



# wwPDB X-ray Structure Validation Summary Report

Oct 18, 2021 – 01:03 pm BST

PDB ID : 7OJP  
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 1  
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 : 2.84 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

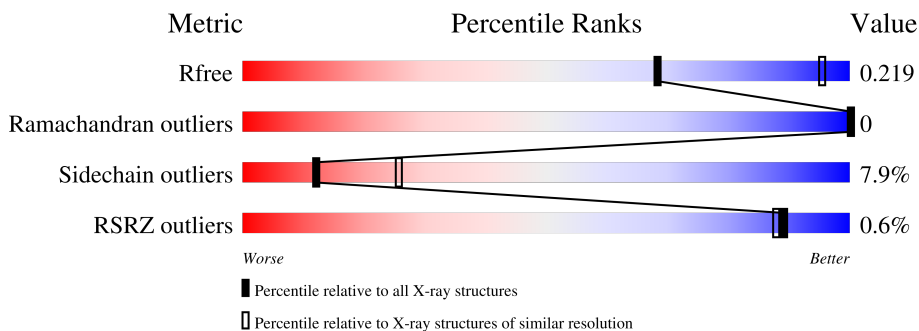
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 Å.

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





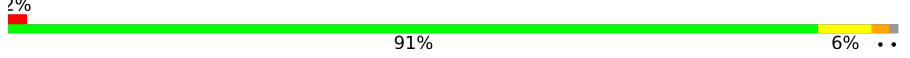


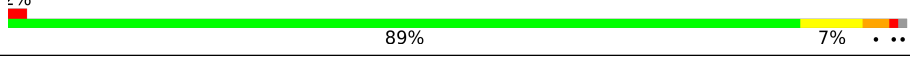
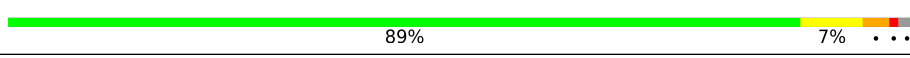

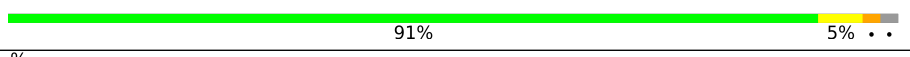

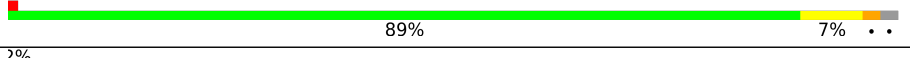
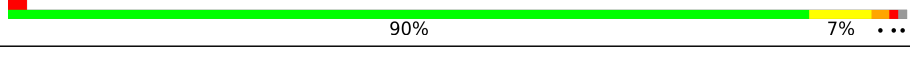

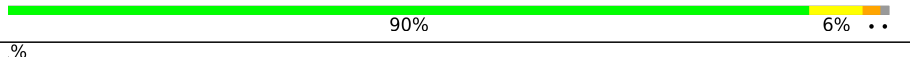


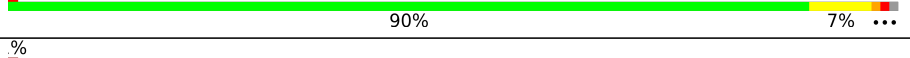

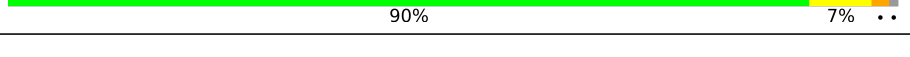
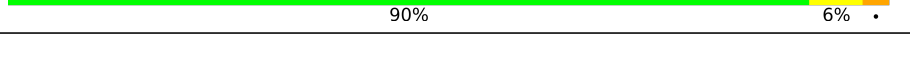

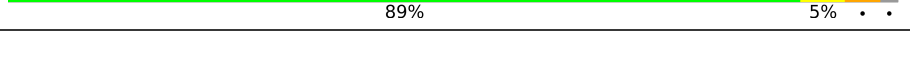
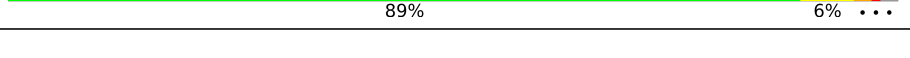
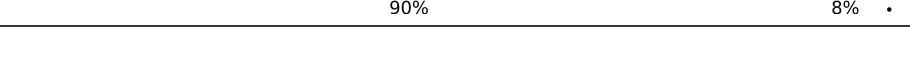
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1031 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	

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Mol	Chain	Length	Quality of chain
1	G	261	 90% 7% ...
1	H	261	 90% 7% ..
1	I	261	 91% 6% ..
1	J	261	 89% 6% . .
1	K	261	 89% 8% ...
1	L	261	 89% 7% ...
1	M	261	 89% 7% ...
1	N	261	 89% 8% ..
1	O	261	 91% 5% ..
1	P	261	 89% 7% ...
1	Q	261	 89% 7% ..
1	R	261	 90% 7% ...
1	S	261	 89% 7% ...
1	T	261	 90% 6% ..
1	U	261	 89% 7% ...
1	V	261	 89% 7% ...
1	W	261	 90% 7% ...
1	X	261	 88% 8% ...
1	Y	261	 90% 7% ..
1	Z	261	 90% 6% .
1	a	261	 88% 8% ..
1	b	261	 89% 5% ..
1	c	261	 89% 6% ...
1	d	261	 90% 8% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 60728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	1982	1240	367	368	7	0	1	0
1	B	258	1982	1240	367	368	7	0	1	0
1	C	257	1974	1235	366	367	6	0	1	0
1	D	257	1974	1235	366	367	6	0	1	0
1	E	258	1982	1240	367	368	7	0	1	0
1	F	257	1974	1235	366	367	6	0	1	0
1	G	258	1982	1240	367	368	7	0	1	0
1	H	258	1982	1240	367	368	7	0	1	0
1	I	258	1982	1240	367	368	7	0	1	0
1	J	257	1974	1235	366	367	6	0	1	0
1	K	258	1982	1240	367	368	7	0	1	0
1	L	258	1982	1240	367	368	7	0	1	0
1	M	257	1974	1235	366	367	6	0	1	0
1	N	257	1974	1235	366	367	6	0	1	0
1	O	257	1974	1235	366	367	6	0	1	0
1	P	257	1974	1235	366	367	6	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	R	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	S	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	T	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	U	259	Total	C	N	O	S	0	1	0
			1992	1246	370	369	7			
1	V	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	W	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	X	259	Total	C	N	O	S	0	2	0
			2003	1252	374	370	7			
1	Y	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	Z	261	Total	C	N	O	S	0	1	0
			2002	1251	372	372	7			
1	a	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	b	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	c	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	d	261	Total	C	N	O	S	0	1	0
			2002	1251	372	372	7			

There are 90 discrepancies between the modelled and reference sequences:

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

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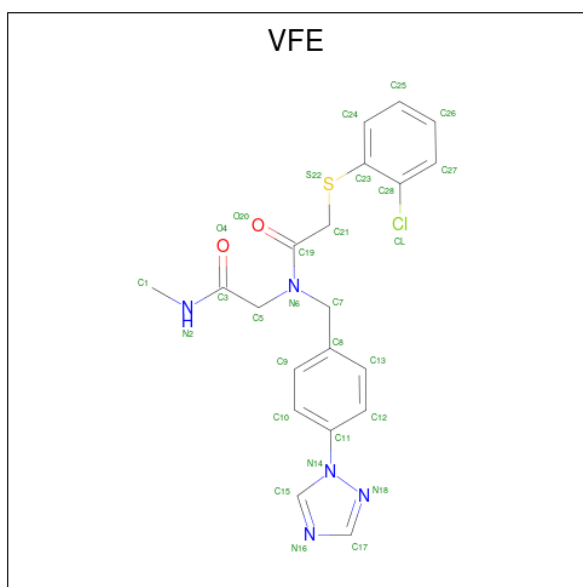
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A6V1E4
E	-2	GLY	-	expression tag	UNP A6V1E4
E	-1	SER	-	expression tag	UNP A6V1E4
E	0	HIS	-	expression tag	UNP A6V1E4
F	-2	GLY	-	expression tag	UNP A6V1E4
F	-1	SER	-	expression tag	UNP A6V1E4
F	0	HIS	-	expression tag	UNP A6V1E4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

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

- Molecule 2 is 2-[2-(2-chlorophenyl)sulfanylethanoyl]-[[4-(1,2,4-triazol-1-yl)phenyl]methyl]amino]-N-methyl-ethanamide (three-letter code: VFE) (formula: C<sub>20</sub>H<sub>20</sub>ClN<sub>5</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	Cl	N	O			S	
2	A	1	Total	29	20	1	5	2	1	0	0
2	B	1	Total	29	20	1	5	2	1	0	0
2	C	1	Total	29	20	1	5	2	1	0	0
2	D	1	Total	29	20	1	5	2	1	0	0
2	E	1	Total	29	20	1	5	2	1	0	0
2	F	1	Total	29	20	1	5	2	1	0	0
2	G	1	Total	29	20	1	5	2	1	0	0
2	H	1	Total	29	20	1	5	2	1	0	0
2	I	1	Total	29	20	1	5	2	1	0	0
2	J	1	Total	29	20	1	5	2	1	0	0
2	K	1	Total	29	20	1	5	2	1	0	0
2	L	1	Total	29	20	1	5	2	1	0	0
2	M	1	Total	29	20	1	5	2	1	0	0
2	N	1	Total	29	20	1	5	2	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	O	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	P	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Q	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	R	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	S	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	T	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	U	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	V	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	W	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	X	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Y	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Z	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	a	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	b	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	c	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	d	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total 13 13	0	0
4	B	19	Total 19 19	0	0
4	C	21	Total 21 21	0	0
4	D	23	Total 23 23	0	0
4	E	16	Total 16 16	0	0
4	F	12	Total 12 12	0	0
4	G	2	Total 2 2	0	0
4	H	7	Total 7 7	0	0
4	I	9	Total 9 9	0	0
4	J	6	Total 6 6	0	0
4	K	9	Total 9 9	0	0
4	L	8	Total 8 8	0	0
4	M	14	Total 14 14	0	0
4	N	8	Total 8 8	0	0
4	O	15	Total 15 15	0	0
4	P	5	Total 5 5	0	0
4	Q	11	Total 11 11	0	0
4	R	10	Total 10 10	0	0
4	S	15	Total 15 15	0	0
4	T	17	Total 17 17	0	0
4	U	19	Total 19 19	0	0
4	V	13	Total 13 13	0	0

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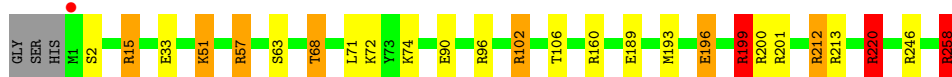
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	W	12	Total O 12 12	0	0
4	X	19	Total O 19 19	0	0
4	Y	24	Total O 24 24	0	0
4	Z	23	Total O 23 23	0	0
4	a	26	Total O 26 26	0	0
4	b	14	Total O 14 14	0	0
4	c	9	Total O 9 9	0	0
4	d	23	Total O 23 23	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A:  89% 6% ..




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

Chain B:  89% 6% ..




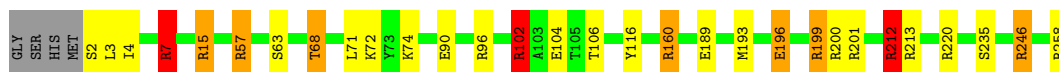
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain C:  89% 6% ..



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

Chain D:  87% 8% ..




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

Chain E:  90% 7% ..



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

Chain F:  89% 7% ..

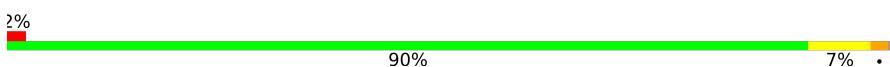


• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain G:  90% 7% ...




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

Chain H:  90% 7% ..




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

Chain I:  91% 6% ..

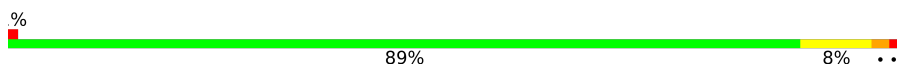


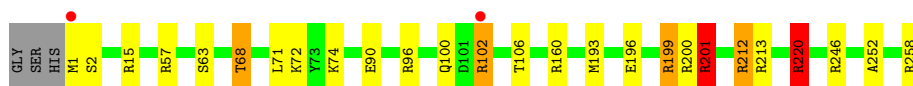
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J:  89% 6% ..




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

Chain K:  89% 8% ...




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

Chain L:  89% 7% ...




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

Chain M:  89% 7% ...




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

Chain N:  89% 8% ..




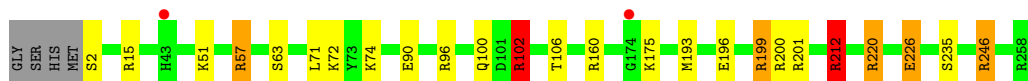
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain O:  91% 5% ..

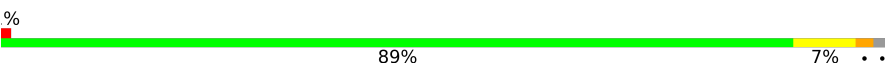


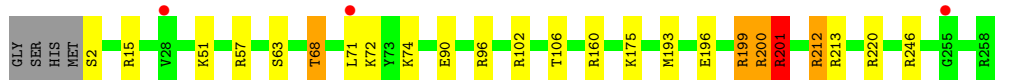
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain P:  89% 7% ...




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

Chain Q:  89% 7% ..




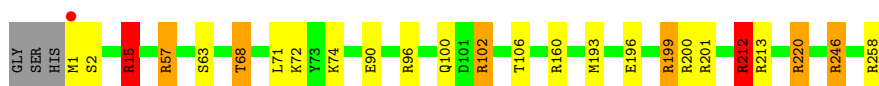
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain R:  90% 7% ...

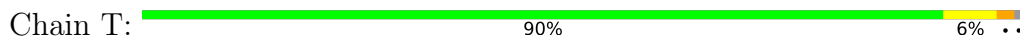


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

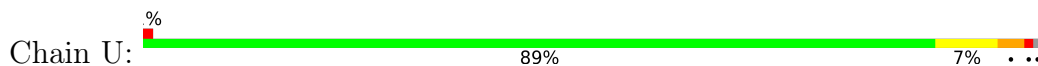
Chain S:  89% 7% ...



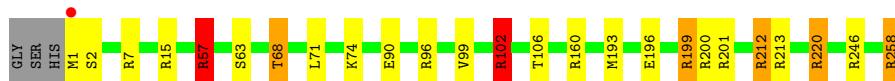
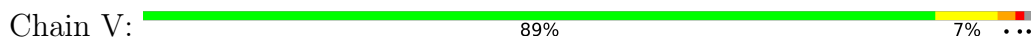
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



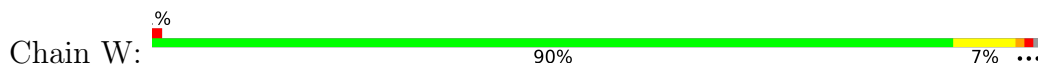
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



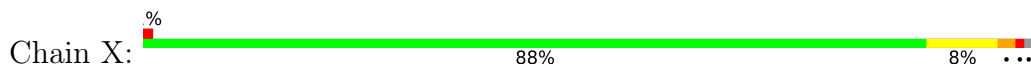
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



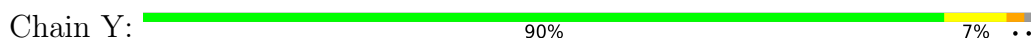
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase




- 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

Chain Z:  90% 6% .




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

Chain a:  88% 8% . .




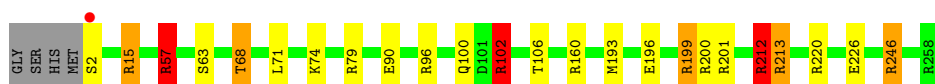
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain b:  89% 5% . . .




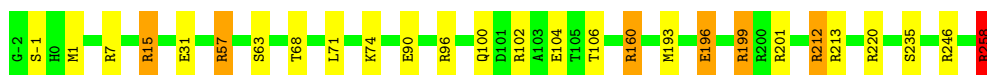
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain c:  89% 6% . . .



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

Chain d:  90% 8% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	245.63Å 367.55Å 370.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.72 – 2.84 105.72 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (105.72-2.84) 99.5 (105.72-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.203 , 0.216 0.206 , 0.219	Depositor DCC
$R_{free}$ test set	19383 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	60728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, VFE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.78	3/2027 (0.1%)	0.95	15/2748 (0.5%)
1	B	0.84	5/2027 (0.2%)	0.98	8/2748 (0.3%)
1	C	0.82	4/2019 (0.2%)	0.92	10/2738 (0.4%)
1	D	0.78	5/2019 (0.2%)	0.92	11/2738 (0.4%)
1	E	0.77	1/2027 (0.0%)	0.91	8/2748 (0.3%)
1	F	0.79	4/2019 (0.2%)	0.92	10/2738 (0.4%)
1	G	0.71	1/2027 (0.0%)	0.92	13/2748 (0.5%)
1	H	0.70	1/2027 (0.0%)	1.00	9/2748 (0.3%)
1	I	0.75	1/2027 (0.0%)	0.97	9/2748 (0.3%)
1	J	0.76	3/2019 (0.1%)	0.91	9/2738 (0.3%)
1	K	0.70	1/2027 (0.0%)	0.84	5/2748 (0.2%)
1	L	0.78	2/2027 (0.1%)	0.94	12/2748 (0.4%)
1	M	0.77	2/2019 (0.1%)	1.04	19/2738 (0.7%)
1	N	0.70	0/2019	0.86	5/2738 (0.2%)
1	O	0.70	1/2019 (0.0%)	0.88	6/2738 (0.2%)
1	P	0.73	1/2019 (0.0%)	0.92	8/2738 (0.3%)
1	Q	0.70	0/2019	0.97	10/2738 (0.4%)
1	R	0.72	1/2027 (0.0%)	0.91	7/2748 (0.3%)
1	S	0.73	0/2027	0.90	7/2748 (0.3%)
1	T	0.74	0/2027	0.90	6/2748 (0.2%)
1	U	0.90	8/2038 (0.4%)	1.05	18/2763 (0.7%)
1	V	0.74	0/2027	0.87	11/2748 (0.4%)
1	W	0.78	2/2027 (0.1%)	1.02	16/2748 (0.6%)
1	X	0.93	9/2049 (0.4%)	1.06	21/2777 (0.8%)
1	Y	0.76	2/2027 (0.1%)	0.98	14/2748 (0.5%)
1	Z	0.86	5/2048 (0.2%)	0.93	9/2776 (0.3%)
1	a	0.88	5/2019 (0.2%)	0.93	9/2738 (0.3%)
1	b	0.82	4/2019 (0.2%)	0.94	12/2738 (0.4%)
1	c	0.73	1/2019 (0.0%)	1.01	16/2738 (0.6%)
1	d	0.84	6/2048 (0.3%)	0.91	7/2776 (0.3%)
All	All	0.78	78/60789 (0.1%)	0.94	320/82420 (0.4%)

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	12
1	B	0	11
1	C	0	10
1	D	0	12
1	E	0	9
1	F	0	10
1	G	0	10
1	H	0	11
1	I	0	7
1	J	0	12
1	K	0	13
1	L	0	11
1	M	0	11
1	N	0	10
1	O	0	10
1	P	0	10
1	Q	0	10
1	R	0	9
1	S	0	12
1	T	0	10
1	U	0	11
1	V	0	10
1	W	0	10
1	X	0	9
1	Y	0	6
1	Z	0	11
1	a	0	12
1	b	0	11
1	c	0	10
1	d	0	10
All	All	0	310

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	33	GLU	CD-OE2	14.72	1.41	1.25
1	Z	206	GLU	CD-OE1	9.15	1.35	1.25
1	X	19	ASP	N-CA	9.11	1.64	1.46
1	L	33	GLU	CD-OE2	8.78	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CD-OE2	-7.86	1.17	1.25

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	CG-CD-NE	-17.93	74.15	111.80
1	H	199	ARG	CG-CD-NE	-17.18	75.72	111.80
1	W	199	ARG	NE-CZ-NH2	17.14	128.87	120.30
1	H	199	ARG	NE-CZ-NH1	-16.52	112.04	120.30
1	Q	201	ARG	NE-CZ-NH1	-15.91	112.34	120.30

There are no chirality outliers.

