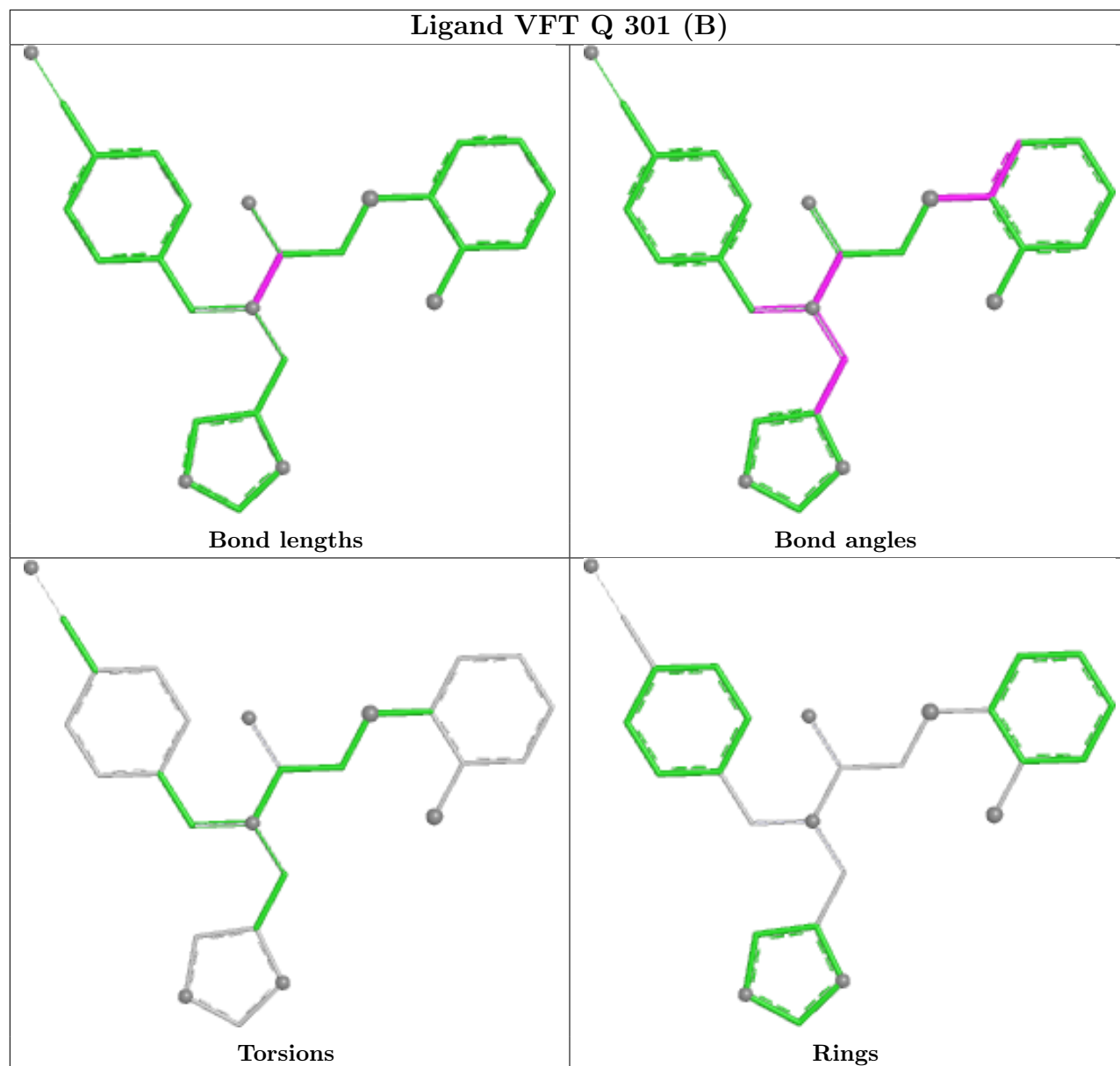
Ligand VFT B 301 (B)

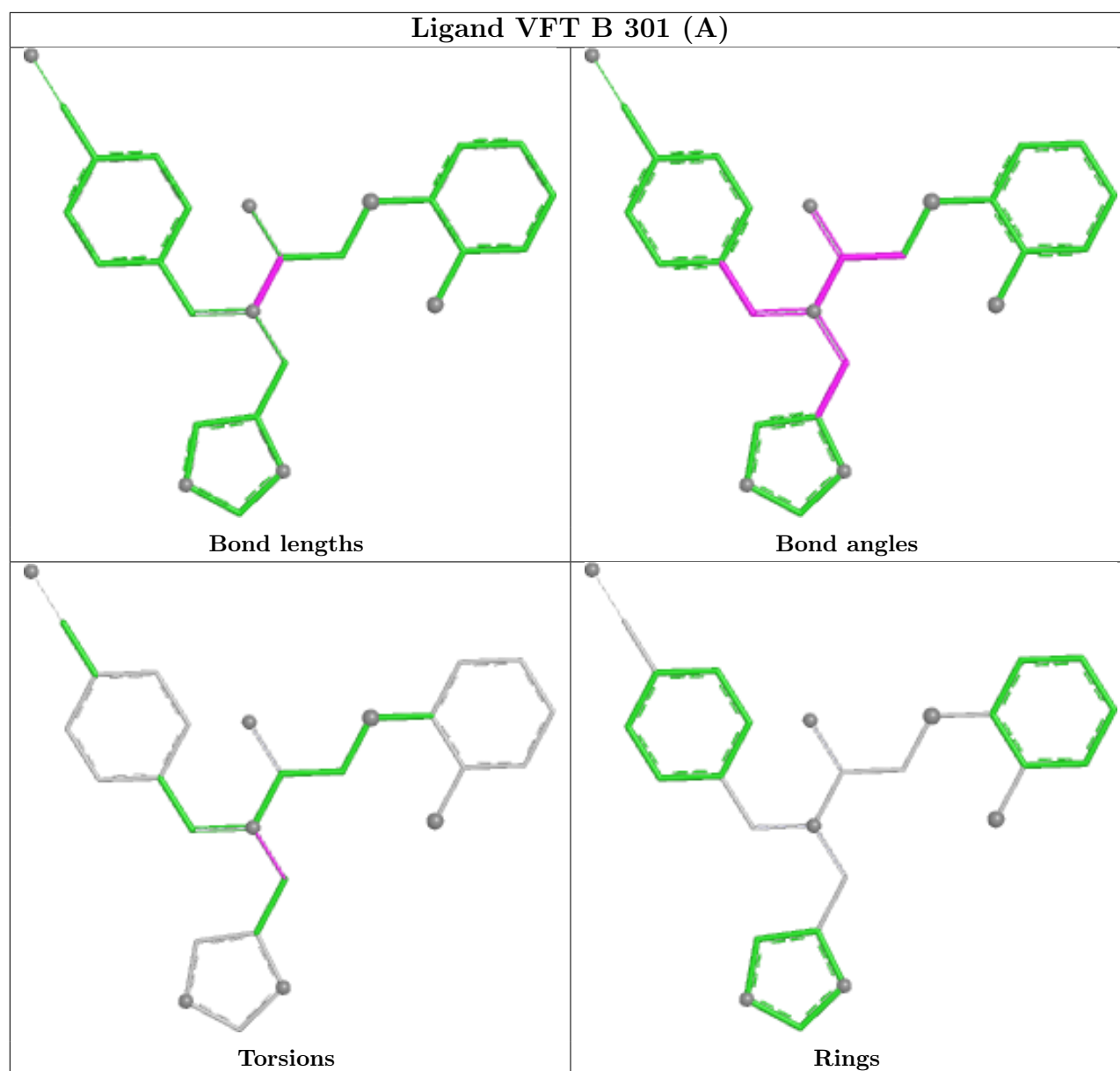












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.47	3 (1%) 76 75	24, 42, 70, 121	3 (1%)
1	B	258/261 (98%)	-0.49	4 (1%) 70 68	22, 41, 66, 102	4 (1%)
1	C	258/261 (98%)	-0.49	7 (2%) 56 53	21, 41, 66, 109	3 (1%)
1	D	258/261 (98%)	-0.50	3 (1%) 76 75	22, 41, 64, 102	1 (0%)
1	E	258/261 (98%)	-0.49	3 (1%) 76 75	30, 41, 66, 121	0
1	F	258/261 (98%)	-0.46	5 (1%) 66 63	22, 42, 68, 106	2 (0%)
1	G	257/261 (98%)	-0.23	7 (2%) 56 53	37, 54, 83, 95	0
1	H	257/261 (98%)	-0.22	7 (2%) 56 53	36, 53, 84, 97	0
1	I	257/261 (98%)	-0.30	6 (2%) 61 58	36, 52, 83, 105	0
1	J	258/261 (98%)	-0.47	6 (2%) 61 58	29, 43, 68, 103	1 (0%)
1	K	258/261 (98%)	-0.39	9 (3%) 47 45	31, 45, 72, 123	0
1	L	258/261 (98%)	-0.43	4 (1%) 70 68	33, 44, 68, 113	0
1	M	257/261 (98%)	-0.22	8 (3%) 51 49	35, 55, 86, 100	0
1	N	257/261 (98%)	-0.22	8 (3%) 51 49	37, 53, 84, 102	0
1	O	257/261 (98%)	-0.18	6 (2%) 61 58	36, 54, 85, 104	0
1	P	257/261 (98%)	-0.26	6 (2%) 61 58	37, 54, 84, 105	0
1	Q	257/261 (98%)	-0.16	12 (4%) 36 36	36, 56, 88, 109	1 (0%)
1	R	257/261 (98%)	-0.17	11 (4%) 40 38	36, 54, 83, 106	0
1	S	258/261 (98%)	-0.45	6 (2%) 61 58	32, 43, 70, 107	0
1	T	258/261 (98%)	-0.45	5 (1%) 66 63	32, 42, 67, 99	0
1	U	258/261 (98%)	-0.44	6 (2%) 61 58	31, 43, 69, 108	0
1	V	257/261 (98%)	-0.24	7 (2%) 56 53	37, 55, 84, 100	0
1	W	257/261 (98%)	-0.20	10 (3%) 43 41	30, 54, 87, 104	1 (0%)
1	X	257/261 (98%)	-0.26	5 (1%) 66 63	25, 53, 84, 110	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	Y	258/261 (98%)	-0.23	5 (1%)	66 63	29, 53, 85, 133	1 (0%)
1	Z	258/261 (98%)	-0.20	10 (3%)	43 41	27, 52, 84, 123	1 (0%)
1	a	257/261 (98%)	-0.28	7 (2%)	56 53	29, 54, 84, 101	1 (0%)
1	b	257/261 (98%)	-0.15	12 (4%)	36 36	29, 53, 87, 110	1 (0%)
1	c	258/261 (98%)	-0.24	8 (3%)	51 49	30, 53, 88, 141	1 (0%)
1	d	257/261 (98%)	-0.25	7 (2%)	56 53	27, 55, 86, 104	1 (0%)
All	All	7725/7830 (98%)	-0.32	203 (2%)	57 54	21, 49, 83, 141	23 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.7
1	C	1	MET	6.7
1	K	1	MET	6.5
1	Y	1	MET	6.1
1	B	1	MET	6.1
1	U	1	MET	6.1
1	Z	1	MET	6.0
1	c	1	MET	5.9
1	L	1	MET	5.7
1	J	1	MET	5.7
1	F	1	MET	5.5
1	M	253	THR	5.4
1	D	1	MET	5.2
1	E	1	MET	5.1
1	S	102	ARG	5.1
1	T	1	MET	5.0
1	R	74	LYS	4.7
1	S	1	MET	4.7
1	K	3	LEU	4.3
1	N	2	SER	4.3
1	b	74	LYS	4.0
1	Z	15	ARG	4.0
1	d	2	SER	3.9
1	b	2	SER	3.8
1	K	220	ARG	3.8
1	G	253	THR	3.7
1	W	253	THR	3.7
1	O	7	ARG	3.7
1	H	2	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	2	SER	3.7
1	H	18	ALA	3.6
1	c	18	ALA	3.6
1	N	18	ALA	3.6
1	X	15	ARG	3.6
1	D	253	THR	3.5
1	O	18	ALA	3.5
1	F	18	ALA	3.5
1	a	2	SER	3.4
1	b	3	LEU	3.4
1	F	226	GLU	3.3
1	U	253	THR	3.3
1	W	47	LYS	3.3
1	I	77	PRO	3.3
1	O	2	SER	3.3
1	V	2	SER	3.3
1	F	253	THR	3.2
1	R	2	SER	3.2
1	H	102	ARG	3.2
1	Q	200[A]	ARG	3.2
1	Y	74	LYS	3.2
1	b	18	ALA	3.2
1	d	18	ALA	3.2
1	W	15	ARG	3.2
1	Q	253	THR	3.2
1	Q	15	ARG	3.1
1	d	253	THR	3.1
1	b	77	PRO	3.0
1	W	2	SER	3.0
1	J	200[A]	ARG	3.0
1	K	2	SER	3.0
1	X	220	ARG	3.0
1	b	102	ARG	3.0
1	E	2	SER	2.9
1	M	2	SER	2.9
1	G	258	ARG	2.9
1	D	220	ARG	2.9
1	G	72	LYS	2.9
1	K	77	PRO	2.9
1	d	77	PRO	2.9
1	V	253	THR	2.8
1	G	77	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	2	SER	2.8
1	A	2	SER	2.8
1	S	18	ALA	2.8
1	V	18	ALA	2.8
1	X	77	PRO	2.8
1	S	77	PRO	2.7
1	I	156	HIS	2.7
1	L	156	HIS	2.7
1	M	258	ARG	2.7
1	O	15	ARG	2.7
1	K	18	ALA	2.7
1	W	220	ARG	2.7
1	a	253	THR	2.7
1	Q	18	ALA	2.7
1	P	220	ARG	2.7
1	B	253	THR	2.7
1	R	18	ALA	2.7
1	R	72	LYS	2.7
1	b	47	LYS	2.7
1	H	157	GLN	2.6
1	T	157	GLN	2.6
1	a	220	ARG	2.6
1	b	51	LYS	2.6
1	c	77	PRO	2.6
1	Y	72	LYS	2.6
1	c	47	LYS	2.6
1	C	102	ARG	2.5
1	c	15	ARG	2.5
1	W	77	PRO	2.5
1	H	253	THR	2.5
1	Z	2	SER	2.5
1	U	220	ARG	2.5
1	S	253	THR	2.5
1	G	102	ARG	2.5
1	Z	200	ARG	2.5
1	P	77	PRO	2.5
1	C	258	ARG	2.5
1	J	102	ARG	2.5
1	Z	102	ARG	2.5
1	c	51	LYS	2.4
1	T	220	ARG	2.4
1	S	2	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	51	LYS	2.4
1	Y	51	LYS	2.4
1	M	7	ARG	2.4
1	R	220	ARG	2.4
1	a	57	ARG	2.4
1	b	220	ARG	2.4
1	Q	226	GLU	2.4
1	N	15	ARG	2.4
1	O	77	PRO	2.4
1	R	77	PRO	2.4
1	Q	102	ARG	2.4
1	U	3	LEU	2.4
1	U	2	SER	2.4
1	X	2	SER	2.4
1	c	2	SER	2.4
1	R	51	LYS	2.4
1	G	254	ARG	2.4
1	V	57	ARG	2.4
1	d	15	ARG	2.4
1	a	47	LYS	2.3
1	Q	220	ARG	2.3
1	E	253	THR	2.3
1	I	253	THR	2.3
1	d	51	LYS	2.3
1	V	70	ASP	2.3
1	U	77	PRO	2.3
1	B	220	ARG	2.3
1	R	15	ARG	2.3
1	W	3	LEU	2.3
1	M	47	LYS	2.3
1	B	254	ARG	2.3
1	P	57	ARG	2.3
1	Y	77	PRO	2.3
1	a	77	PRO	2.3
1	I	18	ALA	2.3
1	G	57	ARG	2.3
1	H	77	PRO	2.3
1	Z	57	ARG	2.3
1	a	15	ARG	2.3
1	b	79	ARG	2.3
1	J	18	ALA	2.2
1	N	47	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	15	ARG	2.2
1	Q	57	ARG	2.2
1	L	77	PRO	2.2
1	J	2	SER	2.2
1	O	72	LYS	2.2
1	T	18	ALA	2.2
1	W	18	ALA	2.2
1	H	258	ARG	2.2
1	M	77	PRO	2.2
1	X	18	ALA	2.2
1	P	253	THR	2.2
1	T	226	GLU	2.2
1	b	15	ARG	2.2
1	Z	77	PRO	2.2
1	P	2	SER	2.2
1	Q	72	LYS	2.2
1	R	47	LYS	2.2
1	C	253	THR	2.2
1	F	254	ARG	2.2
1	I	57	ARG	2.2
1	L	254	ARG	2.2
1	b	57	ARG	2.2
1	J	77	PRO	2.2
1	Q	77	PRO	2.2
1	W	72	LYS	2.2
1	Z	18	ALA	2.1
1	M	102	ARG	2.1
1	K	102	ARG	2.1
1	K	253	THR	2.1
1	R	102	ARG	2.1
1	Z	220	ARG	2.1
1	d	57	ARG	2.1
1	A	77	PRO	2.1
1	N	102	ARG	2.1
1	K	15	ARG	2.1
1	C	200[A]	ARG	2.1
1	Q	258	ARG	2.1
1	R	156	HIS	2.1
1	V	102	ARG	2.1
1	N	74	LYS	2.1
1	C	77	PRO	2.1
1	N	3	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	220	ARG	2.0
1	N	253	THR	2.0
1	W	57	ARG	2.0
1	Z	51	LYS	2.0
1	C	254	ARG	2.0
1	V	15	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	J	303	5/5	0.76	0.24	85,99,117,117	0
4	SO4	U	303	5/5	0.79	0.12	100,100,110,113	0
4	SO4	Q	305	5/5	0.81	0.16	83,88,108,113	0
4	SO4	a	304	5/5	0.82	0.15	71,72,90,96	0
4	SO4	V	302	5/5	0.83	0.16	73,77,95,100	0
4	SO4	P	302	5/5	0.83	0.10	101,104,110,114	0
4	SO4	c	304	5/5	0.83	0.17	75,76,98,114	0
4	SO4	K	302	5/5	0.84	0.20	70,78,96,115	0
4	SO4	E	305	5/5	0.86	0.19	59,86,98,107	0
4	SO4	R	302	5/5	0.86	0.16	70,80,88,103	0
4	SO4	N	303	5/5	0.87	0.17	66,72,90,99	0
4	SO4	G	304	5/5	0.87	0.14	53,60,69,71	5
4	SO4	H	302	5/5	0.88	0.17	59,67,95,98	0
4	SO4	M	305	5/5	0.88	0.23	64,76,90,93	5
4	SO4	V	301	5/5	0.88	0.18	80,85,99,112	0
4	SO4	C	303	5/5	0.88	0.16	68,77,84,98	0
4	SO4	Z	302	5/5	0.88	0.22	66,74,91,95	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	Q	304	5/5	0.88	0.16	63,76,88,94	0
4	SO4	N	304	5/5	0.88	0.25	67,74,91,99	5
4	SO4	A	305	5/5	0.89	0.19	78,79,92,101	0
4	SO4	U	304	5/5	0.89	0.23	83,85,92,94	5
4	SO4	A	307	5/5	0.89	0.22	64,73,93,95	5
3	CL	A	304	1/1	0.89	0.12	75,75,75,75	0
4	SO4	V	303	5/5	0.89	0.27	62,79,90,107	5
4	SO4	J	302	5/5	0.89	0.19	66,78,90,101	0
4	SO4	M	304	5/5	0.89	0.17	75,81,92,94	0
4	SO4	S	303	5/5	0.89	0.21	68,81,101,107	0
4	SO4	d	301	5/5	0.89	0.19	67,69,101,104	0
4	SO4	d	302	5/5	0.89	0.23	63,67,85,96	5
4	SO4	T	303	5/5	0.90	0.16	70,71,88,97	0
4	SO4	G	305	5/5	0.90	0.21	77,82,91,93	0
3	CL	E	302	1/1	0.90	0.15	71,71,71,71	0
4	SO4	D	303	5/5	0.90	0.17	63,67,85,107	0
4	SO4	P	303	5/5	0.90	0.20	73,75,79,79	5
4	SO4	D	304	5/5	0.90	0.23	53,72,80,92	5
4	SO4	W	303	5/5	0.90	0.14	74,79,87,87	0
4	SO4	Y	303	5/5	0.90	0.21	68,75,93,99	5
4	SO4	Z	301	5/5	0.90	0.20	72,75,95,106	0
4	SO4	B	304	5/5	0.90	0.15	60,62,88,95	0
4	SO4	Q	306	5/5	0.90	0.26	69,81,92,102	5
4	SO4	a	305	5/5	0.90	0.20	68,80,85,93	5
4	SO4	b	303	5/5	0.90	0.26	71,75,91,99	5
4	SO4	F	302	5/5	0.90	0.16	65,72,85,89	0
4	SO4	B	305	5/5	0.90	0.21	64,66,87,94	5
4	SO4	S	304	5/5	0.90	0.15	48,51,64,67	5
4	SO4	I	302	5/5	0.91	0.17	61,76,87,98	0
3	CL	G	303	1/1	0.91	0.12	66,66,66,66	0
4	SO4	Y	302	5/5	0.91	0.16	69,72,102,105	0
4	SO4	K	303	5/5	0.91	0.19	57,61,83,90	5
4	SO4	L	303	5/5	0.91	0.16	62,66,96,97	0
4	SO4	P	301	5/5	0.91	0.15	61,82,86,103	0
4	SO4	T	304	5/5	0.91	0.20	69,70,81,91	5
4	SO4	U	302	5/5	0.91	0.18	65,71,87,99	0
4	SO4	A	306	5/5	0.91	0.16	50,54,59,62	5
4	SO4	C	304	5/5	0.91	0.19	64,74,81,97	5
4	SO4	c	305	5/5	0.91	0.18	60,69,79,81	5
4	SO4	G	306	5/5	0.91	0.21	65,74,86,88	5
4	SO4	E	306	5/5	0.91	0.20	67,72,90,94	5
4	SO4	O	304	5/5	0.92	0.20	67,79,93,105	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	303	1/1	0.92	0.11	79,79,79,79	0
3	CL	C	301	1/1	0.92	0.11	69,69,69,69	0
4	SO4	J	304	5/5	0.92	0.19	60,77,84,91	5
4	SO4	a	303	5/5	0.92	0.17	66,84,96,107	0
3	CL	Q	303	1/1	0.92	0.16	74,74,74,74	0
3	CL	S	302	1/1	0.92	0.11	83,83,83,83	0
4	SO4	R	303	5/5	0.92	0.20	74,77,94,101	5
4	SO4	H	303	5/5	0.92	0.24	67,77,85,92	5
4	SO4	O	303	5/5	0.92	0.18	72,74,92,94	0
4	SO4	W	304	5/5	0.92	0.22	72,73,87,91	5
4	SO4	X	304	5/5	0.92	0.17	64,67,90,104	0
3	CL	L	302	1/1	0.93	0.10	67,67,67,67	0
3	CL	C	302	1/1	0.93	0.18	82,82,82,82	0
2	VFT	c	301[B]	27/27	0.93	0.15	44,53,66,70	6
4	SO4	b	302	5/5	0.93	0.14	73,80,92,97	0
4	SO4	X	305	5/5	0.93	0.20	70,76,87,90	5
4	SO4	E	304	5/5	0.93	0.14	45,49,58,69	5
3	CL	X	303	1/1	0.93	0.12	66,66,66,66	0
4	SO4	S	305	5/5	0.93	0.18	61,69,82,92	5
2	VFT	c	301[A]	27/27	0.93	0.15	37,49,57,62	6
2	VFT	Y	301[A]	27/27	0.94	0.15	36,43,63,67	6
2	VFT	Y	301[B]	27/27	0.94	0.15	36,54,64,67	6
3	CL	T	302	1/1	0.94	0.11	66,66,66,66	0
3	CL	B	303	1/1	0.94	0.11	70,70,70,70	0
2	VFT	a	301[A]	27/27	0.94	0.13	33,49,57,58	6
2	VFT	a	301[B]	27/27	0.94	0.13	37,52,65,69	6
2	VFT	W	301[A]	27/27	0.94	0.14	32,45,54,57	6
4	SO4	c	303	5/5	0.94	0.19	72,78,89,92	0
4	SO4	L	304	5/5	0.94	0.18	68,72,79,80	5
2	VFT	W	301[B]	27/27	0.94	0.14	42,48,59,62	6
4	SO4	F	303	5/5	0.94	0.17	62,65,80,84	5
3	CL	A	302	1/1	0.94	0.08	71,71,71,71	0
3	CL	M	302	1/1	0.95	0.10	65,65,65,65	0
3	CL	N	302	1/1	0.95	0.08	64,64,64,64	0
3	CL	O	302	1/1	0.95	0.12	66,66,66,66	0
2	VFT	L	301[A]	27/27	0.95	0.11	26,38,44,45	6
2	VFT	L	301[B]	27/27	0.95	0.11	36,40,57,63	6
2	VFT	R	301[A]	27/27	0.95	0.12	35,47,55,57	6
2	VFT	R	301[B]	27/27	0.95	0.12	41,50,75,78	6
2	VFT	S	301[A]	27/27	0.95	0.12	29,38,42,46	6
2	VFT	S	301[B]	27/27	0.95	0.12	33,39,62,67	6
2	VFT	E	301[A]	27/27	0.95	0.11	27,37,46,50	6