5 of 310 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	15	ARG	Sidechain
1	A	57[A]	ARG	Sidechain
1	A	57[B]	ARG	Sidechain
1	A	96	ARG	Sidechain

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	257/261 (98%)	246 (96%)	11 (4%)	0	100 100
1	B	257/261 (98%)	247 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	D	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	E	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	F	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	G	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	H	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	I	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
1	J	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	K	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	L	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	M	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	N	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	O	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	P	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	Q	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	R	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	S	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	T	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	U	258/261 (99%)	245 (95%)	13 (5%)	0	100	100
1	V	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
1	W	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	X	259/261 (99%)	246 (95%)	13 (5%)	0	100	100
1	Y	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	Z	260/261 (100%)	251 (96%)	9 (4%)	0	100	100
1	a	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	b	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
1	c	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	d	260/261 (100%)	249 (96%)	11 (4%)	0	100	100
All	All	7707/7830 (98%)	7387 (96%)	320 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	207/208 (100%)	191 (92%)	16 (8%)	13	27
1	B	207/208 (100%)	190 (92%)	17 (8%)	11	24
1	C	206/208 (99%)	189 (92%)	17 (8%)	11	24
1	D	206/208 (99%)	186 (90%)	20 (10%)	8	16
1	E	207/208 (100%)	193 (93%)	14 (7%)	16	31
1	F	206/208 (99%)	191 (93%)	15 (7%)	14	29
1	G	207/208 (100%)	188 (91%)	19 (9%)	9	18
1	H	207/208 (100%)	192 (93%)	15 (7%)	14	29
1	I	207/208 (100%)	194 (94%)	13 (6%)	18	34
1	J	206/208 (99%)	188 (91%)	18 (9%)	10	21
1	K	207/208 (100%)	189 (91%)	18 (9%)	10	21
1	L	207/208 (100%)	187 (90%)	20 (10%)	8	16
1	M	206/208 (99%)	188 (91%)	18 (9%)	10	21
1	N	206/208 (99%)	188 (91%)	18 (9%)	10	21
1	O	206/208 (99%)	194 (94%)	12 (6%)	20	38
1	P	206/208 (99%)	187 (91%)	19 (9%)	9	18
1	Q	206/208 (99%)	190 (92%)	16 (8%)	12	26
1	R	207/208 (100%)	187 (90%)	20 (10%)	8	16
1	S	207/208 (100%)	189 (91%)	18 (9%)	10	21
1	T	207/208 (100%)	188 (91%)	19 (9%)	9	18
1	U	208/208 (100%)	196 (94%)	12 (6%)	20	38
1	V	207/208 (100%)	189 (91%)	18 (9%)	10	21
1	W	207/208 (100%)	192 (93%)	15 (7%)	14	29
1	X	209/208 (100%)	191 (91%)	18 (9%)	10	22
1	Y	207/208 (100%)	189 (91%)	18 (9%)	10	21
1	Z	209/208 (100%)	192 (92%)	17 (8%)	11	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	206/208 (99%)	191 (93%)	15 (7%)	14	29
1	b	206/208 (99%)	187 (91%)	19 (9%)	9	18
1	c	206/208 (99%)	189 (92%)	17 (8%)	11	24
1	d	209/208 (100%)	192 (92%)	17 (8%)	11	24
All	All	6205/6240 (99%)	5697 (92%)	508 (8%)	12	24

5 of 508 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	106	THR
1	a	57[B]	ARG
1	R	15	ARG
1	Z	246	ARG
1	b	246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	43	HIS
1	d	100	GLN
1	R	100	GLN
1	c	100	GLN
1	Y	164	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	VFE	S	1001	-	28,31,31	1.30	4 (14%)	35,41,41	1.74	10 (28%)
2	VFE	X	1001	-	28,31,31	1.81	5 (17%)	35,41,41	1.89	9 (25%)
2	VFE	V	1001	-	28,31,31	1.45	3 (10%)	35,41,41	1.89	8 (22%)
2	VFE	I	1001	-	28,31,31	1.50	6 (21%)	35,41,41	2.31	12 (34%)
2	VFE	E	1001	-	28,31,31	1.63	4 (14%)	35,41,41	2.69	16 (45%)
2	VFE	R	1001	-	28,31,31	1.35	3 (10%)	35,41,41	2.30	15 (42%)
2	VFE	D	1001	-	28,31,31	1.90	4 (14%)	35,41,41	2.33	13 (37%)
2	VFE	L	1001	-	28,31,31	1.48	4 (14%)	35,41,41	2.45	17 (48%)
2	VFE	U	1001	-	28,31,31	1.91	6 (21%)	35,41,41	2.14	11 (31%)
2	VFE	W	1001	-	28,31,31	1.30	5 (17%)	35,41,41	2.04	10 (28%)
2	VFE	J	1001	-	28,31,31	1.33	2 (7%)	35,41,41	1.94	11 (31%)
2	VFE	A	1001	-	28,31,31	1.70	4 (14%)	35,41,41	2.36	14 (40%)
2	VFE	B	1001	-	28,31,31	1.18	3 (10%)	35,41,41	1.41	6 (17%)
2	VFE	H	1001	-	28,31,31	1.06	2 (7%)	35,41,41	2.03	9 (25%)
2	VFE	O	1001	-	28,31,31	1.47	4 (14%)	35,41,41	1.63	6 (17%)
2	VFE	Q	1001	-	28,31,31	1.13	3 (10%)	35,41,41	2.14	11 (31%)
2	VFE	Y	1001	-	28,31,31	1.34	3 (10%)	35,41,41	1.64	9 (25%)
2	VFE	Z	1001	-	28,31,31	1.67	4 (14%)	35,41,41	2.36	13 (37%)
2	VFE	F	1001	-	28,31,31	1.20	2 (7%)	35,41,41	1.67	8 (22%)
2	VFE	T	1001	-	28,31,31	1.49	5 (17%)	35,41,41	2.35	14 (40%)
2	VFE	G	1001	-	28,31,31	1.20	2 (7%)	35,41,41	1.86	9 (25%)
2	VFE	K	1001	-	28,31,31	1.53	4 (14%)	35,41,41	1.88	10 (28%)
2	VFE	N	1001	-	28,31,31	1.24	1 (3%)	35,41,41	1.64	7 (20%)
2	VFE	a	1001	-	28,31,31	1.38	5 (17%)	35,41,41	2.17	15 (42%)
2	VFE	b	1001	-	28,31,31	1.22	3 (10%)	35,41,41	1.43	7 (20%)
2	VFE	C	1001	-	28,31,31	1.64	4 (14%)	35,41,41	2.42	13 (37%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	VFE	d	1001	-	28,31,31	1.31	3 (10%)	35,41,41	2.23	15 (42%)
2	VFE	P	1001	-	28,31,31	1.47	4 (14%)	35,41,41	1.42	6 (17%)
2	VFE	c	1001	-	28,31,31	1.05	2 (7%)	35,41,41	1.86	10 (28%)
2	VFE	M	1001	-	28,31,31	1.74	5 (17%)	35,41,41	2.74	13 (37%)

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	VFE	S	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	X	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	V	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	I	1001	-	-	5/23/23/23	0/3/3/3
2	VFE	E	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	R	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	D	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	L	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	U	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	W	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	J	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	A	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	B	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	H	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	O	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	Q	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	Y	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	Z	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	F	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	T	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	G	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	K	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	N	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	a	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	b	1001	-	-	4/23/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFE	C	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	d	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	P	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	c	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	M	1001	-	-	2/23/23/23	0/3/3/3

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	VFE	C23-S22	6.11	1.86	1.77
2	K	1001	VFE	C23-S22	5.90	1.86	1.77
2	E	1001	VFE	C23-S22	5.87	1.86	1.77
2	D	1001	VFE	C27-C28	5.57	1.50	1.38
2	M	1001	VFE	C23-S22	5.57	1.85	1.77

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1001	VFE	C21-S22-C23	9.06	116.51	102.61
2	Z	1001	VFE	C3-C5-N6	-7.46	95.77	113.60
2	E	1001	VFE	C21-S22-C23	6.78	113.02	102.61
2	Q	1001	VFE	C21-S22-C23	6.13	112.02	102.61
2	D	1001	VFE	C24-C23-C28	-6.09	109.43	117.52

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

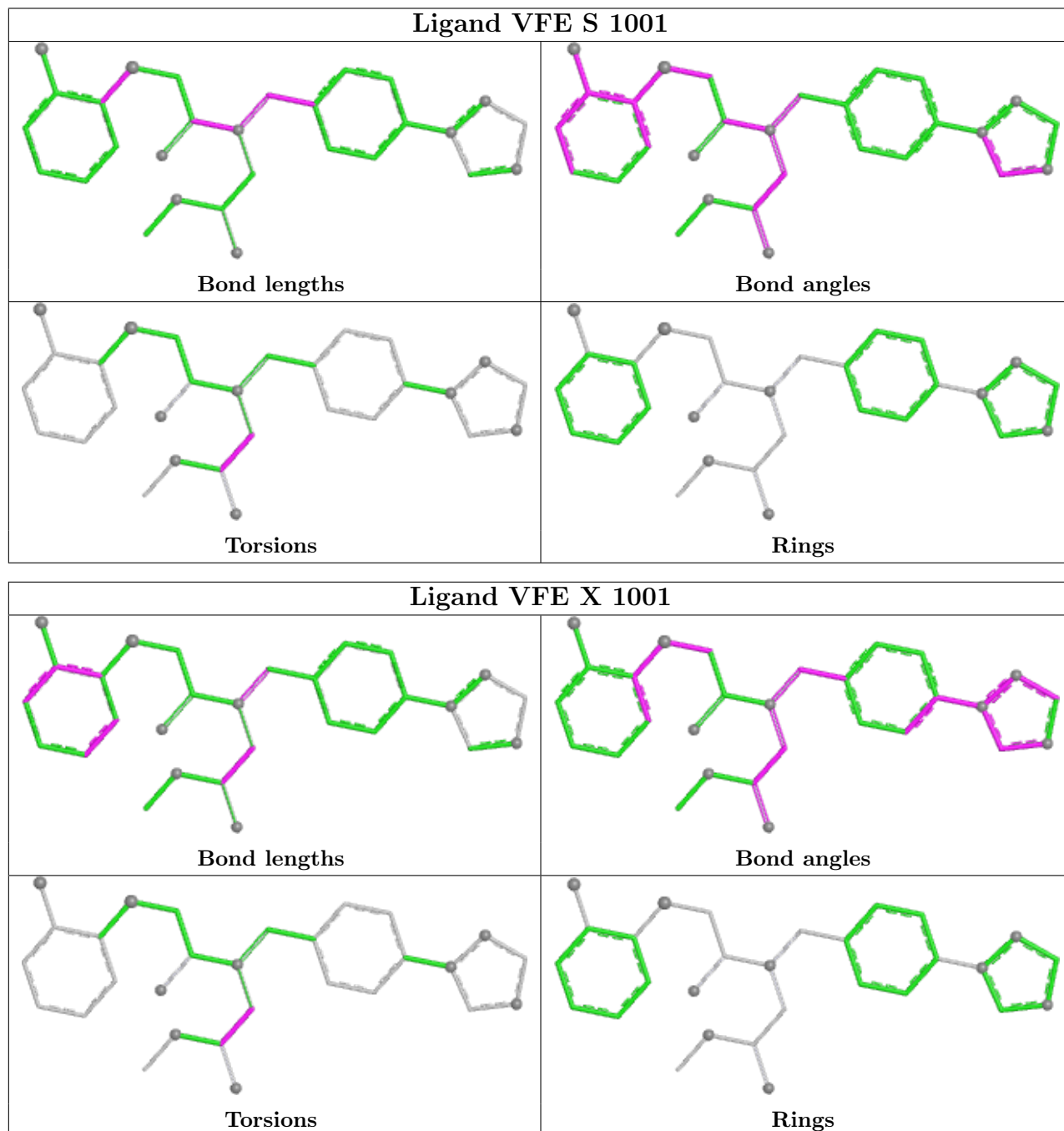
Mol	Chain	Res	Type	Atoms
2	I	1001	VFE	C5-C3-N2-C1
2	I	1001	VFE	C3-C5-N6-C19
2	K	1001	VFE	C5-C3-N2-C1
2	L	1001	VFE	C5-C3-N2-C1
2	O	1001	VFE	C5-C3-N2-C1

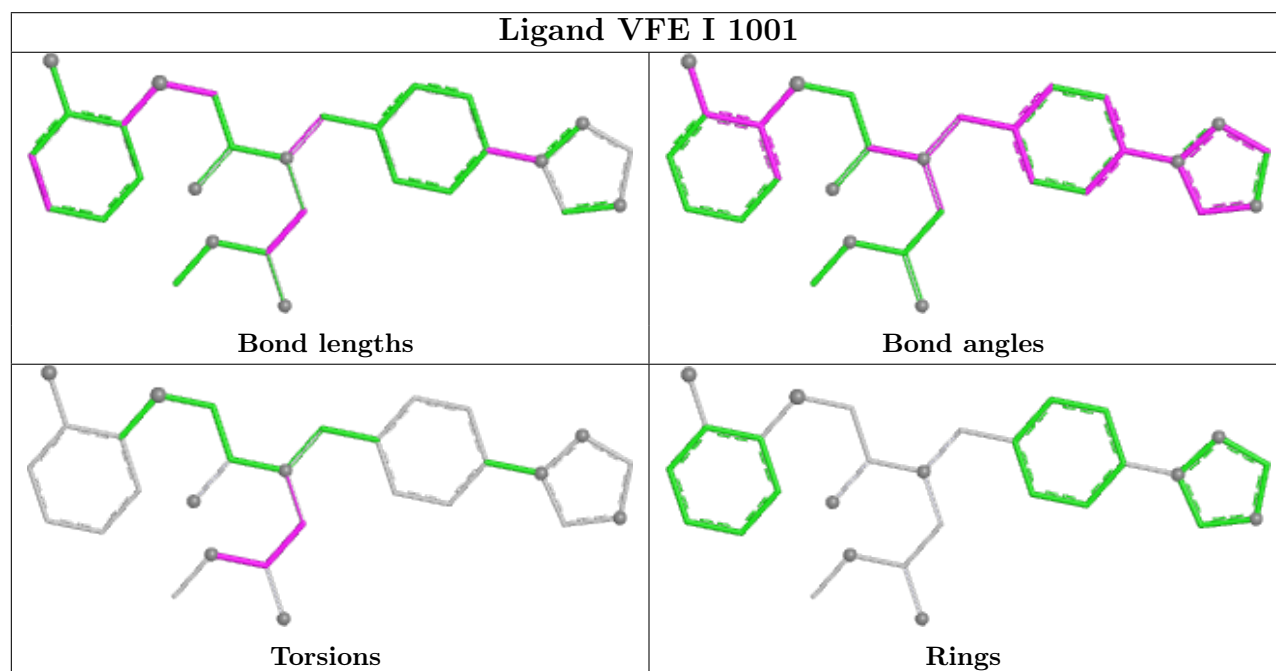
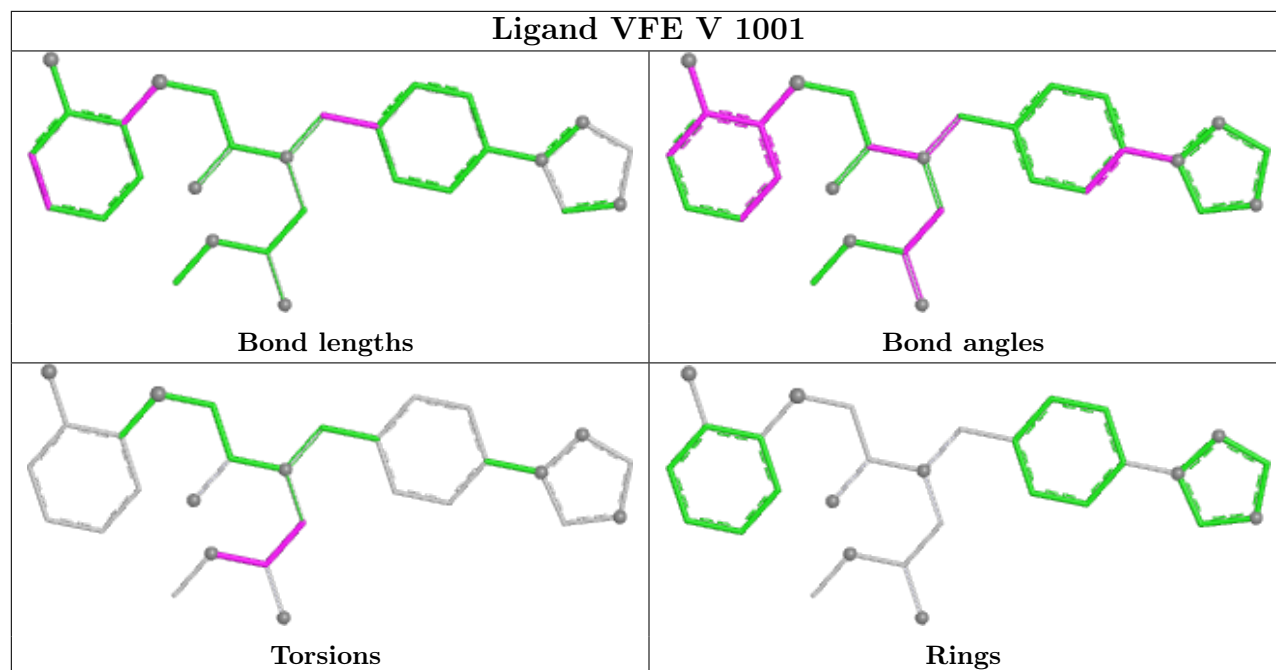
There are no ring outliers.

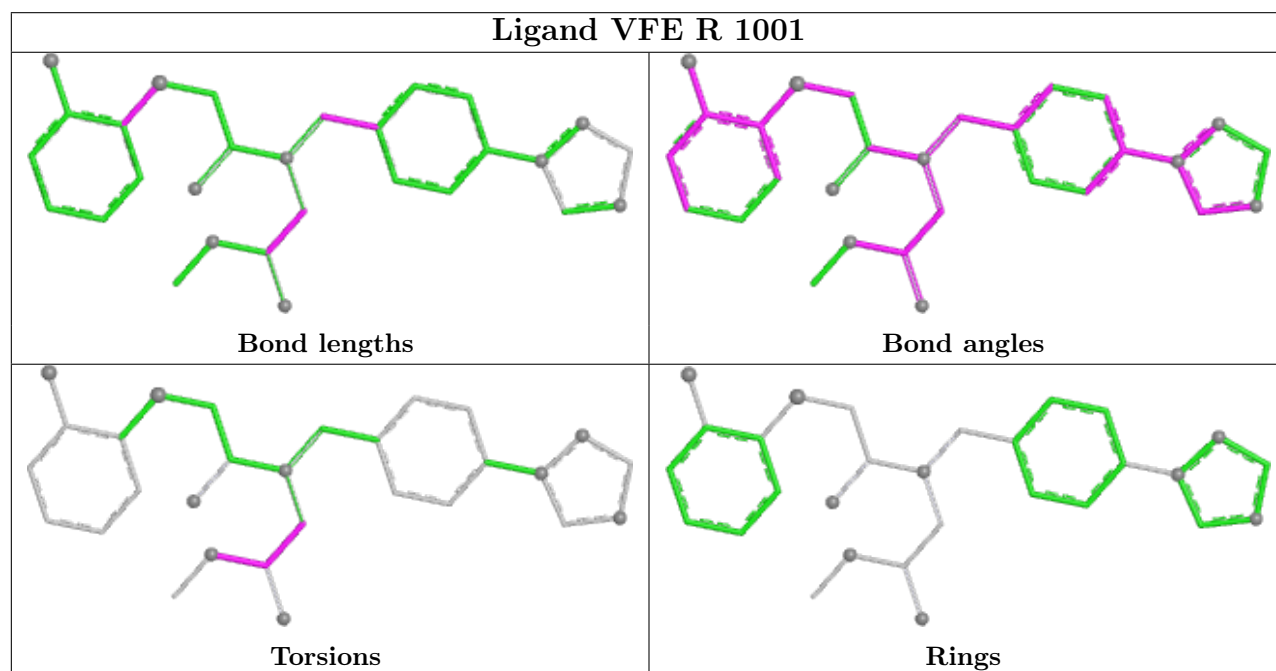
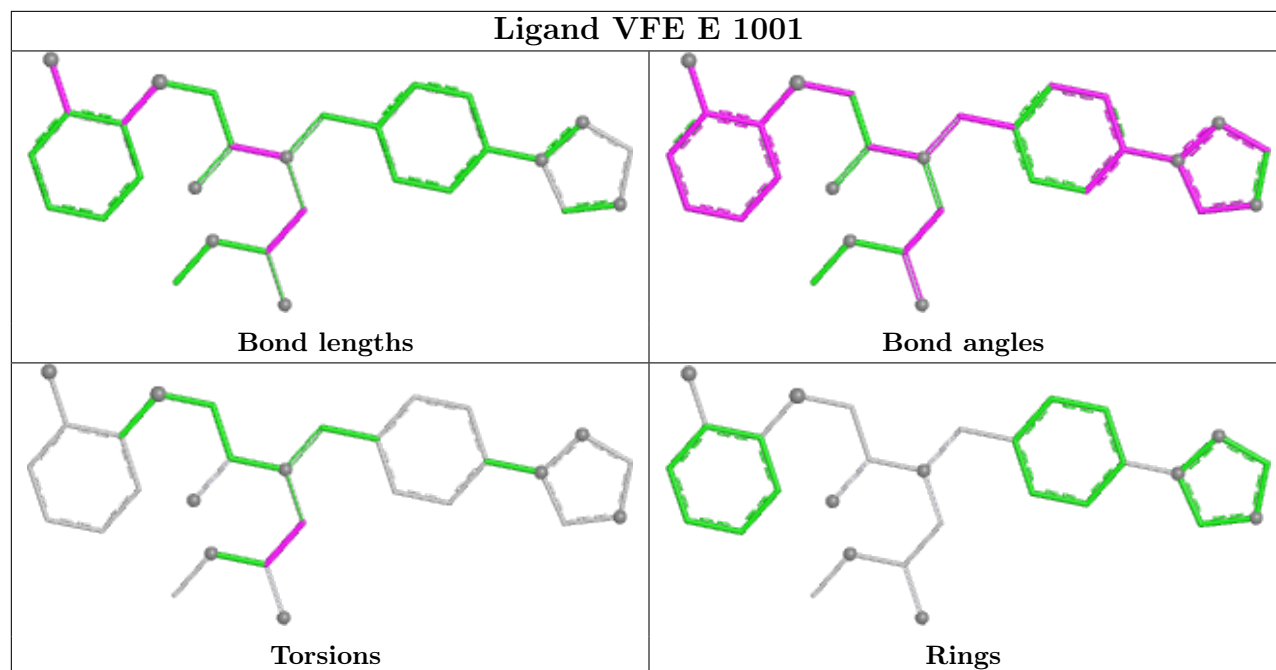
No monomer is involved in short contacts.