Continued on next page...

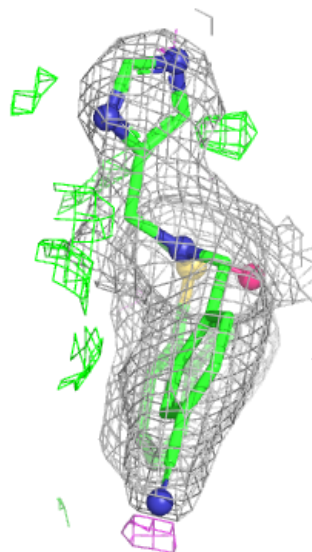
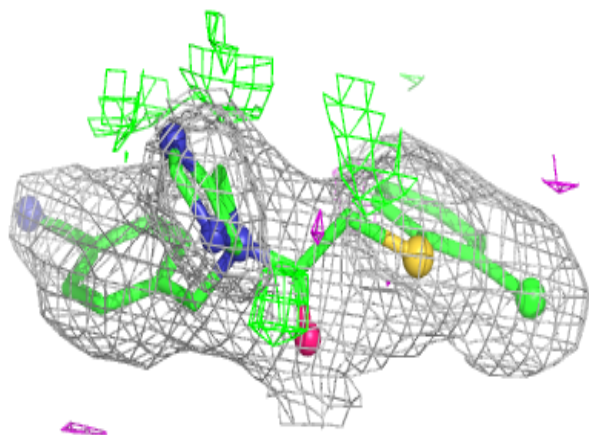
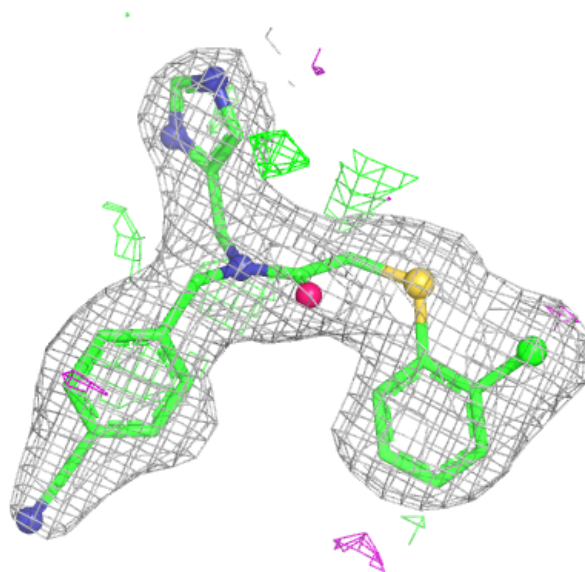
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VFT	E	301[B]	27/27	0.95	0.11	33,41,57,63	6
2	VFT	X	301[A]	27/27	0.95	0.12	31,45,51,60	6
2	VFT	X	301[B]	27/27	0.95	0.12	43,47,65,72	6
4	SO4	I	303	5/5	0.95	0.14	64,74,81,83	5
2	VFT	G	302[A]	27/27	0.95	0.13	34,45,61,63	6
2	VFT	G	302[B]	27/27	0.95	0.13	40,55,63,69	6
2	VFT	A	301[B]	27/27	0.96	0.10	29,44,59,64	6
3	CL	D	302	1/1	0.96	0.08	68,68,68,68	0
2	VFT	G	301[A]	27/27	0.96	0.11	33,46,51,52	6
3	CL	E	303	1/1	0.96	0.10	69,69,69,69	0
2	VFT	G	301[B]	27/27	0.96	0.11	39,49,62,66	6
3	CL	I	301	1/1	0.96	0.07	65,65,65,65	0
2	VFT	U	301[A]	27/27	0.96	0.11	27,37,46,47	6
3	CL	M	303	1/1	0.96	0.08	65,65,65,65	0
2	VFT	U	301[B]	27/27	0.96	0.11	33,42,56,59	6
2	VFT	B	301[A]	27/27	0.96	0.11	27,37,44,47	6
2	VFT	B	301[B]	27/27	0.96	0.11	32,40,60,64	6
2	VFT	W	302	27/27	0.96	0.10	44,52,89,94	0
2	VFT	M	301	27/27	0.96	0.11	36,49,96,97	0
2	VFT	N	301	27/27	0.96	0.10	36,49,83,99	0
3	CL	X	302	1/1	0.96	0.10	66,66,66,66	0
2	VFT	O	301	27/27	0.96	0.10	38,51,78,89	0
2	VFT	J	301[A]	27/27	0.96	0.11	25,38,41,48	6
2	VFT	J	301[B]	27/27	0.96	0.11	35,39,58,63	6
2	VFT	K	301[A]	27/27	0.96	0.10	30,38,43,46	6
2	VFT	a	302	27/27	0.96	0.11	44,48,84,88	0
2	VFT	b	301[A]	27/27	0.96	0.12	30,41,53,61	6
2	VFT	b	301[B]	27/27	0.96	0.12	37,46,69,71	6
2	VFT	K	301[B]	27/27	0.96	0.10	36,39,57,59	6
2	VFT	D	301[A]	27/27	0.96	0.10	25,36,39,46	6
2	VFT	D	301[B]	27/27	0.96	0.10	34,37,64,68	6
2	VFT	Q	301[A]	27/27	0.96	0.12	37,46,55,67	6
2	VFT	Q	301[B]	27/27	0.96	0.12	38,49,64,67	6
2	VFT	Q	302	27/27	0.96	0.11	41,50,84,96	0
2	VFT	A	301[A]	27/27	0.96	0.10	29,37,46,49	6
2	VFT	T	301[B]	27/27	0.97	0.09	33,41,45,47	6
2	VFT	B	302[B]	27/27	0.97	0.09	34,36,39,44	6
2	VFT	F	301	27/27	0.97	0.09	33,41,77,84	0
2	VFT	B	302[A]	27/27	0.97	0.09	34,38,42,44	6
2	VFT	H	301	27/27	0.97	0.09	38,48,85,91	0
2	VFT	c	302	27/27	0.97	0.09	40,48,85,90	0
2	VFT	T	301[A]	27/27	0.97	0.09	33,40,45,47	6

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.

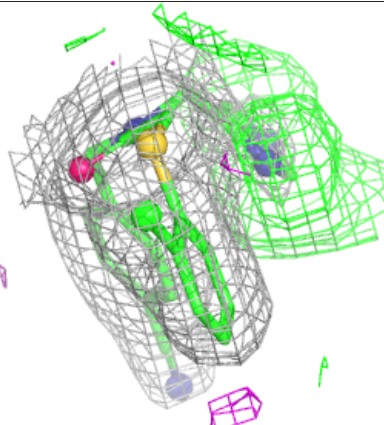
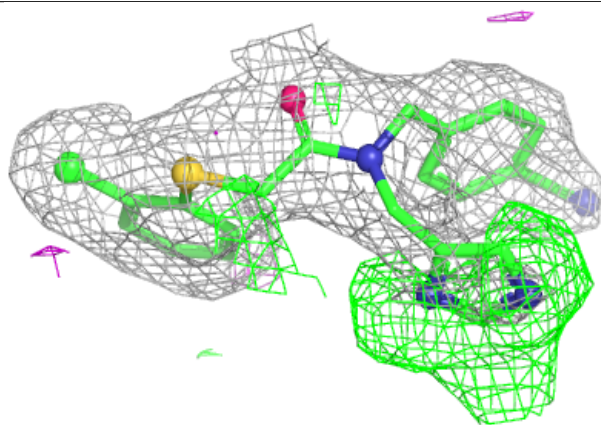
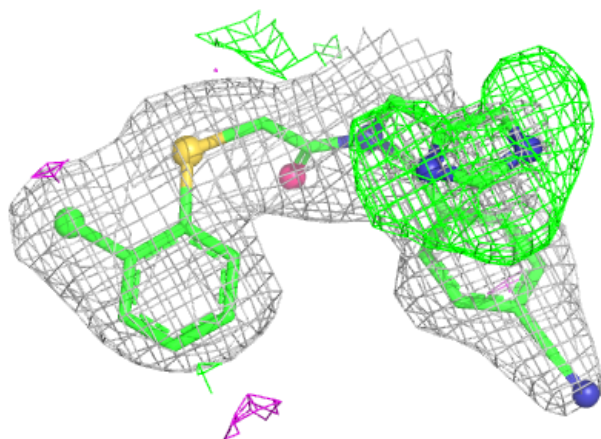
Electron density around VFT c 301 (B):

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



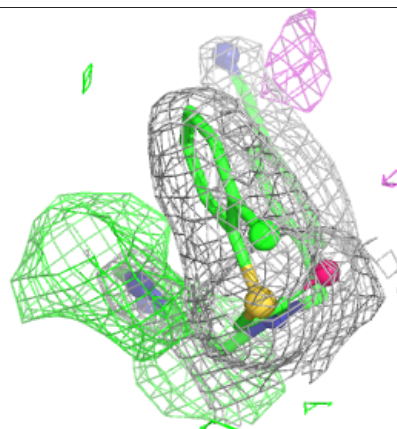
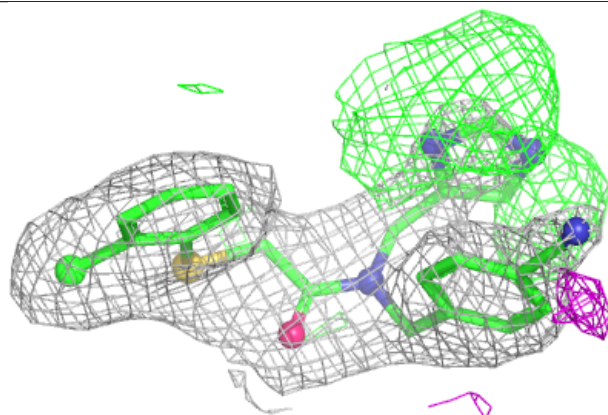
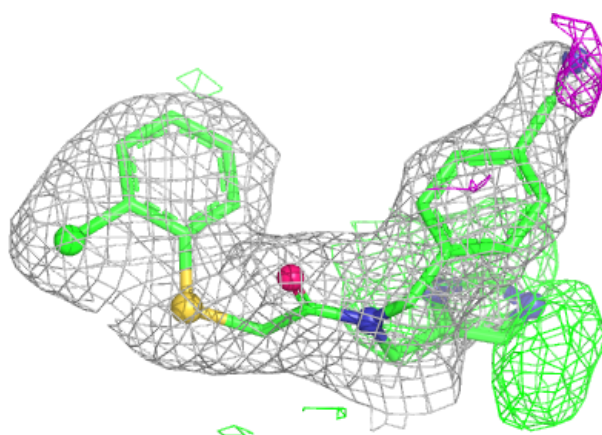
Electron density around VFT c 301 (A):

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



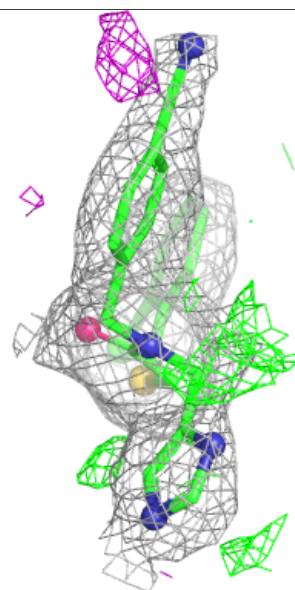
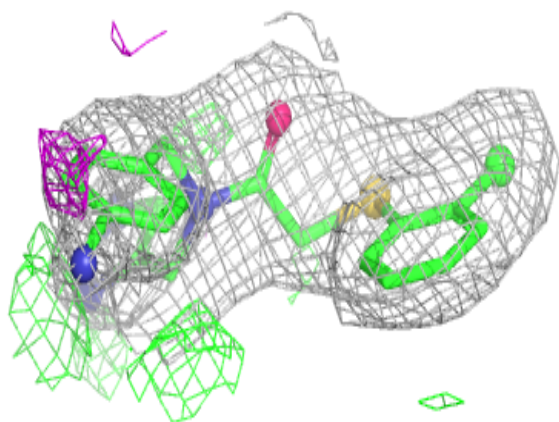
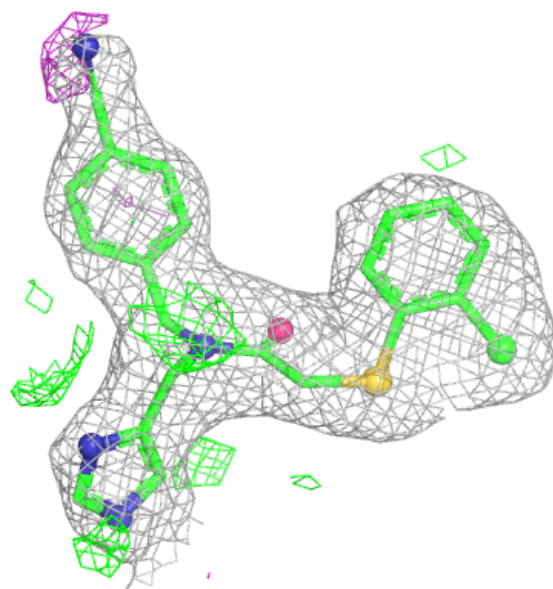
Electron density around VFT Y 301 (A):

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



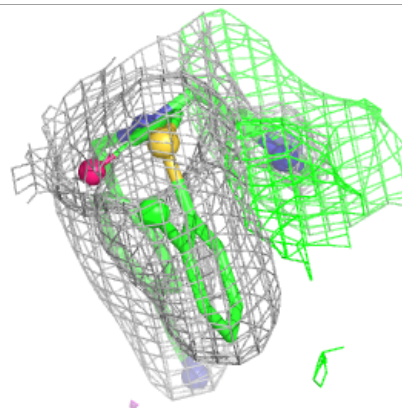
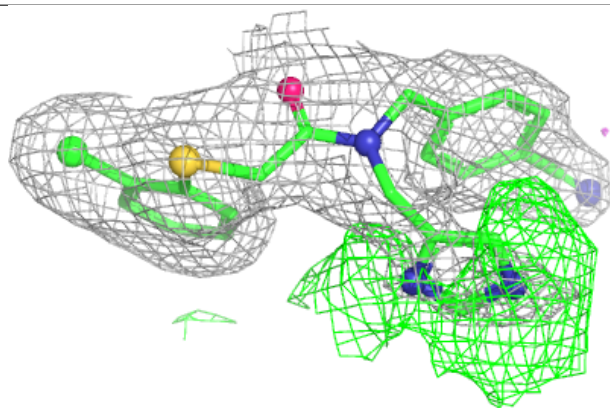
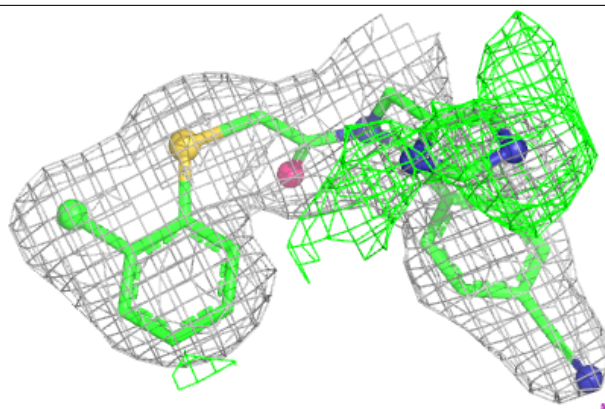
Electron density around VFT Y 301 (B):

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



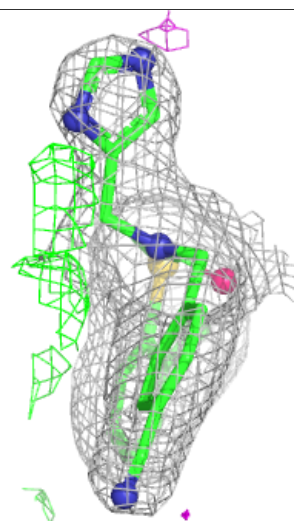
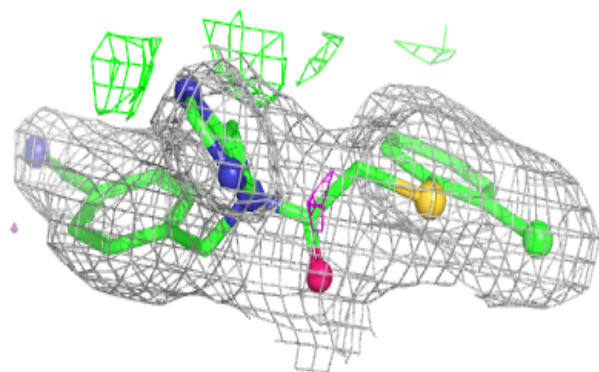
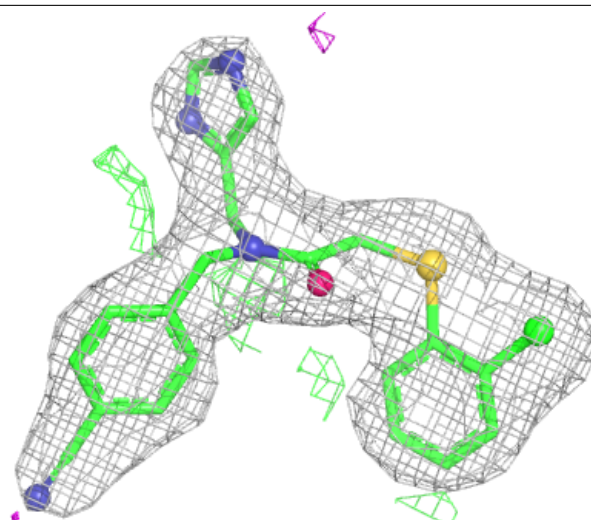
Electron density around VFT a 301 (A):

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



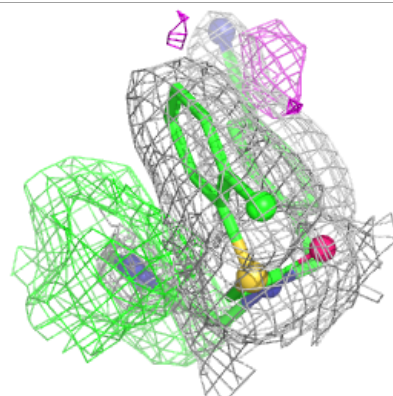
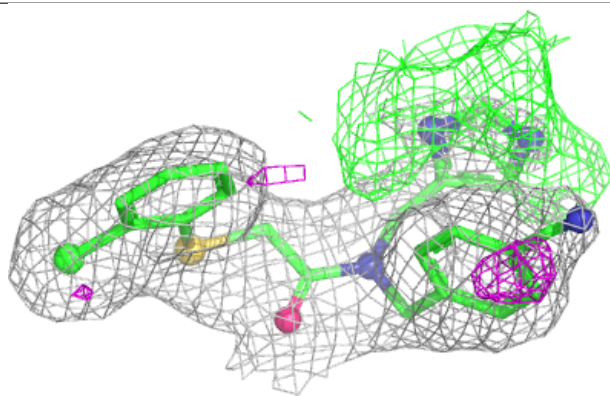
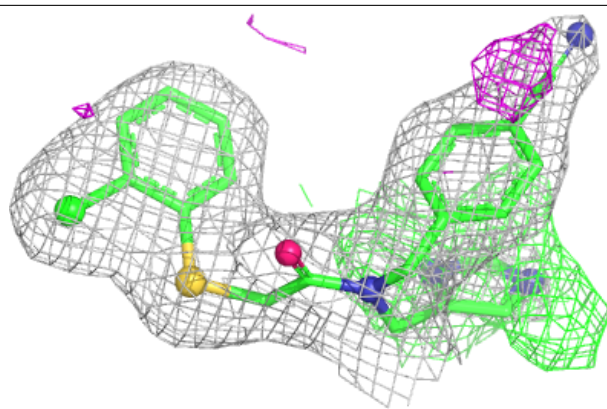
Electron density around VFT a 301 (B):

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



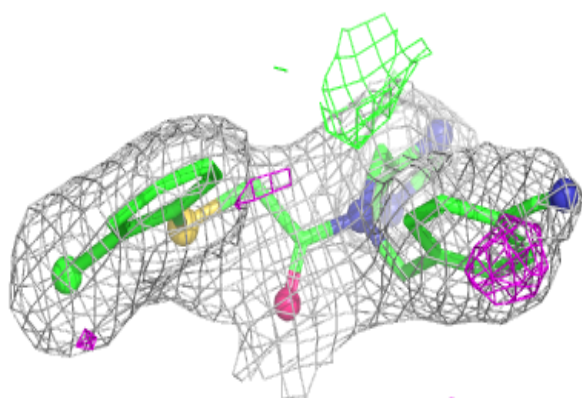
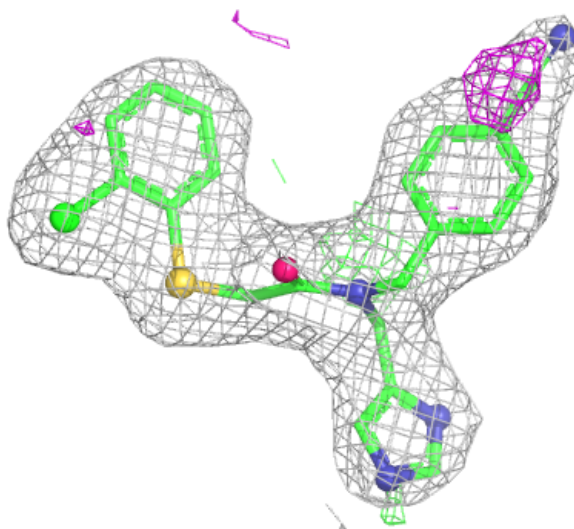
Electron density around VFT W 301 (A):

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



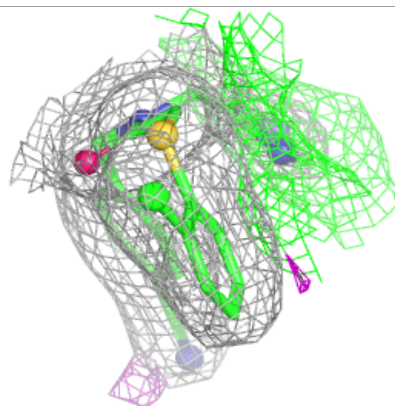
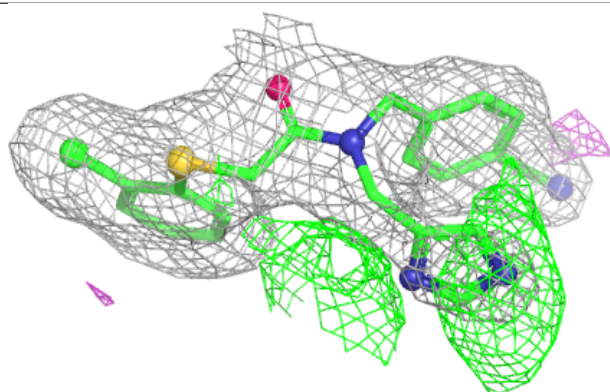
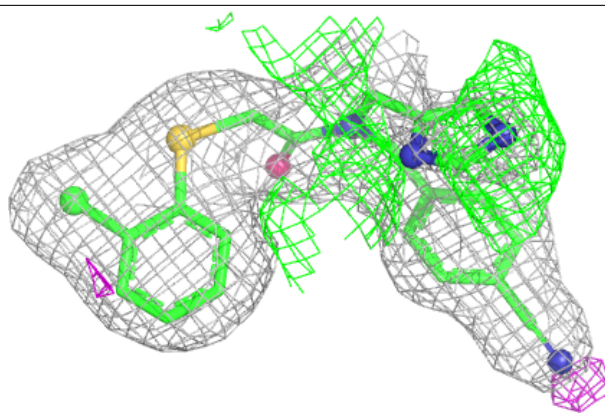
Electron density around VFT W 301 (B):

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



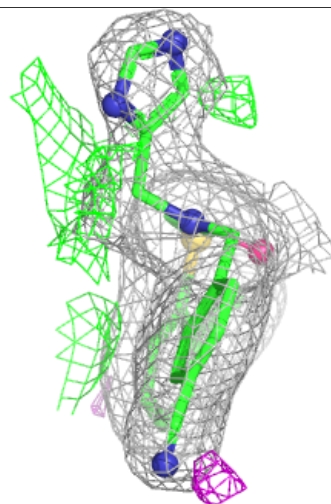
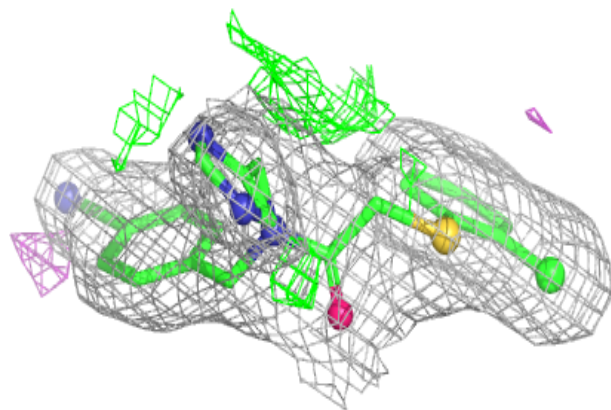
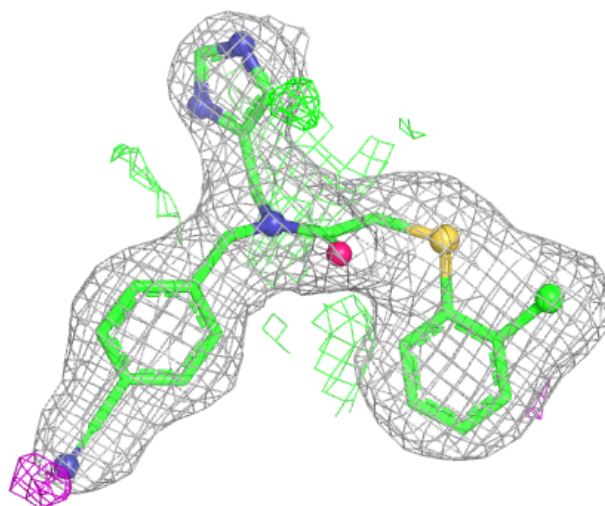
Electron density around VFT L 301 (A):

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



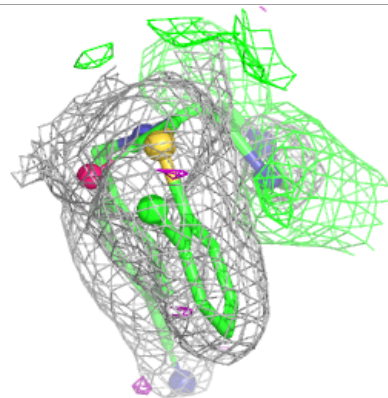
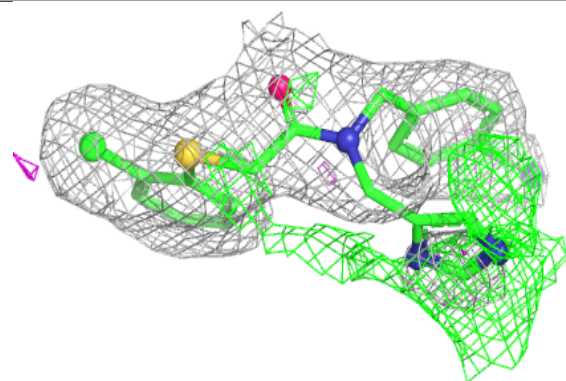
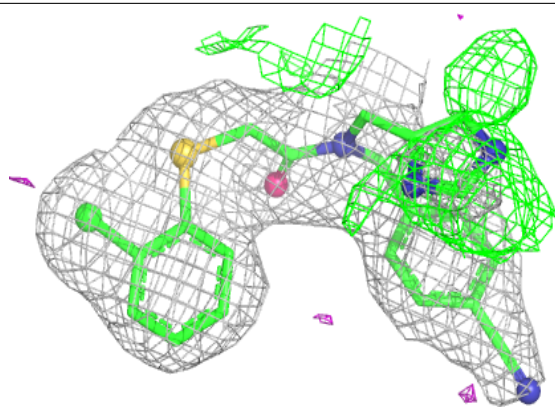
Electron density around VFT L 301 (B):

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



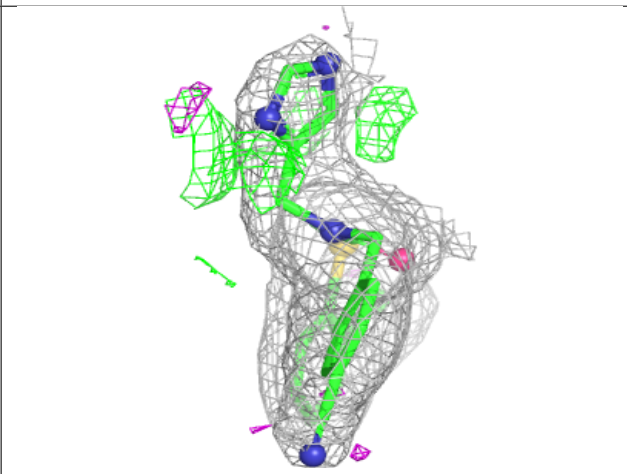
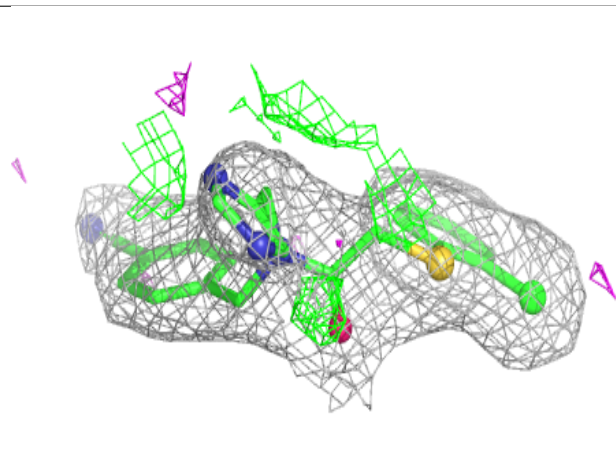
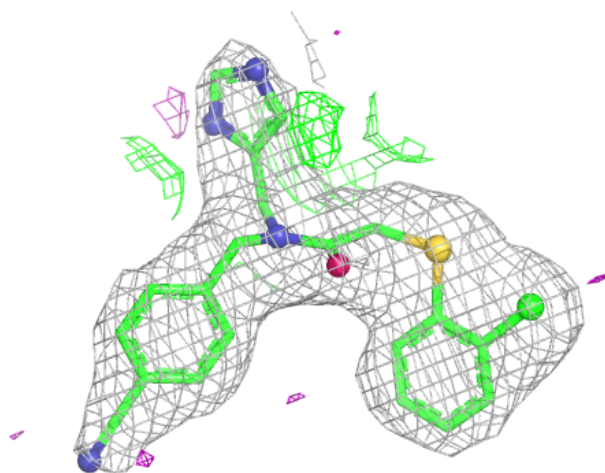
Electron density around VFT R 301 (A):