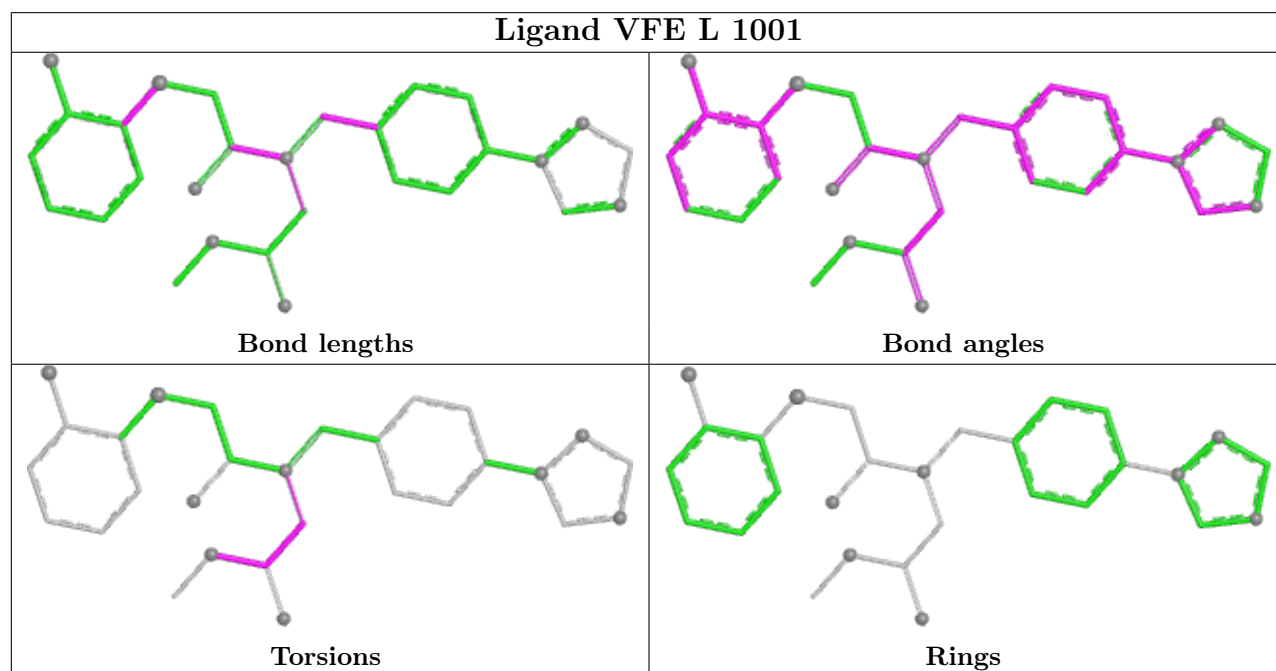
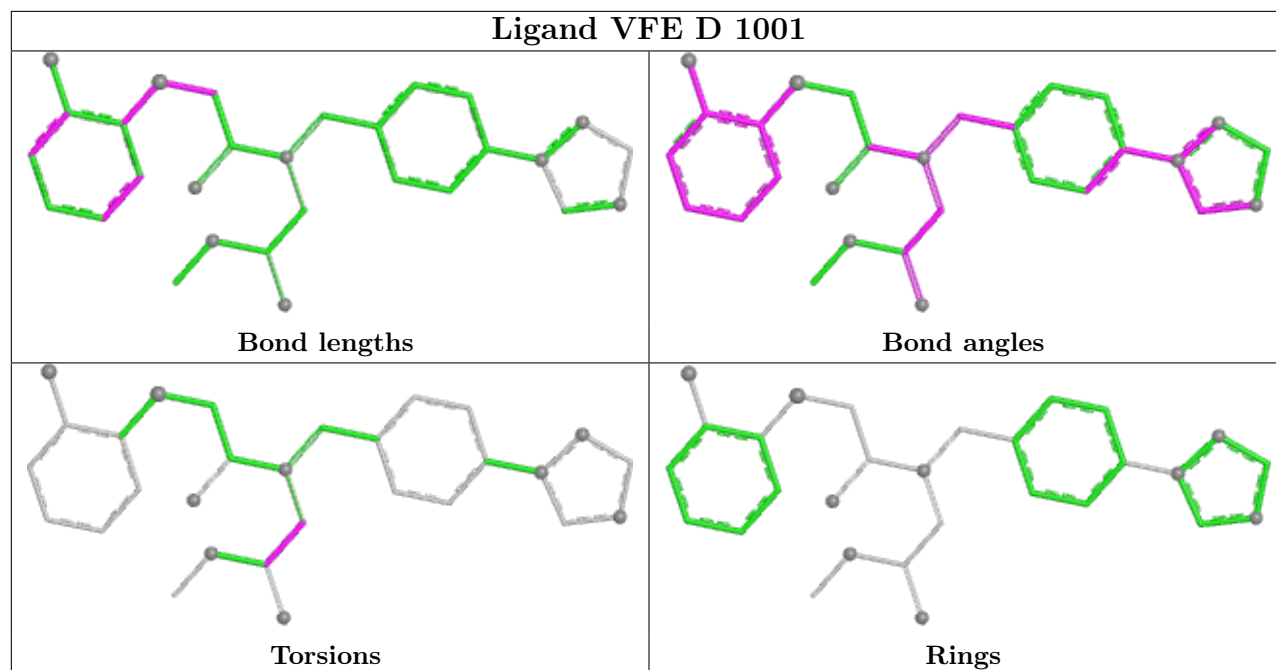
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

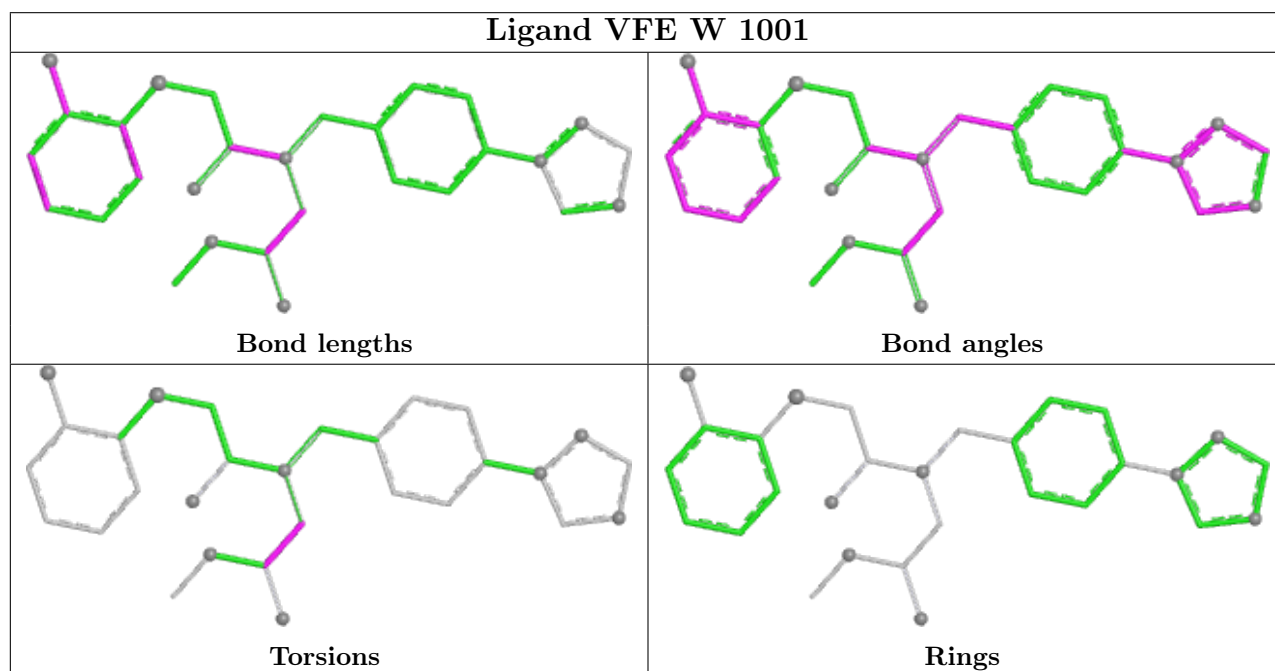
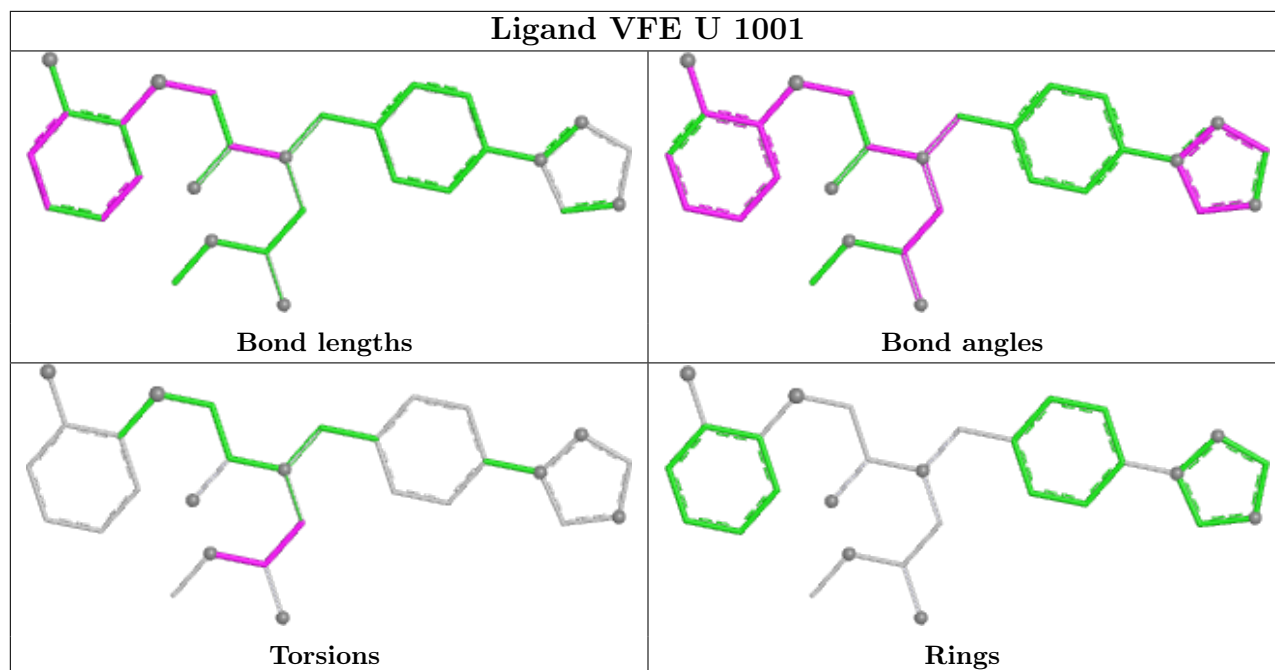
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

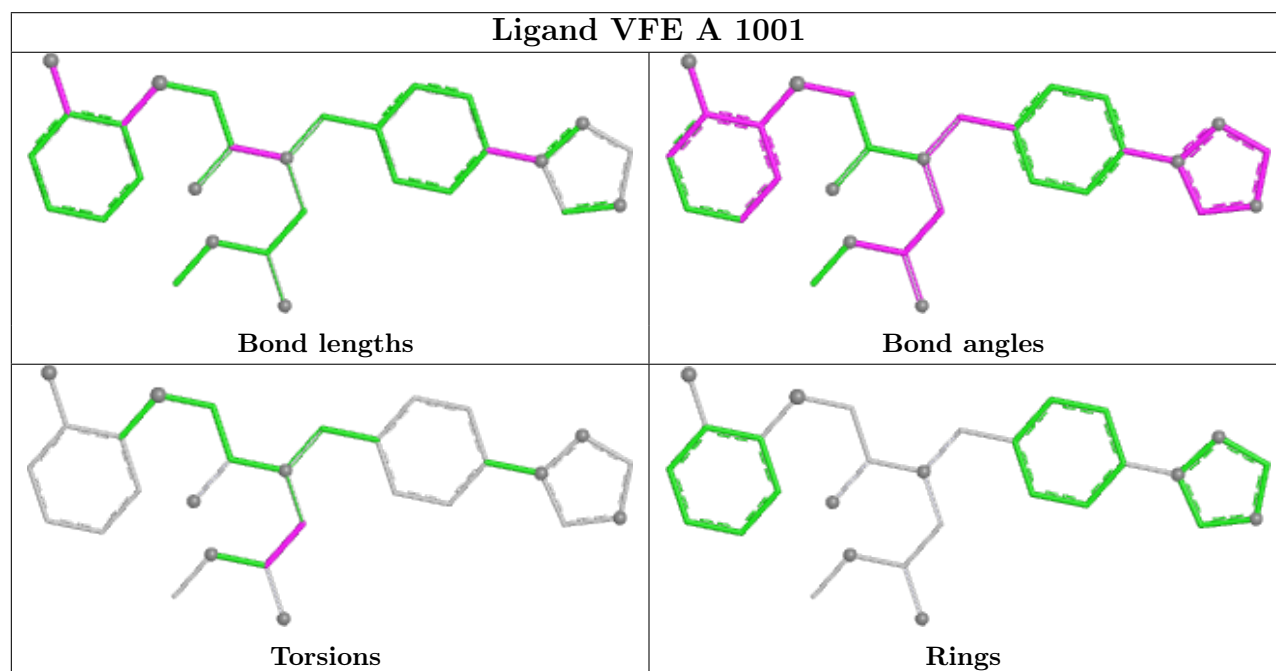
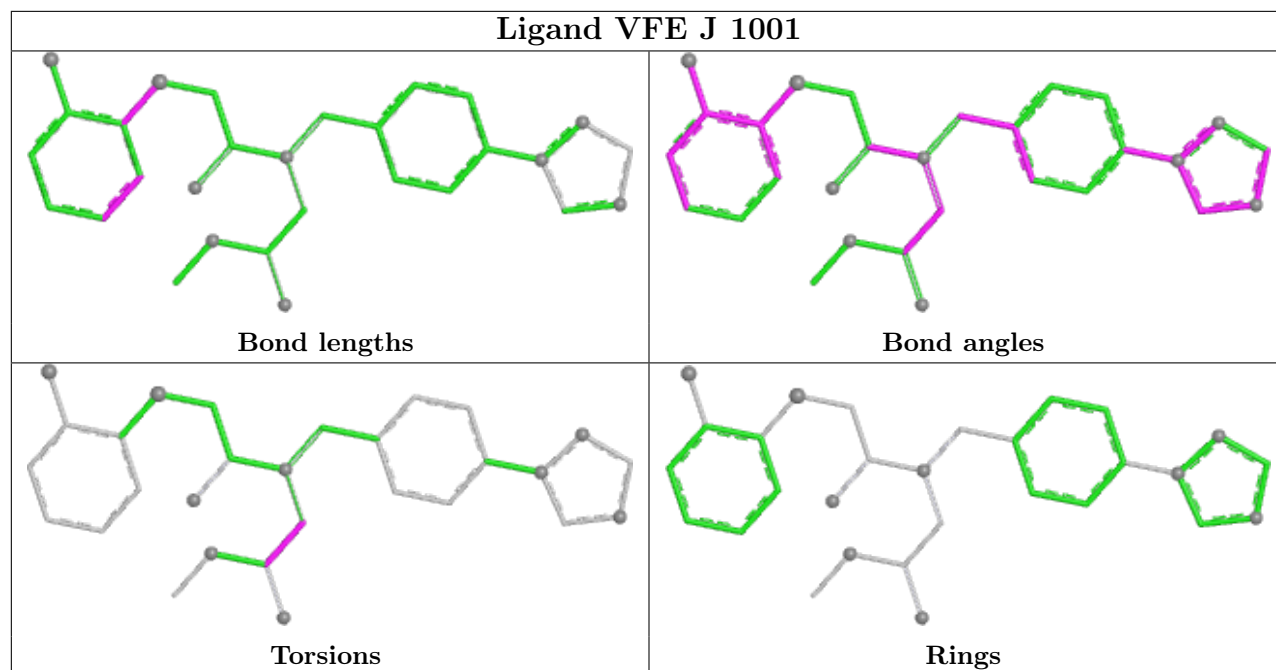




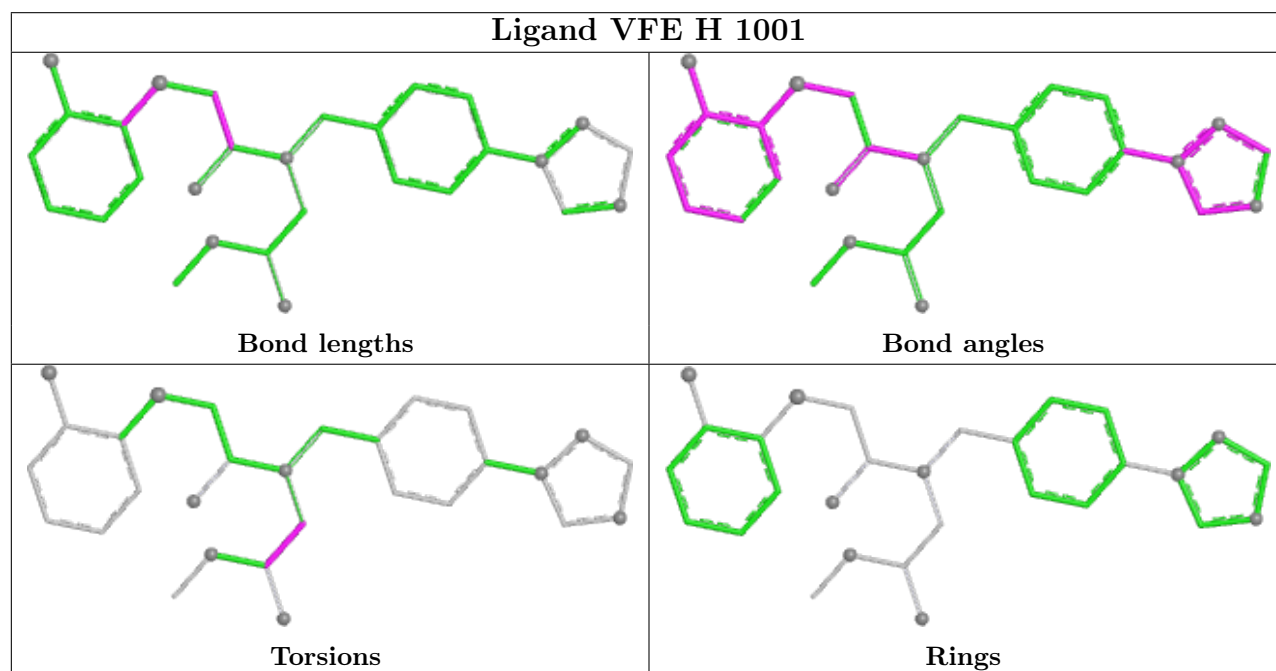
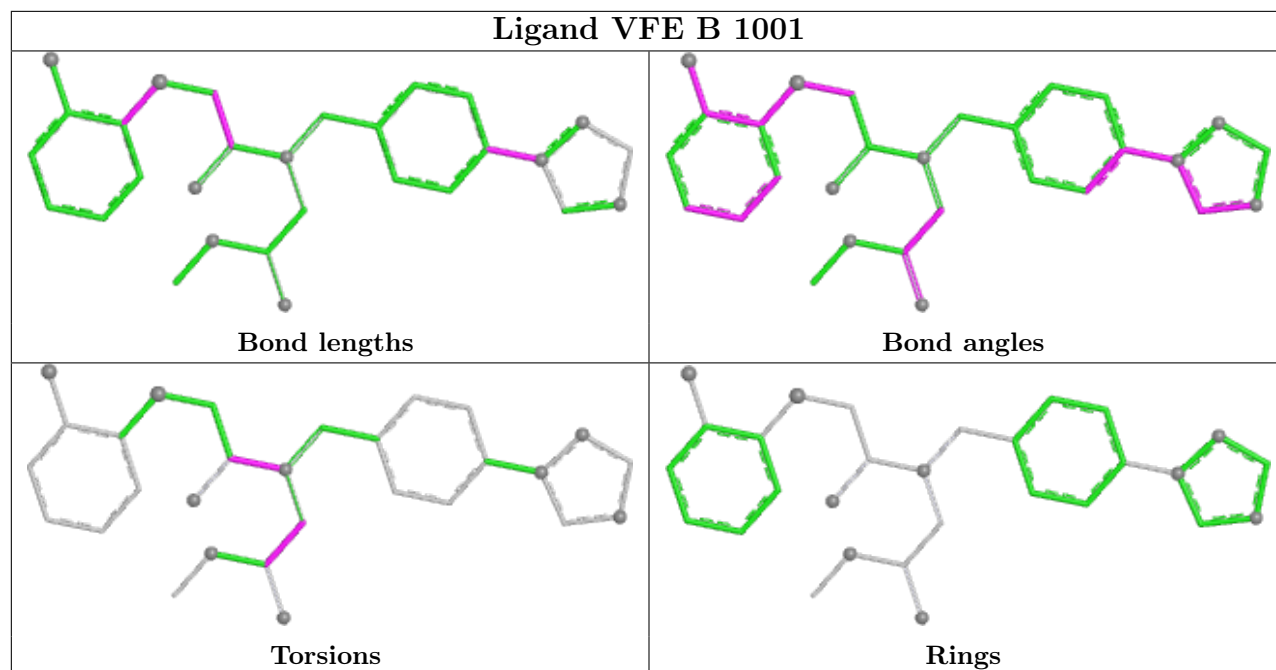


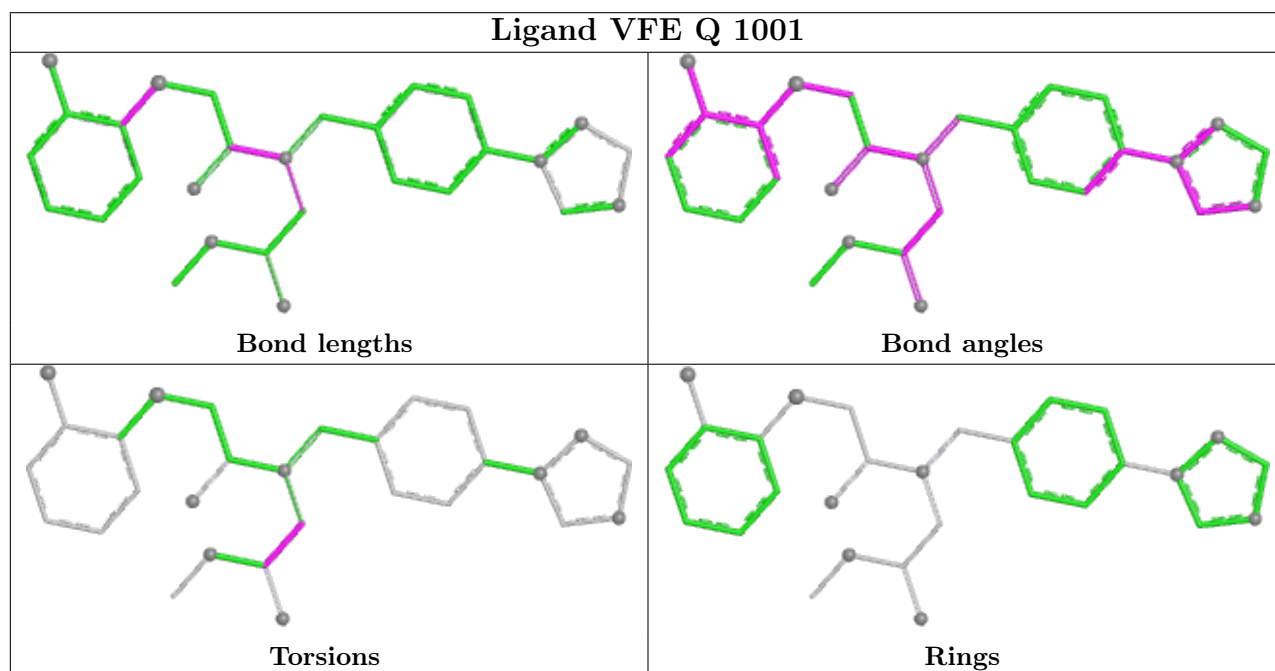
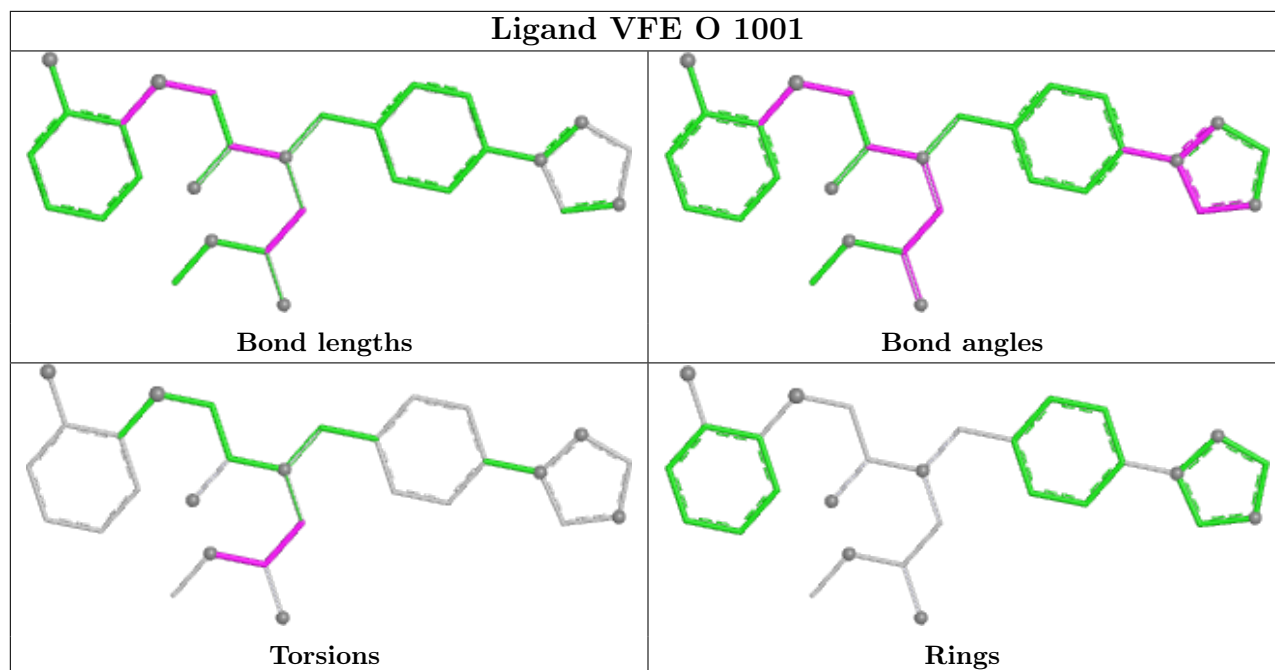


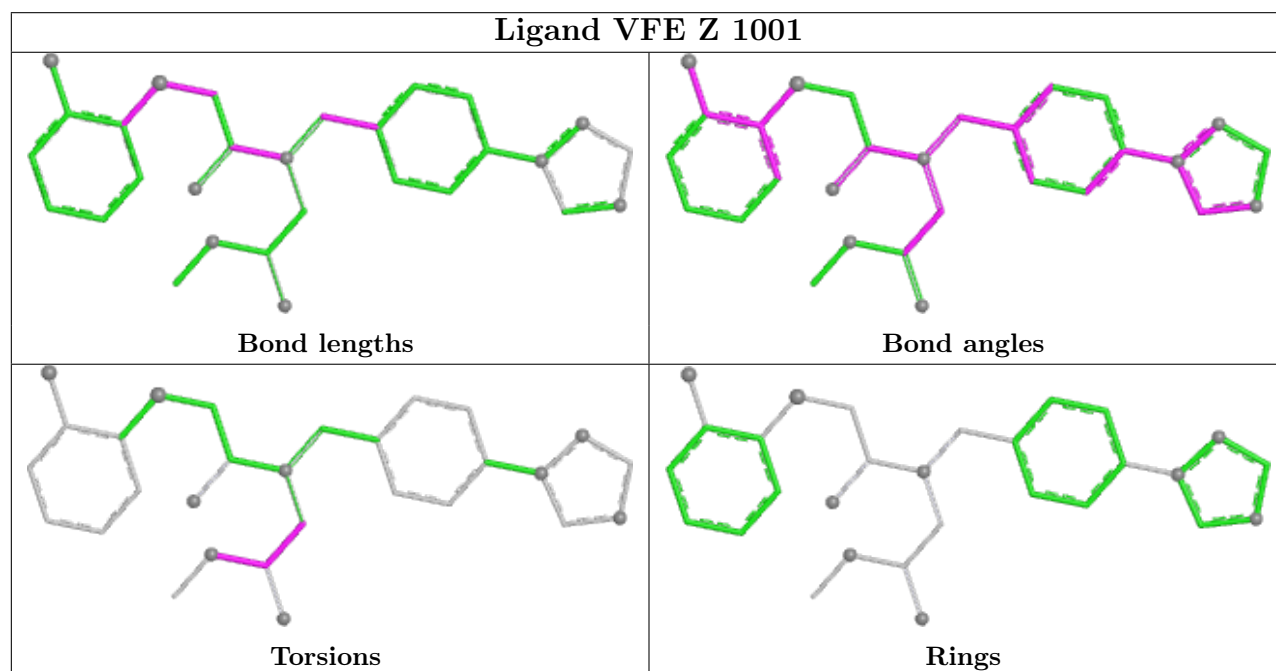
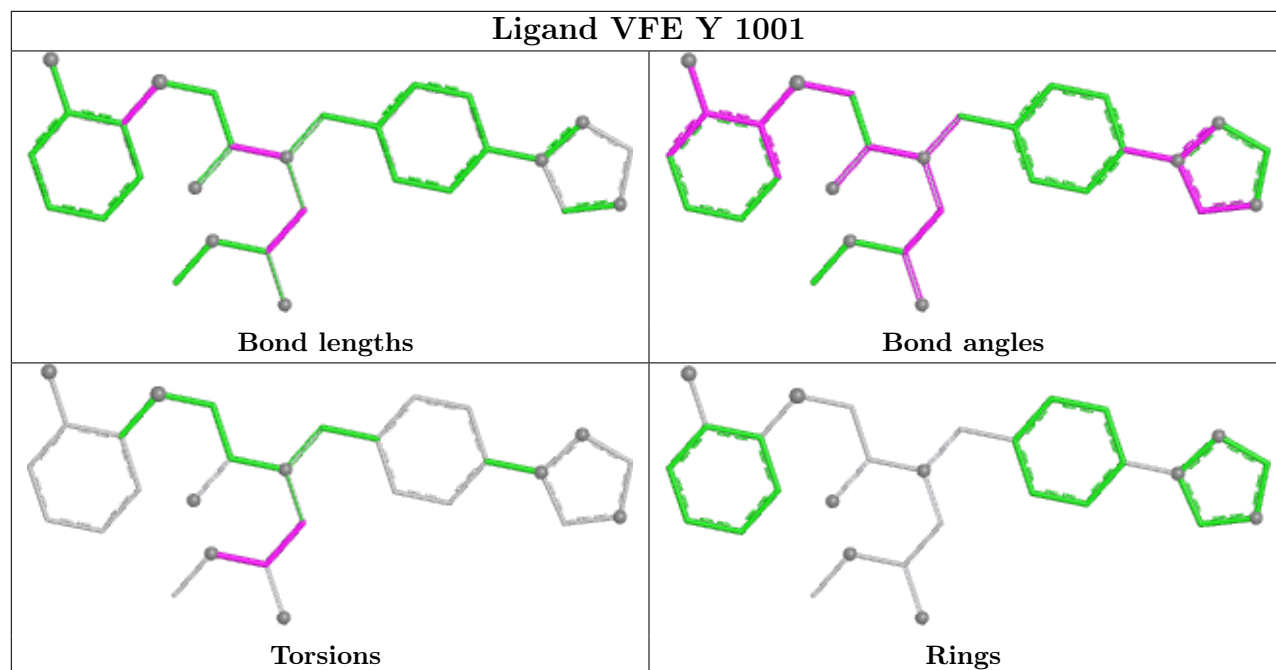


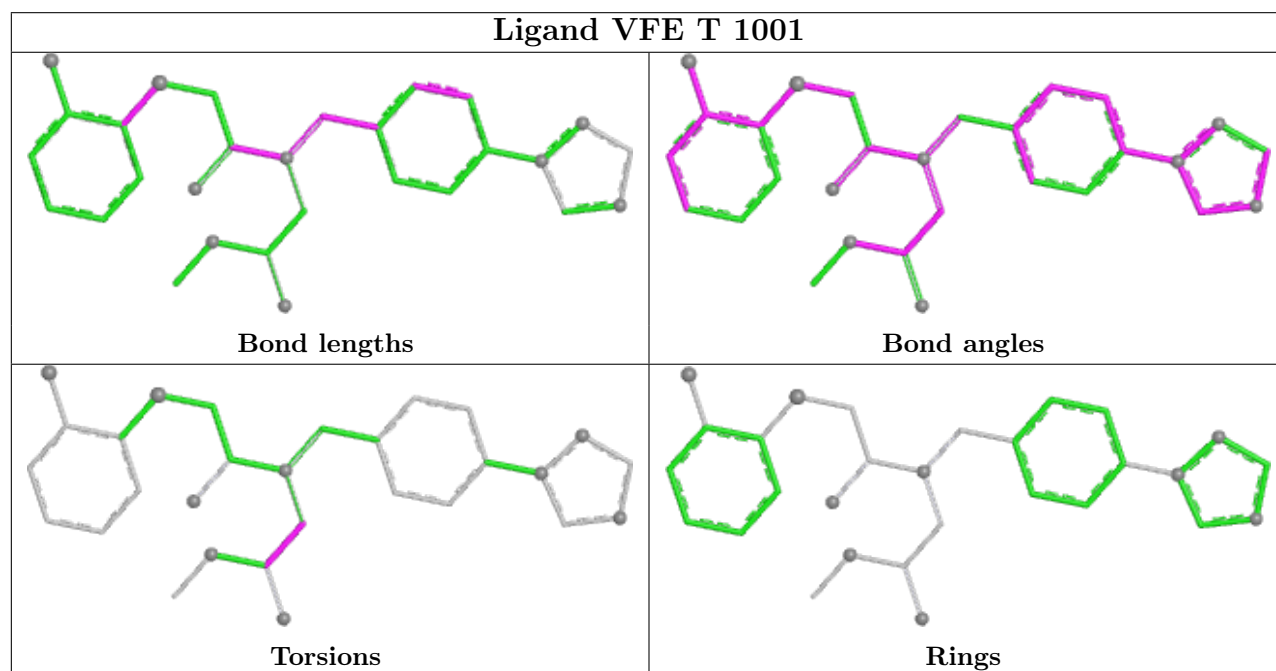
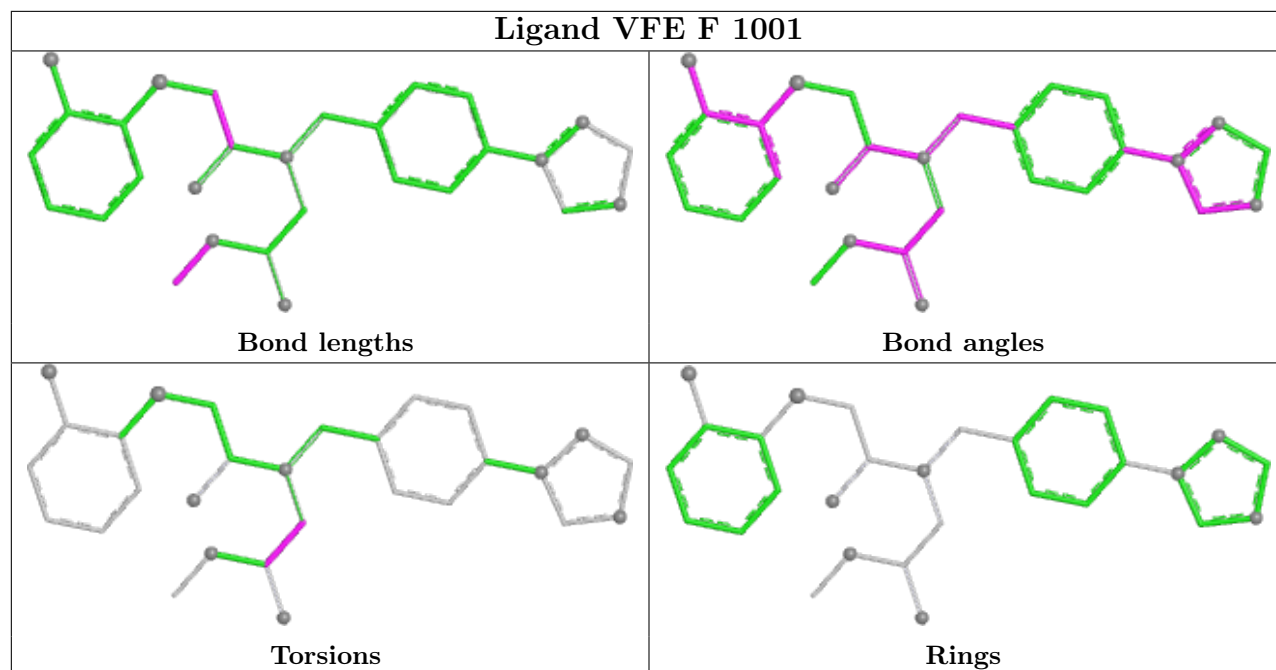