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



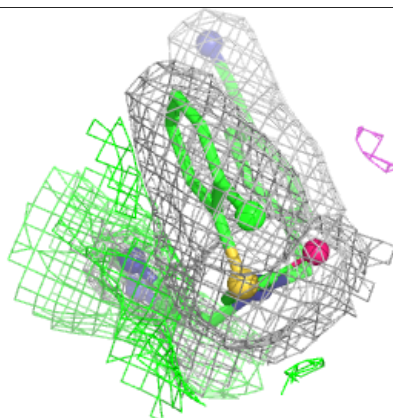
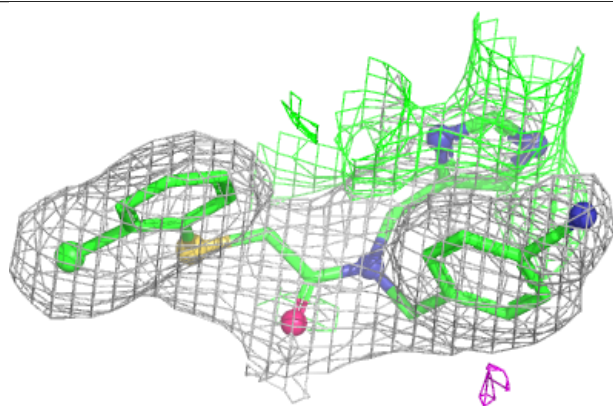
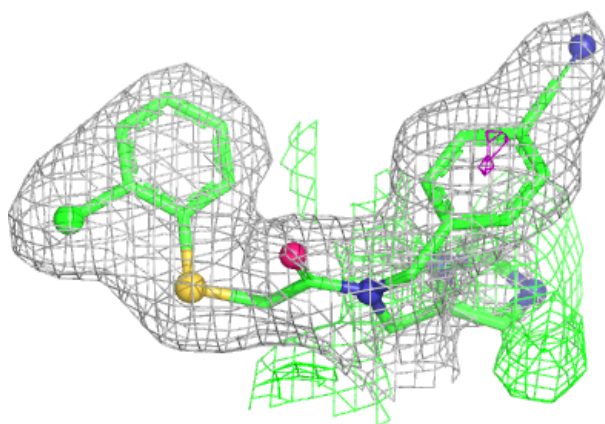
Electron density around VFT R 301 (B):

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



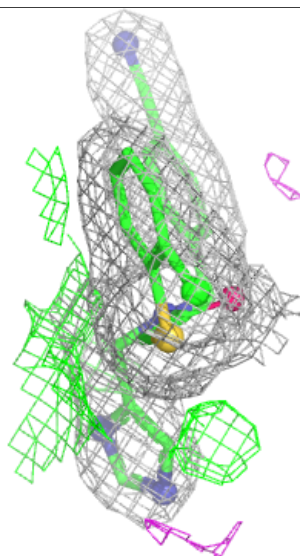
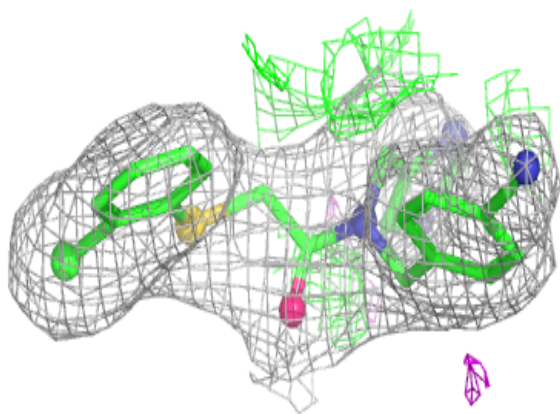
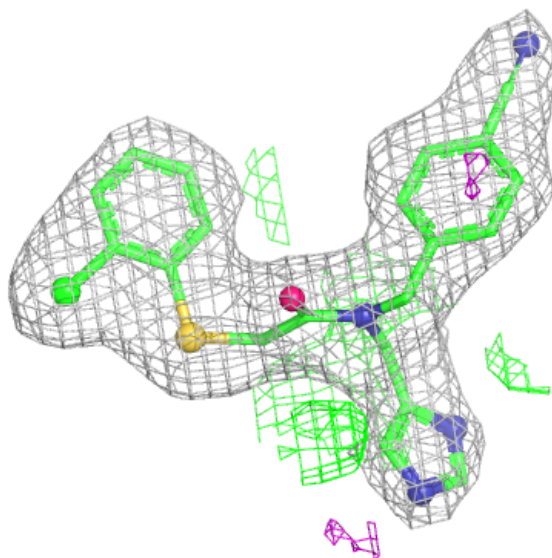
Electron density around VFT S 301 (A):

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



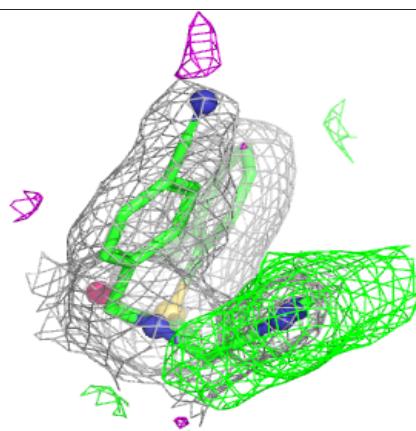
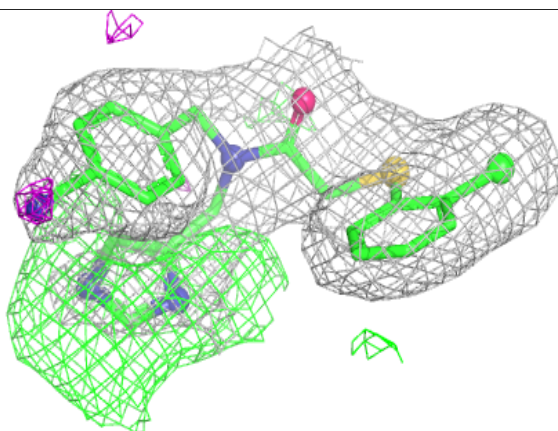
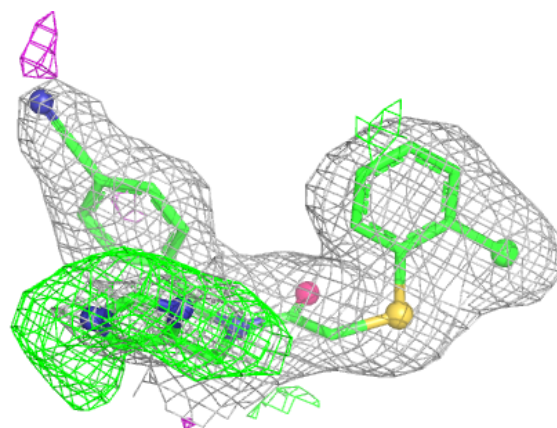
Electron density around VFT S 301 (B):

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



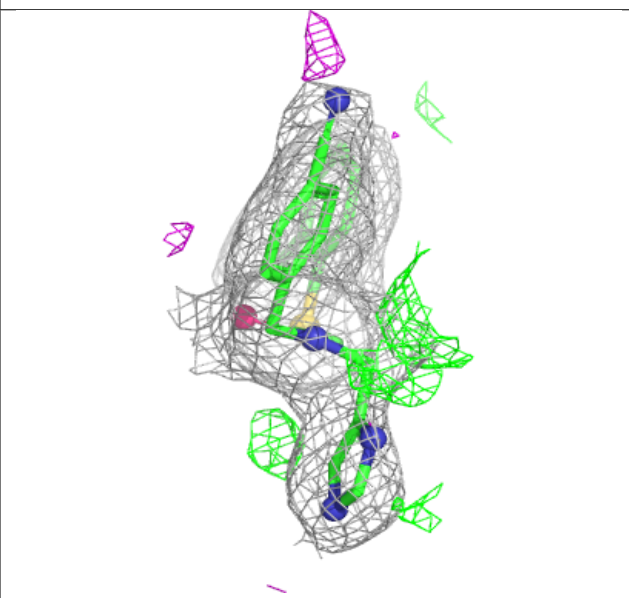
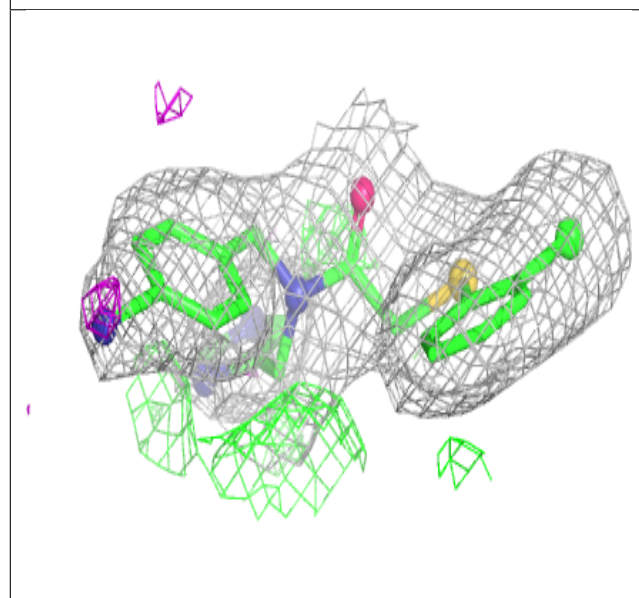
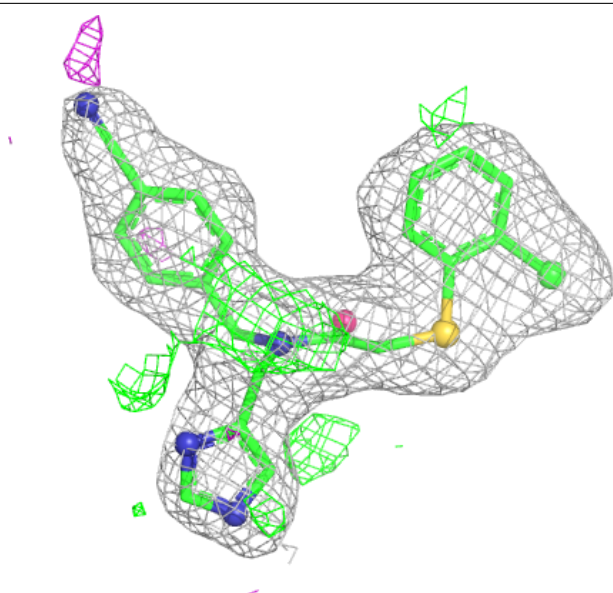
Electron density around VFT E 301 (A):

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



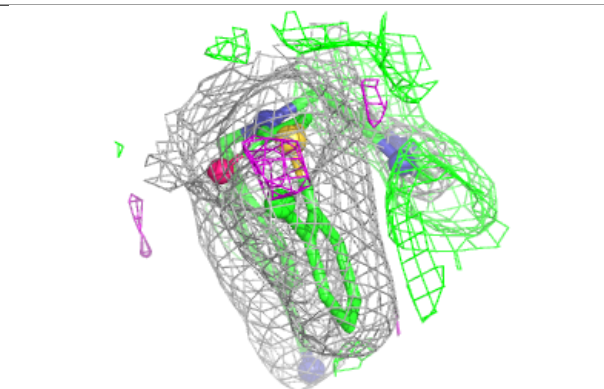
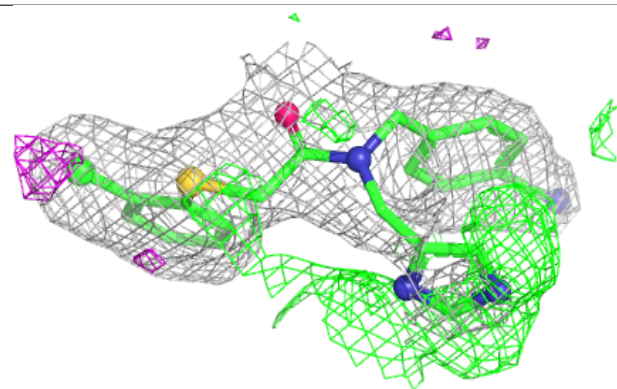
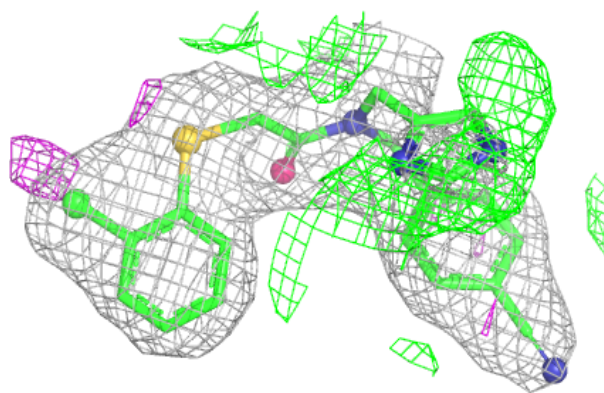
Electron density around VFT E 301 (B):

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



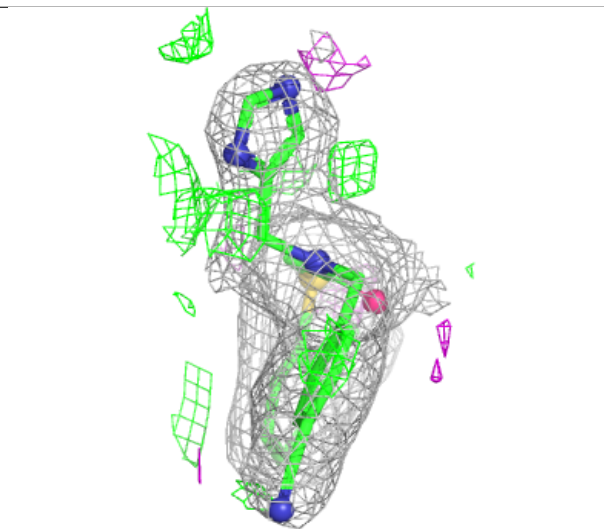
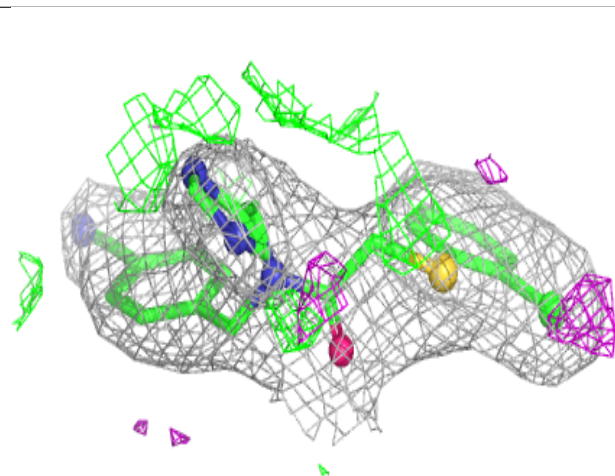
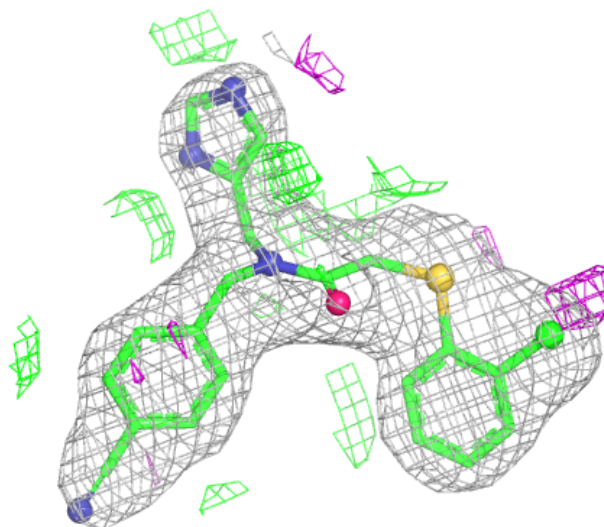
Electron density around VFT X 301 (A):

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



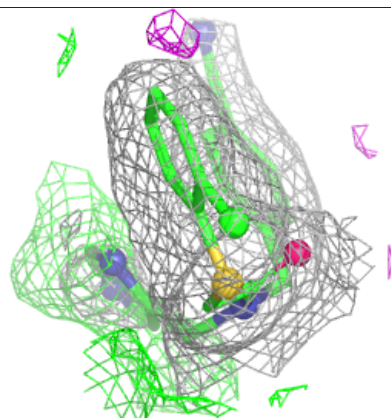
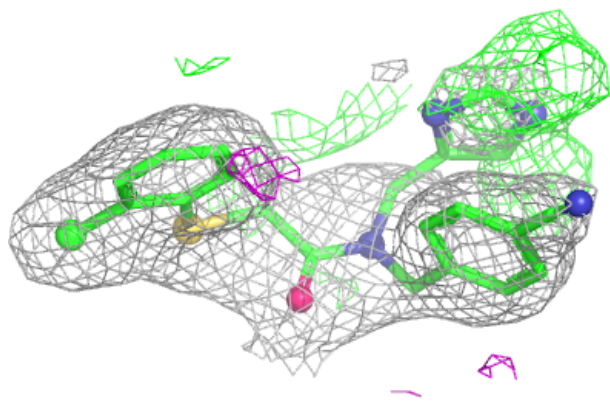
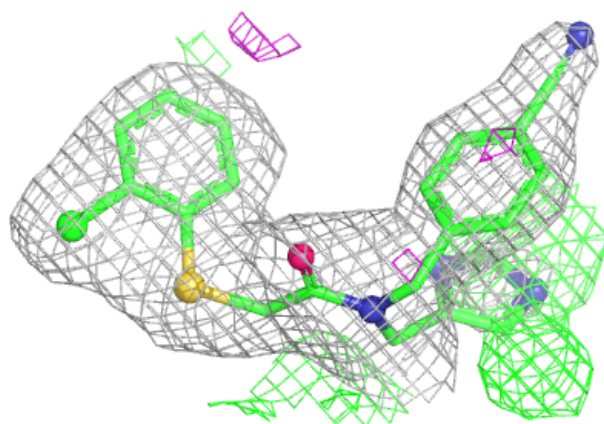
Electron density around VFT X 301 (B):