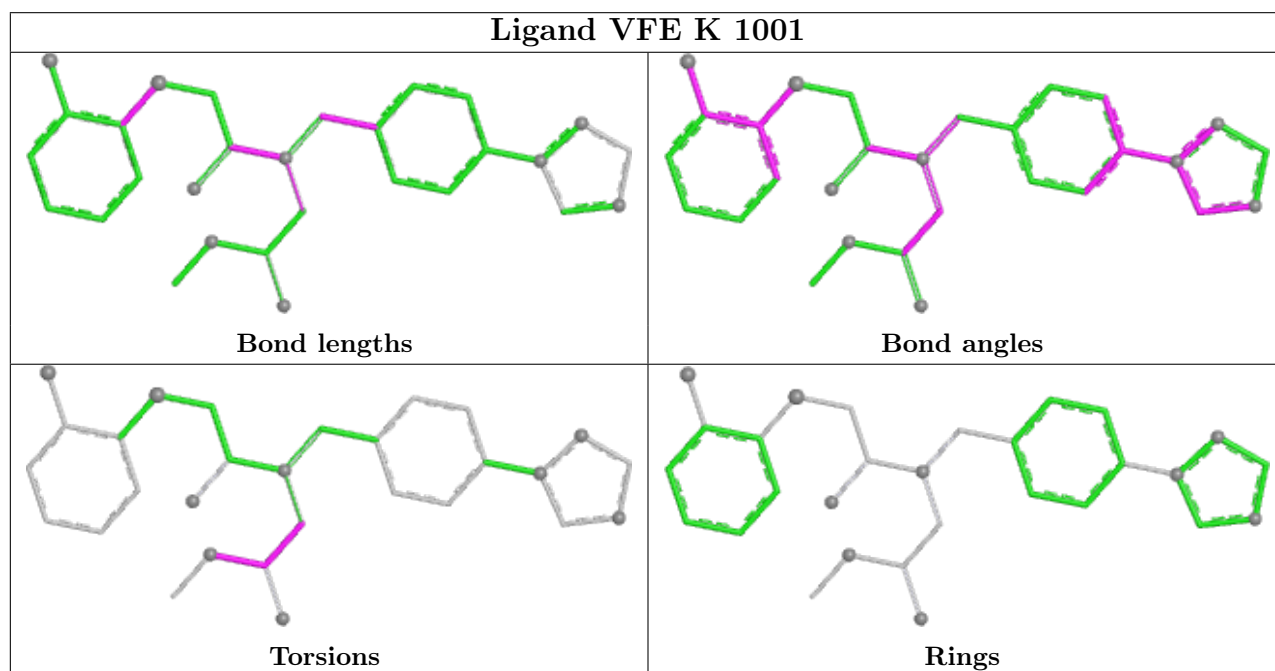
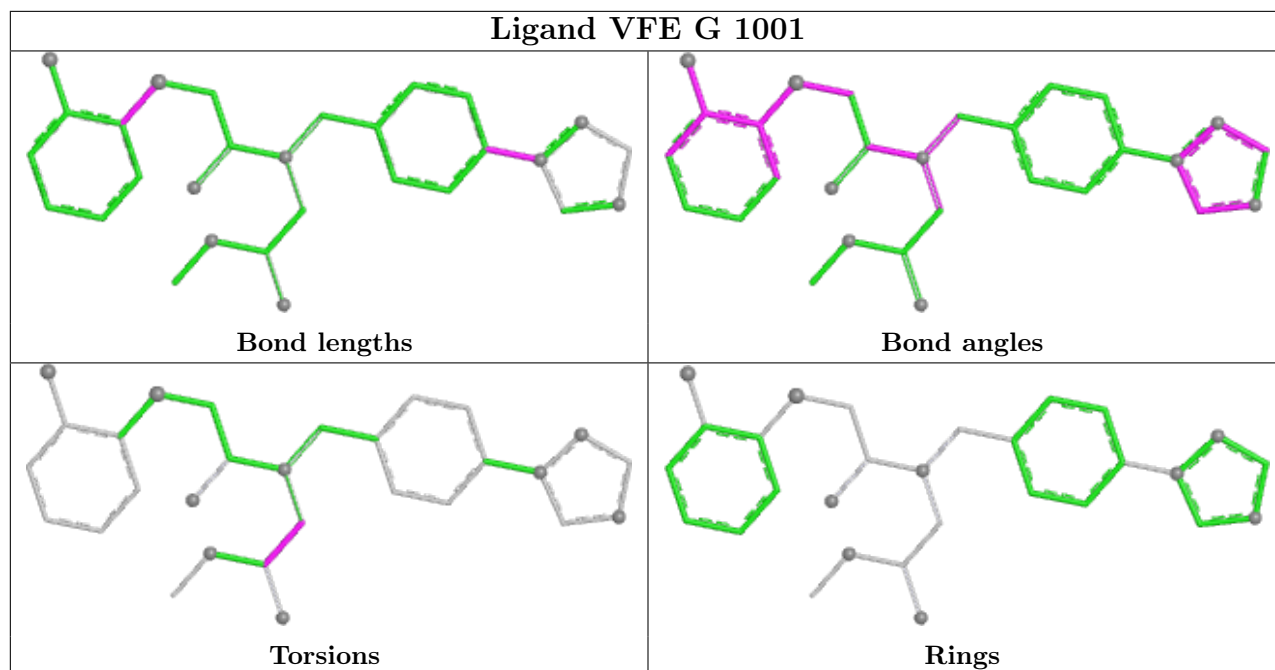


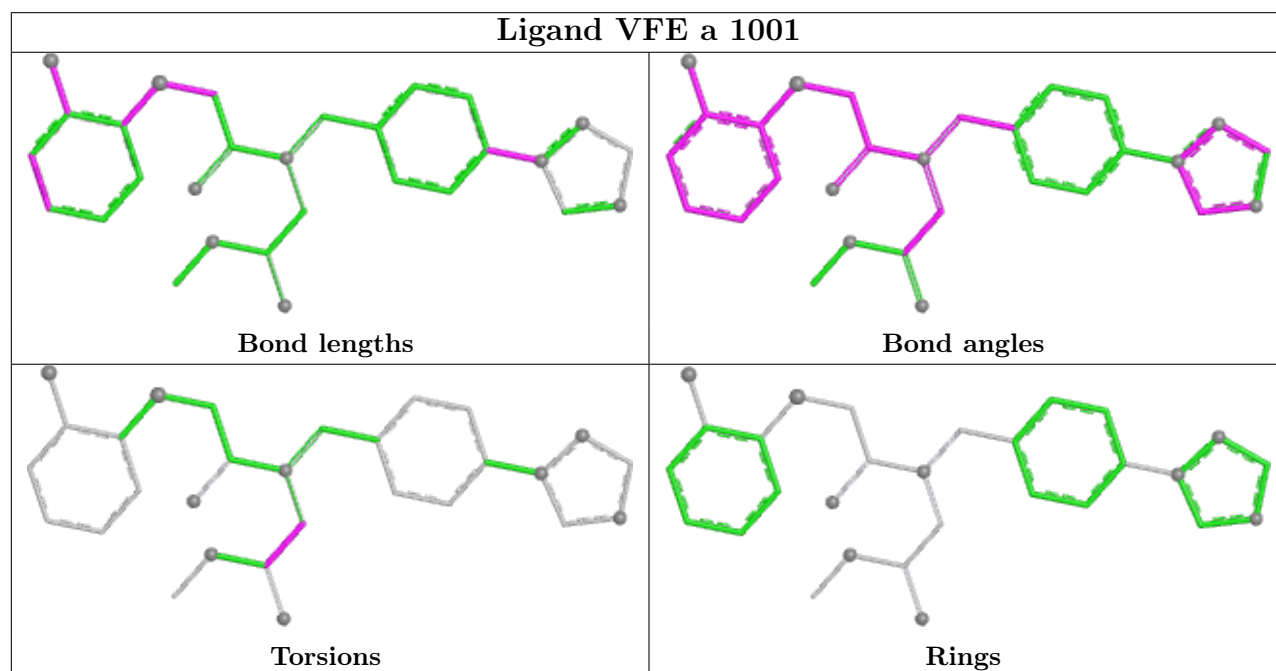
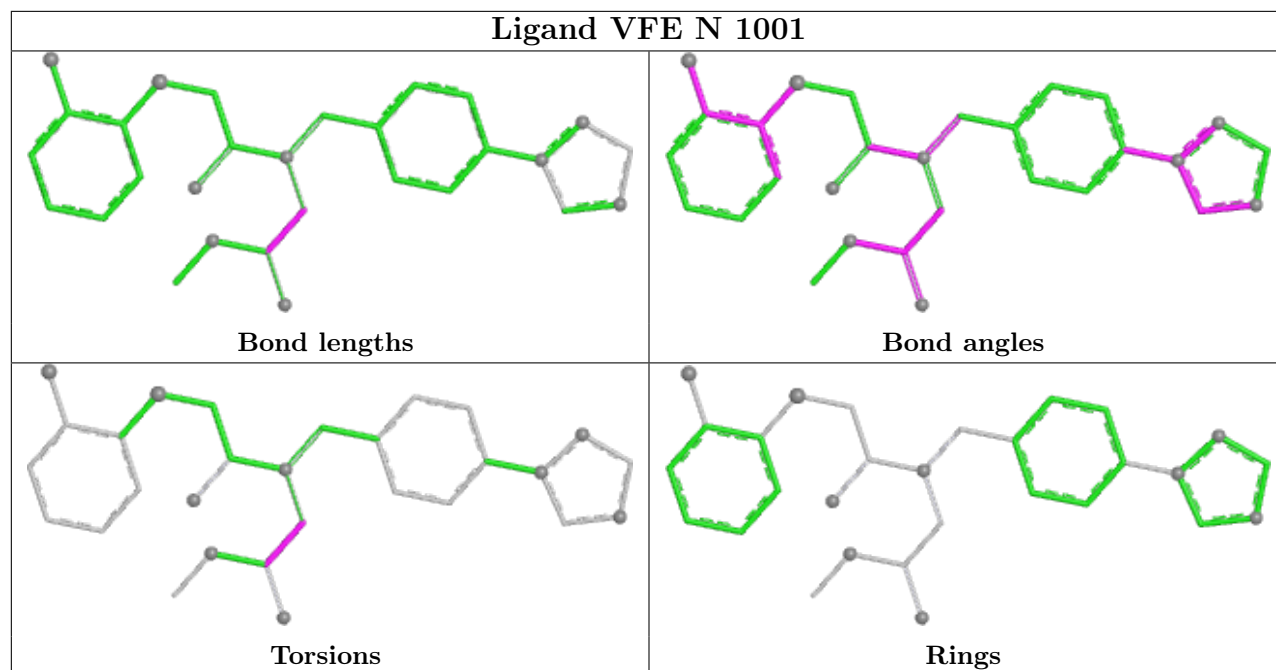


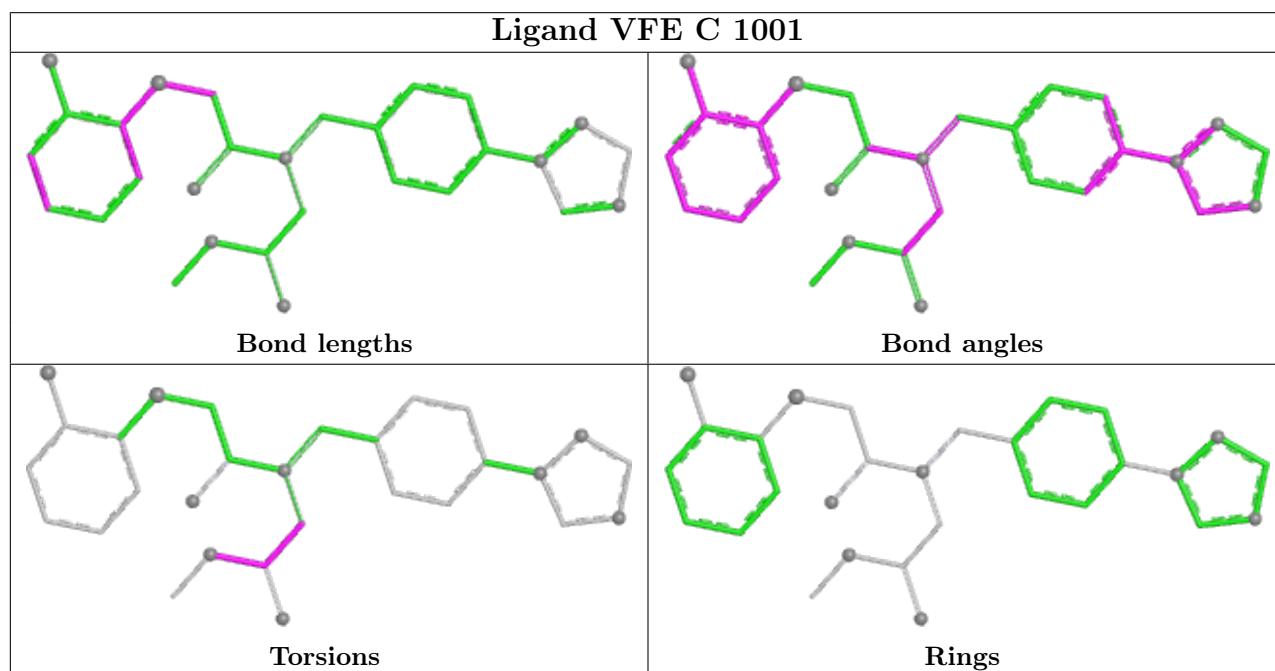
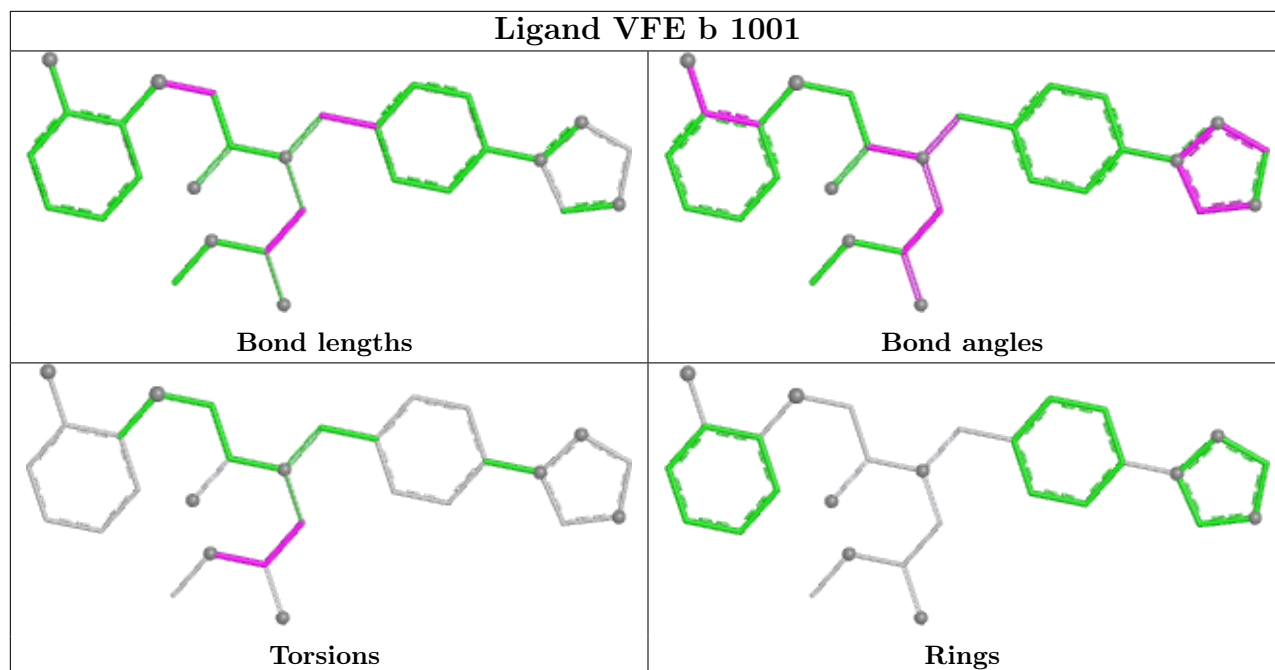


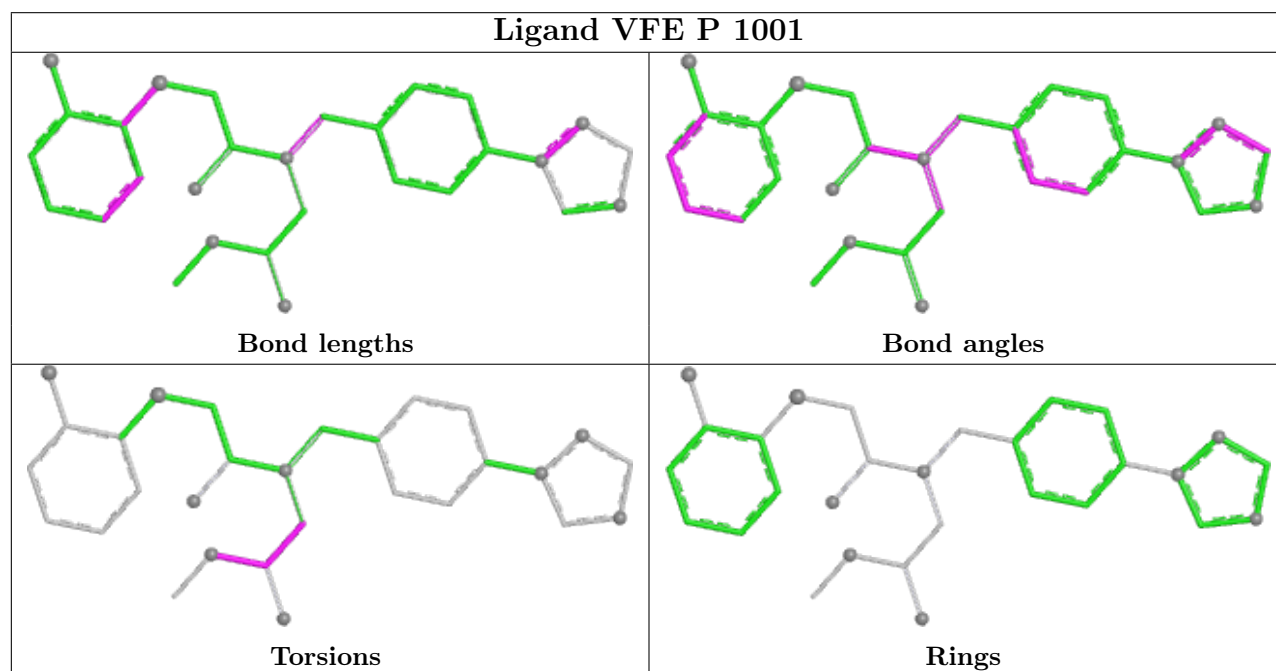
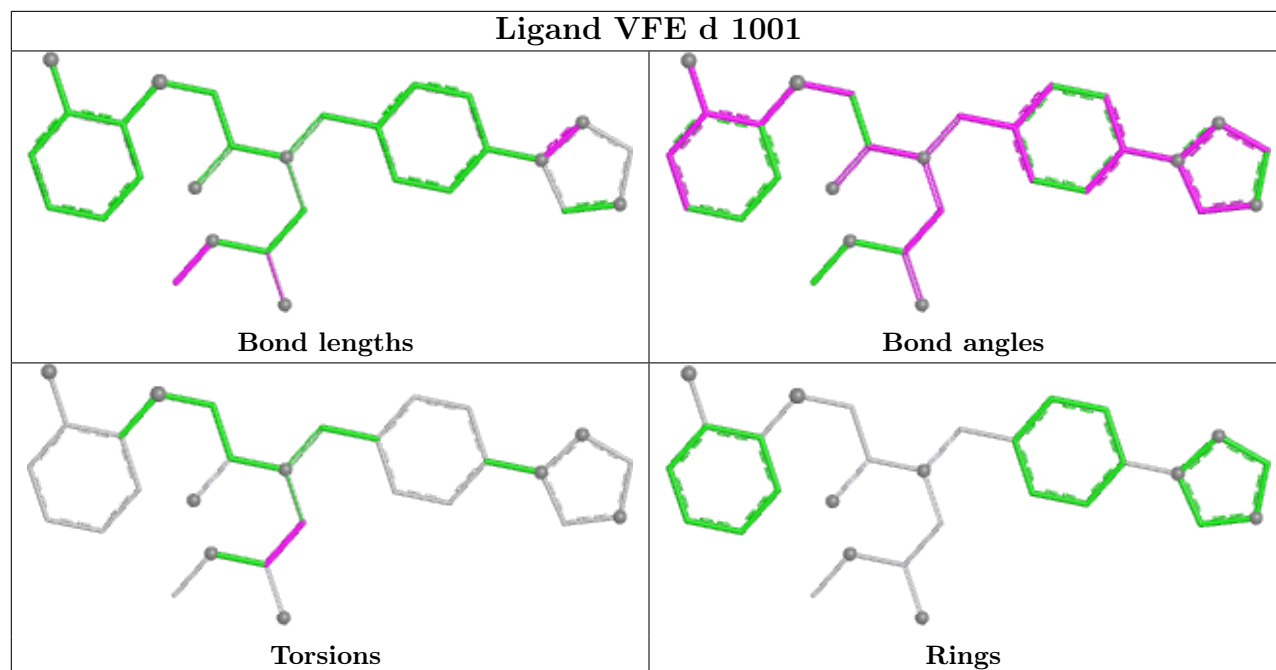