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



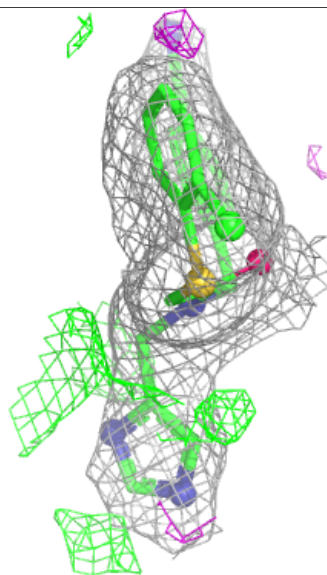
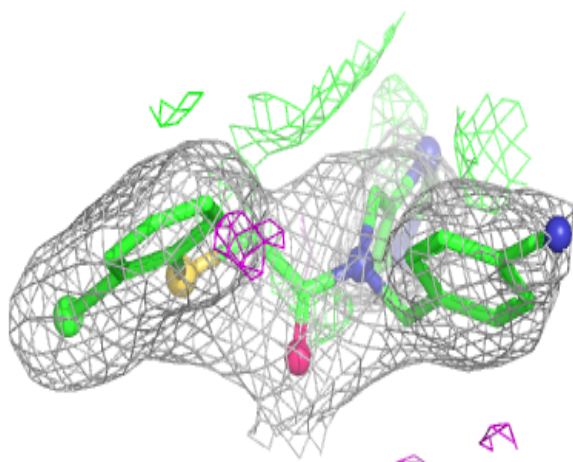
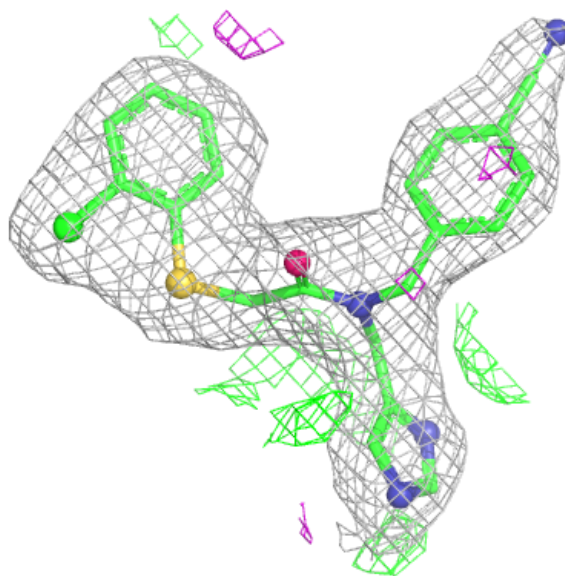
Electron density around VFT G 302 (A):

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



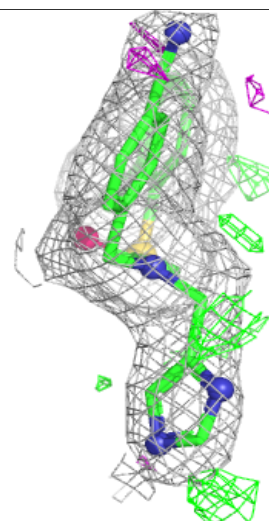
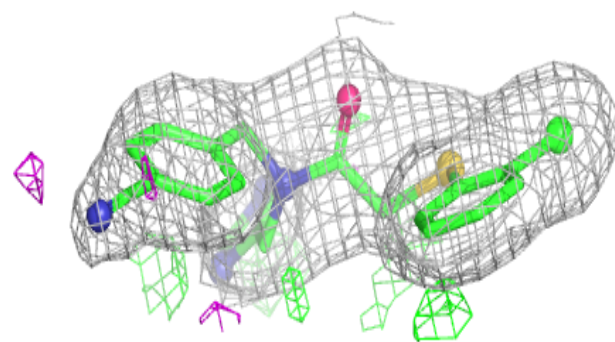
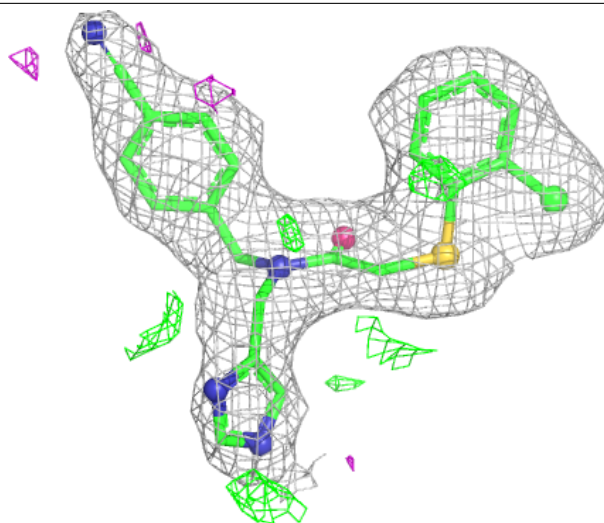
Electron density around VFT G 302 (B):

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



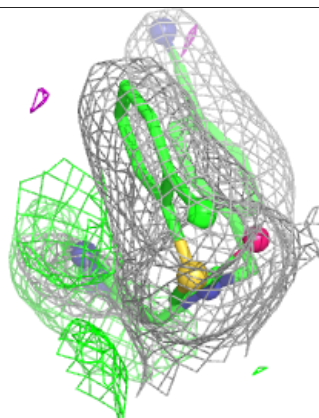
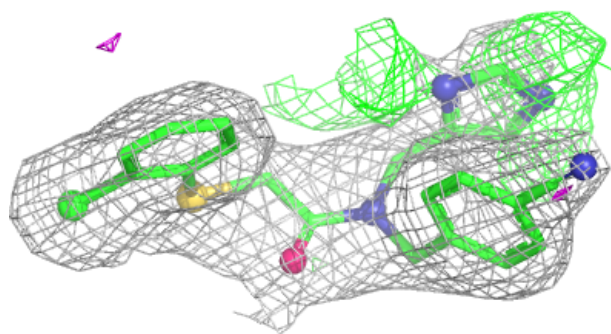
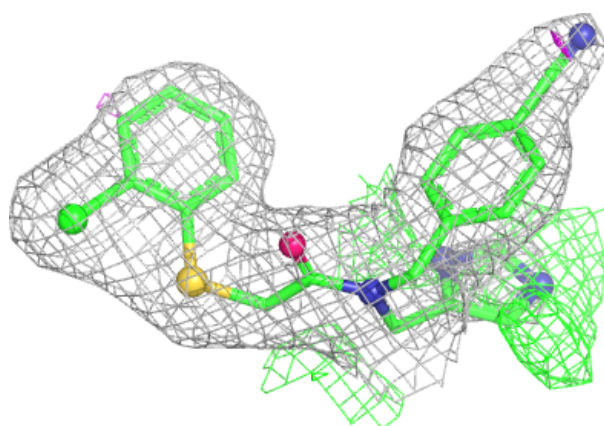
Electron density around VFT A 301 (B):

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



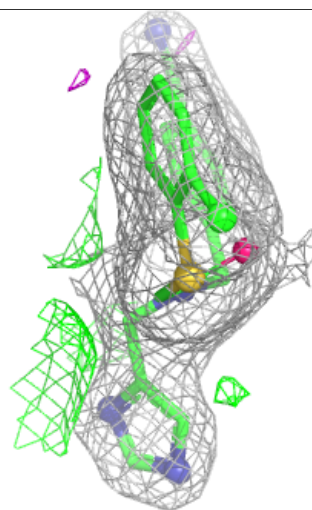
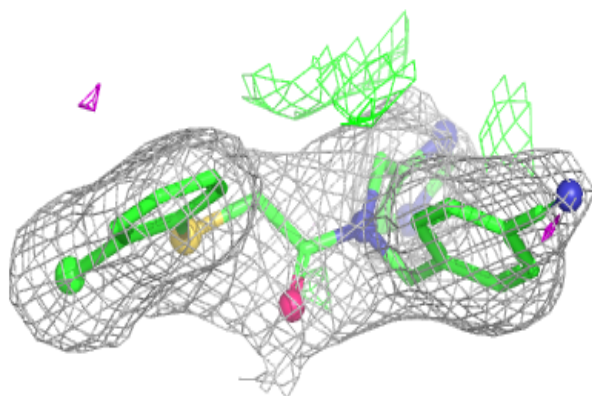
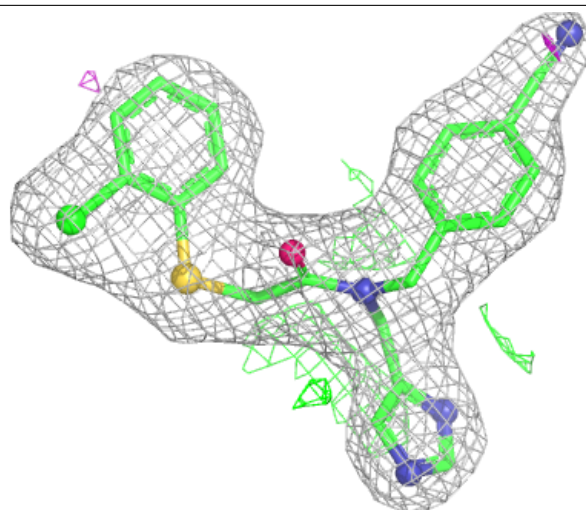
Electron density around VFT G 301 (A):

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



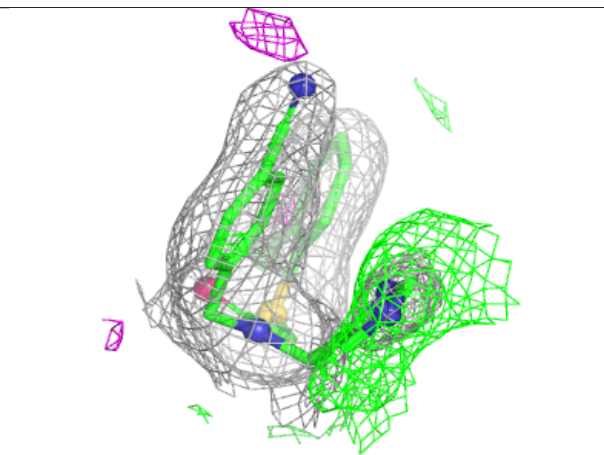
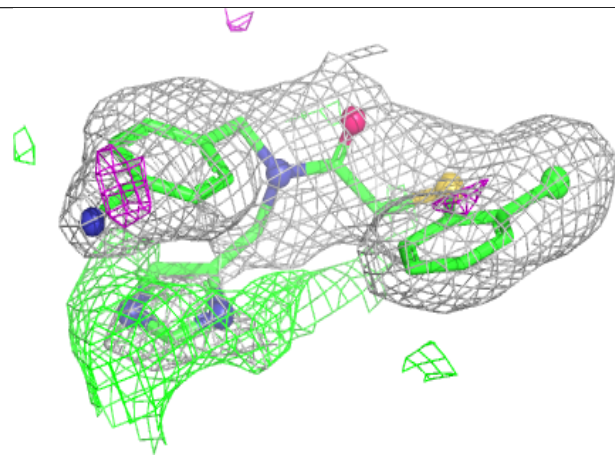
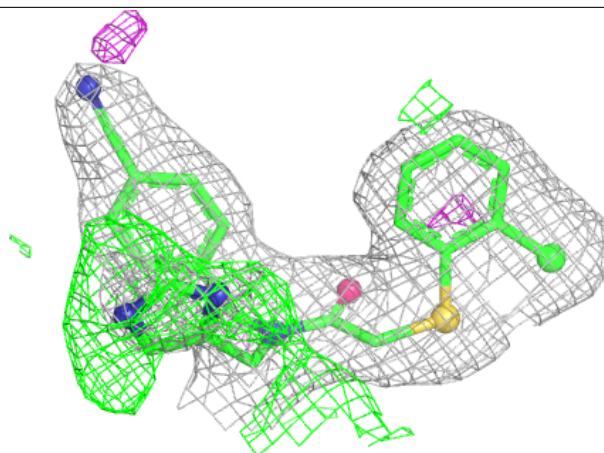
Electron density around VFT G 301 (B):

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



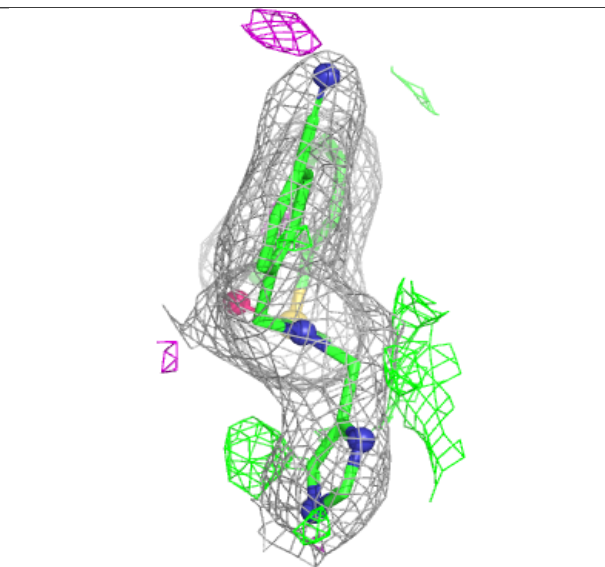
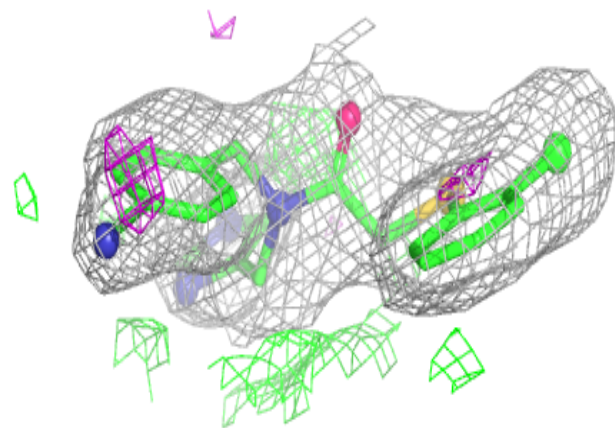
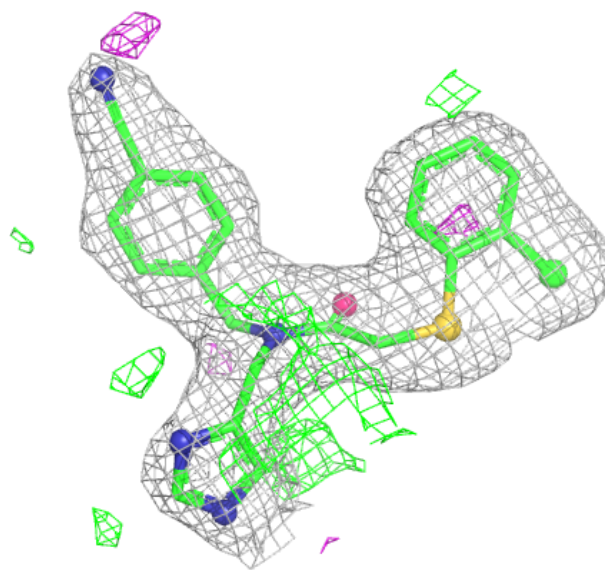
Electron density around VFT U 301 (A):

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



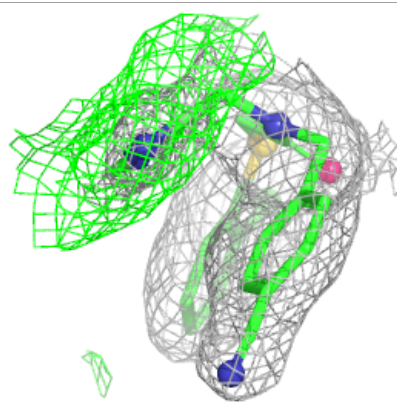
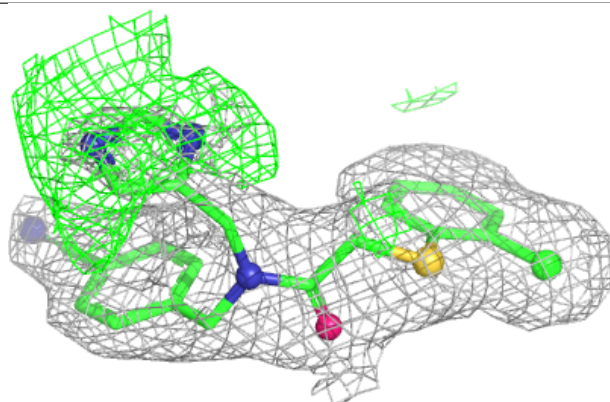
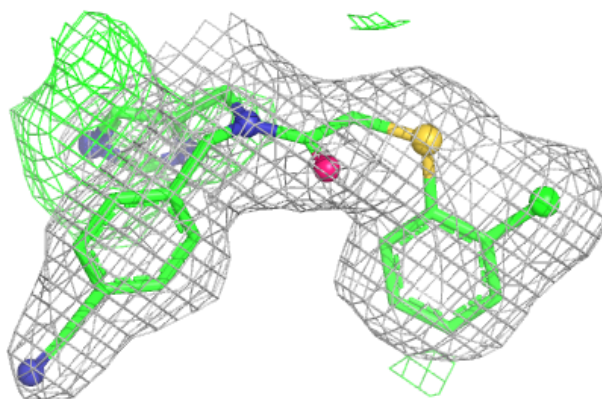
Electron density around VFT U 301 (B):

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



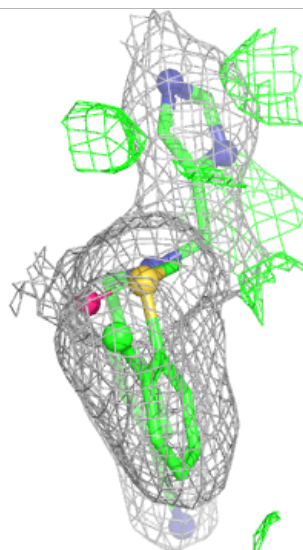
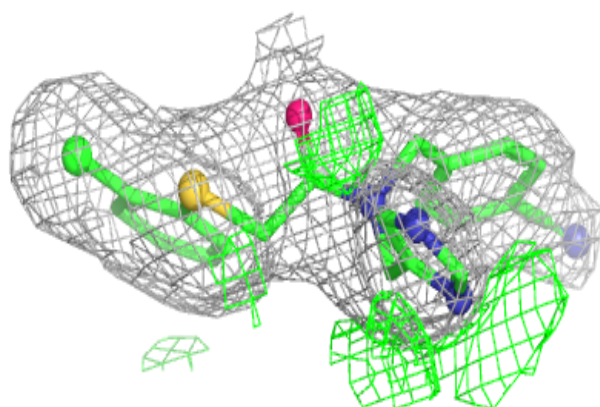
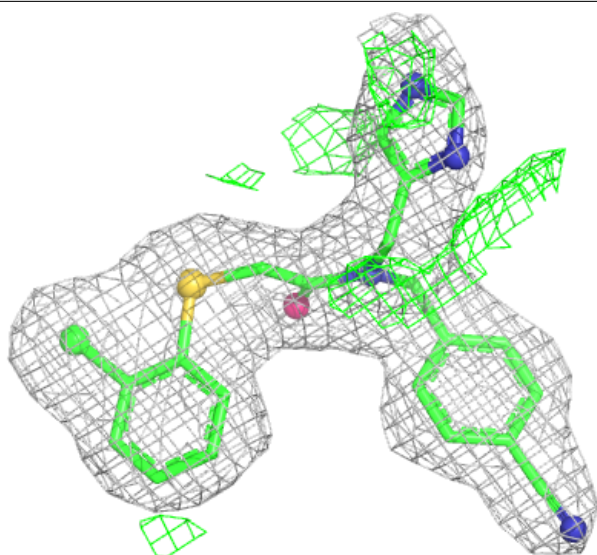
Electron density around VFT B 301 (A):

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



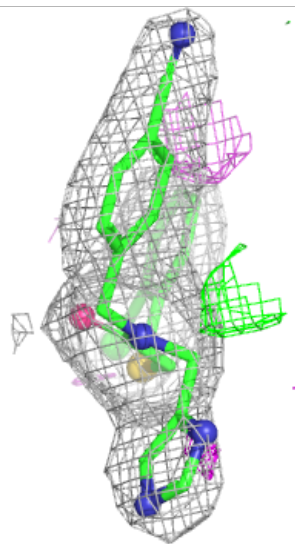
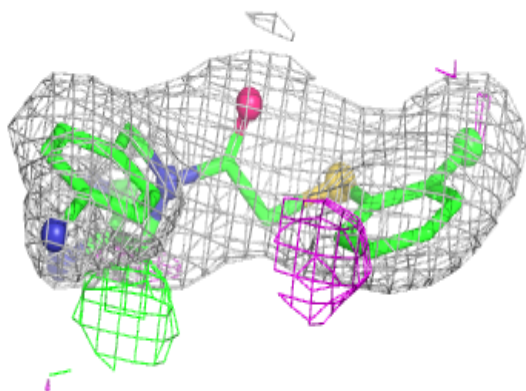
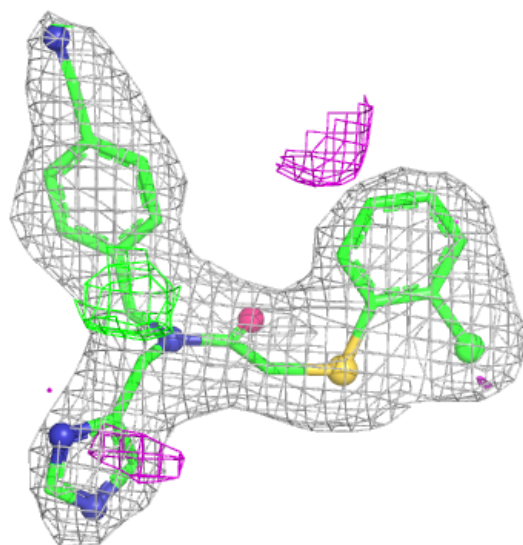
Electron density around VFT B 301 (B):

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



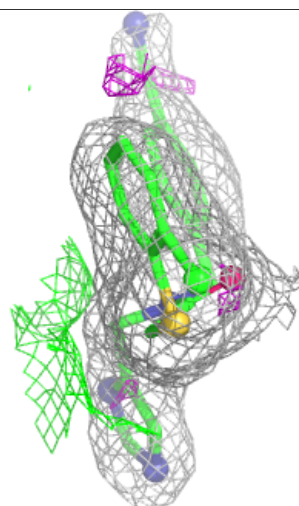
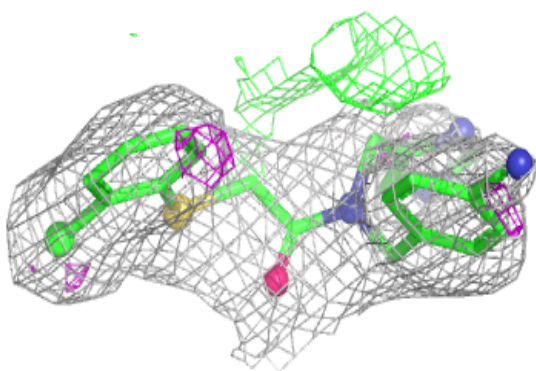
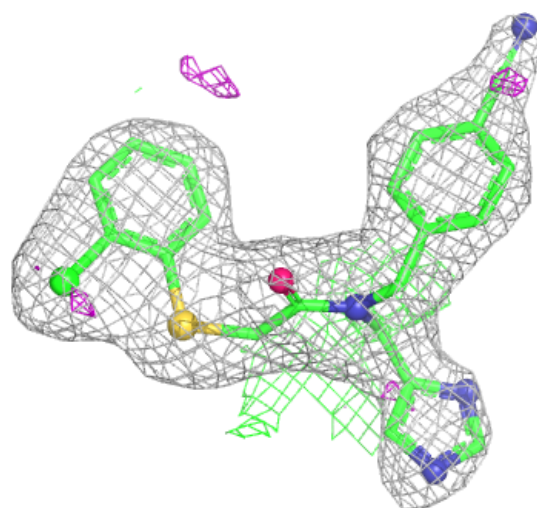
Electron density around VFT W 302:

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



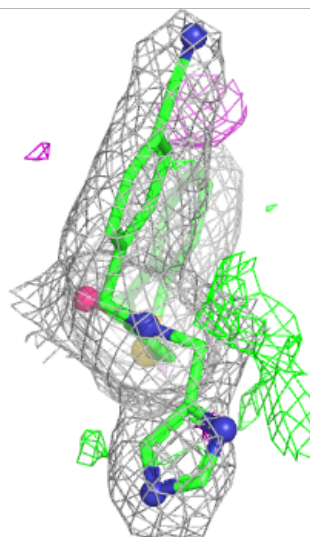
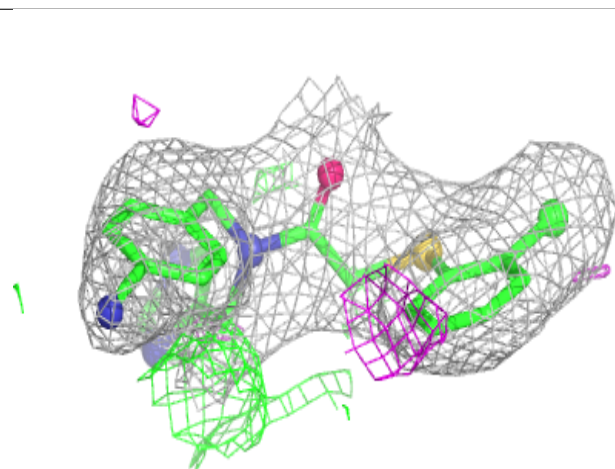
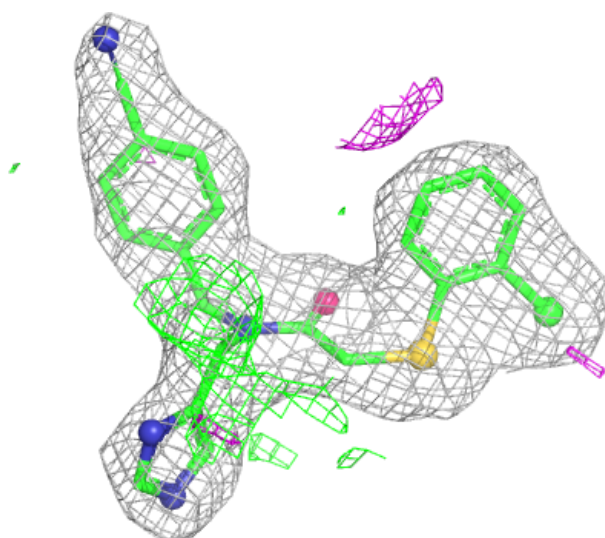
Electron density around VFT M 301:

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



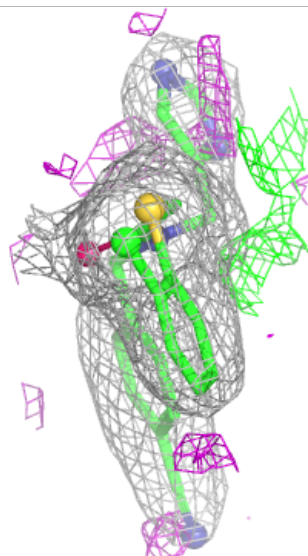
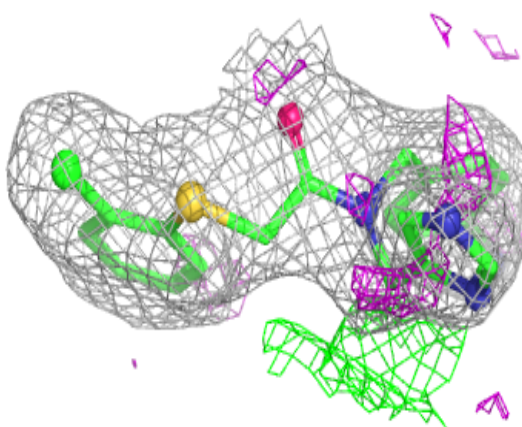
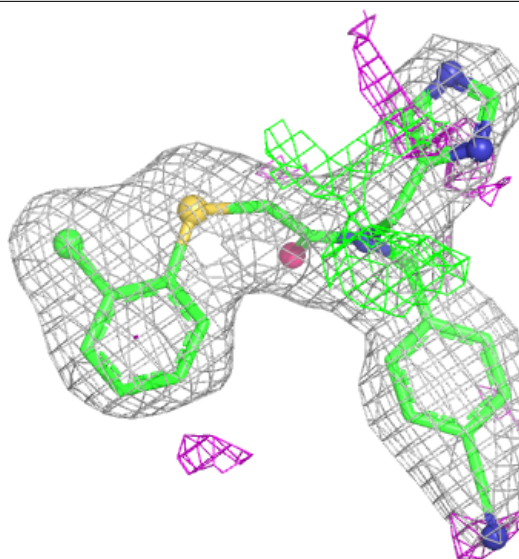
Electron density around VFT N 301:

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



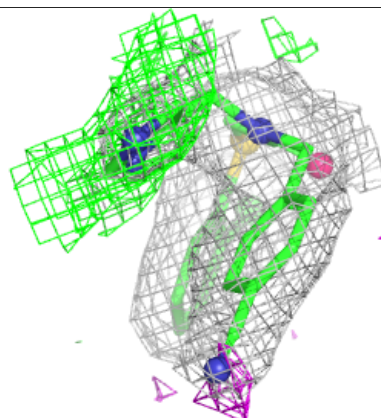
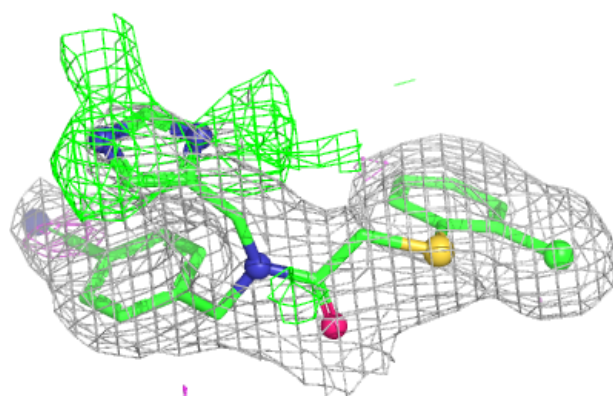
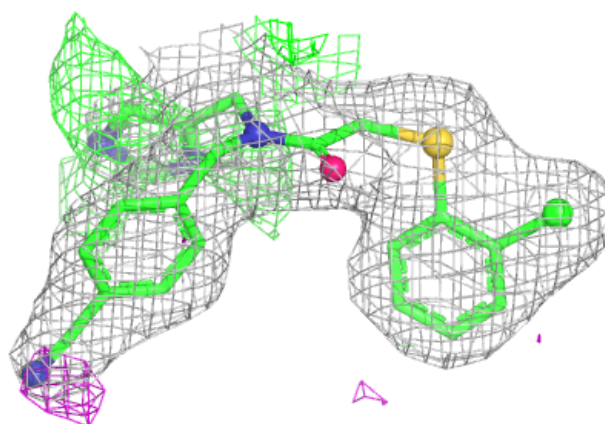
Electron density around VFT O 301:

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



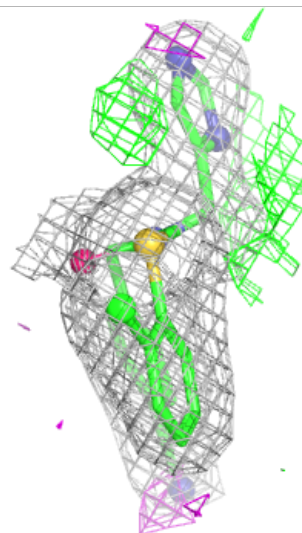
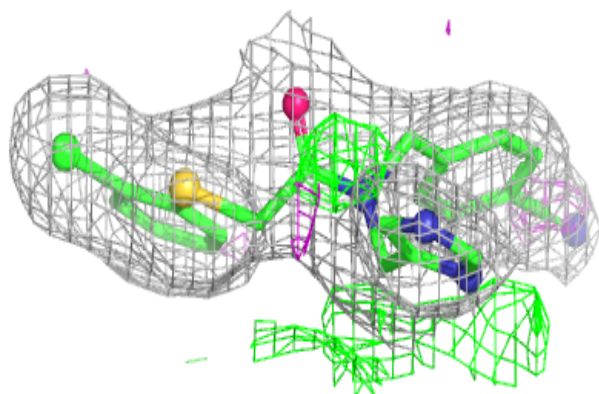
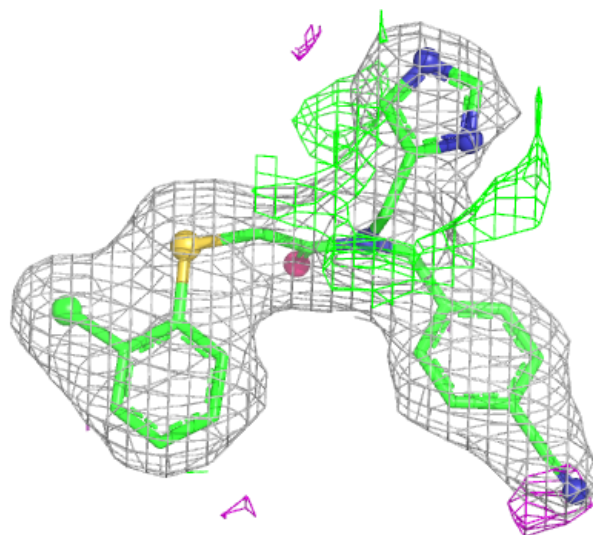
Electron density around VFT J 301 (A):

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



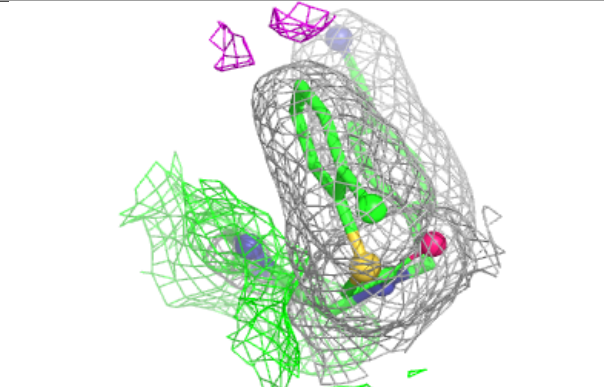
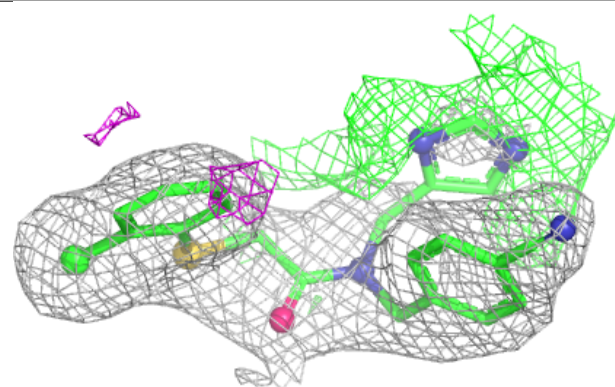
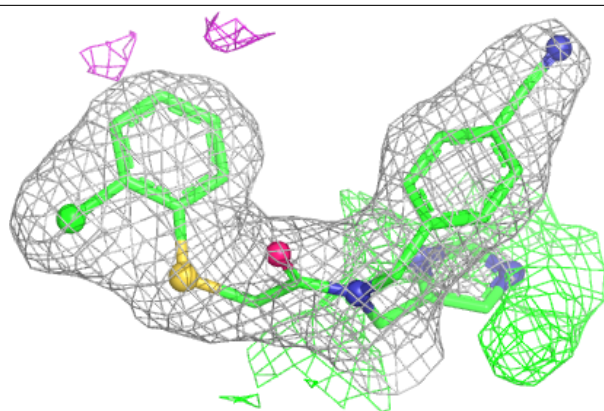
Electron density around VFT J 301 (B):

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



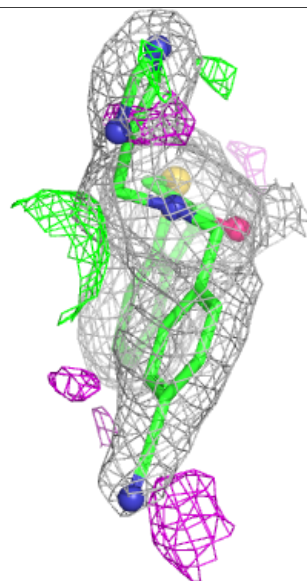
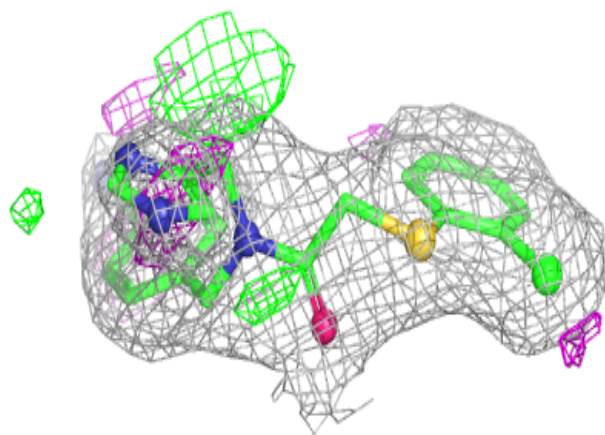
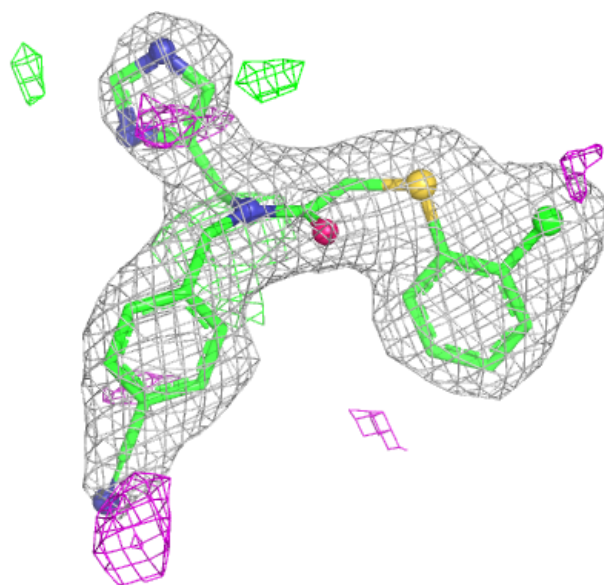
Electron density around VFT K 301 (A):