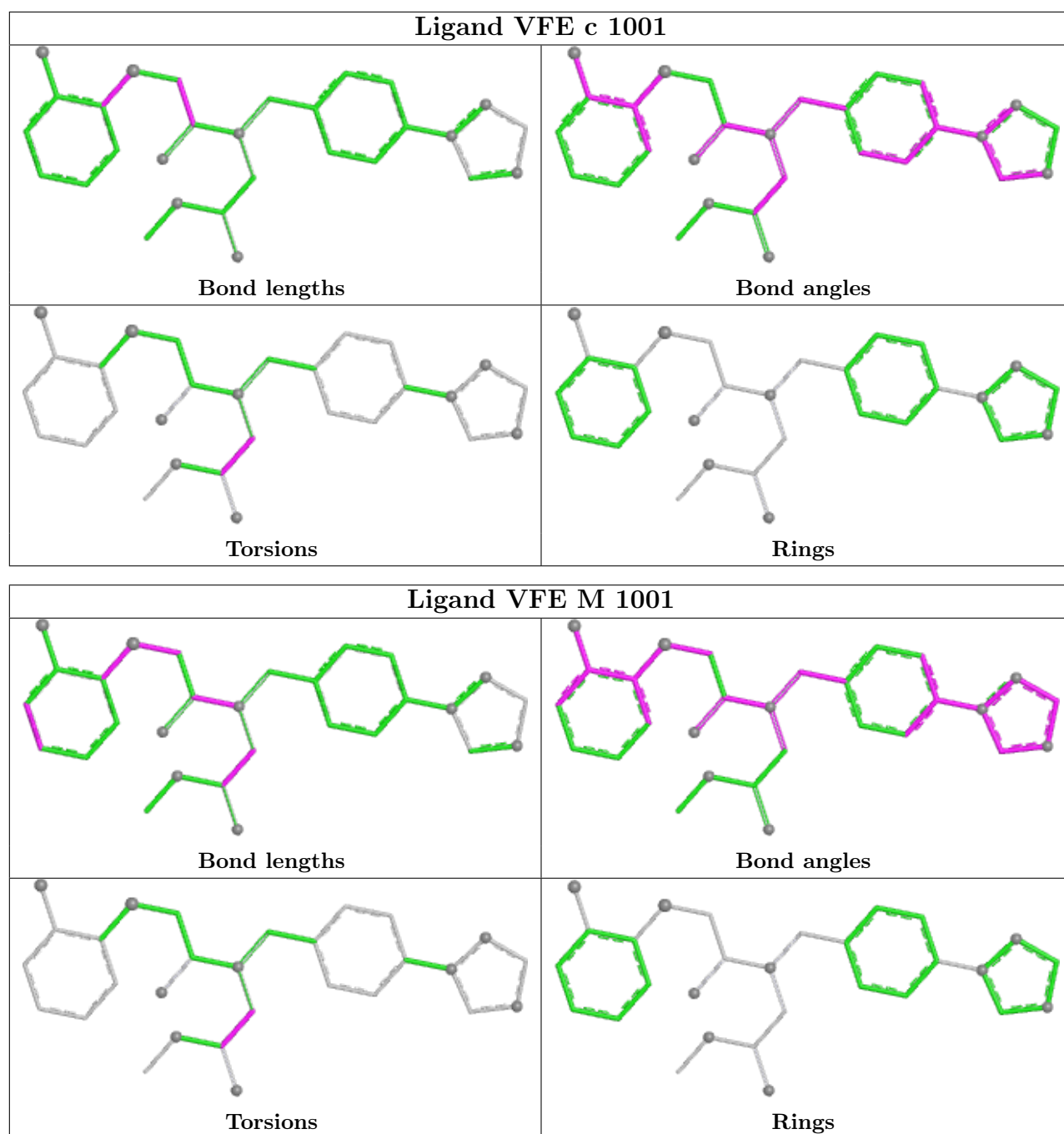












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/261 (98%)	0.28	1 (0%) 92 91	33, 44, 73, 124	0
1	B	258/261 (98%)	0.32	1 (0%) 92 91	32, 43, 71, 105	0
1	C	257/261 (98%)	0.27	0 100 100	31, 42, 69, 84	0
1	D	257/261 (98%)	0.28	0 100 100	30, 42, 69, 84	0
1	E	258/261 (98%)	0.27	2 (0%) 86 85	30, 42, 69, 125	0
1	F	257/261 (98%)	0.30	0 100 100	32, 43, 70, 89	0
1	G	258/261 (98%)	0.43	3 (1%) 79 76	37, 56, 93, 136	0
1	H	258/261 (98%)	0.49	5 (1%) 66 62	39, 55, 93, 127	0
1	I	258/261 (98%)	0.51	5 (1%) 66 62	37, 54, 89, 117	0
1	J	257/261 (98%)	0.36	1 (0%) 92 91	34, 54, 87, 96	0
1	K	258/261 (98%)	0.31	2 (0%) 86 85	35, 54, 88, 140	0
1	L	258/261 (98%)	0.45	5 (1%) 66 62	37, 55, 90, 134	0
1	M	257/261 (98%)	0.30	1 (0%) 92 91	36, 51, 82, 103	0
1	N	257/261 (98%)	0.48	1 (0%) 92 91	36, 54, 88, 103	0
1	O	257/261 (98%)	0.37	1 (0%) 92 91	32, 52, 86, 98	0
1	P	257/261 (98%)	0.55	2 (0%) 86 85	38, 55, 91, 104	0
1	Q	257/261 (98%)	0.53	3 (1%) 79 76	37, 55, 91, 102	0
1	R	258/261 (98%)	0.45	4 (1%) 72 68	33, 52, 90, 122	0
1	S	258/261 (98%)	0.30	1 (0%) 92 91	32, 45, 70, 123	0
1	T	258/261 (98%)	0.43	0 100 100	34, 46, 74, 110	0
1	U	259/261 (99%)	0.29	2 (0%) 86 85	32, 43, 73, 117	0
1	V	258/261 (98%)	0.21	1 (0%) 92 91	33, 46, 73, 121	0
1	W	258/261 (98%)	0.30	2 (0%) 86 85	33, 45, 72, 107	0
1	X	259/261 (99%)	0.31	2 (0%) 86 85	32, 43, 69, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	258/261 (98%)	0.39	1 (0%) 92 91	31, 44, 76, 124	0
1	Z	261/261 (100%)	0.31	0 100 100	30, 42, 69, 81	0
1	a	257/261 (98%)	0.27	0 100 100	33, 44, 71, 91	0
1	b	257/261 (98%)	0.30	1 (0%) 92 91	31, 42, 69, 94	0
1	c	257/261 (98%)	0.35	1 (0%) 92 91	30, 43, 70, 87	0
1	d	261/261 (100%)	0.35	0 100 100	28, 40, 67, 81	0
All	All	7736/7830 (98%)	0.36	48 (0%) 89 88	28, 47, 81, 140	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.9
1	H	1	MET	4.8
1	I	1	MET	4.6
1	L	1	MET	4.3
1	W	1	MET	4.3

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	VFE	I	1001	29/29	0.91	0.29	58,63,70,80	0
2	VFE	U	1001	29/29	0.92	0.29	53,58,66,71	0
2	VFE	d	1001	29/29	0.92	0.26	44,57,66,70	0
2	VFE	M	1001	29/29	0.93	0.30	53,62,70,82	0

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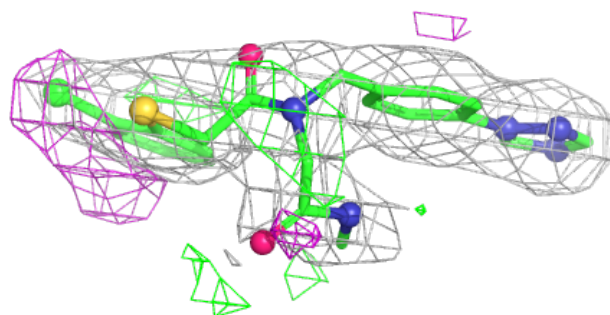
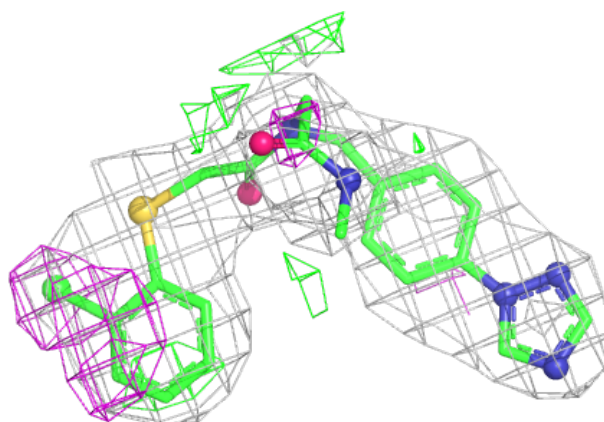
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	VFE	R	1001	29/29	0.93	0.32	52,58,80,80	0
2	VFE	J	1001	29/29	0.93	0.26	55,59,69,71	0
2	VFE	X	1001	29/29	0.93	0.26	51,57,67,72	0
2	VFE	K	1001	29/29	0.93	0.29	61,67,77,82	0
2	VFE	L	1001	29/29	0.94	0.31	59,63,73,81	0
2	VFE	G	1001	29/29	0.94	0.29	56,65,69,74	0
2	VFE	P	1001	29/29	0.94	0.34	56,60,66,77	0
2	VFE	H	1001	29/29	0.94	0.36	61,69,73,82	0
2	VFE	T	1001	29/29	0.94	0.27	47,57,69,72	0
2	VFE	A	1001	29/29	0.94	0.29	46,53,62,69	0
2	VFE	C	1001	29/29	0.94	0.29	49,56,62,81	0
2	VFE	c	1001	29/29	0.94	0.29	47,54,65,78	0
2	VFE	D	1001	29/29	0.94	0.26	47,52,65,68	0
2	VFE	B	1001	29/29	0.95	0.28	46,50,61,63	0
2	VFE	O	1001	29/29	0.95	0.29	56,63,76,78	0
2	VFE	E	1001	29/29	0.95	0.27	49,55,64,72	0
2	VFE	Y	1001	29/29	0.95	0.30	50,58,71,73	0
2	VFE	Z	1001	29/29	0.95	0.28	51,58,72,76	0
2	VFE	a	1001	29/29	0.95	0.28	51,56,67,73	0
2	VFE	b	1001	29/29	0.95	0.30	54,59,73,82	0
2	VFE	Q	1001	29/29	0.95	0.35	57,65,72,78	0
2	VFE	F	1001	29/29	0.95	0.31	46,52,65,76	0
2	VFE	W	1001	29/29	0.96	0.31	52,55,67,72	0
2	VFE	N	1001	29/29	0.96	0.30	50,57,64,73	0
2	VFE	S	1001	29/29	0.96	0.27	45,54,59,71	0
2	VFE	V	1001	29/29	0.96	0.29	49,55,60,73	0
3	MG	D	1002	1/1	0.96	0.10	58,58,58,58	0

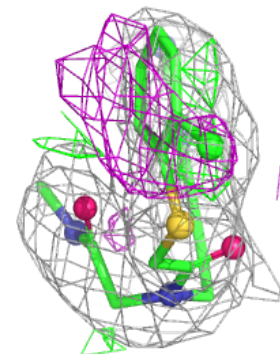
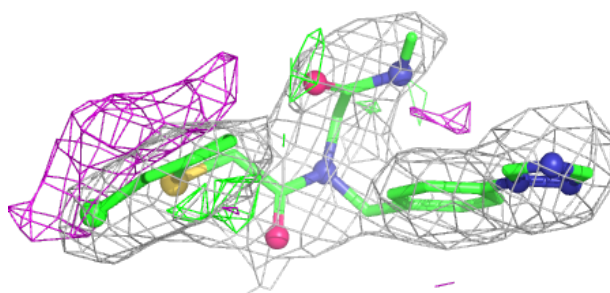
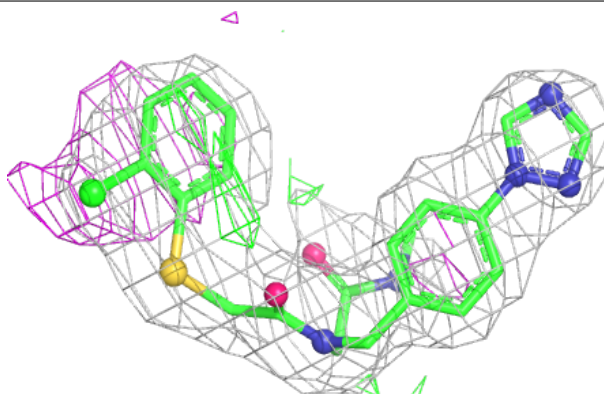
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around VFE I 1001:**

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

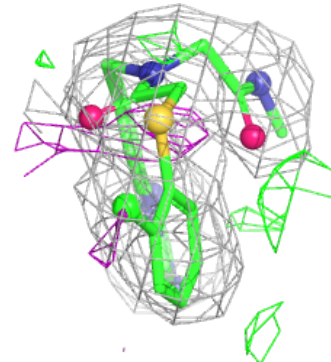
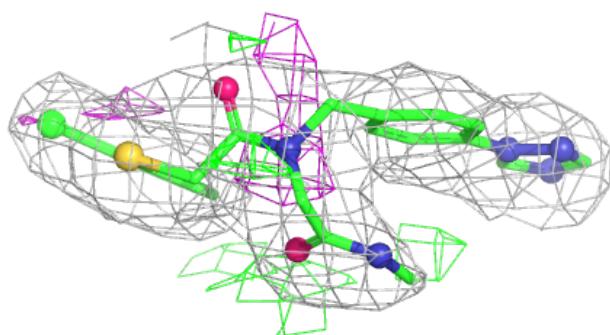
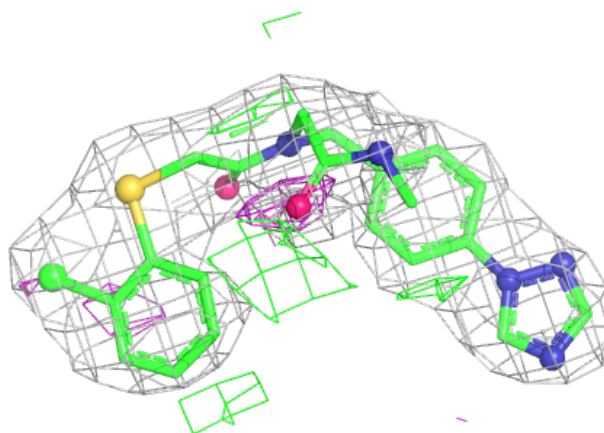
**Electron density around VFE U 1001:**

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

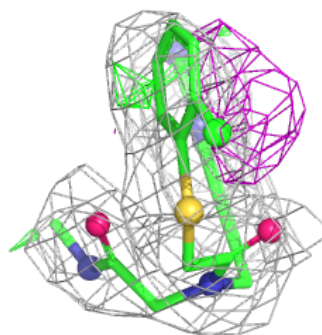
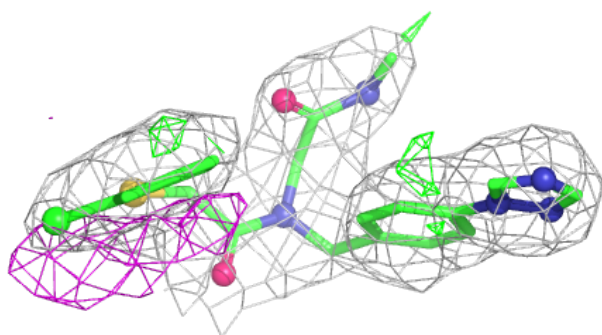
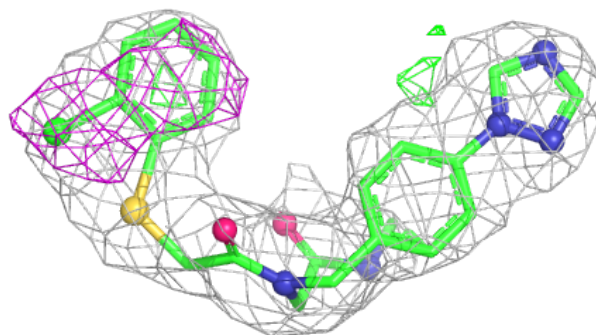


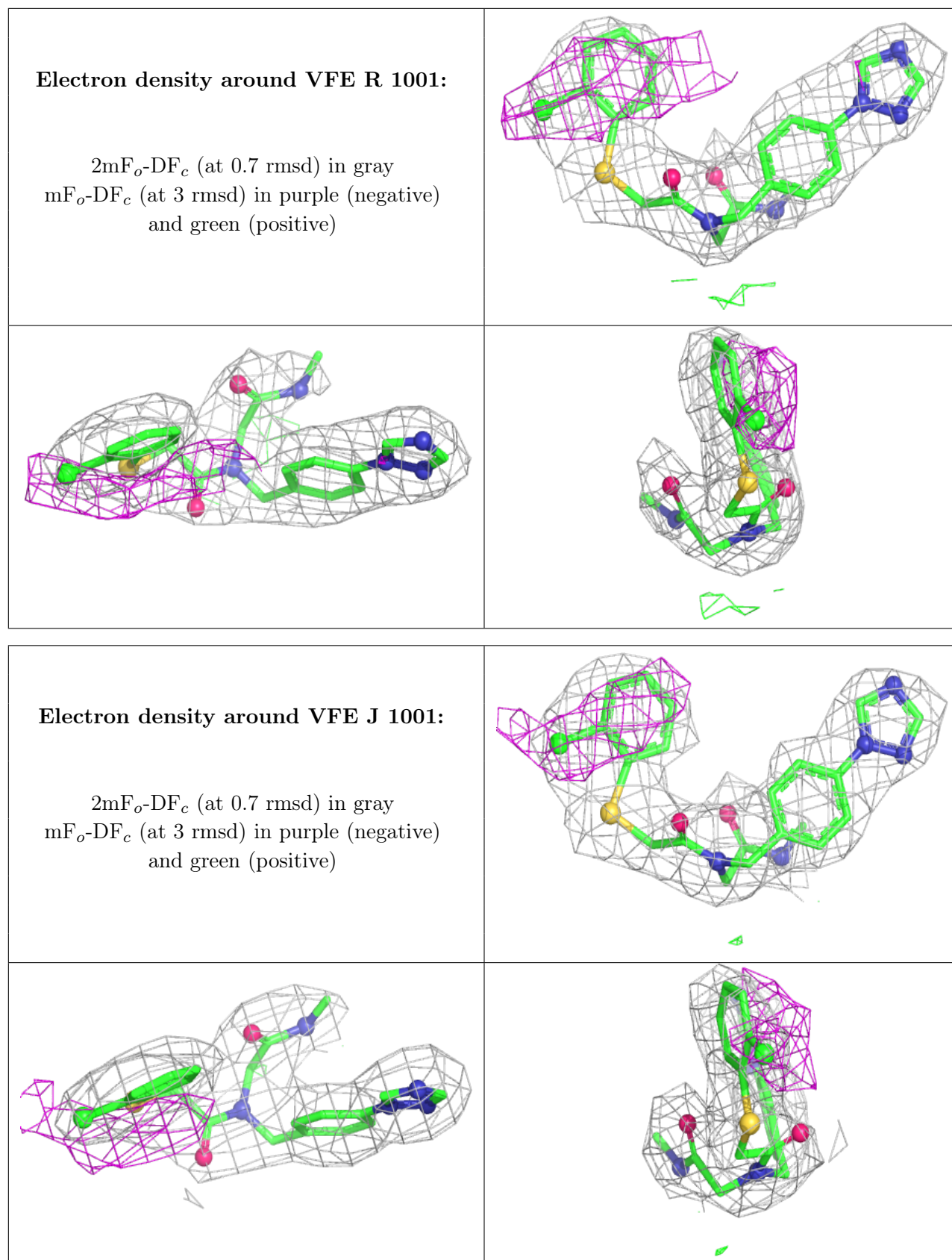
**Electron density around VFE d 1001:**

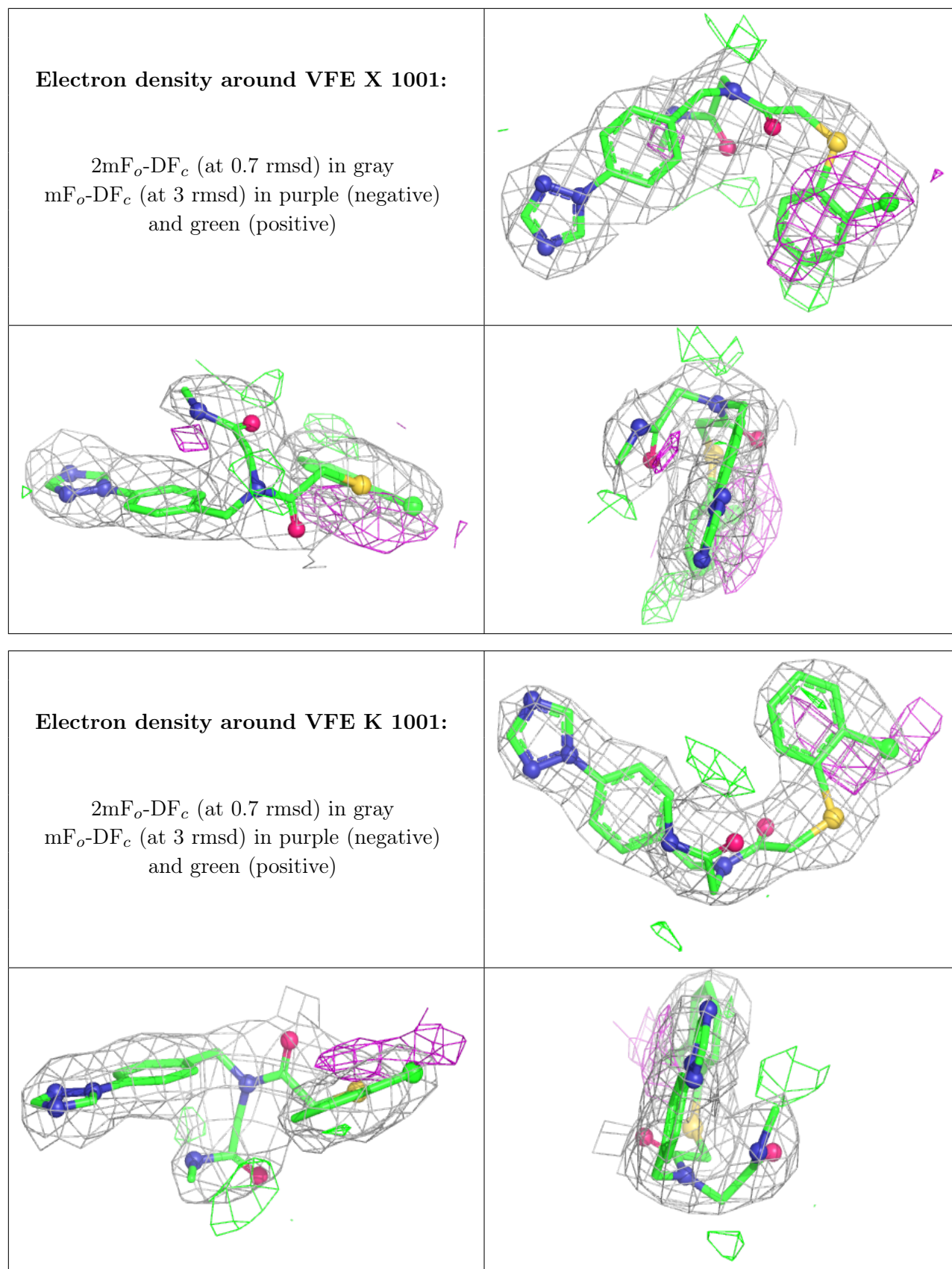
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around VFE M 1001:**