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



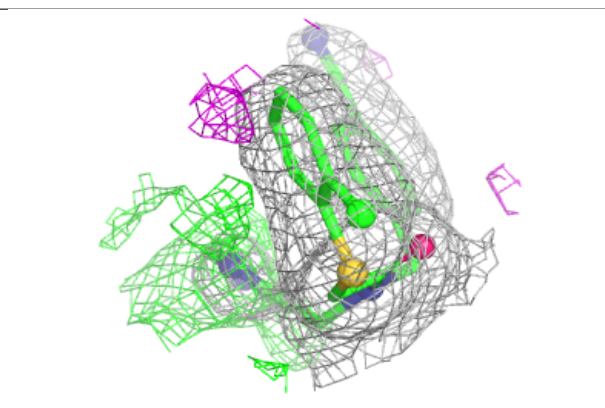
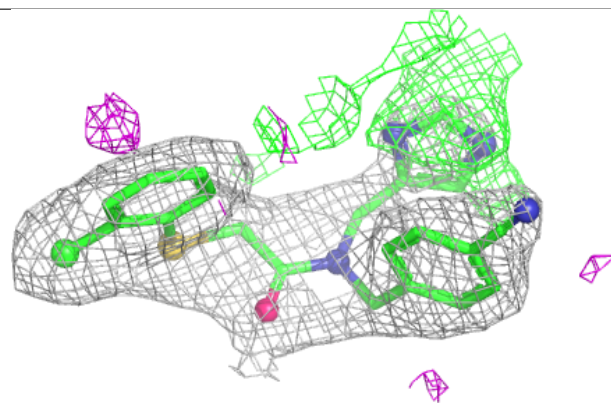
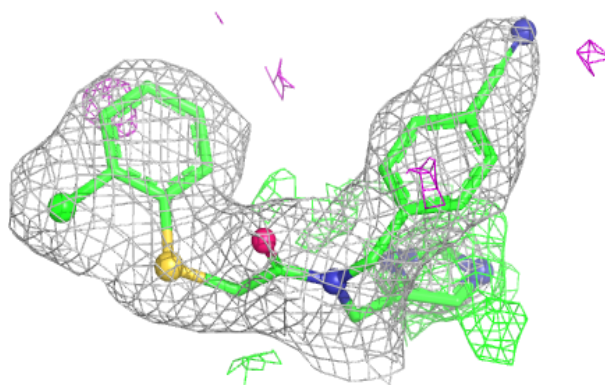
Electron density around VFT a 302:

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



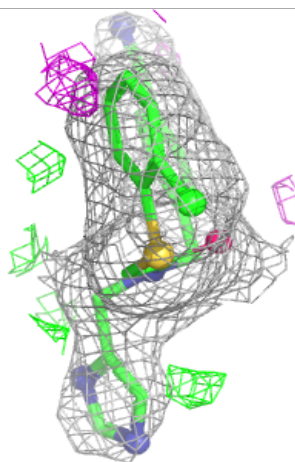
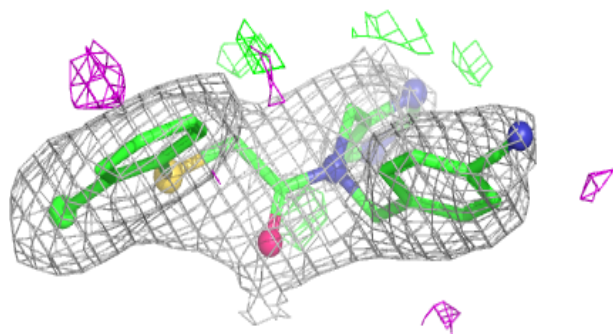
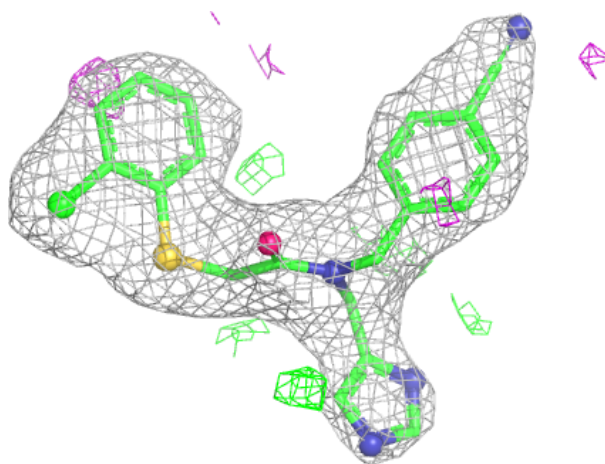
Electron density around VFT b 301 (A):

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



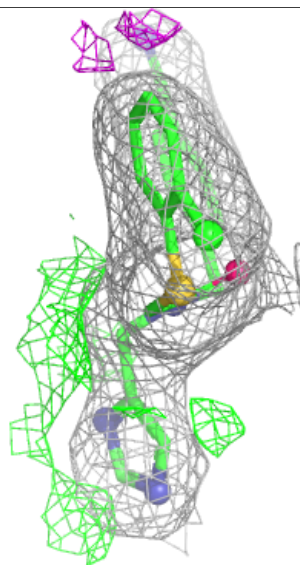
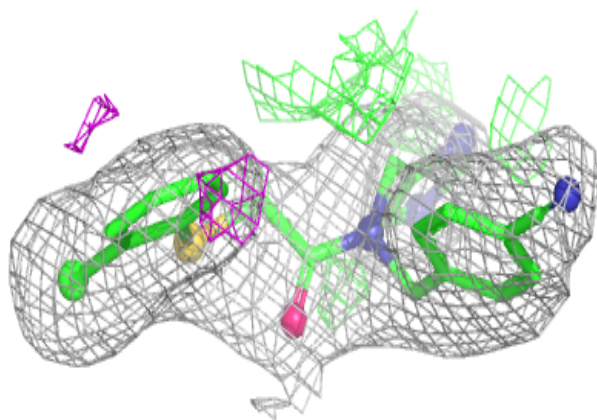
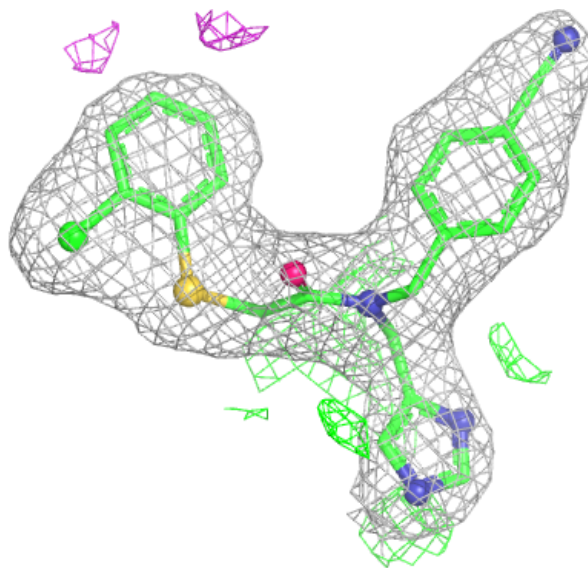
Electron density around VFT b 301 (B):

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



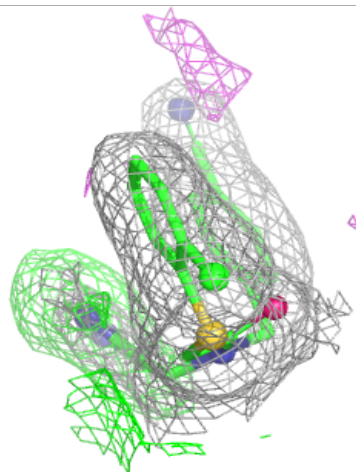
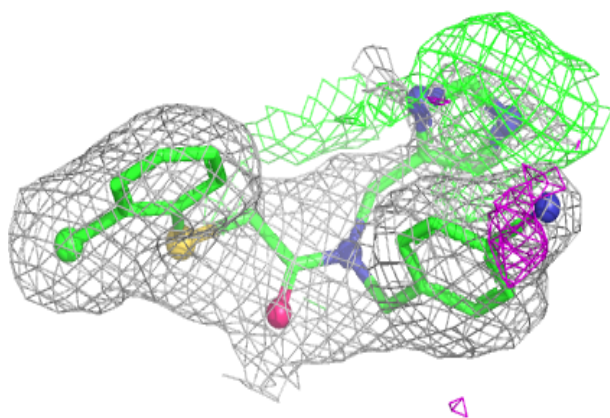
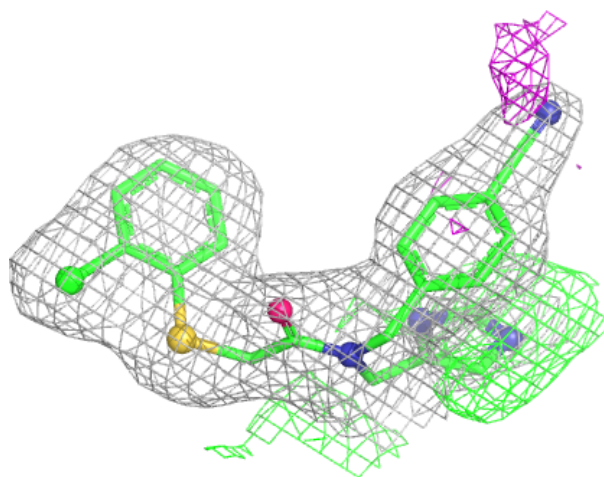
Electron density around VFT K 301 (B):

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



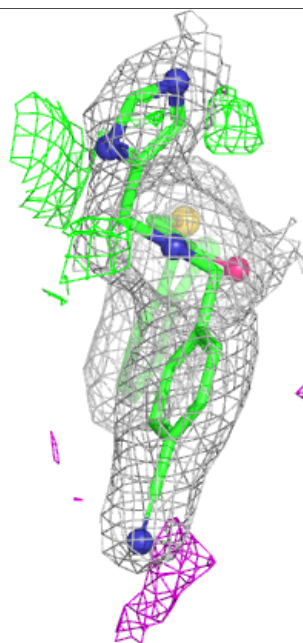
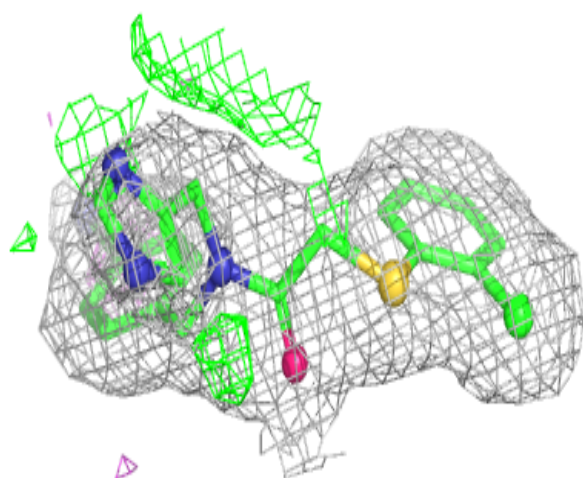
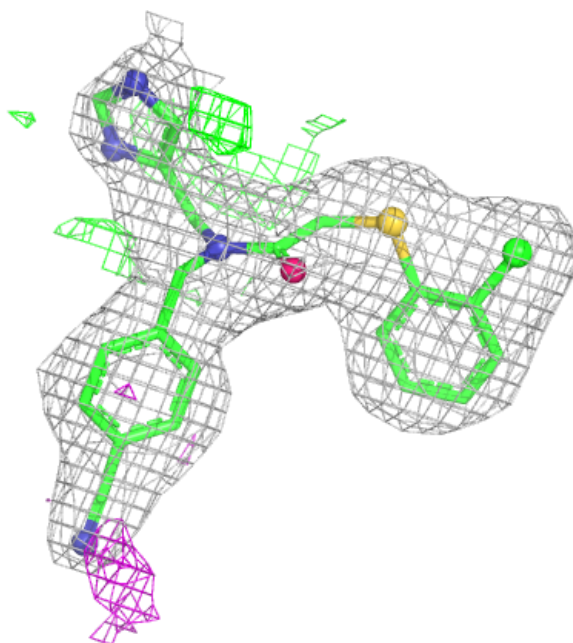
Electron density around VFT D 301 (A):

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



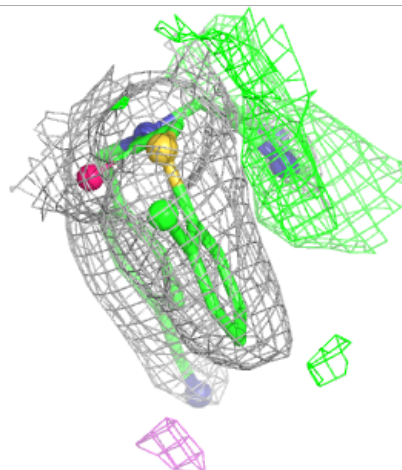
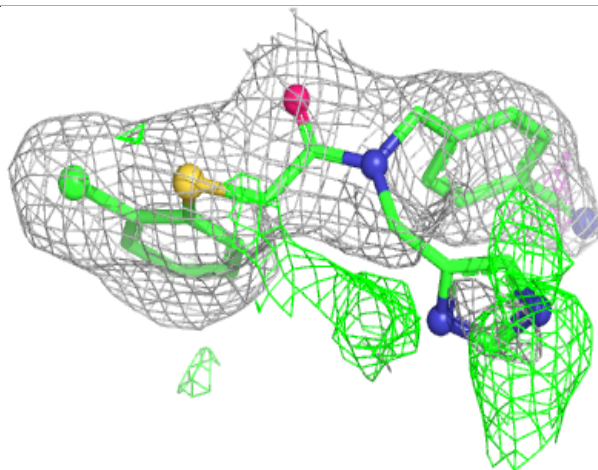
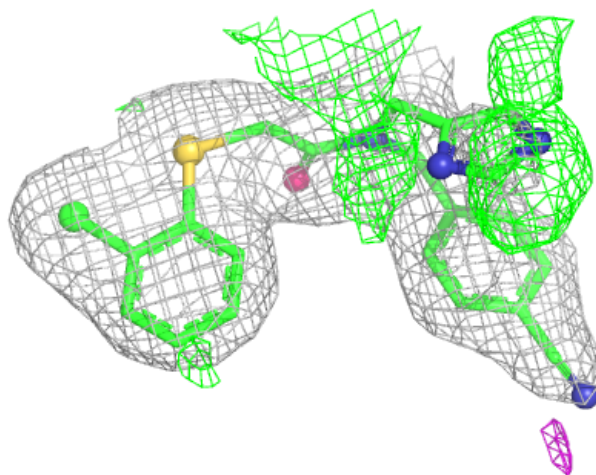
Electron density around VFT D 301 (B):

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



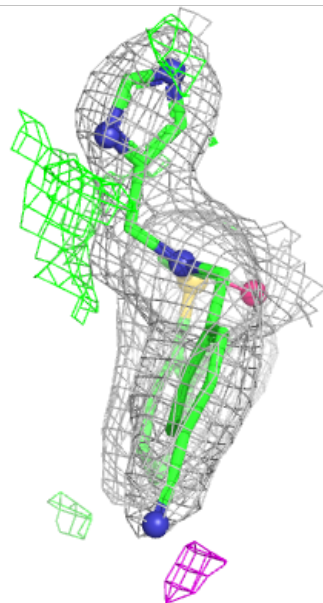
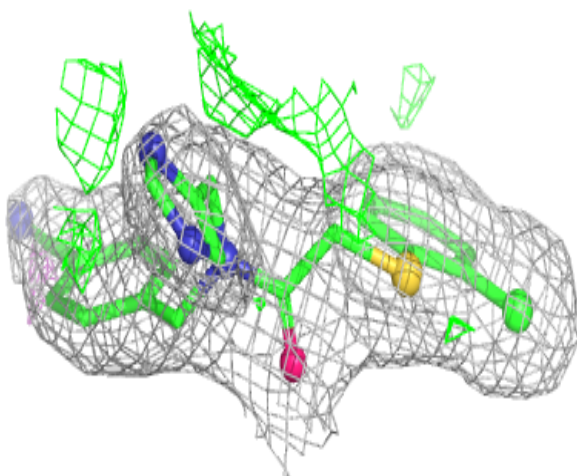
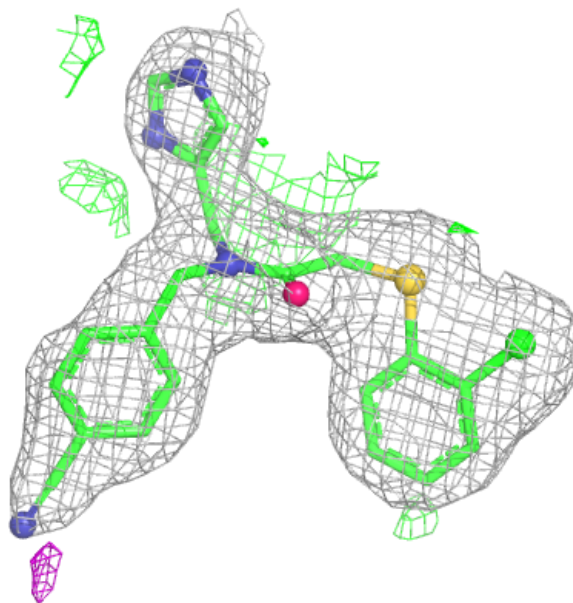
Electron density around VFT Q 301 (A):

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



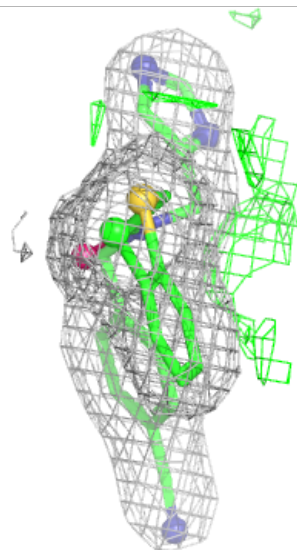
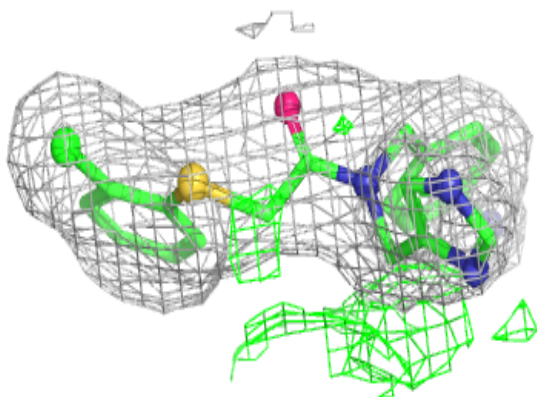
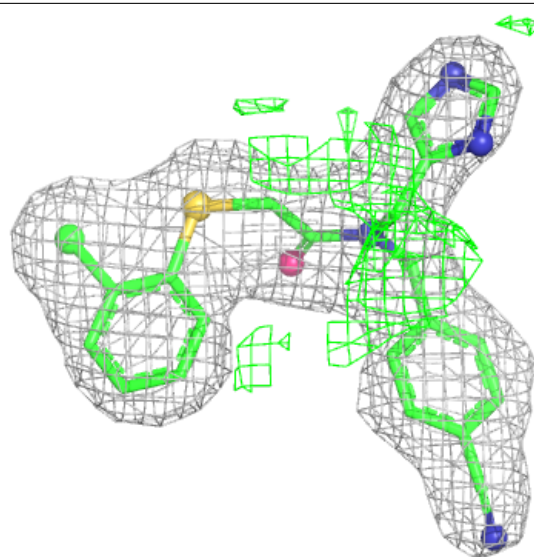
Electron density around VFT Q 301 (B):

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



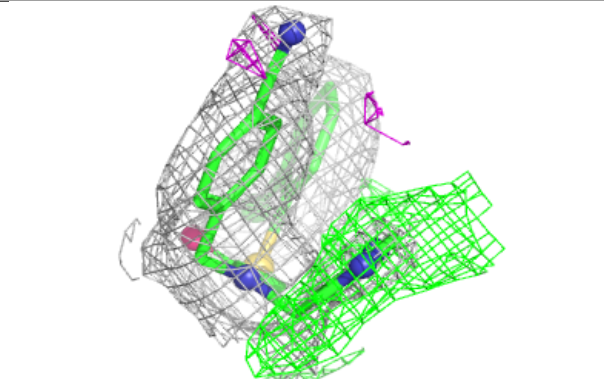
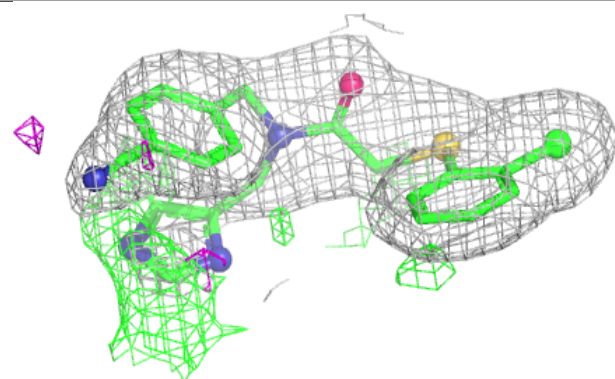
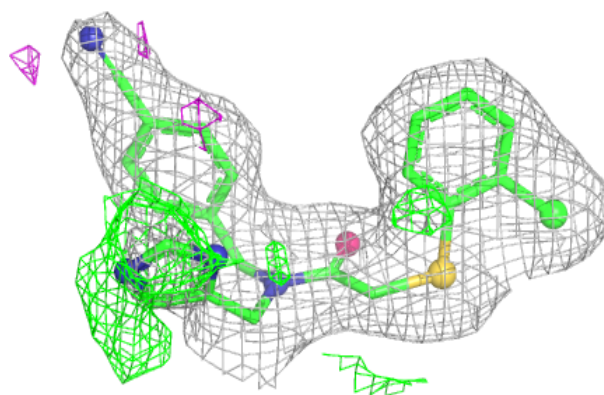
Electron density around VFT Q 302:

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



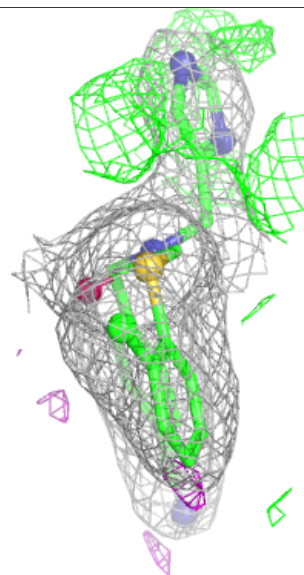
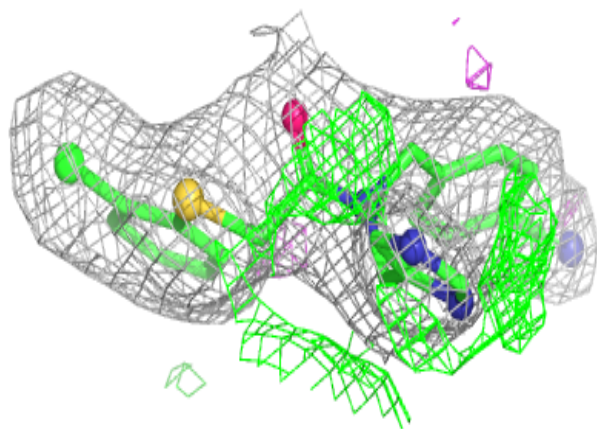
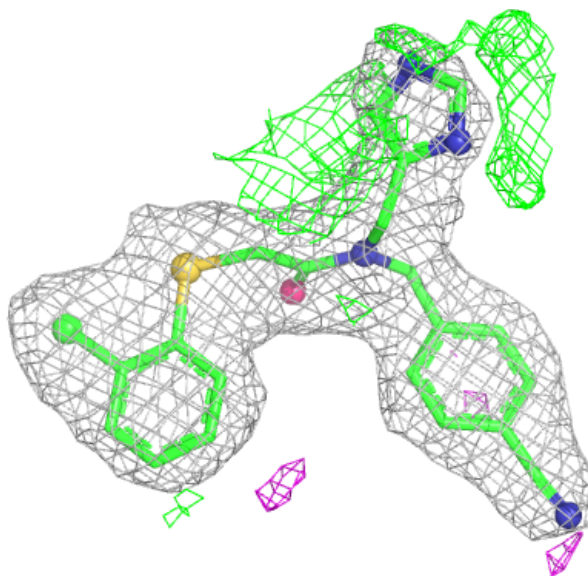
Electron density around VFT A 301 (A):

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



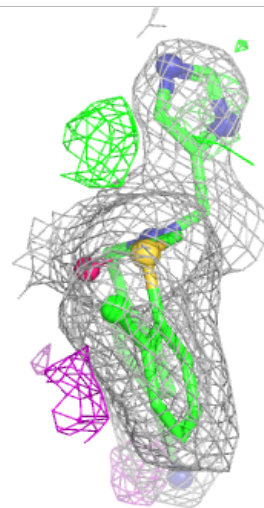
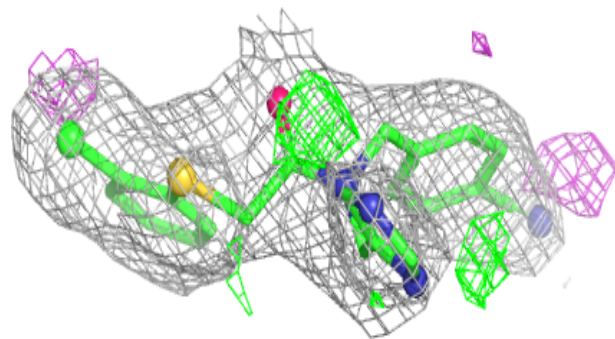
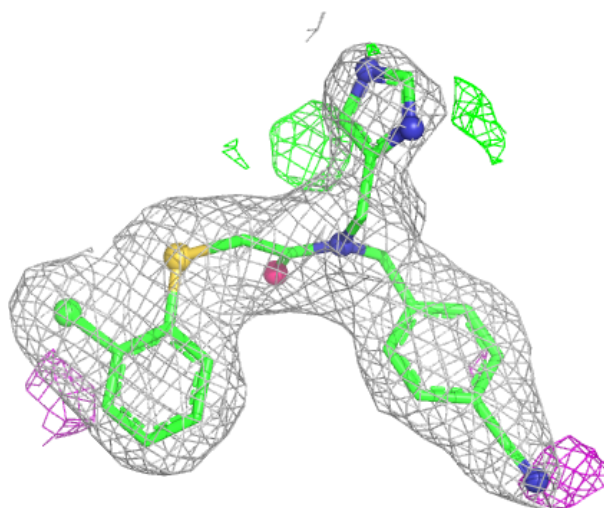
Electron density around VFT T 301 (B):

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



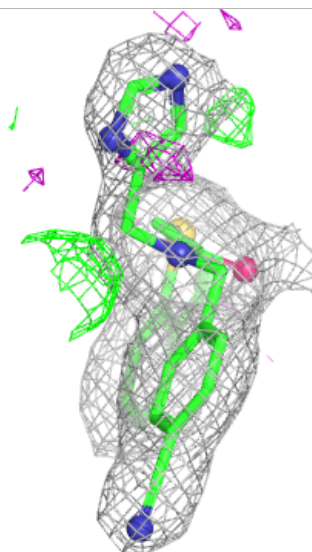
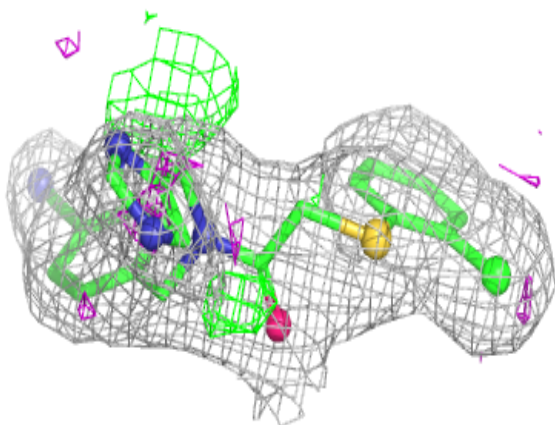
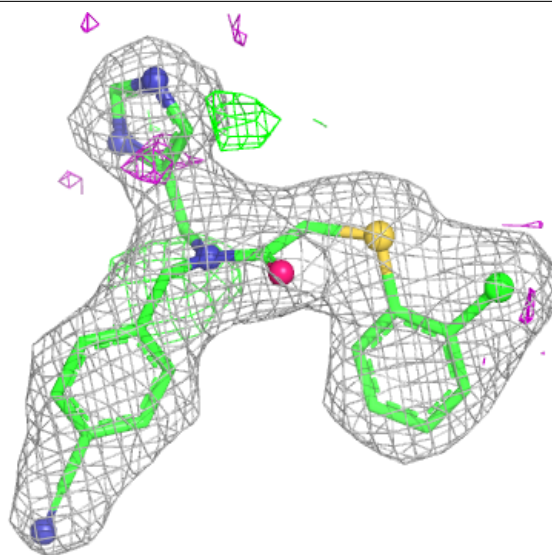
Electron density around VFT B 302 (B):

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



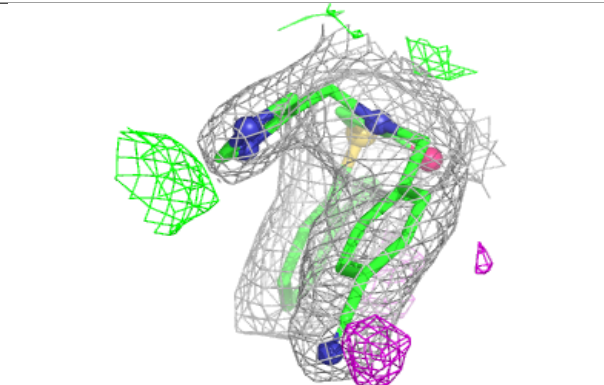
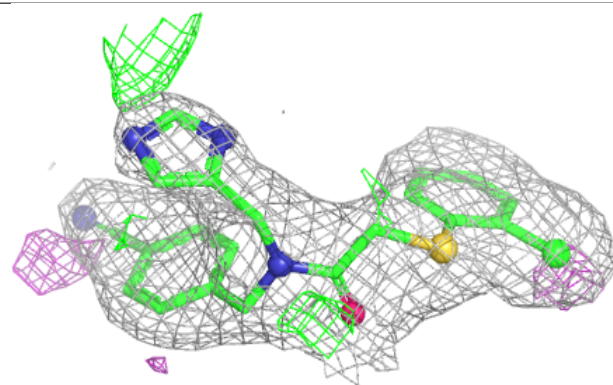
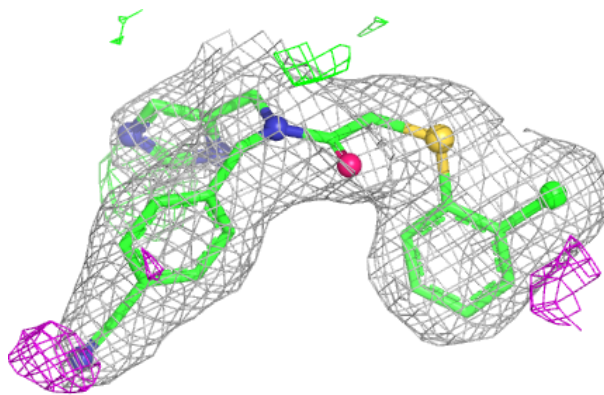
Electron density around VFT F 301:

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



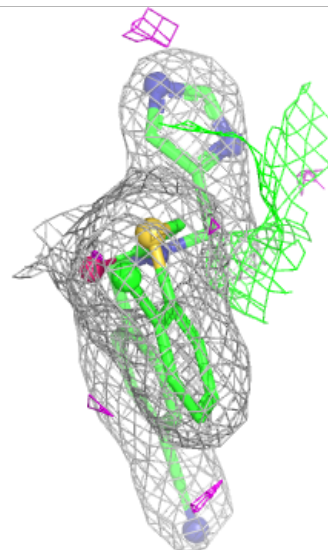
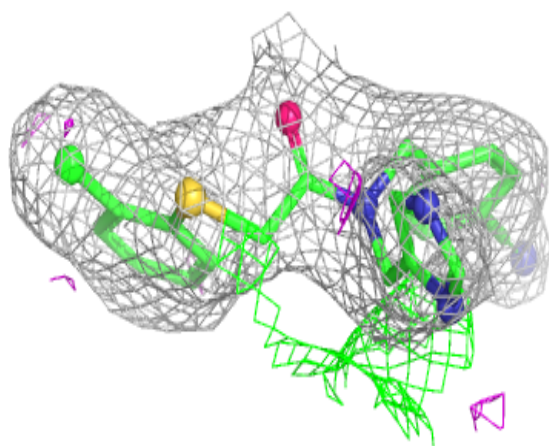
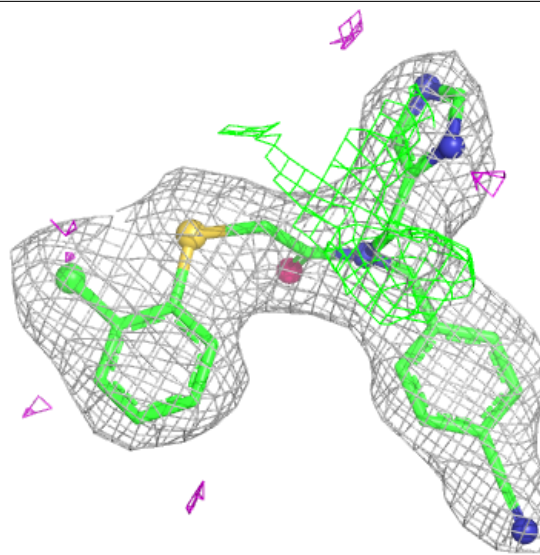
Electron density around VFT B 302 (A):

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



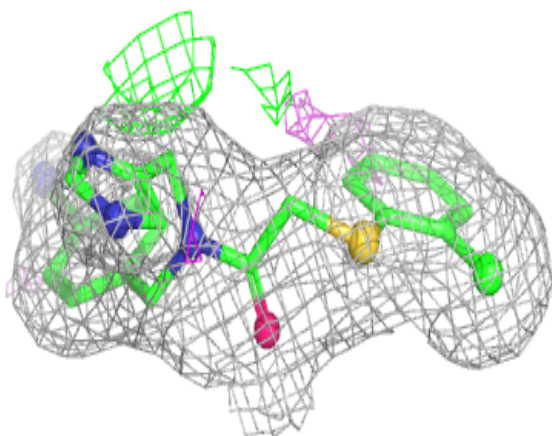
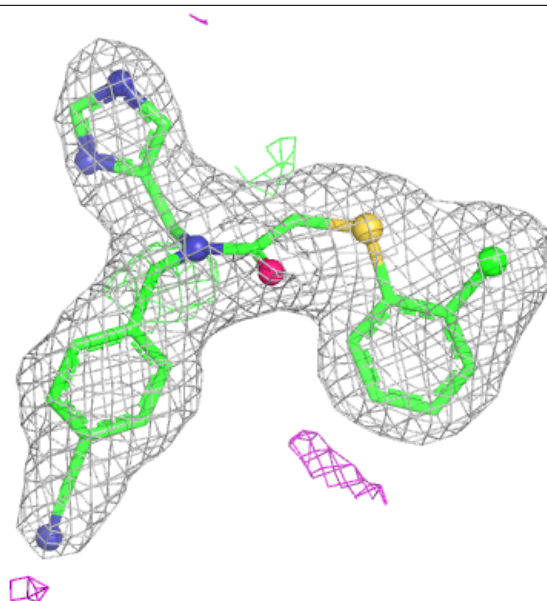
Electron density around VFT H 301:

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



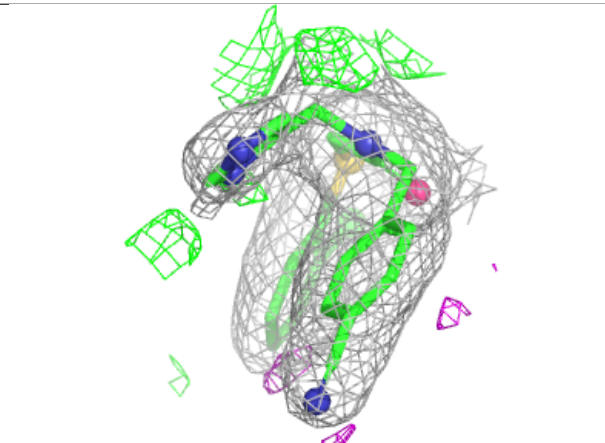
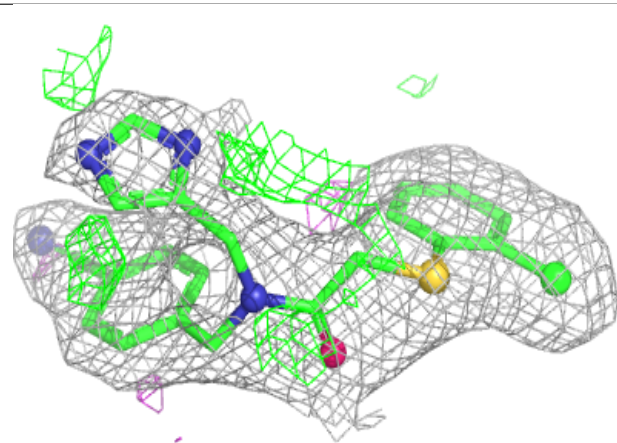
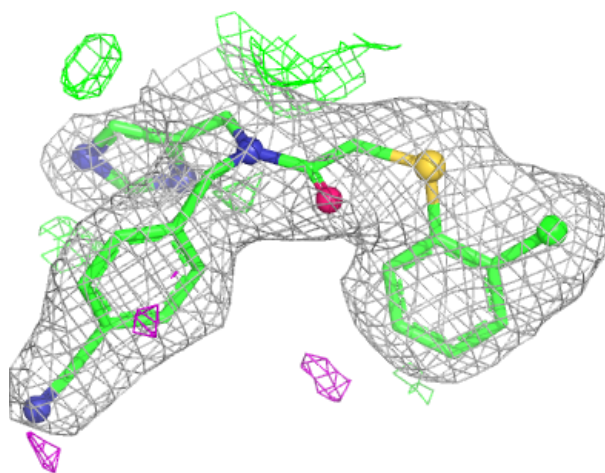
Electron density around VFT c 302:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.