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



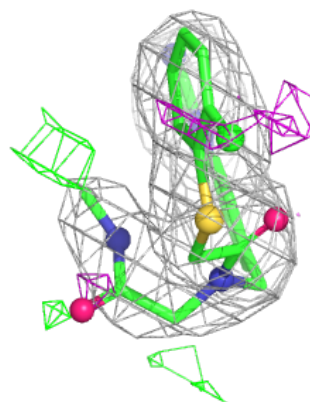
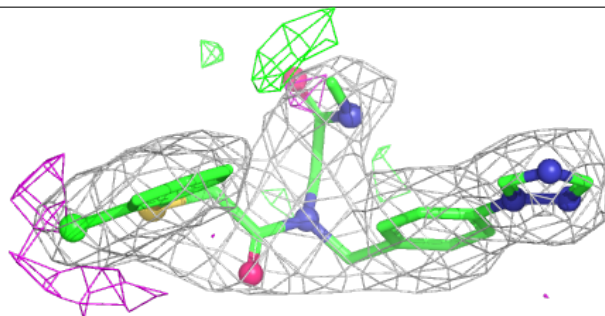
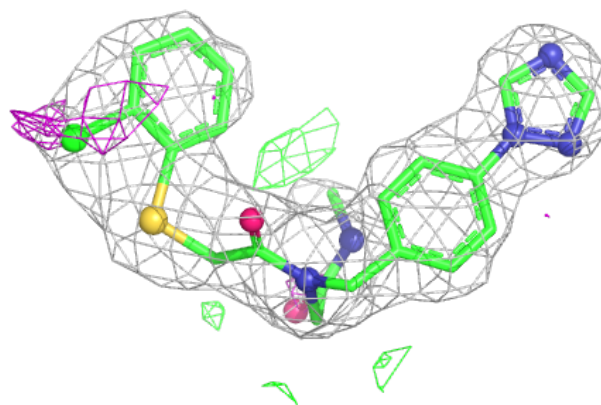




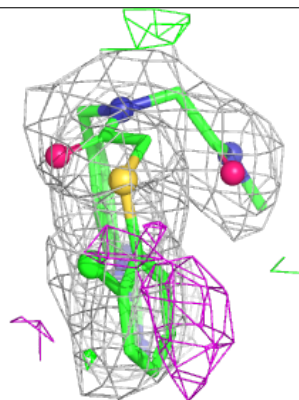
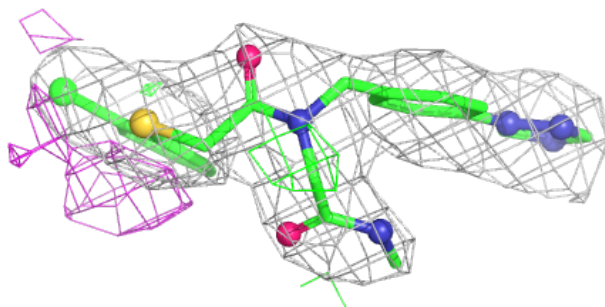
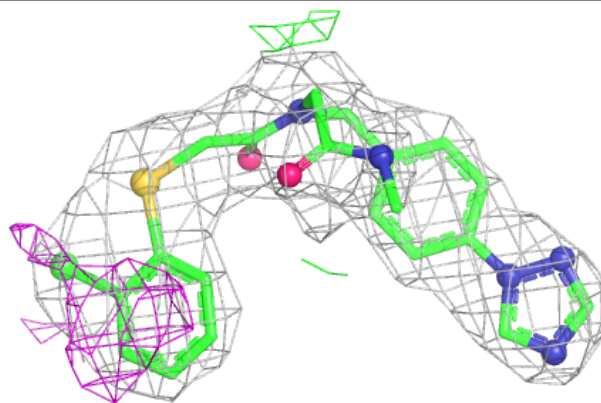


**Electron density around VFE L 1001:**

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

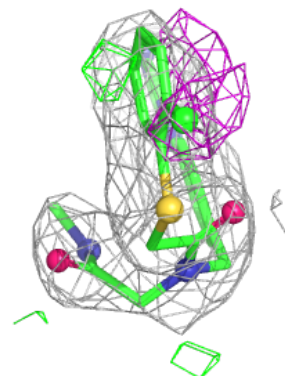
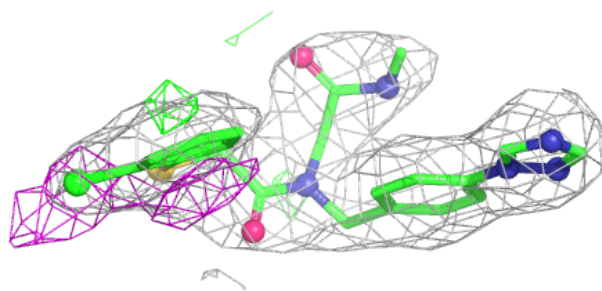
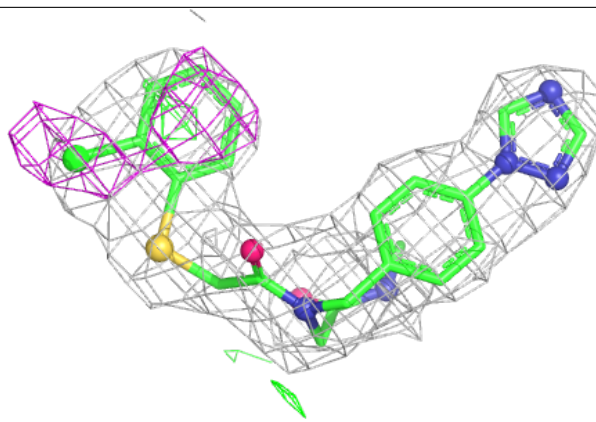
**Electron density around VFE G 1001:**

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

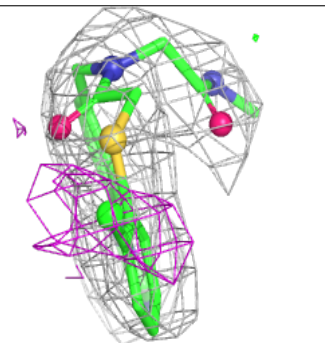
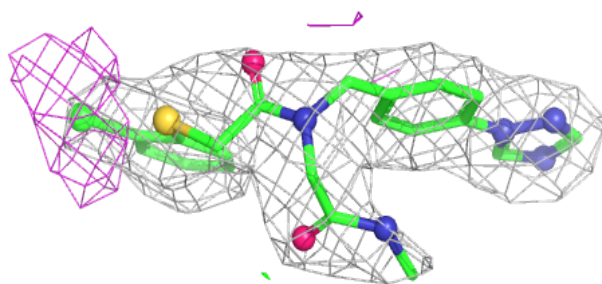
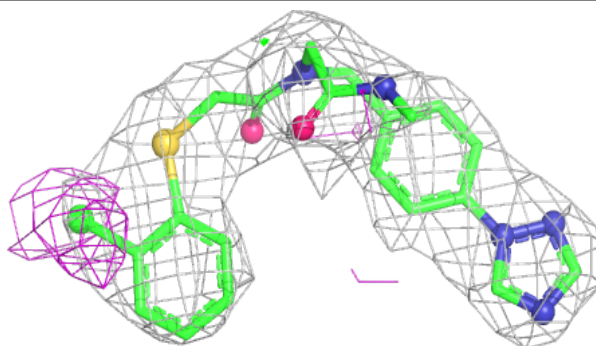


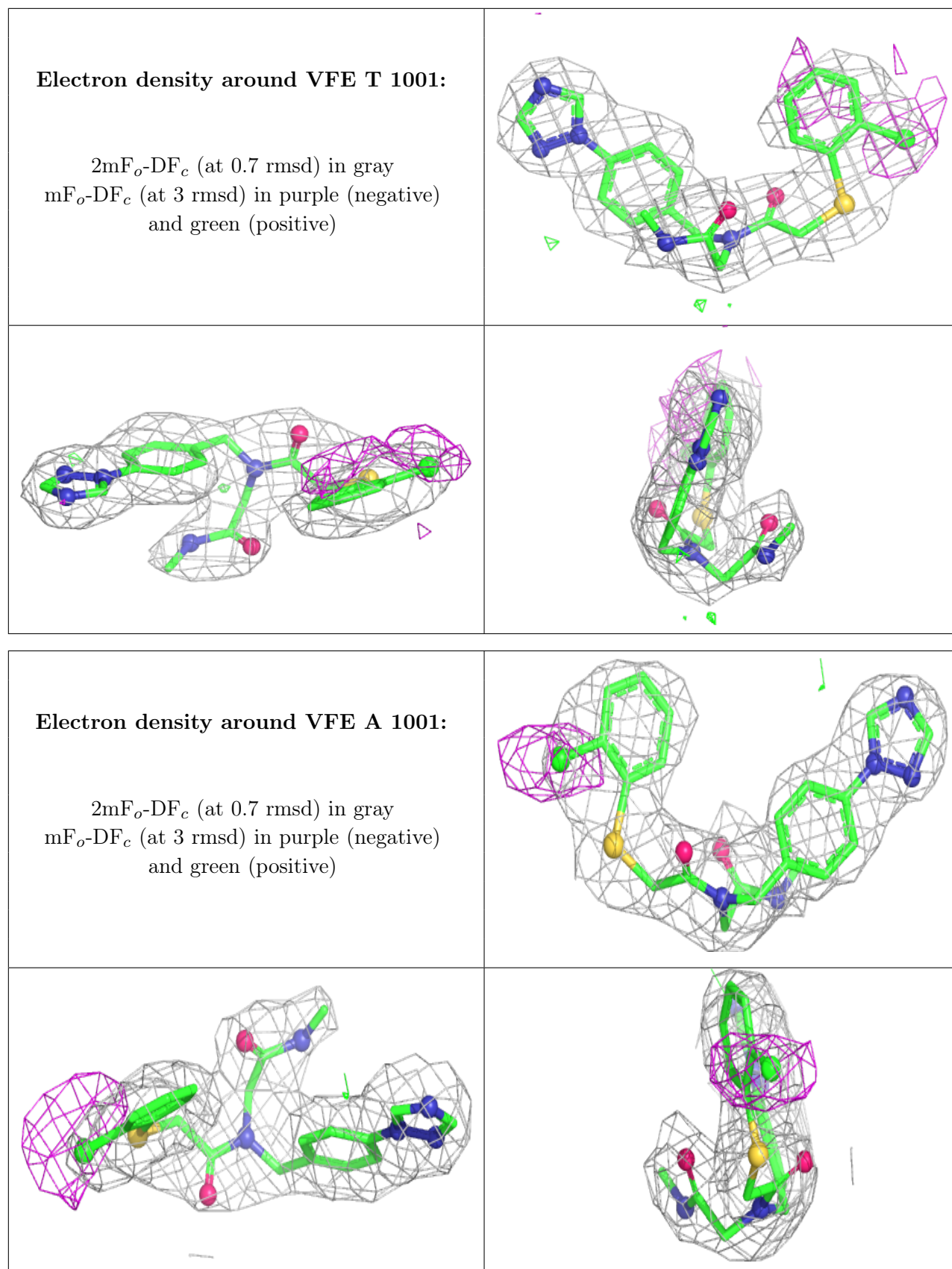
**Electron density around VFE P 1001:**

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

**Electron density around VFE H 1001:**

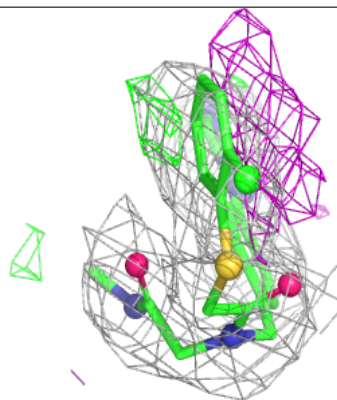
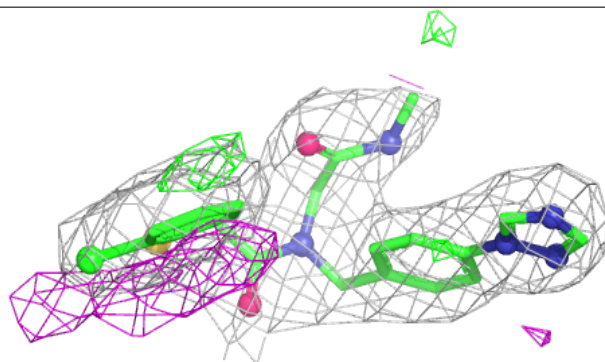
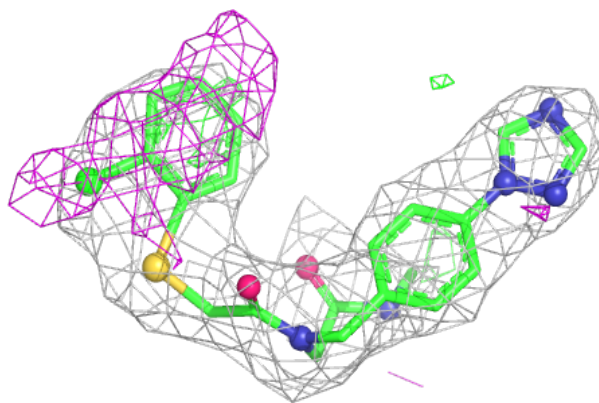
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



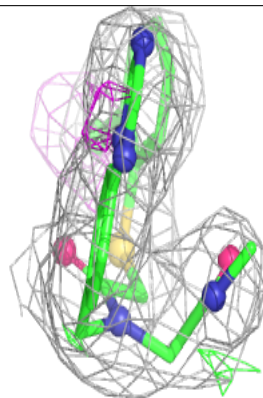
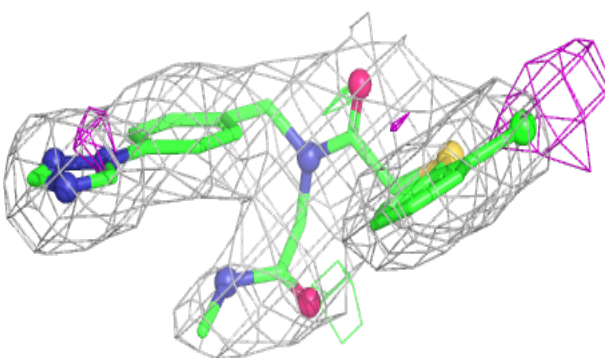
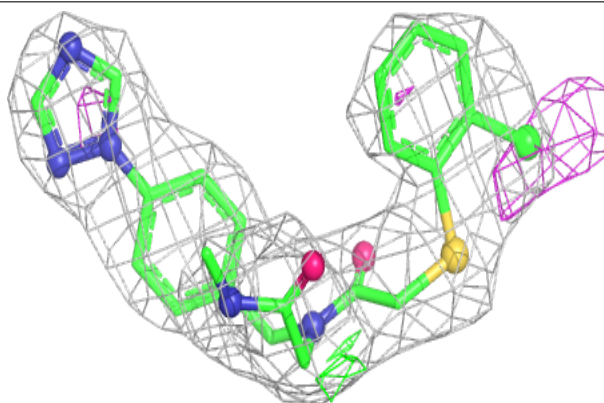


**Electron density around VFE C 1001:**

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

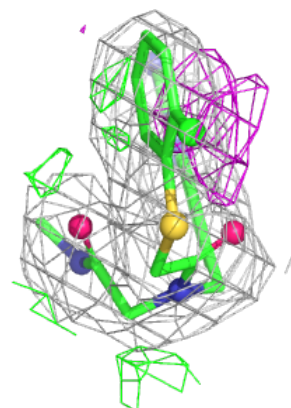
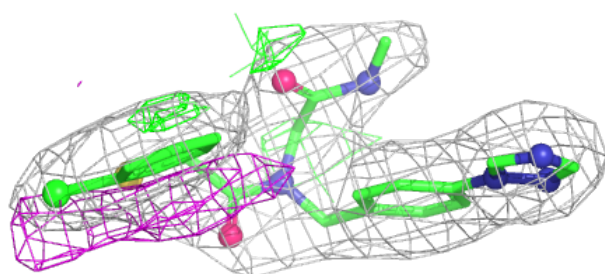
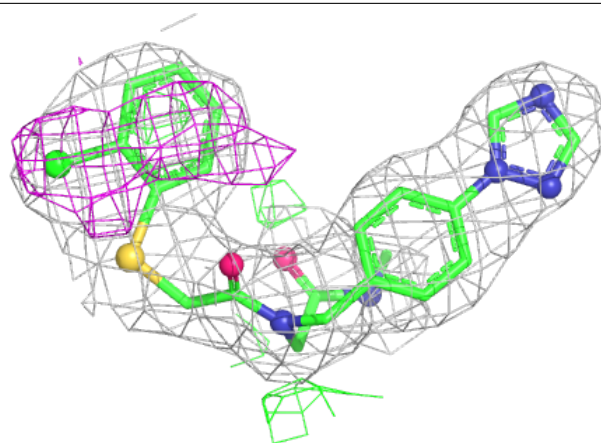
**Electron density around VFE c 1001:**

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

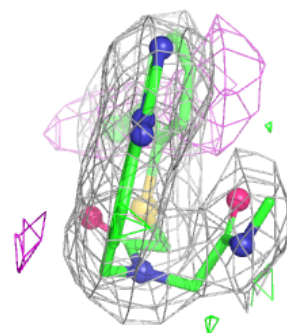
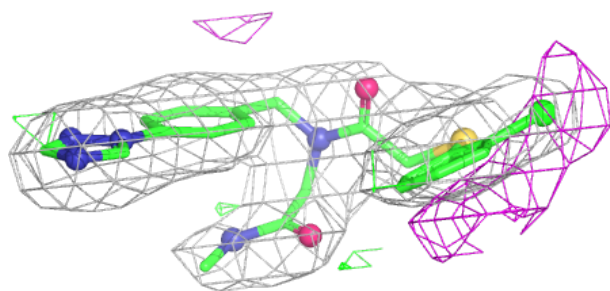
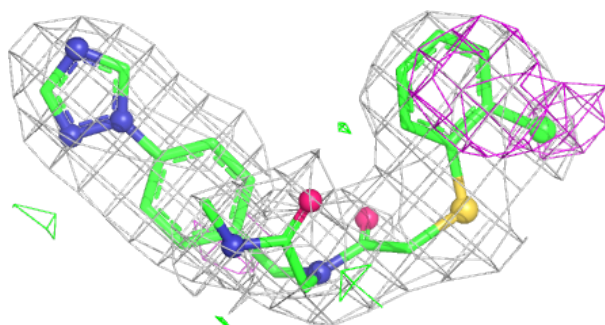


**Electron density around VFE D 1001:**

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

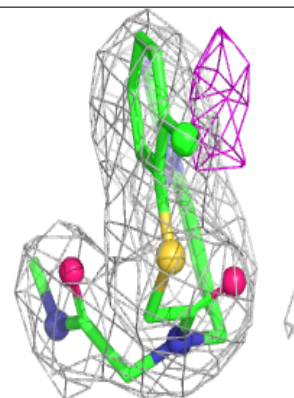
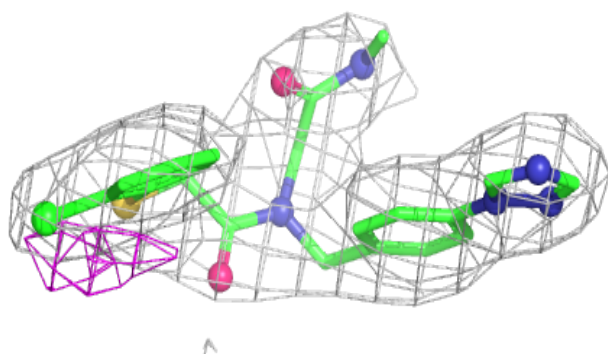
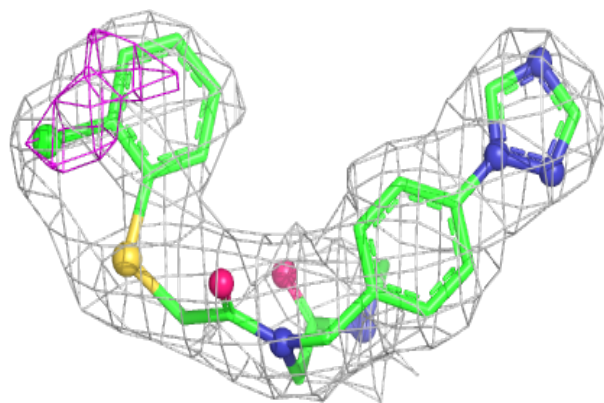
**Electron density around VFE B 1001:**

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

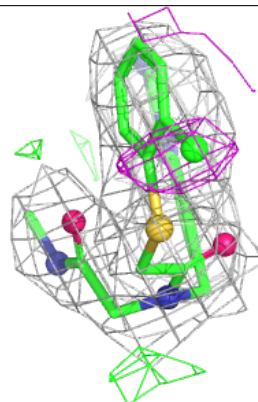
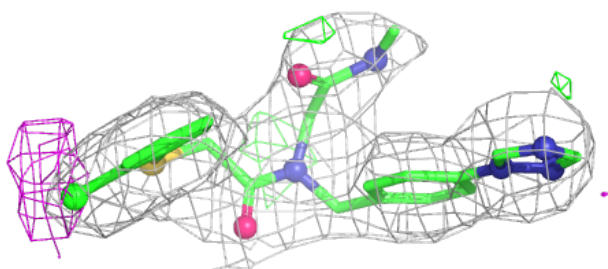
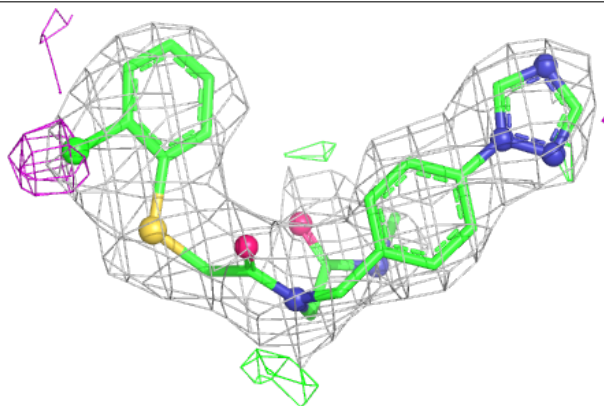


**Electron density around VFE O 1001:**

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

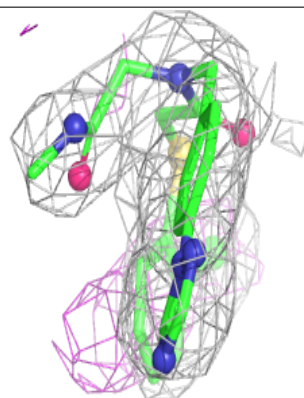
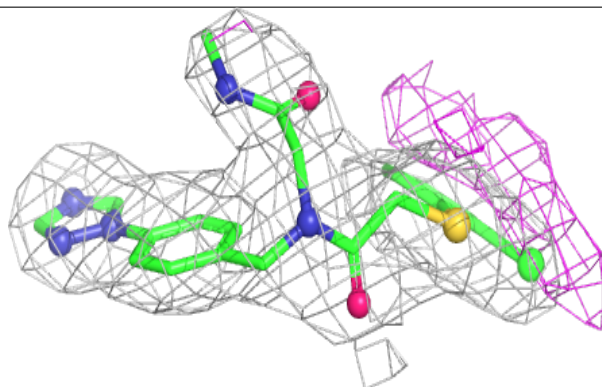
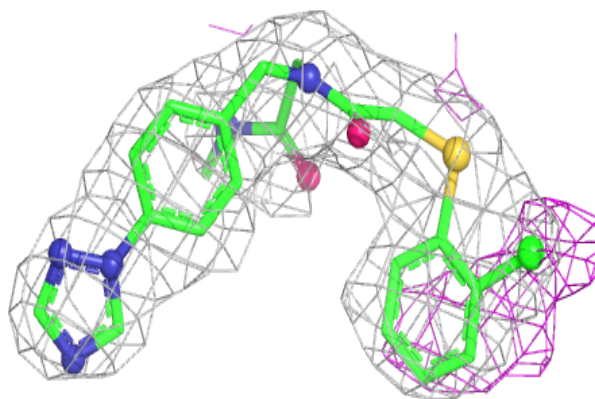
**Electron density around VFE E 1001:**

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

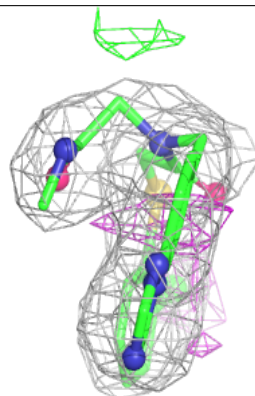
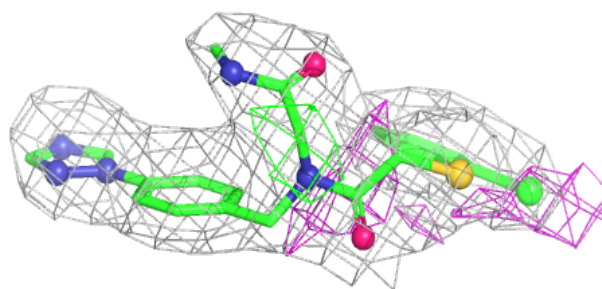
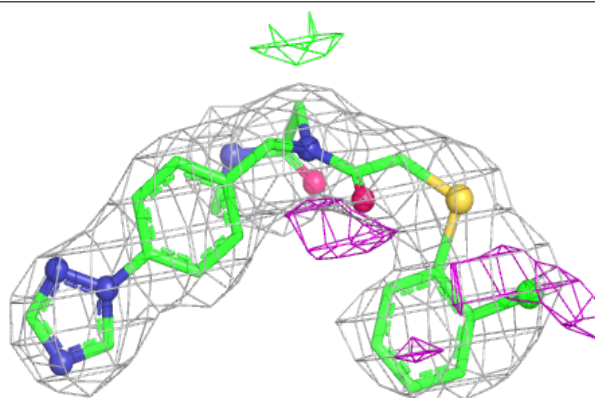


**Electron density around VFE Y 1001:**

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

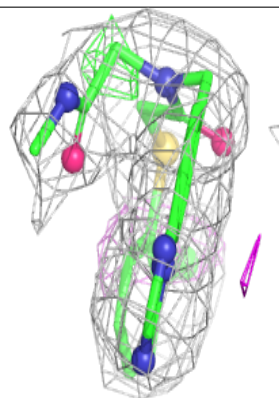
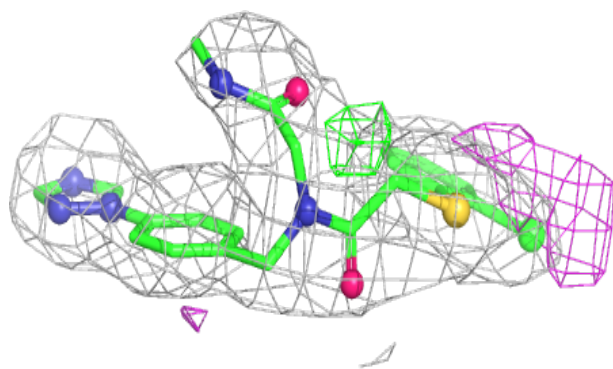
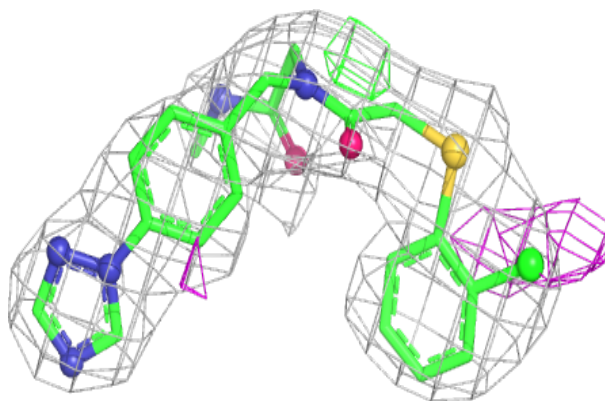
**Electron density around VFE Z 1001:**

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

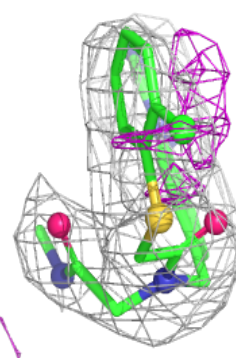
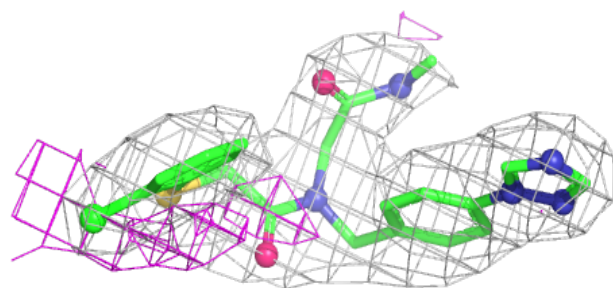
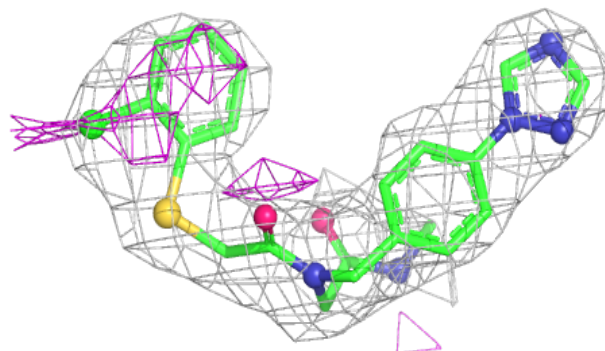


**Electron density around VFE a 1001:**

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

**Electron density around VFE b 1001:**

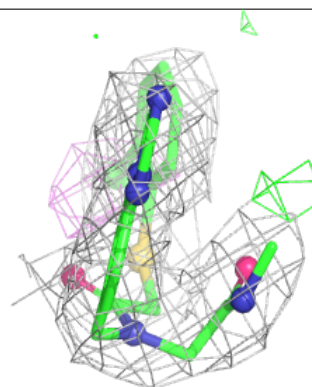
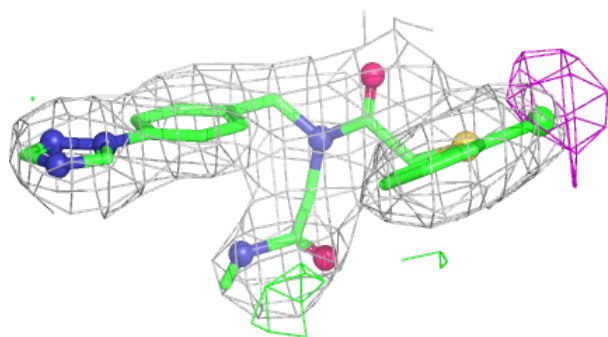
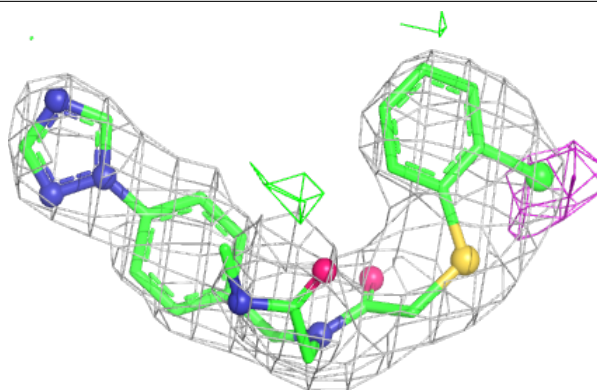
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



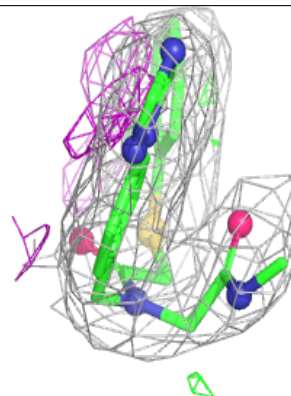
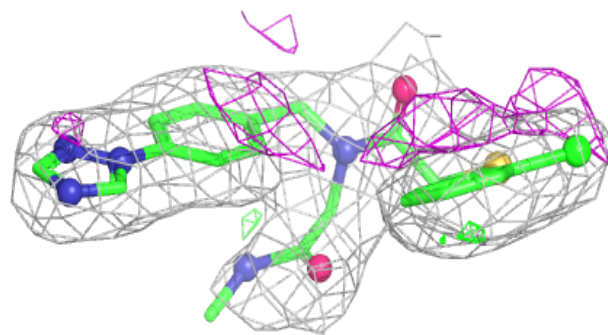
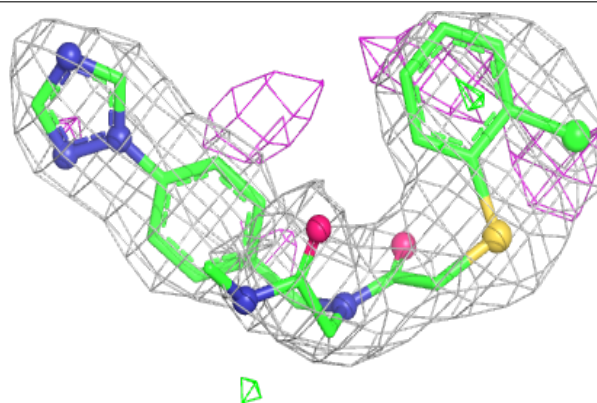


**Electron density around VFE Q 1001:**

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

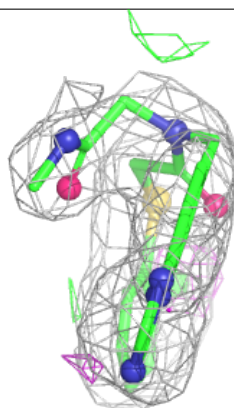
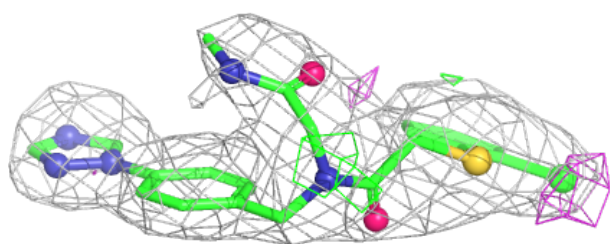
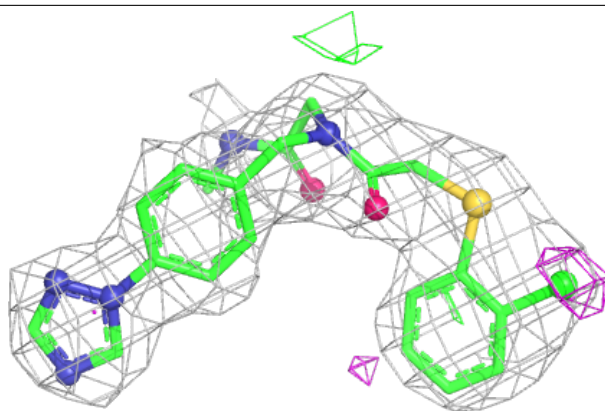
**Electron density around VFE F 1001:**

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

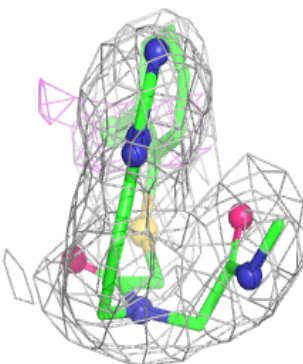
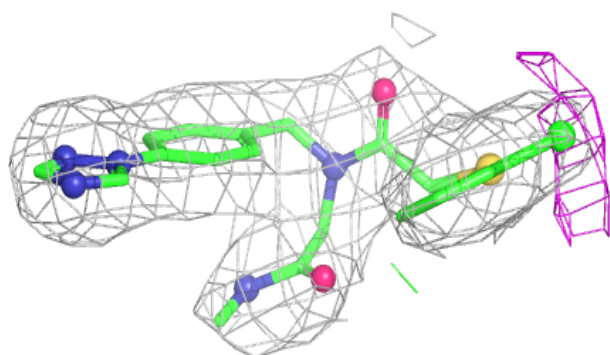
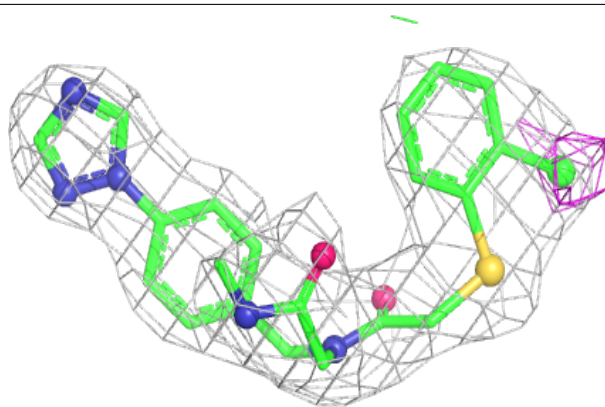


**Electron density around VFE W 1001:**

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

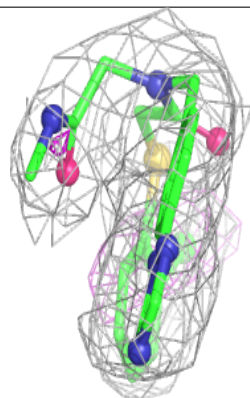
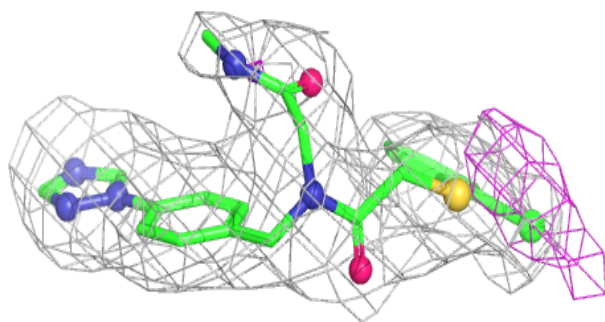
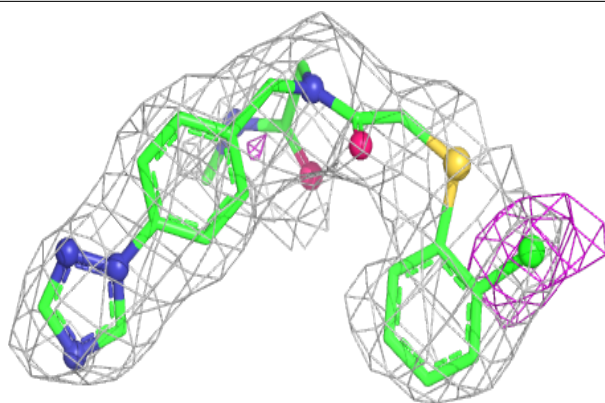
**Electron density around VFE N 1001:**

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

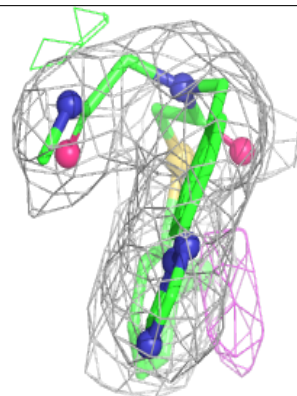
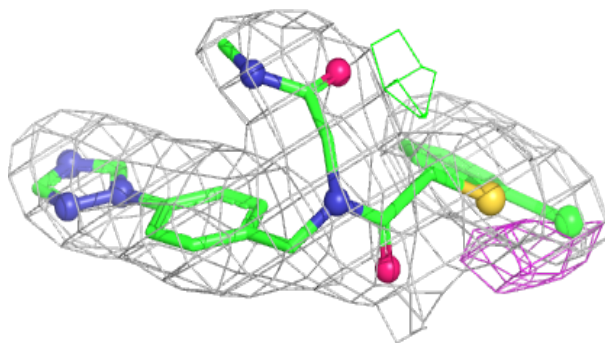
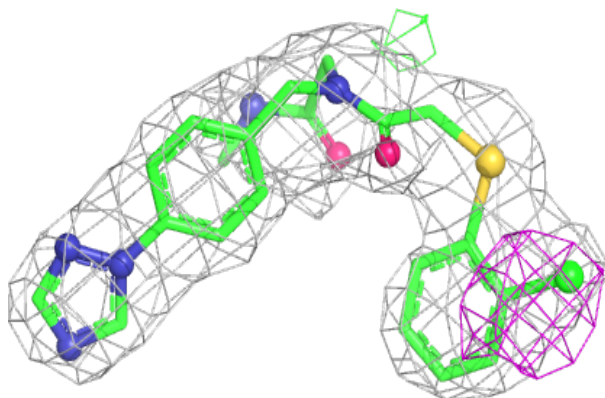


**Electron density around VFE S 1001:**

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

**Electron density around VFE V 1001:**

$2mF_o-DF_c$  (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.